



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 08:26 AM BST

PDB ID : 4XK8
Title : Crystal structure of plant photosystem I-LHCI super-complex at 2.8 angstrom resolution
Authors : Suga, M.; Qin, X.; Kuang, T.; Shen, J.R.
Deposited on : 2015-01-10
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

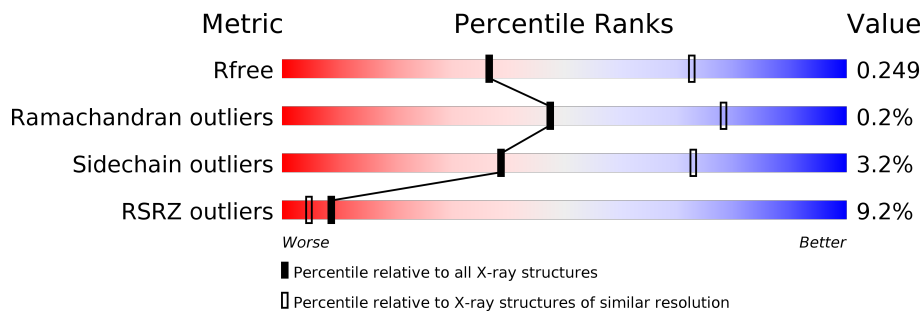
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	742	 4% 98% .
1	a	742	 4% 98% .
2	B	733	 9% 98% .
2	b	733	 7% 98% .
3	C	80	 6% 98% .
3	c	80	 98% .
4	D	141	 8% 96% .

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Mol	Chain	Length	Quality of chain
4	d	141	4% 94% 5%
5	E	64	22% 98%
5	e	64	2% 98%
6	F	151	8% 98%
6	f	151	5% 97%
7	G	95	4% 99%
7	g	95	13% 100%
8	H	90	11% 97%
8	h	90	3% 97%
9	I	30	3% 93%
9	i	30	3% 97%
10	J	39	5% 95% 5%
10	j	39	8% 95% 5%
11	K	84	19% 51% 46%
11	k	84	6% 52% 45%
12	L	153	10% 93% 7%
12	l	153	92% 7%
13	1	195	17% 97%
13	6	195	15% 97%
14	2	206	28% 96%
14	7	206	15% 96%
15	3	218	17% 97%
15	8	218	11% 97%
16	4	196	21% 96%
16	9	196	11% 96%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	1	303	X	-	-	-
17	CLA	1	304	X	-	-	-
17	CLA	1	305	X	-	-	-
17	CLA	1	306	X	-	-	-
17	CLA	1	308	X	-	-	-
17	CLA	1	309	X	-	-	-
17	CLA	1	310	X	-	-	-
17	CLA	1	311	X	-	-	-
17	CLA	1	312	X	-	-	-
17	CLA	1	313	X	-	-	-
17	CLA	1	314	X	-	-	-
17	CLA	1	315	X	-	-	-
17	CLA	2	602	X	-	-	-
17	CLA	2	603	X	-	-	-
17	CLA	2	604	X	-	-	-
17	CLA	2	608	X	-	-	-
17	CLA	2	609	X	-	-	-
17	CLA	2	610	X	-	-	-
17	CLA	2	611	X	-	-	-
17	CLA	2	612	X	-	-	-
17	CLA	2	613	X	-	-	-
17	CLA	3	301	X	-	-	X
17	CLA	3	302	X	-	-	-
17	CLA	3	303	X	-	-	-
17	CLA	3	304	X	-	-	-
17	CLA	3	305	X	-	-	-
17	CLA	3	306	X	-	-	-
17	CLA	3	308	X	-	-	-
17	CLA	3	309	X	-	-	-
17	CLA	3	310	X	-	-	-
17	CLA	3	311	X	-	-	-
17	CLA	3	312	X	-	-	-
17	CLA	3	313	X	-	-	-
17	CLA	3	314	X	-	-	-
17	CLA	3	315	X	-	-	-
17	CLA	4	601	X	-	-	-
17	CLA	4	602	X	-	-	-
17	CLA	4	603	X	-	-	-
17	CLA	4	604	X	-	-	-
17	CLA	4	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	4	609	X	-	-	-
17	CLA	4	610	X	-	-	-
17	CLA	4	611	X	-	-	-
17	CLA	4	612	X	-	-	-
17	CLA	4	613	X	-	-	-
17	CLA	4	614	X	-	-	-
17	CLA	6	304	X	-	-	-
17	CLA	6	305	X	-	-	-
17	CLA	6	306	X	-	-	-
17	CLA	6	307	X	-	-	-
17	CLA	6	309	X	-	-	-
17	CLA	6	310	X	-	-	-
17	CLA	6	311	X	-	-	-
17	CLA	6	312	X	-	-	-
17	CLA	6	313	X	-	-	-
17	CLA	6	314	X	-	-	-
17	CLA	6	315	X	-	-	-
17	CLA	6	316	X	-	-	-
17	CLA	7	602	X	-	-	-
17	CLA	7	603	X	-	-	-
17	CLA	7	604	X	-	-	-
17	CLA	7	608	X	-	-	-
17	CLA	7	609	X	-	-	-
17	CLA	7	610	X	-	-	-
17	CLA	7	611	X	-	-	-
17	CLA	7	612	X	-	-	-
17	CLA	7	613	X	-	-	-
17	CLA	8	301	X	-	-	-
17	CLA	8	302	X	-	-	-
17	CLA	8	303	X	-	-	-
17	CLA	8	304	X	-	-	-
17	CLA	8	305	X	-	-	-
17	CLA	8	307	X	-	-	-
17	CLA	8	308	X	-	-	-
17	CLA	8	309	X	-	-	X
17	CLA	8	310	X	-	-	-
17	CLA	8	311	X	-	-	-
17	CLA	8	312	X	-	-	-
17	CLA	8	313	X	-	-	-
17	CLA	9	601	X	-	-	-
17	CLA	9	602	X	-	-	-
17	CLA	9	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	9	604	X	-	-	-
17	CLA	9	608	X	-	-	-
17	CLA	9	609	X	-	-	-
17	CLA	9	610	X	-	-	-
17	CLA	9	611	X	-	-	-
17	CLA	9	612	X	-	-	-
17	CLA	9	613	X	-	-	-
17	CLA	9	614	X	-	-	-
17	CLA	A	801	X	-	-	-
17	CLA	A	802	X	-	-	-
17	CLA	A	803	X	-	-	-
17	CLA	A	804	X	-	-	-
17	CLA	A	805	X	-	-	-
17	CLA	A	806	X	-	-	-
17	CLA	A	807	X	-	-	-
17	CLA	A	808	X	-	-	-
17	CLA	A	809	X	-	-	-
17	CLA	A	810	X	-	-	-
17	CLA	A	811	X	-	-	-
17	CLA	A	812	X	-	-	-
17	CLA	A	813	X	-	-	-
17	CLA	A	814	X	-	-	-
17	CLA	A	815	X	-	-	-
17	CLA	A	816	X	-	-	-
17	CLA	A	817	X	-	-	-
17	CLA	A	818	X	-	-	-
17	CLA	A	819	X	-	-	-
17	CLA	A	820	X	-	-	-
17	CLA	A	821	X	-	-	-
17	CLA	A	822	X	-	-	-
17	CLA	A	823	X	-	-	-
17	CLA	A	824	X	-	-	-
17	CLA	A	825	X	-	-	-
17	CLA	A	826	X	-	-	-
17	CLA	A	827	X	-	-	-
17	CLA	A	828	X	-	-	-
17	CLA	A	829	X	-	-	-
17	CLA	A	830	X	-	-	-
17	CLA	A	831	X	-	-	-
17	CLA	A	832	X	-	-	-
17	CLA	A	833	X	-	-	-
17	CLA	A	834	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	A	835	X	-	-	-
17	CLA	A	836	X	-	-	-
17	CLA	A	837	X	-	-	-
17	CLA	A	838	X	-	-	-
17	CLA	A	839	X	-	-	-
17	CLA	A	840	X	-	-	-
17	CLA	A	841	X	-	-	-
17	CLA	A	842	X	-	-	-
17	CLA	A	843	X	-	-	-
17	CLA	A	845	X	-	-	-
17	CLA	A	854	X	-	-	-
17	CLA	B	802	X	-	-	-
17	CLA	B	803	X	-	-	-
17	CLA	B	804	X	-	-	-
17	CLA	B	805	X	-	-	-
17	CLA	B	806	X	-	-	-
17	CLA	B	807	X	-	-	-
17	CLA	B	808	X	-	-	-
17	CLA	B	809	X	-	-	-
17	CLA	B	810	X	-	-	-
17	CLA	B	811	X	-	-	-
17	CLA	B	812	X	-	-	-
17	CLA	B	813	X	-	-	-
17	CLA	B	814	X	-	-	-
17	CLA	B	815	X	-	-	-
17	CLA	B	816	X	-	-	-
17	CLA	B	817	X	-	-	-
17	CLA	B	818	X	-	-	-
17	CLA	B	819	X	-	-	-
17	CLA	B	820	X	-	-	-
17	CLA	B	821	X	-	-	-
17	CLA	B	822	X	-	-	-
17	CLA	B	823	X	-	-	-
17	CLA	B	824	X	-	-	-
17	CLA	B	825	X	-	-	-
17	CLA	B	826	X	-	-	-
17	CLA	B	827	X	-	-	-
17	CLA	B	828	X	-	-	-
17	CLA	B	829	X	-	-	-
17	CLA	B	830	X	-	-	-
17	CLA	B	831	X	-	-	-
17	CLA	B	832	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	B	833	X	-	-	-
17	CLA	B	834	X	-	-	-
17	CLA	B	835	X	-	-	-
17	CLA	B	836	X	-	-	-
17	CLA	B	837	X	-	-	-
17	CLA	B	838	X	-	-	-
17	CLA	B	839	X	-	-	-
17	CLA	B	840	X	-	-	-
17	CLA	B	841	X	-	-	-
17	CLA	F	301	X	-	-	-
17	CLA	F	303	X	-	-	-
17	CLA	F	304	X	-	-	-
17	CLA	G	101	X	-	-	-
17	CLA	G	103	X	-	-	-
17	CLA	G	104	X	-	-	-
17	CLA	J	3002	X	-	-	-
17	CLA	K	4002	X	-	-	X
17	CLA	K	4003	X	-	-	-
17	CLA	L	202	X	-	-	-
17	CLA	L	203	X	-	-	-
17	CLA	L	204	X	-	-	-
17	CLA	a	801	X	-	-	-
17	CLA	a	802	X	-	-	-
17	CLA	a	803	X	-	-	-
17	CLA	a	804	X	-	-	-
17	CLA	a	805	X	-	-	-
17	CLA	a	806	X	-	-	-
17	CLA	a	807	X	-	-	-
17	CLA	a	808	X	-	-	-
17	CLA	a	809	X	-	-	-
17	CLA	a	810	X	-	-	-
17	CLA	a	811	X	-	-	-
17	CLA	a	812	X	-	-	-
17	CLA	a	813	X	-	-	-
17	CLA	a	814	X	-	-	-
17	CLA	a	815	X	-	-	-
17	CLA	a	816	X	-	-	-
17	CLA	a	817	X	-	-	-
17	CLA	a	818	X	-	-	-
17	CLA	a	819	X	-	-	-
17	CLA	a	820	X	-	-	-
17	CLA	a	821	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	a	822	X	-	-	-
17	CLA	a	823	X	-	-	-
17	CLA	a	824	X	-	-	-
17	CLA	a	825	X	-	-	-
17	CLA	a	826	X	-	-	-
17	CLA	a	827	X	-	-	-
17	CLA	a	828	X	-	-	-
17	CLA	a	829	X	-	-	-
17	CLA	a	830	X	-	-	-
17	CLA	a	831	X	-	-	-
17	CLA	a	832	X	-	-	-
17	CLA	a	833	X	-	-	-
17	CLA	a	834	X	-	-	-
17	CLA	a	835	X	-	-	-
17	CLA	a	836	X	-	-	-
17	CLA	a	837	X	-	-	-
17	CLA	a	838	X	-	-	-
17	CLA	a	839	X	-	-	-
17	CLA	a	840	X	-	-	-
17	CLA	a	841	X	-	-	-
17	CLA	a	842	X	-	-	-
17	CLA	a	843	X	-	-	-
17	CLA	a	844	X	-	-	-
17	CLA	a	846	X	-	-	-
17	CLA	a	856	X	-	-	-
17	CLA	b	802	X	-	-	-
17	CLA	b	803	X	-	-	-
17	CLA	b	804	X	-	-	-
17	CLA	b	805	X	-	-	-
17	CLA	b	806	X	-	-	-
17	CLA	b	807	X	-	-	-
17	CLA	b	808	X	-	-	-
17	CLA	b	809	X	-	-	-
17	CLA	b	810	X	-	-	-
17	CLA	b	811	X	-	-	-
17	CLA	b	812	X	-	-	-
17	CLA	b	813	X	-	-	-
17	CLA	b	814	X	-	-	-
17	CLA	b	815	X	-	-	-
17	CLA	b	816	X	-	-	-
17	CLA	b	817	X	-	-	-
17	CLA	b	818	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	b	819	X	-	-	-
17	CLA	b	820	X	-	-	-
17	CLA	b	821	X	-	-	-
17	CLA	b	822	X	-	-	-
17	CLA	b	823	X	-	-	-
17	CLA	b	824	X	-	-	-
17	CLA	b	825	X	-	-	-
17	CLA	b	826	X	-	-	-
17	CLA	b	827	X	-	-	-
17	CLA	b	828	X	-	-	-
17	CLA	b	829	X	-	-	-
17	CLA	b	830	X	-	-	-
17	CLA	b	831	X	-	-	-
17	CLA	b	832	X	-	-	-
17	CLA	b	833	X	-	-	-
17	CLA	b	834	X	-	-	-
17	CLA	b	835	X	-	-	-
17	CLA	b	836	X	-	-	-
17	CLA	b	837	X	-	-	-
17	CLA	b	838	X	-	-	-
17	CLA	b	839	X	-	-	-
17	CLA	b	840	X	-	-	-
17	CLA	b	841	X	-	-	-
17	CLA	f	7002	X	-	-	-
17	CLA	f	7003	X	-	-	-
17	CLA	g	101	X	-	-	-
17	CLA	g	102	X	-	-	-
17	CLA	g	103	X	-	-	-
17	CLA	j	3002	X	-	-	-
17	CLA	k	1401	X	-	-	-
17	CLA	k	1402	X	-	-	-
17	CLA	k	1403	X	-	-	-
17	CLA	l	202	X	-	-	-
17	CLA	l	203	X	-	-	-
17	CLA	l	204	X	-	-	-
19	LHG	3	319	-	-	-	X
20	BCR	1	318	-	-	-	X
20	BCR	2	617	-	-	-	X
20	BCR	7	617	-	-	-	X
20	BCR	K	4001	-	-	-	X
20	BCR	K	4004	-	-	-	X
20	BCR	L	206	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	BCR	1	206	-	-	-	X
25	LMG	4	620	-	-	-	X
26	CHL	1	302	X	-	-	-
26	CHL	1	307	X	-	-	-
26	CHL	2	601	X	-	-	-
26	CHL	2	605	X	-	-	-
26	CHL	2	606	X	-	-	-
26	CHL	2	607	X	-	-	-
26	CHL	2	614	X	-	-	-
26	CHL	3	307	X	-	-	-
26	CHL	4	605	X	-	-	-
26	CHL	4	606	X	-	-	-
26	CHL	4	607	X	-	-	-
26	CHL	4	615	X	-	-	-
26	CHL	6	303	X	-	-	-
26	CHL	6	308	X	-	-	-
26	CHL	7	601	X	-	-	-
26	CHL	7	605	X	-	-	-
26	CHL	7	606	X	-	-	-
26	CHL	7	607	X	-	-	-
26	CHL	7	614	X	-	-	-
26	CHL	8	306	X	-	-	-
26	CHL	9	605	X	-	-	-
26	CHL	9	606	X	-	-	-
26	CHL	9	607	X	-	-	-
26	CHL	9	615	X	-	-	-
27	LUT	6	317	-	-	-	X
27	LUT	6	321	-	-	-	X

2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 71157 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	742	5846	3831	994	1003	18	0	0	0
1	a	742	5846	3831	994	1003	18	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	733	5863	3853	1002	994	14	0	0	0
2	b	733	5863	3853	1002	994	14	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	80	611	379	107	114	11	0	0	0
3	c	80	611	379	107	114	11	0	0	0

- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	141	1114	716	193	202	3	0	0	0
4	d	140	1107	712	192	200	3	0	0	0

- Molecule 5 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	63	Total	C	N	O	0	0	0
			507	321	90	96			
5	e	63	Total	C	N	O	0	0	0
			506	322	90	94			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	151	Total	C	N	O	S	0	0	0
			1193	776	204	210	3			
6	f	151	Total	C	N	O	S	0	0	0
			1193	776	204	210	3			

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	95	Total	C	N	O	0	0	0
			741	480	121	140			
7	g	95	Total	C	N	O	0	0	0
			737	478	121	138			

- Molecule 8 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	90	Total	C	N	O	0	0	0
			678	439	110	129			
8	h	90	Total	C	N	O	0	0	0
			682	442	111	129			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	29	Total	C	N	O	S	0	0	0
			221	153	33	34	1			
9	i	30	Total	C	N	O	S	0	0	0
			226	156	34	35	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	39	Total	C	N	O	S	0	0	0
			311	211	48	51	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	j	39	Total	C	N	O	S	0	0	0
			311	211	48	51	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	45	Total	C	N	O	S	0	0	0
			311	204	48	56	3			
11	k	46	Total	C	N	O	S	0	0	0
			316	207	49	57	3			

- Molecule 12 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	153	Total	C	N	O	S	0	0	0
			1136	746	183	206	1			
12	l	151	Total	C	N	O	S	0	0	0
			1122	738	180	203	1			

- Molecule 13 is a protein called Chlorophyll a-b binding protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1	195	Total	C	N	O	S	0	0	0
			1491	969	249	268	5			
13	6	195	Total	C	N	O	S	0	0	0
			1483	963	247	268	5			

- Molecule 14 is a protein called Type II chlorophyll a/b binding protein from photosystem I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	2	206	Total	C	N	O	S	0	0	0
			1610	1055	263	288	4			
14	7	206	Total	C	N	O	S	0	0	0
			1610	1055	263	288	4			

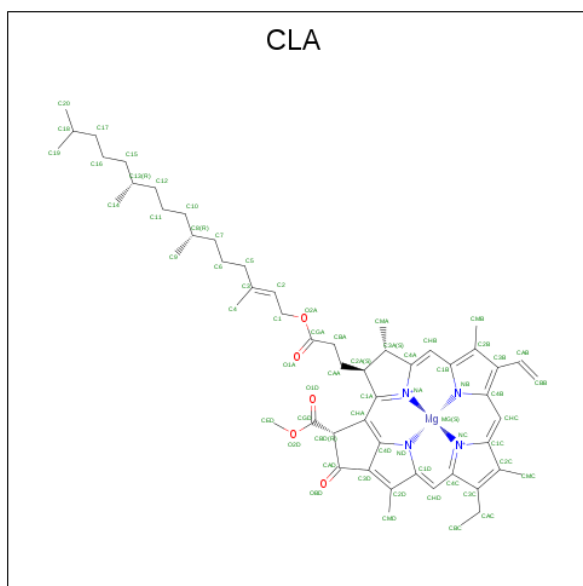
- Molecule 15 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	3	218	Total	C	N	O	S	0	0	0
			1680	1100	273	302	5			
15	8	217	Total	C	N	O	S	0	0	0
			1672	1094	272	301	5			

- Molecule 16 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	4	196	Total	C	N	O	S	0	0	0
			1540	1009	251	277	3			
16	9	196	Total	C	N	O	S	0	0	0
			1540	1009	251	277	3			

- Molecule 17 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
17	A	1	50	40	1	4	5	0	0
17	A	1	65	55	1	4	5	0	0
17	A	1	65	55	1	4	5	0	0
17	A	1	65	55	1	4	5	0	0
17	A	1	50	40	1	4	5	0	0
17	A	1	45	35	1	4	5	0	0
17	A	1	51	41	1	4	5	0	0
17	A	1	65	55	1	4	5	0	0
17	A	1	65	55	1	4	5	0	0
17	A	1	65	55	1	4	5	0	0
17	A	1	65	55	1	4	5	0	0
17	A	1	65	55	1	4	5	0	0
17	A	1	52	42	1	4	5	0	0
17	A	1	65	55	1	4	5	0	0
17	B	1	65	55	1	4	5	0	0
17	B	1	65	55	1	4	5	0	0
17	B	1	45	35	1	4	5	0	0
17	B	1	65	55	1	4	5	0	0
17	B	1	65	55	1	4	5	0	0
17	B	1	65	55	1	4	5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	F	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	G	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	G	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	G	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	J	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
17	K	1	46	36	1	4	5	0	0
17	L	1	Total	C	Mg	N	O		
			65	55	1	4	5	0	0
17	L	1	Total	C	Mg	N	O		
			65	55	1	4	5	0	0
17	L	1	Total	C	Mg	N	O		
			50	40	1	4	5	0	0
17	1	1	Total	C	Mg	N	O		
			65	55	1	4	5	0	0
17	1	1	Total	C	Mg	N	O		
			65	55	1	4	5	0	0
17	1	1	Total	C	Mg	N	O		
			52	42	1	4	5	0	0
17	1	1	Total	C	Mg	N	O		
			52	42	1	4	5	0	0
17	1	1	Total	C	Mg	N	O		
			65	55	1	4	5	0	0
17	1	1	Total	C	Mg	N	O		
			65	55	1	4	5	0	0
17	1	1	Total	C	Mg	N	O		
			60	50	1	4	5	0	0
17	1	1	Total	C	Mg	N	O		
			41	33	1	4	3	0	0
17	1	1	Total	C	Mg	N	O		
			52	42	1	4	5	0	0
17	1	1	Total	C	Mg	N	O		
			65	55	1	4	5	0	0
17	1	1	Total	C	Mg	N	O		
			55	45	1	4	5	0	0
17	1	1	Total	C	Mg	N	O		
			46	36	1	4	5	0	0
17	2	1	Total	C	Mg	N	O		
			65	55	1	4	5	0	0
17	2	1	Total	C	Mg	N	O		
			65	55	1	4	5	0	0
17	2	1	Total	C	Mg	N	O		
			60	50	1	4	5	0	0
17	2	1	Total	C	Mg	N	O		
			50	40	1	4	5	0	0
17	2	1	Total	C	Mg	N	O		
			60	50	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	2	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	2	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			43	35	1	4	3		
17	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	3	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			37	31	1	4	1		
17	3	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
17	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
17	a	1	65	55	1	4	5	0	0
17	a	1	45	35	1	4	5	0	0
17	a	1	50	40	1	4	5	0	0
17	a	1	45	35	1	4	5	0	0
17	a	1	65	55	1	4	5	0	0
17	a	1	65	55	1	4	5	0	0
17	a	1	65	55	1	4	5	0	0
17	a	1	45	35	1	4	5	0	0
17	a	1	65	55	1	4	5	0	0
17	a	1	49	39	1	4	5	0	0
17	a	1	51	41	1	4	5	0	0
17	a	1	55	45	1	4	5	0	0
17	a	1	65	55	1	4	5	0	0
17	a	1	65	55	1	4	5	0	0
17	a	1	65	55	1	4	5	0	0
17	a	1	65	55	1	4	5	0	0
17	a	1	65	55	1	4	5	0	0
17	a	1	65	55	1	4	5	0	0
17	a	1	50	40	1	4	5	0	0
17	a	1	65	55	1	4	5	0	0
17	a	1	65	55	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
17	a	1	65	55	1	4	5	0	0
17	a	1	50	40	1	4	5	0	0
17	a	1	45	35	1	4	5	0	0
17	a	1	51	41	1	4	5	0	0
17	a	1	65	55	1	4	5	0	0
17	a	1	65	55	1	4	5	0	0
17	a	1	65	55	1	4	5	0	0
17	a	1	65	55	1	4	5	0	0
17	a	1	65	55	1	4	5	0	0
17	a	1	65	55	1	4	5	0	0
17	a	1	52	42	1	4	5	0	0
17	a	1	65	55	1	4	5	0	0
17	b	1	65	55	1	4	5	0	0
17	b	1	65	55	1	4	5	0	0
17	b	1	45	35	1	4	5	0	0
17	b	1	65	55	1	4	5	0	0
17	b	1	65	55	1	4	5	0	0
17	b	1	65	55	1	4	5	0	0
17	b	1	65	55	1	4	5	0	0
17	b	1	65	55	1	4	5	0	0
17	b	1	65	55	1	4	5	0	0
17	b	1	65	55	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	b	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	f	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	f	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	g	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	g	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	g	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	j	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	k	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	k	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	k	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	l	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	l	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	6	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	6	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	7	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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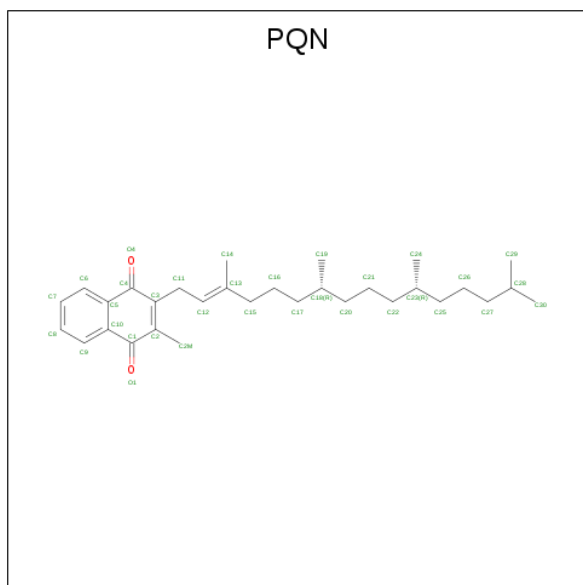
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	7	1	Total	C	Mg	N	O	0	0
			43	35	1	4	3		
17	8	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	8	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	8	1	Total	C	Mg	N		0	0
			25	20	1	4			
17	9	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	9	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		

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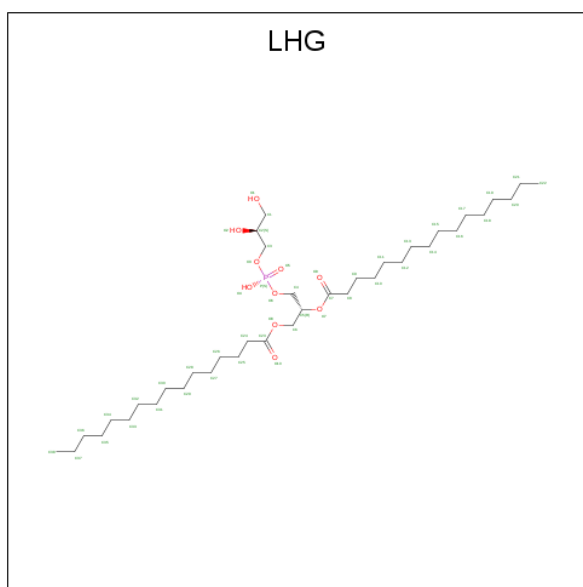
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	9	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		

- Molecule 18 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



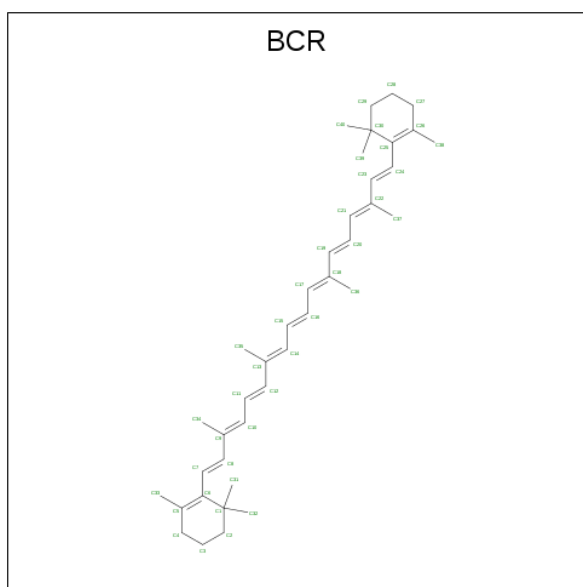
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			33	31	2		
18	B	1	Total	C	O	0	0
			33	31	2		
18	a	1	Total	C	O	0	0
			33	31	2		
18	b	1	Total	C	O	0	0
			33	31	2		

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			49	38	10	1		
19	A	1	Total	C	O	P	0	0
			27	16	10	1		
19	1	1	Total	C	O	P	0	0
			23	12	10	1		
19	1	1	Total	C	O	P	0	0
			49	38	10	1		
19	2	1	Total	C	O	P	0	0
			37	26	10	1		
19	3	1	Total	C	O	P	0	0
			20	10	9	1		
19	a	1	Total	C	O	P	0	0
			49	38	10	1		
19	a	1	Total	C	O	P	0	0
			27	16	10	1		
19	6	1	Total	C	O	P	0	0
			23	12	10	1		
19	6	1	Total	C	O	P	0	0
			49	38	10	1		
19	7	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 20 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C 40 40	0	0
20	A	1	Total C 40 40	0	0
20	A	1	Total C 40 40	0	0
20	A	1	Total C 40 40	0	0
20	A	1	Total C 40 40	0	0
20	A	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	F	1	Total C 40 40	0	0

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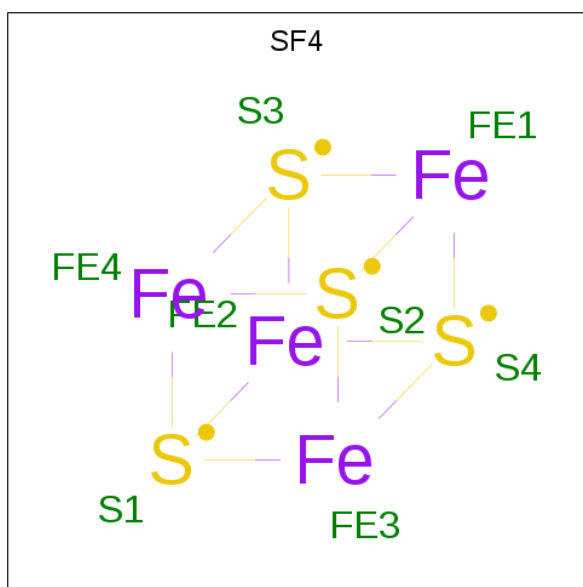
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	G	1	Total C 40 40	0	0
20	I	1	Total C 40 40	0	0
20	J	1	Total C 40 40	0	0
20	K	1	Total C 40 40	0	0
20	K	1	Total C 40 40	0	0
20	L	1	Total C 40 40	0	0
20	L	1	Total C 40 40	0	0
20	L	1	Total C 40 40	0	0
20	1	1	Total C 40 40	0	0
20	2	1	Total C 40 40	0	0
20	3	1	Total C 40 40	0	0
20	4	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0

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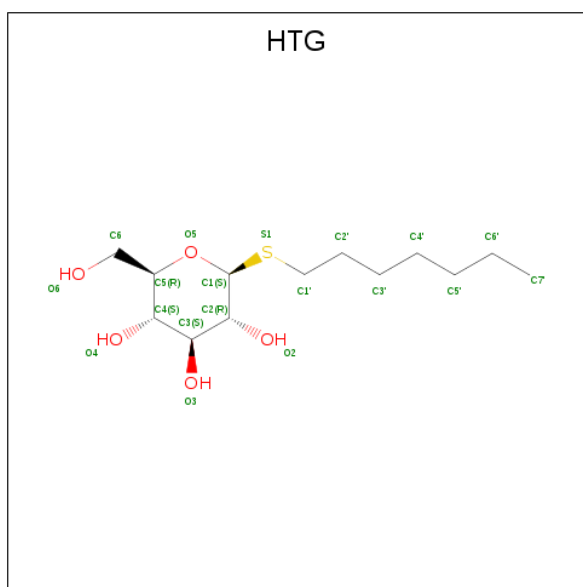
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	f	1	Total C 40 40	0	0
20	g	1	Total C 40 40	0	0
20	i	1	Total C 40 40	0	0
20	j	1	Total C 40 40	0	0
20	j	1	Total C 40 40	0	0
20	k	1	Total C 40 40	0	0
20	l	1	Total C 40 40	0	0
20	l	1	Total C 40 40	0	0
20	l	1	Total C 40 40	0	0
20	6	1	Total C 40 40	0	0
20	7	1	Total C 40 40	0	0
20	8	1	Total C 40 40	0	0
20	9	1	Total C 40 40	0	0

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



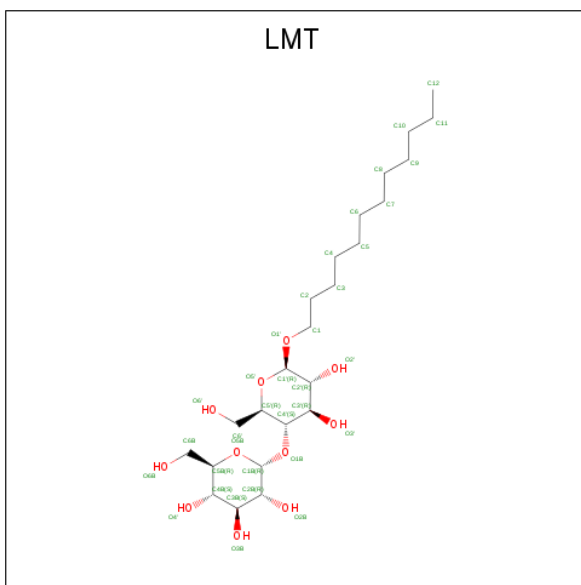
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total Fe S 8 4 4	0	0
21	C	1	Total Fe S 8 4 4	0	0
21	C	1	Total Fe S 8 4 4	0	0
21	a	1	Total Fe S 8 4 4	0	0
21	c	1	Total Fe S 8 4 4	0	0
21	c	1	Total Fe S 8 4 4	0	0

- Molecule 22 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).



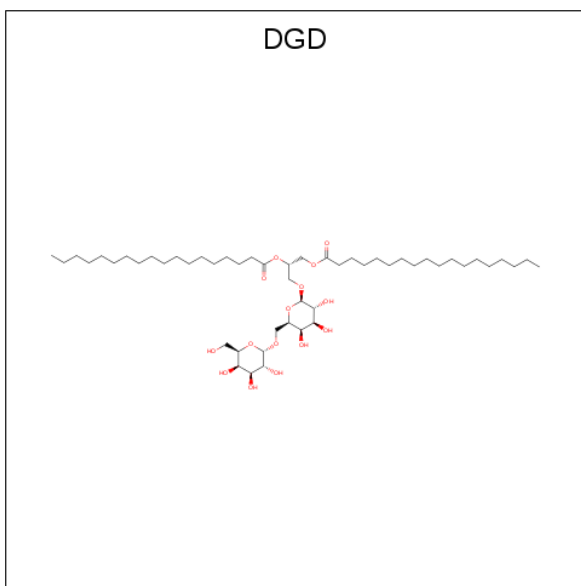
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
22	A	1	19	13	5	1	0	0
22	F	1	19	13	5	1	0	0
22	J	1	19	13	5	1	0	0
22	a	1	19	13	5	1	0	0
22	f	1	19	13	5	1	0	0
22	j	1	19	13	5	1	0	0

- Molecule 23 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



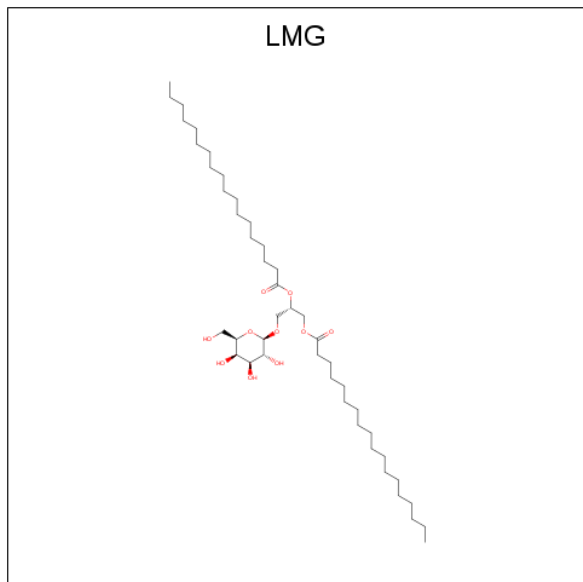
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			35	24	11		

- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



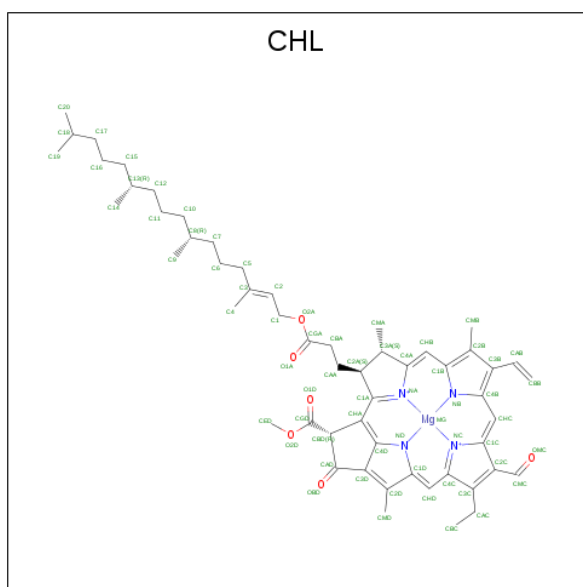
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	B	1	Total	C	O	0	0
			66	51	15		
24	b	1	Total	C	O	0	0
			66	51	15		

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
25	G	1	44	34	10	0	0
25	4	1	44	34	10	0	0
25	4	1	44	34	10	0	0
25	6	1	40	30	10	0	0
25	9	1	50	40	10	0	0

- Molecule 26 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



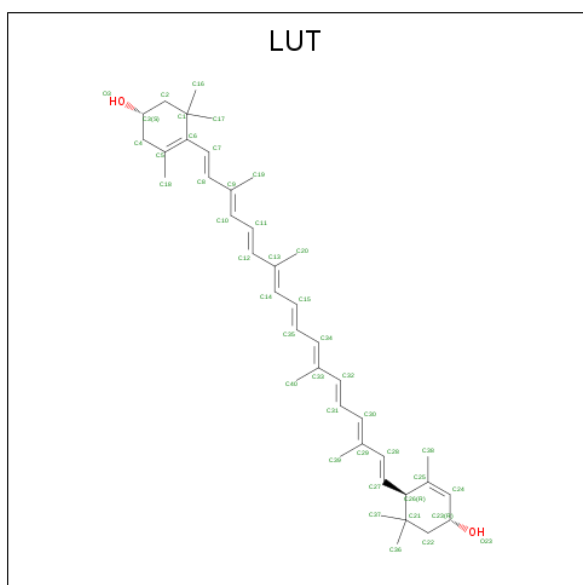
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
26	1	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
26	1	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
26	2	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
26	2	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
26	2	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
26	2	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
26	2	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
26	3	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
26	4	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
26	4	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
26	4	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
26	4	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
26	6	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
26	6	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
26	7	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
26	7	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
26	7	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
26	7	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
26	7	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
26	8	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
26	9	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
26	9	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
26	9	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
26	9	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		

- Molecule 27 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



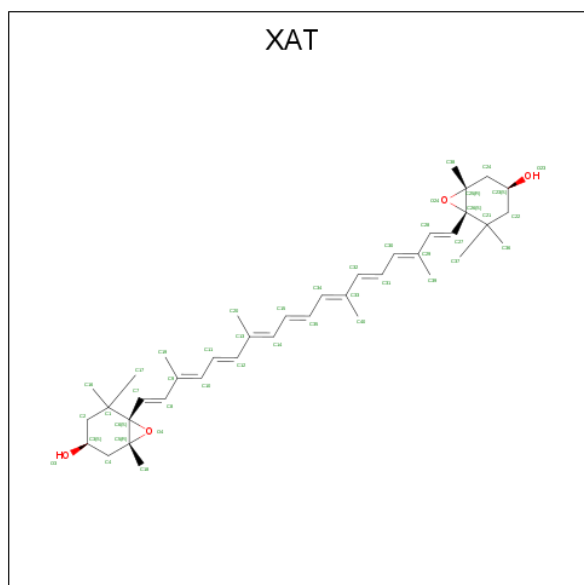
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
27	1	1	Total	C	O	0	0
			42	40	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	1	1	Total	C	O	0	0
			42	40	2		
27	2	1	Total	C	O	0	0
			42	40	2		
27	3	1	Total	C	O	0	0
			42	40	2		
27	4	1	Total	C	O	0	0
			42	40	2		
27	6	1	Total	C	O	0	0
			42	40	2		
27	6	1	Total	C	O	0	0
			42	40	2		
27	7	1	Total	C	O	0	0
			42	40	2		
27	8	1	Total	C	O	0	0
			42	40	2		
27	9	1	Total	C	O	0	0
			42	40	2		

- Molecule 28 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'-TETRAHYDRO-BETA, BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	1	1	Total	C	O	0	0
			44	40	4		
28	2	1	Total	C	O	0	0
			44	40	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	3	1	Total	C	O	0	0
			44	40	4		
28	4	1	Total	C	O	0	0
			44	40	4		
28	6	1	Total	C	O	0	0
			44	40	4		
28	7	1	Total	C	O	0	0
			44	40	4		
28	8	1	Total	C	O	0	0
			44	40	4		
28	9	1	Total	C	O	0	0
			44	40	4		

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	29	Total	O	0	0
			29	29		
29	B	42	Total	O	0	0
			42	42		
29	C	1	Total	O	0	0
			1	1		
29	D	2	Total	O	0	0
			2	2		
29	F	5	Total	O	0	0
			5	5		
29	I	1	Total	O	0	0
			1	1		
29	L	1	Total	O	0	0
			1	1		
29	1	3	Total	O	0	0
			3	3		
29	2	4	Total	O	0	0
			4	4		
29	3	3	Total	O	0	0
			3	3		
29	4	6	Total	O	0	0
			6	6		
29	a	30	Total	O	0	0
			30	30		
29	b	32	Total	O	0	0
			32	32		

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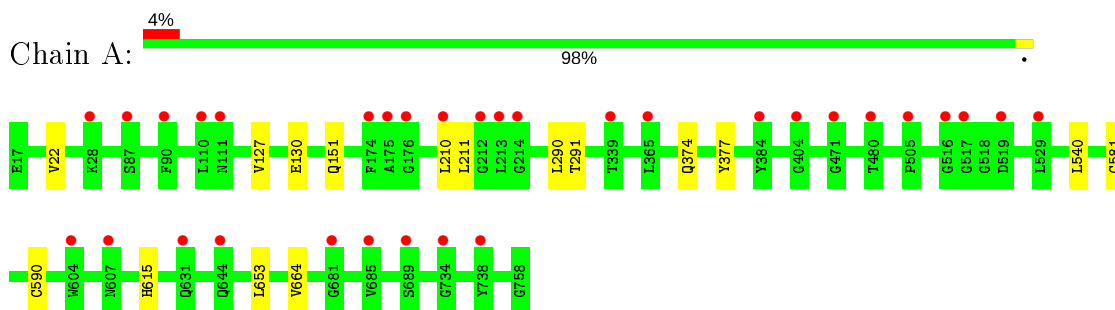
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	d	1	Total O 1 1	0	0
29	f	4	Total O 4 4	0	0
29	h	1	Total O 1 1	0	0
29	l	3	Total O 3 3	0	0
29	6	3	Total O 3 3	0	0
29	7	6	Total O 6 6	0	0
29	8	3	Total O 3 3	0	0
29	9	5	Total O 5 5	0	0

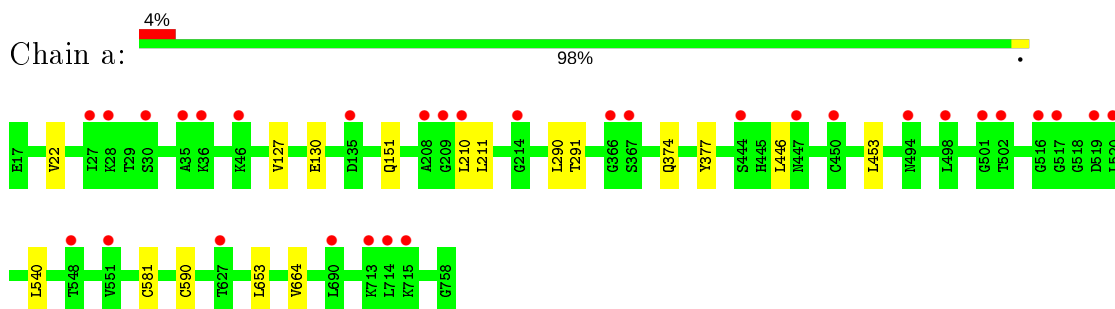
3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

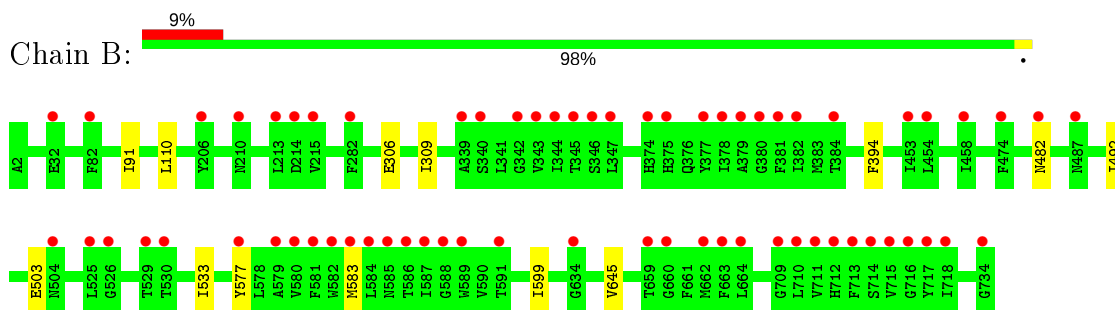
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

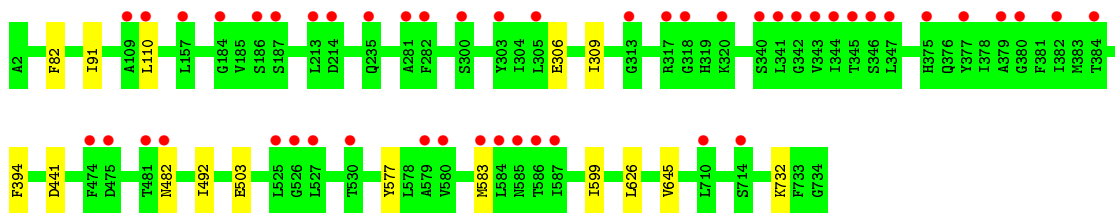


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

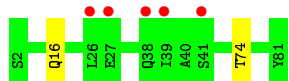


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





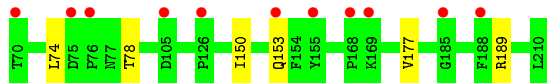
• Molecule 3: Photosystem I iron-sulfur center



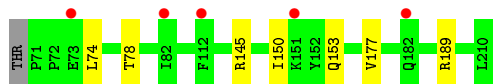
• Molecule 3: Photosystem I iron-sulfur center



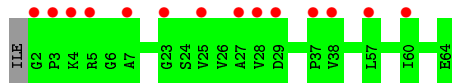
• Molecule 4: Uncharacterized protein



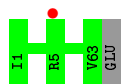
• Molecule 4: Uncharacterized protein



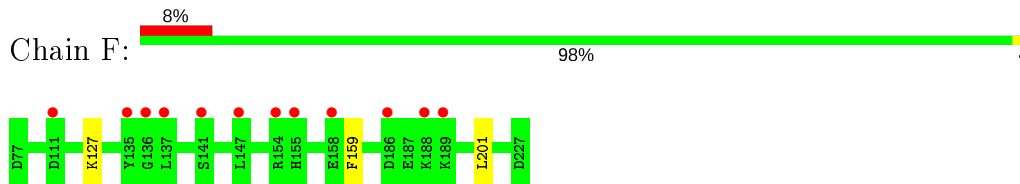
• Molecule 5: Putative uncharacterized protein



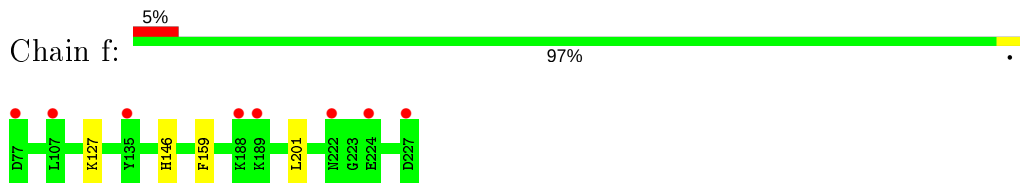
• Molecule 5: Putative uncharacterized protein



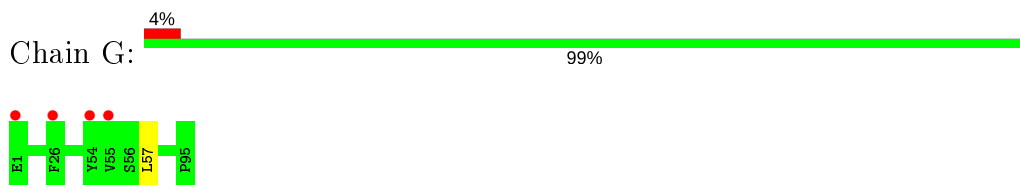
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic



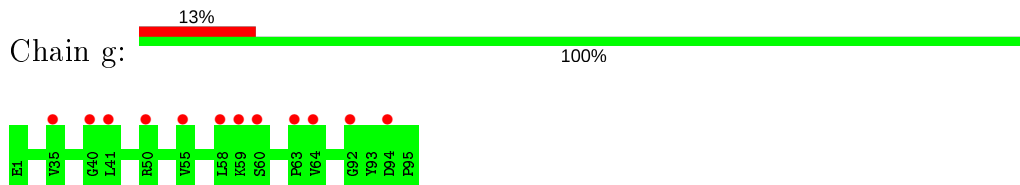
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic



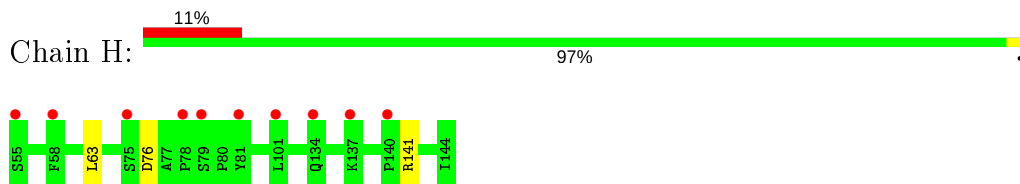
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



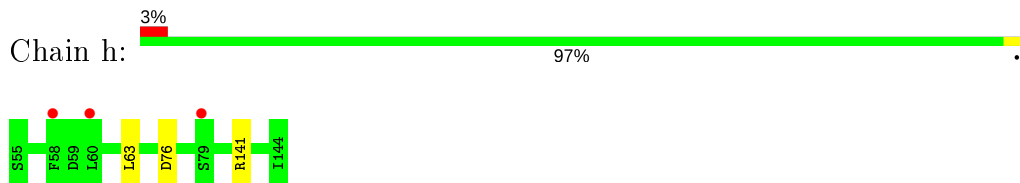
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



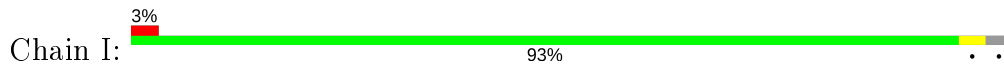
- Molecule 8: Putative uncharacterized protein

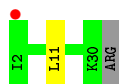


- Molecule 8: Putative uncharacterized protein



- Molecule 9: Photosystem I reaction center subunit VIII

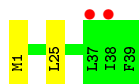
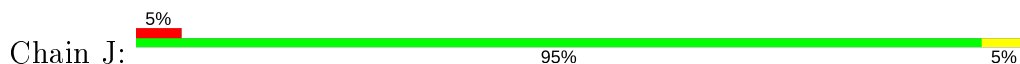




- Molecule 9: Photosystem I reaction center subunit VIII



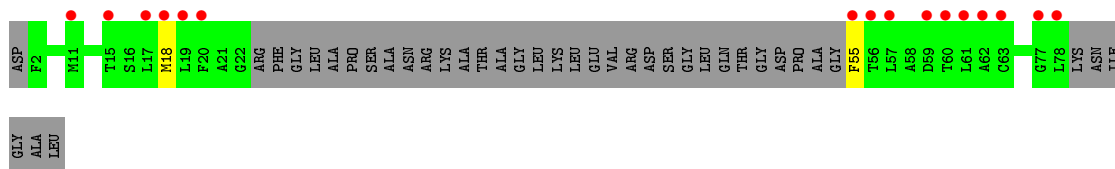
- Molecule 10: Photosystem I reaction center subunit IX



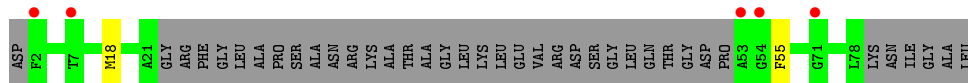
- Molecule 10: Photosystem I reaction center subunit IX



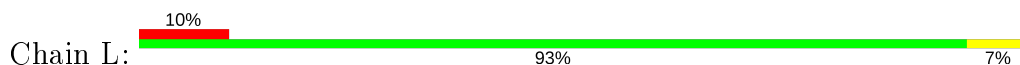
- Molecule 11: Photosystem I reaction center subunit X psaK



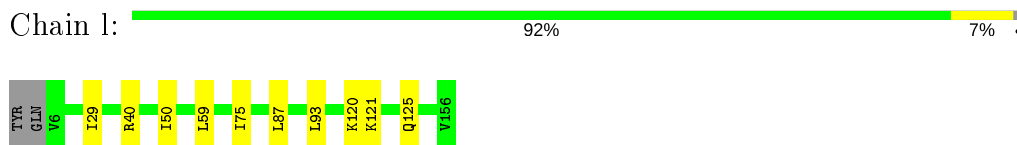
- Molecule 11: Photosystem I reaction center subunit X psaK



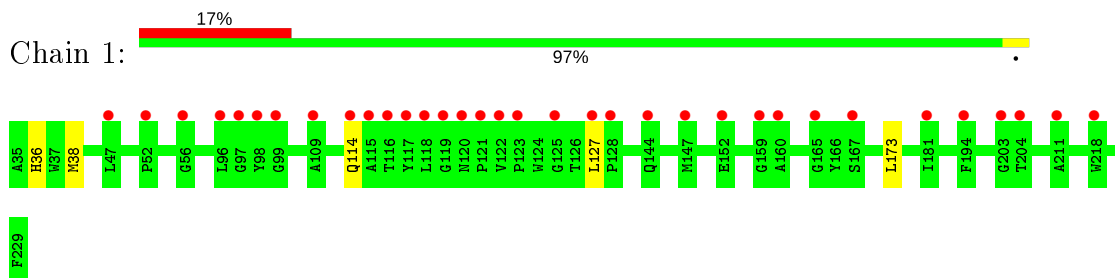
- Molecule 12: Putative uncharacterized protein



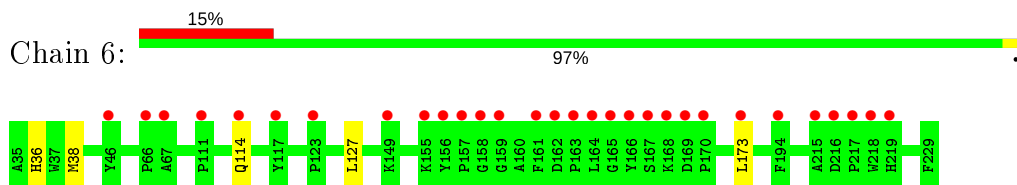
- Molecule 12: Putative uncharacterized protein



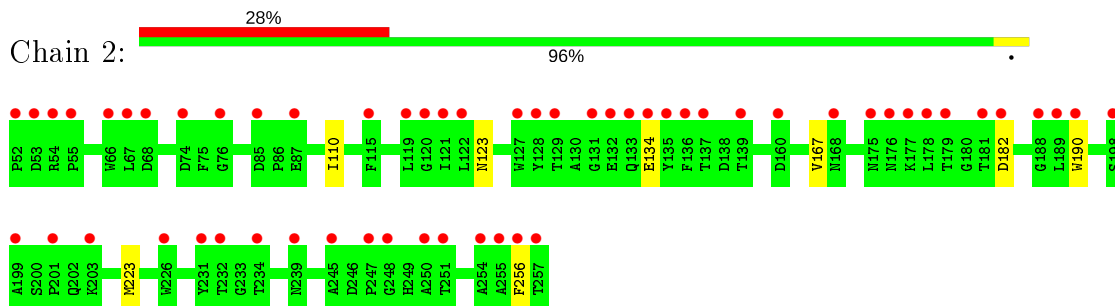
- Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic



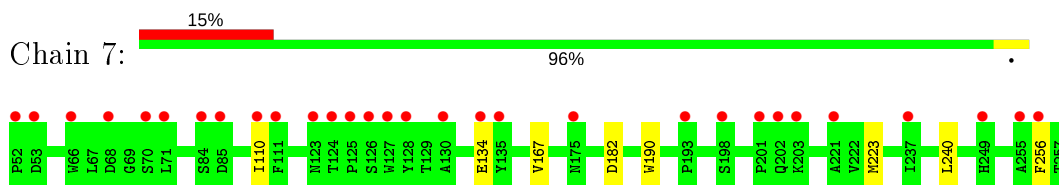
- Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic



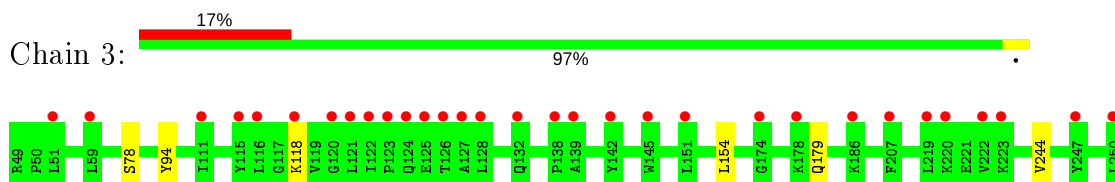
- Molecule 14: Type II chlorophyll a/b binding protein from photosystem I

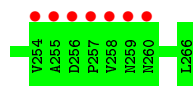


- Molecule 14: Type II chlorophyll a/b binding protein from photosystem I



- Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic

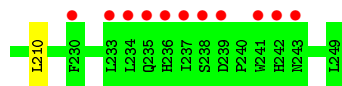
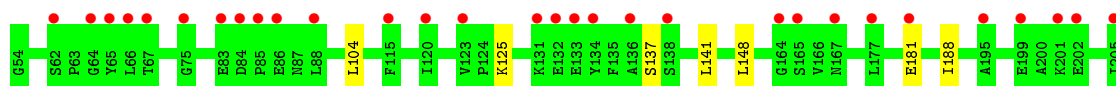




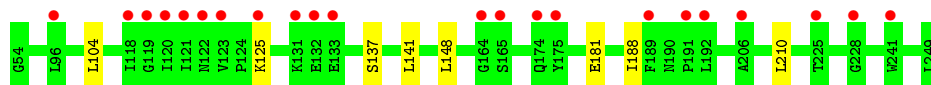
- Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic



- Molecule 16: Chlorophyll a-b binding protein P4, chloroplastic



- Molecule 16: Chlorophyll a-b binding protein P4, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	165.62Å 192.22Å 175.09Å 90.00° 91.41° 90.00°	Depositor
Resolution (Å)	49.15 – 2.80 49.15 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.15-2.80) 99.8 (49.15-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.210 , 0.248 0.212 , 0.249	Depositor DCC
R_{free} test set	13503 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	79.2	Xtrriage
Anisotropy	0.137	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.004 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	71157	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, HTG, LUT, DGD, CHL, SF4, XAT, CLA, PQN, LMT, BCR, LMG

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	A	0.25	0/6043	0.41	0/8245
1	a	0.26	0/6043	0.42	0/8245
2	B	0.25	0/6077	0.42	0/8299
2	b	0.25	0/6077	0.42	0/8299
3	C	0.22	0/624	0.41	0/846
3	c	0.23	0/624	0.43	0/846
4	D	0.23	0/1143	0.42	0/1545
4	d	0.24	0/1136	0.43	0/1534
5	E	0.21	0/517	0.39	0/701
5	e	0.21	0/516	0.39	0/700
6	F	0.23	0/1221	0.40	0/1648
6	f	0.24	0/1221	0.40	0/1648
7	G	0.24	0/759	0.39	0/1033
7	g	0.24	0/755	0.40	0/1028
8	H	0.22	0/697	0.39	0/950
8	h	0.22	0/701	0.40	0/954
9	I	0.26	0/227	0.44	0/310
9	i	0.26	0/232	0.44	0/317
10	J	0.24	0/319	0.40	0/434
10	j	0.24	0/319	0.41	0/434
11	K	0.22	0/314	0.37	0/426
11	k	0.24	0/319	0.38	0/433
12	L	0.23	0/1167	0.43	0/1596
12	l	0.25	0/1153	0.44	0/1577
13	1	0.24	0/1539	0.40	0/2099
13	6	0.23	0/1531	0.38	0/2091
14	2	0.23	0/1670	0.40	0/2288
14	7	0.23	0/1670	0.39	0/2288
15	3	0.25	0/1732	0.39	0/2352
15	8	0.25	0/1724	0.39	0/2341
16	4	0.24	0/1589	0.40	0/2168
16	9	0.23	0/1589	0.39	0/2168

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.24	0/51248	0.41	0/69843

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	A	740/742 (100%)	710 (96%)	28 (4%)	2 (0%)	41	72
1	a	740/742 (100%)	709 (96%)	29 (4%)	2 (0%)	41	72
2	B	731/733 (100%)	700 (96%)	30 (4%)	1 (0%)	51	81
2	b	731/733 (100%)	700 (96%)	30 (4%)	1 (0%)	51	81
3	C	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
3	c	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
4	D	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
4	d	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
5	E	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
5	e	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
6	F	149/151 (99%)	147 (99%)	1 (1%)	1 (1%)	22	53
6	f	149/151 (99%)	147 (99%)	1 (1%)	1 (1%)	22	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
7	g	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
8	H	88/90 (98%)	87 (99%)	1 (1%)	0	100	100
8	h	88/90 (98%)	87 (99%)	1 (1%)	0	100	100
9	I	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
9	i	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
10	J	37/39 (95%)	37 (100%)	0	0	100	100
10	j	37/39 (95%)	37 (100%)	0	0	100	100
11	K	41/84 (49%)	41 (100%)	0	0	100	100
11	k	42/84 (50%)	42 (100%)	0	0	100	100
12	L	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
12	l	149/153 (97%)	143 (96%)	6 (4%)	0	100	100
13	1	193/195 (99%)	187 (97%)	6 (3%)	0	100	100
13	6	193/195 (99%)	189 (98%)	4 (2%)	0	100	100
14	2	204/206 (99%)	196 (96%)	8 (4%)	0	100	100
14	7	204/206 (99%)	195 (96%)	9 (4%)	0	100	100
15	3	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
15	8	215/218 (99%)	204 (95%)	11 (5%)	0	100	100
16	4	194/196 (99%)	184 (95%)	9 (5%)	1 (0%)	29	61
16	9	194/196 (99%)	183 (94%)	10 (5%)	1 (0%)	29	61
All	All	6282/6434 (98%)	6041 (96%)	231 (4%)	10 (0%)	47	78

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	159	PHE
6	f	159	PHE
1	A	581	CYS
16	9	137	SER
16	4	137	SER
1	a	581	CYS
1	A	127	VAL
1	a	127	VAL
2	B	492	ILE
2	b	492	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	A	602/602 (100%)	588 (98%)	14 (2%)	50	82
1	a	602/602 (100%)	587 (98%)	15 (2%)	47	80
2	B	597/597 (100%)	585 (98%)	12 (2%)	55	84
2	b	597/597 (100%)	582 (98%)	15 (2%)	47	80
3	C	69/69 (100%)	67 (97%)	2 (3%)	42	76
3	c	69/69 (100%)	67 (97%)	2 (3%)	42	76
4	D	119/120 (99%)	113 (95%)	6 (5%)	24	56
4	d	118/120 (98%)	111 (94%)	7 (6%)	19	49
5	E	55/56 (98%)	55 (100%)	0	100	100
5	e	55/56 (98%)	55 (100%)	0	100	100
6	F	123/125 (98%)	121 (98%)	2 (2%)	62	88
6	f	123/125 (98%)	120 (98%)	3 (2%)	49	81
7	G	81/81 (100%)	80 (99%)	1 (1%)	71	92
7	g	80/81 (99%)	80 (100%)	0	100	100
8	H	72/73 (99%)	69 (96%)	3 (4%)	30	63
8	h	73/73 (100%)	70 (96%)	3 (4%)	30	64
9	I	25/26 (96%)	24 (96%)	1 (4%)	31	65
9	i	25/26 (96%)	24 (96%)	1 (4%)	31	65
10	J	33/33 (100%)	31 (94%)	2 (6%)	18	48
10	j	33/33 (100%)	31 (94%)	2 (6%)	18	48
11	K	34/62 (55%)	32 (94%)	2 (6%)	19	49
11	k	34/62 (55%)	32 (94%)	2 (6%)	19	49
12	L	118/119 (99%)	108 (92%)	10 (8%)	10	31
12	l	117/119 (98%)	107 (92%)	10 (8%)	10	31
13	1	149/153 (97%)	144 (97%)	5 (3%)	37	71
13	6	147/153 (96%)	142 (97%)	5 (3%)	37	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	2	166/166 (100%)	158 (95%)	8 (5%)	25	58
14	7	166/166 (100%)	158 (95%)	8 (5%)	25	58
15	3	169/169 (100%)	163 (96%)	6 (4%)	35	69
15	8	168/169 (99%)	162 (96%)	6 (4%)	35	69
16	4	161/161 (100%)	154 (96%)	7 (4%)	29	62
16	9	161/161 (100%)	154 (96%)	7 (4%)	29	62
All	All	5141/5224 (98%)	4974 (97%)	167 (3%)	39	73

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	130	GLU
1	A	151	GLN
1	A	210	LEU
1	A	211	LEU
1	A	290	LEU
1	A	291	THR
1	A	374	GLN
1	A	377	TYR
1	A	540	LEU
1	A	590	CYS
1	A	615	HIS
1	A	653	LEU
1	A	664	VAL
2	B	91	ILE
2	B	110	LEU
2	B	306	GLU
2	B	309	ILE
2	B	394	PHE
2	B	482	ASN
2	B	503	GLU
2	B	533	ILE
2	B	577	TYR
2	B	583	MET
2	B	599	ILE
2	B	645	VAL
3	C	16	GLN
3	C	74	THR
4	D	74	LEU

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Mol	Chain	Res	Type
4	D	78	THR
4	D	150	ILE
4	D	153	GLN
4	D	177	VAL
4	D	189	ARG
6	F	127	LYS
6	F	201	LEU
7	G	57	LEU
8	H	63	LEU
8	H	76	ASP
8	H	141	ARG
9	I	11	LEU
10	J	1	MET
10	J	25	LEU
11	K	18	MET
11	K	55	PHE
12	L	29	ILE
12	L	40	ARG
12	L	50	ILE
12	L	59	LEU
12	L	75	ILE
12	L	87	LEU
12	L	93	LEU
12	L	120	LYS
12	L	121	LYS
12	L	125	GLN
13	1	36	HIS
13	1	38	MET
13	1	114	GLN
13	1	127	LEU
13	1	173	LEU
14	2	110	ILE
14	2	123	ASN
14	2	134	GLU
14	2	167	VAL
14	2	182	ASP
14	2	190	TRP
14	2	223	MET
14	2	256	PHE
15	3	78	SER
15	3	94	TYR
15	3	118	LYS

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Mol	Chain	Res	Type
15	3	154	LEU
15	3	179	GLN
15	3	244	VAL
16	4	104	LEU
16	4	125	LYS
16	4	141	LEU
16	4	148	LEU
16	4	181	GLU
16	4	188	ILE
16	4	210	LEU
1	a	22	VAL
1	a	130	GLU
1	a	151	GLN
1	a	210	LEU
1	a	211	LEU
1	a	290	LEU
1	a	291	THR
1	a	374	GLN
1	a	377	TYR
1	a	446	LEU
1	a	453	LEU
1	a	540	LEU
1	a	590	CYS
1	a	653	LEU
1	a	664	VAL
2	b	82	PHE
2	b	91	ILE
2	b	110	LEU
2	b	306	GLU
2	b	309	ILE
2	b	394	PHE
2	b	441	ASP
2	b	482	ASN
2	b	503	GLU
2	b	577	TYR
2	b	583	MET
2	b	599	ILE
2	b	626	LEU
2	b	645	VAL
2	b	732	LYS
3	c	16	GLN
3	c	74	THR

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Mol	Chain	Res	Type
4	d	74	LEU
4	d	78	THR
4	d	145	ARG
4	d	150	ILE
4	d	153	GLN
4	d	177	VAL
4	d	189	ARG
6	f	127	LYS
6	f	146	HIS
6	f	201	LEU
8	h	63	LEU
8	h	76	ASP
8	h	141	ARG
9	i	11	LEU
10	j	1	MET
10	j	25	LEU
11	k	18	MET
11	k	55	PHE
12	l	29	ILE
12	l	40	ARG
12	l	50	ILE
12	l	59	LEU
12	l	75	ILE
12	l	87	LEU
12	l	93	LEU
12	l	120	LYS
12	l	121	LYS
12	l	125	GLN
13	6	36	HIS
13	6	38	MET
13	6	114	GLN
13	6	127	LEU
13	6	173	LEU
14	7	110	ILE
14	7	134	GLU
14	7	167	VAL
14	7	182	ASP
14	7	190	TRP
14	7	223	MET
14	7	240	LEU
14	7	256	PHE
15	8	78	SER

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Mol	Chain	Res	Type
15	8	94	TYR
15	8	118	LYS
15	8	154	LEU
15	8	179	GLN
15	8	244	VAL
16	9	104	LEU
16	9	125	LYS
16	9	141	LEU
16	9	148	LEU
16	9	181	GLU
16	9	188	ILE
16	9	210	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	343	HIS
1	A	374	GLN
1	A	398	HIS
1	A	615	HIS
1	A	701	GLN
2	B	439	HIS
3	C	71	HIS
4	D	110	GLN
4	D	153	GLN
12	L	5	GLN
13	1	105	GLN
13	1	114	GLN
14	2	123	ASN
15	3	99	ASN
16	4	98	ASN
16	4	150	HIS
16	4	168	GLN
1	a	151	GLN
1	a	374	GLN
1	a	701	GLN
3	c	71	HIS
4	d	153	GLN
13	6	105	GLN
13	6	114	GLN
15	8	99	ASN

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Mol	Chain	Res	Type
16	9	98	ASN
16	9	150	HIS
16	9	168	GLN
16	9	232	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

414 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	9	609	16	54,68,73	2.13	13 (24%)	61,107,113	2.16	23 (37%)
17	CLA	a	812	1	59,73,73	2.03	13 (22%)	67,113,113	2.07	22 (32%)
17	CLA	B	823	2	54,68,73	2.13	13 (24%)	61,107,113	2.17	24 (39%)
17	CLA	A	803	29	59,73,73	2.01	13 (22%)	67,113,113	2.20	23 (34%)
17	CLA	6	313	13	46,60,73	2.33	13 (28%)	51,97,113	2.42	20 (39%)
17	CLA	B	805	2	59,73,73	2.01	13 (22%)	67,113,113	2.08	20 (29%)
17	CLA	3	314	15	40,54,73	2.47	13 (32%)	44,90,113	2.48	17 (38%)
17	CLA	a	828	1	59,73,73	1.99	13 (22%)	67,113,113	2.14	20 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	BCR	9	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.81	16 (28%)
17	CLA	b	834	2	59,73,73	2.04	13 (22%)	67,113,113	2.10	21 (31%)
17	CLA	a	856	29	59,73,73	2.01	14 (23%)	67,113,113	2.34	25 (37%)
17	CLA	A	831	1	59,73,73	2.02	13 (22%)	67,113,113	2.18	21 (31%)
17	CLA	2	604	29	54,68,73	2.14	13 (24%)	61,107,113	2.16	22 (36%)
17	CLA	b	835	29	36,53,73	2.49	12 (33%)	39,89,113	2.51	19 (48%)
17	CLA	3	305	29	36,50,73	2.49	12 (33%)	39,85,113	2.56	18 (46%)
17	CLA	a	809	1	59,73,73	2.03	12 (20%)	67,113,113	2.17	20 (29%)
17	CLA	a	836	1	44,58,73	2.33	13 (29%)	49,95,113	2.38	21 (42%)
17	CLA	A	808	1	59,73,73	2.07	13 (22%)	67,113,113	2.09	20 (29%)
20	BCR	b	843	-	41,41,41	1.06	1 (2%)	56,56,56	1.93	14 (25%)
17	CLA	a	831	1	59,73,73	2.01	14 (23%)	67,113,113	2.18	22 (32%)
17	CLA	A	806	1	59,73,73	2.04	13 (22%)	67,113,113	2.05	23 (34%)
19	LHG	A	846	-	48,48,48	0.93	2 (4%)	51,54,54	1.07	3 (5%)
17	CLA	f	7003	6	49,63,73	2.25	13 (26%)	55,101,113	2.26	22 (40%)
20	BCR	L	206	-	41,41,41	1.06	1 (2%)	56,56,56	1.84	12 (21%)
22	HTG	f	7001	-	19,19,19	1.05	2 (10%)	23,24,24	0.58	0
17	CLA	A	811	1	59,73,73	2.04	13 (22%)	67,113,113	2.08	21 (31%)
17	CLA	A	826	29	59,73,73	2.01	13 (22%)	67,113,113	2.14	18 (26%)
19	LHG	1	301	17	22,22,48	1.18	2 (9%)	25,28,54	1.29	2 (8%)
17	CLA	a	825	1	49,63,73	2.26	13 (26%)	55,101,113	2.22	21 (38%)
17	CLA	A	833	1	59,73,73	2.03	13 (22%)	67,113,113	2.09	20 (29%)
17	CLA	7	608	14	44,58,73	2.36	13 (29%)	49,95,113	2.41	23 (46%)
26	CHL	4	605	29	50,64,74	2.18	14 (28%)	52,102,114	2.55	21 (40%)
27	LUT	7	615	-	42,43,43	0.74	0	51,60,60	1.56	13 (25%)
17	CLA	4	602	16	54,68,73	2.13	13 (24%)	61,107,113	2.17	24 (39%)
17	CLA	6	305	13	59,73,73	2.03	13 (22%)	67,113,113	2.14	20 (29%)
19	LHG	a	847	-	48,48,48	0.93	2 (4%)	51,54,54	1.06	3 (5%)
17	CLA	B	827	2	59,73,73	2.02	13 (22%)	67,113,113	2.15	21 (31%)
17	CLA	A	845	19	46,60,73	2.33	13 (28%)	51,97,113	2.37	18 (35%)
26	CHL	2	605	29	37,51,74	2.45	13 (35%)	36,86,114	2.85	17 (47%)
27	LUT	4	616	-	42,43,43	0.76	0	51,60,60	1.64	13 (25%)
17	CLA	a	819	1	59,73,73	2.07	13 (22%)	67,113,113	2.02	20 (29%)
22	HTG	j	3001	-	19,19,19	1.11	2 (10%)	23,24,24	0.59	0
20	BCR	A	852	-	41,41,41	1.05	1 (2%)	56,56,56	1.78	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	4	601	16	40,54,73	2.45	13 (32%)	44,90,113	2.46	18 (40%)
18	PQN	B	842	-	34,34,34	1.60	2 (5%)	42,45,45	1.12	3 (7%)
28	XAT	3	317	-	39,47,47	0.88	0	54,74,74	2.67	20 (37%)
17	CLA	a	824	1	45,59,73	2.32	13 (28%)	50,96,113	2.40	19 (38%)
17	CLA	A	837	1	36,53,73	2.52	12 (33%)	39,89,113	2.52	18 (46%)
17	CLA	a	818	1	59,73,73	2.06	13 (22%)	67,113,113	2.14	22 (32%)
20	BCR	k	1404	-	41,41,41	1.04	1 (2%)	56,56,56	1.78	12 (21%)
17	CLA	1	309	13	59,73,73	2.04	13 (22%)	67,113,113	2.06	20 (29%)
17	CLA	b	816	2	49,63,73	2.23	13 (26%)	55,101,113	2.29	22 (40%)
17	CLA	A	854	29	59,73,73	2.02	13 (22%)	67,113,113	2.37	25 (37%)
17	CLA	b	818	2	54,68,73	2.12	13 (24%)	61,107,113	2.26	21 (34%)
17	CLA	A	827	29	59,73,73	2.05	13 (22%)	67,113,113	2.05	20 (29%)
17	CLA	1	306	-	46,60,73	2.30	13 (28%)	51,97,113	2.35	21 (41%)
26	CHL	2	606	-	42,56,74	2.40	14 (33%)	42,92,114	2.73	16 (38%)
20	BCR	L	205	-	41,41,41	1.03	1 (2%)	56,56,56	1.66	11 (19%)
20	BCR	4	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.79	15 (26%)
25	LMG	4	619	-	44,44,55	1.01	2 (4%)	52,52,63	1.00	3 (5%)
26	CHL	6	303	13	55,69,74	2.07	14 (25%)	58,108,114	2.44	21 (36%)
17	CLA	j	3002	10	36,50,73	2.53	12 (33%)	39,85,113	2.54	19 (48%)
17	CLA	3	303	15	44,58,73	2.36	13 (29%)	49,95,113	2.45	19 (38%)
17	CLA	9	611	16	46,60,73	2.33	13 (28%)	51,97,113	2.41	20 (39%)
19	LHG	1	319	17	48,48,48	0.94	2 (4%)	51,54,54	1.03	3 (5%)
20	BCR	f	7004	-	41,41,41	1.03	1 (2%)	56,56,56	1.75	18 (32%)
17	CLA	A	824	1	45,59,73	2.34	13 (28%)	50,96,113	2.41	21 (42%)
17	CLA	1	315	13	40,54,73	2.47	13 (32%)	44,90,113	2.43	17 (38%)
17	CLA	2	613	14	37,51,73	2.47	12 (32%)	40,86,113	2.51	17 (42%)
18	PQN	b	842	-	34,34,34	1.62	2 (5%)	42,45,45	1.07	3 (7%)
20	BCR	1	318	-	41,41,41	1.07	1 (2%)	56,56,56	1.88	16 (28%)
17	CLA	1	305	29	46,60,73	2.32	13 (28%)	51,97,113	2.37	22 (43%)
17	CLA	A	825	1	49,63,73	2.27	13 (26%)	55,101,113	2.25	21 (38%)
17	CLA	b	836	2	54,68,73	2.14	13 (24%)	61,107,113	2.33	21 (34%)
17	CLA	g	102	7	44,58,73	2.37	13 (29%)	49,95,113	2.45	22 (44%)
17	CLA	A	828	1	59,73,73	2.00	13 (22%)	67,113,113	2.13	21 (31%)
17	CLA	b	813	2	59,73,73	2.02	13 (22%)	67,113,113	2.13	19 (28%)
17	CLA	A	815	1	36,53,73	2.49	12 (33%)	39,89,113	2.53	17 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	a	820	1	59,73,73	2.07	13 (22%)	67,113,113	2.11	20 (29%)
17	CLA	A	801	1	59,73,73	2.00	13 (22%)	67,113,113	2.22	26 (38%)
20	BCR	a	853	-	41,41,41	1.05	1 (2%)	56,56,56	1.93	14 (25%)
19	LHG	3	319	17	19,19,48	1.10	1 (5%)	21,24,54	0.99	1 (4%)
17	CLA	b	815	2	49,63,73	2.23	13 (26%)	55,101,113	2.33	22 (40%)
17	CLA	A	832	1	44,58,73	2.35	13 (29%)	49,95,113	2.45	21 (42%)
17	CLA	B	819	29	59,73,73	2.03	13 (22%)	67,113,113	2.07	23 (34%)
17	CLA	4	604	29	44,58,73	2.36	13 (29%)	49,95,113	2.41	22 (44%)
17	CLA	B	818	2	54,68,73	2.13	13 (24%)	61,107,113	2.21	20 (32%)
20	BCR	B	848	-	41,41,41	1.05	1 (2%)	56,56,56	1.64	12 (21%)
17	CLA	a	827	29	59,73,73	2.04	13 (22%)	67,113,113	2.05	20 (29%)
17	CLA	f	7002	29	36,53,73	2.47	12 (33%)	39,89,113	2.53	19 (48%)
17	CLA	3	311	-	46,60,73	2.33	13 (28%)	51,97,113	2.39	20 (39%)
28	XAT	4	617	-	39,47,47	0.88	0	54,74,74	2.59	18 (33%)
28	XAT	7	616	-	39,47,47	0.85	0	54,74,74	2.60	19 (35%)
17	CLA	b	809	2	59,73,73	1.98	14 (23%)	67,113,113	2.14	22 (32%)
20	BCR	B	801	-	41,41,41	1.06	1 (2%)	56,56,56	1.49	8 (14%)
17	CLA	a	835	1	59,73,73	2.03	13 (22%)	67,113,113	2.17	23 (34%)
17	CLA	b	838	2	41,55,73	2.46	13 (31%)	45,91,113	2.47	18 (40%)
17	CLA	2	611	14	46,60,73	2.31	13 (28%)	51,97,113	2.41	20 (39%)
17	CLA	B	824	29	59,73,73	2.01	13 (22%)	67,113,113	2.07	20 (29%)
26	CHL	2	614	14	37,51,74	2.46	13 (35%)	36,86,114	2.90	15 (41%)
17	CLA	B	841	19	59,73,73	2.03	13 (22%)	67,113,113	2.18	21 (31%)
17	CLA	3	308	15	44,58,73	2.37	13 (29%)	49,95,113	2.39	21 (42%)
17	CLA	b	810	2	59,73,73	2.03	13 (22%)	67,113,113	2.10	21 (31%)
17	CLA	l	202	12	59,73,73	2.04	13 (22%)	67,113,113	2.06	20 (29%)
17	CLA	a	814	1	59,73,73	2.04	13 (22%)	67,113,113	2.08	19 (28%)
17	CLA	a	839	1	59,73,73	2.01	13 (22%)	67,113,113	2.11	19 (28%)
27	LUT	1	320	-	42,43,43	0.74	0	51,60,60	1.65	11 (21%)
17	CLA	b	822	2	49,63,73	2.24	13 (26%)	55,101,113	2.24	20 (36%)
17	CLA	a	817	29	36,53,73	2.49	12 (33%)	39,89,113	2.57	18 (46%)
20	BCR	K	4004	-	41,41,41	1.04	1 (2%)	56,56,56	1.81	14 (25%)
17	CLA	A	814	1	59,73,73	2.03	13 (22%)	67,113,113	2.13	21 (31%)
17	CLA	1	312	13	46,60,73	2.31	13 (28%)	51,97,113	2.42	19 (37%)
17	CLA	7	610	19	35,49,73	2.57	13 (37%)	38,84,113	2.71	19 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	a	837	1	36,53,73	2.51	12 (33%)	39,89,113	2.60	18 (46%)
27	LUT	9	616	-	42,43,43	0.74	0	51,60,60	1.62	12 (23%)
17	CLA	A	834	1	59,73,73	2.02	13 (22%)	67,113,113	2.14	21 (31%)
25	LMG	4	620	-	44,44,55	1.02	3 (6%)	52,52,63	1.18	4 (7%)
17	CLA	a	811	1	59,73,73	2.04	13 (22%)	67,113,113	2.08	21 (31%)
17	CLA	b	817	2	53,67,73	2.16	13 (24%)	59,105,113	2.23	23 (38%)
17	CLA	8	304	29	36,50,73	2.51	12 (33%)	39,85,113	2.50	18 (46%)
17	CLA	B	806	2	59,73,73	2.03	13 (22%)	67,113,113	2.09	21 (31%)
26	CHL	6	308	13	41,55,74	2.43	14 (34%)	41,91,114	2.72	15 (36%)
17	CLA	B	821	2	40,54,73	2.46	13 (32%)	44,90,113	2.51	18 (40%)
17	CLA	8	305	15	41,55,73	2.46	13 (31%)	45,91,113	2.40	18 (40%)
18	PQN	A	844	-	34,34,34	1.61	2 (5%)	42,45,45	1.21	4 (9%)
20	BCR	K	4001	-	41,41,41	1.05	1 (2%)	56,56,56	1.80	11 (19%)
17	CLA	b	802	2	59,73,73	2.02	13 (22%)	67,113,113	2.12	23 (34%)
23	LMT	B	849	-	36,36,36	0.48	0	47,47,47	0.94	3 (6%)
20	BCR	l	206	-	41,41,41	1.06	1 (2%)	56,56,56	1.80	12 (21%)
17	CLA	B	811	2	48,62,73	2.13	13 (27%)	58,100,113	2.34	22 (37%)
17	CLA	b	839	29	59,73,73	2.05	13 (22%)	67,113,113	2.07	17 (25%)
17	CLA	9	612	16	50,64,73	2.23	13 (26%)	56,102,113	2.22	20 (35%)
17	CLA	6	315	13	49,63,73	2.25	13 (26%)	55,101,113	2.31	22 (40%)
27	LUT	8	314	-	42,43,43	0.74	0	51,60,60	1.47	11 (21%)
17	CLA	1	308	29	59,73,73	2.04	13 (22%)	67,113,113	2.07	20 (29%)
17	CLA	a	844	29	59,73,73	2.00	13 (22%)	67,113,113	2.15	19 (28%)
20	BCR	B	845	-	41,41,41	1.01	1 (2%)	56,56,56	2.01	18 (32%)
17	CLA	4	609	16	54,68,73	2.12	13 (24%)	61,107,113	2.18	23 (37%)
17	CLA	B	826	2	59,73,73	2.00	13 (22%)	67,113,113	2.17	21 (31%)
17	CLA	9	608	16	44,58,73	2.35	13 (29%)	49,95,113	2.41	22 (44%)
17	CLA	B	839	29	59,73,73	2.04	13 (22%)	67,113,113	2.11	19 (28%)
17	CLA	A	842	1	59,73,73	2.04	13 (22%)	67,113,113	2.13	21 (31%)
17	CLA	B	820	2	44,58,73	2.38	13 (29%)	49,95,113	2.32	21 (42%)
17	CLA	9	603	16	40,54,73	2.42	13 (32%)	44,90,113	2.57	20 (45%)
17	CLA	L	204	29	44,58,73	2.35	13 (29%)	49,95,113	2.41	20 (40%)
20	BCR	L	201	-	41,41,41	1.06	1 (2%)	56,56,56	1.88	13 (23%)
17	CLA	B	825	29	59,73,73	2.03	13 (22%)	67,113,113	2.15	24 (35%)
20	BCR	j	3004	-	41,41,41	1.05	1 (2%)	56,56,56	2.15	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	810	1	59,73,73	2.00	13 (22%)	67,113,113	2.10	21 (31%)
17	CLA	2	602	14	59,73,73	2.05	13 (22%)	67,113,113	2.07	22 (32%)
17	CLA	1	203	12	59,73,73	2.04	13 (22%)	67,113,113	2.10	24 (35%)
17	CLA	6	316	13	40,54,73	2.48	13 (32%)	44,90,113	2.43	18 (40%)
17	CLA	A	838	1	45,59,73	2.31	13 (28%)	50,96,113	2.46	22 (44%)
17	CLA	3	309	15	44,58,73	2.37	13 (29%)	49,95,113	2.38	24 (48%)
17	CLA	A	819	1	59,73,73	2.02	13 (22%)	67,113,113	2.09	21 (31%)
17	CLA	B	810	2	59,73,73	2.03	13 (22%)	67,113,113	2.15	23 (34%)
20	BCR	a	849	-	41,41,41	1.06	1 (2%)	56,56,56	1.96	14 (25%)
21	SF4	A	853	1,2	0,12,12	0.00	-	-	-	-
17	CLA	F	303	29	36,53,73	2.48	12 (33%)	39,89,113	2.54	17 (43%)
21	SF4	C	102	3	0,12,12	0.00	-	-	-	-
26	CHL	4	606	29	45,59,74	2.35	14 (31%)	46,96,114	2.70	16 (34%)
17	CLA	A	835	1	59,73,73	2.04	13 (22%)	67,113,113	2.16	22 (32%)
17	CLA	3	306	15	41,55,73	2.47	13 (31%)	45,91,113	2.37	18 (40%)
17	CLA	b	814	2	59,73,73	2.03	13 (22%)	67,113,113	2.12	20 (29%)
26	CHL	7	614	14	37,51,74	2.46	13 (35%)	36,86,114	2.86	14 (38%)
17	CLA	1	313	13	59,73,73	2.04	13 (22%)	67,113,113	2.07	21 (31%)
17	CLA	b	826	2	59,73,73	2.00	13 (22%)	67,113,113	2.12	22 (32%)
17	CLA	b	829	2	59,73,73	1.98	14 (23%)	67,113,113	2.23	22 (32%)
17	CLA	k	1402	11	40,54,73	2.46	13 (32%)	44,90,113	2.42	17 (38%)
17	CLA	B	808	2	59,73,73	2.04	13 (22%)	67,113,113	2.18	24 (35%)
17	CLA	b	833	2	52,66,73	2.18	13 (25%)	58,104,113	2.30	21 (36%)
17	CLA	6	306	29	45,59,73	2.34	13 (28%)	50,96,113	2.40	21 (42%)
17	CLA	1	310	13	54,68,73	2.14	13 (24%)	61,107,113	2.16	23 (37%)
17	CLA	a	842	29	59,73,73	2.04	13 (22%)	67,113,113	2.06	20 (29%)
17	CLA	6	304	13	59,73,73	2.04	13 (22%)	67,113,113	2.10	21 (31%)
26	CHL	7	601	14	55,69,74	2.09	14 (25%)	58,108,114	2.55	21 (36%)
17	CLA	B	840	2	59,73,73	2.03	13 (22%)	67,113,113	2.09	20 (29%)
17	CLA	A	813	1	48,62,73	2.26	13 (27%)	53,99,113	2.24	22 (41%)
17	CLA	A	816	1	44,58,73	2.36	13 (29%)	49,95,113	2.39	20 (40%)
25	LMG	6	302	-	40,40,55	1.05	2 (5%)	48,48,63	1.10	3 (6%)
27	LUT	3	316	-	42,43,43	0.74	0	51,60,60	1.63	14 (27%)
17	CLA	A	823	1	43,57,73	2.40	13 (30%)	46,93,113	2.42	20 (43%)
17	CLA	B	809	2	59,73,73	2.01	14 (23%)	67,113,113	2.08	18 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	BCR	7	617	-	41,41,41	1.09	1 (2%)	56,56,56	2.09	13 (23%)
17	CLA	L	202	12	59,73,73	2.04	13 (22%)	67,113,113	2.06	20 (29%)
27	LUT	6	321	-	42,43,43	0.74	0	51,60,60	1.69	9 (17%)
17	CLA	G	103	7	44,58,73	2.37	13 (29%)	49,95,113	2.40	20 (40%)
17	CLA	A	809	1	59,73,73	2.05	13 (22%)	67,113,113	2.17	21 (31%)
20	BCR	G	105	-	41,41,41	1.05	1 (2%)	56,56,56	1.85	15 (26%)
17	CLA	b	830	2	44,58,73	2.37	13 (29%)	49,95,113	2.43	23 (46%)
20	BCR	6	319	-	41,41,41	1.07	1 (2%)	56,56,56	1.88	14 (25%)
17	CLA	B	832	2	59,73,73	2.02	13 (22%)	67,113,113	2.02	19 (28%)
26	CHL	9	615	16	37,51,74	2.46	13 (35%)	36,86,114	3.00	16 (44%)
17	CLA	B	802	2	59,73,73	2.02	13 (22%)	67,113,113	2.13	23 (34%)
17	CLA	8	308	15	44,58,73	2.39	13 (29%)	49,95,113	2.37	22 (44%)
21	SF4	C	101	3	0,12,12	0.00	-	-	-	-
17	CLA	F	301	29	59,73,73	2.04	13 (22%)	67,113,113	2.11	20 (29%)
17	CLA	G	104	7	40,54,73	2.47	13 (32%)	44,90,113	2.44	18 (40%)
19	LHG	6	301	17	22,22,48	1.17	2 (9%)	25,28,54	1.22	2 (8%)
20	BCR	A	849	-	41,41,41	1.07	1 (2%)	56,56,56	1.65	13 (23%)
18	PQN	a	845	-	34,34,34	1.63	2 (5%)	42,45,45	1.09	4 (9%)
21	SF4	c	102	3	0,12,12	0.00	-	-	-	-
17	CLA	A	821	1	36,53,73	2.49	12 (33%)	39,89,113	2.64	19 (48%)
17	CLA	b	841	19	59,73,73	2.04	13 (22%)	67,113,113	2.16	21 (31%)
20	BCR	b	844	-	41,41,41	1.03	1 (2%)	56,56,56	2.08	14 (25%)
17	CLA	A	805	1	49,63,73	2.22	13 (26%)	55,101,113	2.38	23 (41%)
20	BCR	A	850	-	41,41,41	1.04	1 (2%)	56,56,56	1.94	15 (26%)
24	DGD	B	850	-	67,67,67	0.86	2 (2%)	81,81,81	0.93	4 (4%)
26	CHL	9	606	29	45,59,74	2.30	14 (31%)	46,96,114	2.67	18 (39%)
17	CLA	2	608	14	44,58,73	2.38	13 (29%)	49,95,113	2.44	23 (46%)
17	CLA	B	831	2	43,57,73	2.37	13 (30%)	46,93,113	2.34	20 (43%)
17	CLA	a	821	1	36,53,73	2.46	12 (33%)	39,89,113	2.67	18 (46%)
20	BCR	2	617	-	41,41,41	1.07	1 (2%)	56,56,56	1.86	18 (32%)
17	CLA	B	828	2	59,73,73	2.04	13 (22%)	67,113,113	2.09	20 (29%)
20	BCR	j	3003	-	41,41,41	1.02	1 (2%)	56,56,56	1.71	13 (23%)
28	XAT	1	317	-	39,47,47	0.86	0	54,74,74	2.69	21 (38%)
20	BCR	8	316	-	41,41,41	1.07	1 (2%)	56,56,56	1.92	17 (30%)
17	CLA	a	826	29	59,73,73	2.01	13 (22%)	67,113,113	2.15	19 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	XAT	6	318	-	39,47,47	0.89	0	54,74,74	2.62	19 (35%)
17	CLA	a	834	1	59,73,73	2.02	13 (22%)	67,113,113	2.12	22 (32%)
17	CLA	9	602	16	54,68,73	2.12	13 (24%)	61,107,113	2.22	24 (39%)
17	CLA	a	815	1	36,53,73	2.51	12 (33%)	39,89,113	2.49	18 (46%)
26	CHL	4	607	29	45,59,74	2.27	14 (31%)	46,96,114	2.62	18 (39%)
17	CLA	a	833	1	59,73,73	2.05	13 (22%)	67,113,113	2.06	20 (29%)
17	CLA	A	818	1	59,73,73	2.04	13 (22%)	67,113,113	2.14	22 (32%)
17	CLA	A	812	1	59,73,73	2.03	13 (22%)	67,113,113	2.08	22 (32%)
27	LUT	2	615	-	42,43,43	0.75	0	51,60,60	1.62	11 (21%)
17	CLA	A	841	1	59,73,73	2.06	14 (23%)	67,113,113	2.05	17 (25%)
20	BCR	3	318	-	41,41,41	1.06	1 (2%)	56,56,56	1.88	14 (25%)
17	CLA	b	827	2	59,73,73	2.02	13 (22%)	67,113,113	2.14	21 (31%)
17	CLA	2	612	14	59,73,73	2.05	13 (22%)	67,113,113	2.07	21 (31%)
17	CLA	3	301	-	40,54,73	2.48	13 (32%)	44,90,113	2.46	19 (43%)
17	CLA	k	1401	-	36,53,73	2.49	12 (33%)	39,89,113	2.53	18 (46%)
17	CLA	A	822	29	59,73,73	2.04	13 (22%)	67,113,113	2.03	21 (31%)
17	CLA	g	101	-	35,49,73	2.53	13 (37%)	38,84,113	2.66	18 (47%)
17	CLA	7	609	14	54,68,73	2.14	13 (24%)	61,107,113	2.16	23 (37%)
17	CLA	6	309	29	40,54,73	2.47	13 (32%)	44,90,113	2.39	18 (40%)
20	BCR	b	847	-	41,41,41	1.05	1 (2%)	56,56,56	1.82	15 (26%)
28	XAT	8	315	-	39,47,47	0.88	0	54,74,74	2.71	21 (38%)
17	CLA	B	833	2	52,66,73	2.15	13 (25%)	58,104,113	2.25	21 (36%)
17	CLA	B	836	2	54,68,73	2.15	13 (24%)	61,107,113	2.28	20 (32%)
17	CLA	B	822	2	49,63,73	2.26	13 (26%)	55,101,113	2.24	21 (38%)
17	CLA	4	610	29	49,63,73	2.25	13 (26%)	55,101,113	2.23	22 (40%)
20	BCR	b	846	-	41,41,41	1.08	1 (2%)	56,56,56	1.66	13 (23%)
17	CLA	B	813	2	59,73,73	2.02	13 (22%)	67,113,113	2.12	21 (31%)
17	CLA	B	830	2	44,58,73	2.35	13 (29%)	49,95,113	2.41	20 (40%)
17	CLA	J	3002	10	36,50,73	2.54	12 (33%)	39,85,113	2.53	19 (48%)
17	CLA	2	610	19	35,49,73	2.55	13 (37%)	38,84,113	2.73	19 (50%)
28	XAT	2	616	-	39,47,47	0.87	0	54,74,74	2.62	19 (35%)
17	CLA	B	815	2	54,68,73	2.13	13 (24%)	61,107,113	2.18	22 (36%)
17	CLA	a	840	1	59,73,73	2.04	13 (22%)	67,113,113	2.14	20 (29%)
25	LMG	9	619	-	50,50,55	0.93	2 (4%)	58,58,63	0.98	3 (5%)
26	CHL	9	607	29	45,59,74	2.29	14 (31%)	46,96,114	2.60	19 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	BCR	B	847	-	41,41,41	1.06	1 (2%)	56,56,56	1.73	15 (26%)
17	CLA	B	834	2	59,73,73	2.06	13 (22%)	67,113,113	2.01	21 (31%)
17	CLA	7	602	14	59,73,73	2.02	13 (22%)	67,113,113	2.08	21 (31%)
24	DGD	b	849	-	67,67,67	0.86	2 (2%)	81,81,81	1.00	4 (4%)
17	CLA	A	804	1	59,73,73	2.01	13 (22%)	67,113,113	2.16	21 (31%)
17	CLA	b	811	2	48,62,73	2.12	13 (27%)	58,100,113	2.41	22 (37%)
17	CLA	4	613	16	36,53,73	2.51	12 (33%)	39,89,113	2.55	18 (46%)
17	CLA	6	307	-	36,50,73	2.50	12 (33%)	39,85,113	2.53	18 (46%)
17	CLA	B	837	2	59,73,73	2.03	13 (22%)	67,113,113	2.10	23 (34%)
20	BCR	a	850	-	41,41,41	1.01	1 (2%)	56,56,56	1.86	15 (26%)
17	CLA	a	822	29	59,73,73	2.04	13 (22%)	67,113,113	2.05	22 (32%)
17	CLA	9	604	29	44,58,73	2.35	13 (29%)	49,95,113	2.42	22 (44%)
19	LHG	a	848	17	26,26,48	1.26	2 (7%)	29,32,54	1.32	3 (10%)
17	CLA	7	611	14	46,60,73	2.31	13 (28%)	51,97,113	2.40	20 (39%)
20	BCR	b	845	-	41,41,41	1.05	1 (2%)	56,56,56	1.94	13 (23%)
21	SF4	c	101	3	0,12,12	0.00	-	-	-	-
19	LHG	2	618	17	36,36,48	1.08	2 (5%)	39,42,54	1.16	3 (7%)
17	CLA	8	303	29	36,53,73	2.49	12 (33%)	39,89,113	2.57	18 (46%)
17	CLA	l	204	29	44,58,73	2.35	13 (29%)	49,95,113	2.39	22 (44%)
17	CLA	a	810	1	59,73,73	2.04	13 (22%)	67,113,113	2.10	21 (31%)
17	CLA	4	612	16	50,64,73	2.22	13 (26%)	56,102,113	2.26	20 (35%)
20	BCR	B	844	-	41,41,41	1.04	1 (2%)	56,56,56	1.97	13 (23%)
17	CLA	3	315	-	22,32,73	2.68	9 (40%)	26,54,113	4.39	20 (76%)
17	CLA	A	836	1	44,58,73	2.35	13 (29%)	49,95,113	2.39	22 (44%)
17	CLA	b	803	2	59,73,73	2.03	13 (22%)	67,113,113	1.92	20 (29%)
17	CLA	6	312	19	35,49,73	2.56	13 (37%)	38,84,113	2.68	19 (50%)
25	LMG	G	102	-	44,44,55	1.01	2 (4%)	52,52,63	0.98	3 (5%)
17	CLA	b	824	29	59,73,73	2.03	13 (22%)	67,113,113	2.11	21 (31%)
17	CLA	6	310	13	59,73,73	2.05	13 (22%)	67,113,113	2.06	19 (28%)
20	BCR	F	305	-	41,41,41	1.04	1 (2%)	56,56,56	1.74	16 (28%)
17	CLA	b	840	2	59,73,73	2.02	13 (22%)	67,113,113	2.10	21 (31%)
19	LHG	A	847	17	26,26,48	1.28	2 (7%)	29,32,54	1.26	3 (10%)
17	CLA	2	603	14	59,73,73	2.02	13 (22%)	67,113,113	2.09	20 (29%)
17	CLA	2	609	14	54,68,73	2.15	13 (24%)	61,107,113	2.17	24 (39%)
17	CLA	B	835	29	36,53,73	2.49	12 (33%)	39,89,113	2.47	19 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	K	4002	-	36,53,73	2.51	12 (33%)	39,89,113	2.57	18 (46%)
20	BCR	l	201	-	41,41,41	1.04	1 (2%)	56,56,56	1.85	15 (26%)
17	CLA	F	304	6	49,63,73	2.24	13 (26%)	55,101,113	2.23	23 (41%)
17	CLA	a	823	1	43,57,73	2.39	13 (30%)	46,93,113	2.40	19 (41%)
17	CLA	b	823	2	54,68,73	2.12	13 (24%)	61,107,113	2.12	19 (31%)
17	CLA	a	830	1	59,73,73	2.06	13 (22%)	67,113,113	2.12	20 (29%)
22	HTG	J	3001	-	19,19,19	1.05	2 (10%)	23,24,24	0.53	0
17	CLA	b	831	2	43,57,73	2.36	13 (30%)	46,93,113	2.36	20 (43%)
17	CLA	b	819	29	59,73,73	2.04	13 (22%)	67,113,113	2.09	20 (29%)
17	CLA	b	828	2	59,73,73	2.03	13 (22%)	67,113,113	2.08	20 (29%)
20	BCR	b	848	-	41,41,41	1.05	1 (2%)	56,56,56	1.55	10 (17%)
17	CLA	A	802	1	59,73,73	2.05	12 (20%)	67,113,113	2.03	20 (29%)
17	CLA	4	611	16	46,60,73	2.29	13 (28%)	51,97,113	2.39	20 (39%)
17	CLA	b	832	2	59,73,73	2.01	13 (22%)	67,113,113	2.07	21 (31%)
17	CLA	b	837	2	59,73,73	2.03	13 (22%)	67,113,113	2.09	23 (34%)
17	CLA	B	816	2	49,63,73	2.23	13 (26%)	55,101,113	2.32	22 (40%)
26	CHL	2	601	14	55,69,74	2.07	14 (25%)	58,108,114	2.47	19 (32%)
19	LHG	6	320	17	48,48,48	0.94	2 (4%)	51,54,54	1.08	3 (5%)
17	CLA	b	806	2	59,73,73	2.02	13 (22%)	67,113,113	2.07	20 (29%)
17	CLA	a	838	1	45,59,73	2.32	12 (26%)	50,96,113	2.50	24 (48%)
17	CLA	A	820	1	59,73,73	2.04	13 (22%)	67,113,113	2.12	20 (29%)
17	CLA	b	808	2	59,73,73	2.01	13 (22%)	67,113,113	2.23	24 (35%)
22	HTG	A	855	-	19,19,19	1.03	2 (10%)	23,24,24	0.69	0
26	CHL	7	607	29	45,59,74	2.30	14 (31%)	46,96,114	2.65	16 (34%)
26	CHL	3	307	29	41,55,74	2.40	15 (36%)	41,91,114	2.65	17 (41%)
17	CLA	b	825	29	59,73,73	2.03	13 (22%)	67,113,113	2.08	22 (32%)
17	CLA	g	103	7	40,54,73	2.46	13 (32%)	44,90,113	2.49	18 (40%)
17	CLA	B	812	2	49,63,73	2.25	13 (26%)	55,101,113	2.21	19 (34%)
17	CLA	l	303	13	59,73,73	2.03	13 (22%)	67,113,113	2.10	21 (31%)
20	BCR	i	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.60	12 (21%)
17	CLA	9	610	29	35,49,73	2.57	13 (37%)	38,84,113	2.66	18 (47%)
17	CLA	a	803	29	59,73,73	2.00	13 (22%)	67,113,113	2.20	22 (32%)
17	CLA	a	832	1	44,58,73	2.36	13 (29%)	49,95,113	2.43	21 (42%)
26	CHL	1	307	13	42,56,74	2.40	14 (33%)	42,92,114	2.72	15 (35%)
20	BCR	B	846	-	41,41,41	1.04	1 (2%)	56,56,56	1.76	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	BCR	a	851	-	41,41,41	1.03	1 (2%)	56,56,56	1.72	14 (25%)
17	CLA	G	101	29	36,53,73	2.48	12 (33%)	39,89,113	2.54	17 (43%)
17	CLA	B	804	2	36,53,73	2.48	12 (33%)	39,89,113	2.61	19 (48%)
17	CLA	6	311	13	54,68,73	2.14	13 (24%)	61,107,113	2.16	23 (37%)
17	CLA	8	309	-	46,60,73	2.34	13 (28%)	51,97,113	2.36	19 (37%)
17	CLA	1	314	13	49,63,73	2.25	13 (26%)	55,101,113	2.31	22 (40%)
17	CLA	B	803	2	59,73,73	2.04	13 (22%)	67,113,113	1.92	23 (34%)
26	CHL	7	605	29	37,51,74	2.45	13 (35%)	36,86,114	2.91	17 (47%)
17	CLA	b	804	2	36,53,73	2.46	12 (33%)	39,89,113	2.66	18 (46%)
17	CLA	3	310	19	31,45,73	2.54	12 (38%)	31,78,113	2.70	17 (54%)
17	CLA	a	841	1	59,73,73	2.04	13 (22%)	67,113,113	2.04	22 (32%)
17	CLA	7	604	29	54,68,73	2.14	13 (24%)	61,107,113	2.18	22 (36%)
22	HTG	F	302	-	19,19,19	1.01	2 (10%)	23,24,24	0.61	0
17	CLA	A	807	1	59,73,73	2.03	13 (22%)	67,113,113	2.13	22 (32%)
17	CLA	a	843	1	59,73,73	2.00	13 (22%)	67,113,113	2.13	23 (34%)
17	CLA	8	311	15	36,53,73	2.52	12 (33%)	39,89,113	2.55	19 (48%)
20	BCR	g	104	-	41,41,41	1.05	1 (2%)	56,56,56	1.89	16 (28%)
17	CLA	9	614	16	41,55,73	2.42	13 (31%)	45,91,113	2.45	18 (40%)
17	CLA	9	613	16	36,53,73	2.50	12 (33%)	39,89,113	2.55	19 (48%)
17	CLA	B	838	2	41,55,73	2.40	13 (31%)	45,91,113	2.45	20 (44%)
17	CLA	7	613	14	37,51,73	2.46	12 (32%)	40,86,113	2.49	17 (42%)
17	CLA	k	1403	-	40,54,73	2.49	13 (32%)	44,90,113	2.47	20 (45%)
17	CLA	a	801	1	59,73,73	2.02	13 (22%)	67,113,113	2.21	23 (34%)
17	CLA	b	812	2	49,63,73	2.25	13 (26%)	55,101,113	2.25	20 (36%)
17	CLA	b	807	2	59,73,73	2.06	13 (22%)	67,113,113	2.10	20 (29%)
17	CLA	4	608	16	44,58,73	2.37	13 (29%)	49,95,113	2.40	21 (42%)
17	CLA	a	804	1	59,73,73	2.04	13 (22%)	67,113,113	2.12	22 (32%)
17	CLA	3	313	15	36,53,73	2.53	12 (33%)	39,89,113	2.51	18 (46%)
17	CLA	A	839	1	59,73,73	2.00	13 (22%)	67,113,113	2.13	19 (28%)
17	CLA	3	304	29	36,53,73	2.49	12 (33%)	39,89,113	2.55	18 (46%)
17	CLA	1	311	19	35,49,73	2.58	13 (37%)	38,84,113	2.67	18 (47%)
17	CLA	A	817	29	36,53,73	2.50	12 (33%)	39,89,113	2.54	17 (43%)
17	CLA	a	829	1	59,73,73	2.00	13 (22%)	67,113,113	2.12	21 (31%)
17	CLA	b	821	2	40,54,73	2.46	13 (32%)	44,90,113	2.46	19 (43%)
17	CLA	a	802	1	59,73,73	2.05	12 (20%)	67,113,113	2.03	26 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	843	29	59,73,73	2.01	13 (22%)	67,113,113	2.09	19 (28%)
17	CLA	a	808	1	59,73,73	2.03	13 (22%)	67,113,113	2.09	20 (29%)
26	CHL	7	606	-	42,56,74	2.39	14 (33%)	42,92,114	2.74	17 (40%)
26	CHL	8	306	29	41,55,74	2.39	13 (31%)	41,91,114	2.81	16 (39%)
17	CLA	a	813	1	48,62,73	2.30	13 (27%)	53,99,113	2.25	19 (35%)
20	BCR	a	852	-	41,41,41	1.04	1 (2%)	56,56,56	1.94	17 (30%)
17	CLA	A	830	1	59,73,73	2.06	13 (22%)	67,113,113	2.13	21 (31%)
17	CLA	B	817	2	53,67,73	2.13	13 (24%)	59,105,113	2.25	23 (38%)
17	CLA	a	806	1	59,73,73	2.03	13 (22%)	67,113,113	2.16	22 (32%)
17	CLA	8	310	15	49,63,73	2.24	13 (26%)	55,101,113	2.24	21 (38%)
17	CLA	7	612	14	59,73,73	2.04	13 (22%)	67,113,113	2.07	20 (29%)
27	LUT	6	317	-	42,43,43	0.75	0	51,60,60	1.66	14 (27%)
26	CHL	2	607	29	45,59,74	2.27	14 (31%)	46,96,114	2.66	19 (41%)
17	CLA	9	601	16	40,54,73	2.45	13 (32%)	44,90,113	2.46	20 (45%)
17	CLA	L	203	12	59,73,73	2.04	13 (22%)	67,113,113	2.07	22 (32%)
17	CLA	a	805	1	49,63,73	2.22	13 (26%)	55,101,113	2.28	21 (38%)
17	CLA	b	805	2	59,73,73	2.02	13 (22%)	67,113,113	2.12	22 (32%)
19	LHG	7	618	17	36,36,48	1.08	2 (5%)	39,42,54	1.16	4 (10%)
17	CLA	A	829	1	59,73,73	1.99	13 (22%)	67,113,113	2.09	22 (32%)
20	BCR	A	856	-	41,41,41	1.03	1 (2%)	56,56,56	2.03	16 (28%)
17	CLA	8	313	-	22,32,73	2.70	9 (40%)	26,54,113	4.39	20 (76%)
20	BCR	J	3003	-	41,41,41	1.03	1 (2%)	56,56,56	1.76	14 (25%)
26	CHL	9	605	29	50,64,74	2.19	14 (28%)	52,102,114	2.55	21 (40%)
26	CHL	1	302	13	55,69,74	2.07	14 (25%)	58,108,114	2.44	20 (34%)
20	BCR	b	801	-	41,41,41	1.03	1 (2%)	56,56,56	1.43	6 (10%)
20	BCR	A	848	-	41,41,41	1.02	1 (2%)	56,56,56	1.82	13 (23%)
17	CLA	6	314	13	54,68,73	2.13	13 (24%)	61,107,113	2.19	21 (34%)
17	CLA	3	302	15	54,68,73	2.13	13 (24%)	61,107,113	2.20	22 (36%)
20	BCR	a	854	-	41,41,41	1.04	1 (2%)	56,56,56	1.74	12 (21%)
17	CLA	a	816	1	44,58,73	2.36	13 (29%)	49,95,113	2.37	21 (42%)
21	SF4	a	855	1,2	0,12,12	0.00	-	-	-	-
22	HTG	a	857	-	19,19,19	1.05	2 (10%)	23,24,24	0.55	0
17	CLA	8	312	15	40,54,73	2.46	13 (32%)	44,90,113	2.46	19 (43%)
17	CLA	B	814	2	59,73,73	2.01	13 (22%)	67,113,113	2.08	23 (34%)
17	CLA	1	304	13	59,73,73	2.05	13 (22%)	67,113,113	2.14	20 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	BCR	l	205	-	41,41,41	1.02	1 (2%)	56,56,56	1.59	10 (17%)
20	BCR	A	851	-	41,41,41	1.06	1 (2%)	56,56,56	2.02	14 (25%)
28	XAT	9	617	-	39,47,47	0.86	1 (2%)	54,74,74	2.61	17 (31%)
17	CLA	a	846	19	46,60,73	2.33	13 (28%)	51,97,113	2.35	18 (35%)
17	CLA	A	840	1	59,73,73	2.04	13 (22%)	67,113,113	2.13	21 (31%)
20	BCR	B	843	-	41,41,41	1.06	1 (2%)	56,56,56	1.88	14 (25%)
27	LUT	1	316	-	42,43,43	0.74	0	51,60,60	1.55	12 (23%)
26	CHL	4	615	16	37,51,74	2.45	13 (35%)	36,86,114	2.89	13 (36%)
17	CLA	a	807	1	59,73,73	2.03	13 (22%)	67,113,113	2.18	23 (34%)
17	CLA	B	829	2	59,73,73	2.02	13 (22%)	67,113,113	2.21	22 (32%)
17	CLA	b	820	2	44,58,73	2.36	13 (29%)	49,95,113	2.43	21 (42%)
17	CLA	4	614	16	44,58,73	2.36	13 (29%)	49,95,113	2.46	21 (42%)
20	BCR	I	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.93	15 (26%)
17	CLA	4	603	16	40,54,73	2.40	13 (32%)	44,90,113	2.60	19 (43%)
17	CLA	8	301	15	54,68,73	2.14	13 (24%)	61,107,113	2.18	22 (36%)
17	CLA	B	807	2	59,73,73	2.06	13 (22%)	67,113,113	2.13	24 (35%)
17	CLA	3	312	15	49,63,73	2.25	13 (26%)	55,101,113	2.24	21 (38%)
17	CLA	K	4003	11	40,54,73	2.48	13 (32%)	44,90,113	2.47	19 (43%)
17	CLA	8	302	15	44,58,73	2.35	13 (29%)	49,95,113	2.50	21 (42%)
17	CLA	8	307	15	44,58,73	2.36	13 (29%)	49,95,113	2.34	21 (42%)
17	CLA	7	603	14	45,59,73	2.32	13 (28%)	50,96,113	2.41	21 (42%)

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
17	CLA	9	609	16	3/3/19/25	4/31/129/135	-
17	CLA	a	812	1	3/3/20/25	13/37/135/135	-
17	CLA	B	823	2	3/3/19/25	12/31/129/135	-
17	CLA	A	803	29	1/1/20/25	2/37/135/135	-
17	CLA	6	313	13	3/3/17/25	10/22/120/135	-
17	CLA	B	805	2	3/3/20/25	16/37/135/135	-
17	CLA	3	314	15	2/2/16/25	1/15/113/135	-
17	CLA	a	828	1	3/3/20/25	10/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BCR	9	618	-	-	6/29/63/63	0/2/2/2
17	CLA	b	834	2	3/3/20/25	13/37/135/135	-
17	CLA	a	856	29	1/1/20/25	11/37/135/135	-
17	CLA	b	810	2	3/3/20/25	14/37/135/135	-
17	CLA	2	604	29	3/3/19/25	9/31/129/135	-
21	SF4	C	102	3	-	-	0/6/5/5
17	CLA	b	835	29	3/3/16/25	2/11/111/135	-
17	CLA	3	305	29	3/3/15/25	2/10/108/135	-
17	CLA	a	809	1	3/3/20/25	13/37/135/135	-
17	CLA	a	836	1	3/3/17/25	2/19/117/135	-
17	CLA	A	808	1	3/3/20/25	8/37/135/135	-
20	BCR	b	843	-	-	0/29/63/63	0/2/2/2
28	XAT	4	617	-	-	0/31/93/93	0/4/4/4
17	CLA	a	831	1	3/3/20/25	16/37/135/135	-
17	CLA	A	806	1	3/3/20/25	19/37/135/135	-
19	LHG	A	846	-	-	10/53/53/53	-
17	CLA	f	7003	6	1/1/18/25	9/25/123/135	-
20	BCR	L	206	-	-	3/29/63/63	0/2/2/2
17	CLA	A	821	1	3/3/16/25	0/11/111/135	-
17	CLA	A	811	1	3/3/20/25	9/37/135/135	-
17	CLA	A	826	29	3/3/20/25	14/37/135/135	-
20	BCR	B	845	-	-	6/29/63/63	0/2/2/2
19	LHG	1	301	17	-	9/26/26/53	-
17	CLA	a	825	1	3/3/18/25	6/25/123/135	-
17	CLA	b	812	2	3/3/18/25	11/25/123/135	-
17	CLA	7	608	14	3/3/17/25	6/19/117/135	-
26	CHL	4	605	29	2/2/18/26	8/27/125/137	-
27	LUT	7	615	-	-	1/29/67/67	0/2/2/2
17	CLA	4	602	16	3/3/19/25	6/31/129/135	-
17	CLA	6	305	13	3/3/20/25	10/37/135/135	-
19	LHG	a	847	-	-	10/53/53/53	-
20	BCR	I	101	-	-	3/29/63/63	0/2/2/2
17	CLA	B	827	2	1/1/20/25	8/37/135/135	-
17	CLA	A	845	19	3/3/17/25	10/22/120/135	-
26	CHL	2	605	29	2/2/15/26	0/12/110/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LUT	4	616	-	-	2/29/67/67	0/2/2/2
17	CLA	a	819	1	3/3/20/25	14/37/135/135	-
22	HTG	j	3001	-	-	1/10/30/30	0/1/1/1
20	BCR	A	852	-	-	6/29/63/63	0/2/2/2
17	CLA	4	601	16	3/3/16/25	3/15/113/135	-
18	PQN	B	842	-	-	3/23/43/43	0/2/2/2
28	XAT	3	317	-	-	2/31/93/93	0/4/4/4
20	BCR	B	844	-	-	6/29/63/63	0/2/2/2
17	CLA	b	816	2	3/3/18/25	11/25/123/135	-
17	CLA	a	818	1	3/3/20/25	12/37/135/135	-
20	BCR	k	1404	-	-	6/29/63/63	0/2/2/2
17	CLA	1	309	13	3/3/20/25	10/37/135/135	-
17	CLA	A	854	29	1/1/20/25	10/37/135/135	-
17	CLA	b	818	2	3/3/19/25	13/31/129/135	-
17	CLA	A	827	29	3/3/20/25	7/37/135/135	-
17	CLA	1	306	-	3/3/17/25	2/22/120/135	-
26	CHL	2	606	-	3/3/16/26	2/18/116/137	-
20	BCR	L	205	-	-	6/29/63/63	0/2/2/2
20	BCR	B	843	-	-	0/29/63/63	0/2/2/2
25	LMG	4	619	-	-	9/39/59/70	0/1/1/1
26	CHL	6	303	13	3/3/19/26	15/33/131/137	-
17	CLA	j	3002	10	3/3/15/25	1/10/108/135	-
17	CLA	3	303	15	3/3/17/25	2/19/117/135	-
17	CLA	9	611	16	3/3/17/25	6/22/120/135	-
19	LHG	1	319	17	-	10/53/53/53	-
20	BCR	f	7004	-	-	4/29/63/63	0/2/2/2
17	CLA	A	824	1	3/3/17/25	9/21/119/135	-
17	CLA	1	315	13	3/3/16/25	1/15/113/135	-
17	CLA	2	613	14	3/3/15/25	6/11/109/135	-
20	BCR	1	318	-	-	6/29/63/63	0/2/2/2
17	CLA	1	305	29	3/3/17/25	6/22/120/135	-
17	CLA	A	825	1	3/3/18/25	7/25/123/135	-
17	CLA	A	817	29	2/2/16/25	1/11/111/135	-
17	CLA	g	102	7	3/3/17/25	1/19/117/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	828	1	3/3/20/25	13/37/135/135	-
20	BCR	B	801	-	-	1/29/63/63	0/2/2/2
17	CLA	A	815	1	3/3/16/25	1/11/111/135	-
17	CLA	a	820	1	3/3/20/25	11/37/135/135	-
17	CLA	A	801	1	4/4/20/25	7/37/135/135	-
20	BCR	a	853	-	-	7/29/63/63	0/2/2/2
27	LUT	9	616	-	-	2/29/67/67	0/2/2/2
17	CLA	A	834	1	2/2/20/25	10/37/135/135	-
17	CLA	A	832	1	2/2/17/25	2/19/117/135	-
17	CLA	B	819	29	2/2/20/25	9/37/135/135	-
17	CLA	4	604	29	3/3/17/25	5/19/117/135	-
17	CLA	B	818	2	2/2/19/25	10/31/129/135	-
20	BCR	B	848	-	-	2/29/63/63	0/2/2/2
17	CLA	f	7002	29	3/3/16/25	1/11/111/135	-
17	CLA	3	311	-	3/3/17/25	6/22/120/135	-
17	CLA	A	840	1	3/3/20/25	7/37/135/135	-
28	XAT	7	616	-	-	1/31/93/93	0/4/4/4
17	CLA	b	809	2	3/3/20/25	8/37/135/135	-
17	CLA	a	835	1	3/3/20/25	10/37/135/135	-
17	CLA	b	838	2	3/3/16/25	2/16/114/135	-
17	CLA	2	611	14	3/3/17/25	5/22/120/135	-
17	CLA	B	824	29	2/2/20/25	7/37/135/135	-
26	CHL	2	614	14	3/3/15/26	0/12/110/137	-
17	CLA	B	841	19	3/3/20/25	8/37/135/135	-
17	CLA	3	308	15	3/3/17/25	5/19/117/135	-
17	CLA	A	831	1	3/3/20/25	13/37/135/135	-
17	CLA	l	202	12	3/3/20/25	10/37/135/135	-
17	CLA	a	814	1	3/3/20/25	11/37/135/135	-
17	CLA	a	839	1	3/3/20/25	10/37/135/135	-
27	LUT	1	320	-	-	2/29/67/67	0/2/2/2
17	CLA	b	822	2	3/3/18/25	10/25/123/135	-
17	CLA	a	817	29	2/2/16/25	0/11/111/135	-
20	BCR	K	4004	-	-	4/29/63/63	0/2/2/2
17	CLA	A	814	1	3/3/20/25	16/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	1	312	13	3/3/17/25	8/22/120/135	-
28	XAT	6	318	-	-	1/31/93/93	0/4/4/4
17	CLA	7	610	19	3/3/15/25	0/8/106/135	-
17	CLA	a	837	1	2/2/16/25	3/11/111/135	-
17	CLA	b	815	2	3/3/18/25	7/25/123/135	-
17	CLA	2	602	14	3/3/20/25	13/37/135/135	-
17	CLA	a	811	1	3/3/20/25	9/37/135/135	-
17	CLA	A	836	1	3/3/17/25	0/19/117/135	-
17	CLA	8	304	29	3/3/15/25	0/10/108/135	-
17	CLA	B	806	2	3/3/20/25	16/37/135/135	-
26	CHL	6	308	13	3/3/16/26	1/17/115/137	-
17	CLA	B	821	2	3/3/16/25	1/15/113/135	-
17	CLA	8	305	15	3/3/16/25	3/16/114/135	-
18	PQN	A	844	-	-	8/23/43/43	0/2/2/2
20	BCR	K	4001	-	-	1/29/63/63	0/2/2/2
17	CLA	b	802	2	2/2/20/25	5/37/135/135	-
23	LMT	B	849	-	-	3/21/61/61	0/2/2/2
20	BCR	l	206	-	-	0/29/63/63	0/2/2/2
17	CLA	B	811	2	3/3/18/25	4/25/121/135	-
17	CLA	A	818	1	3/3/20/25	12/37/135/135	-
17	CLA	9	612	16	3/3/18/25	10/27/125/135	-
17	CLA	6	315	13	3/3/18/25	6/25/123/135	-
27	LUT	8	314	-	-	2/29/67/67	0/2/2/2
17	CLA	1	308	29	3/3/20/25	5/37/135/135	-
17	CLA	a	844	29	3/3/20/25	12/37/135/135	-
26	CHL	2	601	14	2/2/19/26	11/33/131/137	-
17	CLA	4	609	16	3/3/19/25	5/31/129/135	-
17	CLA	B	826	2	3/3/20/25	10/37/135/135	-
17	CLA	9	608	16	3/3/17/25	4/19/117/135	-
17	CLA	B	839	29	3/3/20/25	7/37/135/135	-
17	CLA	b	823	2	3/3/19/25	6/31/129/135	-
17	CLA	B	820	2	3/3/17/25	3/19/117/135	-
17	CLA	9	603	16	3/3/16/25	4/15/113/135	-
17	CLA	L	204	29	3/3/17/25	3/19/117/135	-
20	BCR	L	201	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	825	29	3/3/20/25	7/37/135/135	-
20	BCR	j	3004	-	-	9/29/63/63	0/2/2/2
17	CLA	A	810	1	3/3/20/25	4/37/135/135	-
25	LMG	4	620	-	-	11/39/59/70	0/1/1/1
17	CLA	l	203	12	3/3/20/25	6/37/135/135	-
17	CLA	6	316	13	3/3/16/25	3/15/113/135	-
17	CLA	b	819	29	3/3/20/25	5/37/135/135	-
17	CLA	3	309	15	3/3/17/25	1/19/117/135	-
17	CLA	A	819	1	3/3/20/25	13/37/135/135	-
20	BCR	a	849	-	-	2/29/63/63	0/2/2/2
21	SF4	A	853	1,2	-	-	0/6/5/5
17	CLA	F	303	29	3/3/16/25	0/11/111/135	-
17	CLA	B	810	2	3/3/20/25	9/37/135/135	-
26	CHL	4	606	29	3/3/17/26	6/21/119/137	-
26	CHL	4	615	16	3/3/15/26	0/12/110/137	-
17	CLA	3	306	15	3/3/16/25	3/16/114/135	-
17	CLA	A	835	1	3/3/20/25	10/37/135/135	-
26	CHL	7	614	14	3/3/15/26	3/12/110/137	-
17	CLA	1	313	13	3/3/20/25	5/37/135/135	-
17	CLA	b	826	2	3/3/20/25	8/37/135/135	-
17	CLA	b	829	2	3/3/20/25	6/37/135/135	-
18	PQN	b	842	-	-	3/23/43/43	0/2/2/2
17	CLA	B	808	2	3/3/20/25	7/37/135/135	-
17	CLA	A	812	1	3/3/20/25	13/37/135/135	-
17	CLA	6	306	29	3/3/17/25	3/21/119/135	-
17	CLA	1	310	13	3/3/19/25	3/31/129/135	-
17	CLA	a	842	29	3/3/20/25	5/37/135/135	-
17	CLA	6	304	13	3/3/20/25	9/37/135/135	-
26	CHL	7	601	14	3/3/19/26	8/33/131/137	-
17	CLA	B	840	2	2/2/20/25	9/37/135/135	-
17	CLA	b	832	2	3/3/20/25	12/37/135/135	-
17	CLA	b	837	2	3/3/20/25	9/37/135/135	-
25	LMG	6	302	-	-	6/35/55/70	0/1/1/1
27	LUT	3	316	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	823	1	3/3/16/25	5/18/116/135	-
17	CLA	B	809	2	3/3/20/25	7/37/135/135	-
22	HTG	f	7001	-	-	1/10/30/30	0/1/1/1
20	BCR	7	617	-	-	4/29/63/63	0/2/2/2
17	CLA	b	806	2	3/3/20/25	9/37/135/135	-
27	LUT	6	321	-	-	2/29/67/67	0/2/2/2
17	CLA	G	103	7	3/3/17/25	1/19/117/135	-
17	CLA	A	809	1	3/3/20/25	18/37/135/135	-
20	BCR	G	105	-	-	3/29/63/63	0/2/2/2
17	CLA	b	830	2	3/3/17/25	3/19/117/135	-
20	BCR	6	319	-	-	4/29/63/63	0/2/2/2
17	CLA	B	832	2	3/3/20/25	14/37/135/135	-
26	CHL	9	615	16	3/3/15/26	0/12/110/137	-
17	CLA	B	802	2	2/2/20/25	13/37/135/135	-
17	CLA	8	308	15	3/3/17/25	1/19/117/135	-
21	SF4	C	101	3	-	-	0/6/5/5
17	CLA	F	301	29	3/3/20/25	8/37/135/135	-
17	CLA	G	104	7	3/3/16/25	2/15/113/135	-
19	LHG	6	301	17	-	7/26/26/53	-
20	BCR	A	849	-	-	2/29/63/63	0/2/2/2
18	PQN	a	845	-	-	5/23/43/43	0/2/2/2
21	SF4	c	102	3	-	-	0/6/5/5
17	CLA	b	840	2	3/3/20/25	5/37/135/135	-
17	CLA	A	820	1	3/3/20/25	12/37/135/135	-
20	BCR	b	844	-	-	6/29/63/63	0/2/2/2
17	CLA	A	805	1	3/3/18/25	8/25/123/135	-
20	BCR	A	850	-	-	3/29/63/63	0/2/2/2
24	DGD	B	850	-	-	12/55/95/95	0/2/2/2
26	CHL	9	606	29	3/3/17/26	4/21/119/137	-
17	CLA	2	608	14	3/3/17/25	3/19/117/135	-
17	CLA	B	831	2	3/3/16/25	8/18/116/135	-
17	CLA	a	821	1	3/3/16/25	2/11/111/135	-
20	BCR	2	617	-	-	3/29/63/63	0/2/2/2
17	CLA	B	828	2	3/3/20/25	5/37/135/135	-
20	BCR	j	3003	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	XAT	1	317	-	-	0/31/93/93	0/4/4/4
20	BCR	8	316	-	-	4/29/63/63	0/2/2/2
17	CLA	a	826	29	3/3/20/25	6/37/135/135	-
17	CLA	k	1402	11	3/3/16/25	0/15/113/135	-
17	CLA	a	834	1	3/3/20/25	10/37/135/135	-
17	CLA	9	602	16	3/3/19/25	10/31/129/135	-
17	CLA	a	815	1	3/3/16/25	3/11/111/135	-
26	CHL	4	607	29	3/3/17/26	3/21/119/137	-
17	CLA	a	833	1	3/3/20/25	5/37/135/135	-
17	CLA	b	839	29	3/3/20/25	9/37/135/135	-
17	CLA	b	833	2	3/3/18/25	8/29/127/135	-
27	LUT	2	615	-	-	2/29/67/67	0/2/2/2
17	CLA	A	841	1	3/3/20/25	10/37/135/135	-
20	BCR	3	318	-	-	6/29/63/63	0/2/2/2
17	CLA	b	827	2	2/2/20/25	14/37/135/135	-
17	CLA	2	612	14	3/3/20/25	9/37/135/135	-
17	CLA	3	301	-	3/3/16/25	2/15/113/135	-
17	CLA	k	1401	-	3/3/16/25	3/11/111/135	-
17	CLA	A	822	29	3/3/20/25	5/37/135/135	-
17	CLA	g	101	-	2/2/15/25	3/8/106/135	-
17	CLA	7	609	14	3/3/19/25	7/31/129/135	-
17	CLA	6	309	29	3/3/16/25	3/15/113/135	-
20	BCR	b	847	-	-	3/29/63/63	0/2/2/2
28	XAT	8	315	-	-	0/31/93/93	0/4/4/4
17	CLA	B	833	2	3/3/18/25	9/29/127/135	-
17	CLA	B	836	2	3/3/19/25	5/31/129/135	-
17	CLA	B	822	2	3/3/18/25	11/25/123/135	-
17	CLA	4	610	29	3/3/18/25	5/25/123/135	-
20	BCR	b	846	-	-	5/29/63/63	0/2/2/2
17	CLA	B	813	2	3/3/20/25	16/37/135/135	-
17	CLA	B	830	2	3/3/17/25	5/19/117/135	-
17	CLA	J	3002	10	3/3/15/25	4/10/108/135	-
17	CLA	2	610	19	2/2/15/25	0/8/106/135	-
28	XAT	2	616	-	-	0/31/93/93	0/4/4/4
17	CLA	B	815	2	3/3/19/25	10/31/129/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	a	840	1	2/2/20/25	9/37/135/135	-
25	LMG	9	619	-	-	10/45/65/70	0/1/1/1
26	CHL	9	607	29	3/3/17/26	3/21/119/137	-
20	BCR	B	847	-	-	5/29/63/63	0/2/2/2
17	CLA	B	834	2	3/3/20/25	16/37/135/135	-
17	CLA	7	602	14	3/3/20/25	8/37/135/135	-
24	DGD	b	849	-	-	10/55/95/95	0/2/2/2
17	CLA	A	804	1	3/3/20/25	7/37/135/135	-
17	CLA	b	811	2	3/3/18/25	10/25/121/135	-
17	CLA	4	613	16	3/3/16/25	0/11/111/135	-
17	CLA	6	307	-	3/3/15/25	4/10/108/135	-
17	CLA	B	837	2	3/3/20/25	9/37/135/135	-
20	BCR	a	850	-	-	6/29/63/63	0/2/2/2
17	CLA	a	822	29	3/3/20/25	3/37/135/135	-
17	CLA	9	604	29	3/3/17/25	5/19/117/135	-
19	LHG	a	848	17	-	12/31/31/53	-
17	CLA	7	611	14	3/3/17/25	5/22/120/135	-
20	BCR	b	845	-	-	6/29/63/63	0/2/2/2
19	LHG	3	319	17	-	11/23/23/53	-
21	SF4	c	101	3	-	-	0/6/5/5
19	LHG	2	618	17	-	9/41/41/53	-
17	CLA	8	303	29	3/3/16/25	1/11/111/135	-
17	CLA	a	832	1	2/2/17/25	4/19/117/135	-
17	CLA	a	810	1	3/3/20/25	2/37/135/135	-
17	CLA	4	612	16	3/3/18/25	9/27/125/135	-
17	CLA	a	824	1	3/3/17/25	8/21/119/135	-
17	CLA	3	315	-	3/3/7/25	-	-
17	CLA	b	817	2	3/3/18/25	11/30/128/135	-
17	CLA	b	803	2	3/3/20/25	6/37/135/135	-
17	CLA	6	312	19	3/3/15/25	0/8/106/135	-
25	LMG	G	102	-	-	10/39/59/70	0/1/1/1
17	CLA	b	824	29	3/3/20/25	10/37/135/135	-
17	CLA	6	310	13	3/3/20/25	7/37/135/135	-
20	BCR	F	305	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LHG	A	847	17	-	9/31/31/53	-
17	CLA	2	603	14	3/3/20/25	11/37/135/135	-
17	CLA	2	609	14	3/3/19/25	8/31/129/135	-
17	CLA	B	835	29	3/3/16/25	1/11/111/135	-
17	CLA	K	4002	-	3/3/16/25	2/11/111/135	-
20	BCR	l	201	-	-	8/29/63/63	0/2/2/2
17	CLA	F	304	6	3/3/18/25	8/25/123/135	-
17	CLA	a	823	1	3/3/16/25	5/18/116/135	-
17	CLA	A	842	1	3/3/20/25	13/37/135/135	-
17	CLA	a	830	1	3/3/20/25	11/37/135/135	-
22	HTG	J	3001	-	-	4/10/30/30	0/1/1/1
17	CLA	b	831	2	2/2/16/25	7/18/116/135	-
17	CLA	A	838	1	3/3/17/25	3/21/119/135	-
20	BCR	B	846	-	-	4/29/63/63	0/2/2/2
17	CLA	b	828	2	3/3/20/25	9/37/135/135	-
20	BCR	b	848	-	-	2/29/63/63	0/2/2/2
17	CLA	A	802	1	3/3/20/25	5/37/135/135	-
17	CLA	4	611	16	3/3/17/25	7/22/120/135	-
17	CLA	A	813	1	3/3/17/25	7/24/122/135	-
17	CLA	A	816	1	3/3/17/25	3/19/117/135	-
17	CLA	B	816	2	3/3/18/25	9/25/123/135	-
19	LHG	6	320	17	-	14/53/53/53	-
17	CLA	L	202	12	3/3/20/25	8/37/135/135	-
17	CLA	a	838	1	3/3/17/25	9/21/119/135	-
20	BCR	4	618	-	-	6/29/63/63	0/2/2/2
17	CLA	b	841	19	3/3/20/25	4/37/135/135	-
17	CLA	b	808	2	3/3/20/25	8/37/135/135	-
22	HTG	A	855	-	-	1/10/30/30	0/1/1/1
26	CHL	7	607	29	3/3/17/26	4/21/119/137	-
26	CHL	3	307	29	3/3/16/26	2/17/115/137	-
17	CLA	b	825	29	3/3/20/25	8/37/135/135	-
17	CLA	b	813	2	3/3/20/25	13/37/135/135	-
17	CLA	g	103	7	3/3/16/25	2/15/113/135	-
17	CLA	B	812	2	3/3/18/25	8/25/123/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	1	303	13	3/3/20/25	9/37/135/135	-
20	BCR	i	101	-	-	1/29/63/63	0/2/2/2
17	CLA	9	610	29	3/3/15/25	0/8/106/135	-
17	CLA	a	803	29	1/1/20/25	1/37/135/135	-
17	CLA	l	204	29	3/3/17/25	4/19/117/135	-
26	CHL	1	307	13	3/3/16/26	3/18/116/137	-
17	CLA	A	837	1	3/3/16/25	3/11/111/135	-
20	BCR	a	851	-	-	1/29/63/63	0/2/2/2
17	CLA	G	101	29	3/3/16/25	2/11/111/135	-
17	CLA	B	804	2	3/3/16/25	6/11/111/135	-
17	CLA	6	311	13	3/3/19/25	9/31/129/135	-
17	CLA	8	309	-	3/3/17/25	5/22/120/135	-
17	CLA	1	314	13	2/2/18/25	4/25/123/135	-
17	CLA	B	803	2	3/3/20/25	5/37/135/135	-
26	CHL	7	605	29	3/3/15/26	4/12/110/137	-
17	CLA	b	804	2	3/3/16/25	4/11/111/135	-
17	CLA	b	807	2	3/3/20/25	6/37/135/135	-
17	CLA	3	310	19	3/3/13/25	0/2/96/135	-
17	CLA	a	841	1	3/3/20/25	12/37/135/135	-
17	CLA	7	604	29	3/3/19/25	11/31/129/135	-
22	HTG	F	302	-	-	2/10/30/30	0/1/1/1
17	CLA	A	807	1	3/3/20/25	12/37/135/135	-
17	CLA	a	843	1	3/3/20/25	14/37/135/135	-
17	CLA	8	311	15	2/2/16/25	1/11/111/135	-
20	BCR	g	104	-	-	2/29/63/63	0/2/2/2
17	CLA	9	614	16	3/3/16/25	4/16/114/135	-
17	CLA	B	838	2	2/2/16/25	0/16/114/135	-
17	CLA	7	613	14	2/2/15/25	0/11/109/135	-
17	CLA	k	1403	-	3/3/16/25	4/15/113/135	-
17	CLA	a	801	1	4/4/20/25	8/37/135/135	-
17	CLA	A	833	1	3/3/20/25	7/37/135/135	-
17	CLA	L	203	12	3/3/20/25	5/37/135/135	-
17	CLA	4	608	16	3/3/17/25	3/19/117/135	-
17	CLA	a	804	1	3/3/20/25	16/37/135/135	-
17	CLA	3	313	15	3/3/16/25	2/11/111/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	839	1	3/3/20/25	5/37/135/135	-
17	CLA	3	304	29	3/3/16/25	1/11/111/135	-
17	CLA	1	311	19	3/3/15/25	0/8/106/135	-
17	CLA	b	836	2	3/3/19/25	5/31/129/135	-
17	CLA	a	829	1	1/1/20/25	12/37/135/135	-
17	CLA	b	821	2	3/3/16/25	3/15/113/135	-
17	CLA	a	802	1	3/3/20/25	16/37/135/135	-
17	CLA	A	843	29	3/3/20/25	16/37/135/135	-
17	CLA	a	808	1	3/3/20/25	8/37/135/135	-
26	CHL	7	606	-	3/3/16/26	0/18/116/137	-
26	CHL	8	306	29	3/3/16/26	3/17/115/137	-
17	CLA	a	813	1	3/3/17/25	6/24/122/135	-
20	BCR	a	852	-	-	6/29/63/63	0/2/2/2
17	CLA	A	830	1	3/3/20/25	13/37/135/135	-
17	CLA	B	817	2	3/3/18/25	10/30/128/135	-
17	CLA	a	806	1	3/3/20/25	16/37/135/135	-
17	CLA	8	310	15	3/3/18/25	8/25/123/135	-
17	CLA	7	612	14	3/3/20/25	8/37/135/135	-
27	LUT	6	317	-	-	2/29/67/67	0/2/2/2
26	CHL	2	607	29	3/3/17/26	5/21/119/137	-
17	CLA	9	601	16	3/3/16/25	5/15/113/135	-
17	CLA	a	805	1	3/3/18/25	9/25/123/135	-
17	CLA	b	805	2	3/3/20/25	19/37/135/135	-
19	LHG	7	618	17	-	10/41/41/53	-
17	CLA	A	829	1	2/2/20/25	11/37/135/135	-
20	BCR	A	856	-	-	4/29/63/63	0/2/2/2
17	CLA	8	313	-	3/3/7/25	-	-
20	BCR	J	3003	-	-	2/29/63/63	0/2/2/2
26	CHL	9	605	29	2/2/18/26	8/27/125/137	-
26	CHL	1	302	13	3/3/19/26	7/33/131/137	-
20	BCR	b	801	-	-	0/29/63/63	0/2/2/2
20	BCR	A	848	-	-	6/29/63/63	0/2/2/2
17	CLA	6	314	13	3/3/19/25	6/31/129/135	-
17	CLA	3	302	15	3/3/19/25	8/31/129/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BCR	a	854	-	-	4/29/63/63	0/2/2/2
17	CLA	a	816	1	3/3/17/25	9/19/117/135	-
17	CLA	b	814	2	3/3/20/25	10/37/135/135	-
21	SF4	a	855	1,2	-	-	0/6/5/5
22	HTG	a	857	-	-	0/10/30/30	0/1/1/1
17	CLA	8	312	15	2/2/16/25	1/15/113/135	-
17	CLA	B	814	2	3/3/20/25	12/37/135/135	-
17	CLA	1	304	13	3/3/20/25	12/37/135/135	-
20	BCR	l	205	-	-	6/29/63/63	0/2/2/2
20	BCR	A	851	-	-	5/29/63/63	0/2/2/2
28	XAT	9	617	-	-	0/31/93/93	0/4/4/4
17	CLA	a	846	19	3/3/17/25	13/22/120/135	-
17	CLA	a	827	29	3/3/20/25	8/37/135/135	-
27	LUT	1	316	-	-	2/29/67/67	0/2/2/2
17	CLA	a	807	1	3/3/20/25	14/37/135/135	-
17	CLA	B	829	2	3/3/20/25	9/37/135/135	-
17	CLA	b	820	2	3/3/17/25	2/19/117/135	-
17	CLA	4	614	16	3/3/17/25	2/19/117/135	-
17	CLA	9	613	16	3/3/16/25	0/11/111/135	-
17	CLA	4	603	16	3/3/16/25	2/15/113/135	-
17	CLA	8	301	15	3/3/19/25	11/31/129/135	-
17	CLA	B	807	2	2/2/20/25	14/37/135/135	-
17	CLA	3	312	15	3/3/18/25	9/25/123/135	-
17	CLA	K	4003	11	3/3/16/25	2/15/113/135	-
17	CLA	8	302	15	3/3/17/25	1/19/117/135	-
17	CLA	8	307	15	3/3/17/25	5/19/117/135	-
17	CLA	7	603	14	3/3/17/25	3/21/119/135	-

All (4107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	845	PQN	C3-C2	7.78	1.49	1.35
18	b	842	PQN	C3-C2	7.70	1.49	1.35
18	A	844	PQN	C3-C2	7.61	1.49	1.35
18	B	842	PQN	C3-C2	7.59	1.49	1.35
17	B	836	CLA	C3B-C2B	6.44	1.49	1.40
17	a	804	CLA	C3B-C2B	6.39	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	838	CLA	C3B-C2B	6.34	1.49	1.40
17	a	830	CLA	C3B-C2B	6.31	1.49	1.40
17	b	836	CLA	C3B-C2B	6.31	1.49	1.40
17	A	808	CLA	C3B-C2B	6.30	1.49	1.40
17	A	830	CLA	C3B-C2B	6.20	1.49	1.40
26	4	606	CHL	C3B-C2B	6.20	1.49	1.40
17	3	306	CLA	C3B-C2B	6.18	1.48	1.40
17	a	818	CLA	C3B-C2B	6.17	1.48	1.40
17	A	854	CLA	C3B-C2B	6.16	1.48	1.40
17	j	3002	CLA	C3B-C2B	6.15	1.48	1.40
17	8	311	CLA	C3B-C2B	6.10	1.48	1.40
17	4	612	CLA	C3B-C2B	6.10	1.48	1.40
17	a	813	CLA	C3B-C2B	6.10	1.48	1.40
17	3	310	CLA	C3B-C2B	6.09	1.48	1.40
17	f	7003	CLA	C3B-C2B	6.09	1.48	1.40
17	1	315	CLA	C3B-C2B	6.08	1.48	1.40
17	8	309	CLA	C3B-C2B	6.08	1.48	1.40
17	3	313	CLA	C3B-C2B	6.08	1.48	1.40
17	6	312	CLA	C3B-C2B	6.08	1.48	1.40
17	J	3002	CLA	C3B-C2B	6.07	1.48	1.40
17	7	612	CLA	C3B-C2B	6.07	1.48	1.40
17	a	802	CLA	C3D-C2D	6.07	1.50	1.39
17	A	837	CLA	C3B-C2B	6.06	1.48	1.40
17	6	310	CLA	C3B-C2B	6.06	1.48	1.40
17	3	314	CLA	C3B-C2B	6.06	1.48	1.40
17	3	312	CLA	C3B-C2B	6.06	1.48	1.40
17	6	316	CLA	C3B-C2B	6.06	1.48	1.40
17	6	315	CLA	C3B-C2B	6.05	1.48	1.40
17	k	1403	CLA	C3B-C2B	6.05	1.48	1.40
17	3	311	CLA	C3B-C2B	6.05	1.48	1.40
17	3	301	CLA	C3B-C2B	6.04	1.48	1.40
17	K	4003	CLA	C3B-C2B	6.04	1.48	1.40
17	A	821	CLA	C3B-C2B	6.04	1.48	1.40
17	B	820	CLA	C3B-C2B	6.03	1.48	1.40
17	K	4002	CLA	C3B-C2B	6.03	1.48	1.40
17	1	311	CLA	C3B-C2B	6.03	1.48	1.40
17	1	309	CLA	C3B-C2B	6.03	1.48	1.40
17	A	806	CLA	C3B-C2B	6.03	1.48	1.40
26	6	308	CHL	C3B-C2B	6.03	1.48	1.40
17	6	309	CLA	C3B-C2B	6.02	1.48	1.40
17	A	818	CLA	C3B-C2B	6.02	1.48	1.40
17	9	612	CLA	C3B-C2B	6.02	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	807	CLA	C3B-C2B	6.02	1.48	1.40
17	g	102	CLA	C3B-C2B	6.02	1.48	1.40
26	2	606	CHL	C3B-C2B	6.02	1.48	1.40
17	A	824	CLA	C3B-C2B	6.02	1.48	1.40
26	7	614	CHL	C3B-C2B	6.01	1.48	1.40
17	b	812	CLA	C3B-C2B	6.01	1.48	1.40
17	8	305	CLA	C3B-C2B	6.01	1.48	1.40
17	A	805	CLA	C3B-C2B	6.01	1.48	1.40
17	B	822	CLA	C3B-C2B	6.01	1.48	1.40
17	4	608	CLA	C3B-C2B	6.01	1.48	1.40
17	A	825	CLA	C3B-C2B	6.00	1.48	1.40
26	9	615	CHL	C3B-C2B	6.00	1.48	1.40
17	1	312	CLA	C3B-C2B	6.00	1.48	1.40
17	A	831	CLA	C3D-C2D	6.00	1.50	1.39
17	a	810	CLA	C3B-C2B	6.00	1.48	1.40
17	7	613	CLA	C3B-C2B	5.99	1.48	1.40
17	b	839	CLA	C3B-C2B	5.99	1.48	1.40
17	a	821	CLA	C3B-C2B	5.99	1.48	1.40
17	8	310	CLA	C3B-C2B	5.99	1.48	1.40
17	B	821	CLA	C3B-C2B	5.99	1.48	1.40
17	4	613	CLA	C3B-C2B	5.99	1.48	1.40
17	B	826	CLA	C3B-C2B	5.99	1.48	1.40
17	1	314	CLA	C3B-C2B	5.99	1.48	1.40
17	8	312	CLA	C3B-C2B	5.99	1.48	1.40
17	8	313	CLA	C3C-C2C	5.99	1.48	1.35
17	1	304	CLA	C3B-C2B	5.98	1.48	1.40
17	g	103	CLA	C3B-C2B	5.98	1.48	1.40
26	7	606	CHL	C3B-C2B	5.98	1.48	1.40
17	7	610	CLA	C3B-C2B	5.98	1.48	1.40
17	a	806	CLA	C3B-C2B	5.98	1.48	1.40
17	k	1401	CLA	C3B-C2B	5.98	1.48	1.40
17	9	601	CLA	C3B-C2B	5.98	1.48	1.40
17	4	610	CLA	C3B-C2B	5.97	1.48	1.40
17	2	611	CLA	C3B-C2B	5.97	1.48	1.40
17	3	315	CLA	C3C-C2C	5.97	1.48	1.35
17	B	810	CLA	C3B-C2B	5.97	1.48	1.40
17	9	613	CLA	C3B-C2B	5.97	1.48	1.40
17	1	313	CLA	C3B-C2B	5.96	1.48	1.40
26	4	615	CHL	C3B-C2B	5.96	1.48	1.40
17	b	834	CLA	C3B-C2B	5.96	1.48	1.40
17	2	603	CLA	C3B-C2B	5.95	1.48	1.40
17	2	613	CLA	C3B-C2B	5.95	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	6	313	CLA	C3B-C2B	5.95	1.48	1.40
26	2	614	CHL	C3B-C2B	5.95	1.48	1.40
17	b	820	CLA	C3B-C2B	5.95	1.48	1.40
17	b	817	CLA	C3B-C2B	5.95	1.48	1.40
17	8	304	CLA	C3B-C2B	5.95	1.48	1.40
17	9	610	CLA	C3B-C2B	5.95	1.48	1.40
17	B	804	CLA	C3B-C2B	5.95	1.48	1.40
17	9	611	CLA	C3B-C2B	5.94	1.48	1.40
17	B	834	CLA	C3B-C2B	5.94	1.48	1.40
17	b	810	CLA	C3B-C2B	5.94	1.48	1.40
17	b	807	CLA	C3B-C2B	5.94	1.48	1.40
17	b	841	CLA	C3B-C2B	5.94	1.48	1.40
17	A	817	CLA	C3B-C2B	5.94	1.48	1.40
17	b	804	CLA	C3B-C2B	5.94	1.48	1.40
17	F	301	CLA	C3B-C2B	5.94	1.48	1.40
17	b	823	CLA	C3B-C2B	5.93	1.48	1.40
17	a	856	CLA	C3B-C2B	5.93	1.48	1.40
17	b	821	CLA	C3B-C2B	5.93	1.48	1.40
17	1	308	CLA	C3B-C2B	5.93	1.48	1.40
17	7	611	CLA	C3B-C2B	5.93	1.48	1.40
26	1	307	CHL	C3B-C2B	5.93	1.48	1.40
17	G	101	CLA	C3B-C2B	5.92	1.48	1.40
17	A	812	CLA	C3B-C2B	5.92	1.48	1.40
17	2	612	CLA	C3B-C2B	5.92	1.48	1.40
26	7	605	CHL	C3B-C2B	5.92	1.48	1.40
17	a	823	CLA	C3B-C2B	5.92	1.48	1.40
17	A	842	CLA	C3B-C2B	5.92	1.48	1.40
17	A	832	CLA	C3B-C2B	5.92	1.48	1.40
17	1	305	CLA	C3B-C2B	5.91	1.48	1.40
26	9	606	CHL	C3B-C2B	5.91	1.48	1.40
17	B	840	CLA	C3B-C2B	5.91	1.48	1.40
17	1	310	CLA	C3B-C2B	5.91	1.48	1.40
17	B	839	CLA	C3B-C2B	5.91	1.48	1.40
17	A	845	CLA	C3B-C2B	5.90	1.48	1.40
17	3	303	CLA	C3B-C2B	5.90	1.48	1.40
26	8	306	CHL	C3B-C2B	5.90	1.48	1.40
17	a	825	CLA	C3B-C2B	5.90	1.48	1.40
17	4	601	CLA	C3B-C2B	5.90	1.48	1.40
17	b	818	CLA	C3D-C2D	5.90	1.50	1.39
17	B	808	CLA	C3B-C2B	5.90	1.48	1.40
17	2	610	CLA	C3B-C2B	5.90	1.48	1.40
17	B	838	CLA	C3B-C2B	5.90	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	825	CLA	C3D-C2D	5.90	1.50	1.39
17	A	803	CLA	C3D-C2D	5.89	1.50	1.39
17	6	307	CLA	C3B-C2B	5.89	1.48	1.40
17	9	608	CLA	C3B-C2B	5.89	1.48	1.40
17	a	819	CLA	C3B-C2B	5.89	1.48	1.40
17	4	611	CLA	C3B-C2B	5.89	1.48	1.40
17	B	817	CLA	C3B-C2B	5.89	1.48	1.40
17	b	840	CLA	C3B-C2B	5.89	1.48	1.40
26	7	601	CHL	C3B-C2B	5.89	1.48	1.40
17	b	806	CLA	C3B-C2B	5.89	1.48	1.40
17	b	822	CLA	C3B-C2B	5.88	1.48	1.40
17	4	603	CLA	C3B-C2B	5.88	1.48	1.40
17	B	812	CLA	C3D-C2D	5.88	1.50	1.39
17	4	614	CLA	C3B-C2B	5.88	1.48	1.40
17	1	304	CLA	C3D-C2D	5.88	1.50	1.39
17	f	7002	CLA	C3B-C2B	5.88	1.48	1.40
17	a	815	CLA	C3B-C2B	5.88	1.48	1.40
17	B	841	CLA	C3B-C2B	5.88	1.48	1.40
17	G	104	CLA	C3B-C2B	5.88	1.48	1.40
17	6	314	CLA	C3B-C2B	5.88	1.48	1.40
17	3	305	CLA	C3B-C2B	5.87	1.48	1.40
17	F	303	CLA	C3B-C2B	5.87	1.48	1.40
17	g	101	CLA	C3B-C2B	5.87	1.48	1.40
17	a	820	CLA	C3B-C2B	5.87	1.48	1.40
17	B	823	CLA	C3B-C2B	5.87	1.48	1.40
17	b	808	CLA	C3B-C2B	5.87	1.48	1.40
17	A	819	CLA	C3B-C2B	5.87	1.48	1.40
17	A	813	CLA	C3B-C2B	5.87	1.48	1.40
17	b	835	CLA	C3B-C2B	5.86	1.48	1.40
17	6	304	CLA	C3B-C2B	5.86	1.48	1.40
17	k	1402	CLA	C3B-C2B	5.86	1.48	1.40
17	a	842	CLA	C3B-C2B	5.86	1.48	1.40
17	2	608	CLA	C3B-C2B	5.86	1.48	1.40
17	A	841	CLA	C3B-C2B	5.86	1.48	1.40
17	A	839	CLA	C3B-C2B	5.86	1.48	1.40
17	a	824	CLA	C3B-C2B	5.86	1.48	1.40
17	G	103	CLA	C3B-C2B	5.85	1.48	1.40
17	a	837	CLA	C3B-C2B	5.85	1.48	1.40
17	B	812	CLA	C3B-C2B	5.85	1.48	1.40
17	a	832	CLA	C3B-C2B	5.85	1.48	1.40
17	a	817	CLA	C3B-C2B	5.85	1.48	1.40
17	A	823	CLA	C3B-C2B	5.85	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	814	CLA	C3B-C2B	5.85	1.48	1.40
17	6	306	CLA	C3B-C2B	5.84	1.48	1.40
17	A	854	CLA	C3D-C2D	5.84	1.49	1.39
17	B	818	CLA	C3D-C2D	5.84	1.49	1.39
17	A	811	CLA	C3B-C2B	5.84	1.48	1.40
17	a	833	CLA	C3B-C2B	5.84	1.48	1.40
17	B	835	CLA	C3B-C2B	5.84	1.48	1.40
17	a	816	CLA	C3B-C2B	5.84	1.48	1.40
17	A	821	CLA	C3D-C2D	5.84	1.49	1.39
17	a	805	CLA	C3B-C2B	5.84	1.48	1.40
17	A	809	CLA	C3B-C2B	5.84	1.48	1.40
17	9	603	CLA	C3B-C2B	5.84	1.48	1.40
17	b	812	CLA	C3D-C2D	5.84	1.49	1.39
17	A	809	CLA	C3D-C2D	5.84	1.49	1.39
17	a	846	CLA	C3B-C2B	5.84	1.48	1.40
17	1	311	CLA	C3D-C2D	5.83	1.49	1.39
26	2	601	CHL	C3B-C2B	5.83	1.48	1.40
17	6	311	CLA	C3B-C2B	5.83	1.48	1.40
17	7	603	CLA	C3B-C2B	5.83	1.48	1.40
17	8	307	CLA	C3D-C2D	5.83	1.49	1.39
17	a	844	CLA	C3D-C2D	5.83	1.49	1.39
17	a	843	CLA	C3B-C2B	5.83	1.48	1.40
17	A	816	CLA	C3B-C2B	5.83	1.48	1.40
17	A	802	CLA	C3D-C2D	5.83	1.49	1.39
17	6	305	CLA	C3B-C2B	5.83	1.48	1.40
17	b	819	CLA	C3D-C2D	5.83	1.49	1.39
17	B	806	CLA	C3B-C2B	5.83	1.48	1.40
17	9	614	CLA	C3B-C2B	5.83	1.48	1.40
17	6	313	CLA	C3D-C2D	5.82	1.49	1.39
17	A	814	CLA	C3D-C2D	5.82	1.49	1.39
17	b	805	CLA	C3D-C2D	5.82	1.49	1.39
17	a	856	CLA	C3D-C2D	5.82	1.49	1.39
17	a	808	CLA	C3B-C2B	5.82	1.48	1.40
17	3	308	CLA	C3D-C2D	5.82	1.49	1.39
17	b	803	CLA	C3B-C2B	5.82	1.48	1.40
17	b	828	CLA	C3B-C2B	5.81	1.48	1.40
26	2	605	CHL	C3B-C2B	5.81	1.48	1.40
17	A	802	CLA	C3B-C2B	5.81	1.48	1.40
17	b	825	CLA	C3B-C2B	5.81	1.48	1.40
17	6	314	CLA	C3D-C2D	5.81	1.49	1.39
17	F	304	CLA	C3B-C2B	5.81	1.48	1.40
17	L	204	CLA	C3B-C2B	5.81	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	825	CLA	C3B-C2B	5.81	1.48	1.40
17	7	609	CLA	C3D-C2D	5.81	1.49	1.39
17	2	608	CLA	C3D-C2D	5.81	1.49	1.39
17	a	838	CLA	C3B-C2B	5.80	1.48	1.40
17	a	803	CLA	C3D-C2D	5.80	1.49	1.39
17	b	807	CLA	C3D-C2D	5.80	1.49	1.39
17	b	833	CLA	C3B-C2B	5.80	1.48	1.40
17	8	302	CLA	C3B-C2B	5.80	1.48	1.40
17	A	836	CLA	C3D-C2D	5.80	1.49	1.39
17	a	836	CLA	C3D-C2D	5.80	1.49	1.39
17	A	827	CLA	C3B-C2B	5.80	1.48	1.40
17	a	801	CLA	C3B-C2B	5.80	1.48	1.40
17	A	815	CLA	C3B-C2B	5.79	1.48	1.40
17	A	830	CLA	C3D-C2D	5.79	1.49	1.39
17	A	835	CLA	C3B-C2B	5.79	1.48	1.40
17	2	609	CLA	C3B-C2B	5.79	1.48	1.40
17	1	306	CLA	C3B-C2B	5.79	1.48	1.40
17	a	811	CLA	C3B-C2B	5.79	1.48	1.40
17	7	610	CLA	C3D-C2D	5.79	1.49	1.39
17	a	809	CLA	C3D-C2D	5.79	1.49	1.39
17	3	302	CLA	C3D-C2D	5.79	1.49	1.39
17	a	823	CLA	C3D-C2D	5.78	1.49	1.39
17	A	820	CLA	C3D-C2D	5.78	1.49	1.39
17	B	833	CLA	C3B-C2B	5.78	1.48	1.40
17	K	4003	CLA	C3D-C2D	5.78	1.49	1.39
17	b	830	CLA	C3B-C2B	5.78	1.48	1.40
17	a	837	CLA	C3D-C2D	5.78	1.49	1.39
17	4	610	CLA	C3D-C2D	5.78	1.49	1.39
17	4	602	CLA	C3B-C2B	5.78	1.48	1.40
17	a	839	CLA	C3B-C2B	5.78	1.48	1.40
17	b	821	CLA	C3D-C2D	5.78	1.49	1.39
17	b	803	CLA	C3D-C2D	5.78	1.49	1.39
17	a	819	CLA	C3D-C2D	5.78	1.49	1.39
17	b	816	CLA	C3D-C2D	5.78	1.49	1.39
17	2	609	CLA	C3D-C2D	5.78	1.49	1.39
17	8	309	CLA	C3D-C2D	5.78	1.49	1.39
17	A	834	CLA	C3B-C2B	5.77	1.48	1.40
17	b	824	CLA	C3B-C2B	5.77	1.48	1.40
17	a	840	CLA	C3B-C2B	5.77	1.48	1.40
17	J	3002	CLA	C3D-C2D	5.77	1.49	1.39
17	B	830	CLA	C3D-C2D	5.77	1.49	1.39
17	2	604	CLA	C3D-C2D	5.77	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	8	310	CLA	C3D-C2D	5.77	1.49	1.39
17	a	833	CLA	C3D-C2D	5.77	1.49	1.39
26	3	307	CHL	C3B-C2B	5.77	1.48	1.40
17	A	805	CLA	C3D-C2D	5.77	1.49	1.39
17	b	826	CLA	C3B-C2B	5.77	1.48	1.40
17	B	815	CLA	C3D-C2D	5.77	1.49	1.39
17	a	813	CLA	C3D-C2D	5.77	1.49	1.39
17	A	840	CLA	C3B-C2B	5.77	1.48	1.40
17	b	831	CLA	C3B-C2B	5.76	1.48	1.40
17	B	828	CLA	C3B-C2B	5.76	1.48	1.40
17	a	827	CLA	C3B-C2B	5.76	1.48	1.40
17	b	815	CLA	C3D-C2D	5.76	1.49	1.39
17	3	310	CLA	C3D-C2D	5.76	1.49	1.39
17	a	820	CLA	C3D-C2D	5.76	1.49	1.39
17	b	833	CLA	C3D-C2D	5.76	1.49	1.39
26	9	607	CHL	C3B-C2B	5.76	1.48	1.40
17	a	807	CLA	C3D-C2D	5.76	1.49	1.39
17	L	203	CLA	C3B-C2B	5.76	1.48	1.40
17	l	203	CLA	C3B-C2B	5.76	1.48	1.40
17	B	819	CLA	C3D-C2D	5.76	1.49	1.39
17	B	815	CLA	C3B-C2B	5.76	1.48	1.40
17	b	809	CLA	C3D-C2D	5.76	1.49	1.39
17	B	807	CLA	C3D-C2D	5.75	1.49	1.39
17	b	815	CLA	C3B-C2B	5.75	1.48	1.40
17	B	818	CLA	C3B-C2B	5.75	1.48	1.40
17	6	312	CLA	C3D-C2D	5.75	1.49	1.39
17	2	602	CLA	C3B-C2B	5.75	1.48	1.40
17	3	309	CLA	C3B-C2B	5.75	1.48	1.40
17	1	315	CLA	C3D-C2D	5.75	1.49	1.39
17	b	836	CLA	C3D-C2D	5.75	1.49	1.39
17	3	304	CLA	C3B-C2B	5.75	1.48	1.40
17	l	202	CLA	C3B-C2B	5.75	1.48	1.40
17	9	610	CLA	C3D-C2D	5.75	1.49	1.39
17	9	608	CLA	C3D-C2D	5.75	1.49	1.39
17	b	811	CLA	C3D-C2D	5.75	1.49	1.39
17	b	830	CLA	C3D-C2D	5.75	1.49	1.39
17	b	813	CLA	C3B-C2B	5.74	1.48	1.40
17	B	809	CLA	C3D-C2D	5.74	1.49	1.39
17	6	310	CLA	C3D-C2D	5.74	1.49	1.39
17	B	813	CLA	C3B-C2B	5.74	1.48	1.40
17	a	802	CLA	C3B-C2B	5.74	1.48	1.40
17	F	301	CLA	C3D-C2D	5.74	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	838	CLA	C3D-C2D	5.74	1.49	1.39
17	B	821	CLA	C3D-C2D	5.74	1.49	1.39
17	a	841	CLA	C3D-C2D	5.74	1.49	1.39
17	j	3002	CLA	C3D-C2D	5.74	1.49	1.39
17	8	308	CLA	C3B-C2B	5.74	1.48	1.40
17	B	803	CLA	C3B-C2B	5.74	1.48	1.40
17	a	825	CLA	C3D-C2D	5.73	1.49	1.39
17	a	814	CLA	C3D-C2D	5.73	1.49	1.39
17	B	830	CLA	C3B-C2B	5.73	1.48	1.40
17	4	604	CLA	C3D-C2D	5.73	1.49	1.39
17	8	303	CLA	C3D-C2D	5.73	1.49	1.39
17	A	808	CLA	C3D-C2D	5.73	1.49	1.39
17	a	846	CLA	C3D-C2D	5.73	1.49	1.39
17	g	102	CLA	C3D-C2D	5.73	1.49	1.39
17	8	301	CLA	C3D-C2D	5.73	1.49	1.39
17	a	835	CLA	C3B-C2B	5.73	1.48	1.40
17	k	1403	CLA	C3D-C2D	5.73	1.49	1.39
17	A	814	CLA	C3B-C2B	5.73	1.48	1.40
17	b	841	CLA	C3D-C2D	5.73	1.49	1.39
17	6	315	CLA	C3D-C2D	5.73	1.49	1.39
17	B	841	CLA	C3D-C2D	5.73	1.49	1.39
17	8	304	CLA	C3D-C2D	5.73	1.49	1.39
17	b	805	CLA	C3B-C2B	5.72	1.48	1.40
17	k	1402	CLA	C3D-C2D	5.72	1.49	1.39
17	G	103	CLA	C3D-C2D	5.72	1.49	1.39
17	a	812	CLA	C3B-C2B	5.72	1.48	1.40
17	7	608	CLA	C3D-C2D	5.72	1.49	1.39
17	a	818	CLA	C3D-C2D	5.72	1.49	1.39
17	a	817	CLA	C3D-C2D	5.72	1.49	1.39
17	A	833	CLA	C3D-C2D	5.72	1.49	1.39
17	a	822	CLA	C3D-C2D	5.72	1.49	1.39
17	2	613	CLA	C3D-C2D	5.72	1.49	1.39
17	b	817	CLA	C3D-C2D	5.72	1.49	1.39
17	6	305	CLA	C3D-C2D	5.72	1.49	1.39
17	B	819	CLA	C3B-C2B	5.72	1.48	1.40
17	3	304	CLA	C3D-C2D	5.72	1.49	1.39
17	4	608	CLA	C3D-C2D	5.72	1.49	1.39
17	8	305	CLA	C3D-C2D	5.72	1.49	1.39
17	B	833	CLA	C3D-C2D	5.72	1.49	1.39
17	l	204	CLA	C3D-C2D	5.72	1.49	1.39
17	6	316	CLA	C3D-C2D	5.71	1.49	1.39
17	8	308	CLA	C3D-C2D	5.71	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	836	CLA	C3D-C2D	5.71	1.49	1.39
17	A	837	CLA	C3D-C2D	5.71	1.49	1.39
17	3	309	CLA	C3D-C2D	5.71	1.49	1.39
17	2	604	CLA	C3B-C2B	5.71	1.48	1.40
17	b	814	CLA	C3B-C2B	5.71	1.48	1.40
17	9	602	CLA	C3B-C2B	5.71	1.48	1.40
17	B	837	CLA	C3D-C2D	5.71	1.49	1.39
17	8	311	CLA	C3D-C2D	5.71	1.49	1.39
26	9	605	CHL	C3B-C2B	5.71	1.48	1.40
17	A	841	CLA	C3D-C2D	5.71	1.49	1.39
17	b	802	CLA	C3D-C2D	5.71	1.49	1.39
17	a	831	CLA	C3D-C2D	5.70	1.49	1.39
17	B	816	CLA	C3D-C2D	5.70	1.49	1.39
17	a	828	CLA	C3B-C2B	5.70	1.48	1.40
17	8	303	CLA	C3B-C2B	5.70	1.48	1.40
17	A	810	CLA	C3B-C2B	5.70	1.48	1.40
17	B	829	CLA	C3D-C2D	5.70	1.49	1.39
17	3	312	CLA	C3D-C2D	5.70	1.49	1.39
17	L	202	CLA	C3B-C2B	5.70	1.48	1.40
17	B	806	CLA	C3D-C2D	5.70	1.49	1.39
17	a	826	CLA	C3B-C2B	5.70	1.48	1.40
17	A	845	CLA	C3D-C2D	5.70	1.49	1.39
26	1	302	CHL	C3B-C2B	5.70	1.48	1.40
17	8	301	CLA	C3B-C2B	5.70	1.48	1.40
17	L	203	CLA	C3D-C2D	5.70	1.49	1.39
17	a	830	CLA	C3D-C2D	5.70	1.49	1.39
17	a	809	CLA	C3B-C2B	5.69	1.48	1.40
17	A	811	CLA	C3D-C2D	5.69	1.49	1.39
17	B	811	CLA	C3D-C2D	5.69	1.49	1.39
17	A	822	CLA	C3D-C2D	5.69	1.49	1.39
17	6	311	CLA	C3D-C2D	5.69	1.49	1.39
17	2	610	CLA	C3D-C2D	5.69	1.49	1.39
17	9	601	CLA	C3D-C2D	5.69	1.49	1.39
17	7	604	CLA	C3D-C2D	5.69	1.49	1.39
17	3	313	CLA	C3D-C2D	5.69	1.49	1.39
17	1	309	CLA	C3D-C2D	5.69	1.49	1.39
17	a	841	CLA	C3B-C2B	5.69	1.48	1.40
26	2	607	CHL	C3B-C2B	5.69	1.48	1.40
17	1	314	CLA	C3D-C2D	5.68	1.49	1.39
17	a	839	CLA	C3D-C2D	5.68	1.49	1.39
17	6	307	CLA	C3D-C2D	5.68	1.49	1.39
17	9	604	CLA	C3D-C2D	5.68	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	310	CLA	C3D-C2D	5.68	1.49	1.39
17	A	804	CLA	C3D-C2D	5.68	1.49	1.39
17	7	611	CLA	C3D-C2D	5.68	1.49	1.39
17	3	308	CLA	C3B-C2B	5.68	1.48	1.40
17	9	603	CLA	C3D-C2D	5.68	1.49	1.39
17	B	820	CLA	C3D-C2D	5.68	1.49	1.39
17	A	832	CLA	C3D-C2D	5.68	1.49	1.39
17	b	837	CLA	C3D-C2D	5.68	1.49	1.39
17	7	609	CLA	C3B-C2B	5.68	1.48	1.40
17	2	602	CLA	C3D-C2D	5.68	1.49	1.39
17	8	302	CLA	C3D-C2D	5.68	1.49	1.39
17	b	835	CLA	C3D-C2D	5.68	1.49	1.39
17	B	837	CLA	C3B-C2B	5.67	1.48	1.40
17	3	303	CLA	C3D-C2D	5.67	1.49	1.39
17	7	604	CLA	C3B-C2B	5.67	1.48	1.40
17	9	611	CLA	C3D-C2D	5.67	1.49	1.39
17	a	834	CLA	C3D-C2D	5.67	1.49	1.39
17	4	609	CLA	C3B-C2B	5.67	1.48	1.40
17	6	306	CLA	C3D-C2D	5.67	1.49	1.39
17	L	202	CLA	C3D-C2D	5.67	1.49	1.39
17	K	4002	CLA	C3D-C2D	5.67	1.49	1.39
17	F	303	CLA	C3D-C2D	5.67	1.49	1.39
17	3	301	CLA	C3D-C2D	5.67	1.49	1.39
17	b	824	CLA	C3D-C2D	5.67	1.49	1.39
17	b	804	CLA	C3D-C2D	5.67	1.49	1.39
17	A	816	CLA	C3D-C2D	5.67	1.49	1.39
17	7	608	CLA	C3B-C2B	5.67	1.48	1.40
17	4	604	CLA	C3B-C2B	5.67	1.48	1.40
17	a	834	CLA	C3B-C2B	5.67	1.48	1.40
17	A	828	CLA	C3B-C2B	5.67	1.48	1.40
17	3	314	CLA	C3D-C2D	5.67	1.49	1.39
17	A	826	CLA	C3D-C2D	5.66	1.49	1.39
17	G	104	CLA	C3D-C2D	5.66	1.49	1.39
17	9	609	CLA	C3B-C2B	5.66	1.48	1.40
17	B	824	CLA	C3D-C2D	5.66	1.49	1.39
17	F	304	CLA	C3D-C2D	5.66	1.49	1.39
17	B	822	CLA	C3D-C2D	5.66	1.49	1.39
17	A	807	CLA	C3B-C2B	5.66	1.48	1.40
17	9	602	CLA	C3D-C2D	5.66	1.49	1.39
17	B	835	CLA	C3D-C2D	5.66	1.49	1.39
17	a	806	CLA	C3D-C2D	5.66	1.49	1.39
17	B	829	CLA	C3B-C2B	5.66	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	817	CLA	C3D-C2D	5.66	1.49	1.39
17	a	826	CLA	C3D-C2D	5.66	1.49	1.39
17	l	202	CLA	C3D-C2D	5.66	1.49	1.39
17	a	816	CLA	C3D-C2D	5.66	1.49	1.39
17	9	612	CLA	C3D-C2D	5.66	1.49	1.39
17	4	612	CLA	C3D-C2D	5.66	1.49	1.39
17	7	603	CLA	C3D-C2D	5.66	1.49	1.39
17	1	303	CLA	C3B-C2B	5.65	1.48	1.40
17	l	203	CLA	C3D-C2D	5.65	1.49	1.39
17	1	313	CLA	C3D-C2D	5.65	1.49	1.39
17	3	311	CLA	C3D-C2D	5.65	1.49	1.39
17	A	827	CLA	C3D-C2D	5.65	1.49	1.39
26	4	607	CHL	C3B-C2B	5.65	1.48	1.40
17	b	819	CLA	C3B-C2B	5.65	1.48	1.40
17	B	803	CLA	C3D-C2D	5.65	1.49	1.39
17	a	811	CLA	C3D-C2D	5.65	1.49	1.39
17	8	313	CLA	C2B-C1B	5.64	1.49	1.39
17	1	305	CLA	C3D-C2D	5.64	1.49	1.39
17	A	843	CLA	C3D-C2D	5.64	1.49	1.39
17	a	807	CLA	C3B-C2B	5.64	1.48	1.40
17	3	315	CLA	C2B-C1B	5.64	1.49	1.39
17	A	801	CLA	C3D-C2D	5.64	1.49	1.39
17	1	312	CLA	C3D-C2D	5.64	1.49	1.39
17	b	813	CLA	C3D-C2D	5.64	1.49	1.39
17	2	612	CLA	C3D-C2D	5.64	1.49	1.39
17	b	831	CLA	C3D-C2D	5.64	1.49	1.39
17	B	805	CLA	C3B-C2B	5.64	1.48	1.40
26	4	605	CHL	C3B-C2B	5.64	1.48	1.40
17	B	834	CLA	C3D-C2D	5.64	1.49	1.39
17	A	841	CLA	C3C-C2C	5.64	1.48	1.36
17	a	801	CLA	C3D-C2D	5.63	1.49	1.39
17	A	840	CLA	C3D-C2D	5.63	1.49	1.39
17	4	614	CLA	C3D-C2D	5.63	1.49	1.39
17	B	831	CLA	C3B-C2B	5.63	1.48	1.40
26	7	607	CHL	C3B-C2B	5.63	1.48	1.40
17	A	818	CLA	C3D-C2D	5.63	1.49	1.39
17	a	808	CLA	C3D-C2D	5.63	1.49	1.39
17	b	822	CLA	C3D-C2D	5.63	1.49	1.39
17	3	302	CLA	C3B-C2B	5.62	1.48	1.40
17	8	312	CLA	C3D-C2D	5.62	1.49	1.39
17	8	307	CLA	C3B-C2B	5.62	1.48	1.40
17	A	823	CLA	C3D-C2D	5.62	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	g	101	CLA	C3D-C2D	5.62	1.49	1.39
17	4	603	CLA	C3D-C2D	5.62	1.49	1.39
17	b	832	CLA	C3B-C2B	5.62	1.48	1.40
17	B	814	CLA	C3B-C2B	5.62	1.48	1.40
17	B	824	CLA	C3B-C2B	5.61	1.48	1.40
17	B	832	CLA	C3B-C2B	5.61	1.48	1.40
17	b	827	CLA	C3B-C2B	5.61	1.48	1.40
17	A	815	CLA	C3D-C2D	5.61	1.49	1.39
17	b	825	CLA	C3D-C2D	5.61	1.49	1.39
17	1	303	CLA	C3D-C2D	5.61	1.49	1.39
17	A	829	CLA	C3B-C2B	5.61	1.48	1.40
17	A	833	CLA	C3B-C2B	5.61	1.48	1.40
17	B	802	CLA	C3D-C2D	5.61	1.49	1.39
17	A	836	CLA	C3B-C2B	5.61	1.48	1.40
17	9	609	CLA	C3D-C2D	5.61	1.49	1.39
17	a	842	CLA	C3D-C2D	5.61	1.49	1.39
17	a	836	CLA	C3B-C2B	5.61	1.48	1.40
17	a	829	CLA	C3B-C2B	5.60	1.48	1.40
17	B	831	CLA	C3D-C2D	5.60	1.49	1.39
17	A	807	CLA	C3D-C2D	5.60	1.49	1.39
17	A	813	CLA	C3D-C2D	5.60	1.49	1.39
17	A	801	CLA	C3B-C2B	5.60	1.48	1.40
17	A	839	CLA	C3D-C2D	5.60	1.49	1.39
17	3	305	CLA	C3D-C2D	5.60	1.49	1.39
17	g	103	CLA	C3D-C2D	5.60	1.49	1.39
17	b	837	CLA	C3B-C2B	5.60	1.48	1.40
17	4	601	CLA	C3D-C2D	5.60	1.49	1.39
17	f	7003	CLA	C3D-C2D	5.60	1.49	1.39
17	b	814	CLA	C3D-C2D	5.59	1.49	1.39
17	a	815	CLA	C3D-C2D	5.59	1.49	1.39
17	A	817	CLA	C3D-C2D	5.59	1.49	1.39
17	A	838	CLA	C3B-C2B	5.59	1.48	1.40
17	A	804	CLA	C3B-C2B	5.59	1.48	1.40
17	a	827	CLA	C3D-C2D	5.59	1.49	1.39
17	A	834	CLA	C3D-C2D	5.59	1.49	1.39
17	4	602	CLA	C3D-C2D	5.59	1.49	1.39
17	B	808	CLA	C3D-C2D	5.59	1.49	1.39
17	b	828	CLA	C3D-C2D	5.59	1.49	1.39
17	3	306	CLA	C3D-C2D	5.59	1.49	1.39
17	2	611	CLA	C3D-C2D	5.59	1.49	1.39
17	B	810	CLA	C3D-C2D	5.59	1.49	1.39
17	k	1401	CLA	C3D-C2D	5.58	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	805	CLA	C3D-C2D	5.58	1.49	1.39
17	A	829	CLA	C3D-C2D	5.58	1.49	1.39
17	4	611	CLA	C3D-C2D	5.58	1.49	1.39
17	A	827	CLA	C3C-C2C	5.58	1.48	1.36
17	B	823	CLA	C3C-C2C	5.58	1.48	1.36
17	A	842	CLA	C3D-C2D	5.58	1.49	1.39
17	B	816	CLA	C3B-C2B	5.58	1.48	1.40
17	B	804	CLA	C3D-C2D	5.58	1.49	1.39
17	b	838	CLA	C3D-C2D	5.58	1.49	1.39
17	1	306	CLA	C3D-C2D	5.58	1.49	1.39
17	B	825	CLA	C3D-C2D	5.58	1.49	1.39
17	a	803	CLA	C3B-C2B	5.58	1.48	1.40
17	A	835	CLA	C3D-C2D	5.58	1.49	1.39
17	B	840	CLA	C3D-C2D	5.57	1.49	1.39
17	b	820	CLA	C3D-C2D	5.57	1.49	1.39
17	B	839	CLA	C3D-C2D	5.57	1.49	1.39
17	7	612	CLA	C3D-C2D	5.57	1.49	1.39
17	A	803	CLA	C3B-C2B	5.57	1.48	1.40
17	7	602	CLA	C3B-C2B	5.57	1.48	1.40
17	a	822	CLA	C3B-C2B	5.56	1.48	1.40
17	4	609	CLA	C3D-C2D	5.56	1.49	1.39
17	9	604	CLA	C3B-C2B	5.56	1.48	1.40
17	b	806	CLA	C3D-C2D	5.56	1.49	1.39
17	A	838	CLA	C3D-C2D	5.56	1.49	1.39
17	A	845	CLA	C3C-C2C	5.56	1.48	1.36
17	G	101	CLA	C3D-C2D	5.56	1.49	1.39
17	b	808	CLA	C3D-C2D	5.56	1.49	1.39
17	b	839	CLA	C3D-C2D	5.56	1.49	1.39
17	6	309	CLA	C3D-C2D	5.55	1.49	1.39
17	a	810	CLA	C3D-C2D	5.55	1.49	1.39
17	f	7002	CLA	C3D-C2D	5.55	1.49	1.39
17	6	304	CLA	C3D-C2D	5.55	1.49	1.39
17	B	840	CLA	C3C-C2C	5.55	1.48	1.36
17	b	834	CLA	C3D-C2D	5.55	1.49	1.39
17	4	613	CLA	C3D-C2D	5.55	1.49	1.39
17	B	823	CLA	C3D-C2D	5.55	1.49	1.39
17	a	829	CLA	C3D-C2D	5.55	1.49	1.39
17	l	204	CLA	C3B-C2B	5.55	1.48	1.40
17	b	827	CLA	C3D-C2D	5.55	1.49	1.39
17	b	810	CLA	C3D-C2D	5.55	1.49	1.39
17	a	827	CLA	C3C-C2C	5.55	1.48	1.36
17	B	813	CLA	C3D-C2D	5.54	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	821	CLA	C3D-C2D	5.54	1.49	1.39
17	a	828	CLA	C3C-C2C	5.54	1.48	1.36
17	B	826	CLA	C3C-C2C	5.54	1.48	1.36
17	A	820	CLA	C3B-C2B	5.54	1.48	1.40
17	b	826	CLA	C3D-C2D	5.54	1.49	1.39
17	A	806	CLA	C3D-C2D	5.54	1.49	1.39
17	A	824	CLA	C3D-C2D	5.54	1.49	1.39
17	9	613	CLA	C3D-C2D	5.54	1.49	1.39
17	A	826	CLA	C3B-C2B	5.54	1.48	1.40
17	a	812	CLA	C3D-C2D	5.54	1.49	1.39
17	B	827	CLA	C3D-C2D	5.54	1.49	1.39
17	b	816	CLA	C3B-C2B	5.53	1.48	1.40
17	A	828	CLA	C3D-C2D	5.53	1.49	1.39
17	7	608	CLA	C3C-C2C	5.52	1.48	1.36
17	b	839	CLA	C3C-C2C	5.52	1.48	1.36
17	9	614	CLA	C3D-C2D	5.52	1.49	1.39
17	a	840	CLA	C3D-C2D	5.52	1.49	1.39
17	A	819	CLA	C3D-C2D	5.52	1.49	1.39
17	7	613	CLA	C3D-C2D	5.52	1.49	1.39
17	k	1403	CLA	C3C-C2C	5.51	1.48	1.36
17	a	835	CLA	C3D-C2D	5.51	1.49	1.39
17	b	840	CLA	C3C-C2C	5.51	1.48	1.36
17	A	810	CLA	C3D-C2D	5.51	1.49	1.39
17	2	603	CLA	C3D-C2D	5.51	1.49	1.39
17	a	809	CLA	C3C-C2C	5.51	1.48	1.36
17	B	814	CLA	C3D-C2D	5.51	1.49	1.39
17	b	837	CLA	C3C-C2C	5.51	1.48	1.36
17	7	602	CLA	C3D-C2D	5.50	1.49	1.39
17	B	828	CLA	C3D-C2D	5.50	1.49	1.39
17	a	846	CLA	C3C-C2C	5.50	1.48	1.36
17	a	844	CLA	C3B-C2B	5.49	1.48	1.40
17	b	840	CLA	C3D-C2D	5.49	1.49	1.39
17	8	309	CLA	C3C-C2C	5.49	1.48	1.36
17	A	812	CLA	C3D-C2D	5.49	1.49	1.39
17	B	838	CLA	C3D-C2D	5.49	1.49	1.39
17	A	822	CLA	C3B-C2B	5.49	1.48	1.40
17	b	810	CLA	C3C-C2C	5.48	1.48	1.36
17	a	815	CLA	C3C-C2C	5.48	1.48	1.36
17	a	832	CLA	C3D-C2D	5.48	1.49	1.39
17	B	802	CLA	C3B-C2B	5.48	1.48	1.40
17	B	836	CLA	C3C-C2C	5.48	1.48	1.36
17	1	308	CLA	C3D-C2D	5.48	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	811	CLA	C3C-C2C	5.47	1.48	1.36
17	a	840	CLA	C3C-C2C	5.47	1.48	1.36
17	B	832	CLA	C3C-C2C	5.47	1.48	1.36
17	a	833	CLA	C3C-C2C	5.47	1.48	1.36
17	B	805	CLA	C3D-C2D	5.47	1.49	1.39
17	4	601	CLA	C3C-C2C	5.47	1.48	1.36
17	a	824	CLA	C3C-C2C	5.47	1.48	1.36
17	B	803	CLA	C3C-C2C	5.47	1.48	1.36
17	3	313	CLA	C3C-C2C	5.46	1.48	1.36
20	A	849	BCR	C23-C22	-5.46	1.34	1.45
17	L	204	CLA	C3C-C2C	5.46	1.48	1.36
17	a	822	CLA	C3C-C2C	5.46	1.48	1.36
17	B	811	CLA	C3C-C2C	5.46	1.48	1.36
17	8	307	CLA	C3C-C2C	5.46	1.48	1.36
17	a	835	CLA	C3C-C2C	5.46	1.48	1.36
17	8	305	CLA	C3C-C2C	5.46	1.48	1.36
17	b	829	CLA	C3D-C2D	5.46	1.49	1.39
17	4	612	CLA	C3C-C2C	5.46	1.48	1.36
17	7	604	CLA	C3C-C2C	5.46	1.48	1.36
26	6	303	CHL	C3B-C2B	5.45	1.47	1.40
17	B	837	CLA	C3C-C2C	5.45	1.48	1.36
17	a	828	CLA	C3D-C2D	5.45	1.49	1.39
17	a	824	CLA	C3D-C2D	5.45	1.49	1.39
17	a	820	CLA	C3C-C2C	5.45	1.48	1.36
17	2	604	CLA	C3C-C2C	5.45	1.48	1.36
17	2	608	CLA	C3C-C2C	5.45	1.48	1.36
17	A	820	CLA	C3C-C2C	5.45	1.48	1.36
17	2	610	CLA	C3C-C2C	5.45	1.48	1.36
17	B	805	CLA	C3C-C2C	5.45	1.48	1.36
17	B	827	CLA	C3B-C2B	5.45	1.47	1.40
17	a	810	CLA	C3C-C2C	5.45	1.48	1.36
17	B	832	CLA	C3D-C2D	5.45	1.49	1.39
17	L	204	CLA	C3D-C2D	5.44	1.49	1.39
17	9	611	CLA	C3C-C2C	5.44	1.48	1.36
17	b	811	CLA	C3C-C2C	5.44	1.48	1.36
17	2	603	CLA	C3C-C2C	5.44	1.48	1.36
17	A	831	CLA	C3C-C2C	5.44	1.48	1.36
17	A	815	CLA	C3C-C2C	5.44	1.48	1.36
17	b	802	CLA	C3B-C2B	5.44	1.47	1.40
17	4	614	CLA	C3C-C2C	5.44	1.48	1.36
17	K	4003	CLA	C3C-C2C	5.44	1.48	1.36
17	b	818	CLA	C3B-C2B	5.44	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	843	CLA	C3B-C2B	5.44	1.47	1.40
17	b	803	CLA	C3C-C2C	5.43	1.48	1.36
17	2	612	CLA	C3C-C2C	5.43	1.48	1.36
17	J	3002	CLA	C3C-C2C	5.43	1.48	1.36
17	A	817	CLA	C3C-C2C	5.43	1.48	1.36
17	9	604	CLA	C3C-C2C	5.43	1.48	1.36
17	a	802	CLA	C3C-C2C	5.43	1.48	1.36
17	4	609	CLA	C3C-C2C	5.43	1.48	1.36
17	a	814	CLA	C3C-C2C	5.43	1.48	1.36
17	b	814	CLA	C3C-C2C	5.43	1.48	1.36
17	a	831	CLA	C3B-C2B	5.43	1.47	1.40
17	a	812	CLA	C3C-C2C	5.42	1.48	1.36
17	3	311	CLA	C3C-C2C	5.42	1.48	1.36
17	b	802	CLA	C3C-C2C	5.42	1.48	1.36
17	A	812	CLA	C3C-C2C	5.42	1.48	1.36
17	A	834	CLA	C3C-C2C	5.42	1.48	1.36
17	b	832	CLA	C3C-C2C	5.42	1.48	1.36
17	1	311	CLA	C3C-C2C	5.42	1.48	1.36
17	3	306	CLA	C3C-C2C	5.42	1.48	1.36
17	1	304	CLA	C3C-C2C	5.42	1.48	1.36
17	a	838	CLA	CHC-C1C	5.42	1.48	1.35
17	B	826	CLA	C3D-C2D	5.42	1.49	1.39
17	a	825	CLA	C3C-C2C	5.42	1.48	1.36
17	B	802	CLA	C3C-C2C	5.41	1.48	1.36
17	A	840	CLA	C3C-C2C	5.41	1.48	1.36
17	B	809	CLA	C3C-C2C	5.41	1.48	1.36
17	A	832	CLA	C3C-C2C	5.41	1.48	1.36
17	6	309	CLA	C3C-C2C	5.41	1.48	1.36
17	A	814	CLA	C3C-C2C	5.41	1.48	1.36
17	3	308	CLA	C3C-C2C	5.41	1.48	1.36
17	a	832	CLA	C3C-C2C	5.41	1.48	1.36
17	2	611	CLA	C3C-C2C	5.41	1.48	1.36
17	9	613	CLA	C3C-C2C	5.41	1.48	1.36
17	9	609	CLA	C3C-C2C	5.41	1.48	1.36
17	1	308	CLA	C3C-C2C	5.41	1.48	1.36
17	1	202	CLA	C3C-C2C	5.41	1.48	1.36
17	2	613	CLA	C3C-C2C	5.41	1.48	1.36
26	2	605	CHL	C2C-C3C	5.41	1.48	1.36
17	j	3002	CLA	C3C-C2C	5.41	1.48	1.36
17	a	804	CLA	C3D-C2D	5.41	1.49	1.39
17	b	834	CLA	C3C-C2C	5.41	1.48	1.36
17	B	831	CLA	C3C-C2C	5.41	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	823	CLA	C3C-C2C	5.41	1.48	1.36
17	b	830	CLA	C3C-C2C	5.40	1.48	1.36
20	b	843	BCR	C23-C22	-5.40	1.34	1.45
17	8	311	CLA	C3C-C2C	5.40	1.48	1.36
17	G	103	CLA	C3C-C2C	5.40	1.48	1.36
20	B	843	BCR	C23-C22	-5.40	1.34	1.45
17	B	806	CLA	C3C-C2C	5.40	1.48	1.36
17	b	832	CLA	C3D-C2D	5.40	1.49	1.39
17	B	819	CLA	C3C-C2C	5.40	1.48	1.36
17	6	315	CLA	C3C-C2C	5.40	1.48	1.36
17	b	822	CLA	C3C-C2C	5.40	1.48	1.36
17	a	842	CLA	C3C-C2C	5.40	1.48	1.36
17	B	814	CLA	C3C-C2C	5.40	1.48	1.36
17	1	305	CLA	C3C-C2C	5.40	1.48	1.36
17	7	610	CLA	C3C-C2C	5.40	1.48	1.36
17	L	202	CLA	C3C-C2C	5.40	1.48	1.36
17	B	828	CLA	C3C-C2C	5.40	1.48	1.36
17	A	818	CLA	C3C-C2C	5.40	1.48	1.36
17	b	816	CLA	C3C-C2C	5.40	1.48	1.36
17	B	835	CLA	C3C-C2C	5.40	1.48	1.36
17	8	301	CLA	C3C-C2C	5.40	1.48	1.36
17	6	307	CLA	C3C-C2C	5.40	1.48	1.36
17	B	834	CLA	C3C-C2C	5.40	1.48	1.36
17	b	807	CLA	C3C-C2C	5.40	1.48	1.36
17	B	820	CLA	C3C-C2C	5.39	1.48	1.36
17	b	826	CLA	C3C-C2C	5.39	1.48	1.36
17	B	822	CLA	C3C-C2C	5.39	1.48	1.36
17	K	4002	CLA	C3C-C2C	5.39	1.48	1.36
17	F	303	CLA	C3C-C2C	5.39	1.48	1.36
17	b	833	CLA	C3C-C2C	5.39	1.48	1.36
17	9	601	CLA	C3C-C2C	5.39	1.48	1.36
17	b	819	CLA	C3C-C2C	5.39	1.48	1.36
17	6	311	CLA	C3C-C2C	5.39	1.48	1.36
17	a	818	CLA	C3C-C2C	5.39	1.48	1.36
17	6	306	CLA	C3C-C2C	5.39	1.48	1.36
17	A	807	CLA	C3C-C2C	5.39	1.48	1.36
17	A	824	CLA	C3C-C2C	5.39	1.48	1.36
17	B	810	CLA	C3C-C2C	5.39	1.48	1.36
17	A	822	CLA	C3C-C2C	5.39	1.48	1.36
17	1	309	CLA	C3C-C2C	5.39	1.48	1.36
17	g	102	CLA	C3C-C2C	5.39	1.48	1.36
17	A	801	CLA	C3C-C2C	5.39	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	808	CLA	C3C-C2C	5.39	1.48	1.36
17	A	811	CLA	C3C-C2C	5.39	1.48	1.36
17	A	825	CLA	C3C-C2C	5.39	1.48	1.36
17	A	838	CLA	C3C-C2C	5.39	1.48	1.36
17	B	838	CLA	C3C-C2C	5.39	1.48	1.36
17	2	602	CLA	C3C-C2C	5.39	1.48	1.36
17	a	826	CLA	C3C-C2C	5.39	1.48	1.36
17	L	203	CLA	C3C-C2C	5.38	1.48	1.36
17	3	305	CLA	C3C-C2C	5.38	1.48	1.36
17	9	612	CLA	C3C-C2C	5.38	1.48	1.36
17	6	314	CLA	C3C-C2C	5.38	1.48	1.36
17	9	608	CLA	C3C-C2C	5.38	1.48	1.36
17	l	204	CLA	C3C-C2C	5.38	1.48	1.36
26	4	605	CHL	C2C-C3C	5.38	1.48	1.36
17	l	203	CLA	C3C-C2C	5.38	1.48	1.36
17	b	835	CLA	C3C-C2C	5.38	1.48	1.36
17	B	827	CLA	C3C-C2C	5.38	1.48	1.36
17	A	804	CLA	C3C-C2C	5.38	1.48	1.36
17	b	828	CLA	C3C-C2C	5.38	1.48	1.36
17	A	816	CLA	C3C-C2C	5.38	1.48	1.36
17	A	838	CLA	CHC-C1C	5.38	1.48	1.35
17	3	304	CLA	C3C-C2C	5.38	1.48	1.36
17	A	835	CLA	C3C-C2C	5.38	1.48	1.36
17	a	830	CLA	C3C-C2C	5.38	1.48	1.36
17	b	823	CLA	C3C-C2C	5.37	1.48	1.36
17	b	820	CLA	C3C-C2C	5.37	1.48	1.36
17	B	829	CLA	C3C-C2C	5.37	1.48	1.36
17	b	841	CLA	C3C-C2C	5.37	1.48	1.36
17	8	308	CLA	C3C-C2C	5.37	1.48	1.36
20	8	316	BCR	C23-C22	-5.37	1.34	1.45
17	b	838	CLA	C3C-C2C	5.37	1.48	1.36
17	1	312	CLA	C3C-C2C	5.37	1.48	1.36
17	3	310	CLA	C3C-C2C	5.37	1.48	1.36
17	b	814	CLA	CHC-C1C	5.37	1.48	1.35
17	b	831	CLA	C3C-C2C	5.37	1.48	1.36
17	a	816	CLA	C3C-C2C	5.37	1.48	1.36
17	F	304	CLA	C3C-C2C	5.37	1.48	1.36
17	A	809	CLA	C3C-C2C	5.37	1.48	1.36
17	9	614	CLA	C3C-C2C	5.36	1.48	1.36
17	B	833	CLA	C3C-C2C	5.36	1.48	1.36
17	7	609	CLA	CHC-C1C	5.36	1.48	1.35
26	7	605	CHL	C2C-C3C	5.36	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	6	305	CLA	C3C-C2C	5.36	1.48	1.36
17	4	602	CLA	C3C-C2C	5.36	1.48	1.36
17	A	836	CLA	C3C-C2C	5.36	1.48	1.36
17	4	613	CLA	C3C-C2C	5.36	1.48	1.36
17	3	303	CLA	C3C-C2C	5.36	1.48	1.36
17	B	815	CLA	C3C-C2C	5.36	1.48	1.36
17	k	1401	CLA	C3C-C2C	5.36	1.48	1.36
20	3	318	BCR	C23-C22	-5.36	1.34	1.45
17	3	314	CLA	C3C-C2C	5.36	1.48	1.36
17	B	807	CLA	C3C-C2C	5.36	1.48	1.36
17	a	823	CLA	C3C-C2C	5.36	1.48	1.36
17	A	828	CLA	C3C-C2C	5.35	1.48	1.36
17	b	815	CLA	C3C-C2C	5.35	1.48	1.36
17	4	610	CLA	C3C-C2C	5.35	1.48	1.36
17	7	609	CLA	C3C-C2C	5.35	1.48	1.36
17	7	611	CLA	C3C-C2C	5.35	1.48	1.36
17	B	818	CLA	C3C-C2C	5.35	1.48	1.36
17	G	104	CLA	C3C-C2C	5.35	1.48	1.36
17	A	837	CLA	C3C-C2C	5.35	1.48	1.36
26	9	605	CHL	C2C-C3C	5.35	1.48	1.36
26	2	601	CHL	C2C-C3C	5.35	1.48	1.36
17	1	310	CLA	C3C-C2C	5.35	1.48	1.36
17	a	839	CLA	C3C-C2C	5.35	1.48	1.36
17	a	835	CLA	O2D-CGD	5.35	1.46	1.33
20	G	105	BCR	C23-C22	-5.35	1.34	1.45
17	1	313	CLA	C3C-C2C	5.35	1.48	1.36
17	a	804	CLA	C3C-C2C	5.35	1.48	1.36
17	3	313	CLA	O2D-CGD	5.34	1.46	1.33
17	3	301	CLA	C3C-C2C	5.34	1.48	1.36
17	8	303	CLA	C3C-C2C	5.34	1.48	1.36
17	G	101	CLA	C3C-C2C	5.34	1.48	1.36
17	8	312	CLA	C3C-C2C	5.34	1.48	1.36
17	a	808	CLA	C3C-C2C	5.34	1.48	1.36
17	1	203	CLA	CHC-C1C	5.34	1.48	1.35
17	2	609	CLA	CHC-C1C	5.34	1.48	1.35
17	b	804	CLA	C3C-C2C	5.34	1.48	1.36
17	A	810	CLA	C3C-C2C	5.34	1.48	1.36
17	B	814	CLA	CHC-C1C	5.34	1.48	1.35
17	B	839	CLA	C3C-C2C	5.34	1.48	1.36
17	1	303	CLA	C3C-C2C	5.34	1.48	1.36
17	7	613	CLA	C3C-C2C	5.34	1.48	1.36
17	9	610	CLA	C3C-C2C	5.34	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	841	CLA	C3C-C2C	5.34	1.48	1.36
17	7	602	CLA	C3C-C2C	5.34	1.48	1.36
20	A	851	BCR	C23-C22	-5.34	1.34	1.45
17	A	808	CLA	C3C-C2C	5.33	1.48	1.36
17	a	831	CLA	C3C-C2C	5.33	1.48	1.36
17	8	310	CLA	C3C-C2C	5.33	1.48	1.36
17	B	821	CLA	C3C-C2C	5.33	1.48	1.36
17	8	302	CLA	C3C-C2C	5.33	1.48	1.36
20	l	206	BCR	C23-C22	-5.33	1.34	1.45
20	6	319	BCR	C23-C22	-5.33	1.34	1.45
17	A	827	CLA	CHC-C1C	5.33	1.48	1.35
17	k	1402	CLA	C3C-C2C	5.33	1.48	1.36
17	b	825	CLA	C3C-C2C	5.33	1.48	1.36
17	A	829	CLA	C3C-C2C	5.33	1.48	1.36
17	B	803	CLA	CHC-C1C	5.33	1.48	1.35
17	9	602	CLA	C3C-C2C	5.33	1.48	1.36
17	1	314	CLA	C3C-C2C	5.33	1.48	1.36
17	b	817	CLA	C3C-C2C	5.33	1.48	1.36
26	2	614	CHL	C2C-C3C	5.33	1.48	1.36
17	3	302	CLA	C3C-C2C	5.33	1.48	1.36
17	6	313	CLA	C3C-C2C	5.33	1.48	1.36
17	a	813	CLA	C3C-C2C	5.33	1.48	1.36
17	f	7003	CLA	C3C-C2C	5.33	1.48	1.36
17	b	806	CLA	C3C-C2C	5.33	1.48	1.36
17	b	836	CLA	C3C-C2C	5.32	1.48	1.36
17	4	611	CLA	C3C-C2C	5.32	1.48	1.36
17	b	829	CLA	C3C-C2C	5.32	1.48	1.36
17	B	824	CLA	C3C-C2C	5.32	1.48	1.36
17	B	817	CLA	C3C-C2C	5.32	1.48	1.36
17	b	805	CLA	C3C-C2C	5.32	1.48	1.36
17	3	312	CLA	C3C-C2C	5.32	1.48	1.36
17	3	309	CLA	C3C-C2C	5.32	1.48	1.36
17	A	830	CLA	C3C-C2C	5.32	1.48	1.36
20	7	617	BCR	C23-C22	-5.32	1.34	1.45
17	8	301	CLA	CHC-C1C	5.32	1.48	1.35
17	A	854	CLA	C3C-C2C	5.32	1.48	1.36
17	A	802	CLA	CHC-C1C	5.32	1.48	1.35
26	1	307	CHL	C2C-C3C	5.32	1.48	1.36
26	4	606	CHL	C2C-C3C	5.32	1.48	1.36
17	a	819	CLA	CHC-C1C	5.32	1.48	1.35
17	a	819	CLA	O2D-CGD	5.32	1.46	1.33
20	b	846	BCR	C23-C22	-5.31	1.34	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	7	606	CHL	C2C-C3C	5.31	1.48	1.36
17	a	817	CLA	C3C-C2C	5.31	1.48	1.36
17	6	316	CLA	C3C-C2C	5.31	1.48	1.36
17	A	826	CLA	C3C-C2C	5.31	1.48	1.36
17	9	602	CLA	CHC-C1C	5.31	1.48	1.35
17	a	819	CLA	C3C-C2C	5.31	1.48	1.36
17	A	843	CLA	C3C-C2C	5.31	1.48	1.36
17	2	609	CLA	C3C-C2C	5.31	1.48	1.36
17	B	832	CLA	CHC-C1C	5.31	1.48	1.35
17	7	612	CLA	C3C-C2C	5.31	1.48	1.36
17	1	303	CLA	CHC-C1C	5.31	1.48	1.35
17	B	825	CLA	C3C-C2C	5.31	1.48	1.36
17	a	815	CLA	CHC-C1C	5.31	1.48	1.35
17	3	302	CLA	CHC-C1C	5.31	1.48	1.35
20	A	850	BCR	C23-C22	-5.30	1.34	1.45
17	3	309	CLA	CHC-C1C	5.30	1.48	1.35
17	B	813	CLA	C3C-C2C	5.30	1.48	1.36
17	a	837	CLA	C3C-C2C	5.30	1.48	1.36
17	a	816	CLA	O2D-CGD	5.30	1.46	1.33
17	a	827	CLA	CHC-C1C	5.30	1.48	1.35
17	8	308	CLA	CHC-C1C	5.30	1.48	1.35
17	A	803	CLA	C3C-C2C	5.30	1.48	1.36
17	A	805	CLA	C3C-C2C	5.30	1.48	1.36
20	L	206	BCR	C23-C22	-5.30	1.34	1.45
20	g	104	BCR	C23-C22	-5.30	1.34	1.45
20	B	847	BCR	C23-C22	-5.30	1.34	1.45
17	b	827	CLA	C3C-C2C	5.30	1.48	1.36
17	1	315	CLA	C3C-C2C	5.30	1.48	1.36
17	b	809	CLA	C3C-C2C	5.30	1.48	1.36
17	a	807	CLA	C3C-C2C	5.30	1.48	1.36
17	a	825	CLA	O2D-CGD	5.30	1.46	1.33
17	g	103	CLA	C3C-C2C	5.30	1.48	1.36
17	A	839	CLA	C3C-C2C	5.30	1.48	1.36
17	7	602	CLA	CHC-C1C	5.30	1.48	1.35
17	A	841	CLA	CHC-C1C	5.30	1.48	1.35
17	a	806	CLA	O2D-CGD	5.29	1.46	1.33
17	B	812	CLA	C3C-C2C	5.29	1.48	1.36
17	A	831	CLA	C3B-C2B	5.29	1.47	1.40
20	k	1404	BCR	C23-C22	-5.29	1.34	1.45
17	6	312	CLA	C3C-C2C	5.29	1.48	1.36
17	8	308	CLA	O2D-CGD	5.29	1.46	1.33
20	A	852	BCR	C23-C22	-5.29	1.34	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	F	301	CLA	C3C-C2C	5.29	1.48	1.36
17	a	805	CLA	C3C-C2C	5.29	1.48	1.36
26	7	614	CHL	C2C-C3C	5.29	1.48	1.36
17	1	306	CLA	C3C-C2C	5.29	1.48	1.36
17	A	819	CLA	C3C-C2C	5.29	1.48	1.36
17	A	802	CLA	C3C-C2C	5.29	1.48	1.36
17	b	827	CLA	CHC-C1C	5.29	1.48	1.35
20	K	4001	BCR	C23-C22	-5.29	1.34	1.45
20	b	845	BCR	C23-C22	-5.29	1.34	1.45
17	2	602	CLA	CHC-C1C	5.29	1.48	1.35
17	b	808	CLA	C3C-C2C	5.29	1.48	1.36
17	a	843	CLA	C3D-C2D	5.28	1.48	1.39
17	b	821	CLA	C3C-C2C	5.28	1.48	1.36
17	6	311	CLA	CHC-C1C	5.28	1.48	1.35
20	1	318	BCR	C23-C22	-5.28	1.34	1.45
17	B	841	CLA	C3C-C2C	5.28	1.48	1.36
26	2	606	CHL	C2C-C3C	5.28	1.48	1.36
17	a	833	CLA	CHC-C1C	5.28	1.48	1.35
26	4	615	CHL	C2C-C3C	5.28	1.48	1.36
17	L	203	CLA	CHC-C1C	5.28	1.48	1.35
17	a	829	CLA	C3C-C2C	5.28	1.48	1.36
17	b	823	CLA	C3D-C2D	5.28	1.48	1.39
17	A	821	CLA	C3C-C2C	5.28	1.48	1.36
17	B	827	CLA	CHC-C1C	5.28	1.48	1.35
17	A	828	CLA	CHC-C1C	5.28	1.48	1.35
17	a	814	CLA	CHC-C1C	5.28	1.48	1.35
17	9	612	CLA	O2D-CGD	5.27	1.46	1.33
17	b	803	CLA	CHC-C1C	5.27	1.48	1.35
17	b	818	CLA	C3C-C2C	5.27	1.47	1.36
17	6	310	CLA	C3C-C2C	5.27	1.47	1.36
20	L	201	BCR	C23-C22	-5.27	1.34	1.45
17	B	804	CLA	C3C-C2C	5.27	1.47	1.36
20	4	618	BCR	C23-C22	-5.27	1.34	1.45
20	K	4004	BCR	C23-C22	-5.27	1.34	1.45
20	a	852	BCR	C23-C22	-5.27	1.34	1.45
17	A	813	CLA	C3C-C2C	5.27	1.47	1.36
17	A	815	CLA	CHC-C1C	5.27	1.48	1.35
17	7	613	CLA	O2D-CGD	5.27	1.46	1.33
20	b	847	BCR	C23-C22	-5.27	1.34	1.45
17	b	829	CLA	C3B-C2B	5.27	1.47	1.40
17	2	612	CLA	O2D-CGD	5.27	1.46	1.33
17	J	3002	CLA	O2D-CGD	5.27	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	g	101	CLA	C3C-C2C	5.27	1.47	1.36
17	b	824	CLA	CHC-C1C	5.27	1.48	1.35
17	f	7002	CLA	C3C-C2C	5.26	1.47	1.36
17	8	304	CLA	C3C-C2C	5.26	1.47	1.36
26	9	615	CHL	C2C-C3C	5.26	1.48	1.36
20	a	851	BCR	C23-C22	-5.26	1.34	1.45
17	B	806	CLA	CHC-C1C	5.26	1.48	1.35
17	b	832	CLA	CHC-C1C	5.26	1.48	1.35
17	A	833	CLA	C3C-C2C	5.26	1.47	1.36
26	6	308	CHL	C2C-C3C	5.26	1.48	1.36
17	A	842	CLA	C3C-C2C	5.26	1.47	1.36
20	F	305	BCR	C23-C22	-5.25	1.34	1.45
17	a	829	CLA	CHC-C1C	5.25	1.48	1.35
17	4	602	CLA	O2D-CGD	5.25	1.46	1.33
17	j	3002	CLA	O2D-CGD	5.25	1.46	1.33
17	a	808	CLA	CHC-C1C	5.25	1.48	1.35
26	7	601	CHL	C2C-C3C	5.25	1.48	1.36
17	6	304	CLA	C3C-C2C	5.25	1.47	1.36
17	a	811	CLA	O2D-CGD	5.25	1.46	1.33
17	1	306	CLA	CHC-C1C	5.25	1.48	1.35
17	A	806	CLA	C3C-C2C	5.25	1.47	1.36
17	A	825	CLA	O2D-CGD	5.25	1.46	1.33
17	B	807	CLA	CHC-C1C	5.25	1.48	1.35
17	4	604	CLA	C3C-C2C	5.25	1.47	1.36
26	7	601	CHL	CHC-C1C	5.25	1.48	1.35
17	a	801	CLA	C3C-C2C	5.25	1.47	1.36
17	4	608	CLA	C3C-C2C	5.25	1.47	1.36
17	b	841	CLA	CHC-C1C	5.25	1.48	1.35
17	B	816	CLA	C3C-C2C	5.24	1.47	1.36
17	a	834	CLA	C3C-C2C	5.24	1.47	1.36
17	a	837	CLA	O2D-CGD	5.24	1.46	1.33
20	a	854	BCR	C23-C22	-5.24	1.34	1.45
17	a	820	CLA	O2D-CGD	5.24	1.46	1.33
20	B	848	BCR	C23-C22	-5.24	1.34	1.45
17	A	833	CLA	CHC-C1C	5.24	1.48	1.35
17	6	311	CLA	O2D-CGD	5.24	1.46	1.33
17	7	612	CLA	O2D-CGD	5.24	1.46	1.33
17	4	609	CLA	O2D-CGD	5.24	1.46	1.33
17	b	812	CLA	C3C-C2C	5.24	1.47	1.36
17	a	836	CLA	C3C-C2C	5.24	1.47	1.36
17	B	813	CLA	CHC-C1C	5.24	1.48	1.35
17	a	830	CLA	O2D-CGD	5.24	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	822	CLA	CHC-C1C	5.23	1.48	1.35
17	a	822	CLA	O2D-CGD	5.23	1.46	1.33
17	f	7002	CLA	O2D-CGD	5.23	1.46	1.33
17	1	313	CLA	O2D-CGD	5.23	1.46	1.33
17	2	609	CLA	O2D-CGD	5.23	1.46	1.33
17	9	609	CLA	CHC-C1C	5.23	1.48	1.35
17	4	609	CLA	CHC-C1C	5.23	1.48	1.35
17	2	611	CLA	O2D-CGD	5.23	1.46	1.33
17	6	312	CLA	O2D-CGD	5.23	1.46	1.33
20	f	7004	BCR	C23-C22	-5.23	1.34	1.45
17	A	823	CLA	CHC-C1C	5.23	1.48	1.35
17	8	311	CLA	O2D-CGD	5.23	1.46	1.33
26	4	606	CHL	CHC-C1C	5.23	1.48	1.35
20	a	853	BCR	C23-C22	-5.23	1.34	1.45
17	A	822	CLA	O2D-CGD	5.23	1.46	1.33
17	A	806	CLA	CHC-C1C	5.23	1.48	1.35
26	1	302	CHL	C2C-C3C	5.23	1.47	1.36
17	F	304	CLA	O2D-CGD	5.23	1.45	1.33
17	b	806	CLA	CHC-C1C	5.22	1.48	1.35
17	B	830	CLA	C3C-C2C	5.22	1.47	1.36
17	B	837	CLA	CHC-C1C	5.22	1.48	1.35
20	a	849	BCR	C23-C22	-5.22	1.34	1.45
17	A	811	CLA	O2D-CGD	5.22	1.45	1.33
17	A	812	CLA	O2D-CGD	5.22	1.45	1.33
26	4	615	CHL	O2D-CGD	5.22	1.45	1.33
17	A	826	CLA	CHC-C1C	5.22	1.48	1.35
17	a	824	CLA	O2D-CGD	5.22	1.45	1.33
17	B	807	CLA	O2D-CGD	5.22	1.45	1.33
26	2	606	CHL	O2D-CGD	5.22	1.45	1.33
17	A	841	CLA	O2D-CGD	5.22	1.45	1.33
17	K	4003	CLA	O2D-CGD	5.22	1.45	1.33
17	6	306	CLA	O2D-CGD	5.22	1.45	1.33
17	1	310	CLA	O2D-CGD	5.22	1.45	1.33
26	9	615	CHL	O2D-CGD	5.22	1.45	1.33
17	B	824	CLA	CHC-C1C	5.22	1.48	1.35
17	B	802	CLA	CHC-C1C	5.22	1.48	1.35
17	B	825	CLA	CHC-C1C	5.22	1.48	1.35
17	4	602	CLA	CHC-C1C	5.22	1.48	1.35
17	a	821	CLA	C3C-C2C	5.21	1.47	1.36
17	1	305	CLA	O2D-CGD	5.21	1.45	1.33
17	A	843	CLA	O2D-CGD	5.21	1.45	1.33
17	8	310	CLA	O2D-CGD	5.21	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	611	CLA	O2D-CGD	5.21	1.45	1.33
17	4	613	CLA	O2D-CGD	5.21	1.45	1.33
17	b	837	CLA	CHC-C1C	5.21	1.48	1.35
17	a	807	CLA	CHC-C1C	5.21	1.48	1.35
17	a	823	CLA	O2D-CGD	5.21	1.45	1.33
17	A	809	CLA	CHC-C1C	5.21	1.48	1.35
17	b	823	CLA	CHC-C1C	5.21	1.48	1.35
17	b	825	CLA	CHC-C1C	5.21	1.48	1.35
26	3	307	CHL	O2D-CGD	5.21	1.45	1.33
26	7	614	CHL	O2D-CGD	5.21	1.45	1.33
17	A	837	CLA	O2D-CGD	5.21	1.45	1.33
17	B	841	CLA	CHC-C1C	5.21	1.48	1.35
17	B	823	CLA	O2D-CGD	5.21	1.45	1.33
17	A	807	CLA	CHC-C1C	5.21	1.48	1.35
17	3	309	CLA	O2D-CGD	5.21	1.45	1.33
17	6	314	CLA	O2D-CGD	5.21	1.45	1.33
26	9	606	CHL	C2C-C3C	5.21	1.47	1.36
17	a	832	CLA	O2D-CGD	5.21	1.45	1.33
17	4	608	CLA	O2D-CGD	5.21	1.45	1.33
17	8	313	CLA	C3B-C4B	5.21	1.49	1.39
17	1	308	CLA	O2D-CGD	5.21	1.45	1.33
17	2	608	CLA	O2D-CGD	5.20	1.45	1.33
17	B	816	CLA	O2D-CGD	5.20	1.45	1.33
17	8	305	CLA	O2D-CGD	5.20	1.45	1.33
17	8	301	CLA	O2D-CGD	5.20	1.45	1.33
17	3	312	CLA	O2D-CGD	5.20	1.45	1.33
17	b	839	CLA	O2D-CGD	5.20	1.45	1.33
17	G	104	CLA	O2D-CGD	5.20	1.45	1.33
17	7	611	CLA	O2D-CGD	5.20	1.45	1.33
17	A	842	CLA	CHC-C1C	5.20	1.48	1.35
17	A	813	CLA	O2D-CGD	5.20	1.45	1.33
20	9	618	BCR	C23-C22	-5.20	1.34	1.45
17	8	309	CLA	O2D-CGD	5.20	1.45	1.33
17	b	838	CLA	O2D-CGD	5.20	1.45	1.33
17	b	826	CLA	CHC-C1C	5.20	1.48	1.35
17	3	311	CLA	O2D-CGD	5.20	1.45	1.33
26	2	614	CHL	O2D-CGD	5.20	1.45	1.33
17	6	316	CLA	O2D-CGD	5.20	1.45	1.33
17	A	824	CLA	O2D-CGD	5.20	1.45	1.33
17	1	202	CLA	O2D-CGD	5.20	1.45	1.33
17	b	813	CLA	C3C-C2C	5.20	1.47	1.36
17	3	314	CLA	O2D-CGD	5.20	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	308	CHL	O2D-CGD	5.20	1.45	1.33
17	7	603	CLA	O2D-CGD	5.20	1.45	1.33
17	l	204	CLA	CHC-C1C	5.20	1.48	1.35
26	7	607	CHL	C2C-C3C	5.20	1.47	1.36
17	A	819	CLA	CHC-C1C	5.20	1.48	1.35
17	B	809	CLA	C3B-C2B	5.20	1.47	1.40
17	3	308	CLA	CHC-C1C	5.19	1.48	1.35
17	L	203	CLA	O2D-CGD	5.19	1.45	1.33
17	b	828	CLA	O2D-CGD	5.19	1.45	1.33
17	b	810	CLA	CHC-C1C	5.19	1.48	1.35
17	3	306	CLA	O2D-CGD	5.19	1.45	1.33
17	B	826	CLA	CHC-C1C	5.19	1.48	1.35
17	b	807	CLA	CHC-C1C	5.19	1.48	1.35
17	L	204	CLA	O2D-CGD	5.19	1.45	1.33
17	A	823	CLA	O2D-CGD	5.19	1.45	1.33
17	6	310	CLA	O2D-CGD	5.19	1.45	1.33
17	A	807	CLA	O2D-CGD	5.19	1.45	1.33
17	b	824	CLA	C3C-C2C	5.19	1.47	1.36
17	a	816	CLA	CHC-C1C	5.19	1.48	1.35
17	a	805	CLA	CHC-C1C	5.19	1.48	1.35
17	7	603	CLA	C3C-C2C	5.19	1.47	1.36
17	8	304	CLA	O2D-CGD	5.19	1.45	1.33
17	a	841	CLA	O2D-CGD	5.19	1.45	1.33
17	b	835	CLA	O2D-CGD	5.19	1.45	1.33
20	A	856	BCR	C23-C22	-5.19	1.34	1.45
17	9	610	CLA	O2D-CGD	5.19	1.45	1.33
17	8	307	CLA	O2D-CGD	5.19	1.45	1.33
17	3	303	CLA	O2D-CGD	5.19	1.45	1.33
17	8	307	CLA	CHC-C1C	5.19	1.48	1.35
26	9	606	CHL	O2D-CGD	5.19	1.45	1.33
17	4	612	CLA	O2D-CGD	5.19	1.45	1.33
17	B	821	CLA	CHC-C1C	5.19	1.48	1.35
26	6	303	CHL	C2C-C3C	5.19	1.47	1.36
17	b	809	CLA	C3B-C2B	5.19	1.47	1.40
26	2	607	CHL	C2C-C3C	5.19	1.47	1.36
17	b	823	CLA	O2D-CGD	5.18	1.45	1.33
17	7	603	CLA	CHC-C1C	5.18	1.48	1.35
17	A	808	CLA	O2D-CGD	5.18	1.45	1.33
17	3	308	CLA	O2D-CGD	5.18	1.45	1.33
17	l	204	CLA	O2D-CGD	5.18	1.45	1.33
26	9	605	CHL	O2D-CGD	5.18	1.45	1.33
17	6	307	CLA	O2D-CGD	5.18	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	k	1402	CLA	O2D-CGD	5.18	1.45	1.33
17	b	813	CLA	CHC-C1C	5.18	1.48	1.35
17	8	303	CLA	CHC-C1C	5.18	1.48	1.35
26	4	606	CHL	O2D-CGD	5.18	1.45	1.33
17	b	830	CLA	O2D-CGD	5.18	1.45	1.33
17	9	609	CLA	O2D-CGD	5.18	1.45	1.33
17	B	811	CLA	O2D-CGD	5.18	1.45	1.33
17	9	608	CLA	O2D-CGD	5.18	1.45	1.33
17	l	203	CLA	O2D-CGD	5.18	1.45	1.33
17	a	842	CLA	O2D-CGD	5.18	1.45	1.33
17	G	103	CLA	O2D-CGD	5.18	1.45	1.33
17	A	801	CLA	CHC-C1C	5.18	1.48	1.35
17	F	304	CLA	CHC-C1C	5.18	1.48	1.35
17	6	313	CLA	O2D-CGD	5.17	1.45	1.33
17	a	846	CLA	O2D-CGD	5.17	1.45	1.33
17	a	843	CLA	CHC-C1C	5.17	1.48	1.35
17	b	840	CLA	O2D-CGD	5.17	1.45	1.33
17	G	104	CLA	CHC-C1C	5.17	1.48	1.35
26	7	607	CHL	C3D-C2D	5.17	1.48	1.39
20	I	101	BCR	C23-C22	-5.17	1.34	1.45
17	6	307	CLA	CHC-C1C	5.17	1.48	1.35
17	B	835	CLA	CHC-C1C	5.17	1.48	1.35
17	a	843	CLA	C3C-C2C	5.17	1.47	1.36
17	b	818	CLA	O2D-CGD	5.17	1.45	1.33
17	B	840	CLA	O2D-CGD	5.17	1.45	1.33
17	a	813	CLA	O2D-CGD	5.17	1.45	1.33
17	a	809	CLA	CHC-C1C	5.17	1.48	1.35
17	a	846	CLA	CHC-C1C	5.17	1.48	1.35
17	3	315	CLA	C3B-C4B	5.17	1.49	1.39
17	2	604	CLA	O2D-CGD	5.17	1.45	1.33
17	9	613	CLA	O2D-CGD	5.17	1.45	1.33
20	2	617	BCR	C23-C22	-5.17	1.34	1.45
17	a	856	CLA	C3C-C2C	5.17	1.47	1.36
17	A	830	CLA	CHC-C1C	5.17	1.48	1.35
26	7	605	CHL	C3D-C2D	5.17	1.48	1.39
17	a	830	CLA	CHC-C1C	5.17	1.48	1.35
17	a	802	CLA	CHC-C1C	5.17	1.48	1.35
17	A	836	CLA	O2D-CGD	5.17	1.45	1.33
17	A	818	CLA	CHC-C1C	5.17	1.48	1.35
26	3	307	CHL	C2C-C3C	5.17	1.47	1.36
17	9	604	CLA	CHC-C1C	5.17	1.48	1.35
17	A	809	CLA	O2D-CGD	5.17	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	810	CLA	CHC-C1C	5.17	1.48	1.35
17	B	830	CLA	CHC-C1C	5.17	1.48	1.35
17	6	309	CLA	O2D-CGD	5.17	1.45	1.33
17	1	315	CLA	O2D-CGD	5.16	1.45	1.33
17	a	812	CLA	CHC-C1C	5.16	1.48	1.35
17	2	603	CLA	CHC-C1C	5.16	1.48	1.35
17	b	831	CLA	O2D-CGD	5.16	1.45	1.33
17	a	823	CLA	CHC-C1C	5.16	1.48	1.35
17	B	835	CLA	O2D-CGD	5.16	1.45	1.33
17	F	303	CLA	O2D-CGD	5.16	1.45	1.33
17	4	610	CLA	O2D-CGD	5.16	1.45	1.33
17	a	803	CLA	C3C-C2C	5.16	1.47	1.36
17	B	819	CLA	O2D-CGD	5.16	1.45	1.33
17	2	610	CLA	O2D-CGD	5.16	1.45	1.33
26	7	606	CHL	O2D-CGD	5.16	1.45	1.33
17	B	805	CLA	O2D-CGD	5.16	1.45	1.33
17	B	812	CLA	CHC-C1C	5.16	1.48	1.35
17	3	305	CLA	O2D-CGD	5.16	1.45	1.33
17	b	827	CLA	O2D-CGD	5.16	1.45	1.33
17	b	819	CLA	O2D-CGD	5.16	1.45	1.33
20	B	844	BCR	C23-C22	-5.16	1.34	1.45
17	A	803	CLA	O2D-CGD	5.16	1.45	1.33
17	k	1403	CLA	O2D-CGD	5.16	1.45	1.33
17	K	4002	CLA	CHC-C1C	5.16	1.48	1.35
17	1	309	CLA	O2D-CGD	5.16	1.45	1.33
26	8	306	CHL	O2D-CGD	5.16	1.45	1.33
17	a	803	CLA	O2D-CGD	5.16	1.45	1.33
17	3	302	CLA	O2D-CGD	5.16	1.45	1.33
17	3	306	CLA	CHC-C1C	5.16	1.48	1.35
17	b	817	CLA	O2D-CGD	5.15	1.45	1.33
17	a	831	CLA	CHC-C1C	5.15	1.48	1.35
17	7	604	CLA	O2D-CGD	5.15	1.45	1.33
17	1	311	CLA	O2D-CGD	5.15	1.45	1.33
17	B	822	CLA	CHC-C1C	5.15	1.48	1.35
17	A	815	CLA	O2D-CGD	5.15	1.45	1.33
17	9	613	CLA	CHC-C1C	5.15	1.48	1.35
17	2	602	CLA	O2D-CGD	5.15	1.45	1.33
17	b	802	CLA	O2D-CGD	5.15	1.45	1.33
17	f	7003	CLA	CHC-C1C	5.15	1.48	1.35
17	a	826	CLA	CHC-C1C	5.15	1.48	1.35
17	9	603	CLA	C3C-C2C	5.15	1.47	1.36
17	k	1401	CLA	CHC-C1C	5.15	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	303	CHL	C3D-C2D	5.15	1.48	1.39
17	A	817	CLA	O2D-CGD	5.15	1.45	1.33
26	4	607	CHL	C2C-C3C	5.15	1.47	1.36
17	4	611	CLA	O2D-CGD	5.15	1.45	1.33
20	A	848	BCR	C23-C22	-5.15	1.34	1.45
17	7	608	CLA	O2D-CGD	5.15	1.45	1.33
17	6	305	CLA	O2D-CGD	5.15	1.45	1.33
17	B	839	CLA	O2D-CGD	5.15	1.45	1.33
17	B	828	CLA	O2D-CGD	5.14	1.45	1.33
17	8	312	CLA	CHC-C1C	5.14	1.48	1.35
17	B	831	CLA	O2D-CGD	5.14	1.45	1.33
17	A	830	CLA	O2D-CGD	5.14	1.45	1.33
17	8	304	CLA	CHC-C1C	5.14	1.48	1.35
17	a	836	CLA	O2D-CGD	5.14	1.45	1.33
17	f	7003	CLA	O2D-CGD	5.14	1.45	1.33
17	A	829	CLA	CHC-C1C	5.14	1.48	1.35
17	A	833	CLA	O2D-CGD	5.14	1.45	1.33
17	A	812	CLA	CHC-C1C	5.14	1.48	1.35
17	G	103	CLA	CHC-C1C	5.14	1.48	1.35
17	L	202	CLA	O2D-CGD	5.14	1.45	1.33
17	A	818	CLA	O2D-CGD	5.14	1.45	1.33
26	7	607	CHL	O2D-CGD	5.14	1.45	1.33
17	1	310	CLA	CHC-C1C	5.14	1.48	1.35
17	G	101	CLA	CHC-C1C	5.14	1.48	1.35
17	6	309	CLA	CHC-C1C	5.14	1.48	1.35
17	A	822	CLA	CHC-C1C	5.14	1.48	1.35
17	B	811	CLA	CHC-C1C	5.14	1.48	1.35
17	1	308	CLA	CHC-C1C	5.14	1.48	1.35
17	b	830	CLA	CHC-C1C	5.14	1.48	1.35
17	b	826	CLA	O2D-CGD	5.14	1.45	1.33
17	7	609	CLA	O2D-CGD	5.14	1.45	1.33
17	a	808	CLA	O2D-CGD	5.14	1.45	1.33
26	1	302	CHL	CHC-C1C	5.14	1.48	1.35
17	b	833	CLA	O2D-CGD	5.13	1.45	1.33
17	a	802	CLA	O2D-CGD	5.13	1.45	1.33
17	a	810	CLA	CHC-C1C	5.13	1.48	1.35
17	b	822	CLA	O2D-CGD	5.13	1.45	1.33
17	3	304	CLA	CHC-C1C	5.13	1.48	1.35
20	B	801	BCR	C23-C22	-5.13	1.34	1.45
17	A	845	CLA	O2D-CGD	5.13	1.45	1.33
17	b	805	CLA	O2D-CGD	5.13	1.45	1.33
17	4	604	CLA	O2D-CGD	5.13	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	204	CLA	CHC-C1C	5.13	1.48	1.35
17	3	301	CLA	O2D-CGD	5.13	1.45	1.33
17	J	3002	CLA	CHC-C1C	5.13	1.48	1.35
17	6	304	CLA	O2D-CGD	5.13	1.45	1.33
17	a	840	CLA	O2D-CGD	5.13	1.45	1.33
17	A	816	CLA	CHC-C1C	5.13	1.48	1.35
17	A	820	CLA	CHC-C1C	5.13	1.48	1.35
17	a	804	CLA	CHC-C1C	5.13	1.48	1.35
17	6	304	CLA	CHC-C1C	5.13	1.48	1.35
17	A	805	CLA	CHC-C1C	5.13	1.48	1.35
17	b	828	CLA	CHC-C1C	5.13	1.48	1.35
26	1	307	CHL	O2D-CGD	5.13	1.45	1.33
20	J	3003	BCR	C23-C22	-5.13	1.34	1.45
17	b	811	CLA	O2D-CGD	5.13	1.45	1.33
17	A	845	CLA	CHC-C1C	5.13	1.48	1.35
17	1	305	CLA	CHC-C1C	5.13	1.48	1.35
17	g	102	CLA	O2D-CGD	5.13	1.45	1.33
17	A	816	CLA	O2D-CGD	5.13	1.45	1.33
17	B	817	CLA	CHC-C1C	5.12	1.48	1.35
20	b	848	BCR	C23-C22	-5.12	1.34	1.45
17	A	832	CLA	CHC-C1C	5.12	1.48	1.35
17	A	837	CLA	CHC-C1C	5.12	1.48	1.35
17	3	311	CLA	CHC-C1C	5.12	1.48	1.35
17	B	827	CLA	O2D-CGD	5.12	1.45	1.33
17	b	835	CLA	CHC-C1C	5.12	1.48	1.35
17	A	814	CLA	CHC-C1C	5.12	1.48	1.35
17	7	604	CLA	CHC-C1C	5.12	1.48	1.35
17	b	816	CLA	O2D-CGD	5.12	1.45	1.33
17	A	842	CLA	O2D-CGD	5.12	1.45	1.33
17	8	312	CLA	O2D-CGD	5.12	1.45	1.33
17	1	304	CLA	O2D-CGD	5.12	1.45	1.33
20	l	201	BCR	C23-C22	-5.12	1.34	1.45
26	4	607	CHL	O2D-CGD	5.12	1.45	1.33
17	B	816	CLA	CHC-C1C	5.12	1.48	1.35
17	9	610	CLA	CHC-C1C	5.12	1.48	1.35
17	a	832	CLA	CHC-C1C	5.12	1.48	1.35
17	a	834	CLA	CHC-C1C	5.12	1.48	1.35
17	b	836	CLA	O2D-CGD	5.12	1.45	1.33
17	A	810	CLA	O2D-CGD	5.12	1.45	1.33
17	A	840	CLA	O2D-CGD	5.12	1.45	1.33
17	4	601	CLA	O2D-CGD	5.12	1.45	1.33
17	A	840	CLA	CHC-C1C	5.12	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	822	CLA	CHC-C1C	5.12	1.48	1.35
26	2	605	CHL	O2D-CGD	5.12	1.45	1.33
17	a	817	CLA	O2D-CGD	5.12	1.45	1.33
17	b	834	CLA	CHC-C1C	5.12	1.48	1.35
17	3	304	CLA	O2D-CGD	5.12	1.45	1.33
17	b	836	CLA	CHC-C1C	5.12	1.48	1.35
17	g	101	CLA	O2D-CGD	5.12	1.45	1.33
17	9	604	CLA	O2D-CGD	5.12	1.45	1.33
17	k	1402	CLA	CHC-C1C	5.12	1.48	1.35
26	2	605	CHL	C3D-C2D	5.12	1.48	1.39
17	B	834	CLA	CHC-C1C	5.12	1.48	1.35
17	a	813	CLA	CHC-C1C	5.12	1.48	1.35
26	4	605	CHL	O2D-CGD	5.12	1.45	1.33
17	7	610	CLA	O2D-CGD	5.12	1.45	1.33
17	3	305	CLA	CHC-C1C	5.12	1.48	1.35
17	9	603	CLA	O2D-CGD	5.11	1.45	1.33
17	2	613	CLA	CHC-C1C	5.11	1.48	1.35
17	4	613	CLA	CHC-C1C	5.11	1.48	1.35
17	A	831	CLA	CHC-C1C	5.11	1.48	1.35
17	a	844	CLA	O2D-CGD	5.11	1.45	1.33
17	A	819	CLA	O2D-CGD	5.11	1.45	1.33
17	1	311	CLA	CHC-C1C	5.11	1.48	1.35
17	a	818	CLA	O2D-CGD	5.11	1.45	1.33
17	A	820	CLA	O2D-CGD	5.11	1.45	1.33
17	a	844	CLA	C3C-C2C	5.11	1.47	1.36
17	A	811	CLA	CHC-C1C	5.11	1.48	1.35
17	B	820	CLA	CHC-C1C	5.11	1.48	1.35
17	1	306	CLA	O2D-CGD	5.11	1.45	1.33
17	g	102	CLA	CHC-C1C	5.11	1.48	1.35
17	1	312	CLA	O2D-CGD	5.11	1.45	1.33
17	B	805	CLA	CHC-C1C	5.11	1.48	1.35
17	8	311	CLA	CHC-C1C	5.11	1.48	1.35
17	8	303	CLA	O2D-CGD	5.11	1.45	1.33
17	B	828	CLA	CHC-C1C	5.11	1.48	1.35
17	B	830	CLA	O2D-CGD	5.11	1.45	1.33
17	a	838	CLA	C3C-C2C	5.11	1.47	1.36
17	g	103	CLA	CHC-C1C	5.11	1.48	1.35
17	B	806	CLA	O2D-CGD	5.11	1.45	1.33
17	6	315	CLA	O2D-CGD	5.11	1.45	1.33
17	3	314	CLA	CHC-C1C	5.11	1.48	1.35
17	B	831	CLA	CHC-C1C	5.11	1.48	1.35
17	b	804	CLA	CHC-C1C	5.11	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	820	CLA	CHC-C1C	5.11	1.48	1.35
20	a	850	BCR	C23-C22	-5.11	1.35	1.45
17	2	611	CLA	CHC-C1C	5.11	1.48	1.35
17	b	809	CLA	CHC-C1C	5.10	1.48	1.35
17	7	613	CLA	CHC-C1C	5.10	1.48	1.35
17	b	815	CLA	CHC-C1C	5.10	1.48	1.35
17	a	844	CLA	CHC-C1C	5.10	1.48	1.35
17	a	840	CLA	CHC-C1C	5.10	1.48	1.35
17	a	810	CLA	O2D-CGD	5.10	1.45	1.33
17	a	841	CLA	CHC-C1C	5.10	1.48	1.35
17	8	302	CLA	O2D-CGD	5.10	1.45	1.33
26	4	605	CHL	C3D-C2D	5.10	1.48	1.39
17	A	804	CLA	CHC-C1C	5.10	1.48	1.35
17	7	602	CLA	O2D-CGD	5.10	1.45	1.33
17	a	833	CLA	O2D-CGD	5.10	1.45	1.33
17	j	3002	CLA	CHC-C1C	5.10	1.48	1.35
17	B	823	CLA	CHC-C1C	5.10	1.48	1.35
20	b	844	BCR	C23-C22	-5.10	1.35	1.45
17	2	612	CLA	CHC-C1C	5.10	1.48	1.35
17	3	310	CLA	CHC-C1C	5.10	1.48	1.35
17	A	831	CLA	O2D-CGD	5.10	1.45	1.33
17	b	821	CLA	O2D-CGD	5.10	1.45	1.33
26	9	607	CHL	O2D-CGD	5.10	1.45	1.33
17	a	842	CLA	CHC-C1C	5.10	1.48	1.35
17	B	810	CLA	O2D-CGD	5.10	1.45	1.33
17	4	603	CLA	C3C-C2C	5.10	1.47	1.36
17	K	4002	CLA	O2D-CGD	5.10	1.45	1.33
17	B	818	CLA	CHC-C1C	5.09	1.48	1.35
17	4	614	CLA	CHC-C1C	5.09	1.48	1.35
26	6	303	CHL	CHC-C1C	5.09	1.48	1.35
26	9	605	CHL	CHC-C1C	5.09	1.48	1.35
17	b	812	CLA	CHC-C1C	5.09	1.48	1.35
20	i	101	BCR	C23-C22	-5.09	1.35	1.45
26	1	302	CHL	C3D-C2D	5.09	1.48	1.39
17	B	836	CLA	CHC-C1C	5.09	1.48	1.35
17	B	817	CLA	O2D-CGD	5.09	1.45	1.33
17	3	301	CLA	CHC-C1C	5.09	1.48	1.35
17	B	818	CLA	O2D-CGD	5.09	1.45	1.33
26	2	607	CHL	O2D-CGD	5.09	1.45	1.33
17	A	806	CLA	O2D-CGD	5.09	1.45	1.33
17	B	815	CLA	CHC-C1C	5.09	1.48	1.35
17	g	103	CLA	O2D-CGD	5.09	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	806	CLA	C3C-C2C	5.09	1.47	1.36
17	6	316	CLA	CHC-C1C	5.09	1.48	1.35
17	b	834	CLA	O2D-CGD	5.09	1.45	1.33
17	B	804	CLA	CHC-C1C	5.09	1.48	1.35
26	9	605	CHL	C3D-C2D	5.09	1.48	1.39
17	a	801	CLA	CHC-C1C	5.09	1.48	1.35
17	2	604	CLA	CHC-C1C	5.08	1.48	1.35
17	a	809	CLA	O2D-CGD	5.08	1.45	1.33
17	B	839	CLA	CHC-C1C	5.08	1.48	1.35
17	6	306	CLA	CHC-C1C	5.08	1.48	1.35
26	2	606	CHL	CHC-C1C	5.08	1.48	1.35
17	a	812	CLA	O2D-CGD	5.08	1.45	1.33
17	A	835	CLA	CHC-C1C	5.08	1.48	1.35
17	B	809	CLA	O2D-CGD	5.08	1.45	1.33
17	a	806	CLA	CHC-C1C	5.08	1.48	1.35
17	A	826	CLA	O2D-CGD	5.08	1.45	1.33
17	a	828	CLA	CHC-C1C	5.08	1.48	1.35
17	b	820	CLA	O2D-CGD	5.08	1.45	1.33
17	8	309	CLA	CHC-C1C	5.08	1.48	1.35
20	j	3004	BCR	C23-C22	-5.08	1.35	1.45
17	9	602	CLA	O2D-CGD	5.08	1.45	1.33
26	2	605	CHL	CHC-C1C	5.08	1.48	1.35
17	K	4003	CLA	CHC-C1C	5.08	1.48	1.35
17	B	802	CLA	O2D-CGD	5.08	1.45	1.33
17	A	808	CLA	CHC-C1C	5.08	1.48	1.35
17	9	614	CLA	CHC-C1C	5.08	1.48	1.35
17	1	303	CLA	O2D-CGD	5.08	1.45	1.33
17	4	603	CLA	O2D-CGD	5.08	1.45	1.33
17	B	804	CLA	O2D-CGD	5.07	1.45	1.33
17	4	610	CLA	CHC-C1C	5.07	1.48	1.35
17	4	604	CLA	CHC-C1C	5.07	1.48	1.35
17	1	315	CLA	CHC-C1C	5.07	1.48	1.35
26	7	605	CHL	O2D-CGD	5.07	1.45	1.33
17	B	808	CLA	O2D-CGD	5.07	1.45	1.33
17	F	301	CLA	CHC-C1C	5.07	1.48	1.35
17	B	834	CLA	O2D-CGD	5.07	1.45	1.33
17	b	818	CLA	CHC-C1C	5.07	1.48	1.35
17	1	314	CLA	O2D-CGD	5.07	1.45	1.33
26	4	615	CHL	CHC-C1C	5.07	1.48	1.35
17	A	835	CLA	O2D-CGD	5.07	1.45	1.33
17	b	807	CLA	O2D-CGD	5.07	1.45	1.33
17	a	827	CLA	O2D-CGD	5.07	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	9	615	CHL	C3D-C2D	5.07	1.48	1.39
17	9	611	CLA	CHC-C1C	5.07	1.48	1.35
17	f	7002	CLA	CHC-C1C	5.07	1.48	1.35
17	b	821	CLA	CHC-C1C	5.07	1.48	1.35
17	b	833	CLA	CHC-C1C	5.07	1.48	1.35
26	7	614	CHL	C3D-C2D	5.07	1.48	1.39
17	A	827	CLA	O2D-CGD	5.07	1.45	1.33
17	B	836	CLA	O2D-CGD	5.07	1.45	1.33
17	b	803	CLA	O2D-CGD	5.07	1.45	1.33
17	a	843	CLA	O2D-CGD	5.07	1.45	1.33
17	a	839	CLA	CHC-C1C	5.07	1.48	1.35
17	a	826	CLA	O2D-CGD	5.06	1.45	1.33
17	A	832	CLA	O2D-CGD	5.06	1.45	1.33
20	b	801	BCR	C23-C22	-5.06	1.35	1.45
17	3	313	CLA	CHC-C1C	5.06	1.48	1.35
17	b	831	CLA	CHC-C1C	5.06	1.47	1.35
26	1	307	CHL	CHC-C1C	5.06	1.47	1.35
17	B	820	CLA	O2D-CGD	5.06	1.45	1.33
17	b	817	CLA	CHC-C1C	5.06	1.47	1.35
17	A	802	CLA	O2D-CGD	5.06	1.45	1.33
17	a	837	CLA	CHC-C1C	5.06	1.47	1.35
20	B	846	BCR	C23-C22	-5.06	1.35	1.45
17	1	313	CLA	CHC-C1C	5.06	1.47	1.35
26	6	308	CHL	C3D-C2D	5.06	1.48	1.39
17	A	813	CLA	CHC-C1C	5.06	1.47	1.35
17	A	821	CLA	CHC-C1C	5.06	1.47	1.35
17	b	811	CLA	CHC-C1C	5.06	1.47	1.35
17	6	312	CLA	CHC-C1C	5.06	1.47	1.35
17	k	1401	CLA	O2D-CGD	5.06	1.45	1.33
26	8	306	CHL	CHC-C1C	5.06	1.47	1.35
26	7	605	CHL	CHC-C1C	5.05	1.47	1.35
17	A	836	CLA	CHC-C1C	5.05	1.47	1.35
18	A	844	PQN	C10-C5	5.05	1.49	1.40
26	2	614	CHL	C3D-C2D	5.05	1.48	1.39
26	4	607	CHL	C3D-C2D	5.05	1.48	1.39
17	F	301	CLA	O2D-CGD	5.05	1.45	1.33
26	9	607	CHL	C2C-C3C	5.05	1.47	1.36
17	B	833	CLA	CHC-C1C	5.05	1.47	1.35
17	B	821	CLA	O2D-CGD	5.05	1.45	1.33
17	B	815	CLA	O2D-CGD	5.05	1.45	1.33
17	A	834	CLA	O2D-CGD	5.05	1.45	1.33
20	B	845	BCR	C23-C22	-5.05	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	l	205	BCR	C23-C22	-5.05	1.35	1.45
17	1	314	CLA	CHC-C1C	5.05	1.47	1.35
26	3	307	CHL	C3D-C2D	5.05	1.48	1.39
17	A	817	CLA	CHC-C1C	5.05	1.47	1.35
17	k	1403	CLA	CHC-C1C	5.05	1.47	1.35
17	b	816	CLA	CHC-C1C	5.05	1.47	1.35
26	6	308	CHL	CHC-C1C	5.05	1.47	1.35
17	b	838	CLA	CHC-C1C	5.04	1.47	1.35
17	B	840	CLA	CHC-C1C	5.04	1.47	1.35
17	a	821	CLA	CHC-C1C	5.04	1.47	1.35
17	b	839	CLA	CHC-C1C	5.04	1.47	1.35
17	6	315	CLA	CHC-C1C	5.04	1.47	1.35
17	B	833	CLA	O2D-CGD	5.04	1.45	1.33
17	A	803	CLA	CHC-C1C	5.04	1.47	1.35
17	a	835	CLA	CHC-C1C	5.04	1.47	1.35
17	a	814	CLA	O2D-CGD	5.04	1.45	1.33
20	j	3003	BCR	C23-C22	-5.04	1.35	1.45
17	B	813	CLA	O2D-CGD	5.04	1.45	1.33
17	6	314	CLA	CHC-C1C	5.04	1.47	1.35
26	7	606	CHL	CHC-C1C	5.04	1.47	1.35
17	6	313	CLA	CHC-C1C	5.04	1.47	1.35
17	9	612	CLA	CHC-C1C	5.04	1.47	1.35
17	8	305	CLA	CHC-C1C	5.04	1.47	1.35
17	B	824	CLA	O2D-CGD	5.03	1.45	1.33
20	L	205	BCR	C23-C22	-5.03	1.35	1.45
17	B	803	CLA	O2D-CGD	5.03	1.45	1.33
17	B	808	CLA	CHC-C1C	5.03	1.47	1.35
17	a	805	CLA	O2D-CGD	5.03	1.45	1.33
17	9	603	CLA	CHC-C1C	5.03	1.47	1.35
17	B	822	CLA	O2D-CGD	5.03	1.45	1.33
17	A	821	CLA	O2D-CGD	5.03	1.45	1.33
17	a	821	CLA	O2D-CGD	5.03	1.45	1.33
17	9	601	CLA	O2D-CGD	5.03	1.45	1.33
17	4	601	CLA	CHC-C1C	5.03	1.47	1.35
17	4	608	CLA	CHC-C1C	5.03	1.47	1.35
17	4	611	CLA	CHC-C1C	5.02	1.47	1.35
17	l	202	CLA	CHC-C1C	5.02	1.47	1.35
17	6	305	CLA	CHC-C1C	5.02	1.47	1.35
17	A	810	CLA	CHC-C1C	5.02	1.47	1.35
18	b	842	PQN	C10-C5	5.02	1.49	1.40
17	2	610	CLA	CHC-C1C	5.02	1.47	1.35
26	6	303	CHL	O2D-CGD	5.02	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	825	CLA	CHC-C1C	5.02	1.47	1.35
17	B	841	CLA	O2D-CGD	5.02	1.45	1.33
17	8	310	CLA	CHC-C1C	5.02	1.47	1.35
26	1	307	CHL	C3D-C2D	5.02	1.48	1.39
17	A	829	CLA	O2D-CGD	5.02	1.45	1.33
17	a	807	CLA	O2D-CGD	5.02	1.45	1.33
17	2	613	CLA	O2D-CGD	5.02	1.45	1.33
17	b	812	CLA	O2D-CGD	5.02	1.45	1.33
17	B	812	CLA	O2D-CGD	5.02	1.45	1.33
17	a	815	CLA	O2D-CGD	5.01	1.45	1.33
17	6	310	CLA	CHC-C1C	5.01	1.47	1.35
26	2	607	CHL	C3D-C2D	5.01	1.48	1.39
17	A	825	CLA	CHC-C1C	5.01	1.47	1.35
17	A	839	CLA	CHC-C1C	5.01	1.47	1.35
17	a	811	CLA	CHC-C1C	5.01	1.47	1.35
17	B	838	CLA	CHC-C1C	5.01	1.47	1.35
17	a	829	CLA	O2D-CGD	5.01	1.45	1.33
17	7	612	CLA	CHC-C1C	5.01	1.47	1.35
17	9	601	CLA	CHC-C1C	5.01	1.47	1.35
17	7	608	CLA	CHC-C1C	5.01	1.47	1.35
17	1	312	CLA	CHC-C1C	5.01	1.47	1.35
17	b	805	CLA	CHC-C1C	5.01	1.47	1.35
17	a	820	CLA	CHC-C1C	5.01	1.47	1.35
26	2	614	CHL	CHC-C1C	5.01	1.47	1.35
17	2	603	CLA	O2D-CGD	5.01	1.45	1.33
17	b	824	CLA	O2D-CGD	5.00	1.45	1.33
26	7	606	CHL	C3D-C2D	5.00	1.48	1.39
17	a	824	CLA	CHC-C1C	5.00	1.47	1.35
17	4	612	CLA	CHC-C1C	5.00	1.47	1.35
17	A	824	CLA	CHC-C1C	5.00	1.47	1.35
26	4	605	CHL	CHC-C1C	5.00	1.47	1.35
17	2	608	CLA	CHC-C1C	5.00	1.47	1.35
17	A	838	CLA	O2D-CGD	5.00	1.45	1.33
17	a	818	CLA	CHC-C1C	5.00	1.47	1.35
26	8	306	CHL	C3D-C2D	5.00	1.48	1.39
17	7	610	CLA	CHC-C1C	5.00	1.47	1.35
17	a	831	CLA	O2D-CGD	5.00	1.45	1.33
17	b	802	CLA	CHC-C1C	5.00	1.47	1.35
17	a	817	CLA	CHC-C1C	5.00	1.47	1.35
17	L	202	CLA	CHC-C1C	5.00	1.47	1.35
17	4	614	CLA	O2D-CGD	4.99	1.45	1.33
26	2	601	CHL	CHC-C1C	4.99	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	843	CLA	CHC-C1C	4.99	1.47	1.35
17	B	838	CLA	O2D-CGD	4.99	1.45	1.33
17	a	801	CLA	O2D-CGD	4.99	1.45	1.33
26	2	601	CHL	C3D-C2D	4.99	1.48	1.39
17	B	809	CLA	CHC-C1C	4.99	1.47	1.35
17	G	101	CLA	O2D-CGD	4.99	1.45	1.33
17	g	101	CLA	CHC-C1C	4.99	1.47	1.35
17	9	608	CLA	CHC-C1C	4.99	1.47	1.35
26	9	615	CHL	CHC-C1C	4.99	1.47	1.35
26	9	607	CHL	C3D-C2D	4.99	1.48	1.39
17	b	819	CLA	CHC-C1C	4.99	1.47	1.35
17	b	841	CLA	O2D-CGD	4.98	1.45	1.33
26	7	601	CHL	C3D-C2D	4.98	1.48	1.39
17	a	815	CLA	OBD-CAD	4.98	1.29	1.22
17	b	829	CLA	CHC-C1C	4.98	1.47	1.35
26	8	306	CHL	C2C-C3C	4.98	1.47	1.36
17	A	854	CLA	CHC-C1C	4.98	1.47	1.35
17	4	603	CLA	CHC-C1C	4.98	1.47	1.35
17	7	611	CLA	CHC-C1C	4.98	1.47	1.35
26	4	607	CHL	CHC-C1C	4.98	1.47	1.35
17	a	834	CLA	O2D-CGD	4.97	1.45	1.33
17	B	829	CLA	O2D-CGD	4.97	1.45	1.33
26	7	607	CHL	CHC-C1C	4.97	1.47	1.35
17	1	304	CLA	CHC-C1C	4.97	1.47	1.35
17	3	312	CLA	CHC-C1C	4.97	1.47	1.35
17	B	832	CLA	O2D-CGD	4.97	1.45	1.33
26	9	606	CHL	CHC-C1C	4.97	1.47	1.35
17	A	839	CLA	O2D-CGD	4.97	1.45	1.33
17	A	834	CLA	CHC-C1C	4.96	1.47	1.35
26	2	606	CHL	C3D-C2D	4.96	1.48	1.39
17	a	836	CLA	CHC-C1C	4.96	1.47	1.35
17	a	804	CLA	O2D-CGD	4.96	1.45	1.33
17	b	810	CLA	O2D-CGD	4.96	1.45	1.33
26	7	614	CHL	CHC-C1C	4.96	1.47	1.35
17	F	303	CLA	CHC-C1C	4.96	1.47	1.35
26	9	607	CHL	CHC-C1C	4.95	1.47	1.35
26	2	607	CHL	CHC-C1C	4.95	1.47	1.35
26	9	606	CHL	C3D-C2D	4.95	1.48	1.39
17	B	822	CLA	OBD-CAD	4.95	1.29	1.22
17	A	828	CLA	O2D-CGD	4.95	1.45	1.33
17	b	814	CLA	O2D-CGD	4.95	1.45	1.33
17	b	840	CLA	CHC-C1C	4.95	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	309	CLA	CHC-C1C	4.95	1.47	1.35
17	B	826	CLA	O2D-CGD	4.95	1.45	1.33
26	4	615	CHL	C3D-C2D	4.94	1.48	1.39
26	1	302	CHL	O2D-CGD	4.94	1.45	1.33
17	a	801	CLA	OBD-CAD	4.94	1.29	1.22
17	b	806	CLA	O2D-CGD	4.94	1.45	1.33
17	B	819	CLA	CHC-C1C	4.94	1.47	1.35
17	a	838	CLA	O2D-CGD	4.94	1.45	1.33
17	9	614	CLA	O2D-CGD	4.94	1.45	1.33
17	a	813	CLA	OBD-CAD	4.94	1.29	1.22
18	B	842	PQN	C10-C5	4.93	1.48	1.40
17	b	815	CLA	O2D-CGD	4.93	1.45	1.33
17	b	825	CLA	O2D-CGD	4.93	1.45	1.33
17	b	808	CLA	CHC-C1C	4.93	1.47	1.35
17	A	801	CLA	O2D-CGD	4.93	1.45	1.33
17	b	832	CLA	O2D-CGD	4.93	1.45	1.33
17	3	303	CLA	CHC-C1C	4.92	1.47	1.35
17	a	828	CLA	O2D-CGD	4.91	1.45	1.33
17	a	803	CLA	CHC-C1C	4.91	1.47	1.35
18	a	845	PQN	C10-C5	4.91	1.48	1.40
17	8	302	CLA	CHC-C1C	4.91	1.47	1.35
17	A	835	CLA	OBD-CAD	4.90	1.29	1.22
17	B	829	CLA	CHC-C1C	4.90	1.47	1.35
17	a	839	CLA	O2D-CGD	4.90	1.45	1.33
17	6	313	CLA	OBD-CAD	4.90	1.29	1.22
17	A	830	CLA	OBD-CAD	4.89	1.29	1.22
26	2	601	CHL	O2D-CGD	4.89	1.45	1.33
26	4	606	CHL	C3D-C2D	4.88	1.48	1.39
17	b	829	CLA	O2D-CGD	4.88	1.45	1.33
17	a	856	CLA	CHC-C1C	4.88	1.47	1.35
26	4	606	CHL	OBD-CAD	4.88	1.29	1.22
17	A	814	CLA	O2D-CGD	4.88	1.45	1.33
17	b	808	CLA	O2D-CGD	4.88	1.45	1.33
26	3	307	CHL	CHC-C1C	4.87	1.47	1.35
26	7	601	CHL	O2D-CGD	4.87	1.45	1.33
17	b	815	CLA	OBD-CAD	4.86	1.29	1.22
17	b	837	CLA	O2D-CGD	4.86	1.45	1.33
17	a	837	CLA	OBD-CAD	4.85	1.29	1.22
17	B	825	CLA	O2D-CGD	4.85	1.45	1.33
17	a	820	CLA	OBD-CAD	4.85	1.29	1.22
17	A	805	CLA	OBD-CAD	4.84	1.29	1.22
17	B	814	CLA	O2D-CGD	4.84	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	306	CLA	OBD-CAD	4.84	1.29	1.22
17	A	806	CLA	OBD-CAD	4.84	1.29	1.22
17	a	834	CLA	OBD-CAD	4.84	1.29	1.22
17	b	804	CLA	O2D-CGD	4.83	1.45	1.33
17	B	815	CLA	OBD-CAD	4.83	1.29	1.22
17	b	802	CLA	OBD-CAD	4.83	1.29	1.22
17	b	813	CLA	O2D-CGD	4.83	1.45	1.33
17	1	312	CLA	OBD-CAD	4.83	1.29	1.22
17	A	854	CLA	O2D-CGD	4.83	1.45	1.33
17	b	809	CLA	O2D-CGD	4.83	1.45	1.33
17	b	812	CLA	OBD-CAD	4.83	1.29	1.22
17	b	834	CLA	OBD-CAD	4.82	1.29	1.22
17	6	306	CLA	OBD-CAD	4.82	1.29	1.22
17	b	832	CLA	OBD-CAD	4.82	1.29	1.22
17	9	611	CLA	OBD-CAD	4.82	1.29	1.22
17	A	805	CLA	O2D-CGD	4.82	1.45	1.33
26	8	306	CHL	OBD-CAD	4.81	1.29	1.22
17	J	3002	CLA	OBD-CAD	4.81	1.29	1.22
17	a	842	CLA	OBD-CAD	4.81	1.29	1.22
17	A	825	CLA	OBD-CAD	4.81	1.29	1.22
17	l	202	CLA	OBD-CAD	4.81	1.29	1.22
17	7	611	CLA	OBD-CAD	4.81	1.29	1.22
17	b	840	CLA	OBD-CAD	4.80	1.29	1.22
17	A	840	CLA	OBD-CAD	4.80	1.29	1.22
17	3	301	CLA	OBD-CAD	4.80	1.29	1.22
17	3	313	CLA	OBD-CAD	4.80	1.29	1.22
17	8	305	CLA	OBD-CAD	4.80	1.29	1.22
17	B	837	CLA	O2D-CGD	4.80	1.44	1.33
17	B	802	CLA	OBD-CAD	4.80	1.29	1.22
17	K	4003	CLA	OBD-CAD	4.80	1.29	1.22
17	b	824	CLA	OBD-CAD	4.80	1.29	1.22
17	8	304	CLA	OBD-CAD	4.80	1.29	1.22
17	2	613	CLA	OBD-CAD	4.80	1.29	1.22
17	G	104	CLA	OBD-CAD	4.80	1.29	1.22
17	8	311	CLA	OBD-CAD	4.79	1.29	1.22
17	B	820	CLA	OBD-CAD	4.79	1.29	1.22
17	a	841	CLA	OBD-CAD	4.79	1.29	1.22
17	B	834	CLA	OBD-CAD	4.79	1.29	1.22
17	4	604	CLA	OBD-CAD	4.79	1.29	1.22
17	a	810	CLA	OBD-CAD	4.79	1.29	1.22
17	a	814	CLA	OBD-CAD	4.79	1.29	1.22
17	B	808	CLA	OBD-CAD	4.79	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	8	303	CLA	OBD-CAD	4.79	1.29	1.22
17	a	805	CLA	OBD-CAD	4.79	1.29	1.22
17	a	819	CLA	OBD-CAD	4.79	1.29	1.22
17	B	828	CLA	OBD-CAD	4.79	1.29	1.22
17	A	826	CLA	OBD-CAD	4.78	1.29	1.22
17	L	202	CLA	OBD-CAD	4.78	1.29	1.22
17	a	846	CLA	OBD-CAD	4.78	1.29	1.22
17	8	307	CLA	OBD-CAD	4.78	1.29	1.22
17	6	310	CLA	OBD-CAD	4.78	1.29	1.22
17	a	806	CLA	OBD-CAD	4.78	1.29	1.22
17	b	821	CLA	OBD-CAD	4.78	1.29	1.22
17	A	804	CLA	O2D-CGD	4.78	1.44	1.33
17	f	7003	CLA	OBD-CAD	4.77	1.29	1.22
17	A	836	CLA	OBD-CAD	4.77	1.29	1.22
17	4	608	CLA	OBD-CAD	4.77	1.29	1.22
26	7	601	CHL	OBD-CAD	4.77	1.29	1.22
26	9	606	CHL	OBD-CAD	4.77	1.29	1.22
17	A	837	CLA	OBD-CAD	4.77	1.29	1.22
17	7	604	CLA	OBD-CAD	4.77	1.29	1.22
17	1	314	CLA	OBD-CAD	4.77	1.29	1.22
26	7	605	CHL	OBD-CAD	4.77	1.29	1.22
17	B	827	CLA	OBD-CAD	4.77	1.29	1.22
17	2	609	CLA	OBD-CAD	4.77	1.29	1.22
17	B	809	CLA	OBD-CAD	4.77	1.29	1.22
17	2	611	CLA	OBD-CAD	4.76	1.29	1.22
17	K	4002	CLA	OBD-CAD	4.76	1.29	1.22
17	8	308	CLA	OBD-CAD	4.76	1.29	1.22
26	3	307	CHL	OBD-CAD	4.76	1.29	1.22
17	b	830	CLA	OBD-CAD	4.76	1.29	1.22
17	A	818	CLA	OBD-CAD	4.76	1.29	1.22
17	1	306	CLA	OBD-CAD	4.76	1.29	1.22
17	k	1403	CLA	OBD-CAD	4.76	1.29	1.22
26	2	614	CHL	OBD-CAD	4.76	1.29	1.22
17	a	817	CLA	OBD-CAD	4.76	1.29	1.22
17	a	808	CLA	OBD-CAD	4.76	1.29	1.22
17	G	103	CLA	OBD-CAD	4.76	1.29	1.22
26	4	605	CHL	OBD-CAD	4.76	1.29	1.22
26	2	605	CHL	OBD-CAD	4.76	1.28	1.22
17	1	313	CLA	OBD-CAD	4.76	1.28	1.22
17	k	1401	CLA	OBD-CAD	4.75	1.28	1.22
17	b	813	CLA	OBD-CAD	4.75	1.28	1.22
17	a	840	CLA	OBD-CAD	4.75	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	614	CLA	OBD-CAD	4.75	1.28	1.22
26	7	614	CHL	OBD-CAD	4.75	1.28	1.22
17	A	845	CLA	OBD-CAD	4.75	1.28	1.22
17	j	3002	CLA	OBD-CAD	4.75	1.28	1.22
17	9	612	CLA	OBD-CAD	4.75	1.28	1.22
17	a	827	CLA	OBD-CAD	4.75	1.28	1.22
17	a	818	CLA	OBD-CAD	4.74	1.28	1.22
17	A	823	CLA	OBD-CAD	4.74	1.28	1.22
17	a	825	CLA	OBD-CAD	4.74	1.28	1.22
17	b	804	CLA	OBD-CAD	4.74	1.28	1.22
17	3	308	CLA	OBD-CAD	4.74	1.28	1.22
17	8	309	CLA	OBD-CAD	4.74	1.28	1.22
17	8	301	CLA	OBD-CAD	4.74	1.28	1.22
17	A	822	CLA	OBD-CAD	4.74	1.28	1.22
17	6	316	CLA	OBD-CAD	4.74	1.28	1.22
17	a	832	CLA	OBD-CAD	4.74	1.28	1.22
17	b	833	CLA	OBD-CAD	4.74	1.28	1.22
17	a	830	CLA	OBD-CAD	4.74	1.28	1.22
17	a	821	CLA	OBD-CAD	4.73	1.28	1.22
17	3	311	CLA	OBD-CAD	4.73	1.28	1.22
26	6	308	CHL	OBD-CAD	4.73	1.28	1.22
17	B	818	CLA	OBD-CAD	4.73	1.28	1.22
17	4	613	CLA	OBD-CAD	4.73	1.28	1.22
17	9	614	CLA	OBD-CAD	4.73	1.28	1.22
26	2	606	CHL	OBD-CAD	4.73	1.28	1.22
17	a	809	CLA	OBD-CAD	4.73	1.28	1.22
17	B	812	CLA	OBD-CAD	4.73	1.28	1.22
17	B	819	CLA	OBD-CAD	4.73	1.28	1.22
17	B	841	CLA	OBD-CAD	4.73	1.28	1.22
26	7	606	CHL	OBD-CAD	4.73	1.28	1.22
17	3	302	CLA	OBD-CAD	4.73	1.28	1.22
17	a	823	CLA	OBD-CAD	4.73	1.28	1.22
17	g	102	CLA	OBD-CAD	4.72	1.28	1.22
17	2	604	CLA	OBD-CAD	4.72	1.28	1.22
26	6	303	CHL	OBD-CAD	4.72	1.28	1.22
17	9	609	CLA	OBD-CAD	4.72	1.28	1.22
17	b	831	CLA	OBD-CAD	4.72	1.28	1.22
17	7	612	CLA	OBD-CAD	4.72	1.28	1.22
17	A	813	CLA	OBD-CAD	4.72	1.28	1.22
17	g	101	CLA	OBD-CAD	4.72	1.28	1.22
26	1	307	CHL	OBD-CAD	4.72	1.28	1.22
17	6	304	CLA	OBD-CAD	4.72	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	303	CLA	OBD-CAD	4.72	1.28	1.22
17	b	822	CLA	OBD-CAD	4.72	1.28	1.22
17	A	832	CLA	OBD-CAD	4.72	1.28	1.22
17	A	804	CLA	OBD-CAD	4.72	1.28	1.22
17	1	311	CLA	OBD-CAD	4.72	1.28	1.22
17	b	819	CLA	OBD-CAD	4.72	1.28	1.22
17	A	810	CLA	OBD-CAD	4.71	1.28	1.22
17	B	831	CLA	OBD-CAD	4.71	1.28	1.22
17	b	827	CLA	OBD-CAD	4.71	1.28	1.22
17	A	817	CLA	OBD-CAD	4.71	1.28	1.22
17	b	820	CLA	OBD-CAD	4.71	1.28	1.22
17	a	802	CLA	OBD-CAD	4.71	1.28	1.22
17	A	820	CLA	OBD-CAD	4.71	1.28	1.22
17	A	843	CLA	OBD-CAD	4.71	1.28	1.22
17	1	315	CLA	OBD-CAD	4.71	1.28	1.22
17	b	837	CLA	OBD-CAD	4.71	1.28	1.22
17	A	827	CLA	OBD-CAD	4.71	1.28	1.22
17	B	804	CLA	OBD-CAD	4.71	1.28	1.22
26	9	615	CHL	OBD-CAD	4.71	1.28	1.22
17	A	833	CLA	OBD-CAD	4.71	1.28	1.22
17	A	816	CLA	OBD-CAD	4.71	1.28	1.22
17	9	604	CLA	OBD-CAD	4.71	1.28	1.22
17	1	204	CLA	OBD-CAD	4.71	1.28	1.22
17	a	856	CLA	O2D-CGD	4.71	1.44	1.33
17	2	612	CLA	OBD-CAD	4.71	1.28	1.22
17	2	602	CLA	OBD-CAD	4.70	1.28	1.22
17	F	301	CLA	OBD-CAD	4.70	1.28	1.22
17	1	203	CLA	OBD-CAD	4.70	1.28	1.22
17	3	304	CLA	OBD-CAD	4.70	1.28	1.22
17	1	305	CLA	OBD-CAD	4.70	1.28	1.22
17	A	834	CLA	OBD-CAD	4.70	1.28	1.22
17	b	807	CLA	OBD-CAD	4.70	1.28	1.22
17	b	838	CLA	OBD-CAD	4.70	1.28	1.22
17	B	821	CLA	OBD-CAD	4.70	1.28	1.22
17	B	835	CLA	OBD-CAD	4.70	1.28	1.22
17	b	816	CLA	OBD-CAD	4.70	1.28	1.22
17	4	610	CLA	OBD-CAD	4.70	1.28	1.22
17	B	805	CLA	OBD-CAD	4.70	1.28	1.22
17	A	802	CLA	OBD-CAD	4.70	1.28	1.22
17	A	821	CLA	OBD-CAD	4.69	1.28	1.22
17	3	312	CLA	OBD-CAD	4.69	1.28	1.22
26	7	607	CHL	OBD-CAD	4.69	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	812	CLA	OBD-CAD	4.69	1.28	1.22
17	3	305	CLA	OBD-CAD	4.69	1.28	1.22
17	B	825	CLA	OBD-CAD	4.69	1.28	1.22
17	4	612	CLA	OBD-CAD	4.69	1.28	1.22
26	2	601	CHL	OBD-CAD	4.69	1.28	1.22
17	6	311	CLA	OBD-CAD	4.69	1.28	1.22
26	1	302	CHL	OBD-CAD	4.69	1.28	1.22
17	1	309	CLA	OBD-CAD	4.69	1.28	1.22
17	L	204	CLA	OBD-CAD	4.69	1.28	1.22
17	A	808	CLA	OBD-CAD	4.69	1.28	1.22
17	9	610	CLA	OBD-CAD	4.69	1.28	1.22
17	F	303	CLA	OBD-CAD	4.68	1.28	1.22
17	g	103	CLA	OBD-CAD	4.68	1.28	1.22
17	1	304	CLA	OBD-CAD	4.68	1.28	1.22
26	4	615	CHL	OBD-CAD	4.68	1.28	1.22
17	b	841	CLA	OBD-CAD	4.68	1.28	1.22
17	A	841	CLA	OBD-CAD	4.68	1.28	1.22
17	b	818	CLA	OBD-CAD	4.68	1.28	1.22
17	f	7002	CLA	OBD-CAD	4.68	1.28	1.22
17	8	312	CLA	OBD-CAD	4.68	1.28	1.22
17	b	808	CLA	OBD-CAD	4.68	1.28	1.22
17	a	811	CLA	OBD-CAD	4.67	1.28	1.22
17	7	609	CLA	OBD-CAD	4.67	1.28	1.22
17	B	811	CLA	OBD-CAD	4.67	1.28	1.22
17	3	309	CLA	OBD-CAD	4.67	1.28	1.22
17	B	807	CLA	OBD-CAD	4.67	1.28	1.22
17	A	814	CLA	OBD-CAD	4.67	1.28	1.22
17	6	309	CLA	OBD-CAD	4.67	1.28	1.22
17	A	819	CLA	OBD-CAD	4.67	1.28	1.22
17	A	809	CLA	OBD-CAD	4.66	1.28	1.22
17	9	602	CLA	OBD-CAD	4.66	1.28	1.22
17	L	203	CLA	OBD-CAD	4.66	1.28	1.22
17	4	609	CLA	OBD-CAD	4.66	1.28	1.22
17	a	835	CLA	OBD-CAD	4.66	1.28	1.22
17	B	837	CLA	OBD-CAD	4.65	1.28	1.22
17	b	811	CLA	OBD-CAD	4.65	1.28	1.22
17	3	314	CLA	OBD-CAD	4.65	1.28	1.22
17	a	824	CLA	OBD-CAD	4.65	1.28	1.22
17	2	608	CLA	OBD-CAD	4.65	1.28	1.22
17	B	829	CLA	OBD-CAD	4.65	1.28	1.22
17	B	832	CLA	OBD-CAD	4.65	1.28	1.22
17	6	307	CLA	OBD-CAD	4.65	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	G	101	CLA	OBD-CAD	4.64	1.28	1.22
17	B	816	CLA	OBD-CAD	4.64	1.28	1.22
17	B	833	CLA	OBD-CAD	4.64	1.28	1.22
17	9	613	CLA	OBD-CAD	4.64	1.28	1.22
26	9	605	CHL	OBD-CAD	4.64	1.28	1.22
17	4	602	CLA	OBD-CAD	4.64	1.28	1.22
26	9	607	CHL	OBD-CAD	4.64	1.28	1.22
17	4	601	CLA	OBD-CAD	4.64	1.28	1.22
17	1	303	CLA	OBD-CAD	4.64	1.28	1.22
17	a	816	CLA	OBD-CAD	4.64	1.28	1.22
17	a	844	CLA	OBD-CAD	4.63	1.28	1.22
17	B	814	CLA	OBD-CAD	4.63	1.28	1.22
17	a	822	CLA	OBD-CAD	4.63	1.28	1.22
17	6	312	CLA	OBD-CAD	4.63	1.28	1.22
17	7	602	CLA	OBD-CAD	4.63	1.28	1.22
17	a	807	CLA	OBD-CAD	4.63	1.28	1.22
17	A	812	CLA	OBD-CAD	4.63	1.28	1.22
17	B	803	CLA	OBD-CAD	4.63	1.28	1.22
17	1	308	CLA	OBD-CAD	4.63	1.28	1.22
17	9	601	CLA	OBD-CAD	4.63	1.28	1.22
17	B	839	CLA	OBD-CAD	4.63	1.28	1.22
17	A	842	CLA	OBD-CAD	4.62	1.28	1.22
17	8	302	CLA	OBD-CAD	4.62	1.28	1.22
17	A	815	CLA	OBD-CAD	4.62	1.28	1.22
17	B	813	CLA	OBD-CAD	4.62	1.28	1.22
17	4	603	CLA	OBD-CAD	4.62	1.28	1.22
17	B	830	CLA	OBD-CAD	4.62	1.28	1.22
17	6	315	CLA	OBD-CAD	4.62	1.28	1.22
17	a	836	CLA	OBD-CAD	4.61	1.28	1.22
17	4	611	CLA	OBD-CAD	4.61	1.28	1.22
17	B	810	CLA	OBD-CAD	4.61	1.28	1.22
17	9	608	CLA	OBD-CAD	4.61	1.28	1.22
17	k	1402	CLA	OBD-CAD	4.61	1.28	1.22
17	b	825	CLA	OBD-CAD	4.61	1.28	1.22
17	A	824	CLA	OBD-CAD	4.60	1.28	1.22
17	b	809	CLA	OBD-CAD	4.60	1.28	1.22
17	a	856	CLA	OBD-CAD	4.60	1.28	1.22
17	a	833	CLA	OBD-CAD	4.60	1.28	1.22
17	A	801	CLA	OBD-CAD	4.60	1.28	1.22
17	b	810	CLA	OBD-CAD	4.59	1.28	1.22
17	a	826	CLA	OBD-CAD	4.58	1.28	1.22
17	a	831	CLA	OBD-CAD	4.58	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	8	310	CLA	OBD-CAD	4.58	1.28	1.22
17	b	814	CLA	OBD-CAD	4.58	1.28	1.22
17	b	828	CLA	OBD-CAD	4.58	1.28	1.22
17	a	839	CLA	OBD-CAD	4.58	1.28	1.22
17	A	831	CLA	OBD-CAD	4.57	1.28	1.22
17	B	823	CLA	OBD-CAD	4.57	1.28	1.22
17	b	835	CLA	OBD-CAD	4.57	1.28	1.22
17	F	304	CLA	OBD-CAD	4.57	1.28	1.22
17	1	310	CLA	OBD-CAD	4.56	1.28	1.22
17	A	807	CLA	OBD-CAD	4.56	1.28	1.22
17	b	839	CLA	OBD-CAD	4.56	1.28	1.22
17	2	610	CLA	OBD-CAD	4.55	1.28	1.22
17	7	610	CLA	OBD-CAD	4.55	1.28	1.22
17	A	854	CLA	OBD-CAD	4.55	1.28	1.22
17	a	804	CLA	OBD-CAD	4.55	1.28	1.22
17	B	824	CLA	OBD-CAD	4.54	1.28	1.22
17	7	613	CLA	OBD-CAD	4.54	1.28	1.22
17	7	608	CLA	OBD-CAD	4.53	1.28	1.22
17	b	803	CLA	OBD-CAD	4.53	1.28	1.22
17	b	805	CLA	OBD-CAD	4.53	1.28	1.22
17	a	838	CLA	OBD-CAD	4.52	1.28	1.22
17	b	829	CLA	OBD-CAD	4.52	1.28	1.22
17	b	823	CLA	OBD-CAD	4.51	1.28	1.22
17	6	314	CLA	OBD-CAD	4.51	1.28	1.22
17	A	811	CLA	OBD-CAD	4.51	1.28	1.22
17	7	603	CLA	OBD-CAD	4.51	1.28	1.22
17	B	840	CLA	OBD-CAD	4.50	1.28	1.22
17	6	305	CLA	OBD-CAD	4.50	1.28	1.22
17	l	204	CLA	O2A-CGA	4.49	1.46	1.33
17	A	803	CLA	OBD-CAD	4.49	1.28	1.22
17	b	817	CLA	OBD-CAD	4.49	1.28	1.22
17	b	839	CLA	O2A-CGA	4.49	1.46	1.33
17	a	818	CLA	O2A-CGA	4.49	1.46	1.33
17	B	839	CLA	O2A-CGA	4.47	1.46	1.33
17	B	836	CLA	OBD-CAD	4.46	1.28	1.22
17	b	816	CLA	O2A-CGA	4.46	1.46	1.33
17	l	202	CLA	O2A-CGA	4.46	1.46	1.33
17	a	843	CLA	OBD-CAD	4.46	1.28	1.22
17	a	829	CLA	OBD-CAD	4.46	1.28	1.22
17	A	813	CLA	O2A-CGA	4.46	1.46	1.33
17	B	838	CLA	OBD-CAD	4.46	1.28	1.22
17	B	815	CLA	O2A-CGA	4.45	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	828	CLA	O2A-CGA	4.45	1.46	1.33
26	4	607	CHL	OBD-CAD	4.45	1.28	1.22
17	a	812	CLA	O2A-CGA	4.45	1.46	1.33
17	A	829	CLA	OBD-CAD	4.45	1.28	1.22
17	A	828	CLA	OBD-CAD	4.44	1.28	1.22
17	A	839	CLA	OBD-CAD	4.44	1.28	1.22
17	b	807	CLA	O2A-CGA	4.43	1.46	1.33
17	b	824	CLA	O2A-CGA	4.43	1.46	1.33
17	a	843	CLA	O2A-CGA	4.42	1.46	1.33
17	A	823	CLA	O2A-CGA	4.42	1.46	1.33
17	a	840	CLA	O2A-CGA	4.42	1.46	1.33
17	a	838	CLA	O2A-CGA	4.42	1.46	1.33
17	A	822	CLA	O2A-CGA	4.42	1.46	1.33
17	2	608	CLA	O2A-CGA	4.42	1.46	1.33
17	b	806	CLA	OBD-CAD	4.41	1.28	1.22
17	B	812	CLA	O2A-CGA	4.41	1.46	1.33
17	b	814	CLA	O2A-CGA	4.41	1.46	1.33
17	A	842	CLA	O2A-CGA	4.41	1.46	1.33
17	b	825	CLA	O2A-CGA	4.41	1.46	1.33
17	9	611	CLA	O2A-CGA	4.41	1.46	1.33
17	8	305	CLA	O2A-CGA	4.41	1.46	1.33
17	b	808	CLA	O2A-CGA	4.40	1.46	1.33
17	b	806	CLA	O2A-CGA	4.40	1.46	1.33
17	B	829	CLA	O2A-CGA	4.40	1.46	1.33
17	B	808	CLA	O2A-CGA	4.40	1.46	1.33
17	1	310	CLA	O2A-CGA	4.40	1.46	1.33
17	A	807	CLA	O2A-CGA	4.40	1.46	1.33
17	a	820	CLA	O2A-CGA	4.40	1.46	1.33
17	a	839	CLA	O2A-CGA	4.40	1.46	1.33
17	A	839	CLA	O2A-CGA	4.40	1.46	1.33
17	A	840	CLA	O2A-CGA	4.40	1.46	1.33
17	9	603	CLA	OBD-CAD	4.40	1.28	1.22
17	a	816	CLA	O2A-CGA	4.40	1.46	1.33
17	B	837	CLA	O2A-CGA	4.40	1.46	1.33
17	2	602	CLA	O2A-CGA	4.39	1.46	1.33
17	4	610	CLA	O2A-CGA	4.39	1.46	1.33
17	A	825	CLA	O2A-CGA	4.39	1.46	1.33
17	L	202	CLA	O2A-CGA	4.39	1.46	1.33
17	L	204	CLA	O2A-CGA	4.39	1.46	1.33
17	b	836	CLA	O2A-CGA	4.39	1.46	1.33
17	2	609	CLA	O2A-CGA	4.39	1.46	1.33
17	B	836	CLA	O2A-CGA	4.39	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	816	CLA	O2A-CGA	4.39	1.46	1.33
17	3	312	CLA	O2A-CGA	4.39	1.46	1.33
17	A	824	CLA	O2A-CGA	4.38	1.46	1.33
17	8	302	CLA	O2A-CGA	4.38	1.46	1.33
17	b	815	CLA	O2A-CGA	4.38	1.46	1.33
26	2	607	CHL	OBD-CAD	4.38	1.28	1.22
17	8	308	CLA	O2A-CGA	4.38	1.46	1.33
17	b	820	CLA	O2A-CGA	4.38	1.46	1.33
17	3	306	CLA	O2A-CGA	4.38	1.46	1.33
17	a	803	CLA	O2A-CGA	4.38	1.46	1.33
17	a	835	CLA	O2A-CGA	4.38	1.46	1.33
17	b	812	CLA	O2A-CGA	4.37	1.46	1.33
17	b	828	CLA	O2A-CGA	4.37	1.46	1.33
17	A	818	CLA	O2A-CGA	4.37	1.46	1.33
17	4	608	CLA	O2A-CGA	4.37	1.46	1.33
17	4	602	CLA	O2A-CGA	4.37	1.46	1.33
17	7	604	CLA	O2A-CGA	4.37	1.46	1.33
17	b	822	CLA	O2A-CGA	4.37	1.46	1.33
17	A	841	CLA	O2A-CGA	4.37	1.46	1.33
17	2	612	CLA	O2A-CGA	4.37	1.46	1.33
17	a	813	CLA	O2A-CGA	4.37	1.46	1.33
17	B	817	CLA	OBD-CAD	4.37	1.28	1.22
17	B	832	CLA	O2A-CGA	4.37	1.46	1.33
17	2	603	CLA	O2A-CGA	4.36	1.46	1.33
17	b	838	CLA	O2A-CGA	4.36	1.46	1.33
17	G	103	CLA	O2A-CGA	4.36	1.46	1.33
17	B	833	CLA	O2A-CGA	4.36	1.46	1.33
17	8	309	CLA	O2A-CGA	4.36	1.46	1.33
17	A	845	CLA	O2A-CGA	4.36	1.46	1.33
17	A	808	CLA	O2A-CGA	4.36	1.46	1.33
17	a	823	CLA	O2A-CGA	4.36	1.46	1.33
17	A	828	CLA	O2A-CGA	4.36	1.46	1.33
17	4	604	CLA	O2A-CGA	4.36	1.46	1.33
17	A	816	CLA	O2A-CGA	4.36	1.46	1.33
17	9	614	CLA	O2A-CGA	4.36	1.46	1.33
17	A	820	CLA	O2A-CGA	4.35	1.46	1.33
17	6	306	CLA	O2A-CGA	4.35	1.46	1.33
17	a	836	CLA	O2A-CGA	4.35	1.46	1.33
17	8	310	CLA	O2A-CGA	4.35	1.46	1.33
17	b	837	CLA	O2A-CGA	4.35	1.46	1.33
17	b	833	CLA	O2A-CGA	4.35	1.46	1.33
17	9	609	CLA	O2A-CGA	4.35	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	809	CLA	O2A-CGA	4.35	1.46	1.33
17	2	604	CLA	O2A-CGA	4.35	1.46	1.33
17	B	811	CLA	O2A-CGA	4.35	1.46	1.33
17	1	306	CLA	O2A-CGA	4.34	1.46	1.33
17	B	826	CLA	O2A-CGA	4.34	1.46	1.33
17	A	835	CLA	O2A-CGA	4.34	1.46	1.33
17	3	303	CLA	O2A-CGA	4.34	1.46	1.33
17	3	309	CLA	O2A-CGA	4.34	1.46	1.33
17	6	311	CLA	O2A-CGA	4.34	1.46	1.33
17	4	609	CLA	O2A-CGA	4.34	1.46	1.33
17	a	808	CLA	O2A-CGA	4.34	1.46	1.33
17	4	612	CLA	O2A-CGA	4.33	1.46	1.33
17	7	602	CLA	O2A-CGA	4.33	1.46	1.33
17	8	301	CLA	O2A-CGA	4.33	1.46	1.33
17	1	309	CLA	O2A-CGA	4.33	1.46	1.33
17	A	805	CLA	O2A-CGA	4.33	1.46	1.33
17	6	310	CLA	O2A-CGA	4.33	1.46	1.33
17	f	7003	CLA	O2A-CGA	4.33	1.46	1.33
17	a	825	CLA	O2A-CGA	4.33	1.46	1.33
17	A	819	CLA	O2A-CGA	4.33	1.46	1.33
17	b	819	CLA	O2A-CGA	4.33	1.46	1.33
17	6	304	CLA	O2A-CGA	4.33	1.46	1.33
17	F	304	CLA	O2A-CGA	4.33	1.46	1.33
17	L	203	CLA	O2A-CGA	4.33	1.46	1.33
17	A	838	CLA	O2A-CGA	4.32	1.46	1.33
17	F	301	CLA	O2A-CGA	4.32	1.46	1.33
17	6	313	CLA	O2A-CGA	4.32	1.46	1.33
17	B	840	CLA	O2A-CGA	4.32	1.46	1.33
17	B	807	CLA	O2A-CGA	4.32	1.46	1.33
17	7	609	CLA	O2A-CGA	4.32	1.46	1.33
17	b	811	CLA	O2A-CGA	4.32	1.46	1.33
17	7	612	CLA	O2A-CGA	4.32	1.46	1.33
17	A	854	CLA	O2A-CGA	4.32	1.46	1.33
17	l	203	CLA	O2A-CGA	4.32	1.46	1.33
17	a	819	CLA	O2A-CGA	4.32	1.46	1.33
17	a	824	CLA	O2A-CGA	4.31	1.45	1.33
17	b	817	CLA	O2A-CGA	4.31	1.45	1.33
17	4	611	CLA	O2A-CGA	4.31	1.45	1.33
17	a	805	CLA	O2A-CGA	4.31	1.45	1.33
17	B	814	CLA	O2A-CGA	4.31	1.45	1.33
17	1	314	CLA	O2A-CGA	4.31	1.45	1.33
26	1	307	CHL	O2A-CGA	4.31	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	311	CLA	O2A-CGA	4.31	1.45	1.33
17	a	832	CLA	O2A-CGA	4.31	1.45	1.33
17	a	846	CLA	O2A-CGA	4.31	1.45	1.33
17	7	603	CLA	O2A-CGA	4.31	1.45	1.33
17	b	831	CLA	O2A-CGA	4.31	1.45	1.33
17	1	305	CLA	O2A-CGA	4.31	1.45	1.33
17	B	830	CLA	O2A-CGA	4.31	1.45	1.33
17	B	824	CLA	O2A-CGA	4.30	1.45	1.33
17	A	802	CLA	O2A-CGA	4.30	1.45	1.33
17	7	611	CLA	O2A-CGA	4.30	1.45	1.33
17	7	608	CLA	O2A-CGA	4.30	1.45	1.33
17	B	834	CLA	O2A-CGA	4.30	1.45	1.33
17	2	603	CLA	OBD-CAD	4.30	1.28	1.22
26	2	606	CHL	O2A-CGA	4.30	1.45	1.33
17	B	820	CLA	O2A-CGA	4.30	1.45	1.33
17	B	806	CLA	OBD-CAD	4.30	1.28	1.22
17	8	307	CLA	O2A-CGA	4.30	1.45	1.33
17	B	841	CLA	O2A-CGA	4.30	1.45	1.33
26	7	607	CHL	O2A-CGA	4.30	1.45	1.33
17	B	827	CLA	O2A-CGA	4.30	1.45	1.33
17	A	838	CLA	OBD-CAD	4.30	1.28	1.22
19	2	618	LHG	O8-C23	4.30	1.45	1.33
17	A	836	CLA	O2A-CGA	4.29	1.45	1.33
17	A	814	CLA	O2A-CGA	4.29	1.45	1.33
17	6	314	CLA	O2A-CGA	4.29	1.45	1.33
17	B	818	CLA	O2A-CGA	4.29	1.45	1.33
25	6	302	LMG	O8-C28	4.29	1.45	1.33
26	4	607	CHL	O2A-CGA	4.29	1.45	1.33
17	A	809	CLA	O2A-CGA	4.28	1.45	1.33
17	b	827	CLA	O2A-CGA	4.28	1.45	1.33
17	A	832	CLA	O2A-CGA	4.28	1.45	1.33
17	6	305	CLA	O2A-CGA	4.28	1.45	1.33
17	4	614	CLA	O2A-CGA	4.28	1.45	1.33
26	4	606	CHL	O2A-CGA	4.28	1.45	1.33
19	A	847	LHG	O8-C23	4.28	1.45	1.33
17	B	803	CLA	O2A-CGA	4.28	1.45	1.33
17	a	822	CLA	O2A-CGA	4.28	1.45	1.33
17	9	612	CLA	O2A-CGA	4.28	1.45	1.33
17	9	608	CLA	O2A-CGA	4.28	1.45	1.33
26	9	607	CHL	O2A-CGA	4.28	1.45	1.33
17	2	611	CLA	O2A-CGA	4.27	1.45	1.33
17	1	308	CLA	O2A-CGA	4.27	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	6	315	CLA	O2A-CGA	4.27	1.45	1.33
17	1	304	CLA	O2A-CGA	4.27	1.45	1.33
17	B	831	CLA	O2A-CGA	4.27	1.45	1.33
17	a	826	CLA	O2A-CGA	4.27	1.45	1.33
17	B	825	CLA	O2A-CGA	4.27	1.45	1.33
17	B	838	CLA	O2A-CGA	4.27	1.45	1.33
17	a	856	CLA	O2A-CGA	4.27	1.45	1.33
17	B	806	CLA	O2A-CGA	4.27	1.45	1.33
17	a	834	CLA	O2A-CGA	4.27	1.45	1.33
25	G	102	LMG	O8-C28	4.27	1.45	1.33
17	b	810	CLA	O2A-CGA	4.26	1.45	1.33
17	b	803	CLA	O2A-CGA	4.26	1.45	1.33
17	a	842	CLA	O2A-CGA	4.26	1.45	1.33
17	b	830	CLA	O2A-CGA	4.26	1.45	1.33
17	B	802	CLA	O2A-CGA	4.26	1.45	1.33
17	1	312	CLA	O2A-CGA	4.26	1.45	1.33
26	1	302	CHL	O2A-CGA	4.25	1.45	1.33
17	a	807	CLA	O2A-CGA	4.25	1.45	1.33
17	g	102	CLA	O2A-CGA	4.25	1.45	1.33
17	A	833	CLA	O2A-CGA	4.25	1.45	1.33
26	2	607	CHL	O2A-CGA	4.25	1.45	1.33
17	a	804	CLA	O2A-CGA	4.24	1.45	1.33
17	b	823	CLA	O2A-CGA	4.24	1.45	1.33
17	b	818	CLA	O2A-CGA	4.24	1.45	1.33
17	A	812	CLA	O2A-CGA	4.24	1.45	1.33
26	7	606	CHL	O2A-CGA	4.24	1.45	1.33
17	B	823	CLA	O2A-CGA	4.24	1.45	1.33
17	a	827	CLA	O2A-CGA	4.24	1.45	1.33
26	6	303	CHL	O2A-CGA	4.24	1.45	1.33
17	A	810	CLA	O2A-CGA	4.24	1.45	1.33
17	b	836	CLA	OBD-CAD	4.24	1.28	1.22
17	B	822	CLA	O2A-CGA	4.24	1.45	1.33
17	1	313	CLA	O2A-CGA	4.23	1.45	1.33
17	a	841	CLA	O2A-CGA	4.23	1.45	1.33
17	a	811	CLA	O2A-CGA	4.23	1.45	1.33
17	9	604	CLA	O2A-CGA	4.23	1.45	1.33
19	6	320	LHG	O8-C23	4.23	1.45	1.33
25	4	620	LMG	O8-C28	4.23	1.45	1.33
17	B	819	CLA	O2A-CGA	4.23	1.45	1.33
17	a	833	CLA	O2A-CGA	4.23	1.45	1.33
17	b	841	CLA	O2A-CGA	4.23	1.45	1.33
17	A	827	CLA	O2A-CGA	4.23	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	834	CLA	O2A-CGA	4.22	1.45	1.33
17	1	303	CLA	O2A-CGA	4.22	1.45	1.33
17	3	302	CLA	O2A-CGA	4.22	1.45	1.33
17	b	809	CLA	O2A-CGA	4.22	1.45	1.33
19	1	319	LHG	O8-C23	4.22	1.45	1.33
17	a	828	CLA	OBD-CAD	4.22	1.28	1.22
17	b	840	CLA	O2A-CGA	4.21	1.45	1.33
17	a	830	CLA	O2A-CGA	4.21	1.45	1.33
26	2	601	CHL	O2A-CGA	4.21	1.45	1.33
17	A	830	CLA	O2A-CGA	4.21	1.45	1.33
19	7	618	LHG	O8-C23	4.21	1.45	1.33
17	3	308	CLA	O2A-CGA	4.21	1.45	1.33
17	B	813	CLA	O2A-CGA	4.21	1.45	1.33
19	A	847	LHG	O7-C7	4.21	1.46	1.34
17	A	803	CLA	O2A-CGA	4.21	1.45	1.33
17	a	814	CLA	O2A-CGA	4.21	1.45	1.33
17	A	826	CLA	O2A-CGA	4.21	1.45	1.33
17	A	811	CLA	O2A-CGA	4.20	1.45	1.33
17	b	826	CLA	O2A-CGA	4.20	1.45	1.33
26	9	606	CHL	O2A-CGA	4.20	1.45	1.33
17	a	801	CLA	O2A-CGA	4.20	1.45	1.33
24	b	849	DGD	O1G-C1A	4.20	1.45	1.33
17	b	826	CLA	OBD-CAD	4.20	1.28	1.22
25	4	619	LMG	O8-C28	4.20	1.45	1.33
17	9	602	CLA	O2A-CGA	4.20	1.45	1.33
17	a	809	CLA	O2A-CGA	4.20	1.45	1.33
17	A	804	CLA	O2A-CGA	4.19	1.45	1.33
17	b	813	CLA	O2A-CGA	4.19	1.45	1.33
17	A	801	CLA	O2A-CGA	4.19	1.45	1.33
17	a	806	CLA	O2A-CGA	4.19	1.45	1.33
25	4	620	LMG	O7-C10	4.19	1.46	1.34
17	A	834	CLA	O2A-CGA	4.19	1.45	1.33
25	4	619	LMG	O7-C10	4.19	1.46	1.34
26	9	605	CHL	O2A-CGA	4.19	1.45	1.33
17	a	828	CLA	O2A-CGA	4.19	1.45	1.33
25	9	619	LMG	O8-C28	4.18	1.45	1.33
17	A	829	CLA	O2A-CGA	4.18	1.45	1.33
19	a	848	LHG	O8-C23	4.18	1.45	1.33
19	1	301	LHG	O7-C7	4.18	1.46	1.34
19	3	319	LHG	O8-C23	4.18	1.45	1.33
19	a	847	LHG	O7-C7	4.18	1.46	1.34
24	B	850	DGD	O2G-C1B	4.18	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	831	CLA	O2A-CGA	4.17	1.45	1.33
19	A	846	LHG	O8-C23	4.17	1.45	1.33
17	a	803	CLA	OBD-CAD	4.16	1.28	1.22
19	a	848	LHG	O7-C7	4.16	1.46	1.34
17	3	310	CLA	OBD-CAD	4.16	1.29	1.22
17	B	817	CLA	O2A-CGA	4.16	1.45	1.33
19	6	320	LHG	O7-C7	4.15	1.46	1.34
17	a	831	CLA	O2A-CGA	4.14	1.45	1.33
17	b	805	CLA	O2A-CGA	4.14	1.45	1.33
26	4	605	CHL	O2A-CGA	4.14	1.45	1.33
17	a	829	CLA	O2A-CGA	4.14	1.45	1.33
17	1	315	CLA	O2A-CGA	4.13	1.46	1.33
25	G	102	LMG	O7-C10	4.13	1.45	1.34
17	a	810	CLA	O2A-CGA	4.13	1.45	1.33
19	A	846	LHG	O7-C7	4.12	1.45	1.34
17	b	829	CLA	O2A-CGA	4.12	1.45	1.33
17	B	805	CLA	O2A-CGA	4.12	1.45	1.33
24	b	849	DGD	O2G-C1B	4.12	1.45	1.34
19	6	301	LHG	O7-C7	4.12	1.45	1.34
17	B	821	CLA	O2A-CGA	4.12	1.46	1.33
26	7	601	CHL	O2A-CGA	4.11	1.45	1.33
17	g	103	CLA	O2A-CGA	4.11	1.46	1.33
17	B	810	CLA	O2A-CGA	4.11	1.45	1.33
24	B	850	DGD	O1G-C1A	4.10	1.45	1.33
19	1	319	LHG	O7-C7	4.10	1.45	1.34
26	3	307	CHL	O2A-CGA	4.10	1.46	1.33
19	7	618	LHG	O7-C7	4.10	1.45	1.34
17	9	603	CLA	O2A-CGA	4.09	1.46	1.33
17	b	832	CLA	O2A-CGA	4.09	1.45	1.33
17	A	806	CLA	O2A-CGA	4.09	1.45	1.33
17	a	802	CLA	O2A-CGA	4.09	1.45	1.33
17	b	821	CLA	O2A-CGA	4.09	1.46	1.33
17	k	1402	CLA	O2A-CGA	4.09	1.46	1.33
17	6	309	CLA	O2A-CGA	4.08	1.46	1.33
17	6	316	CLA	O2A-CGA	4.08	1.46	1.33
17	A	843	CLA	O2A-CGA	4.08	1.45	1.33
25	6	302	LMG	O7-C10	4.07	1.45	1.34
17	k	1403	CLA	O2A-CGA	4.07	1.46	1.33
19	2	618	LHG	O7-C7	4.07	1.45	1.34
17	4	603	CLA	O2A-CGA	4.06	1.45	1.33
17	3	301	CLA	O2A-CGA	4.06	1.45	1.33
17	a	844	CLA	O2A-CGA	4.06	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	314	CLA	O2A-CGA	4.06	1.45	1.33
17	b	802	CLA	O2A-CGA	4.06	1.45	1.33
17	B	826	CLA	OBD-CAD	4.05	1.28	1.22
25	9	619	LMG	O7-C10	4.05	1.45	1.34
19	a	847	LHG	O8-C23	4.05	1.45	1.33
17	G	104	CLA	O2A-CGA	4.05	1.45	1.33
17	4	601	CLA	O2A-CGA	4.05	1.45	1.33
26	6	308	CHL	O2A-CGA	4.05	1.45	1.33
17	K	4003	CLA	O2A-CGA	4.04	1.45	1.33
17	8	312	CLA	O2A-CGA	4.02	1.45	1.33
26	8	306	CHL	O2A-CGA	4.01	1.45	1.33
17	9	601	CLA	O2A-CGA	3.98	1.45	1.33
22	j	3001	HTG	C1 ¹ -S1	-3.91	1.76	1.81
22	f	7001	HTG	C1 ¹ -S1	-3.79	1.76	1.81
22	J	3001	HTG	C1 ¹ -S1	-3.71	1.76	1.81
22	a	857	HTG	C1 ¹ -S1	-3.67	1.76	1.81
22	A	855	HTG	C1 ¹ -S1	-3.62	1.76	1.81
22	F	302	HTG	C1 ¹ -S1	-3.55	1.76	1.81
17	8	313	CLA	CHC-C1C	3.52	1.48	1.39
17	3	315	CLA	CHC-C1C	3.51	1.48	1.39
17	2	602	CLA	C1D-C2D	3.16	1.49	1.42
17	7	613	CLA	C1D-C2D	3.16	1.49	1.42
17	A	823	CLA	C1D-C2D	3.14	1.49	1.42
17	1	314	CLA	C1D-C2D	3.14	1.49	1.42
17	6	304	CLA	C1D-C2D	3.14	1.49	1.42
17	B	822	CLA	C1D-C2D	3.13	1.49	1.42
17	4	613	CLA	C1D-C2D	3.13	1.49	1.42
17	b	830	CLA	C1D-C2D	3.12	1.49	1.42
17	a	803	CLA	C1D-C2D	3.11	1.49	1.42
17	A	845	CLA	C1D-C2D	3.11	1.49	1.42
17	A	820	CLA	C1D-C2D	3.11	1.49	1.42
17	3	301	CLA	C1D-C2D	3.10	1.49	1.42
17	B	834	CLA	C1D-C2D	3.10	1.49	1.42
17	9	604	CLA	C1D-C2D	3.10	1.49	1.42
17	g	103	CLA	C1D-C2D	3.10	1.49	1.42
17	A	811	CLA	C1D-C2D	3.10	1.49	1.42
17	7	602	CLA	C1D-C2D	3.09	1.49	1.42
17	b	837	CLA	C1D-C2D	3.09	1.49	1.42
17	f	7003	CLA	C1D-C2D	3.09	1.49	1.42
17	B	811	CLA	C1D-C2D	3.09	1.49	1.42
17	7	604	CLA	C1D-C2D	3.09	1.49	1.42
17	A	827	CLA	C1D-C2D	3.09	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	604	CLA	C1D-C2D	3.08	1.49	1.42
17	4	609	CLA	C1D-C2D	3.08	1.49	1.42
17	6	311	CLA	C1D-C2D	3.08	1.49	1.42
17	9	609	CLA	C1D-C2D	3.08	1.49	1.42
17	2	608	CLA	C1D-C2D	3.08	1.49	1.42
17	b	822	CLA	C1D-C2D	3.08	1.49	1.42
17	A	817	CLA	C1D-C2D	3.08	1.49	1.42
17	A	816	CLA	C1D-C2D	3.08	1.49	1.42
17	k	1403	CLA	C1D-C2D	3.08	1.49	1.42
17	2	604	CLA	C1D-C2D	3.08	1.49	1.42
17	b	814	CLA	C1D-C2D	3.07	1.49	1.42
17	1	305	CLA	C1D-C2D	3.07	1.49	1.42
17	8	304	CLA	C1D-C2D	3.07	1.49	1.42
17	j	3002	CLA	C1D-C2D	3.07	1.49	1.42
17	b	841	CLA	C1D-C2D	3.07	1.49	1.42
17	b	834	CLA	C1D-C2D	3.07	1.49	1.42
17	3	304	CLA	C1D-C2D	3.06	1.49	1.42
17	4	602	CLA	C1D-C2D	3.06	1.49	1.42
17	b	817	CLA	C1D-C2D	3.05	1.49	1.42
17	8	309	CLA	C1D-C2D	3.05	1.49	1.42
17	A	825	CLA	C1D-C2D	3.05	1.49	1.42
17	1	304	CLA	C1D-C2D	3.05	1.49	1.42
17	B	816	CLA	C1D-C2D	3.05	1.49	1.42
17	8	308	CLA	C1D-C2D	3.05	1.49	1.42
17	8	303	CLA	C1D-C2D	3.05	1.49	1.42
17	9	612	CLA	C1D-C2D	3.05	1.49	1.42
17	1	303	CLA	C1D-C2D	3.05	1.49	1.42
17	9	613	CLA	C1D-C2D	3.05	1.49	1.42
17	A	813	CLA	C1D-C2D	3.04	1.49	1.42
17	6	316	CLA	C1D-C2D	3.04	1.49	1.42
17	a	820	CLA	C1D-C2D	3.04	1.49	1.42
17	A	835	CLA	C1D-C2D	3.04	1.49	1.42
17	g	101	CLA	C1D-C2D	3.04	1.49	1.42
17	a	833	CLA	C1D-C2D	3.04	1.49	1.42
26	9	605	CHL	C1D-C2D	3.04	1.49	1.42
17	4	614	CLA	C1D-C2D	3.04	1.49	1.42
17	a	813	CLA	C1D-C2D	3.03	1.49	1.42
17	B	830	CLA	C1D-C2D	3.03	1.49	1.42
17	a	818	CLA	C1D-C2D	3.03	1.49	1.42
17	J	3002	CLA	C1D-C2D	3.03	1.49	1.42
17	B	803	CLA	C1D-C2D	3.03	1.49	1.42
17	a	846	CLA	C1D-C2D	3.03	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	835	CLA	C1D-C2D	3.03	1.49	1.42
17	K	4002	CLA	C1D-C2D	3.03	1.49	1.42
17	a	811	CLA	C1D-C2D	3.03	1.49	1.42
17	B	812	CLA	C1D-C2D	3.03	1.49	1.42
17	k	1402	CLA	C1D-C2D	3.03	1.49	1.42
17	3	302	CLA	C1D-C2D	3.03	1.49	1.42
17	3	311	CLA	C1D-C2D	3.03	1.49	1.42
17	7	608	CLA	C1D-C2D	3.02	1.49	1.42
17	B	807	CLA	C1D-C2D	3.02	1.49	1.42
17	F	304	CLA	C1D-C2D	3.02	1.49	1.42
17	1	313	CLA	C1D-C2D	3.02	1.49	1.42
17	2	613	CLA	C1D-C2D	3.02	1.49	1.42
17	G	104	CLA	C1D-C2D	3.02	1.49	1.42
17	A	815	CLA	C1D-C2D	3.02	1.49	1.42
17	a	834	CLA	C1D-C2D	3.02	1.49	1.42
17	3	313	CLA	C1D-C2D	3.02	1.49	1.42
17	b	807	CLA	C1D-C2D	3.02	1.49	1.42
17	9	611	CLA	C1D-C2D	3.02	1.49	1.42
17	8	301	CLA	C1D-C2D	3.02	1.49	1.42
17	3	310	CLA	C1D-C2D	3.01	1.49	1.42
17	B	805	CLA	C1D-C2D	3.01	1.49	1.42
17	a	817	CLA	C1D-C2D	3.01	1.49	1.42
17	A	833	CLA	C1D-C2D	3.01	1.49	1.42
17	1	306	CLA	C1D-C2D	3.01	1.49	1.42
26	2	605	CHL	C1D-C2D	3.01	1.49	1.42
17	6	305	CLA	C1D-C2D	3.01	1.49	1.42
17	A	843	CLA	C1D-C2D	3.01	1.49	1.42
26	4	605	CHL	C1D-C2D	3.01	1.49	1.42
17	6	306	CLA	C1D-C2D	3.01	1.49	1.42
17	B	840	CLA	C1D-C2D	3.01	1.49	1.42
17	B	837	CLA	C1D-C2D	3.01	1.49	1.42
17	B	806	CLA	C1D-C2D	3.01	1.49	1.42
17	8	311	CLA	C1D-C2D	3.01	1.49	1.42
17	9	614	CLA	C1D-C2D	3.01	1.49	1.42
17	B	817	CLA	C1D-C2D	3.01	1.49	1.42
17	6	315	CLA	C1D-C2D	3.01	1.49	1.42
17	G	101	CLA	C1D-C2D	3.00	1.49	1.42
17	g	102	CLA	C1D-C2D	3.00	1.49	1.42
17	L	202	CLA	C1D-C2D	3.00	1.49	1.42
17	1	308	CLA	C1D-C2D	3.00	1.49	1.42
17	6	307	CLA	C1D-C2D	3.00	1.49	1.42
17	a	815	CLA	C1D-C2D	3.00	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	821	CLA	C1D-C2D	3.00	1.49	1.42
17	b	832	CLA	C1D-C2D	3.00	1.49	1.42
17	a	812	CLA	C1D-C2D	3.00	1.49	1.42
17	1	310	CLA	C1D-C2D	3.00	1.49	1.42
17	b	805	CLA	C1D-C2D	3.00	1.49	1.42
17	3	303	CLA	C1D-C2D	3.00	1.49	1.42
17	2	612	CLA	C1D-C2D	3.00	1.49	1.42
17	7	610	CLA	C1D-C2D	3.00	1.49	1.42
17	A	837	CLA	C1D-C2D	3.00	1.49	1.42
17	2	610	CLA	C1D-C2D	3.00	1.49	1.42
17	8	310	CLA	C1D-C2D	2.99	1.49	1.42
17	3	305	CLA	C1D-C2D	2.99	1.49	1.42
17	A	834	CLA	C1D-C2D	2.99	1.49	1.42
17	6	309	CLA	C1D-C2D	2.99	1.49	1.42
17	2	603	CLA	C1D-C2D	2.99	1.49	1.42
17	A	842	CLA	C1D-C2D	2.99	1.49	1.42
17	G	103	CLA	C1D-C2D	2.99	1.49	1.42
17	L	204	CLA	C1D-C2D	2.99	1.49	1.42
17	9	601	CLA	C1D-C2D	2.99	1.49	1.42
26	4	606	CHL	C1D-C2D	2.99	1.49	1.42
17	B	835	CLA	C1D-C2D	2.99	1.49	1.42
17	b	818	CLA	C1D-C2D	2.99	1.49	1.42
17	2	609	CLA	C1D-C2D	2.99	1.49	1.42
26	6	303	CHL	C1D-C2D	2.99	1.49	1.42
17	8	305	CLA	C1D-C2D	2.99	1.49	1.42
17	9	603	CLA	C1D-C2D	2.99	1.49	1.42
17	a	805	CLA	C1D-C2D	2.99	1.49	1.42
17	b	831	CLA	C1D-C2D	2.98	1.49	1.42
17	8	312	CLA	C1D-C2D	2.98	1.49	1.42
17	a	837	CLA	C1D-C2D	2.98	1.49	1.42
17	7	612	CLA	C1D-C2D	2.98	1.49	1.42
17	B	819	CLA	C1D-C2D	2.98	1.49	1.42
17	4	612	CLA	C1D-C2D	2.98	1.49	1.42
17	a	804	CLA	C1D-C2D	2.98	1.49	1.42
17	B	841	CLA	C1D-C2D	2.98	1.49	1.42
17	L	203	CLA	C1D-C2D	2.98	1.49	1.42
17	B	839	CLA	C1D-C2D	2.98	1.49	1.42
17	K	4003	CLA	C1D-C2D	2.98	1.49	1.42
17	B	827	CLA	C1D-C2D	2.97	1.49	1.42
17	9	602	CLA	C1D-C2D	2.97	1.49	1.42
17	B	820	CLA	C1D-C2D	2.97	1.49	1.42
17	b	816	CLA	C1D-C2D	2.97	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	819	CLA	C1D-C2D	2.97	1.49	1.42
17	a	835	CLA	C1D-C2D	2.97	1.49	1.42
17	B	821	CLA	C1D-C2D	2.97	1.49	1.42
17	A	824	CLA	C1D-C2D	2.97	1.49	1.42
17	A	832	CLA	C1D-C2D	2.96	1.49	1.42
17	B	804	CLA	C1D-C2D	2.96	1.49	1.42
26	9	615	CHL	C1D-C2D	2.96	1.49	1.42
17	B	810	CLA	C1D-C2D	2.96	1.49	1.42
17	4	601	CLA	C1D-C2D	2.96	1.49	1.42
17	A	804	CLA	C1D-C2D	2.96	1.49	1.42
17	A	808	CLA	C1D-C2D	2.96	1.49	1.42
17	l	202	CLA	C1D-C2D	2.96	1.49	1.42
17	A	805	CLA	C1D-C2D	2.95	1.49	1.42
17	A	806	CLA	C1D-C2D	2.95	1.49	1.42
17	3	312	CLA	C1D-C2D	2.95	1.49	1.42
17	3	314	CLA	C1D-C2D	2.95	1.49	1.42
17	k	1401	CLA	C1D-C2D	2.95	1.49	1.42
17	b	813	CLA	C1D-C2D	2.95	1.49	1.42
17	B	831	CLA	C1D-C2D	2.95	1.49	1.42
26	7	605	CHL	C1D-C2D	2.95	1.49	1.42
17	a	832	CLA	C1D-C2D	2.95	1.49	1.42
17	1	312	CLA	C1D-C2D	2.94	1.49	1.42
17	3	308	CLA	C1D-C2D	2.94	1.49	1.42
17	4	611	CLA	C1D-C2D	2.94	1.49	1.42
17	a	840	CLA	C1D-C2D	2.94	1.49	1.42
17	a	841	CLA	C1D-C2D	2.94	1.49	1.42
17	b	838	CLA	C1D-C2D	2.94	1.49	1.42
17	A	822	CLA	C1D-C2D	2.94	1.49	1.42
17	4	610	CLA	C1D-C2D	2.94	1.49	1.42
17	8	302	CLA	C1D-C2D	2.94	1.49	1.42
17	3	306	CLA	C1D-C2D	2.94	1.49	1.42
26	2	614	CHL	C1D-C2D	2.94	1.49	1.42
17	b	812	CLA	C1D-C2D	2.94	1.49	1.42
17	a	823	CLA	C1D-C2D	2.94	1.49	1.42
17	9	610	CLA	C1D-C2D	2.94	1.49	1.42
17	1	309	CLA	C1D-C2D	2.94	1.49	1.42
17	B	829	CLA	C1D-C2D	2.94	1.49	1.42
26	6	308	CHL	C1D-C2D	2.93	1.49	1.42
17	a	816	CLA	C1D-C2D	2.93	1.49	1.42
17	A	812	CLA	C1D-C2D	2.93	1.49	1.42
17	b	811	CLA	C1D-C2D	2.93	1.49	1.42
26	7	614	CHL	C1D-C2D	2.93	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	7	609	CLA	C1D-C2D	2.93	1.49	1.42
17	a	808	CLA	C1D-C2D	2.93	1.49	1.42
17	A	809	CLA	C1D-C2D	2.93	1.49	1.42
17	b	806	CLA	C1D-C2D	2.93	1.49	1.42
17	3	309	CLA	C1D-C2D	2.92	1.49	1.42
17	6	313	CLA	C1D-C2D	2.92	1.49	1.42
17	b	802	CLA	C1D-C2D	2.92	1.49	1.42
26	3	307	CHL	C1D-C2D	2.92	1.49	1.42
17	7	603	CLA	C1D-C2D	2.92	1.49	1.42
17	a	819	CLA	C1D-C2D	2.92	1.49	1.42
26	7	601	CHL	C1D-C2D	2.92	1.49	1.42
26	7	607	CHL	C1D-C2D	2.92	1.49	1.42
17	2	611	CLA	C1D-C2D	2.92	1.49	1.42
17	b	808	CLA	C1D-C2D	2.91	1.49	1.42
17	1	311	CLA	C1D-C2D	2.91	1.49	1.42
17	B	838	CLA	C1D-C2D	2.91	1.49	1.42
17	a	809	CLA	C1D-C2D	2.91	1.49	1.42
17	a	824	CLA	C1D-C2D	2.91	1.49	1.42
17	A	814	CLA	C1D-C2D	2.91	1.49	1.42
26	2	601	CHL	C1D-C2D	2.91	1.49	1.42
17	B	833	CLA	C1D-C2D	2.91	1.49	1.42
26	8	306	CHL	C1D-C2D	2.91	1.49	1.42
17	1	315	CLA	C1D-C2D	2.91	1.49	1.42
17	A	821	CLA	C1D-C2D	2.90	1.49	1.42
26	9	607	CHL	C1D-C2D	2.90	1.49	1.42
17	b	823	CLA	C1D-C2D	2.90	1.49	1.42
17	l	204	CLA	C1D-C2D	2.90	1.49	1.42
17	a	825	CLA	C1D-C2D	2.90	1.49	1.42
26	4	615	CHL	C1D-C2D	2.90	1.49	1.42
17	a	822	CLA	C1D-C2D	2.90	1.49	1.42
17	A	840	CLA	C1D-C2D	2.90	1.49	1.42
17	b	829	CLA	C1D-C2D	2.90	1.49	1.42
17	B	809	CLA	C1D-C2D	2.90	1.49	1.42
17	a	829	CLA	C1D-C2D	2.89	1.49	1.42
17	B	813	CLA	C1D-C2D	2.89	1.49	1.42
17	B	814	CLA	C1D-C2D	2.89	1.49	1.42
17	7	611	CLA	C1D-C2D	2.89	1.49	1.42
17	a	826	CLA	C1D-C2D	2.89	1.49	1.42
17	B	828	CLA	C1D-C2D	2.89	1.49	1.42
17	A	819	CLA	C1D-C2D	2.89	1.49	1.42
17	b	839	CLA	C1D-C2D	2.89	1.49	1.42
17	A	803	CLA	C1D-C2D	2.88	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	820	CLA	C1D-C2D	2.88	1.49	1.42
17	6	312	CLA	C1D-C2D	2.88	1.49	1.42
17	A	838	CLA	C1D-C2D	2.87	1.49	1.42
17	b	804	CLA	C1D-C2D	2.87	1.49	1.42
17	a	827	CLA	C1D-C2D	2.87	1.49	1.42
17	F	301	CLA	C1D-C2D	2.87	1.49	1.42
17	b	833	CLA	C1D-C2D	2.87	1.49	1.42
17	B	818	CLA	C1D-C2D	2.87	1.49	1.42
17	F	303	CLA	C1D-C2D	2.87	1.49	1.42
17	b	824	CLA	C1D-C2D	2.87	1.49	1.42
26	7	606	CHL	C1D-C2D	2.87	1.49	1.42
17	B	836	CLA	C1D-C2D	2.86	1.49	1.42
17	A	807	CLA	C1D-C2D	2.86	1.49	1.42
26	2	606	CHL	C1D-C2D	2.86	1.49	1.42
17	8	307	CLA	C1D-C2D	2.86	1.49	1.42
17	a	814	CLA	C1D-C2D	2.86	1.49	1.42
17	A	829	CLA	C1D-C2D	2.86	1.49	1.42
17	6	314	CLA	C1D-C2D	2.86	1.49	1.42
17	a	810	CLA	C1D-C2D	2.86	1.49	1.42
17	A	818	CLA	C1D-C2D	2.86	1.49	1.42
26	1	307	CHL	C1D-C2D	2.85	1.49	1.42
17	b	810	CLA	C1D-C2D	2.85	1.49	1.42
17	a	843	CLA	C1D-C2D	2.85	1.49	1.42
17	b	825	CLA	C1D-C2D	2.85	1.49	1.42
17	B	808	CLA	C1D-C2D	2.84	1.49	1.42
17	A	839	CLA	C1D-C2D	2.84	1.49	1.42
26	9	606	CHL	C1D-C2D	2.84	1.49	1.42
17	B	802	CLA	C1D-C2D	2.84	1.49	1.42
17	a	831	CLA	C1D-C2D	2.84	1.49	1.42
17	b	809	CLA	C1D-C2D	2.84	1.49	1.42
26	1	302	CHL	C1D-C2D	2.83	1.49	1.42
17	6	310	CLA	C1D-C2D	2.83	1.49	1.42
17	4	603	CLA	C1D-C2D	2.83	1.49	1.42
17	B	832	CLA	C1D-C2D	2.83	1.49	1.42
17	B	824	CLA	C1D-C2D	2.82	1.49	1.42
17	a	836	CLA	C1D-C2D	2.82	1.49	1.42
17	a	806	CLA	C1D-C2D	2.82	1.48	1.42
17	f	7002	CLA	C1D-C2D	2.82	1.48	1.42
26	4	607	CHL	C1D-C2D	2.81	1.48	1.42
17	A	841	CLA	C1D-C2D	2.81	1.48	1.42
17	a	844	CLA	C1D-C2D	2.81	1.48	1.42
26	7	601	CHL	MG-NA	-2.80	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	l	203	CLA	C1D-C2D	2.80	1.48	1.42
17	a	839	CLA	C1D-C2D	2.80	1.48	1.42
17	A	828	CLA	C1D-C2D	2.80	1.48	1.42
26	2	607	CHL	C1D-C2D	2.79	1.48	1.42
17	A	831	CLA	C1D-C2D	2.79	1.48	1.42
17	b	828	CLA	C1D-C2D	2.78	1.48	1.42
17	a	802	CLA	C1D-C2D	2.78	1.48	1.42
17	b	840	CLA	C1D-C2D	2.78	1.48	1.42
17	b	826	CLA	C1D-C2D	2.78	1.48	1.42
17	a	821	CLA	C1D-C2D	2.78	1.48	1.42
17	B	815	CLA	C1D-C2D	2.78	1.48	1.42
17	b	815	CLA	C1D-C2D	2.78	1.48	1.42
17	B	825	CLA	C1D-C2D	2.77	1.48	1.42
17	a	838	CLA	C1C-C2C	2.77	1.49	1.44
17	A	826	CLA	C1D-C2D	2.76	1.48	1.42
17	2	602	CLA	CHD-C4C	2.76	1.49	1.41
17	b	836	CLA	C1D-C2D	2.76	1.48	1.42
17	A	802	CLA	C1D-C2D	2.76	1.48	1.42
17	A	836	CLA	C1D-C2D	2.76	1.48	1.42
17	A	831	CLA	C4C-C3C	2.76	1.49	1.45
17	a	807	CLA	C1D-C2D	2.75	1.48	1.42
17	b	827	CLA	C1D-C2D	2.75	1.48	1.42
17	8	313	CLA	CHA-C1A	2.75	1.49	1.41
17	a	842	CLA	C1D-C2D	2.75	1.48	1.42
17	a	813	CLA	CHD-C4C	2.74	1.49	1.41
17	4	608	CLA	C1D-C2D	2.74	1.48	1.42
17	A	830	CLA	C1D-C2D	2.74	1.48	1.42
17	a	856	CLA	C1D-C2D	2.74	1.48	1.42
17	B	834	CLA	CHD-C4C	2.73	1.49	1.41
17	A	831	CLA	CHD-C4C	2.73	1.49	1.41
17	3	315	CLA	CHD-C4C	2.73	1.48	1.41
17	7	604	CLA	CHD-C4C	2.73	1.48	1.41
17	b	821	CLA	CHD-C4C	2.73	1.48	1.41
17	B	829	CLA	CHD-C4C	2.73	1.48	1.41
17	8	313	CLA	CHD-C4C	2.73	1.48	1.41
17	6	304	CLA	CHD-C4C	2.73	1.48	1.41
17	4	602	CLA	CHD-C4C	2.72	1.48	1.41
17	A	824	CLA	C4C-C3C	2.72	1.49	1.45
17	a	834	CLA	CHD-C4C	2.72	1.48	1.41
17	k	1403	CLA	CHD-C4C	2.72	1.48	1.41
17	B	822	CLA	CHD-C4C	2.72	1.48	1.41
17	3	315	CLA	CHA-C1A	2.72	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	8	308	CLA	CHD-C4C	2.72	1.48	1.41
17	9	613	CLA	CHD-C4C	2.72	1.48	1.41
17	8	313	CLA	C3C-C4C	2.72	1.49	1.43
17	9	604	CLA	CHD-C4C	2.72	1.48	1.41
17	A	801	CLA	C1D-C2D	2.72	1.48	1.42
17	9	609	CLA	CHD-C4C	2.72	1.48	1.41
17	a	803	CLA	C4C-C3C	2.71	1.49	1.45
17	B	826	CLA	C1D-C2D	2.71	1.48	1.42
17	3	315	CLA	C3C-C4C	2.71	1.49	1.43
17	a	828	CLA	C1D-C2D	2.71	1.48	1.42
17	A	817	CLA	CHD-C4C	2.71	1.48	1.41
17	b	837	CLA	CHD-C4C	2.71	1.48	1.41
17	a	838	CLA	C1D-C2D	2.71	1.48	1.42
17	9	608	CLA	C1D-C2D	2.70	1.48	1.42
17	L	204	CLA	CHD-C4C	2.70	1.48	1.41
17	b	817	CLA	CHD-C4C	2.70	1.48	1.41
17	f	7003	CLA	CHD-C4C	2.70	1.48	1.41
17	b	803	CLA	C1D-C2D	2.70	1.48	1.42
17	2	604	CLA	CHD-C4C	2.70	1.48	1.41
17	B	810	CLA	CHD-C4C	2.70	1.48	1.41
17	a	812	CLA	CHD-C4C	2.70	1.48	1.41
17	a	820	CLA	CHD-C4C	2.69	1.48	1.41
17	a	807	CLA	C1C-C2C	2.69	1.49	1.44
17	g	103	CLA	CHD-C4C	2.69	1.48	1.41
17	2	613	CLA	CHD-C4C	2.69	1.48	1.41
17	3	301	CLA	CHD-C4C	2.69	1.48	1.41
17	1	314	CLA	CHD-C4C	2.69	1.48	1.41
17	a	822	CLA	CHD-C4C	2.69	1.48	1.41
17	a	801	CLA	C1D-C2D	2.69	1.48	1.42
17	a	846	CLA	CHD-C4C	2.69	1.48	1.41
17	B	834	CLA	C4C-C3C	2.68	1.49	1.45
17	b	819	CLA	CHD-C4C	2.68	1.48	1.41
17	b	813	CLA	C4C-C3C	2.68	1.49	1.45
17	3	308	CLA	CHD-C4C	2.68	1.48	1.41
17	B	820	CLA	CHD-C4C	2.68	1.48	1.41
17	8	309	CLA	CHD-C4C	2.68	1.48	1.41
17	F	304	CLA	CHD-C4C	2.68	1.48	1.41
17	3	310	CLA	CHD-C4C	2.68	1.48	1.41
17	B	823	CLA	C1D-C2D	2.68	1.48	1.42
17	A	823	CLA	CHD-C4C	2.68	1.48	1.41
17	A	835	CLA	CHD-C4C	2.68	1.48	1.41
17	b	816	CLA	CHD-C4C	2.67	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	803	CLA	CHD-C4C	2.67	1.48	1.41
17	8	311	CLA	CHD-C4C	2.67	1.48	1.41
17	4	613	CLA	CHD-C4C	2.67	1.48	1.41
17	B	821	CLA	CHD-C4C	2.67	1.48	1.41
17	2	612	CLA	CHD-C4C	2.67	1.48	1.41
17	3	312	CLA	CHD-C4C	2.67	1.48	1.41
17	k	1403	CLA	C4C-C3C	2.67	1.49	1.45
17	8	303	CLA	CHD-C4C	2.67	1.48	1.41
17	b	805	CLA	CHD-C4C	2.67	1.48	1.41
17	B	819	CLA	CHD-C4C	2.67	1.48	1.41
17	3	305	CLA	CHD-C4C	2.67	1.48	1.41
17	8	312	CLA	CHD-C4C	2.67	1.48	1.41
17	A	814	CLA	CHD-C4C	2.67	1.48	1.41
17	7	609	CLA	CHD-C4C	2.67	1.48	1.41
17	A	816	CLA	CHD-C4C	2.66	1.48	1.41
17	A	802	CLA	CHD-C4C	2.66	1.48	1.41
17	7	613	CLA	CHD-C4C	2.66	1.48	1.41
17	A	813	CLA	CHD-C4C	2.66	1.48	1.41
17	A	842	CLA	CHD-C4C	2.66	1.48	1.41
17	A	843	CLA	CHD-C4C	2.66	1.48	1.41
17	b	822	CLA	CHD-C4C	2.66	1.48	1.41
17	7	608	CLA	CHD-C4C	2.66	1.48	1.41
17	2	609	CLA	CHD-C4C	2.66	1.48	1.41
17	a	818	CLA	CHD-C4C	2.66	1.48	1.41
17	1	305	CLA	CHD-C4C	2.66	1.48	1.41
17	L	202	CLA	CHD-C4C	2.66	1.48	1.41
17	J	3002	CLA	CHD-C4C	2.66	1.48	1.41
17	1	308	CLA	CHD-C4C	2.66	1.48	1.41
17	6	315	CLA	CHD-C4C	2.66	1.48	1.41
17	A	833	CLA	CHD-C4C	2.66	1.48	1.41
17	b	841	CLA	CHD-C4C	2.66	1.48	1.41
17	a	837	CLA	CHD-C4C	2.66	1.48	1.41
17	9	612	CLA	CHD-C4C	2.66	1.48	1.41
17	2	610	CLA	CHD-C4C	2.66	1.48	1.41
17	B	816	CLA	CHD-C4C	2.66	1.48	1.41
17	A	811	CLA	CHD-C4C	2.65	1.48	1.41
17	a	813	CLA	C4C-C3C	2.65	1.49	1.45
17	A	845	CLA	CHD-C4C	2.65	1.48	1.41
17	j	3002	CLA	CHD-C4C	2.65	1.48	1.41
17	a	805	CLA	CHD-C4C	2.65	1.48	1.41
17	8	304	CLA	CHD-C4C	2.65	1.48	1.41
17	3	302	CLA	CHD-C4C	2.65	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	303	CLA	CHD-C4C	2.65	1.48	1.41
17	K	4003	CLA	CHD-C4C	2.65	1.48	1.41
17	7	610	CLA	CHD-C4C	2.65	1.48	1.41
17	6	309	CLA	CHD-C4C	2.65	1.48	1.41
17	k	1402	CLA	CHD-C4C	2.65	1.48	1.41
17	a	811	CLA	CHD-C4C	2.65	1.48	1.41
17	8	301	CLA	CHD-C4C	2.65	1.48	1.41
17	3	314	CLA	CHD-C4C	2.65	1.48	1.41
17	B	835	CLA	CHD-C4C	2.65	1.48	1.41
17	B	803	CLA	CHD-C4C	2.65	1.48	1.41
17	A	834	CLA	CHD-C4C	2.65	1.48	1.41
17	A	814	CLA	C4C-C3C	2.65	1.49	1.45
17	A	854	CLA	C1D-C2D	2.65	1.48	1.42
17	1	311	CLA	CHD-C4C	2.65	1.48	1.41
17	3	304	CLA	CHD-C4C	2.65	1.48	1.41
22	j	3001	HTG	C1-S1	-2.65	1.76	1.80
17	B	841	CLA	CHD-C4C	2.65	1.48	1.41
17	3	309	CLA	CHD-C4C	2.65	1.48	1.41
17	A	837	CLA	CHD-C4C	2.65	1.48	1.41
17	A	826	CLA	C1C-C2C	2.65	1.49	1.44
17	4	604	CLA	CHD-C4C	2.64	1.48	1.41
17	6	311	CLA	CHD-C4C	2.64	1.48	1.41
17	b	806	CLA	CHD-C4C	2.64	1.48	1.41
17	a	823	CLA	CHD-C4C	2.64	1.48	1.41
17	A	822	CLA	CHD-C4C	2.64	1.48	1.41
17	b	807	CLA	CHD-C4C	2.64	1.48	1.41
17	l	203	CLA	CHD-C4C	2.64	1.48	1.41
17	A	827	CLA	CHD-C4C	2.64	1.48	1.41
17	6	316	CLA	CHD-C4C	2.64	1.48	1.41
17	A	824	CLA	CHD-C4C	2.64	1.48	1.41
17	A	838	CLA	C1C-C2C	2.64	1.49	1.44
17	b	827	CLA	C1C-C2C	2.64	1.49	1.44
17	b	829	CLA	CHD-C4C	2.64	1.48	1.41
17	b	830	CLA	CHD-C4C	2.64	1.48	1.41
17	B	807	CLA	CHD-C4C	2.64	1.48	1.41
17	1	310	CLA	CHD-C4C	2.64	1.48	1.41
17	7	602	CLA	CHD-C4C	2.64	1.48	1.41
17	3	311	CLA	CHD-C4C	2.64	1.48	1.41
17	A	832	CLA	CHD-C4C	2.64	1.48	1.41
17	1	315	CLA	CHD-C4C	2.63	1.48	1.41
17	b	814	CLA	CHD-C4C	2.63	1.48	1.41
17	3	313	CLA	CHD-C4C	2.63	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	308	CHL	MG-NA	-2.63	2.00	2.06
17	b	835	CLA	CHD-C4C	2.63	1.48	1.41
17	A	820	CLA	CHD-C4C	2.63	1.48	1.41
17	A	840	CLA	CHD-C4C	2.63	1.48	1.41
17	a	829	CLA	C1C-C2C	2.63	1.49	1.44
17	1	313	CLA	CHD-C4C	2.63	1.48	1.41
17	a	815	CLA	CHD-C4C	2.63	1.48	1.41
17	6	307	CLA	CHD-C4C	2.63	1.48	1.41
17	B	804	CLA	CHD-C4C	2.63	1.48	1.41
17	b	829	CLA	C4C-C3C	2.63	1.49	1.45
17	k	1401	CLA	CHD-C4C	2.63	1.48	1.41
17	L	203	CLA	CHD-C4C	2.63	1.48	1.41
17	9	601	CLA	CHD-C4C	2.63	1.48	1.41
17	A	803	CLA	CHD-C4C	2.63	1.48	1.41
17	b	824	CLA	CHD-C4C	2.63	1.48	1.41
17	B	831	CLA	CHD-C4C	2.63	1.48	1.41
17	4	610	CLA	CHD-C4C	2.63	1.48	1.41
17	8	302	CLA	CHD-C4C	2.63	1.48	1.41
17	A	815	CLA	CHD-C4C	2.62	1.48	1.41
17	6	306	CLA	CHD-C4C	2.62	1.48	1.41
17	a	829	CLA	CHD-C4C	2.62	1.48	1.41
17	G	104	CLA	CHD-C4C	2.62	1.48	1.41
17	B	839	CLA	CHD-C4C	2.62	1.48	1.41
17	B	812	CLA	CHD-C4C	2.62	1.48	1.41
17	b	818	CLA	CHD-C4C	2.62	1.48	1.41
17	8	301	CLA	C4B-CHC	2.62	1.48	1.41
17	b	813	CLA	CHD-C4C	2.62	1.48	1.41
17	K	4002	CLA	CHD-C4C	2.62	1.48	1.41
17	a	830	CLA	C1C-C2C	2.62	1.49	1.44
17	4	614	CLA	CHD-C4C	2.62	1.48	1.41
17	6	313	CLA	CHD-C4C	2.62	1.48	1.41
17	a	840	CLA	C4C-C3C	2.62	1.49	1.45
17	B	813	CLA	CHD-C4C	2.62	1.48	1.41
17	a	810	CLA	CHD-C4C	2.62	1.48	1.41
17	1	306	CLA	CHD-C4C	2.62	1.48	1.41
17	A	841	CLA	C4B-CHC	2.62	1.48	1.41
17	2	603	CLA	CHD-C4C	2.61	1.48	1.41
17	A	810	CLA	C1D-C2D	2.61	1.48	1.42
17	3	303	CLA	CHD-C4C	2.61	1.48	1.41
17	b	812	CLA	CHD-C4C	2.61	1.48	1.41
17	6	305	CLA	CHD-C4C	2.61	1.48	1.41
17	A	830	CLA	C1C-C2C	2.61	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	823	CLA	CHD-C4C	2.61	1.48	1.41
17	2	608	CLA	CHD-C4C	2.61	1.48	1.41
17	B	831	CLA	C4C-C3C	2.61	1.49	1.45
17	9	602	CLA	CHD-C4C	2.61	1.48	1.41
17	B	837	CLA	CHD-C4C	2.61	1.48	1.41
17	a	832	CLA	CHD-C4C	2.61	1.48	1.41
17	4	609	CLA	CHD-C4C	2.61	1.48	1.41
17	a	830	CLA	C1D-C2D	2.61	1.48	1.42
17	a	841	CLA	CHD-C4C	2.61	1.48	1.41
17	a	828	CLA	C1C-C2C	2.61	1.49	1.44
17	A	838	CLA	CHD-C4C	2.61	1.48	1.41
17	g	102	CLA	CHD-C4C	2.61	1.48	1.41
17	7	611	CLA	CHD-C4C	2.61	1.48	1.41
17	B	826	CLA	C1C-C2C	2.61	1.49	1.44
17	8	305	CLA	CHD-C4C	2.60	1.48	1.41
17	a	819	CLA	C4B-CHC	2.60	1.48	1.41
17	l	202	CLA	CHD-C4C	2.60	1.48	1.41
17	A	806	CLA	CHD-C4C	2.60	1.48	1.41
17	4	611	CLA	CHD-C4C	2.60	1.48	1.41
17	G	101	CLA	CHD-C4C	2.60	1.48	1.41
17	8	310	CLA	CHD-C4C	2.60	1.48	1.41
17	6	314	CLA	CHD-C4C	2.60	1.48	1.41
17	b	823	CLA	C4C-C3C	2.60	1.49	1.45
17	B	812	CLA	C4C-C3C	2.60	1.49	1.45
17	A	825	CLA	CHD-C4C	2.60	1.48	1.41
17	7	612	CLA	CHD-C4C	2.60	1.48	1.41
17	1	304	CLA	CHD-C4C	2.60	1.48	1.41
17	B	817	CLA	CHD-C4C	2.60	1.48	1.41
17	b	817	CLA	C4C-C3C	2.60	1.49	1.45
17	b	834	CLA	CHD-C4C	2.60	1.48	1.41
17	A	837	CLA	C4C-C3C	2.60	1.49	1.45
17	B	808	CLA	CHD-C4C	2.60	1.48	1.41
17	A	809	CLA	CHD-C4C	2.60	1.48	1.41
17	b	819	CLA	C4C-C3C	2.60	1.49	1.45
17	B	805	CLA	CHD-C4C	2.60	1.48	1.41
17	A	822	CLA	C4C-C3C	2.60	1.49	1.45
17	a	814	CLA	CHD-C4C	2.60	1.48	1.41
17	3	310	CLA	C4C-C3C	2.60	1.49	1.45
17	b	810	CLA	C1C-C2C	2.60	1.49	1.44
17	a	836	CLA	CHD-C4C	2.59	1.48	1.41
17	l	204	CLA	CHD-C4C	2.59	1.48	1.41
17	a	838	CLA	C4B-CHC	2.59	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	824	CLA	CHD-C4C	2.59	1.48	1.41
17	F	301	CLA	CHD-C4C	2.59	1.48	1.41
17	4	612	CLA	CHD-C4C	2.59	1.48	1.41
17	2	611	CLA	CHD-C4C	2.59	1.48	1.41
17	6	312	CLA	CHD-C4C	2.59	1.48	1.41
17	a	802	CLA	CHD-C4C	2.59	1.48	1.41
17	2	610	CLA	C4C-C3C	2.59	1.49	1.45
17	B	832	CLA	CHD-C4C	2.59	1.48	1.41
17	A	821	CLA	CHD-C4C	2.59	1.48	1.41
17	b	827	CLA	C4B-CHC	2.59	1.48	1.41
17	a	840	CLA	CHD-C4C	2.59	1.48	1.41
17	B	806	CLA	CHD-C4C	2.59	1.48	1.41
17	4	601	CLA	CHD-C4C	2.59	1.48	1.41
17	a	804	CLA	CHD-C4C	2.59	1.48	1.41
17	a	835	CLA	CHD-C4C	2.59	1.48	1.41
17	a	820	CLA	C4C-C3C	2.59	1.49	1.45
17	b	831	CLA	CHD-C4C	2.59	1.48	1.41
17	B	832	CLA	C4C-C3C	2.59	1.49	1.45
17	B	811	CLA	CHD-C4C	2.59	1.48	1.41
17	g	101	CLA	CHD-C4C	2.59	1.48	1.41
17	b	802	CLA	CHD-C4C	2.59	1.48	1.41
17	A	804	CLA	CHD-C4C	2.58	1.48	1.41
17	b	828	CLA	CHD-C4C	2.58	1.48	1.41
26	3	307	CHL	MG-NA	-2.58	2.00	2.06
17	a	827	CLA	CHD-C4C	2.58	1.48	1.41
17	A	807	CLA	CHD-C4C	2.58	1.48	1.41
17	G	103	CLA	CHD-C4C	2.58	1.48	1.41
17	7	610	CLA	C4C-C3C	2.58	1.49	1.45
17	B	830	CLA	C4C-C3C	2.58	1.49	1.45
17	B	829	CLA	C4C-C3C	2.58	1.49	1.45
17	9	614	CLA	CHD-C4C	2.58	1.48	1.41
17	1	309	CLA	CHD-C4C	2.58	1.48	1.41
17	b	838	CLA	CHD-C4C	2.58	1.48	1.41
17	a	826	CLA	C1C-C2C	2.58	1.49	1.44
17	a	814	CLA	C1C-C2C	2.58	1.49	1.44
17	a	856	CLA	CHD-C4C	2.57	1.48	1.41
17	a	838	CLA	CHD-C4C	2.57	1.48	1.41
17	6	304	CLA	C4C-C3C	2.57	1.49	1.45
17	B	828	CLA	CHD-C4C	2.57	1.48	1.41
26	2	601	CHL	MG-NA	-2.57	2.00	2.06
17	4	604	CLA	C4C-C3C	2.57	1.49	1.45
17	J	3002	CLA	C4C-C3C	2.57	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	801	CLA	CHD-C4C	2.57	1.48	1.41
17	A	838	CLA	C4B-CHC	2.57	1.48	1.41
17	B	830	CLA	CHD-C4C	2.57	1.48	1.41
17	8	309	CLA	C4C-C3C	2.57	1.49	1.45
17	9	610	CLA	CHD-C4C	2.57	1.48	1.41
17	b	818	CLA	C4C-C3C	2.57	1.49	1.45
17	a	846	CLA	C4C-C3C	2.57	1.49	1.45
17	A	808	CLA	CHD-C4C	2.57	1.48	1.41
17	a	824	CLA	CHD-C4C	2.57	1.48	1.41
17	7	603	CLA	CHD-C4C	2.57	1.48	1.41
17	B	840	CLA	CHD-C4C	2.57	1.48	1.41
17	a	833	CLA	C4B-CHC	2.57	1.48	1.41
17	A	845	CLA	C4C-C3C	2.57	1.49	1.45
17	a	843	CLA	CHD-C4C	2.57	1.48	1.41
17	F	304	CLA	C4C-C3C	2.57	1.49	1.45
17	8	307	CLA	CHD-C4C	2.57	1.48	1.41
17	a	808	CLA	C1C-C2C	2.57	1.49	1.44
17	3	306	CLA	CHD-C4C	2.57	1.48	1.41
17	b	825	CLA	CHD-C4C	2.57	1.48	1.41
17	A	802	CLA	C4B-CHC	2.57	1.48	1.41
17	b	816	CLA	C4C-C3C	2.57	1.49	1.45
17	1	312	CLA	CHD-C4C	2.56	1.48	1.41
17	7	610	CLA	C3A-C2A	-2.56	1.52	1.54
17	L	203	CLA	C1C-C2C	2.56	1.49	1.44
17	b	808	CLA	CHD-C4C	2.56	1.48	1.41
17	B	833	CLA	CHD-C4C	2.56	1.48	1.41
17	9	603	CLA	CHD-C4C	2.56	1.48	1.41
17	A	833	CLA	C4B-CHC	2.56	1.48	1.41
17	7	609	CLA	C4B-CHC	2.56	1.48	1.41
17	b	803	CLA	CHD-C4C	2.56	1.48	1.41
17	3	313	CLA	C4C-C3C	2.56	1.49	1.45
17	a	817	CLA	CHD-C4C	2.56	1.48	1.41
17	7	602	CLA	C4B-CHC	2.56	1.48	1.41
17	A	830	CLA	CHD-C4C	2.56	1.48	1.41
17	b	832	CLA	CHD-C4C	2.56	1.48	1.41
17	B	827	CLA	C1C-C2C	2.56	1.49	1.44
17	3	315	CLA	C2C-C1C	2.56	1.49	1.43
17	A	807	CLA	C4B-CHC	2.56	1.48	1.41
17	B	826	CLA	C4B-CHC	2.55	1.48	1.41
17	a	819	CLA	CHD-C4C	2.55	1.48	1.41
17	B	814	CLA	C4B-CHC	2.55	1.48	1.41
17	B	841	CLA	C4B-CHC	2.55	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	814	CLA	C4B-CHC	2.55	1.48	1.41
17	6	310	CLA	CHD-C4C	2.55	1.48	1.41
17	b	803	CLA	C4B-CHC	2.55	1.48	1.41
17	a	807	CLA	CHD-C4C	2.55	1.48	1.41
17	B	802	CLA	C1C-C2C	2.55	1.49	1.44
17	a	839	CLA	CHD-C4C	2.55	1.48	1.41
17	a	825	CLA	CHD-C4C	2.55	1.48	1.41
17	8	313	CLA	C2C-C1C	2.55	1.49	1.43
17	A	812	CLA	CHD-C4C	2.55	1.48	1.41
17	A	836	CLA	CHD-C4C	2.55	1.48	1.41
17	6	315	CLA	C4C-C3C	2.55	1.49	1.45
17	A	818	CLA	CHD-C4C	2.55	1.48	1.41
17	A	810	CLA	C1B-CHB	2.55	1.48	1.41
17	b	832	CLA	C4C-C3C	2.55	1.49	1.45
17	B	832	CLA	C4B-CHC	2.55	1.48	1.41
17	B	832	CLA	C1C-C2C	2.55	1.49	1.44
17	a	842	CLA	CHD-C4C	2.55	1.48	1.41
19	6	301	LHG	O8-C23	2.55	1.45	1.33
26	2	605	CHL	MG-NA	-2.55	2.00	2.06
17	B	825	CLA	C1C-C2C	2.54	1.49	1.44
17	B	802	CLA	CHD-C4C	2.54	1.48	1.41
17	g	103	CLA	C4C-C3C	2.54	1.49	1.45
26	9	605	CHL	MG-NA	-2.54	2.00	2.06
17	B	825	CLA	CHD-C4C	2.54	1.48	1.41
17	b	823	CLA	C1C-C2C	2.54	1.49	1.44
17	a	841	CLA	C4B-CHC	2.54	1.48	1.41
17	3	301	CLA	C4C-C3C	2.54	1.49	1.45
17	B	816	CLA	C4C-C3C	2.54	1.49	1.45
17	B	827	CLA	CHD-C4C	2.54	1.48	1.41
26	7	614	CHL	MG-NA	-2.54	2.00	2.06
17	B	815	CLA	CHD-C4C	2.54	1.48	1.41
17	B	841	CLA	C1C-C2C	2.54	1.49	1.44
17	B	827	CLA	C4B-CHC	2.54	1.48	1.41
17	A	825	CLA	C4C-C3C	2.54	1.49	1.45
17	A	835	CLA	C4C-C3C	2.54	1.49	1.45
17	a	831	CLA	CHD-C4C	2.53	1.48	1.41
17	B	818	CLA	CHD-C4C	2.53	1.48	1.41
17	F	301	CLA	C1C-C2C	2.53	1.49	1.44
17	9	611	CLA	CHD-C4C	2.53	1.48	1.41
17	A	839	CLA	CHD-C4C	2.53	1.48	1.41
17	b	810	CLA	C4B-CHC	2.53	1.48	1.41
22	a	857	HTG	C1-S1	-2.53	1.76	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	306	CLA	C4B-CHC	2.53	1.48	1.41
17	9	612	CLA	C4C-C3C	2.53	1.49	1.45
17	b	830	CLA	C4C-C3C	2.53	1.49	1.45
17	B	814	CLA	CHD-C4C	2.53	1.48	1.41
17	a	806	CLA	CHD-C4C	2.53	1.48	1.41
17	2	610	CLA	C3A-C2A	-2.53	1.52	1.54
17	B	819	CLA	C4C-C3C	2.53	1.49	1.45
17	b	804	CLA	CHD-C4C	2.53	1.48	1.41
17	A	817	CLA	C4C-C3C	2.53	1.49	1.45
17	b	814	CLA	C1C-C2C	2.53	1.49	1.44
17	b	833	CLA	CHD-C4C	2.53	1.48	1.41
17	a	828	CLA	C4B-CHC	2.53	1.48	1.41
17	B	804	CLA	C4C-C3C	2.53	1.49	1.45
17	k	1401	CLA	C4B-CHC	2.53	1.48	1.41
26	4	607	CHL	MG-NA	-2.52	2.00	2.06
17	B	809	CLA	CHD-C4C	2.52	1.48	1.41
17	2	613	CLA	C4C-C3C	2.52	1.49	1.45
17	8	303	CLA	C4C-C3C	2.52	1.49	1.45
17	a	826	CLA	CHD-C4C	2.52	1.48	1.41
17	a	830	CLA	CHD-C4C	2.52	1.48	1.41
26	1	307	CHL	MG-NA	-2.52	2.00	2.06
17	b	810	CLA	CHD-C4C	2.52	1.48	1.41
17	6	311	CLA	C4B-CHC	2.52	1.48	1.41
26	4	606	CHL	C2C-C1C	2.52	1.49	1.44
17	1	304	CLA	C4C-C3C	2.52	1.49	1.45
17	b	828	CLA	C1C-C2C	2.52	1.49	1.44
17	3	311	CLA	C4C-C3C	2.52	1.49	1.45
17	A	819	CLA	CHD-C4C	2.52	1.48	1.41
17	B	807	CLA	C4B-CHC	2.52	1.48	1.41
17	b	805	CLA	C4C-C3C	2.52	1.49	1.45
17	A	833	CLA	C1C-C2C	2.52	1.49	1.44
17	A	811	CLA	C4C-C3C	2.52	1.49	1.45
17	B	813	CLA	C4C-C3C	2.52	1.49	1.45
17	8	301	CLA	C1C-C2C	2.52	1.49	1.44
17	A	805	CLA	CHD-C4C	2.52	1.48	1.41
17	b	826	CLA	CHD-C4C	2.52	1.48	1.41
17	A	841	CLA	CHD-C4C	2.52	1.48	1.41
17	a	815	CLA	C4B-CHC	2.52	1.48	1.41
26	1	307	CHL	C2C-C1C	2.52	1.49	1.44
17	a	809	CLA	CHD-C4C	2.52	1.48	1.41
26	9	607	CHL	MG-NA	-2.52	2.00	2.06
17	l	203	CLA	C4B-CHC	2.52	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	819	CLA	C4B-CHC	2.52	1.48	1.41
17	7	612	CLA	C4C-C3C	2.52	1.49	1.45
17	a	810	CLA	C4C-C3C	2.51	1.49	1.45
17	a	807	CLA	C4B-CHC	2.51	1.48	1.41
17	B	823	CLA	CHD-C4C	2.51	1.48	1.41
17	A	829	CLA	CHD-C4C	2.51	1.48	1.41
17	B	838	CLA	CHD-C4C	2.51	1.48	1.41
17	a	801	CLA	CHD-C4C	2.51	1.48	1.41
17	2	609	CLA	C4B-CHC	2.51	1.48	1.41
26	8	306	CHL	C2C-C1C	2.51	1.49	1.44
17	8	308	CLA	C4B-CHC	2.51	1.48	1.41
17	b	820	CLA	CHD-C4C	2.51	1.48	1.41
17	B	803	CLA	C4B-CHC	2.51	1.48	1.41
17	A	828	CLA	C4B-CHC	2.51	1.48	1.41
26	7	601	CHL	C4B-CHC	2.51	1.48	1.41
17	a	808	CLA	CHD-C4C	2.51	1.48	1.41
17	A	827	CLA	C1C-C2C	2.51	1.49	1.44
17	L	202	CLA	C4C-C3C	2.51	1.49	1.45
17	6	305	CLA	C4C-C3C	2.51	1.49	1.45
17	b	836	CLA	CHD-C4C	2.51	1.48	1.41
26	4	606	CHL	MG-NA	-2.51	2.00	2.06
17	A	823	CLA	C4C-C3C	2.51	1.49	1.45
17	3	314	CLA	C4B-CHC	2.51	1.48	1.41
17	2	612	CLA	C4C-C3C	2.51	1.49	1.45
26	7	606	CHL	MG-NA	-2.51	2.00	2.06
17	9	613	CLA	C4C-C3C	2.51	1.49	1.45
17	F	303	CLA	CHD-C4C	2.50	1.48	1.41
17	B	808	CLA	C4C-C3C	2.50	1.49	1.45
17	8	302	CLA	C4C-C3C	2.50	1.49	1.45
26	4	615	CHL	C2C-C1C	2.50	1.49	1.44
17	B	831	CLA	C4B-CHC	2.50	1.47	1.41
17	6	306	CLA	C4C-C3C	2.50	1.49	1.45
17	4	608	CLA	CHD-C4C	2.50	1.48	1.41
17	9	602	CLA	C1C-C2C	2.50	1.49	1.44
17	a	837	CLA	C4C-C3C	2.50	1.49	1.45
17	a	821	CLA	CHD-C4C	2.50	1.48	1.41
17	A	820	CLA	C4C-C3C	2.50	1.49	1.45
17	1	313	CLA	C4C-C3C	2.50	1.49	1.45
17	9	601	CLA	C4C-C3C	2.50	1.49	1.45
17	a	844	CLA	CHD-C4C	2.50	1.48	1.41
17	b	826	CLA	C4B-CHC	2.50	1.47	1.41
17	j	3002	CLA	C4C-C3C	2.50	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	314	CLA	C4C-C3C	2.50	1.49	1.45
17	1	203	CLA	C1C-C2C	2.50	1.49	1.44
17	9	602	CLA	C4B-CHC	2.50	1.47	1.41
17	b	832	CLA	C4B-CHC	2.50	1.47	1.41
17	4	603	CLA	CHD-C4C	2.50	1.48	1.41
26	2	606	CHL	C2C-C1C	2.50	1.49	1.44
17	A	827	CLA	C4B-CHC	2.50	1.47	1.41
26	2	614	CHL	MG-NA	-2.49	2.00	2.06
17	b	836	CLA	C1C-C2C	2.49	1.49	1.44
17	b	827	CLA	CHD-C4C	2.49	1.48	1.41
17	2	604	CLA	C4C-C3C	2.49	1.49	1.45
19	1	301	LHG	O8-C23	2.49	1.45	1.33
26	4	607	CHL	C2C-C1C	2.49	1.49	1.44
17	8	307	CLA	C4B-CHC	2.49	1.47	1.41
17	a	833	CLA	CHD-C4C	2.49	1.48	1.41
17	9	608	CLA	CHD-C4C	2.49	1.48	1.41
17	B	838	CLA	C1B-CHB	2.49	1.47	1.41
17	a	808	CLA	C4B-CHC	2.49	1.47	1.41
17	a	816	CLA	C4B-CHC	2.49	1.47	1.41
17	G	103	CLA	C4B-CHC	2.49	1.47	1.41
17	6	314	CLA	C4C-C3C	2.49	1.49	1.45
17	a	842	CLA	C4B-CHC	2.49	1.47	1.41
17	b	809	CLA	CHD-C4C	2.49	1.48	1.41
17	A	828	CLA	C1C-C2C	2.49	1.49	1.44
17	B	828	CLA	C4B-CHC	2.49	1.47	1.41
17	A	842	CLA	C4B-CHC	2.49	1.47	1.41
17	b	832	CLA	C1C-C2C	2.49	1.49	1.44
17	b	825	CLA	C1C-C2C	2.49	1.49	1.44
17	L	203	CLA	C4B-CHC	2.49	1.47	1.41
17	F	304	CLA	C4B-CHC	2.49	1.47	1.41
17	3	309	CLA	C4B-CHC	2.49	1.47	1.41
17	A	813	CLA	C4C-C3C	2.49	1.49	1.45
17	K	4002	CLA	C4C-C3C	2.49	1.49	1.45
17	a	832	CLA	C4C-C3C	2.49	1.49	1.45
26	2	606	CHL	MG-NA	-2.49	2.00	2.06
17	a	809	CLA	C4B-CHC	2.49	1.47	1.41
17	7	613	CLA	C4C-C3C	2.49	1.49	1.45
17	B	836	CLA	C1C-C2C	2.49	1.49	1.44
17	B	824	CLA	C4B-CHC	2.48	1.47	1.41
26	6	308	CHL	C2C-C1C	2.48	1.49	1.44
17	3	303	CLA	C4C-C3C	2.48	1.49	1.45
17	3	312	CLA	C4C-C3C	2.48	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	839	CLA	C1C-C2C	2.48	1.49	1.44
17	B	822	CLA	C4C-C3C	2.48	1.49	1.45
17	1	312	CLA	C4C-C3C	2.48	1.49	1.45
17	A	809	CLA	C1C-C2C	2.48	1.49	1.44
26	4	615	CHL	MG-NA	-2.48	2.00	2.06
17	6	309	CLA	C4B-CHC	2.48	1.47	1.41
17	b	824	CLA	C1C-C2C	2.48	1.49	1.44
17	2	609	CLA	C1C-C2C	2.48	1.49	1.44
17	a	856	CLA	C4C-C3C	2.48	1.49	1.45
22	J	3001	HTG	C1-S1	-2.48	1.76	1.80
17	B	812	CLA	C4B-CHC	2.48	1.47	1.41
17	A	840	CLA	C1C-C2C	2.48	1.49	1.44
26	2	607	CHL	MG-NA	-2.48	2.00	2.06
17	f	7002	CLA	C1C-C2C	2.48	1.49	1.44
17	b	839	CLA	CHD-C4C	2.48	1.48	1.41
17	9	611	CLA	C4C-C3C	2.48	1.49	1.45
17	f	7003	CLA	C4B-CHC	2.48	1.47	1.41
17	b	806	CLA	C4B-CHC	2.48	1.47	1.41
17	A	804	CLA	C4B-CHC	2.48	1.47	1.41
17	K	4003	CLA	C4C-C3C	2.48	1.49	1.45
17	b	841	CLA	C4B-CHC	2.48	1.47	1.41
17	2	608	CLA	C4C-C3C	2.48	1.49	1.45
17	b	815	CLA	CHD-C4C	2.48	1.48	1.41
17	b	806	CLA	C1C-C2C	2.48	1.49	1.44
17	b	840	CLA	CHD-C4C	2.48	1.48	1.41
17	a	843	CLA	C4B-CHC	2.48	1.47	1.41
17	b	835	CLA	C4C-C3C	2.48	1.49	1.45
17	9	613	CLA	C4B-CHC	2.48	1.47	1.41
17	A	808	CLA	C1C-C2C	2.48	1.49	1.44
17	a	811	CLA	C4C-C3C	2.48	1.49	1.45
17	4	614	CLA	C4B-CHC	2.48	1.47	1.41
17	a	819	CLA	C1C-C2C	2.48	1.49	1.44
17	A	841	CLA	C1C-C2C	2.48	1.49	1.44
17	B	837	CLA	C4B-CHC	2.48	1.47	1.41
17	6	307	CLA	C4C-C3C	2.47	1.49	1.45
17	7	604	CLA	C4C-C3C	2.47	1.49	1.45
17	1	308	CLA	C4C-C3C	2.47	1.49	1.45
17	3	311	CLA	C4B-CHC	2.47	1.47	1.41
26	4	605	CHL	MG-NA	-2.47	2.00	2.06
17	b	811	CLA	CHD-C4C	2.47	1.48	1.41
17	B	817	CLA	C4C-C3C	2.47	1.49	1.45
17	B	834	CLA	C4B-CHC	2.47	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	7	609	CLA	C1C-C2C	2.47	1.49	1.44
17	B	806	CLA	C4B-CHC	2.47	1.47	1.41
17	B	836	CLA	CHD-C4C	2.47	1.48	1.41
17	G	104	CLA	C4C-C3C	2.47	1.49	1.45
17	f	7002	CLA	CHD-C4C	2.47	1.48	1.41
17	a	818	CLA	C4C-C3C	2.47	1.49	1.45
17	8	311	CLA	C4C-C3C	2.47	1.49	1.45
17	1	303	CLA	C4C-C3C	2.47	1.49	1.45
17	a	814	CLA	C4B-CHC	2.47	1.47	1.41
17	A	843	CLA	C4C-C3C	2.47	1.49	1.45
17	A	828	CLA	CHD-C4C	2.47	1.48	1.41
26	2	607	CHL	C2C-C1C	2.47	1.49	1.44
26	9	606	CHL	MG-NA	-2.47	2.00	2.06
17	b	812	CLA	C4C-C3C	2.47	1.49	1.45
26	7	605	CHL	MG-NA	-2.47	2.00	2.06
26	1	302	CHL	MG-NA	-2.47	2.00	2.06
17	9	603	CLA	C4B-CHC	2.47	1.47	1.41
17	8	311	CLA	C4B-CHC	2.47	1.47	1.41
17	B	826	CLA	CHD-C4C	2.46	1.48	1.41
17	1	303	CLA	C4B-CHC	2.46	1.47	1.41
17	a	816	CLA	CHD-C4C	2.46	1.48	1.41
17	b	822	CLA	C1C-C2C	2.46	1.49	1.44
17	A	816	CLA	C4B-CHC	2.46	1.47	1.41
17	b	841	CLA	C1C-C2C	2.46	1.49	1.44
17	B	830	CLA	C1C-C2C	2.46	1.49	1.44
17	7	608	CLA	C4B-CHC	2.46	1.47	1.41
17	A	834	CLA	C4C-C3C	2.46	1.49	1.45
17	9	610	CLA	C3A-C2A	-2.46	1.52	1.54
17	7	603	CLA	C4B-CHC	2.46	1.47	1.41
17	g	102	CLA	C4C-C3C	2.46	1.49	1.45
17	A	840	CLA	C4B-CHC	2.46	1.47	1.41
17	A	815	CLA	C4B-CHC	2.46	1.47	1.41
17	1	308	CLA	C4B-CHC	2.46	1.47	1.41
17	8	305	CLA	C4C-C3C	2.46	1.49	1.45
17	4	613	CLA	C4C-C3C	2.46	1.49	1.45
17	A	802	CLA	C1C-C2C	2.46	1.49	1.44
17	B	807	CLA	C1C-C2C	2.46	1.49	1.44
17	1	306	CLA	C4B-CHC	2.46	1.47	1.41
17	b	820	CLA	C4B-CHC	2.46	1.47	1.41
17	3	304	CLA	C4C-C3C	2.46	1.49	1.45
17	8	310	CLA	C4C-C3C	2.46	1.49	1.45
17	4	609	CLA	C4B-CHC	2.46	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	7	607	CHL	MG-NA	-2.46	2.00	2.06
17	a	833	CLA	C1C-C2C	2.46	1.49	1.44
17	8	309	CLA	C4B-CHC	2.46	1.47	1.41
17	B	823	CLA	C4C-C3C	2.46	1.49	1.45
17	B	818	CLA	C4B-CHC	2.46	1.47	1.41
17	A	812	CLA	C1C-C2C	2.46	1.49	1.44
17	f	7002	CLA	C4B-CHC	2.46	1.47	1.41
17	a	821	CLA	C1B-CHB	2.46	1.47	1.41
17	A	808	CLA	C4C-C3C	2.46	1.49	1.45
17	G	101	CLA	C4B-CHC	2.46	1.47	1.41
17	a	829	CLA	C4C-C3C	2.46	1.49	1.45
17	B	833	CLA	C4B-CHC	2.46	1.47	1.41
17	2	613	CLA	C4B-CHC	2.46	1.47	1.41
17	8	312	CLA	C4B-CHC	2.46	1.47	1.41
17	b	833	CLA	C4C-C3C	2.46	1.49	1.45
17	1	311	CLA	C4C-C3C	2.46	1.49	1.45
17	b	833	CLA	C4B-CHC	2.46	1.47	1.41
17	b	834	CLA	C4C-C3C	2.45	1.49	1.45
17	a	839	CLA	C4B-CHC	2.45	1.47	1.41
17	B	813	CLA	C4B-CHC	2.45	1.47	1.41
17	A	807	CLA	C1C-C2C	2.45	1.49	1.44
17	B	821	CLA	C4C-C3C	2.45	1.49	1.45
17	B	835	CLA	C4B-CHC	2.45	1.47	1.41
17	3	314	CLA	C4C-C3C	2.45	1.49	1.45
17	j	3002	CLA	C4B-CHC	2.45	1.47	1.41
17	a	824	CLA	C4C-C3C	2.45	1.49	1.45
17	1	315	CLA	C4B-CHC	2.45	1.47	1.41
17	b	834	CLA	C4B-CHC	2.45	1.47	1.41
17	b	822	CLA	C4B-CHC	2.45	1.47	1.41
17	f	7003	CLA	C4C-C3C	2.45	1.49	1.45
17	4	608	CLA	C4C-C3C	2.45	1.49	1.45
17	A	837	CLA	C4B-CHC	2.45	1.47	1.41
17	b	821	CLA	C4C-C3C	2.45	1.49	1.45
17	B	807	CLA	C4C-C3C	2.45	1.49	1.45
17	B	810	CLA	C4B-CHC	2.45	1.47	1.41
17	A	805	CLA	C4B-CHC	2.45	1.47	1.41
17	a	813	CLA	C4B-CHC	2.45	1.47	1.41
17	6	309	CLA	C4C-C3C	2.45	1.49	1.45
17	3	309	CLA	C1C-C2C	2.45	1.49	1.44
17	L	204	CLA	C4B-CHC	2.45	1.47	1.41
26	9	615	CHL	MG-NA	-2.45	2.00	2.06
17	a	812	CLA	C4B-CHC	2.45	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	838	CLA	C4C-C3C	2.45	1.49	1.45
17	b	841	CLA	C4C-C3C	2.45	1.49	1.45
17	a	830	CLA	C4B-CHC	2.45	1.47	1.41
17	8	304	CLA	C4B-CHC	2.45	1.47	1.41
17	a	834	CLA	C1C-C2C	2.45	1.49	1.44
17	b	826	CLA	C1C-C2C	2.45	1.49	1.44
17	A	804	CLA	C1C-C2C	2.45	1.49	1.44
17	A	830	CLA	C4B-CHC	2.45	1.47	1.41
17	3	308	CLA	C4B-CHC	2.45	1.47	1.41
17	B	839	CLA	C4B-CHC	2.45	1.47	1.41
17	B	820	CLA	C4B-CHC	2.44	1.47	1.41
17	2	602	CLA	C4B-CHC	2.44	1.47	1.41
26	7	607	CHL	C2C-C1C	2.44	1.49	1.44
17	4	601	CLA	C4C-C3C	2.44	1.49	1.45
17	b	838	CLA	C1C-C2C	2.44	1.49	1.44
17	G	104	CLA	C4B-CHC	2.44	1.47	1.41
17	a	804	CLA	C4B-CHC	2.44	1.47	1.41
17	b	816	CLA	C4B-CHC	2.44	1.47	1.41
17	A	801	CLA	C4B-CHC	2.44	1.47	1.41
17	3	305	CLA	C4C-C3C	2.44	1.49	1.45
17	6	307	CLA	C4B-CHC	2.44	1.47	1.41
17	B	820	CLA	C4C-C3C	2.44	1.49	1.45
17	J	3002	CLA	C4B-CHC	2.44	1.47	1.41
26	2	614	CHL	C4C-C3C	2.44	1.49	1.45
17	8	305	CLA	C4B-CHC	2.44	1.47	1.41
17	3	302	CLA	C4B-CHC	2.44	1.47	1.41
17	6	313	CLA	C4C-C3C	2.44	1.49	1.45
17	4	609	CLA	C1C-C2C	2.44	1.49	1.44
17	6	316	CLA	C4B-CHC	2.44	1.47	1.41
26	6	303	CHL	MG-NA	-2.44	2.00	2.06
17	A	826	CLA	C4B-CHC	2.44	1.47	1.41
17	6	316	CLA	C4C-C3C	2.44	1.49	1.45
17	k	1402	CLA	C4C-C3C	2.44	1.49	1.45
17	b	804	CLA	C1C-C2C	2.44	1.49	1.44
17	4	602	CLA	C4B-CHC	2.44	1.47	1.41
17	a	835	CLA	C4B-CHC	2.44	1.47	1.41
17	k	1401	CLA	C1C-C2C	2.44	1.49	1.44
17	a	834	CLA	C4B-CHC	2.44	1.47	1.41
17	F	304	CLA	C1C-C2C	2.44	1.49	1.44
17	B	821	CLA	C4B-CHC	2.44	1.47	1.41
17	9	614	CLA	C4B-CHC	2.44	1.47	1.41
17	4	608	CLA	C4B-CHC	2.44	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	824	CLA	C4C-C3C	2.44	1.49	1.45
17	9	614	CLA	C4C-C3C	2.44	1.49	1.45
17	7	602	CLA	C1C-C2C	2.44	1.49	1.44
17	2	608	CLA	C4B-CHC	2.44	1.47	1.41
17	3	304	CLA	C4B-CHC	2.44	1.47	1.41
17	b	839	CLA	C4C-C3C	2.44	1.49	1.45
17	6	312	CLA	C4B-CHC	2.44	1.47	1.41
17	3	305	CLA	C4B-CHC	2.43	1.47	1.41
17	3	301	CLA	C4B-CHC	2.43	1.47	1.41
17	B	806	CLA	C1C-C2C	2.43	1.49	1.44
17	8	307	CLA	C1C-C2C	2.43	1.49	1.44
17	K	4002	CLA	C4B-CHC	2.43	1.47	1.41
17	4	611	CLA	C4C-C3C	2.43	1.49	1.45
17	2	604	CLA	C4B-CHC	2.43	1.47	1.41
17	a	817	CLA	C4C-C3C	2.43	1.49	1.45
17	F	301	CLA	C4B-CHC	2.43	1.47	1.41
17	4	613	CLA	C4B-CHC	2.43	1.47	1.41
17	A	836	CLA	C4C-C3C	2.43	1.49	1.45
17	a	839	CLA	C1C-C2C	2.43	1.49	1.44
17	B	803	CLA	C1C-C2C	2.43	1.49	1.44
17	g	102	CLA	C4B-CHC	2.43	1.47	1.41
17	A	810	CLA	C1C-C2C	2.43	1.49	1.44
17	7	611	CLA	C4C-C3C	2.43	1.49	1.45
17	3	308	CLA	C4C-C3C	2.43	1.49	1.45
17	2	603	CLA	C4C-C3C	2.43	1.49	1.45
17	B	804	CLA	C1C-C2C	2.43	1.49	1.44
17	a	822	CLA	C4B-CHC	2.43	1.47	1.41
17	B	816	CLA	C4B-CHC	2.43	1.47	1.41
17	A	823	CLA	C1C-C2C	2.43	1.49	1.44
17	A	806	CLA	C4C-C3C	2.43	1.49	1.45
17	9	609	CLA	C4B-CHC	2.43	1.47	1.41
17	A	803	CLA	C1C-C2C	2.43	1.49	1.44
17	b	839	CLA	C4B-CHC	2.43	1.47	1.41
17	A	818	CLA	C4B-CHC	2.43	1.47	1.41
17	b	837	CLA	C4B-CHC	2.43	1.47	1.41
17	B	839	CLA	C4C-C3C	2.43	1.49	1.45
17	A	806	CLA	C4B-CHC	2.43	1.47	1.41
17	L	202	CLA	C4B-CHC	2.43	1.47	1.41
17	a	802	CLA	C4B-CHC	2.43	1.47	1.41
17	1	310	CLA	C4C-C3C	2.43	1.49	1.45
17	a	846	CLA	C4B-CHC	2.43	1.47	1.41
17	a	840	CLA	C1B-CHB	2.43	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	601	CLA	C4B-CHC	2.43	1.47	1.41
17	a	827	CLA	C1C-C2C	2.43	1.49	1.44
17	8	308	CLA	C1C-C2C	2.43	1.49	1.44
17	a	823	CLA	C1C-C2C	2.43	1.49	1.44
17	B	803	CLA	C4C-C3C	2.43	1.49	1.45
26	4	605	CHL	CHD-C4C	2.42	1.48	1.41
17	4	612	CLA	C1B-CHB	2.42	1.47	1.41
17	a	804	CLA	C1B-CHB	2.42	1.47	1.41
17	b	838	CLA	C4B-CHC	2.42	1.47	1.41
17	k	1401	CLA	C4C-C3C	2.42	1.49	1.45
17	3	302	CLA	C1C-C2C	2.42	1.49	1.44
17	9	604	CLA	C4B-CHC	2.42	1.47	1.41
17	1	305	CLA	C4B-CHC	2.42	1.47	1.41
17	K	4003	CLA	C4B-CHC	2.42	1.47	1.41
17	b	811	CLA	C1C-C2C	2.42	1.49	1.44
17	A	825	CLA	C1B-CHB	2.42	1.47	1.41
17	9	609	CLA	C4C-C3C	2.42	1.49	1.45
17	A	836	CLA	C4B-CHC	2.42	1.47	1.41
17	b	828	CLA	C4B-CHC	2.42	1.47	1.41
17	9	612	CLA	C4B-CHC	2.42	1.47	1.41
17	1	313	CLA	C4B-CHC	2.42	1.47	1.41
17	4	612	CLA	C4C-C3C	2.42	1.49	1.45
17	b	807	CLA	C4B-CHC	2.42	1.47	1.41
26	8	306	CHL	MG-NA	-2.42	2.00	2.06
17	a	810	CLA	C4B-CHC	2.42	1.47	1.41
26	2	601	CHL	C4C-C3C	2.42	1.49	1.45
17	F	303	CLA	C4B-CHC	2.42	1.47	1.41
17	A	812	CLA	C4B-CHC	2.42	1.47	1.41
17	A	813	CLA	C4B-CHC	2.42	1.47	1.41
17	A	823	CLA	C4B-CHC	2.42	1.47	1.41
17	B	813	CLA	C1C-C2C	2.42	1.49	1.44
17	3	302	CLA	C4C-C3C	2.42	1.49	1.45
17	a	815	CLA	C1C-C2C	2.42	1.49	1.44
17	3	313	CLA	C4B-CHC	2.42	1.47	1.41
17	7	612	CLA	C1B-CHB	2.42	1.47	1.41
17	3	311	CLA	C1C-C2C	2.42	1.49	1.44
17	b	820	CLA	C1C-C2C	2.42	1.49	1.44
17	a	804	CLA	C1C-C2C	2.42	1.49	1.44
17	a	816	CLA	C1C-C2C	2.42	1.49	1.44
17	k	1402	CLA	C4B-CHC	2.42	1.47	1.41
17	A	826	CLA	CHD-C4C	2.42	1.48	1.41
17	A	810	CLA	CHD-C4C	2.42	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	310	CLA	C4B-CHC	2.42	1.47	1.41
26	4	615	CHL	CHD-C4C	2.42	1.48	1.41
17	F	301	CLA	C4C-C3C	2.42	1.49	1.45
17	a	832	CLA	C1C-C2C	2.41	1.49	1.44
17	B	823	CLA	C1C-C2C	2.41	1.49	1.44
17	B	832	CLA	C1B-CHB	2.41	1.47	1.41
17	8	304	CLA	C4C-C3C	2.41	1.49	1.45
26	4	606	CHL	CHD-C4C	2.41	1.48	1.41
17	b	840	CLA	C1B-CHB	2.41	1.47	1.41
17	A	815	CLA	C4C-C3C	2.41	1.49	1.45
17	a	839	CLA	C4C-C3C	2.41	1.49	1.45
17	a	829	CLA	C4B-CHC	2.41	1.47	1.41
17	3	312	CLA	C4B-CHC	2.41	1.47	1.41
17	A	842	CLA	C4C-C3C	2.41	1.49	1.45
17	2	602	CLA	C4C-C3C	2.41	1.49	1.45
17	B	828	CLA	C1C-C2C	2.41	1.49	1.44
17	B	836	CLA	C4B-CHC	2.41	1.47	1.41
17	K	4002	CLA	C1C-C2C	2.41	1.49	1.44
17	2	611	CLA	C4C-C3C	2.41	1.49	1.45
17	7	613	CLA	C4B-CHC	2.41	1.47	1.41
17	F	303	CLA	C1C-C2C	2.41	1.49	1.44
17	a	842	CLA	C1C-C2C	2.41	1.49	1.44
17	2	611	CLA	C4B-CHC	2.41	1.47	1.41
17	B	815	CLA	C1C-C2C	2.41	1.49	1.44
26	9	607	CHL	C2C-C1C	2.41	1.49	1.44
17	b	813	CLA	C4B-CHC	2.41	1.47	1.41
17	b	812	CLA	C4B-CHC	2.41	1.47	1.41
17	B	823	CLA	C4B-CHC	2.41	1.47	1.41
26	1	302	CHL	C4B-CHC	2.41	1.47	1.41
17	a	831	CLA	C4C-C3C	2.41	1.49	1.45
17	8	308	CLA	C4C-C3C	2.41	1.49	1.45
17	B	811	CLA	C1B-CHB	2.41	1.47	1.41
17	b	825	CLA	C4B-CHC	2.41	1.47	1.41
17	9	610	CLA	C4B-CHC	2.41	1.47	1.41
17	A	854	CLA	CHD-C4C	2.41	1.48	1.41
17	A	801	CLA	C1C-C2C	2.41	1.49	1.44
17	a	809	CLA	C1C-C2C	2.41	1.49	1.44
26	2	605	CHL	CHD-C4C	2.41	1.48	1.41
17	G	104	CLA	C1C-C2C	2.41	1.49	1.44
17	6	304	CLA	C4B-CHC	2.41	1.47	1.41
17	6	314	CLA	C4B-CHC	2.41	1.47	1.41
17	1	308	CLA	C1C-C2C	2.41	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	817	CLA	C4B-CHC	2.40	1.47	1.41
17	4	608	CLA	C1C-C2C	2.40	1.49	1.44
17	7	603	CLA	C1C-C2C	2.40	1.49	1.44
17	2	612	CLA	C4B-CHC	2.40	1.47	1.41
17	4	611	CLA	C4B-CHC	2.40	1.47	1.41
17	a	823	CLA	C4B-CHC	2.40	1.47	1.41
17	1	311	CLA	C4B-CHC	2.40	1.47	1.41
17	2	611	CLA	C1C-C2C	2.40	1.49	1.44
17	B	821	CLA	C1C-C2C	2.40	1.49	1.44
26	6	303	CHL	CHD-C4C	2.40	1.48	1.41
22	A	855	HTG	C1-S1	-2.40	1.77	1.80
17	G	103	CLA	C4C-C3C	2.40	1.49	1.45
17	a	825	CLA	C1C-C2C	2.40	1.49	1.44
17	b	835	CLA	C4B-CHC	2.40	1.47	1.41
17	A	809	CLA	C4C-C3C	2.40	1.49	1.45
17	a	826	CLA	C4C-C3C	2.40	1.49	1.45
17	A	829	CLA	C1C-C2C	2.40	1.49	1.44
17	6	306	CLA	C4B-CHC	2.40	1.47	1.41
17	a	830	CLA	C1B-CHB	2.40	1.47	1.41
17	2	603	CLA	C4B-CHC	2.40	1.47	1.41
17	8	312	CLA	C1C-C2C	2.40	1.49	1.44
17	B	814	CLA	C1C-C2C	2.40	1.49	1.44
17	b	840	CLA	C1C-C2C	2.40	1.49	1.44
26	4	606	CHL	C4C-C3C	2.40	1.49	1.45
17	6	315	CLA	C4B-CHC	2.40	1.47	1.41
17	B	808	CLA	C1C-C2C	2.40	1.49	1.44
17	k	1402	CLA	C1B-CHB	2.40	1.47	1.41
17	B	840	CLA	C4B-CHC	2.40	1.47	1.41
26	7	606	CHL	C2C-C1C	2.40	1.49	1.44
17	4	610	CLA	C1C-C2C	2.40	1.49	1.44
17	b	802	CLA	C4C-C3C	2.40	1.49	1.45
17	6	309	CLA	C1C-C2C	2.40	1.49	1.44
17	6	311	CLA	C1C-C2C	2.40	1.49	1.44
17	b	823	CLA	C4B-CHC	2.40	1.47	1.41
17	b	818	CLA	C4B-CHC	2.40	1.47	1.41
17	1	310	CLA	C4B-CHC	2.40	1.47	1.41
17	L	204	CLA	C4C-C3C	2.40	1.49	1.45
17	9	604	CLA	C4C-C3C	2.40	1.49	1.45
17	B	824	CLA	C4C-C3C	2.40	1.49	1.45
17	A	814	CLA	C4B-CHC	2.40	1.47	1.41
17	b	824	CLA	C4B-CHC	2.40	1.47	1.41
17	7	612	CLA	C4B-CHC	2.40	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	309	CLA	C4C-C3C	2.40	1.49	1.45
17	b	834	CLA	C1B-CHB	2.40	1.47	1.41
17	a	840	CLA	C1C-C2C	2.40	1.49	1.44
17	B	802	CLA	C4B-CHC	2.40	1.47	1.41
17	l	202	CLA	C4C-C3C	2.40	1.49	1.45
17	A	811	CLA	C4B-CHC	2.40	1.47	1.41
17	A	845	CLA	C4B-CHC	2.39	1.47	1.41
17	B	825	CLA	C4B-CHC	2.39	1.47	1.41
17	4	604	CLA	C4B-CHC	2.39	1.47	1.41
26	9	615	CHL	C4C-C3C	2.39	1.49	1.45
17	A	807	CLA	C4C-C3C	2.39	1.49	1.45
17	a	844	CLA	C4B-CHC	2.39	1.47	1.41
17	B	809	CLA	C4C-C3C	2.39	1.49	1.45
17	6	310	CLA	C4C-C3C	2.39	1.49	1.45
17	A	820	CLA	C1C-C2C	2.39	1.49	1.44
26	9	615	CHL	CHD-C4C	2.39	1.48	1.41
17	A	815	CLA	C1C-C2C	2.39	1.49	1.44
17	A	840	CLA	C4C-C3C	2.39	1.49	1.45
17	A	808	CLA	C1B-CHB	2.39	1.47	1.41
17	B	823	CLA	C1B-CHB	2.39	1.47	1.41
17	b	839	CLA	C1B-CHB	2.39	1.47	1.41
17	B	830	CLA	C4B-CHC	2.39	1.47	1.41
17	a	816	CLA	C1B-CHB	2.39	1.47	1.41
17	g	102	CLA	C1C-C2C	2.39	1.49	1.44
17	a	821	CLA	C4B-CHC	2.39	1.47	1.41
17	l	204	CLA	C4B-CHC	2.39	1.47	1.41
26	2	605	CHL	C4B-CHC	2.39	1.47	1.41
17	a	826	CLA	C1B-CHB	2.39	1.47	1.41
17	4	601	CLA	C1C-C2C	2.39	1.49	1.44
17	a	826	CLA	C4B-CHC	2.39	1.47	1.41
17	9	603	CLA	C1C-C2C	2.39	1.49	1.44
17	8	303	CLA	C4B-CHC	2.39	1.47	1.41
17	B	837	CLA	C1C-C2C	2.39	1.49	1.44
17	b	807	CLA	C1C-C2C	2.39	1.49	1.44
26	2	605	CHL	C4C-C3C	2.39	1.49	1.45
17	B	839	CLA	C1C-C2C	2.39	1.49	1.44
17	1	312	CLA	C4B-CHC	2.39	1.47	1.41
17	9	609	CLA	C1C-C2C	2.39	1.49	1.44
17	1	306	CLA	C4C-C3C	2.39	1.49	1.45
17	g	103	CLA	C4B-CHC	2.39	1.47	1.41
17	G	101	CLA	C1B-CHB	2.39	1.47	1.41
17	b	830	CLA	C4B-CHC	2.38	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	814	CLA	C1C-C2C	2.38	1.49	1.44
17	B	822	CLA	C1C-C2C	2.38	1.49	1.44
17	a	825	CLA	C1B-CHB	2.38	1.47	1.41
17	a	827	CLA	C4B-CHC	2.38	1.47	1.41
17	a	837	CLA	C4B-CHC	2.38	1.47	1.41
17	a	846	CLA	C1C-C2C	2.38	1.49	1.44
17	b	833	CLA	C1B-CHB	2.38	1.47	1.41
17	g	101	CLA	C1B-CHB	2.38	1.47	1.41
17	8	310	CLA	C4B-CHC	2.38	1.47	1.41
17	4	601	CLA	C4B-CHC	2.38	1.47	1.41
17	8	301	CLA	C4C-C3C	2.38	1.49	1.45
17	a	812	CLA	C1C-C2C	2.38	1.49	1.44
17	A	839	CLA	C1B-CHB	2.38	1.47	1.41
17	1	303	CLA	C1C-C2C	2.38	1.49	1.44
17	4	610	CLA	C4C-C3C	2.38	1.49	1.45
26	4	615	CHL	C4B-CHC	2.38	1.47	1.41
17	1	315	CLA	C4C-C3C	2.38	1.49	1.45
17	B	811	CLA	C4C-C3C	2.38	1.49	1.45
17	3	308	CLA	C1C-C2C	2.38	1.49	1.44
17	a	825	CLA	C4B-CHC	2.38	1.47	1.41
17	9	611	CLA	C4B-CHC	2.38	1.47	1.41
17	b	831	CLA	C4B-CHC	2.38	1.47	1.41
17	1	305	CLA	C4C-C3C	2.38	1.49	1.45
26	9	607	CHL	CHD-C4C	2.38	1.47	1.41
17	a	801	CLA	C1C-C2C	2.38	1.49	1.44
17	b	811	CLA	C4B-CHC	2.38	1.47	1.41
17	b	826	CLA	C4C-C3C	2.38	1.49	1.45
17	F	303	CLA	C1B-CHB	2.38	1.47	1.41
17	a	801	CLA	C4B-CHC	2.38	1.47	1.41
17	b	818	CLA	C1C-C2C	2.38	1.49	1.44
17	a	840	CLA	C4B-CHC	2.38	1.47	1.41
17	j	3002	CLA	C1C-C2C	2.38	1.49	1.44
17	7	602	CLA	C4C-C3C	2.38	1.49	1.45
17	a	806	CLA	C1B-CHB	2.38	1.47	1.41
17	3	306	CLA	C1C-C2C	2.38	1.49	1.44
17	a	828	CLA	CHD-C4C	2.38	1.47	1.41
17	a	817	CLA	C4B-CHC	2.37	1.47	1.41
17	6	316	CLA	C1B-CHB	2.37	1.47	1.41
17	a	827	CLA	C4C-C3C	2.37	1.49	1.45
17	A	832	CLA	C4C-C3C	2.37	1.49	1.45
17	a	839	CLA	C1B-CHB	2.37	1.47	1.41
17	A	817	CLA	C4B-CHC	2.37	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	840	CLA	C1B-CHB	2.37	1.47	1.41
17	a	823	CLA	C1B-CHB	2.37	1.47	1.41
26	9	606	CHL	C2C-C1C	2.37	1.49	1.44
17	a	812	CLA	C4C-C3C	2.37	1.49	1.45
17	b	810	CLA	C4C-C3C	2.37	1.49	1.45
17	a	807	CLA	C4C-C3C	2.37	1.49	1.45
17	1	314	CLA	C4B-CHC	2.37	1.47	1.41
17	A	843	CLA	C1B-CHB	2.37	1.47	1.41
17	9	610	CLA	C1C-C2C	2.37	1.49	1.44
17	b	807	CLA	C4C-C3C	2.37	1.49	1.45
17	a	817	CLA	C1B-CHB	2.37	1.47	1.41
17	A	810	CLA	C4B-CHC	2.37	1.47	1.41
17	a	824	CLA	C4B-CHC	2.37	1.47	1.41
17	3	306	CLA	C1B-CHB	2.37	1.47	1.41
17	1	202	CLA	C1B-CHB	2.37	1.47	1.41
17	B	822	CLA	C4B-CHC	2.37	1.47	1.41
17	b	815	CLA	C4B-CHC	2.37	1.47	1.41
17	b	811	CLA	C1B-CHB	2.37	1.47	1.41
17	A	820	CLA	C4B-CHC	2.37	1.47	1.41
17	7	604	CLA	C4B-CHC	2.37	1.47	1.41
17	1	310	CLA	C1C-C2C	2.37	1.49	1.44
17	B	824	CLA	C1C-C2C	2.37	1.49	1.44
17	a	822	CLA	C1C-C2C	2.37	1.49	1.44
17	a	841	CLA	C4C-C3C	2.37	1.49	1.45
17	a	836	CLA	C1B-CHB	2.37	1.47	1.41
17	8	302	CLA	C4B-CHC	2.37	1.47	1.41
17	3	313	CLA	C1B-CHB	2.37	1.47	1.41
17	b	821	CLA	C1C-C2C	2.37	1.49	1.44
17	b	836	CLA	C1B-CHB	2.37	1.47	1.41
26	7	606	CHL	C4B-CHC	2.37	1.47	1.41
17	1	304	CLA	C4B-CHC	2.37	1.47	1.41
17	a	836	CLA	C4C-C3C	2.37	1.49	1.45
17	A	816	CLA	C4C-C3C	2.37	1.49	1.45
17	a	833	CLA	C1B-CHB	2.37	1.47	1.41
17	b	806	CLA	C1B-CHB	2.36	1.47	1.41
17	6	314	CLA	C1C-C2C	2.36	1.49	1.44
17	A	804	CLA	C4C-C3C	2.36	1.49	1.45
17	6	310	CLA	C4B-CHC	2.36	1.47	1.41
17	B	815	CLA	C4C-C3C	2.36	1.49	1.45
17	6	313	CLA	C4B-CHC	2.36	1.47	1.41
17	9	608	CLA	C4C-C3C	2.36	1.49	1.45
17	7	603	CLA	C4C-C3C	2.36	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	810	CLA	C1C-C2C	2.36	1.49	1.44
17	B	815	CLA	C4B-CHC	2.36	1.47	1.41
17	a	831	CLA	C1C-C2C	2.36	1.49	1.44
26	1	307	CHL	CHD-C4C	2.36	1.47	1.41
17	a	824	CLA	C1B-CHB	2.36	1.47	1.41
17	B	810	CLA	C4C-C3C	2.36	1.49	1.45
17	3	305	CLA	C1B-CHB	2.36	1.47	1.41
17	A	822	CLA	C4B-CHC	2.36	1.47	1.41
17	4	610	CLA	C4B-CHC	2.36	1.47	1.41
17	L	204	CLA	C1C-C2C	2.36	1.49	1.44
17	a	819	CLA	C4C-C3C	2.36	1.49	1.45
26	6	303	CHL	C4C-C3C	2.36	1.49	1.45
17	b	835	CLA	C1C-C2C	2.36	1.49	1.44
17	B	816	CLA	C1C-C2C	2.36	1.49	1.44
17	a	808	CLA	C1B-CHB	2.36	1.47	1.41
17	B	805	CLA	C4C-C3C	2.36	1.49	1.45
17	A	854	CLA	C1C-C2C	2.36	1.49	1.44
17	b	815	CLA	C1C-C2C	2.36	1.49	1.44
26	7	605	CHL	C4B-CHC	2.36	1.47	1.41
17	2	603	CLA	C1C-C2C	2.36	1.49	1.44
17	B	817	CLA	C1C-C2C	2.36	1.49	1.44
17	A	819	CLA	C1B-CHB	2.36	1.47	1.41
17	a	805	CLA	C4B-CHC	2.36	1.47	1.41
17	9	608	CLA	C4B-CHC	2.36	1.47	1.41
17	A	824	CLA	C4B-CHC	2.35	1.47	1.41
17	A	845	CLA	C1C-C2C	2.35	1.49	1.44
17	6	312	CLA	C1C-C2C	2.35	1.49	1.44
17	a	805	CLA	C1C-C2C	2.35	1.49	1.44
17	3	306	CLA	C4C-C3C	2.35	1.49	1.45
17	a	836	CLA	C4B-CHC	2.35	1.47	1.41
17	A	818	CLA	C1C-C2C	2.35	1.49	1.44
17	4	602	CLA	C4C-C3C	2.35	1.49	1.45
26	6	303	CHL	C4B-CHC	2.35	1.47	1.41
17	9	610	CLA	C4C-C3C	2.35	1.49	1.45
17	8	312	CLA	C4C-C3C	2.35	1.49	1.45
17	B	833	CLA	C1B-CHB	2.35	1.47	1.41
17	J	3002	CLA	C1C-C2C	2.35	1.49	1.44
17	b	821	CLA	C4B-CHC	2.35	1.47	1.41
17	A	804	CLA	C1B-CHB	2.35	1.47	1.41
17	b	815	CLA	C4C-C3C	2.35	1.49	1.45
17	l	202	CLA	C4B-CHC	2.35	1.47	1.41
17	3	310	CLA	C1B-CHB	2.35	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	603	CLA	C4B-CHC	2.35	1.47	1.41
17	B	812	CLA	C1C-C2C	2.35	1.49	1.44
17	7	611	CLA	C4B-CHC	2.35	1.47	1.41
17	A	824	CLA	C1C-C2C	2.35	1.49	1.44
17	6	310	CLA	C1C-C2C	2.35	1.49	1.44
17	a	841	CLA	C1C-C2C	2.35	1.49	1.44
17	a	815	CLA	C4C-C3C	2.35	1.49	1.45
17	g	101	CLA	C4C-C3C	2.35	1.49	1.45
17	b	836	CLA	C4B-CHC	2.35	1.47	1.41
17	A	834	CLA	C1B-CHB	2.35	1.47	1.41
17	b	831	CLA	C1B-CHB	2.35	1.47	1.41
17	2	602	CLA	C1C-C2C	2.35	1.49	1.44
17	B	835	CLA	C1C-C2C	2.35	1.49	1.44
17	B	811	CLA	C4B-CHC	2.35	1.47	1.41
17	b	817	CLA	C4B-CHC	2.35	1.47	1.41
26	9	605	CHL	CHD-C4C	2.35	1.47	1.41
17	k	1403	CLA	C4B-CHC	2.35	1.47	1.41
17	a	835	CLA	C1C-C2C	2.35	1.49	1.44
17	6	307	CLA	C1C-C2C	2.35	1.49	1.44
17	A	832	CLA	C4B-CHC	2.35	1.47	1.41
17	4	602	CLA	C1C-C2C	2.35	1.49	1.44
17	A	805	CLA	C1B-CHB	2.35	1.47	1.41
26	7	614	CHL	CHD-C4C	2.35	1.47	1.41
17	4	601	CLA	C1B-CHB	2.35	1.47	1.41
17	a	822	CLA	C4C-C3C	2.35	1.49	1.45
17	a	802	CLA	C4C-C3C	2.35	1.49	1.45
17	4	614	CLA	C4C-C3C	2.35	1.49	1.45
26	2	606	CHL	C4B-CHC	2.35	1.47	1.41
17	6	309	CLA	C1B-CHB	2.34	1.47	1.41
17	6	305	CLA	C4B-CHC	2.34	1.47	1.41
26	9	605	CHL	C4B-CHC	2.34	1.47	1.41
17	7	608	CLA	C4C-C3C	2.34	1.49	1.45
17	B	827	CLA	C4C-C3C	2.34	1.49	1.45
17	A	830	CLA	C1B-CHB	2.34	1.47	1.41
22	F	302	HTG	C1-S1	-2.34	1.77	1.80
17	b	841	CLA	C1B-CHB	2.34	1.47	1.41
26	2	601	CHL	C4B-CHC	2.34	1.47	1.41
17	A	817	CLA	C1B-CHB	2.34	1.47	1.41
17	K	4003	CLA	C1B-CHB	2.34	1.47	1.41
17	A	833	CLA	C4C-C3C	2.34	1.49	1.45
17	b	840	CLA	C4B-CHC	2.34	1.47	1.41
26	7	607	CHL	C4B-CHC	2.34	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	821	CLA	C1C-C2C	2.34	1.49	1.44
17	B	821	CLA	C1B-CHB	2.34	1.47	1.41
17	3	303	CLA	C4B-CHC	2.34	1.47	1.41
17	a	810	CLA	C1B-CHB	2.34	1.47	1.41
17	6	312	CLA	C3A-C2A	-2.34	1.52	1.54
17	1	312	CLA	C1C-C2C	2.34	1.49	1.44
17	a	806	CLA	C1C-C2C	2.34	1.49	1.44
17	1	315	CLA	C1B-CHB	2.34	1.47	1.41
26	7	607	CHL	C4C-C3C	2.34	1.49	1.45
17	b	810	CLA	C1B-CHB	2.34	1.47	1.41
17	B	834	CLA	C1B-CHB	2.34	1.47	1.41
17	b	809	CLA	C1B-NB	-2.34	1.33	1.35
17	B	820	CLA	C1C-C2C	2.34	1.49	1.44
17	b	803	CLA	C1C-C2C	2.34	1.49	1.44
17	8	310	CLA	C1C-C2C	2.34	1.49	1.44
17	B	806	CLA	C1B-CHB	2.34	1.47	1.41
26	6	308	CHL	CHD-C4C	2.34	1.47	1.41
17	b	805	CLA	C4B-CHC	2.34	1.47	1.41
17	3	301	CLA	C1C-C2C	2.34	1.49	1.44
26	2	614	CHL	CHD-C4C	2.34	1.47	1.41
17	G	103	CLA	C1C-C2C	2.34	1.49	1.44
17	A	835	CLA	C4B-CHC	2.34	1.47	1.41
17	F	304	CLA	C1B-CHB	2.34	1.47	1.41
17	B	804	CLA	C4B-CHC	2.34	1.47	1.41
17	A	834	CLA	C4B-CHC	2.34	1.47	1.41
17	A	821	CLA	C4B-CHC	2.34	1.47	1.41
17	3	310	CLA	C1C-C2C	2.34	1.49	1.44
17	3	312	CLA	C1B-CHB	2.34	1.47	1.41
17	f	7003	CLA	C1C-C2C	2.34	1.49	1.44
17	9	611	CLA	C1C-C2C	2.34	1.49	1.44
17	1	309	CLA	C4B-CHC	2.34	1.47	1.41
17	A	837	CLA	C1B-CHB	2.34	1.47	1.41
26	1	302	CHL	C2C-C1C	2.33	1.49	1.44
17	7	611	CLA	C1B-CHB	2.33	1.47	1.41
17	A	827	CLA	C4C-C3C	2.33	1.49	1.45
17	9	614	CLA	C1C-C2C	2.33	1.49	1.44
17	B	805	CLA	C4B-CHC	2.33	1.47	1.41
17	1	303	CLA	C1B-CHB	2.33	1.47	1.41
17	a	832	CLA	C4B-CHC	2.33	1.47	1.41
17	4	614	CLA	C1C-C2C	2.33	1.49	1.44
17	9	612	CLA	C1B-CHB	2.33	1.47	1.41
17	b	823	CLA	C1B-CHB	2.33	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	820	CLA	C4B-CHC	2.33	1.47	1.41
17	6	310	CLA	C1B-CHB	2.33	1.47	1.41
17	4	603	CLA	C1B-CHB	2.33	1.47	1.41
17	b	830	CLA	C1C-C2C	2.33	1.49	1.44
17	A	803	CLA	C4C-C3C	2.33	1.49	1.45
17	l	204	CLA	C4C-C3C	2.33	1.49	1.45
17	a	837	CLA	C1C-C2C	2.33	1.49	1.44
17	A	839	CLA	C4B-CHC	2.33	1.47	1.41
17	B	840	CLA	C1C-C2C	2.33	1.49	1.44
17	b	812	CLA	C1C-C2C	2.33	1.49	1.44
17	a	828	CLA	C1B-CHB	2.33	1.47	1.41
17	1	311	CLA	C1C-C2C	2.33	1.49	1.44
17	B	820	CLA	C1B-CHB	2.33	1.47	1.41
17	B	810	CLA	C1C-C2C	2.33	1.49	1.44
17	A	802	CLA	C4C-C3C	2.33	1.49	1.45
17	b	807	CLA	C1B-CHB	2.33	1.47	1.41
17	b	833	CLA	C1C-C2C	2.33	1.49	1.44
17	a	831	CLA	C1B-NB	-2.33	1.33	1.35
26	4	615	CHL	C4C-C3C	2.33	1.49	1.45
17	3	303	CLA	C1B-CHB	2.33	1.47	1.41
17	a	815	CLA	C1B-CHB	2.33	1.47	1.41
17	l	202	CLA	C1C-C2C	2.33	1.49	1.44
17	1	311	CLA	C3A-C2A	-2.33	1.52	1.54
17	8	305	CLA	C1C-C2C	2.33	1.49	1.44
17	2	613	CLA	C1C-C2C	2.33	1.49	1.44
17	9	604	CLA	C1C-C2C	2.33	1.49	1.44
17	7	611	CLA	C1C-C2C	2.33	1.49	1.44
26	9	615	CHL	C2C-C1C	2.33	1.49	1.44
17	3	314	CLA	C1C-C2C	2.33	1.49	1.44
26	6	308	CHL	C4B-CHC	2.33	1.47	1.41
26	2	601	CHL	CHD-C4C	2.32	1.47	1.41
17	B	829	CLA	C1B-CHB	2.32	1.47	1.41
26	7	605	CHL	CHD-C4C	2.32	1.47	1.41
22	f	7001	HTG	C1-S1	-2.32	1.77	1.80
17	A	826	CLA	C4C-C3C	2.32	1.49	1.45
17	b	811	CLA	C4C-C3C	2.32	1.49	1.45
17	1	313	CLA	C1B-CHB	2.32	1.47	1.41
17	8	310	CLA	C1B-CHB	2.32	1.47	1.41
17	b	834	CLA	C1C-C2C	2.32	1.49	1.44
17	B	818	CLA	C1C-C2C	2.32	1.49	1.44
17	A	843	CLA	C4B-CHC	2.32	1.47	1.41
17	f	7002	CLA	C1B-CHB	2.32	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	4	606	CHL	C4B-CHC	2.32	1.47	1.41
17	k	1403	CLA	C1B-CHB	2.32	1.47	1.41
26	2	607	CHL	C4B-CHC	2.32	1.47	1.41
17	2	611	CLA	C1B-CHB	2.32	1.47	1.41
17	B	838	CLA	C4B-CHC	2.32	1.47	1.41
17	b	838	CLA	C4C-C3C	2.32	1.49	1.45
17	B	831	CLA	C1C-C2C	2.32	1.49	1.44
17	A	837	CLA	C1C-C2C	2.32	1.49	1.44
17	A	809	CLA	C4B-CHC	2.32	1.47	1.41
26	9	606	CHL	C4B-CHC	2.32	1.47	1.41
17	4	612	CLA	C4B-CHC	2.32	1.47	1.41
17	8	309	CLA	C1C-C2C	2.32	1.49	1.44
17	A	801	CLA	C4C-C3C	2.32	1.49	1.45
26	7	601	CHL	CHD-C4C	2.32	1.47	1.41
17	8	304	CLA	C1B-CHB	2.32	1.47	1.41
17	A	806	CLA	C1B-CHB	2.32	1.47	1.41
17	1	308	CLA	C1B-CHB	2.32	1.47	1.41
17	b	804	CLA	C4B-CHC	2.32	1.47	1.41
17	9	603	CLA	C4C-C3C	2.32	1.49	1.45
17	A	839	CLA	C4C-C3C	2.32	1.49	1.45
17	6	316	CLA	C1C-C2C	2.32	1.49	1.44
17	7	612	CLA	C1C-C2C	2.32	1.49	1.44
17	a	844	CLA	C4C-C3C	2.32	1.49	1.45
17	b	813	CLA	C1B-CHB	2.32	1.47	1.41
17	b	812	CLA	C1B-CHB	2.32	1.47	1.41
17	K	4002	CLA	C1B-CHB	2.32	1.47	1.41
17	a	819	CLA	C1B-CHB	2.32	1.47	1.41
26	1	307	CHL	C4C-C3C	2.32	1.49	1.45
17	a	844	CLA	C1C-C2C	2.32	1.49	1.44
17	b	835	CLA	C1B-CHB	2.32	1.47	1.41
17	G	103	CLA	C1B-CHB	2.32	1.47	1.41
17	g	101	CLA	C4B-CHC	2.32	1.47	1.41
26	1	307	CHL	C4B-CHC	2.32	1.47	1.41
17	b	821	CLA	C1B-CHB	2.31	1.47	1.41
17	7	610	CLA	C4B-CHC	2.31	1.47	1.41
17	B	840	CLA	C1B-CHB	2.31	1.47	1.41
17	a	836	CLA	C1C-C2C	2.31	1.49	1.44
17	a	806	CLA	C4B-CHC	2.31	1.47	1.41
17	9	601	CLA	C1C-C2C	2.31	1.49	1.44
26	7	614	CHL	C2C-C1C	2.31	1.49	1.44
17	a	805	CLA	C4C-C3C	2.31	1.49	1.45
26	4	607	CHL	C4B-CHC	2.31	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	809	CLA	C1C-C2C	2.31	1.49	1.44
17	g	101	CLA	C3A-C2A	-2.31	1.52	1.54
17	1	304	CLA	C1B-CHB	2.31	1.47	1.41
17	A	830	CLA	C4C-C3C	2.31	1.49	1.45
17	2	604	CLA	C1C-C2C	2.31	1.49	1.44
26	7	607	CHL	CHD-C4C	2.31	1.47	1.41
17	a	844	CLA	C1B-CHB	2.31	1.47	1.41
17	2	612	CLA	C1B-CHB	2.31	1.47	1.41
17	G	101	CLA	C1C-C2C	2.31	1.49	1.44
26	3	307	CHL	CHD-C4C	2.31	1.47	1.41
17	b	832	CLA	C1B-CHB	2.31	1.47	1.41
17	l	204	CLA	C1C-C2C	2.31	1.49	1.44
17	g	103	CLA	C1C-C2C	2.31	1.49	1.44
26	6	303	CHL	C2C-C1C	2.31	1.49	1.44
17	b	808	CLA	C4B-CHC	2.31	1.47	1.41
17	A	813	CLA	C1C-C2C	2.31	1.49	1.44
17	2	610	CLA	C4B-CHC	2.31	1.47	1.41
17	6	313	CLA	C1C-C2C	2.31	1.49	1.44
17	3	313	CLA	C1C-C2C	2.31	1.49	1.44
17	a	811	CLA	C4B-CHC	2.31	1.47	1.41
17	A	807	CLA	C1B-CHB	2.31	1.47	1.41
26	9	607	CHL	C4B-CHC	2.31	1.47	1.41
17	A	832	CLA	C1C-C2C	2.31	1.49	1.44
26	7	614	CHL	C4C-C3C	2.31	1.49	1.45
17	A	829	CLA	C4B-CHC	2.31	1.47	1.41
26	2	614	CHL	C4B-CHC	2.31	1.47	1.41
26	2	607	CHL	CHD-C4C	2.31	1.47	1.41
26	1	302	CHL	CHD-C4C	2.31	1.47	1.41
17	9	601	CLA	C1B-CHB	2.31	1.47	1.41
17	9	602	CLA	C4C-C3C	2.31	1.49	1.45
17	A	821	CLA	C1B-CHB	2.31	1.47	1.41
17	A	816	CLA	C1C-C2C	2.31	1.49	1.44
17	A	836	CLA	C1B-CHB	2.31	1.47	1.41
17	b	828	CLA	C1B-CHB	2.31	1.47	1.41
17	A	825	CLA	C4B-CHC	2.31	1.47	1.41
17	3	311	CLA	C1B-CHB	2.31	1.47	1.41
17	B	811	CLA	C1C-C2C	2.31	1.49	1.44
17	a	820	CLA	C1C-C2C	2.30	1.49	1.44
17	g	102	CLA	C1B-CHB	2.30	1.47	1.41
17	a	806	CLA	C4C-C3C	2.30	1.49	1.45
17	1	315	CLA	C1C-C2C	2.30	1.49	1.44
17	2	603	CLA	C1B-CHB	2.30	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	805	CLA	C1C-C2C	2.30	1.49	1.44
17	g	101	CLA	C1C-C2C	2.30	1.49	1.44
17	7	609	CLA	C4C-C3C	2.30	1.49	1.45
17	b	838	CLA	C1B-CHB	2.30	1.47	1.41
17	a	813	CLA	C1B-CHB	2.30	1.47	1.41
17	A	817	CLA	C1C-C2C	2.30	1.49	1.44
17	a	842	CLA	C4C-C3C	2.30	1.49	1.45
26	8	306	CHL	C4B-CHC	2.30	1.47	1.41
17	F	303	CLA	C4C-C3C	2.30	1.49	1.45
17	B	838	CLA	C4C-C3C	2.30	1.49	1.45
17	6	306	CLA	C1C-C2C	2.30	1.49	1.44
17	b	837	CLA	C4C-C3C	2.30	1.49	1.45
17	k	1401	CLA	C1B-CHB	2.30	1.47	1.41
17	8	309	CLA	C1B-CHB	2.30	1.47	1.41
17	2	609	CLA	C4C-C3C	2.30	1.49	1.45
17	7	608	CLA	C1C-C2C	2.30	1.49	1.44
26	2	606	CHL	CHD-C4C	2.30	1.47	1.41
17	B	806	CLA	C4C-C3C	2.30	1.49	1.45
26	9	605	CHL	C4C-C3C	2.30	1.49	1.45
17	A	811	CLA	C1B-CHB	2.30	1.47	1.41
17	b	820	CLA	C1B-CHB	2.30	1.47	1.41
17	A	808	CLA	C4B-CHC	2.30	1.47	1.41
26	2	614	CHL	C2C-C1C	2.30	1.49	1.44
17	1	311	CLA	C1B-CHB	2.30	1.47	1.41
17	B	813	CLA	C1B-CHB	2.30	1.47	1.41
17	a	843	CLA	C1C-C2C	2.30	1.49	1.44
17	b	804	CLA	C1B-CHB	2.29	1.47	1.41
17	9	608	CLA	C1C-C2C	2.29	1.49	1.44
17	g	103	CLA	C1B-CHB	2.29	1.47	1.41
17	4	611	CLA	C1C-C2C	2.29	1.49	1.44
17	B	837	CLA	C1B-CHB	2.29	1.47	1.41
17	A	836	CLA	C1C-C2C	2.29	1.49	1.44
17	A	826	CLA	C1B-CHB	2.29	1.47	1.41
26	3	307	CHL	C2C-C1C	2.29	1.49	1.44
17	B	838	CLA	C1C-C2C	2.29	1.49	1.44
17	3	304	CLA	C1C-C2C	2.29	1.49	1.44
17	A	828	CLA	C1B-CHB	2.29	1.47	1.41
17	A	813	CLA	C1B-CHB	2.29	1.47	1.41
17	A	829	CLA	C1B-CHB	2.29	1.47	1.41
17	B	840	CLA	C4C-C3C	2.29	1.49	1.45
17	6	305	CLA	C1C-C2C	2.29	1.49	1.44
17	b	831	CLA	C4C-C3C	2.29	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	818	CLA	C4B-CHC	2.29	1.47	1.41
17	J	3002	CLA	C1B-CHB	2.29	1.47	1.41
17	B	828	CLA	C1B-CHB	2.29	1.47	1.41
17	2	612	CLA	C1C-C2C	2.29	1.49	1.44
17	6	312	CLA	C4C-C3C	2.29	1.49	1.45
17	6	307	CLA	C1B-CHB	2.29	1.47	1.41
17	b	802	CLA	C4B-CHC	2.29	1.47	1.41
17	b	816	CLA	C1C-C2C	2.29	1.49	1.44
17	a	802	CLA	C1C-C2C	2.29	1.49	1.44
17	a	801	CLA	C1B-CHB	2.29	1.47	1.41
17	a	805	CLA	C1B-CHB	2.29	1.47	1.41
26	9	615	CHL	C4B-CHC	2.29	1.47	1.41
26	7	601	CHL	C2C-C1C	2.29	1.49	1.44
17	B	825	CLA	C1B-CHB	2.29	1.47	1.41
17	6	304	CLA	C1B-CHB	2.29	1.47	1.41
17	b	824	CLA	C1B-CHB	2.29	1.47	1.41
17	G	101	CLA	C4C-C3C	2.29	1.49	1.45
26	7	605	CHL	C4C-C3C	2.29	1.49	1.45
17	8	302	CLA	C1C-C2C	2.29	1.49	1.44
17	a	816	CLA	C4C-C3C	2.29	1.49	1.45
17	a	837	CLA	C1B-CHB	2.29	1.47	1.41
17	6	312	CLA	C1B-CHB	2.29	1.47	1.41
17	4	604	CLA	C1C-C2C	2.29	1.49	1.44
26	4	607	CHL	CHD-C4C	2.29	1.47	1.41
17	a	820	CLA	C1B-CHB	2.29	1.47	1.41
17	b	829	CLA	C1B-CHB	2.29	1.47	1.41
26	7	614	CHL	C4B-CHC	2.29	1.47	1.41
17	8	311	CLA	C1C-C2C	2.28	1.49	1.44
17	b	817	CLA	C1C-C2C	2.28	1.49	1.44
17	8	311	CLA	C1B-CHB	2.28	1.47	1.41
17	7	613	CLA	C1C-C2C	2.28	1.49	1.44
17	a	831	CLA	C4B-CHC	2.28	1.47	1.41
17	A	822	CLA	C1C-C2C	2.28	1.49	1.44
17	a	856	CLA	C1B-NB	-2.28	1.33	1.35
17	A	824	CLA	C1B-CHB	2.28	1.47	1.41
17	8	304	CLA	C1C-C2C	2.28	1.49	1.44
17	a	825	CLA	C4C-C3C	2.28	1.49	1.45
17	B	819	CLA	C4B-CHC	2.28	1.47	1.41
17	B	808	CLA	C4B-CHC	2.28	1.47	1.41
17	9	612	CLA	C1C-C2C	2.28	1.49	1.44
17	a	824	CLA	C1C-C2C	2.28	1.49	1.44
17	8	307	CLA	C4C-C3C	2.28	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	303	CLA	C1C-C2C	2.28	1.49	1.44
17	4	603	CLA	C1C-C2C	2.28	1.49	1.44
17	6	306	CLA	C1B-CHB	2.28	1.47	1.41
17	7	603	CLA	C1B-CHB	2.28	1.47	1.41
17	B	818	CLA	C1B-CHB	2.28	1.47	1.41
26	9	606	CHL	CHD-C4C	2.28	1.47	1.41
17	a	801	CLA	C4C-C3C	2.28	1.49	1.45
17	a	808	CLA	C4C-C3C	2.28	1.49	1.45
17	b	837	CLA	C1B-CHB	2.28	1.47	1.41
17	A	838	CLA	C1B-CHB	2.28	1.47	1.41
17	4	613	CLA	C1B-CHB	2.28	1.47	1.41
17	A	819	CLA	C1C-C2C	2.28	1.49	1.44
17	b	837	CLA	C1C-C2C	2.28	1.49	1.44
17	3	301	CLA	C1B-CHB	2.28	1.47	1.41
17	A	815	CLA	C1B-CHB	2.28	1.47	1.41
17	6	311	CLA	C4C-C3C	2.28	1.49	1.45
26	7	614	CHL	C1B-CHB	2.28	1.47	1.41
17	F	301	CLA	C1B-CHB	2.27	1.47	1.41
17	9	604	CLA	C1B-CHB	2.27	1.47	1.41
17	b	813	CLA	C1C-C2C	2.27	1.49	1.44
17	4	613	CLA	C1C-C2C	2.27	1.49	1.44
17	B	835	CLA	C4C-C3C	2.27	1.49	1.45
17	B	828	CLA	C4C-C3C	2.27	1.49	1.45
17	9	613	CLA	C1B-CHB	2.27	1.47	1.41
17	b	815	CLA	C1B-CHB	2.27	1.47	1.41
17	A	845	CLA	C1B-CHB	2.27	1.47	1.41
17	1	305	CLA	C1C-C2C	2.27	1.49	1.44
17	a	811	CLA	C1C-C2C	2.27	1.49	1.44
26	4	605	CHL	C4C-C3C	2.27	1.49	1.45
17	a	814	CLA	C4C-C3C	2.27	1.49	1.45
17	a	843	CLA	C4C-C3C	2.27	1.49	1.45
17	B	839	CLA	C1B-CHB	2.27	1.47	1.41
17	K	4003	CLA	C1C-C2C	2.27	1.49	1.44
17	9	613	CLA	C1C-C2C	2.27	1.49	1.44
26	8	306	CHL	CHD-C4C	2.27	1.47	1.41
17	7	610	CLA	C1B-CHB	2.27	1.47	1.41
17	B	810	CLA	C1B-CHB	2.27	1.47	1.41
17	3	305	CLA	C1C-C2C	2.27	1.49	1.44
17	B	815	CLA	C1B-CHB	2.27	1.47	1.41
17	A	811	CLA	C1C-C2C	2.27	1.49	1.44
17	A	842	CLA	C1B-CHB	2.27	1.47	1.41
17	A	832	CLA	C1B-CHB	2.27	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	610	CLA	C1B-CHB	2.27	1.47	1.41
17	a	846	CLA	C1B-CHB	2.27	1.47	1.41
17	1	313	CLA	C1C-C2C	2.27	1.49	1.44
17	8	305	CLA	C1B-CHB	2.27	1.47	1.41
17	6	314	CLA	C1B-CHB	2.27	1.47	1.41
17	a	834	CLA	C4C-C3C	2.27	1.48	1.45
17	b	819	CLA	C4B-CHC	2.27	1.47	1.41
17	A	803	CLA	C4B-CHC	2.27	1.47	1.41
17	9	603	CLA	C1B-CHB	2.26	1.47	1.41
17	b	826	CLA	C1B-CHB	2.26	1.47	1.41
17	a	842	CLA	C1B-CHB	2.26	1.47	1.41
17	A	854	CLA	C4B-CHC	2.26	1.47	1.41
17	B	819	CLA	C1B-CHB	2.26	1.47	1.41
17	A	816	CLA	C1B-CHB	2.26	1.47	1.41
17	A	825	CLA	C1C-C2C	2.26	1.48	1.44
17	a	818	CLA	C1B-CHB	2.26	1.47	1.41
17	A	821	CLA	C1C-C2C	2.26	1.48	1.44
17	B	836	CLA	C1B-CHB	2.26	1.47	1.41
17	8	303	CLA	C1C-C2C	2.26	1.48	1.44
17	f	7003	CLA	C1B-CHB	2.26	1.47	1.41
17	A	818	CLA	C1B-CHB	2.26	1.47	1.41
17	6	305	CLA	C1B-CHB	2.26	1.47	1.41
17	a	835	CLA	C4C-C3C	2.26	1.48	1.45
17	1	306	CLA	C1C-C2C	2.26	1.48	1.44
17	6	315	CLA	C1C-C2C	2.26	1.48	1.44
26	7	606	CHL	CHD-C4C	2.26	1.47	1.41
17	a	834	CLA	C1B-CHB	2.26	1.47	1.41
17	1	312	CLA	C1B-CHB	2.26	1.47	1.41
17	A	812	CLA	C1B-CHB	2.26	1.47	1.41
17	B	804	CLA	C1B-CHB	2.26	1.47	1.41
17	A	823	CLA	C1B-CHB	2.26	1.47	1.41
17	4	610	CLA	C1B-CHB	2.26	1.47	1.41
26	7	607	CHL	C1B-CHB	2.26	1.47	1.41
26	9	605	CHL	C2C-C1C	2.26	1.49	1.44
17	2	610	CLA	C1C-C2C	2.26	1.48	1.44
17	B	809	CLA	C1B-CHB	2.26	1.47	1.41
17	L	202	CLA	C1B-CHB	2.26	1.47	1.41
17	4	611	CLA	C1B-CHB	2.26	1.47	1.41
17	L	204	CLA	C1B-CHB	2.26	1.47	1.41
17	B	809	CLA	C4B-CHC	2.26	1.47	1.41
17	a	838	CLA	C1B-CHB	2.26	1.47	1.41
17	a	827	CLA	C1B-CHB	2.26	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	309	CLA	C1C-C2C	2.26	1.48	1.44
17	a	811	CLA	C1B-CHB	2.26	1.47	1.41
17	b	814	CLA	C4C-C3C	2.26	1.48	1.45
17	B	841	CLA	C1B-CHB	2.26	1.47	1.41
17	9	614	CLA	C1B-CHB	2.26	1.47	1.41
17	a	841	CLA	C1B-CHB	2.25	1.47	1.41
17	b	805	CLA	C1B-CHB	2.25	1.47	1.41
17	B	818	CLA	C4C-C3C	2.25	1.48	1.45
17	B	809	CLA	C1C-C2C	2.25	1.48	1.44
17	3	304	CLA	C1B-CHB	2.25	1.47	1.41
17	3	312	CLA	C1C-C2C	2.25	1.48	1.44
17	1	305	CLA	C1B-CHB	2.25	1.47	1.41
17	a	823	CLA	C4C-C3C	2.25	1.48	1.45
17	b	820	CLA	C4C-C3C	2.25	1.48	1.45
17	a	813	CLA	C1C-C2C	2.25	1.48	1.44
17	1	306	CLA	C1B-CHB	2.25	1.47	1.41
17	6	315	CLA	C1B-CHB	2.25	1.47	1.41
17	b	836	CLA	C4C-C3C	2.25	1.48	1.45
17	A	820	CLA	C1B-CHB	2.25	1.47	1.41
17	7	613	CLA	C1B-CHB	2.25	1.47	1.41
17	7	610	CLA	C1C-C2C	2.25	1.48	1.44
17	3	309	CLA	C4C-C3C	2.25	1.48	1.45
26	7	601	CHL	C1B-CHB	2.25	1.47	1.41
17	B	812	CLA	C1B-CHB	2.24	1.47	1.41
17	8	303	CLA	C1B-CHB	2.24	1.47	1.41
26	4	615	CHL	C1B-CHB	2.24	1.47	1.41
26	4	605	CHL	C4B-CHC	2.24	1.47	1.41
17	b	802	CLA	C1B-CHB	2.24	1.47	1.41
17	A	839	CLA	C1C-C2C	2.24	1.48	1.44
17	B	826	CLA	C1B-CHB	2.24	1.47	1.41
17	a	843	CLA	C1B-CHB	2.24	1.47	1.41
17	B	830	CLA	C1B-CHB	2.24	1.47	1.41
26	7	605	CHL	C1B-CHB	2.24	1.47	1.41
17	2	602	CLA	C1B-CHB	2.24	1.47	1.41
17	A	842	CLA	C1C-C2C	2.24	1.48	1.44
17	A	831	CLA	C4B-CHC	2.24	1.47	1.41
17	B	824	CLA	C1B-CHB	2.24	1.47	1.41
17	6	304	CLA	C1C-C2C	2.24	1.48	1.44
17	A	818	CLA	C4C-C3C	2.24	1.48	1.45
17	1	314	CLA	C1B-CHB	2.24	1.47	1.41
17	B	841	CLA	C4C-C3C	2.24	1.48	1.45
17	B	807	CLA	C1B-CHB	2.23	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	806	CLA	C4C-C3C	2.23	1.48	1.45
17	B	805	CLA	C1C-C2C	2.23	1.48	1.44
17	b	830	CLA	C1B-CHB	2.23	1.47	1.41
26	7	605	CHL	C2C-C1C	2.23	1.49	1.44
17	1	309	CLA	C1B-CHB	2.23	1.47	1.41
17	2	613	CLA	C1B-CHB	2.23	1.47	1.41
17	6	313	CLA	C1B-CHB	2.23	1.47	1.41
17	j	3002	CLA	C1B-CHB	2.23	1.47	1.41
17	B	819	CLA	C1C-C2C	2.23	1.48	1.44
17	A	833	CLA	C1B-CHB	2.23	1.47	1.41
17	l	203	CLA	C1B-CHB	2.23	1.47	1.41
17	a	817	CLA	C1C-C2C	2.22	1.48	1.44
17	9	608	CLA	C1B-CHB	2.22	1.47	1.41
17	G	104	CLA	C1B-CHB	2.22	1.47	1.41
17	2	610	CLA	C1B-CHB	2.22	1.47	1.41
17	2	604	CLA	C1B-CHB	2.22	1.47	1.41
17	1	314	CLA	C1C-C2C	2.22	1.48	1.44
26	8	306	CHL	C1B-CHB	2.22	1.47	1.41
17	3	314	CLA	C1B-CHB	2.22	1.47	1.41
17	B	802	CLA	C4C-C3C	2.22	1.48	1.45
26	1	307	CHL	C1B-CHB	2.22	1.47	1.41
17	L	203	CLA	C4C-C3C	2.22	1.48	1.45
17	7	604	CLA	C1C-C2C	2.22	1.48	1.44
17	l	204	CLA	C1B-CHB	2.22	1.47	1.41
17	4	612	CLA	C1C-C2C	2.22	1.48	1.44
17	k	1403	CLA	C1C-C2C	2.22	1.48	1.44
26	6	308	CHL	C4C-C3C	2.22	1.48	1.45
17	3	310	CLA	C3A-C2A	-2.22	1.52	1.54
17	B	802	CLA	C1B-CHB	2.22	1.47	1.41
17	7	602	CLA	C1B-CHB	2.22	1.47	1.41
17	b	808	CLA	C4C-C3C	2.22	1.48	1.45
17	A	843	CLA	C1C-C2C	2.22	1.48	1.44
17	A	831	CLA	C1C-C2C	2.21	1.48	1.44
17	A	821	CLA	C4C-C3C	2.21	1.48	1.45
17	A	854	CLA	C4C-C3C	2.21	1.48	1.45
17	b	818	CLA	C1B-CHB	2.21	1.47	1.41
17	8	312	CLA	C1B-CHB	2.21	1.47	1.41
17	a	831	CLA	C1B-CHB	2.21	1.47	1.41
17	a	856	CLA	C1C-C2C	2.21	1.48	1.44
17	L	202	CLA	C1C-C2C	2.21	1.48	1.44
17	B	805	CLA	C1B-CHB	2.21	1.47	1.41
17	4	608	CLA	C1B-CHB	2.21	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	835	CLA	C1B-CHB	2.21	1.47	1.41
17	A	829	CLA	C4C-C3C	2.21	1.48	1.45
17	B	817	CLA	C1B-CHB	2.21	1.47	1.41
17	4	614	CLA	C1B-CHB	2.21	1.47	1.41
17	a	803	CLA	C1B-CHB	2.20	1.47	1.41
17	b	809	CLA	C4B-CHC	2.20	1.47	1.41
17	4	609	CLA	C4C-C3C	2.20	1.48	1.45
17	A	812	CLA	C4C-C3C	2.20	1.48	1.45
17	b	825	CLA	C4C-C3C	2.20	1.48	1.45
17	a	818	CLA	C1C-C2C	2.20	1.48	1.44
17	b	819	CLA	C1C-C2C	2.20	1.48	1.44
26	6	308	CHL	C1B-CHB	2.20	1.47	1.41
17	a	832	CLA	C1B-CHB	2.20	1.47	1.41
17	b	829	CLA	C1B-NB	-2.20	1.33	1.35
17	4	602	CLA	C1B-CHB	2.20	1.47	1.41
17	b	840	CLA	C4C-C3C	2.20	1.48	1.45
17	b	809	CLA	C1B-CHB	2.20	1.47	1.41
17	9	611	CLA	C1B-CHB	2.20	1.47	1.41
17	B	822	CLA	C1B-CHB	2.20	1.47	1.41
17	b	831	CLA	C1C-C2C	2.20	1.48	1.44
17	b	827	CLA	C4C-C3C	2.20	1.48	1.45
17	B	834	CLA	C1C-C2C	2.20	1.48	1.44
17	1	310	CLA	C1B-CHB	2.20	1.47	1.41
17	A	834	CLA	C1C-C2C	2.19	1.48	1.44
17	B	833	CLA	C4C-C3C	2.19	1.48	1.45
17	1	304	CLA	C1C-C2C	2.19	1.48	1.44
17	l	203	CLA	C4C-C3C	2.19	1.48	1.45
17	9	602	CLA	C1B-CHB	2.19	1.47	1.41
17	k	1402	CLA	C1C-C2C	2.19	1.48	1.44
17	B	836	CLA	C4C-C3C	2.19	1.48	1.45
17	4	604	CLA	C1B-CHB	2.19	1.47	1.41
17	L	203	CLA	C1B-CHB	2.19	1.47	1.41
17	a	807	CLA	C1B-CHB	2.19	1.47	1.41
17	b	808	CLA	C1B-CHB	2.19	1.47	1.41
17	A	819	CLA	C4C-C3C	2.19	1.48	1.45
17	a	829	CLA	C1B-CHB	2.19	1.47	1.41
17	B	814	CLA	C1B-CHB	2.19	1.47	1.41
17	B	808	CLA	C1B-CHB	2.18	1.47	1.41
17	b	822	CLA	C4C-C3C	2.18	1.48	1.45
17	a	809	CLA	C1B-CHB	2.18	1.47	1.41
17	a	803	CLA	C1C-C2C	2.18	1.48	1.44
17	A	801	CLA	C1B-CHB	2.18	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	309	CLA	C1B-CHB	2.18	1.47	1.41
17	b	817	CLA	C1B-CHB	2.18	1.47	1.41
17	a	804	CLA	C4C-C3C	2.18	1.48	1.45
17	2	608	CLA	C1B-CHB	2.18	1.47	1.41
17	a	830	CLA	C4C-C3C	2.18	1.48	1.45
17	A	841	CLA	C1B-CHB	2.17	1.47	1.41
17	B	825	CLA	C4C-C3C	2.17	1.48	1.45
17	B	814	CLA	C4C-C3C	2.17	1.48	1.45
17	b	805	CLA	C1C-C2C	2.17	1.48	1.44
17	A	831	CLA	C1B-CHB	2.17	1.47	1.41
26	4	607	CHL	C1B-CHB	2.17	1.47	1.41
17	A	806	CLA	C1C-C2C	2.17	1.48	1.44
17	b	819	CLA	C1B-CHB	2.17	1.47	1.41
26	3	307	CHL	C1B-CHB	2.17	1.47	1.41
26	2	601	CHL	C1B-CHB	2.17	1.47	1.41
26	7	606	CHL	C1B-CHB	2.17	1.47	1.41
17	b	822	CLA	C1B-CHB	2.16	1.47	1.41
17	8	301	CLA	C1B-CHB	2.16	1.47	1.41
17	A	809	CLA	C1B-CHB	2.16	1.47	1.41
17	A	822	CLA	C1B-CHB	2.16	1.47	1.41
26	9	606	CHL	C4C-C3C	2.16	1.48	1.45
17	b	803	CLA	C4C-C3C	2.16	1.48	1.45
17	B	837	CLA	C4C-C3C	2.16	1.48	1.45
17	4	603	CLA	C4C-C3C	2.16	1.48	1.45
17	A	814	CLA	C1B-CHB	2.16	1.47	1.41
17	A	835	CLA	C1B-CHB	2.16	1.47	1.41
17	a	812	CLA	C1B-CHB	2.16	1.47	1.41
17	6	311	CLA	C1B-CHB	2.16	1.47	1.41
26	2	606	CHL	C1B-CHB	2.16	1.47	1.41
17	a	856	CLA	C4B-CHC	2.16	1.47	1.41
17	b	802	CLA	C1C-C2C	2.16	1.48	1.44
26	2	614	CHL	C1B-CHB	2.16	1.47	1.41
26	2	607	CHL	C4C-C3C	2.16	1.48	1.45
26	9	607	CHL	C1B-CHB	2.16	1.47	1.41
17	b	808	CLA	C1C-C2C	2.16	1.48	1.44
17	A	854	CLA	C1B-CHB	2.16	1.47	1.41
17	a	828	CLA	C4C-C3C	2.15	1.48	1.45
17	9	609	CLA	C1B-CHB	2.15	1.47	1.41
17	8	302	CLA	C1B-CHB	2.15	1.47	1.41
17	3	308	CLA	C1B-CHB	2.15	1.47	1.41
17	7	604	CLA	C1B-CHB	2.15	1.47	1.41
17	A	835	CLA	C1C-C2C	2.15	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	302	CHL	C1B-CHB	2.15	1.47	1.41
26	9	607	CHL	C4C-C3C	2.15	1.48	1.45
26	3	307	CHL	C4B-CHC	2.15	1.47	1.41
17	b	804	CLA	C4C-C3C	2.15	1.48	1.45
17	4	609	CLA	C1B-CHB	2.15	1.47	1.41
26	7	606	CHL	C4C-C3C	2.15	1.48	1.45
17	b	814	CLA	C1B-CHB	2.14	1.47	1.41
17	A	827	CLA	C1B-CHB	2.14	1.46	1.41
17	2	609	CLA	C1B-CHB	2.14	1.46	1.41
17	a	814	CLA	C1B-CHB	2.14	1.46	1.41
17	b	829	CLA	C4B-CHC	2.14	1.46	1.41
17	b	827	CLA	C1B-CHB	2.14	1.46	1.41
17	8	307	CLA	C1B-CHB	2.14	1.46	1.41
17	b	829	CLA	C1C-C2C	2.14	1.48	1.44
26	2	605	CHL	C1B-CHB	2.13	1.46	1.41
17	8	308	CLA	C1B-CHB	2.13	1.46	1.41
17	A	810	CLA	C4C-C3C	2.13	1.48	1.45
17	a	803	CLA	C4B-CHC	2.13	1.46	1.41
26	9	615	CHL	C1B-CHB	2.13	1.46	1.41
17	B	816	CLA	C1B-CHB	2.13	1.46	1.41
17	B	835	CLA	C1B-CHB	2.13	1.46	1.41
17	a	833	CLA	C4C-C3C	2.12	1.48	1.45
17	2	608	CLA	C1C-C2C	2.12	1.48	1.44
26	4	606	CHL	C1B-CHB	2.12	1.46	1.41
17	b	828	CLA	C4C-C3C	2.12	1.48	1.45
17	3	315	CLA	C3D-C2D	2.12	1.49	1.39
26	3	307	CHL	C1B-NB	-2.12	1.33	1.35
17	A	803	CLA	C1B-CHB	2.12	1.46	1.41
17	3	302	CLA	C1B-CHB	2.12	1.46	1.41
17	B	809	CLA	C1B-NB	-2.12	1.33	1.35
17	B	833	CLA	C1C-C2C	2.12	1.48	1.44
17	f	7002	CLA	C4C-C3C	2.11	1.48	1.45
26	2	601	CHL	C2C-C1C	2.11	1.49	1.44
17	B	829	CLA	C4B-CHC	2.11	1.46	1.41
26	2	607	CHL	C1B-CHB	2.11	1.46	1.41
17	A	828	CLA	C4C-C3C	2.11	1.48	1.45
17	a	822	CLA	C1B-CHB	2.11	1.46	1.41
26	9	605	CHL	C1B-CHB	2.10	1.46	1.41
17	7	609	CLA	C1B-CHB	2.10	1.46	1.41
26	6	303	CHL	C1B-CHB	2.10	1.46	1.41
17	b	825	CLA	C1B-CHB	2.10	1.46	1.41
26	7	601	CHL	C4C-C3C	2.10	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	831	CLA	C1B-CHB	2.10	1.46	1.41
26	3	307	CHL	C4C-C3C	2.09	1.48	1.45
17	a	856	CLA	C1B-CHB	2.09	1.46	1.41
17	A	805	CLA	C4C-C3C	2.09	1.48	1.45
17	8	313	CLA	C3D-C2D	2.09	1.49	1.39
26	2	605	CHL	C2C-C1C	2.09	1.49	1.44
26	2	606	CHL	C4C-C3C	2.08	1.48	1.45
26	9	606	CHL	C1B-CHB	2.08	1.46	1.41
17	B	827	CLA	C1B-CHB	2.08	1.46	1.41
17	B	826	CLA	C4C-C3C	2.08	1.48	1.45
26	1	302	CHL	C4C-C3C	2.08	1.48	1.45
26	4	605	CHL	C1B-CHB	2.08	1.46	1.41
28	9	617	XAT	O4-C5	-2.08	1.43	1.46
17	7	608	CLA	C1B-CHB	2.07	1.46	1.41
17	b	816	CLA	C1B-CHB	2.07	1.46	1.41
17	b	811	CLA	C3B-C2B	2.06	1.48	1.41
17	B	803	CLA	C1B-CHB	2.06	1.46	1.41
17	b	809	CLA	C4C-C3C	2.06	1.48	1.45
25	4	620	LMG	O1-C1	2.05	1.43	1.40
17	A	841	CLA	C4C-C3C	2.04	1.48	1.45
26	4	605	CHL	C2C-C1C	2.04	1.48	1.44
17	B	829	CLA	C1C-C2C	2.03	1.48	1.44
17	b	803	CLA	C1B-CHB	2.03	1.46	1.41
17	a	821	CLA	C4C-C3C	2.03	1.48	1.45
17	B	811	CLA	C3B-C2B	2.02	1.48	1.41
26	4	607	CHL	C4C-C3C	2.02	1.48	1.45
17	A	841	CLA	C1B-NB	-2.01	1.33	1.35

All (7347) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	8	306	CHL	C4A-NA-C1A	-9.69	102.35	106.71
26	9	615	CHL	C4A-NA-C1A	-9.19	102.57	106.71
26	7	605	CHL	C4A-NA-C1A	-8.75	102.77	106.71
26	7	601	CHL	C4A-NA-C1A	-8.69	102.80	106.71
26	4	606	CHL	C4A-NA-C1A	-8.62	102.83	106.71
26	4	615	CHL	C4A-NA-C1A	-8.55	102.86	106.71
26	2	614	CHL	C4A-NA-C1A	-8.54	102.87	106.71
26	2	601	CHL	C4A-NA-C1A	-8.49	102.89	106.71
26	6	303	CHL	C4A-NA-C1A	-8.46	102.90	106.71
26	2	605	CHL	C4A-NA-C1A	-8.45	102.91	106.71
28	4	617	XAT	O4-C5-C4	8.42	119.70	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	8	315	XAT	O4-C5-C4	8.37	119.67	113.38
28	3	317	XAT	O4-C5-C4	8.36	119.66	113.38
26	4	605	CHL	C4A-NA-C1A	-8.33	102.96	106.71
26	1	302	CHL	C4A-NA-C1A	-8.31	102.97	106.71
26	9	605	CHL	C4A-NA-C1A	-8.27	102.99	106.71
26	9	607	CHL	C4A-NA-C1A	-8.22	103.01	106.71
17	3	315	CLA	C3D-C4D-ND	8.14	117.22	110.14
26	7	607	CHL	C4A-NA-C1A	-8.11	103.06	106.71
26	2	607	CHL	C4A-NA-C1A	-8.08	103.08	106.71
17	8	313	CLA	C3D-C4D-ND	8.02	117.11	110.14
26	1	307	CHL	C4A-NA-C1A	-8.01	103.10	106.71
26	7	606	CHL	C4A-NA-C1A	-7.98	103.12	106.71
26	2	606	CHL	C4A-NA-C1A	-7.91	103.15	106.71
26	4	607	CHL	C4A-NA-C1A	-7.91	103.15	106.71
26	7	614	CHL	C4A-NA-C1A	-7.90	103.16	106.71
26	6	308	CHL	C4A-NA-C1A	-7.89	103.16	106.71
26	9	606	CHL	C4A-NA-C1A	-7.81	103.19	106.71
28	1	317	XAT	O24-C25-C24	7.65	119.13	113.38
26	3	307	CHL	C4A-NA-C1A	-7.61	103.28	106.71
28	2	616	XAT	O24-C25-C24	7.52	119.03	113.38
17	8	313	CLA	C3D-C2D-C1D	-7.46	99.87	106.30
17	3	315	CLA	C3D-C2D-C1D	-7.36	99.96	106.30
28	7	616	XAT	O24-C25-C24	7.28	118.85	113.38
17	8	313	CLA	C3B-C2B-C1B	-7.24	100.09	106.29
17	3	315	CLA	C3B-C2B-C1B	-7.20	100.13	106.29
28	9	617	XAT	O4-C5-C4	6.87	118.54	113.38
17	8	302	CLA	C4A-NA-C1A	-6.82	103.64	106.71
28	6	318	XAT	C18-C5-C6	-6.71	111.01	122.26
28	1	317	XAT	C18-C5-C6	-6.67	111.08	122.26
28	9	617	XAT	O24-C25-C24	6.64	118.37	113.38
17	9	603	CLA	C4A-NA-C1A	-6.61	103.73	106.71
17	b	804	CLA	O2D-CGD-CBD	6.60	122.99	111.27
17	3	315	CLA	C2B-C1B-NB	6.58	115.88	110.11
17	8	313	CLA	C2B-C1B-NB	6.58	115.87	110.11
28	6	318	XAT	O4-C5-C4	6.58	118.32	113.38
26	7	601	CHL	O2D-CGD-CBD	6.58	122.95	111.27
28	2	616	XAT	C38-C25-C26	-6.56	111.27	122.26
28	6	318	XAT	O24-C25-C24	6.53	118.28	113.38
28	7	616	XAT	C18-C5-C6	-6.52	111.33	122.26
17	3	303	CLA	C4A-NA-C1A	-6.52	103.78	106.71
28	2	616	XAT	C18-C5-C6	-6.51	111.35	122.26
20	a	849	BCR	C15-C14-C13	-6.48	118.06	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	854	CLA	O2D-CGD-CBD	6.47	122.77	111.27
28	6	318	XAT	C38-C25-C26	-6.46	111.44	122.26
17	A	805	CLA	O2D-CGD-CBD	6.45	122.73	111.27
28	8	315	XAT	C38-C25-C26	-6.45	111.45	122.26
28	4	617	XAT	O24-C25-C24	6.42	118.21	113.38
28	8	315	XAT	O24-C25-C24	6.41	118.20	113.38
28	7	616	XAT	C38-C25-C26	-6.41	111.51	122.26
17	b	808	CLA	O2D-CGD-CBD	6.40	122.64	111.27
28	9	617	XAT	C38-C25-C26	-6.39	111.55	122.26
17	a	838	CLA	C4A-NA-C1A	-6.39	103.83	106.71
28	9	617	XAT	C18-C5-C6	-6.38	111.56	122.26
28	8	315	XAT	C18-C5-C6	-6.37	111.58	122.26
17	4	603	CLA	C4A-NA-C1A	-6.36	103.85	106.71
28	3	317	XAT	C18-C5-C6	-6.34	111.63	122.26
28	1	317	XAT	C38-C25-C26	-6.33	111.66	122.26
17	B	826	CLA	CHD-C4C-C3C	-6.32	115.54	124.84
28	3	317	XAT	O24-C25-C24	6.32	118.13	113.38
17	b	829	CLA	O2D-CGD-CBD	6.32	122.49	111.27
17	3	315	CLA	C3A-C4A-CHB	-6.29	116.20	123.91
17	B	808	CLA	O2D-CGD-CBD	6.29	122.45	111.27
17	a	856	CLA	O2D-CGD-CBD	6.29	122.45	111.27
17	8	313	CLA	C2D-C1D-ND	6.28	115.60	110.14
17	a	828	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
17	A	831	CLA	O2D-CGD-CBD	6.24	122.35	111.27
17	8	313	CLA	C3A-C4A-CHB	-6.21	116.31	123.91
17	3	315	CLA	C2D-C1D-ND	6.20	115.53	110.14
17	a	838	CLA	CHD-C4C-C3C	-6.18	115.76	124.84
26	2	601	CHL	O2D-CGD-CBD	6.17	122.24	111.27
17	A	828	CLA	CHD-C4C-C3C	-6.17	115.77	124.84
17	A	835	CLA	O2D-CGD-CBD	6.17	122.23	111.27
20	7	617	BCR	C24-C23-C22	-6.15	116.94	126.23
17	A	820	CLA	C4A-NA-C1A	-6.15	103.94	106.71
28	4	617	XAT	C38-C25-C26	-6.15	111.95	122.26
17	a	831	CLA	O2D-CGD-CBD	6.15	122.19	111.27
17	a	826	CLA	O2D-CGD-CBD	6.11	122.12	111.27
28	4	617	XAT	C18-C5-C6	-6.10	112.05	122.26
17	a	821	CLA	CHD-C4C-C3C	-6.09	115.89	124.84
17	B	829	CLA	O2D-CGD-CBD	6.09	122.08	111.27
17	b	815	CLA	O2D-CGD-CBD	6.08	122.07	111.27
17	B	836	CLA	CHD-C4C-C3C	-6.07	115.92	124.84
17	b	841	CLA	O2D-CGD-CBD	6.05	122.02	111.27
17	A	838	CLA	C4A-NA-C1A	-6.04	103.99	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	1	317	XAT	O4-C5-C4	6.02	117.91	113.38
17	B	806	CLA	C4A-NA-C1A	-6.02	104.00	106.71
17	a	856	CLA	C4A-NA-C1A	-6.01	104.00	106.71
28	3	317	XAT	C38-C25-C26	-6.01	112.19	122.26
17	B	829	CLA	C4A-NA-C1A	-6.01	104.01	106.71
17	B	841	CLA	O2D-CGD-CBD	5.99	121.92	111.27
17	B	827	CLA	C4A-NA-C1A	-5.99	104.01	106.71
28	2	616	XAT	O4-C5-C4	5.98	117.87	113.38
17	a	809	CLA	CHD-C4C-C3C	-5.97	116.06	124.84
17	b	829	CLA	C2C-C1C-NC	5.97	115.57	109.97
17	B	829	CLA	C2C-C1C-NC	5.97	115.57	109.97
17	A	854	CLA	C4A-NA-C1A	-5.96	104.03	106.71
17	b	827	CLA	C4A-NA-C1A	-5.96	104.03	106.71
17	b	837	CLA	O2D-CGD-CBD	5.96	121.85	111.27
17	a	820	CLA	C4A-NA-C1A	-5.95	104.03	106.71
17	B	804	CLA	O2D-CGD-CBD	5.95	121.85	111.27
17	b	809	CLA	C4A-NA-C1A	-5.95	104.03	106.71
17	A	840	CLA	O2D-CGD-CBD	5.95	121.84	111.27
20	a	849	BCR	C24-C23-C22	-5.94	117.26	126.23
17	a	856	CLA	C2C-C1C-NC	5.94	115.54	109.97
17	b	827	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
17	A	804	CLA	O2D-CGD-CBD	5.94	121.81	111.27
26	3	307	CHL	C1C-C2C-C3C	-5.93	102.40	107.11
17	A	810	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
17	A	841	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
17	B	836	CLA	C4A-NA-C1A	-5.93	104.04	106.71
17	A	818	CLA	O2D-CGD-CBD	5.93	121.80	111.27
17	f	7002	CLA	CHD-C4C-C3C	-5.92	116.13	124.84
20	b	845	BCR	C7-C8-C9	-5.92	117.28	126.23
17	B	841	CLA	C4A-NA-C1A	-5.92	104.04	106.71
17	B	837	CLA	O2D-CGD-CBD	5.92	121.79	111.27
17	A	821	CLA	C2C-C1C-NC	5.91	115.51	109.97
17	B	811	CLA	C1B-C2B-C3B	-5.91	101.42	106.92
17	6	305	CLA	C4A-NA-C1A	-5.91	104.05	106.71
17	B	802	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
17	A	803	CLA	C4A-NA-C1A	-5.89	104.06	106.71
17	4	603	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
17	a	830	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
17	A	805	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
17	a	803	CLA	C4A-NA-C1A	-5.89	104.06	106.71
17	A	826	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
20	B	844	BCR	C7-C8-C9	-5.88	117.34	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	840	CLA	CHD-C4C-C3C	-5.88	116.19	124.84
17	A	836	CLA	C2C-C1C-NC	5.88	115.48	109.97
17	a	803	CLA	C2C-C1C-NC	5.88	115.48	109.97
17	a	808	CLA	CHD-C4C-C3C	-5.88	116.20	124.84
17	b	811	CLA	C1B-C2B-C3B	-5.88	101.45	106.92
20	b	844	BCR	C7-C8-C9	-5.87	117.36	126.23
17	b	824	CLA	O2D-CGD-CBD	5.87	121.69	111.27
17	b	836	CLA	CHD-C4C-C3C	-5.86	116.22	124.84
17	b	836	CLA	C4A-NA-C1A	-5.86	104.07	106.71
17	a	818	CLA	O2D-CGD-CBD	5.86	121.68	111.27
17	B	841	CLA	CHD-C4C-C3C	-5.86	116.23	124.84
17	b	814	CLA	C4A-NA-C1A	-5.86	104.07	106.71
26	6	303	CHL	O2D-CGD-CBD	5.85	121.67	111.27
17	b	806	CLA	C4A-NA-C1A	-5.85	104.08	106.71
17	b	828	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
17	A	809	CLA	O2D-CGD-CBD	5.84	121.65	111.27
17	6	304	CLA	C4A-NA-C1A	-5.84	104.08	106.71
20	j	3004	BCR	C20-C21-C22	-5.84	118.97	127.31
17	3	302	CLA	C4A-NA-C1A	-5.84	104.08	106.71
17	1	304	CLA	C4A-NA-C1A	-5.83	104.08	106.71
17	a	835	CLA	O2D-CGD-CBD	5.83	121.64	111.27
17	2	610	CLA	C4A-NA-C1A	-5.83	104.08	106.71
17	a	826	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
17	B	814	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
17	b	829	CLA	C4A-NA-C1A	-5.82	104.09	106.71
17	a	807	CLA	CHD-C4C-C3C	-5.82	116.29	124.84
17	a	821	CLA	C2C-C1C-NC	5.81	115.42	109.97
17	b	813	CLA	C4A-NA-C1A	-5.81	104.09	106.71
17	b	806	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
17	B	838	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
17	G	104	CLA	C4A-NA-C1A	-5.81	104.09	106.71
26	9	607	CHL	C1C-C2C-C3C	-5.80	102.51	107.11
17	a	839	CLA	O2D-CGD-CBD	5.80	121.58	111.27
17	B	825	CLA	C4A-NA-C1A	-5.80	104.10	106.71
17	A	819	CLA	CHD-C4C-C3C	-5.80	116.31	124.84
17	b	826	CLA	CHD-C4C-C3C	-5.80	116.31	124.84
17	4	601	CLA	O2D-CGD-CBD	5.80	121.57	111.27
26	7	605	CHL	C2C-C3C-C4C	-5.80	102.36	106.49
17	A	826	CLA	O2D-CGD-CBD	5.79	121.56	111.27
17	k	1403	CLA	O2D-CGD-CBD	5.79	121.56	111.27
17	a	807	CLA	C4A-NA-C1A	-5.79	104.10	106.71
17	A	818	CLA	CHD-C4C-C3C	-5.79	116.33	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	813	CLA	C4A-NA-C1A	-5.79	104.10	106.71
20	b	843	BCR	C16-C17-C18	-5.79	119.05	127.31
17	a	809	CLA	O2D-CGD-CBD	5.79	121.55	111.27
17	7	610	CLA	C4A-NA-C1A	-5.78	104.11	106.71
17	A	830	CLA	CHD-C4C-C3C	-5.78	116.35	124.84
17	A	854	CLA	CHD-C4C-C3C	-5.77	116.35	124.84
17	B	837	CLA	CHD-C4C-C3C	-5.77	116.35	124.84
17	8	302	CLA	C2C-C1C-NC	5.77	115.38	109.97
17	B	828	CLA	C4A-NA-C1A	-5.77	104.11	106.71
17	b	811	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
17	b	804	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
17	a	801	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
17	3	306	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
17	a	823	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
17	A	829	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
17	A	828	CLA	O2D-CGD-CBD	5.76	121.50	111.27
17	8	303	CLA	O2D-CGD-CBD	5.76	121.50	111.27
17	a	836	CLA	C2C-C1C-NC	5.76	115.36	109.97
17	b	839	CLA	CHD-C4C-C3C	-5.75	116.38	124.84
17	3	314	CLA	C4A-NA-C1A	-5.75	104.12	106.71
17	A	839	CLA	O2D-CGD-CBD	5.75	121.48	111.27
17	b	817	CLA	C4A-NA-C1A	-5.74	104.12	106.71
17	B	825	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
17	b	822	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
17	a	816	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
26	8	306	CHL	CHD-C4C-C3C	-5.74	116.41	124.84
17	b	818	CLA	C4A-NA-C1A	-5.73	104.13	106.71
17	A	821	CLA	CHD-C4C-C3C	-5.73	116.41	124.84
20	A	852	BCR	C7-C8-C9	-5.73	117.57	126.23
17	a	817	CLA	C2C-C1C-NC	5.72	115.33	109.97
17	b	830	CLA	O2D-CGD-CBD	5.72	121.44	111.27
26	1	302	CHL	O2D-CGD-CBD	5.72	121.44	111.27
26	4	606	CHL	C2C-C3C-C4C	-5.72	102.41	106.49
17	B	806	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
17	g	103	CLA	C4A-NA-C1A	-5.71	104.14	106.71
17	9	602	CLA	O2D-CGD-CBD	5.71	121.42	111.27
17	2	603	CLA	C4A-NA-C1A	-5.71	104.14	106.71
17	3	303	CLA	C2C-C1C-NC	5.71	115.32	109.97
17	B	827	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
17	9	602	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
26	2	601	CHL	C2C-C3C-C4C	-5.70	102.42	106.49
17	a	829	CLA	C4A-NA-C1A	-5.70	104.14	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	821	CLA	O2D-CGD-CBD	5.70	121.40	111.27
17	A	834	CLA	C2C-C1C-NC	5.70	115.31	109.97
17	a	831	CLA	C4A-NA-C1A	-5.70	104.14	106.71
20	j	3004	BCR	C24-C23-C22	-5.70	117.63	126.23
17	a	815	CLA	CHD-C4C-C3C	-5.70	116.47	124.84
17	A	854	CLA	C2C-C1C-NC	5.69	115.31	109.97
17	a	805	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
17	6	312	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
17	b	825	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
17	a	835	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
17	b	814	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
20	7	617	BCR	C15-C14-C13	-5.69	119.19	127.31
17	a	833	CLA	CHD-C4C-C3C	-5.69	116.48	124.84
17	a	804	CLA	CHD-C4C-C3C	-5.69	116.48	124.84
26	8	306	CHL	C1C-C2C-C3C	-5.68	102.60	107.11
17	A	814	CLA	O2D-CGD-CBD	5.68	121.37	111.27
17	8	301	CLA	C4A-NA-C1A	-5.67	104.16	106.71
17	b	809	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
17	a	843	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
17	l	204	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
17	B	818	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
17	9	603	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
17	a	806	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
17	A	838	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
17	A	831	CLA	C4A-NA-C1A	-5.66	104.16	106.71
17	b	820	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
17	A	833	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
17	B	840	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
17	A	807	CLA	O2D-CGD-CBD	5.65	121.32	111.27
17	B	815	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
17	l	203	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
26	4	607	CHL	C1C-C2C-C3C	-5.65	102.63	107.11
17	b	810	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
17	B	828	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
17	9	601	CLA	O2D-CGD-CBD	5.64	121.29	111.27
17	a	814	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
17	6	309	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
17	7	603	CLA	C4A-NA-C1A	-5.63	104.17	106.71
17	a	837	CLA	C2C-C1C-NC	5.63	115.25	109.97
17	A	804	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
17	a	840	CLA	O2D-CGD-CBD	5.63	121.27	111.27
17	2	611	CLA	C4A-NA-C1A	-5.63	104.18	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	824	CLA	CHD-C4C-C3C	-5.63	116.57	124.84
17	a	825	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
17	b	841	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
17	a	827	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
26	4	607	CHL	CHD-C4C-C3C	-5.62	116.58	124.84
17	2	602	CLA	C4A-NA-C1A	-5.62	104.18	106.71
17	2	613	CLA	O2D-CGD-CBD	5.61	121.25	111.27
17	a	834	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
17	F	303	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
17	A	840	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
17	3	309	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
17	A	834	CLA	CHD-C4C-C3C	-5.61	116.60	124.84
17	G	101	CLA	CHD-C4C-C3C	-5.60	116.60	124.84
17	1	308	CLA	C4A-NA-C1A	-5.60	104.19	106.71
17	A	825	CLA	C2C-C1C-NC	5.60	115.22	109.97
17	8	312	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
17	2	603	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
17	G	103	CLA	C4A-NA-C1A	-5.60	104.19	106.71
17	A	809	CLA	C4A-NA-C1A	-5.60	104.19	106.71
17	a	842	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
17	1	306	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
17	B	823	CLA	CHD-C4C-C3C	-5.59	116.61	124.84
17	6	313	CLA	C4A-NA-C1A	-5.59	104.19	106.71
17	B	822	CLA	C4A-NA-C1A	-5.59	104.19	106.71
17	4	609	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
17	A	836	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
17	G	103	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
17	A	815	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
17	B	820	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
17	6	310	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
17	b	831	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
17	B	802	CLA	C4A-NA-C1A	-5.59	104.19	106.71
17	a	836	CLA	CHD-C4C-C3C	-5.59	116.63	124.84
17	b	834	CLA	CHD-C4C-C3C	-5.58	116.63	124.84
17	b	838	CLA	CHD-C4C-C3C	-5.58	116.63	124.84
17	7	608	CLA	C4A-NA-C1A	-5.58	104.20	106.71
17	a	818	CLA	C2C-C1C-NC	5.58	115.20	109.97
17	A	845	CLA	C4A-NA-C1A	-5.58	104.20	106.71
17	A	822	CLA	C4A-NA-C1A	-5.58	104.20	106.71
26	1	302	CHL	CHD-C4C-C3C	-5.58	116.64	124.84
17	b	833	CLA	O2D-CGD-CBD	5.58	121.18	111.27
26	2	605	CHL	C2C-C3C-C4C	-5.57	102.52	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	803	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
17	l	312	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
17	g	101	CLA	C2C-C1C-NC	5.56	115.18	109.97
17	g	102	CLA	C4A-NA-C1A	-5.56	104.21	106.71
17	A	812	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
17	k	1401	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
17	a	819	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
17	b	824	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
17	l	311	CLA	C4A-NA-C1A	-5.56	104.21	106.71
17	a	844	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
17	4	614	CLA	CHD-C4C-C3C	-5.55	116.67	124.84
17	b	818	CLA	O2D-CGD-CBD	5.55	121.14	111.27
17	L	204	CLA	C4A-NA-C1A	-5.55	104.21	106.71
17	A	808	CLA	CHD-C4C-C3C	-5.55	116.67	124.84
17	A	827	CLA	CHD-C4C-C3C	-5.55	116.67	124.84
17	B	833	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
17	3	314	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
17	A	823	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
17	l	312	CLA	C4A-NA-C1A	-5.55	104.21	106.71
17	b	828	CLA	C4A-NA-C1A	-5.55	104.21	106.71
17	B	809	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
26	7	606	CHL	CHD-C4C-C3C	-5.55	116.69	124.84
17	F	301	CLA	C4A-NA-C1A	-5.55	104.21	106.71
17	l	303	CLA	C4A-NA-C1A	-5.55	104.21	106.71
17	7	610	CLA	C2C-C1C-NC	5.54	115.16	109.97
17	4	609	CLA	C4A-NA-C1A	-5.54	104.22	106.71
17	l	304	CLA	C2C-C1C-NC	5.54	115.16	109.97
17	4	611	CLA	C4A-NA-C1A	-5.54	104.22	106.71
17	A	801	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
26	2	614	CHL	C2C-C3C-C4C	-5.54	102.54	106.49
17	B	830	CLA	O2D-CGD-CBD	5.54	121.11	111.27
26	7	614	CHL	C1C-C2C-C3C	-5.54	102.72	107.11
17	a	824	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
26	2	607	CHL	C1C-C2C-C3C	-5.53	102.72	107.11
17	b	819	CLA	C4A-NA-C1A	-5.53	104.22	106.71
17	B	819	CLA	C2C-C1C-NC	5.53	115.16	109.97
17	a	810	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
17	3	314	CLA	C2C-C1C-NC	5.53	115.15	109.97
17	B	811	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
17	a	840	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
17	B	821	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
17	K	4003	CLA	CHD-C4C-C3C	-5.53	116.71	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	830	CLA	C4A-NA-C1A	-5.53	104.22	106.71
20	A	851	BCR	C24-C23-C22	-5.53	117.88	126.23
17	3	313	CLA	C2C-C1C-NC	5.53	115.15	109.97
17	8	301	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
17	A	824	CLA	C2C-C1C-NC	5.52	115.15	109.97
17	7	603	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
26	4	605	CHL	C2C-C3C-C4C	-5.52	102.55	106.49
17	3	301	CLA	O2D-CGD-CBD	5.52	121.08	111.27
17	L	204	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
17	3	305	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
17	a	839	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
17	B	821	CLA	C2C-C1C-NC	5.52	115.14	109.97
17	B	835	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
17	9	610	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
17	a	832	CLA	C2C-C1C-NC	5.51	115.14	109.97
17	A	842	CLA	C4A-NA-C1A	-5.51	104.23	106.71
17	a	838	CLA	O2D-CGD-CBD	5.51	121.06	111.27
17	4	601	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
17	A	803	CLA	C2C-C1C-NC	5.51	115.14	109.97
17	A	816	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
17	b	832	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
17	B	832	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
17	B	807	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
17	A	802	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
17	G	104	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
17	8	307	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
17	7	602	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
17	8	311	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
17	4	610	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
17	a	829	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
17	A	815	CLA	C4A-NA-C1A	-5.50	104.23	106.71
17	l	203	CLA	O2D-CGD-CBD	5.50	121.05	111.27
17	b	833	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
17	l	202	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
17	1	315	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
17	a	846	CLA	C4A-NA-C1A	-5.50	104.23	106.71
17	2	610	CLA	C2C-C1C-NC	5.50	115.12	109.97
28	7	616	XAT	O4-C5-C4	5.50	117.51	113.38
20	K	4001	BCR	C15-C14-C13	-5.50	119.46	127.31
17	L	203	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
17	9	608	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
26	2	607	CHL	CHD-C4C-C3C	-5.49	116.76	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	807	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
17	8	312	CLA	C2C-C1C-NC	5.49	115.12	109.97
17	2	611	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
17	b	835	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
17	B	824	CLA	O2D-CGD-CBD	5.49	121.02	111.27
17	b	814	CLA	O2D-CGD-CBD	5.49	121.02	111.27
26	2	606	CHL	CHD-C4C-C3C	-5.49	116.77	124.84
17	K	4002	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
17	7	602	CLA	C4A-NA-C1A	-5.49	104.24	106.71
17	4	614	CLA	C4A-NA-C1A	-5.49	104.24	106.71
17	4	611	CLA	CHD-C4C-C3C	-5.48	116.78	124.84
26	7	601	CHL	C2C-C3C-C4C	-5.48	102.58	106.49
17	F	301	CLA	CHD-C4C-C3C	-5.48	116.78	124.84
17	8	308	CLA	CHD-C4C-C3C	-5.48	116.78	124.84
17	b	821	CLA	C2C-C1C-NC	5.48	115.11	109.97
17	A	802	CLA	C4A-NA-C1A	-5.48	104.24	106.71
17	b	841	CLA	C4A-NA-C1A	-5.48	104.24	106.71
17	4	602	CLA	CHD-C4C-C3C	-5.48	116.79	124.84
20	7	617	BCR	C11-C10-C9	-5.48	119.50	127.31
17	B	805	CLA	CHD-C4C-C3C	-5.48	116.79	124.84
17	B	838	CLA	C2C-C1C-NC	5.47	115.10	109.97
26	7	606	CHL	C2C-C3C-C4C	-5.47	102.59	106.49
17	b	830	CLA	C4A-NA-C1A	-5.47	104.25	106.71
17	b	825	CLA	C4A-NA-C1A	-5.47	104.25	106.71
17	A	820	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
17	B	804	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
17	a	837	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
17	9	611	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
17	6	311	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
20	j	3004	BCR	C16-C17-C18	-5.47	119.51	127.31
17	9	608	CLA	C2C-C1C-NC	5.47	115.09	109.97
17	a	828	CLA	O2D-CGD-CBD	5.47	120.98	111.27
17	K	4003	CLA	C2C-C1C-NC	5.47	115.09	109.97
17	g	102	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
26	9	606	CHL	CHD-C4C-C3C	-5.46	116.81	124.84
17	6	307	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
17	7	611	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
17	b	819	CLA	C2C-C1C-NC	5.46	115.09	109.97
17	8	302	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
17	A	839	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
17	b	811	CLA	O2D-CGD-CBD	5.46	120.97	111.27
17	9	614	CLA	CHD-C4C-C3C	-5.46	116.81	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	302	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
17	7	609	CLA	C4A-NA-C1A	-5.46	104.25	106.71
17	2	609	CLA	CHD-C4C-C3C	-5.46	116.82	124.84
17	a	812	CLA	C4A-NA-C1A	-5.46	104.25	106.71
17	3	311	CLA	CHD-C4C-C3C	-5.46	116.82	124.84
17	b	834	CLA	C2C-C1C-NC	5.45	115.08	109.97
26	9	605	CHL	C2C-C3C-C4C	-5.45	102.60	106.49
17	A	823	CLA	O2D-CGD-CBD	5.45	120.96	111.27
17	B	818	CLA	C4A-NA-C1A	-5.45	104.25	106.71
17	b	808	CLA	CHD-C4C-C3C	-5.45	116.82	124.84
17	8	305	CLA	CHD-C4C-C3C	-5.45	116.82	124.84
17	B	839	CLA	CHD-C4C-C3C	-5.45	116.82	124.84
17	A	817	CLA	C2C-C1C-NC	5.45	115.08	109.97
17	A	830	CLA	C4A-NA-C1A	-5.45	104.26	106.71
17	3	303	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
17	9	604	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
17	a	832	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
17	6	312	CLA	C2C-C1C-NC	5.45	115.08	109.97
17	A	801	CLA	C4A-NA-C1A	-5.45	104.26	106.71
17	B	816	CLA	C4A-NA-C1A	-5.45	104.26	106.71
17	a	824	CLA	C2C-C1C-NC	5.45	115.08	109.97
17	8	311	CLA	C2C-C1C-NC	5.45	115.07	109.97
17	A	832	CLA	CHD-C4C-C3C	-5.44	116.83	124.84
17	b	815	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
17	6	313	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
17	1	308	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
17	A	809	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
17	k	1403	CLA	C2C-C1C-NC	5.44	115.07	109.97
17	8	312	CLA	C4A-NA-C1A	-5.44	104.26	106.71
17	B	817	CLA	C4A-NA-C1A	-5.44	104.26	106.71
17	a	816	CLA	C4A-NA-C1A	-5.44	104.26	106.71
17	b	803	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
17	A	831	CLA	C2C-C1C-NC	5.44	115.06	109.97
17	4	612	CLA	CHD-C4C-C3C	-5.44	116.85	124.84
17	K	4002	CLA	O2D-CGD-CBD	5.44	120.93	111.27
17	6	306	CLA	CHD-C4C-C3C	-5.44	116.85	124.84
17	b	818	CLA	C2C-C1C-NC	5.44	115.06	109.97
17	2	609	CLA	C4A-NA-C1A	-5.43	104.26	106.71
17	A	806	CLA	CHD-C4C-C3C	-5.43	116.86	124.84
17	A	807	CLA	C4A-NA-C1A	-5.43	104.27	106.71
17	b	805	CLA	C4A-NA-C1A	-5.43	104.27	106.71
17	B	813	CLA	CHD-C4C-C3C	-5.43	116.86	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	8	304	CLA	CHD-C4C-C3C	-5.43	116.86	124.84
17	b	840	CLA	C2C-C1C-NC	5.43	115.06	109.97
17	b	821	CLA	CHD-C4C-C3C	-5.43	116.86	124.84
17	B	839	CLA	C4A-NA-C1A	-5.43	104.27	106.71
17	7	602	CLA	O2D-CGD-CBD	5.42	120.91	111.27
17	a	835	CLA	C4A-NA-C1A	-5.42	104.27	106.71
17	J	3002	CLA	C2C-C1C-NC	5.42	115.05	109.97
17	a	821	CLA	O2D-CGD-CBD	5.42	120.90	111.27
17	g	103	CLA	O2D-CGD-CBD	5.42	120.90	111.27
17	1	309	CLA	CHD-C4C-C3C	-5.42	116.87	124.84
17	b	802	CLA	CHD-C4C-C3C	-5.42	116.88	124.84
17	A	845	CLA	O2D-CGD-CBD	5.42	120.89	111.27
17	a	818	CLA	CHD-C4C-C3C	-5.42	116.88	124.84
17	b	810	CLA	C4A-NA-C1A	-5.41	104.27	106.71
17	8	308	CLA	C4A-NA-C1A	-5.41	104.27	106.71
17	A	832	CLA	C2C-C1C-NC	5.41	115.04	109.97
17	6	310	CLA	C2C-C1C-NC	5.41	115.04	109.97
17	7	608	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
17	B	810	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
17	1	311	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
17	a	826	CLA	C4A-NA-C1A	-5.41	104.27	106.71
17	b	812	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
17	6	305	CLA	C2C-C1C-NC	5.41	115.04	109.97
17	F	301	CLA	C2C-C1C-NC	5.41	115.04	109.97
17	6	315	CLA	O2D-CGD-CBD	5.40	120.87	111.27
17	2	608	CLA	C2C-C1C-NC	5.40	115.03	109.97
17	7	611	CLA	C2C-C1C-NC	5.40	115.03	109.97
17	a	846	CLA	C2C-C1C-NC	5.40	115.03	109.97
26	6	308	CHL	C1C-C2C-C3C	-5.40	102.83	107.11
17	4	603	CLA	O2D-CGD-CBD	5.40	120.87	111.27
17	A	825	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
17	6	316	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
26	4	615	CHL	C2C-C3C-C4C	-5.40	102.64	106.49
17	6	305	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
17	a	841	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
17	8	305	CLA	C2C-C1C-NC	5.40	115.03	109.97
17	7	609	CLA	CHD-C4C-C3C	-5.40	116.91	124.84
17	1	303	CLA	CHD-C4C-C3C	-5.40	116.91	124.84
17	a	801	CLA	O2D-CGD-CBD	5.39	120.85	111.27
17	a	840	CLA	C2C-C1C-NC	5.39	115.03	109.97
17	2	612	CLA	CHD-C4C-C3C	-5.39	116.91	124.84
17	3	308	CLA	C4A-NA-C1A	-5.39	104.28	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	j	3002	CLA	CHD-C4C-C3C	-5.39	116.91	124.84
17	L	202	CLA	C2C-C1C-NC	5.39	115.02	109.97
17	4	608	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
17	9	611	CLA	C2C-C1C-NC	5.39	115.02	109.97
17	b	802	CLA	C4A-NA-C1A	-5.39	104.28	106.71
26	1	302	CHL	C2C-C3C-C4C	-5.38	102.65	106.49
17	8	305	CLA	C4A-NA-C1A	-5.38	104.29	106.71
17	A	842	CLA	CHD-C4C-C3C	-5.38	116.93	124.84
17	a	801	CLA	C2C-C1C-NC	5.38	115.01	109.97
17	1	310	CLA	CHD-C4C-C3C	-5.38	116.93	124.84
17	A	837	CLA	C2C-C1C-NC	5.38	115.01	109.97
17	B	810	CLA	C4A-NA-C1A	-5.38	104.29	106.71
17	a	827	CLA	C4A-NA-C1A	-5.38	104.29	106.71
17	B	821	CLA	C4A-NA-C1A	-5.38	104.29	106.71
17	1	314	CLA	C4A-NA-C1A	-5.38	104.29	106.71
26	9	606	CHL	O2D-CGD-CBD	5.38	120.82	111.27
17	6	314	CLA	C4A-NA-C1A	-5.37	104.29	106.71
17	A	845	CLA	C2C-C1C-NC	5.37	115.01	109.97
17	a	843	CLA	O2D-CGD-CBD	5.37	120.82	111.27
17	a	831	CLA	CHD-C4C-C3C	-5.37	116.94	124.84
17	a	822	CLA	CHD-C4C-C3C	-5.37	116.94	124.84
17	3	315	CLA	C4A-NA-C1A	-5.37	104.29	106.71
17	a	817	CLA	CHD-C4C-C3C	-5.37	116.94	124.84
17	a	813	CLA	C2C-C1C-NC	5.37	115.00	109.97
17	A	808	CLA	C2C-C1C-NC	5.37	115.00	109.97
17	F	303	CLA	C4A-NA-C1A	-5.37	104.29	106.71
17	b	823	CLA	C4A-NA-C1A	-5.37	104.29	106.71
17	3	304	CLA	CHD-C4C-C3C	-5.37	116.95	124.84
17	1	314	CLA	C2C-C1C-NC	5.37	115.00	109.97
17	1	303	CLA	O2D-CGD-CBD	5.37	120.80	111.27
17	A	827	CLA	C4A-NA-C1A	-5.37	104.29	106.71
17	a	834	CLA	C4A-NA-C1A	-5.37	104.29	106.71
17	4	613	CLA	CHD-C4C-C3C	-5.36	116.95	124.84
17	B	822	CLA	CHD-C4C-C3C	-5.36	116.95	124.84
17	9	609	CLA	C4A-NA-C1A	-5.36	104.30	106.71
17	3	309	CLA	C4A-NA-C1A	-5.36	104.30	106.71
17	a	822	CLA	C4A-NA-C1A	-5.36	104.30	106.71
26	3	307	CHL	CHD-C4C-C3C	-5.36	116.96	124.84
17	b	813	CLA	O2D-CGD-CBD	5.36	120.79	111.27
17	1	314	CLA	O2D-CGD-CBD	5.36	120.79	111.27
17	a	811	CLA	C2C-C1C-NC	5.36	114.99	109.97
17	B	809	CLA	C4A-NA-C1A	-5.36	104.30	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	310	CLA	C2C-C1C-NC	5.36	114.99	109.97
17	b	807	CLA	CHD-C4C-C3C	-5.36	116.96	124.84
26	9	615	CHL	C1C-C2C-C3C	-5.36	102.86	107.11
17	L	203	CLA	C4A-NA-C1A	-5.36	104.30	106.71
17	7	610	CLA	CHD-C4C-C3C	-5.36	116.97	124.84
17	2	602	CLA	CHD-C4C-C3C	-5.36	116.97	124.84
17	8	310	CLA	CHD-C4C-C3C	-5.35	116.97	124.84
17	A	810	CLA	C2C-C1C-NC	5.35	114.99	109.97
26	4	606	CHL	CHD-C4C-C3C	-5.35	116.97	124.84
17	4	608	CLA	C2C-C1C-NC	5.35	114.99	109.97
17	a	846	CLA	CHD-C4C-C3C	-5.35	116.97	124.84
17	B	826	CLA	C4A-NA-C1A	-5.35	104.30	106.71
17	9	602	CLA	C4A-NA-C1A	-5.35	104.30	106.71
17	1	312	CLA	C2C-C1C-NC	5.35	114.98	109.97
17	6	306	CLA	C2C-C1C-NC	5.35	114.98	109.97
17	1	305	CLA	CHD-C4C-C3C	-5.35	116.97	124.84
26	7	605	CHL	CHD-C4C-C3C	-5.35	116.97	124.84
17	a	825	CLA	C2C-C1C-NC	5.35	114.98	109.97
17	B	818	CLA	C2C-C1C-NC	5.35	114.98	109.97
17	A	814	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
17	A	843	CLA	C4A-NA-C1A	-5.35	104.30	106.71
17	k	1402	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
17	3	312	CLA	C2C-C1C-NC	5.35	114.98	109.97
26	9	606	CHL	C2C-C3C-C4C	-5.35	102.68	106.49
17	B	807	CLA	C4A-NA-C1A	-5.34	104.30	106.71
26	7	607	CHL	C1C-C2C-C3C	-5.34	102.87	107.11
17	b	837	CLA	CHD-C4C-C3C	-5.34	116.98	124.84
17	1	309	CLA	C2C-C1C-NC	5.34	114.98	109.97
17	a	814	CLA	O2D-CGD-CBD	5.34	120.76	111.27
17	2	613	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
17	F	304	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
17	9	613	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
17	B	808	CLA	C2C-C1C-NC	5.34	114.97	109.97
17	4	612	CLA	C2C-C1C-NC	5.34	114.97	109.97
17	B	833	CLA	O2D-CGD-CBD	5.34	120.76	111.27
17	6	315	CLA	C2C-C1C-NC	5.34	114.97	109.97
17	f	7003	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
17	8	310	CLA	C2C-C1C-NC	5.34	114.97	109.97
17	F	303	CLA	C2C-C1C-NC	5.34	114.97	109.97
17	a	809	CLA	C4A-NA-C1A	-5.33	104.31	106.71
17	b	838	CLA	C2C-C1C-NC	5.33	114.97	109.97
17	a	856	CLA	CHD-C4C-C3C	-5.33	117.00	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	7	613	CLA	CHD-C4C-C3C	-5.33	117.00	124.84
17	b	821	CLA	O2D-CGD-CBD	5.33	120.74	111.27
17	4	604	CLA	C4A-NA-C1A	-5.33	104.31	106.71
17	A	845	CLA	CHD-C4C-C3C	-5.33	117.00	124.84
17	b	805	CLA	O2D-CGD-CBD	5.33	120.74	111.27
17	9	601	CLA	CHD-C4C-C3C	-5.33	117.00	124.84
26	2	606	CHL	C2C-C3C-C4C	-5.33	102.69	106.49
26	9	615	CHL	C2C-C3C-C4C	-5.33	102.69	106.49
17	g	101	CLA	CHD-C4C-C3C	-5.33	117.00	124.84
17	b	805	CLA	C2C-C1C-NC	5.33	114.96	109.97
17	A	843	CLA	C2C-C1C-NC	5.33	114.96	109.97
17	g	102	CLA	C2C-C1C-NC	5.33	114.96	109.97
26	7	601	CHL	CHD-C4C-C3C	-5.33	117.01	124.84
17	b	816	CLA	C2C-C1C-NC	5.33	114.96	109.97
17	J	3002	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
26	1	307	CHL	C1C-C2C-C3C	-5.33	102.89	107.11
17	7	612	CLA	CHD-C4C-C3C	-5.32	117.01	124.84
17	1	313	CLA	C2C-C1C-NC	5.32	114.96	109.97
17	A	832	CLA	O2D-CGD-CBD	5.32	120.73	111.27
17	L	202	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
17	3	313	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
17	B	817	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
17	3	310	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
17	2	610	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
17	3	311	CLA	C2C-C1C-NC	5.32	114.95	109.97
17	6	314	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
17	A	837	CLA	O2D-CGD-CBD	5.32	120.72	111.27
17	9	601	CLA	C2C-C1C-NC	5.32	114.95	109.97
17	2	608	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
17	3	310	CLA	C4A-NA-C1A	-5.31	104.32	106.71
17	7	604	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
26	4	615	CHL	CHD-C4C-C3C	-5.31	117.03	124.84
17	8	313	CLA	C4A-NA-C1A	-5.31	104.32	106.71
26	2	606	CHL	C1C-C2C-C3C	-5.31	102.90	107.11
17	2	604	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
17	2	604	CLA	C4A-NA-C1A	-5.31	104.32	106.71
17	4	601	CLA	C2C-C1C-NC	5.31	114.94	109.97
17	6	314	CLA	C2C-C1C-NC	5.31	114.94	109.97
17	9	614	CLA	C4A-NA-C1A	-5.31	104.32	106.71
17	9	609	CLA	CHD-C4C-C3C	-5.31	117.04	124.84
17	4	602	CLA	C4A-NA-C1A	-5.30	104.32	106.71
17	b	818	CLA	CHD-C4C-C3C	-5.30	117.04	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	9	612	CLA	C2C-C1C-NC	5.30	114.94	109.97
17	B	809	CLA	C2C-C1C-NC	5.30	114.94	109.97
17	b	816	CLA	CHD-C4C-C3C	-5.30	117.04	124.84
17	A	835	CLA	CHD-C4C-C3C	-5.30	117.04	124.84
17	B	816	CLA	O2D-CGD-CBD	5.30	120.69	111.27
26	1	307	CHL	C2C-C3C-C4C	-5.30	102.71	106.49
17	A	835	CLA	C2C-C1C-NC	5.30	114.94	109.97
17	9	604	CLA	O2D-CGD-CBD	5.30	120.69	111.27
17	B	812	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
17	6	311	CLA	C4A-NA-C1A	-5.30	104.32	106.71
17	7	604	CLA	C4A-NA-C1A	-5.30	104.32	106.71
17	3	305	CLA	C2C-C1C-NC	5.30	114.94	109.97
17	a	842	CLA	C2C-C1C-NC	5.30	114.94	109.97
17	A	839	CLA	C2C-C1C-NC	5.30	114.94	109.97
17	7	611	CLA	C4A-NA-C1A	-5.30	104.32	106.71
17	2	603	CLA	C2C-C1C-NC	5.30	114.94	109.97
17	4	611	CLA	C2C-C1C-NC	5.30	114.94	109.97
20	B	845	BCR	C24-C23-C22	-5.30	118.23	126.23
17	A	837	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
17	a	812	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
17	1	304	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
17	k	1401	CLA	O2D-CGD-CBD	5.29	120.68	111.27
17	4	613	CLA	C2C-C1C-NC	5.29	114.93	109.97
17	B	819	CLA	CHD-C4C-C3C	-5.29	117.06	124.84
17	A	804	CLA	C4A-NA-C1A	-5.29	104.33	106.71
17	4	608	CLA	C4A-NA-C1A	-5.29	104.33	106.71
17	2	608	CLA	C4A-NA-C1A	-5.29	104.33	106.71
17	B	808	CLA	CHD-C4C-C3C	-5.29	117.06	124.84
17	A	817	CLA	CHD-C4C-C3C	-5.29	117.07	124.84
17	b	839	CLA	C2C-C1C-NC	5.28	114.92	109.97
17	b	820	CLA	O2D-CGD-CBD	5.28	120.66	111.27
17	3	301	CLA	C4A-NA-C1A	-5.28	104.33	106.71
17	a	843	CLA	C4A-NA-C1A	-5.28	104.33	106.71
26	9	606	CHL	C1C-C2C-C3C	-5.28	102.92	107.11
17	a	820	CLA	CHD-C4C-C3C	-5.28	117.08	124.84
17	b	823	CLA	CHD-C4C-C3C	-5.28	117.08	124.84
26	1	307	CHL	CHD-C4C-C3C	-5.28	117.08	124.84
17	8	309	CLA	C2C-C1C-NC	5.28	114.92	109.97
17	j	3002	CLA	C2C-C1C-NC	5.28	114.92	109.97
17	A	813	CLA	CHD-C4C-C3C	-5.28	117.08	124.84
17	B	826	CLA	O2D-CGD-CBD	5.28	120.64	111.27
17	6	313	CLA	C2C-C1C-NC	5.28	114.91	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	9	614	CLA	O2D-CGD-CBD	5.27	120.64	111.27
26	9	605	CHL	O2D-CGD-CBD	5.27	120.64	111.27
17	9	612	CLA	CHD-C4C-C3C	-5.27	117.08	124.84
17	f	7003	CLA	C2C-C1C-NC	5.27	114.91	109.97
17	A	824	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
26	7	607	CHL	CHD-C4C-C3C	-5.27	117.09	124.84
17	b	809	CLA	C2C-C1C-NC	5.27	114.91	109.97
17	b	831	CLA	C2C-C1C-NC	5.27	114.91	109.97
17	b	816	CLA	C4A-NA-C1A	-5.27	104.34	106.71
17	A	832	CLA	C4A-NA-C1A	-5.27	104.34	106.71
17	B	831	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
17	3	312	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
17	b	815	CLA	C2C-C1C-NC	5.26	114.90	109.97
17	B	820	CLA	C2C-C1C-NC	5.26	114.90	109.97
26	7	614	CHL	O2D-CGD-CBD	5.26	120.62	111.27
26	2	614	CHL	C1C-C2C-C3C	-5.26	102.94	107.11
20	a	854	BCR	C7-C8-C9	-5.26	118.28	126.23
28	7	616	XAT	C6-C7-C8	-5.26	114.87	125.99
26	9	605	CHL	CHD-C4C-C3C	-5.26	117.10	124.84
20	A	851	BCR	C20-C21-C22	-5.26	119.80	127.31
17	B	815	CLA	O2D-CGD-CBD	5.26	120.62	111.27
17	6	315	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
17	A	843	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
17	a	802	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
17	b	822	CLA	C4A-NA-C1A	-5.26	104.34	106.71
26	4	605	CHL	CHD-C4C-C3C	-5.26	117.11	124.84
17	B	839	CLA	C2C-C1C-NC	5.26	114.89	109.97
17	9	613	CLA	C2C-C1C-NC	5.26	114.89	109.97
17	b	807	CLA	O2D-CGD-CBD	5.25	120.61	111.27
17	K	4002	CLA	C2C-C1C-NC	5.25	114.89	109.97
17	7	603	CLA	C2C-C1C-NC	5.25	114.89	109.97
17	A	833	CLA	C4A-NA-C1A	-5.25	104.34	106.71
26	2	601	CHL	CHD-C4C-C3C	-5.25	117.12	124.84
17	1	311	CLA	C2C-C1C-NC	5.25	114.89	109.97
17	7	612	CLA	C2C-C1C-NC	5.25	114.89	109.97
17	8	309	CLA	CHD-C4C-C3C	-5.25	117.12	124.84
26	7	606	CHL	C1C-C2C-C3C	-5.25	102.95	107.11
17	9	614	CLA	C2C-C1C-NC	5.24	114.89	109.97
17	k	1402	CLA	C2C-C1C-NC	5.24	114.88	109.97
17	B	834	CLA	C2C-C1C-NC	5.24	114.88	109.97
17	3	304	CLA	O2D-CGD-CBD	5.24	120.58	111.27
17	9	604	CLA	C4A-NA-C1A	-5.24	104.35	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	8	303	CLA	CHD-C4C-C3C	-5.24	117.13	124.84
28	1	317	XAT	C6-C7-C8	-5.24	114.91	125.99
17	A	813	CLA	C2C-C1C-NC	5.24	114.88	109.97
17	3	311	CLA	C4A-NA-C1A	-5.24	104.35	106.71
17	1	310	CLA	C4A-NA-C1A	-5.24	104.35	106.71
17	A	823	CLA	C4A-NA-C1A	-5.24	104.35	106.71
17	a	823	CLA	O2D-CGD-CBD	5.24	120.58	111.27
26	2	614	CHL	CHD-C4C-C3C	-5.24	117.14	124.84
17	6	310	CLA	C4A-NA-C1A	-5.24	104.35	106.71
17	B	807	CLA	O2D-CGD-CBD	5.24	120.57	111.27
17	l	202	CLA	C2C-C1C-NC	5.23	114.88	109.97
17	B	805	CLA	O2D-CGD-CBD	5.23	120.57	111.27
17	g	101	CLA	C4A-NA-C1A	-5.23	104.35	106.71
17	b	813	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
17	A	816	CLA	C2C-C1C-NC	5.23	114.87	109.97
17	g	103	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
17	a	837	CLA	C4A-NA-C1A	-5.23	104.36	106.71
17	7	604	CLA	C2C-C1C-NC	5.23	114.87	109.97
17	8	307	CLA	C4A-NA-C1A	-5.23	104.36	106.71
17	a	813	CLA	CHD-C4C-C3C	-5.23	117.16	124.84
17	3	301	CLA	C2C-C1C-NC	5.22	114.87	109.97
17	4	604	CLA	C2C-C1C-NC	5.22	114.86	109.97
17	G	101	CLA	C2C-C1C-NC	5.22	114.86	109.97
17	9	611	CLA	C4A-NA-C1A	-5.22	104.36	106.71
26	6	308	CHL	CHD-C4C-C3C	-5.22	117.17	124.84
26	4	605	CHL	C1C-C2C-C3C	-5.22	102.97	107.11
17	b	835	CLA	C2C-C1C-NC	5.22	114.86	109.97
17	a	811	CLA	CHD-C4C-C3C	-5.22	117.17	124.84
17	l	202	CLA	O2D-CGD-CBD	5.22	120.54	111.27
26	7	614	CHL	C2C-C3C-C4C	-5.22	102.77	106.49
17	3	301	CLA	CHD-C4C-C3C	-5.21	117.17	124.84
26	9	615	CHL	O2D-CGD-CBD	5.21	120.53	111.27
17	A	824	CLA	C4A-NA-C1A	-5.21	104.36	106.71
17	9	610	CLA	C4A-NA-C1A	-5.21	104.36	106.71
17	1	315	CLA	C2C-C1C-NC	5.21	114.86	109.97
26	4	606	CHL	O2D-CGD-CBD	5.21	120.53	111.27
17	1	313	CLA	CHD-C4C-C3C	-5.21	117.17	124.84
17	b	817	CLA	C2C-C1C-NC	5.21	114.85	109.97
17	b	833	CLA	C2C-C1C-NC	5.21	114.85	109.97
17	B	804	CLA	C2C-C1C-NC	5.21	114.85	109.97
17	7	613	CLA	C2C-C1C-NC	5.21	114.85	109.97
17	3	308	CLA	CHD-C4C-C3C	-5.21	117.19	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	9	607	CHL	CHD-C4C-C3C	-5.21	117.19	124.84
17	A	840	CLA	C2C-C1C-NC	5.20	114.85	109.97
17	B	815	CLA	C2C-C1C-NC	5.20	114.85	109.97
17	A	823	CLA	C2C-C1C-NC	5.20	114.84	109.97
17	2	611	CLA	C2C-C1C-NC	5.20	114.84	109.97
17	A	813	CLA	C4A-NA-C1A	-5.20	104.37	106.71
17	b	836	CLA	O2D-CGD-CBD	5.20	120.51	111.27
17	4	613	CLA	O2D-CGD-CBD	5.20	120.51	111.27
17	b	830	CLA	CHD-C4C-C3C	-5.20	117.20	124.84
26	9	605	CHL	C1C-C2C-C3C	-5.19	102.99	107.11
17	a	810	CLA	C2C-C1C-NC	5.19	114.84	109.97
17	K	4003	CLA	O2D-CGD-CBD	5.19	120.50	111.27
17	B	818	CLA	O2D-CGD-CBD	5.19	120.50	111.27
17	B	816	CLA	CHD-C4C-C3C	-5.19	117.21	124.84
17	9	613	CLA	O2D-CGD-CBD	5.19	120.49	111.27
26	7	607	CHL	C2C-C3C-C4C	-5.19	102.79	106.49
17	a	823	CLA	C2C-C1C-NC	5.19	114.83	109.97
17	A	804	CLA	C2C-C1C-NC	5.19	114.83	109.97
17	1	311	CLA	O2D-CGD-CBD	5.19	120.49	111.27
17	6	315	CLA	C4A-NA-C1A	-5.19	104.37	106.71
17	6	307	CLA	C4A-NA-C1A	-5.19	104.37	106.71
17	4	614	CLA	O2D-CGD-CBD	5.19	120.48	111.27
17	a	830	CLA	C2C-C1C-NC	5.19	114.83	109.97
17	A	815	CLA	O2D-CGD-CBD	5.18	120.48	111.27
20	7	617	BCR	C16-C17-C18	-5.18	119.91	127.31
17	A	811	CLA	CHD-C4C-C3C	-5.18	117.22	124.84
26	6	303	CHL	C2C-C3C-C4C	-5.18	102.80	106.49
17	B	813	CLA	O2D-CGD-CBD	5.18	120.47	111.27
17	2	604	CLA	C2C-C1C-NC	5.18	114.82	109.97
17	f	7003	CLA	O2D-CGD-CBD	5.18	120.47	111.27
17	a	820	CLA	C2C-C1C-NC	5.18	114.82	109.97
17	6	309	CLA	C2C-C1C-NC	5.18	114.82	109.97
17	g	103	CLA	C2C-C1C-NC	5.18	114.82	109.97
17	A	811	CLA	C4A-NA-C1A	-5.18	104.38	106.71
17	8	311	CLA	C4A-NA-C1A	-5.18	104.38	106.71
17	4	604	CLA	CHD-C4C-C3C	-5.18	117.23	124.84
26	2	606	CHL	O2D-CGD-CBD	5.17	120.46	111.27
17	A	801	CLA	O2D-CGD-CBD	5.17	120.46	111.27
17	B	831	CLA	C4A-NA-C1A	-5.17	104.38	106.71
17	9	603	CLA	O2D-CGD-CBD	5.17	120.46	111.27
17	B	832	CLA	O2D-CGD-CBD	5.17	120.46	111.27
17	3	306	CLA	C2C-C1C-NC	5.17	114.81	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	829	CLA	C4A-NA-C1A	-5.17	104.38	106.71
17	4	603	CLA	C2C-C1C-NC	5.17	114.81	109.97
26	7	614	CHL	CHD-C4C-C3C	-5.17	117.24	124.84
17	8	304	CLA	C4A-NA-C1A	-5.17	104.38	106.71
17	6	309	CLA	C4A-NA-C1A	-5.17	104.38	106.71
17	4	614	CLA	C2C-C1C-NC	5.17	114.81	109.97
17	B	830	CLA	CHD-C4C-C3C	-5.17	117.24	124.84
17	A	822	CLA	C2C-C1C-NC	5.16	114.81	109.97
17	A	830	CLA	C2C-C1C-NC	5.16	114.81	109.97
17	a	804	CLA	O2D-CGD-CBD	5.16	120.44	111.27
17	A	816	CLA	C4A-NA-C1A	-5.16	104.39	106.71
17	a	831	CLA	C2C-C1C-NC	5.16	114.81	109.97
17	A	822	CLA	CHD-C4C-C3C	-5.16	117.25	124.84
17	A	817	CLA	C4A-NA-C1A	-5.16	104.39	106.71
26	4	605	CHL	O2D-CGD-CBD	5.16	120.44	111.27
20	l	201	BCR	C7-C8-C9	-5.16	118.44	126.23
17	1	308	CLA	C2C-C1C-NC	5.16	114.80	109.97
17	a	814	CLA	C4A-NA-C1A	-5.16	104.39	106.71
17	a	844	CLA	C4A-NA-C1A	-5.16	104.39	106.71
17	b	812	CLA	C2C-C1C-NC	5.16	114.80	109.97
26	9	615	CHL	CHD-C4C-C3C	-5.16	117.26	124.84
17	6	316	CLA	C2C-C1C-NC	5.15	114.80	109.97
28	2	616	XAT	O4-C5-C18	5.15	121.23	115.06
17	8	303	CLA	C4A-NA-C1A	-5.15	104.39	106.71
17	A	811	CLA	C2C-C1C-NC	5.15	114.80	109.97
17	b	808	CLA	C2C-C1C-NC	5.15	114.80	109.97
17	K	4002	CLA	C4A-NA-C1A	-5.15	104.39	106.71
17	8	301	CLA	O2D-CGD-CBD	5.15	120.42	111.27
17	k	1403	CLA	CHD-C4C-C3C	-5.15	117.27	124.84
17	a	835	CLA	C2C-C1C-NC	5.15	114.80	109.97
17	6	316	CLA	C4A-NA-C1A	-5.15	104.39	106.71
17	B	832	CLA	C4A-NA-C1A	-5.14	104.39	106.71
17	A	841	CLA	C4A-NA-C1A	-5.14	104.39	106.71
17	b	831	CLA	C4A-NA-C1A	-5.14	104.39	106.71
17	A	821	CLA	O2D-CGD-CBD	5.14	120.41	111.27
17	B	812	CLA	C2C-C1C-NC	5.14	114.79	109.97
17	9	610	CLA	C2C-C1C-NC	5.14	114.79	109.97
17	B	834	CLA	CHD-C4C-C3C	-5.14	117.28	124.84
26	6	303	CHL	CHD-C4C-C3C	-5.14	117.29	124.84
17	2	612	CLA	C2C-C1C-NC	5.14	114.78	109.97
17	a	819	CLA	C4A-NA-C1A	-5.14	104.40	106.71
17	b	821	CLA	C4A-NA-C1A	-5.14	104.40	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	826	CLA	C4A-NA-C1A	-5.14	104.40	106.71
17	6	304	CLA	CHD-C4C-C3C	-5.14	117.29	124.84
17	b	811	CLA	C2C-C1C-NC	5.13	114.78	109.97
17	b	817	CLA	CHD-C4C-C3C	-5.13	117.29	124.84
17	f	7002	CLA	C2C-C1C-NC	5.13	114.78	109.97
17	3	304	CLA	C2C-C1C-NC	5.13	114.78	109.97
17	A	818	CLA	C2C-C1C-NC	5.13	114.78	109.97
17	2	613	CLA	C4A-NA-C1A	-5.13	104.40	106.71
20	K	4001	BCR	C16-C17-C18	-5.13	119.99	127.31
17	b	802	CLA	C2C-C1C-NC	5.13	114.78	109.97
17	B	811	CLA	C2C-C1C-NC	5.13	114.77	109.97
17	B	828	CLA	C2C-C1C-NC	5.13	114.77	109.97
17	A	812	CLA	C2C-C1C-NC	5.13	114.77	109.97
17	B	836	CLA	C2C-C1C-NC	5.13	114.77	109.97
20	a	852	BCR	C16-C17-C18	-5.12	120.00	127.31
17	8	313	CLA	C3C-C4C-NC	5.12	114.70	109.97
17	b	819	CLA	CHD-C4C-C3C	-5.12	117.31	124.84
17	a	837	CLA	O2D-CGD-CBD	5.12	120.37	111.27
17	a	822	CLA	C2C-C1C-NC	5.12	114.77	109.97
28	3	317	XAT	C26-C27-C28	-5.12	115.16	125.99
17	3	304	CLA	C4A-NA-C1A	-5.12	104.40	106.71
26	6	303	CHL	C1C-C2C-C3C	-5.12	103.05	107.11
17	b	816	CLA	O2D-CGD-CBD	5.12	120.37	111.27
17	a	807	CLA	O2D-CGD-CBD	5.12	120.37	111.27
17	F	304	CLA	C2C-C1C-NC	5.12	114.77	109.97
17	B	814	CLA	O2D-CGD-CBD	5.12	120.37	111.27
26	2	607	CHL	C2C-C3C-C4C	-5.12	102.84	106.49
20	a	853	BCR	C24-C23-C22	-5.12	118.50	126.23
20	3	318	BCR	C15-C14-C13	-5.12	120.00	127.31
17	B	812	CLA	C4A-NA-C1A	-5.12	104.41	106.71
17	b	804	CLA	C2C-C1C-NC	5.12	114.77	109.97
17	a	805	CLA	C2C-C1C-NC	5.11	114.76	109.97
17	a	830	CLA	C4A-NA-C1A	-5.11	104.41	106.71
26	6	308	CHL	C2C-C3C-C4C	-5.11	102.84	106.49
17	2	613	CLA	C2C-C1C-NC	5.11	114.76	109.97
17	a	811	CLA	C4A-NA-C1A	-5.11	104.41	106.71
17	k	1401	CLA	C2C-C1C-NC	5.11	114.76	109.97
17	8	309	CLA	O2D-CGD-CBD	5.11	120.35	111.27
17	1	314	CLA	CHD-C4C-C3C	-5.11	117.33	124.84
17	a	839	CLA	C2C-C1C-NC	5.11	114.76	109.97
17	A	801	CLA	C2C-C1C-NC	5.11	114.76	109.97
17	3	315	CLA	C3C-C4C-NC	5.10	114.68	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	4	615	CHL	C1C-C2C-C3C	-5.10	103.06	107.11
17	A	814	CLA	C2C-C1C-NC	5.10	114.75	109.97
17	b	835	CLA	C4A-NA-C1A	-5.10	104.41	106.71
17	a	808	CLA	C4A-NA-C1A	-5.10	104.41	106.71
17	4	610	CLA	C2C-C1C-NC	5.10	114.75	109.97
17	a	803	CLA	CHD-C4C-C3C	-5.10	117.34	124.84
17	a	829	CLA	C2C-C1C-NC	5.10	114.75	109.97
17	b	820	CLA	C2C-C1C-NC	5.10	114.75	109.97
17	B	805	CLA	C4A-NA-C1A	-5.10	104.41	106.71
26	2	605	CHL	CHD-C4C-C3C	-5.10	117.34	124.84
26	2	605	CHL	C1C-C2C-C3C	-5.10	103.07	107.11
17	9	603	CLA	C2C-C1C-NC	5.10	114.75	109.97
26	1	307	CHL	O2D-CGD-CBD	5.10	120.33	111.27
17	6	307	CLA	C2C-C1C-NC	5.10	114.75	109.97
17	6	304	CLA	O2D-CGD-CBD	5.09	120.32	111.27
17	B	831	CLA	C2C-C1C-NC	5.09	114.74	109.97
17	9	612	CLA	C4A-NA-C1A	-5.09	104.42	106.71
17	3	302	CLA	O2D-CGD-CBD	5.09	120.31	111.27
17	b	836	CLA	C2C-C1C-NC	5.09	114.74	109.97
17	A	807	CLA	C2C-C1C-NC	5.09	114.74	109.97
17	a	815	CLA	C4A-NA-C1A	-5.09	104.42	106.71
17	G	103	CLA	C2C-C1C-NC	5.09	114.74	109.97
17	B	840	CLA	C2C-C1C-NC	5.09	114.74	109.97
17	8	303	CLA	C2C-C1C-NC	5.08	114.73	109.97
17	k	1403	CLA	C4A-NA-C1A	-5.08	104.42	106.71
17	b	807	CLA	C2C-C1C-NC	5.08	114.73	109.97
17	B	823	CLA	C2C-C1C-NC	5.08	114.73	109.97
17	B	817	CLA	C2C-C1C-NC	5.08	114.73	109.97
17	4	602	CLA	O2D-CGD-CBD	5.08	120.29	111.27
17	1	305	CLA	C2C-C1C-NC	5.07	114.73	109.97
17	8	304	CLA	C2C-C1C-NC	5.07	114.73	109.97
17	6	305	CLA	O2D-CGD-CBD	5.07	120.28	111.27
17	1	304	CLA	O2D-CGD-CBD	5.07	120.28	111.27
17	b	815	CLA	C4A-NA-C1A	-5.07	104.42	106.71
17	B	816	CLA	C2C-C1C-NC	5.07	114.72	109.97
26	2	601	CHL	C1C-C2C-C3C	-5.07	103.09	107.11
17	b	838	CLA	C4A-NA-C1A	-5.07	104.43	106.71
17	B	840	CLA	C4A-NA-C1A	-5.07	104.43	106.71
17	A	812	CLA	C4A-NA-C1A	-5.07	104.43	106.71
26	1	302	CHL	C1C-C2C-C3C	-5.07	103.09	107.11
26	7	606	CHL	O2D-CGD-CBD	5.07	120.28	111.27
17	b	827	CLA	O2D-CGD-CBD	5.07	120.28	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	313	CLA	C4A-NA-C1A	-5.07	104.43	106.71
17	b	820	CLA	C4A-NA-C1A	-5.07	104.43	106.71
17	B	807	CLA	C2C-C1C-NC	5.07	114.72	109.97
20	B	843	BCR	C15-C14-C13	-5.06	120.08	127.31
17	1	309	CLA	C4A-NA-C1A	-5.06	104.43	106.71
17	B	815	CLA	C4A-NA-C1A	-5.06	104.43	106.71
17	l	204	CLA	C4A-NA-C1A	-5.06	104.43	106.71
17	B	802	CLA	C2C-C1C-NC	5.06	114.71	109.97
17	b	826	CLA	O2D-CGD-CBD	5.06	120.25	111.27
17	B	834	CLA	C4A-NA-C1A	-5.06	104.43	106.71
17	7	613	CLA	C4A-NA-C1A	-5.06	104.43	106.71
17	B	814	CLA	C4A-NA-C1A	-5.06	104.43	106.71
17	7	608	CLA	C2C-C1C-NC	5.05	114.71	109.97
17	B	833	CLA	C2C-C1C-NC	5.05	114.71	109.97
17	1	305	CLA	C4A-NA-C1A	-5.05	104.44	106.71
17	B	823	CLA	C4A-NA-C1A	-5.05	104.44	106.71
17	3	305	CLA	O2D-CGD-CBD	5.05	120.24	111.27
17	A	829	CLA	C2C-C1C-NC	5.05	114.70	109.97
17	a	842	CLA	C4A-NA-C1A	-5.05	104.44	106.71
17	B	835	CLA	C4A-NA-C1A	-5.05	104.44	106.71
17	1	315	CLA	O2D-CGD-CBD	5.05	120.23	111.27
17	B	835	CLA	C2C-C1C-NC	5.04	114.70	109.97
17	l	203	CLA	C4A-NA-C1A	-5.04	104.44	106.71
17	k	1401	CLA	C4A-NA-C1A	-5.04	104.44	106.71
17	1	305	CLA	O2D-CGD-CBD	5.04	120.23	111.27
26	6	308	CHL	O2D-CGD-CBD	5.04	120.23	111.27
17	a	812	CLA	C2C-C1C-NC	5.04	114.70	109.97
17	B	810	CLA	C2C-C1C-NC	5.04	114.70	109.97
17	9	601	CLA	C4A-NA-C1A	-5.04	104.44	106.71
17	a	826	CLA	C2C-C1C-NC	5.04	114.69	109.97
20	I	101	BCR	C24-C23-C22	-5.03	118.63	126.23
17	b	823	CLA	C2C-C1C-NC	5.03	114.69	109.97
17	l	204	CLA	C2C-C1C-NC	5.03	114.69	109.97
27	6	321	LUT	C15-C14-C13	-5.03	120.13	127.31
17	J	3002	CLA	O2D-CGD-CBD	5.03	120.21	111.27
17	9	611	CLA	O2D-CGD-CBD	5.03	120.20	111.27
17	b	812	CLA	C4A-NA-C1A	-5.02	104.45	106.71
17	a	834	CLA	C2C-C1C-NC	5.02	114.67	109.97
17	b	805	CLA	CHD-C4C-C3C	-5.02	117.46	124.84
17	b	832	CLA	O2D-CGD-CBD	5.02	120.18	111.27
17	3	311	CLA	O2D-CGD-CBD	5.01	120.18	111.27
17	b	824	CLA	C2C-C1C-NC	5.01	114.67	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	830	CLA	C2C-C1C-NC	5.01	114.67	109.97
17	B	803	CLA	CHD-C4C-C3C	-5.01	117.47	124.84
17	A	805	CLA	C2C-C1C-NC	5.01	114.67	109.97
17	4	610	CLA	C4A-NA-C1A	-5.00	104.46	106.71
17	6	304	CLA	C2C-C1C-NC	5.00	114.66	109.97
17	b	838	CLA	O2D-CGD-CBD	5.00	120.16	111.27
20	j	3004	BCR	C38-C26-C25	-5.00	118.91	124.53
17	b	832	CLA	C4A-NA-C1A	-5.00	104.46	106.71
17	6	316	CLA	O2D-CGD-CBD	5.00	120.15	111.27
17	B	805	CLA	C2C-C1C-NC	5.00	114.66	109.97
17	9	604	CLA	C2C-C1C-NC	5.00	114.65	109.97
17	L	202	CLA	C4A-NA-C1A	-5.00	104.46	106.71
17	3	305	CLA	C4A-NA-C1A	-4.99	104.46	106.71
17	B	822	CLA	C2C-C1C-NC	4.99	114.65	109.97
17	a	841	CLA	C2C-C1C-NC	4.99	114.65	109.97
17	L	202	CLA	O2D-CGD-CBD	4.99	120.13	111.27
17	b	830	CLA	C2C-C1C-NC	4.98	114.64	109.97
17	B	808	CLA	C4A-NA-C1A	-4.98	104.47	106.71
17	2	602	CLA	O2D-CGD-CBD	4.98	120.12	111.27
17	A	803	CLA	O2D-CGD-CBD	4.98	120.11	111.27
17	A	820	CLA	C2C-C1C-NC	4.98	114.64	109.97
17	b	813	CLA	C2C-C1C-NC	4.98	114.63	109.97
17	a	832	CLA	O2D-CGD-CBD	4.98	120.11	111.27
17	A	819	CLA	O2D-CGD-CBD	4.97	120.11	111.27
17	A	826	CLA	C4A-NA-C1A	-4.97	104.47	106.71
17	1	306	CLA	C4A-NA-C1A	-4.97	104.47	106.71
17	b	837	CLA	C2C-C1C-NC	4.97	114.63	109.97
17	B	827	CLA	C2C-C1C-NC	4.97	114.63	109.97
20	B	845	BCR	C7-C8-C9	-4.97	118.72	126.23
17	G	104	CLA	C2C-C1C-NC	4.97	114.63	109.97
17	A	842	CLA	C2C-C1C-NC	4.97	114.63	109.97
17	A	826	CLA	C2C-C1C-NC	4.97	114.62	109.97
17	a	804	CLA	C2C-C1C-NC	4.96	114.62	109.97
17	b	826	CLA	C2C-C1C-NC	4.96	114.62	109.97
17	G	101	CLA	C4A-NA-C1A	-4.96	104.48	106.71
17	2	612	CLA	C4A-NA-C1A	-4.95	104.48	106.71
20	a	850	BCR	C15-C14-C13	-4.95	120.24	127.31
17	L	204	CLA	C2C-C1C-NC	4.95	114.61	109.97
17	A	833	CLA	C2C-C1C-NC	4.95	114.61	109.97
20	B	845	BCR	C16-C17-C18	-4.95	120.25	127.31
17	a	828	CLA	C2C-C1C-NC	4.94	114.60	109.97
28	8	315	XAT	C26-C27-C28	-4.94	115.55	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	9	618	BCR	C15-C14-C13	-4.94	120.26	127.31
17	A	806	CLA	C4A-NA-C1A	-4.94	104.48	106.71
17	7	604	CLA	O2D-CGD-CBD	4.94	120.05	111.27
17	B	824	CLA	C2C-C1C-NC	4.94	114.60	109.97
17	7	613	CLA	O2D-CGD-CBD	4.94	120.04	111.27
17	a	844	CLA	C2C-C1C-NC	4.94	114.60	109.97
17	b	811	CLA	C4A-NA-C1A	-4.94	104.49	106.71
17	1	312	CLA	O2D-CGD-CBD	4.93	120.03	111.27
17	K	4003	CLA	C4A-NA-C1A	-4.93	104.49	106.71
17	A	828	CLA	C4A-NA-C1A	-4.93	104.49	106.71
28	7	616	XAT	O4-C5-C18	4.92	120.96	115.06
17	a	816	CLA	C2C-C1C-NC	4.92	114.58	109.97
17	2	611	CLA	O2D-CGD-CBD	4.92	120.01	111.27
17	B	837	CLA	C2C-C1C-NC	4.92	114.58	109.97
26	2	614	CHL	O2D-CGD-CBD	4.92	120.01	111.27
17	a	824	CLA	C4A-NA-C1A	-4.92	104.50	106.71
17	3	308	CLA	C2C-C1C-NC	4.92	114.58	109.97
17	a	813	CLA	C4A-NA-C1A	-4.92	104.50	106.71
17	6	312	CLA	O2D-CGD-CBD	4.92	120.00	111.27
17	B	827	CLA	O2D-CGD-CBD	4.91	120.00	111.27
17	3	312	CLA	C4A-NA-C1A	-4.91	104.50	106.71
17	A	809	CLA	C2C-C1C-NC	4.91	114.57	109.97
28	1	317	XAT	O4-C5-C18	4.91	120.94	115.06
17	k	1402	CLA	C4A-NA-C1A	-4.91	104.50	106.71
17	G	104	CLA	O2D-CGD-CBD	4.90	119.98	111.27
17	A	834	CLA	C4A-NA-C1A	-4.90	104.50	106.71
17	a	840	CLA	C4A-NA-C1A	-4.90	104.50	106.71
17	A	819	CLA	C2C-C1C-NC	4.90	114.56	109.97
17	a	815	CLA	O2D-CGD-CBD	4.90	119.98	111.27
17	a	817	CLA	O2D-CGD-CBD	4.90	119.97	111.27
17	b	833	CLA	C4A-NA-C1A	-4.90	104.50	106.71
17	b	828	CLA	C2C-C1C-NC	4.90	114.56	109.97
17	A	838	CLA	O2D-CGD-CBD	4.90	119.97	111.27
17	a	806	CLA	C2C-C1C-NC	4.89	114.56	109.97
17	3	306	CLA	O2D-CGD-CBD	4.89	119.96	111.27
17	A	831	CLA	CHD-C4C-C3C	-4.89	117.65	124.84
17	a	833	CLA	C4A-NA-C1A	-4.89	104.51	106.71
28	6	318	XAT	C6-C7-C8	-4.89	115.65	125.99
20	L	201	BCR	C7-C8-C9	-4.89	118.85	126.23
17	b	812	CLA	O2D-CGD-CBD	4.89	119.96	111.27
17	4	613	CLA	C4A-NA-C1A	-4.89	104.51	106.71
17	2	610	CLA	O2D-CGD-CBD	4.89	119.95	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	825	CLA	C4A-NA-C1A	-4.89	104.51	106.71
17	4	604	CLA	O2D-CGD-CBD	4.89	119.95	111.27
17	L	204	CLA	O2D-CGD-CBD	4.89	119.95	111.27
17	A	815	CLA	C2C-C1C-NC	4.89	114.55	109.97
17	a	817	CLA	C4A-NA-C1A	-4.88	104.51	106.71
17	1	313	CLA	C4A-NA-C1A	-4.88	104.51	106.71
17	8	309	CLA	C4A-NA-C1A	-4.88	104.51	106.71
17	a	834	CLA	O2D-CGD-CBD	4.88	119.94	111.27
17	6	306	CLA	C4A-NA-C1A	-4.88	104.51	106.71
17	A	840	CLA	C4A-NA-C1A	-4.88	104.51	106.71
17	3	314	CLA	O2D-CGD-CBD	4.88	119.94	111.27
17	B	812	CLA	O2D-CGD-CBD	4.87	119.92	111.27
20	K	4004	BCR	C16-C17-C18	-4.87	120.36	127.31
17	b	810	CLA	C2C-C1C-NC	4.87	114.53	109.97
26	4	615	CHL	O2D-CGD-CBD	4.87	119.92	111.27
17	4	612	CLA	C4A-NA-C1A	-4.87	104.52	106.71
17	b	829	CLA	CHD-C4C-C3C	-4.87	117.69	124.84
17	j	3002	CLA	O2D-CGD-CBD	4.86	119.91	111.27
17	A	814	CLA	C4A-NA-C1A	-4.86	104.52	106.71
17	B	813	CLA	C2C-C1C-NC	4.86	114.53	109.97
17	6	306	CLA	O2D-CGD-CBD	4.86	119.90	111.27
20	L	206	BCR	C20-C21-C22	-4.86	120.38	127.31
17	7	611	CLA	O2D-CGD-CBD	4.86	119.90	111.27
17	1	310	CLA	C2C-C1C-NC	4.85	114.52	109.97
17	a	806	CLA	O2D-CGD-CBD	4.85	119.89	111.27
17	b	827	CLA	C2C-C1C-NC	4.85	114.52	109.97
17	9	613	CLA	C4A-NA-C1A	-4.85	104.53	106.71
17	A	817	CLA	O2D-CGD-CBD	4.85	119.88	111.27
17	a	807	CLA	C2C-C1C-NC	4.85	114.51	109.97
17	A	818	CLA	C4A-NA-C1A	-4.85	104.53	106.71
17	l	202	CLA	C4A-NA-C1A	-4.84	104.53	106.71
26	4	607	CHL	C2C-C3C-C4C	-4.84	103.04	106.49
17	2	602	CLA	C2C-C1C-NC	4.84	114.51	109.97
17	g	102	CLA	O2D-CGD-CBD	4.84	119.86	111.27
26	7	605	CHL	C1C-C2C-C3C	-4.83	103.28	107.11
17	4	601	CLA	C4A-NA-C1A	-4.82	104.54	106.71
17	8	313	CLA	C1C-NC-C4C	-4.82	104.54	106.71
17	B	826	CLA	C2C-C1C-NC	4.82	114.49	109.97
17	A	806	CLA	C2C-C1C-NC	4.82	114.49	109.97
17	A	824	CLA	O2D-CGD-CBD	4.82	119.83	111.27
17	a	846	CLA	O2D-CGD-CBD	4.82	119.83	111.27
17	B	804	CLA	C4A-NA-C1A	-4.81	104.54	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	824	CLA	O2D-CGD-CBD	4.81	119.81	111.27
17	L	203	CLA	O2D-CGD-CBD	4.81	119.81	111.27
17	6	313	CLA	O2D-CGD-CBD	4.80	119.81	111.27
20	8	316	BCR	C15-C14-C13	-4.80	120.46	127.31
17	B	817	CLA	O2D-CGD-CBD	4.80	119.79	111.27
17	9	608	CLA	C4A-NA-C1A	-4.80	104.55	106.71
17	b	822	CLA	C2C-C1C-NC	4.80	114.47	109.97
17	B	832	CLA	C2C-C1C-NC	4.80	114.47	109.97
17	a	841	CLA	C4A-NA-C1A	-4.79	104.55	106.71
17	B	806	CLA	C2C-C1C-NC	4.79	114.46	109.97
17	f	7003	CLA	C4A-NA-C1A	-4.79	104.55	106.71
20	A	856	BCR	C15-C14-C13	-4.79	120.47	127.31
17	l	315	CLA	C4A-NA-C1A	-4.79	104.55	106.71
17	a	803	CLA	O2D-CGD-CBD	4.78	119.77	111.27
17	a	832	CLA	C4A-NA-C1A	-4.78	104.56	106.71
17	k	1402	CLA	O2D-CGD-CBD	4.78	119.76	111.27
17	B	838	CLA	O2D-CGD-CBD	4.78	119.76	111.27
17	j	3002	CLA	C4A-NA-C1A	-4.78	104.56	106.71
20	4	618	BCR	C15-C14-C13	-4.78	120.49	127.31
17	A	838	CLA	C2C-C1C-NC	4.78	114.45	109.97
17	a	808	CLA	C2C-C1C-NC	4.78	114.45	109.97
17	A	808	CLA	C4A-NA-C1A	-4.77	104.56	106.71
17	a	805	CLA	C4A-NA-C1A	-4.77	104.56	106.71
17	2	604	CLA	O2D-CGD-CBD	4.77	119.75	111.27
17	1	306	CLA	O2D-CGD-CBD	4.77	119.74	111.27
20	B	843	BCR	C16-C17-C18	-4.77	120.51	127.31
17	a	802	CLA	C4A-NA-C1A	-4.76	104.56	106.71
17	a	802	CLA	C2C-C1C-NC	4.76	114.43	109.97
17	7	612	CLA	C4A-NA-C1A	-4.76	104.57	106.71
17	8	305	CLA	O2D-CGD-CBD	4.76	119.72	111.27
17	a	809	CLA	C2C-C1C-NC	4.76	114.43	109.97
17	7	610	CLA	O2D-CGD-CBD	4.76	119.72	111.27
17	A	816	CLA	O2D-CGD-CBD	4.76	119.72	111.27
17	B	819	CLA	C4A-NA-C1A	-4.76	104.57	106.71
17	A	833	CLA	O2D-CGD-CBD	4.76	119.72	111.27
17	6	312	CLA	C4A-NA-C1A	-4.76	104.57	106.71
17	8	310	CLA	C4A-NA-C1A	-4.76	104.57	106.71
17	b	841	CLA	C2C-C1C-NC	4.75	114.43	109.97
17	A	841	CLA	C2C-C1C-NC	4.75	114.43	109.97
17	a	805	CLA	O2D-CGD-CBD	4.75	119.71	111.27
17	b	832	CLA	C2C-C1C-NC	4.75	114.42	109.97
17	B	836	CLA	O2D-CGD-CBD	4.75	119.70	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	f	7002	CLA	C4A-NA-C1A	-4.74	104.57	106.71
17	a	804	CLA	C4A-NA-C1A	-4.74	104.57	106.71
20	B	801	BCR	C16-C15-C14	-4.74	113.76	123.47
17	b	809	CLA	O2D-CGD-CBD	4.74	119.69	111.27
17	B	833	CLA	C4A-NA-C1A	-4.74	104.57	106.71
17	1	303	CLA	C2C-C1C-NC	4.74	114.41	109.97
17	a	828	CLA	C4A-NA-C1A	-4.74	104.58	106.71
17	a	818	CLA	C4A-NA-C1A	-4.74	104.58	106.71
17	3	315	CLA	C1C-NC-C4C	-4.74	104.58	106.71
17	a	815	CLA	C2C-C1C-NC	4.74	114.41	109.97
26	4	606	CHL	C1C-C2C-C3C	-4.73	103.36	107.11
17	8	307	CLA	C2C-C1C-NC	4.73	114.41	109.97
17	3	302	CLA	C2C-C1C-NC	4.73	114.40	109.97
17	L	203	CLA	C2C-C1C-NC	4.73	114.40	109.97
17	a	833	CLA	C2C-C1C-NC	4.72	114.39	109.97
17	b	834	CLA	O2D-CGD-CBD	4.72	119.65	111.27
26	7	601	CHL	C1C-C2C-C3C	-4.72	103.37	107.11
17	B	811	CLA	C4A-NA-C1A	-4.72	104.59	106.71
17	a	814	CLA	C2C-C1C-NC	4.71	114.39	109.97
17	a	806	CLA	C1-C2-C3	-4.71	117.89	126.04
17	9	609	CLA	C2C-C1C-NC	4.71	114.39	109.97
17	A	808	CLA	O2D-CGD-CBD	4.71	119.64	111.27
17	F	304	CLA	C4A-NA-C1A	-4.71	104.59	106.71
17	A	842	CLA	O2D-CGD-CBD	4.70	119.63	111.27
17	b	825	CLA	C2C-C1C-NC	4.70	114.38	109.97
17	B	811	CLA	O2D-CGD-CBD	4.70	119.61	111.27
17	a	827	CLA	C2C-C1C-NC	4.70	114.37	109.97
17	a	808	CLA	O2D-CGD-CBD	4.70	119.61	111.27
26	7	607	CHL	O2D-CGD-CBD	4.69	119.61	111.27
17	4	612	CLA	O2D-CGD-CBD	4.69	119.60	111.27
17	b	804	CLA	C4A-NA-C1A	-4.69	104.60	106.71
17	B	825	CLA	C2C-C1C-NC	4.69	114.36	109.97
17	G	101	CLA	O2D-CGD-CBD	4.69	119.60	111.27
17	B	829	CLA	CHD-C4C-C3C	-4.69	117.95	124.84
20	6	319	BCR	C15-C14-C13	-4.68	120.63	127.31
17	B	810	CLA	O2D-CGD-CBD	4.68	119.58	111.27
17	B	841	CLA	C2C-C1C-NC	4.68	114.36	109.97
17	A	820	CLA	O2D-CGD-CBD	4.67	119.57	111.27
17	a	843	CLA	C2C-C1C-NC	4.67	114.35	109.97
17	b	834	CLA	C4A-NA-C1A	-4.67	104.61	106.71
17	A	835	CLA	C4A-NA-C1A	-4.66	104.61	106.71
17	A	843	CLA	O2D-CGD-CBD	4.66	119.55	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	801	CLA	C4A-NA-C1A	-4.66	104.61	106.71
17	A	839	CLA	C4A-NA-C1A	-4.66	104.61	106.71
17	A	825	CLA	O2D-CGD-CBD	4.66	119.54	111.27
17	b	839	CLA	C4A-NA-C1A	-4.65	104.61	106.71
26	3	307	CHL	O2D-CGD-CBD	4.65	119.53	111.27
17	1	306	CLA	C2C-C1C-NC	4.65	114.32	109.97
20	L	201	BCR	C15-C14-C13	-4.64	120.69	127.31
17	7	602	CLA	C2C-C1C-NC	4.64	114.32	109.97
17	b	806	CLA	C2C-C1C-NC	4.64	114.32	109.97
26	7	605	CHL	O2D-CGD-CBD	4.63	119.50	111.27
17	a	810	CLA	C4A-NA-C1A	-4.63	104.62	106.71
17	9	610	CLA	O2D-CGD-CBD	4.63	119.50	111.27
26	2	607	CHL	O2D-CGD-CBD	4.63	119.49	111.27
17	4	602	CLA	C2C-C1C-NC	4.63	114.31	109.97
17	A	834	CLA	O2D-CGD-CBD	4.62	119.48	111.27
17	a	811	CLA	O2D-CGD-CBD	4.62	119.48	111.27
20	a	853	BCR	C28-C27-C26	-4.62	105.83	114.08
20	a	853	BCR	C20-C21-C22	-4.62	120.72	127.31
17	a	819	CLA	C2C-C1C-NC	4.61	114.30	109.97
17	b	807	CLA	C4A-NA-C1A	-4.61	104.63	106.71
28	6	318	XAT	O24-C25-C38	4.61	120.58	115.06
17	a	813	CLA	O2D-CGD-CBD	4.61	119.45	111.27
17	A	827	CLA	O2D-CGD-CBD	4.61	119.45	111.27
17	6	307	CLA	O2D-CGD-CBD	4.60	119.45	111.27
17	4	609	CLA	C2C-C1C-NC	4.60	114.28	109.97
28	2	616	XAT	C6-C7-C8	-4.60	116.27	125.99
17	1	204	CLA	O2D-CGD-CBD	4.60	119.44	111.27
17	a	810	CLA	O2D-CGD-CBD	4.60	119.44	111.27
17	1	313	CLA	O2D-CGD-CBD	4.59	119.43	111.27
17	B	839	CLA	O2D-CGD-CBD	4.59	119.43	111.27
17	b	817	CLA	O2D-CGD-CBD	4.59	119.42	111.27
17	a	839	CLA	C4A-NA-C1A	-4.58	104.64	106.71
17	2	608	CLA	O2D-CGD-CBD	4.58	119.41	111.27
17	3	313	CLA	O2D-CGD-CBD	4.58	119.40	111.27
20	A	850	BCR	C16-C17-C18	-4.57	120.79	127.31
20	b	843	BCR	C15-C14-C13	-4.56	120.80	127.31
17	8	312	CLA	O2D-CGD-CBD	4.56	119.38	111.27
17	8	304	CLA	O2D-CGD-CBD	4.56	119.37	111.27
17	3	312	CLA	O2D-CGD-CBD	4.56	119.37	111.27
17	A	828	CLA	C2C-C1C-NC	4.56	114.24	109.97
17	a	833	CLA	O2D-CGD-CBD	4.56	119.37	111.27
20	A	851	BCR	C28-C27-C26	-4.56	105.94	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	840	CLA	O2D-CGD-CBD	4.55	119.36	111.27
17	6	314	CLA	O2D-CGD-CBD	4.55	119.35	111.27
17	A	827	CLA	C2C-C1C-NC	4.55	114.23	109.97
17	l	203	CLA	C2C-C1C-NC	4.55	114.23	109.97
20	j	3003	BCR	C28-C27-C26	-4.54	105.97	114.08
17	8	302	CLA	O2D-CGD-CBD	4.54	119.34	111.27
20	a	850	BCR	C3-C4-C5	-4.54	105.97	114.08
20	2	617	BCR	C15-C14-C13	-4.54	120.83	127.31
17	8	310	CLA	O2D-CGD-CBD	4.54	119.33	111.27
20	B	844	BCR	C28-C27-C26	-4.54	105.98	114.08
17	B	837	CLA	C4A-NA-C1A	-4.54	104.67	106.71
17	7	612	CLA	O2D-CGD-CBD	4.53	119.33	111.27
17	A	802	CLA	C2C-C1C-NC	4.53	114.22	109.97
17	a	844	CLA	O2D-CGD-CBD	4.53	119.31	111.27
17	8	311	CLA	O2D-CGD-CBD	4.53	119.31	111.27
17	6	311	CLA	C2C-C1C-NC	4.53	114.21	109.97
17	8	308	CLA	C2C-C1C-NC	4.52	114.21	109.97
17	a	806	CLA	C4A-NA-C1A	-4.52	104.68	106.71
17	b	840	CLA	C4A-NA-C1A	-4.51	104.68	106.71
17	2	612	CLA	O2D-CGD-CBD	4.51	119.28	111.27
26	9	607	CHL	C2C-C3C-C4C	-4.51	103.28	106.49
17	8	301	CLA	C2C-C1C-NC	4.50	114.19	109.97
17	A	825	CLA	C4A-NA-C1A	-4.50	104.68	106.71
28	6	318	XAT	O4-C5-C18	4.50	120.45	115.06
17	4	610	CLA	O2D-CGD-CBD	4.50	119.27	111.27
17	B	803	CLA	C2C-C1C-NC	4.49	114.18	109.97
17	9	612	CLA	O2D-CGD-CBD	4.49	119.25	111.27
17	3	309	CLA	C2C-C1C-NC	4.49	114.18	109.97
17	b	803	CLA	C2C-C1C-NC	4.49	114.18	109.97
17	4	611	CLA	O2D-CGD-CBD	4.49	119.25	111.27
17	J	3002	CLA	C4A-NA-C1A	-4.49	104.69	106.71
17	f	7002	CLA	O2D-CGD-CBD	4.49	119.24	111.27
28	8	315	XAT	C35-C34-C33	-4.49	120.91	127.31
17	3	306	CLA	C4A-NA-C1A	-4.48	104.69	106.71
17	a	812	CLA	O2D-CGD-CBD	4.48	119.23	111.27
17	b	808	CLA	C4A-NA-C1A	-4.48	104.69	106.71
20	7	617	BCR	C20-C21-C22	-4.48	120.92	127.31
17	F	304	CLA	O2D-CGD-CBD	4.48	119.23	111.27
17	7	609	CLA	O2D-CGD-CBD	4.47	119.22	111.27
17	b	814	CLA	C2C-C1C-NC	4.47	114.16	109.97
17	b	835	CLA	O2D-CGD-CBD	4.47	119.21	111.27
26	3	307	CHL	C2C-C3C-C4C	-4.47	103.31	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	830	CLA	O2D-CGD-CBD	4.46	119.20	111.27
17	2	609	CLA	C2C-C1C-NC	4.46	114.15	109.97
28	4	617	XAT	C26-C27-C28	-4.46	116.56	125.99
20	1	206	BCR	C20-C21-C22	-4.46	120.95	127.31
27	6	317	LUT	C35-C34-C33	-4.46	120.95	127.31
26	8	306	CHL	C2C-C3C-C4C	-4.45	103.31	106.49
17	9	608	CLA	O2D-CGD-CBD	4.45	119.18	111.27
17	B	828	CLA	O2D-CGD-CBD	4.45	119.18	111.27
17	9	602	CLA	C2C-C1C-NC	4.45	114.14	109.97
17	2	609	CLA	O2D-CGD-CBD	4.45	119.17	111.27
17	B	809	CLA	O2D-CGD-CBD	4.45	119.17	111.27
27	1	320	LUT	C15-C14-C13	-4.45	120.96	127.31
17	4	608	CLA	O2D-CGD-CBD	4.45	119.17	111.27
17	G	103	CLA	O2D-CGD-CBD	4.44	119.16	111.27
17	b	803	CLA	C4A-NA-C1A	-4.44	104.71	106.71
28	9	617	XAT	C26-C27-C28	-4.44	116.61	125.99
17	B	820	CLA	C4A-NA-C1A	-4.44	104.71	106.71
17	7	609	CLA	C2C-C1C-NC	4.44	114.13	109.97
17	a	838	CLA	C2C-C1C-NC	4.43	114.12	109.97
17	A	811	CLA	O2D-CGD-CBD	4.43	119.14	111.27
20	B	847	BCR	C15-C14-C13	-4.43	120.99	127.31
20	I	101	BCR	C20-C21-C22	-4.43	120.99	127.31
17	7	603	CLA	O2D-CGD-CBD	4.43	119.13	111.27
20	b	845	BCR	C24-C23-C22	-4.42	119.55	126.23
17	B	831	CLA	O2D-CGD-CBD	4.42	119.11	111.27
17	B	838	CLA	C4A-NA-C1A	-4.41	104.72	106.71
17	b	837	CLA	C4A-NA-C1A	-4.40	104.73	106.71
17	A	819	CLA	C4A-NA-C1A	-4.40	104.73	106.71
17	A	830	CLA	O2D-CGD-CBD	4.40	119.09	111.27
17	A	806	CLA	O2D-CGD-CBD	4.40	119.09	111.27
17	A	810	CLA	O2D-CGD-CBD	4.40	119.08	111.27
17	b	831	CLA	O2D-CGD-CBD	4.39	119.07	111.27
17	A	836	CLA	C4A-NA-C1A	-4.39	104.73	106.71
17	b	824	CLA	C4A-NA-C1A	-4.39	104.73	106.71
26	8	306	CHL	O2D-CGD-CBD	4.38	119.05	111.27
28	9	617	XAT	O24-C25-C38	4.38	120.30	115.06
17	A	837	CLA	C4A-NA-C1A	-4.38	104.74	106.71
20	A	850	BCR	C3-C4-C5	-4.38	106.27	114.08
28	7	616	XAT	O24-C25-C38	4.37	120.30	115.06
20	1	318	BCR	C15-C14-C13	-4.37	121.07	127.31
26	7	606	CHL	C3C-C4C-NC	4.37	115.47	110.57
28	8	315	XAT	O24-C25-C38	4.36	120.28	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	1	317	XAT	C26-C27-C28	-4.36	116.77	125.99
20	A	848	BCR	C16-C17-C18	-4.35	121.10	127.31
26	2	606	CHL	C3C-C4C-NC	4.35	115.45	110.57
17	g	101	CLA	O2D-CGD-CBD	4.35	119.00	111.27
17	a	819	CLA	O2D-CGD-CBD	4.35	118.99	111.27
28	9	617	XAT	C35-C34-C33	-4.35	121.11	127.31
17	a	836	CLA	C4A-NA-C1A	-4.34	104.75	106.71
19	1	301	LHG	O7-C7-C8	4.34	120.86	111.50
26	2	607	CHL	C3C-C4C-NC	4.33	115.43	110.57
17	A	805	CLA	C4A-NA-C1A	-4.33	104.76	106.71
17	a	823	CLA	C4A-NA-C1A	-4.33	104.76	106.71
20	b	845	BCR	C28-C27-C26	-4.33	106.35	114.08
17	3	309	CLA	O2D-CGD-CBD	4.33	118.96	111.27
17	A	821	CLA	C4A-NA-C1A	-4.33	104.76	106.71
17	B	814	CLA	C2C-C1C-NC	4.32	114.02	109.97
17	A	842	CLA	C1-C2-C3	-4.32	118.58	126.04
17	a	836	CLA	O2D-CGD-CBD	4.31	118.93	111.27
20	b	847	BCR	C3-C4-C5	-4.31	106.38	114.08
17	a	816	CLA	O2D-CGD-CBD	4.31	118.92	111.27
17	b	839	CLA	O2D-CGD-CBD	4.30	118.91	111.27
20	k	1404	BCR	C16-C17-C18	-4.30	121.17	127.31
17	b	822	CLA	O2D-CGD-CBD	4.29	118.89	111.27
26	4	607	CHL	C3C-C4C-NC	4.29	115.38	110.57
17	a	841	CLA	O2D-CGD-CBD	4.29	118.89	111.27
17	B	824	CLA	C4A-NA-C1A	-4.29	104.78	106.71
20	a	849	BCR	C20-C21-C22	-4.29	121.19	127.31
17	7	608	CLA	O2D-CGD-CBD	4.28	118.88	111.27
17	a	828	CLA	C3C-C4C-NC	4.28	115.37	110.57
17	3	308	CLA	C1-C2-C3	-4.27	119.84	126.75
26	4	607	CHL	O2D-CGD-CBD	4.27	118.85	111.27
26	9	606	CHL	C3C-C4C-NC	4.27	115.36	110.57
17	B	822	CLA	O2D-CGD-CBD	4.27	118.85	111.27
26	1	302	CHL	C3C-C4C-NC	4.26	115.35	110.57
17	1	308	CLA	O2D-CGD-CBD	4.26	118.84	111.27
26	4	606	CHL	C3C-C4C-NC	4.26	115.35	110.57
17	F	303	CLA	O2D-CGD-CBD	4.26	118.84	111.27
17	8	307	CLA	O2D-CGD-CBD	4.26	118.84	111.27
28	4	617	XAT	O24-C25-C38	4.26	120.16	115.06
17	A	813	CLA	O2D-CGD-CBD	4.25	118.82	111.27
20	g	104	BCR	C16-C17-C18	-4.25	121.24	127.31
17	A	854	CLA	C1-C2-C3	-4.25	118.70	126.04
17	B	823	CLA	C1-C2-C3	-4.25	118.70	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	840	CLA	O2D-CGD-CBD	4.24	118.81	111.27
17	A	854	CLA	C3C-C4C-NC	4.24	115.33	110.57
17	b	819	CLA	O2D-CGD-CBD	4.24	118.80	111.27
17	B	803	CLA	C4A-NA-C1A	-4.24	104.80	106.71
28	2	616	XAT	O24-C25-C38	4.24	120.13	115.06
20	g	104	BCR	C28-C27-C26	-4.24	106.52	114.08
26	4	615	CHL	C3C-C4C-NC	4.23	115.32	110.57
17	a	820	CLA	O2D-CGD-CBD	4.23	118.79	111.27
17	a	827	CLA	O2D-CGD-CBD	4.23	118.79	111.27
17	6	309	CLA	O2D-CGD-CBD	4.23	118.79	111.27
20	B	844	BCR	C3-C4-C5	-4.23	106.52	114.08
26	1	307	CHL	C3C-C4C-NC	4.23	115.32	110.57
26	7	605	CHL	C3C-C4C-NC	4.23	115.31	110.57
28	6	318	XAT	C26-C27-C28	-4.22	117.06	125.99
17	B	826	CLA	C3C-C4C-NC	4.22	115.31	110.57
26	2	605	CHL	O2D-CGD-CBD	4.22	118.77	111.27
24	b	849	DGD	O2G-C1B-C2B	4.22	120.59	111.50
20	b	844	BCR	C3-C4-C5	-4.22	106.54	114.08
17	B	834	CLA	O2D-CGD-CBD	4.22	118.76	111.27
20	B	843	BCR	C20-C21-C22	-4.22	121.29	127.31
26	7	607	CHL	C3C-C4C-NC	4.21	115.30	110.57
17	6	311	CLA	O2D-CGD-CBD	4.21	118.75	111.27
20	I	101	BCR	C16-C17-C18	-4.21	121.30	127.31
17	3	308	CLA	O2D-CGD-CBD	4.21	118.74	111.27
28	8	315	XAT	C6-C7-C8	-4.21	117.10	125.99
17	A	829	CLA	O2D-CGD-CBD	4.20	118.74	111.27
20	g	104	BCR	C20-C21-C22	-4.20	121.31	127.31
17	B	819	CLA	O2D-CGD-CBD	4.20	118.73	111.27
17	9	609	CLA	O2D-CGD-CBD	4.20	118.73	111.27
20	A	850	BCR	C11-C10-C9	-4.20	121.32	127.31
17	b	828	CLA	O2D-CGD-CBD	4.20	118.72	111.27
17	a	824	CLA	C1-C2-C3	-4.19	118.80	126.04
28	4	617	XAT	C6-C7-C8	-4.18	117.15	125.99
17	4	609	CLA	O2D-CGD-CBD	4.18	118.70	111.27
20	b	844	BCR	C28-C27-C26	-4.17	106.62	114.08
26	9	605	CHL	C3C-C4C-NC	4.17	115.25	110.57
26	2	601	CHL	C3C-C4C-NC	4.17	115.25	110.57
20	G	105	BCR	C20-C21-C22	-4.17	121.36	127.31
19	a	847	LHG	O7-C7-C8	4.17	120.48	111.50
26	2	614	CHL	C3C-C4C-NC	4.17	115.24	110.57
17	2	610	CLA	CAA-C2A-C3A	-4.16	106.39	116.10
20	J	3003	BCR	C15-C14-C13	-4.16	121.38	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	G	105	BCR	C16-C17-C18	-4.16	121.38	127.31
26	7	614	CHL	C3C-C4C-NC	4.16	115.23	110.57
26	9	615	CHL	C3C-C4C-NC	4.16	115.23	110.57
17	B	829	CLA	C1C-C2C-C3C	-4.16	102.59	106.96
17	A	839	CLA	C1D-CHD-C4C	-4.15	117.08	122.56
17	A	822	CLA	O2D-CGD-CBD	4.15	118.63	111.27
20	j	3004	BCR	C3-C4-C5	-4.14	106.68	114.08
20	A	856	BCR	C3-C4-C5	-4.14	106.68	114.08
19	A	846	LHG	O7-C7-C8	4.14	120.43	111.50
20	b	844	BCR	C24-C23-C22	-4.14	119.98	126.23
19	a	848	LHG	O7-C7-C8	4.13	120.41	111.50
20	A	851	BCR	C15-C14-C13	-4.13	121.41	127.31
26	4	605	CHL	C3C-C4C-NC	4.13	115.20	110.57
28	1	317	XAT	O24-C25-C38	4.13	120.00	115.06
17	a	844	CLA	C1-C2-C3	-4.13	118.90	126.04
17	7	610	CLA	CAA-C2A-C3A	-4.13	106.47	116.10
17	A	821	CLA	C1C-C2C-C3C	-4.12	102.62	106.96
17	a	842	CLA	C1D-CHD-C4C	-4.12	117.12	122.56
19	7	618	LHG	O7-C7-C8	4.12	120.39	111.50
17	a	821	CLA	C1C-C2C-C3C	-4.12	102.62	106.96
20	G	105	BCR	C28-C27-C26	-4.12	106.73	114.08
26	8	306	CHL	C3C-C4C-NC	4.11	115.18	110.57
20	b	843	BCR	C11-C10-C9	-4.11	121.44	127.31
20	l	201	BCR	C15-C14-C13	-4.11	121.44	127.31
17	a	821	CLA	C1D-CHD-C4C	-4.11	117.14	122.56
17	a	822	CLA	O2D-CGD-CBD	4.11	118.56	111.27
28	1	317	XAT	C35-C34-C33	-4.11	121.45	127.31
17	A	836	CLA	O2D-CGD-CBD	4.10	118.56	111.27
17	a	856	CLA	C3C-C4C-NC	4.10	115.17	110.57
17	g	101	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
20	L	206	BCR	C11-C10-C9	-4.10	121.46	127.31
20	b	801	BCR	C16-C17-C18	-4.10	121.47	127.31
17	A	836	CLA	C3C-C4C-NC	4.10	115.16	110.57
26	6	308	CHL	C3C-C4C-NC	4.09	115.16	110.57
17	A	812	CLA	C1D-CHD-C4C	-4.09	117.16	122.56
17	b	810	CLA	C1-C2-C3	-4.09	118.97	126.04
20	B	848	BCR	C16-C17-C18	-4.09	121.48	127.31
20	b	844	BCR	C15-C14-C13	-4.09	121.48	127.31
17	A	812	CLA	O2D-CGD-CBD	4.09	118.53	111.27
17	1	310	CLA	O2D-CGD-CBD	4.08	118.52	111.27
17	A	834	CLA	C1-C2-C3	-4.08	118.99	126.04
20	l	206	BCR	C24-C23-C22	-4.07	120.08	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	826	CLA	C3C-C4C-NC	4.07	115.14	110.57
28	3	317	XAT	C35-C34-C33	-4.07	121.50	127.31
20	A	856	BCR	C38-C26-C25	-4.07	119.96	124.53
26	2	605	CHL	C3C-C4C-NC	4.06	115.13	110.57
28	9	617	XAT	C6-C7-C8	-4.06	117.40	125.99
17	B	820	CLA	O2D-CGD-CBD	4.06	118.49	111.27
20	A	856	BCR	C28-C27-C26	-4.06	106.83	114.08
17	a	821	CLA	C3C-C4C-NC	4.06	115.12	110.57
20	A	851	BCR	C16-C17-C18	-4.06	121.52	127.31
25	4	619	LMG	O7-C10-C11	4.06	120.24	111.50
28	3	317	XAT	O24-C25-C38	4.06	119.92	115.06
20	2	617	BCR	C16-C17-C18	-4.05	121.52	127.31
17	b	829	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
17	a	832	CLA	C3C-C4C-NC	4.05	115.11	110.57
19	6	320	LHG	O7-C7-C8	4.05	120.23	111.50
17	A	810	CLA	C3C-C4C-NC	4.05	115.11	110.57
17	9	610	CLA	CAA-C2A-C3A	-4.04	106.67	116.10
17	4	614	CLA	C1-C2-C3	-4.04	120.22	126.75
26	7	601	CHL	C3C-C4C-NC	4.04	115.10	110.57
20	k	1404	BCR	C15-C14-C13	-4.04	121.55	127.31
17	8	308	CLA	O2D-CGD-CBD	4.03	118.43	111.27
20	a	854	BCR	C16-C17-C18	-4.03	121.56	127.31
20	l	206	BCR	C15-C14-C13	-4.03	121.56	127.31
17	b	839	CLA	C3C-C4C-NC	4.03	115.09	110.57
17	b	838	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
19	A	847	LHG	O7-C7-C8	4.03	120.18	111.50
20	l	205	BCR	C38-C26-C25	-4.03	120.01	124.53
26	9	607	CHL	O2D-CGD-CBD	4.03	118.42	111.27
17	b	840	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
17	a	829	CLA	O2D-CGD-CBD	4.02	118.41	111.27
17	b	827	CLA	C3C-C4C-NC	4.01	115.07	110.57
27	7	615	LUT	C35-C34-C33	-4.01	121.59	127.31
17	a	830	CLA	C3C-C4C-NC	4.01	115.07	110.57
17	a	809	CLA	C1-C2-C3	-4.01	119.11	126.04
20	i	101	BCR	C16-C17-C18	-4.01	121.59	127.31
20	L	206	BCR	C16-C17-C18	-4.01	121.59	127.31
20	I	101	BCR	C28-C27-C26	-4.00	106.93	114.08
20	B	843	BCR	C28-C27-C26	-4.00	106.93	114.08
17	A	830	CLA	C3C-C4C-NC	4.00	115.06	110.57
20	4	618	BCR	C28-C27-C26	-4.00	106.94	114.08
20	B	847	BCR	C24-C23-C22	-4.00	120.19	126.23
26	6	303	CHL	C3C-C4C-NC	3.99	115.05	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	8	316	BCR	C28-C27-C26	-3.99	106.95	114.08
20	a	850	BCR	C11-C10-C9	-3.99	121.61	127.31
20	A	850	BCR	C15-C14-C13	-3.99	121.61	127.31
20	A	850	BCR	C7-C8-C9	-3.99	120.20	126.23
28	2	616	XAT	C26-C27-C28	-3.99	117.56	125.99
17	a	804	CLA	C1-C2-C3	-3.99	119.15	126.04
28	7	616	XAT	C26-C27-C28	-3.99	117.56	125.99
20	B	848	BCR	C33-C5-C6	-3.99	120.05	124.53
20	L	206	BCR	C24-C23-C22	-3.99	120.21	126.23
20	a	851	BCR	C16-C17-C18	-3.98	121.63	127.31
20	b	843	BCR	C28-C27-C26	-3.98	106.97	114.08
20	6	319	BCR	C28-C27-C26	-3.98	106.97	114.08
17	4	603	CLA	C1D-CHD-C4C	-3.98	117.30	122.56
17	b	806	CLA	O2D-CGD-CBD	3.98	118.33	111.27
17	a	856	CLA	C3B-C4B-NB	3.98	114.35	109.21
20	k	1404	BCR	C20-C21-C22	-3.97	121.64	127.31
28	3	317	XAT	C6-C7-C8	-3.97	117.60	125.99
17	b	809	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
19	6	301	LHG	O7-C7-C8	3.97	120.05	111.50
20	g	104	BCR	C24-C23-C22	-3.96	120.25	126.23
20	A	852	BCR	C20-C21-C22	-3.96	121.66	127.31
20	1	318	BCR	C16-C17-C18	-3.96	121.66	127.31
26	2	606	CHL	C1D-CHD-C4C	-3.96	117.33	122.56
17	a	829	CLA	C3C-C4C-NC	3.96	115.01	110.57
17	b	810	CLA	O2D-CGD-CBD	3.96	118.30	111.27
17	a	831	CLA	C3C-C4C-NC	3.96	115.01	110.57
20	1	318	BCR	C11-C10-C9	-3.95	121.67	127.31
17	9	608	CLA	C1D-CHD-C4C	-3.95	117.34	122.56
17	B	836	CLA	C3C-C4C-NC	3.95	115.00	110.57
17	a	817	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
27	6	321	LUT	C11-C10-C9	-3.95	121.68	127.31
20	b	845	BCR	C15-C14-C13	-3.95	121.68	127.31
19	1	319	LHG	O7-C7-C8	3.95	120.00	111.50
17	b	836	CLA	C3C-C4C-NC	3.95	115.00	110.57
17	a	836	CLA	C3C-C4C-NC	3.94	114.99	110.57
17	B	827	CLA	C3C-C4C-NC	3.94	114.99	110.57
17	A	854	CLA	C1D-CHD-C4C	-3.94	117.36	122.56
17	b	807	CLA	C1-C2-C3	-3.94	119.24	126.04
17	9	611	CLA	C1D-CHD-C4C	-3.94	117.36	122.56
17	b	823	CLA	O2D-CGD-CBD	3.94	118.26	111.27
20	B	845	BCR	C3-C4-C5	-3.93	107.06	114.08
17	A	810	CLA	C4A-NA-C1A	-3.93	104.94	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	101	CLA	C1D-CHD-C4C	-3.93	117.37	122.56
17	A	829	CLA	C3C-C4C-NC	3.93	114.97	110.57
17	b	836	CLA	C1D-CHD-C4C	-3.93	117.38	122.56
17	b	826	CLA	C3C-C4C-NC	3.93	114.97	110.57
17	b	813	CLA	CAC-C3C-C4C	3.92	129.89	124.81
17	b	810	CLA	C3C-C4C-NC	3.92	114.96	110.57
17	F	301	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
17	a	801	CLA	C3C-C4C-NC	3.91	114.96	110.57
17	A	821	CLA	C3C-C4C-NC	3.91	114.96	110.57
26	9	607	CHL	C3C-C4C-NC	3.91	114.96	110.57
17	4	608	CLA	C1D-CHD-C4C	-3.91	117.40	122.56
17	A	828	CLA	C3C-C4C-NC	3.91	114.95	110.57
20	k	1404	BCR	C38-C26-C25	-3.91	120.14	124.53
20	A	856	BCR	C16-C17-C18	-3.91	121.73	127.31
17	b	804	CLA	C1D-CHD-C4C	-3.91	117.40	122.56
20	a	852	BCR	C15-C14-C13	-3.91	121.73	127.31
17	B	825	CLA	O2D-CGD-CBD	3.91	118.21	111.27
20	B	844	BCR	C24-C23-C22	-3.91	120.33	126.23
26	1	307	CHL	C1D-CHD-C4C	-3.90	117.41	122.56
17	A	803	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
17	1	309	CLA	O2D-CGD-CBD	3.90	118.20	111.27
17	B	835	CLA	O2D-CGD-CBD	3.90	118.20	111.27
17	a	818	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
17	B	806	CLA	O2D-CGD-CBD	3.90	118.19	111.27
17	B	815	CLA	C1D-CHD-C4C	-3.89	117.42	122.56
17	1	304	CLA	C1C-C2C-C3C	-3.89	102.86	106.96
17	8	302	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
17	a	821	CLA	C4A-NA-C1A	-3.89	104.96	106.71
17	F	301	CLA	C1D-CHD-C4C	-3.89	117.42	122.56
17	A	808	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
17	F	301	CLA	O2D-CGD-CBD	3.89	118.17	111.27
17	3	309	CLA	C1-C2-C3	-3.89	120.46	126.75
17	a	812	CLA	C1D-CHD-C4C	-3.89	117.43	122.56
20	F	305	BCR	C11-C10-C9	-3.89	121.77	127.31
17	a	825	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
17	a	830	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
17	A	817	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
17	1	306	CLA	C1-C2-C3	-3.88	119.33	126.04
17	3	303	CLA	O2D-CGD-CBD	3.88	118.17	111.27
20	A	852	BCR	C16-C17-C18	-3.88	121.77	127.31
17	7	612	CLA	C1-C2-C3	-3.88	119.33	126.04
26	7	606	CHL	C1D-CHD-C4C	-3.88	117.44	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	828	CLA	C1D-CHD-C4C	-3.88	117.44	122.56
20	B	846	BCR	C15-C14-C13	-3.88	121.78	127.31
17	3	303	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
17	a	801	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
17	6	312	CLA	CAA-C2A-C3A	-3.88	107.06	116.10
17	a	807	CLA	CAA-C2A-C3A	-3.88	102.17	112.78
17	B	823	CLA	C3C-C4C-NC	3.88	114.92	110.57
17	8	312	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
20	b	847	BCR	C15-C14-C13	-3.87	121.78	127.31
17	A	841	CLA	C3C-C4C-NC	3.87	114.91	110.57
17	b	803	CLA	C1D-CHD-C4C	-3.87	117.45	122.56
17	b	814	CLA	C1D-CHD-C4C	-3.87	117.45	122.56
17	B	802	CLA	C3C-C4C-NC	3.87	114.91	110.57
17	A	836	CLA	C1C-C2C-C3C	-3.86	102.89	106.96
17	7	611	CLA	C1D-CHD-C4C	-3.86	117.46	122.56
17	A	812	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
17	3	314	CLA	C3C-C4C-NC	3.86	114.90	110.57
17	A	834	CLA	C3C-C4C-NC	3.86	114.90	110.57
17	a	836	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
26	4	607	CHL	C1D-CHD-C4C	-3.86	117.47	122.56
17	a	826	CLA	C3C-C4C-NC	3.86	114.89	110.57
17	B	808	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
17	A	854	CLA	C1C-C2C-C3C	-3.85	102.90	106.96
17	A	819	CLA	C1D-CHD-C4C	-3.85	117.47	122.56
17	A	854	CLA	O2D-CGD-O1D	-3.85	116.31	123.84
17	B	819	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
19	2	618	LHG	O7-C7-C8	3.85	119.80	111.50
17	A	803	CLA	C3C-C4C-NC	3.85	114.89	110.57
17	A	825	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
26	9	606	CHL	C1D-CHD-C4C	-3.84	117.49	122.56
17	6	310	CLA	C1D-CHD-C4C	-3.84	117.49	122.56
20	A	856	BCR	C20-C21-C22	-3.84	121.83	127.31
20	2	617	BCR	C3-C4-C5	-3.84	107.22	114.08
20	b	847	BCR	C24-C23-C22	-3.84	120.43	126.23
28	9	617	XAT	O4-C5-C18	3.84	119.66	115.06
17	B	824	CLA	C3C-C4C-NC	3.84	114.88	110.57
26	3	307	CHL	C3C-C4C-NC	3.84	114.88	110.57
17	a	816	CLA	C3C-C4C-NC	3.84	114.88	110.57
20	3	318	BCR	C33-C5-C6	-3.84	120.22	124.53
20	a	852	BCR	C3-C4-C5	-3.83	107.23	114.08
17	B	802	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
17	b	818	CLA	C1C-C2C-C3C	-3.83	102.93	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	838	CLA	C1D-CHD-C4C	-3.83	117.51	122.56
17	6	312	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
20	6	319	BCR	C16-C17-C18	-3.83	121.85	127.31
17	a	814	CLA	C3C-C4C-NC	3.83	114.86	110.57
17	B	808	CLA	C1D-CHD-C4C	-3.82	117.51	122.56
17	F	303	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
17	a	808	CLA	C3C-C4C-NC	3.82	114.86	110.57
17	4	601	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
25	6	302	LMG	O7-C10-C11	3.82	119.74	111.50
17	6	310	CLA	O2D-CGD-CBD	3.82	118.06	111.27
17	8	305	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
17	3	310	CLA	CAA-C2A-C3A	-3.82	107.19	116.10
17	1	311	CLA	CAA-C2A-C3A	-3.82	107.19	116.10
17	3	306	CLA	C3C-C4C-NC	3.82	114.85	110.57
17	g	102	CLA	C1-C2-C3	-3.81	120.58	126.75
17	4	612	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
17	a	803	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
20	L	205	BCR	C38-C26-C25	-3.81	120.25	124.53
17	f	7002	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
17	a	807	CLA	C3C-C4C-NC	3.81	114.84	110.57
17	a	856	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
17	B	818	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
17	9	608	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
17	B	821	CLA	C3C-C4C-NC	3.81	114.84	110.57
17	2	608	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
17	1	314	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
17	A	841	CLA	O2D-CGD-CBD	3.81	118.04	111.27
17	a	842	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
17	B	825	CLA	C3C-C4C-NC	3.81	114.84	110.57
17	A	830	CLA	C1-C2-C3	-3.80	119.47	126.04
26	7	607	CHL	C1D-CHD-C4C	-3.80	117.54	122.56
17	b	825	CLA	C3C-C4C-NC	3.80	114.83	110.57
17	3	315	CLA	C3C-C4C-CHD	-3.80	116.90	125.22
17	3	308	CLA	C1D-CHD-C4C	-3.80	117.54	122.56
17	l	202	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
17	b	815	CLA	C3C-C4C-NC	3.80	114.83	110.57
17	A	832	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
20	A	849	BCR	C15-C14-C13	-3.80	121.89	127.31
20	B	844	BCR	C15-C14-C13	-3.80	121.89	127.31
26	1	302	CHL	C1D-CHD-C4C	-3.80	117.55	122.56
17	B	838	CLA	C3C-C4C-NC	3.80	114.83	110.57
17	f	7002	CLA	C3C-C4C-NC	3.80	114.83	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	805	CLA	C3C-C4C-NC	3.80	114.83	110.57
17	9	608	CLA	C3C-C4C-NC	3.80	114.83	110.57
20	9	618	BCR	C11-C10-C9	-3.80	121.89	127.31
20	a	849	BCR	C16-C17-C18	-3.80	121.89	127.31
25	9	619	LMG	O7-C10-C11	3.80	119.68	111.50
17	2	610	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
17	B	836	CLA	C1D-CHD-C4C	-3.79	117.55	122.56
17	a	833	CLA	C1-C2-C3	-3.79	119.49	126.04
17	b	808	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
17	1	313	CLA	C1-C2-C3	-3.79	119.49	126.04
17	a	837	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
17	3	313	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
26	6	308	CHL	C1D-CHD-C4C	-3.79	117.56	122.56
17	b	840	CLA	C3C-C4C-NC	3.79	114.82	110.57
17	6	305	CLA	C1C-C2C-C3C	-3.79	102.98	106.96
27	3	316	LUT	C35-C34-C33	-3.78	121.91	127.31
17	B	828	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
17	B	815	CLA	C3C-C4C-NC	3.78	114.81	110.57
17	9	604	CLA	C1-C2-C3	-3.78	120.63	126.75
17	9	610	CLA	C1D-CHD-C4C	-3.78	117.57	122.56
17	b	819	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
17	4	608	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
17	8	313	CLA	C3C-C4C-CHD	-3.78	116.94	125.22
20	b	848	BCR	C33-C5-C6	-3.78	120.28	124.53
17	A	818	CLA	C1D-CHD-C4C	-3.78	117.57	122.56
17	f	7003	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
17	1	309	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
17	8	312	CLA	C3C-C4C-NC	3.78	114.81	110.57
25	4	620	LMG	O7-C10-C11	3.78	119.64	111.50
17	4	611	CLA	C1D-CHD-C4C	-3.77	117.58	122.56
17	b	804	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
17	a	824	CLA	C3C-C4C-NC	3.77	114.80	110.57
17	9	601	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
17	a	838	CLA	C3C-C4C-NC	3.77	114.80	110.57
17	A	838	CLA	C1-C2-C3	-3.77	119.52	126.04
17	8	310	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
17	B	839	CLA	C1-C2-C3	-3.77	119.52	126.04
17	b	834	CLA	C3C-C4C-NC	3.77	114.80	110.57
17	B	838	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
17	a	835	CLA	C1D-CHD-C4C	-3.77	117.58	122.56
17	A	833	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
17	a	809	CLA	C1C-C2C-C3C	-3.77	102.99	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	821	CLA	C1C-C2C-C3C	-3.77	103.00	106.96
17	a	842	CLA	C3C-C4C-NC	3.77	114.79	110.57
17	A	810	CLA	C1C-C2C-C3C	-3.77	103.00	106.96
26	7	601	CHL	C1D-CHD-C4C	-3.76	117.59	122.56
17	7	609	CLA	C1D-CHD-C4C	-3.76	117.59	122.56
17	B	823	CLA	O2D-CGD-CBD	3.76	117.95	111.27
17	G	101	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
20	K	4001	BCR	C15-C16-C17	-3.76	115.77	123.47
17	2	611	CLA	C1D-CHD-C4C	-3.76	117.60	122.56
20	K	4004	BCR	C15-C14-C13	-3.76	121.95	127.31
17	9	612	CLA	C1C-C2C-C3C	-3.76	103.01	106.96
17	a	823	CLA	C1C-C2C-C3C	-3.76	103.01	106.96
17	7	610	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
17	L	202	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
17	1	312	CLA	C3C-C4C-NC	3.75	114.78	110.57
17	b	804	CLA	C3C-C4C-NC	3.75	114.78	110.57
17	7	613	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
27	2	615	LUT	C35-C34-C33	-3.75	121.96	127.31
17	A	804	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
17	A	823	CLA	C3C-C4C-NC	3.75	114.78	110.57
17	a	822	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
17	6	310	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
17	A	834	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
17	b	821	CLA	C3C-C4C-NC	3.75	114.77	110.57
20	6	319	BCR	C33-C5-C6	-3.75	120.32	124.53
17	6	315	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
17	1	309	CLA	C1D-CHD-C4C	-3.75	117.61	122.56
17	b	809	CLA	C3C-C4C-NC	3.75	114.77	110.57
17	a	823	CLA	C3C-C4C-NC	3.75	114.77	110.57
17	b	841	CLA	C1-C2-C3	-3.74	119.57	126.04
17	a	825	CLA	C3C-C4C-NC	3.74	114.77	110.57
17	8	313	CLA	C2C-C3C-C4C	-3.74	102.73	107.21
26	3	307	CHL	C1D-CHD-C4C	-3.74	117.62	122.56
17	6	311	CLA	C1-C2-C3	-3.74	119.57	126.04
20	J	3003	BCR	C28-C27-C26	-3.74	107.39	114.08
17	J	3002	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
17	a	803	CLA	C3C-C4C-NC	3.74	114.77	110.57
17	A	824	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
17	A	843	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
17	a	805	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
17	a	824	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
17	1	313	CLA	C1C-C2C-C3C	-3.74	103.02	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	837	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
17	a	837	CLA	C3C-C4C-NC	3.74	114.77	110.57
17	a	810	CLA	C3C-C4C-NC	3.74	114.77	110.57
17	a	811	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
17	B	818	CLA	C3C-C4C-NC	3.74	114.77	110.57
17	8	311	CLA	C3C-C4C-NC	3.74	114.76	110.57
17	2	612	CLA	C1-C2-C3	-3.74	119.58	126.04
28	8	315	XAT	C35-C15-C14	-3.74	115.82	123.47
17	A	813	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
17	B	809	CLA	C3C-C4C-NC	3.73	114.76	110.57
17	7	611	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
17	b	834	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
17	6	306	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
17	A	845	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
17	3	312	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
17	A	818	CLA	C3C-C4C-NC	3.73	114.75	110.57
17	A	854	CLA	C3B-C4B-NB	3.73	114.03	109.21
17	B	831	CLA	C3C-C4C-NC	3.73	114.75	110.57
17	b	829	CLA	C1D-CHD-C4C	-3.73	117.64	122.56
17	6	313	CLA	C1-C2-C3	-3.73	119.59	126.04
17	a	839	CLA	C3C-C4C-NC	3.73	114.75	110.57
17	b	811	CLA	C3C-C4C-NC	3.73	114.75	110.57
17	K	4002	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
26	7	605	CHL	C1D-CHD-C4C	-3.73	117.64	122.56
17	B	804	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
17	b	836	CLA	C1-C2-C3	-3.73	119.60	126.04
17	B	820	CLA	C3C-C4C-NC	3.73	114.75	110.57
17	A	832	CLA	C3C-C4C-NC	3.73	114.75	110.57
17	a	816	CLA	C1-C2-C3	-3.72	120.73	126.75
17	2	603	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
17	9	603	CLA	C3C-C4C-NC	3.72	114.75	110.57
17	4	613	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
17	B	813	CLA	C3C-C4C-NC	3.72	114.75	110.57
17	3	315	CLA	C2C-C3C-C4C	-3.72	102.75	107.21
17	B	825	CLA	C1D-CHD-C4C	-3.72	117.65	122.56
17	A	816	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
17	A	838	CLA	C3C-C4C-NC	3.72	114.74	110.57
17	6	312	CLA	C1D-CHD-C4C	-3.72	117.65	122.56
20	L	205	BCR	C28-C27-C26	-3.72	107.44	114.08
17	3	310	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
17	B	807	CLA	C3C-C4C-NC	3.72	114.74	110.57
17	b	820	CLA	C3C-C4C-NC	3.72	114.74	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	6	312	CLA	C3C-C4C-NC	3.71	114.74	110.57
17	K	4003	CLA	C3C-C4C-NC	3.71	114.74	110.57
20	l	206	BCR	C11-C10-C9	-3.71	122.01	127.31
17	7	608	CLA	C1-C2-C3	-3.71	120.74	126.75
17	B	836	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
17	B	814	CLA	C1D-CHD-C4C	-3.71	117.66	122.56
17	F	303	CLA	C3C-C4C-NC	3.71	114.73	110.57
26	2	607	CHL	C1D-CHD-C4C	-3.71	117.66	122.56
17	a	846	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
28	4	617	XAT	C35-C34-C33	-3.71	122.01	127.31
20	1	318	BCR	C28-C27-C26	-3.71	107.45	114.08
17	a	825	CLA	O2D-CGD-CBD	3.71	117.86	111.27
17	9	608	CLA	C1-C2-C3	-3.71	120.75	126.75
17	6	310	CLA	C3C-C4C-NC	3.71	114.73	110.57
20	b	844	BCR	C16-C17-C18	-3.71	122.01	127.31
17	k	1403	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
17	a	840	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
17	A	840	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
17	A	807	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
20	3	318	BCR	C16-C17-C18	-3.71	122.02	127.31
17	A	837	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
17	B	802	CLA	O2D-CGD-CBD	3.71	117.86	111.27
17	A	821	CLA	C1D-CHD-C4C	-3.71	117.67	122.56
20	L	201	BCR	C33-C5-C6	-3.71	120.37	124.53
17	3	311	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
17	b	821	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
26	4	606	CHL	C1D-CHD-C4C	-3.71	117.67	122.56
17	6	313	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
17	B	809	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
17	a	843	CLA	C1D-CHD-C4C	-3.70	117.67	122.56
17	B	837	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
17	a	812	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
17	g	103	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
17	8	309	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
17	b	807	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
17	b	815	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
17	A	801	CLA	CAA-C2A-C3A	-3.70	102.64	112.78
17	b	808	CLA	C1D-CHD-C4C	-3.70	117.67	122.56
17	4	603	CLA	C3C-C4C-NC	3.70	114.72	110.57
17	1	315	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
17	2	603	CLA	O2D-CGD-CBD	3.70	117.84	111.27
17	B	826	CLA	C1D-CHD-C4C	-3.70	117.68	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	8	307	CLA	C1D-CHD-C4C	-3.70	117.68	122.56
17	1	305	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
17	b	811	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
17	9	614	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
17	a	833	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
17	4	614	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
17	B	813	CLA	CAC-C3C-C4C	3.70	129.60	124.81
17	b	811	CLA	C1D-CHD-C4C	-3.70	117.68	122.56
17	7	611	CLA	C3C-C4C-NC	3.70	114.72	110.57
17	a	806	CLA	C3C-C4C-NC	3.70	114.72	110.57
17	7	603	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
17	A	828	CLA	C1D-CHD-C4C	-3.69	117.68	122.56
17	B	840	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
17	9	610	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
17	A	830	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
17	b	833	CLA	C3C-C4C-NC	3.69	114.71	110.57
17	9	611	CLA	C3C-C4C-NC	3.69	114.71	110.57
17	B	832	CLA	C3C-C4C-NC	3.69	114.71	110.57
17	A	811	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
17	a	804	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
17	6	309	CLA	C3C-C4C-NC	3.69	114.71	110.57
17	3	314	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
17	g	102	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
17	B	835	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
17	a	804	CLA	C3C-C4C-NC	3.69	114.71	110.57
17	a	840	CLA	C3C-C4C-NC	3.69	114.71	110.57
17	9	611	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
17	B	839	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
17	b	835	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
17	a	834	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
17	b	817	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
26	9	615	CHL	C1D-CHD-C4C	-3.68	117.70	122.56
17	B	814	CLA	C3C-C4C-NC	3.68	114.70	110.57
17	B	838	CLA	C1D-CHD-C4C	-3.68	117.70	122.56
17	1	312	CLA	C1D-CHD-C4C	-3.68	117.70	122.56
17	b	820	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
17	a	832	CLA	C1-C2-C3	-3.68	120.80	126.75
17	8	302	CLA	C3C-C4C-NC	3.68	114.70	110.57
20	L	201	BCR	C38-C26-C25	-3.68	120.40	124.53
17	A	801	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
17	l	204	CLA	C1-C2-C3	-3.68	120.80	126.75
17	7	603	CLA	C1D-CHD-C4C	-3.68	117.71	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	840	CLA	C3C-C4C-NC	3.68	114.69	110.57
17	A	836	CLA	C1D-CHD-C4C	-3.67	117.71	122.56
20	l	201	BCR	C33-C5-C6	-3.67	120.40	124.53
17	a	834	CLA	C1-C2-C3	-3.67	119.69	126.04
17	3	304	CLA	C1C-C2C-C3C	-3.67	103.09	106.96
17	6	314	CLA	C1-C2-C3	-3.67	119.69	126.04
17	6	313	CLA	C1D-CHD-C4C	-3.67	117.71	122.56
17	F	303	CLA	C1D-CHD-C4C	-3.67	117.71	122.56
17	A	801	CLA	C3C-C4C-NC	3.67	114.69	110.57
17	A	818	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
17	A	839	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
17	6	314	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
17	b	831	CLA	C3C-C4C-NC	3.67	114.69	110.57
17	9	604	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
17	7	604	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
17	4	608	CLA	C1-C2-C3	-3.67	120.81	126.75
17	3	303	CLA	C3C-C4C-NC	3.67	114.68	110.57
26	8	306	CHL	C1D-CHD-C4C	-3.67	117.72	122.56
17	F	304	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
20	1	318	BCR	C33-C5-C6	-3.67	120.41	124.53
17	2	611	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
17	b	816	CLA	C1C-C2C-C3C	-3.66	103.10	106.96
17	3	301	CLA	C1C-C2C-C3C	-3.66	103.10	106.96
17	A	820	CLA	C1C-C2C-C3C	-3.66	103.10	106.96
17	K	4003	CLA	C1C-C2C-C3C	-3.66	103.10	106.96
17	G	103	CLA	C3C-C4C-NC	3.66	114.68	110.57
17	a	846	CLA	C3C-C4C-NC	3.66	114.68	110.57
17	b	813	CLA	C1-C2-C3	-3.66	119.71	126.04
17	a	818	CLA	C3B-C4B-NB	3.66	113.94	109.21
17	8	311	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
20	a	854	BCR	C20-C21-C22	-3.66	122.09	127.31
17	b	828	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
27	1	316	LUT	C35-C34-C33	-3.66	122.09	127.31
17	j	3002	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
20	a	850	BCR	C16-C17-C18	-3.66	122.09	127.31
17	b	815	CLA	C1D-CHD-C4C	-3.66	117.73	122.56
26	7	614	CHL	C1D-CHD-C4C	-3.66	117.73	122.56
17	b	828	CLA	C3C-C4C-NC	3.66	114.67	110.57
17	b	832	CLA	C3C-C4C-NC	3.66	114.67	110.57
17	A	808	CLA	C3C-C4C-NC	3.65	114.67	110.57
17	A	804	CLA	C3C-C4C-NC	3.65	114.67	110.57
17	B	811	CLA	C1C-C2C-C3C	-3.65	103.11	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	6	314	CLA	C1D-CHD-C4C	-3.65	117.74	122.56
17	a	856	CLA	C1D-CHD-C4C	-3.65	117.74	122.56
17	4	604	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
17	a	817	CLA	C3C-C4C-NC	3.65	114.67	110.57
20	4	618	BCR	C11-C10-C9	-3.65	122.10	127.31
17	F	301	CLA	C3C-C4C-NC	3.65	114.66	110.57
17	k	1401	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
17	a	828	CLA	C1-C2-C3	-3.65	119.73	126.04
17	2	604	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
20	J	3003	BCR	C20-C21-C22	-3.65	122.11	127.31
17	b	805	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
17	a	833	CLA	C3C-C4C-NC	3.65	114.66	110.57
20	A	848	BCR	C20-C21-C22	-3.65	122.11	127.31
17	a	835	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
17	b	803	CLA	C3C-C4C-NC	3.65	114.66	110.57
26	4	605	CHL	C1D-CHD-C4C	-3.64	117.75	122.56
17	9	613	CLA	C1C-C2C-C3C	-3.64	103.12	106.96
17	k	1401	CLA	C3C-C4C-NC	3.64	114.66	110.57
17	a	856	CLA	O2D-CGD-O1D	-3.64	116.71	123.84
17	3	305	CLA	C3C-C4C-NC	3.64	114.66	110.57
17	B	828	CLA	C3C-C4C-NC	3.64	114.66	110.57
17	4	611	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
17	a	818	CLA	C3C-C4C-NC	3.64	114.66	110.57
17	2	613	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
17	b	839	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
17	1	306	CLA	C1D-CHD-C4C	-3.64	117.75	122.56
17	j	3002	CLA	C3C-C4C-NC	3.64	114.65	110.57
17	1	311	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
17	B	839	CLA	C1D-CHD-C4C	-3.64	117.75	122.56
17	A	825	CLA	C3C-C4C-NC	3.64	114.65	110.57
17	b	822	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
20	3	318	BCR	C28-C27-C26	-3.64	107.58	114.08
17	9	603	CLA	C1D-CHD-C4C	-3.64	117.76	122.56
17	A	831	CLA	C3C-C4C-NC	3.64	114.65	110.57
17	B	830	CLA	C1-C2-C3	-3.64	120.87	126.75
17	b	824	CLA	C1D-CHD-C4C	-3.64	117.76	122.56
17	A	839	CLA	C3C-C4C-NC	3.63	114.65	110.57
25	G	102	LMG	O7-C10-C11	3.63	119.33	111.50
17	7	608	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
17	g	102	CLA	C3C-C4C-NC	3.63	114.65	110.57
17	L	203	CLA	C3C-C4C-NC	3.63	114.65	110.57
17	A	841	CLA	C1C-C2C-C3C	-3.63	103.14	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	308	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
26	4	615	CHL	C1D-CHD-C4C	-3.63	117.77	122.56
17	A	832	CLA	C1-C2-C3	-3.63	120.88	126.75
17	b	824	CLA	C3C-C4C-NC	3.63	114.64	110.57
17	b	802	CLA	O2D-CGD-CBD	3.63	117.72	111.27
17	2	610	CLA	C3B-C4B-NB	3.63	113.90	109.21
17	A	819	CLA	C3C-C4C-NC	3.63	114.64	110.57
17	B	838	CLA	C3B-C4B-NB	3.63	113.90	109.21
17	3	313	CLA	C3C-C4C-NC	3.63	114.64	110.57
17	3	306	CLA	C1D-CHD-C4C	-3.63	117.77	122.56
26	2	601	CHL	C1D-CHD-C4C	-3.63	117.77	122.56
17	A	814	CLA	C3C-C4C-NC	3.63	114.64	110.57
17	B	839	CLA	C3C-C4C-NC	3.63	114.64	110.57
17	1	311	CLA	C3C-C4C-NC	3.63	114.64	110.57
17	8	309	CLA	C1D-CHD-C4C	-3.63	117.77	122.56
17	a	820	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
17	l	203	CLA	C3C-C4C-NC	3.63	114.64	110.57
17	a	815	CLA	C3C-C4C-NC	3.63	114.64	110.57
20	8	316	BCR	C33-C5-C6	-3.63	120.46	124.53
17	4	609	CLA	C1D-CHD-C4C	-3.62	117.78	122.56
17	8	313	CLA	C3C-C2C-C1C	-3.62	102.87	107.21
17	l	204	CLA	C3C-C4C-NC	3.62	114.64	110.57
17	4	611	CLA	C3C-C4C-NC	3.62	114.64	110.57
24	B	850	DGD	O2G-C1B-C2B	3.62	119.31	111.50
17	A	812	CLA	C3C-C4C-NC	3.62	114.63	110.57
17	A	815	CLA	C3C-C4C-NC	3.62	114.63	110.57
17	B	830	CLA	C3C-C4C-NC	3.62	114.63	110.57
17	b	812	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
17	A	802	CLA	C3C-C4C-NC	3.62	114.63	110.57
17	A	845	CLA	C3C-C4C-NC	3.62	114.63	110.57
17	B	810	CLA	CAA-C2A-C3A	-3.62	102.87	112.78
17	k	1402	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
20	L	206	BCR	C15-C14-C13	-3.62	122.15	127.31
26	6	303	CHL	C1D-CHD-C4C	-3.61	117.79	122.56
17	A	810	CLA	C1D-CHD-C4C	-3.61	117.79	122.56
17	b	840	CLA	C1-C2-C3	-3.61	119.79	126.04
17	2	603	CLA	C3C-C4C-NC	3.61	114.62	110.57
17	4	608	CLA	C3C-C4C-NC	3.61	114.62	110.57
17	4	610	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
17	a	839	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
17	a	835	CLA	C3C-C4C-NC	3.61	114.62	110.57
17	A	805	CLA	C1C-C2C-C3C	-3.61	103.16	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	815	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
17	4	612	CLA	C1-C2-C3	-3.61	119.80	126.04
17	a	811	CLA	C1D-CHD-C4C	-3.61	117.80	122.56
17	a	844	CLA	C1D-CHD-C4C	-3.61	117.80	122.56
17	B	825	CLA	CAA-C2A-C3A	-3.61	102.90	112.78
17	4	612	CLA	C1D-CHD-C4C	-3.61	117.80	122.56
17	B	811	CLA	C3C-C4C-NC	3.61	114.62	110.57
17	a	843	CLA	C3C-C4C-NC	3.61	114.62	110.57
17	3	315	CLA	C3C-C2C-C1C	-3.61	102.89	107.21
17	B	820	CLA	C1C-C2C-C3C	-3.61	103.17	106.96
17	2	609	CLA	C1D-CHD-C4C	-3.61	117.80	122.56
17	A	829	CLA	C1D-CHD-C4C	-3.61	117.80	122.56
17	a	809	CLA	C3C-C4C-NC	3.61	114.61	110.57
17	7	610	CLA	C1D-CHD-C4C	-3.60	117.80	122.56
17	B	805	CLA	C3C-C4C-NC	3.60	114.61	110.57
17	7	608	CLA	C1D-CHD-C4C	-3.60	117.80	122.56
17	3	305	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
17	6	316	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
17	a	836	CLA	C1D-CHD-C4C	-3.60	117.80	122.56
20	a	851	BCR	C3-C4-C5	-3.60	107.65	114.08
17	f	7002	CLA	C1D-CHD-C4C	-3.60	117.81	122.56
28	3	317	XAT	O4-C5-C18	3.60	119.37	115.06
17	b	834	CLA	C1-C2-C3	-3.60	119.81	126.04
17	a	824	CLA	C4-C3-C5	3.60	120.10	115.98
17	B	840	CLA	C3C-C4C-NC	3.60	114.61	110.57
17	B	802	CLA	C1D-CHD-C4C	-3.60	117.81	122.56
17	g	101	CLA	C1D-CHD-C4C	-3.60	117.81	122.56
17	a	832	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
17	g	101	CLA	CAA-C2A-C3A	-3.60	107.70	116.10
28	3	317	XAT	C10-C11-C12	-3.60	111.99	123.22
17	7	612	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
17	B	841	CLA	C3C-C4C-NC	3.60	114.61	110.57
17	b	832	CLA	C1-C2-C3	-3.60	119.82	126.04
26	2	614	CHL	C1D-CHD-C4C	-3.60	117.81	122.56
17	A	807	CLA	C3C-C4C-NC	3.60	114.60	110.57
17	1	312	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
17	1	306	CLA	C3C-C4C-NC	3.59	114.60	110.57
17	a	822	CLA	C3C-C4C-NC	3.59	114.60	110.57
17	b	806	CLA	C1-C2-C3	-3.59	119.83	126.04
17	2	612	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
17	4	603	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
17	1	310	CLA	C1D-CHD-C4C	-3.59	117.82	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	810	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
17	B	812	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
20	b	844	BCR	C34-C9-C10	-3.59	117.90	122.92
17	B	817	CLA	C1C-C2C-C3C	-3.59	103.19	106.96
17	b	813	CLA	C3C-C4C-NC	3.59	114.59	110.57
17	G	101	CLA	C3C-C4C-NC	3.59	114.59	110.57
17	B	816	CLA	C1C-C2C-C3C	-3.59	103.19	106.96
20	A	848	BCR	C28-C27-C26	-3.59	107.67	114.08
17	l	204	CLA	C1D-CHD-C4C	-3.58	117.83	122.56
17	8	307	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
20	G	105	BCR	C15-C14-C13	-3.58	122.19	127.31
17	J	3002	CLA	C3C-C4C-NC	3.58	114.59	110.57
17	B	837	CLA	C3C-C4C-NC	3.58	114.59	110.57
17	a	820	CLA	C1-C2-C3	-3.58	119.85	126.04
17	2	611	CLA	C3C-C4C-NC	3.58	114.59	110.57
17	a	829	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
17	3	311	CLA	C3C-C4C-NC	3.58	114.59	110.57
17	b	802	CLA	C3C-C4C-NC	3.58	114.59	110.57
17	B	833	CLA	C3C-C4C-NC	3.58	114.59	110.57
17	b	833	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
17	a	827	CLA	C3C-C4C-NC	3.58	114.58	110.57
17	A	808	CLA	C3B-C4B-NB	3.58	113.84	109.21
17	B	822	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
17	9	602	CLA	C3C-C4C-NC	3.58	114.58	110.57
17	6	314	CLA	C3C-C4C-NC	3.58	114.58	110.57
20	k	1404	BCR	C33-C5-C6	-3.58	120.51	124.53
20	B	845	BCR	C15-C14-C13	-3.58	122.20	127.31
17	6	307	CLA	C3C-C4C-NC	3.57	114.58	110.57
17	1	308	CLA	C3C-C4C-NC	3.57	114.58	110.57
17	b	828	CLA	C1D-CHD-C4C	-3.57	117.84	122.56
17	3	306	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
17	B	804	CLA	C1D-CHD-C4C	-3.57	117.84	122.56
17	b	825	CLA	C1D-CHD-C4C	-3.57	117.84	122.56
17	a	844	CLA	C3C-C4C-NC	3.57	114.58	110.57
17	K	4003	CLA	C1D-CHD-C4C	-3.57	117.84	122.56
25	6	302	LMG	O8-C28-C29	3.57	120.75	111.38
17	a	842	CLA	C1-C2-C3	-3.57	119.87	126.04
17	8	308	CLA	C1-C2-C3	-3.57	120.97	126.75
17	6	309	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
17	b	823	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
17	b	831	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
17	a	819	CLA	C3C-C4C-NC	3.57	114.57	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	823	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
17	B	833	CLA	C1D-CHD-C4C	-3.57	117.85	122.56
17	7	603	CLA	C3C-C4C-NC	3.57	114.57	110.57
17	9	609	CLA	C1-C2-C3	-3.57	119.87	126.04
17	a	826	CLA	C1C-C2C-C3C	-3.57	103.21	106.96
17	A	826	CLA	C1D-CHD-C4C	-3.57	117.85	122.56
17	B	806	CLA	C1C-C2C-C3C	-3.57	103.21	106.96
17	8	304	CLA	C1C-C2C-C3C	-3.57	103.21	106.96
17	B	836	CLA	C1-C2-C3	-3.56	119.88	126.04
26	2	605	CHL	C1D-CHD-C4C	-3.56	117.86	122.56
17	a	807	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
17	1	309	CLA	C1-C2-C3	-3.56	119.88	126.04
17	A	809	CLA	C3C-C4C-NC	3.56	114.57	110.57
17	B	829	CLA	C3B-C4B-NB	3.56	113.81	109.21
17	A	835	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
17	A	827	CLA	C3C-C4C-NC	3.56	114.56	110.57
17	a	841	CLA	C1-C2-C3	-3.56	119.89	126.04
17	a	813	CLA	C3C-C4C-NC	3.56	114.56	110.57
17	L	203	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
17	L	204	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
17	B	835	CLA	C3C-C4C-NC	3.56	114.56	110.57
17	a	819	CLA	C1D-CHD-C4C	-3.56	117.86	122.56
17	b	839	CLA	C1D-CHD-C4C	-3.56	117.86	122.56
17	a	841	CLA	C1C-C2C-C3C	-3.56	103.22	106.96
20	B	845	BCR	C37-C22-C21	-3.56	117.94	122.92
17	7	610	CLA	C3C-C4C-NC	3.56	114.56	110.57
17	7	609	CLA	C1-C2-C3	-3.56	119.89	126.04
17	b	802	CLA	C1C-C2C-C3C	-3.56	103.22	106.96
17	8	303	CLA	C1C-C2C-C3C	-3.56	103.22	106.96
17	B	818	CLA	C1D-CHD-C4C	-3.56	117.86	122.56
17	b	833	CLA	C1D-CHD-C4C	-3.56	117.86	122.56
17	A	841	CLA	C1D-CHD-C4C	-3.56	117.86	122.56
17	a	821	CLA	CBC-CAC-C3C	-3.56	102.63	112.43
17	b	829	CLA	C3C-C4C-NC	3.56	114.56	110.57
17	A	816	CLA	C3C-C4C-NC	3.56	114.56	110.57
17	A	809	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
17	a	813	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
20	K	4004	BCR	C20-C21-C22	-3.55	122.24	127.31
17	4	601	CLA	C3C-C4C-NC	3.55	114.55	110.57
17	a	805	CLA	C1D-CHD-C4C	-3.55	117.87	122.56
17	A	824	CLA	C3C-C4C-NC	3.55	114.55	110.57
17	3	303	CLA	C3B-C4B-NB	3.55	113.80	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	L	204	CLA	C1-C2-C3	-3.55	121.01	126.75
17	b	836	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
17	l	204	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
17	b	808	CLA	O2A-CGA-CBA	3.55	123.04	111.91
17	6	304	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
17	A	806	CLA	C3C-C4C-NC	3.55	114.55	110.57
17	B	823	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
17	a	807	CLA	O2A-CGA-CBA	3.54	123.03	111.91
17	4	609	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
17	b	818	CLA	C3C-C4C-NC	3.54	114.55	110.57
17	a	811	CLA	C3C-C4C-NC	3.54	114.55	110.57
17	A	822	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
17	b	824	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
17	3	308	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
17	2	612	CLA	C1D-CHD-C4C	-3.54	117.89	122.56
20	a	853	BCR	C38-C26-C25	-3.54	120.55	124.53
17	4	609	CLA	C1-C2-C3	-3.54	119.92	126.04
17	A	815	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
17	a	839	CLA	O2D-CGD-O1D	-3.54	116.92	123.84
20	l	201	BCR	C38-C26-C25	-3.54	120.55	124.53
20	b	847	BCR	C7-C8-C9	-3.54	120.89	126.23
17	b	839	CLA	C1-C2-C3	-3.54	119.92	126.04
17	b	823	CLA	C3C-C4C-NC	3.54	114.54	110.57
17	a	841	CLA	C3C-C4C-NC	3.54	114.54	110.57
17	2	603	CLA	C1D-CHD-C4C	-3.54	117.89	122.56
17	6	306	CLA	C3C-C4C-NC	3.54	114.54	110.57
20	a	851	BCR	C15-C14-C13	-3.54	122.26	127.31
17	9	609	CLA	C1D-CHD-C4C	-3.54	117.89	122.56
17	f	7003	CLA	C1D-CHD-C4C	-3.54	117.89	122.56
17	8	307	CLA	C3C-C4C-NC	3.54	114.54	110.57
17	B	803	CLA	C1D-CHD-C4C	-3.53	117.89	122.56
17	K	4002	CLA	C3C-C4C-NC	3.53	114.53	110.57
17	9	614	CLA	C3C-C4C-NC	3.53	114.53	110.57
17	B	820	CLA	C1D-CHD-C4C	-3.53	117.90	122.56
17	6	307	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
17	8	302	CLA	C3B-C4B-NB	3.53	113.78	109.21
17	6	311	CLA	C1D-CHD-C4C	-3.53	117.90	122.56
20	I	101	BCR	C3-C4-C5	-3.53	107.77	114.08
17	A	829	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
17	A	811	CLA	C1D-CHD-C4C	-3.53	117.90	122.56
20	B	844	BCR	C34-C9-C10	-3.53	117.98	122.92
17	G	104	CLA	C1D-CHD-C4C	-3.53	117.90	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	8	305	CLA	C3C-C4C-NC	3.53	114.53	110.57
17	4	614	CLA	C3C-C4C-NC	3.53	114.53	110.57
20	9	618	BCR	C28-C27-C26	-3.53	107.78	114.08
17	B	806	CLA	C3C-C4C-NC	3.53	114.53	110.57
17	a	812	CLA	C3C-C4C-NC	3.53	114.53	110.57
17	G	103	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
17	4	610	CLA	C1D-CHD-C4C	-3.53	117.90	122.56
17	4	604	CLA	C1-C2-C3	-3.53	121.05	126.75
17	9	610	CLA	C3C-C4C-NC	3.52	114.52	110.57
17	a	802	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
20	4	618	BCR	C7-C8-C9	-3.52	120.91	126.23
17	7	612	CLA	C3C-C4C-NC	3.52	114.52	110.57
17	a	810	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
17	B	807	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
20	1	201	BCR	C16-C17-C18	-3.52	122.28	127.31
17	2	602	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
26	7	601	CHL	O2D-CGD-O1D	-3.52	116.95	123.84
17	4	610	CLA	C3C-C4C-NC	3.52	114.52	110.57
26	9	607	CHL	C1D-CHD-C4C	-3.52	117.91	122.56
17	B	806	CLA	C1-C2-C3	-3.52	119.95	126.04
17	g	101	CLA	C3B-C4B-NB	3.52	113.76	109.21
17	b	835	CLA	C3C-C4C-NC	3.52	114.52	110.57
17	A	837	CLA	C3C-C4C-NC	3.52	114.52	110.57
20	b	845	BCR	C33-C5-C6	-3.52	120.58	124.53
17	A	831	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
17	2	608	CLA	C1D-CHD-C4C	-3.52	117.91	122.56
17	B	810	CLA	C1D-CHD-C4C	-3.52	117.91	122.56
17	b	807	CLA	C3C-C4C-NC	3.52	114.52	110.57
20	8	316	BCR	C11-C10-C9	-3.52	122.29	127.31
17	a	829	CLA	C1-C2-C3	-3.52	119.96	126.04
17	b	830	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
17	1	315	CLA	C3C-C4C-NC	3.52	114.52	110.57
17	F	304	CLA	C3C-C4C-NC	3.52	114.52	110.57
20	6	319	BCR	C11-C10-C9	-3.52	122.29	127.31
17	a	834	CLA	C3C-C4C-NC	3.52	114.51	110.57
17	K	4002	CLA	C1D-CHD-C4C	-3.52	117.92	122.56
17	3	309	CLA	C3C-C4C-NC	3.51	114.51	110.57
17	b	841	CLA	C3C-C4C-NC	3.51	114.51	110.57
17	l	202	CLA	C3C-C4C-NC	3.51	114.51	110.57
17	b	825	CLA	O2D-CGD-CBD	3.51	117.51	111.27
20	i	101	BCR	C28-C27-C26	-3.51	107.80	114.08
17	a	826	CLA	C1D-CHD-C4C	-3.51	117.92	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	F	305	BCR	C3-C4-C5	-3.51	107.80	114.08
17	A	803	CLA	C1D-CHD-C4C	-3.51	117.92	122.56
17	b	822	CLA	C1D-CHD-C4C	-3.51	117.92	122.56
17	B	804	CLA	C3C-C4C-NC	3.51	114.51	110.57
17	B	831	CLA	CAC-C3C-C4C	3.51	129.37	124.81
17	b	827	CLA	C1D-CHD-C4C	-3.51	117.92	122.56
17	g	103	CLA	CAC-C3C-C4C	3.51	129.37	124.81
17	b	834	CLA	C1D-CHD-C4C	-3.51	117.92	122.56
17	b	822	CLA	C3C-C4C-NC	3.51	114.51	110.57
17	B	827	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
20	b	846	BCR	C38-C26-C25	-3.51	120.59	124.53
20	8	316	BCR	C7-C8-C9	-3.51	120.94	126.23
17	a	839	CLA	C1D-CHD-C4C	-3.51	117.93	122.56
17	A	809	CLA	C1-C2-C3	-3.51	119.98	126.04
17	B	833	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
28	6	318	XAT	C35-C34-C33	-3.51	122.31	127.31
17	A	833	CLA	C1-C2-C3	-3.51	119.98	126.04
17	A	814	CLA	C1D-CHD-C4C	-3.51	117.93	122.56
17	b	827	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
17	f	7003	CLA	C3C-C4C-NC	3.50	114.50	110.57
17	2	612	CLA	C3C-C4C-NC	3.50	114.50	110.57
17	a	823	CLA	C1D-CHD-C4C	-3.50	117.94	122.56
17	B	817	CLA	C3C-C4C-NC	3.50	114.50	110.57
17	3	302	CLA	C3C-C4C-NC	3.50	114.49	110.57
17	1	303	CLA	C1-C2-C3	-3.50	120.00	126.04
17	A	829	CLA	C1-C2-C3	-3.50	120.00	126.04
17	b	830	CLA	C3C-C4C-NC	3.50	114.49	110.57
17	a	805	CLA	C3C-C4C-NC	3.50	114.49	110.57
20	A	851	BCR	C38-C26-C25	-3.50	120.60	124.53
17	a	809	CLA	C1D-CHD-C4C	-3.49	117.95	122.56
20	1	318	BCR	C7-C8-C9	-3.49	120.96	126.23
17	b	814	CLA	C3C-C4C-NC	3.49	114.49	110.57
17	b	802	CLA	C1D-CHD-C4C	-3.49	117.95	122.56
17	b	820	CLA	C1D-CHD-C4C	-3.49	117.95	122.56
17	b	838	CLA	C3C-C4C-NC	3.49	114.49	110.57
17	G	104	CLA	C3C-C4C-NC	3.49	114.49	110.57
17	A	820	CLA	C1-C2-C3	-3.49	120.01	126.04
17	B	841	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
17	A	831	CLA	C1D-CHD-C4C	-3.49	117.95	122.56
27	1	316	LUT	C18-C5-C6	-3.49	120.61	124.53
17	B	819	CLA	C3C-C4C-NC	3.49	114.48	110.57
17	b	812	CLA	C3C-C4C-NC	3.49	114.48	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	838	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
17	b	816	CLA	C3C-C4C-NC	3.49	114.48	110.57
17	F	304	CLA	C1D-CHD-C4C	-3.49	117.96	122.56
17	6	316	CLA	C3C-C4C-NC	3.48	114.48	110.57
17	7	610	CLA	C3B-C4B-NB	3.48	113.72	109.21
17	a	831	CLA	C1C-C2C-C3C	-3.48	103.29	106.96
17	b	806	CLA	C1C-C2C-C3C	-3.48	103.29	106.96
17	A	822	CLA	C3C-C4C-NC	3.48	114.48	110.57
20	3	318	BCR	C38-C26-C25	-3.48	120.62	124.53
17	G	104	CLA	C1C-C2C-C3C	-3.48	103.29	106.96
17	k	1402	CLA	C1D-CHD-C4C	-3.48	117.96	122.56
17	1	304	CLA	C1D-CHD-C4C	-3.48	117.96	122.56
17	a	808	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
17	6	313	CLA	C3C-C4C-NC	3.48	114.47	110.57
17	B	812	CLA	C3C-C4C-NC	3.48	114.47	110.57
17	a	831	CLA	C1D-CHD-C4C	-3.48	117.96	122.56
17	a	806	CLA	C1D-CHD-C4C	-3.48	117.96	122.56
17	2	609	CLA	C1-C2-C3	-3.48	120.02	126.04
18	A	844	PQN	C11-C12-C13	-3.48	121.00	126.79
17	6	309	CLA	C1D-CHD-C4C	-3.48	117.97	122.56
17	b	806	CLA	C3C-C4C-NC	3.48	114.47	110.57
17	A	805	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
17	b	840	CLA	C1D-CHD-C4C	-3.48	117.97	122.56
28	4	617	XAT	O4-C5-C18	3.48	119.22	115.06
17	A	842	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
17	3	311	CLA	C1D-CHD-C4C	-3.48	117.97	122.56
17	A	834	CLA	C1D-CHD-C4C	-3.48	117.97	122.56
27	6	321	LUT	C7-C8-C9	-3.48	120.98	126.23
17	7	602	CLA	C3C-C4C-NC	3.48	114.47	110.57
17	b	816	CLA	C1D-CHD-C4C	-3.48	117.97	122.56
17	A	842	CLA	C1D-CHD-C4C	-3.47	117.97	122.56
17	B	810	CLA	C1-C2-C3	-3.47	120.03	126.04
17	b	810	CLA	C1D-CHD-C4C	-3.47	117.97	122.56
17	b	825	CLA	CAA-C2A-C3A	-3.47	103.27	112.78
17	k	1401	CLA	C1D-CHD-C4C	-3.47	117.97	122.56
17	B	827	CLA	O2A-CGA-CBA	3.47	122.81	111.91
17	B	813	CLA	C1D-CHD-C4C	-3.47	117.98	122.56
17	8	310	CLA	C1D-CHD-C4C	-3.47	117.98	122.56
17	6	305	CLA	C3C-C4C-NC	3.47	114.46	110.57
20	L	205	BCR	C16-C17-C18	-3.47	122.36	127.31
17	A	831	CLA	CAC-C3C-C4C	3.47	129.31	124.81
17	6	316	CLA	C1D-CHD-C4C	-3.47	117.98	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	803	CLA	C1D-CHD-C4C	-3.47	117.98	122.56
17	a	811	CLA	C1-C2-C3	-3.47	120.05	126.04
17	B	802	CLA	C1-C2-C3	-3.47	120.05	126.04
17	1	309	CLA	C3C-C4C-NC	3.47	114.46	110.57
17	3	310	CLA	C3C-C4C-NC	3.47	114.46	110.57
17	b	802	CLA	C3B-C4B-NB	3.47	113.69	109.21
17	8	311	CLA	C1D-CHD-C4C	-3.47	117.98	122.56
17	A	827	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
17	B	830	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
26	7	614	CHL	C3B-C4B-NB	3.47	113.69	109.21
26	9	605	CHL	C1D-CHD-C4C	-3.47	117.98	122.56
17	b	808	CLA	O2D-CGD-O1D	-3.46	117.06	123.84
20	f	7004	BCR	C3-C4-C5	-3.46	107.89	114.08
17	7	613	CLA	C1D-CHD-C4C	-3.46	117.99	122.56
17	2	610	CLA	C1D-CHD-C4C	-3.46	117.99	122.56
17	b	838	CLA	C3B-C4B-NB	3.46	113.69	109.21
17	a	844	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
17	b	832	CLA	O2A-CGA-CBA	3.46	122.77	111.91
17	8	310	CLA	C3C-C4C-NC	3.46	114.45	110.57
17	a	816	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
17	3	312	CLA	C3C-C4C-NC	3.46	114.45	110.57
17	b	829	CLA	C1-C2-C3	-3.46	120.06	126.04
17	a	841	CLA	C1D-CHD-C4C	-3.46	117.99	122.56
17	k	1402	CLA	C3C-C4C-NC	3.46	114.45	110.57
27	4	616	LUT	C35-C34-C33	-3.46	122.38	127.31
17	A	835	CLA	C3C-C4C-NC	3.46	114.45	110.57
17	a	815	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
17	A	841	CLA	C1-C2-C3	-3.46	120.07	126.04
17	a	815	CLA	C1D-CHD-C4C	-3.45	118.00	122.56
17	6	304	CLA	CAC-C3C-C4C	3.45	129.29	124.81
17	L	204	CLA	C3C-C4C-NC	3.45	114.44	110.57
17	4	613	CLA	C3C-C4C-NC	3.45	114.44	110.57
17	9	601	CLA	C3C-C4C-NC	3.45	114.44	110.57
17	b	826	CLA	C1D-CHD-C4C	-3.45	118.00	122.56
17	b	805	CLA	C3C-C4C-NC	3.45	114.44	110.57
17	b	820	CLA	C1-C2-C3	-3.45	121.17	126.75
17	1	315	CLA	C1D-CHD-C4C	-3.45	118.00	122.56
17	8	302	CLA	C1D-CHD-C4C	-3.45	118.00	122.56
20	a	852	BCR	C33-C5-C6	-3.45	120.65	124.53
17	a	843	CLA	C1-C2-C3	-3.45	120.07	126.04
17	8	301	CLA	C3C-C4C-NC	3.45	114.44	110.57
17	A	843	CLA	C1D-CHD-C4C	-3.45	118.00	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	310	CLA	C3C-C4C-NC	3.45	114.44	110.57
20	a	853	BCR	C16-C17-C18	-3.45	122.39	127.31
17	8	310	CLA	C1-C2-C3	-3.45	120.08	126.04
20	9	618	BCR	C16-C17-C18	-3.45	122.39	127.31
17	b	806	CLA	C1D-CHD-C4C	-3.45	118.01	122.56
17	1	310	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
17	A	817	CLA	C3C-C4C-NC	3.45	114.44	110.57
20	l	205	BCR	C28-C27-C26	-3.45	107.92	114.08
17	B	805	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
20	A	848	BCR	C38-C26-C25	-3.45	120.66	124.53
17	l	203	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
17	3	308	CLA	C3C-C4C-NC	3.45	114.44	110.57
17	B	810	CLA	C3C-C4C-NC	3.45	114.44	110.57
17	B	808	CLA	C3C-C4C-NC	3.45	114.44	110.57
17	b	821	CLA	C1D-CHD-C4C	-3.44	118.01	122.56
17	B	834	CLA	C3C-C4C-NC	3.44	114.43	110.57
17	A	826	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
17	A	819	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
17	7	608	CLA	C3C-C4C-NC	3.44	114.43	110.57
17	8	304	CLA	C3C-C4C-NC	3.44	114.43	110.57
17	A	826	CLA	C1-C2-C3	-3.44	120.09	126.04
17	A	842	CLA	C3C-C4C-NC	3.44	114.43	110.57
17	a	828	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
17	A	824	CLA	C1-C2-C3	-3.44	120.10	126.04
17	6	307	CLA	C1D-CHD-C4C	-3.44	118.02	122.56
17	9	601	CLA	C1D-CHD-C4C	-3.44	118.02	122.56
17	a	842	CLA	O2D-CGD-CBD	3.44	117.37	111.27
20	l	206	BCR	C3-C4-C5	-3.43	107.94	114.08
17	9	603	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
17	2	610	CLA	C3C-C4C-NC	3.43	114.42	110.57
17	a	818	CLA	C1D-CHD-C4C	-3.43	118.03	122.56
17	B	840	CLA	C1D-CHD-C4C	-3.43	118.03	122.56
20	A	856	BCR	C33-C5-C6	-3.43	120.67	124.53
20	f	7004	BCR	C11-C10-C9	-3.43	122.41	127.31
17	B	811	CLA	C1D-CHD-C4C	-3.43	118.03	122.56
17	7	612	CLA	C1D-CHD-C4C	-3.43	118.03	122.56
17	B	830	CLA	CAC-C3C-C4C	3.43	129.26	124.81
17	3	305	CLA	C1D-CHD-C4C	-3.43	118.03	122.56
17	9	602	CLA	C1D-CHD-C4C	-3.43	118.03	122.56
17	A	843	CLA	C1-C2-C3	-3.43	120.11	126.04
17	A	802	CLA	O2D-CGD-CBD	3.43	117.36	111.27
26	2	614	CHL	C3B-C4B-NB	3.43	113.64	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	602	CLA	C3C-C4C-NC	3.43	114.42	110.57
17	8	301	CLA	C1-C2-C3	-3.43	120.11	126.04
20	F	305	BCR	C15-C14-C13	-3.43	122.42	127.31
17	9	609	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
17	B	829	CLA	C1D-CHD-C4C	-3.43	118.04	122.56
17	a	817	CLA	C1D-CHD-C4C	-3.43	118.04	122.56
26	6	303	CHL	CAC-C3C-C4C	3.43	129.25	124.81
26	3	307	CHL	C3B-C4B-NB	3.43	113.64	109.21
17	1	313	CLA	C1D-CHD-C4C	-3.42	118.04	122.56
17	A	828	CLA	C1-C2-C3	-3.42	120.12	126.04
17	3	303	CLA	C1D-CHD-C4C	-3.42	118.04	122.56
26	7	607	CHL	C1-C2-C3	-3.42	121.21	126.75
17	A	817	CLA	C1D-CHD-C4C	-3.42	118.04	122.56
17	3	312	CLA	C1D-CHD-C4C	-3.42	118.04	122.56
17	A	840	CLA	C1D-CHD-C4C	-3.42	118.04	122.56
17	2	604	CLA	C3C-C4C-NC	3.42	114.41	110.57
17	1	303	CLA	C3C-C4C-NC	3.42	114.41	110.57
17	9	613	CLA	C3C-C4C-NC	3.42	114.41	110.57
17	b	805	CLA	CAC-C3C-C4C	3.42	129.25	124.81
17	6	311	CLA	C3C-C4C-NC	3.42	114.41	110.57
17	3	302	CLA	C1-C2-C3	-3.42	120.13	126.04
17	L	202	CLA	C3C-C4C-NC	3.42	114.41	110.57
17	7	604	CLA	C3C-C4C-NC	3.42	114.41	110.57
20	J	3003	BCR	C16-C17-C18	-3.42	122.43	127.31
17	k	1403	CLA	C3B-C4B-NB	3.42	113.63	109.21
17	B	824	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
20	j	3003	BCR	C16-C17-C18	-3.42	122.43	127.31
17	B	806	CLA	C1D-CHD-C4C	-3.42	118.05	122.56
20	K	4004	BCR	C38-C26-C25	-3.42	120.69	124.53
17	3	301	CLA	C3C-C4C-NC	3.42	114.40	110.57
17	8	305	CLA	C1D-CHD-C4C	-3.42	118.05	122.56
17	a	810	CLA	C1D-CHD-C4C	-3.42	118.05	122.56
17	a	803	CLA	C3B-C4B-NB	3.42	113.63	109.21
17	B	834	CLA	C1C-C2C-C3C	-3.42	103.37	106.96
17	6	305	CLA	C1D-CHD-C4C	-3.41	118.05	122.56
17	G	103	CLA	C1D-CHD-C4C	-3.41	118.05	122.56
17	a	816	CLA	C1D-CHD-C4C	-3.41	118.05	122.56
17	A	833	CLA	C3C-C4C-NC	3.41	114.40	110.57
17	a	830	CLA	C1-C2-C3	-3.41	120.14	126.04
17	L	203	CLA	C1-C2-C3	-3.41	120.14	126.04
17	a	814	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
17	B	803	CLA	C1C-C2C-C3C	-3.41	103.37	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	828	CLA	C1D-CHD-C4C	-3.41	118.06	122.56
17	A	833	CLA	C1D-CHD-C4C	-3.41	118.06	122.56
17	1	313	CLA	C3C-C4C-NC	3.41	114.39	110.57
17	A	812	CLA	C1-C2-C3	-3.41	120.15	126.04
17	a	831	CLA	C1-C2-C3	-3.41	120.15	126.04
17	a	838	CLA	C1C-C2C-C3C	-3.41	103.38	106.96
17	A	804	CLA	O2D-CGD-O1D	-3.41	117.18	123.84
17	A	821	CLA	C3B-C4B-NB	3.40	113.61	109.21
17	B	816	CLA	C1D-CHD-C4C	-3.40	118.06	122.56
17	A	801	CLA	C1D-CHD-C4C	-3.40	118.07	122.56
17	a	846	CLA	C1D-CHD-C4C	-3.40	118.07	122.56
17	B	825	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
17	B	822	CLA	C3C-C4C-NC	3.40	114.39	110.57
27	1	320	LUT	C18-C5-C6	-3.40	120.71	124.53
17	a	837	CLA	C1D-CHD-C4C	-3.40	118.07	122.56
17	8	308	CLA	C1D-CHD-C4C	-3.40	118.07	122.56
17	9	612	CLA	C3C-C4C-NC	3.40	114.39	110.57
17	6	315	CLA	C1D-CHD-C4C	-3.40	118.07	122.56
17	b	810	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
17	B	826	CLA	C1C-C2C-C3C	-3.40	103.39	106.96
17	a	814	CLA	C1-C2-C3	-3.40	120.17	126.04
17	B	834	CLA	CAC-C3C-C4C	3.40	129.22	124.81
17	B	841	CLA	C1D-CHD-C4C	-3.40	118.08	122.56
17	B	821	CLA	C1D-CHD-C4C	-3.39	118.08	122.56
17	b	831	CLA	C1D-CHD-C4C	-3.39	118.08	122.56
17	8	309	CLA	C3C-C4C-NC	3.39	114.38	110.57
17	A	806	CLA	C1D-CHD-C4C	-3.39	118.08	122.56
20	j	3004	BCR	C15-C14-C13	-3.39	122.47	127.31
17	b	841	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
17	8	308	CLA	C3C-C4C-NC	3.39	114.37	110.57
17	g	103	CLA	C1D-CHD-C4C	-3.39	118.08	122.56
17	8	303	CLA	C3C-C4C-NC	3.39	114.37	110.57
17	b	819	CLA	C3C-C4C-NC	3.39	114.37	110.57
17	4	612	CLA	C3C-C4C-NC	3.39	114.37	110.57
17	a	827	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
17	a	827	CLA	C1D-CHD-C4C	-3.39	118.09	122.56
17	b	812	CLA	C1D-CHD-C4C	-3.39	118.09	122.56
17	A	809	CLA	C1D-CHD-C4C	-3.39	118.09	122.56
17	a	825	CLA	C1D-CHD-C4C	-3.38	118.09	122.56
17	a	802	CLA	O2D-CGD-CBD	3.38	117.28	111.27
17	1	312	CLA	C1-C2-C3	-3.38	120.19	126.04
17	1	311	CLA	C1D-CHD-C4C	-3.38	118.09	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	829	CLA	C1D-CHD-C4C	-3.38	118.09	122.56
17	b	814	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
17	4	601	CLA	C1D-CHD-C4C	-3.38	118.10	122.56
17	l	202	CLA	C1D-CHD-C4C	-3.38	118.10	122.56
25	4	620	LMG	O1-C1-C2	3.38	113.58	108.30
17	3	314	CLA	C1D-CHD-C4C	-3.38	118.10	122.56
17	L	202	CLA	C1D-CHD-C4C	-3.38	118.10	122.56
17	A	813	CLA	C3C-C4C-NC	3.38	114.36	110.57
17	B	819	CLA	C1-C2-C3	-3.38	120.20	126.04
17	2	613	CLA	C3C-C4C-NC	3.38	114.36	110.57
17	B	816	CLA	CAC-C3C-C4C	3.38	129.19	124.81
17	L	204	CLA	C1D-CHD-C4C	-3.38	118.10	122.56
27	6	321	LUT	C18-C5-C6	-3.38	120.74	124.53
17	A	838	CLA	C1D-CHD-C4C	-3.38	118.10	122.56
17	a	832	CLA	C1D-CHD-C4C	-3.38	118.10	122.56
17	b	826	CLA	C1C-C2C-C3C	-3.38	103.41	106.96
20	I	101	BCR	C29-C30-C25	3.37	115.68	110.48
17	A	811	CLA	C1-C2-C3	-3.37	120.21	126.04
17	b	813	CLA	C1D-CHD-C4C	-3.37	118.11	122.56
17	4	604	CLA	CAC-C3C-C4C	3.37	129.19	124.81
17	b	829	CLA	CAC-C3C-C4C	3.37	129.19	124.81
17	b	838	CLA	C1D-CHD-C4C	-3.37	118.11	122.56
20	a	852	BCR	C28-C27-C26	-3.37	108.06	114.08
20	i	101	BCR	C29-C30-C25	3.37	115.67	110.48
17	A	837	CLA	C1D-CHD-C4C	-3.37	118.11	122.56
17	8	304	CLA	C1D-CHD-C4C	-3.37	118.11	122.56
17	a	807	CLA	C1D-CHD-C4C	-3.37	118.11	122.56
17	1	305	CLA	C1-C2-C3	-3.37	120.22	126.04
17	a	820	CLA	C3C-C4C-NC	3.37	114.35	110.57
17	B	834	CLA	C1D-CHD-C4C	-3.37	118.11	122.56
17	a	808	CLA	C1D-CHD-C4C	-3.37	118.11	122.56
20	A	849	BCR	C33-C5-C6	-3.37	120.75	124.53
17	A	843	CLA	C3C-C4C-NC	3.37	114.35	110.57
27	2	615	LUT	C18-C5-C6	-3.37	120.75	124.53
17	3	309	CLA	C1D-CHD-C4C	-3.37	118.12	122.56
17	2	609	CLA	C3C-C4C-NC	3.37	114.34	110.57
17	1	304	CLA	C3C-C4C-NC	3.37	114.34	110.57
17	A	835	CLA	O2D-CGD-O1D	-3.36	117.26	123.84
17	1	308	CLA	C1D-CHD-C4C	-3.36	118.12	122.56
26	2	607	CHL	C1-C2-C3	-3.36	121.31	126.75
17	b	807	CLA	C1D-CHD-C4C	-3.36	118.12	122.56
17	A	814	CLA	C1C-C2C-C3C	-3.36	103.42	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	609	CLA	C3C-C4C-NC	3.36	114.34	110.57
28	8	315	XAT	C10-C11-C12	-3.36	112.73	123.22
17	A	820	CLA	C1D-CHD-C4C	-3.36	118.12	122.56
17	4	614	CLA	C1D-CHD-C4C	-3.36	118.12	122.56
17	B	835	CLA	C1D-CHD-C4C	-3.36	118.12	122.56
17	2	608	CLA	C3C-C4C-NC	3.36	114.34	110.57
17	A	814	CLA	CAC-C3C-C4C	3.36	129.17	124.81
17	9	603	CLA	C3B-C4B-NB	3.36	113.55	109.21
17	a	806	CLA	C1C-C2C-C3C	-3.36	103.43	106.96
17	B	809	CLA	C1D-CHD-C4C	-3.36	118.13	122.56
17	3	315	CLA	C3A-C4A-NA	3.36	116.96	109.92
17	3	312	CLA	C1-C2-C3	-3.36	120.24	126.04
17	g	101	CLA	C3C-C4C-NC	3.36	114.33	110.57
17	b	808	CLA	C3B-C4B-NB	3.36	113.55	109.21
17	1	305	CLA	C3C-C4C-NC	3.36	114.33	110.57
17	A	815	CLA	C1D-CHD-C4C	-3.36	118.13	122.56
20	b	844	BCR	C20-C21-C22	-3.35	122.52	127.31
17	7	612	CLA	CAC-C3C-C4C	3.35	129.16	124.81
17	6	311	CLA	C1C-C2C-C3C	-3.35	103.43	106.96
17	B	812	CLA	C1D-CHD-C4C	-3.35	118.13	122.56
17	3	304	CLA	C3C-C4C-NC	3.35	114.33	110.57
17	6	306	CLA	C1D-CHD-C4C	-3.35	118.13	122.56
20	b	846	BCR	C15-C14-C13	-3.35	122.53	127.31
17	a	804	CLA	C3B-C4B-NB	3.35	113.54	109.21
17	a	801	CLA	C3B-C4B-NB	3.35	113.54	109.21
17	k	1403	CLA	C3C-C4C-NC	3.35	114.33	110.57
17	7	611	CLA	C3B-C4B-NB	3.35	113.54	109.21
17	a	802	CLA	C3C-C4C-NC	3.35	114.33	110.57
17	8	301	CLA	C1C-C2C-C3C	-3.35	103.44	106.96
17	9	604	CLA	C3C-C4C-NC	3.35	114.33	110.57
20	b	847	BCR	C11-C10-C9	-3.35	122.53	127.31
17	F	301	CLA	C1-C2-C3	-3.35	120.25	126.04
17	B	829	CLA	CAC-C3C-C4C	3.35	129.15	124.81
20	B	847	BCR	C15-C16-C17	-3.35	116.62	123.47
17	b	835	CLA	C1D-CHD-C4C	-3.34	118.14	122.56
17	b	836	CLA	C3B-C4B-NB	3.34	113.53	109.21
17	B	829	CLA	C3C-C4C-NC	3.34	114.32	110.57
17	A	814	CLA	C1-C2-C3	-3.34	120.26	126.04
17	6	315	CLA	C3C-C4C-NC	3.34	114.32	110.57
17	b	811	CLA	C1-C2-C3	-3.34	120.26	126.04
17	6	306	CLA	C4-C3-C5	3.34	119.80	115.98
17	B	805	CLA	C1D-CHD-C4C	-3.34	118.15	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	304	CLA	C3B-C4B-NB	3.34	113.53	109.21
26	9	607	CHL	C1-C2-C3	-3.34	121.35	126.75
17	7	609	CLA	C1C-C2C-C3C	-3.34	103.44	106.96
17	A	832	CLA	C1D-CHD-C4C	-3.34	118.15	122.56
17	7	602	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
17	A	804	CLA	C1-C2-C3	-3.34	120.27	126.04
17	2	609	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
17	8	313	CLA	C2C-C1C-NC	3.34	115.17	109.51
17	B	831	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
17	b	823	CLA	C1D-CHD-C4C	-3.33	118.16	122.56
17	A	830	CLA	C1D-CHD-C4C	-3.33	118.16	122.56
17	B	824	CLA	C1D-CHD-C4C	-3.33	118.16	122.56
17	B	837	CLA	C1D-CHD-C4C	-3.33	118.16	122.56
17	b	825	CLA	C1C-C2C-C3C	-3.33	103.45	106.96
20	b	847	BCR	C38-C26-C25	-3.33	120.78	124.53
17	3	304	CLA	C1D-CHD-C4C	-3.33	118.16	122.56
19	a	848	LHG	O8-C23-C24	3.33	120.12	111.38
17	9	611	CLA	C3B-C4B-NB	3.33	113.52	109.21
17	g	101	CLA	CBC-CAC-C3C	-3.33	103.25	112.43
17	b	829	CLA	C3B-C4B-NB	3.33	113.52	109.21
17	b	805	CLA	C3B-C4B-NB	3.33	113.52	109.21
17	3	302	CLA	C1C-C2C-C3C	-3.33	103.45	106.96
17	B	822	CLA	C1-C2-C3	-3.33	120.28	126.04
17	a	821	CLA	C3B-C4B-NB	3.33	113.52	109.21
17	b	817	CLA	C3C-C4C-NC	3.33	114.31	110.57
17	B	832	CLA	C1C-C2C-C3C	-3.33	103.45	106.96
17	8	313	CLA	C3A-C4A-NA	3.33	116.91	109.92
17	k	1403	CLA	C1D-CHD-C4C	-3.33	118.16	122.56
17	a	801	CLA	O2A-CGA-CBA	3.33	122.36	111.91
17	3	315	CLA	C3B-C4B-NB	3.33	113.02	110.11
26	4	605	CHL	C3B-C4B-NB	3.33	113.51	109.21
17	a	801	CLA	C1-C2-C3	-3.33	120.29	126.04
17	B	823	CLA	C1D-CHD-C4C	-3.33	118.17	122.56
20	a	852	BCR	C24-C23-C22	-3.33	121.21	126.23
17	A	824	CLA	C3B-C4B-NB	3.33	113.51	109.21
17	1	303	CLA	C1D-CHD-C4C	-3.32	118.17	122.56
17	B	816	CLA	C4-C3-C5	3.32	120.86	115.27
17	A	810	CLA	C3B-C4B-NB	3.32	113.51	109.21
17	a	810	CLA	O2A-CGA-CBA	3.32	122.34	111.91
17	A	816	CLA	C1-C2-C3	-3.32	121.38	126.75
18	A	844	PQN	C14-C13-C15	3.32	120.86	115.27
17	b	832	CLA	C1C-C2C-C3C	-3.32	103.46	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	604	CLA	C3C-C4C-NC	3.32	114.30	110.57
20	a	853	BCR	C15-C14-C13	-3.32	122.57	127.31
20	b	845	BCR	C34-C9-C10	-3.32	118.27	122.92
17	a	840	CLA	C3B-C4B-NB	3.32	113.50	109.21
17	4	603	CLA	C3B-C4B-NB	3.32	113.50	109.21
17	b	808	CLA	C3C-C4C-NC	3.32	114.30	110.57
20	K	4001	BCR	C11-C10-C9	-3.32	122.57	127.31
17	a	819	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
20	B	846	BCR	C28-C27-C26	-3.32	108.15	114.08
17	a	803	CLA	CAC-C3C-C4C	3.32	129.12	124.81
17	3	309	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
17	A	825	CLA	C1D-CHD-C4C	-3.32	118.18	122.56
17	l	203	CLA	C1D-CHD-C4C	-3.32	118.18	122.56
17	9	613	CLA	C1D-CHD-C4C	-3.32	118.18	122.56
17	a	838	CLA	CHD-C4C-NC	3.32	129.43	124.20
17	9	609	CLA	C3C-C4C-NC	3.32	114.29	110.57
17	a	801	CLA	CAA-C2A-C3A	-3.32	103.70	112.78
17	1	303	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
17	b	833	CLA	C1-C2-C3	-3.32	120.31	126.04
26	7	607	CHL	CAC-C3C-C4C	3.32	129.11	124.81
17	A	819	CLA	C1-C2-C3	-3.31	120.31	126.04
17	8	308	CLA	C1C-C2C-C3C	-3.31	103.47	106.96
17	A	807	CLA	C1D-CHD-C4C	-3.31	118.19	122.56
17	1	305	CLA	C1D-CHD-C4C	-3.31	118.19	122.56
17	9	612	CLA	C1D-CHD-C4C	-3.31	118.19	122.56
17	3	310	CLA	C1D-CHD-C4C	-3.31	118.19	122.56
20	L	201	BCR	C34-C9-C10	-3.31	118.28	122.92
17	4	602	CLA	C1C-C2C-C3C	-3.31	103.47	106.96
27	9	616	LUT	C35-C34-C33	-3.31	122.58	127.31
17	7	609	CLA	C3C-C4C-NC	3.31	114.28	110.57
26	9	605	CHL	C4-C3-C5	3.31	120.84	115.27
17	a	824	CLA	C3B-C4B-NB	3.31	113.49	109.21
17	8	312	CLA	C1D-CHD-C4C	-3.31	118.19	122.56
17	8	301	CLA	C1D-CHD-C4C	-3.31	118.19	122.56
17	2	613	CLA	C1D-CHD-C4C	-3.31	118.19	122.56
27	1	320	LUT	C11-C10-C9	-3.31	122.59	127.31
17	2	602	CLA	C3C-C4C-NC	3.31	114.28	110.57
17	A	820	CLA	C3C-C4C-NC	3.31	114.28	110.57
17	B	803	CLA	C3C-C4C-NC	3.31	114.28	110.57
17	A	804	CLA	C1D-CHD-C4C	-3.31	118.19	122.56
20	8	316	BCR	C16-C17-C18	-3.31	122.59	127.31
20	f	7004	BCR	C15-C14-C13	-3.31	122.59	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	613	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
17	a	829	CLA	CAC-C3C-C4C	3.30	129.10	124.81
17	a	819	CLA	C1-C2-C3	-3.30	120.33	126.04
17	b	833	CLA	C3B-C4B-NB	3.30	113.48	109.21
17	1	314	CLA	C3B-C4B-NB	3.30	113.48	109.21
17	b	811	CLA	C4B-C3B-C2B	-3.30	103.85	106.92
17	A	827	CLA	C1-C2-C3	-3.30	120.33	126.04
17	b	837	CLA	C1D-CHD-C4C	-3.30	118.20	122.56
17	6	313	CLA	C3B-C4B-NB	3.30	113.48	109.21
26	9	606	CHL	C3B-C4B-NB	3.30	113.48	109.21
17	b	817	CLA	CAC-C3C-C4C	3.30	129.09	124.81
17	9	614	CLA	C1D-CHD-C4C	-3.30	118.20	122.56
17	k	1402	CLA	C3B-C4B-NB	3.30	113.47	109.21
20	a	852	BCR	C11-C10-C9	-3.30	122.60	127.31
17	A	828	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
20	b	845	BCR	C16-C17-C18	-3.30	122.61	127.31
20	g	104	BCR	C3-C4-C5	-3.30	108.19	114.08
17	b	819	CLA	C1-C2-C3	-3.30	120.34	126.04
20	A	850	BCR	C28-C27-C26	-3.30	108.19	114.08
17	3	315	CLA	C2C-C1C-NC	3.30	115.10	109.51
17	4	612	CLA	C3B-C4B-NB	3.29	113.47	109.21
17	a	837	CLA	CAC-C3C-C4C	3.29	129.08	124.81
17	A	805	CLA	C1D-CHD-C4C	-3.29	118.21	122.56
17	6	304	CLA	C1-C2-C3	-3.29	120.35	126.04
17	4	611	CLA	C3B-C4B-NB	3.29	113.47	109.21
26	7	606	CHL	C3B-C4B-NB	3.29	113.47	109.21
17	a	838	CLA	CMC-C2C-C1C	3.29	130.05	125.04
17	A	806	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
17	B	812	CLA	CAC-C3C-C4C	3.29	129.08	124.81
17	A	845	CLA	C1D-CHD-C4C	-3.29	118.21	122.56
17	A	823	CLA	C1D-CHD-C4C	-3.29	118.22	122.56
17	B	802	CLA	C3B-C4B-NB	3.29	113.46	109.21
17	9	603	CLA	CAC-C3C-C4C	3.29	129.08	124.81
17	b	817	CLA	C1D-CHD-C4C	-3.29	118.22	122.56
17	B	836	CLA	C3B-C4B-NB	3.29	113.46	109.21
17	A	811	CLA	C3C-C4C-NC	3.29	114.26	110.57
17	A	806	CLA	C3B-C4B-NB	3.29	113.46	109.21
17	A	831	CLA	C1-C2-C3	-3.29	120.36	126.04
20	A	848	BCR	C3-C4-C5	-3.29	108.21	114.08
17	B	816	CLA	C3C-C4C-NC	3.28	114.25	110.57
17	B	817	CLA	C1D-CHD-C4C	-3.28	118.22	122.56
17	B	803	CLA	O2D-CGD-CBD	3.28	117.10	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	848	BCR	C15-C14-C13	-3.28	122.62	127.31
28	8	315	XAT	O4-C5-C18	3.28	118.99	115.06
17	l	202	CLA	C3B-C4B-NB	3.28	113.45	109.21
17	A	835	CLA	C1D-CHD-C4C	-3.28	118.23	122.56
17	J	3002	CLA	C1D-CHD-C4C	-3.28	118.23	122.56
17	1	314	CLA	C3C-C4C-NC	3.28	114.25	110.57
17	7	612	CLA	C3B-C4B-NB	3.28	113.45	109.21
17	A	802	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
26	1	307	CHL	C3B-C4B-NB	3.28	113.45	109.21
17	A	839	CLA	C3B-C4B-NB	3.28	113.45	109.21
17	B	819	CLA	C1D-CHD-C4C	-3.28	118.23	122.56
17	A	810	CLA	O2A-CGA-CBA	3.28	122.19	111.91
17	B	822	CLA	C1D-CHD-C4C	-3.28	118.23	122.56
17	a	830	CLA	C1D-CHD-C4C	-3.28	118.23	122.56
17	g	102	CLA	C1D-CHD-C4C	-3.28	118.23	122.56
28	1	317	XAT	C10-C11-C12	-3.27	113.00	123.22
26	2	606	CHL	C3B-C4B-NB	3.27	113.44	109.21
17	A	808	CLA	C1D-CHD-C4C	-3.27	118.24	122.56
17	A	816	CLA	C1D-CHD-C4C	-3.27	118.24	122.56
17	7	603	CLA	C4-C3-C5	3.27	119.72	115.98
17	B	824	CLA	C1-C2-C3	-3.27	120.38	126.04
17	1	313	CLA	C3B-C4B-NB	3.27	113.44	109.21
17	4	613	CLA	C1D-CHD-C4C	-3.27	118.24	122.56
17	b	832	CLA	C1D-CHD-C4C	-3.27	118.24	122.56
17	b	812	CLA	CAC-C3C-C4C	3.27	129.05	124.81
17	7	602	CLA	C1D-CHD-C4C	-3.27	118.25	122.56
17	b	840	CLA	C3B-C4B-NB	3.27	113.44	109.21
17	b	809	CLA	C1D-CHD-C4C	-3.27	118.25	122.56
17	b	837	CLA	C3C-C4C-NC	3.27	114.23	110.57
17	B	832	CLA	C1D-CHD-C4C	-3.27	118.25	122.56
17	A	825	CLA	C3B-C4B-NB	3.27	113.43	109.21
20	A	848	BCR	C33-C5-C6	-3.27	120.86	124.53
17	A	824	CLA	C4-C3-C5	3.27	119.72	115.98
17	1	314	CLA	C1D-CHD-C4C	-3.26	118.25	122.56
20	K	4004	BCR	C33-C5-C6	-3.26	120.86	124.53
17	8	313	CLA	C3B-C4B-NB	3.26	112.97	110.11
17	b	824	CLA	CAC-C3C-C4C	3.26	129.04	124.81
17	4	604	CLA	C1D-CHD-C4C	-3.26	118.25	122.56
17	B	820	CLA	C1-C2-C3	-3.26	121.47	126.75
20	g	104	BCR	C15-C14-C13	-3.26	122.66	127.31
26	6	308	CHL	C3B-C4B-NB	3.26	113.42	109.21
17	1	314	CLA	CAC-C3C-C4C	3.26	129.04	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	9	607	CHL	C3B-C4B-NB	3.26	113.42	109.21
17	a	829	CLA	O2A-CGA-CBA	3.26	122.13	111.91
17	3	301	CLA	CAC-C3C-C4C	3.26	129.04	124.81
17	4	601	CLA	C3B-C4B-NB	3.26	113.42	109.21
20	a	849	BCR	C11-C10-C9	-3.26	122.66	127.31
17	B	827	CLA	C1D-CHD-C4C	-3.26	118.26	122.56
20	b	843	BCR	C7-C8-C9	-3.25	121.32	126.23
17	a	809	CLA	CHD-C4C-NC	3.25	129.33	124.20
17	8	309	CLA	C3B-C4B-NB	3.25	113.42	109.21
17	B	837	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
17	a	813	CLA	C1D-CHD-C4C	-3.25	118.27	122.56
17	b	819	CLA	C1D-CHD-C4C	-3.25	118.27	122.56
17	b	824	CLA	C3B-C4B-NB	3.25	113.41	109.21
17	b	823	CLA	CAC-C3C-C4C	3.25	129.03	124.81
17	g	103	CLA	C3C-C4C-NC	3.25	114.22	110.57
17	1	312	CLA	C3B-C4B-NB	3.25	113.41	109.21
17	b	829	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
17	b	837	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
17	9	604	CLA	C1D-CHD-C4C	-3.25	118.27	122.56
17	B	807	CLA	C1D-CHD-C4C	-3.25	118.27	122.56
17	3	301	CLA	C3B-C4B-NB	3.25	113.41	109.21
17	b	830	CLA	C1-C2-C3	-3.25	121.50	126.75
17	A	843	CLA	CAC-C3C-C4C	3.24	129.02	124.81
17	A	824	CLA	C1D-CHD-C4C	-3.24	118.28	122.56
17	9	601	CLA	C3B-C4B-NB	3.24	113.40	109.21
17	9	602	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
20	A	849	BCR	C16-C17-C18	-3.24	122.68	127.31
17	a	817	CLA	C3B-C4B-NB	3.24	113.40	109.21
20	1	318	BCR	C38-C26-C25	-3.24	120.89	124.53
17	3	312	CLA	C3B-C4B-NB	3.24	113.40	109.21
17	B	829	CLA	CHC-C1C-C2C	-3.24	117.75	126.72
17	a	808	CLA	C1-C2-C3	-3.24	120.44	126.04
27	6	321	LUT	C35-C34-C33	-3.24	122.69	127.31
17	7	613	CLA	C3C-C4C-NC	3.24	114.20	110.57
17	a	837	CLA	C3B-C4B-NB	3.24	113.40	109.21
17	a	823	CLA	C3B-C4B-NB	3.24	113.40	109.21
17	A	806	CLA	CAC-C3C-C4C	3.24	129.01	124.81
17	B	829	CLA	C1-C2-C3	-3.24	120.44	126.04
17	A	811	CLA	C3B-C4B-NB	3.24	113.40	109.21
17	1	303	CLA	CAC-C3C-C4C	3.24	129.01	124.81
20	L	206	BCR	C7-C8-C9	-3.24	121.34	126.23
20	6	319	BCR	C7-C8-C9	-3.24	121.34	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	101	CLA	C3B-C4B-NB	3.24	113.39	109.21
17	6	304	CLA	C1D-CHD-C4C	-3.24	118.29	122.56
17	a	801	CLA	C1D-CHD-C4C	-3.24	118.29	122.56
17	g	103	CLA	C3B-C4B-NB	3.24	113.39	109.21
17	6	305	CLA	C3B-C4B-NB	3.23	113.39	109.21
17	A	820	CLA	C3B-C4B-NB	3.23	113.39	109.21
17	8	310	CLA	C3B-C4B-NB	3.23	113.39	109.21
17	A	809	CLA	C3B-C4B-NB	3.23	113.39	109.21
20	B	801	BCR	C20-C21-C22	-3.23	122.70	127.31
17	6	316	CLA	C3B-C4B-NB	3.23	113.39	109.21
27	4	616	LUT	C18-C5-C6	-3.23	120.90	124.53
17	j	3002	CLA	C1D-CHD-C4C	-3.23	118.29	122.56
17	a	820	CLA	C1D-CHD-C4C	-3.23	118.29	122.56
17	1	309	CLA	C3B-C4B-NB	3.23	113.39	109.21
17	a	811	CLA	C3B-C4B-NB	3.23	113.39	109.21
17	B	840	CLA	C1-C2-C3	-3.23	120.45	126.04
20	B	847	BCR	C11-C10-C9	-3.23	122.70	127.31
17	6	315	CLA	C3B-C4B-NB	3.23	113.39	109.21
18	B	842	PQN	C14-C13-C15	3.23	120.70	115.27
17	A	830	CLA	C3B-C4B-NB	3.23	113.38	109.21
17	7	604	CLA	C1D-CHD-C4C	-3.23	118.30	122.56
20	b	848	BCR	C16-C17-C18	-3.23	122.71	127.31
17	A	802	CLA	C1D-CHD-C4C	-3.22	118.30	122.56
20	L	205	BCR	C20-C21-C22	-3.22	122.71	127.31
17	a	844	CLA	CAC-C3C-C4C	3.22	128.99	124.81
17	b	803	CLA	C1C-C2C-C3C	-3.22	103.57	106.96
17	a	806	CLA	C3B-C4B-NB	3.22	113.38	109.21
17	b	805	CLA	C4-C3-C5	3.22	120.69	115.27
17	B	836	CLA	CMB-C2B-C3B	3.22	130.70	124.68
17	2	611	CLA	C3B-C4B-NB	3.22	113.37	109.21
17	B	817	CLA	C4-C3-C5	3.22	120.69	115.27
17	A	828	CLA	CHD-C4C-NC	3.22	129.28	124.20
17	B	811	CLA	C4B-C3B-C2B	-3.22	103.93	106.92
27	9	616	LUT	C18-C5-C6	-3.22	120.91	124.53
26	7	601	CHL	C4-C3-C5	3.22	120.68	115.27
17	6	310	CLA	C3B-C4B-NB	3.22	113.37	109.21
20	1	205	BCR	C20-C21-C22	-3.22	122.72	127.31
17	2	602	CLA	C1D-CHD-C4C	-3.22	118.31	122.56
17	A	805	CLA	O2A-CGA-CBA	3.22	122.00	111.91
27	8	314	LUT	C18-C5-C6	-3.22	120.92	124.53
17	A	840	CLA	C3B-C4B-NB	3.22	113.37	109.21
17	a	825	CLA	C1-C2-C3	-3.22	120.48	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	830	CLA	C3B-C4B-NB	3.21	113.37	109.21
20	K	4004	BCR	C3-C4-C5	-3.21	108.34	114.08
17	b	839	CLA	C3B-C4B-NB	3.21	113.36	109.21
17	b	841	CLA	C1D-CHD-C4C	-3.21	118.32	122.56
17	a	840	CLA	C1D-CHD-C4C	-3.21	118.32	122.56
17	L	203	CLA	C1D-CHD-C4C	-3.21	118.32	122.56
18	b	842	PQN	C11-C12-C13	-3.21	121.44	126.79
26	9	615	CHL	C3B-C4B-NB	3.21	113.36	109.21
17	a	843	CLA	C1C-C2C-C3C	-3.21	103.58	106.96
20	j	3004	BCR	C33-C5-C6	-3.21	120.92	124.53
17	a	804	CLA	CMB-C2B-C3B	3.21	130.69	124.68
20	l	206	BCR	C16-C17-C18	-3.21	122.73	127.31
17	L	202	CLA	C3B-C4B-NB	3.21	113.36	109.21
17	3	313	CLA	C3B-C4B-NB	3.21	113.36	109.21
17	a	828	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
27	3	316	LUT	C31-C30-C29	-3.21	122.73	127.31
26	4	607	CHL	C3B-C4B-NB	3.21	113.36	109.21
17	a	814	CLA	C1D-CHD-C4C	-3.21	118.33	122.56
20	G	105	BCR	C24-C23-C22	-3.21	121.39	126.23
17	b	819	CLA	C3B-C4B-NB	3.21	113.35	109.21
17	b	818	CLA	CAC-C3C-C4C	3.20	128.97	124.81
17	2	604	CLA	C1D-CHD-C4C	-3.20	118.33	122.56
17	a	822	CLA	C1D-CHD-C4C	-3.20	118.33	122.56
17	b	802	CLA	C1-C2-C3	-3.20	120.50	126.04
17	1	315	CLA	C3B-C4B-NB	3.20	113.35	109.21
17	B	825	CLA	O2A-CGA-CBA	3.20	121.96	111.91
17	A	822	CLA	C1D-CHD-C4C	-3.20	118.33	122.56
17	2	608	CLA	C1-C2-C3	-3.20	121.57	126.75
17	A	831	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
17	3	310	CLA	C3B-C4B-NB	3.20	113.35	109.21
17	A	825	CLA	CHC-C1C-C2C	-3.20	117.88	126.72
17	A	837	CLA	C3B-C4B-NB	3.20	113.34	109.21
20	4	618	BCR	C16-C17-C18	-3.20	122.75	127.31
27	8	314	LUT	C35-C34-C33	-3.19	122.75	127.31
17	B	817	CLA	C1-C2-C3	-3.19	120.52	126.04
17	a	824	CLA	C1D-CHD-C4C	-3.19	118.34	122.56
17	a	834	CLA	C1D-CHD-C4C	-3.19	118.34	122.56
17	A	834	CLA	C3B-C4B-NB	3.19	113.34	109.21
17	A	821	CLA	CBC-CAC-C3C	-3.19	103.63	112.43
17	A	831	CLA	C3B-C4B-NB	3.19	113.33	109.21
27	7	615	LUT	C18-C5-C6	-3.19	120.95	124.53
20	B	844	BCR	C8-C9-C10	3.19	123.83	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	608	CLA	C3B-C4B-NB	3.19	113.33	109.21
17	b	806	CLA	CHD-C4C-NC	3.19	129.23	124.20
17	b	826	CLA	C1-C2-C3	-3.19	120.53	126.04
17	2	612	CLA	C3B-C4B-NB	3.19	113.33	109.21
17	1	305	CLA	C3B-C4B-NB	3.19	113.33	109.21
17	A	843	CLA	C3B-C4B-NB	3.19	113.33	109.21
20	8	316	BCR	C38-C26-C25	-3.19	120.95	124.53
17	9	612	CLA	C3B-C4B-NB	3.19	113.33	109.21
17	9	614	CLA	C3B-C4B-NB	3.19	113.33	109.21
17	7	603	CLA	CAC-C3C-C4C	3.19	128.94	124.81
17	8	311	CLA	C3B-C4B-NB	3.18	113.33	109.21
23	B	849	LMT	C1B-O1B-C4'	-3.18	110.08	117.96
17	A	813	CLA	C1D-CHD-C4C	-3.18	118.36	122.56
17	9	613	CLA	C3B-C4B-NB	3.18	113.32	109.21
17	3	302	CLA	C1D-CHD-C4C	-3.18	118.36	122.56
17	b	830	CLA	CAC-C3C-C4C	3.18	128.94	124.81
17	B	819	CLA	C3B-C4B-NB	3.18	113.32	109.21
28	9	617	XAT	C35-C15-C14	-3.18	116.96	123.47
17	a	806	CLA	CAC-C3C-C4C	3.18	128.93	124.81
17	6	316	CLA	CAC-C3C-C4C	3.18	128.93	124.81
17	B	831	CLA	C1D-CHD-C4C	-3.17	118.37	122.56
20	k	1404	BCR	C24-C23-C22	-3.17	121.44	126.23
26	9	615	CHL	CAC-C3C-C4C	3.17	128.93	124.81
17	1	310	CLA	C1-C2-C3	-3.17	120.55	126.04
17	3	313	CLA	C1D-CHD-C4C	-3.17	118.37	122.56
26	1	302	CHL	O2D-CGD-O1D	-3.17	117.63	123.84
17	A	801	CLA	C1-C2-C3	-3.17	120.56	126.04
17	3	303	CLA	C1-C2-C3	-3.17	121.62	126.75
17	b	831	CLA	C3B-C4B-NB	3.17	113.31	109.21
17	4	602	CLA	C1D-CHD-C4C	-3.17	118.37	122.56
20	b	844	BCR	C8-C9-C10	3.17	123.81	118.94
17	a	805	CLA	C1-C2-C3	-3.17	120.56	126.04
26	2	605	CHL	C3B-C4B-NB	3.17	113.31	109.21
17	a	820	CLA	C3B-C4B-NB	3.17	113.31	109.21
17	K	4003	CLA	C3B-C4B-NB	3.17	113.31	109.21
17	b	818	CLA	C1D-CHD-C4C	-3.17	118.38	122.56
17	A	801	CLA	C3B-C4B-NB	3.17	113.31	109.21
17	B	804	CLA	C3B-C4B-NB	3.17	113.31	109.21
17	g	102	CLA	C3B-C4B-NB	3.17	113.31	109.21
17	b	809	CLA	C3B-C4B-NB	3.17	113.31	109.21
26	7	607	CHL	C3B-C4B-NB	3.17	113.30	109.21
17	b	835	CLA	C3B-C4B-NB	3.17	113.30	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	827	CLA	C1-C2-C3	-3.17	120.57	126.04
27	2	615	LUT	C15-C14-C13	-3.17	122.79	127.31
17	a	805	CLA	C3B-C4B-NB	3.16	113.30	109.21
17	B	833	CLA	C3B-C4B-NB	3.16	113.30	109.21
17	b	819	CLA	CHC-C1C-C2C	-3.16	117.97	126.72
17	3	302	CLA	CAC-C3C-C4C	3.16	128.91	124.81
17	K	4002	CLA	C3B-C4B-NB	3.16	113.30	109.21
17	a	846	CLA	C3B-C4B-NB	3.16	113.30	109.21
17	b	829	CLA	CHC-C1C-C2C	-3.16	117.97	126.72
17	a	856	CLA	C4D-C3D-CAD	-3.16	106.71	108.47
17	A	817	CLA	C3B-C4B-NB	3.16	113.30	109.21
17	A	839	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
17	b	816	CLA	CAC-C3C-C4C	3.16	128.91	124.81
17	a	810	CLA	C3B-C4B-NB	3.16	113.29	109.21
17	4	613	CLA	C3B-C4B-NB	3.16	113.29	109.21
17	B	826	CLA	C4C-C3C-C2C	-3.16	102.30	106.90
17	b	836	CLA	CMB-C2B-C3B	3.16	130.58	124.68
17	a	802	CLA	C1D-CHD-C4C	-3.16	118.39	122.56
17	1	310	CLA	C3B-C4B-NB	3.16	113.29	109.21
17	a	813	CLA	CAC-C3C-C4C	3.16	128.90	124.81
17	2	613	CLA	C3B-C4B-NB	3.16	113.29	109.21
17	B	822	CLA	C3B-C4B-NB	3.16	113.29	109.21
17	A	809	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
17	6	304	CLA	C3C-C4C-NC	3.15	114.11	110.57
17	1	308	CLA	C3B-C4B-NB	3.15	113.29	109.21
17	8	303	CLA	CAC-C3C-C4C	3.15	128.90	124.81
17	A	812	CLA	C3B-C4B-NB	3.15	113.29	109.21
20	F	305	BCR	C38-C26-C25	-3.15	120.99	124.53
17	b	812	CLA	C3B-C4B-NB	3.15	113.28	109.21
17	a	803	CLA	CHC-C1C-C2C	-3.15	118.01	126.72
17	a	839	CLA	C1-C2-C3	-3.15	120.59	126.04
17	a	826	CLA	C1-C2-C3	-3.15	120.59	126.04
17	3	305	CLA	C3B-C4B-NB	3.15	113.28	109.21
17	j	3002	CLA	C3B-C4B-NB	3.15	113.28	109.21
17	B	841	CLA	CHD-C4C-NC	3.15	129.17	124.20
17	A	827	CLA	C1D-CHD-C4C	-3.15	118.40	122.56
17	B	819	CLA	CHC-C1C-C2C	-3.15	118.01	126.72
17	3	312	CLA	CAC-C3C-C4C	3.15	128.90	124.81
17	a	836	CLA	C3B-C4B-NB	3.15	113.28	109.21
17	G	103	CLA	C1-C2-C3	-3.15	121.66	126.75
17	1	310	CLA	O2A-CGA-CBA	3.15	121.78	111.91
17	A	822	CLA	CAC-C3C-C4C	3.15	128.89	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	820	CLA	C3B-C4B-NB	3.15	113.28	109.21
17	b	834	CLA	C3B-C4B-NB	3.14	113.28	109.21
17	6	306	CLA	C3B-C4B-NB	3.14	113.28	109.21
20	3	318	BCR	C7-C8-C9	-3.14	121.48	126.23
17	a	831	CLA	C3B-C4B-NB	3.14	113.27	109.21
26	6	303	CHL	C3B-C4B-NB	3.14	113.27	109.21
20	f	7004	BCR	C16-C17-C18	-3.14	122.83	127.31
17	A	854	CLA	CMB-C2B-C3B	3.14	130.56	124.68
17	B	813	CLA	C1C-C2C-C3C	-3.14	103.66	106.96
17	a	844	CLA	C4-C3-C5	3.14	120.55	115.27
17	B	814	CLA	C1C-C2C-C3C	-3.14	103.66	106.96
17	B	826	CLA	CHD-C4C-NC	3.14	129.15	124.20
17	B	808	CLA	C3B-C4B-NB	3.14	113.27	109.21
17	A	826	CLA	C4-C3-C5	3.14	120.55	115.27
17	a	817	CLA	CHC-C1C-C2C	-3.14	118.05	126.72
26	9	605	CHL	C3B-C4B-NB	3.14	113.27	109.21
17	6	314	CLA	C3B-C4B-NB	3.14	113.27	109.21
17	a	831	CLA	CAC-C3C-C4C	3.14	128.88	124.81
17	k	1403	CLA	CAC-C3C-C4C	3.14	128.88	124.81
17	b	828	CLA	C3B-C4B-NB	3.14	113.26	109.21
17	B	840	CLA	C3B-C4B-NB	3.13	113.26	109.21
17	9	602	CLA	O2A-CGA-CBA	3.13	121.74	111.91
17	6	314	CLA	CAC-C3C-C4C	3.13	128.88	124.81
17	A	834	CLA	CHC-C1C-C2C	-3.13	118.05	126.72
17	A	836	CLA	CHC-C1C-C2C	-3.13	118.05	126.72
17	b	813	CLA	C3B-C4B-NB	3.13	113.26	109.21
17	A	805	CLA	C3B-C4B-NB	3.13	113.26	109.21
17	A	818	CLA	C3B-C4B-NB	3.13	113.26	109.21
17	B	839	CLA	C3B-C4B-NB	3.13	113.26	109.21
17	B	808	CLA	O2A-CGA-CBA	3.13	121.73	111.91
20	F	305	BCR	C16-C17-C18	-3.13	122.84	127.31
17	B	832	CLA	CAC-C3C-C4C	3.13	128.87	124.81
20	9	618	BCR	C38-C26-C25	-3.13	121.01	124.53
17	8	305	CLA	C3B-C4B-NB	3.13	113.26	109.21
17	8	302	CLA	CAC-C3C-C4C	3.13	128.87	124.81
17	A	845	CLA	C3B-C4B-NB	3.13	113.25	109.21
17	A	842	CLA	C3B-C4B-NB	3.13	113.25	109.21
17	3	301	CLA	C1D-CHD-C4C	-3.13	118.43	122.56
17	a	820	CLA	CAC-C3C-C4C	3.13	128.87	124.81
17	6	306	CLA	C1-C2-C3	-3.13	120.63	126.04
17	B	805	CLA	C3B-C4B-NB	3.13	113.25	109.21
20	b	846	BCR	C16-C17-C18	-3.13	122.85	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	818	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
17	B	805	CLA	C4-C3-C5	3.13	120.53	115.27
17	b	804	CLA	C3B-C4B-NB	3.13	113.25	109.21
17	7	613	CLA	C3B-C4B-NB	3.13	113.25	109.21
17	1	311	CLA	C3B-C4B-NB	3.13	113.25	109.21
17	4	604	CLA	C3B-C4B-NB	3.12	113.25	109.21
17	G	103	CLA	C3B-C4B-NB	3.12	113.25	109.21
17	b	813	CLA	C1C-C2C-C3C	-3.12	103.67	106.96
17	A	821	CLA	CHC-C1C-C2C	-3.12	118.08	126.72
17	9	610	CLA	C3B-C4B-NB	3.12	113.25	109.21
17	6	311	CLA	O2A-CGA-CBA	3.12	121.70	111.91
17	9	602	CLA	C1-C2-C3	-3.12	120.65	126.04
17	A	835	CLA	CAC-C3C-C4C	3.12	128.86	124.81
17	A	836	CLA	C3B-C4B-NB	3.12	113.24	109.21
17	F	303	CLA	C3B-C4B-NB	3.12	113.24	109.21
26	2	601	CHL	O2D-CGD-O1D	-3.12	117.74	123.84
17	B	833	CLA	C4-C3-C5	3.12	120.51	115.27
26	9	615	CHL	C2A-C1A-CHA	-3.12	118.41	123.86
17	7	602	CLA	CAC-C3C-C4C	3.12	128.85	124.81
17	3	314	CLA	C3B-C4B-NB	3.11	113.24	109.21
17	b	822	CLA	C1-C2-C3	-3.11	120.66	126.04
27	9	616	LUT	C15-C14-C13	-3.11	122.87	127.31
27	6	317	LUT	C18-C5-C6	-3.11	121.03	124.53
17	B	809	CLA	C3B-C4B-NB	3.11	113.23	109.21
17	a	846	CLA	C1-C2-C3	-3.11	120.66	126.04
17	B	813	CLA	C1-C2-C3	-3.11	120.66	126.04
17	b	804	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
17	6	309	CLA	C3B-C4B-NB	3.11	113.23	109.21
26	8	306	CHL	C3B-C4B-NB	3.11	113.23	109.21
17	B	828	CLA	O2A-CGA-CBA	3.11	121.66	111.91
17	a	819	CLA	CAC-C3C-C4C	3.11	128.84	124.81
26	4	606	CHL	CAC-C3C-C4C	3.11	128.84	124.81
17	1	304	CLA	CAC-C3C-C4C	3.11	128.84	124.81
17	b	807	CLA	C3B-C4B-NB	3.11	113.22	109.21
17	8	307	CLA	C1-C2-C3	-3.10	121.73	126.75
17	b	832	CLA	CAC-C3C-C4C	3.10	128.84	124.81
17	a	802	CLA	O2A-CGA-CBA	3.10	121.65	111.91
20	a	852	BCR	C20-C21-C22	-3.10	122.88	127.31
17	4	603	CLA	CHD-C4C-NC	3.10	129.09	124.20
28	2	616	XAT	C35-C34-C33	-3.10	122.88	127.31
17	b	821	CLA	C3B-C4B-NB	3.10	113.22	109.21
17	f	7003	CLA	C3B-C4B-NB	3.10	113.22	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	828	CLA	C1-C2-C3	-3.10	120.68	126.04
17	b	822	CLA	CHD-C4C-NC	3.10	129.09	124.20
17	b	828	CLA	CHD-C4C-NC	3.10	129.09	124.20
17	3	311	CLA	C3B-C4B-NB	3.10	113.22	109.21
17	B	829	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
20	B	843	BCR	C24-C23-C22	-3.10	121.55	126.23
20	9	618	BCR	C21-C20-C19	-3.10	113.54	123.22
17	a	825	CLA	C3B-C4B-NB	3.10	113.22	109.21
17	4	608	CLA	C3B-C4B-NB	3.10	113.22	109.21
17	b	802	CLA	O2A-CGA-CBA	3.10	121.64	111.91
17	9	608	CLA	C3B-C4B-NB	3.10	113.22	109.21
17	A	835	CLA	C3B-C4B-NB	3.10	113.22	109.21
17	6	305	CLA	CAC-C3C-C4C	3.10	128.83	124.81
17	b	817	CLA	C3B-C4B-NB	3.10	113.22	109.21
17	b	805	CLA	CHC-C1C-C2C	-3.10	118.15	126.72
17	A	834	CLA	C4-C3-C5	3.10	120.48	115.27
17	b	808	CLA	CBC-CAC-C3C	-3.10	103.89	112.43
17	a	856	CLA	CHC-C1C-C2C	-3.10	118.16	126.72
17	A	802	CLA	CMB-C2B-C3B	3.10	130.47	124.68
17	2	612	CLA	CAC-C3C-C4C	3.10	128.83	124.81
17	b	824	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
20	1	318	BCR	C21-C20-C19	-3.09	113.56	123.22
17	8	303	CLA	C3B-C4B-NB	3.09	113.21	109.21
20	a	852	BCR	C38-C26-C25	-3.09	121.05	124.53
17	A	833	CLA	CHD-C4C-NC	3.09	129.08	124.20
17	8	303	CLA	C1D-CHD-C4C	-3.09	118.48	122.56
17	A	831	CLA	CHC-C1C-C2C	-3.09	118.17	126.72
17	7	604	CLA	C3B-C4B-NB	3.09	113.21	109.21
17	B	836	CLA	CHD-C4C-NC	3.09	129.07	124.20
17	9	609	CLA	O2A-CGA-CBA	3.09	121.61	111.91
17	A	829	CLA	C3B-C4B-NB	3.09	113.20	109.21
17	8	308	CLA	CAC-C3C-C4C	3.09	128.82	124.81
17	B	828	CLA	C3B-C4B-NB	3.09	113.20	109.21
17	j	3002	CLA	CAC-C3C-C4C	3.09	128.82	124.81
19	A	847	LHG	O8-C23-C24	3.09	119.48	111.38
26	2	614	CHL	CAC-C3C-C4C	3.09	128.82	124.81
17	a	832	CLA	CAC-C3C-C4C	3.09	128.82	124.81
17	4	614	CLA	C3B-C4B-NB	3.09	113.20	109.21
17	J	3002	CLA	C3B-C4B-NB	3.09	113.20	109.21
17	a	813	CLA	CHC-C1C-C2C	-3.09	118.18	126.72
17	2	604	CLA	C3B-C4B-NB	3.09	113.20	109.21
17	b	805	CLA	C1D-CHD-C4C	-3.09	118.49	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	802	CLA	C1-C2-C3	-3.09	120.71	126.04
17	6	307	CLA	C3B-C4B-NB	3.08	113.20	109.21
17	9	604	CLA	C3B-C4B-NB	3.08	113.20	109.21
17	a	835	CLA	C3B-C4B-NB	3.08	113.20	109.21
17	a	844	CLA	C3B-C4B-NB	3.08	113.20	109.21
26	4	615	CHL	C3B-C4B-NB	3.08	113.19	109.21
20	2	617	BCR	C11-C10-C9	-3.08	122.91	127.31
26	6	303	CHL	O2D-CGD-O1D	-3.08	117.81	123.84
17	A	813	CLA	C3B-C4B-NB	3.08	113.19	109.21
17	B	837	CLA	CHD-C4C-NC	3.08	129.06	124.20
17	k	1402	CLA	CHC-C1C-C2C	-3.08	118.20	126.72
17	F	301	CLA	O2A-CGA-CBA	3.08	121.57	111.91
17	G	104	CLA	C3B-C4B-NB	3.08	113.19	109.21
17	1	304	CLA	CHC-C1C-C2C	-3.08	118.20	126.72
20	j	3003	BCR	C15-C14-C13	-3.08	122.92	127.31
17	b	819	CLA	CAC-C3C-C4C	3.08	128.80	124.81
17	b	830	CLA	C3B-C4B-NB	3.08	113.19	109.21
17	b	836	CLA	CAC-C3C-C4C	3.08	128.80	124.81
17	A	803	CLA	C3B-C4B-NB	3.08	113.19	109.21
28	2	616	XAT	C10-C11-C12	-3.08	113.62	123.22
17	B	824	CLA	C4-C3-C5	3.08	120.44	115.27
17	J	3002	CLA	CHC-C1C-C2C	-3.08	118.21	126.72
17	6	304	CLA	C3B-C4B-NB	3.07	113.18	109.21
17	b	820	CLA	C3B-C4B-NB	3.07	113.18	109.21
17	b	821	CLA	CHC-C1C-C2C	-3.07	118.22	126.72
17	A	835	CLA	CHC-C1C-C2C	-3.07	118.22	126.72
28	4	617	XAT	C24-C23-C22	-3.07	104.84	110.77
17	A	819	CLA	CHD-C4C-NC	3.07	129.04	124.20
17	7	609	CLA	O2A-CGA-CBA	3.07	121.55	111.91
17	k	1401	CLA	C3B-C4B-NB	3.07	113.18	109.21
20	j	3003	BCR	C24-C23-C22	-3.07	121.59	126.23
17	B	809	CLA	CHC-C1C-C2C	-3.07	118.23	126.72
17	8	304	CLA	C3B-C4B-NB	3.07	113.18	109.21
17	f	7002	CLA	CHD-C4C-NC	3.07	129.04	124.20
17	A	803	CLA	C4D-C3D-CAD	-3.07	106.76	108.47
17	6	312	CLA	C3B-C4B-NB	3.07	113.18	109.21
17	4	609	CLA	CHD-C4C-NC	3.07	129.04	124.20
17	1	306	CLA	C1C-C2C-C3C	-3.07	103.73	106.96
17	B	810	CLA	C3B-C4B-NB	3.07	113.18	109.21
17	b	838	CLA	CMB-C2B-C3B	3.07	130.42	124.68
17	B	821	CLA	CAC-C3C-C4C	3.07	128.79	124.81
17	a	805	CLA	CHD-C4C-NC	3.07	129.04	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	2	601	CHL	C3B-C4B-NB	3.07	113.18	109.21
17	2	608	CLA	CHC-C1C-C2C	-3.07	118.24	126.72
17	B	813	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
17	A	831	CLA	C4-C3-C5	3.07	120.43	115.27
17	a	817	CLA	CAC-C3C-C4C	3.07	128.79	124.81
17	3	310	CLA	CAC-C3C-C4C	3.07	128.79	124.81
17	A	801	CLA	O2A-CGA-CBA	3.07	121.53	111.91
17	A	825	CLA	CAC-C3C-C4C	3.07	128.79	124.81
17	b	814	CLA	CHD-C4C-NC	3.07	129.03	124.20
17	b	805	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
17	3	304	CLA	C3B-C4B-NB	3.06	113.17	109.21
17	B	806	CLA	CHD-C4C-NC	3.06	129.03	124.20
17	1	309	CLA	CHC-C1C-C2C	-3.06	118.25	126.72
17	4	604	CLA	CHC-C1C-C2C	-3.06	118.25	126.72
17	A	837	CLA	CAC-C3C-C4C	3.06	128.78	124.81
26	7	605	CHL	C3B-C4B-NB	3.06	113.17	109.21
17	6	313	CLA	C4-C3-C5	3.06	120.42	115.27
17	7	609	CLA	CAC-C3C-C4C	3.06	128.78	124.81
17	4	612	CLA	CHC-C1C-C2C	-3.06	118.25	126.72
17	a	810	CLA	C1-C2-C3	-3.06	120.75	126.04
17	B	802	CLA	O2A-CGA-CBA	3.06	121.51	111.91
17	B	834	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
20	7	617	BCR	C7-C8-C9	-3.06	121.61	126.23
20	b	846	BCR	C33-C5-C6	-3.06	121.09	124.53
17	9	611	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
17	A	832	CLA	C3B-C4B-NB	3.06	113.16	109.21
17	b	821	CLA	CAC-C3C-C4C	3.06	128.78	124.81
17	a	821	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
17	B	808	CLA	C1-C2-C3	-3.06	120.75	126.04
17	A	837	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
17	B	814	CLA	CHD-C4C-NC	3.06	129.02	124.20
17	B	808	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
20	L	201	BCR	C20-C21-C22	-3.06	122.95	127.31
17	A	832	CLA	CHC-C1C-C2C	-3.06	118.27	126.72
17	a	828	CLA	CHD-C4C-NC	3.06	129.02	124.20
17	b	839	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
18	a	845	PQN	C14-C13-C15	3.06	120.41	115.27
17	b	815	CLA	C3B-C4B-NB	3.06	113.16	109.21
17	a	813	CLA	C3B-C4B-NB	3.06	113.16	109.21
17	A	824	CLA	CAC-C3C-C4C	3.06	128.78	124.81
17	a	804	CLA	C1D-CHD-C4C	-3.06	118.53	122.56
17	A	817	CLA	CHC-C1C-C2C	-3.06	118.27	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	319	LHG	O8-C23-C24	3.06	119.39	111.38
17	a	822	CLA	C3B-C4B-NB	3.05	113.16	109.21
17	A	838	CLA	C4-C3-C5	3.05	119.47	115.98
17	1	306	CLA	CAC-C3C-C4C	3.05	128.77	124.81
17	B	831	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
17	6	305	CLA	CHC-C1C-C2C	-3.05	118.27	126.72
17	7	604	CLA	CHC-C1C-C2C	-3.05	118.28	126.72
17	a	856	CLA	O2A-CGA-CBA	3.05	121.49	111.91
20	6	319	BCR	C38-C26-C25	-3.05	121.10	124.53
17	A	814	CLA	C3B-C4B-NB	3.05	113.16	109.21
17	b	810	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
17	8	313	CLA	C2C-C1C-CHC	-3.05	118.36	125.67
17	A	811	CLA	CHC-C1C-C2C	-3.05	118.28	126.72
17	a	836	CLA	CHC-C1C-C2C	-3.05	118.28	126.72
17	f	7002	CLA	C3B-C4B-NB	3.05	113.15	109.21
17	b	808	CLA	O2A-CGA-O1A	-3.05	115.89	123.59
17	B	841	CLA	CMC-C2C-C1C	3.05	129.68	125.04
20	f	7004	BCR	C38-C26-C25	-3.05	121.10	124.53
17	9	612	CLA	CHC-C1C-C2C	-3.05	118.29	126.72
17	K	4003	CLA	CHC-C1C-C2C	-3.05	118.29	126.72
17	b	826	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
17	b	841	CLA	CAC-C3C-C4C	3.05	128.76	124.81
17	3	305	CLA	CHC-C1C-C2C	-3.05	118.30	126.72
17	9	609	CLA	CAC-C3C-C4C	3.05	128.76	124.81
17	A	814	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
17	4	609	CLA	O2A-CGA-CBA	3.05	121.47	111.91
17	b	831	CLA	CHC-C1C-C2C	-3.05	118.30	126.72
17	2	603	CLA	C4-C3-C5	3.05	120.39	115.27
17	B	826	CLA	C1-C2-C3	-3.04	120.78	126.04
17	7	612	CLA	CHC-C1C-C2C	-3.04	118.31	126.72
17	b	805	CLA	O2A-CGA-CBA	3.04	121.45	111.91
20	A	850	BCR	C20-C21-C22	-3.04	122.97	127.31
17	3	313	CLA	CHC-C1C-C2C	-3.04	118.31	126.72
17	1	202	CLA	CHC-C1C-C2C	-3.04	118.31	126.72
17	3	312	CLA	CHC-C1C-C2C	-3.04	118.31	126.72
17	1	306	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
17	a	832	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
17	2	609	CLA	O2A-CGA-CBA	3.04	121.45	111.91
17	B	813	CLA	C3B-C4B-NB	3.04	113.14	109.21
17	1	310	CLA	CAC-C3C-C4C	3.04	128.75	124.81
17	b	823	CLA	C1-C2-C3	-3.04	120.79	126.04
17	B	823	CLA	C4C-C3C-C2C	-3.04	102.47	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	834	CLA	C3B-C4B-NB	3.04	113.14	109.21
17	a	836	CLA	C1-C2-C3	-3.04	121.84	126.75
17	2	613	CLA	CAC-C3C-C4C	3.04	128.75	124.81
20	A	849	BCR	C24-C23-C22	-3.04	121.65	126.23
17	9	601	CLA	CHC-C1C-C2C	-3.04	118.32	126.72
17	b	840	CLA	CHD-C4C-NC	3.04	128.99	124.20
17	A	841	CLA	O2A-CGA-CBA	3.04	121.44	111.91
17	B	808	CLA	CHC-C1C-C2C	-3.04	118.32	126.72
20	a	853	BCR	C38-C26-C27	3.04	119.45	113.62
17	A	805	CLA	CHD-C4C-NC	3.04	128.99	124.20
17	a	842	CLA	O2A-CGA-CBA	3.03	121.43	111.91
17	b	810	CLA	C3B-C4B-NB	3.03	113.13	109.21
17	3	315	CLA	C2C-C1C-CHC	-3.03	118.41	125.67
17	3	302	CLA	O2A-CGA-CBA	3.03	121.43	111.91
20	8	316	BCR	C23-C24-C25	-3.03	118.68	127.20
17	3	308	CLA	C3B-C4B-NB	3.03	113.13	109.21
17	4	610	CLA	C3B-C4B-NB	3.03	113.13	109.21
17	B	826	CLA	O2A-CGA-CBA	3.03	121.42	111.91
17	B	810	CLA	O2A-CGA-CBA	3.03	121.42	111.91
17	b	817	CLA	C4-C3-C5	3.03	120.37	115.27
20	i	101	BCR	C15-C16-C17	-3.03	117.26	123.47
17	a	821	CLA	CHD-C4C-NC	3.03	128.98	124.20
17	a	834	CLA	C3B-C4B-NB	3.03	113.13	109.21
17	L	204	CLA	C3B-C4B-NB	3.03	113.13	109.21
17	g	102	CLA	CAC-C3C-C4C	3.03	128.74	124.81
17	1	313	CLA	CHC-C1C-C2C	-3.03	118.34	126.72
17	b	813	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
17	a	820	CLA	CHC-C1C-C2C	-3.03	118.34	126.72
17	B	812	CLA	C3B-C4B-NB	3.03	113.13	109.21
17	3	311	CLA	C1-C2-C3	-3.03	120.80	126.04
17	1	204	CLA	C3B-C4B-NB	3.03	113.13	109.21
17	3	303	CLA	CAC-C3C-C4C	3.03	128.74	124.81
17	9	602	CLA	CAC-C3C-C4C	3.03	128.74	124.81
17	6	313	CLA	CHC-C1C-C2C	-3.03	118.34	126.72
27	9	616	LUT	C10-C11-C12	-3.03	113.76	123.22
17	A	808	CLA	C4-C3-C5	3.03	120.37	115.27
17	8	310	CLA	CAC-C3C-C4C	3.03	128.74	124.81
20	L	201	BCR	C16-C17-C18	-3.03	122.99	127.31
17	B	817	CLA	CAC-C3C-C4C	3.03	128.74	124.81
17	a	844	CLA	CBC-CAC-C3C	-3.03	104.08	112.43
17	B	819	CLA	CAC-C3C-C4C	3.03	128.74	124.81
17	b	833	CLA	CAC-C3C-C4C	3.03	128.74	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	818	CLA	CHC-C1C-C2C	-3.03	118.35	126.72
17	4	613	CLA	CHC-C1C-C2C	-3.03	118.35	126.72
17	3	310	CLA	CHC-C1C-C2C	-3.03	118.35	126.72
17	k	1403	CLA	CHC-C1C-C2C	-3.03	118.35	126.72
17	b	808	CLA	CHC-C1C-C2C	-3.03	118.35	126.72
26	4	606	CHL	C3B-C4B-NB	3.03	113.12	109.21
17	a	832	CLA	C3B-C4B-NB	3.03	113.12	109.21
17	9	602	CLA	CHD-C4C-NC	3.03	128.97	124.20
17	A	842	CLA	CAC-C3C-C4C	3.02	128.73	124.81
17	a	818	CLA	CHC-C1C-C2C	-3.02	118.36	126.72
17	4	603	CLA	CAC-C3C-C4C	3.02	128.73	124.81
17	B	817	CLA	O2A-CGA-CBA	3.02	121.39	111.91
17	b	817	CLA	CHC-C1C-C2C	-3.02	118.36	126.72
17	6	304	CLA	CHC-C1C-C2C	-3.02	118.36	126.72
17	A	843	CLA	CHC-C1C-C2C	-3.02	118.36	126.72
17	A	841	CLA	CHD-C4C-NC	3.02	128.96	124.20
28	2	616	XAT	C15-C14-C13	-3.02	123.00	127.31
17	b	837	CLA	O2A-CGA-CBA	3.02	121.39	111.91
17	b	815	CLA	CAC-C3C-C4C	3.02	128.73	124.81
17	8	310	CLA	CHC-C1C-C2C	-3.02	118.37	126.72
17	6	306	CLA	CHC-C1C-C2C	-3.02	118.38	126.72
17	A	810	CLA	C4-C3-C5	3.02	120.35	115.27
17	a	837	CLA	CHC-C1C-C2C	-3.02	118.38	126.72
20	B	801	BCR	C33-C5-C6	-3.02	121.14	124.53
20	b	847	BCR	C21-C20-C19	-3.02	113.81	123.22
17	3	303	CLA	CHC-C1C-C2C	-3.02	118.38	126.72
17	3	315	CLA	C1D-CHD-C4C	-3.02	118.64	126.10
17	7	610	CLA	CHC-C1C-C2C	-3.01	118.38	126.72
17	7	611	CLA	CHC-C1C-C2C	-3.01	118.38	126.72
17	8	313	CLA	C1D-CHD-C4C	-3.01	118.64	126.10
17	B	821	CLA	C3B-C4B-NB	3.01	113.11	109.21
17	2	603	CLA	C3B-C4B-NB	3.01	113.11	109.21
20	L	201	BCR	C24-C23-C22	-3.01	121.68	126.23
17	A	824	CLA	CHC-C1C-C2C	-3.01	118.39	126.72
17	B	803	CLA	C1-C2-C3	-3.01	120.83	126.04
17	a	841	CLA	C3B-C4B-NB	3.01	113.10	109.21
17	6	312	CLA	CHC-C1C-C2C	-3.01	118.39	126.72
17	B	839	CLA	CAC-C3C-C4C	3.01	128.72	124.81
17	A	801	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
17	a	811	CLA	CHC-C1C-C2C	-3.01	118.40	126.72
17	b	816	CLA	C4-C3-C5	3.01	120.33	115.27
17	b	822	CLA	C3B-C4B-NB	3.01	113.10	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	827	CLA	CAA-C2A-C3A	-3.01	104.54	112.78
17	9	608	CLA	CHC-C1C-C2C	-3.01	118.40	126.72
17	2	604	CLA	CHC-C1C-C2C	-3.01	118.40	126.72
17	2	602	CLA	C3B-C4B-NB	3.01	113.10	109.21
17	B	807	CLA	CAC-C3C-C4C	3.01	128.71	124.81
17	A	814	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
28	3	317	XAT	C38-C25-C24	3.01	117.66	114.28
17	B	831	CLA	CHC-C1C-C2C	-3.01	118.40	126.72
17	a	808	CLA	CHD-C4C-NC	3.01	128.94	124.20
17	4	603	CLA	CBC-CAC-C3C	-3.01	104.14	112.43
17	8	309	CLA	CHC-C1C-C2C	-3.01	118.40	126.72
17	a	818	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
17	a	856	CLA	CAA-C2A-C3A	-3.01	104.54	112.78
20	L	206	BCR	C33-C5-C6	-3.01	121.15	124.53
20	A	852	BCR	C20-C19-C18	-3.01	117.97	126.42
17	8	311	CLA	CHC-C1C-C2C	-3.01	118.41	126.72
17	b	815	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
17	8	301	CLA	CAC-C3C-C4C	3.01	128.71	124.81
17	a	812	CLA	C3B-C4B-NB	3.01	113.09	109.21
17	a	840	CLA	CHC-C1C-C2C	-3.00	118.41	126.72
17	4	613	CLA	CAC-C3C-C4C	3.00	128.71	124.81
17	1	312	CLA	C4-C3-C5	3.00	120.32	115.27
17	A	845	CLA	CHC-C1C-C2C	-3.00	118.41	126.72
17	b	809	CLA	CHC-C1C-C2C	-3.00	118.42	126.72
17	b	835	CLA	CHC-C1C-C2C	-3.00	118.42	126.72
17	b	834	CLA	CHC-C1C-C2C	-3.00	118.42	126.72
17	2	610	CLA	CAC-C3C-C4C	3.00	128.70	124.81
17	A	822	CLA	C3B-C4B-NB	3.00	113.09	109.21
17	b	837	CLA	C3B-C4B-NB	3.00	113.09	109.21
17	A	822	CLA	CHC-C1C-C2C	-3.00	118.42	126.72
17	B	814	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
17	4	611	CLA	CHC-C1C-C2C	-3.00	118.42	126.72
17	a	807	CLA	C1-C2-C3	-3.00	120.86	126.04
17	1	313	CLA	CAC-C3C-C4C	3.00	128.70	124.81
17	L	202	CLA	CHC-C1C-C2C	-3.00	118.42	126.72
17	2	610	CLA	CHC-C1C-C2C	-3.00	118.42	126.72
17	9	612	CLA	CAC-C3C-C4C	3.00	128.70	124.81
17	B	825	CLA	C3B-C4B-NB	3.00	113.09	109.21
17	B	835	CLA	C3B-C4B-NB	3.00	113.09	109.21
26	1	302	CHL	C3B-C4B-NB	3.00	113.09	109.21
17	2	612	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
17	9	611	CLA	O2A-CGA-CBA	3.00	121.32	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	807	CLA	O2A-CGA-CBA	3.00	121.32	111.91
17	J	3002	CLA	CAC-C3C-C4C	3.00	128.70	124.81
17	9	613	CLA	CAC-C3C-C4C	3.00	128.70	124.81
17	b	840	CLA	O2A-CGA-CBA	3.00	121.31	111.91
17	1	315	CLA	CAC-C3C-C4C	3.00	128.70	124.81
17	b	810	CLA	CAC-C3C-C4C	3.00	128.70	124.81
17	8	305	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
27	3	316	LUT	C15-C14-C13	-3.00	123.03	127.31
17	A	820	CLA	CHD-C4C-NC	3.00	128.93	124.20
17	a	839	CLA	C3B-C4B-NB	3.00	113.08	109.21
17	9	614	CLA	CHC-C1C-C2C	-3.00	118.44	126.72
28	1	317	XAT	C35-C15-C14	-3.00	117.34	123.47
17	B	802	CLA	CHD-C4C-NC	3.00	128.92	124.20
17	A	816	CLA	C3B-C4B-NB	2.99	113.08	109.21
17	b	825	CLA	C3B-C4B-NB	2.99	113.08	109.21
17	B	820	CLA	CHC-C1C-C2C	-2.99	118.44	126.72
17	k	1402	CLA	CAC-C3C-C4C	2.99	128.69	124.81
17	7	613	CLA	CHC-C1C-C2C	-2.99	118.44	126.72
17	3	304	CLA	CHC-C1C-C2C	-2.99	118.44	126.72
17	a	831	CLA	C4C-C3C-C2C	-2.99	102.53	106.90
17	1	314	CLA	CHC-C1C-C2C	-2.99	118.44	126.72
17	B	815	CLA	C3B-C4B-NB	2.99	113.08	109.21
17	a	843	CLA	C3B-C4B-NB	2.99	113.08	109.21
17	B	817	CLA	C3B-C4B-NB	2.99	113.08	109.21
17	b	841	CLA	C3B-C4B-NB	2.99	113.08	109.21
17	b	832	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
17	A	827	CLA	CAA-C2A-C3A	-2.99	104.59	112.78
17	3	314	CLA	CAC-C3C-C4C	2.99	128.69	124.81
17	7	613	CLA	CAC-C3C-C4C	2.99	128.69	124.81
17	1	306	CLA	C3B-C4B-NB	2.99	113.08	109.21
17	B	818	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
17	6	315	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
17	B	831	CLA	C3B-C4B-NB	2.99	113.08	109.21
17	6	315	CLA	CAC-C3C-C4C	2.99	128.69	124.81
17	b	817	CLA	O2A-CGA-CBA	2.99	121.29	111.91
17	B	833	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
17	A	818	CLA	CHD-C4C-NC	2.99	128.91	124.20
17	3	315	CLA	C2A-C3A-C4A	-2.99	99.49	104.18
17	B	803	CLA	CAC-C3C-C4C	2.99	128.69	124.81
17	b	841	CLA	CHD-C4C-NC	2.99	128.91	124.20
17	b	802	CLA	CHC-C1C-C2C	-2.99	118.46	126.72
17	F	301	CLA	C3B-C4B-NB	2.99	113.07	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	616	LUT	C11-C10-C9	-2.99	123.05	127.31
17	a	824	CLA	CHC-C1C-C2C	-2.99	118.46	126.72
17	B	824	CLA	CAC-C3C-C4C	2.99	128.69	124.81
17	a	843	CLA	CAC-C3C-C4C	2.99	128.69	124.81
17	b	802	CLA	CAA-C2A-C3A	-2.99	104.60	112.78
17	b	809	CLA	CBC-CAC-C3C	-2.99	104.20	112.43
17	a	842	CLA	C3B-C4B-NB	2.98	113.07	109.21
17	B	832	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
17	A	825	CLA	C1-C2-C3	-2.98	120.88	126.04
20	L	205	BCR	C3-C4-C5	-2.98	108.75	114.08
17	A	831	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
17	A	828	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
17	6	310	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
17	b	825	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
26	2	607	CHL	C3B-C4B-NB	2.98	113.07	109.21
20	A	856	BCR	C38-C26-C27	2.98	119.35	113.62
20	B	845	BCR	C38-C26-C25	-2.98	121.18	124.53
20	l	205	BCR	C23-C24-C25	-2.98	118.82	127.20
17	2	613	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
17	7	603	CLA	C3B-C4B-NB	2.98	113.07	109.21
18	B	842	PQN	C11-C12-C13	-2.98	121.83	126.79
17	8	303	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
17	A	839	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
26	1	302	CHL	C4-C3-C5	2.98	120.29	115.27
17	B	804	CLA	CAC-C3C-C4C	2.98	128.68	124.81
17	A	823	CLA	C3B-C4B-NB	2.98	113.06	109.21
17	a	835	CLA	CHD-C4C-NC	2.98	128.90	124.20
17	A	803	CLA	CHC-C1C-C2C	-2.98	118.48	126.72
17	a	856	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
17	b	841	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
20	2	617	BCR	C33-C5-C6	-2.98	121.18	124.53
17	a	826	CLA	C3B-C4B-NB	2.98	113.06	109.21
17	a	833	CLA	C4-C3-C5	2.98	120.28	115.27
17	7	608	CLA	C3B-C4B-NB	2.98	113.06	109.21
17	g	103	CLA	CHC-C1C-C2C	-2.98	118.48	126.72
17	a	834	CLA	CHD-C4C-NC	2.98	128.90	124.20
17	a	815	CLA	CHD-C4C-NC	2.98	128.90	124.20
17	B	825	CLA	CAC-C3C-C4C	2.98	128.67	124.81
17	f	7003	CLA	CHC-C1C-C2C	-2.98	118.48	126.72
17	9	613	CLA	CHC-C1C-C2C	-2.98	118.48	126.72
27	2	615	LUT	C11-C10-C9	-2.98	123.06	127.31
17	B	827	CLA	C4C-C3C-C2C	-2.98	102.56	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	847	BCR	C33-C5-C6	-2.98	121.18	124.53
17	A	808	CLA	CMB-C2B-C3B	2.98	130.25	124.68
17	1	312	CLA	CHC-C1C-C2C	-2.98	118.48	126.72
17	A	826	CLA	CAC-C3C-C4C	2.98	128.67	124.81
17	3	309	CLA	CHD-C4C-NC	2.98	128.89	124.20
26	4	615	CHL	CAC-C3C-C4C	2.98	128.67	124.81
17	a	818	CLA	CMB-C2B-C3B	2.98	130.25	124.68
17	A	840	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
20	G	105	BCR	C3-C4-C5	-2.98	108.76	114.08
17	F	303	CLA	CHC-C1C-C2C	-2.98	118.49	126.72
17	a	833	CLA	C1D-CHD-C4C	-2.97	118.63	122.56
17	b	811	CLA	CHD-C4C-NC	2.97	128.89	124.20
24	b	849	DGD	C2G-O2G-C1B	-2.97	110.47	117.79
17	b	803	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
17	6	307	CLA	CAC-C3C-C4C	2.97	128.67	124.81
17	B	805	CLA	CHC-C1C-C2C	-2.97	118.50	126.72
17	b	813	CLA	CHC-C1C-C2C	-2.97	118.50	126.72
17	B	807	CLA	O2A-CGA-CBA	2.97	121.23	111.91
17	9	609	CLA	C3B-C4B-NB	2.97	113.05	109.21
17	a	832	CLA	CHC-C1C-C2C	-2.97	118.50	126.72
17	B	805	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
17	A	809	CLA	CAC-C3C-C4C	2.97	128.66	124.81
17	a	813	CLA	C1-C2-C3	-2.97	120.91	126.04
17	a	843	CLA	CHD-C4C-NC	2.97	128.88	124.20
17	3	313	CLA	CAC-C3C-C4C	2.97	128.66	124.81
17	3	306	CLA	C3B-C4B-NB	2.97	113.05	109.21
17	b	808	CLA	CHD-C4C-NC	2.97	128.88	124.20
17	A	826	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
17	b	837	CLA	CHC-C1C-C2C	-2.97	118.51	126.72
17	b	838	CLA	CHD-C4C-NC	2.97	128.88	124.20
26	9	607	CHL	CAC-C3C-C4C	2.97	128.66	124.81
17	9	604	CLA	CHC-C1C-C2C	-2.97	118.51	126.72
17	A	854	CLA	O2A-CGA-CBA	2.97	121.22	111.91
17	a	805	CLA	CHC-C1C-C2C	-2.97	118.52	126.72
17	3	301	CLA	CHC-C1C-C2C	-2.97	118.52	126.72
17	B	811	CLA	CHC-C1C-C2C	-2.97	118.52	126.72
28	9	617	XAT	C18-C5-C4	2.97	117.62	114.28
27	9	616	LUT	C31-C30-C29	-2.97	123.08	127.31
17	1	315	CLA	CHC-C1C-C2C	-2.97	118.52	126.72
17	A	820	CLA	CHC-C1C-C2C	-2.96	118.52	126.72
17	a	814	CLA	CAC-C3C-C4C	2.96	128.66	124.81
17	7	604	CLA	CAC-C3C-C4C	2.96	128.66	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	849	BCR	C20-C21-C22	-2.96	123.08	127.31
17	b	828	CLA	O2A-CGA-CBA	2.96	121.21	111.91
17	F	304	CLA	C3B-C4B-NB	2.96	113.04	109.21
20	9	618	BCR	C33-C5-C6	-2.96	121.20	124.53
17	B	826	CLA	OBD-CAD-C3D	-2.96	123.06	127.98
17	j	3002	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
17	6	307	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
17	4	614	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
17	B	840	CLA	CHD-C4C-NC	2.96	128.87	124.20
17	B	838	CLA	CHD-C4C-NC	2.96	128.87	124.20
17	A	804	CLA	C3B-C4B-NB	2.96	113.04	109.21
17	a	808	CLA	C3B-C4B-NB	2.96	113.04	109.21
26	4	606	CHL	C1-C2-C3	-2.96	121.96	126.75
17	b	833	CLA	O2A-CGA-CBA	2.96	121.20	111.91
17	2	609	CLA	CAC-C3C-C4C	2.96	128.65	124.81
17	B	807	CLA	C3B-C4B-NB	2.96	113.04	109.21
17	a	833	CLA	CHD-C4C-NC	2.96	128.86	124.20
17	a	807	CLA	CHD-C4C-NC	2.96	128.86	124.20
17	1	305	CLA	CHC-C1C-C2C	-2.96	118.54	126.72
17	A	823	CLA	CHC-C1C-C2C	-2.96	118.54	126.72
17	A	811	CLA	CAC-C3C-C4C	2.96	128.65	124.81
17	6	306	CLA	CAC-C3C-C4C	2.96	128.65	124.81
17	B	827	CLA	C3B-C4B-NB	2.96	113.03	109.21
17	b	807	CLA	CHC-C1C-C2C	-2.96	118.54	126.72
17	B	821	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
17	b	825	CLA	O2A-CGA-CBA	2.96	121.18	111.91
17	6	316	CLA	CHC-C1C-C2C	-2.96	118.55	126.72
17	B	840	CLA	CHC-C1C-C2C	-2.96	118.55	126.72
17	3	305	CLA	CAC-C3C-C4C	2.95	128.64	124.81
17	a	823	CLA	CHD-C4C-NC	2.95	128.86	124.20
17	B	824	CLA	C4C-C3C-C2C	-2.95	102.59	106.90
17	a	808	CLA	C4-C3-C5	2.95	120.24	115.27
17	b	813	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
17	4	610	CLA	CAC-C3C-C4C	2.95	128.64	124.81
17	l	204	CLA	CHD-C4C-NC	2.95	128.86	124.20
17	a	830	CLA	O2A-CGA-CBA	2.95	121.18	111.91
17	a	801	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
17	A	854	CLA	CHC-C1C-C2C	-2.95	118.55	126.72
27	2	615	LUT	C7-C8-C9	-2.95	121.77	126.23
17	b	804	CLA	CHD-C4C-NC	2.95	128.86	124.20
17	6	310	CLA	C4-C3-C5	2.95	120.24	115.27
17	9	610	CLA	CHC-C1C-C2C	-2.95	118.55	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	856	CLA	CMB-C2B-C3B	2.95	130.20	124.68
17	b	818	CLA	C3B-C4B-NB	2.95	113.03	109.21
17	A	805	CLA	C1-C2-C3	-2.95	120.94	126.04
17	a	802	CLA	CMB-C2B-C3B	2.95	130.20	124.68
17	8	303	CLA	CHC-C1C-C2C	-2.95	118.56	126.72
17	B	821	CLA	CHC-C1C-C2C	-2.95	118.56	126.72
17	3	314	CLA	CHC-C1C-C2C	-2.95	118.56	126.72
17	1	308	CLA	CAC-C3C-C4C	2.95	128.64	124.81
17	2	603	CLA	CHC-C1C-C2C	-2.95	118.56	126.72
17	A	854	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
17	B	805	CLA	O2A-CGA-CBA	2.95	121.16	111.91
17	2	604	CLA	CAC-C3C-C4C	2.95	128.64	124.81
17	a	840	CLA	CAC-C3C-C4C	2.95	128.64	124.81
17	B	812	CLA	CHC-C1C-C2C	-2.95	118.56	126.72
17	1	314	CLA	O2A-CGA-CBA	2.95	121.16	111.91
17	A	813	CLA	CHC-C1C-C2C	-2.95	118.57	126.72
17	2	611	CLA	CHC-C1C-C2C	-2.95	118.57	126.72
28	7	616	XAT	C35-C34-C33	-2.95	123.10	127.31
17	b	825	CLA	C1-C2-C3	-2.95	120.94	126.04
17	B	814	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
17	4	602	CLA	C3B-C4B-NB	2.95	113.02	109.21
20	b	844	BCR	C33-C5-C6	-2.95	121.22	124.53
17	B	839	CLA	O2A-CGA-CBA	2.95	121.16	111.91
17	a	831	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
17	9	604	CLA	CHD-C4C-NC	2.95	128.84	124.20
17	B	810	CLA	CAC-C3C-C4C	2.95	128.63	124.81
17	B	832	CLA	C3B-C4B-NB	2.95	113.02	109.21
17	B	839	CLA	CHC-C1C-C2C	-2.95	118.57	126.72
17	8	308	CLA	CHD-C4C-NC	2.95	128.84	124.20
17	g	101	CLA	CHC-C1C-C2C	-2.95	118.58	126.72
17	8	304	CLA	CHC-C1C-C2C	-2.94	118.58	126.72
17	a	812	CLA	O2A-CGA-CBA	2.94	121.15	111.91
17	4	601	CLA	CHC-C1C-C2C	-2.94	118.58	126.72
17	B	841	CLA	C3B-C4B-NB	2.94	113.02	109.21
17	A	802	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
17	a	841	CLA	CAC-C3C-C4C	2.94	128.63	124.81
17	4	608	CLA	CAC-C3C-C4C	2.94	128.63	124.81
17	8	301	CLA	CHD-C4C-NC	2.94	128.84	124.20
17	8	302	CLA	CHC-C1C-C2C	-2.94	118.58	126.72
17	A	836	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
17	b	833	CLA	C4-C3-C5	2.94	120.22	115.27
17	2	602	CLA	O2A-CGA-CBA	2.94	121.14	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	823	CLA	CAC-C3C-C4C	2.94	128.63	124.81
17	1	306	CLA	CHC-C1C-C2C	-2.94	118.58	126.72
17	a	834	CLA	C4-C3-C5	2.94	120.22	115.27
17	9	614	CLA	CAC-C3C-C4C	2.94	128.63	124.81
17	3	306	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
17	A	841	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
17	8	312	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
17	a	827	CLA	CHD-C4C-NC	2.94	128.84	124.20
17	2	609	CLA	CHD-C4C-NC	2.94	128.84	124.20
17	b	812	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
17	b	824	CLA	C4-C3-C5	2.94	120.22	115.27
17	b	833	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
20	3	318	BCR	C11-C10-C9	-2.94	123.11	127.31
17	a	834	CLA	O2A-CGA-CBA	2.94	121.13	111.91
17	1	308	CLA	O2A-CGA-CBA	2.94	121.13	111.91
17	1	312	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
17	F	301	CLA	CAC-C3C-C4C	2.94	128.62	124.81
17	A	839	CLA	CAC-C3C-C4C	2.94	128.62	124.81
17	g	102	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
17	A	834	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
17	B	823	CLA	C3B-C4B-NB	2.94	113.01	109.21
17	L	204	CLA	CHD-C4C-NC	2.94	128.83	124.20
17	a	826	CLA	CHD-C4C-NC	2.94	128.83	124.20
17	b	836	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
20	B	846	BCR	C33-C5-C6	-2.94	121.23	124.53
17	1	303	CLA	O2A-CGA-CBA	2.94	121.12	111.91
17	4	602	CLA	CAC-C3C-C4C	2.94	128.62	124.81
17	b	827	CLA	C1-C2-C3	-2.94	120.97	126.04
17	a	810	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
28	2	616	XAT	C4-C3-C2	-2.94	105.10	110.77
17	1	311	CLA	CHC-C1C-C2C	-2.94	118.60	126.72
17	a	844	CLA	CMC-C2C-C1C	2.94	129.51	125.04
17	4	602	CLA	O2A-CGA-CBA	2.94	121.12	111.91
20	b	843	BCR	C20-C21-C22	-2.94	123.12	127.31
17	6	314	CLA	CHC-C1C-C2C	-2.93	118.60	126.72
17	b	829	CLA	O2A-CGA-CBA	2.93	121.12	111.91
17	l	203	CLA	CHD-C4C-NC	2.93	128.83	124.20
17	a	829	CLA	CMC-C2C-C1C	2.93	129.51	125.04
17	8	307	CLA	C3B-C4B-NB	2.93	113.00	109.21
17	A	854	CLA	CAA-C2A-C3A	-2.93	104.75	112.78
17	B	825	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
17	a	809	CLA	C3B-C4B-NB	2.93	113.00	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	810	CLA	CHC-C1C-C2C	-2.93	118.61	126.72
17	B	817	CLA	CHC-C1C-C2C	-2.93	118.61	126.72
17	b	818	CLA	O2A-CGA-CBA	2.93	121.11	111.91
17	a	816	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
26	7	601	CHL	C1-C2-C3	-2.93	120.97	126.04
26	2	601	CHL	C4-C3-C5	2.93	120.20	115.27
17	A	813	CLA	CAC-C3C-C4C	2.93	128.61	124.81
17	A	819	CLA	O2A-CGA-CBA	2.93	121.11	111.91
20	8	316	BCR	C21-C20-C19	-2.93	114.07	123.22
17	G	104	CLA	CAC-C3C-C4C	2.93	128.61	124.81
17	l	203	CLA	C1-C2-C3	-2.93	120.97	126.04
17	A	806	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
17	1	305	CLA	CAC-C3C-C4C	2.93	128.61	124.81
17	9	609	CLA	CHC-C1C-C2C	-2.93	118.62	126.72
17	A	814	CLA	CHC-C1C-C2C	-2.93	118.62	126.72
17	3	311	CLA	CHC-C1C-C2C	-2.93	118.62	126.72
17	B	818	CLA	C3B-C4B-NB	2.93	113.00	109.21
17	a	801	CLA	CHC-C1C-C2C	-2.93	118.62	126.72
17	A	810	CLA	CHC-C1C-C2C	-2.93	118.62	126.72
17	8	304	CLA	CAC-C3C-C4C	2.93	128.61	124.81
17	3	306	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
17	b	827	CLA	CHD-C4C-NC	2.93	128.82	124.20
17	a	825	CLA	O2A-CGA-CBA	2.93	121.10	111.91
17	8	313	CLA	C2A-C3A-C4A	-2.93	99.59	104.18
28	7	616	XAT	C24-C23-C22	-2.93	105.12	110.77
17	a	824	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
17	8	312	CLA	C3B-C4B-NB	2.93	112.99	109.21
17	A	816	CLA	CHC-C1C-C2C	-2.93	118.63	126.72
17	a	823	CLA	CHC-C1C-C2C	-2.93	118.63	126.72
17	a	804	CLA	CHD-C4C-NC	2.93	128.81	124.20
17	A	836	CLA	C1-C2-C3	-2.93	122.02	126.75
20	K	4001	BCR	C20-C19-C18	-2.93	118.20	126.42
17	8	311	CLA	CAC-C3C-C4C	2.93	128.61	124.81
17	A	842	CLA	CHC-C1C-C2C	-2.93	118.63	126.72
17	a	805	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
17	B	822	CLA	CHC-C1C-C2C	-2.92	118.63	126.72
17	1	308	CLA	C1-C2-C3	-2.92	120.99	126.04
26	2	614	CHL	C2A-C1A-CHA	-2.92	118.75	123.86
17	7	609	CLA	CHD-C4C-NC	2.92	128.81	124.20
17	a	806	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
17	a	826	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
27	4	616	LUT	C21-C26-C27	-2.92	109.01	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	610	CLA	CHC-C1C-C2C	-2.92	118.64	126.72
17	a	835	CLA	CHC-C1C-C2C	-2.92	118.64	126.72
17	4	603	CLA	CHC-C1C-C2C	-2.92	118.64	126.72
20	3	318	BCR	C23-C24-C25	-2.92	119.00	127.20
20	A	848	BCR	C7-C8-C9	-2.92	121.82	126.23
17	a	840	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
27	1	320	LUT	C35-C34-C33	-2.92	123.14	127.31
17	a	825	CLA	CHC-C1C-C2C	-2.92	118.65	126.72
17	b	815	CLA	CHC-C1C-C2C	-2.92	118.65	126.72
17	b	802	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
17	7	611	CLA	CAC-C3C-C4C	2.92	128.59	124.81
17	B	841	CLA	C1-C2-C3	-2.92	121.00	126.04
28	6	318	XAT	C10-C11-C12	-2.92	114.11	123.22
17	a	827	CLA	C4C-C3C-C2C	-2.92	102.65	106.90
17	2	608	CLA	O2A-CGA-CBA	2.92	121.06	111.91
17	A	826	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
17	a	843	CLA	C4C-C3C-C2C	-2.92	102.65	106.90
17	B	835	CLA	CHC-C1C-C2C	-2.92	118.66	126.72
17	l	203	CLA	C3B-C4B-NB	2.92	112.98	109.21
17	B	828	CLA	CHD-C4C-NC	2.92	128.80	124.20
17	G	101	CLA	CHD-C4C-NC	2.92	128.80	124.20
17	6	309	CLA	CHC-C1C-C2C	-2.92	118.66	126.72
17	A	807	CLA	C3B-C4B-NB	2.92	112.98	109.21
17	4	614	CLA	CHD-C4C-NC	2.92	128.80	124.20
17	a	856	CLA	CAC-C3C-C4C	2.91	128.59	124.81
26	4	607	CHL	C1-C2-C3	-2.91	122.04	126.75
17	4	602	CLA	CHD-C4C-NC	2.91	128.80	124.20
17	b	814	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
17	7	613	CLA	CHD-C4C-NC	2.91	128.79	124.20
17	B	837	CLA	O2A-CGA-CBA	2.91	121.05	111.91
17	a	814	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
17	b	823	CLA	C3B-C4B-NB	2.91	112.98	109.21
17	A	829	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
17	B	802	CLA	CAA-C2A-C3A	-2.91	104.80	112.78
17	a	807	CLA	CMC-C2C-C1C	2.91	129.47	125.04
17	6	312	CLA	CHD-C4C-NC	2.91	128.79	124.20
27	6	317	LUT	C7-C8-C9	-2.91	121.83	126.23
17	F	304	CLA	CHC-C1C-C2C	-2.91	118.67	126.72
17	6	311	CLA	CHD-C4C-NC	2.91	128.79	124.20
17	b	806	CLA	C3B-C4B-NB	2.91	112.97	109.21
20	a	853	BCR	C3-C4-C5	-2.91	108.88	114.08
17	b	840	CLA	CHC-C1C-C2C	-2.91	118.67	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	306	CLA	O2A-CGA-CBA	2.91	121.04	111.91
17	3	306	CLA	CHD-C4C-NC	2.91	128.79	124.20
17	2	604	CLA	C1-C2-C3	-2.91	121.01	126.04
17	A	833	CLA	C3B-C4B-NB	2.91	112.97	109.21
20	G	105	BCR	C7-C8-C9	-2.91	121.84	126.23
17	3	314	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
17	l	204	CLA	CHC-C1C-C2C	-2.91	118.68	126.72
17	1	306	CLA	CHD-C4C-NC	2.91	128.78	124.20
17	B	807	CLA	C1-C2-C3	-2.91	121.02	126.04
17	7	602	CLA	CHD-C4C-NC	2.91	128.78	124.20
17	b	837	CLA	CHD-C4C-NC	2.91	128.78	124.20
17	B	804	CLA	CMC-C2C-C1C	2.91	129.47	125.04
17	A	819	CLA	CHC-C1C-C2C	-2.91	118.68	126.72
18	A	844	PQN	C2M-C2-C3	-2.91	119.66	124.40
17	B	820	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
17	B	833	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
17	b	836	CLA	CHD-C4C-NC	2.91	128.78	124.20
17	B	824	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
17	1	303	CLA	CHC-C1C-C2C	-2.91	118.68	126.72
17	4	612	CLA	CHD-C4C-NC	2.91	128.78	124.20
17	a	828	CLA	C3B-C4B-NB	2.90	112.96	109.21
17	b	816	CLA	CHC-C1C-C2C	-2.90	118.69	126.72
20	a	850	BCR	C24-C23-C22	-2.90	121.85	126.23
17	B	815	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
17	B	806	CLA	C3B-C4B-NB	2.90	112.96	109.21
17	3	309	CLA	C3B-C4B-NB	2.90	112.96	109.21
20	g	104	BCR	C7-C8-C9	-2.90	121.85	126.23
17	a	833	CLA	C3B-C4B-NB	2.90	112.96	109.21
17	a	856	CLA	C1-C2-C3	-2.90	121.03	126.04
17	1	308	CLA	C4-C3-C5	2.90	120.15	115.27
17	8	309	CLA	O2A-CGA-CBA	2.90	121.01	111.91
17	a	846	CLA	CHC-C1C-C2C	-2.90	118.70	126.72
20	A	851	BCR	C38-C26-C27	2.90	119.19	113.62
17	2	602	CLA	CHC-C1C-C2C	-2.90	118.70	126.72
17	A	810	CLA	CHD-C4C-NC	2.90	128.77	124.20
17	a	803	CLA	C4D-C3D-CAD	-2.90	106.85	108.47
17	b	830	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
17	b	811	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
17	K	4002	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
17	G	104	CLA	CHD-C4C-NC	2.90	128.77	124.20
17	A	804	CLA	CHD-C4C-NC	2.90	128.77	124.20
28	7	616	XAT	C10-C11-C12	-2.90	114.17	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	603	CLA	CHD-C4C-NC	2.90	128.77	124.20
17	B	830	CLA	C3B-C4B-NB	2.90	112.95	109.21
17	B	837	CLA	C3B-C4B-NB	2.90	112.95	109.21
17	A	828	CLA	O2A-CGA-CBA	2.90	121.00	111.91
17	6	309	CLA	C4C-C3C-C2C	-2.90	102.68	106.90
17	B	834	CLA	C4C-C3C-C2C	-2.90	102.68	106.90
17	f	7002	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
17	B	810	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
17	A	838	CLA	CAC-C3C-C4C	2.90	128.57	124.81
17	a	806	CLA	CHD-C4C-NC	2.90	128.77	124.20
17	b	833	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
17	8	307	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
17	2	604	CLA	O2A-CGA-CBA	2.90	120.99	111.91
17	A	806	CLA	CHC-C1C-C2C	-2.89	118.72	126.72
17	b	827	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
17	K	4003	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
17	B	814	CLA	C1-C2-C3	-2.89	121.04	126.04
17	A	810	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
17	3	311	CLA	O2A-CGA-CBA	2.89	120.99	111.91
17	A	836	CLA	CAC-C3C-C4C	2.89	128.56	124.81
17	B	836	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
17	a	806	CLA	O2A-CGA-CBA	2.89	120.98	111.91
17	a	822	CLA	CHC-C1C-C2C	-2.89	118.72	126.72
17	A	827	CLA	CHD-C4C-NC	2.89	128.76	124.20
20	b	845	BCR	C8-C9-C10	2.89	123.38	118.94
28	8	315	XAT	C24-C23-C22	-2.89	105.19	110.77
17	B	825	CLA	CHD-C4C-NC	2.89	128.76	124.20
17	b	839	CLA	CHC-C1C-C2C	-2.89	118.73	126.72
17	B	841	CLA	C4-C3-C5	2.89	120.13	115.27
17	a	811	CLA	CAC-C3C-C4C	2.89	128.56	124.81
17	A	802	CLA	CAC-C3C-C4C	2.89	128.56	124.81
17	b	802	CLA	C4-C3-C5	2.89	120.13	115.27
17	b	834	CLA	CAC-C3C-C4C	2.89	128.56	124.81
17	A	830	CLA	CAC-C3C-C4C	2.89	128.56	124.81
28	7	616	XAT	C4-C3-C2	-2.89	105.20	110.77
17	B	817	CLA	CMB-C2B-C3B	2.89	130.08	124.68
17	B	837	CLA	CHC-C1C-C2C	-2.89	118.73	126.72
27	7	615	LUT	C15-C14-C13	-2.89	123.19	127.31
17	6	315	CLA	O2A-CGA-CBA	2.89	120.97	111.91
17	a	829	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
17	a	819	CLA	CHD-C4C-NC	2.89	128.75	124.20
17	6	309	CLA	CAC-C3C-C4C	2.89	128.56	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	7	611	CLA	O2A-CGA-CBA	2.89	120.97	111.91
17	A	818	CLA	CHC-C1C-C2C	-2.89	118.74	126.72
17	a	844	CLA	CHD-C4C-NC	2.89	128.75	124.20
17	2	611	CLA	O2A-CGA-CBA	2.89	120.97	111.91
20	B	845	BCR	C11-C10-C9	-2.89	123.19	127.31
17	a	827	CLA	C3B-C4B-NB	2.89	112.94	109.21
26	6	308	CHL	CAC-C3C-C4C	2.89	128.55	124.81
17	2	602	CLA	CHD-C4C-NC	2.89	128.75	124.20
17	a	830	CLA	CHD-C4C-NC	2.89	128.75	124.20
17	a	808	CLA	CMC-C2C-C1C	2.89	129.43	125.04
17	G	103	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
17	9	602	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
17	F	301	CLA	CHC-C1C-C2C	-2.88	118.74	126.72
17	1	305	CLA	O2A-CGA-CBA	2.88	120.96	111.91
17	7	602	CLA	O2A-CGA-CBA	2.88	120.96	111.91
17	a	841	CLA	O2A-CGA-CBA	2.88	120.96	111.91
17	B	840	CLA	O2A-CGA-CBA	2.88	120.96	111.91
17	a	813	CLA	C4C-C3C-C2C	-2.88	102.69	106.90
20	B	847	BCR	C29-C30-C25	2.88	114.92	110.48
20	a	850	BCR	C38-C26-C25	-2.88	121.29	124.53
17	A	815	CLA	CHD-C4C-NC	2.88	128.75	124.20
17	a	820	CLA	CMB-C2B-C3B	2.88	130.07	124.68
17	b	808	CLA	C1-C2-C3	-2.88	121.06	126.04
17	7	608	CLA	CHC-C1C-C2C	-2.88	118.75	126.72
17	a	808	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
17	9	610	CLA	CHD-C4C-NC	2.88	128.75	124.20
20	K	4004	BCR	C24-C23-C22	-2.88	121.88	126.23
17	B	807	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
17	A	832	CLA	CAC-C3C-C4C	2.88	128.55	124.81
17	a	831	CLA	CHC-C1C-C2C	-2.88	118.75	126.72
17	8	308	CLA	O2A-CGA-CBA	2.88	120.95	111.91
17	b	826	CLA	C4-C3-C5	2.88	120.12	115.27
17	8	302	CLA	C1-C2-C3	-2.88	122.09	126.75
17	a	807	CLA	C3B-C4B-NB	2.88	112.93	109.21
17	6	307	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
17	g	102	CLA	O2A-CGA-CBA	2.88	120.95	111.91
17	B	824	CLA	CHC-C1C-C2C	-2.88	118.75	126.72
17	B	815	CLA	CHC-C1C-C2C	-2.88	118.75	126.72
17	B	838	CLA	CHC-C1C-C2C	-2.88	118.75	126.72
17	b	832	CLA	C3B-C4B-NB	2.88	112.93	109.21
17	b	820	CLA	CHD-C4C-NC	2.88	128.74	124.20
17	1	308	CLA	CHC-C1C-C2C	-2.88	118.76	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	9	611	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
17	9	603	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
17	9	603	CLA	CHD-C4C-NC	2.88	128.74	124.20
17	A	838	CLA	CHD-C4C-NC	2.88	128.74	124.20
17	2	602	CLA	CAC-C3C-C4C	2.88	128.54	124.81
17	4	608	CLA	CHC-C1C-C2C	-2.88	118.76	126.72
17	b	834	CLA	O2A-CGA-CBA	2.88	120.94	111.91
17	b	815	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
17	8	311	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
17	6	309	CLA	CHD-C4C-NC	2.88	128.74	124.20
17	b	818	CLA	C4-C3-C5	2.88	120.11	115.27
17	a	841	CLA	CHC-C1C-C2C	-2.88	118.76	126.72
17	1	303	CLA	C3B-C4B-NB	2.88	112.93	109.21
17	B	833	CLA	CHD-C4C-NC	2.88	128.74	124.20
17	A	819	CLA	CAC-C3C-C4C	2.88	128.54	124.81
17	a	846	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
17	a	829	CLA	C3B-C4B-NB	2.88	112.93	109.21
17	7	602	CLA	C1-C2-C3	-2.88	121.07	126.04
17	B	822	CLA	CAC-C3C-C4C	2.88	128.54	124.81
17	A	804	CLA	CHC-C1C-C2C	-2.88	118.77	126.72
17	3	308	CLA	O2A-CGA-CBA	2.88	120.93	111.91
17	l	202	CLA	CHD-C4C-NC	2.88	128.74	124.20
17	a	819	CLA	C4C-C3C-C2C	-2.88	102.71	106.90
17	G	101	CLA	CHC-C1C-C2C	-2.88	118.77	126.72
28	6	318	XAT	C31-C30-C29	-2.88	123.21	127.31
20	l	201	BCR	C34-C9-C10	-2.88	118.89	122.92
17	6	311	CLA	C3B-C4B-NB	2.88	112.93	109.21
20	2	617	BCR	C2-C1-C6	2.88	114.91	110.48
20	J	3003	BCR	C24-C23-C22	-2.87	121.89	126.23
17	B	829	CLA	O2A-CGA-CBA	2.87	120.93	111.91
17	3	302	CLA	C3B-C4B-NB	2.87	112.93	109.21
17	1	315	CLA	CHD-C4C-NC	2.87	128.73	124.20
17	G	103	CLA	CHC-C1C-C2C	-2.87	118.77	126.72
26	4	615	CHL	C2A-C1A-CHA	-2.87	118.83	123.86
27	6	317	LUT	C35-C15-C14	-2.87	117.59	123.47
17	4	610	CLA	CHD-C4C-NC	2.87	128.73	124.20
17	A	815	CLA	C3B-C4B-NB	2.87	112.92	109.21
17	2	602	CLA	C1-C2-C3	-2.87	121.08	126.04
17	A	845	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
17	b	831	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
17	a	802	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
28	1	317	XAT	C4-C3-C2	-2.87	105.23	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	854	CLA	C4D-C3D-CAD	-2.87	106.87	108.47
17	b	809	CLA	CHD-C4C-NC	2.87	128.73	124.20
27	2	615	LUT	C31-C30-C29	-2.87	123.21	127.31
20	a	854	BCR	C28-C27-C26	-2.87	108.95	114.08
17	1	312	CLA	CAC-C3C-C4C	2.87	128.53	124.81
17	B	818	CLA	CHD-C4C-NC	2.87	128.73	124.20
17	8	301	CLA	O2A-CGA-CBA	2.87	120.91	111.91
17	A	827	CLA	C4-C3-C5	2.87	120.10	115.27
17	9	601	CLA	CAC-C3C-C4C	2.87	128.53	124.81
17	A	817	CLA	CAA-CBA-CGA	-2.87	107.42	113.59
17	L	204	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
17	7	603	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
17	b	830	CLA	C1D-CHD-C4C	-2.87	118.77	122.56
17	2	603	CLA	CAC-C3C-C4C	2.87	128.53	124.81
17	3	304	CLA	CHD-C4C-NC	2.87	128.72	124.20
26	7	606	CHL	O2A-CGA-CBA	2.87	120.90	111.91
17	6	313	CLA	CAC-C3C-C4C	2.87	128.53	124.81
17	B	813	CLA	CHC-C1C-C2C	-2.87	118.79	126.72
17	3	302	CLA	CHC-C1C-C2C	-2.87	118.79	126.72
17	b	838	CLA	O2A-CGA-CBA	2.87	120.90	111.91
17	3	305	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
17	a	815	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
17	b	824	CLA	CMC-C2C-C1C	2.87	129.40	125.04
27	9	616	LUT	C8-C7-C6	-2.87	119.15	127.20
17	A	812	CLA	CHC-C1C-C2C	-2.87	118.80	126.72
17	a	812	CLA	CHC-C1C-C2C	-2.87	118.80	126.72
17	k	1401	CLA	CHC-C1C-C2C	-2.87	118.80	126.72
17	8	307	CLA	CHD-C4C-NC	2.87	128.72	124.20
17	b	814	CLA	C1-C2-C3	-2.86	121.09	126.04
17	a	811	CLA	C4C-C3C-C2C	-2.86	102.72	106.90
17	a	816	CLA	CHD-C4C-NC	2.86	128.72	124.20
28	4	617	XAT	C15-C14-C13	-2.86	123.22	127.31
20	b	843	BCR	C29-C30-C25	2.86	114.89	110.48
20	L	206	BCR	C38-C26-C25	-2.86	121.31	124.53
17	B	833	CLA	O2A-CGA-CBA	2.86	120.89	111.91
17	A	819	CLA	C3B-C4B-NB	2.86	112.91	109.21
20	A	852	BCR	C28-C27-C26	-2.86	108.96	114.08
17	A	840	CLA	CHD-C4C-NC	2.86	128.72	124.20
27	2	615	LUT	C21-C26-C27	-2.86	109.08	112.70
28	4	617	XAT	C10-C11-C12	-2.86	114.28	123.22
17	3	309	CLA	O2A-CGA-CBA	2.86	120.89	111.91
17	A	829	CLA	CHC-C1C-C2C	-2.86	118.81	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	9	608	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
17	A	823	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
17	b	823	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
26	4	607	CHL	O2A-CGA-CBA	2.86	120.89	111.91
17	b	835	CLA	CHD-C4C-NC	2.86	128.71	124.20
17	b	826	CLA	CHD-C4C-NC	2.86	128.71	124.20
17	a	816	CLA	C3B-C4B-NB	2.86	112.91	109.21
17	4	601	CLA	CHD-C4C-NC	2.86	128.71	124.20
17	3	315	CLA	C2A-C1A-CHA	-2.86	117.76	122.63
17	B	818	CLA	C4-C3-C5	2.86	120.08	115.27
17	f	7003	CLA	CAC-C3C-C4C	2.86	128.52	124.81
17	1	309	CLA	O2A-CGA-CBA	2.86	120.88	111.91
28	9	617	XAT	C4-C3-C2	-2.86	105.25	110.77
20	B	848	BCR	C15-C14-C13	-2.86	123.23	127.31
17	A	835	CLA	C4-C3-C5	2.86	120.08	115.27
17	B	838	CLA	O2A-CGA-CBA	2.86	120.88	111.91
17	8	304	CLA	CHD-C4C-NC	2.86	128.71	124.20
17	B	835	CLA	CHD-C4C-NC	2.86	128.71	124.20
17	7	603	CLA	CHD-C4C-NC	2.86	128.71	124.20
20	4	618	BCR	C33-C5-C6	-2.86	121.32	124.53
17	b	807	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
17	A	819	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
17	A	835	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
17	A	830	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
17	B	804	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
17	b	827	CLA	CMC-C2C-C1C	2.86	129.39	125.04
17	b	807	CLA	CAC-C3C-C4C	2.86	128.52	124.81
20	a	854	BCR	C34-C9-C10	-2.86	118.92	122.92
17	b	838	CLA	CHC-C1C-C2C	-2.86	118.82	126.72
17	2	609	CLA	C3B-C4B-NB	2.86	112.90	109.21
17	3	309	CLA	CAC-C3C-C4C	2.86	128.52	124.81
17	A	810	CLA	C1-C2-C3	-2.86	121.10	126.04
17	4	609	CLA	C3B-C4B-NB	2.86	112.90	109.21
17	A	816	CLA	CHD-C4C-NC	2.86	128.70	124.20
17	8	309	CLA	CAC-C3C-C4C	2.86	128.51	124.81
17	A	838	CLA	C4C-C3C-C2C	-2.86	102.74	106.90
17	1	311	CLA	C4C-C3C-C2C	-2.86	102.74	106.90
17	A	808	CLA	CHC-C1C-C2C	-2.86	118.82	126.72
17	b	826	CLA	CHC-C1C-C2C	-2.86	118.82	126.72
17	A	801	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
20	K	4001	BCR	C20-C21-C22	-2.85	123.24	127.31
17	a	838	CLA	C1-C2-C3	-2.85	121.11	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	103	CLA	CAC-C3C-C4C	2.85	128.51	124.81
17	A	803	CLA	C1-C2-C3	-2.85	121.11	126.04
17	G	103	CLA	CHD-C4C-NC	2.85	128.70	124.20
17	4	602	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
17	B	804	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
20	a	854	BCR	C15-C14-C13	-2.85	123.24	127.31
17	A	815	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
17	b	834	CLA	C4-C3-C5	2.85	120.07	115.27
17	l	204	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
17	6	310	CLA	CAC-C3C-C4C	2.85	128.51	124.81
17	A	812	CLA	CHD-C4C-NC	2.85	128.69	124.20
17	3	302	CLA	CHD-C4C-NC	2.85	128.69	124.20
17	B	823	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
17	b	824	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
17	b	820	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
17	1	305	CLA	CHD-C4C-NC	2.85	128.69	124.20
20	B	844	BCR	C33-C5-C6	-2.85	121.33	124.53
17	b	825	CLA	CHD-C4C-NC	2.85	128.69	124.20
17	A	827	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
17	l	203	CLA	C4-C3-C5	2.85	120.06	115.27
17	K	4002	CLA	CHD-C4C-NC	2.85	128.69	124.20
17	A	818	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
26	7	601	CHL	C2A-C1A-CHA	-2.85	118.88	123.86
17	A	807	CLA	CHC-C1C-C2C	-2.85	118.85	126.72
27	1	316	LUT	C21-C26-C27	-2.85	109.10	112.70
17	B	841	CLA	O2A-CGA-CBA	2.85	120.84	111.91
17	b	831	CLA	CHD-C4C-NC	2.85	128.69	124.20
17	B	804	CLA	CHD-C4C-NC	2.85	128.69	124.20
20	I	101	BCR	C2-C1-C6	2.85	114.86	110.48
17	a	808	CLA	CAC-C3C-C4C	2.85	128.50	124.81
17	B	838	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
28	3	317	XAT	C35-C15-C14	-2.85	117.64	123.47
28	9	617	XAT	C24-C23-C22	-2.85	105.28	110.77
20	8	316	BCR	C15-C16-C17	-2.85	117.64	123.47
20	g	104	BCR	C11-C10-C9	-2.85	123.25	127.31
17	a	839	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
17	B	840	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
17	b	824	CLA	CHD-C4C-NC	2.85	128.69	124.20
17	b	816	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
28	6	318	XAT	C24-C23-C22	-2.84	105.28	110.77
17	b	814	CLA	C3B-C4B-NB	2.84	112.89	109.21
17	6	313	CLA	CHD-C4C-NC	2.84	128.69	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	311	CLA	CAC-C3C-C4C	2.84	128.50	124.81
17	1	303	CLA	CHD-C4C-NC	2.84	128.68	124.20
26	1	307	CHL	CAC-C3C-C4C	2.84	128.50	124.81
17	1	310	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
17	7	608	CLA	CHD-C4C-NC	2.84	128.68	124.20
17	B	827	CLA	CAC-C3C-C4C	2.84	128.50	124.81
26	2	607	CHL	CAC-C3C-C4C	2.84	128.50	124.81
20	B	846	BCR	C29-C30-C25	2.84	114.86	110.48
17	4	604	CLA	O2A-CGA-CBA	2.84	120.83	111.91
17	a	826	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
17	A	805	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
17	b	815	CLA	C1-C2-C3	-2.84	121.13	126.04
17	a	801	CLA	CHD-C4C-NC	2.84	128.68	124.20
17	a	812	CLA	CAA-C2A-C3A	-2.84	105.00	112.78
17	A	840	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
17	l	202	CLA	C4-C3-C5	2.84	120.05	115.27
17	B	810	CLA	CHD-C4C-NC	2.84	128.68	124.20
17	8	308	CLA	C3B-C4B-NB	2.84	112.88	109.21
17	B	828	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
17	b	807	CLA	O2A-CGA-CBA	2.84	120.82	111.91
20	B	846	BCR	C11-C10-C9	-2.84	123.26	127.31
20	A	848	BCR	C11-C10-C9	-2.84	123.26	127.31
17	B	814	CLA	C3B-C4B-NB	2.84	112.88	109.21
17	K	4002	CLA	CAC-C3C-C4C	2.84	128.49	124.81
17	B	809	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
17	A	826	CLA	CHD-C4C-NC	2.84	128.68	124.20
17	8	313	CLA	C2A-C1A-CHA	-2.84	117.79	122.63
17	6	311	CLA	CAC-C3C-C4C	2.84	128.49	124.81
17	k	1401	CLA	CHD-C4C-NC	2.84	128.68	124.20
20	a	850	BCR	C33-C5-C6	-2.84	121.34	124.53
17	b	822	CLA	CHC-C1C-C2C	-2.84	118.87	126.72
17	9	602	CLA	C3B-C4B-NB	2.84	112.88	109.21
17	2	611	CLA	CAC-C3C-C4C	2.84	128.49	124.81
17	3	308	CLA	CHC-C1C-C2C	-2.84	118.87	126.72
17	A	825	CLA	O2A-CGA-CBA	2.84	120.81	111.91
17	a	826	CLA	C4-C3-C5	2.84	120.04	115.27
17	4	602	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
20	b	845	BCR	C20-C21-C22	-2.84	123.26	127.31
20	a	851	BCR	C2-C1-C6	2.84	114.85	110.48
17	B	811	CLA	CHD-C4C-NC	2.84	128.67	124.20
17	A	838	CLA	C3B-C4B-NB	2.84	112.88	109.21
17	F	303	CLA	CHD-C4C-NC	2.84	128.67	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	834	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
17	a	835	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
17	2	612	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
17	A	822	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
17	a	834	CLA	CHC-C1C-C2C	-2.84	118.88	126.72
17	3	309	CLA	C4C-C3C-C2C	-2.84	102.77	106.90
17	a	840	CLA	C4C-C3C-C2C	-2.84	102.77	106.90
17	a	807	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
17	9	609	CLA	CHD-C4C-NC	2.83	128.67	124.20
17	B	815	CLA	CAC-C3C-C4C	2.83	128.49	124.81
20	2	617	BCR	C38-C26-C25	-2.83	121.35	124.53
17	1	309	CLA	CHD-C4C-NC	2.83	128.67	124.20
17	B	830	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
17	B	807	CLA	CHC-C1C-C2C	-2.83	118.89	126.72
26	8	306	CHL	C2A-C1A-CHA	-2.83	118.91	123.86
17	A	833	CLA	CHC-C1C-C2C	-2.83	118.89	126.72
17	a	844	CLA	CHC-C1C-C2C	-2.83	118.89	126.72
17	B	816	CLA	CHC-C1C-C2C	-2.83	118.89	126.72
17	b	808	CLA	CAA-C2A-C3A	-2.83	105.03	112.78
17	1	310	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
17	a	810	CLA	CAC-C3C-C4C	2.83	128.48	124.81
17	7	603	CLA	O2A-CGA-CBA	2.83	120.79	111.91
17	B	813	CLA	O2A-CGA-CBA	2.83	120.79	111.91
17	A	827	CLA	C3B-C4B-NB	2.83	112.87	109.21
17	4	611	CLA	C4-C3-C5	2.83	120.03	115.27
17	a	839	CLA	CHC-C1C-C2C	-2.83	118.89	126.72
17	7	610	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
17	6	314	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
17	g	101	CLA	CHD-C4C-NC	2.83	128.66	124.20
17	B	822	CLA	CHD-C4C-NC	2.83	128.66	124.20
17	7	612	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
17	a	830	CLA	CMC-C2C-C1C	2.83	129.34	125.04
17	B	811	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
28	3	317	XAT	C24-C23-C22	-2.83	105.31	110.77
17	a	815	CLA	C3B-C4B-NB	2.83	112.86	109.21
17	A	808	CLA	CHD-C4C-NC	2.83	128.66	124.20
17	B	815	CLA	CHD-C4C-NC	2.83	128.66	124.20
17	j	3002	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
17	a	803	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
17	B	811	CLA	C4-C3-C5	2.83	120.02	115.27
17	A	816	CLA	O2A-CGA-CBA	2.82	120.77	111.91
17	b	830	CLA	C4C-C3C-C2C	-2.82	102.78	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	828	CLA	C3B-C4B-NB	2.82	112.86	109.21
17	A	808	CLA	CAC-C3C-C4C	2.82	128.47	124.81
17	2	613	CLA	CHD-C4C-NC	2.82	128.65	124.20
17	a	825	CLA	CHD-C4C-NC	2.82	128.65	124.20
17	A	829	CLA	CHD-C4C-NC	2.82	128.65	124.20
17	3	302	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
17	a	802	CLA	C3B-C4B-NB	2.82	112.86	109.21
17	4	611	CLA	CAC-C3C-C4C	2.82	128.47	124.81
17	6	315	CLA	C1-C2-C3	-2.82	121.16	126.04
17	9	614	CLA	CHD-C4C-NC	2.82	128.65	124.20
17	a	842	CLA	CHC-C1C-C2C	-2.82	118.91	126.72
17	b	825	CLA	CAC-C3C-C4C	2.82	128.47	124.81
17	G	104	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
17	7	608	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
17	8	308	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
20	f	7004	BCR	C28-C27-C26	-2.82	109.04	114.08
20	a	851	BCR	C28-C27-C26	-2.82	109.04	114.08
17	a	836	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
17	a	806	CLA	CMC-C2C-C1C	2.82	129.34	125.04
17	3	308	CLA	CAC-C3C-C4C	2.82	128.47	124.81
17	7	611	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
17	F	304	CLA	CAC-C3C-C4C	2.82	128.47	124.81
17	6	304	CLA	O2A-CGA-CBA	2.82	120.76	111.91
17	a	841	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
17	8	305	CLA	CHD-C4C-NC	2.82	128.65	124.20
17	a	818	CLA	CAC-C3C-C4C	2.82	128.47	124.81
20	A	852	BCR	C34-C9-C10	-2.82	118.97	122.92
17	A	842	CLA	CHD-C4C-NC	2.82	128.65	124.20
17	G	103	CLA	O2A-CGA-CBA	2.82	120.75	111.91
17	7	609	CLA	C3B-C4B-NB	2.82	112.85	109.21
17	b	832	CLA	CHC-C1C-C2C	-2.82	118.93	126.72
17	2	611	CLA	CHD-C4C-NC	2.82	128.64	124.20
20	A	851	BCR	C33-C5-C6	-2.82	121.36	124.53
17	g	102	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
17	b	805	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
26	9	607	CHL	C2A-C1A-CHA	-2.82	118.93	123.86
17	6	310	CLA	CHD-C4C-NC	2.82	128.64	124.20
17	a	837	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
17	a	842	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
17	6	305	CLA	CHD-C4C-NC	2.81	128.64	124.20
26	2	606	CHL	O2A-CGA-CBA	2.81	120.74	111.91
17	L	203	CLA	C3B-C4B-NB	2.81	112.85	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	817	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
17	b	817	CLA	CMB-C2B-C3B	2.81	129.94	124.68
28	8	315	XAT	C38-C25-C24	2.81	117.45	114.28
17	a	816	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
17	B	825	CLA	C1-C2-C3	-2.81	121.18	126.04
20	b	843	BCR	C24-C23-C22	-2.81	121.98	126.23
17	2	608	CLA	CHD-C4C-NC	2.81	128.64	124.20
17	8	301	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
17	b	823	CLA	C4-C3-C5	2.81	120.00	115.27
17	A	840	CLA	C4-C3-C5	2.81	120.00	115.27
17	9	601	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
27	1	316	LUT	C15-C14-C13	-2.81	123.30	127.31
17	3	311	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
17	4	611	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
20	6	319	BCR	C21-C20-C19	-2.81	114.45	123.22
17	a	843	CLA	O2A-C1-C2	2.81	116.02	108.64
17	A	834	CLA	O2A-CGA-CBA	2.81	120.73	111.91
17	b	816	CLA	C3B-C4B-NB	2.81	112.84	109.21
17	A	842	CLA	O2A-CGA-CBA	2.81	120.73	111.91
17	g	103	CLA	CHD-C4C-NC	2.81	128.63	124.20
17	A	815	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
17	A	842	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
17	A	805	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
17	a	805	CLA	O2A-CGA-CBA	2.81	120.72	111.91
17	B	820	CLA	CHD-C4C-NC	2.81	128.63	124.20
17	A	833	CLA	CMC-C2C-C1C	2.81	129.32	125.04
17	b	841	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
17	b	820	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
17	A	807	CLA	CHD-C4C-NC	2.81	128.63	124.20
17	b	812	CLA	CHD-C4C-NC	2.81	128.63	124.20
17	B	832	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
17	a	843	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
17	1	310	CLA	CHD-C4C-NC	2.81	128.63	124.20
17	3	304	CLA	CAC-C3C-C4C	2.81	128.45	124.81
17	G	104	CLA	C4C-C3C-C2C	-2.81	102.81	106.90
17	B	812	CLA	C4C-C3C-C2C	-2.81	102.81	106.90
17	a	815	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
26	7	607	CHL	O2A-CGA-CBA	2.81	120.72	111.91
17	k	1402	CLA	C4C-C3C-C2C	-2.81	102.81	106.90
17	A	802	CLA	CHD-C4C-NC	2.81	128.63	124.20
17	l	203	CLA	C4C-C3C-C2C	-2.81	102.81	106.90
17	b	826	CLA	C3B-C4B-NB	2.81	112.84	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	841	CLA	CHC-C1C-C2C	-2.81	118.96	126.72
17	A	830	CLA	CMB-C2B-C3B	2.81	129.93	124.68
20	B	848	BCR	C10-C11-C12	-2.81	114.46	123.22
17	a	805	CLA	CBC-CAC-C3C	-2.81	104.70	112.43
17	1	303	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
26	2	607	CHL	O2A-CGA-CBA	2.80	120.71	111.91
17	b	828	CLA	CHC-C1C-C2C	-2.80	118.96	126.72
17	b	828	CLA	C4-C3-C5	2.80	119.99	115.27
26	7	614	CHL	CAC-C3C-C4C	2.80	128.45	124.81
17	a	833	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
17	B	818	CLA	O2A-CGA-CBA	2.80	120.70	111.91
17	7	604	CLA	O2A-CGA-CBA	2.80	120.70	111.91
17	A	824	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
17	6	316	CLA	CHD-C4C-NC	2.80	128.62	124.20
17	1	304	CLA	C4-C3-C5	2.80	119.98	115.27
17	A	821	CLA	CHD-C4C-NC	2.80	128.62	124.20
17	3	305	CLA	CHD-C4C-NC	2.80	128.62	124.20
17	A	839	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
17	B	841	CLA	CAC-C3C-C4C	2.80	128.44	124.81
17	A	845	CLA	C1-C2-C3	-2.80	121.20	126.04
17	A	811	CLA	C4-C3-C5	2.80	119.98	115.27
20	I	101	BCR	C8-C7-C6	-2.80	119.34	127.20
17	b	830	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
17	A	826	CLA	C3B-C4B-NB	2.80	112.83	109.21
17	B	816	CLA	C3B-C4B-NB	2.80	112.83	109.21
26	4	605	CHL	C4-C3-C5	2.80	119.98	115.27
17	6	306	CLA	CHD-C4C-NC	2.80	128.62	124.20
17	6	307	CLA	CHD-C4C-NC	2.80	128.61	124.20
17	a	827	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
17	2	603	CLA	O2A-CGA-CBA	2.80	120.69	111.91
17	B	839	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
17	a	822	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
17	7	610	CLA	CAC-C3C-C4C	2.80	128.44	124.81
17	A	801	CLA	CHD-C4C-NC	2.80	128.61	124.20
26	4	606	CHL	C2A-C1A-CHA	-2.80	118.97	123.86
17	2	612	CLA	O2A-CGA-CBA	2.80	120.69	111.91
17	A	803	CLA	CAA-C2A-C3A	-2.80	105.12	112.78
17	b	804	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
20	a	849	BCR	C35-C13-C14	-2.80	119.00	122.92
17	3	312	CLA	O2A-CGA-CBA	2.80	120.69	111.91
20	L	205	BCR	C23-C24-C25	-2.80	119.35	127.20
17	b	831	CLA	CAC-C3C-C4C	2.80	128.44	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	824	CLA	C1-C2-C3	-2.80	121.21	126.04
17	k	1401	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
17	B	840	CLA	C4-C3-C5	2.80	119.97	115.27
17	J	3002	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
17	7	602	CLA	CHC-C1C-C2C	-2.80	118.99	126.72
17	a	806	CLA	CHC-C1C-C2C	-2.80	118.99	126.72
17	4	609	CLA	CHC-C1C-C2C	-2.79	118.99	126.72
17	A	806	CLA	C4-C3-C5	2.79	119.97	115.27
17	B	808	CLA	CAC-C3C-C4C	2.79	128.44	124.81
17	b	803	CLA	CAC-C3C-C4C	2.79	128.44	124.81
17	b	813	CLA	O2A-CGA-CBA	2.79	120.67	111.91
17	b	841	CLA	O2A-CGA-CBA	2.79	120.67	111.91
17	9	613	CLA	CHD-C4C-NC	2.79	128.60	124.20
17	a	816	CLA	CAC-C3C-C4C	2.79	128.43	124.81
17	3	311	CLA	C4-C3-C5	2.79	119.97	115.27
17	4	613	CLA	CHD-C4C-NC	2.79	128.60	124.20
17	7	602	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
28	2	616	XAT	C24-C23-C22	-2.79	105.38	110.77
17	B	810	CLA	C4-C3-C5	2.79	119.97	115.27
17	b	814	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
17	6	304	CLA	CHD-C4C-NC	2.79	128.60	124.20
20	f	7004	BCR	C35-C13-C14	-2.79	119.01	122.92
17	1	309	CLA	CAC-C3C-C4C	2.79	128.43	124.81
17	a	804	CLA	CHC-C1C-C2C	-2.79	119.00	126.72
17	B	823	CLA	O2A-CGA-CBA	2.79	120.66	111.91
17	9	611	CLA	CAC-C3C-C4C	2.79	128.43	124.81
17	1	308	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
17	6	310	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
17	9	604	CLA	O2A-CGA-CBA	2.79	120.66	111.91
17	k	1403	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
17	1	304	CLA	CHD-C4C-NC	2.79	128.60	124.20
27	1	320	LUT	C7-C8-C9	-2.79	122.02	126.23
17	9	612	CLA	C1-C2-C3	-2.79	121.22	126.04
17	6	306	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
17	B	805	CLA	CHD-C4C-NC	2.79	128.59	124.20
17	A	830	CLA	CHD-C4C-NC	2.79	128.59	124.20
17	L	203	CLA	C4C-C3C-C2C	-2.79	102.84	106.90
17	A	809	CLA	CHC-C1C-C2C	-2.79	119.01	126.72
17	3	311	CLA	CHD-C4C-NC	2.79	128.59	124.20
17	2	611	CLA	C4C-C3C-C2C	-2.79	102.84	106.90
17	b	811	CLA	C4C-C3C-C2C	-2.79	102.84	106.90
17	b	823	CLA	C4C-C3C-C2C	-2.79	102.84	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	806	CLA	CHD-C4C-NC	2.79	128.59	124.20
17	A	809	CLA	CHD-C4C-NC	2.79	128.59	124.20
17	a	838	CLA	O2A-CGA-CBA	2.79	120.65	111.91
26	7	614	CHL	C2A-C1A-CHA	-2.79	118.99	123.86
17	L	203	CLA	CHD-C4C-NC	2.79	128.59	124.20
17	a	825	CLA	C4C-C3C-C2C	-2.79	102.84	106.90
26	4	606	CHL	CMB-C2B-C3B	2.78	129.89	124.68
17	a	819	CLA	O2A-CGA-CBA	2.78	120.65	111.91
17	A	840	CLA	CAC-C3C-C4C	2.78	128.42	124.81
17	7	602	CLA	C3B-C4B-NB	2.78	112.81	109.21
17	a	814	CLA	CHD-C4C-NC	2.78	128.59	124.20
17	a	842	CLA	CHD-C4C-NC	2.78	128.59	124.20
17	2	612	CLA	CHD-C4C-NC	2.78	128.59	124.20
17	A	827	CLA	CHC-C1C-C2C	-2.78	119.02	126.72
17	a	830	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
17	8	302	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
17	b	803	CLA	O2A-CGA-CBA	2.78	120.64	111.91
17	B	834	CLA	C4-C3-C5	2.78	119.95	115.27
17	3	308	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
17	A	840	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
17	4	611	CLA	O2A-CGA-CBA	2.78	120.64	111.91
17	4	610	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
26	8	306	CHL	CAC-C3C-C4C	2.78	128.42	124.81
17	a	814	CLA	C3B-C4B-NB	2.78	112.81	109.21
17	6	316	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
17	A	808	CLA	CMC-C2C-C1C	2.78	129.27	125.04
17	2	611	CLA	C4-C3-C5	2.78	119.95	115.27
17	B	841	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
17	A	807	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
17	B	816	CLA	O2A-CGA-CBA	2.78	120.63	111.91
17	8	312	CLA	CHD-C4C-NC	2.78	128.59	124.20
20	K	4004	BCR	C11-C10-C9	-2.78	123.34	127.31
17	B	821	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
17	9	614	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
17	3	313	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
17	b	817	CLA	C1-C2-C3	-2.78	121.23	126.04
28	3	317	XAT	C15-C14-C13	-2.78	123.34	127.31
20	b	844	BCR	C29-C30-C25	2.78	114.76	110.48
17	4	611	CLA	CHD-C4C-NC	2.78	128.58	124.20
17	b	832	CLA	CHD-C4C-NC	2.78	128.58	124.20
17	3	303	CLA	O2A-CGA-CBA	2.78	120.63	111.91
17	1	308	CLA	CHD-C4C-NC	2.78	128.58	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	8	310	CLA	CHD-C4C-NC	2.78	128.58	124.20
17	b	827	CLA	C3B-C4B-NB	2.78	112.80	109.21
17	a	808	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
17	b	826	CLA	CAC-C3C-C4C	2.78	128.41	124.81
17	K	4003	CLA	CAC-C3C-C4C	2.78	128.41	124.81
17	A	825	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
17	L	202	CLA	CHD-C4C-NC	2.78	128.58	124.20
17	a	840	CLA	CHD-C4C-NC	2.78	128.58	124.20
17	7	609	CLA	CMB-C2B-C3B	2.78	129.87	124.68
26	7	606	CHL	C2A-C1A-CHA	-2.78	119.00	123.86
20	4	618	BCR	C21-C20-C19	-2.78	114.55	123.22
17	4	612	CLA	CAC-C3C-C4C	2.78	128.41	124.81
17	b	827	CLA	CAA-C2A-C3A	-2.78	105.18	112.78
17	B	828	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
17	b	836	CLA	CMC-C2C-C1C	2.77	129.26	125.04
19	2	618	LHG	O8-C23-C24	2.77	120.62	111.91
17	A	822	CLA	C4-C3-C5	2.77	119.94	115.27
17	B	802	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
27	3	316	LUT	C18-C5-C6	-2.77	121.41	124.53
17	B	806	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
17	B	830	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
17	a	820	CLA	CHD-C4C-NC	2.77	128.57	124.20
17	b	821	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
26	2	606	CHL	C2A-C1A-CHA	-2.77	119.01	123.86
17	6	315	CLA	CHD-C4C-NC	2.77	128.57	124.20
17	a	826	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
24	b	849	DGD	O1G-C1A-C2A	2.77	120.61	111.91
17	k	1402	CLA	CHD-C4C-NC	2.77	128.57	124.20
17	a	831	CLA	O2A-CGA-CBA	2.77	120.61	111.91
17	6	311	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
17	1	314	CLA	C4-C3-C5	2.77	119.93	115.27
17	b	835	CLA	CAC-C3C-C4C	2.77	128.41	124.81
17	2	603	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
17	7	604	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
20	A	849	BCR	C8-C7-C6	-2.77	119.42	127.20
17	1	312	CLA	CHD-C4C-NC	2.77	128.57	124.20
17	8	308	CLA	CHC-C1C-C2C	-2.77	119.06	126.72
17	9	603	CLA	CMC-C2C-C1C	2.77	129.26	125.04
26	9	606	CHL	CAC-C3C-C4C	2.77	128.40	124.81
17	B	802	CLA	CMA-C3A-C4A	-2.77	104.33	111.77
17	b	834	CLA	CHD-C4C-NC	2.77	128.56	124.20
17	b	810	CLA	CHC-C1C-C2C	-2.77	119.06	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	847	BCR	C15-C16-C17	-2.77	117.80	123.47
17	8	303	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
20	l	205	BCR	C29-C30-C25	2.77	114.74	110.48
17	8	308	CLA	CAA-C2A-C3A	-2.77	105.20	112.78
17	7	604	CLA	CHD-C4C-NC	2.77	128.56	124.20
17	b	802	CLA	CMA-C3A-C4A	-2.77	104.34	111.77
17	B	810	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
17	A	834	CLA	CAC-C3C-C4C	2.77	128.40	124.81
17	a	841	CLA	CHD-C4C-NC	2.77	128.56	124.20
27	6	317	LUT	C21-C26-C27	-2.77	109.20	112.70
17	a	802	CLA	CHD-C4C-NC	2.77	128.56	124.20
17	2	610	CLA	C4C-C3C-C2C	-2.77	102.87	106.90
17	A	804	CLA	C4C-C3C-C2C	-2.77	102.87	106.90
17	b	804	CLA	CMC-C2C-C1C	2.77	129.25	125.04
27	4	616	LUT	C15-C14-C13	-2.76	123.36	127.31
17	6	311	CLA	CHC-C1C-C2C	-2.76	119.07	126.72
17	B	803	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
17	2	604	CLA	CHD-C4C-NC	2.76	128.56	124.20
17	B	827	CLA	CHD-C4C-NC	2.76	128.56	124.20
17	A	828	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
17	A	813	CLA	CHD-C4C-NC	2.76	128.56	124.20
17	2	610	CLA	CHD-C4C-NC	2.76	128.56	124.20
17	9	612	CLA	C4-C3-C5	2.76	119.92	115.27
17	7	611	CLA	C4-C3-C5	2.76	119.92	115.27
17	A	809	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
17	9	613	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
17	4	601	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
17	B	809	CLA	CHD-C4C-NC	2.76	128.56	124.20
17	9	601	CLA	CHD-C4C-NC	2.76	128.55	124.20
17	A	803	CLA	C4-C3-C5	2.76	119.92	115.27
17	2	604	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
17	L	204	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
17	a	809	CLA	CHC-C1C-C2C	-2.76	119.09	126.72
17	8	301	CLA	CHC-C1C-C2C	-2.76	119.09	126.72
17	B	824	CLA	CHD-C4C-NC	2.76	128.55	124.20
26	1	302	CHL	CAC-C3C-C4C	2.76	128.39	124.81
20	a	852	BCR	C7-C8-C9	-2.76	122.06	126.23
17	A	837	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
17	a	829	CLA	CHC-C1C-C2C	-2.76	119.09	126.72
26	2	605	CHL	CAC-C3C-C4C	2.76	128.39	124.81
17	F	301	CLA	CHD-C4C-NC	2.76	128.55	124.20
20	B	843	BCR	C7-C8-C9	-2.76	122.07	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	7	612	CLA	O2A-CGA-CBA	2.76	120.56	111.91
27	8	314	LUT	C15-C14-C13	-2.76	123.37	127.31
17	K	4003	CLA	CHD-C4C-NC	2.76	128.55	124.20
24	B	850	DGD	O1G-C1A-C2A	2.76	120.56	111.91
17	j	3002	CLA	CAA-C2A-C3A	-2.76	107.37	114.26
17	a	826	CLA	CAC-C3C-C4C	2.76	128.39	124.81
17	g	102	CLA	CHD-C4C-NC	2.76	128.55	124.20
17	B	802	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
17	a	802	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
17	B	826	CLA	C4-C3-C5	2.76	119.91	115.27
17	a	812	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
17	B	806	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
17	3	312	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
17	A	816	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
17	A	843	CLA	CHD-C4C-NC	2.76	128.54	124.20
17	A	802	CLA	CAA-C2A-C3A	-2.75	105.23	112.78
20	7	617	BCR	C11-C12-C13	-2.75	118.68	126.42
17	4	603	CLA	C4C-C3C-C2C	-2.75	102.88	106.90
17	B	832	CLA	CHD-C4C-NC	2.75	128.54	124.20
17	L	202	CLA	C4C-C3C-C2C	-2.75	102.88	106.90
17	B	807	CLA	C4-C3-C5	2.75	119.90	115.27
17	8	309	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
17	A	823	CLA	CHD-C4C-NC	2.75	128.54	124.20
20	4	618	BCR	C23-C24-C25	-2.75	119.47	127.20
17	A	841	CLA	CHC-C1C-C2C	-2.75	119.11	126.72
17	4	614	CLA	CAC-C3C-C4C	2.75	128.38	124.81
17	2	613	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
17	4	614	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
17	A	830	CLA	CHC-C1C-C2C	-2.75	119.11	126.72
17	9	609	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
17	a	818	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
17	2	608	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
17	A	812	CLA	O2A-CGA-CBA	2.75	120.54	111.91
17	B	830	CLA	CMC-C2C-C1C	2.75	129.23	125.04
17	3	303	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
17	b	833	CLA	CHD-C4C-NC	2.75	128.54	124.20
17	A	833	CLA	CBC-CAC-C3C	-2.75	104.85	112.43
17	B	839	CLA	CHD-C4C-NC	2.75	128.54	124.20
17	B	816	CLA	CHD-C4C-NC	2.75	128.54	124.20
17	A	839	CLA	CHD-C4C-NC	2.75	128.54	124.20
17	b	835	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
17	3	310	CLA	C4C-C3C-C2C	-2.75	102.89	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	802	CLA	CHD-C4C-NC	2.75	128.53	124.20
20	L	201	BCR	C3-C4-C5	-2.75	109.17	114.08
20	a	854	BCR	C3-C4-C5	-2.75	109.17	114.08
17	A	817	CLA	CAC-C3C-C4C	2.75	128.38	124.81
20	b	846	BCR	C21-C20-C19	-2.75	114.64	123.22
17	b	839	CLA	CHD-C4C-NC	2.75	128.53	124.20
26	7	601	CHL	CAC-C3C-C4C	2.75	128.37	124.81
17	B	836	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
28	1	317	XAT	C24-C23-C22	-2.75	105.47	110.77
17	A	818	CLA	C1-C2-C3	-2.75	121.29	126.04
17	a	814	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
17	a	828	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
17	B	820	CLA	CAC-C3C-C4C	2.75	128.37	124.81
17	2	609	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
17	K	4002	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
17	F	304	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
17	b	828	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
20	1	318	BCR	C23-C24-C25	-2.75	119.49	127.20
17	9	603	CLA	CHC-C1C-C2C	-2.75	119.13	126.72
17	B	827	CLA	C1-C2-C3	-2.75	121.29	126.04
17	9	612	CLA	CHD-C4C-NC	2.75	128.53	124.20
17	b	803	CLA	CHC-C1C-C2C	-2.74	119.13	126.72
17	A	833	CLA	C4-C3-C5	2.74	119.89	115.27
27	6	317	LUT	C15-C14-C13	-2.74	123.39	127.31
17	B	841	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
17	8	312	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
17	L	202	CLA	CAC-C3C-C4C	2.74	128.37	124.81
26	7	605	CHL	C2A-C1A-CHA	-2.74	119.06	123.86
17	a	810	CLA	CHD-C4C-NC	2.74	128.53	124.20
17	a	834	CLA	CAC-C3C-C4C	2.74	128.37	124.81
17	b	836	CLA	CHC-C1C-C2C	-2.74	119.13	126.72
20	B	847	BCR	C28-C27-C26	-2.74	109.18	114.08
17	8	305	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
17	a	801	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
28	6	318	XAT	C4-C3-C2	-2.74	105.48	110.77
17	F	303	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
17	a	839	CLA	CHD-C4C-NC	2.74	128.52	124.20
17	3	310	CLA	CHD-C4C-NC	2.74	128.52	124.20
17	8	301	CLA	C3B-C4B-NB	2.74	112.75	109.21
17	b	812	CLA	C1-C2-C3	-2.74	121.30	126.04
17	b	836	CLA	O2A-CGA-CBA	2.74	120.51	111.91
17	b	840	CLA	C4C-C3C-C2C	-2.74	102.90	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	F	303	CLA	CAC-C3C-C4C	2.74	128.37	124.81
17	A	839	CLA	C1-C2-C3	-2.74	121.30	126.04
17	A	811	CLA	CHD-C4C-NC	2.74	128.52	124.20
17	8	304	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
20	j	3003	BCR	C11-C10-C9	-2.74	123.40	127.31
17	b	807	CLA	CHD-C4C-NC	2.74	128.52	124.20
17	a	843	CLA	O2A-CGA-CBA	2.74	120.50	111.91
17	B	807	CLA	CHD-C4C-NC	2.74	128.52	124.20
17	A	802	CLA	C4-C3-C5	2.74	119.88	115.27
17	a	801	CLA	CMA-C3A-C4A	-2.74	104.41	111.77
17	f	7003	CLA	C4-C3-C5	2.74	119.88	115.27
17	4	612	CLA	O2A-CGA-CBA	2.74	120.50	111.91
17	1	309	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
17	g	103	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
20	b	846	BCR	C3-C4-C5	-2.74	109.19	114.08
26	9	606	CHL	O2A-CGA-CBA	2.74	120.50	111.91
17	b	807	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
17	b	836	CLA	C4-C3-C5	2.74	119.87	115.27
26	9	607	CHL	O2A-CGA-CBA	2.74	120.49	111.91
17	a	844	CLA	O2A-CGA-CBA	2.74	120.49	111.91
17	a	844	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
17	4	613	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
17	A	830	CLA	CMC-C2C-C1C	2.73	129.20	125.04
17	A	826	CLA	CHC-C1C-C2C	-2.73	119.16	126.72
17	a	838	CLA	CBC-CAC-C3C	-2.73	104.89	112.43
17	1	315	CLA	C4C-C3C-C2C	-2.73	102.91	106.90
17	b	802	CLA	CMA-C3A-C2A	-2.73	102.80	113.83
17	A	835	CLA	CHD-C4C-NC	2.73	128.51	124.20
17	B	802	CLA	CMC-C2C-C1C	2.73	129.20	125.04
17	7	609	CLA	CMC-C2C-C1C	2.73	129.20	125.04
17	B	836	CLA	O2A-CGA-CBA	2.73	120.48	111.91
17	f	7003	CLA	CHD-C4C-NC	2.73	128.51	124.20
17	G	101	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
17	A	814	CLA	C4-C3-C5	2.73	119.87	115.27
20	4	618	BCR	C38-C26-C25	-2.73	121.46	124.53
20	j	3004	BCR	C37-C22-C21	-2.73	119.10	122.92
17	6	313	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
17	a	820	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
27	6	317	LUT	C30-C31-C32	-2.73	114.69	123.22
17	b	808	CLA	CAC-C3C-C4C	2.73	128.35	124.81
17	9	610	CLA	CAC-C3C-C4C	2.73	128.35	124.81
17	a	804	CLA	O2D-CGD-O1D	-2.73	118.50	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	307	CHL	O2A-CGA-CBA	2.73	120.48	111.91
17	b	815	CLA	C4-C3-C5	2.73	119.86	115.27
17	A	814	CLA	O2A-CGA-CBA	2.73	120.48	111.91
26	6	308	CHL	O2D-CGD-O1D	-2.73	118.50	123.84
17	b	811	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
17	B	822	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
17	a	823	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
17	3	315	CLA	CHD-C4C-NC	2.73	128.42	124.21
17	A	834	CLA	CHD-C4C-NC	2.73	128.50	124.20
17	b	806	CLA	CMC-C2C-C1C	2.73	129.20	125.04
26	7	601	CHL	C3B-C4B-NB	2.73	112.74	109.21
17	a	809	CLA	O2A-CGA-CBA	2.73	120.47	111.91
17	3	301	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
17	7	609	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
17	a	810	CLA	C4-C3-C5	2.73	119.86	115.27
17	B	835	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
17	a	804	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
17	A	807	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
17	B	824	CLA	C3B-C4B-NB	2.73	112.74	109.21
17	b	810	CLA	CHD-C4C-NC	2.73	128.50	124.20
17	9	612	CLA	O2A-CGA-CBA	2.73	120.47	111.91
17	A	820	CLA	CAC-C3C-C4C	2.73	128.35	124.81
17	A	810	CLA	CAA-CBA-CGA	-2.73	105.28	113.25
17	b	804	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
26	2	601	CHL	CAC-C3C-C4C	2.73	128.35	124.81
26	7	601	CHL	C2A-C3A-C4A	-2.73	97.47	101.87
17	8	309	CLA	CHD-C4C-NC	2.73	128.50	124.20
17	4	608	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
17	A	838	CLA	CHC-C1C-C2C	-2.72	119.18	126.72
17	F	304	CLA	CHD-C4C-NC	2.72	128.50	124.20
17	8	312	CLA	CAC-C3C-C4C	2.72	128.34	124.81
17	b	828	CLA	C1-C2-C3	-2.72	121.33	126.04
17	B	808	CLA	CHD-C4C-NC	2.72	128.50	124.20
17	8	303	CLA	CHD-C4C-NC	2.72	128.50	124.20
17	A	817	CLA	CHD-C4C-NC	2.72	128.50	124.20
20	J	3003	BCR	C33-C5-C6	-2.72	121.47	124.53
17	4	601	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
17	6	312	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
17	9	602	CLA	CHC-C1C-C2C	-2.72	119.19	126.72
17	A	801	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
17	B	819	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
17	b	809	CLA	O2D-CGD-O1D	-2.72	118.51	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	824	CLA	CHD-C4C-NC	2.72	128.49	124.20
17	b	803	CLA	CHD-C4C-NC	2.72	128.49	124.20
17	a	838	CLA	C3B-C4B-NB	2.72	112.73	109.21
20	2	617	BCR	C7-C8-C9	-2.72	122.12	126.23
17	B	822	CLA	C4-C3-C5	2.72	119.85	115.27
17	A	832	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
17	9	610	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
17	1	312	CLA	O2A-CGA-CBA	2.72	120.45	111.91
17	a	811	CLA	O2A-CGA-CBA	2.72	120.45	111.91
17	b	826	CLA	O2A-CGA-CBA	2.72	120.45	111.91
17	b	837	CLA	CBC-CAC-C3C	-2.72	104.93	112.43
20	B	847	BCR	C8-C7-C6	-2.72	119.56	127.20
17	B	806	CLA	O2A-CGA-CBA	2.72	120.45	111.91
17	B	818	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
17	b	819	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
17	a	838	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
17	b	812	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
17	A	840	CLA	O2A-CGA-CBA	2.72	120.44	111.91
17	8	311	CLA	CHD-C4C-NC	2.72	128.49	124.20
17	8	302	CLA	CHD-C4C-NC	2.72	128.49	124.20
17	b	829	CLA	CBC-CAC-C3C	-2.72	104.93	112.43
26	7	607	CHL	C2A-C1A-CHA	-2.72	119.11	123.86
20	B	845	BCR	C29-C30-C25	2.72	114.67	110.48
17	9	601	CLA	C4C-C3C-C2C	-2.72	102.94	106.90
17	B	809	CLA	C4-C3-C5	2.72	119.84	115.27
17	B	817	CLA	CHD-C4C-NC	2.72	128.49	124.20
17	a	836	CLA	CAC-C3C-C4C	2.72	128.34	124.81
17	B	823	CLA	CAC-C3C-C4C	2.72	128.34	124.81
17	4	602	CLA	C1-C2-C3	-2.72	121.34	126.04
17	b	805	CLA	C1-C2-C3	-2.72	121.34	126.04
17	2	609	CLA	CMC-C2C-C1C	2.72	129.18	125.04
17	B	837	CLA	C4C-C3C-C2C	-2.72	102.94	106.90
17	b	822	CLA	O2A-CGA-CBA	2.72	120.44	111.91
17	6	306	CLA	O2A-CGA-CBA	2.72	120.43	111.91
17	b	837	CLA	C1-C2-C3	-2.72	121.34	126.04
17	A	845	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
26	9	606	CHL	O2D-CGD-O1D	-2.72	118.53	123.84
17	A	816	CLA	CAC-C3C-C4C	2.72	128.34	124.81
17	9	611	CLA	C4-C3-C5	2.72	119.84	115.27
17	a	840	CLA	C4-C3-C5	2.72	119.84	115.27
17	3	303	CLA	CHD-C4C-NC	2.72	128.48	124.20
17	9	611	CLA	CHD-C4C-NC	2.72	128.48	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	824	CLA	C4C-C3C-C2C	-2.72	102.94	106.90
17	4	612	CLA	C4C-C3C-C2C	-2.72	102.94	106.90
17	b	819	CLA	O2A-CGA-CBA	2.72	120.43	111.91
26	9	605	CHL	C2A-C1A-CHA	-2.72	119.11	123.86
17	A	828	CLA	CHC-C1C-C2C	-2.71	119.21	126.72
17	A	809	CLA	O2A-CGA-CBA	2.71	120.43	111.91
17	4	603	CLA	CMC-C2C-C1C	2.71	129.17	125.04
17	b	827	CLA	CAC-C3C-C4C	2.71	128.33	124.81
17	b	806	CLA	C4C-C3C-C2C	-2.71	102.94	106.90
20	g	104	BCR	C33-C5-C6	-2.71	121.48	124.53
27	4	616	LUT	C8-C7-C6	-2.71	119.58	127.20
17	F	304	CLA	O2A-CGA-CBA	2.71	120.42	111.91
17	a	818	CLA	O2A-CGA-CBA	2.71	120.42	111.91
17	1	313	CLA	C4C-C3C-C2C	-2.71	102.94	106.90
17	3	304	CLA	C4C-C3C-C2C	-2.71	102.94	106.90
17	b	819	CLA	CMB-C2B-C3B	2.71	129.75	124.68
17	B	812	CLA	CHD-C4C-NC	2.71	128.48	124.20
17	a	817	CLA	C4C-C3C-C2C	-2.71	102.94	106.90
17	9	612	CLA	C4C-C3C-C2C	-2.71	102.94	106.90
17	B	834	CLA	O2A-CGA-CBA	2.71	120.42	111.91
17	a	812	CLA	CAC-C3C-C4C	2.71	128.33	124.81
17	b	822	CLA	CBC-CAC-C3C	-2.71	104.95	112.43
17	b	816	CLA	CHD-C4C-NC	2.71	128.48	124.20
17	6	315	CLA	C4C-C3C-C2C	-2.71	102.94	106.90
17	a	802	CLA	CAA-C2A-C3A	-2.71	105.35	112.78
17	A	803	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
20	b	846	BCR	C7-C8-C9	-2.71	122.14	126.23
17	A	804	CLA	CAC-C3C-C4C	2.71	128.33	124.81
20	F	305	BCR	C35-C13-C14	-2.71	119.13	122.92
17	3	309	CLA	CHC-C1C-C2C	-2.71	119.22	126.72
20	B	846	BCR	C21-C20-C19	-2.71	114.76	123.22
17	8	310	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
17	8	307	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
17	7	611	CLA	CHD-C4C-NC	2.71	128.47	124.20
17	1	311	CLA	CHD-C4C-NC	2.71	128.47	124.20
17	L	204	CLA	O2A-CGA-CBA	2.71	120.41	111.91
20	b	848	BCR	C28-C27-C26	-2.71	109.24	114.08
17	4	604	CLA	CHD-C4C-NC	2.71	128.47	124.20
17	A	802	CLA	C1-C2-C3	-2.71	121.36	126.04
20	a	851	BCR	C29-C30-C25	2.71	114.65	110.48
17	3	302	CLA	C4-C3-C5	2.71	119.83	115.27
17	b	806	CLA	CHC-C1C-C2C	-2.71	119.23	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	7	610	CLA	CHD-C4C-NC	2.71	128.47	124.20
17	a	833	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
17	1	304	CLA	C1-C2-C3	-2.71	121.36	126.04
17	l	202	CLA	CAC-C3C-C4C	2.71	128.32	124.81
17	g	101	CLA	CAC-C3C-C4C	2.71	128.32	124.81
17	b	812	CLA	O2A-CGA-CBA	2.71	120.40	111.91
17	B	827	CLA	CHC-C1C-C2C	-2.71	119.23	126.72
17	B	823	CLA	CHD-C4C-NC	2.71	128.47	124.20
17	k	1401	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
26	7	605	CHL	CAC-C3C-C4C	2.71	128.32	124.81
17	9	604	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
17	2	611	CLA	C1-C2-C3	-2.71	121.36	126.04
17	A	818	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
17	b	839	CLA	O2A-CGA-CBA	2.70	120.40	111.91
17	B	822	CLA	CMB-C2B-C3B	2.70	129.74	124.68
17	a	818	CLA	CHD-C4C-NC	2.70	128.47	124.20
17	7	612	CLA	CHD-C4C-NC	2.70	128.47	124.20
20	J	3003	BCR	C29-C30-C25	2.70	114.64	110.48
17	b	820	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
17	2	609	CLA	CHC-C1C-C2C	-2.70	119.24	126.72
17	a	819	CLA	CMC-C2C-C1C	2.70	129.16	125.04
17	B	812	CLA	O2A-CGA-CBA	2.70	120.39	111.91
28	7	616	XAT	C18-C5-C4	2.70	117.32	114.28
26	4	606	CHL	O2D-CGD-O1D	-2.70	118.55	123.84
26	4	605	CHL	C2A-C1A-CHA	-2.70	119.13	123.86
17	a	809	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
17	A	803	CLA	CHD-C4C-NC	2.70	128.46	124.20
17	b	836	CLA	C4D-C3D-CAD	-2.70	106.96	108.47
17	B	818	CLA	CAC-C3C-C4C	2.70	128.32	124.81
17	1	305	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
17	A	804	CLA	CAA-C2A-C3A	-2.70	105.38	112.78
20	6	319	BCR	C23-C24-C25	-2.70	119.62	127.20
17	f	7002	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
17	a	827	CLA	C4-C3-C5	2.70	119.81	115.27
17	B	819	CLA	CHD-C4C-NC	2.70	128.46	124.20
17	a	822	CLA	CHD-C4C-NC	2.70	128.46	124.20
17	4	608	CLA	CHD-C4C-NC	2.70	128.46	124.20
17	b	812	CLA	C4-C3-C5	2.70	119.81	115.27
17	2	609	CLA	CAA-C2A-C3A	-2.70	105.39	112.78
17	a	822	CLA	C1-C2-C3	-2.70	121.38	126.04
17	b	841	CLA	CMC-C2C-C1C	2.70	129.15	125.04
17	a	827	CLA	CMB-C2B-C3B	2.70	129.73	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	808	CLA	CHC-C1C-C2C	-2.70	119.26	126.72
17	3	312	CLA	CHD-C4C-NC	2.70	128.46	124.20
17	6	305	CLA	C4C-C3C-C2C	-2.70	102.97	106.90
27	3	316	LUT	C8-C7-C6	-2.70	119.63	127.20
17	a	830	CLA	CMB-C2B-C3B	2.70	129.72	124.68
20	b	848	BCR	C24-C23-C22	-2.70	122.16	126.23
17	k	1403	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
17	A	825	CLA	CHD-C4C-NC	2.70	128.45	124.20
17	a	803	CLA	C1-C2-C3	-2.70	121.38	126.04
20	b	846	BCR	C11-C10-C9	-2.70	123.46	127.31
17	B	816	CLA	C4C-C3C-C2C	-2.70	102.97	106.90
17	b	817	CLA	C4C-C3C-C2C	-2.70	102.97	106.90
17	l	202	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
17	A	832	CLA	O2A-CGA-CBA	2.69	120.36	111.91
17	a	834	CLA	CMC-C2C-C1C	2.69	129.14	125.04
17	a	804	CLA	O2A-CGA-CBA	2.69	120.36	111.91
17	b	810	CLA	O2A-CGA-CBA	2.69	120.36	111.91
17	B	825	CLA	CMC-C2C-C1C	2.69	129.14	125.04
17	B	805	CLA	CAC-C3C-C4C	2.69	128.30	124.81
17	B	819	CLA	C4-C3-C5	2.69	119.80	115.27
17	B	835	CLA	CMB-C2B-C3B	2.69	129.72	124.68
17	F	301	CLA	CMC-C2C-C1C	2.69	129.14	125.04
26	2	607	CHL	C2A-C1A-CHA	-2.69	119.15	123.86
17	a	828	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
17	l	204	CLA	CAC-C3C-C4C	2.69	128.30	124.81
17	B	821	CLA	CHD-C4C-NC	2.69	128.44	124.20
17	A	807	CLA	CAC-C3C-C4C	2.69	128.30	124.81
17	2	603	CLA	C1-C2-C3	-2.69	121.39	126.04
17	a	833	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
20	B	844	BCR	C16-C17-C18	-2.69	123.47	127.31
17	8	313	CLA	CHD-C4C-NC	2.69	128.36	124.21
17	a	856	CLA	O2A-C1-C2	2.69	115.70	108.64
17	A	845	CLA	O2A-CGA-CBA	2.69	120.34	111.91
17	4	614	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
17	8	302	CLA	O2A-CGA-CBA	2.69	120.34	111.91
17	a	834	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
17	A	842	CLA	O2A-C1-C2	2.69	115.69	108.64
17	a	837	CLA	CHD-C4C-NC	2.68	128.43	124.20
17	6	310	CLA	O2A-CGA-CBA	2.68	120.33	111.91
17	1	304	CLA	CBC-CAC-C3C	-2.68	105.03	112.43
17	B	841	CLA	CHC-C1C-C2C	-2.68	119.30	126.72
17	b	839	CLA	CAC-C3C-C4C	2.68	128.29	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	j	3002	CLA	CHD-C4C-NC	2.68	128.43	124.20
27	8	314	LUT	C10-C11-C12	-2.68	114.84	123.22
17	a	830	CLA	CHC-C1C-C2C	-2.68	119.30	126.72
20	B	848	BCR	C21-C20-C19	-2.68	114.84	123.22
17	7	609	CLA	CHC-C1C-C2C	-2.68	119.30	126.72
17	l	203	CLA	CHC-C1C-C2C	-2.68	119.30	126.72
17	A	845	CLA	CAC-C3C-C4C	2.68	128.29	124.81
17	F	301	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
17	1	304	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
17	L	203	CLA	C2A-C1A-CHA	-2.68	119.17	123.86
17	A	837	CLA	CHD-C4C-NC	2.68	128.43	124.20
17	b	816	CLA	O2A-CGA-CBA	2.68	120.32	111.91
17	A	813	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
20	B	847	BCR	C21-C20-C19	-2.68	114.85	123.22
17	B	826	CLA	C3B-C4B-NB	2.68	112.68	109.21
17	b	814	CLA	CHC-C1C-C2C	-2.68	119.31	126.72
17	a	835	CLA	C4-C3-C5	2.68	119.78	115.27
17	1	313	CLA	CHD-C4C-NC	2.68	128.43	124.20
17	3	301	CLA	CHD-C4C-NC	2.68	128.43	124.20
17	b	802	CLA	CAC-C3C-C4C	2.68	128.29	124.81
17	f	7003	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
18	b	842	PQN	C14-C13-C15	2.68	119.78	115.27
17	A	812	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
17	3	314	CLA	CHD-C4C-NC	2.68	128.42	124.20
17	1	314	CLA	CHD-C4C-NC	2.68	128.42	124.20
19	A	846	LHG	C5-O7-C7	-2.68	111.20	117.79
17	A	830	CLA	C4-C3-C5	2.68	119.77	115.27
17	A	838	CLA	O2A-CGA-CBA	2.68	120.31	111.91
17	K	4002	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
17	A	811	CLA	C4C-C3C-C2C	-2.68	103.00	106.90
17	a	806	CLA	CAA-C2A-C3A	-2.68	105.45	112.78
17	1	310	CLA	CAA-C2A-C3A	-2.68	105.45	112.78
25	G	102	LMG	O8-C28-C29	2.68	120.30	111.91
17	2	608	CLA	CAC-C3C-C4C	2.68	128.28	124.81
17	b	814	CLA	C2A-C1A-CHA	-2.67	119.18	123.86
17	L	203	CLA	CHC-C1C-C2C	-2.67	119.32	126.72
17	3	301	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
17	b	818	CLA	CMC-C2C-C1C	2.67	129.11	125.04
17	A	832	CLA	CHD-C4C-NC	2.67	128.42	124.20
17	A	838	CLA	CMC-C2C-C1C	2.67	129.11	125.04
17	2	602	CLA	C4C-C3C-C2C	-2.67	103.00	106.90
20	B	843	BCR	C3-C4-C5	-2.67	109.30	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	843	BCR	C2-C1-C6	2.67	114.60	110.48
20	b	848	BCR	C10-C11-C12	-2.67	114.88	123.22
17	a	811	CLA	C4-C3-C5	2.67	119.77	115.27
17	a	812	CLA	CHD-C4C-NC	2.67	128.41	124.20
17	b	818	CLA	CHD-C4C-NC	2.67	128.41	124.20
17	A	801	CLA	CMA-C3A-C4A	-2.67	104.59	111.77
17	B	804	CLA	C4C-C3C-C2C	-2.67	103.00	106.90
17	9	608	CLA	CHD-C4C-NC	2.67	128.41	124.20
26	2	605	CHL	C2A-C1A-CHA	-2.67	119.19	123.86
17	3	309	CLA	CAA-C2A-C3A	-2.67	105.47	112.78
20	J	3003	BCR	C38-C26-C25	-2.67	121.53	124.53
17	A	808	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
17	b	829	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
17	A	854	CLA	C4-C3-C5	2.67	119.76	115.27
20	B	846	BCR	C38-C26-C25	-2.67	121.53	124.53
17	b	812	CLA	CMC-C2C-C1C	2.67	129.10	125.04
17	4	604	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
17	A	821	CLA	CAC-C3C-C4C	2.67	128.27	124.81
17	7	603	CLA	CMC-C2C-C1C	2.67	129.10	125.04
17	a	839	CLA	C4-C3-C5	2.67	119.76	115.27
17	a	813	CLA	CMB-C2B-C3B	2.67	129.67	124.68
17	B	811	CLA	C1-C2-C3	-2.67	121.43	126.04
26	8	306	CHL	CHD-C4C-NC	2.67	128.41	124.20
17	6	307	CLA	CAA-C2A-C3A	-2.67	107.60	114.26
26	1	307	CHL	C2A-C1A-CHA	-2.67	119.20	123.86
17	a	812	CLA	C4-C3-C5	2.67	119.76	115.27
17	8	310	CLA	O2A-CGA-CBA	2.67	120.27	111.91
17	A	817	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
17	9	614	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
17	b	817	CLA	CHD-C4C-NC	2.67	128.40	124.20
17	A	839	CLA	C4-C3-C5	2.66	119.75	115.27
17	B	826	CLA	CHC-C1C-C2C	-2.66	119.35	126.72
17	k	1403	CLA	CHD-C4C-NC	2.66	128.40	124.20
17	a	807	CLA	CAC-C3C-C4C	2.66	128.27	124.81
20	2	617	BCR	C31-C1-C6	-2.66	105.98	110.30
17	1	311	CLA	CAC-C3C-C4C	2.66	128.27	124.81
17	A	843	CLA	C4C-C3C-C2C	-2.66	103.02	106.90
17	A	802	CLA	CHC-C1C-C2C	-2.66	119.35	126.72
17	J	3002	CLA	CHD-C4C-NC	2.66	128.40	124.20
20	B	843	BCR	C2-C1-C6	2.66	114.58	110.48
17	B	830	CLA	C1D-CHD-C4C	-2.66	119.04	122.56
19	6	320	LHG	O8-C23-C24	2.66	120.26	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	845	CLA	C4-C3-C5	2.66	119.75	115.27
17	B	825	CLA	CHC-C1C-C2C	-2.66	119.36	126.72
17	A	821	CLA	C4C-C3C-C2C	-2.66	103.02	106.90
17	2	604	CLA	C4-C3-C5	2.66	119.75	115.27
17	a	809	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
20	3	318	BCR	C21-C20-C19	-2.66	114.92	123.22
26	6	303	CHL	C4-C3-C5	2.66	119.75	115.27
17	B	825	CLA	C4-C3-C5	2.66	119.75	115.27
17	b	809	CLA	C1-C2-C3	-2.66	121.44	126.04
17	4	609	CLA	C4C-C3C-C2C	-2.66	103.02	106.90
17	a	817	CLA	CHD-C4C-NC	2.66	128.39	124.20
17	B	813	CLA	CHD-C4C-NC	2.66	128.39	124.20
17	B	830	CLA	O2A-CGA-CBA	2.66	120.25	111.91
17	a	846	CLA	O2A-CGA-CBA	2.66	120.25	111.91
17	6	314	CLA	CHD-C4C-NC	2.66	128.39	124.20
17	B	830	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
17	J	3002	CLA	CAA-C2A-C3A	-2.66	107.62	114.26
17	L	202	CLA	C1-C2-C3	-2.66	121.45	126.04
17	a	840	CLA	C1-O2A-CGA	2.66	123.42	116.44
17	7	603	CLA	C4C-C3C-C2C	-2.66	103.02	106.90
17	8	309	CLA	C4-C3-C5	2.66	119.74	115.27
17	b	825	CLA	CHC-C1C-C2C	-2.66	119.37	126.72
17	b	813	CLA	C4-C3-C5	2.66	119.74	115.27
17	a	819	CLA	CHC-C1C-C2C	-2.66	119.37	126.72
17	b	818	CLA	C4C-C3C-C2C	-2.66	103.03	106.90
17	a	803	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
17	b	822	CLA	C4C-C3C-C2C	-2.66	103.03	106.90
17	A	835	CLA	C1-C2-C3	-2.66	121.45	126.04
17	B	803	CLA	O2A-CGA-CBA	2.65	120.24	111.91
27	1	320	LUT	C8-C7-C6	-2.65	119.75	127.20
17	G	101	CLA	CAC-C3C-C4C	2.65	128.25	124.81
20	b	845	BCR	C37-C22-C21	-2.65	119.20	122.92
17	b	823	CLA	CHD-C4C-NC	2.65	128.38	124.20
28	3	317	XAT	C31-C30-C29	-2.65	123.52	127.31
17	b	803	CLA	CMB-C2B-C3B	2.65	129.64	124.68
17	A	818	CLA	C4-C3-C5	2.65	119.73	115.27
17	A	801	CLA	CAC-C3C-C4C	2.65	128.25	124.81
17	A	808	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
17	A	820	CLA	C4C-C3C-C2C	-2.65	103.03	106.90
17	A	814	CLA	CHD-C4C-NC	2.65	128.38	124.20
17	B	803	CLA	CMB-C2B-C3B	2.65	129.64	124.68
17	A	841	CLA	C3B-C4B-NB	2.65	112.64	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	814	CLA	CMC-C2C-C1C	2.65	129.08	125.04
17	a	834	CLA	C4C-C3C-C2C	-2.65	103.03	106.90
17	a	836	CLA	CHD-C4C-NC	2.65	128.38	124.20
17	3	308	CLA	CHD-C4C-NC	2.65	128.38	124.20
26	1	302	CHL	C2A-C1A-CHA	-2.65	119.22	123.86
17	A	815	CLA	CAC-C3C-C4C	2.65	128.25	124.81
17	A	829	CLA	CAC-C3C-C4C	2.65	128.25	124.81
20	B	846	BCR	C3-C4-C5	-2.65	109.35	114.08
17	A	835	CLA	O2A-CGA-CBA	2.65	120.22	111.91
17	B	808	CLA	C4C-C3C-C2C	-2.65	103.04	106.90
17	a	832	CLA	O2A-CGA-CBA	2.65	120.22	111.91
17	a	839	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
17	4	601	CLA	CAC-C3C-C4C	2.65	128.25	124.81
17	b	822	CLA	C4-C3-C5	2.65	119.73	115.27
17	A	812	CLA	C4-C3-C5	2.65	119.73	115.27
20	B	844	BCR	C29-C30-C25	2.65	114.56	110.48
17	g	103	CLA	CMC-C2C-C1C	2.65	129.07	125.04
20	a	850	BCR	C20-C21-C22	-2.65	123.53	127.31
17	9	602	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
17	a	803	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
20	b	801	BCR	C33-C5-C6	-2.65	121.56	124.53
20	F	305	BCR	C28-C27-C26	-2.65	109.35	114.08
26	3	307	CHL	C2A-C1A-CHA	-2.65	119.23	123.86
28	4	617	XAT	C38-C25-C24	2.65	117.26	114.28
17	a	801	CLA	CBC-CAC-C3C	-2.65	105.13	112.43
17	B	803	CLA	CHC-C1C-C2C	-2.65	119.40	126.72
20	A	849	BCR	C38-C26-C25	-2.65	121.56	124.53
17	A	813	CLA	O2A-CGA-CBA	2.65	120.21	111.91
17	A	818	CLA	O2A-CGA-CBA	2.65	120.21	111.91
17	A	807	CLA	C1-C2-C3	-2.65	121.47	126.04
17	b	833	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
28	1	317	XAT	C19-C9-C8	2.65	122.25	118.08
20	G	105	BCR	C33-C5-C6	-2.64	121.56	124.53
17	a	821	CLA	C4C-C3C-C2C	-2.64	103.04	106.90
17	a	822	CLA	CAC-C3C-C4C	2.64	128.24	124.81
17	b	833	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
20	7	617	BCR	C3-C4-C5	-2.64	109.36	114.08
17	A	845	CLA	CHD-C4C-NC	2.64	128.37	124.20
17	7	604	CLA	C1-C2-C3	-2.64	121.47	126.04
17	f	7003	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
17	g	103	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
17	1	314	CLA	C4C-C3C-C2C	-2.64	103.05	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	808	CLA	CBC-CAC-C3C	-2.64	105.15	112.43
20	G	105	BCR	C10-C11-C12	-2.64	114.97	123.22
26	9	606	CHL	C1-C2-C3	-2.64	122.48	126.75
17	1	314	CLA	C1-C2-C3	-2.64	121.47	126.04
28	7	616	XAT	C35-C15-C14	-2.64	118.06	123.47
17	b	820	CLA	CAC-C3C-C4C	2.64	128.24	124.81
17	b	821	CLA	CHD-C4C-NC	2.64	128.36	124.20
17	3	305	CLA	CAA-C2A-C3A	-2.64	107.66	114.26
17	4	608	CLA	CMC-C2C-C1C	2.64	129.06	125.04
20	a	851	BCR	C20-C21-C22	-2.64	123.54	127.31
17	A	824	CLA	CHD-C4C-NC	2.64	128.36	124.20
17	f	7002	CLA	CMC-C2C-C1C	2.64	129.06	125.04
17	g	103	CLA	CBC-CAC-C3C	-2.64	105.16	112.43
17	b	814	CLA	O2A-CGA-CBA	2.64	120.18	111.91
17	A	823	CLA	O2A-CGA-CBA	2.64	120.18	111.91
17	J	3002	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
27	4	616	LUT	C7-C8-C9	-2.64	122.25	126.23
17	b	841	CLA	C4-C3-C5	2.64	119.71	115.27
17	A	811	CLA	O2A-CGA-CBA	2.64	120.18	111.91
17	a	836	CLA	CBC-CAC-C3C	-2.64	105.17	112.43
17	L	202	CLA	C4-C3-C5	2.64	119.70	115.27
20	9	618	BCR	C23-C24-C25	-2.64	119.80	127.20
17	A	803	CLA	CBC-CAC-C3C	-2.63	105.17	112.43
17	6	304	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
17	A	802	CLA	C3B-C4B-NB	2.63	112.62	109.21
17	1	311	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
17	b	830	CLA	O2A-CGA-CBA	2.63	120.17	111.91
17	A	830	CLA	O2A-CGA-CBA	2.63	120.17	111.91
17	a	839	CLA	CAC-C3C-C4C	2.63	128.23	124.81
20	A	856	BCR	C33-C5-C4	2.63	118.67	113.62
17	a	846	CLA	CHD-C4C-NC	2.63	128.35	124.20
17	b	837	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
17	B	820	CLA	O2A-CGA-CBA	2.63	120.16	111.91
20	B	843	BCR	C27-C26-C25	-2.63	118.91	122.73
17	6	312	CLA	CAC-C3C-C4C	2.63	128.22	124.81
17	A	807	CLA	CAA-C2A-C3A	-2.63	105.58	112.78
17	7	602	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
17	9	604	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
17	b	808	CLA	C4C-C3C-C2C	-2.63	103.07	106.90
20	B	845	BCR	C34-C9-C10	-2.63	119.24	122.92
26	6	303	CHL	C2A-C1A-CHA	-2.63	119.26	123.86
17	4	610	CLA	C4-C3-C5	2.63	119.69	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	609	CLA	CAA-C2A-C3A	-2.63	105.58	112.78
17	9	608	CLA	CAC-C3C-C4C	2.63	128.22	124.81
17	B	814	CLA	CHC-C1C-C2C	-2.63	119.46	126.72
17	A	826	CLA	CMC-C2C-C1C	2.63	129.04	125.04
17	3	313	CLA	CHD-C4C-NC	2.63	128.34	124.20
17	B	839	CLA	CMB-C2B-C3B	2.63	129.59	124.68
20	l	201	BCR	C24-C23-C22	-2.63	122.27	126.23
17	a	805	CLA	C4C-C3C-C2C	-2.63	103.07	106.90
20	j	3004	BCR	C7-C8-C9	-2.62	122.27	126.23
17	6	313	CLA	O2A-CGA-CBA	2.62	120.14	111.91
17	a	834	CLA	CBC-CAC-C3C	-2.62	105.20	112.43
17	B	832	CLA	O2A-CGA-CBA	2.62	120.14	111.91
27	6	317	LUT	C8-C7-C6	-2.62	119.83	127.20
27	9	616	LUT	C21-C26-C27	-2.62	109.39	112.70
17	8	305	CLA	CAC-C3C-C4C	2.62	128.21	124.81
17	L	204	CLA	CAC-C3C-C4C	2.62	128.21	124.81
17	b	822	CLA	CMB-C2B-C3B	2.62	129.59	124.68
17	a	813	CLA	O2A-CGA-CBA	2.62	120.14	111.91
17	1	314	CLA	CBC-CAC-C3C	-2.62	105.20	112.43
17	7	604	CLA	C4-C3-C5	2.62	119.68	115.27
20	b	843	BCR	C36-C18-C17	-2.62	119.25	122.92
17	a	807	CLA	CHC-C1C-C2C	-2.62	119.47	126.72
26	9	605	CHL	CAC-C3C-C4C	2.62	128.21	124.81
26	4	607	CHL	C2A-C1A-CHA	-2.62	119.28	123.86
20	7	617	BCR	C34-C9-C10	-2.62	119.25	122.92
17	a	819	CLA	C3B-C4B-NB	2.62	112.60	109.21
20	J	3003	BCR	C3-C4-C5	-2.62	109.40	114.08
17	b	809	CLA	O2A-CGA-CBA	2.62	120.13	111.91
26	1	307	CHL	O2D-CGD-O1D	-2.62	118.72	123.84
17	7	613	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
17	b	815	CLA	CHD-C4C-NC	2.62	128.33	124.20
26	7	606	CHL	CBC-CAC-C3C	-2.62	105.21	112.43
17	7	602	CLA	CMC-C2C-C1C	2.62	129.03	125.04
17	a	804	CLA	CMC-C2C-C1C	2.62	129.03	125.04
17	9	608	CLA	CMB-C2B-C3B	2.62	129.57	124.68
17	9	604	CLA	CAC-C3C-C4C	2.62	128.21	124.81
20	l	205	BCR	C16-C17-C18	-2.62	123.58	127.31
17	A	843	CLA	C4-C3-C5	2.62	119.67	115.27
17	A	809	CLA	CMC-C2C-C1C	2.62	129.02	125.04
17	A	806	CLA	O2A-CGA-CBA	2.62	120.11	111.91
17	1	313	CLA	O2A-CGA-CBA	2.62	120.11	111.91
17	6	305	CLA	C1-C2-C3	-2.62	121.52	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	827	CLA	CAC-C3C-C4C	2.62	128.20	124.81
17	b	832	CLA	C4-C3-C5	2.62	119.67	115.27
17	a	846	CLA	C4-C3-C5	2.62	119.67	115.27
17	B	833	CLA	C1-C2-C3	-2.61	121.52	126.04
27	3	316	LUT	C21-C26-C27	-2.61	109.40	112.70
17	b	809	CLA	C4C-C3C-C2C	-2.61	103.09	106.90
17	8	307	CLA	O2A-CGA-CBA	2.61	120.11	111.91
17	6	312	CLA	CBC-CAC-C3C	-2.61	105.23	112.43
25	4	619	LMG	O8-C28-C29	2.61	120.11	111.91
17	A	854	CLA	CHD-C4C-NC	2.61	128.32	124.20
17	b	819	CLA	CHD-C4C-NC	2.61	128.32	124.20
20	b	848	BCR	C21-C20-C19	-2.61	115.06	123.22
18	a	845	PQN	C2M-C2-C3	-2.61	120.14	124.40
17	B	837	CLA	C1-C2-C3	-2.61	121.53	126.04
17	A	802	CLA	CHB-C4A-NA	2.61	128.12	124.51
17	B	809	CLA	CAC-C3C-C4C	2.61	128.20	124.81
17	B	828	CLA	CAC-C3C-C4C	2.61	128.20	124.81
17	B	813	CLA	C4-C3-C5	2.61	119.66	115.27
17	2	609	CLA	CBC-CAC-C3C	-2.61	105.23	112.43
17	a	831	CLA	C4-C3-C5	2.61	119.66	115.27
17	B	807	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
17	a	829	CLA	C4-C3-C5	2.61	119.66	115.27
17	l	203	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
17	2	609	CLA	CMB-C2B-C3B	2.61	129.56	124.68
20	B	846	BCR	C16-C17-C18	-2.61	123.59	127.31
17	b	837	CLA	C4-C3-C5	2.61	119.66	115.27
17	B	829	CLA	CBC-CAC-C3C	-2.61	105.24	112.43
17	A	831	CLA	O2A-CGA-CBA	2.61	120.09	111.91
17	A	824	CLA	O2A-CGA-CBA	2.61	120.09	111.91
17	A	819	CLA	CMB-C2B-C3B	2.61	129.56	124.68
20	b	843	BCR	C3-C4-C5	-2.61	109.42	114.08
27	1	320	LUT	C30-C31-C32	-2.61	115.08	123.22
17	a	838	CLA	CAC-C3C-C4C	2.61	128.19	124.81
17	a	840	CLA	O2A-CGA-CBA	2.61	120.09	111.91
17	b	819	CLA	C4-C3-C5	2.61	119.66	115.27
17	b	830	CLA	CHD-C4C-NC	2.61	128.31	124.20
17	j	3002	CLA	CMB-C2B-C3B	2.61	129.56	124.68
17	B	805	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
17	A	832	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
26	9	605	CHL	C1-C2-C3	-2.61	121.54	126.04
26	9	615	CHL	CMB-C2B-C3B	2.61	129.55	124.68
17	a	826	CLA	CMC-C2C-C1C	2.60	129.01	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	847	LHG	C5-O7-C7	-2.60	111.38	117.79
28	9	617	XAT	C38-C25-C24	2.60	117.21	114.28
17	7	608	CLA	CAC-C3C-C4C	2.60	128.19	124.81
17	6	315	CLA	C4-C3-C5	2.60	119.65	115.27
17	B	802	CLA	CBC-CAC-C3C	-2.60	105.26	112.43
17	b	827	CLA	CHC-C1C-C2C	-2.60	119.52	126.72
17	A	825	CLA	C4-C3-C5	2.60	119.65	115.27
17	B	816	CLA	CMB-C2B-C3B	2.60	129.55	124.68
20	2	617	BCR	C33-C5-C4	2.60	118.61	113.62
20	a	851	BCR	C11-C10-C9	-2.60	123.60	127.31
17	a	844	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
17	k	1402	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
20	A	850	BCR	C24-C23-C22	-2.60	122.31	126.23
17	a	821	CLA	CMC-C2C-C1C	2.60	129.00	125.04
28	8	315	XAT	C19-C9-C8	2.60	122.17	118.08
17	b	806	CLA	CAC-C3C-C4C	2.60	128.18	124.81
17	A	809	CLA	C4-C3-C5	2.60	119.64	115.27
17	b	823	CLA	CMC-C2C-C1C	2.60	129.00	125.04
17	b	816	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
17	B	807	CLA	CMB-C2B-C3B	2.60	129.54	124.68
20	B	844	BCR	C33-C5-C4	2.60	118.61	113.62
17	B	822	CLA	O2A-CGA-CBA	2.60	120.06	111.91
17	a	828	CLA	O2A-CGA-CBA	2.60	120.05	111.91
26	9	615	CHL	O2D-CGD-O1D	-2.59	118.77	123.84
17	A	841	CLA	CMB-C2B-C3B	2.59	129.53	124.68
26	4	607	CHL	CAC-C3C-C4C	2.59	128.18	124.81
17	B	811	CLA	CAC-C3C-C4C	2.59	128.18	124.81
20	b	847	BCR	C20-C21-C22	-2.59	123.61	127.31
17	4	614	CLA	O2A-CGA-CBA	2.59	120.05	111.91
17	A	832	CLA	CMB-C2B-C3B	2.59	129.53	124.68
17	6	311	CLA	CAA-C2A-C3A	-2.59	105.68	112.78
17	A	805	CLA	CBC-CAC-C3C	-2.59	105.28	112.43
20	j	3003	BCR	C20-C21-C22	-2.59	123.61	127.31
17	A	833	CLA	CAC-C3C-C4C	2.59	128.17	124.81
17	B	804	CLA	CBC-CAC-C3C	-2.59	105.29	112.43
17	B	803	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
17	A	822	CLA	C1-C2-C3	-2.59	121.56	126.04
17	9	602	CLA	CMC-C2C-C1C	2.59	128.98	125.04
17	B	811	CLA	CAB-C3B-C2B	2.59	129.76	124.69
17	a	840	CLA	C1-C2-C3	-2.59	121.57	126.04
17	A	842	CLA	CMB-C2B-C3B	2.59	129.52	124.68
17	7	608	CLA	CAA-C2A-C3A	-2.59	105.69	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	7	609	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
17	a	811	CLA	CHD-C4C-NC	2.59	128.28	124.20
26	4	605	CHL	CAC-C3C-C4C	2.59	128.17	124.81
17	a	842	CLA	CAC-C3C-C4C	2.59	128.17	124.81
17	B	834	CLA	CHD-C4C-NC	2.59	128.28	124.20
17	3	302	CLA	CMB-C2B-C3B	2.59	129.52	124.68
17	B	833	CLA	CAC-C3C-C4C	2.59	128.17	124.81
17	4	602	CLA	CMB-C2B-C3B	2.59	129.52	124.68
20	B	846	BCR	C7-C8-C9	-2.59	122.33	126.23
17	1	303	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
17	a	813	CLA	CHD-C4C-NC	2.59	128.28	124.20
17	b	811	CLA	CAB-C3B-C2B	2.59	129.75	124.69
17	8	301	CLA	C4-C3-C5	2.58	119.62	115.27
17	3	301	CLA	CMB-C2B-C3B	2.58	129.51	124.68
17	B	814	CLA	C4-C3-C5	2.58	119.62	115.27
17	a	802	CLA	CGD-CBD-CAD	2.58	119.10	110.73
17	a	835	CLA	CAA-C2A-C3A	-2.58	105.70	112.78
27	7	615	LUT	C21-C26-C27	-2.58	109.44	112.70
17	f	7003	CLA	CBC-CAC-C3C	-2.58	105.31	112.43
17	b	817	CLA	CAA-C2A-C3A	-2.58	105.71	112.78
17	A	819	CLA	C4-C3-C5	2.58	119.61	115.27
17	L	203	CLA	CBC-CAC-C3C	-2.58	105.31	112.43
17	9	609	CLA	CAA-C2A-C3A	-2.58	105.71	112.78
17	a	827	CLA	CAC-C3C-C4C	2.58	128.16	124.81
17	b	803	CLA	CAA-C2A-C3A	-2.58	105.71	112.78
20	a	851	BCR	C7-C8-C9	-2.58	122.33	126.23
24	B	850	DGD	O6D-C5D-C6D	2.58	111.88	106.67
17	A	822	CLA	CHD-C4C-NC	2.58	128.27	124.20
17	6	314	CLA	C4D-C3D-CAD	-2.58	107.03	108.47
20	l	205	BCR	C38-C26-C27	2.58	118.57	113.62
20	l	201	BCR	C3-C4-C5	-2.58	109.47	114.08
17	a	833	CLA	CMC-C2C-C1C	2.58	128.97	125.04
17	8	301	CLA	CMC-C2C-C1C	2.58	128.97	125.04
17	8	305	CLA	O2A-CGA-CBA	2.58	120.00	111.91
26	6	308	CHL	CMB-C2B-C3B	2.58	129.50	124.68
17	B	814	CLA	CAC-C3C-C4C	2.58	128.15	124.81
27	3	316	LUT	C7-C8-C9	-2.58	122.34	126.23
17	b	814	CLA	C4-C3-C5	2.58	119.61	115.27
17	B	829	CLA	C4C-C3C-C2C	-2.58	103.14	106.90
17	A	806	CLA	CMB-C2B-C3B	2.58	129.50	124.68
26	7	606	CHL	CAC-C3C-C4C	2.58	128.15	124.81
17	B	808	CLA	CAA-C2A-C3A	-2.58	105.72	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	839	CLA	O2A-CGA-CBA	2.58	119.99	111.91
17	a	801	CLA	O2A-CGA-O1A	-2.58	117.09	123.59
17	k	1401	CLA	CAC-C3C-C4C	2.57	128.15	124.81
17	8	312	CLA	CMC-C2C-C1C	2.57	128.96	125.04
26	6	308	CHL	C2A-C1A-CHA	-2.57	119.36	123.86
17	4	610	CLA	O2A-CGA-CBA	2.57	119.98	111.91
17	b	820	CLA	O2A-CGA-CBA	2.57	119.98	111.91
17	a	825	CLA	C4-C3-C5	2.57	119.60	115.27
17	4	610	CLA	CMC-C2C-C1C	2.57	128.96	125.04
17	b	806	CLA	C2A-C1A-CHA	-2.57	119.36	123.86
17	b	828	CLA	CBC-CAC-C3C	-2.57	105.34	112.43
17	B	829	CLA	C2A-C1A-CHA	-2.57	119.36	123.86
17	b	813	CLA	CHD-C4C-NC	2.57	128.26	124.20
17	f	7003	CLA	O2A-CGA-CBA	2.57	119.98	111.91
17	A	829	CLA	C4-C3-C5	2.57	119.60	115.27
20	B	845	BCR	C23-C22-C21	2.57	122.89	118.94
28	4	617	XAT	C4-C3-C2	-2.57	105.81	110.77
28	9	617	XAT	C31-C30-C29	-2.57	123.64	127.31
17	l	203	CLA	C2A-C1A-CHA	-2.57	119.37	123.86
17	9	610	CLA	CBC-CAC-C3C	-2.57	105.35	112.43
20	a	849	BCR	C8-C7-C6	-2.57	119.99	127.20
26	2	606	CHL	CAC-C3C-C4C	2.57	128.14	124.81
17	4	611	CLA	C1-C2-C3	-2.57	121.60	126.04
17	B	837	CLA	C4-C3-C5	2.57	119.59	115.27
17	B	818	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
19	7	618	LHG	C5-O7-C7	-2.57	111.47	117.79
17	B	821	CLA	CMC-C2C-C1C	2.57	128.95	125.04
17	A	833	CLA	C4C-C3C-C2C	-2.57	103.16	106.90
17	a	846	CLA	CAC-C3C-C4C	2.57	128.14	124.81
17	a	814	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
17	B	803	CLA	CHD-C4C-NC	2.57	128.25	124.20
17	a	824	CLA	CAC-C3C-C4C	2.56	128.14	124.81
17	B	817	CLA	CAA-C2A-C3A	-2.56	105.75	112.78
17	3	304	CLA	O2D-CGD-O1D	-2.56	118.82	123.84
17	6	310	CLA	C1-C2-C3	-2.56	121.61	126.04
17	b	838	CLA	C4C-C3C-C2C	-2.56	103.16	106.90
26	7	605	CHL	OMC-CMC-C2C	-2.56	119.89	125.69
17	a	829	CLA	CHD-C4C-NC	2.56	128.24	124.20
17	a	826	CLA	O2A-CGA-CBA	2.56	119.95	111.91
17	a	856	CLA	C4-C3-C5	2.56	119.58	115.27
17	a	825	CLA	CAC-C3C-C4C	2.56	128.13	124.81
17	A	805	CLA	CMC-C2C-C1C	2.56	128.94	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	7	618	LHG	O8-C23-C24	2.56	119.95	111.91
26	1	307	CHL	CMB-C2B-C3B	2.56	129.47	124.68
17	a	817	CLA	CBC-CAC-C3C	-2.56	105.37	112.43
17	b	818	CLA	C1-C2-C3	-2.56	121.61	126.04
17	a	833	CLA	CMB-C2B-C3B	2.56	129.47	124.68
17	9	602	CLA	C4-C3-C5	2.56	119.58	115.27
17	a	856	CLA	CHA-C1A-NA	-2.56	120.53	126.40
17	B	833	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
17	3	314	CLA	CMB-C2B-C3B	2.56	129.47	124.68
17	6	304	CLA	CMB-C2B-C3B	2.56	129.47	124.68
17	a	830	CLA	C4-C3-C5	2.56	119.58	115.27
17	a	815	CLA	CAC-C3C-C4C	2.56	128.13	124.81
17	6	314	CLA	O2A-CGA-CBA	2.56	119.94	111.91
17	b	838	CLA	CBC-CAC-C3C	-2.56	105.38	112.43
17	b	804	CLA	O1D-CGD-CBD	-2.56	119.25	124.48
17	2	602	CLA	C4-C3-C5	2.56	119.57	115.27
17	A	804	CLA	CMC-C2C-C1C	2.56	128.93	125.04
17	a	801	CLA	CMC-C2C-C1C	2.56	128.93	125.04
20	I	101	BCR	C15-C14-C13	-2.56	123.66	127.31
17	b	811	CLA	CAC-C3C-C4C	2.56	128.13	124.81
17	B	816	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
17	b	838	CLA	CMC-C2C-C1C	2.56	128.93	125.04
17	A	843	CLA	CMC-C2C-C1C	2.56	128.93	125.04
20	A	852	BCR	C15-C14-C13	-2.56	123.66	127.31
17	8	308	CLA	CMC-C2C-C1C	2.56	128.93	125.04
17	a	805	CLA	CAC-C3C-C4C	2.55	128.12	124.81
27	3	316	LUT	C11-C10-C9	-2.55	123.66	127.31
17	2	608	CLA	CMA-C3A-C4A	-2.55	104.91	111.77
17	a	823	CLA	CBC-CAC-C3C	-2.55	105.39	112.43
20	F	305	BCR	C7-C8-C9	-2.55	122.38	126.23
17	4	609	CLA	CAC-C3C-C4C	2.55	128.12	124.81
17	b	838	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
17	B	825	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
17	b	803	CLA	C1-C2-C3	-2.55	121.63	126.04
19	1	319	LHG	O8-C23-C24	2.55	119.91	111.91
17	8	309	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
17	1	314	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
17	3	308	CLA	CMB-C2B-C3B	2.55	129.45	124.68
20	G	105	BCR	C2-C1-C6	2.55	114.41	110.48
17	B	816	CLA	CMC-C2C-C1C	2.55	128.92	125.04
17	b	812	CLA	CMB-C2B-C3B	2.55	129.45	124.68
17	2	611	CLA	O2D-CGD-O1D	-2.55	118.86	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	a	853	BCR	C33-C5-C6	-2.55	121.67	124.53
17	6	311	CLA	CMB-C2B-C3B	2.55	129.44	124.68
17	A	837	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
20	A	849	BCR	C28-C27-C26	-2.55	109.53	114.08
17	A	804	CLA	C4-C3-C5	2.55	119.55	115.27
17	A	836	CLA	CHD-C4C-NC	2.55	128.22	124.20
17	l	204	CLA	O2A-CGA-CBA	2.55	119.89	111.91
17	6	305	CLA	O2A-CGA-CBA	2.54	119.89	111.91
20	j	3004	BCR	C2-C1-C6	2.54	114.40	110.48
17	a	803	CLA	C4-C3-C5	2.54	119.55	115.27
17	F	301	CLA	CMB-C2B-C3B	2.54	129.44	124.68
20	a	853	BCR	C7-C8-C9	-2.54	122.39	126.23
17	a	828	CLA	C4-C3-C5	2.54	119.55	115.27
26	6	308	CHL	CBC-CAC-C3C	-2.54	105.42	112.43
17	6	315	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
17	l	203	CLA	CMC-C2C-C1C	2.54	128.91	125.04
17	1	310	CLA	CMC-C2C-C1C	2.54	128.91	125.04
17	9	608	CLA	O2A-CGA-CBA	2.54	119.88	111.91
17	9	609	CLA	C4-C3-C5	2.54	119.55	115.27
17	7	603	CLA	CBC-CAC-C3C	-2.54	105.43	112.43
17	a	823	CLA	CAC-C3C-C4C	2.54	128.10	124.81
17	a	801	CLA	C4-C3-C5	2.54	119.54	115.27
17	B	809	CLA	O2A-CGA-CBA	2.54	119.87	111.91
17	g	101	CLA	CMA-C3A-C2A	-2.54	110.18	116.10
17	a	803	CLA	O2A-CGA-CBA	2.54	119.87	111.91
18	a	845	PQN	C11-C12-C13	-2.54	122.57	126.79
17	A	823	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
17	6	304	CLA	C4-C3-C5	2.54	119.54	115.27
17	b	832	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
17	A	802	CLA	CMC-C2C-C1C	2.53	128.90	125.04
26	2	601	CHL	C2A-C1A-CHA	-2.53	119.43	123.86
17	f	7003	CLA	CMB-C2B-C3B	2.53	129.42	124.68
20	L	205	BCR	C2-C1-C6	2.53	114.38	110.48
20	L	205	BCR	C15-C14-C13	-2.53	123.69	127.31
20	B	844	BCR	C20-C21-C22	-2.53	123.69	127.31
26	9	606	CHL	C2A-C1A-CHA	-2.53	119.43	123.86
17	A	808	CLA	CBC-CAC-C3C	-2.53	105.45	112.43
17	3	309	CLA	CMC-C2C-C1C	2.53	128.90	125.04
17	4	609	CLA	C4-C3-C5	2.53	119.53	115.27
17	B	827	CLA	CMC-C2C-C1C	2.53	128.89	125.04
17	a	828	CLA	OBD-CAD-C3D	-2.53	123.78	127.98
17	6	305	CLA	CBC-CAC-C3C	-2.53	105.46	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	828	CLA	CMC-C2C-C1C	2.53	128.89	125.04
17	1	310	CLA	CMB-C2B-C3B	2.53	129.41	124.68
20	B	843	BCR	C29-C30-C25	2.53	114.37	110.48
26	7	614	CHL	O2D-CGD-O1D	-2.53	118.90	123.84
17	8	311	CLA	CMB-C2B-C3B	2.53	129.41	124.68
17	L	203	CLA	CAC-C3C-C4C	2.53	128.09	124.81
17	a	835	CLA	O2A-CGA-CBA	2.53	119.84	111.91
17	7	613	CLA	CBC-CAC-C3C	-2.53	105.47	112.43
17	1	303	CLA	C4-C3-C5	2.53	119.52	115.27
17	a	802	CLA	CAC-C3C-C4C	2.53	128.09	124.81
17	1	305	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
17	B	817	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
17	1	315	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
17	B	818	CLA	CMB-C2B-C3B	2.52	129.40	124.68
20	A	850	BCR	C33-C5-C6	-2.52	121.69	124.53
26	9	606	CHL	CBC-CAC-C3C	-2.52	105.47	112.43
17	B	814	CLA	O2A-CGA-CBA	2.52	119.83	111.91
17	7	610	CLA	CMB-C2B-C3B	2.52	129.40	124.68
17	A	822	CLA	CMB-C2B-C3B	2.52	129.40	124.68
17	b	809	CLA	C4-C3-C5	2.52	119.52	115.27
17	a	839	CLA	O2A-CGA-CBA	2.52	119.82	111.91
17	B	824	CLA	CMC-C2C-C1C	2.52	128.88	125.04
17	b	803	CLA	C3B-C4B-NB	2.52	112.47	109.21
17	A	826	CLA	O2A-CGA-CBA	2.52	119.82	111.91
17	b	827	CLA	O2A-CGA-CBA	2.52	119.82	111.91
17	a	830	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
17	1	305	CLA	C4-C3-C5	2.52	119.51	115.27
17	a	802	CLA	CHB-C4A-NA	2.52	128.00	124.51
17	B	819	CLA	CBC-CAC-C3C	-2.52	105.48	112.43
17	A	823	CLA	CMB-C2B-C3B	2.52	129.39	124.68
17	b	823	CLA	CMB-C2B-C3B	2.52	129.39	124.68
17	b	804	CLA	CAC-C3C-C4C	2.52	128.08	124.81
17	2	602	CLA	CBC-CAC-C3C	-2.52	105.49	112.43
26	2	606	CHL	CBC-CAC-C3C	-2.52	105.49	112.43
17	a	819	CLA	CMB-C2B-C3B	2.52	129.39	124.68
28	2	616	XAT	C19-C9-C8	2.52	122.05	118.08
17	l	202	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
20	b	844	BCR	C33-C5-C4	2.52	118.45	113.62
17	A	805	CLA	CAC-C3C-C4C	2.52	128.07	124.81
17	A	803	CLA	CMC-C2C-C1C	2.52	128.87	125.04
17	g	101	CLA	CMC-C2C-C1C	2.52	128.87	125.04
17	6	311	CLA	CMC-C2C-C1C	2.52	128.87	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	318	BCR	C29-C30-C25	2.52	114.35	110.48
20	K	4001	BCR	C33-C5-C6	-2.52	121.70	124.53
17	B	825	CLA	O2A-CGA-O1A	-2.52	117.24	123.59
26	3	307	CHL	CHD-C4C-NC	2.52	128.17	124.20
17	A	827	CLA	CMB-C2B-C3B	2.52	129.38	124.68
17	a	810	CLA	CAA-CBA-CGA	-2.51	105.91	113.25
17	A	803	CLA	CAC-C3C-C4C	2.51	128.07	124.81
17	a	835	CLA	O1D-CGD-CBD	-2.51	119.34	124.48
17	1	315	CLA	CBC-CAC-C3C	-2.51	105.50	112.43
17	b	811	CLA	CBC-CAC-C3C	-2.51	105.50	112.43
17	8	309	CLA	CMB-C2B-C3B	2.51	129.38	124.68
17	8	312	CLA	CBC-CAC-C3C	-2.51	105.50	112.43
17	8	301	CLA	CMB-C2B-C3B	2.51	129.38	124.68
17	a	801	CLA	CHB-C4A-NA	2.51	127.98	124.51
17	B	834	CLA	C1-C2-C3	-2.51	121.70	126.04
17	a	819	CLA	C4-C3-C5	2.51	119.50	115.27
26	7	601	CHL	OMC-CMC-C2C	-2.51	120.01	125.69
17	1	305	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
20	1	201	BCR	C11-C10-C9	-2.51	123.73	127.31
17	B	819	CLA	CMB-C2B-C3B	2.51	129.38	124.68
17	b	811	CLA	C4-C3-C5	2.51	119.49	115.27
17	l	203	CLA	CAC-C3C-C4C	2.51	128.07	124.81
17	a	820	CLA	O2A-CGA-CBA	2.51	119.78	111.91
17	4	612	CLA	CBC-CAC-C3C	-2.51	105.51	112.43
17	b	821	CLA	CMB-C2B-C3B	2.51	129.37	124.68
17	4	609	CLA	CMB-C2B-C3B	2.51	129.37	124.68
17	1	311	CLA	CMB-C2B-C3B	2.51	129.37	124.68
17	A	838	CLA	CBA-CAA-C2A	-2.51	106.46	113.86
17	B	830	CLA	CMB-C2B-C3B	2.51	129.37	124.68
17	4	608	CLA	CMB-C2B-C3B	2.51	129.37	124.68
17	B	832	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
17	a	801	CLA	CAC-C3C-C4C	2.51	128.06	124.81
17	A	840	CLA	CMC-C2C-C1C	2.51	128.86	125.04
17	a	821	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
17	3	311	CLA	CMB-C2B-C3B	2.51	129.37	124.68
28	1	317	XAT	C18-C5-C4	2.51	117.10	114.28
27	7	615	LUT	C35-C15-C14	-2.51	118.34	123.47
17	K	4003	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
17	B	831	CLA	CHD-C4C-NC	2.51	128.15	124.20
17	3	306	CLA	CAC-C3C-C4C	2.51	128.06	124.81
17	A	818	CLA	CAC-C3C-C4C	2.51	128.06	124.81
17	B	835	CLA	CAC-C3C-C4C	2.51	128.06	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	818	CLA	CMC-C2C-C1C	2.51	128.85	125.04
17	a	842	CLA	CMC-C2C-C1C	2.51	128.85	125.04
17	b	823	CLA	O2A-CGA-CBA	2.51	119.77	111.91
17	8	302	CLA	CMB-C2B-C3B	2.50	129.36	124.68
17	8	307	CLA	CMB-C2B-C3B	2.50	129.36	124.68
20	a	850	BCR	C28-C27-C26	-2.50	109.61	114.08
17	a	812	CLA	C1-C2-C3	-2.50	121.71	126.04
17	l	202	CLA	C1-C2-C3	-2.50	121.71	126.04
25	9	619	LMG	O8-C28-C29	2.50	119.76	111.91
17	3	311	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
17	a	804	CLA	CAC-C3C-C4C	2.50	128.06	124.81
28	8	315	XAT	C18-C5-C4	2.50	117.09	114.28
17	a	827	CLA	O2A-CGA-CBA	2.50	119.76	111.91
17	B	806	CLA	CAC-C3C-C4C	2.50	128.06	124.81
20	8	316	BCR	C20-C21-C22	-2.50	123.74	127.31
17	a	837	CLA	CMC-C2C-C1C	2.50	128.85	125.04
17	7	608	CLA	CMB-C2B-C3B	2.50	129.35	124.68
17	2	602	CLA	CMB-C2B-C3B	2.50	129.35	124.68
20	B	845	BCR	C39-C30-C25	-2.50	106.25	110.30
17	g	102	CLA	CMB-C2B-C3B	2.50	129.35	124.68
17	F	301	CLA	CBC-CAC-C3C	-2.50	105.54	112.43
17	B	838	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
17	b	814	CLA	CAC-C3C-C4C	2.50	128.05	124.81
26	4	615	CHL	CMB-C2B-C3B	2.50	129.35	124.68
17	A	807	CLA	CMC-C2C-C1C	2.50	128.84	125.04
17	A	836	CLA	O2A-CGA-CBA	2.50	119.74	111.91
17	a	833	CLA	CAC-C3C-C4C	2.50	128.05	124.81
20	b	848	BCR	C8-C7-C6	-2.50	120.19	127.20
17	A	820	CLA	CMB-C2B-C3B	2.50	129.35	124.68
17	B	826	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
17	9	613	CLA	CMB-C2B-C3B	2.49	129.34	124.68
17	a	814	CLA	C4-C3-C5	2.49	119.47	115.27
17	7	602	CLA	C2A-C1A-CHA	-2.49	119.50	123.86
17	3	309	CLA	CMB-C2B-C3B	2.49	129.34	124.68
17	G	101	CLA	C2A-C1A-CHA	-2.49	119.50	123.86
17	l	203	CLA	CBC-CAC-C3C	-2.49	105.56	112.43
17	a	837	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
17	B	816	CLA	C2A-C1A-CHA	-2.49	119.50	123.86
17	2	611	CLA	CMB-C2B-C3B	2.49	129.34	124.68
20	K	4004	BCR	C28-C27-C26	-2.49	109.63	114.08
17	6	315	CLA	CMB-C2B-C3B	2.49	129.34	124.68
17	A	829	CLA	O2A-CGA-CBA	2.49	119.73	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	f	7004	BCR	C11-C12-C13	-2.49	119.42	126.42
17	9	613	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
17	1	309	CLA	C4-C3-C5	2.49	119.46	115.27
20	j	3003	BCR	C38-C26-C27	2.49	118.40	113.62
20	l	205	BCR	C15-C14-C13	-2.49	123.76	127.31
17	g	101	CLA	C4C-C3C-C2C	-2.49	103.27	106.90
20	j	3003	BCR	C33-C5-C6	-2.49	121.73	124.53
17	B	807	CLA	CMC-C2C-C1C	2.49	128.83	125.04
17	B	835	CLA	CAA-C2A-C3A	-2.49	105.96	112.78
17	B	830	CLA	CHD-C4C-NC	2.49	128.12	124.20
17	B	812	CLA	CMB-C2B-C3B	2.49	129.33	124.68
17	2	602	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
17	A	803	CLA	O2A-CGA-CBA	2.49	119.71	111.91
20	B	848	BCR	C3-C4-C5	-2.49	109.64	114.08
28	6	318	XAT	C18-C5-C4	2.49	117.08	114.28
17	a	823	CLA	CMC-C2C-C1C	2.49	128.82	125.04
27	6	317	LUT	C11-C10-C9	-2.49	123.76	127.31
17	b	829	CLA	C4-C3-C5	2.49	119.45	115.27
19	6	320	LHG	C6-C5-C4	-2.48	105.91	111.79
17	B	825	CLA	CMB-C2B-C3B	2.48	129.33	124.68
17	G	101	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
26	8	306	CHL	CBC-CAC-C3C	-2.48	105.58	112.43
20	a	851	BCR	C23-C24-C25	-2.48	120.23	127.20
17	j	3002	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
17	3	302	CLA	CMC-C2C-C1C	2.48	128.82	125.04
17	B	810	CLA	CMC-C2C-C1C	2.48	128.82	125.04
19	A	846	LHG	O8-C23-C24	2.48	119.69	111.91
20	f	7004	BCR	C33-C5-C6	-2.48	121.74	124.53
17	A	821	CLA	CMC-C2C-C1C	2.48	128.82	125.04
17	F	301	CLA	C4-C3-C5	2.48	119.44	115.27
17	B	803	CLA	C3B-C4B-NB	2.48	112.42	109.21
26	4	606	CHL	O2A-CGA-CBA	2.48	119.69	111.91
17	a	835	CLA	C1-C2-C3	-2.48	121.75	126.04
17	4	604	CLA	CBC-CAC-C3C	-2.48	105.59	112.43
17	b	831	CLA	O2A-CGA-CBA	2.48	119.69	111.91
17	B	838	CLA	CAC-C3C-C4C	2.48	128.03	124.81
17	B	807	CLA	C2A-C1A-CHA	-2.48	119.52	123.86
17	J	3002	CLA	CMB-C2B-C3B	2.48	129.32	124.68
17	6	311	CLA	C4-C3-C5	2.48	119.44	115.27
17	f	7003	CLA	CMC-C2C-C1C	2.48	128.81	125.04
17	A	854	CLA	CAC-C3C-C4C	2.48	128.03	124.81
25	9	619	LMG	C8-O7-C10	-2.48	111.69	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	846	BCR	C15-C16-C17	-2.48	118.40	123.47
26	9	607	CHL	C5-C3-C4	2.48	120.07	114.60
17	F	304	CLA	CBC-CAC-C3C	-2.48	105.60	112.43
17	a	838	CLA	CHC-C1C-C2C	-2.48	119.87	126.72
20	k	1404	BCR	C7-C8-C9	-2.48	122.49	126.23
26	3	307	CHL	CAC-C3C-C4C	2.48	128.02	124.81
17	A	809	CLA	CMB-C2B-C3B	2.48	129.31	124.68
27	3	316	LUT	C35-C15-C14	-2.48	118.40	123.47
17	b	830	CLA	C2A-C1A-CHA	-2.48	119.53	123.86
17	a	823	CLA	O2A-CGA-CBA	2.48	119.68	111.91
17	b	808	CLA	CHB-C4A-NA	2.48	127.94	124.51
20	A	856	BCR	C8-C7-C6	-2.47	120.25	127.20
17	A	843	CLA	CBC-CAC-C3C	-2.47	105.61	112.43
17	a	846	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
17	1	315	CLA	CMC-C2C-C1C	2.47	128.81	125.04
17	9	604	CLA	CBC-CAC-C3C	-2.47	105.61	112.43
20	F	305	BCR	C15-C16-C17	-2.47	118.41	123.47
17	A	833	CLA	CMB-C2B-C3B	2.47	129.30	124.68
17	B	815	CLA	C4-C3-C5	2.47	119.43	115.27
20	B	846	BCR	C24-C23-C22	-2.47	122.50	126.23
25	6	302	LMG	C8-O7-C10	-2.47	111.71	117.79
20	j	3004	BCR	C33-C5-C4	2.47	118.36	113.62
17	b	805	CLA	CHD-C4C-NC	2.47	128.10	124.20
20	A	850	BCR	C38-C26-C25	-2.47	121.75	124.53
26	2	606	CHL	CMB-C2B-C3B	2.47	129.30	124.68
17	3	310	CLA	CMB-C2B-C3B	2.47	129.30	124.68
17	9	614	CLA	O2A-CGA-CBA	2.47	119.66	111.91
17	7	603	CLA	CMB-C2B-C3B	2.47	129.30	124.68
20	B	848	BCR	C23-C24-C25	-2.47	120.27	127.20
17	9	612	CLA	CMB-C2B-C3B	2.47	129.30	124.68
20	a	850	BCR	C7-C8-C9	-2.47	122.50	126.23
17	b	808	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
17	B	831	CLA	O2A-CGA-CBA	2.47	119.66	111.91
17	b	815	CLA	O2A-CGA-CBA	2.47	119.65	111.91
17	L	203	CLA	CMC-C2C-C1C	2.47	128.80	125.04
17	B	806	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
20	b	801	BCR	C8-C7-C6	-2.47	120.27	127.20
17	a	805	CLA	CMC-C2C-C1C	2.47	128.80	125.04
17	A	819	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
17	B	821	CLA	CMB-C2B-C3B	2.47	129.29	124.68
20	6	319	BCR	C29-C30-C25	2.47	114.28	110.48
17	A	801	CLA	C4-C3-C5	2.47	119.42	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	7	612	CLA	C4-C3-C5	2.47	119.42	115.27
26	9	605	CHL	O2D-CGD-O1D	-2.47	119.02	123.84
17	A	854	CLA	CHA-C1A-NA	-2.47	120.75	126.40
26	9	606	CHL	CMB-C2B-C3B	2.47	129.29	124.68
20	A	850	BCR	C33-C5-C4	2.46	118.35	113.62
17	A	812	CLA	CAC-C3C-C4C	2.46	128.01	124.81
17	b	840	CLA	C4-C3-C5	2.46	119.42	115.27
17	8	305	CLA	CMB-C2B-C3B	2.46	129.29	124.68
17	A	821	CLA	CMB-C2B-C3B	2.46	129.29	124.68
17	4	614	CLA	CMB-C2B-C3B	2.46	129.29	124.68
20	1	318	BCR	C38-C26-C27	2.46	118.35	113.62
28	6	318	XAT	C35-C15-C14	-2.46	118.43	123.47
17	a	831	CLA	CMC-C2C-C1C	2.46	128.79	125.04
17	b	812	CLA	CBC-CAC-C3C	-2.46	105.64	112.43
17	b	806	CLA	O2A-CGA-CBA	2.46	119.64	111.91
20	B	846	BCR	C20-C21-C22	-2.46	123.80	127.31
17	a	835	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
20	I	101	BCR	C27-C26-C25	-2.46	119.16	122.73
17	A	802	CLA	O2A-CGA-CBA	2.46	119.63	111.91
17	A	816	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
17	7	604	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
17	9	610	CLA	CMB-C2B-C3B	2.46	129.28	124.68
17	1	314	CLA	CMB-C2B-C3B	2.46	129.28	124.68
20	9	618	BCR	C7-C8-C9	-2.46	122.52	126.23
20	K	4001	BCR	C28-C27-C26	-2.46	109.69	114.08
17	4	610	CLA	CMB-C2B-C3B	2.46	129.28	124.68
17	7	611	CLA	C1-C2-C3	-2.46	121.79	126.04
20	B	847	BCR	C38-C26-C25	-2.46	121.77	124.53
27	8	314	LUT	C30-C31-C32	-2.46	115.54	123.22
20	L	205	BCR	C29-C30-C25	2.46	114.27	110.48
17	a	813	CLA	C4-C3-C5	2.46	119.41	115.27
17	g	103	CLA	CMB-C2B-C3B	2.46	129.28	124.68
17	A	811	CLA	CBC-CAC-C3C	-2.46	105.65	112.43
17	B	836	CLA	CMC-C2C-C1C	2.46	128.78	125.04
17	a	843	CLA	CBC-CAC-C3C	-2.46	105.65	112.43
20	8	316	BCR	C38-C26-C27	2.46	118.34	113.62
17	L	203	CLA	O2A-CGA-CBA	2.46	119.62	111.91
17	a	816	CLA	O2A-CGA-CBA	2.46	119.62	111.91
20	l	205	BCR	C3-C4-C5	-2.46	109.69	114.08
20	G	105	BCR	C29-C30-C25	2.46	114.26	110.48
17	2	608	CLA	CAA-C2A-C3A	-2.46	106.05	112.78
20	b	801	BCR	C20-C19-C18	-2.46	119.52	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	6	319	BCR	C38-C26-C27	2.46	118.33	113.62
26	2	605	CHL	CMB-C2B-C3B	2.46	129.27	124.68
17	a	810	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
20	A	856	BCR	C2-C1-C6	2.46	114.26	110.48
17	a	833	CLA	CBC-CAC-C3C	-2.46	105.66	112.43
17	a	816	CLA	CMC-C2C-C1C	2.46	128.78	125.04
17	A	801	CLA	CMC-C2C-C1C	2.46	128.78	125.04
20	b	801	BCR	C35-C13-C12	2.45	121.94	118.08
17	7	613	CLA	CMB-C2B-C3B	2.45	129.27	124.68
17	6	316	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
20	9	618	BCR	C37-C22-C23	2.45	121.94	118.08
17	b	803	CLA	O2D-CGD-CBD	2.45	115.63	111.27
17	G	101	CLA	CMC-C2C-C1C	2.45	128.78	125.04
17	L	204	CLA	CMB-C2B-C3B	2.45	129.27	124.68
17	B	810	CLA	CMB-C2B-C3B	2.45	129.27	124.68
17	4	602	CLA	C4-C3-C5	2.45	119.40	115.27
17	a	810	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
17	1	309	CLA	CMB-C2B-C3B	2.45	129.26	124.68
17	L	203	CLA	CMB-C2B-C3B	2.45	129.26	124.68
17	B	804	CLA	CMB-C2B-C3B	2.45	129.26	124.68
17	8	312	CLA	CMB-C2B-C3B	2.45	129.26	124.68
17	l	204	CLA	C5-C3-C4	2.45	120.02	114.60
17	A	813	CLA	C1-C2-C3	-2.45	121.80	126.04
17	a	823	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
19	a	847	LHG	O8-C23-C24	2.45	119.60	111.91
17	b	838	CLA	CAC-C3C-C4C	2.45	127.99	124.81
17	a	822	CLA	CMB-C2B-C3B	2.45	129.26	124.68
17	a	832	CLA	CMB-C2B-C3B	2.45	129.26	124.68
17	3	306	CLA	O2A-CGA-CBA	2.45	119.60	111.91
17	b	821	CLA	CBC-CAC-C3C	-2.45	105.68	112.43
17	B	827	CLA	C4-C3-C5	2.45	119.39	115.27
17	A	824	CLA	CMB-C2B-C3B	2.45	129.26	124.68
17	B	828	CLA	CMC-C2C-C1C	2.45	128.77	125.04
17	7	604	CLA	CAA-C2A-C3A	-2.45	106.07	112.78
20	4	618	BCR	C3-C4-C5	-2.45	109.70	114.08
20	f	7004	BCR	C7-C8-C9	-2.45	122.53	126.23
17	b	822	CLA	CMC-C2C-C1C	2.45	128.77	125.04
17	b	837	CLA	CAC-C3C-C4C	2.45	127.99	124.81
17	A	822	CLA	O2A-CGA-CBA	2.45	119.59	111.91
28	8	315	XAT	C4-C3-C2	-2.45	106.05	110.77
28	7	616	XAT	C15-C14-C13	-2.45	123.82	127.31
17	A	801	CLA	CBC-CAC-C3C	-2.45	105.68	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	820	CLA	CBC-CAC-C3C	-2.45	105.68	112.43
27	3	316	LUT	C10-C11-C12	-2.45	115.58	123.22
17	a	833	CLA	O2A-CGA-CBA	2.45	119.59	111.91
17	7	603	CLA	C1-C2-C3	-2.45	121.81	126.04
17	B	826	CLA	CMB-C2B-C3B	2.45	129.25	124.68
17	9	611	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
20	K	4001	BCR	C29-C30-C25	2.45	114.25	110.48
17	1	306	CLA	C4-C3-C5	2.45	119.39	115.27
17	2	610	CLA	CMA-C3A-C2A	-2.45	110.39	116.10
17	A	809	CLA	C2A-C1A-CHA	-2.44	119.58	123.86
17	b	824	CLA	O2A-CGA-CBA	2.44	119.58	111.91
28	4	617	XAT	C35-C15-C14	-2.44	118.47	123.47
17	a	842	CLA	CMB-C2B-C3B	2.44	129.25	124.68
17	b	803	CLA	CHB-C4A-NA	2.44	127.89	124.51
17	B	803	CLA	C4-C3-C5	2.44	119.38	115.27
17	b	812	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
17	4	609	CLA	CMC-C2C-C1C	2.44	128.76	125.04
26	2	607	CHL	C5-C3-C4	2.44	120.00	114.60
20	a	850	BCR	C33-C5-C4	2.44	118.31	113.62
17	a	832	CLA	CHD-C4C-NC	2.44	128.05	124.20
17	a	822	CLA	C4-C3-C5	2.44	119.38	115.27
17	B	815	CLA	CMC-C2C-C1C	2.44	128.76	125.04
20	L	201	BCR	C15-C16-C17	-2.44	118.47	123.47
26	4	607	CHL	C5-C3-C4	2.44	119.99	114.60
17	8	308	CLA	CMB-C2B-C3B	2.44	129.24	124.68
17	a	816	CLA	C5-C3-C4	2.44	119.99	114.60
20	B	847	BCR	C39-C30-C25	-2.44	106.34	110.30
20	L	206	BCR	C3-C4-C5	-2.44	109.72	114.08
17	F	303	CLA	CMC-C2C-C1C	2.44	128.75	125.04
17	a	812	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
17	A	806	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
17	A	815	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
17	A	839	CLA	CBC-CAC-C3C	-2.44	105.71	112.43
17	7	608	CLA	O2A-CGA-CBA	2.44	119.56	111.91
17	B	816	CLA	CBC-CAC-C3C	-2.44	105.71	112.43
17	B	837	CLA	C2A-C1A-CHA	-2.44	119.60	123.86
17	B	836	CLA	C4-C3-C5	2.44	119.37	115.27
17	F	304	CLA	C4-C3-C5	2.44	119.37	115.27
20	K	4001	BCR	C8-C7-C6	-2.44	120.36	127.20
17	A	801	CLA	CHB-C4A-NA	2.44	127.88	124.51
17	1	305	CLA	CMB-C2B-C3B	2.44	129.24	124.68
17	b	821	CLA	O2D-CGD-O1D	-2.44	119.08	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	831	CLA	CHD-C4C-NC	2.44	128.04	124.20
17	a	808	CLA	C2A-C1A-CHA	-2.44	119.60	123.86
17	1	315	CLA	CMB-C2B-C3B	2.44	129.23	124.68
17	6	307	CLA	CMB-C2B-C3B	2.44	129.23	124.68
17	6	313	CLA	CBC-CAC-C3C	-2.44	105.72	112.43
20	B	843	BCR	C11-C10-C9	-2.43	123.83	127.31
17	a	830	CLA	CAC-C3C-C4C	2.43	127.97	124.81
17	3	308	CLA	CAA-C2A-C3A	-2.43	106.11	112.78
26	4	605	CHL	O2D-CGD-O1D	-2.43	119.08	123.84
17	A	810	CLA	CAC-C3C-C4C	2.43	127.97	124.81
17	b	825	CLA	C4-C3-C5	2.43	119.36	115.27
17	A	820	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
26	4	607	CHL	CHD-C4C-NC	2.43	128.04	124.20
20	K	4004	BCR	C7-C8-C9	-2.43	122.56	126.23
17	B	819	CLA	O2A-CGA-CBA	2.43	119.54	111.91
17	4	603	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
27	7	615	LUT	C7-C8-C9	-2.43	122.56	126.23
17	A	836	CLA	CBC-CAC-C3C	-2.43	105.73	112.43
27	7	615	LUT	C11-C10-C9	-2.43	123.84	127.31
27	4	616	LUT	C31-C30-C29	-2.43	123.84	127.31
20	7	617	BCR	C20-C19-C18	-2.43	119.59	126.42
17	b	830	CLA	CMC-C2C-C1C	2.43	128.74	125.04
17	4	611	CLA	CMB-C2B-C3B	2.43	129.23	124.68
17	8	310	CLA	C4-C3-C5	2.43	119.36	115.27
17	4	613	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
17	2	604	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
17	6	316	CLA	CMC-C2C-C1C	2.43	128.74	125.04
17	B	803	CLA	CMC-C2C-C1C	2.43	128.74	125.04
28	6	318	XAT	C38-C25-C24	2.43	117.01	114.28
17	L	204	CLA	C5-C3-C4	2.43	119.97	114.60
17	a	815	CLA	CMC-C2C-C1C	2.43	128.74	125.04
20	B	847	BCR	C20-C21-C22	-2.43	123.84	127.31
20	L	201	BCR	C8-C9-C10	2.43	122.67	118.94
17	8	304	CLA	CBC-CAC-C3C	-2.43	105.74	112.43
17	4	612	CLA	C4-C3-C5	2.43	119.36	115.27
20	A	852	BCR	C8-C9-C10	2.43	122.67	118.94
17	a	806	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
17	b	841	CLA	CMB-C2B-C3B	2.43	129.22	124.68
17	b	836	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
17	6	305	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
17	L	202	CLA	O2A-CGA-CBA	2.43	119.52	111.91
27	1	320	LUT	C15-C35-C34	-2.43	118.50	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	7	614	CHL	CMB-C2B-C3B	2.43	129.22	124.68
17	b	810	CLA	C2A-C1A-CHA	-2.43	119.62	123.86
17	b	813	CLA	CMC-C2C-C1C	2.43	128.73	125.04
17	A	817	CLA	O2D-CGD-O1D	-2.43	119.10	123.84
17	B	806	CLA	C4-C3-C5	2.43	119.35	115.27
17	a	824	CLA	O2A-CGA-CBA	2.43	119.52	111.91
17	a	843	CLA	CMC-C2C-C1C	2.42	128.73	125.04
17	a	803	CLA	CMB-C2B-C3B	2.42	129.22	124.68
17	7	610	CLA	CMA-C3A-C2A	-2.42	110.44	116.10
17	l	203	CLA	CMB-C2B-C3B	2.42	129.21	124.68
26	4	606	CHL	C5-C3-C4	2.42	119.96	114.60
26	7	607	CHL	C5-C3-C4	2.42	119.96	114.60
17	a	838	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
17	6	313	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
20	3	318	BCR	C15-C16-C17	-2.42	118.51	123.47
17	2	609	CLA	C4-C3-C5	2.42	119.35	115.27
17	A	812	CLA	CMC-C2C-C1C	2.42	128.73	125.04
17	b	828	CLA	CMB-C2B-C3B	2.42	129.21	124.68
17	a	806	CLA	CBC-CAC-C3C	-2.42	105.76	112.43
27	6	317	LUT	C18-C5-C4	2.42	118.84	114.36
17	2	602	CLA	C2A-C1A-CHA	-2.42	119.63	123.86
17	A	838	CLA	CMB-C2B-C3B	2.42	129.21	124.68
17	B	810	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
20	a	854	BCR	C8-C9-C10	2.42	122.65	118.94
17	a	808	CLA	O2A-CGA-CBA	2.42	119.50	111.91
17	B	835	CLA	CBC-CAC-C3C	-2.42	105.76	112.43
17	9	602	CLA	CMB-C2B-C3B	2.42	129.20	124.68
17	3	314	CLA	CMC-C2C-C1C	2.42	128.72	125.04
20	8	316	BCR	C29-C30-C25	2.42	114.20	110.48
17	9	602	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
17	8	301	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
28	7	616	XAT	C19-C9-C8	2.42	121.89	118.08
25	4	620	LMG	C1-O6-C5	-2.42	108.94	113.69
17	B	806	CLA	CMB-C2B-C3B	2.42	129.20	124.68
17	B	840	CLA	C2A-C1A-CHA	-2.42	119.63	123.86
20	f	7004	BCR	C21-C20-C19	-2.42	115.67	123.22
17	A	841	CLA	CED-O2D-CGD	2.42	121.40	115.94
17	G	104	CLA	CMC-C2C-C1C	2.42	128.72	125.04
17	B	812	CLA	CMC-C2C-C1C	2.42	128.72	125.04
17	a	836	CLA	O2A-CGA-CBA	2.42	119.49	111.91
17	B	813	CLA	CMC-C2C-C1C	2.42	128.72	125.04
20	7	617	BCR	C35-C13-C14	-2.42	119.54	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	806	CLA	CMC-C2C-C1C	2.42	128.72	125.04
17	A	843	CLA	O2A-CGA-CBA	2.41	119.49	111.91
17	a	823	CLA	CMB-C2B-C3B	2.41	129.20	124.68
17	a	804	CLA	C4-C3-C5	2.41	119.33	115.27
20	B	845	BCR	C2-C1-C6	2.41	114.20	110.48
26	1	302	CHL	CHD-C4C-NC	2.41	128.01	124.20
17	b	815	CLA	CMC-C2C-C1C	2.41	128.72	125.04
17	B	814	CLA	CMC-C2C-C1C	2.41	128.72	125.04
17	a	817	CLA	CAA-CBA-CGA	-2.41	108.40	113.59
17	1	304	CLA	O2A-CGA-CBA	2.41	119.48	111.91
17	B	815	CLA	O2A-CGA-CBA	2.41	119.48	111.91
20	F	305	BCR	C11-C12-C13	-2.41	119.64	126.42
17	G	103	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
28	6	318	XAT	C19-C9-C8	2.41	121.88	118.08
17	6	316	CLA	CBC-CAC-C3C	-2.41	105.78	112.43
17	a	805	CLA	C4-C3-C5	2.41	119.33	115.27
17	1	312	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
17	b	825	CLA	CMB-C2B-C3B	2.41	129.19	124.68
17	4	611	CLA	CBC-CAC-C3C	-2.41	105.78	112.43
17	A	817	CLA	CBC-CAC-C3C	-2.41	105.78	112.43
17	6	304	CLA	CMC-C2C-C1C	2.41	128.71	125.04
17	3	306	CLA	CMB-C2B-C3B	2.41	129.19	124.68
17	4	613	CLA	CMB-C2B-C3B	2.41	129.19	124.68
17	2	608	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
17	B	803	CLA	CHB-C4A-NA	2.41	127.84	124.51
17	A	827	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
17	3	306	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
17	A	833	CLA	O2A-CGA-CBA	2.41	119.47	111.91
17	B	814	CLA	CMB-C2B-C3B	2.41	129.19	124.68
17	4	612	CLA	C2A-C1A-CHA	-2.41	119.65	123.86
17	3	302	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
17	6	313	CLA	CMB-C2B-C3B	2.41	129.18	124.68
17	1	312	CLA	CMB-C2B-C3B	2.41	129.18	124.68
26	7	606	CHL	CMB-C2B-C3B	2.41	129.18	124.68
17	a	814	CLA	CMB-C2B-C3B	2.41	129.18	124.68
17	1	203	CLA	O2A-CGA-CBA	2.41	119.46	111.91
17	A	812	CLA	CBC-CAC-C3C	-2.41	105.80	112.43
17	A	820	CLA	O2A-CGA-CBA	2.41	119.46	111.91
17	B	839	CLA	CMC-C2C-C1C	2.41	128.70	125.04
17	3	301	CLA	CMC-C2C-C1C	2.41	128.70	125.04
17	b	827	CLA	C4-C3-C5	2.41	119.32	115.27
18	B	842	PQN	C2M-C2-C3	-2.41	120.47	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	6	311	CLA	CBC-CAC-C3C	-2.41	105.80	112.43
17	B	808	CLA	CMB-C2B-C3B	2.41	129.18	124.68
17	K	4002	CLA	CMB-C2B-C3B	2.40	129.18	124.68
17	A	845	CLA	CMB-C2B-C3B	2.40	129.18	124.68
17	a	846	CLA	CMB-C2B-C3B	2.40	129.18	124.68
17	6	315	CLA	CBC-CAC-C3C	-2.40	105.80	112.43
17	B	833	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
17	a	835	CLA	CMB-C2B-C3B	2.40	129.18	124.68
17	b	808	CLA	CMB-C2B-C3B	2.40	129.18	124.68
17	B	827	CLA	CAA-C2A-C3A	-2.40	106.20	112.78
17	A	804	CLA	O2A-CGA-CBA	2.40	119.45	111.91
20	i	101	BCR	C8-C7-C6	-2.40	120.45	127.20
17	8	304	CLA	CMB-C2B-C3B	2.40	129.17	124.68
17	b	814	CLA	CMC-C2C-C1C	2.40	128.70	125.04
17	2	603	CLA	CMB-C2B-C3B	2.40	129.17	124.68
17	K	4003	CLA	CMB-C2B-C3B	2.40	129.17	124.68
18	A	844	PQN	C2M-C2-C1	2.40	120.25	116.27
17	a	842	CLA	C4-C3-C5	2.40	119.31	115.27
17	A	827	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
17	k	1402	CLA	CBC-CAC-C3C	-2.40	105.81	112.43
17	1	310	CLA	C4-C3-C5	2.40	119.31	115.27
17	6	314	CLA	C4-C3-C5	2.40	119.31	115.27
17	2	603	CLA	CBC-CAC-C3C	-2.40	105.81	112.43
27	1	316	LUT	C8-C7-C6	-2.40	120.46	127.20
17	6	310	CLA	CMC-C2C-C1C	2.40	128.69	125.04
27	4	616	LUT	C35-C15-C14	-2.40	118.56	123.47
17	8	307	CLA	C5-C3-C4	2.40	119.90	114.60
28	9	617	XAT	C15-C14-C13	-2.40	123.89	127.31
17	A	813	CLA	C4-C3-C5	2.40	119.31	115.27
17	3	305	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
26	4	605	CHL	CBC-CAC-C3C	-2.40	105.82	112.43
17	a	822	CLA	C2A-C1A-CHA	-2.40	119.67	123.86
27	2	615	LUT	C35-C15-C14	-2.40	118.56	123.47
17	A	828	CLA	OBD-CAD-C3D	-2.40	124.00	127.98
17	a	809	CLA	CMC-C2C-C1C	2.40	128.69	125.04
17	A	808	CLA	O2A-CGA-CBA	2.40	119.43	111.91
17	A	815	CLA	CMC-C2C-C1C	2.40	128.69	125.04
17	B	837	CLA	CBC-CAC-C3C	-2.40	105.82	112.43
17	3	314	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
17	B	815	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
17	6	309	CLA	CMB-C2B-C3B	2.40	129.16	124.68
17	B	809	CLA	C1-C2-C3	-2.40	121.90	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	803	CLA	CBC-CAC-C3C	-2.40	105.82	112.43
17	9	603	CLA	C2A-C1A-CHA	-2.40	119.67	123.86
17	6	316	CLA	CMB-C2B-C3B	2.40	129.16	124.68
17	F	304	CLA	C1-C2-C3	-2.40	121.90	126.04
17	9	610	CLA	CMC-C2C-C1C	2.40	128.69	125.04
17	a	809	CLA	CBC-CAC-C3C	-2.39	105.83	112.43
17	b	824	CLA	CMB-C2B-C3B	2.39	129.16	124.68
17	b	816	CLA	CMC-C2C-C1C	2.39	128.69	125.04
17	3	303	CLA	CBC-CAC-C3C	-2.39	105.83	112.43
20	3	318	BCR	C38-C26-C27	2.39	118.21	113.62
20	b	846	BCR	C23-C24-C25	-2.39	120.48	127.20
17	2	610	CLA	CMB-C2B-C3B	2.39	129.16	124.68
17	8	303	CLA	C2A-C1A-CHA	-2.39	119.67	123.86
20	2	617	BCR	C28-C27-C26	-2.39	109.80	114.08
17	7	604	CLA	CMB-C2B-C3B	2.39	129.16	124.68
17	b	837	CLA	C2A-C1A-CHA	-2.39	119.67	123.86
17	a	810	CLA	CMB-C2B-C3B	2.39	129.15	124.68
17	A	828	CLA	CMC-C2C-C1C	2.39	128.68	125.04
20	a	851	BCR	C33-C5-C6	-2.39	121.84	124.53
17	A	819	CLA	CBC-CAC-C3C	-2.39	105.84	112.43
17	3	303	CLA	CMB-C2B-C3B	2.39	129.15	124.68
17	F	304	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
20	A	851	BCR	C3-C4-C5	-2.39	109.81	114.08
17	2	608	CLA	CHB-C4A-NA	2.39	127.82	124.51
17	1	303	CLA	CMC-C2C-C1C	2.39	128.68	125.04
17	a	812	CLA	CMB-C2B-C3B	2.39	129.15	124.68
17	B	833	CLA	CBC-CAC-C3C	-2.39	105.84	112.43
17	B	811	CLA	O2A-CGA-CBA	2.39	119.41	111.91
17	B	821	CLA	CBC-CAC-C3C	-2.39	105.84	112.43
20	3	318	BCR	C29-C30-C25	2.39	114.16	110.48
17	A	819	CLA	CMC-C2C-C1C	2.39	128.68	125.04
17	9	611	CLA	CMB-C2B-C3B	2.39	129.15	124.68
17	a	837	CLA	CBC-CAC-C3C	-2.39	105.85	112.43
17	b	829	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
17	4	602	CLA	CMC-C2C-C1C	2.39	128.68	125.04
17	6	312	CLA	CMB-C2B-C3B	2.39	129.14	124.68
20	A	851	BCR	C11-C10-C9	-2.39	123.90	127.31
20	1	318	BCR	C37-C22-C23	2.39	121.84	118.08
20	g	104	BCR	C2-C1-C6	2.39	114.15	110.48
17	7	608	CLA	CHB-C4A-NA	2.39	127.81	124.51
17	8	302	CLA	CMC-C2C-C1C	2.38	128.67	125.04
17	B	813	CLA	O2D-CGD-O1D	-2.38	119.18	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	j	3003	BCR	C38-C26-C25	-2.38	121.85	124.53
20	A	848	BCR	C24-C23-C22	-2.38	122.63	126.23
17	a	815	CLA	CMB-C2B-C3B	2.38	129.14	124.68
17	A	832	CLA	CBC-CAC-C3C	-2.38	105.86	112.43
20	b	848	BCR	C29-C30-C25	2.38	114.15	110.48
17	b	810	CLA	C4-C3-C5	2.38	119.28	115.27
17	B	826	CLA	CMC-C2C-C1C	2.38	128.67	125.04
17	8	312	CLA	CAA-C2A-C3A	-2.38	106.25	112.78
20	A	856	BCR	C29-C30-C25	2.38	114.15	110.48
20	4	618	BCR	C29-C30-C25	2.38	114.15	110.48
17	b	809	CLA	CMC-C2C-C1C	2.38	128.67	125.04
17	9	609	CLA	CMB-C2B-C3B	2.38	129.13	124.68
17	8	310	CLA	CBC-CAC-C3C	-2.38	105.86	112.43
17	a	809	CLA	C2A-C1A-CHA	-2.38	119.69	123.86
17	a	807	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
17	b	839	CLA	CMB-C2B-C3B	2.38	129.13	124.68
17	B	831	CLA	CMB-C2B-C3B	2.38	129.13	124.68
26	3	307	CHL	CMB-C2B-C3B	2.38	129.13	124.68
17	A	835	CLA	CAA-C2A-C3A	-2.38	106.26	112.78
20	2	617	BCR	C36-C18-C17	-2.38	119.59	122.92
17	4	601	CLA	CBC-CAC-C3C	-2.38	105.87	112.43
17	b	825	CLA	CMC-C2C-C1C	2.38	128.66	125.04
17	B	827	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
17	A	810	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
26	1	307	CHL	CBC-CAC-C3C	-2.38	105.87	112.43
17	3	312	CLA	C4-C3-C5	2.38	119.27	115.27
17	G	104	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
17	B	828	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
17	f	7002	CLA	CAC-C3C-C4C	2.38	127.90	124.81
17	4	608	CLA	C5-C3-C4	2.38	119.86	114.60
23	B	849	LMT	O5B-C1B-C2B	2.38	115.38	110.35
17	6	312	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
26	7	601	CHL	O2A-CGA-CBA	2.38	119.37	111.91
17	9	603	CLA	CBC-CAC-C3C	-2.38	105.88	112.43
17	b	804	CLA	CBC-CAC-C3C	-2.38	105.88	112.43
17	B	812	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
17	a	833	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
20	A	852	BCR	C33-C5-C6	-2.38	121.86	124.53
20	i	101	BCR	C21-C20-C19	-2.37	115.81	123.22
17	a	818	CLA	C1-C2-C3	-2.37	121.94	126.04
17	4	601	CLA	CMB-C2B-C3B	2.37	129.12	124.68
17	B	814	CLA	CMA-C3A-C4A	-2.37	105.39	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	k	1404	BCR	C8-C7-C6	-2.37	120.53	127.20
17	F	304	CLA	C1-O2A-CGA	2.37	122.67	116.44
26	7	601	CHL	CMB-C2B-C3B	2.37	129.12	124.68
17	G	103	CLA	CMB-C2B-C3B	2.37	129.12	124.68
17	B	808	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
17	a	835	CLA	CAC-C3C-C4C	2.37	127.89	124.81
20	B	843	BCR	C36-C18-C17	-2.37	119.60	122.92
17	2	610	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
20	A	856	BCR	C23-C24-C25	-2.37	120.54	127.20
17	A	842	CLA	CBC-CAC-C3C	-2.37	105.89	112.43
17	1	304	CLA	C2A-C1A-CHA	-2.37	119.71	123.86
17	A	813	CLA	CMC-C2C-C1C	2.37	128.65	125.04
17	F	304	CLA	CMC-C2C-C1C	2.37	128.65	125.04
17	b	820	CLA	CBC-CAC-C3C	-2.37	105.89	112.43
17	B	822	CLA	CAA-C2A-C3A	-2.37	106.29	112.78
17	b	806	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
17	b	832	CLA	CMC-C2C-C1C	2.37	128.65	125.04
17	9	613	CLA	CBC-CAC-C3C	-2.37	105.90	112.43
17	a	834	CLA	CAA-C2A-C3A	-2.37	106.29	112.78
20	b	848	BCR	C15-C14-C13	-2.37	123.93	127.31
17	A	805	CLA	C4-C3-C5	2.37	119.26	115.27
17	9	601	CLA	CMB-C2B-C3B	2.37	129.11	124.68
27	6	321	LUT	C15-C35-C34	-2.37	118.62	123.47
28	1	317	XAT	C31-C30-C29	-2.37	123.93	127.31
17	b	816	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
20	l	201	BCR	C29-C30-C25	2.37	114.13	110.48
17	a	832	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
17	b	824	CLA	CBC-CAC-C3C	-2.37	105.90	112.43
17	6	306	CLA	CMB-C2B-C3B	2.37	129.11	124.68
17	3	303	CLA	CMC-C2C-C1C	2.37	128.64	125.04
17	a	839	CLA	CMC-C2C-C1C	2.37	128.64	125.04
17	A	818	CLA	CMC-C2C-C1C	2.37	128.64	125.04
17	B	828	CLA	CBC-CAC-C3C	-2.37	105.91	112.43
27	4	616	LUT	C18-C5-C4	2.37	118.74	114.36
17	4	601	CLA	CMC-C2C-C1C	2.37	128.64	125.04
20	7	617	BCR	C36-C18-C17	-2.37	119.61	122.92
20	a	852	BCR	C16-C15-C14	-2.37	118.63	123.47
17	b	807	CLA	CMB-C2B-C3B	2.37	129.10	124.68
27	1	316	LUT	C31-C30-C29	-2.37	123.93	127.31
17	4	614	CLA	C5-C3-C4	2.37	119.83	114.60
20	k	1404	BCR	C3-C4-C5	-2.37	109.85	114.08
17	B	823	CLA	C4-C3-C5	2.36	119.25	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	8	306	CHL	CMB-C2B-C3B	2.36	129.10	124.68
17	A	813	CLA	CBC-CAC-C3C	-2.36	105.91	112.43
17	b	826	CLA	C4D-C3D-CAD	-2.36	107.15	108.47
26	2	614	CHL	CMB-C2B-C3B	2.36	129.10	124.68
20	a	854	BCR	C20-C19-C18	-2.36	119.78	126.42
17	a	814	CLA	CHB-C4A-NA	2.36	127.78	124.51
17	A	818	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
26	2	607	CHL	CMB-C2B-C3B	2.36	129.10	124.68
17	6	305	CLA	C4-C3-C5	2.36	119.25	115.27
17	B	841	CLA	CBC-CAC-C3C	-2.36	105.92	112.43
17	6	305	CLA	CMC-C2C-C1C	2.36	128.64	125.04
17	A	810	CLA	CMC-C2C-C1C	2.36	128.64	125.04
17	3	305	CLA	CMB-C2B-C3B	2.36	129.10	124.68
17	6	306	CLA	CBC-CAC-C3C	-2.36	105.92	112.43
17	b	820	CLA	C5-C3-C4	2.36	119.82	114.60
17	A	834	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
17	B	841	CLA	CMB-C2B-C3B	2.36	129.09	124.68
17	b	826	CLA	CMB-C2B-C3B	2.36	129.09	124.68
17	b	811	CLA	O2A-CGA-CBA	2.36	119.31	111.91
17	a	812	CLA	CMC-C2C-C1C	2.36	128.63	125.04
17	K	4002	CLA	CMC-C2C-C1C	2.36	128.63	125.04
20	A	850	BCR	C29-C30-C25	2.36	114.11	110.48
17	b	809	CLA	CAC-C3C-C4C	2.36	127.87	124.81
26	9	615	CHL	CBC-CAC-C3C	-2.36	105.92	112.43
17	b	840	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
17	1	305	CLA	CBC-CAC-C3C	-2.36	105.93	112.43
17	b	832	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
17	l	202	CLA	CBC-CAC-C3C	-2.36	105.93	112.43
17	B	820	CLA	C5-C3-C4	2.36	119.81	114.60
17	a	818	CLA	C4-C3-C5	2.36	119.24	115.27
17	B	832	CLA	C4-C3-C5	2.36	119.24	115.27
17	L	204	CLA	CBC-CAC-C3C	-2.36	105.93	112.43
17	A	837	CLA	CMB-C2B-C3B	2.36	129.09	124.68
20	J	3003	BCR	C38-C26-C27	2.36	118.15	113.62
17	A	854	CLA	CMC-C2C-C1C	2.36	128.63	125.04
17	6	312	CLA	CMC-C2C-C1C	2.36	128.63	125.04
17	b	831	CLA	C2A-C1A-CHA	-2.36	119.74	123.86
26	4	605	CHL	CBA-CAA-C2A	-2.36	106.90	113.86
26	2	606	CHL	O2D-CGD-O1D	-2.36	119.23	123.84
17	A	806	CLA	CMC-C2C-C1C	2.36	128.63	125.04
17	L	202	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
17	g	102	CLA	C5-C3-C4	2.36	119.81	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	608	CLA	C5-C3-C4	2.36	119.81	114.60
17	a	806	CLA	C2A-C1A-CHA	-2.36	119.74	123.86
20	A	849	BCR	C3-C4-C5	-2.36	109.87	114.08
20	f	7004	BCR	C8-C7-C6	-2.36	120.58	127.20
17	4	612	CLA	CMB-C2B-C3B	2.36	129.09	124.68
17	B	836	CLA	C2A-C1A-CHA	-2.36	119.74	123.86
17	a	821	CLA	CAC-C3C-C4C	2.35	127.86	124.81
17	b	828	CLA	CAC-C3C-C4C	2.35	127.86	124.81
17	a	836	CLA	CMC-C2C-C1C	2.35	128.62	125.04
20	I	101	BCR	C34-C9-C8	2.35	121.78	118.08
17	6	304	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
17	g	102	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
17	b	829	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
17	B	822	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
17	b	817	CLA	CMC-C2C-C1C	2.35	128.62	125.04
17	a	811	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
17	b	835	CLA	CBC-CAC-C3C	-2.35	105.95	112.43
17	B	838	CLA	CBC-CAC-C3C	-2.35	105.95	112.43
17	9	612	CLA	CBC-CAC-C3C	-2.35	105.95	112.43
17	B	819	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
26	2	607	CHL	O2D-CGD-O1D	-2.35	119.24	123.84
17	b	805	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
17	B	839	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
17	a	825	CLA	CMB-C2B-C3B	2.35	129.07	124.68
17	a	811	CLA	CAA-C2A-C3A	-2.35	106.34	112.78
17	a	832	CLA	CAA-C2A-C3A	-2.35	106.34	112.78
17	a	812	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
17	6	305	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
17	B	841	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
26	2	614	CHL	O2D-CGD-O1D	-2.35	119.25	123.84
17	2	613	CLA	CMB-C2B-C3B	2.35	129.07	124.68
17	a	818	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
17	A	804	CLA	CBC-CAC-C3C	-2.35	105.96	112.43
17	a	840	CLA	CMC-C2C-C1C	2.35	128.61	125.04
17	b	808	CLA	CMC-C2C-C1C	2.35	128.61	125.04
27	8	314	LUT	C35-C15-C14	-2.35	118.67	123.47
17	B	811	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
17	B	808	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
17	6	309	CLA	CMC-C2C-C1C	2.35	128.61	125.04
17	B	837	CLA	CMC-C2C-C1C	2.35	128.61	125.04
17	4	609	CLA	CBC-CAC-C3C	-2.35	105.96	112.43
17	8	302	CLA	CBC-CAC-C3C	-2.35	105.96	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	3	317	XAT	C19-C9-C8	2.35	121.77	118.08
17	4	608	CLA	O2A-CGA-CBA	2.35	119.27	111.91
20	2	617	BCR	C20-C21-C22	-2.35	123.96	127.31
17	B	809	CLA	CBC-CAC-C3C	-2.35	105.96	112.43
27	1	320	LUT	C18-C5-C4	2.35	118.70	114.36
27	4	616	LUT	C30-C31-C32	-2.35	115.90	123.22
17	4	612	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
17	B	805	CLA	CHB-C4A-NA	2.35	127.75	124.51
20	j	3004	BCR	C20-C19-C18	-2.35	119.83	126.42
17	b	803	CLA	CED-O2D-CGD	2.35	121.24	115.94
17	a	807	CLA	CMB-C2B-C3B	2.34	129.06	124.68
17	9	602	CLA	C2A-C1A-CHA	-2.34	119.76	123.86
17	7	611	CLA	O2D-CGD-O1D	-2.34	119.25	123.84
17	1	308	CLA	CMB-C2B-C3B	2.34	129.06	124.68
17	3	308	CLA	C5-C3-C4	2.34	119.78	114.60
17	L	203	CLA	C4-C3-C5	2.34	119.21	115.27
17	b	827	CLA	CMB-C2B-C3B	2.34	129.06	124.68
17	a	838	CLA	CMB-C2B-C3B	2.34	129.06	124.68
28	1	317	XAT	C20-C13-C12	2.34	121.77	118.08
17	a	803	CLA	CHD-C4C-NC	2.34	127.89	124.20
17	A	825	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
17	2	611	CLA	CBC-CAC-C3C	-2.34	105.98	112.43
20	i	101	BCR	C10-C11-C12	-2.34	115.91	123.22
17	7	611	CLA	CMB-C2B-C3B	2.34	129.06	124.68
28	9	617	XAT	C10-C11-C12	-2.34	115.91	123.22
17	b	839	CLA	C2A-C1A-CHA	-2.34	119.77	123.86
26	9	605	CHL	CBA-CAA-C2A	-2.34	106.95	113.86
27	7	615	LUT	C10-C11-C12	-2.34	115.91	123.22
17	B	814	CLA	CHB-C4A-NA	2.34	127.75	124.51
17	9	610	CLA	CMA-C3A-C2A	-2.34	110.64	116.10
17	b	820	CLA	CMC-C2C-C1C	2.34	128.60	125.04
17	L	204	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
17	9	603	CLA	CMB-C2B-C3B	2.34	129.05	124.68
20	g	104	BCR	C10-C11-C12	-2.34	115.92	123.22
17	b	819	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
17	8	307	CLA	CAC-C3C-C4C	2.34	127.84	124.81
17	b	820	CLA	CMB-C2B-C3B	2.34	129.05	124.68
26	7	601	CHL	CHD-C4C-NC	2.34	127.89	124.20
17	2	613	CLA	CBC-CAC-C3C	-2.34	105.99	112.43
17	g	102	CLA	CMC-C2C-C1C	2.34	128.60	125.04
17	B	830	CLA	C5-C3-C4	2.34	119.77	114.60
17	A	835	CLA	CMB-C2B-C3B	2.34	129.05	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	6	310	CLA	CMB-C2B-C3B	2.34	129.05	124.68
17	3	304	CLA	CBC-CAC-C3C	-2.34	105.99	112.43
17	a	809	CLA	C4-C3-C5	2.34	119.20	115.27
17	B	827	CLA	CMB-C2B-C3B	2.34	129.05	124.68
20	A	851	BCR	C37-C22-C21	-2.34	119.65	122.92
17	B	811	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
17	9	614	CLA	CMB-C2B-C3B	2.34	129.05	124.68
17	b	820	CLA	C2A-C1A-CHA	-2.34	119.77	123.86
20	A	856	BCR	C11-C12-C13	-2.34	119.86	126.42
19	1	301	LHG	C5-O7-C7	-2.34	112.04	117.79
20	1	206	BCR	C7-C8-C9	-2.33	122.71	126.23
17	A	806	CLA	C1-O2A-CGA	2.33	122.57	116.44
26	7	605	CHL	O2D-CGD-O1D	-2.33	119.27	123.84
17	a	856	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
17	A	813	CLA	CMB-C2B-C3B	2.33	129.04	124.68
17	8	307	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
17	2	603	CLA	CMC-C2C-C1C	2.33	128.59	125.04
17	1	306	CLA	CMB-C2B-C3B	2.33	129.04	124.68
17	A	812	CLA	CMB-C2B-C3B	2.33	129.04	124.68
17	2	609	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
17	a	825	CLA	CED-O2D-CGD	2.33	121.21	115.94
17	B	824	CLA	CMB-C2B-C3B	2.33	129.04	124.68
17	a	825	CLA	CMC-C2C-C1C	2.33	128.59	125.04
17	6	306	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
20	1	206	BCR	C38-C26-C25	-2.33	121.91	124.53
27	1	316	LUT	C18-C5-C4	2.33	118.67	114.36
17	a	843	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
17	G	104	CLA	CMB-C2B-C3B	2.33	129.04	124.68
17	a	831	CLA	CMB-C2B-C3B	2.33	129.04	124.68
17	8	305	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
17	6	304	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
17	1	303	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
17	k	1401	CLA	CMB-C2B-C3B	2.33	129.04	124.68
17	b	826	CLA	OBD-CAD-C3D	-2.33	124.11	127.98
17	A	803	CLA	CMB-C2B-C3B	2.33	129.04	124.68
17	A	839	CLA	CMC-C2C-C1C	2.33	128.59	125.04
17	A	840	CLA	C1-C2-C3	-2.33	122.02	126.04
17	B	830	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
17	B	838	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
17	b	811	CLA	CMC-C2C-C1C	2.33	128.58	125.04
17	7	610	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
20	a	849	BCR	C20-C19-C18	-2.33	119.88	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	816	CLA	C5-C3-C4	2.33	119.74	114.60
17	a	831	CLA	O1D-CGD-CBD	-2.33	119.72	124.48
17	b	807	CLA	CBC-CAC-C3C	-2.33	106.02	112.43
17	B	824	CLA	O2A-CGA-CBA	2.33	119.21	111.91
27	8	314	LUT	C8-C7-C6	-2.33	120.67	127.20
20	a	852	BCR	C33-C5-C4	2.33	118.09	113.62
17	a	832	CLA	C5-C3-C4	2.33	119.74	114.60
17	4	610	CLA	C1-C2-C3	-2.33	122.02	126.04
17	A	811	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
17	7	612	CLA	CMC-C2C-C1C	2.33	128.58	125.04
17	j	3002	CLA	CHB-C4A-NA	2.32	127.73	124.51
17	B	841	CLA	C2A-C1A-CHA	-2.32	119.79	123.86
17	b	817	CLA	O2D-CGD-O1D	-2.32	119.29	123.84
17	a	843	CLA	O2D-CGD-O1D	-2.32	119.29	123.84
17	2	613	CLA	CMC-C2C-C1C	2.32	128.58	125.04
17	j	3002	CLA	CBC-CAC-C3C	-2.32	106.03	112.43
17	4	602	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
17	b	823	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
17	a	826	CLA	O1D-CGD-CBD	-2.32	119.73	124.48
17	A	818	CLA	CMB-C2B-C3B	2.32	129.03	124.68
17	b	829	CLA	CMC-C2C-C1C	2.32	128.58	125.04
17	6	314	CLA	CMC-C2C-C1C	2.32	128.58	125.04
17	G	103	CLA	C5-C3-C4	2.32	119.73	114.60
17	2	610	CLA	CBC-CAC-C3C	-2.32	106.03	112.43
17	A	804	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
27	4	616	LUT	C38-C25-C24	-2.32	118.59	123.56
17	1	305	CLA	CMC-C2C-C1C	2.32	128.57	125.04
27	9	616	LUT	C7-C8-C9	-2.32	122.73	126.23
17	4	602	CLA	CBC-CAC-C3C	-2.32	106.03	112.43
17	a	807	CLA	C4-C3-C5	2.32	119.18	115.27
17	A	832	CLA	CMC-C2C-C1C	2.32	128.57	125.04
17	b	830	CLA	C5-C3-C4	2.32	119.73	114.60
19	6	301	LHG	C5-O7-C7	-2.32	112.08	117.79
17	A	839	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
17	a	840	CLA	CMB-C2B-C3B	2.32	129.02	124.68
17	A	823	CLA	CMC-C2C-C1C	2.32	128.57	125.04
17	a	837	CLA	CMB-C2B-C3B	2.32	129.02	124.68
17	8	310	CLA	CMC-C2C-C1C	2.32	128.57	125.04
20	b	847	BCR	C2-C1-C6	2.32	114.05	110.48
17	4	610	CLA	CBC-CAC-C3C	-2.32	106.04	112.43
20	K	4001	BCR	C35-C13-C14	-2.32	119.67	122.92
17	k	1401	CLA	CBC-CAC-C3C	-2.32	106.04	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	614	CLA	CBC-CAC-C3C	-2.32	106.04	112.43
20	b	847	BCR	C33-C5-C4	2.32	118.07	113.62
26	9	607	CHL	CHD-C4C-NC	2.32	127.86	124.20
17	A	813	CLA	C2A-C1A-CHA	-2.32	119.81	123.86
20	a	849	BCR	C33-C5-C6	-2.32	121.92	124.53
17	b	817	CLA	CBC-CAC-C3C	-2.32	106.04	112.43
17	B	808	CLA	CMC-C2C-C1C	2.32	128.57	125.04
17	a	841	CLA	C4-C3-C5	2.32	119.17	115.27
17	2	612	CLA	CMB-C2B-C3B	2.32	129.01	124.68
17	a	829	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
20	j	3003	BCR	C3-C4-C5	-2.32	109.94	114.08
17	a	829	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
17	1	304	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
20	A	852	BCR	C29-C30-C25	2.32	114.05	110.48
26	6	303	CHL	O2A-CGA-CBA	2.32	119.18	111.91
17	b	841	CLA	CBC-CAC-C3C	-2.32	106.05	112.43
17	7	612	CLA	CBC-CAC-C3C	-2.32	106.05	112.43
17	a	803	CLA	CMC-C2C-C1C	2.32	128.57	125.04
17	1	314	CLA	CMC-C2C-C1C	2.32	128.57	125.04
17	7	613	CLA	CMC-C2C-C1C	2.32	128.57	125.04
17	7	608	CLA	C5-C3-C4	2.32	119.72	114.60
17	b	810	CLA	CAA-C2A-C3A	-2.32	106.44	112.78
17	A	811	CLA	C2A-C1A-CHA	-2.32	119.81	123.86
17	B	840	CLA	CAC-C3C-C4C	2.31	127.81	124.81
17	a	817	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
17	a	843	CLA	CMB-C2B-C3B	2.31	129.01	124.68
17	A	816	CLA	CBC-CAC-C3C	-2.31	106.05	112.43
17	9	602	CLA	CAA-C2A-C3A	-2.31	106.44	112.78
17	A	854	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
17	A	812	CLA	C2A-C1A-CHA	-2.31	119.81	123.86
28	8	315	XAT	C30-C31-C32	-2.31	116.00	123.22
17	b	816	CLA	C1-C2-C3	-2.31	122.04	126.04
17	g	103	CLA	C2A-C1A-CHA	-2.31	119.81	123.86
17	b	826	CLA	CMC-C2C-C1C	2.31	128.56	125.04
17	b	839	CLA	CMC-C2C-C1C	2.31	128.56	125.04
17	3	310	CLA	CMA-C3A-C2A	-2.31	110.70	116.10
17	b	814	CLA	CMB-C2B-C3B	2.31	129.00	124.68
17	4	603	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
17	8	304	CLA	CAA-C2A-C3A	-2.31	108.48	114.26
20	B	848	BCR	C37-C22-C23	2.31	121.72	118.08
17	L	203	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
17	b	810	CLA	CMB-C2B-C3B	2.31	129.00	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	608	CLA	CMB-C2B-C3B	2.31	129.00	124.68
17	8	301	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
26	2	601	CHL	OMC-CMC-C2C	-2.31	120.46	125.69
17	3	312	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
27	9	616	LUT	C18-C5-C4	2.31	118.63	114.36
17	1	308	CLA	CMC-C2C-C1C	2.31	128.56	125.04
17	9	608	CLA	C5-C3-C4	2.31	119.70	114.60
20	B	846	BCR	C38-C26-C27	2.31	118.05	113.62
17	b	840	CLA	CMC-C2C-C1C	2.31	128.56	125.04
17	3	311	CLA	CMC-C2C-C1C	2.31	128.56	125.04
17	A	820	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
17	b	816	CLA	CMB-C2B-C3B	2.31	129.00	124.68
20	f	7004	BCR	C24-C23-C22	-2.31	122.75	126.23
17	7	604	CLA	CBC-CAC-C3C	-2.31	106.07	112.43
27	2	615	LUT	C8-C7-C6	-2.31	120.72	127.20
20	b	847	BCR	C36-C18-C19	2.31	121.71	118.08
17	b	810	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
26	3	307	CHL	O2D-CGD-O1D	-2.31	119.33	123.84
26	4	615	CHL	O2D-CGD-O1D	-2.31	119.33	123.84
17	7	609	CLA	CBC-CAC-C3C	-2.31	106.07	112.43
17	1	303	CLA	CMB-C2B-C3B	2.31	128.99	124.68
17	a	832	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
20	F	305	BCR	C33-C5-C6	-2.31	121.94	124.53
26	3	307	CHL	CBC-CAC-C3C	-2.31	106.08	112.43
20	b	847	BCR	C29-C30-C25	2.30	114.03	110.48
17	A	833	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
26	7	606	CHL	CHD-C4C-NC	2.30	127.83	124.20
17	1	312	CLA	CMC-C2C-C1C	2.30	128.55	125.04
17	A	805	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
17	7	602	CLA	C4-C3-C5	2.30	119.15	115.27
17	a	807	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
28	7	616	XAT	C38-C25-C24	2.30	116.87	114.28
26	9	606	CHL	CHD-C4C-NC	2.30	127.83	124.20
17	b	822	CLA	CAC-C3C-C4C	2.30	127.80	124.81
17	B	836	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
27	9	616	LUT	C38-C25-C24	-2.30	118.63	123.56
17	B	836	CLA	C4D-C3D-CAD	-2.30	107.19	108.47
17	A	818	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
17	4	609	CLA	CED-O2D-CGD	2.30	121.14	115.94
26	4	605	CHL	C1-O2A-CGA	2.30	122.48	116.44
17	A	829	CLA	CMC-C2C-C1C	2.30	128.54	125.04
17	B	818	CLA	CBC-CAC-C3C	-2.30	106.09	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	856	CLA	CHD-C4C-NC	2.30	127.83	124.20
17	L	203	CLA	CAA-C2A-C3A	-2.30	106.48	112.78
17	3	301	CLA	CBC-CAC-C3C	-2.30	106.09	112.43
17	3	310	CLA	CBC-CAC-C3C	-2.30	106.09	112.43
17	3	312	CLA	CBC-CAC-C3C	-2.30	106.09	112.43
17	a	856	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
17	B	822	CLA	CMC-C2C-C1C	2.30	128.54	125.04
17	B	820	CLA	CMB-C2B-C3B	2.30	128.98	124.68
17	3	313	CLA	CMB-C2B-C3B	2.30	128.98	124.68
17	6	315	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
17	l	203	CLA	C4D-C3D-CAD	-2.30	107.19	108.47
17	a	822	CLA	CBC-CAC-C3C	-2.30	106.09	112.43
17	b	821	CLA	CMC-C2C-C1C	2.30	128.54	125.04
17	7	613	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
17	A	801	CLA	CMA-C3A-C2A	-2.30	104.56	113.83
17	a	836	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
17	6	312	CLA	CMA-C3A-C2A	-2.30	110.74	116.10
17	b	825	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
18	b	842	PQN	C2M-C2-C3	-2.30	120.65	124.40
17	A	824	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
17	9	614	CLA	CMC-C2C-C1C	2.30	128.54	125.04
20	4	618	BCR	C15-C16-C17	-2.30	118.77	123.47
17	A	854	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
17	2	604	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
17	2	604	CLA	CMB-C2B-C3B	2.30	128.97	124.68
17	8	309	CLA	CBC-CAC-C3C	-2.30	106.10	112.43
17	k	1401	CLA	CMC-C2C-C1C	2.30	128.53	125.04
17	F	304	CLA	CMB-C2B-C3B	2.30	128.97	124.68
26	7	605	CHL	CMB-C2B-C3B	2.30	128.97	124.68
17	1	311	CLA	CMA-C3A-C2A	-2.30	110.74	116.10
17	8	303	CLA	CBC-CAC-C3C	-2.30	106.10	112.43
17	6	307	CLA	CMC-C2C-C1C	2.29	128.53	125.04
17	1	311	CLA	C2A-C1A-CHA	-2.29	119.85	123.85
17	b	819	CLA	CAA-C2A-C3A	-2.29	106.50	112.78
17	3	312	CLA	CMB-C2B-C3B	2.29	128.97	124.68
17	B	828	CLA	C2A-C1A-CHA	-2.29	119.85	123.86
17	b	840	CLA	CBC-CAC-C3C	-2.29	106.11	112.43
26	9	606	CHL	C5-C3-C4	2.29	119.67	114.60
17	6	313	CLA	CMC-C2C-C1C	2.29	128.53	125.04
17	A	820	CLA	CMC-C2C-C1C	2.29	128.53	125.04
17	a	805	CLA	CMB-C2B-C3B	2.29	128.97	124.68
17	3	303	CLA	C5-C3-C4	2.29	119.67	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	6	319	BCR	C37-C22-C23	2.29	121.69	118.08
28	3	317	XAT	C4-C3-C2	-2.29	106.35	110.77
17	b	802	CLA	CBC-CAC-C3C	-2.29	106.11	112.43
17	K	4002	CLA	CBC-CAC-C3C	-2.29	106.11	112.43
17	1	314	CLA	C2A-C1A-CHA	-2.29	119.85	123.86
17	3	309	CLA	CBC-CAC-C3C	-2.29	106.11	112.43
20	b	845	BCR	C29-C30-C25	2.29	114.01	110.48
17	2	611	CLA	CMC-C2C-C1C	2.29	128.53	125.04
17	B	802	CLA	CMA-C3A-C2A	-2.29	104.59	113.83
17	B	832	CLA	CMC-C2C-C1C	2.29	128.53	125.04
17	A	816	CLA	CMB-C2B-C3B	2.29	128.96	124.68
17	B	808	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
20	g	104	BCR	C38-C26-C27	2.29	118.01	113.62
17	b	841	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
17	9	604	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
20	a	853	BCR	C37-C22-C21	-2.29	119.72	122.92
17	A	827	CLA	O2A-CGA-CBA	2.29	119.09	111.91
17	A	854	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
17	A	835	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
26	7	607	CHL	O2D-CGD-O1D	-2.29	119.37	123.84
17	a	809	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
17	9	602	CLA	CBC-CAC-C3C	-2.29	106.13	112.43
17	8	304	CLA	CMC-C2C-C1C	2.29	128.52	125.04
20	A	856	BCR	C15-C16-C17	-2.29	118.79	123.47
17	A	842	CLA	CMC-C2C-C1C	2.29	128.52	125.04
17	6	306	CLA	CMC-C2C-C1C	2.29	128.52	125.04
27	7	615	LUT	C38-C25-C24	-2.29	118.67	123.56
17	A	825	CLA	CBC-CAC-C3C	-2.29	106.13	112.43
26	2	607	CHL	CHD-C4C-NC	2.29	127.81	124.20
17	a	802	CLA	C1-O2A-CGA	2.29	122.44	116.44
17	A	836	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
26	6	303	CHL	OMC-CMC-C2C	-2.28	120.52	125.69
17	6	316	CLA	C2A-C1A-CHA	-2.28	119.86	123.86
17	3	305	CLA	CBC-CAC-C3C	-2.28	106.13	112.43
17	A	832	CLA	C5-C3-C4	2.28	119.65	114.60
17	a	819	CLA	CBC-CAC-C3C	-2.28	106.13	112.43
17	3	306	CLA	CBC-CAC-C3C	-2.28	106.13	112.43
17	b	825	CLA	CHB-C4A-NA	2.28	127.67	124.51
17	b	835	CLA	CMB-C2B-C3B	2.28	128.95	124.68
17	B	829	CLA	CMB-C2B-C3B	2.28	128.95	124.68
17	b	833	CLA	CMC-C2C-C1C	2.28	128.52	125.04
17	8	310	CLA	C2A-C1A-CHA	-2.28	119.87	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	8	314	LUT	C31-C30-C29	-2.28	124.05	127.31
26	7	606	CHL	O2D-CGD-O1D	-2.28	119.38	123.84
17	b	835	CLA	CMC-C2C-C1C	2.28	128.51	125.04
17	A	822	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
26	9	607	CHL	CMB-C2B-C3B	2.28	128.95	124.68
17	2	602	CLA	CMC-C2C-C1C	2.28	128.51	125.04
17	b	830	CLA	CMB-C2B-C3B	2.28	128.94	124.68
17	a	803	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
17	A	842	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
17	9	604	CLA	C5-C3-C4	2.28	119.64	114.60
17	b	811	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
27	7	615	LUT	C30-C31-C32	-2.28	116.11	123.22
17	A	833	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
17	A	816	CLA	CMC-C2C-C1C	2.28	128.51	125.04
17	b	824	CLA	CGD-CBD-CAD	-2.28	103.36	110.73
17	a	838	CLA	O1D-CGD-CBD	-2.28	119.82	124.48
17	b	810	CLA	CMC-C2C-C1C	2.28	128.51	125.04
20	2	617	BCR	C15-C16-C17	-2.28	118.81	123.47
17	8	302	CLA	C5-C3-C4	2.28	119.63	114.60
17	A	831	CLA	C2A-C1A-CHA	-2.28	119.88	123.86
17	a	842	CLA	CBC-CAC-C3C	-2.28	106.16	112.43
17	3	309	CLA	O2A-CGA-O1A	-2.28	117.85	123.59
17	1	313	CLA	CMC-C2C-C1C	2.28	128.50	125.04
17	G	103	CLA	CMC-C2C-C1C	2.28	128.50	125.04
20	f	7004	BCR	C20-C21-C22	-2.28	124.06	127.31
17	A	808	CLA	C1-C2-C3	-2.28	122.11	126.04
17	9	612	CLA	C2A-C1A-CHA	-2.28	119.88	123.86
17	G	104	CLA	CBC-CAC-C3C	-2.28	106.16	112.43
17	7	602	CLA	CBC-CAC-C3C	-2.28	106.16	112.43
17	B	832	CLA	C6-C7-C8	-2.27	108.57	115.92
17	7	612	CLA	C2A-C1A-CHA	-2.27	119.88	123.86
20	j	3003	BCR	C10-C11-C12	-2.27	116.12	123.22
17	6	305	CLA	CMB-C2B-C3B	2.27	128.93	124.68
17	9	614	CLA	CBC-CAC-C3C	-2.27	106.16	112.43
17	B	837	CLA	CAA-C2A-C3A	-2.27	106.55	112.78
20	g	104	BCR	C29-C30-C25	2.27	113.98	110.48
17	4	613	CLA	CBC-CAC-C3C	-2.27	106.17	112.43
27	6	321	LUT	C30-C31-C32	-2.27	116.12	123.22
17	a	841	CLA	CMC-C2C-C1C	2.27	128.50	125.04
17	6	314	CLA	CBC-CAC-C3C	-2.27	106.17	112.43
17	a	841	CLA	CMB-C2B-C3B	2.27	128.93	124.68
20	B	801	BCR	C21-C20-C19	-2.27	116.13	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	807	CLA	CMC-C2C-C1C	2.27	128.50	125.04
17	8	308	CLA	CED-O2D-CGD	2.27	121.07	115.94
17	L	202	CLA	CBC-CAC-C3C	-2.27	106.17	112.43
17	B	813	CLA	CMB-C2B-C3B	2.27	128.93	124.68
17	7	602	CLA	CMB-C2B-C3B	2.27	128.93	124.68
17	9	601	CLA	O2A-CGA-CBA	2.27	121.20	112.23
17	a	827	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
17	a	804	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
17	a	856	CLA	CBC-CAC-C3C	-2.27	106.17	112.43
20	9	618	BCR	C29-C30-C25	2.27	113.98	110.48
20	L	205	BCR	C38-C26-C27	2.27	117.98	113.62
17	3	312	CLA	CMC-C2C-C1C	2.27	128.50	125.04
17	7	611	CLA	CBC-CAC-C3C	-2.27	106.17	112.43
17	b	826	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
17	a	830	CLA	CBC-CAC-C3C	-2.27	106.17	112.43
17	b	808	CLA	C4-C3-C5	2.27	119.09	115.27
17	k	1403	CLA	CMB-C2B-C3B	2.27	128.92	124.68
17	a	829	CLA	C4D-C3D-CAD	-2.27	107.20	108.47
26	2	605	CHL	OMC-CMC-C2C	-2.27	120.56	125.69
27	9	616	LUT	C30-C31-C32	-2.27	116.14	123.22
17	g	102	CLA	CBC-CAC-C3C	-2.27	106.18	112.43
26	2	606	CHL	CHD-C4C-NC	2.27	127.78	124.20
17	7	611	CLA	CMC-C2C-C1C	2.27	128.49	125.04
27	6	321	LUT	C31-C30-C29	-2.27	124.08	127.31
26	1	302	CHL	CBC-CAC-C3C	-2.27	106.18	112.43
20	9	618	BCR	C36-C18-C19	2.27	121.65	118.08
28	8	315	XAT	C39-C29-C28	2.27	121.65	118.08
17	8	310	CLA	CMB-C2B-C3B	2.27	128.92	124.68
17	2	609	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
17	6	304	CLA	CBC-CAC-C3C	-2.26	106.19	112.43
17	A	821	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
18	a	845	PQN	C2M-C2-C1	2.26	120.02	116.27
17	b	828	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
17	4	604	CLA	CMC-C2C-C1C	2.26	128.49	125.04
20	l	201	BCR	C8-C9-C10	2.26	122.42	118.94
17	a	820	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
17	B	823	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
17	B	834	CLA	CMB-C2B-C3B	2.26	128.91	124.68
17	a	817	CLA	CMC-C2C-C1C	2.26	128.49	125.04
17	l	202	CLA	CMC-C2C-C1C	2.26	128.49	125.04
20	l	206	BCR	C2-C1-C6	2.26	113.97	110.48
17	8	309	CLA	C1-C2-C3	-2.26	122.13	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	l	202	CLA	O2A-CGA-CBA	2.26	119.01	111.91
17	8	303	CLA	CMC-C2C-C1C	2.26	128.49	125.04
17	9	613	CLA	CMC-C2C-C1C	2.26	128.49	125.04
17	b	835	CLA	CAA-C2A-C3A	-2.26	106.58	112.78
17	J	3002	CLA	CHB-C4A-NA	2.26	127.64	124.51
26	4	607	CHL	CBC-CAC-C3C	-2.26	106.19	112.43
17	2	612	CLA	C4-C3-C5	2.26	119.08	115.27
17	G	104	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
17	A	814	CLA	CMC-C2C-C1C	2.26	128.48	125.04
17	a	806	CLA	CMB-C2B-C3B	2.26	128.91	124.68
17	B	808	CLA	C4-C3-C5	2.26	119.08	115.27
17	G	101	CLA	CBC-CAC-C3C	-2.26	106.20	112.43
17	3	302	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
17	b	830	CLA	CBC-CAC-C3C	-2.26	106.20	112.43
17	l	204	CLA	CBC-CAC-C3C	-2.26	106.20	112.43
17	b	837	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
17	B	823	CLA	CMB-C2B-C3B	2.26	128.91	124.68
17	3	310	CLA	C2A-C1A-CHA	-2.26	119.91	123.85
20	A	850	BCR	C23-C24-C25	-2.26	120.86	127.20
20	6	319	BCR	C15-C16-C17	-2.26	118.85	123.47
17	a	835	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
17	A	814	CLA	CHB-C4A-NA	2.26	127.64	124.51
17	a	820	CLA	CMC-C2C-C1C	2.26	128.48	125.04
17	1	308	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
17	7	613	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
17	B	817	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
17	A	829	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
17	7	609	CLA	C4-C3-C5	2.26	119.07	115.27
17	3	310	CLA	CMC-C2C-C1C	2.26	128.48	125.04
17	a	818	CLA	CBC-CAC-C3C	-2.26	106.21	112.43
17	9	612	CLA	CMC-C2C-C1C	2.26	128.47	125.04
17	K	4003	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
17	A	812	CLA	CAA-C2A-C3A	-2.26	106.60	112.78
17	7	608	CLA	CMA-C3A-C4A	-2.26	105.71	111.77
20	b	848	BCR	C34-C9-C8	2.26	121.63	118.08
17	k	1403	CLA	O1D-CGD-CBD	-2.25	119.87	124.48
17	4	613	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
17	3	308	CLA	CMC-C2C-C1C	2.25	128.47	125.04
17	g	101	CLA	C2A-C1A-CHA	-2.25	119.92	123.85
17	6	306	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
17	j	3002	CLA	CMC-C2C-C1C	2.25	128.47	125.04
17	A	831	CLA	C4D-C3D-CAD	-2.25	107.21	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	306	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
17	1	313	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
17	B	823	CLA	CED-O2D-CGD	2.25	121.03	115.94
20	B	845	BCR	C33-C5-C4	2.25	117.94	113.62
17	F	303	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
17	A	808	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
17	2	603	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
17	A	843	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
17	A	843	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
17	a	831	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
17	B	825	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
17	b	834	CLA	CMC-C2C-C1C	2.25	128.47	125.04
17	B	802	CLA	CAC-C3C-C4C	2.25	127.73	124.81
17	a	814	CLA	O2A-CGA-CBA	2.25	118.97	111.91
17	a	829	CLA	CMB-C2B-C3B	2.25	128.89	124.68
17	b	813	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
17	b	837	CLA	CAA-C2A-C3A	-2.25	106.62	112.78
26	9	605	CHL	CMB-C2B-C3B	2.25	128.89	124.68
17	a	812	CLA	CBC-CAC-C3C	-2.25	106.23	112.43
17	6	307	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
17	8	302	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
17	a	822	CLA	O2A-CGA-CBA	2.25	118.97	111.91
17	B	821	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
17	A	832	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
17	B	819	CLA	CMC-C2C-C1C	2.25	128.47	125.04
17	a	841	CLA	CBC-CAC-C3C	-2.25	106.23	112.43
17	a	829	CLA	C11-C10-C8	-2.25	108.65	115.92
17	8	301	CLA	CBC-CAC-C3C	-2.25	106.23	112.43
17	4	602	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
17	4	613	CLA	CMC-C2C-C1C	2.25	128.46	125.04
17	b	836	CLA	C2A-C1A-CHA	-2.25	119.93	123.86
17	a	832	CLA	CHB-C4A-NA	2.25	127.62	124.51
17	a	843	CLA	O1D-CGD-CBD	-2.25	119.89	124.48
17	L	202	CLA	CMB-C2B-C3B	2.25	128.88	124.68
17	6	314	CLA	CMB-C2B-C3B	2.25	128.88	124.68
17	F	304	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
17	B	817	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
20	j	3004	BCR	C16-C15-C14	-2.25	118.87	123.47
17	a	816	CLA	CBC-CAC-C3C	-2.25	106.24	112.43
20	B	801	BCR	C10-C11-C12	-2.25	116.21	123.22
27	1	316	LUT	C35-C15-C14	-2.25	118.87	123.47
17	k	1402	CLA	CAA-C2A-C3A	-2.25	106.63	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	1	317	XAT	C15-C14-C13	-2.24	124.11	127.31
17	a	837	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
17	a	838	CLA	CAA-C2A-C3A	-2.24	106.63	112.78
26	9	606	CHL	CHB-C4A-NA	2.24	127.61	124.51
17	a	806	CLA	CHB-C4A-NA	2.24	127.61	124.51
17	A	803	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
17	b	818	CLA	CMB-C2B-C3B	2.24	128.87	124.68
17	8	307	CLA	CAA-C2A-C3A	-2.24	106.64	112.78
17	A	837	CLA	CMC-C2C-C1C	2.24	128.45	125.04
20	b	844	BCR	C2-C1-C6	2.24	113.93	110.48
17	B	804	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
28	6	318	XAT	C20-C13-C12	2.24	121.61	118.08
17	B	811	CLA	CMB-C2B-C3B	2.24	129.08	124.69
17	3	304	CLA	CMB-C2B-C3B	2.24	128.87	124.68
17	9	601	CLA	CBC-CAC-C3C	-2.24	106.25	112.43
20	a	849	BCR	C37-C22-C21	-2.24	119.78	122.92
17	B	827	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
26	7	605	CHL	CBC-CAC-C3C	-2.24	106.25	112.43
17	1	311	CLA	CMC-C2C-C1C	2.24	128.45	125.04
20	L	206	BCR	C28-C27-C26	-2.24	110.08	114.08
20	k	1404	BCR	C11-C10-C9	-2.24	124.11	127.31
17	A	834	CLA	CBC-CAC-C3C	-2.24	106.26	112.43
17	b	829	CLA	CHD-C4C-NC	2.24	127.73	124.20
20	b	843	BCR	C11-C12-C13	-2.24	120.13	126.42
17	b	815	CLA	CMB-C2B-C3B	2.24	128.87	124.68
17	4	609	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
27	8	314	LUT	C7-C8-C9	-2.24	122.85	126.23
17	A	828	CLA	C4-C3-C5	2.24	119.04	115.27
17	B	825	CLA	CBC-CAC-C3C	-2.24	106.26	112.43
20	a	852	BCR	C29-C30-C25	2.24	113.93	110.48
17	1	309	CLA	CED-O2D-CGD	2.24	121.00	115.94
17	A	842	CLA	C2A-C1A-CHA	-2.24	119.95	123.86
27	6	317	LUT	C39-C29-C28	2.24	121.60	118.08
26	9	605	CHL	CBC-CAC-C3C	-2.24	106.27	112.43
20	B	846	BCR	C37-C22-C23	2.24	121.60	118.08
17	b	837	CLA	CMC-C2C-C1C	2.24	128.44	125.04
17	l	202	CLA	C2A-C1A-CHA	-2.23	119.95	123.86
20	i	101	BCR	C33-C5-C6	-2.23	122.02	124.53
26	9	607	CHL	CBC-CAC-C3C	-2.23	106.27	112.43
20	j	3004	BCR	C8-C7-C6	-2.23	120.93	127.20
17	B	817	CLA	CHB-C4A-NA	2.23	127.60	124.51
17	A	842	CLA	C4-C3-C5	2.23	119.03	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	838	CLA	CMC-C2C-C1C	2.23	128.44	125.04
17	b	802	CLA	CHB-C4A-NA	2.23	127.60	124.51
17	9	602	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
26	1	302	CHL	C1-O2A-CGA	2.23	122.30	116.44
17	B	813	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
17	A	828	CLA	CAC-C3C-C4C	2.23	127.71	124.81
17	2	604	CLA	CBC-CAC-C3C	-2.23	106.28	112.43
17	B	810	CLA	CBC-CAC-C3C	-2.23	106.28	112.43
17	B	814	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
17	4	603	CLA	CMB-C2B-C3B	2.23	128.85	124.68
17	a	823	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
17	6	311	CLA	CED-O2D-CGD	2.23	120.98	115.94
17	a	818	CLA	CMC-C2C-C1C	2.23	128.44	125.04
17	3	306	CLA	CMC-C2C-C1C	2.23	128.44	125.04
17	b	827	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
17	a	840	CLA	CBC-CAC-C3C	-2.23	106.29	112.43
17	4	611	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
26	7	605	CHL	CHD-C4C-NC	2.23	127.72	124.20
17	B	829	CLA	CHD-C4C-NC	2.23	127.72	124.20
20	F	305	BCR	C37-C22-C23	2.23	121.59	118.08
17	b	833	CLA	CBC-CAC-C3C	-2.23	106.29	112.43
17	B	822	CLA	CBC-CAC-C3C	-2.23	106.29	112.43
17	6	310	CLA	CBC-CAC-C3C	-2.23	106.29	112.43
17	b	802	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
17	3	309	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
17	A	820	CLA	C4-C3-C5	2.23	119.02	115.27
17	b	802	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
17	k	1402	CLA	CMB-C2B-C3B	2.23	128.84	124.68
17	L	202	CLA	C2A-C1A-CHA	-2.23	119.97	123.86
26	7	614	CHL	CBC-CAC-C3C	-2.23	106.29	112.43
17	b	806	CLA	CBC-CAC-C3C	-2.23	106.29	112.43
17	a	802	CLA	CBC-CAC-C3C	-2.23	106.29	112.43
20	4	618	BCR	C36-C18-C19	2.23	121.58	118.08
17	B	840	CLA	CMB-C2B-C3B	2.23	128.84	124.68
20	A	851	BCR	C8-C7-C6	-2.23	120.95	127.20
17	1	313	CLA	C2A-C1A-CHA	-2.23	119.97	123.86
17	3	313	CLA	CED-O2D-CGD	2.23	120.97	115.94
20	9	618	BCR	C3-C4-C5	-2.23	110.10	114.08
17	a	808	CLA	CBC-CAC-C3C	-2.23	106.30	112.43
17	1	304	CLA	CMB-C2B-C3B	2.22	128.84	124.68
17	B	802	CLA	CHB-C4A-NA	2.22	127.59	124.51
17	7	609	CLA	O2A-CGA-O1A	-2.22	117.98	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	2	616	XAT	C38-C25-C24	2.22	116.78	114.28
28	6	318	XAT	C15-C14-C13	-2.22	124.14	127.31
17	A	811	CLA	CMB-C2B-C3B	2.22	128.84	124.68
20	7	617	BCR	C33-C5-C6	-2.22	122.03	124.53
20	9	618	BCR	C15-C16-C17	-2.22	118.92	123.47
17	9	614	CLA	C2A-C1A-CHA	-2.22	119.97	123.86
26	6	303	CHL	CBC-CAC-C3C	-2.22	106.31	112.43
17	1	203	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
17	B	819	CLA	C2A-C1A-CHA	-2.22	119.97	123.86
27	1	316	LUT	C7-C8-C9	-2.22	122.88	126.23
17	9	604	CLA	CMC-C2C-C1C	2.22	128.42	125.04
17	B	829	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
17	B	839	CLA	C2A-C1A-CHA	-2.22	119.98	123.86
28	1	317	XAT	C38-C25-C24	2.22	116.78	114.28
17	B	807	CLA	CBC-CAC-C3C	-2.22	106.31	112.43
17	4	614	CLA	CMC-C2C-C1C	2.22	128.42	125.04
17	8	308	CLA	CBC-CAC-C3C	-2.22	106.31	112.43
17	b	822	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
17	4	604	CLA	C5-C3-C4	2.22	119.50	114.60
17	L	204	CLA	CMC-C2C-C1C	2.22	128.42	125.04
17	1	313	CLA	CMB-C2B-C3B	2.22	128.83	124.68
20	b	843	BCR	C27-C26-C25	-2.22	119.51	122.73
17	b	817	CLA	C2A-C1A-CHA	-2.22	119.98	123.86
20	G	105	BCR	C16-C15-C14	-2.22	118.93	123.47
17	1	308	CLA	CBC-CAC-C3C	-2.22	106.32	112.43
17	3	304	CLA	C2A-C1A-CHA	-2.22	119.98	123.86
17	B	814	CLA	CAA-C2A-C3A	-2.22	106.71	112.78
17	B	809	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
20	I	101	BCR	C11-C10-C9	-2.22	124.15	127.31
17	A	831	CLA	CHD-C4C-NC	2.22	127.70	124.20
17	b	813	CLA	CMB-C2B-C3B	2.22	128.82	124.68
17	A	815	CLA	CMB-C2B-C3B	2.22	128.82	124.68
19	2	618	LHG	C5-O7-C7	-2.22	112.34	117.79
17	A	806	CLA	O2A-C1-C2	2.22	114.46	108.64
20	K	4004	BCR	C8-C7-C6	-2.22	120.98	127.20
17	a	818	CLA	CHB-C4A-NA	2.22	127.58	124.51
17	A	825	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
17	8	311	CLA	CBC-CAC-C3C	-2.21	106.33	112.43
17	B	815	CLA	CBC-CAC-C3C	-2.21	106.33	112.43
17	b	841	CLA	O1D-CGD-CBD	-2.21	119.95	124.48
17	6	307	CLA	CBC-CAC-C3C	-2.21	106.33	112.43
26	4	605	CHL	CHC-C1C-C2C	-2.21	118.08	126.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	l	206	BCR	C33-C5-C6	-2.21	122.04	124.53
17	8	305	CLA	CBC-CAC-C3C	-2.21	106.33	112.43
17	9	608	CLA	CHB-C4A-NA	2.21	127.57	124.51
17	6	314	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
27	1	316	LUT	C30-C31-C32	-2.21	116.31	123.22
17	3	308	CLA	CHB-C4A-NA	2.21	127.57	124.51
17	b	840	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
17	B	832	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
27	1	320	LUT	C38-C25-C24	-2.21	118.83	123.56
26	9	605	CHL	OMC-CMC-C2C	-2.21	120.69	125.69
17	A	829	CLA	C4D-C3D-CAD	-2.21	107.24	108.47
26	4	605	CHL	C1-C2-C3	-2.21	122.22	126.04
27	2	615	LUT	C38-C25-C24	-2.21	118.83	123.56
17	a	802	CLA	C4-C3-C5	2.21	118.99	115.27
20	I	101	BCR	C37-C22-C21	-2.21	119.83	122.92
17	b	816	CLA	CHB-C4A-NA	2.21	127.57	124.51
17	b	818	CLA	CBC-CAC-C3C	-2.21	106.34	112.43
17	A	814	CLA	CMB-C2B-C3B	2.21	128.81	124.68
27	1	316	LUT	C10-C11-C12	-2.21	116.32	123.22
17	2	613	CLA	C2A-C1A-CHA	-2.21	120.00	123.86
17	b	815	CLA	O1D-CGD-CBD	-2.21	119.97	124.48
17	g	101	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
17	3	313	CLA	CMC-C2C-C1C	2.21	128.40	125.04
17	A	830	CLA	CBC-CAC-C3C	-2.21	106.34	112.43
28	3	317	XAT	C20-C13-C12	2.21	121.56	118.08
26	2	605	CHL	CBC-CAC-C3C	-2.21	106.35	112.43
17	b	819	CLA	C2A-C1A-CHA	-2.21	120.00	123.86
17	A	831	CLA	CMB-C2B-C3B	2.21	128.81	124.68
26	7	601	CHL	CBC-CAC-C3C	-2.21	106.35	112.43
17	8	308	CLA	CHB-C4A-NA	2.21	127.56	124.51
17	8	310	CLA	O2D-CGD-O1D	-2.21	119.53	123.84
17	4	614	CLA	C2A-C1A-CHA	-2.21	120.00	123.86
17	8	307	CLA	CHB-C4A-NA	2.21	127.56	124.51
17	8	311	CLA	O2D-CGD-O1D	-2.21	119.53	123.84
20	b	843	BCR	C34-C9-C10	-2.21	119.83	122.92
17	A	824	CLA	CMC-C2C-C1C	2.21	128.40	125.04
20	I	101	BCR	C33-C5-C6	-2.20	122.05	124.53
17	8	303	CLA	CHB-C4A-NA	2.20	127.56	124.51
26	4	605	CHL	CHD-C4C-NC	2.20	127.68	124.20
17	3	305	CLA	CMC-C2C-C1C	2.20	128.40	125.04
17	6	311	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
20	B	848	BCR	C38-C26-C25	-2.20	122.05	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	a	851	BCR	C38-C26-C25	-2.20	122.05	124.53
20	a	852	BCR	C8-C7-C6	-2.20	121.01	127.20
17	A	810	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
17	a	810	CLA	CMC-C2C-C1C	2.20	128.40	125.04
17	B	817	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
24	B	850	DGD	C2G-O2G-C1B	-2.20	112.37	117.79
17	B	818	CLA	C1-C2-C3	-2.20	122.23	126.04
17	1	310	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
17	1	303	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
17	b	819	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
17	a	813	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
20	B	844	BCR	C2-C1-C6	2.20	113.87	110.48
26	6	308	CHL	CHD-C4C-NC	2.20	127.67	124.20
26	4	606	CHL	CHD-C4C-NC	2.20	127.67	124.20
17	a	838	CLA	O2A-C1-C2	2.20	114.42	108.64
17	J	3002	CLA	CBC-CAC-C3C	-2.20	106.37	112.43
20	L	205	BCR	C37-C22-C21	-2.20	119.84	122.92
17	4	604	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
17	b	818	CLA	C4D-C3D-CAD	-2.20	107.24	108.47
17	A	824	CLA	CBC-CAC-C3C	-2.20	106.37	112.43
17	4	611	CLA	CMC-C2C-C1C	2.20	128.39	125.04
17	L	204	CLA	C2A-C1A-CHA	-2.20	120.02	123.86
17	3	313	CLA	C2A-C1A-CHA	-2.20	120.02	123.86
17	9	603	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
17	B	831	CLA	CHB-C4A-NA	2.20	127.55	124.51
17	B	824	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
20	B	847	BCR	C36-C18-C19	2.20	121.54	118.08
17	A	827	CLA	CMC-C2C-C1C	2.20	128.38	125.04
17	b	805	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
17	b	821	CLA	C4D-C3D-CAD	-2.20	107.25	108.47
17	B	838	CLA	CMB-C2B-C3B	2.20	128.79	124.68
17	A	836	CLA	C5-C3-C4	2.20	119.45	114.60
17	k	1402	CLA	C2A-C1A-CHA	-2.20	120.02	123.86
17	4	604	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
17	a	839	CLA	CBC-CAC-C3C	-2.20	106.38	112.43
20	G	105	BCR	C11-C10-C9	-2.20	124.18	127.31
17	B	837	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
17	7	612	CLA	O2D-CGD-O1D	-2.20	119.55	123.84
17	1	313	CLA	CBC-CAC-C3C	-2.20	106.38	112.43
17	A	818	CLA	CBC-CAC-C3C	-2.20	106.38	112.43
20	2	617	BCR	C36-C18-C19	2.20	121.54	118.08
26	6	303	CHL	CHD-C4C-NC	2.20	127.66	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	9	609	CLA	CMC-C2C-C1C	2.20	128.38	125.04
17	7	608	CLA	C2A-C1A-CHA	-2.19	120.02	123.86
17	4	601	CLA	O1D-CGD-CBD	-2.19	119.99	124.48
17	B	837	CLA	CHB-C4A-NA	2.19	127.55	124.51
17	9	610	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
26	2	605	CHL	CHC-C1C-C2C	-2.19	118.15	126.11
17	a	824	CLA	CMB-C2B-C3B	2.19	128.78	124.68
27	7	615	LUT	C8-C7-C6	-2.19	121.04	127.20
20	A	852	BCR	C19-C18-C17	2.19	122.31	118.94
17	9	609	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
17	a	813	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
20	A	849	BCR	C10-C11-C12	-2.19	116.38	123.22
20	B	846	BCR	C10-C11-C12	-2.19	116.38	123.22
17	9	603	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
17	b	807	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
17	b	834	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
17	1	310	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
17	a	816	CLA	CMB-C2B-C3B	2.19	128.78	124.68
28	8	315	XAT	C20-C13-C12	2.19	121.53	118.08
26	1	302	CHL	CMB-C2B-C3B	2.19	128.78	124.68
17	b	837	CLA	CHB-C4A-NA	2.19	127.54	124.51
17	a	835	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
17	3	314	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
26	2	601	CHL	CMB-C2B-C3B	2.19	128.78	124.68
20	B	846	BCR	C36-C18-C19	2.19	121.53	118.08
17	A	812	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
17	a	838	CLA	C4D-C3D-CAD	-2.19	107.25	108.47
17	8	308	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
25	4	619	LMG	C8-O7-C10	-2.19	112.40	117.79
17	8	307	CLA	CMC-C2C-C1C	2.19	128.37	125.04
17	2	608	CLA	CBC-CAC-C3C	-2.19	106.40	112.43
17	a	832	CLA	CMC-C2C-C1C	2.19	128.37	125.04
17	b	829	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
17	3	302	CLA	CBC-CAC-C3C	-2.19	106.40	112.43
17	b	814	CLA	CBC-CAC-C3C	-2.19	106.40	112.43
17	B	803	CLA	CED-O2D-CGD	2.19	120.88	115.94
17	a	816	CLA	CED-O2D-CGD	2.19	120.88	115.94
17	B	807	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
17	B	828	CLA	CMB-C2B-C3B	2.19	128.77	124.68
26	4	615	CHL	CHD-C4C-NC	2.19	127.65	124.20
17	B	826	CLA	C4D-C3D-CAD	-2.19	107.25	108.47
17	6	315	CLA	CMC-C2C-C1C	2.19	128.37	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	304	CLA	CMC-C2C-C1C	2.19	128.37	125.04
17	b	809	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
17	A	822	CLA	C11-C10-C8	-2.19	108.86	115.92
17	A	841	CLA	C2A-C1A-CHA	-2.19	120.04	123.86
17	6	315	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
26	2	601	CHL	CHC-C1C-C2C	-2.19	118.19	126.11
17	A	817	CLA	CMB-C2B-C3B	2.18	128.77	124.68
26	6	303	CHL	C4D-C3D-CAD	-2.18	107.25	108.47
17	A	838	CLA	C4D-C3D-CAD	-2.18	107.25	108.47
26	2	601	CHL	O1D-CGD-CBD	-2.18	120.02	124.48
17	2	611	CLA	C2A-C1A-CHA	-2.18	120.04	123.86
17	A	810	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
26	9	605	CHL	CHD-C4C-NC	2.18	127.64	124.20
17	9	609	CLA	CHB-C4A-NA	2.18	127.53	124.51
20	j	3004	BCR	C36-C18-C17	-2.18	119.87	122.92
17	A	840	CLA	CBC-CAC-C3C	-2.18	106.42	112.43
20	b	846	BCR	C20-C21-C22	-2.18	124.20	127.31
17	b	825	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
17	3	302	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
17	A	812	CLA	CHB-C4A-NA	2.18	127.53	124.51
27	3	316	LUT	C38-C25-C24	-2.18	118.89	123.56
17	K	4002	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
17	B	812	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
17	A	811	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
17	4	608	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
20	j	3004	BCR	C11-C10-C9	-2.18	124.20	127.31
17	B	805	CLA	CMB-C2B-C3B	2.18	128.75	124.68
20	F	305	BCR	C21-C20-C19	-2.18	116.42	123.22
17	b	835	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
17	a	810	CLA	CBC-CAC-C3C	-2.18	106.43	112.43
17	9	608	CLA	CMC-C2C-C1C	2.18	128.36	125.04
20	a	851	BCR	C33-C5-C4	2.18	117.80	113.62
17	1	309	CLA	CHB-C4A-NA	2.18	127.52	124.51
17	B	810	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
17	b	832	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
20	a	849	BCR	C2-C1-C6	2.18	113.83	110.48
17	b	831	CLA	CBC-CAC-C3C	-2.18	106.43	112.43
17	K	4003	CLA	CBC-CAC-C3C	-2.18	106.43	112.43
17	4	608	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
26	1	302	CHL	OMC-CMC-C2C	-2.18	120.77	125.69
17	a	836	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
20	B	801	BCR	C8-C7-C6	-2.17	121.09	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	7	609	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
26	2	601	CHL	CHD-C4C-NC	2.17	127.63	124.20
17	B	817	CLA	CMC-C2C-C1C	2.17	128.35	125.04
28	2	616	XAT	C30-C31-C32	-2.17	116.43	123.22
28	4	617	XAT	O4-C5-C6	-2.17	57.16	58.96
27	3	316	LUT	C18-C5-C4	2.17	118.38	114.36
20	b	801	BCR	C20-C21-C22	-2.17	124.21	127.31
20	j	3004	BCR	C38-C26-C27	2.17	117.79	113.62
17	3	308	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
17	b	828	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
17	f	7002	CLA	CMB-C2B-C3B	2.17	128.74	124.68
20	A	849	BCR	C34-C9-C8	2.17	121.50	118.08
17	B	823	CLA	CMC-C2C-C1C	2.17	128.35	125.04
17	2	612	CLA	CMC-C2C-C1C	2.17	128.35	125.04
17	J	3002	CLA	CMC-C2C-C1C	2.17	128.35	125.04
17	B	835	CLA	CHB-C4A-NA	2.17	127.52	124.51
17	B	829	CLA	CMC-C2C-C1C	2.17	128.35	125.04
17	B	816	CLA	CHB-C4A-NA	2.17	127.52	124.51
17	2	610	CLA	CMC-C2C-C1C	2.17	128.35	125.04
17	A	807	CLA	C2A-C1A-CHA	-2.17	120.06	123.86
17	3	311	CLA	CBC-CAC-C3C	-2.17	106.44	112.43
17	b	837	CLA	CMB-C2B-C3B	2.17	128.74	124.68
17	G	103	CLA	C2A-C1A-CHA	-2.17	120.06	123.86
17	a	828	CLA	CMC-C2C-C1C	2.17	128.34	125.04
17	B	837	CLA	CMB-C2B-C3B	2.17	128.74	124.68
17	A	836	CLA	CMC-C2C-C1C	2.17	128.34	125.04
26	2	601	CHL	O2A-CGA-CBA	2.17	118.72	111.91
17	f	7002	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
17	A	813	CLA	C1-O2A-CGA	2.17	122.14	116.44
17	B	832	CLA	C1-O2A-CGA	2.17	122.14	116.44
17	A	814	CLA	C1-O2A-CGA	2.17	122.14	116.44
17	4	603	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
17	B	819	CLA	CHB-C4A-NA	2.17	127.51	124.51
20	1	318	BCR	C15-C16-C17	-2.17	119.03	123.47
19	1	319	LHG	C5-O7-C7	-2.17	112.45	117.79
17	a	819	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
17	2	612	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
17	A	836	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
20	a	851	BCR	C21-C20-C19	-2.17	116.45	123.22
26	2	614	CHL	CHD-C4C-NC	2.17	127.62	124.20
17	B	835	CLA	CED-O2D-CGD	2.17	120.84	115.94
17	a	809	CLA	CAA-C2A-C1A	-2.17	104.88	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	825	CLA	CAA-C2A-C1A	-2.17	104.88	111.97
28	2	616	XAT	C18-C5-C4	2.17	116.72	114.28
17	A	801	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
17	6	314	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
26	6	303	CHL	C1-C2-C3	-2.17	122.30	126.04
17	8	305	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
27	2	615	LUT	C30-C31-C32	-2.16	116.46	123.22
17	2	608	CLA	C2A-C1A-CHA	-2.16	120.07	123.86
17	B	837	CLA	CAC-C3C-C4C	2.16	127.62	124.81
28	2	616	XAT	C35-C15-C14	-2.16	119.04	123.47
26	4	605	CHL	OMC-CMC-C2C	-2.16	120.79	125.69
17	3	301	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
20	F	305	BCR	C8-C7-C6	-2.16	121.13	127.20
17	B	806	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
20	b	845	BCR	C27-C26-C25	-2.16	119.59	122.73
17	4	611	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
17	9	613	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
17	b	805	CLA	CMC-C2C-C1C	2.16	128.33	125.04
17	2	609	CLA	CHB-C4A-NA	2.16	127.50	124.51
17	A	805	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
28	4	617	XAT	C19-C9-C8	2.16	121.48	118.08
17	A	834	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
17	1	310	CLA	CHB-C4A-NA	2.16	127.50	124.51
17	A	831	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
17	8	308	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
17	4	612	CLA	CMC-C2C-C1C	2.16	128.33	125.04
17	b	816	CLA	C1-O2A-CGA	2.16	122.11	116.44
17	A	828	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
26	6	303	CHL	CHB-C4A-NA	2.16	127.50	124.51
17	b	822	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
17	1	310	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
20	2	617	BCR	C8-C7-C6	-2.16	121.14	127.20
26	4	605	CHL	CMB-C2B-C3B	2.16	128.72	124.68
20	8	316	BCR	C37-C22-C23	2.16	121.48	118.08
20	4	618	BCR	C38-C26-C27	2.16	117.77	113.62
26	7	607	CHL	CHD-C4C-NC	2.16	127.61	124.20
26	1	307	CHL	CHD-C4C-NC	2.16	127.61	124.20
17	A	825	CLA	CMC-C2C-C1C	2.16	128.33	125.04
17	a	821	CLA	CMB-C2B-C3B	2.16	128.72	124.68
26	7	607	CHL	C4D-C3D-CAD	-2.16	107.27	108.47
17	l	204	CLA	CMC-C2C-C1C	2.16	128.33	125.04
17	a	815	CLA	C2A-C1A-CHA	-2.16	120.08	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	804	CLA	CBC-CAC-C3C	-2.16	106.48	112.43
17	b	834	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
17	a	836	CLA	CAA-C2A-C3A	-2.16	106.87	112.78
17	7	603	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
17	b	823	CLA	CBC-CAC-C3C	-2.16	106.48	112.43
17	3	311	CLA	C2A-C1A-CHA	-2.16	120.09	123.86
27	3	316	LUT	C30-C31-C32	-2.16	116.49	123.22
20	B	845	BCR	C4-C5-C6	-2.16	119.60	122.73
17	1	309	CLA	CMC-C2C-C1C	2.16	128.32	125.04
17	B	815	CLA	CMB-C2B-C3B	2.16	128.71	124.68
17	l	204	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
28	1	317	XAT	C8-C9-C10	-2.16	115.63	118.94
17	A	837	CLA	CBC-CAC-C3C	-2.16	106.49	112.43
17	B	818	CLA	C4D-C3D-CAD	-2.16	107.27	108.47
17	F	303	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
26	9	605	CHL	CHC-C1C-C2C	-2.16	118.30	126.11
17	8	311	CLA	CMC-C2C-C1C	2.16	128.32	125.04
17	9	613	CLA	CHB-C4A-NA	2.16	127.49	124.51
17	b	831	CLA	O2D-CGD-O1D	-2.15	119.62	123.84
17	B	831	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
27	1	316	LUT	C38-C25-C24	-2.15	118.95	123.56
17	a	822	CLA	CMC-C2C-C1C	2.15	128.32	125.04
17	B	805	CLA	C1-C2-C3	-2.15	122.32	126.04
17	f	7003	CLA	C1-C2-C3	-2.15	122.32	126.04
17	A	816	CLA	C2A-C1A-CHA	-2.15	120.09	123.86
17	4	602	CLA	CAA-C2A-C3A	-2.15	106.88	112.78
27	8	314	LUT	C38-C25-C24	-2.15	118.95	123.56
17	1	310	CLA	CED-O2D-CGD	2.15	120.81	115.94
17	a	820	CLA	C4-C3-C5	2.15	118.89	115.27
17	a	804	CLA	CAA-C2A-C3A	-2.15	106.88	112.78
17	B	810	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
17	a	837	CLA	CED-O2D-CGD	2.15	120.80	115.94
17	a	842	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
17	4	613	CLA	CHB-C4A-NA	2.15	127.49	124.51
17	A	835	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
17	3	309	CLA	CHB-C4A-NA	2.15	127.48	124.51
17	1	306	CLA	CBC-CAC-C3C	-2.15	106.50	112.43
17	B	811	CLA	CBC-CAC-C3C	-2.15	106.50	112.43
17	4	601	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
17	4	609	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
17	A	840	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
17	B	824	CLA	CHB-C4A-NA	2.15	127.48	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	f	7002	CLA	CBC-CAC-C3C	-2.15	106.51	112.43
26	7	601	CHL	O1D-CGD-CBD	-2.15	120.09	124.48
17	a	838	CLA	C4-C3-C5	2.15	118.44	115.98
26	1	302	CHL	O2A-CGA-CBA	2.15	118.65	111.91
19	a	848	LHG	C5-O7-C7	-2.15	112.50	117.79
17	1	315	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
17	A	803	CLA	CHA-C1A-NA	-2.15	121.48	126.40
20	a	850	BCR	C11-C12-C13	-2.15	120.39	126.42
17	b	803	CLA	C4-C3-C5	2.15	118.88	115.27
17	4	604	CLA	CMB-C2B-C3B	2.15	128.69	124.68
17	b	809	CLA	CMB-C2B-C3B	2.15	128.69	124.68
17	b	820	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
17	8	305	CLA	CMC-C2C-C1C	2.15	128.31	125.04
17	a	831	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
26	4	607	CHL	C4D-C3D-CAD	-2.14	107.27	108.47
17	B	819	CLA	CAA-C2A-C3A	-2.14	106.91	112.78
20	B	848	BCR	C35-C13-C12	2.14	121.46	118.08
20	A	849	BCR	C15-C16-C17	-2.14	119.08	123.47
17	a	844	CLA	C2A-C1A-CHA	-2.14	120.11	123.86
28	7	616	XAT	O4-C5-C6	-2.14	57.18	58.96
17	B	834	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
17	A	854	CLA	C4-C3-C2	-2.14	118.18	123.68
17	B	820	CLA	C2A-C1A-CHA	-2.14	120.11	123.86
17	1	308	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
17	B	814	CLA	CBC-CAC-C3C	-2.14	106.52	112.43
17	g	102	CLA	C2A-C1A-CHA	-2.14	120.11	123.86
17	a	828	CLA	CMB-C2B-C3B	2.14	128.69	124.68
20	3	318	BCR	C37-C22-C23	2.14	121.45	118.08
26	9	605	CHL	CHB-C4A-NA	2.14	127.47	124.51
17	B	820	CLA	CMC-C2C-C1C	2.14	128.30	125.04
17	6	309	CLA	C2A-C1A-CHA	-2.14	120.11	123.86
17	9	601	CLA	C2A-C1A-CHA	-2.14	120.11	123.86
20	b	845	BCR	C38-C26-C27	2.14	117.73	113.62
17	4	610	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
17	a	802	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
17	B	835	CLA	CMC-C2C-C1C	2.14	128.30	125.04
17	a	825	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
17	k	1401	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
17	A	819	CLA	CHB-C4A-NA	2.14	127.47	124.51
17	7	608	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
17	k	1401	CLA	CAA-CBA-CGA	-2.14	108.99	113.59
17	a	822	CLA	CED-O2D-CGD	2.14	120.78	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	L	202	CLA	CMC-C2C-C1C	2.14	128.30	125.04
17	7	609	CLA	CHB-C4A-NA	2.14	127.47	124.51
17	b	804	CLA	CHB-C4A-NA	2.14	127.47	124.51
17	8	304	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
17	3	304	CLA	CHB-C4A-NA	2.14	127.47	124.51
17	3	306	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
17	9	609	CLA	CBC-CAC-C3C	-2.14	106.54	112.43
17	6	307	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
26	7	601	CHL	C4D-C3D-CAD	-2.14	107.28	108.47
17	b	803	CLA	CMC-C2C-C1C	2.14	128.29	125.04
17	b	805	CLA	CMB-C2B-C3B	2.14	128.68	124.68
17	a	841	CLA	CHB-C4A-NA	2.14	127.47	124.51
17	a	830	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
17	F	303	CLA	CBC-CAC-C3C	-2.14	106.54	112.43
17	l	204	CLA	CMB-C2B-C3B	2.14	128.68	124.68
17	9	601	CLA	CMC-C2C-C1C	2.14	128.29	125.04
17	1	313	CLA	C4-C3-C5	2.14	118.86	115.27
17	9	603	CLA	C4D-C3D-CAD	-2.14	107.28	108.47
17	8	304	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
17	A	807	CLA	CBC-CAC-C3C	-2.14	106.54	112.43
20	j	3004	BCR	C10-C11-C12	-2.13	116.56	123.22
17	7	612	CLA	CMB-C2B-C3B	2.13	128.67	124.68
20	A	848	BCR	C29-C30-C25	2.13	113.77	110.48
17	A	822	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
17	a	808	CLA	CMB-C2B-C3B	2.13	128.67	124.68
17	B	829	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
17	4	604	CLA	CHB-C4A-NA	2.13	127.46	124.51
17	a	824	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
17	9	608	CLA	C4D-C3D-CAD	-2.13	107.28	108.47
17	G	101	CLA	CMB-C2B-C3B	2.13	128.67	124.68
17	9	609	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
17	a	834	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
17	b	806	CLA	CMB-C2B-C3B	2.13	128.67	124.68
17	7	604	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
17	b	834	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
20	A	849	BCR	C23-C24-C25	-2.13	121.22	127.20
20	a	852	BCR	C38-C26-C27	2.13	117.71	113.62
20	l	205	BCR	C8-C7-C6	-2.13	121.22	127.20
17	a	856	CLA	CMC-C2C-C1C	2.13	128.28	125.04
17	4	608	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
17	B	812	CLA	C4-C3-C5	2.13	118.86	115.27
17	3	309	CLA	O2D-CGD-O1D	-2.13	119.67	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	9	607	CHL	CHB-C4A-NA	2.13	127.46	124.51
26	8	306	CHL	O2A-CGA-CBA	2.13	120.64	112.23
17	A	836	CLA	CHB-C4A-NA	2.13	127.45	124.51
17	A	806	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
17	b	806	CLA	C4-C3-C5	2.13	118.85	115.27
17	a	826	CLA	C2A-C1A-CHA	-2.13	120.14	123.86
17	a	831	CLA	CBC-CAC-C3C	-2.13	106.57	112.43
17	A	805	CLA	CMB-C2B-C3B	2.13	128.66	124.68
19	A	847	LHG	C5-O7-C7	-2.13	112.56	117.79
20	B	845	BCR	C36-C18-C17	-2.13	119.95	122.92
20	b	846	BCR	C2-C1-C6	2.12	113.75	110.48
17	b	834	CLA	C2A-C1A-CHA	-2.12	120.14	123.86
20	A	856	BCR	C34-C9-C8	2.12	121.42	118.08
17	A	837	CLA	C2A-C1A-CHA	-2.12	120.14	123.86
20	8	316	BCR	C10-C11-C12	-2.12	116.59	123.22
17	A	840	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
17	6	309	CLA	CBC-CAC-C3C	-2.12	106.58	112.43
17	f	7002	CLA	CAA-C2A-C3A	-2.12	106.96	112.78
17	A	829	CLA	C6-C7-C8	-2.12	109.06	115.92
17	L	203	CLA	CHB-C4A-NA	2.12	127.45	124.51
17	9	608	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
26	2	601	CHL	CBC-CAC-C3C	-2.12	106.58	112.43
17	a	822	CLA	CAA-C2A-C3A	-2.12	106.96	112.78
17	2	609	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
17	B	831	CLA	C2A-C1A-CHA	-2.12	120.15	123.86
17	a	836	CLA	C5-C3-C4	2.12	119.29	114.60
17	a	807	CLA	CHB-C4A-NA	2.12	127.45	124.51
28	2	616	XAT	O4-C5-C6	-2.12	57.20	58.96
17	a	811	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
28	3	317	XAT	C18-C5-C4	2.12	116.67	114.28
17	3	303	CLA	C2A-C1A-CHA	-2.12	120.15	123.86
17	B	836	CLA	CAC-C3C-C4C	2.12	127.56	124.81
17	3	309	CLA	C5-C3-C4	2.12	119.29	114.60
17	A	830	CLA	C2A-C1A-CHA	-2.12	120.15	123.86
17	B	806	CLA	C4D-C3D-CAD	-2.12	107.29	108.47
17	4	602	CLA	CHB-C4A-NA	2.12	127.44	124.51
17	a	804	CLA	CAA-CBA-CGA	-2.12	107.06	113.25
17	9	608	CLA	CBC-CAC-C3C	-2.12	106.59	112.43
17	9	613	CLA	CAA-CBA-CGA	-2.12	109.03	113.59
20	J	3003	BCR	C23-C24-C25	-2.12	121.25	127.20
17	A	815	CLA	CBC-CAC-C3C	-2.12	106.59	112.43
17	A	822	CLA	CMC-C2C-C1C	2.12	128.26	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	811	CLA	CMB-C2B-C3B	2.12	128.64	124.68
17	A	832	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
20	A	852	BCR	C10-C11-C12	-2.12	116.61	123.22
17	B	802	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
17	3	302	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
17	9	611	CLA	CBC-CAC-C3C	-2.12	106.60	112.43
23	B	849	LMT	C1B-C2B-C3B	2.12	114.40	110.00
20	2	617	BCR	C24-C23-C22	-2.12	123.04	126.23
17	B	839	CLA	CBC-CAC-C3C	-2.12	106.60	112.43
17	b	833	CLA	O1D-CGD-CBD	-2.12	120.16	124.48
20	A	851	BCR	C20-C19-C18	-2.12	120.47	126.42
20	f	7004	BCR	C37-C22-C23	2.12	121.41	118.08
17	a	819	CLA	O2D-CGD-O1D	-2.11	119.70	123.84
20	L	206	BCR	C11-C12-C13	-2.11	120.47	126.42
17	l	202	CLA	CMB-C2B-C3B	2.11	128.63	124.68
17	3	313	CLA	CBC-CAC-C3C	-2.11	106.60	112.43
17	A	823	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
17	A	845	CLA	C2A-C1A-CHA	-2.11	120.16	123.86
26	3	307	CHL	CHC-C1C-C2C	-2.11	118.45	126.11
17	2	604	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
27	6	317	LUT	C10-C11-C12	-2.11	116.62	123.22
17	6	310	CLA	CED-O2D-CGD	2.11	120.71	115.94
20	a	850	BCR	C8-C7-C6	-2.11	121.27	127.20
17	A	835	CLA	CHB-C4A-NA	2.11	127.43	124.51
20	G	105	BCR	C27-C26-C25	-2.11	119.67	122.73
17	b	821	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
17	9	604	CLA	CAA-C2A-C3A	-2.11	107.00	112.78
17	9	609	CLA	CED-O2D-CGD	2.11	120.71	115.94
26	2	605	CHL	CHD-C4C-NC	2.11	127.53	124.20
17	F	303	CLA	CMB-C2B-C3B	2.11	128.62	124.68
17	B	809	CLA	CMC-C2C-C1C	2.11	128.25	125.04
17	b	812	CLA	C2A-C1A-CHA	-2.11	120.17	123.86
17	a	821	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
17	2	609	CLA	CED-O2D-CGD	2.11	120.70	115.94
17	A	809	CLA	CHB-C4A-NA	2.11	127.43	124.51
17	8	301	CLA	CAA-C2A-C3A	-2.11	107.01	112.78
17	A	806	CLA	CED-O2D-CGD	2.11	120.70	115.94
20	b	844	BCR	C37-C22-C21	-2.11	119.97	122.92
26	7	614	CHL	CHD-C4C-NC	2.11	127.52	124.20
17	b	804	CLA	CMB-C2B-C3B	2.11	128.62	124.68
26	8	306	CHL	O2D-CGD-O1D	-2.11	119.72	123.84
17	B	829	CLA	C4-C3-C5	2.11	118.81	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	815	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
17	3	304	CLA	CMC-C2C-C1C	2.11	128.25	125.04
17	4	609	CLA	CHB-C4A-NA	2.11	127.42	124.51
24	b	849	DGD	O6D-C5D-C6D	2.10	110.91	106.67
17	a	841	CLA	O2D-CGD-O1D	-2.10	119.72	123.84
17	1	309	CLA	CBC-CAC-C3C	-2.10	106.63	112.43
17	9	601	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
17	B	819	CLA	CED-O2D-CGD	2.10	120.70	115.94
17	7	603	CLA	C2A-C1A-CHA	-2.10	120.18	123.86
17	F	304	CLA	CHB-C4A-NA	2.10	127.42	124.51
17	F	301	CLA	C4D-C3D-CAD	-2.10	107.30	108.47
17	8	311	CLA	CED-O2D-CGD	2.10	120.69	115.94
20	2	617	BCR	C10-C11-C12	-2.10	116.65	123.22
17	A	838	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
17	A	821	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
17	3	313	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
17	7	608	CLA	CBC-CAC-C3C	-2.10	106.64	112.43
17	a	802	CLA	CED-O2D-CGD	2.10	120.69	115.94
20	g	104	BCR	C38-C26-C25	-2.10	122.17	124.53
17	a	801	CLA	CGD-CBD-CAD	-2.10	103.93	110.73
17	l	204	CLA	C2A-C1A-CHA	-2.10	120.19	123.86
17	1	305	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
17	A	841	CLA	CHB-C4A-NA	2.10	127.42	124.51
20	L	201	BCR	C11-C10-C9	-2.10	124.31	127.31
17	F	301	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
20	4	618	BCR	C37-C22-C23	2.10	121.39	118.08
20	B	801	BCR	C36-C18-C19	2.10	121.39	118.08
17	G	103	CLA	CBC-CAC-C3C	-2.10	106.64	112.43
20	i	101	BCR	C37-C22-C23	2.10	121.38	118.08
17	A	829	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
17	a	843	CLA	C4-C3-C5	2.10	118.80	115.27
26	2	614	CHL	C4D-C3D-CAD	-2.10	107.30	108.47
17	B	815	CLA	C4D-C3D-CAD	-2.10	107.30	108.47
17	B	820	CLA	CBC-CAC-C3C	-2.10	106.65	112.43
20	L	206	BCR	C37-C22-C21	-2.10	119.98	122.92
17	8	309	CLA	CMC-C2C-C1C	2.10	128.23	125.04
17	A	805	CLA	CHB-C4A-NA	2.10	127.41	124.51
17	6	311	CLA	CHB-C4A-NA	2.10	127.41	124.51
26	9	615	CHL	CHD-C4C-NC	2.10	127.51	124.20
17	B	834	CLA	CMC-C2C-C1C	2.10	128.23	125.04
17	7	604	CLA	CHB-C4A-NA	2.10	127.41	124.51
17	B	803	CLA	CBC-CAC-C3C	-2.10	106.65	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	827	CLA	CMC-C2C-C1C	2.10	128.23	125.04
17	b	802	CLA	CMC-C2C-C1C	2.10	128.23	125.04
17	7	610	CLA	C2A-C1A-CHA	-2.10	120.19	123.85
26	8	306	CHL	CED-O2D-CGD	2.10	120.68	115.94
17	B	808	CLA	CHB-C4A-NA	2.09	127.41	124.51
17	B	823	CLA	O2D-CGD-O1D	-2.09	119.74	123.84
17	f	7003	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
17	b	830	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
17	A	821	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
17	6	306	CLA	CHB-C4A-NA	2.09	127.41	124.51
17	a	846	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
17	A	829	CLA	CBC-CAC-C3C	-2.09	106.66	112.43
17	A	830	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
17	A	811	CLA	CMC-C2C-C1C	2.09	128.22	125.04
17	a	843	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
17	4	604	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
20	A	848	BCR	C23-C24-C25	-2.09	121.33	127.20
17	a	811	CLA	CBC-CAC-C3C	-2.09	106.67	112.43
17	8	312	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
17	B	807	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
17	a	815	CLA	CBC-CAC-C3C	-2.09	106.67	112.43
28	4	617	XAT	C18-C5-C4	2.09	116.63	114.28
17	b	830	CLA	CHB-C4A-NA	2.09	127.40	124.51
17	a	836	CLA	C1-O2A-CGA	2.09	121.93	116.44
17	B	802	CLA	C4-C3-C5	2.09	118.79	115.27
20	B	846	BCR	C8-C7-C6	-2.09	121.33	127.20
26	2	607	CHL	CHB-C4A-NA	2.09	127.40	124.51
17	A	806	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
17	j	3002	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
17	A	830	CLA	CED-O2D-CGD	2.09	120.66	115.94
17	l	203	CLA	CHB-C4A-NA	2.09	127.40	124.51
17	f	7003	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
17	7	611	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
17	b	825	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
17	B	823	CLA	CMA-C3A-C4A	-2.09	106.16	111.77
17	b	835	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
17	b	807	CLA	CHB-C4A-NA	2.09	127.40	124.51
17	a	817	CLA	CMB-C2B-C3B	2.09	128.58	124.68
17	b	827	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
20	A	850	BCR	C2-C1-C6	2.09	113.69	110.48
17	B	826	CLA	CAC-C3C-C4C	2.09	127.52	124.81
17	b	834	CLA	CMB-C2B-C3B	2.09	128.58	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	848	BCR	C38-C26-C27	2.09	117.62	113.62
17	3	312	CLA	O2D-CGD-O1D	-2.09	119.76	123.84
17	A	817	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
17	A	834	CLA	CMB-C2B-C3B	2.09	128.58	124.68
26	2	607	CHL	CBC-CAC-C3C	-2.08	106.68	112.43
17	l	203	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
17	B	815	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
17	B	804	CLA	CHB-C4A-NA	2.08	127.39	124.51
17	9	611	CLA	C1-C2-C3	-2.08	122.44	126.04
17	b	811	CLA	CMB-C2B-C3B	2.08	128.77	124.69
17	3	314	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
17	a	817	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
20	b	846	BCR	C31-C1-C6	-2.08	106.92	110.30
17	b	805	CLA	CHB-C4A-NA	2.08	127.39	124.51
17	1	306	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
17	2	612	CLA	CED-O2D-CGD	2.08	120.65	115.94
20	J	3003	BCR	C8-C7-C6	-2.08	121.36	127.20
20	k	1404	BCR	C28-C27-C26	-2.08	110.36	114.08
17	A	818	CLA	CHB-C4A-NA	2.08	127.39	124.51
17	3	305	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
20	J	3003	BCR	C11-C10-C9	-2.08	124.34	127.31
17	a	838	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
17	8	312	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
17	B	820	CLA	CHB-C4A-NA	2.08	127.39	124.51
17	A	805	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
20	a	850	BCR	C2-C1-C6	2.08	113.68	110.48
17	8	307	CLA	CBC-CAC-C3C	-2.08	106.70	112.43
17	B	811	CLA	CMC-C2C-C1C	2.08	128.21	125.04
17	a	806	CLA	C4-C3-C5	2.08	118.77	115.27
20	G	105	BCR	C38-C26-C27	2.08	117.61	113.62
26	1	302	CHL	C4D-C3D-CAD	-2.08	107.31	108.47
17	b	817	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
17	A	823	CLA	C2A-C1A-CHA	-2.08	120.23	123.86
17	a	820	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
20	b	847	BCR	C33-C5-C6	-2.08	122.19	124.53
17	b	815	CLA	CBC-CAC-C3C	-2.08	106.70	112.43
27	6	317	LUT	C38-C25-C24	-2.08	119.11	123.56
20	J	3003	BCR	C10-C11-C12	-2.08	116.74	123.22
17	B	822	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
17	b	830	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
17	B	805	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
17	1	314	CLA	CHB-C4A-NA	2.08	127.38	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	g	102	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
17	a	824	CLA	C2A-C1A-CHA	-2.07	120.23	123.86
17	a	827	CLA	C2A-C1A-CHA	-2.07	120.23	123.86
26	4	607	CHL	O2D-CGD-O1D	-2.07	119.78	123.84
26	6	308	CHL	O2A-CGA-CBA	2.07	120.43	112.23
17	k	1403	CLA	CBC-CAC-C3C	-2.07	106.71	112.43
17	l	313	CLA	CHB-C4A-NA	2.07	127.38	124.51
17	4	608	CLA	CHB-C4A-NA	2.07	127.38	124.51
20	B	801	BCR	C2-C1-C6	2.07	113.67	110.48
17	A	821	CLA	CHB-C4A-NA	2.07	127.38	124.51
17	b	840	CLA	CAC-C3C-C4C	2.07	127.50	124.81
17	J	3002	CLA	C2A-C1A-CHA	-2.07	120.23	123.86
17	A	840	CLA	C1-O2A-CGA	2.07	121.88	116.44
17	B	830	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
17	4	610	CLA	C2A-C1A-CHA	-2.07	120.24	123.86
17	A	801	CLA	C6-C7-C8	-2.07	109.22	115.92
17	B	821	CLA	C4D-C3D-CAD	-2.07	107.31	108.47
20	B	843	BCR	C15-C16-C17	-2.07	119.23	123.47
20	l	318	BCR	C8-C7-C6	-2.07	121.39	127.20
20	L	201	BCR	C21-C20-C19	-2.07	116.76	123.22
17	B	840	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
20	g	104	BCR	C8-C7-C6	-2.07	121.39	127.20
27	6	317	LUT	C3-C4-C5	-2.07	107.73	111.85
17	B	816	CLA	C4D-C3D-CAD	-2.07	107.32	108.47
17	B	838	CLA	C2A-C1A-CHA	-2.07	120.24	123.86
17	A	831	CLA	CHB-C4A-NA	2.07	127.37	124.51
17	a	820	CLA	CBC-CAC-C3C	-2.07	106.73	112.43
17	k	1403	CLA	C2A-C1A-CHA	-2.07	120.24	123.86
17	g	103	CLA	O2A-CGA-CBA	2.07	120.40	112.23
17	A	813	CLA	O2D-CGD-O1D	-2.07	119.80	123.84
17	2	610	CLA	C2A-C1A-CHA	-2.07	120.24	123.85
20	f	7004	BCR	C2-C1-C6	2.07	113.66	110.48
17	B	828	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
28	7	616	XAT	C30-C31-C32	-2.07	116.77	123.22
17	B	834	CLA	C2A-C1A-CHA	-2.07	120.24	123.86
17	8	312	CLA	O2A-CGA-CBA	2.07	120.40	112.23
17	8	301	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
17	8	303	CLA	CMB-C2B-C3B	2.07	128.54	124.68
17	6	315	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
20	l	206	BCR	C8-C7-C6	-2.07	121.40	127.20
17	4	602	CLA	O1D-CGD-CBD	-2.07	120.26	124.48
17	b	821	CLA	O2A-CGA-CBA	2.07	120.39	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	9	615	CHL	C1B-CHB-C4A	-2.07	126.03	130.12
17	A	823	CLA	CBC-CAC-C3C	-2.07	106.74	112.43
26	3	307	CHL	O2A-CGA-CBA	2.07	120.39	112.23
26	9	607	CHL	CED-O2D-CGD	2.07	120.61	115.94
17	K	4002	CLA	CAA-CBA-CGA	-2.07	109.15	113.59
17	1	305	CLA	CHB-C4A-NA	2.07	127.37	124.51
17	6	313	CLA	C2A-C1A-CHA	-2.07	120.25	123.86
17	9	608	CLA	CAA-C2A-C3A	-2.06	107.12	112.78
17	a	802	CLA	C6-C7-C8	-2.06	109.25	115.92
20	b	846	BCR	C36-C18-C19	2.06	121.33	118.08
20	K	4004	BCR	C16-C15-C14	-2.06	119.25	123.47
20	a	853	BCR	C8-C7-C6	-2.06	121.40	127.20
20	b	847	BCR	C4-C5-C6	-2.06	119.73	122.73
20	A	850	BCR	C16-C15-C14	-2.06	119.25	123.47
17	B	835	CLA	C2A-C1A-CHA	-2.06	120.25	123.86
17	a	825	CLA	CBC-CAC-C3C	-2.06	106.74	112.43
26	1	302	CHL	CHB-C4A-NA	2.06	127.37	124.51
17	2	604	CLA	CMC-C2C-C1C	2.06	128.18	125.04
17	7	609	CLA	C2A-C1A-CHA	-2.06	120.25	123.86
17	8	302	CLA	C2A-C1A-CHA	-2.06	120.25	123.86
17	7	604	CLA	CMC-C2C-C1C	2.06	128.18	125.04
17	1	306	CLA	CHB-C4A-NA	2.06	127.36	124.51
20	a	854	BCR	C24-C23-C22	-2.06	123.12	126.23
17	B	806	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
17	4	610	CLA	CHB-C4A-NA	2.06	127.36	124.51
17	B	834	CLA	CHB-C4A-NA	2.06	127.36	124.51
17	A	809	CLA	CBC-CAC-C3C	-2.06	106.75	112.43
17	b	829	CLA	CMB-C2B-C3B	2.06	128.54	124.68
17	l	204	CLA	C1-O2A-CGA	2.06	121.85	116.44
17	a	805	CLA	CHB-C4A-NA	2.06	127.36	124.51
26	9	607	CHL	O2D-CGD-O1D	-2.06	119.81	123.84
17	4	603	CLA	O2A-CGA-CBA	2.06	120.38	112.23
17	A	802	CLA	C6-C7-C8	-2.06	109.26	115.92
17	a	834	CLA	CMB-C2B-C3B	2.06	128.53	124.68
20	B	848	BCR	C7-C8-C9	-2.06	123.12	126.23
20	A	852	BCR	C37-C22-C23	2.06	121.32	118.08
17	a	841	CLA	CED-O2D-CGD	2.06	120.60	115.94
17	A	815	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
20	k	1404	BCR	C23-C24-C25	-2.06	121.42	127.20
20	i	101	BCR	C2-C1-C6	2.06	113.65	110.48
17	K	4003	CLA	C4D-C3D-CAD	-2.06	107.32	108.47
27	9	616	LUT	C15-C35-C34	-2.06	119.25	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	610	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
17	a	802	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
17	b	809	CLA	CHA-C1A-NA	-2.06	121.68	126.40
17	8	311	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
17	a	816	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
17	k	1403	CLA	O2A-CGA-CBA	2.06	120.36	112.23
17	f	7003	CLA	C1-O2A-CGA	2.06	121.84	116.44
17	A	801	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
17	b	810	CLA	C4D-C3D-CAD	-2.06	107.32	108.47
28	1	317	XAT	C30-C31-C32	-2.06	116.80	123.22
20	B	845	BCR	C8-C9-C10	2.06	122.10	118.94
17	a	821	CLA	CHB-C4A-NA	2.06	127.36	124.51
20	A	852	BCR	C23-C24-C25	-2.06	121.43	127.20
17	B	831	CLA	CED-O2D-CGD	2.06	120.59	115.94
20	l	201	BCR	C15-C16-C17	-2.06	119.26	123.47
17	A	826	CLA	O1D-CGD-CBD	-2.06	120.28	124.48
20	j	3003	BCR	C27-C26-C25	-2.05	119.75	122.73
17	b	816	CLA	CBC-CAC-C3C	-2.05	106.77	112.43
17	a	807	CLA	CBC-CAC-C3C	-2.05	106.77	112.43
17	A	807	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
17	9	612	CLA	O2D-CGD-O1D	-2.05	119.82	123.84
17	9	604	CLA	CMB-C2B-C3B	2.05	128.52	124.68
17	b	835	CLA	CHB-C4A-NA	2.05	127.35	124.51
17	9	604	CLA	CHB-C4A-NA	2.05	127.35	124.51
20	6	319	BCR	C8-C7-C6	-2.05	121.44	127.20
17	4	602	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
17	6	312	CLA	C2A-C1A-CHA	-2.05	120.27	123.85
17	a	812	CLA	CHB-C4A-NA	2.05	127.35	124.51
17	b	832	CLA	CHB-C4A-NA	2.05	127.35	124.51
17	b	809	CLA	C4D-C3D-CAD	-2.05	107.33	108.47
27	4	616	LUT	C10-C11-C12	-2.05	116.81	123.22
17	3	301	CLA	O2A-CGA-CBA	2.05	120.34	112.23
20	9	618	BCR	C8-C7-C6	-2.05	121.44	127.20
17	6	311	CLA	C2A-C1A-CHA	-2.05	120.27	123.86
17	B	840	CLA	CBC-CAC-C3C	-2.05	106.78	112.43
17	7	608	CLA	CMC-C2C-C1C	2.05	128.16	125.04
17	A	824	CLA	C2A-C1A-CHA	-2.05	120.28	123.86
17	A	814	CLA	OBD-CAD-C3D	-2.05	124.58	127.98
26	6	303	CHL	CMB-C2B-C3B	2.05	128.51	124.68
20	F	305	BCR	C2-C1-C6	2.05	113.64	110.48
17	2	608	CLA	CMC-C2C-C1C	2.05	128.16	125.04
17	a	835	CLA	CHB-C4A-NA	2.05	127.34	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	3	307	CHL	CHB-C4A-NA	2.05	127.34	124.51
17	B	813	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
17	1	306	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
20	a	854	BCR	C29-C30-C25	2.05	113.63	110.48
17	2	612	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
17	b	815	CLA	C2A-C1A-CHA	-2.05	120.28	123.86
20	B	847	BCR	C38-C26-C27	2.05	117.55	113.62
26	4	607	CHL	O2A-CGA-O1A	-2.05	118.43	123.59
20	a	854	BCR	C37-C22-C23	2.05	121.30	118.08
17	a	822	CLA	O2D-CGD-O1D	-2.05	119.84	123.84
26	2	606	CHL	O1D-CGD-CBD	-2.05	120.30	124.48
17	g	102	CLA	C4D-C3D-CAD	-2.05	107.33	108.47
17	b	808	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
17	l	204	CLA	CHB-C4A-NA	2.05	127.34	124.51
17	1	312	CLA	C2A-C1A-CHA	-2.05	120.28	123.86
20	i	101	BCR	C27-C26-C25	-2.05	119.76	122.73
27	1	320	LUT	C39-C29-C28	2.05	121.30	118.08
17	A	807	CLA	CMB-C2B-C3B	2.05	128.50	124.68
20	1	318	BCR	C39-C30-C25	-2.05	106.98	110.30
17	A	803	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
17	A	838	CLA	C2A-C1A-CHA	-2.04	120.28	123.86
17	6	309	CLA	O2A-CGA-CBA	2.04	120.31	112.23
17	B	815	CLA	CHB-C4A-NA	2.04	127.34	124.51
20	a	853	BCR	C2-C1-C6	2.04	113.63	110.48
17	A	838	CLA	O2D-CGD-O1D	-2.04	119.84	123.84
17	B	840	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
26	7	605	CHL	CHC-C1C-C2C	-2.04	118.70	126.11
26	2	607	CHL	C4D-C3D-CAD	-2.04	107.33	108.47
20	a	849	BCR	C15-C16-C17	-2.04	119.29	123.47
17	a	816	CLA	C2A-C1A-CHA	-2.04	120.29	123.86
17	A	806	CLA	CHB-C4A-NA	2.04	127.33	124.51
17	b	815	CLA	CHB-C4A-NA	2.04	127.33	124.51
28	8	315	XAT	C8-C9-C10	-2.04	115.81	118.94
17	a	802	CLA	CMC-C2C-C1C	2.04	128.15	125.04
17	a	841	CLA	C2A-C1A-CHA	-2.04	120.29	123.86
17	a	815	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
17	b	818	CLA	O2A-C1-C2	2.04	114.00	108.64
17	k	1403	CLA	CHB-C4A-NA	2.04	127.33	124.51
20	a	852	BCR	C23-C24-C25	-2.04	121.47	127.20
17	A	828	CLA	CMB-C2B-C3B	2.04	128.49	124.68
17	4	614	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
17	3	301	CLA	O1D-CGD-CBD	-2.04	120.31	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	834	CLA	CMC-C2C-C1C	2.04	128.14	125.04
26	2	614	CHL	CHC-C1C-C2C	-2.04	118.72	126.11
17	B	803	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
17	B	827	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
26	6	303	CHL	CHC-C1C-C2C	-2.04	118.72	126.11
26	9	615	CHL	C4D-C3D-CAD	-2.04	107.33	108.47
19	7	618	LHG	O7-C7-O9	-2.04	118.78	123.70
17	F	304	CLA	C2A-C1A-CHA	-2.04	120.30	123.86
20	f	7004	BCR	C12-C13-C14	2.04	122.06	118.94
17	B	815	CLA	C1-C2-C3	-2.04	122.52	126.04
17	b	832	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
27	8	314	LUT	C19-C9-C8	2.04	121.28	118.08
28	3	317	XAT	C39-C29-C28	2.04	121.28	118.08
17	B	804	CLA	C2A-C1A-CHA	-2.04	120.30	123.86
17	B	812	CLA	CBC-CAC-C3C	-2.04	106.82	112.43
20	8	316	BCR	C3-C4-C5	-2.04	110.44	114.08
20	j	3003	BCR	C29-C30-C25	2.04	113.61	110.48
17	b	836	CLA	OBD-CAD-C3D	-2.04	124.60	127.98
17	A	837	CLA	CHB-C4A-NA	2.03	127.33	124.51
17	A	807	CLA	C4-C3-C5	2.03	118.69	115.27
20	F	305	BCR	C20-C21-C22	-2.03	124.41	127.31
17	B	816	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
20	a	849	BCR	C29-C30-C25	2.03	113.61	110.48
17	B	831	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
17	2	602	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
17	a	828	CLA	CAC-C3C-C4C	2.03	127.45	124.81
17	b	805	CLA	CBC-CAC-C3C	-2.03	106.83	112.43
17	a	813	CLA	CMC-C2C-C1C	2.03	128.13	125.04
17	A	836	CLA	CED-O2D-CGD	2.03	120.53	115.94
20	a	850	BCR	C39-C30-C25	-2.03	107.00	110.30
17	B	820	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
20	B	848	BCR	C34-C9-C8	2.03	121.28	118.08
20	l	201	BCR	C39-C30-C25	-2.03	107.00	110.30
20	l	206	BCR	C15-C16-C17	-2.03	119.31	123.47
17	2	612	CLA	CBC-CAC-C3C	-2.03	106.83	112.43
26	2	605	CHL	O2D-CGD-O1D	-2.03	119.87	123.84
17	b	833	CLA	C4D-C3D-CAD	-2.03	107.34	108.47
17	2	603	CLA	C4D-C3D-CAD	-2.03	107.34	108.47
17	A	835	CLA	CMC-C2C-C1C	2.03	128.13	125.04
17	B	831	CLA	CMC-C2C-C1C	2.03	128.13	125.04
17	B	823	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
17	1	303	CLA	O2A-CGA-O1A	-2.03	118.47	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	7	606	CHL	O1D-CGD-CBD	-2.03	120.33	124.48
17	a	805	CLA	C2A-C1A-CHA	-2.03	120.31	123.86
17	B	825	CLA	CHB-C4A-NA	2.03	127.32	124.51
17	b	827	CLA	C4D-C3D-CAD	-2.03	107.34	108.47
17	b	838	CLA	C2A-C1A-CHA	-2.03	120.31	123.86
17	b	824	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
17	b	840	CLA	CHB-C4A-NA	2.03	127.31	124.51
26	9	605	CHL	O1D-CGD-CBD	-2.03	120.34	124.48
27	3	316	LUT	C3-C4-C5	-2.03	107.82	111.85
20	I	101	BCR	C10-C11-C12	-2.03	116.89	123.22
20	K	4004	BCR	C23-C24-C25	-2.03	121.51	127.20
17	2	602	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
20	i	101	BCR	C35-C13-C12	2.03	121.27	118.08
20	B	847	BCR	C16-C17-C18	-2.03	124.42	127.31
17	b	831	CLA	CMB-C2B-C3B	2.03	128.47	124.68
26	4	605	CHL	CHB-C4A-NA	2.03	127.31	124.51
17	b	840	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
26	2	605	CHL	C4D-C3D-CAD	-2.02	107.34	108.47
17	a	825	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
20	l	201	BCR	C20-C21-C22	-2.02	124.42	127.31
17	A	804	CLA	CHB-C4A-NA	2.02	127.31	124.51
17	a	818	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
17	b	826	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
17	A	822	CLA	CAA-C2A-C3A	-2.02	107.24	112.78
17	B	802	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
17	6	309	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
27	7	615	LUT	C19-C9-C8	2.02	121.26	118.08
17	a	842	CLA	CAA-C2A-C3A	-2.02	107.24	112.78
17	1	314	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
17	9	603	CLA	O2A-CGA-CBA	2.02	120.22	112.23
20	9	618	BCR	C38-C26-C27	2.02	117.50	113.62
25	4	620	LMG	O1-C7-C8	-2.02	106.02	110.90
17	B	803	CLA	CHA-C1A-NA	-2.02	121.77	126.40
17	K	4003	CLA	CMC-C2C-C1C	2.02	128.12	125.04
20	1	318	BCR	C16-C15-C14	-2.02	119.34	123.47
17	B	813	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
20	l	201	BCR	C21-C20-C19	-2.02	116.92	123.22
20	B	843	BCR	C33-C5-C6	-2.02	122.26	124.53
17	b	831	CLA	CMC-C2C-C1C	2.02	128.11	125.04
20	K	4004	BCR	C33-C5-C4	2.02	117.49	113.62
17	3	308	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
17	A	825	CLA	CHB-C4A-NA	2.02	127.30	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	851	BCR	C7-C8-C9	-2.02	123.19	126.23
17	a	811	CLA	CHB-C4A-NA	2.02	127.30	124.51
17	A	823	CLA	CHB-C4A-NA	2.02	127.30	124.51
17	B	805	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
17	f	7002	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
17	9	601	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
17	A	836	CLA	CAA-C2A-C3A	-2.02	107.26	112.78
20	8	316	BCR	C36-C18-C19	2.02	121.25	118.08
17	A	829	CLA	CHB-C4A-NA	2.02	127.30	124.51
17	A	824	CLA	CED-O2D-CGD	2.02	120.50	115.94
17	a	835	CLA	CMC-C2C-C1C	2.02	128.11	125.04
26	7	605	CHL	C2A-C3A-C4A	-2.02	98.61	101.87
26	7	606	CHL	CHB-C4A-NA	2.02	127.30	124.51
20	B	845	BCR	C16-C15-C14	-2.02	119.35	123.47
17	A	828	CLA	CHB-C4A-NA	2.01	127.30	124.51
17	k	1403	CLA	CMC-C2C-C1C	2.01	128.11	125.04
25	G	102	LMG	C8-O7-C10	-2.01	112.83	117.79
17	a	807	CLA	C2A-C1A-CHA	-2.01	120.34	123.86
17	7	610	CLA	CMC-C2C-C1C	2.01	128.11	125.04
17	2	604	CLA	CHB-C4A-NA	2.01	127.30	124.51
28	8	315	XAT	C15-C14-C13	-2.01	124.44	127.31
17	6	316	CLA	O2A-CGA-CBA	2.01	120.18	112.23
17	K	4003	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
20	a	853	BCR	C11-C10-C9	-2.01	124.44	127.31
17	B	833	CLA	C4D-C3D-CAD	-2.01	107.35	108.47
17	9	602	CLA	CHB-C4A-NA	2.01	127.29	124.51
17	b	817	CLA	CHB-C4A-NA	2.01	127.29	124.51
17	8	311	CLA	CHB-C4A-NA	2.01	127.29	124.51
17	3	312	CLA	CED-O2D-CGD	2.01	120.49	115.94
17	b	826	CLA	C2A-C1A-CHA	-2.01	120.34	123.86
17	8	310	CLA	CED-O2D-CGD	2.01	120.48	115.94
17	7	603	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
17	a	823	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
17	a	834	CLA	CHB-C4A-NA	2.01	127.29	124.51
17	B	823	CLA	CHB-C4A-NA	2.01	127.29	124.51
17	B	810	CLA	CHB-C4A-NA	2.01	127.29	124.51
20	a	852	BCR	C36-C18-C17	-2.01	120.11	122.92
27	6	321	LUT	C38-C25-C24	-2.01	119.26	123.56
17	3	309	CLA	CED-O2D-CGD	2.01	120.48	115.94
17	B	807	CLA	C4D-C3D-CAD	-2.01	107.35	108.47
17	A	801	CLA	CGD-CBD-CAD	-2.01	104.23	110.73
17	f	7002	CLA	CHB-C4A-NA	2.01	127.29	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	318	BCR	C20-C21-C22	-2.01	124.44	127.31
17	a	828	CLA	C2A-C1A-CHA	-2.01	120.35	123.86
17	B	826	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
17	A	819	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
17	a	824	CLA	CED-O2D-CGD	2.01	120.48	115.94
17	A	825	CLA	CMB-C2B-C3B	2.01	128.43	124.68
17	6	304	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
20	g	104	BCR	C27-C26-C25	-2.01	119.82	122.73
17	G	104	CLA	O2A-CGA-CBA	2.01	120.16	112.23
20	a	849	BCR	C3-C4-C5	-2.00	110.50	114.08
17	B	833	CLA	CMB-C2B-C3B	2.00	128.43	124.68
17	B	823	CLA	O2A-C1-C2	2.00	113.90	108.64
17	9	611	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
17	A	810	CLA	OBD-CAD-C3D	-2.00	124.66	127.98
17	b	831	CLA	CED-O2D-CGD	2.00	120.47	115.94
17	B	834	CLA	CBC-CAC-C3C	-2.00	106.91	112.43
17	9	611	CLA	CHB-C4A-NA	2.00	127.28	124.51
27	7	615	LUT	C39-C29-C28	2.00	121.23	118.08
17	A	813	CLA	CAA-C2A-C3A	-2.00	107.30	112.78
17	B	833	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
17	7	602	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
17	7	610	CLA	C4D-C3D-CAD	-2.00	107.35	108.47
17	B	838	CLA	CGD-CBD-CAD	-2.00	104.25	110.73
17	8	302	CLA	CHA-C1A-NA	-2.00	121.81	126.40
17	A	834	CLA	CHB-C4A-NA	2.00	127.28	124.51
17	b	831	CLA	CAA-C2A-C3A	-2.00	107.30	112.78
17	B	807	CLA	CHB-C4A-NA	2.00	127.28	124.51
20	f	7004	BCR	C29-C30-C25	2.00	113.56	110.48

All (886) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	9	609	CLA	NC
17	9	609	CLA	ND
17	9	609	CLA	NA
17	a	812	CLA	NC
17	a	812	CLA	ND
17	a	812	CLA	NA
17	A	803	CLA	ND
17	6	313	CLA	NC
17	6	313	CLA	ND
17	6	313	CLA	NA

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Mol	Chain	Res	Type	Atom
17	B	805	CLA	NC
17	B	805	CLA	ND
17	B	805	CLA	NA
17	3	314	CLA	ND
17	3	314	CLA	NA
17	a	828	CLA	NC
17	a	828	CLA	ND
17	a	828	CLA	NA
17	A	815	CLA	NC
17	A	815	CLA	ND
17	A	815	CLA	NA
17	a	856	CLA	ND
17	A	831	CLA	NC
17	A	831	CLA	ND
17	A	831	CLA	NA
17	2	604	CLA	NC
17	2	604	CLA	ND
17	2	604	CLA	NA
17	b	835	CLA	NC
17	b	835	CLA	ND
17	b	835	CLA	NA
17	3	305	CLA	NC
17	3	305	CLA	ND
17	3	305	CLA	NA
17	a	809	CLA	NC
17	a	809	CLA	ND
17	a	809	CLA	NA
17	a	836	CLA	NC
17	a	836	CLA	ND
17	a	836	CLA	NA
17	A	808	CLA	NC
17	A	808	CLA	ND
17	A	808	CLA	NA
17	a	831	CLA	NC
17	a	831	CLA	ND
17	a	831	CLA	NA
17	A	806	CLA	NC
17	A	806	CLA	ND
17	A	806	CLA	NA
17	f	7003	CLA	NA
17	b	840	CLA	NC
17	b	840	CLA	ND

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Mol	Chain	Res	Type	Atom
17	b	840	CLA	NA
17	A	811	CLA	NC
17	A	811	CLA	ND
17	A	811	CLA	NA
17	A	826	CLA	NC
17	A	826	CLA	ND
17	A	826	CLA	NA
17	a	825	CLA	NC
17	a	825	CLA	ND
17	a	825	CLA	NA
17	A	833	CLA	NC
17	A	833	CLA	ND
17	A	833	CLA	NA
17	7	608	CLA	NC
17	7	608	CLA	ND
17	7	608	CLA	NA
26	4	605	CHL	NC
26	4	605	CHL	ND
17	4	602	CLA	NC
17	4	602	CLA	ND
17	4	602	CLA	NA
17	6	305	CLA	NC
17	6	305	CLA	ND
17	6	305	CLA	NA
17	B	827	CLA	ND
17	A	845	CLA	NC
17	A	845	CLA	ND
17	A	845	CLA	NA
26	2	605	CHL	NC
26	2	605	CHL	ND
17	a	819	CLA	NC
17	a	819	CLA	ND
17	a	819	CLA	NA
17	4	601	CLA	NC
17	4	601	CLA	ND
17	4	601	CLA	NA
17	a	824	CLA	NC
17	a	824	CLA	ND
17	a	824	CLA	NA
17	b	816	CLA	NC
17	b	816	CLA	ND
17	b	816	CLA	NA

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Mol	Chain	Res	Type	Atom
17	a	818	CLA	NC
17	a	818	CLA	ND
17	a	818	CLA	NA
17	1	309	CLA	NC
17	1	309	CLA	ND
17	1	309	CLA	NA
17	A	854	CLA	ND
17	b	818	CLA	NC
17	b	818	CLA	ND
17	b	818	CLA	NA
17	A	827	CLA	NC
17	A	827	CLA	ND
17	A	827	CLA	NA
17	1	306	CLA	NC
17	1	306	CLA	ND
17	1	306	CLA	NA
26	2	606	CHL	NC
26	2	606	CHL	ND
26	2	606	CHL	NA
26	6	303	CHL	NC
26	6	303	CHL	ND
26	6	303	CHL	NA
17	j	3002	CLA	NC
17	j	3002	CLA	ND
17	j	3002	CLA	NA
17	3	303	CLA	NA
17	3	303	CLA	NC
17	3	303	CLA	ND
17	9	611	CLA	NC
17	9	611	CLA	ND
17	9	611	CLA	NA
17	A	824	CLA	NC
17	A	824	CLA	ND
17	A	824	CLA	NA
17	1	315	CLA	NC
17	1	315	CLA	ND
17	1	315	CLA	NA
17	2	613	CLA	NC
17	2	613	CLA	ND
17	2	613	CLA	NA
17	1	305	CLA	NC
17	1	305	CLA	ND

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Mol	Chain	Res	Type	Atom
17	1	305	CLA	NA
17	A	825	CLA	NC
17	A	825	CLA	ND
17	A	825	CLA	NA
17	b	836	CLA	NC
17	b	836	CLA	ND
17	b	836	CLA	NA
17	g	102	CLA	NC
17	g	102	CLA	ND
17	g	102	CLA	NA
17	A	828	CLA	NC
17	A	828	CLA	ND
17	A	828	CLA	NA
17	b	813	CLA	NC
17	b	813	CLA	ND
17	b	813	CLA	NA
17	b	834	CLA	NC
17	b	834	CLA	ND
17	b	834	CLA	NA
17	a	820	CLA	NC
17	a	820	CLA	ND
17	a	820	CLA	NA
17	A	801	CLA	CBD
17	A	801	CLA	NC
17	A	801	CLA	ND
17	A	801	CLA	NA
17	b	815	CLA	NC
17	b	815	CLA	ND
17	b	815	CLA	NA
17	B	819	CLA	ND
17	B	819	CLA	NA
17	4	604	CLA	NC
17	4	604	CLA	ND
17	4	604	CLA	NA
17	B	818	CLA	ND
17	B	818	CLA	NA
17	a	827	CLA	NC
17	a	827	CLA	ND
17	a	827	CLA	NA
17	f	7002	CLA	NC
17	f	7002	CLA	ND
17	f	7002	CLA	NA

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Mol	Chain	Res	Type	Atom
17	3	311	CLA	NC
17	3	311	CLA	ND
17	3	311	CLA	NA
17	b	821	CLA	NC
17	b	821	CLA	ND
17	b	821	CLA	NA
17	b	809	CLA	NC
17	b	809	CLA	ND
17	b	809	CLA	NA
17	a	835	CLA	NC
17	a	835	CLA	ND
17	a	835	CLA	NA
17	b	838	CLA	NC
17	b	838	CLA	ND
17	b	838	CLA	NA
17	2	611	CLA	NC
17	2	611	CLA	ND
17	2	611	CLA	NA
17	B	824	CLA	NC
17	B	824	CLA	NA
26	2	614	CHL	NC
26	2	614	CHL	ND
26	2	614	CHL	NA
17	B	841	CLA	NC
17	B	841	CLA	ND
17	B	841	CLA	NA
17	3	308	CLA	NC
17	3	308	CLA	ND
17	3	308	CLA	NA
17	b	810	CLA	NC
17	b	810	CLA	ND
17	b	810	CLA	NA
17	a	834	CLA	NC
17	a	834	CLA	ND
17	a	834	CLA	NA
17	a	814	CLA	NC
17	a	814	CLA	ND
17	a	814	CLA	NA
17	a	839	CLA	NC
17	a	839	CLA	ND
17	a	839	CLA	NA
17	b	822	CLA	NC

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Mol	Chain	Res	Type	Atom
17	b	822	CLA	ND
17	b	822	CLA	NA
17	a	817	CLA	ND
17	a	817	CLA	NA
17	A	814	CLA	NC
17	A	814	CLA	ND
17	A	814	CLA	NA
17	1	312	CLA	NC
17	1	312	CLA	ND
17	1	312	CLA	NA
17	7	610	CLA	NC
17	7	610	CLA	ND
17	7	610	CLA	NA
17	a	837	CLA	ND
17	a	837	CLA	NA
17	A	834	CLA	ND
17	A	834	CLA	NA
17	a	811	CLA	NC
17	a	811	CLA	ND
17	a	811	CLA	NA
17	A	836	CLA	NC
17	A	836	CLA	ND
17	A	836	CLA	NA
17	8	304	CLA	NC
17	8	304	CLA	ND
17	8	304	CLA	NA
17	B	806	CLA	NC
17	B	806	CLA	ND
17	B	806	CLA	NA
26	6	308	CHL	NC
26	6	308	CHL	ND
26	6	308	CHL	NA
17	B	821	CLA	NC
17	B	821	CLA	ND
17	B	821	CLA	NA
17	8	305	CLA	NC
17	8	305	CLA	ND
17	8	305	CLA	NA
17	b	802	CLA	NC
17	b	802	CLA	ND
17	L	203	CLA	NC
17	L	203	CLA	ND

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Mol	Chain	Res	Type	Atom
17	L	203	CLA	NA
17	B	811	CLA	NC
17	B	811	CLA	ND
17	B	811	CLA	NA
17	b	839	CLA	NC
17	b	839	CLA	ND
17	b	839	CLA	NA
17	9	612	CLA	NC
17	9	612	CLA	ND
17	9	612	CLA	NA
17	6	315	CLA	NC
17	6	315	CLA	ND
17	6	315	CLA	NA
17	B	823	CLA	NC
17	B	823	CLA	ND
17	B	823	CLA	NA
17	1	308	CLA	NC
17	1	308	CLA	ND
17	1	308	CLA	NA
17	a	844	CLA	NC
17	a	844	CLA	ND
17	a	844	CLA	NA
17	4	609	CLA	NC
17	4	609	CLA	ND
17	4	609	CLA	NA
17	B	826	CLA	NC
17	B	826	CLA	ND
17	B	826	CLA	NA
17	9	608	CLA	NC
17	9	608	CLA	ND
17	9	608	CLA	NA
17	B	839	CLA	NC
17	B	839	CLA	ND
17	B	839	CLA	NA
17	A	842	CLA	NC
17	A	842	CLA	ND
17	A	842	CLA	NA
17	B	820	CLA	NC
17	B	820	CLA	ND
17	B	820	CLA	NA
17	9	603	CLA	NA
17	9	603	CLA	NC

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Mol	Chain	Res	Type	Atom
17	9	603	CLA	ND
17	L	204	CLA	NC
17	L	204	CLA	ND
17	L	204	CLA	NA
17	B	825	CLA	NC
17	B	825	CLA	ND
17	B	825	CLA	NA
17	A	810	CLA	NC
17	A	810	CLA	ND
17	A	810	CLA	NA
17	2	602	CLA	NC
17	2	602	CLA	ND
17	2	602	CLA	NA
17	1	203	CLA	NC
17	1	203	CLA	ND
17	1	203	CLA	NA
17	6	316	CLA	NC
17	6	316	CLA	ND
17	6	316	CLA	NA
17	A	838	CLA	NC
17	A	838	CLA	ND
17	A	838	CLA	NA
17	3	309	CLA	NC
17	3	309	CLA	ND
17	3	309	CLA	NA
17	A	819	CLA	NC
17	A	819	CLA	ND
17	A	819	CLA	NA
17	F	303	CLA	NC
17	F	303	CLA	ND
17	F	303	CLA	NA
17	B	810	CLA	NC
17	B	810	CLA	ND
17	B	810	CLA	NA
26	4	606	CHL	NC
26	4	606	CHL	ND
26	4	606	CHL	NA
17	A	835	CLA	NC
17	A	835	CLA	ND
17	A	835	CLA	NA
17	3	306	CLA	NC
17	3	306	CLA	ND

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Mol	Chain	Res	Type	Atom
17	3	306	CLA	NA
17	b	814	CLA	NC
17	b	814	CLA	ND
17	b	814	CLA	NA
26	7	614	CHL	NC
26	7	614	CHL	ND
26	7	614	CHL	NA
17	1	313	CLA	NC
17	1	313	CLA	ND
17	1	313	CLA	NA
17	b	826	CLA	NC
17	b	826	CLA	ND
17	b	826	CLA	NA
17	b	829	CLA	NC
17	b	829	CLA	ND
17	b	829	CLA	NA
17	k	1402	CLA	NC
17	k	1402	CLA	ND
17	k	1402	CLA	NA
17	B	808	CLA	NC
17	B	808	CLA	ND
17	B	808	CLA	NA
17	b	833	CLA	NC
17	b	833	CLA	ND
17	b	833	CLA	NA
17	6	306	CLA	NC
17	6	306	CLA	ND
17	6	306	CLA	NA
17	1	310	CLA	NC
17	1	310	CLA	ND
17	1	310	CLA	NA
17	a	842	CLA	NC
17	a	842	CLA	ND
17	a	842	CLA	NA
17	6	304	CLA	NC
17	6	304	CLA	ND
17	6	304	CLA	NA
26	7	601	CHL	NC
26	7	601	CHL	ND
26	7	601	CHL	NA
17	B	840	CLA	NC
17	B	840	CLA	NA

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Mol	Chain	Res	Type	Atom
17	A	813	CLA	NC
17	A	813	CLA	ND
17	A	813	CLA	NA
17	A	816	CLA	NC
17	A	816	CLA	ND
17	A	816	CLA	NA
17	A	823	CLA	NC
17	A	823	CLA	ND
17	A	823	CLA	NA
17	B	809	CLA	NC
17	B	809	CLA	ND
17	B	809	CLA	NA
17	L	202	CLA	NC
17	L	202	CLA	ND
17	L	202	CLA	NA
17	G	103	CLA	NC
17	G	103	CLA	ND
17	G	103	CLA	NA
17	A	809	CLA	NC
17	A	809	CLA	ND
17	A	809	CLA	NA
17	b	830	CLA	NC
17	b	830	CLA	ND
17	b	830	CLA	NA
17	B	832	CLA	NC
17	B	832	CLA	ND
17	B	832	CLA	NA
26	9	615	CHL	NC
26	9	615	CHL	ND
26	9	615	CHL	NA
17	B	802	CLA	NC
17	B	802	CLA	ND
17	8	308	CLA	NC
17	8	308	CLA	ND
17	8	308	CLA	NA
17	F	301	CLA	NC
17	F	301	CLA	ND
17	F	301	CLA	NA
17	G	104	CLA	NC
17	G	104	CLA	ND
17	G	104	CLA	NA
17	A	821	CLA	NC

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Mol	Chain	Res	Type	Atom
17	A	821	CLA	ND
17	A	821	CLA	NA
17	b	841	CLA	NC
17	b	841	CLA	ND
17	b	841	CLA	NA
17	A	805	CLA	NC
17	A	805	CLA	ND
17	A	805	CLA	NA
26	9	606	CHL	NC
26	9	606	CHL	ND
26	9	606	CHL	NA
17	2	608	CLA	NC
17	2	608	CLA	ND
17	2	608	CLA	NA
17	B	831	CLA	NC
17	B	831	CLA	ND
17	B	831	CLA	NA
17	a	821	CLA	NC
17	a	821	CLA	ND
17	a	821	CLA	NA
17	B	828	CLA	NC
17	B	828	CLA	ND
17	B	828	CLA	NA
17	a	826	CLA	NA
17	a	826	CLA	NC
17	a	826	CLA	ND
17	l	202	CLA	NC
17	l	202	CLA	ND
17	l	202	CLA	NA
17	9	602	CLA	NC
17	9	602	CLA	ND
17	9	602	CLA	NA
17	a	815	CLA	NC
17	a	815	CLA	ND
17	a	815	CLA	NA
26	4	607	CHL	NC
26	4	607	CHL	ND
26	4	607	CHL	NA
17	a	833	CLA	NC
17	a	833	CLA	ND
17	a	833	CLA	NA
17	A	818	CLA	NC

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Mol	Chain	Res	Type	Atom
17	A	818	CLA	ND
17	A	818	CLA	NA
17	A	812	CLA	NC
17	A	812	CLA	ND
17	A	812	CLA	NA
17	A	841	CLA	NC
17	A	841	CLA	ND
17	A	841	CLA	NA
17	b	827	CLA	NC
17	b	827	CLA	ND
17	2	612	CLA	NC
17	2	612	CLA	ND
17	2	612	CLA	NA
17	A	832	CLA	ND
17	A	832	CLA	NA
17	3	301	CLA	NC
17	3	301	CLA	ND
17	3	301	CLA	NA
17	k	1401	CLA	NC
17	k	1401	CLA	ND
17	k	1401	CLA	NA
17	A	822	CLA	NC
17	A	822	CLA	ND
17	A	822	CLA	NA
17	g	101	CLA	NC
17	g	101	CLA	NA
17	7	609	CLA	NC
17	7	609	CLA	ND
17	7	609	CLA	NA
17	6	309	CLA	NC
17	6	309	CLA	ND
17	6	309	CLA	NA
17	B	833	CLA	NC
17	B	833	CLA	ND
17	B	833	CLA	NA
17	B	836	CLA	NC
17	B	836	CLA	ND
17	B	836	CLA	NA
17	A	837	CLA	NC
17	A	837	CLA	ND
17	A	837	CLA	NA
17	B	822	CLA	NC

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Mol	Chain	Res	Type	Atom
17	B	822	CLA	ND
17	B	822	CLA	NA
17	4	610	CLA	NC
17	4	610	CLA	ND
17	4	610	CLA	NA
17	B	813	CLA	NC
17	B	813	CLA	ND
17	B	813	CLA	NA
17	B	830	CLA	NC
17	B	830	CLA	ND
17	B	830	CLA	NA
17	J	3002	CLA	NC
17	J	3002	CLA	ND
17	J	3002	CLA	NA
17	2	610	CLA	NC
17	2	610	CLA	ND
17	B	815	CLA	NC
17	B	815	CLA	ND
17	B	815	CLA	NA
17	a	840	CLA	ND
17	a	840	CLA	NA
26	9	607	CHL	NC
26	9	607	CHL	ND
26	9	607	CHL	NA
17	B	834	CLA	NC
17	B	834	CLA	ND
17	B	834	CLA	NA
17	7	602	CLA	NC
17	7	602	CLA	ND
17	7	602	CLA	NA
17	A	804	CLA	NC
17	A	804	CLA	ND
17	A	804	CLA	NA
17	b	811	CLA	NC
17	b	811	CLA	ND
17	b	811	CLA	NA
17	4	613	CLA	NC
17	4	613	CLA	ND
17	4	613	CLA	NA
17	6	307	CLA	NC
17	6	307	CLA	ND
17	6	307	CLA	NA

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Mol	Chain	Res	Type	Atom
17	a	822	CLA	NC
17	a	822	CLA	ND
17	a	822	CLA	NA
17	9	604	CLA	NC
17	9	604	CLA	ND
17	9	604	CLA	NA
17	7	611	CLA	NC
17	7	611	CLA	ND
17	7	611	CLA	NA
17	8	303	CLA	NC
17	8	303	CLA	ND
17	8	303	CLA	NA
17	1	204	CLA	NC
17	1	204	CLA	ND
17	1	204	CLA	NA
17	a	810	CLA	NC
17	a	810	CLA	ND
17	a	810	CLA	NA
17	4	612	CLA	NC
17	4	612	CLA	ND
17	4	612	CLA	NA
17	3	315	CLA	NC
17	3	315	CLA	ND
17	3	315	CLA	NA
17	b	803	CLA	NC
17	b	803	CLA	ND
17	b	803	CLA	NA
17	6	312	CLA	NC
17	6	312	CLA	ND
17	6	312	CLA	NA
17	b	824	CLA	NC
17	b	824	CLA	ND
17	b	824	CLA	NA
17	6	310	CLA	NC
17	6	310	CLA	ND
17	6	310	CLA	NA
17	2	603	CLA	NC
17	2	603	CLA	ND
17	2	603	CLA	NA
17	2	609	CLA	NC
17	2	609	CLA	ND
17	2	609	CLA	NA

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Mol	Chain	Res	Type	Atom
17	B	835	CLA	NC
17	B	835	CLA	ND
17	B	835	CLA	NA
17	K	4002	CLA	NC
17	K	4002	CLA	ND
17	K	4002	CLA	NA
17	F	304	CLA	NC
17	F	304	CLA	ND
17	F	304	CLA	NA
17	a	823	CLA	NC
17	a	823	CLA	ND
17	a	823	CLA	NA
17	b	823	CLA	NC
17	b	823	CLA	ND
17	b	823	CLA	NA
17	a	830	CLA	NC
17	a	830	CLA	ND
17	a	830	CLA	NA
17	b	831	CLA	ND
17	b	831	CLA	NA
17	b	819	CLA	NC
17	b	819	CLA	ND
17	b	819	CLA	NA
17	b	828	CLA	NC
17	b	828	CLA	ND
17	b	828	CLA	NA
17	A	802	CLA	NC
17	A	802	CLA	ND
17	A	802	CLA	NA
17	4	611	CLA	NC
17	4	611	CLA	ND
17	4	611	CLA	NA
17	b	832	CLA	NC
17	b	832	CLA	ND
17	b	832	CLA	NA
17	b	837	CLA	NC
17	b	837	CLA	ND
17	b	837	CLA	NA
17	B	816	CLA	NC
17	B	816	CLA	ND
17	B	816	CLA	NA
26	2	601	CHL	NC

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Mol	Chain	Res	Type	Atom
26	2	601	CHL	ND
17	b	806	CLA	NC
17	b	806	CLA	ND
17	b	806	CLA	NA
17	a	838	CLA	NC
17	a	838	CLA	ND
17	a	838	CLA	NA
17	A	820	CLA	NC
17	A	820	CLA	ND
17	A	820	CLA	NA
17	b	808	CLA	NC
17	b	808	CLA	ND
17	b	808	CLA	NA
26	7	607	CHL	NC
26	7	607	CHL	ND
26	7	607	CHL	NA
26	3	307	CHL	NC
26	3	307	CHL	ND
26	3	307	CHL	NA
17	b	825	CLA	NC
17	b	825	CLA	ND
17	b	825	CLA	NA
17	b	817	CLA	NC
17	b	817	CLA	ND
17	b	817	CLA	NA
17	g	103	CLA	NC
17	g	103	CLA	ND
17	g	103	CLA	NA
17	B	812	CLA	NC
17	B	812	CLA	ND
17	B	812	CLA	NA
17	1	303	CLA	NC
17	1	303	CLA	ND
17	1	303	CLA	NA
17	9	610	CLA	NC
17	9	610	CLA	ND
17	9	610	CLA	NA
17	a	803	CLA	ND
17	a	832	CLA	ND
17	a	832	CLA	NA
26	1	307	CHL	NC
26	1	307	CHL	ND

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Mol	Chain	Res	Type	Atom
26	1	307	CHL	NA
17	G	101	CLA	NC
17	G	101	CLA	ND
17	G	101	CLA	NA
17	B	804	CLA	NC
17	B	804	CLA	ND
17	B	804	CLA	NA
17	6	311	CLA	NC
17	6	311	CLA	ND
17	6	311	CLA	NA
17	8	309	CLA	NC
17	8	309	CLA	ND
17	8	309	CLA	NA
17	1	314	CLA	NC
17	1	314	CLA	NA
17	B	803	CLA	NC
17	B	803	CLA	NA
17	B	803	CLA	ND
26	7	605	CHL	NC
26	7	605	CHL	ND
26	7	605	CHL	NA
17	b	804	CLA	NC
17	b	804	CLA	ND
17	b	804	CLA	NA
17	3	310	CLA	NC
17	3	310	CLA	ND
17	3	310	CLA	NA
17	a	841	CLA	NC
17	a	841	CLA	ND
17	a	841	CLA	NA
17	7	604	CLA	NC
17	7	604	CLA	ND
17	7	604	CLA	NA
17	A	807	CLA	NC
17	A	807	CLA	ND
17	A	807	CLA	NA
17	a	843	CLA	NC
17	a	843	CLA	ND
17	a	843	CLA	NA
17	8	311	CLA	ND
17	8	311	CLA	NA
17	9	614	CLA	NC

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Mol	Chain	Res	Type	Atom
17	9	614	CLA	ND
17	9	614	CLA	NA
17	9	613	CLA	NC
17	9	613	CLA	ND
17	9	613	CLA	NA
17	B	838	CLA	ND
17	B	838	CLA	NA
17	7	613	CLA	NC
17	7	613	CLA	NA
17	k	1403	CLA	NC
17	k	1403	CLA	ND
17	k	1403	CLA	NA
17	a	801	CLA	CBD
17	a	801	CLA	NC
17	a	801	CLA	ND
17	a	801	CLA	NA
17	b	812	CLA	NC
17	b	812	CLA	ND
17	b	812	CLA	NA
17	b	807	CLA	NC
17	b	807	CLA	ND
17	b	807	CLA	NA
17	4	608	CLA	NC
17	4	608	CLA	ND
17	4	608	CLA	NA
17	a	804	CLA	NC
17	a	804	CLA	ND
17	a	804	CLA	NA
17	3	313	CLA	NC
17	3	313	CLA	ND
17	3	313	CLA	NA
17	A	839	CLA	NC
17	A	839	CLA	ND
17	A	839	CLA	NA
17	3	304	CLA	NC
17	3	304	CLA	ND
17	3	304	CLA	NA
17	1	311	CLA	NC
17	1	311	CLA	ND
17	1	311	CLA	NA
17	A	817	CLA	NC
17	A	817	CLA	NA

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Mol	Chain	Res	Type	Atom
17	a	829	CLA	ND
17	A	840	CLA	NC
17	A	840	CLA	ND
17	A	840	CLA	NA
17	a	802	CLA	NC
17	a	802	CLA	ND
17	a	802	CLA	NA
17	A	843	CLA	NC
17	A	843	CLA	ND
17	A	843	CLA	NA
17	a	808	CLA	NC
17	a	808	CLA	ND
17	a	808	CLA	NA
26	7	606	CHL	NC
26	7	606	CHL	ND
26	7	606	CHL	NA
26	8	306	CHL	NA
26	8	306	CHL	NC
26	8	306	CHL	ND
17	a	813	CLA	NC
17	a	813	CLA	ND
17	a	813	CLA	NA
17	A	830	CLA	NC
17	A	830	CLA	ND
17	A	830	CLA	NA
17	B	817	CLA	NC
17	B	817	CLA	ND
17	B	817	CLA	NA
17	a	806	CLA	NC
17	a	806	CLA	ND
17	a	806	CLA	NA
17	8	310	CLA	NC
17	8	310	CLA	ND
17	8	310	CLA	NA
17	7	612	CLA	NC
17	7	612	CLA	ND
17	7	612	CLA	NA
26	2	607	CHL	NC
26	2	607	CHL	ND
26	2	607	CHL	NA
17	9	601	CLA	NC
17	9	601	CLA	ND

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Mol	Chain	Res	Type	Atom
17	9	601	CLA	NA
17	a	805	CLA	NC
17	a	805	CLA	ND
17	a	805	CLA	NA
17	b	805	CLA	NC
17	b	805	CLA	ND
17	b	805	CLA	NA
17	A	829	CLA	NC
17	A	829	CLA	ND
17	8	313	CLA	NC
17	8	313	CLA	ND
17	8	313	CLA	NA
26	9	605	CHL	NC
26	9	605	CHL	ND
26	1	302	CHL	NC
26	1	302	CHL	ND
26	1	302	CHL	NA
17	6	314	CLA	NC
17	6	314	CLA	ND
17	6	314	CLA	NA
17	3	302	CLA	NC
17	3	302	CLA	ND
17	3	302	CLA	NA
17	a	816	CLA	NC
17	a	816	CLA	ND
17	a	816	CLA	NA
17	8	312	CLA	ND
17	8	312	CLA	NA
17	B	814	CLA	NC
17	B	814	CLA	ND
17	B	814	CLA	NA
17	1	304	CLA	NC
17	1	304	CLA	ND
17	1	304	CLA	NA
17	a	846	CLA	NC
17	a	846	CLA	ND
17	a	846	CLA	NA
26	4	615	CHL	NC
26	4	615	CHL	ND
26	4	615	CHL	NA
17	a	807	CLA	NC
17	a	807	CLA	ND

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Mol	Chain	Res	Type	Atom
17	a	807	CLA	NA
17	B	829	CLA	NC
17	B	829	CLA	ND
17	B	829	CLA	NA
17	b	820	CLA	NC
17	b	820	CLA	ND
17	b	820	CLA	NA
17	4	614	CLA	NC
17	4	614	CLA	ND
17	4	614	CLA	NA
17	B	837	CLA	NC
17	B	837	CLA	ND
17	B	837	CLA	NA
17	4	603	CLA	NA
17	4	603	CLA	NC
17	4	603	CLA	ND
17	8	301	CLA	NC
17	8	301	CLA	ND
17	8	301	CLA	NA
17	B	807	CLA	ND
17	B	807	CLA	NA
17	3	312	CLA	NC
17	3	312	CLA	ND
17	3	312	CLA	NA
17	K	4003	CLA	NC
17	K	4003	CLA	ND
17	K	4003	CLA	NA
17	8	302	CLA	NA
17	8	302	CLA	NC
17	8	302	CLA	ND
17	8	307	CLA	NC
17	8	307	CLA	ND
17	8	307	CLA	NA
17	7	603	CLA	NC
17	7	603	CLA	ND
17	7	603	CLA	NA

All (2517) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	B	805	CLA	C3A-C2A-CAA-CBA
20	9	618	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
20	9	618	BCR	C7-C8-C9-C34
17	A	831	CLA	CHA-CBD-CGD-O1D
17	A	831	CLA	CHA-CBD-CGD-O2D
17	A	831	CLA	C4-C3-C5-C6
17	a	809	CLA	C3A-C2A-CAA-CBA
17	a	809	CLA	CHA-CBD-CGD-O2D
17	a	831	CLA	CHA-CBD-CGD-O1D
17	a	831	CLA	CHA-CBD-CGD-O2D
19	A	846	LHG	C4-O6-P-O4
17	f	7003	CLA	C2-C1-O2A-CGA
20	L	206	BCR	C11-C12-C13-C14
20	L	206	BCR	C11-C12-C13-C35
17	A	811	CLA	CHA-CBD-CGD-O1D
17	A	811	CLA	CHA-CBD-CGD-O2D
19	1	301	LHG	C3-O3-P-O5
19	1	301	LHG	C4-O6-P-O4
19	1	301	LHG	C8-C7-O7-C5
17	a	825	CLA	CHA-CBD-CGD-O1D
17	a	825	CLA	CHA-CBD-CGD-O2D
26	4	605	CHL	C1C-C2C-CMC-OMC
19	a	847	LHG	C3-O3-P-O6
19	a	847	LHG	C4-O6-P-O3
17	B	827	CLA	C1A-C2A-CAA-CBA
17	B	827	CLA	C3A-C2A-CAA-CBA
17	A	845	CLA	CBA-CGA-O2A-C1
17	A	845	CLA	O1A-CGA-O2A-C1
17	a	819	CLA	C3A-C2A-CAA-CBA
17	a	824	CLA	CHA-CBD-CGD-O1D
17	a	824	CLA	CHA-CBD-CGD-O2D
17	a	818	CLA	CHA-CBD-CGD-O2D
20	k	1404	BCR	C21-C22-C23-C24
20	k	1404	BCR	C37-C22-C23-C24
20	k	1404	BCR	C23-C24-C25-C30
17	1	309	CLA	C1A-C2A-CAA-CBA
17	1	309	CLA	C3A-C2A-CAA-CBA
17	A	854	CLA	CHA-CBD-CGD-O1D
17	A	854	CLA	CHA-CBD-CGD-O2D
17	b	818	CLA	C1A-C2A-CAA-CBA
17	b	818	CLA	C3A-C2A-CAA-CBA
17	b	818	CLA	C4-C3-C5-C6
20	L	205	BCR	C7-C8-C9-C10
20	L	205	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
26	6	303	CHL	C1C-C2C-CMC-OMC
26	6	303	CHL	C3C-C2C-CMC-OMC
19	1	319	LHG	C3-O3-P-O4
19	1	319	LHG	O10-C23-O8-C6
19	1	319	LHG	C24-C23-O8-C6
17	A	824	CLA	C1A-C2A-CAA-CBA
17	2	613	CLA	CHA-CBD-CGD-O1D
17	2	613	CLA	CHA-CBD-CGD-O2D
17	2	613	CLA	CAD-CBD-CGD-O1D
20	1	318	BCR	C23-C24-C25-C30
17	A	825	CLA	CHA-CBD-CGD-O1D
17	A	825	CLA	CHA-CBD-CGD-O2D
17	a	820	CLA	C1A-C2A-CAA-CBA
17	a	820	CLA	C3A-C2A-CAA-CBA
20	a	853	BCR	C21-C22-C23-C24
20	a	853	BCR	C37-C22-C23-C24
19	3	319	LHG	C3-O3-P-O4
19	3	319	LHG	C4-O6-P-O3
17	b	815	CLA	CHA-CBD-CGD-O1D
17	b	815	CLA	CHA-CBD-CGD-O2D
17	B	818	CLA	C1A-C2A-CAA-CBA
17	B	818	CLA	C3A-C2A-CAA-CBA
17	B	818	CLA	C2-C3-C5-C6
17	B	818	CLA	C4-C3-C5-C6
20	B	848	BCR	C1-C6-C7-C8
17	a	835	CLA	CHA-CBD-CGD-O1D
17	a	835	CLA	CHA-CBD-CGD-O2D
17	B	841	CLA	C2-C3-C5-C6
17	B	841	CLA	C4-C3-C5-C6
17	3	308	CLA	C1A-C2A-CAA-CBA
17	a	834	CLA	C2-C3-C5-C6
17	a	834	CLA	C4-C3-C5-C6
17	a	814	CLA	C4-C3-C5-C6
17	a	839	CLA	C2-C3-C5-C6
17	a	839	CLA	C4-C3-C5-C6
17	b	822	CLA	C4-C3-C5-C6
20	K	4004	BCR	C1-C6-C7-C8
17	A	814	CLA	C2-C3-C5-C6
17	A	814	CLA	C4-C3-C5-C6
17	1	312	CLA	C4-C3-C5-C6
17	a	837	CLA	CHA-CBD-CGD-O1D
17	a	837	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	A	834	CLA	C2-C3-C5-C6
17	A	834	CLA	C4-C3-C5-C6
25	4	620	LMG	C2-C1-O1-C7
17	8	305	CLA	C1A-C2A-CAA-CBA
17	8	305	CLA	C3A-C2A-CAA-CBA
17	6	315	CLA	CHA-CBD-CGD-O1D
17	6	315	CLA	CHA-CBD-CGD-O2D
20	B	845	BCR	C7-C8-C9-C10
20	B	845	BCR	C7-C8-C9-C34
17	9	608	CLA	C1A-C2A-CAA-CBA
17	9	608	CLA	C3A-C2A-CAA-CBA
20	j	3004	BCR	C1-C6-C7-C8
20	j	3004	BCR	C21-C22-C23-C24
20	j	3004	BCR	C37-C22-C23-C24
17	A	819	CLA	C3A-C2A-CAA-CBA
17	B	810	CLA	C1A-C2A-CAA-CBA
26	4	606	CHL	C3A-C2A-CAA-CBA
17	A	835	CLA	C2-C3-C5-C6
17	A	835	CLA	C4-C3-C5-C6
17	3	306	CLA	C1A-C2A-CAA-CBA
17	3	306	CLA	C3A-C2A-CAA-CBA
17	3	306	CLA	C2A-CAA-CBA-CGA
17	B	808	CLA	CHA-CBD-CGD-O2D
17	b	833	CLA	CHA-CBD-CGD-O1D
17	b	833	CLA	CHA-CBD-CGD-O2D
17	6	306	CLA	C2-C3-C5-C6
17	6	306	CLA	C4-C3-C5-C6
26	7	601	CHL	C1C-C2C-CMC-OMC
26	7	601	CHL	C3C-C2C-CMC-OMC
26	7	601	CHL	C2-C3-C5-C6
26	7	601	CHL	C4-C3-C5-C6
17	B	840	CLA	C4-C3-C5-C6
17	A	823	CLA	C1A-C2A-CAA-CBA
17	A	823	CLA	C3A-C2A-CAA-CBA
20	7	617	BCR	C7-C8-C9-C10
20	7	617	BCR	C7-C8-C9-C34
20	7	617	BCR	C21-C22-C23-C24
20	7	617	BCR	C37-C22-C23-C24
17	L	202	CLA	C1A-C2A-CAA-CBA
17	L	202	CLA	C3A-C2A-CAA-CBA
17	A	809	CLA	C3A-C2A-CAA-CBA
17	A	809	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
17	A	809	CLA	CHA-CBD-CGD-O2D
17	B	832	CLA	C1A-C2A-CAA-CBA
19	6	301	LHG	C3-O3-P-O4
19	6	301	LHG	C4-O6-P-O3
17	b	841	CLA	C2-C3-C5-C6
17	b	841	CLA	C4-C3-C5-C6
17	A	805	CLA	CHA-CBD-CGD-O1D
24	B	850	DGD	O6D-C1D-O3G-C3G
26	9	606	CHL	C1A-C2A-CAA-CBA
26	9	606	CHL	C3A-C2A-CAA-CBA
17	B	831	CLA	C1A-C2A-CAA-CBA
17	B	831	CLA	C3A-C2A-CAA-CBA
17	B	828	CLA	C1A-C2A-CAA-CBA
17	B	828	CLA	C3A-C2A-CAA-CBA
20	8	316	BCR	C1-C6-C7-C8
20	8	316	BCR	C23-C24-C25-C30
17	l	202	CLA	C1A-C2A-CAA-CBA
17	l	202	CLA	C3A-C2A-CAA-CBA
17	a	833	CLA	C4-C3-C5-C6
17	A	818	CLA	CHA-CBD-CGD-O1D
17	A	818	CLA	CHA-CBD-CGD-O2D
17	A	818	CLA	C2-C3-C5-C6
17	A	818	CLA	C4-C3-C5-C6
17	A	841	CLA	CHA-CBD-CGD-O1D
17	A	841	CLA	CHA-CBD-CGD-O2D
20	3	318	BCR	C23-C24-C25-C30
17	A	832	CLA	C2A-CAA-CBA-CGA
17	B	836	CLA	C2-C3-C5-C6
17	B	836	CLA	C4-C3-C5-C6
17	A	837	CLA	C2A-CAA-CBA-CGA
17	A	837	CLA	CHA-CBD-CGD-O1D
17	A	837	CLA	CHA-CBD-CGD-O2D
17	B	822	CLA	C2-C3-C5-C6
17	B	822	CLA	C4-C3-C5-C6
17	B	830	CLA	C1A-C2A-CAA-CBA
17	B	830	CLA	C3A-C2A-CAA-CBA
17	J	3002	CLA	CHA-CBD-CGD-O1D
17	J	3002	CLA	CHA-CBD-CGD-O2D
17	J	3002	CLA	CAD-CBD-CGD-O1D
17	B	815	CLA	C1A-C2A-CAA-CBA
17	a	840	CLA	CHA-CBD-CGD-O1D
17	a	840	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	B	847	BCR	C7-C8-C9-C34
17	b	811	CLA	CHA-CBD-CGD-O1D
17	b	811	CLA	CHA-CBD-CGD-O2D
20	I	101	BCR	C21-C22-C23-C24
20	I	101	BCR	C37-C22-C23-C24
20	a	850	BCR	C1-C6-C7-C8
20	a	850	BCR	C7-C8-C9-C10
20	a	850	BCR	C7-C8-C9-C34
19	a	848	LHG	C3-O3-P-O5
19	a	848	LHG	C4-O6-P-O5
19	2	618	LHG	C4-O6-P-O4
19	A	847	LHG	C3-O3-P-O5
17	2	603	CLA	CBD-CGD-O2D-CED
17	2	603	CLA	C2-C3-C5-C6
17	2	603	CLA	C4-C3-C5-C6
20	l	201	BCR	C1-C6-C7-C8
17	F	304	CLA	C2-C1-O2A-CGA
17	a	823	CLA	C1A-C2A-CAA-CBA
17	a	823	CLA	C3A-C2A-CAA-CBA
17	b	823	CLA	CHA-CBD-CGD-O1D
17	b	823	CLA	CHA-CBD-CGD-O2D
17	b	828	CLA	C1A-C2A-CAA-CBA
17	b	828	CLA	C3A-C2A-CAA-CBA
17	b	828	CLA	C2-C3-C5-C6
17	b	828	CLA	C4-C3-C5-C6
20	b	848	BCR	C1-C6-C7-C8
26	2	601	CHL	C1C-C2C-CMC-OMC
19	6	320	LHG	C3-O3-P-O4
19	6	320	LHG	C4-O6-P-O3
17	a	838	CLA	C1A-C2A-CAA-CBA
17	A	820	CLA	C1A-C2A-CAA-CBA
17	A	820	CLA	C3A-C2A-CAA-CBA
17	b	808	CLA	CHA-CBD-CGD-O1D
17	b	808	CLA	CHA-CBD-CGD-O2D
17	B	804	CLA	C1A-C2A-CAA-CBA
17	B	804	CLA	CHA-CBD-CGD-O2D
26	7	605	CHL	C1C-C2C-CMC-OMC
26	7	605	CHL	C3C-C2C-CMC-OMC
17	b	804	CLA	C1A-C2A-CAA-CBA
17	7	604	CLA	CHA-CBD-CGD-O1D
17	7	604	CLA	CHA-CBD-CGD-O2D
17	4	608	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	4	608	CLA	C3A-C2A-CAA-CBA
17	a	829	CLA	C1A-C2A-CAA-CBA
17	a	829	CLA	C3A-C2A-CAA-CBA
17	a	829	CLA	C2-C3-C5-C6
17	a	829	CLA	C4-C3-C5-C6
17	A	840	CLA	CHA-CBD-CGD-O1D
17	A	840	CLA	CHA-CBD-CGD-O2D
17	a	806	CLA	CHA-CBD-CGD-O1D
17	a	806	CLA	CHA-CBD-CGD-O2D
17	a	806	CLA	CAD-CBD-CGD-O1D
17	b	805	CLA	C3A-C2A-CAA-CBA
19	7	618	LHG	C3-O3-P-O4
19	7	618	LHG	C4-O6-P-O3
26	1	302	CHL	C1C-C2C-CMC-OMC
26	1	302	CHL	C3C-C2C-CMC-OMC
20	A	848	BCR	C1-C6-C7-C8
20	A	848	BCR	C23-C24-C25-C30
17	3	302	CLA	C2-C3-C5-C6
17	3	302	CLA	C4-C3-C5-C6
17	a	816	CLA	C3A-C2A-CAA-CBA
17	a	816	CLA	CHA-CBD-CGD-O1D
17	a	816	CLA	CHA-CBD-CGD-O2D
20	l	205	BCR	C7-C8-C9-C10
20	l	205	BCR	C7-C8-C9-C34
20	l	205	BCR	C23-C24-C25-C26
17	a	846	CLA	CHA-CBD-CGD-O1D
17	a	846	CLA	CHA-CBD-CGD-O2D
17	a	846	CLA	CAD-CBD-CGD-O1D
20	4	618	BCR	C7-C8-C9-C10
20	4	618	BCR	C7-C8-C9-C34
17	a	807	CLA	C1A-C2A-CAA-CBA
17	K	4003	CLA	CHA-CBD-CGD-O1D
17	K	4003	CLA	CHA-CBD-CGD-O2D
17	8	307	CLA	C2-C1-O2A-CGA
17	2	603	CLA	O1D-CGD-O2D-CED
17	b	810	CLA	CBD-CGD-O2D-CED
17	b	822	CLA	CBD-CGD-O2D-CED
17	B	806	CLA	CBD-CGD-O2D-CED
26	4	607	CHL	CBD-CGD-O2D-CED
17	g	101	CLA	CBD-CGD-O2D-CED
26	9	607	CHL	CBD-CGD-O2D-CED
17	G	101	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	b	811	CLA	O1A-CGA-O2A-C1
17	B	806	CLA	O1D-CGD-O2D-CED
17	b	811	CLA	CBA-CGA-O2A-C1
17	a	818	CLA	CBD-CGD-O2D-CED
17	B	840	CLA	CBD-CGD-O2D-CED
26	8	306	CHL	CBD-CGD-O2D-CED
26	2	607	CHL	CBD-CGD-O2D-CED
17	a	802	CLA	O1A-CGA-O2A-C1
19	7	618	LHG	O10-C23-O8-C6
17	a	846	CLA	O1A-CGA-O2A-C1
17	8	307	CLA	O1A-CGA-O2A-C1
19	1	301	LHG	O9-C7-O7-C5
17	a	856	CLA	C3-C5-C6-C7
17	2	604	CLA	C3-C5-C6-C7
17	A	808	CLA	C3-C5-C6-C7
17	a	831	CLA	C3-C5-C6-C7
17	A	806	CLA	C3-C5-C6-C7
17	f	7003	CLA	C3-C5-C6-C7
17	A	826	CLA	C3-C5-C6-C7
17	A	833	CLA	C3-C5-C6-C7
17	6	305	CLA	C3-C5-C6-C7
17	b	816	CLA	C3-C5-C6-C7
17	a	818	CLA	C3-C5-C6-C7
17	A	854	CLA	C3-C5-C6-C7
17	A	825	CLA	C3-C5-C6-C7
17	B	818	CLA	C3-C5-C6-C7
17	B	824	CLA	C3-C5-C6-C7
17	a	839	CLA	C3-C5-C6-C7
17	b	822	CLA	C3-C5-C6-C7
17	B	806	CLA	C3-C5-C6-C7
17	b	839	CLA	C3-C5-C6-C7
17	A	819	CLA	C3-C5-C6-C7
17	6	304	CLA	C3-C5-C6-C7
26	7	601	CHL	C3-C5-C6-C7
17	B	809	CLA	C3-C5-C6-C7
17	A	818	CLA	C3-C5-C6-C7
17	b	827	CLA	C3-C5-C6-C7
17	7	609	CLA	C3-C5-C6-C7
17	4	610	CLA	C3-C5-C6-C7
17	a	840	CLA	C3-C5-C6-C7
17	b	824	CLA	C3-C5-C6-C7
26	2	601	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
17	b	806	CLA	C3-C5-C6-C7
17	b	808	CLA	C3-C5-C6-C7
17	7	604	CLA	C3-C5-C6-C7
17	A	840	CLA	C3-C5-C6-C7
17	a	802	CLA	C3-C5-C6-C7
17	A	843	CLA	C3-C5-C6-C7
17	a	808	CLA	C3-C5-C6-C7
17	8	310	CLA	C3-C5-C6-C7
17	7	612	CLA	C3-C5-C6-C7
17	A	829	CLA	C3-C5-C6-C7
17	B	807	CLA	C3-C5-C6-C7
17	A	812	CLA	CBA-CGA-O2A-C1
17	F	304	CLA	CBA-CGA-O2A-C1
17	b	825	CLA	CBA-CGA-O2A-C1
19	7	618	LHG	C24-C23-O8-C6
17	B	817	CLA	C5-C6-C7-C8
17	A	818	CLA	CBD-CGD-O2D-CED
17	a	846	CLA	C3-C5-C6-C7
17	a	831	CLA	C4-C3-C5-C6
17	9	611	CLA	C4-C3-C5-C6
17	b	836	CLA	C4-C3-C5-C6
17	3	311	CLA	C4-C3-C5-C6
17	2	611	CLA	C4-C3-C5-C6
17	2	602	CLA	C4-C3-C5-C6
17	6	304	CLA	C4-C3-C5-C6
17	7	611	CLA	C4-C3-C5-C6
17	4	611	CLA	C4-C3-C5-C6
17	8	309	CLA	C4-C3-C5-C6
17	A	839	CLA	C4-C3-C5-C6
17	A	829	CLA	C4-C3-C5-C6
17	6	314	CLA	C4-C3-C5-C6
17	8	301	CLA	C4-C3-C5-C6
17	A	831	CLA	C2-C3-C5-C6
17	b	818	CLA	C2-C3-C5-C6
17	a	814	CLA	C2-C3-C5-C6
17	b	822	CLA	C2-C3-C5-C6
17	1	312	CLA	C2-C3-C5-C6
17	B	840	CLA	C2-C3-C5-C6
17	A	829	CLA	C2-C3-C5-C6
17	6	314	CLA	C2-C3-C5-C6
17	8	301	CLA	C2-C3-C5-C6
17	a	831	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	a	835	CLA	CBD-CGD-O2D-CED
17	b	823	CLA	CBD-CGD-O2D-CED
17	a	825	CLA	C2A-CAA-CBA-CGA
17	A	825	CLA	C2A-CAA-CBA-CGA
17	g	102	CLA	C2A-CAA-CBA-CGA
17	8	305	CLA	C2A-CAA-CBA-CGA
17	b	839	CLA	C2A-CAA-CBA-CGA
17	B	839	CLA	C2A-CAA-CBA-CGA
26	4	606	CHL	C2A-CAA-CBA-CGA
17	G	103	CLA	C2A-CAA-CBA-CGA
17	b	830	CLA	C2A-CAA-CBA-CGA
17	a	830	CLA	C2A-CAA-CBA-CGA
17	a	816	CLA	C2A-CAA-CBA-CGA
17	f	7003	CLA	O1A-CGA-O2A-C1
17	a	812	CLA	C3-C5-C6-C7
17	A	804	CLA	C3-C5-C6-C7
17	A	807	CLA	C3-C5-C6-C7
17	b	812	CLA	C3-C5-C6-C7
17	b	807	CLA	C3-C5-C6-C7
17	a	812	CLA	CBA-CGA-O2A-C1
17	A	806	CLA	CBA-CGA-O2A-C1
17	a	824	CLA	CBA-CGA-O2A-C1
17	b	810	CLA	CBA-CGA-O2A-C1
17	B	823	CLA	CBA-CGA-O2A-C1
17	B	825	CLA	CBA-CGA-O2A-C1
17	b	833	CLA	CBA-CGA-O2A-C1
17	l	202	CLA	CBA-CGA-O2A-C1
17	B	833	CLA	CBA-CGA-O2A-C1
17	B	834	CLA	CBA-CGA-O2A-C1
17	A	820	CLA	CBA-CGA-O2A-C1
17	a	846	CLA	CBA-CGA-O2A-C1
17	8	307	CLA	CBA-CGA-O2A-C1
17	B	823	CLA	CBD-CGD-O2D-CED
26	4	607	CHL	O1D-CGD-O2D-CED
17	A	806	CLA	O1A-CGA-O2A-C1
17	B	818	CLA	O1A-CGA-O2A-C1
17	b	810	CLA	O1A-CGA-O2A-C1
17	B	823	CLA	O1A-CGA-O2A-C1
17	A	812	CLA	O1A-CGA-O2A-C1
17	6	310	CLA	O1A-CGA-O2A-C1
17	F	304	CLA	O1A-CGA-O2A-C1
17	b	825	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	B	804	CLA	C2A-CAA-CBA-CGA
17	4	604	CLA	CBD-CGD-O2D-CED
17	F	301	CLA	CBD-CGD-O2D-CED
17	b	827	CLA	CBD-CGD-O2D-CED
17	B	822	CLA	CBD-CGD-O2D-CED
17	B	815	CLA	CBD-CGD-O2D-CED
17	6	307	CLA	CBD-CGD-O2D-CED
17	b	813	CLA	C3-C5-C6-C7
17	B	808	CLA	C3-C5-C6-C7
17	A	809	CLA	C3-C5-C6-C7
17	B	802	CLA	C3-C5-C6-C7
17	A	805	CLA	C3-C5-C6-C7
17	B	813	CLA	C3-C5-C6-C7
17	7	602	CLA	C3-C5-C6-C7
17	F	304	CLA	C3-C5-C6-C7
17	A	839	CLA	C3-C5-C6-C7
17	a	807	CLA	C3-C5-C6-C7
17	8	301	CLA	C3-C5-C6-C7
17	b	818	CLA	CBA-CGA-O2A-C1
17	B	818	CLA	CBA-CGA-O2A-C1
17	6	310	CLA	CBA-CGA-O2A-C1
17	a	838	CLA	CBA-CGA-O2A-C1
17	B	812	CLA	CBA-CGA-O2A-C1
17	a	802	CLA	CBA-CGA-O2A-C1
17	a	805	CLA	CBA-CGA-O2A-C1
17	A	829	CLA	CBA-CGA-O2A-C1
17	B	825	CLA	O1A-CGA-O2A-C1
17	b	833	CLA	O1A-CGA-O2A-C1
17	A	829	CLA	O1A-CGA-O2A-C1
17	g	101	CLA	O1D-CGD-O2D-CED
26	9	607	CHL	O1D-CGD-O2D-CED
17	b	811	CLA	CBD-CGD-O2D-CED
26	3	307	CHL	CBD-CGD-O2D-CED
17	B	803	CLA	CBD-CGD-O2D-CED
17	8	301	CLA	CBD-CGD-O2D-CED
17	B	833	CLA	O1A-CGA-O2A-C1
17	A	831	CLA	C3-C5-C6-C7
17	a	834	CLA	C3-C5-C6-C7
17	L	202	CLA	C3-C5-C6-C7
17	2	612	CLA	C3-C5-C6-C7
17	B	833	CLA	C3-C5-C6-C7
17	B	822	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
17	a	804	CLA	C3-C5-C6-C7
17	a	829	CLA	C3-C5-C6-C7
26	9	605	CHL	C3-C5-C6-C7
17	3	312	CLA	C3-C5-C6-C7
17	f	7003	CLA	CBA-CGA-O2A-C1
17	a	812	CLA	O1A-CGA-O2A-C1
17	a	824	CLA	O1A-CGA-O2A-C1
17	B	834	CLA	O1A-CGA-O2A-C1
17	8	309	CLA	C3-C5-C6-C7
17	6	313	CLA	C4-C3-C5-C6
17	a	856	CLA	C4-C3-C5-C6
17	A	808	CLA	C4-C3-C5-C6
17	A	833	CLA	C4-C3-C5-C6
17	b	816	CLA	C4-C3-C5-C6
17	a	844	CLA	C4-C3-C5-C6
17	A	842	CLA	C4-C3-C5-C6
17	b	833	CLA	C4-C3-C5-C6
17	B	833	CLA	C4-C3-C5-C6
17	B	816	CLA	C4-C3-C5-C6
17	b	817	CLA	C4-C3-C5-C6
17	a	843	CLA	C4-C3-C5-C6
17	a	804	CLA	C4-C3-C5-C6
17	A	843	CLA	C4-C3-C5-C6
17	a	808	CLA	C4-C3-C5-C6
17	B	817	CLA	C4-C3-C5-C6
17	a	806	CLA	C4-C3-C5-C6
17	1	304	CLA	C4-C3-C5-C6
17	6	313	CLA	C2-C3-C5-C6
17	a	856	CLA	C2-C3-C5-C6
17	A	808	CLA	C2-C3-C5-C6
17	A	833	CLA	C2-C3-C5-C6
17	b	816	CLA	C2-C3-C5-C6
17	9	611	CLA	C2-C3-C5-C6
17	b	836	CLA	C2-C3-C5-C6
17	a	844	CLA	C2-C3-C5-C6
17	A	842	CLA	C2-C3-C5-C6
17	b	833	CLA	C2-C3-C5-C6
17	a	833	CLA	C2-C3-C5-C6
17	B	833	CLA	C2-C3-C5-C6
17	B	816	CLA	C2-C3-C5-C6
17	b	817	CLA	C2-C3-C5-C6
17	a	843	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
17	a	804	CLA	C2-C3-C5-C6
17	A	839	CLA	C2-C3-C5-C6
17	A	843	CLA	C2-C3-C5-C6
17	a	808	CLA	C2-C3-C5-C6
17	B	817	CLA	C2-C3-C5-C6
17	a	806	CLA	C2-C3-C5-C6
17	1	304	CLA	C2-C3-C5-C6
17	b	818	CLA	O1A-CGA-O2A-C1
17	1	202	CLA	O1A-CGA-O2A-C1
17	2	603	CLA	O1A-CGA-O2A-C1
17	a	838	CLA	O1A-CGA-O2A-C1
17	A	820	CLA	O1A-CGA-O2A-C1
17	B	812	CLA	O1A-CGA-O2A-C1
17	a	805	CLA	O1A-CGA-O2A-C1
17	b	817	CLA	C5-C6-C7-C8
17	a	819	CLA	C3-C5-C6-C7
17	b	815	CLA	C3-C5-C6-C7
17	B	811	CLA	C3-C5-C6-C7
17	2	603	CLA	CBA-CGA-O2A-C1
17	A	807	CLA	CBA-CGA-O2A-C1
17	a	824	CLA	CBD-CGD-O2D-CED
17	b	810	CLA	O1D-CGD-O2D-CED
17	G	101	CLA	O1D-CGD-O2D-CED
17	A	807	CLA	O1A-CGA-O2A-C1
17	b	822	CLA	O1D-CGD-O2D-CED
17	B	805	CLA	O1A-CGA-O2A-C1
17	B	825	CLA	C3-C5-C6-C7
17	a	842	CLA	C3-C5-C6-C7
17	2	609	CLA	C3-C5-C6-C7
17	3	302	CLA	C3-C5-C6-C7
26	2	607	CHL	O1D-CGD-O2D-CED
17	B	805	CLA	CBA-CGA-O2A-C1
17	2	604	CLA	CBA-CGA-O2A-C1
17	A	824	CLA	CBA-CGA-O2A-C1
17	A	825	CLA	CBA-CGA-O2A-C1
17	a	820	CLA	CBA-CGA-O2A-C1
17	A	814	CLA	CBA-CGA-O2A-C1
17	B	811	CLA	CBA-CGA-O2A-C1
17	a	844	CLA	CBA-CGA-O2A-C1
17	b	829	CLA	CBA-CGA-O2A-C1
17	L	202	CLA	CBA-CGA-O2A-C1
17	A	809	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	b	827	CLA	CBA-CGA-O2A-C1
17	B	830	CLA	CBA-CGA-O2A-C1
17	1	303	CLA	CBA-CGA-O2A-C1
17	a	843	CLA	CBA-CGA-O2A-C1
17	A	843	CLA	CBA-CGA-O2A-C1
17	b	805	CLA	CBA-CGA-O2A-C1
17	7	603	CLA	CBA-CGA-O2A-C1
17	b	835	CLA	CBD-CGD-O2D-CED
17	b	821	CLA	CBD-CGD-O2D-CED
17	k	1401	CLA	CBD-CGD-O2D-CED
17	a	838	CLA	CBD-CGD-O2D-CED
26	7	607	CHL	CBD-CGD-O2D-CED
17	a	837	CLA	C2A-CAA-CBA-CGA
17	3	313	CLA	C2A-CAA-CBA-CGA
26	4	605	CHL	C5-C6-C7-C8
17	B	803	CLA	C10-C11-C12-C13
17	A	829	CLA	C15-C16-C17-C18
17	l	202	CLA	C3-C5-C6-C7
25	9	619	LMG	C10-C11-C12-C13
17	6	313	CLA	C3-C5-C6-C7
17	A	845	CLA	C3-C5-C6-C7
17	9	611	CLA	C3-C5-C6-C7
17	3	311	CLA	C3-C5-C6-C7
17	2	611	CLA	C3-C5-C6-C7
17	1	312	CLA	C3-C5-C6-C7
17	7	611	CLA	C3-C5-C6-C7
17	4	611	CLA	C3-C5-C6-C7
25	4	620	LMG	O7-C8-C9-O8
17	b	829	CLA	O1A-CGA-O2A-C1
17	a	843	CLA	O1A-CGA-O2A-C1
17	a	831	CLA	C2-C3-C5-C6
17	3	311	CLA	C2-C3-C5-C6
17	2	611	CLA	C2-C3-C5-C6
17	2	602	CLA	C2-C3-C5-C6
17	6	304	CLA	C2-C3-C5-C6
17	A	806	CLA	C11-C10-C8-C9
17	a	819	CLA	C11-C10-C8-C9
17	b	818	CLA	C6-C7-C8-C9
17	A	827	CLA	C6-C7-C8-C9
17	B	818	CLA	C6-C7-C8-C9
17	a	827	CLA	C6-C7-C8-C9
17	b	809	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
17	l	203	CLA	C6-C7-C8-C9
17	A	812	CLA	C14-C13-C15-C16
26	2	601	CHL	C6-C7-C8-C9
17	b	808	CLA	C14-C13-C15-C16
17	a	841	CLA	C14-C13-C15-C16
17	a	829	CLA	C6-C7-C8-C9
17	b	805	CLA	C6-C7-C8-C9
17	2	602	CLA	CBD-CGD-O2D-CED
17	b	803	CLA	C10-C11-C12-C13
17	a	812	CLA	C2A-CAA-CBA-CGA
17	1	309	CLA	C2A-CAA-CBA-CGA
17	A	812	CLA	C2A-CAA-CBA-CGA
17	a	802	CLA	C2A-CAA-CBA-CGA
28	3	317	XAT	C27-C28-C29-C39
20	L	205	BCR	C37-C22-C23-C24
20	a	853	BCR	C36-C18-C19-C20
20	L	201	BCR	C11-C12-C13-C35
20	a	849	BCR	C37-C22-C23-C24
20	b	844	BCR	C37-C22-C23-C24
20	j	3003	BCR	C7-C8-C9-C34
20	j	3003	BCR	C36-C18-C19-C20
20	3	318	BCR	C7-C8-C9-C34
20	b	847	BCR	C37-C22-C23-C24
20	B	847	BCR	C37-C22-C23-C24
20	b	845	BCR	C37-C22-C23-C24
20	l	205	BCR	C37-C22-C23-C24
20	A	851	BCR	C37-C22-C23-C24
20	4	618	BCR	C11-C12-C13-C35
20	L	205	BCR	C21-C22-C23-C24
20	a	849	BCR	C21-C22-C23-C24
20	b	844	BCR	C21-C22-C23-C24
20	l	205	BCR	C21-C22-C23-C24
20	A	851	BCR	C21-C22-C23-C24
17	2	604	CLA	O1A-CGA-O2A-C1
17	A	824	CLA	O1A-CGA-O2A-C1
17	a	820	CLA	O1A-CGA-O2A-C1
17	A	814	CLA	O1A-CGA-O2A-C1
17	B	811	CLA	O1A-CGA-O2A-C1
17	A	843	CLA	O1A-CGA-O2A-C1
17	7	603	CLA	O1A-CGA-O2A-C1
17	a	839	CLA	C10-C11-C12-C13
17	B	839	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
26	2	601	CHL	C10-C11-C12-C13
17	B	833	CLA	CBD-CGD-O2D-CED
25	4	620	LMG	O6-C5-C6-O5
17	a	806	CLA	C3-C5-C6-C7
17	A	842	CLA	CBA-CGA-O2A-C1
17	A	805	CLA	CBA-CGA-O2A-C1
17	b	812	CLA	CBA-CGA-O2A-C1
17	a	818	CLA	C10-C11-C12-C13
17	1	308	CLA	C5-C6-C7-C8
17	b	814	CLA	C13-C15-C16-C17
17	b	824	CLA	C8-C10-C11-C12
17	b	819	CLA	C8-C10-C11-C12
17	a	841	CLA	C5-C6-C7-C8
17	B	840	CLA	O1D-CGD-O2D-CED
17	B	805	CLA	C10-C11-C12-C13
17	A	808	CLA	C10-C11-C12-C13
17	b	840	CLA	C15-C16-C17-C18
17	A	826	CLA	C10-C11-C12-C13
17	A	826	CLA	C13-C15-C16-C17
17	a	814	CLA	C8-C10-C11-C12
17	A	814	CLA	C8-C10-C11-C12
17	B	832	CLA	C15-C16-C17-C18
17	B	834	CLA	C13-C15-C16-C17
17	7	602	CLA	C13-C15-C16-C17
17	b	837	CLA	C13-C15-C16-C17
17	a	801	CLA	C8-C10-C11-C12
17	a	808	CLA	C10-C11-C12-C13
17	a	806	CLA	C13-C15-C16-C17
17	a	806	CLA	C15-C16-C17-C18
17	b	805	CLA	O1A-CGA-O2A-C1
19	6	320	LHG	C23-C24-C25-C26
26	8	306	CHL	O1D-CGD-O2D-CED
17	a	831	CLA	C13-C15-C16-C17
17	a	843	CLA	C10-C11-C12-C13
17	B	829	CLA	C5-C6-C7-C8
17	a	809	CLA	CBA-CGA-O2A-C1
17	A	806	CLA	C2-C1-O2A-CGA
17	a	840	CLA	C2-C1-O2A-CGA
17	a	814	CLA	C13-C15-C16-C17
26	7	601	CHL	C5-C6-C7-C8
17	a	844	CLA	O1A-CGA-O2A-C1
17	B	820	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	a	843	CLA	CBD-CGD-O2D-CED
17	b	804	CLA	C2A-CAA-CBA-CGA
17	b	818	CLA	C8-C10-C11-C12
17	b	810	CLA	C5-C6-C7-C8
17	A	834	CLA	C5-C6-C7-C8
17	b	839	CLA	C15-C16-C17-C18
17	B	825	CLA	C13-C15-C16-C17
17	A	822	CLA	C5-C6-C7-C8
17	a	819	CLA	C6-C7-C8-C10
17	B	806	CLA	C11-C10-C8-C7
17	A	842	CLA	C6-C7-C8-C10
17	b	806	CLA	C11-C12-C13-C15
17	A	829	CLA	C12-C13-C15-C16
17	B	814	CLA	C11-C10-C8-C7
17	A	822	CLA	C3-C5-C6-C7
17	B	830	CLA	O1A-CGA-O2A-C1
17	1	303	CLA	O1A-CGA-O2A-C1
17	3	314	CLA	C2A-CAA-CBA-CGA
17	A	814	CLA	C2A-CAA-CBA-CGA
17	B	840	CLA	C2A-CAA-CBA-CGA
17	B	828	CLA	C2A-CAA-CBA-CGA
17	A	831	CLA	C8-C10-C11-C12
17	a	839	CLA	C13-C15-C16-C17
17	B	829	CLA	C13-C15-C16-C17
17	L	202	CLA	O1A-CGA-O2A-C1
17	A	805	CLA	O1A-CGA-O2A-C1
17	K	4002	CLA	CBD-CGD-O2D-CED
17	B	834	CLA	C10-C11-C12-C13
17	2	603	CLA	C10-C11-C12-C13
17	A	839	CLA	C13-C15-C16-C17
17	B	810	CLA	C3-C5-C6-C7
17	a	841	CLA	C3-C5-C6-C7
17	a	843	CLA	C3-C5-C6-C7
17	B	818	CLA	C8-C10-C11-C12
17	B	806	CLA	C10-C11-C12-C13
17	B	802	CLA	C5-C6-C7-C8
17	b	832	CLA	C10-C11-C12-C13
17	b	837	CLA	C15-C16-C17-C18
17	a	825	CLA	CBA-CGA-O2A-C1
17	4	611	CLA	CBA-CGA-O2A-C1
17	a	818	CLA	O1D-CGD-O2D-CED
17	A	825	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	A	809	CLA	O1A-CGA-O2A-C1
17	b	827	CLA	O1A-CGA-O2A-C1
17	b	814	CLA	C8-C10-C11-C12
17	B	837	CLA	C15-C16-C17-C18
17	b	812	CLA	O1A-CGA-O2A-C1
17	1	308	CLA	C15-C16-C17-C18
17	2	602	CLA	C13-C15-C16-C17
17	6	304	CLA	C13-C15-C16-C17
17	A	818	CLA	C10-C11-C12-C13
17	B	837	CLA	C13-C15-C16-C17
19	A	846	LHG	C4-O6-P-O3
19	1	301	LHG	C4-O6-P-O3
19	1	319	LHG	C3-O3-P-O6
19	3	319	LHG	C3-O3-P-O6
19	6	301	LHG	C3-O3-P-O6
19	2	618	LHG	C4-O6-P-O3
19	6	320	LHG	C3-O3-P-O6
19	7	618	LHG	C3-O3-P-O6
17	a	844	CLA	C3-C5-C6-C7
17	B	814	CLA	C3-C5-C6-C7
17	B	810	CLA	CBA-CGA-O2A-C1
17	6	304	CLA	CBA-CGA-O2A-C1
17	B	813	CLA	CBA-CGA-O2A-C1
22	F	302	HTG	O5-C5-C6-O6
17	a	856	CLA	C10-C11-C12-C13
17	B	815	CLA	C10-C11-C12-C13
17	1	303	CLA	C13-C15-C16-C17
17	A	818	CLA	O1D-CGD-O2D-CED
17	B	819	CLA	C4-C3-C5-C6
17	9	602	CLA	C4-C3-C5-C6
17	4	611	CLA	C2-C3-C5-C6
17	a	834	CLA	C5-C6-C7-C8
17	A	803	CLA	C2A-CAA-CBA-CGA
17	a	809	CLA	C2A-CAA-CBA-CGA
17	b	840	CLA	C2A-CAA-CBA-CGA
17	b	810	CLA	C2A-CAA-CBA-CGA
17	A	834	CLA	C2A-CAA-CBA-CGA
17	L	204	CLA	C2A-CAA-CBA-CGA
17	6	316	CLA	C2A-CAA-CBA-CGA
17	1	204	CLA	C2A-CAA-CBA-CGA
17	b	828	CLA	C2A-CAA-CBA-CGA
26	6	303	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
17	9	602	CLA	C3-C5-C6-C7
17	4	602	CLA	CBA-CGA-O2A-C1
25	4	620	LMG	C29-C28-O8-C9
26	7	607	CHL	CBA-CGA-O2A-C1
17	B	814	CLA	CBA-CGA-O2A-C1
18	b	842	PQN	C20-C21-C22-C23
25	G	102	LMG	C19-C20-C21-C22
26	2	601	CHL	C5-C6-C7-C8
17	b	823	CLA	O1D-CGD-O2D-CED
25	4	620	LMG	C11-C10-O7-C8
19	A	847	LHG	C8-C7-O7-C5
17	6	315	CLA	C3-C5-C6-C7
17	F	301	CLA	C3-C5-C6-C7
17	A	802	CLA	C3-C5-C6-C7
22	J	3001	HTG	C2'-C3'-C4'-C5'
17	A	842	CLA	O1A-CGA-O2A-C1
17	a	839	CLA	CBA-CGA-O2A-C1
17	7	611	CLA	CBA-CGA-O2A-C1
25	9	619	LMG	C19-C20-C21-C22
17	a	835	CLA	O1D-CGD-O2D-CED
25	4	620	LMG	O9-C10-O7-C8
19	A	847	LHG	O9-C7-O7-C5
17	a	856	CLA	C8-C10-C11-C12
17	b	832	CLA	C15-C16-C17-C18
19	a	847	LHG	C10-C11-C12-C13
25	9	619	LMG	C22-C23-C24-C25
19	7	618	LHG	C9-C10-C11-C12
17	a	831	CLA	O1D-CGD-O2D-CED
17	1	303	CLA	C3-C5-C6-C7
17	A	831	CLA	C10-C11-C12-C13
17	B	813	CLA	O1A-CGA-O2A-C1
26	7	607	CHL	O1A-CGA-O2A-C1
17	B	814	CLA	O1A-CGA-O2A-C1
17	b	810	CLA	C16-C17-C18-C20
26	6	303	CHL	C4-C3-C5-C6
17	4	612	CLA	C4-C3-C5-C6
17	b	823	CLA	C4-C3-C5-C6
17	a	841	CLA	C4-C3-C5-C6
17	8	309	CLA	C2-C3-C5-C6
17	a	831	CLA	C11-C10-C8-C9
18	B	842	PQN	C21-C22-C23-C24
17	a	818	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
17	b	834	CLA	C11-C10-C8-C9
17	a	814	CLA	C6-C7-C8-C9
17	B	826	CLA	C11-C10-C8-C9
17	F	301	CLA	C11-C10-C8-C9
17	8	301	CLA	C6-C7-C8-C9
17	B	823	CLA	O1D-CGD-O2D-CED
17	a	844	CLA	C15-C16-C17-C18
17	A	842	CLA	C5-C6-C7-C8
17	A	809	CLA	C2A-CAA-CBA-CGA
17	9	604	CLA	C2A-CAA-CBA-CGA
17	a	803	CLA	C2A-CAA-CBA-CGA
17	A	830	CLA	C2A-CAA-CBA-CGA
17	a	809	CLA	O1A-CGA-O2A-C1
17	a	825	CLA	O1A-CGA-O2A-C1
20	B	844	BCR	C37-C22-C23-C24
19	A	847	LHG	O1-C1-C2-C3
20	B	847	BCR	C7-C8-C9-C10
20	B	844	BCR	C21-C22-C23-C24
18	A	844	PQN	C13-C15-C16-C17
17	b	833	CLA	C3-C5-C6-C7
17	A	841	CLA	C8-C10-C11-C12
17	A	807	CLA	C5-C6-C7-C8
24	B	850	DGD	C2B-C1B-O2G-C2G
19	a	848	LHG	C8-C7-O7-C5
24	b	849	DGD	C8A-C9A-CAA-CBA
19	a	847	LHG	C23-C24-C25-C26
19	A	846	LHG	C27-C28-C29-C30
24	b	849	DGD	O6E-C5E-C6E-O5E
17	A	828	CLA	C16-C17-C18-C20
17	a	805	CLA	C6-C7-C8-C9
17	a	805	CLA	C6-C7-C8-C10
17	1	304	CLA	C15-C16-C17-C18
17	F	301	CLA	O1D-CGD-O2D-CED
17	b	832	CLA	CBD-CGD-O2D-CED
19	7	618	LHG	C24-C25-C26-C27
18	a	845	PQN	C18-C20-C21-C22
17	b	825	CLA	C10-C11-C12-C13
17	B	810	CLA	O1A-CGA-O2A-C1
17	4	611	CLA	O1A-CGA-O2A-C1
24	B	850	DGD	CAA-CBA-CCA-CDA
17	B	816	CLA	C3-C5-C6-C7
17	7	608	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	4	606	CHL	CBA-CGA-O2A-C1
17	b	814	CLA	CBA-CGA-O2A-C1
17	8	301	CLA	CBA-CGA-O2A-C1
17	6	313	CLA	C3A-C2A-CAA-CBA
17	f	7003	CLA	C3A-C2A-CAA-CBA
17	A	824	CLA	C3A-C2A-CAA-CBA
17	b	813	CLA	C3A-C2A-CAA-CBA
17	a	834	CLA	C3A-C2A-CAA-CBA
17	1	312	CLA	C3A-C2A-CAA-CBA
17	A	834	CLA	C3A-C2A-CAA-CBA
17	B	832	CLA	C3A-C2A-CAA-CBA
17	B	813	CLA	C3A-C2A-CAA-CBA
17	B	815	CLA	C3A-C2A-CAA-CBA
17	A	804	CLA	C3A-C2A-CAA-CBA
17	F	304	CLA	C3A-C2A-CAA-CBA
17	a	838	CLA	C3A-C2A-CAA-CBA
17	B	804	CLA	C3A-C2A-CAA-CBA
17	b	804	CLA	C3A-C2A-CAA-CBA
17	A	807	CLA	C3A-C2A-CAA-CBA
17	a	804	CLA	C3A-C2A-CAA-CBA
17	a	807	CLA	C3A-C2A-CAA-CBA
17	B	839	CLA	C13-C15-C16-C17
17	a	808	CLA	C13-C15-C16-C17
17	6	304	CLA	O1A-CGA-O2A-C1
26	9	605	CHL	C6-C7-C8-C9
19	A	846	LHG	C4-C5-C6-O8
17	B	834	CLA	CBD-CGD-O2D-CED
17	9	604	CLA	CBD-CGD-O2D-CED
17	b	827	CLA	O1D-CGD-O2D-CED
17	b	818	CLA	C3-C5-C6-C7
17	a	814	CLA	C3-C5-C6-C7
17	A	834	CLA	C3-C5-C6-C7
17	6	314	CLA	C3-C5-C6-C7
25	9	619	LMG	C33-C34-C35-C36
17	A	820	CLA	C13-C15-C16-C17
17	f	7003	CLA	C4-C3-C5-C6
18	A	844	PQN	C14-C13-C15-C16
17	a	826	CLA	C4-C3-C5-C6
17	a	822	CLA	C4-C3-C5-C6
17	F	304	CLA	C4-C3-C5-C6
17	b	832	CLA	C4-C3-C5-C6
17	a	828	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
17	f	7003	CLA	C2-C3-C5-C6
17	B	823	CLA	C2-C3-C5-C6
17	a	826	CLA	C2-C3-C5-C6
17	a	822	CLA	C2-C3-C5-C6
17	7	611	CLA	C2-C3-C5-C6
17	4	612	CLA	C2-C3-C5-C6
17	b	823	CLA	C2-C3-C5-C6
17	a	841	CLA	C2-C3-C5-C6
26	9	606	CHL	C2A-CAA-CBA-CGA
25	4	620	LMG	C14-C15-C16-C17
17	4	604	CLA	O1D-CGD-O2D-CED
25	4	620	LMG	O10-C28-O8-C9
17	7	611	CLA	O1A-CGA-O2A-C1
17	B	806	CLA	C8-C10-C11-C12
17	7	612	CLA	C8-C10-C11-C12
17	A	814	CLA	C3-C5-C6-C7
17	4	602	CLA	O1A-CGA-O2A-C1
17	a	839	CLA	O1A-CGA-O2A-C1
19	a	848	LHG	O9-C7-O7-C5
17	B	833	CLA	C2-C1-O2A-CGA
17	B	834	CLA	C2-C1-O2A-CGA
17	A	829	CLA	C2-C1-O2A-CGA
17	2	604	CLA	C5-C6-C7-C8
17	a	806	CLA	C10-C11-C12-C13
26	4	606	CHL	O1A-CGA-O2A-C1
17	2	613	CLA	CBD-CGD-O2D-CED
20	k	1404	BCR	C23-C24-C25-C26
20	L	205	BCR	C23-C24-C25-C26
20	L	205	BCR	C23-C24-C25-C30
20	1	318	BCR	C23-C24-C25-C26
20	a	853	BCR	C23-C24-C25-C26
20	a	853	BCR	C23-C24-C25-C30
20	B	848	BCR	C5-C6-C7-C8
27	1	320	LUT	C1-C6-C7-C8
27	1	320	LUT	C5-C6-C7-C8
27	9	616	LUT	C1-C6-C7-C8
20	j	3004	BCR	C5-C6-C7-C8
20	j	3004	BCR	C23-C24-C25-C26
20	j	3004	BCR	C23-C24-C25-C30
20	6	319	BCR	C23-C24-C25-C30
20	8	316	BCR	C23-C24-C25-C26
20	3	318	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	3	318	BCR	C23-C24-C25-C26
20	a	850	BCR	C5-C6-C7-C8
20	l	201	BCR	C5-C6-C7-C8
20	b	848	BCR	C5-C6-C7-C8
20	a	852	BCR	C1-C6-C7-C8
20	a	852	BCR	C5-C6-C7-C8
20	A	856	BCR	C1-C6-C7-C8
20	A	856	BCR	C5-C6-C7-C8
20	A	856	BCR	C23-C24-C25-C26
20	A	856	BCR	C23-C24-C25-C30
20	A	848	BCR	C23-C24-C25-C26
20	l	205	BCR	C23-C24-C25-C30
20	A	851	BCR	C23-C24-C25-C26
20	A	851	BCR	C23-C24-C25-C30
17	B	822	CLA	O1D-CGD-O2D-CED
26	3	307	CHL	O1D-CGD-O2D-CED
17	A	811	CLA	CBA-CGA-O2A-C1
17	2	611	CLA	CBA-CGA-O2A-C1
17	a	834	CLA	CBA-CGA-O2A-C1
17	b	819	CLA	CBA-CGA-O2A-C1
17	A	833	CLA	C10-C11-C12-C13
17	1	305	CLA	C3-C5-C6-C7
25	9	619	LMG	O6-C5-C6-O5
17	9	602	CLA	C8-C10-C11-C12
17	a	828	CLA	C4-C3-C5-C6
17	B	834	CLA	C4-C3-C5-C6
17	a	831	CLA	C11-C10-C8-C7
18	B	842	PQN	C21-C22-C23-C25
26	6	303	CHL	C2-C3-C5-C6
17	b	834	CLA	C11-C10-C8-C7
17	B	826	CLA	C11-C10-C8-C7
17	b	826	CLA	C11-C10-C8-C7
17	A	809	CLA	C11-C12-C13-C15
17	F	301	CLA	C11-C10-C8-C7
18	a	845	PQN	C21-C22-C23-C25
17	9	602	CLA	C2-C3-C5-C6
17	B	813	CLA	C11-C12-C13-C15
17	B	834	CLA	C11-C10-C8-C7
17	F	304	CLA	C2-C3-C5-C6
17	b	828	CLA	C6-C7-C8-C10
17	b	832	CLA	C2-C3-C5-C6
17	a	841	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
17	a	801	CLA	C12-C13-C15-C16
17	a	801	CLA	C3-C5-C6-C7
17	7	608	CLA	O1A-CGA-O2A-C1
17	b	814	CLA	O1A-CGA-O2A-C1
17	b	819	CLA	O1A-CGA-O2A-C1
17	8	301	CLA	O1A-CGA-O2A-C1
17	a	804	CLA	C10-C11-C12-C13
17	b	805	CLA	C10-C11-C12-C13
17	B	829	CLA	C10-C11-C12-C13
17	B	815	CLA	O1D-CGD-O2D-CED
17	6	307	CLA	O1D-CGD-O2D-CED
25	4	619	LMG	O9-C10-O7-C8
24	B	850	DGD	O1B-C1B-O2G-C2G
26	4	605	CHL	CBA-CGA-O2A-C1
17	7	602	CLA	CBA-CGA-O2A-C1
17	B	807	CLA	CBA-CGA-O2A-C1
17	B	824	CLA	C13-C15-C16-C17
17	A	840	CLA	C10-C11-C12-C13
24	B	850	DGD	C3B-C4B-C5B-C6B
22	f	7001	HTG	C1'-C2'-C3'-C4'
17	2	611	CLA	O1A-CGA-O2A-C1
25	4	620	LMG	C15-C16-C17-C18
25	9	619	LMG	C29-C30-C31-C32
25	G	102	LMG	C17-C18-C19-C20
17	a	834	CLA	O1A-CGA-O2A-C1
17	B	819	CLA	CBA-CGA-O2A-C1
17	8	309	CLA	CBA-CGA-O2A-C1
17	a	807	CLA	CBA-CGA-O2A-C1
17	a	809	CLA	C8-C10-C11-C12
17	1	308	CLA	C13-C15-C16-C17
17	A	841	CLA	C15-C16-C17-C18
24	B	850	DGD	C4B-C5B-C6B-C7B
25	4	619	LMG	C11-C10-O7-C8
25	9	619	LMG	C11-C10-O7-C8
17	b	824	CLA	C10-C11-C12-C13
17	b	840	CLA	CBD-CGD-O2D-CED
17	A	824	CLA	CBD-CGD-O2D-CED
17	b	836	CLA	C3-C5-C6-C7
17	a	805	CLA	C3-C5-C6-C7
17	A	806	CLA	C8-C10-C11-C12
19	A	846	LHG	O7-C5-C6-O8
19	a	847	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
17	6	315	CLA	CBA-CGA-O2A-C1
17	2	602	CLA	CBA-CGA-O2A-C1
25	9	619	LMG	C35-C36-C37-C38
17	b	810	CLA	C16-C17-C18-C19
24	b	849	DGD	CAA-CBA-CCA-CDA
17	B	823	CLA	C4-C3-C5-C6
17	B	819	CLA	C2-C3-C5-C6
18	A	844	PQN	C12-C13-C15-C16
17	B	834	CLA	C2-C3-C5-C6
17	a	819	CLA	C6-C7-C8-C9
17	a	839	CLA	C14-C13-C15-C16
17	B	826	CLA	C11-C12-C13-C14
17	A	819	CLA	C11-C10-C8-C9
17	b	826	CLA	C11-C10-C8-C9
17	6	304	CLA	C6-C7-C8-C9
17	A	841	CLA	C11-C10-C8-C9
17	B	834	CLA	C11-C10-C8-C9
17	b	828	CLA	C6-C7-C8-C9
17	b	832	CLA	C6-C7-C8-C9
17	b	806	CLA	C11-C12-C13-C14
17	a	843	CLA	C11-C12-C13-C14
17	A	829	CLA	C14-C13-C15-C16
17	B	814	CLA	C11-C10-C8-C9
17	9	609	CLA	C3-C5-C6-C7
17	B	815	CLA	C3-C5-C6-C7
17	A	819	CLA	C2A-CAA-CBA-CGA
17	8	310	CLA	C2A-CAA-CBA-CGA
17	7	612	CLA	C2A-CAA-CBA-CGA
17	b	811	CLA	O1D-CGD-O2D-CED
17	A	843	CLA	C13-C15-C16-C17
17	a	812	CLA	C1A-C2A-CAA-CBA
17	6	313	CLA	C1A-C2A-CAA-CBA
17	B	805	CLA	C1A-C2A-CAA-CBA
17	a	809	CLA	C1A-C2A-CAA-CBA
17	f	7003	CLA	C1A-C2A-CAA-CBA
17	a	819	CLA	C1A-C2A-CAA-CBA
26	2	606	CHL	C1A-C2A-CAA-CBA
17	4	604	CLA	C1A-C2A-CAA-CBA
17	a	834	CLA	C1A-C2A-CAA-CBA
17	1	312	CLA	C1A-C2A-CAA-CBA
17	A	834	CLA	C1A-C2A-CAA-CBA
17	a	811	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	4	609	CLA	C1A-C2A-CAA-CBA
17	3	309	CLA	C1A-C2A-CAA-CBA
17	A	819	CLA	C1A-C2A-CAA-CBA
26	4	606	CHL	C1A-C2A-CAA-CBA
17	A	809	CLA	C1A-C2A-CAA-CBA
17	8	308	CLA	C1A-C2A-CAA-CBA
17	A	812	CLA	C1A-C2A-CAA-CBA
17	b	827	CLA	C1A-C2A-CAA-CBA
17	B	822	CLA	C1A-C2A-CAA-CBA
26	9	607	CHL	C1A-C2A-CAA-CBA
17	A	804	CLA	C1A-C2A-CAA-CBA
17	9	604	CLA	C1A-C2A-CAA-CBA
17	F	304	CLA	C1A-C2A-CAA-CBA
26	1	307	CHL	C1A-C2A-CAA-CBA
17	6	311	CLA	C1A-C2A-CAA-CBA
17	7	604	CLA	C1A-C2A-CAA-CBA
17	A	807	CLA	C1A-C2A-CAA-CBA
17	a	804	CLA	C1A-C2A-CAA-CBA
17	b	805	CLA	C1A-C2A-CAA-CBA
17	a	816	CLA	C1A-C2A-CAA-CBA
25	9	619	LMG	O9-C10-O7-C8
19	A	846	LHG	C24-C25-C26-C27
17	a	812	CLA	C10-C11-C12-C13
17	A	833	CLA	C8-C10-C11-C12
18	B	842	PQN	C20-C21-C22-C23
17	b	809	CLA	C10-C11-C12-C13
17	b	802	CLA	C13-C15-C16-C17
17	a	841	CLA	C10-C11-C12-C13
17	7	604	CLA	C10-C11-C12-C13
17	A	830	CLA	C5-C6-C7-C8
19	1	319	LHG	C33-C34-C35-C36
24	b	849	DGD	C1B-C2B-C3B-C4B
17	A	811	CLA	O1A-CGA-O2A-C1
17	b	807	CLA	C5-C6-C7-C8
17	a	802	CLA	C15-C16-C17-C18
17	6	314	CLA	C5-C6-C7-C8
17	b	813	CLA	CBA-CGA-O2A-C1
17	A	813	CLA	CBA-CGA-O2A-C1
22	j	3001	HTG	O5-C5-C6-O6
25	4	619	LMG	O6-C5-C6-O5
17	a	830	CLA	C13-C15-C16-C17
17	A	828	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
17	a	809	CLA	C5-C6-C7-C8
17	B	814	CLA	C13-C15-C16-C17
17	A	831	CLA	CBA-CGA-O2A-C1
17	1	305	CLA	CBA-CGA-O2A-C1
17	B	806	CLA	C4-C3-C5-C6
17	B	808	CLA	C2-C3-C5-C6
17	A	801	CLA	C15-C16-C17-C18
17	b	828	CLA	C10-C11-C12-C13
26	4	605	CHL	O1A-CGA-O2A-C1
17	B	819	CLA	O1A-CGA-O2A-C1
17	B	807	CLA	O1A-CGA-O2A-C1
26	2	606	CHL	C2A-CAA-CBA-CGA
17	B	830	CLA	C2A-CAA-CBA-CGA
25	4	620	LMG	C7-C8-C9-O8
17	b	818	CLA	C10-C11-C12-C13
17	A	809	CLA	C13-C15-C16-C17
17	B	803	CLA	O1D-CGD-O2D-CED
26	7	607	CHL	O1D-CGD-O2D-CED
17	a	802	CLA	C10-C11-C12-C13
17	A	819	CLA	CAA-CBA-CGA-O2A
17	b	805	CLA	CAA-CBA-CGA-O2A
17	A	813	CLA	O1A-CGA-O2A-C1
17	8	309	CLA	O1A-CGA-O2A-C1
17	6	309	CLA	CBA-CGA-O2A-C1
17	B	810	CLA	C13-C15-C16-C17
25	4	619	LMG	C22-C23-C24-C25
18	A	844	PQN	C18-C20-C21-C22
17	7	604	CLA	C5-C6-C7-C8
17	b	817	CLA	C11-C12-C13-C14
17	B	817	CLA	C11-C12-C13-C14
17	A	845	CLA	C4-C3-C5-C6
17	B	839	CLA	C4-C3-C5-C6
17	A	810	CLA	C4-C3-C5-C6
17	B	808	CLA	C4-C3-C5-C6
17	L	202	CLA	C4-C3-C5-C6
17	B	828	CLA	C4-C3-C5-C6
17	6	310	CLA	C4-C3-C5-C6
17	b	806	CLA	C4-C3-C5-C6
17	6	315	CLA	O1A-CGA-O2A-C1
17	7	602	CLA	O1A-CGA-O2A-C1
17	B	839	CLA	C2-C3-C5-C6
17	8	301	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	6	313	CLA	CBA-CGA-O2A-C1
17	A	826	CLA	CBA-CGA-O2A-C1
17	9	611	CLA	CBA-CGA-O2A-C1
17	9	602	CLA	CBA-CGA-O2A-C1
26	9	605	CHL	CBA-CGA-O2A-C1
17	b	813	CLA	C15-C16-C17-C18
17	4	609	CLA	C10-C11-C12-C13
17	A	835	CLA	C5-C6-C7-C8
17	1	304	CLA	C5-C6-C7-C8
24	B	850	DGD	O6E-C5E-C6E-O5E
17	A	854	CLA	C2A-CAA-CBA-CGA
17	a	844	CLA	C2A-CAA-CBA-CGA
17	A	810	CLA	C2A-CAA-CBA-CGA
17	A	823	CLA	C2A-CAA-CBA-CGA
17	b	817	CLA	C2A-CAA-CBA-CGA
26	1	307	CHL	C2A-CAA-CBA-CGA
17	7	604	CLA	C2A-CAA-CBA-CGA
17	3	312	CLA	C2A-CAA-CBA-CGA
17	b	834	CLA	C10-C11-C12-C13
17	l	203	CLA	C5-C6-C7-C8
17	B	834	CLA	C5-C6-C7-C8
17	A	807	CLA	C8-C10-C11-C12
17	A	843	CLA	C15-C16-C17-C18
17	a	831	CLA	C2-C1-O2A-CGA
17	A	854	CLA	C2-C1-O2A-CGA
17	b	802	CLA	C2-C1-O2A-CGA
17	b	833	CLA	C2-C1-O2A-CGA
17	B	832	CLA	C2-C1-O2A-CGA
17	B	831	CLA	C2-C1-O2A-CGA
17	B	812	CLA	C2-C1-O2A-CGA
17	A	840	CLA	C2-C1-O2A-CGA
17	b	817	CLA	C3-C5-C6-C7
25	4	619	LMG	C12-C13-C14-C15
17	b	835	CLA	O1D-CGD-O2D-CED
26	6	303	CHL	CBA-CGA-O2A-C1
17	1	312	CLA	CBA-CGA-O2A-C1
17	A	835	CLA	CBA-CGA-O2A-C1
17	A	831	CLA	O1A-CGA-O2A-C1
17	b	813	CLA	O1A-CGA-O2A-C1
17	4	602	CLA	C10-C11-C12-C13
17	9	611	CLA	O1A-CGA-O2A-C1
17	1	305	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	a	807	CLA	O1A-CGA-O2A-C1
17	B	841	CLA	C13-C15-C16-C17
17	a	826	CLA	C10-C11-C12-C13
17	A	822	CLA	C10-C11-C12-C13
17	b	806	CLA	C10-C11-C12-C13
17	2	602	CLA	O1A-CGA-O2A-C1
17	A	835	CLA	O1A-CGA-O2A-C1
17	k	1401	CLA	O1D-CGD-O2D-CED
17	A	826	CLA	C4-C3-C5-C6
17	b	839	CLA	C4-C3-C5-C6
17	l	202	CLA	C4-C3-C5-C6
17	2	612	CLA	C4-C3-C5-C6
17	9	612	CLA	C5-C6-C7-C8
17	a	844	CLA	C5-C6-C7-C8
17	b	814	CLA	C15-C16-C17-C18
17	a	809	CLA	C11-C10-C8-C7
17	A	808	CLA	C12-C13-C15-C16
17	A	845	CLA	C2-C3-C5-C6
17	a	819	CLA	C11-C10-C8-C7
17	A	854	CLA	C6-C7-C8-C10
17	A	827	CLA	C6-C7-C8-C10
26	6	303	CHL	C6-C7-C8-C10
17	b	809	CLA	C11-C12-C13-C15
17	a	835	CLA	C6-C7-C8-C10
17	a	814	CLA	C6-C7-C8-C10
17	A	814	CLA	C12-C13-C15-C16
17	B	806	CLA	C2-C3-C5-C6
17	B	826	CLA	C11-C12-C13-C15
17	B	839	CLA	C12-C13-C15-C16
17	2	602	CLA	C12-C13-C15-C16
17	l	203	CLA	C6-C7-C8-C10
17	L	202	CLA	C2-C3-C5-C6
17	B	828	CLA	C2-C3-C5-C6
17	l	202	CLA	C2-C3-C5-C6
17	A	812	CLA	C12-C13-C15-C16
17	A	841	CLA	C11-C10-C8-C7
17	7	609	CLA	C6-C7-C8-C10
17	B	813	CLA	C11-C10-C8-C7
17	6	310	CLA	C2-C3-C5-C6
17	b	832	CLA	C6-C7-C8-C10
17	b	806	CLA	C2-C3-C5-C6
17	A	807	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
17	a	806	CLA	C12-C13-C15-C16
17	b	805	CLA	C6-C7-C8-C10
17	B	807	CLA	C6-C7-C8-C10
17	B	805	CLA	CAA-CBA-CGA-O2A
17	A	801	CLA	C3-C5-C6-C7
17	A	812	CLA	C3-C5-C6-C7
17	A	826	CLA	C6-C7-C8-C9
26	6	303	CHL	C6-C7-C8-C9
17	A	828	CLA	C11-C12-C13-C14
17	A	814	CLA	C6-C7-C8-C9
17	b	839	CLA	C14-C13-C15-C16
17	9	612	CLA	C6-C7-C8-C9
17	A	819	CLA	C6-C7-C8-C9
17	A	835	CLA	C6-C7-C8-C9
17	b	826	CLA	C11-C12-C13-C14
17	B	809	CLA	C6-C7-C8-C9
17	B	802	CLA	C6-C7-C8-C9
17	B	813	CLA	C11-C10-C8-C9
17	A	820	CLA	C11-C12-C13-C14
17	A	807	CLA	C11-C12-C13-C14
17	B	807	CLA	C6-C7-C8-C9
17	a	818	CLA	CBA-CGA-O2A-C1
17	4	612	CLA	CBA-CGA-O2A-C1
17	7	604	CLA	CBA-CGA-O2A-C1
17	8	310	CLA	CBA-CGA-O2A-C1
17	3	302	CLA	CBA-CGA-O2A-C1
18	b	842	PQN	C18-C20-C21-C22
17	a	856	CLA	C2A-CAA-CBA-CGA
17	B	827	CLA	C2A-CAA-CBA-CGA
20	j	3004	BCR	C36-C18-C19-C20
20	G	105	BCR	C37-C22-C23-C24
20	3	318	BCR	C7-C8-C9-C10
20	b	847	BCR	C21-C22-C23-C24
17	a	809	CLA	C3-C5-C6-C7
17	1	313	CLA	C3-C5-C6-C7
17	b	825	CLA	C3-C5-C6-C7
17	1	314	CLA	C3-C5-C6-C7
17	b	821	CLA	O1D-CGD-O2D-CED
17	B	820	CLA	O1D-CGD-O2D-CED
17	a	838	CLA	O1D-CGD-O2D-CED
17	2	604	CLA	C10-C11-C12-C13
17	A	814	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
17	b	827	CLA	C15-C16-C17-C18
17	B	812	CLA	C5-C6-C7-C8
17	a	806	CLA	C8-C10-C11-C12
25	6	302	LMG	C11-C10-O7-C8
17	b	817	CLA	C10-C11-C12-C13
17	9	608	CLA	CBA-CGA-O2A-C1
17	B	816	CLA	CBA-CGA-O2A-C1
26	2	601	CHL	CBA-CGA-O2A-C1
17	1	314	CLA	CBA-CGA-O2A-C1
26	2	607	CHL	CBA-CGA-O2A-C1
17	b	826	CLA	C10-C11-C12-C13
17	A	809	CLA	C5-C6-C7-C8
17	A	806	CLA	C10-C11-C12-C13
17	b	818	CLA	C5-C6-C7-C8
17	B	806	CLA	C5-C6-C7-C8
17	b	814	CLA	C3-C5-C6-C7
17	4	601	CLA	CAA-CBA-CGA-O2A
17	3	308	CLA	CAA-CBA-CGA-O2A
17	a	830	CLA	C4-C3-C5-C6
17	b	808	CLA	C4-C3-C5-C6
17	a	802	CLA	C4-C3-C5-C6
17	a	805	CLA	C4-C3-C5-C6
17	A	826	CLA	C2-C3-C5-C6
17	b	839	CLA	C2-C3-C5-C6
17	2	612	CLA	C2-C3-C5-C6
17	b	808	CLA	C2-C3-C5-C6
17	a	824	CLA	O1D-CGD-O2D-CED
17	B	819	CLA	C8-C10-C11-C12
17	B	802	CLA	C8-C10-C11-C12
17	a	843	CLA	O1D-CGD-O2D-CED
17	A	838	CLA	CBA-CGA-O2A-C1
17	A	819	CLA	CBA-CGA-O2A-C1
17	2	608	CLA	CBA-CGA-O2A-C1
17	L	204	CLA	CAA-CBA-CGA-O2A
17	7	608	CLA	C3A-C2A-CAA-CBA
17	b	815	CLA	C3A-C2A-CAA-CBA
17	B	819	CLA	C3A-C2A-CAA-CBA
17	B	841	CLA	C3A-C2A-CAA-CBA
17	3	308	CLA	C3A-C2A-CAA-CBA
17	a	815	CLA	C3A-C2A-CAA-CBA
17	B	834	CLA	C3A-C2A-CAA-CBA
17	b	811	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	a	830	CLA	C3A-C2A-CAA-CBA
17	b	831	CLA	C3A-C2A-CAA-CBA
17	B	812	CLA	C3A-C2A-CAA-CBA
17	A	829	CLA	C3A-C2A-CAA-CBA
17	8	307	CLA	C3A-C2A-CAA-CBA
17	B	836	CLA	C3-C5-C6-C7
17	A	818	CLA	CBA-CGA-O2A-C1
17	B	807	CLA	C5-C6-C7-C8
19	1	301	LHG	C4-C5-C6-O8
19	a	847	LHG	C4-C5-C6-O8
19	6	301	LHG	C4-C5-C6-O8
26	6	303	CHL	O1A-CGA-O2A-C1
17	2	602	CLA	O1D-CGD-O2D-CED
17	B	826	CLA	C10-C11-C12-C13
17	a	830	CLA	C2-C3-C5-C6
17	a	805	CLA	C2-C3-C5-C6
17	B	834	CLA	O1D-CGD-O2D-CED
19	1	301	LHG	C3-O3-P-O6
26	4	605	CHL	C3C-C2C-CMC-OMC
26	7	614	CHL	C3C-C2C-CMC-OMC
26	2	601	CHL	C3C-C2C-CMC-OMC
17	A	826	CLA	O1A-CGA-O2A-C1
26	9	605	CHL	O1A-CGA-O2A-C1
17	B	833	CLA	O1D-CGD-O2D-CED
17	4	604	CLA	C2A-CAA-CBA-CGA
17	b	839	CLA	C10-C11-C12-C13
17	6	313	CLA	O1A-CGA-O2A-C1
17	1	312	CLA	O1A-CGA-O2A-C1
17	4	612	CLA	O1A-CGA-O2A-C1
17	8	310	CLA	O1A-CGA-O2A-C1
17	B	817	CLA	CAA-CBA-CGA-O2A
17	9	602	CLA	O1A-CGA-O2A-C1
19	1	319	LHG	C11-C10-C9-C8
19	6	301	LHG	O7-C5-C6-O8
17	b	816	CLA	CBA-CGA-O2A-C1
17	1	204	CLA	CAA-CBA-CGA-O2A
17	b	812	CLA	C5-C6-C7-C8
25	6	302	LMG	O9-C10-O7-C8
17	a	833	CLA	C3-C5-C6-C7
17	A	833	CLA	C2-C1-O2A-CGA
26	4	605	CHL	C2-C1-O2A-CGA
17	1	305	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
17	A	810	CLA	C2-C1-O2A-CGA
17	B	802	CLA	C2-C1-O2A-CGA
17	a	833	CLA	C2-C1-O2A-CGA
17	a	843	CLA	C2-C1-O2A-CGA
17	b	812	CLA	C2-C1-O2A-CGA
17	a	805	CLA	C2-C1-O2A-CGA
17	7	603	CLA	C2-C1-O2A-CGA
17	a	856	CLA	C15-C16-C17-C18
17	a	812	CLA	C14-C13-C15-C16
17	B	805	CLA	C6-C7-C8-C9
17	a	831	CLA	C6-C7-C8-C9
17	A	828	CLA	C11-C10-C8-C9
17	a	820	CLA	C11-C12-C13-C14
17	a	835	CLA	C6-C7-C8-C9
17	1	310	CLA	C11-C10-C8-C9
17	9	602	CLA	C6-C7-C8-C9
17	B	834	CLA	C11-C12-C13-C14
17	A	802	CLA	C11-C10-C8-C9
17	B	825	CLA	C10-C11-C12-C13
17	b	806	CLA	C5-C6-C7-C8
17	7	604	CLA	O1A-CGA-O2A-C1
17	a	819	CLA	C2A-CAA-CBA-CGA
17	a	810	CLA	C2A-CAA-CBA-CGA
17	A	842	CLA	C16-C17-C18-C20
20	9	618	BCR	C23-C24-C25-C26
20	9	618	BCR	C23-C24-C25-C30
27	4	616	LUT	C1-C6-C7-C8
27	4	616	LUT	C5-C6-C7-C8
20	k	1404	BCR	C1-C6-C7-C8
20	k	1404	BCR	C5-C6-C7-C8
20	1	318	BCR	C1-C6-C7-C8
20	1	318	BCR	C5-C6-C7-C8
20	K	4004	BCR	C5-C6-C7-C8
20	K	4004	BCR	C23-C24-C25-C26
20	K	4004	BCR	C23-C24-C25-C30
27	9	616	LUT	C5-C6-C7-C8
20	L	201	BCR	C1-C6-C7-C8
20	L	201	BCR	C5-C6-C7-C8
27	6	321	LUT	C1-C6-C7-C8
27	6	321	LUT	C5-C6-C7-C8
20	6	319	BCR	C1-C6-C7-C8
20	6	319	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	b	844	BCR	C1-C6-C7-C8
20	A	850	BCR	C5-C6-C7-C8
20	2	617	BCR	C1-C6-C7-C8
20	2	617	BCR	C5-C6-C7-C8
20	j	3003	BCR	C23-C24-C25-C26
20	j	3003	BCR	C23-C24-C25-C30
20	8	316	BCR	C5-C6-C7-C8
20	3	318	BCR	C5-C6-C7-C8
20	b	846	BCR	C23-C24-C25-C30
20	a	850	BCR	C23-C24-C25-C26
20	a	850	BCR	C23-C24-C25-C30
20	B	844	BCR	C5-C6-C7-C8
20	l	201	BCR	C23-C24-C25-C26
20	l	201	BCR	C23-C24-C25-C30
20	B	846	BCR	C23-C24-C25-C26
20	B	846	BCR	C23-C24-C25-C30
27	6	317	LUT	C1-C6-C7-C8
20	J	3003	BCR	C23-C24-C25-C26
20	J	3003	BCR	C23-C24-C25-C30
20	A	848	BCR	C5-C6-C7-C8
20	4	618	BCR	C23-C24-C25-C26
20	4	618	BCR	C23-C24-C25-C30
27	1	316	LUT	C1-C6-C7-C8
27	1	316	LUT	C5-C6-C7-C8
20	a	853	BCR	C17-C18-C19-C20
20	j	3003	BCR	C17-C18-C19-C20
20	B	847	BCR	C21-C22-C23-C24
17	a	804	CLA	C15-C16-C17-C18
17	A	843	CLA	C16-C17-C18-C20
26	9	605	CHL	C6-C7-C8-C10
17	a	820	CLA	C3-C5-C6-C7
17	9	608	CLA	O1A-CGA-O2A-C1
26	2	601	CHL	O1A-CGA-O2A-C1
26	2	607	CHL	O1A-CGA-O2A-C1
19	2	618	LHG	O6-C4-C5-C6
17	7	612	CLA	C4-C3-C5-C6
17	a	828	CLA	C11-C12-C13-C15
17	b	818	CLA	C6-C7-C8-C10
17	A	828	CLA	C11-C12-C13-C15
17	a	820	CLA	C11-C12-C13-C15
17	a	827	CLA	C6-C7-C8-C10
17	A	814	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
17	b	839	CLA	C12-C13-C15-C16
17	A	835	CLA	C6-C7-C8-C10
17	b	814	CLA	C11-C10-C8-C7
17	b	826	CLA	C11-C12-C13-C15
17	1	310	CLA	C11-C10-C8-C7
17	A	809	CLA	C11-C10-C8-C7
17	A	809	CLA	C12-C13-C15-C16
17	B	802	CLA	C6-C7-C8-C10
17	F	301	CLA	C12-C13-C15-C16
17	2	603	CLA	C11-C12-C13-C15
17	a	830	CLA	C12-C13-C15-C16
17	A	802	CLA	C11-C10-C8-C7
17	A	820	CLA	C11-C12-C13-C15
17	b	808	CLA	C12-C13-C15-C16
17	b	825	CLA	C12-C13-C15-C16
17	a	829	CLA	C11-C12-C13-C15
17	A	843	CLA	C6-C7-C8-C10
17	A	830	CLA	C12-C13-C15-C16
17	1	304	CLA	C6-C7-C8-C10
17	a	807	CLA	C11-C10-C8-C7
17	a	818	CLA	O1A-CGA-O2A-C1
24	b	849	DGD	C2A-C1A-O1G-C1G
17	b	824	CLA	CBA-CGA-O2A-C1
17	2	612	CLA	C2A-CAA-CBA-CGA
26	9	605	CHL	C2A-CAA-CBA-CGA
17	A	842	CLA	C3-C5-C6-C7
17	B	817	CLA	C3-C5-C6-C7
17	A	806	CLA	C15-C16-C17-C18
17	B	841	CLA	C15-C16-C17-C18
17	9	612	CLA	CBA-CGA-O2A-C1
17	a	819	CLA	CAA-CBA-CGA-O2A
17	9	601	CLA	CAA-CBA-CGA-O2A
17	a	812	CLA	CAD-CBD-CGD-O2D
17	b	816	CLA	CAD-CBD-CGD-O2D
26	6	303	CHL	CAD-CBD-CGD-O2D
17	3	303	CLA	CAD-CBD-CGD-O2D
17	9	611	CLA	CAD-CBD-CGD-O2D
17	2	613	CLA	CAD-CBD-CGD-O2D
17	f	7002	CLA	CAD-CBD-CGD-O2D
17	3	311	CLA	CAD-CBD-CGD-O2D
17	a	834	CLA	CAD-CBD-CGD-O2D
17	B	825	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	2	602	CLA	CAD-CBD-CGD-O2D
17	a	821	CLA	CAD-CBD-CGD-O2D
17	a	826	CLA	CAD-CBD-CGD-O2D
17	a	815	CLA	CAD-CBD-CGD-O2D
17	A	812	CLA	CAD-CBD-CGD-O2D
17	A	832	CLA	CAD-CBD-CGD-O2D
17	6	309	CLA	CAD-CBD-CGD-O2D
17	9	604	CLA	CAD-CBD-CGD-O2D
17	l	204	CLA	CAD-CBD-CGD-O2D
17	a	810	CLA	CAD-CBD-CGD-O2D
17	2	609	CLA	CAD-CBD-CGD-O2D
17	B	835	CLA	CAD-CBD-CGD-O2D
17	a	823	CLA	CAD-CBD-CGD-O2D
17	g	103	CLA	CAD-CBD-CGD-O2D
17	1	303	CLA	CAD-CBD-CGD-O2D
17	a	832	CLA	CAD-CBD-CGD-O2D
17	8	311	CLA	CAD-CBD-CGD-O2D
17	3	313	CLA	CAD-CBD-CGD-O2D
26	8	306	CHL	CAD-CBD-CGD-O2D
26	1	302	CHL	CAD-CBD-CGD-O2D
17	K	4002	CLA	O1D-CGD-O2D-CED
17	a	814	CLA	C10-C11-C12-C13
17	B	832	CLA	C10-C11-C12-C13
17	1	314	CLA	O1A-CGA-O2A-C1
17	2	612	CLA	CBA-CGA-O2A-C1
17	B	822	CLA	CBA-CGA-O2A-C1
17	A	842	CLA	C16-C17-C18-C19
24	b	849	DGD	C2A-C3A-C4A-C5A
17	7	612	CLA	C2-C3-C5-C6
19	a	848	LHG	C4-C5-C6-O8
19	6	320	LHG	C4-C5-C6-O8
17	a	804	CLA	CBD-CGD-O2D-CED
17	b	820	CLA	CBD-CGD-O2D-CED
17	2	612	CLA	O1A-CGA-O2A-C1
17	B	816	CLA	O1A-CGA-O2A-C1
17	a	827	CLA	C15-C16-C17-C18
17	b	834	CLA	C3-C5-C6-C7
17	b	832	CLA	CAA-CBA-CGA-O2A
17	a	823	CLA	C2A-CAA-CBA-CGA
17	B	817	CLA	C2A-CAA-CBA-CGA
17	a	804	CLA	C5-C6-C7-C8
17	A	801	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
17	B	805	CLA	CHA-CBD-CGD-O1D
17	a	856	CLA	CHA-CBD-CGD-O1D
17	a	856	CLA	CHA-CBD-CGD-O2D
17	a	809	CLA	CHA-CBD-CGD-O1D
17	A	806	CLA	CHA-CBD-CGD-O1D
17	A	806	CLA	CHA-CBD-CGD-O2D
17	6	305	CLA	CHA-CBD-CGD-O1D
17	6	305	CLA	CHA-CBD-CGD-O2D
17	A	845	CLA	CHA-CBD-CGD-O1D
17	A	845	CLA	CHA-CBD-CGD-O2D
17	a	818	CLA	CHA-CBD-CGD-O1D
17	b	813	CLA	CHA-CBD-CGD-O1D
17	A	814	CLA	CHA-CBD-CGD-O1D
17	A	814	CLA	CHA-CBD-CGD-O2D
17	9	603	CLA	CHA-CBD-CGD-O1D
17	9	603	CLA	CHA-CBD-CGD-O2D
17	b	829	CLA	CHA-CBD-CGD-O1D
17	b	829	CLA	CHA-CBD-CGD-O2D
17	B	808	CLA	CHA-CBD-CGD-O1D
17	A	805	CLA	CHA-CBD-CGD-O2D
17	3	301	CLA	CHA-CBD-CGD-O1D
17	3	301	CLA	CHA-CBD-CGD-O2D
17	4	610	CLA	CHA-CBD-CGD-O1D
17	B	815	CLA	CHA-CBD-CGD-O1D
17	B	815	CLA	CHA-CBD-CGD-O2D
17	b	824	CLA	CHA-CBD-CGD-O1D
17	b	824	CLA	CHA-CBD-CGD-O2D
17	B	804	CLA	CHA-CBD-CGD-O1D
17	k	1403	CLA	CHA-CBD-CGD-O1D
17	k	1403	CLA	CHA-CBD-CGD-O2D
17	a	804	CLA	CHA-CBD-CGD-O1D
17	a	804	CLA	CHA-CBD-CGD-O2D
17	9	601	CLA	CHA-CBD-CGD-O1D
17	b	805	CLA	CHA-CBD-CGD-O1D
17	b	805	CLA	CHA-CBD-CGD-O2D
17	B	829	CLA	CHA-CBD-CGD-O1D
17	B	829	CLA	CHA-CBD-CGD-O2D
17	a	842	CLA	C8-C10-C11-C12
17	b	816	CLA	O1A-CGA-O2A-C1
17	A	838	CLA	O1A-CGA-O2A-C1
17	A	819	CLA	O1A-CGA-O2A-C1
17	A	818	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	3	302	CLA	O1A-CGA-O2A-C1
19	1	301	LHG	O7-C5-C6-O8
19	3	319	LHG	O7-C5-C6-O8
24	B	850	DGD	O2G-C2G-C3G-O3G
24	b	849	DGD	O2G-C2G-C3G-O3G
19	6	320	LHG	O7-C5-C6-O8
17	a	816	CLA	CBD-CGD-O2D-CED
17	2	608	CLA	O1A-CGA-O2A-C1
25	6	302	LMG	C19-C20-C21-C22
17	4	609	CLA	C3-C5-C6-C7
17	b	826	CLA	C3-C5-C6-C7
17	b	827	CLA	C4-C3-C5-C6
17	b	824	CLA	O1A-CGA-O2A-C1
18	A	844	PQN	C15-C16-C17-C18
17	b	834	CLA	C6-C7-C8-C9
17	A	842	CLA	C6-C7-C8-C9
17	b	814	CLA	C11-C10-C8-C9
17	B	802	CLA	C11-C10-C8-C9
25	4	620	LMG	C4-C5-C6-O5
17	9	612	CLA	O1A-CGA-O2A-C1
24	b	849	DGD	O1A-C1A-O1G-C1G
19	6	320	LHG	C11-C10-C9-C8
17	B	824	CLA	C2A-CAA-CBA-CGA
17	B	807	CLA	C2A-CAA-CBA-CGA
17	a	836	CLA	CBD-CGD-O2D-CED
25	9	619	LMG	C36-C37-C38-C39
17	A	830	CLA	O1A-CGA-O2A-C1
17	a	811	CLA	CBA-CGA-O2A-C1
17	b	827	CLA	C13-C15-C16-C17
20	L	201	BCR	C11-C12-C13-C14
20	j	3003	BCR	C7-C8-C9-C10
20	b	845	BCR	C21-C22-C23-C24
17	9	609	CLA	C1A-C2A-CAA-CBA
17	2	604	CLA	C1A-C2A-CAA-CBA
17	a	815	CLA	C1A-C2A-CAA-CBA
26	4	607	CHL	C1A-C2A-CAA-CBA
17	B	813	CLA	C1A-C2A-CAA-CBA
17	b	811	CLA	C1A-C2A-CAA-CBA
17	2	609	CLA	C1A-C2A-CAA-CBA
17	A	826	CLA	C16-C17-C18-C19
18	A	844	PQN	C26-C27-C28-C30
17	A	808	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
17	a	820	CLA	C8-C10-C11-C12
17	3	311	CLA	CBA-CGA-O2A-C1
19	A	846	LHG	C3-O3-P-O6
19	a	848	LHG	C3-O3-P-O6
19	2	618	LHG	C3-O3-P-O6
17	b	840	CLA	O1D-CGD-O2D-CED
17	b	832	CLA	O1D-CGD-O2D-CED
17	9	612	CLA	C4-C3-C5-C6
17	B	810	CLA	C4-C3-C5-C6
17	1	303	CLA	C4-C3-C5-C6
17	9	604	CLA	O1D-CGD-O2D-CED
17	A	810	CLA	C2-C3-C5-C6
19	1	301	LHG	C3-O3-P-O4
19	a	847	LHG	C3-O3-P-O4
19	a	847	LHG	C4-O6-P-O4
19	3	319	LHG	C4-O6-P-O4
19	6	301	LHG	C4-O6-P-O4
19	6	320	LHG	C4-O6-P-O4
19	7	618	LHG	C4-O6-P-O4
17	a	840	CLA	C16-C17-C18-C20
17	b	812	CLA	C6-C7-C8-C10
17	1	304	CLA	C16-C17-C18-C20
25	G	102	LMG	C21-C22-C23-C24
17	a	819	CLA	CBA-CGA-O2A-C1
17	A	830	CLA	CBA-CGA-O2A-C1
17	B	805	CLA	C15-C16-C17-C18
17	1	315	CLA	C2A-CAA-CBA-CGA
17	6	310	CLA	C3-C5-C6-C7
17	B	805	CLA	CAD-CBD-CGD-O1D
17	a	828	CLA	CAD-CBD-CGD-O1D
17	a	856	CLA	CAD-CBD-CGD-O1D
17	A	806	CLA	CAD-CBD-CGD-O1D
17	6	305	CLA	CAD-CBD-CGD-O1D
17	A	845	CLA	CAD-CBD-CGD-O1D
17	A	854	CLA	CAD-CBD-CGD-O1D
17	b	813	CLA	CAD-CBD-CGD-O1D
17	A	814	CLA	CAD-CBD-CGD-O1D
17	b	829	CLA	CAD-CBD-CGD-O1D
17	9	601	CLA	CAD-CBD-CGD-O1D
17	b	805	CLA	CAD-CBD-CGD-O1D
17	B	829	CLA	CAD-CBD-CGD-O1D
17	A	801	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
17	A	804	CLA	C13-C15-C16-C17
17	7	612	CLA	C10-C11-C12-C13
17	B	814	CLA	C8-C10-C11-C12
19	6	320	LHG	C11-C12-C13-C14
17	1	309	CLA	C8-C10-C11-C12
17	A	804	CLA	C8-C10-C11-C12
17	7	609	CLA	CBA-CGA-O2A-C1
17	A	831	CLA	C11-C10-C8-C7
17	A	806	CLA	C11-C10-C8-C7
17	a	824	CLA	C3A-C2A-CAA-CBA
17	a	818	CLA	C12-C13-C15-C16
17	A	854	CLA	C12-C13-C15-C16
17	B	810	CLA	C3A-C2A-CAA-CBA
17	B	840	CLA	C12-C13-C15-C16
17	B	802	CLA	C11-C10-C8-C7
17	A	812	CLA	C11-C10-C8-C7
17	B	813	CLA	C12-C13-C15-C16
19	2	618	LHG	O6-C4-C5-O7
17	a	843	CLA	C6-C7-C8-C10
17	a	829	CLA	C6-C7-C8-C10
17	a	808	CLA	C12-C13-C15-C16
17	a	806	CLA	C11-C12-C13-C15
17	a	807	CLA	C11-C12-C13-C15
17	b	805	CLA	C3-C5-C6-C7
17	3	311	CLA	O1A-CGA-O2A-C1
17	A	845	CLA	C2C-C3C-CAC-CBC
19	3	319	LHG	O2-C2-C3-O3
17	a	828	CLA	C5-C6-C7-C8
17	b	829	CLA	C10-C11-C12-C13
17	a	838	CLA	C2A-CAA-CBA-CGA
17	b	803	CLA	C16-C17-C18-C20
26	2	601	CHL	C11-C12-C13-C15
26	7	614	CHL	C1C-C2C-CMC-OMC
17	a	819	CLA	O1A-CGA-O2A-C1
26	7	601	CHL	CAA-CBA-CGA-O2A
17	1	313	CLA	C10-C11-C12-C13
17	B	822	CLA	O1A-CGA-O2A-C1
17	B	813	CLA	C5-C6-C7-C8
17	a	840	CLA	C10-C11-C12-C13
17	a	820	CLA	C4-C3-C5-C6
17	A	820	CLA	C4-C3-C5-C6
17	2	609	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	b	817	CLA	CAA-CBA-CGA-O2A
17	a	828	CLA	C11-C12-C13-C14
17	a	809	CLA	C11-C10-C8-C9
17	1	309	CLA	C14-C13-C15-C16
17	a	839	CLA	C11-C10-C8-C9
17	2	602	CLA	C6-C7-C8-C9
17	B	810	CLA	C14-C13-C15-C16
17	B	808	CLA	C14-C13-C15-C16
17	a	842	CLA	C11-C12-C13-C14
17	A	809	CLA	C11-C10-C8-C9
17	A	809	CLA	C14-C13-C15-C16
18	a	845	PQN	C24-C23-C25-C26
17	B	815	CLA	C11-C10-C8-C9
17	7	602	CLA	C6-C7-C8-C9
17	2	603	CLA	C11-C12-C13-C14
17	b	825	CLA	C14-C13-C15-C16
17	1	303	CLA	C6-C7-C8-C9
17	a	802	CLA	C14-C13-C15-C16
17	A	843	CLA	C6-C7-C8-C9
17	A	830	CLA	C14-C13-C15-C16
17	a	806	CLA	C14-C13-C15-C16
17	1	304	CLA	C6-C7-C8-C9
17	a	807	CLA	C11-C10-C8-C9
17	B	837	CLA	O1A-CGA-O2A-C1
17	A	826	CLA	C16-C17-C18-C20
17	A	801	CLA	O1A-CGA-O2A-C1
17	a	811	CLA	O1A-CGA-O2A-C1
17	a	804	CLA	O1A-CGA-O2A-C1
20	A	852	BCR	C7-C8-C9-C34
17	A	827	CLA	C3-C5-C6-C7
20	j	3004	BCR	C17-C18-C19-C20
17	2	608	CLA	CAA-CBA-CGA-O2A
25	G	102	LMG	C11-C12-C13-C14
17	6	305	CLA	C10-C11-C12-C13
17	a	807	CLA	C8-C10-C11-C12
17	L	203	CLA	C4-C3-C5-C6
17	b	814	CLA	C4-C3-C5-C6
17	B	810	CLA	C2-C3-C5-C6
17	B	814	CLA	C15-C16-C17-C18
17	1	304	CLA	C8-C10-C11-C12
17	A	823	CLA	C1-C2-C3-C4
17	B	831	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
17	a	823	CLA	C1-C2-C3-C4
17	b	831	CLA	C1-C2-C3-C4
25	6	302	LMG	C14-C15-C16-C17
17	a	801	CLA	CAA-CBA-CGA-O2A
17	a	820	CLA	C13-C15-C16-C17
17	4	602	CLA	C2A-CAA-CBA-CGA
17	b	826	CLA	C2A-CAA-CBA-CGA
17	A	813	CLA	C2A-CAA-CBA-CGA
17	4	612	CLA	C2A-CAA-CBA-CGA
17	8	312	CLA	C2A-CAA-CBA-CGA
25	G	102	LMG	C29-C28-O8-C9
17	B	805	CLA	C2-C1-O2A-CGA
17	a	856	CLA	C2-C1-O2A-CGA
17	A	831	CLA	C2-C1-O2A-CGA
17	a	825	CLA	C2-C1-O2A-CGA
17	b	818	CLA	C2-C1-O2A-CGA
17	1	306	CLA	C2-C1-O2A-CGA
26	6	303	CHL	C2-C1-O2A-CGA
17	b	836	CLA	C2-C1-O2A-CGA
17	b	834	CLA	C2-C1-O2A-CGA
17	a	827	CLA	C2-C1-O2A-CGA
17	b	810	CLA	C2-C1-O2A-CGA
17	1	312	CLA	C2-C1-O2A-CGA
17	A	834	CLA	C2-C1-O2A-CGA
17	L	203	CLA	C2-C1-O2A-CGA
26	7	601	CHL	C2-C1-O2A-CGA
17	B	836	CLA	C2-C1-O2A-CGA
17	2	603	CLA	C2-C1-O2A-CGA
17	a	830	CLA	C2-C1-O2A-CGA
17	4	611	CLA	C2-C1-O2A-CGA
17	B	816	CLA	C2-C1-O2A-CGA
17	A	807	CLA	C2-C1-O2A-CGA
17	A	830	CLA	C2-C1-O2A-CGA
17	8	310	CLA	C2-C1-O2A-CGA
17	b	805	CLA	C2-C1-O2A-CGA
17	3	312	CLA	C2-C1-O2A-CGA
19	7	618	LHG	C11-C10-C9-C8
17	6	309	CLA	O1A-CGA-O2A-C1
17	A	824	CLA	O1D-CGD-O2D-CED
17	7	609	CLA	O1A-CGA-O2A-C1
25	G	102	LMG	O10-C28-O8-C9
17	a	832	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	L	203	CLA	CBA-CGA-O2A-C1
17	A	828	CLA	C10-C11-C12-C13
27	8	314	LUT	C1-C6-C7-C8
27	3	316	LUT	C1-C6-C7-C8
20	6	319	BCR	C23-C24-C25-C26
20	A	849	BCR	C1-C6-C7-C8
20	A	849	BCR	C5-C6-C7-C8
20	b	844	BCR	C5-C6-C7-C8
20	A	850	BCR	C1-C6-C7-C8
27	2	615	LUT	C1-C6-C7-C8
27	2	615	LUT	C5-C6-C7-C8
20	b	846	BCR	C1-C6-C7-C8
20	b	846	BCR	C23-C24-C25-C26
20	B	844	BCR	C1-C6-C7-C8
27	6	317	LUT	C5-C6-C7-C8
17	a	836	CLA	O1D-CGD-O2D-CED
22	A	855	HTG	C3'-C4'-C5'-C6'
17	a	832	CLA	CBA-CGA-O2A-C1
17	a	844	CLA	C13-C15-C16-C17
17	b	812	CLA	C6-C7-C8-C9
17	A	843	CLA	C16-C17-C18-C19
17	A	805	CLA	C2A-CAA-CBA-CGA
23	B	849	LMT	C2'-C1'-O1'-C1
19	2	618	LHG	O7-C5-C6-O8
17	A	843	CLA	C8-C10-C11-C12
17	A	801	CLA	CBA-CGA-O2A-C1
19	1	319	LHG	C4-O6-P-O3
19	a	848	LHG	C4-O6-P-O3
19	A	847	LHG	C3-O3-P-O6
19	A	847	LHG	C4-O6-P-O3
24	B	850	DGD	C1G-C2G-C3G-O3G
19	2	618	LHG	C4-C5-C6-O8
26	1	302	CHL	C4-C3-C5-C6
17	a	846	CLA	C4-C3-C5-C6
17	3	312	CLA	C4-C3-C5-C6
17	B	806	CLA	C11-C12-C13-C15
17	A	819	CLA	C11-C10-C8-C7
17	b	827	CLA	C2-C3-C5-C6
17	A	831	CLA	C11-C10-C8-C9
17	A	808	CLA	C14-C13-C15-C16
17	A	854	CLA	C14-C13-C15-C16
17	B	806	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
17	B	839	CLA	C14-C13-C15-C16
17	2	602	CLA	C14-C13-C15-C16
17	B	840	CLA	C14-C13-C15-C16
17	l	202	CLA	C14-C13-C15-C16
17	a	830	CLA	C14-C13-C15-C16
17	a	808	CLA	C14-C13-C15-C16
17	a	807	CLA	C11-C12-C13-C14
17	2	612	CLA	C10-C11-C12-C13
17	L	203	CLA	O1A-CGA-O2A-C1
17	2	609	CLA	O1A-CGA-O2A-C1
17	9	612	CLA	C2A-CAA-CBA-CGA
17	1	303	CLA	C2A-CAA-CBA-CGA
17	a	835	CLA	O1A-CGA-O2A-C1
20	9	618	BCR	C11-C12-C13-C35
20	l	201	BCR	C11-C12-C13-C35
17	a	804	CLA	CBA-CGA-O2A-C1
19	1	319	LHG	O1-C1-C2-C3
17	a	830	CLA	CAA-CBA-CGA-O2A
17	a	828	CLA	C10-C11-C12-C13
17	b	827	CLA	C10-C11-C12-C13
17	2	609	CLA	C10-C11-C12-C13
19	3	319	LHG	C1-C2-C3-O3
17	A	812	CLA	C10-C11-C12-C13
17	b	819	CLA	C4-C3-C5-C6
17	a	802	CLA	C2-C3-C5-C6
17	a	840	CLA	C16-C17-C18-C19
17	1	304	CLA	C16-C17-C18-C19
17	B	837	CLA	CBA-CGA-O2A-C1
17	a	841	CLA	O1A-CGA-O2A-C1
17	b	822	CLA	CBA-CGA-O2A-C1
17	8	301	CLA	C2A-CAA-CBA-CGA
26	1	302	CHL	C11-C12-C13-C14
20	b	846	BCR	C19-C20-C21-C22
17	B	812	CLA	C3-C5-C6-C7
17	b	837	CLA	O1A-CGA-O2A-C1
17	a	841	CLA	C15-C16-C17-C18
17	B	817	CLA	C10-C11-C12-C13
17	A	820	CLA	C16-C17-C18-C19
17	B	827	CLA	CAA-CBA-CGA-O2A
17	a	835	CLA	C3-C5-C6-C7
17	A	806	CLA	C4-C3-C5-C6
17	B	827	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
17	6	311	CLA	C4-C3-C5-C6
17	a	804	CLA	O1D-CGD-O2D-CED
17	a	816	CLA	O1D-CGD-O2D-CED
17	A	828	CLA	C5-C6-C7-C8
17	a	812	CLA	C2-C1-O2A-CGA
17	B	827	CLA	C2-C1-O2A-CGA
17	A	801	CLA	C2-C1-O2A-CGA
17	9	612	CLA	C2-C1-O2A-CGA
17	4	609	CLA	C2-C1-O2A-CGA
17	A	842	CLA	C2-C1-O2A-CGA
26	2	607	CHL	C2-C1-O2A-CGA
17	A	841	CLA	C2C-C3C-CAC-CBC
17	3	308	CLA	C2A-CAA-CBA-CGA
17	a	834	CLA	C2A-CAA-CBA-CGA
17	4	609	CLA	C2A-CAA-CBA-CGA
17	1	313	CLA	C2A-CAA-CBA-CGA
17	6	304	CLA	C2A-CAA-CBA-CGA
17	b	827	CLA	C2A-CAA-CBA-CGA
17	7	609	CLA	C2A-CAA-CBA-CGA
17	B	816	CLA	C2A-CAA-CBA-CGA
17	a	843	CLA	C2A-CAA-CBA-CGA
17	A	843	CLA	C2A-CAA-CBA-CGA
17	A	819	CLA	CAA-CBA-CGA-O1A
17	A	833	CLA	C3A-C2A-CAA-CBA
17	a	833	CLA	C3A-C2A-CAA-CBA
17	a	822	CLA	C3A-C2A-CAA-CBA
17	b	812	CLA	C3A-C2A-CAA-CBA
17	A	830	CLA	C3A-C2A-CAA-CBA
17	B	802	CLA	CAA-CBA-CGA-O2A
17	A	845	CLA	C4C-C3C-CAC-CBC
17	B	831	CLA	CBA-CGA-O2A-C1
17	B	802	CLA	C4-C3-C5-C6
26	2	601	CHL	C4-C3-C5-C6
19	7	618	LHG	C25-C26-C27-C28
17	9	612	CLA	C2-C3-C5-C6
17	a	812	CLA	C11-C10-C8-C9
17	a	818	CLA	C11-C12-C13-C14
17	a	818	CLA	C14-C13-C15-C16
17	B	819	CLA	C11-C12-C13-C14
17	b	803	CLA	C14-C13-C15-C16
17	6	310	CLA	C14-C13-C15-C16
17	b	816	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
17	A	843	CLA	C10-C11-C12-C13
17	6	314	CLA	C10-C11-C12-C13
20	A	852	BCR	C11-C10-C9-C34
20	A	852	BCR	C16-C17-C18-C36
20	f	7004	BCR	C35-C13-C14-C15
20	B	845	BCR	C11-C10-C9-C34
20	B	845	BCR	C20-C21-C22-C37
20	L	201	BCR	C11-C10-C9-C34
20	b	844	BCR	C11-C10-C9-C34
24	b	849	DGD	C1G-C2G-C3G-O3G
20	b	845	BCR	C11-C10-C9-C34
20	b	845	BCR	C20-C21-C22-C37
20	B	844	BCR	C11-C10-C9-C34
20	F	305	BCR	C35-C13-C14-C15
20	l	201	BCR	C11-C10-C9-C34
20	a	854	BCR	C11-C10-C9-C34
20	a	854	BCR	C16-C17-C18-C36
17	a	827	CLA	C3-C5-C6-C7
19	1	319	LHG	C25-C26-C27-C28
26	2	601	CHL	C11-C12-C13-C14
17	A	806	CLA	O2A-C1-C2-C3
17	a	835	CLA	CBA-CGA-O2A-C1
23	B	849	LMT	O5'-C1'-O1'-C1
20	1	318	BCR	C7-C8-C9-C34
20	A	848	BCR	C37-C22-C23-C24
17	1	309	CLA	C10-C11-C12-C13
17	B	807	CLA	C15-C16-C17-C18
17	A	805	CLA	C4-C3-C5-C6
17	A	840	CLA	C4-C3-C5-C6
17	A	830	CLA	C4-C3-C5-C6
17	A	811	CLA	C1A-C2A-CAA-CBA
17	b	813	CLA	C1A-C2A-CAA-CBA
17	b	822	CLA	C1A-C2A-CAA-CBA
17	b	830	CLA	C1A-C2A-CAA-CBA
17	7	609	CLA	C1A-C2A-CAA-CBA
17	b	831	CLA	C1A-C2A-CAA-CBA
17	8	301	CLA	C1A-C2A-CAA-CBA
17	2	604	CLA	C6-C7-C8-C10
17	a	809	CLA	C6-C7-C8-C10
17	A	827	CLA	C12-C13-C15-C16
17	b	834	CLA	C6-C7-C8-C10
17	a	827	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
17	b	810	CLA	C11-C12-C13-C15
17	B	806	CLA	C12-C13-C15-C16
17	1	308	CLA	C12-C13-C15-C16
17	A	819	CLA	C6-C7-C8-C10
17	B	832	CLA	C11-C10-C8-C7
18	b	842	PQN	C17-C18-C20-C21
17	B	834	CLA	C11-C12-C13-C15
17	2	609	CLA	C6-C7-C8-C10
17	7	604	CLA	C6-C7-C8-C10
17	a	843	CLA	C11-C12-C13-C15
17	a	804	CLA	C6-C7-C8-C10
17	a	807	CLA	C12-C13-C15-C16
17	B	829	CLA	C11-C10-C8-C7
17	B	837	CLA	C12-C13-C15-C16
17	f	7003	CLA	C5-C6-C7-C8
25	6	302	LMG	O8-C28-C29-C30
17	a	841	CLA	CBA-CGA-O2A-C1
17	b	822	CLA	O1A-CGA-O2A-C1
17	B	831	CLA	O1A-CGA-O2A-C1
17	a	839	CLA	C8-C10-C11-C12
17	b	805	CLA	CAA-CBA-CGA-O1A
17	2	602	CLA	C2A-CAA-CBA-CGA
17	B	832	CLA	C2A-CAA-CBA-CGA
17	7	602	CLA	C2A-CAA-CBA-CGA
17	b	831	CLA	C2A-CAA-CBA-CGA
17	a	832	CLA	C2A-CAA-CBA-CGA
17	b	805	CLA	C15-C16-C17-C18
19	1	319	LHG	C9-C10-C11-C12
17	A	816	CLA	CBA-CGA-O2A-C1
17	9	614	CLA	CBA-CGA-O2A-C1
17	b	805	CLA	C16-C17-C18-C20
17	b	820	CLA	O1D-CGD-O2D-CED
17	B	829	CLA	C15-C16-C17-C18
17	b	834	CLA	O1A-CGA-O2A-C1
19	2	618	LHG	C23-C24-C25-C26
25	G	102	LMG	C10-C11-C12-C13
17	a	846	CLA	C2C-C3C-CAC-CBC
20	A	852	BCR	C11-C10-C9-C8
20	A	852	BCR	C16-C17-C18-C19
20	f	7004	BCR	C12-C13-C14-C15
20	B	845	BCR	C11-C10-C9-C8
20	B	845	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
20	L	201	BCR	C11-C10-C9-C8
20	b	844	BCR	C11-C10-C9-C8
20	b	845	BCR	C11-C10-C9-C8
20	b	845	BCR	C20-C21-C22-C23
20	B	844	BCR	C11-C10-C9-C8
20	F	305	BCR	C12-C13-C14-C15
20	l	201	BCR	C11-C10-C9-C8
20	a	854	BCR	C11-C10-C9-C8
20	a	854	BCR	C16-C17-C18-C19
17	b	817	CLA	O1A-CGA-O2A-C1
25	4	619	LMG	O7-C8-C9-O8
17	b	817	CLA	CBA-CGA-O2A-C1
25	G	102	LMG	C12-C13-C14-C15
25	4	619	LMG	C10-C11-C12-C13
20	B	801	BCR	C15-C16-C17-C18
20	K	4001	BCR	C15-C16-C17-C18
20	B	846	BCR	C19-C20-C21-C22
17	A	816	CLA	O1A-CGA-O2A-C1
17	b	837	CLA	C8-C10-C11-C12
17	b	813	CLA	C4-C3-C5-C6
17	a	813	CLA	C4-C3-C5-C6
17	B	837	CLA	C4-C3-C5-C6
17	9	609	CLA	C2-C1-O2A-CGA
17	2	604	CLA	C2-C1-O2A-CGA
17	a	802	CLA	C2-C1-O2A-CGA
17	a	813	CLA	C2-C1-O2A-CGA
17	B	827	CLA	C2-C3-C5-C6
17	L	203	CLA	C2-C3-C5-C6
17	B	802	CLA	C2-C3-C5-C6
17	A	805	CLA	C2-C3-C5-C6
26	1	302	CHL	C2-C3-C5-C6
17	A	826	CLA	C8-C10-C11-C12
17	B	819	CLA	C15-C16-C17-C18
17	6	305	CLA	C6-C7-C8-C9
17	b	825	CLA	C6-C7-C8-C9
17	9	614	CLA	O1A-CGA-O2A-C1
17	9	609	CLA	C2A-CAA-CBA-CGA
17	A	841	CLA	C2A-CAA-CBA-CGA
17	a	831	CLA	O1A-CGA-O2A-C1
20	L	206	BCR	C1-C6-C7-C8
27	7	615	LUT	C1-C6-C7-C8
20	f	7004	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	f	7004	BCR	C23-C24-C25-C30
20	L	201	BCR	C23-C24-C25-C30
20	G	105	BCR	C1-C6-C7-C8
20	b	846	BCR	C5-C6-C7-C8
20	I	101	BCR	C1-C6-C7-C8
20	a	851	BCR	C1-C6-C7-C8
20	F	305	BCR	C23-C24-C25-C30
20	B	846	BCR	C1-C6-C7-C8
20	g	104	BCR	C1-C6-C7-C8
20	a	852	BCR	C23-C24-C25-C30
20	A	851	BCR	C1-C6-C7-C8
17	a	829	CLA	C15-C16-C17-C18
17	2	613	CLA	O1D-CGD-O2D-CED
17	b	802	CLA	CAA-CBA-CGA-O2A
22	J	3001	HTG	C1'-C2'-C3'-C4'
19	6	320	LHG	O1-C1-C2-C3
22	F	302	HTG	C1'-C2'-C3'-C4'
19	6	320	LHG	C30-C31-C32-C33
20	a	853	BCR	C19-C20-C21-C22
28	7	616	XAT	C29-C30-C31-C32
17	1	309	CLA	C4-C3-C5-C6
17	b	809	CLA	C4-C3-C5-C6
17	a	811	CLA	C4-C3-C5-C6
17	B	826	CLA	C4-C3-C5-C6
17	a	840	CLA	C4-C3-C5-C6
17	B	814	CLA	C4-C3-C5-C6
26	7	614	CHL	C1A-C2A-CAA-CBA
20	4	618	BCR	C11-C12-C13-C14
17	A	820	CLA	C16-C17-C18-C20
17	a	820	CLA	C2-C3-C5-C6
17	b	814	CLA	C2-C3-C5-C6
17	A	820	CLA	C2-C3-C5-C6
17	1	303	CLA	C2-C3-C5-C6
17	a	846	CLA	C2-C3-C5-C6
17	3	312	CLA	C2-C3-C5-C6
26	4	606	CHL	CAA-CBA-CGA-O2A
17	4	612	CLA	C3-C5-C6-C7
17	b	802	CLA	C5-C6-C7-C8
17	A	818	CLA	C13-C15-C16-C17
17	a	830	CLA	C15-C16-C17-C18
17	b	815	CLA	CBD-CGD-O2D-CED
17	B	818	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
17	4	612	CLA	C5-C6-C7-C8
17	6	310	CLA	C10-C11-C12-C13
19	3	319	LHG	O6-C4-C5-O7
17	A	841	CLA	C4C-C3C-CAC-CBC
19	3	319	LHG	C4-C5-O7-C7
19	3	319	LHG	C6-C5-O7-C7
17	B	820	CLA	C2A-CAA-CBA-CGA
17	b	812	CLA	C2A-CAA-CBA-CGA
17	A	809	CLA	C8-C10-C11-C12
17	1	309	CLA	C3-C5-C6-C7
17	b	803	CLA	C3-C5-C6-C7
23	B	849	LMT	C2-C3-C4-C5
17	1	306	CLA	C4-C3-C5-C6
17	b	810	CLA	C4-C3-C5-C6
17	A	822	CLA	C4-C3-C5-C6
17	8	310	CLA	C4-C3-C5-C6
17	b	805	CLA	C4-C3-C5-C6
17	3	308	CLA	CAA-CBA-CGA-O1A
19	A	846	LHG	C16-C17-C18-C19
17	A	806	CLA	C2-C3-C5-C6
17	A	828	CLA	C2-C3-C5-C6
17	b	809	CLA	C2-C3-C5-C6
17	B	815	CLA	C11-C10-C8-C7
17	A	840	CLA	C2-C3-C5-C6
17	a	813	CLA	C2-C3-C5-C6
17	B	814	CLA	C2-C3-C5-C6
17	b	834	CLA	CBA-CGA-O2A-C1
17	b	831	CLA	CBA-CGA-O2A-C1
17	b	808	CLA	C13-C15-C16-C17
17	4	601	CLA	CAA-CBA-CGA-O1A
20	2	617	BCR	C13-C14-C15-C16
17	b	810	CLA	C13-C15-C16-C17
17	6	311	CLA	CBD-CGD-O2D-CED
17	b	839	CLA	C13-C15-C16-C17
17	A	830	CLA	C13-C15-C16-C17
17	B	831	CLA	C2A-CAA-CBA-CGA
17	1	304	CLA	C10-C11-C12-C13
19	2	618	LHG	C25-C26-C27-C28
17	a	831	CLA	CBA-CGA-O2A-C1
17	6	311	CLA	CBA-CGA-O2A-C1
17	A	811	CLA	C4-C3-C5-C6
17	B	824	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
17	a	842	CLA	C4-C3-C5-C6
17	A	813	CLA	C4-C3-C5-C6
17	B	809	CLA	C4-C3-C5-C6
17	A	809	CLA	C4-C3-C5-C6
17	F	301	CLA	C4-C3-C5-C6
17	b	837	CLA	C4-C3-C5-C6
17	a	807	CLA	C4-C3-C5-C6
17	B	807	CLA	C4-C3-C5-C6
17	b	813	CLA	C13-C15-C16-C17
17	A	802	CLA	C15-C16-C17-C18
17	b	815	CLA	O1D-CGD-O2D-CED
17	1	304	CLA	CAA-CBA-CGA-O2A
19	a	847	LHG	C16-C17-C18-C19
17	6	305	CLA	C11-C10-C8-C9
17	a	827	CLA	C14-C13-C15-C16
17	B	806	CLA	C11-C12-C13-C14
17	B	806	CLA	C14-C13-C15-C16
17	1	308	CLA	C14-C13-C15-C16
17	A	809	CLA	C11-C12-C13-C14
17	F	301	CLA	C14-C13-C15-C16
18	a	845	PQN	C21-C22-C23-C24
17	A	812	CLA	C11-C10-C8-C9
17	B	813	CLA	C11-C12-C13-C14
17	B	813	CLA	C14-C13-C15-C16
17	7	604	CLA	C6-C7-C8-C9
17	a	843	CLA	C6-C7-C8-C9
17	a	829	CLA	C11-C12-C13-C14
17	a	806	CLA	C11-C12-C13-C14
25	6	302	LMG	C17-C18-C19-C20
17	A	815	CLA	C3A-C2A-CAA-CBA
17	B	811	CLA	C3A-C2A-CAA-CBA
17	B	823	CLA	C3A-C2A-CAA-CBA
17	6	306	CLA	C3A-C2A-CAA-CBA
17	4	610	CLA	C3A-C2A-CAA-CBA
17	b	831	CLA	O1A-CGA-O2A-C1
26	4	605	CHL	CAA-CBA-CGA-O2A
17	a	811	CLA	CAA-CBA-CGA-O2A
17	A	830	CLA	CAA-CBA-CGA-O2A
17	a	846	CLA	CAA-CBA-CGA-O2A
17	4	614	CLA	CAA-CBA-CGA-O2A
17	A	808	CLA	CAD-CBD-CGD-O2D
17	A	826	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	A	827	CLA	CAD-CBD-CGD-O2D
17	j	3002	CLA	CAD-CBD-CGD-O2D
17	1	305	CLA	CAD-CBD-CGD-O2D
17	4	604	CLA	CAD-CBD-CGD-O2D
17	a	827	CLA	CAD-CBD-CGD-O2D
17	a	814	CLA	CAD-CBD-CGD-O2D
17	A	834	CLA	CAD-CBD-CGD-O2D
26	6	308	CHL	CAD-CBD-CGD-O2D
17	B	826	CLA	CAD-CBD-CGD-O2D
17	A	838	CLA	CAD-CBD-CGD-O2D
17	b	826	CLA	CAD-CBD-CGD-O2D
17	A	813	CLA	CAD-CBD-CGD-O2D
17	l	202	CLA	CAD-CBD-CGD-O2D
17	9	602	CLA	CAD-CBD-CGD-O2D
17	k	1401	CLA	CAD-CBD-CGD-O2D
17	g	101	CLA	CAD-CBD-CGD-O2D
17	B	813	CLA	CAD-CBD-CGD-O2D
17	J	3002	CLA	CAD-CBD-CGD-O2D
17	7	602	CLA	CAD-CBD-CGD-O2D
17	A	804	CLA	CAD-CBD-CGD-O2D
17	8	303	CLA	CAD-CBD-CGD-O2D
17	4	611	CLA	CAD-CBD-CGD-O2D
17	a	838	CLA	CAD-CBD-CGD-O2D
26	1	307	CHL	CAD-CBD-CGD-O2D
26	7	605	CHL	CAD-CBD-CGD-O2D
17	b	804	CLA	CAD-CBD-CGD-O2D
17	A	839	CLA	CAD-CBD-CGD-O2D
17	a	808	CLA	CAD-CBD-CGD-O2D
17	a	806	CLA	CAD-CBD-CGD-O2D
17	a	846	CLA	CAD-CBD-CGD-O2D
17	B	837	CLA	CAD-CBD-CGD-O2D
24	b	849	DGD	C8B-C9B-CAB-CBB
17	2	603	CLA	C8-C10-C11-C12
17	b	832	CLA	C8-C10-C11-C12
17	A	804	CLA	C2A-CAA-CBA-CGA
17	b	816	CLA	C2-C1-O2A-CGA
17	a	801	CLA	C2-C1-O2A-CGA
17	3	302	CLA	C2-C1-O2A-CGA
17	B	829	CLA	C2-C1-O2A-CGA
25	4	619	LMG	O7-C10-C11-C12
17	a	844	CLA	CAA-CBA-CGA-O2A
17	L	204	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
17	B	804	CLA	CBD-CGD-O2D-CED
17	a	812	CLA	C5-C6-C7-C8
17	A	803	CLA	C4-C3-C5-C6
17	B	805	CLA	C4-C3-C5-C6
17	1	305	CLA	C4-C3-C5-C6
17	b	824	CLA	C4-C3-C5-C6
17	A	807	CLA	C4-C3-C5-C6
17	b	807	CLA	C4-C3-C5-C6
17	1	309	CLA	C2-C3-C5-C6
17	a	811	CLA	C2-C3-C5-C6
17	A	807	CLA	C2-C3-C5-C6
17	A	830	CLA	C2-C3-C5-C6
17	a	807	CLA	C2-C3-C5-C6
17	B	807	CLA	C2-C3-C5-C6
17	A	806	CLA	CAA-CBA-CGA-O2A
17	B	813	CLA	CAA-CBA-CGA-O2A
20	A	852	BCR	C7-C8-C9-C10
28	3	317	XAT	C27-C28-C29-C30
20	1	318	BCR	C7-C8-C9-C10
20	G	105	BCR	C21-C22-C23-C24
28	6	318	XAT	O4-C6-C7-C8
25	G	102	LMG	O1-C7-C8-C9
19	a	848	LHG	O6-C4-C5-O7
17	A	811	CLA	CAA-CBA-CGA-O2A
26	6	303	CHL	CAA-CBA-CGA-O2A
17	B	832	CLA	CAA-CBA-CGA-O2A
17	a	802	CLA	CAA-CBA-CGA-O2A
17	B	832	CLA	O2A-C1-C2-C3
26	9	606	CHL	O2A-C1-C2-C3
17	a	802	CLA	O2A-C1-C2-C3
17	2	609	CLA	C2A-CAA-CBA-CGA
17	B	803	CLA	C2A-CAA-CBA-CGA
17	a	841	CLA	C2A-CAA-CBA-CGA
17	b	809	CLA	CAA-CBA-CGA-O2A
17	B	841	CLA	CAA-CBA-CGA-O2A
17	a	814	CLA	CAA-CBA-CGA-O2A
17	7	612	CLA	CAA-CBA-CGA-O2A
17	b	816	CLA	C6-C7-C8-C9
19	A	846	LHG	C15-C16-C17-C18
17	B	805	CLA	CHA-CBD-CGD-O2D
17	a	828	CLA	CHA-CBD-CGD-O1D
17	3	305	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
17	3	305	CLA	CHA-CBD-CGD-O2D
17	4	602	CLA	CHA-CBD-CGD-O2D
17	A	824	CLA	CHA-CBD-CGD-O1D
17	A	824	CLA	CHA-CBD-CGD-O2D
17	b	813	CLA	CHA-CBD-CGD-O2D
17	B	824	CLA	CHA-CBD-CGD-O1D
17	B	824	CLA	CHA-CBD-CGD-O2D
17	a	811	CLA	CHA-CBD-CGD-O1D
17	a	811	CLA	CHA-CBD-CGD-O2D
17	b	802	CLA	CHA-CBD-CGD-O2D
17	B	823	CLA	CHA-CBD-CGD-O1D
17	B	823	CLA	CHA-CBD-CGD-O2D
20	j	3004	BCR	C19-C20-C21-C22
17	l	203	CLA	CHA-CBD-CGD-O1D
17	l	203	CLA	CHA-CBD-CGD-O2D
17	A	835	CLA	CHA-CBD-CGD-O1D
17	A	835	CLA	CHA-CBD-CGD-O2D
17	6	304	CLA	CHA-CBD-CGD-O2D
17	G	104	CLA	CHA-CBD-CGD-O2D
17	B	833	CLA	CHA-CBD-CGD-O2D
17	4	610	CLA	CHA-CBD-CGD-O2D
17	6	307	CLA	CHA-CBD-CGD-O1D
17	6	307	CLA	CHA-CBD-CGD-O2D
17	b	837	CLA	CHA-CBD-CGD-O1D
17	a	802	CLA	CHA-CBD-CGD-O1D
17	a	802	CLA	CHA-CBD-CGD-O2D
17	9	601	CLA	CHA-CBD-CGD-O2D
17	3	302	CLA	CHA-CBD-CGD-O2D
17	8	301	CLA	CHA-CBD-CGD-O2D
17	9	614	CLA	CAA-CBA-CGA-O2A
17	b	812	CLA	CAA-CBA-CGA-O2A
17	3	312	CLA	CAA-CBA-CGA-O2A
17	b	824	CLA	C2-C3-C5-C6
22	J	3001	HTG	C3'-C4'-C5'-C6'
17	a	846	CLA	C4C-C3C-CAC-CBC
24	B	850	DGD	C9A-CAA-CBA-CCA
17	b	809	CLA	C16-C17-C18-C20
17	a	829	CLA	C16-C17-C18-C19
17	B	840	CLA	C5-C6-C7-C8
17	A	828	CLA	CAA-CBA-CGA-O2A
17	B	806	CLA	CAA-CBA-CGA-O2A
17	B	809	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
17	B	822	CLA	CAA-CBA-CGA-O2A
25	G	102	LMG	O1-C7-C8-O7
17	b	828	CLA	C5-C6-C7-C8
17	b	822	CLA	CAA-CBA-CGA-O2A
17	9	612	CLA	CAA-CBA-CGA-O2A
17	9	603	CLA	CAA-CBA-CGA-O2A
17	1	313	CLA	CAA-CBA-CGA-O2A
17	B	816	CLA	CAA-CBA-CGA-O2A
26	9	605	CHL	CAA-CBA-CGA-O2A
17	B	805	CLA	CAA-CBA-CGA-O1A
17	A	816	CLA	C2A-CAA-CBA-CGA
17	b	807	CLA	C2A-CAA-CBA-CGA
17	b	837	CLA	CBA-CGA-O2A-C1
24	B	850	DGD	C8A-C9A-CAA-CBA
17	1	204	CLA	CAA-CBA-CGA-O1A
17	B	817	CLA	CAA-CBA-CGA-O1A
17	b	811	CLA	CAA-CBA-CGA-O2A
17	4	603	CLA	CAA-CBA-CGA-O2A
17	6	315	CLA	C4-C3-C5-C6
17	4	610	CLA	C4-C3-C5-C6
17	A	811	CLA	C2-C3-C5-C6
17	6	305	CLA	C6-C7-C8-C10
17	b	834	CLA	C11-C12-C13-C15
17	B	824	CLA	C2-C3-C5-C6
17	B	832	CLA	C2-C3-C5-C6
17	b	819	CLA	C2-C3-C5-C6
17	b	837	CLA	C2-C3-C5-C6
17	b	807	CLA	C2-C3-C5-C6
17	B	814	CLA	C12-C13-C15-C16
26	1	302	CHL	C11-C12-C13-C15
17	A	813	CLA	CAA-CBA-CGA-O2A
19	A	847	LHG	O7-C7-C8-C9
17	B	807	CLA	CAA-CBA-CGA-O2A
19	A	846	LHG	C10-C11-C12-C13
17	2	604	CLA	C6-C7-C8-C9
17	A	806	CLA	C6-C7-C8-C9
17	A	827	CLA	C14-C13-C15-C16
17	B	826	CLA	C6-C7-C8-C9
17	B	832	CLA	C11-C10-C8-C9
17	b	827	CLA	C11-C10-C8-C9
17	7	609	CLA	C6-C7-C8-C9
17	6	311	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
17	b	805	CLA	C11-C12-C13-C14
17	a	807	CLA	C14-C13-C15-C16
17	B	837	CLA	C14-C13-C15-C16
17	B	807	CLA	C11-C10-C8-C9
17	A	817	CLA	C2C-C3C-CAC-CBC
19	a	848	LHG	C24-C23-O8-C6
17	6	313	CLA	CAA-CBA-CGA-O2A
17	b	816	CLA	CAA-CBA-CGA-O2A
19	6	320	LHG	O7-C7-C8-C9
17	a	802	CLA	CAA-CBA-CGA-O1A
17	b	838	CLA	CAA-CBA-CGA-O2A
17	a	821	CLA	C2A-CAA-CBA-CGA
20	a	852	BCR	C7-C8-C9-C34
17	A	842	CLA	C13-C15-C16-C17
17	b	832	CLA	C13-C15-C16-C17
17	A	825	CLA	C6-C7-C8-C9
17	B	832	CLA	C2C-C3C-CAC-CBC
17	A	828	CLA	C4-C3-C5-C6
17	A	841	CLA	O1A-CGA-O2A-C1
17	A	822	CLA	C2-C3-C5-C6
20	l	201	BCR	C11-C12-C13-C14
20	A	848	BCR	C21-C22-C23-C24
17	A	806	CLA	C1A-C2A-CAA-CBA
17	7	608	CLA	C1A-C2A-CAA-CBA
17	a	824	CLA	C1A-C2A-CAA-CBA
17	b	815	CLA	C1A-C2A-CAA-CBA
17	B	819	CLA	C1A-C2A-CAA-CBA
17	B	841	CLA	C1A-C2A-CAA-CBA
17	B	823	CLA	C1A-C2A-CAA-CBA
17	B	825	CLA	C1A-C2A-CAA-CBA
17	B	834	CLA	C1A-C2A-CAA-CBA
17	7	602	CLA	C1A-C2A-CAA-CBA
17	a	830	CLA	C1A-C2A-CAA-CBA
17	b	817	CLA	C1A-C2A-CAA-CBA
17	B	812	CLA	C1A-C2A-CAA-CBA
17	A	830	CLA	C1A-C2A-CAA-CBA
17	a	806	CLA	C1A-C2A-CAA-CBA
17	A	829	CLA	C1A-C2A-CAA-CBA
17	8	307	CLA	C1A-C2A-CAA-CBA
17	a	844	CLA	C16-C17-C18-C20
17	4	614	CLA	CAA-CBA-CGA-O1A
17	3	312	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	6	313	CLA	C2-C1-O2A-CGA
17	B	813	CLA	C2-C1-O2A-CGA
19	a	847	LHG	C24-C25-C26-C27
17	A	806	CLA	CAA-CBA-CGA-O1A
17	B	841	CLA	CAA-CBA-CGA-O1A
17	1	304	CLA	CAA-CBA-CGA-O1A
17	3	312	CLA	CAA-CBA-CGA-O1A
19	6	320	LHG	C29-C30-C31-C32
19	3	319	LHG	C4-C5-C6-O8
17	A	842	CLA	C2A-CAA-CBA-CGA
17	A	812	CLA	C16-C17-C18-C19
17	b	812	CLA	CAA-CBA-CGA-O1A
17	a	846	CLA	CAA-CBA-CGA-O1A
17	B	807	CLA	CAA-CBA-CGA-O1A
17	A	827	CLA	C13-C15-C16-C17
17	a	826	CLA	CAA-CBA-CGA-O2A
17	B	812	CLA	CAA-CBA-CGA-O2A
17	6	314	CLA	CAA-CBA-CGA-O2A
17	a	831	CLA	C10-C11-C12-C13
17	B	802	CLA	C13-C15-C16-C17
25	4	619	LMG	O9-C10-C11-C12
17	B	806	CLA	CAA-CBA-CGA-O1A
17	9	614	CLA	CAA-CBA-CGA-O1A
17	a	840	CLA	C2-C3-C5-C6
17	6	311	CLA	O1A-CGA-O2A-C1
17	B	817	CLA	O1A-CGA-O2A-C1
17	a	819	CLA	C8-C10-C11-C12
17	b	803	CLA	C15-C16-C17-C18
17	B	822	CLA	C6-C7-C8-C10
24	B	850	DGD	CCA-CDA-CEA-CFA
26	6	303	CHL	CAA-CBA-CGA-O1A
17	9	603	CLA	CAA-CBA-CGA-O1A
17	B	832	CLA	CAA-CBA-CGA-O1A
17	B	822	CLA	CAA-CBA-CGA-O1A
17	B	813	CLA	CAA-CBA-CGA-O1A
17	7	612	CLA	CAA-CBA-CGA-O1A
26	9	605	CHL	CAA-CBA-CGA-O1A
17	b	806	CLA	CAA-CBA-CGA-O2A
17	b	813	CLA	C5-C6-C7-C8
19	a	848	LHG	O10-C23-O8-C6
27	8	314	LUT	C5-C6-C7-C8
20	L	201	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
27	3	316	LUT	C5-C6-C7-C8
20	A	850	BCR	C23-C24-C25-C30
20	B	847	BCR	C1-C6-C7-C8
20	F	305	BCR	C23-C24-C25-C26
20	g	104	BCR	C5-C6-C7-C8
20	a	852	BCR	C23-C24-C25-C26
17	b	840	CLA	C13-C15-C16-C17
18	a	845	PQN	C23-C25-C26-C27
17	A	811	CLA	CAA-CBA-CGA-O1A
17	a	814	CLA	CAA-CBA-CGA-O1A
17	a	811	CLA	CAA-CBA-CGA-O1A
17	9	612	CLA	CAA-CBA-CGA-O1A
17	B	809	CLA	CAA-CBA-CGA-O1A
19	A	847	LHG	O9-C7-C8-C9
19	6	320	LHG	O9-C7-C8-C9
17	4	603	CLA	CAA-CBA-CGA-O1A
17	A	814	CLA	CAA-CBA-CGA-O2A
19	a	848	LHG	O7-C7-C8-C9
17	1	310	CLA	C2A-CAA-CBA-CGA
17	9	602	CLA	C2A-CAA-CBA-CGA
17	6	311	CLA	C2A-CAA-CBA-CGA
17	a	813	CLA	C2A-CAA-CBA-CGA
17	b	809	CLA	CAA-CBA-CGA-O1A
17	a	844	CLA	CAA-CBA-CGA-O1A
17	B	836	CLA	O1A-CGA-O2A-C1
17	3	303	CLA	CAA-CBA-CGA-O2A
17	b	834	CLA	CAA-CBA-CGA-O2A
17	a	838	CLA	CAA-CBA-CGA-O2A
17	B	803	CLA	CAA-CBA-CGA-O2A
17	a	841	CLA	CAA-CBA-CGA-O2A
17	k	1403	CLA	CAA-CBA-CGA-O2A
17	a	816	CLA	CAA-CBA-CGA-O2A
17	4	602	CLA	CBD-CGD-O2D-CED
17	3	312	CLA	CBA-CGA-O2A-C1
17	4	601	CLA	CAD-CBD-CGD-O1D
17	A	824	CLA	CAD-CBD-CGD-O1D
17	b	836	CLA	CAD-CBD-CGD-O1D
17	A	828	CLA	CAD-CBD-CGD-O1D
17	b	821	CLA	CAD-CBD-CGD-O1D
17	B	821	CLA	CAD-CBD-CGD-O1D
17	A	823	CLA	CAD-CBD-CGD-O1D
17	L	202	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
17	b	830	CLA	CAD-CBD-CGD-O1D
17	A	818	CLA	CAD-CBD-CGD-O1D
17	b	837	CLA	CAD-CBD-CGD-O1D
26	7	605	CHL	CAD-CBD-CGD-O1D
17	3	304	CLA	CAD-CBD-CGD-O1D
17	a	819	CLA	CBD-CGD-O2D-CED
26	4	605	CHL	CAA-CBA-CGA-O1A
17	a	819	CLA	CAA-CBA-CGA-O1A
17	1	313	CLA	CAA-CBA-CGA-O1A
17	a	802	CLA	C5-C6-C7-C8
17	B	805	CLA	C11-C12-C13-C14
17	B	827	CLA	C6-C7-C8-C9
17	A	854	CLA	C6-C7-C8-C9
17	b	834	CLA	C11-C12-C13-C14
17	a	835	CLA	C11-C10-C8-C9
18	A	844	PQN	C19-C18-C20-C21
17	B	809	CLA	C11-C12-C13-C14
17	B	802	CLA	C14-C13-C15-C16
17	a	801	CLA	C11-C12-C13-C14
17	a	801	CLA	C14-C13-C15-C16
19	A	847	LHG	O1-C1-C2-O2
26	6	303	CHL	C10-C11-C12-C13
17	A	826	CLA	CAA-CBA-CGA-O2A
17	7	608	CLA	CAA-CBA-CGA-O2A
17	2	612	CLA	CAA-CBA-CGA-O2A
17	a	804	CLA	CAA-CBA-CGA-O2A
17	A	843	CLA	CAA-CBA-CGA-O2A
17	B	840	CLA	C15-C16-C17-C18
17	B	816	CLA	CAA-CBA-CGA-O1A
17	9	602	CLA	C10-C11-C12-C13
17	b	824	CLA	C2A-CAA-CBA-CGA
17	3	302	CLA	C2A-CAA-CBA-CGA
17	a	828	CLA	CAA-CBA-CGA-O2A
17	b	810	CLA	CAA-CBA-CGA-O2A
17	4	612	CLA	CAA-CBA-CGA-O2A
17	1	314	CLA	CAA-CBA-CGA-O2A
17	b	807	CLA	CAA-CBA-CGA-O2A
17	a	813	CLA	CAA-CBA-CGA-O2A
17	8	310	CLA	CAA-CBA-CGA-O2A
17	B	814	CLA	CAA-CBA-CGA-O2A
17	8	302	CLA	CAA-CBA-CGA-O2A
17	A	834	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	6	301	LHG	C1-C2-C3-O3
17	a	812	CLA	C13-C15-C16-C17
17	B	832	CLA	C13-C15-C16-C17
17	b	841	CLA	CAA-CBA-CGA-O1A
17	b	811	CLA	CAA-CBA-CGA-O1A
17	a	812	CLA	C12-C13-C15-C16
17	B	805	CLA	C11-C12-C13-C15
17	A	831	CLA	C12-C13-C15-C16
17	a	831	CLA	C6-C7-C8-C10
17	1	309	CLA	C12-C13-C15-C16
17	A	828	CLA	C11-C10-C8-C7
18	A	844	PQN	C17-C18-C20-C21
17	B	826	CLA	C2-C3-C5-C6
17	B	826	CLA	C6-C7-C8-C10
17	2	602	CLA	C6-C7-C8-C10
17	A	835	CLA	C12-C13-C15-C16
17	B	808	CLA	C12-C13-C15-C16
17	a	842	CLA	C12-C13-C15-C16
17	B	809	CLA	C11-C12-C13-C15
17	l	202	CLA	C12-C13-C15-C16
17	b	827	CLA	C11-C10-C8-C7
17	b	803	CLA	C11-C10-C8-C7
22	J	3001	HTG	C2-C1-S1-C1'
17	b	825	CLA	C6-C7-C8-C10
17	6	311	CLA	C2-C3-C5-C6
17	6	311	CLA	C11-C10-C8-C7
17	a	801	CLA	C11-C12-C13-C15
17	b	805	CLA	C11-C12-C13-C15
17	B	807	CLA	C11-C10-C8-C7
17	6	313	CLA	CAA-CBA-CGA-O1A
17	b	816	CLA	CAA-CBA-CGA-O1A
17	A	828	CLA	CAA-CBA-CGA-O1A
17	b	822	CLA	CAA-CBA-CGA-O1A
17	6	316	CLA	CAA-CBA-CGA-O1A
17	k	1403	CLA	CAA-CBA-CGA-O1A
17	8	310	CLA	CAA-CBA-CGA-O1A
17	9	601	CLA	CAA-CBA-CGA-O1A
17	6	305	CLA	CAA-CBA-CGA-O2A
17	B	823	CLA	CAA-CBA-CGA-O2A
17	G	104	CLA	CAA-CBA-CGA-O2A
17	b	841	CLA	CAA-CBA-CGA-O2A
17	b	831	CLA	CAA-CBA-CGA-O2A

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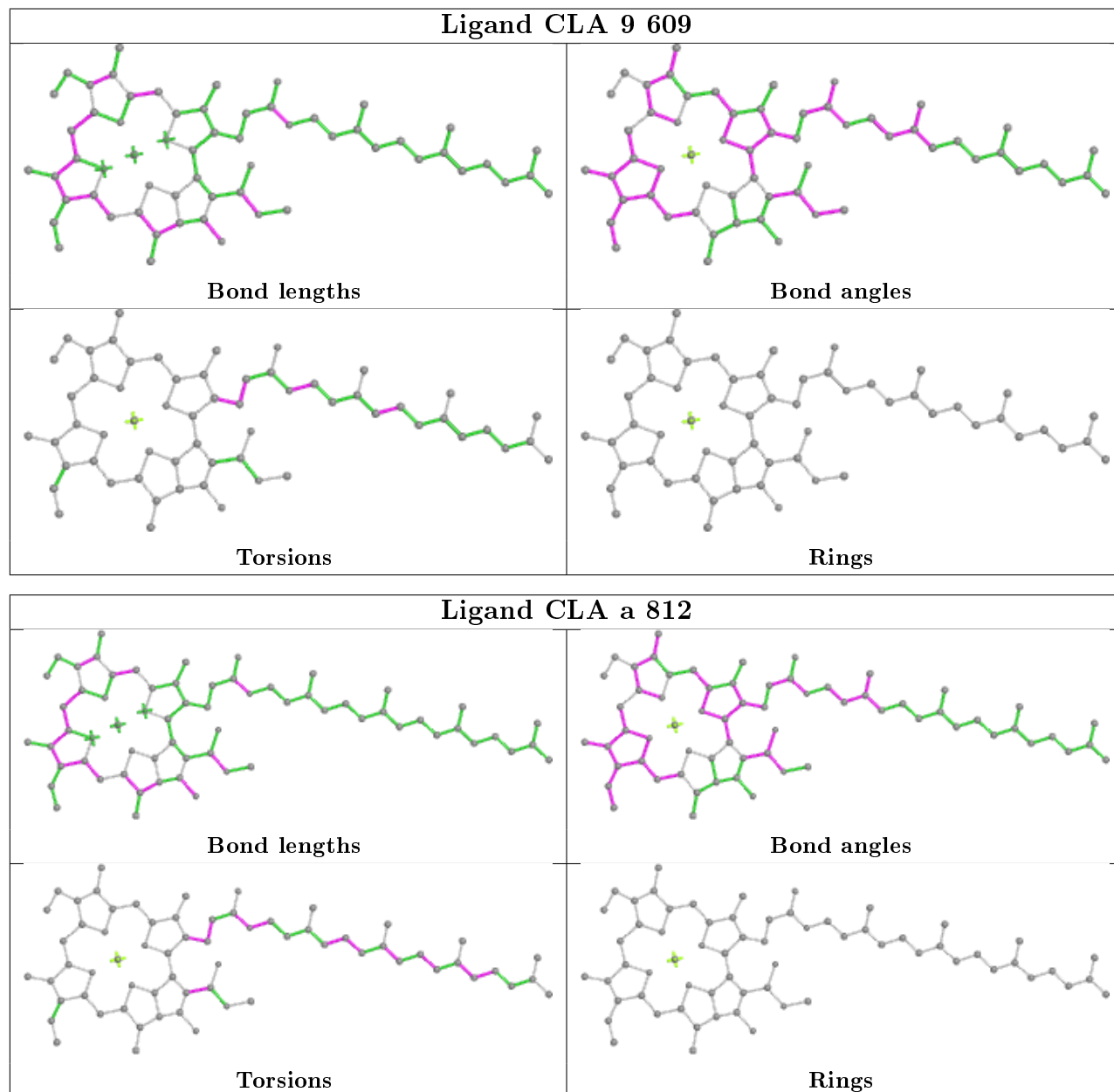
Mol	Chain	Res	Type	Atoms
20	9	618	BCR	C11-C12-C13-C14
20	i	101	BCR	C21-C22-C23-C24
20	a	852	BCR	C7-C8-C9-C10
17	A	826	CLA	CAA-CBA-CGA-O1A
17	b	838	CLA	CAA-CBA-CGA-O1A
17	A	813	CLA	CAA-CBA-CGA-O1A
20	b	847	BCR	C19-C20-C21-C22
17	l	203	CLA	CAA-CBA-CGA-O2A
17	A	820	CLA	C8-C10-C11-C12
17	a	828	CLA	CAA-CBA-CGA-O1A
17	6	305	CLA	CAA-CBA-CGA-O1A
17	b	810	CLA	CAA-CBA-CGA-O1A
17	B	823	CLA	CAA-CBA-CGA-O1A
19	a	848	LHG	O9-C7-C8-C9
17	A	843	CLA	CAA-CBA-CGA-O1A
17	a	816	CLA	CAA-CBA-CGA-O1A
17	6	316	CLA	CAA-CBA-CGA-O2A
17	B	831	CLA	CAA-CBA-CGA-O2A
17	g	103	CLA	CAA-CBA-CGA-O2A
17	4	608	CLA	CAA-CBA-CGA-O2A
17	7	608	CLA	CAA-CBA-CGA-O1A
17	A	814	CLA	CAA-CBA-CGA-O1A
17	a	826	CLA	CAA-CBA-CGA-O1A
17	4	612	CLA	CAA-CBA-CGA-O1A
17	b	806	CLA	CAA-CBA-CGA-O1A
26	6	303	CHL	C2A-CAA-CBA-CGA
17	A	819	CLA	C10-C11-C12-C13
17	A	812	CLA	C8-C10-C11-C12
17	a	829	CLA	C5-C6-C7-C8
17	a	805	CLA	C5-C6-C7-C8
17	B	837	CLA	C5-C6-C7-C8
17	b	834	CLA	CAA-CBA-CGA-O1A
17	2	612	CLA	CAA-CBA-CGA-O1A
17	b	832	CLA	CAA-CBA-CGA-O1A
17	a	813	CLA	CAA-CBA-CGA-O1A
17	b	813	CLA	CAA-CBA-CGA-O2A
17	A	802	CLA	CAA-CBA-CGA-O2A

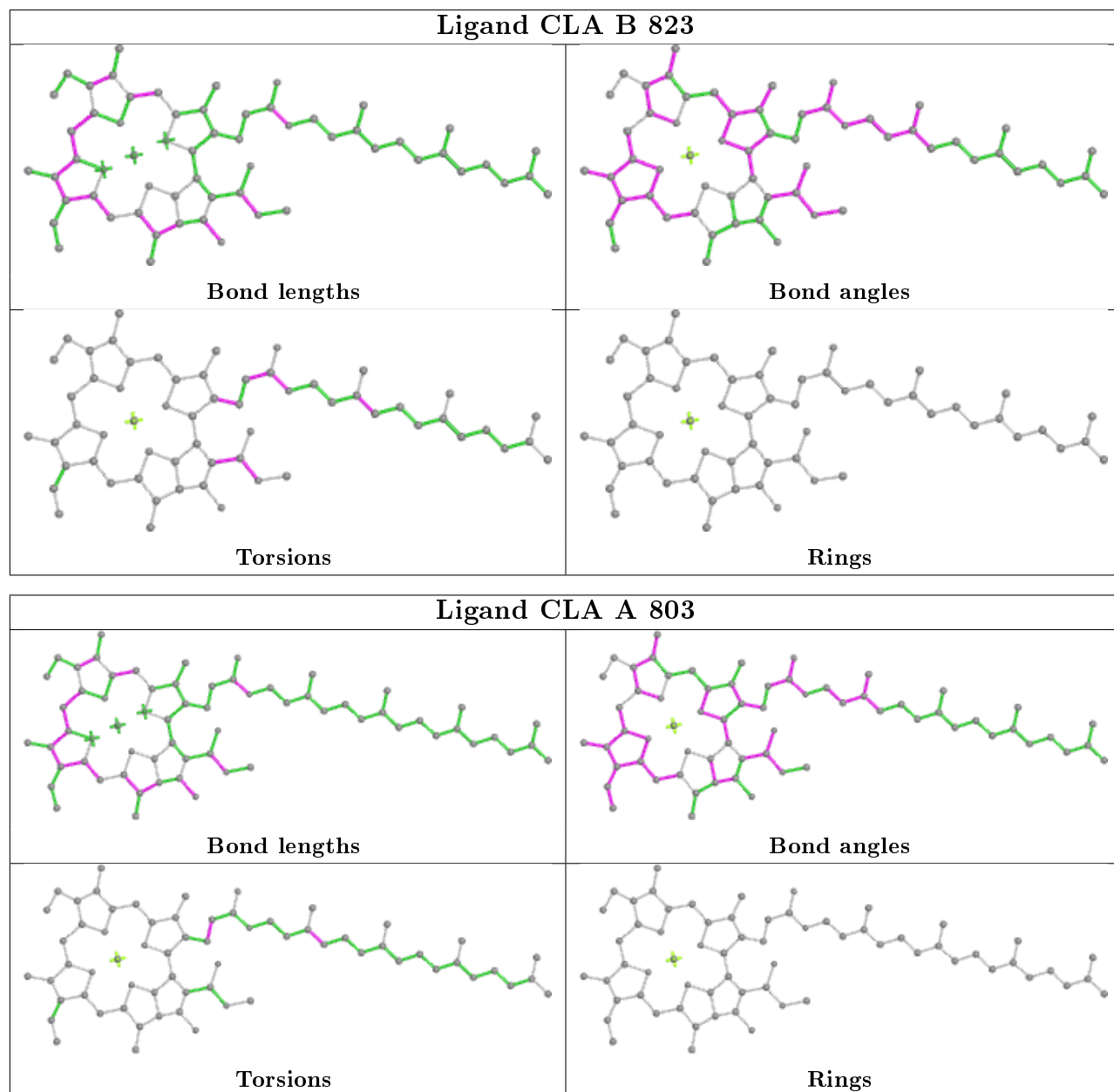
There are no ring outliers.

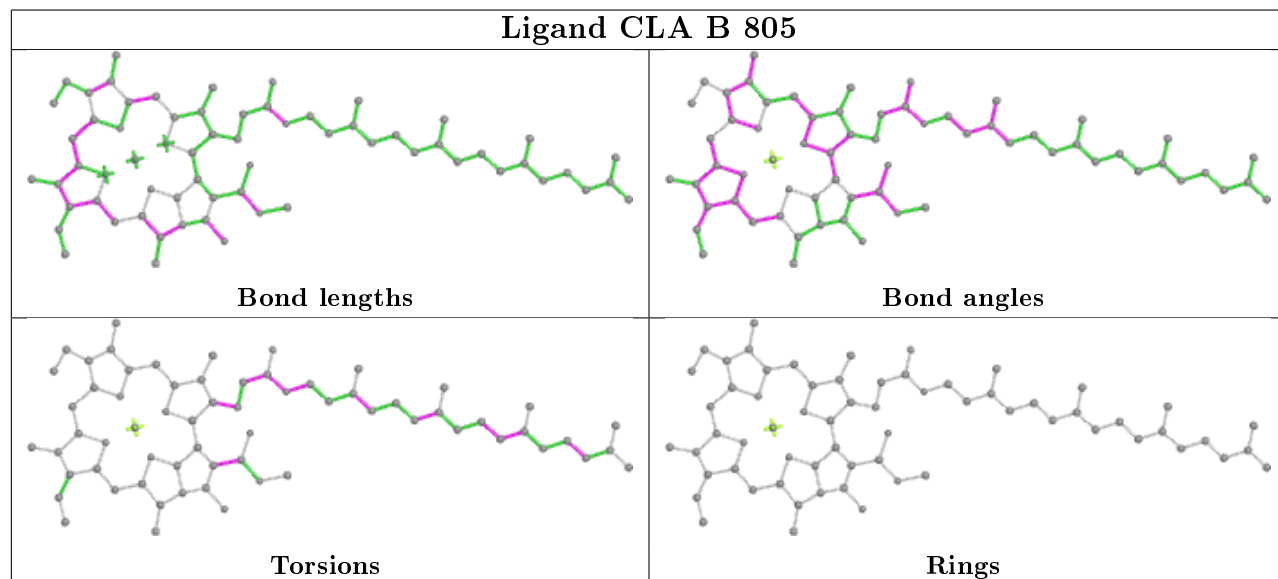
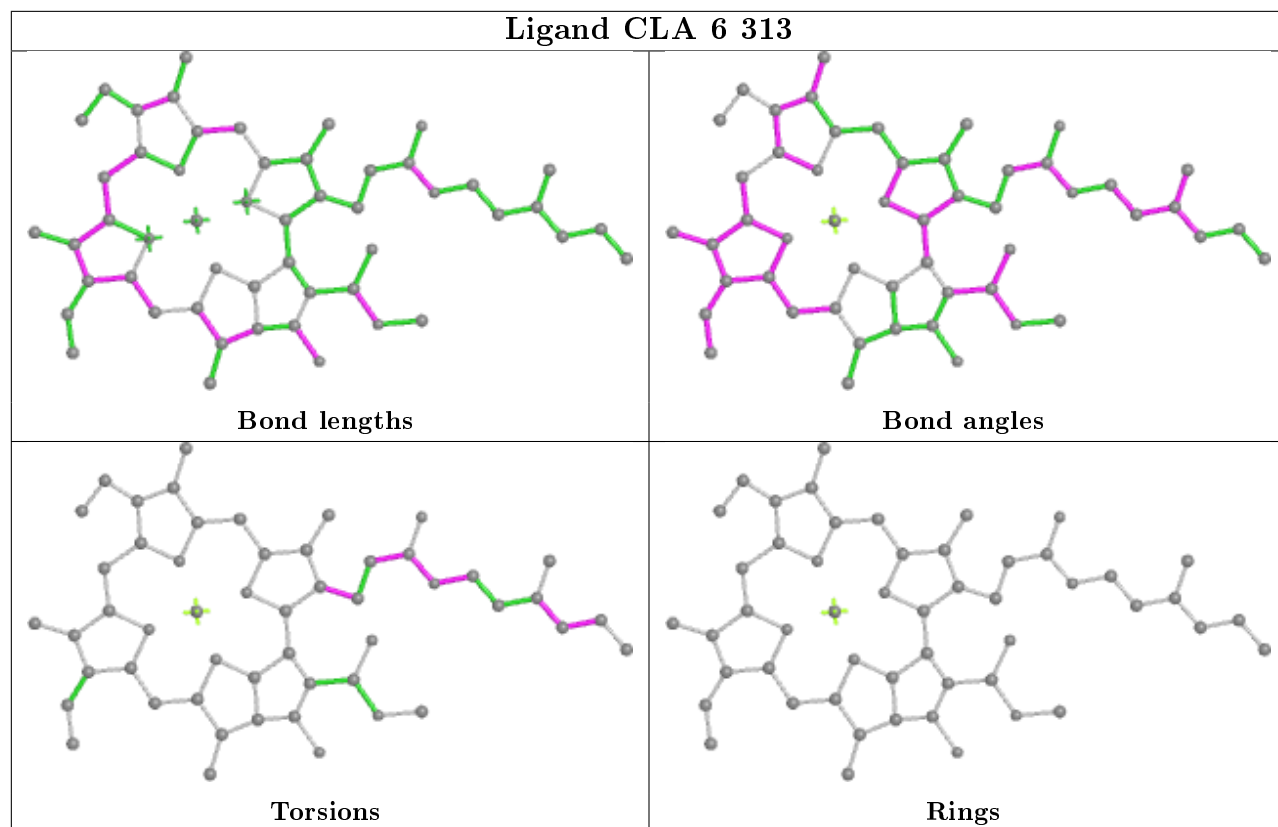
No monomer is involved in short contacts.

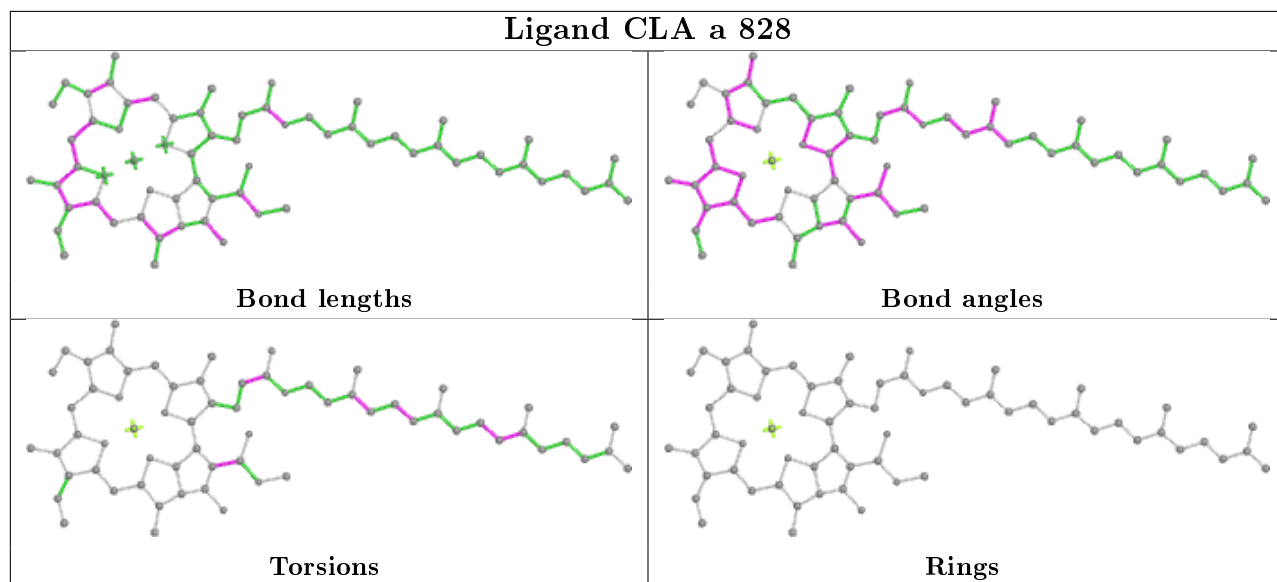
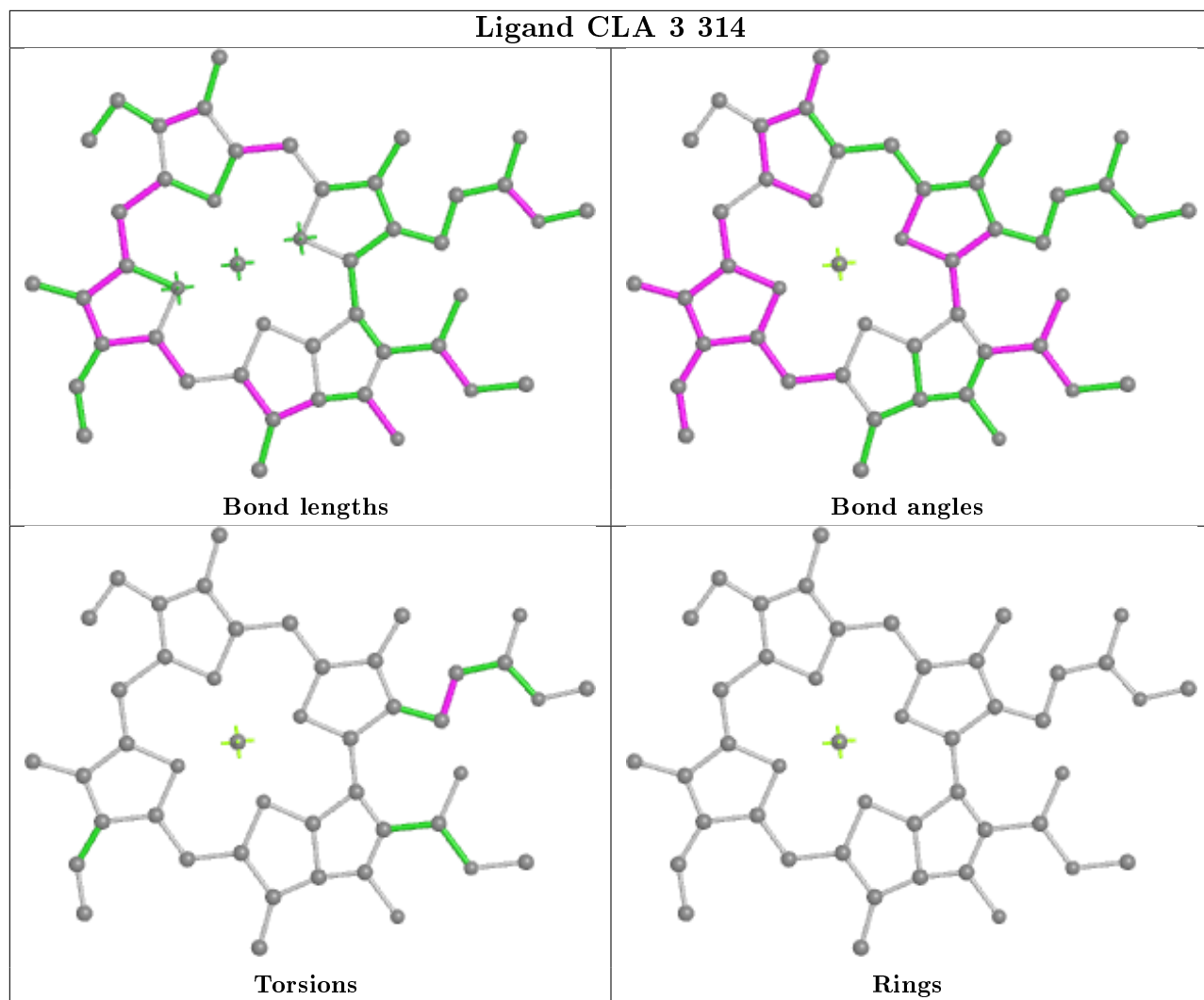
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

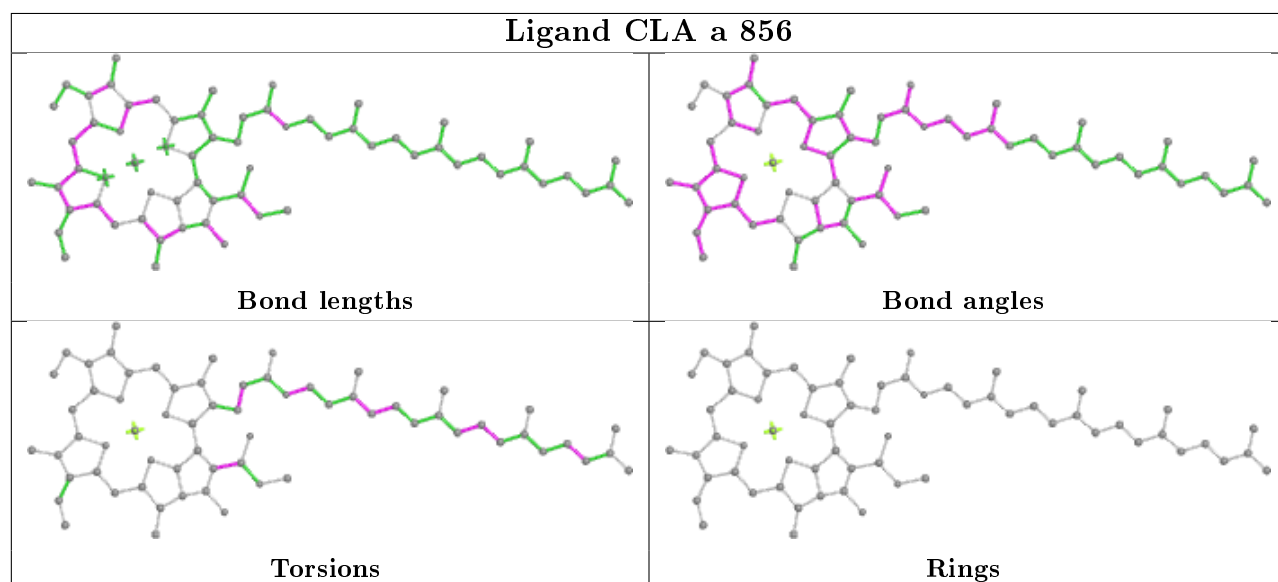
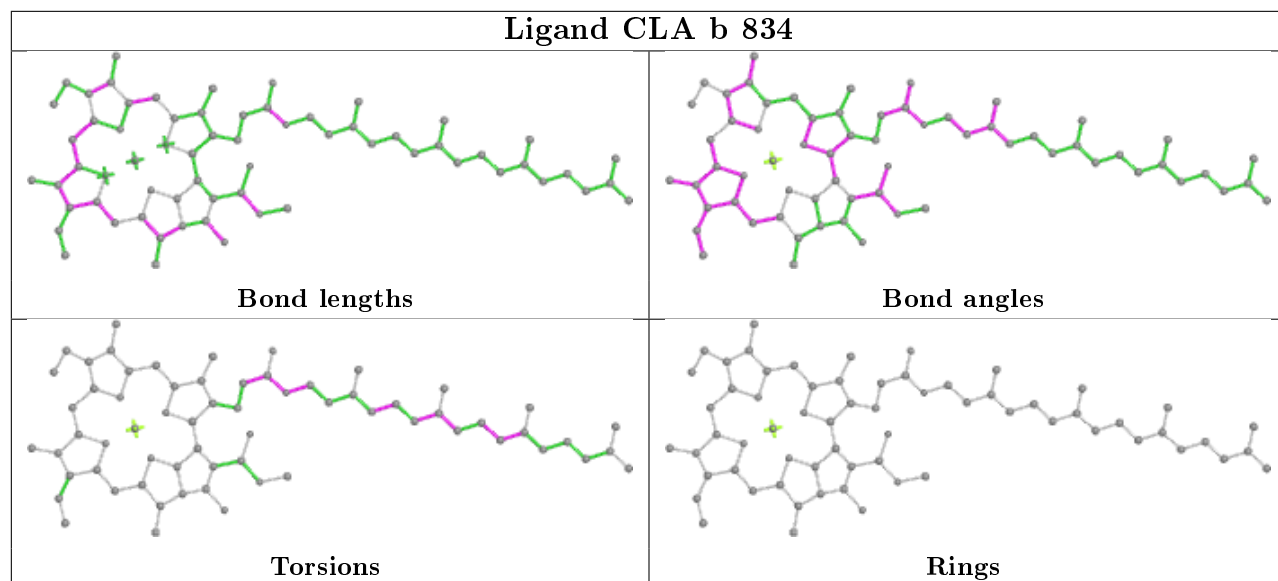
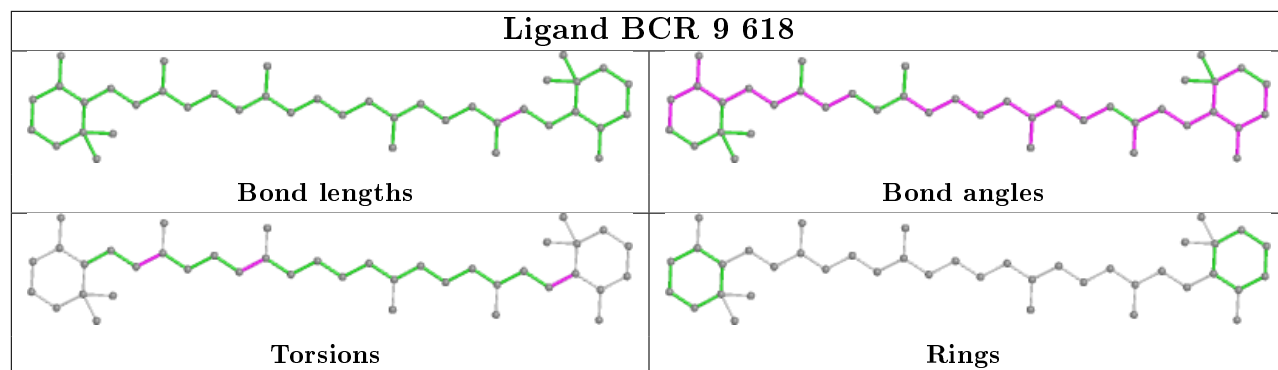
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

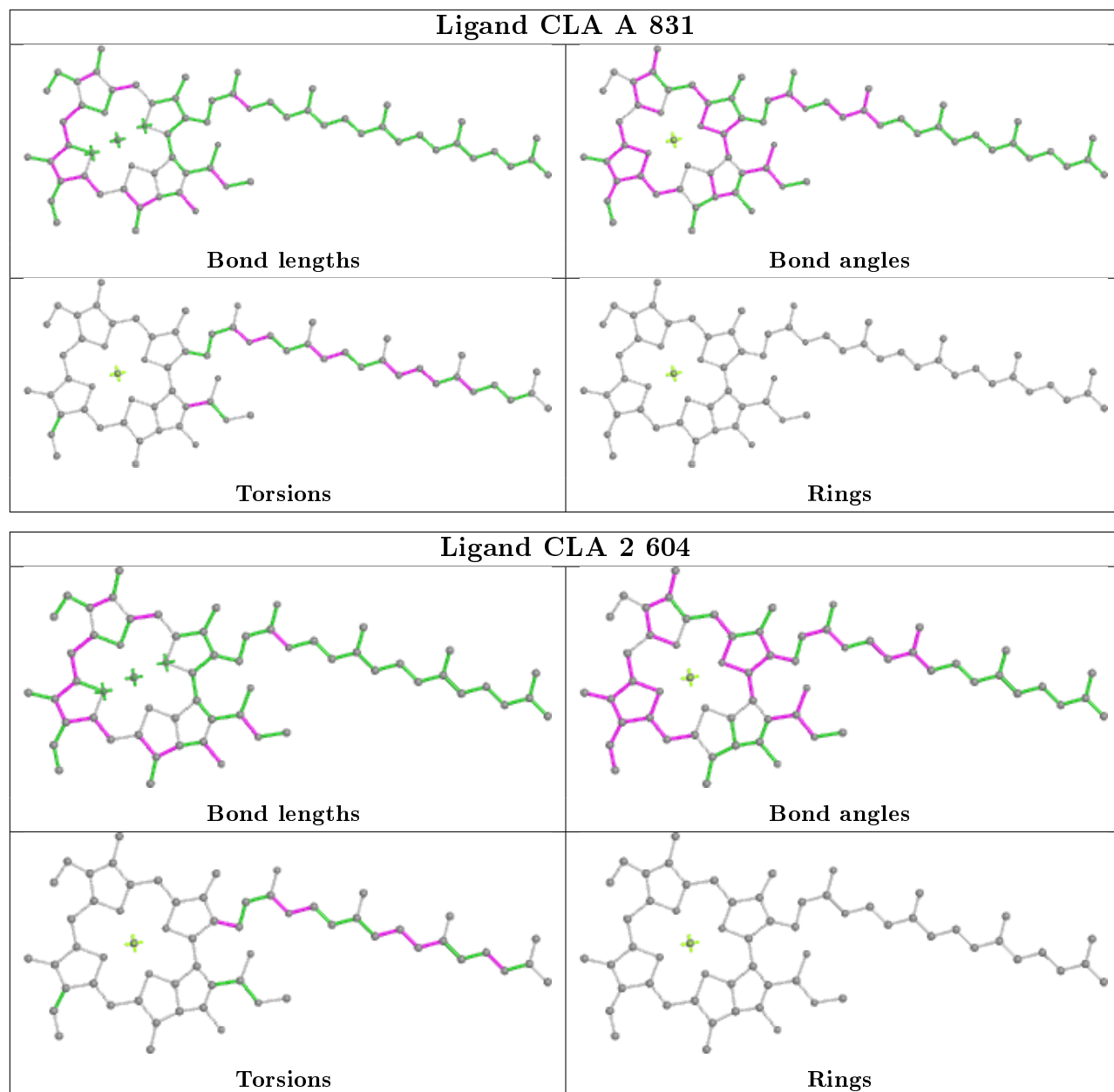


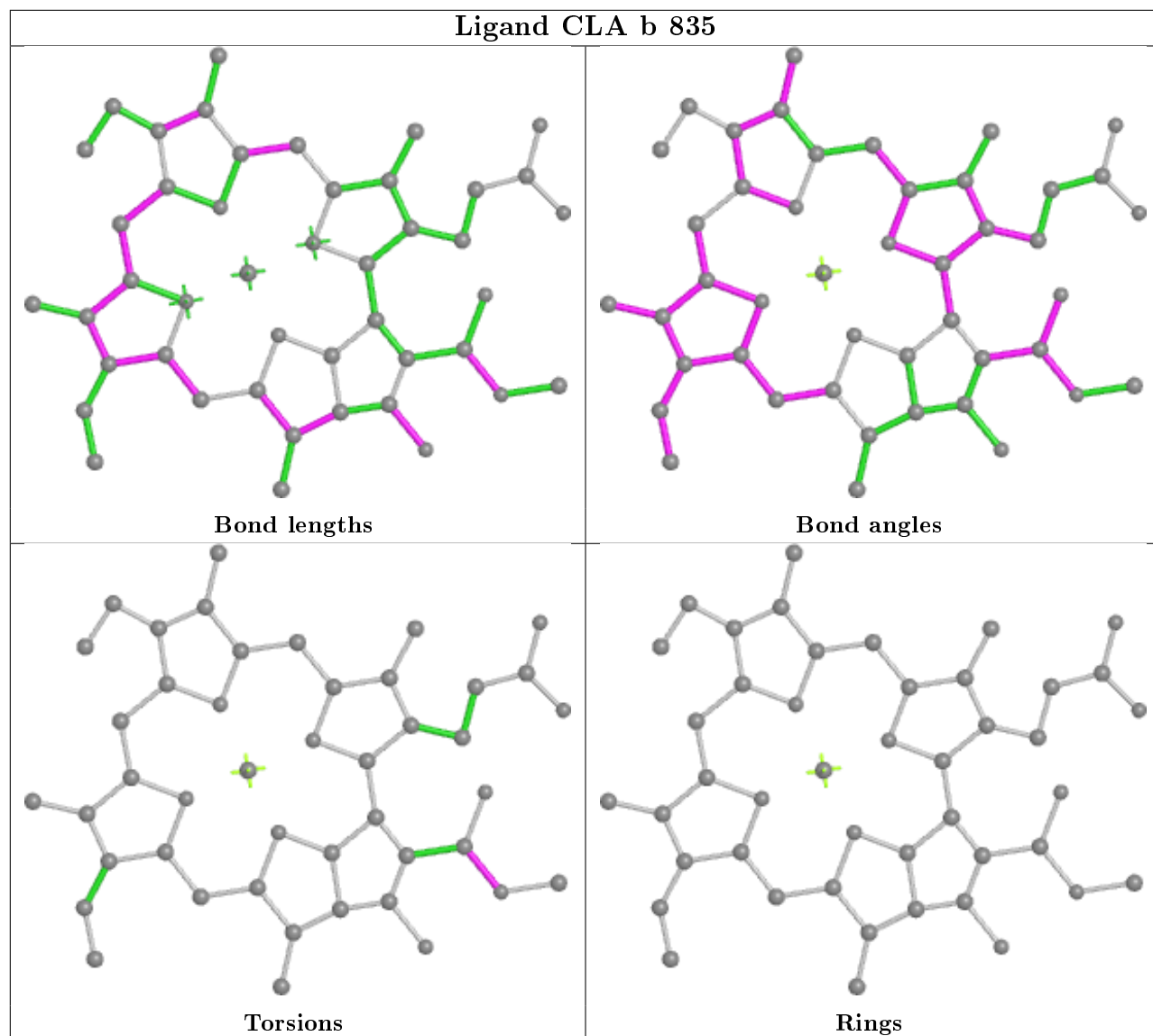


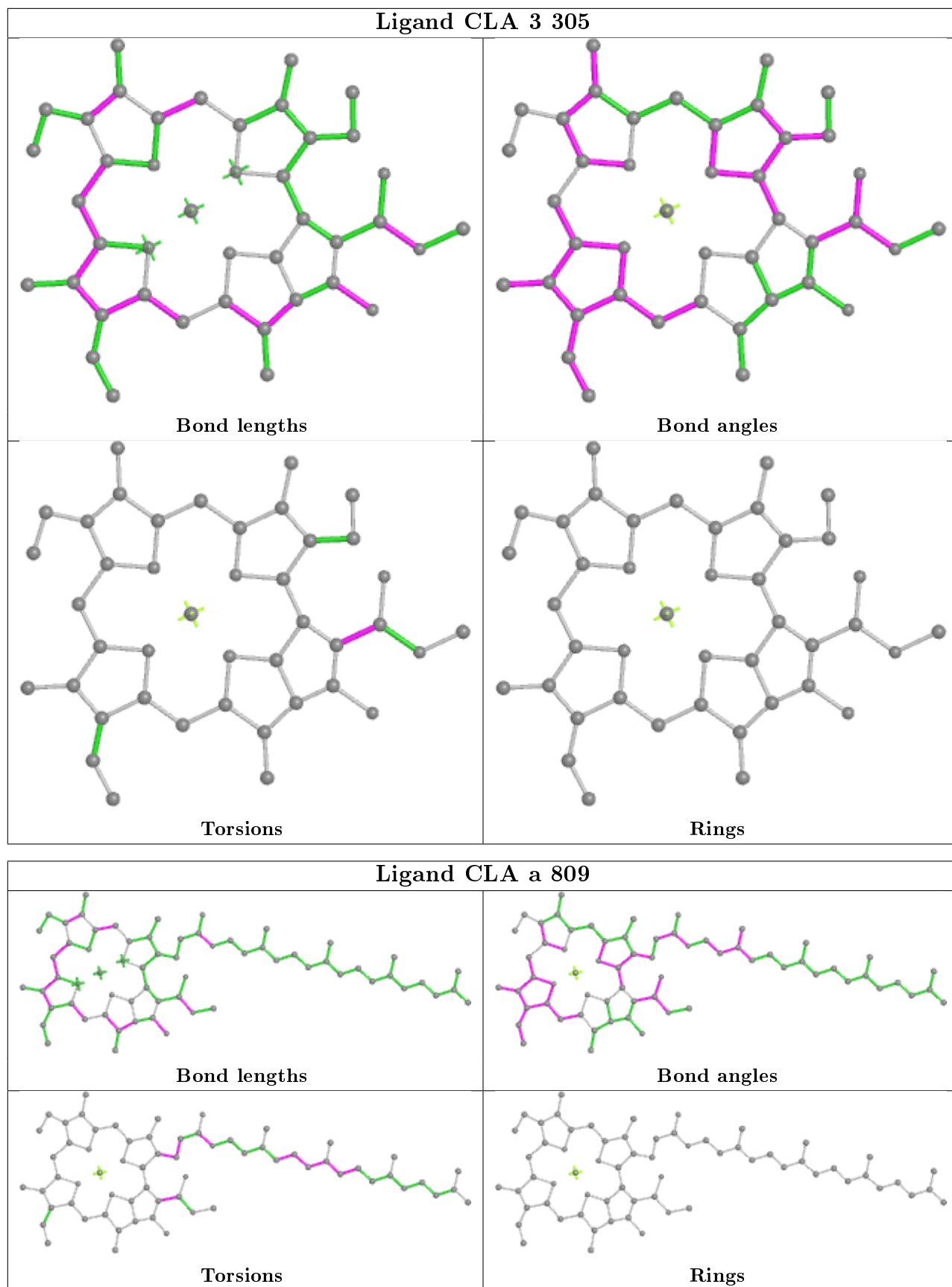


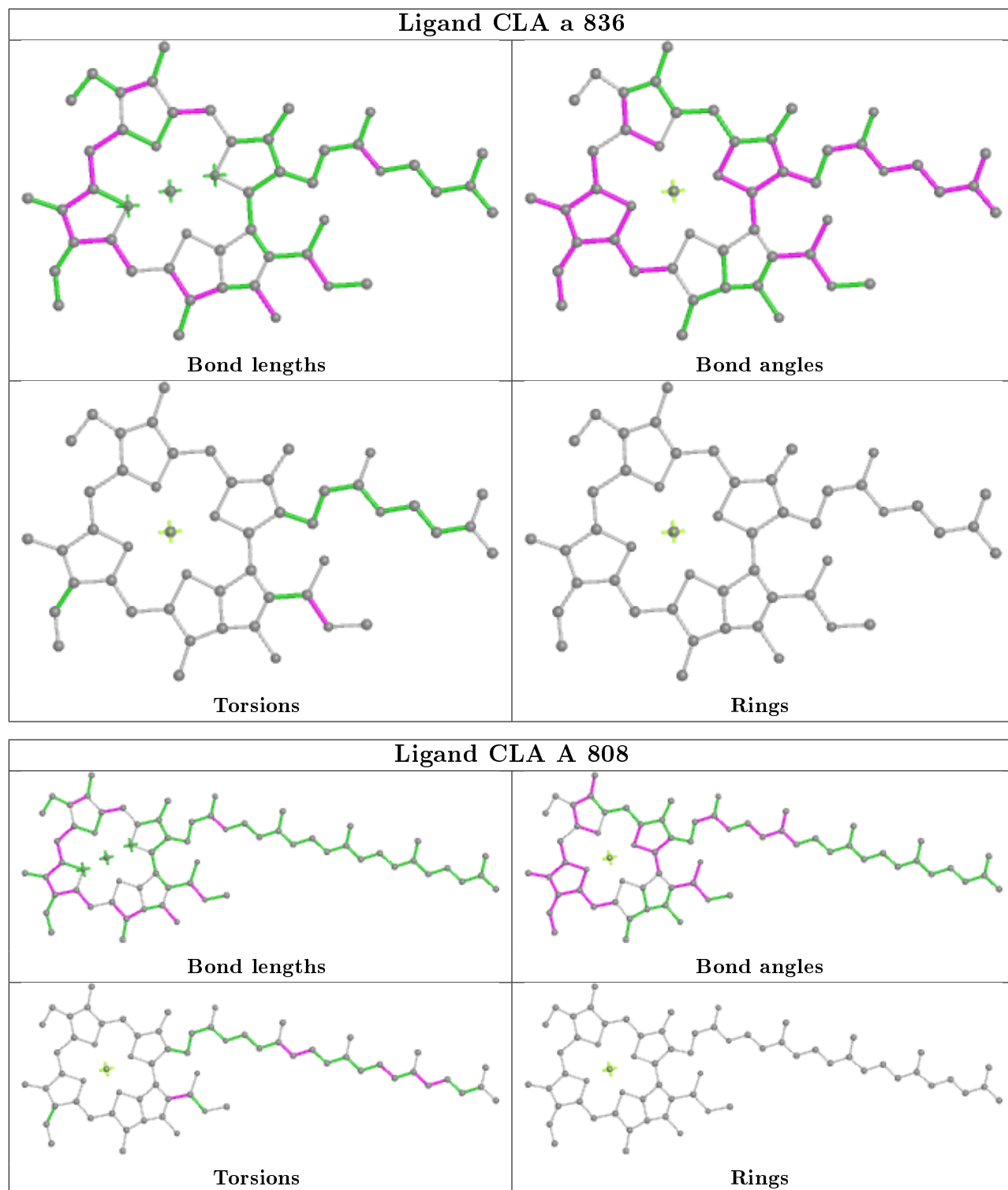


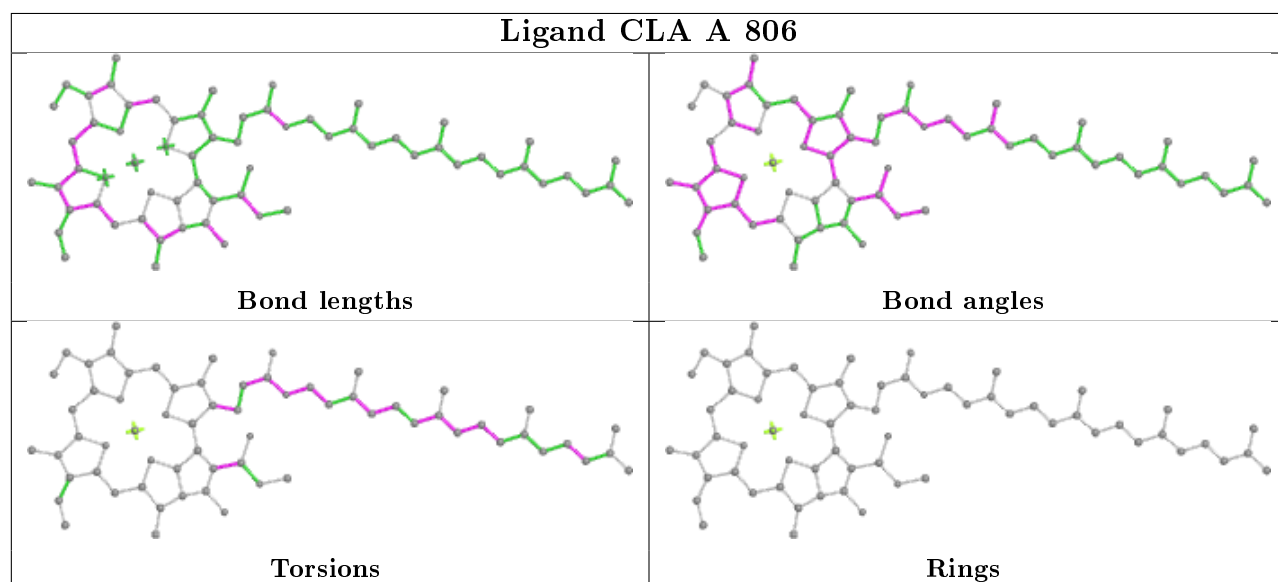
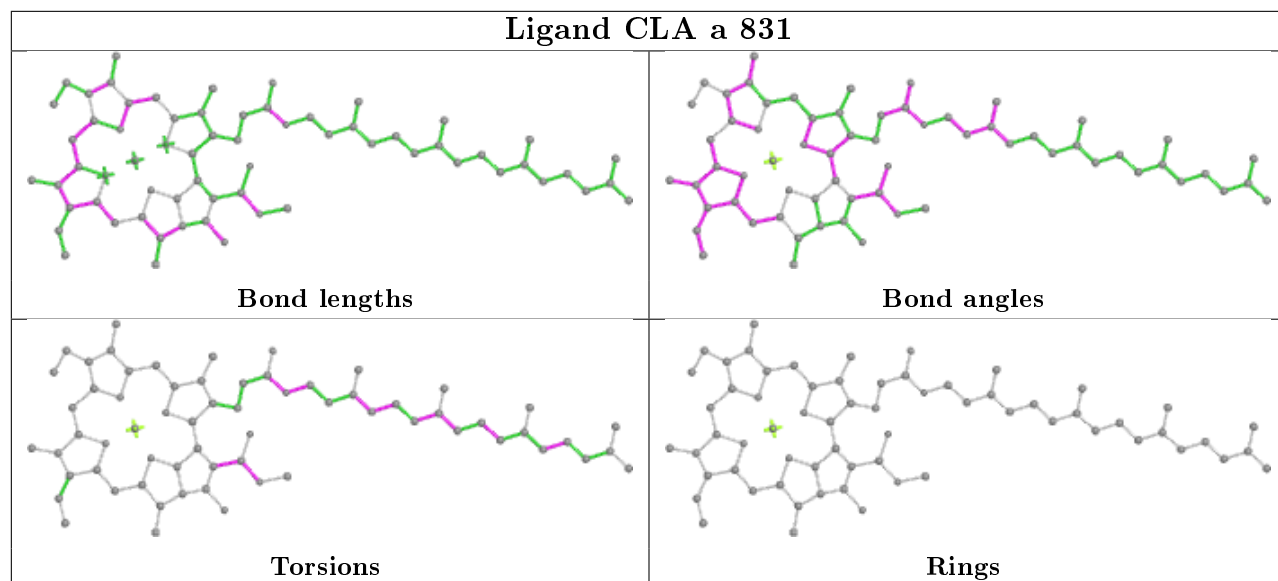
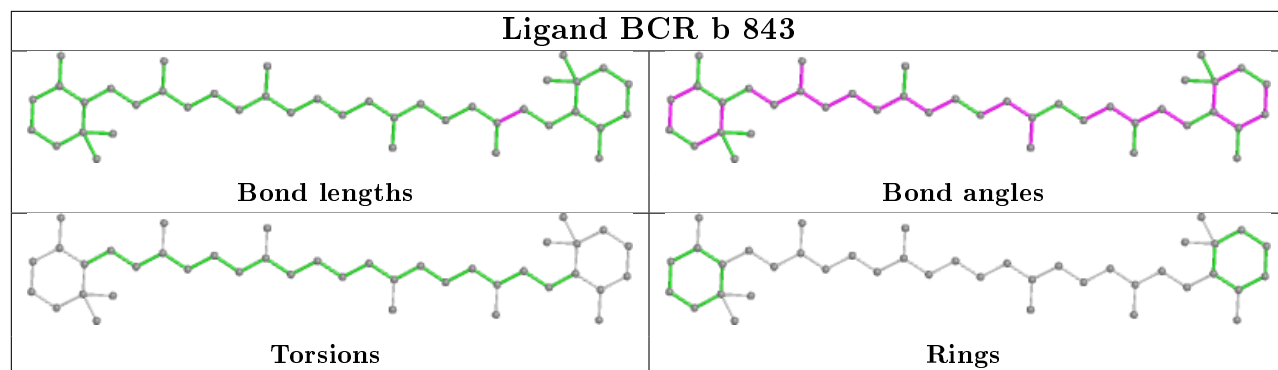


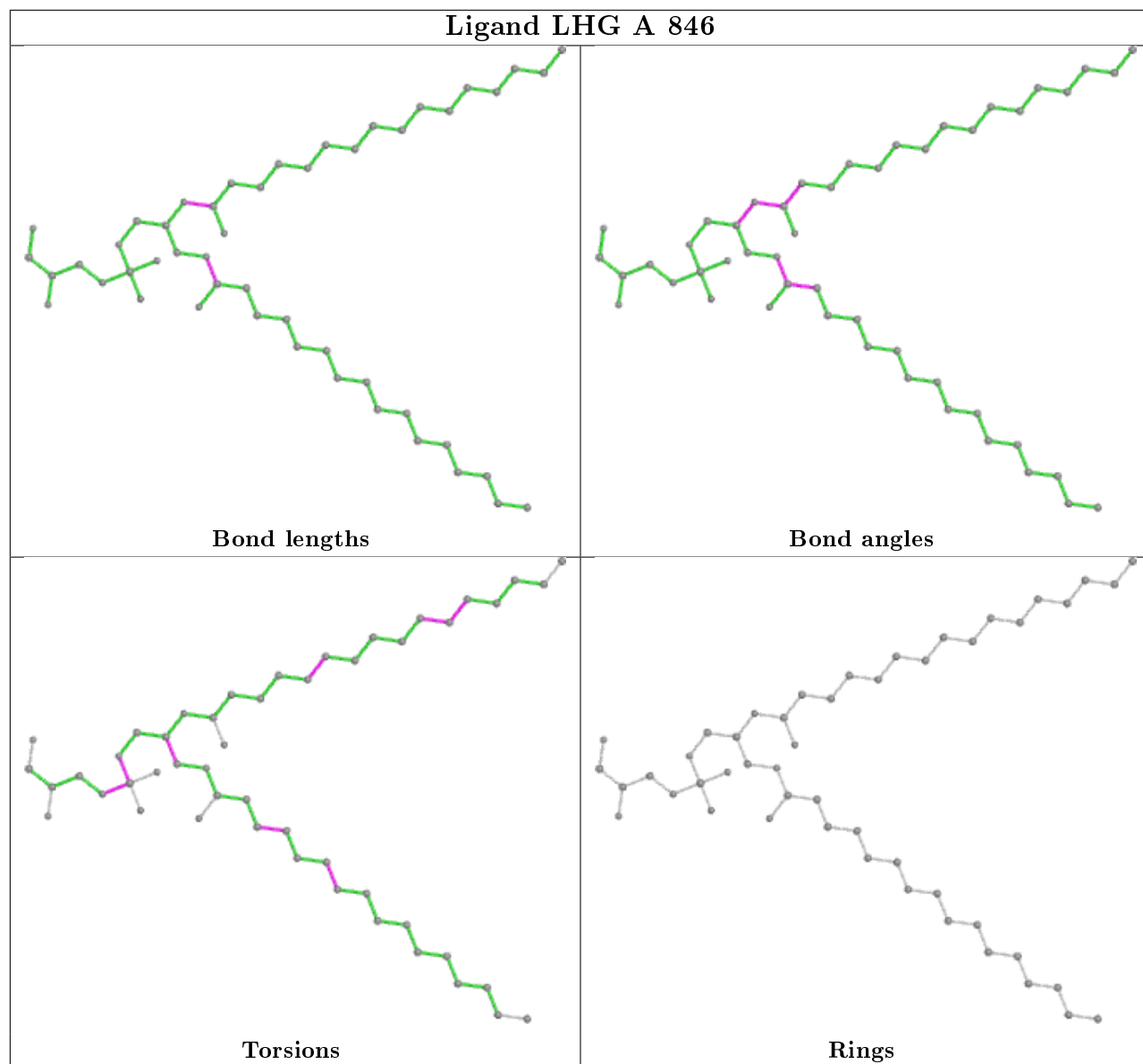


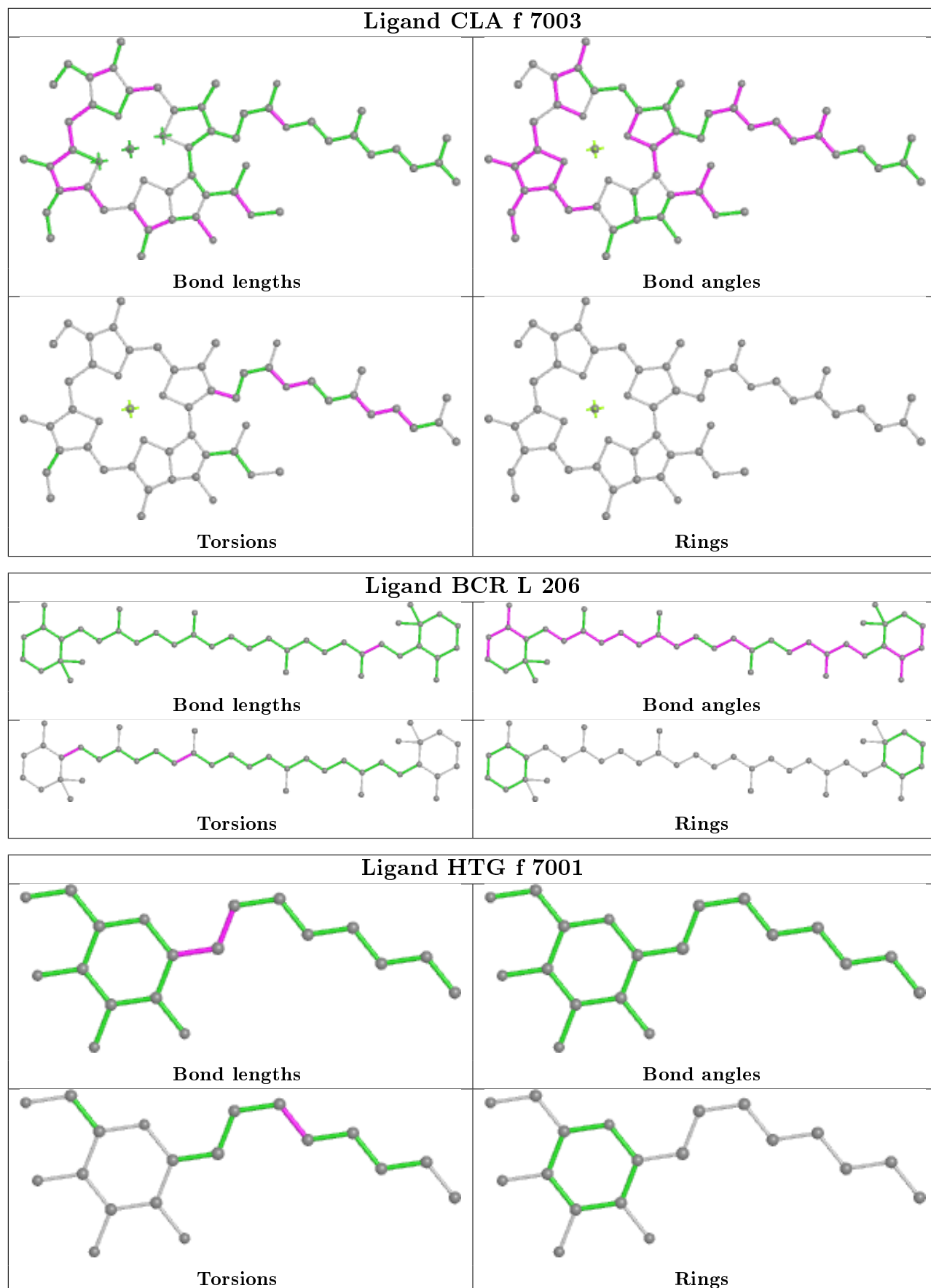


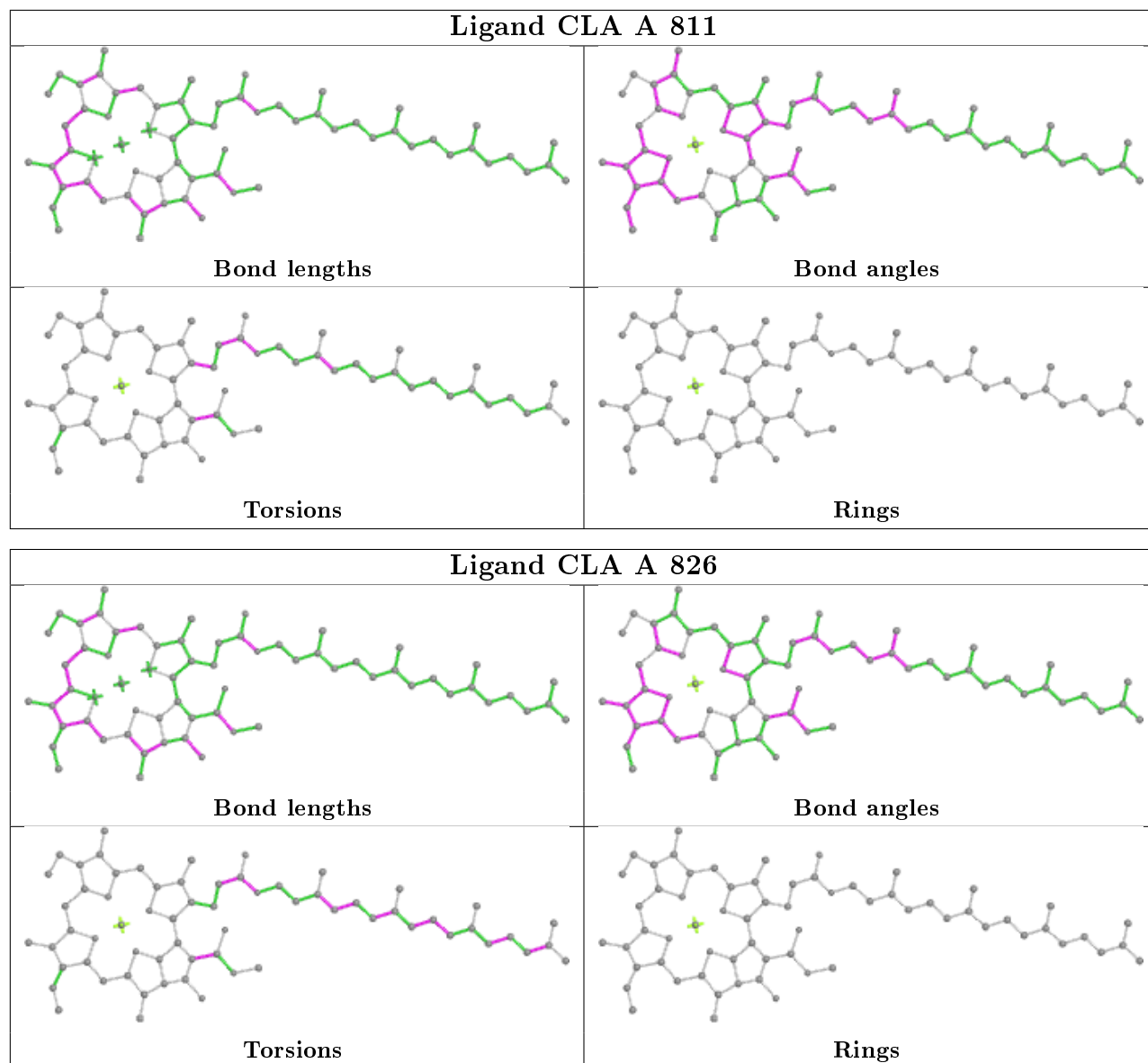


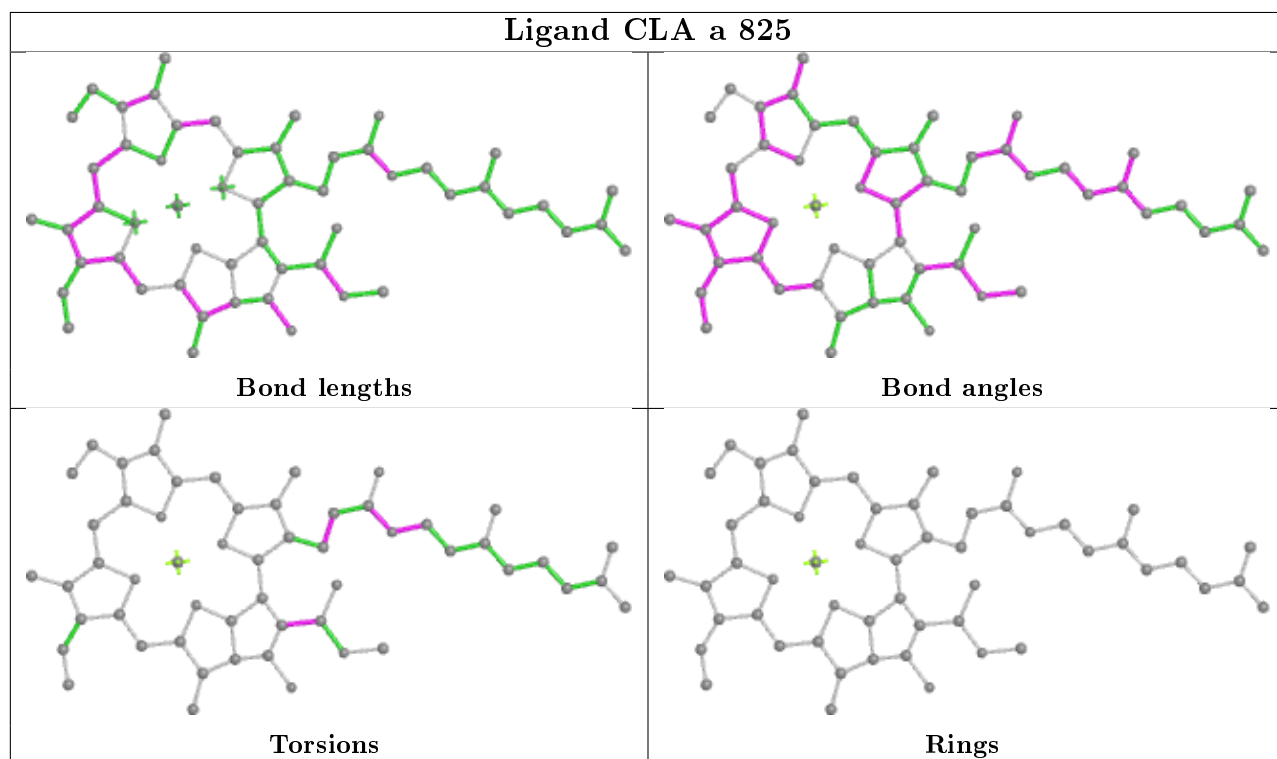
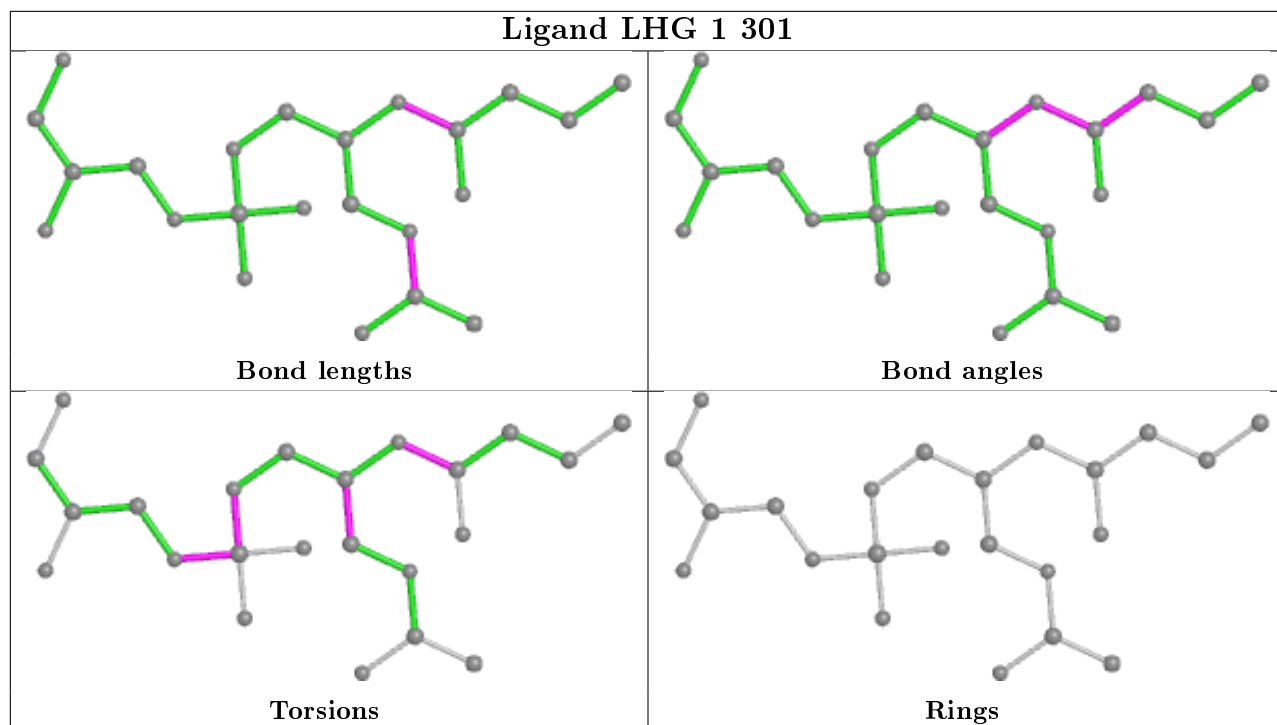


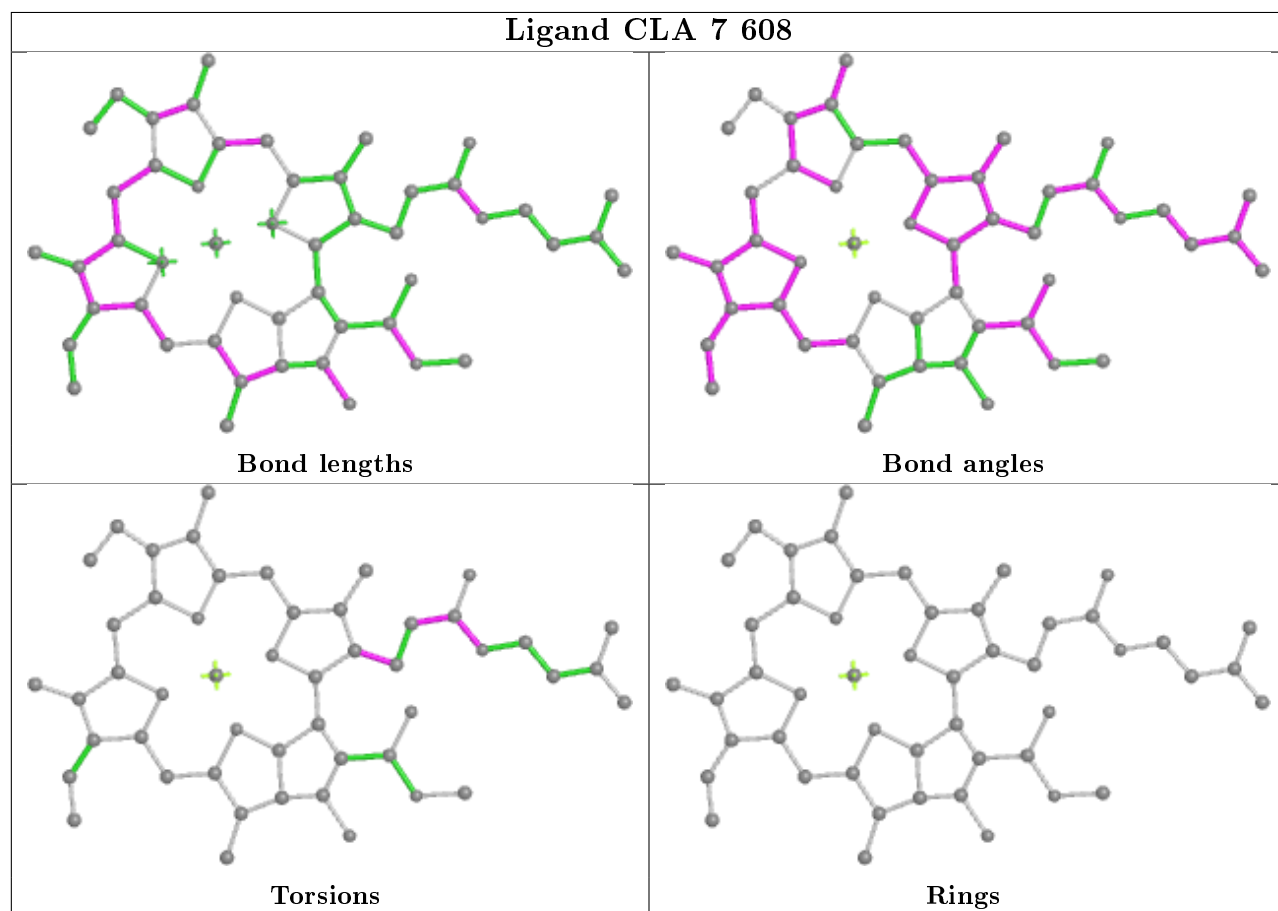
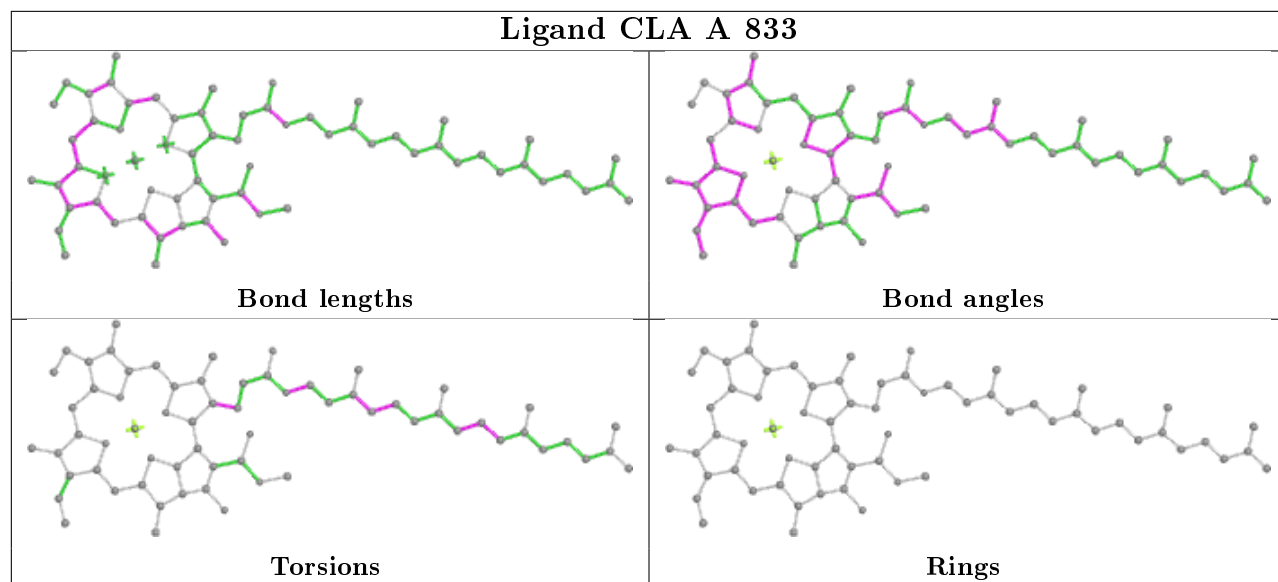


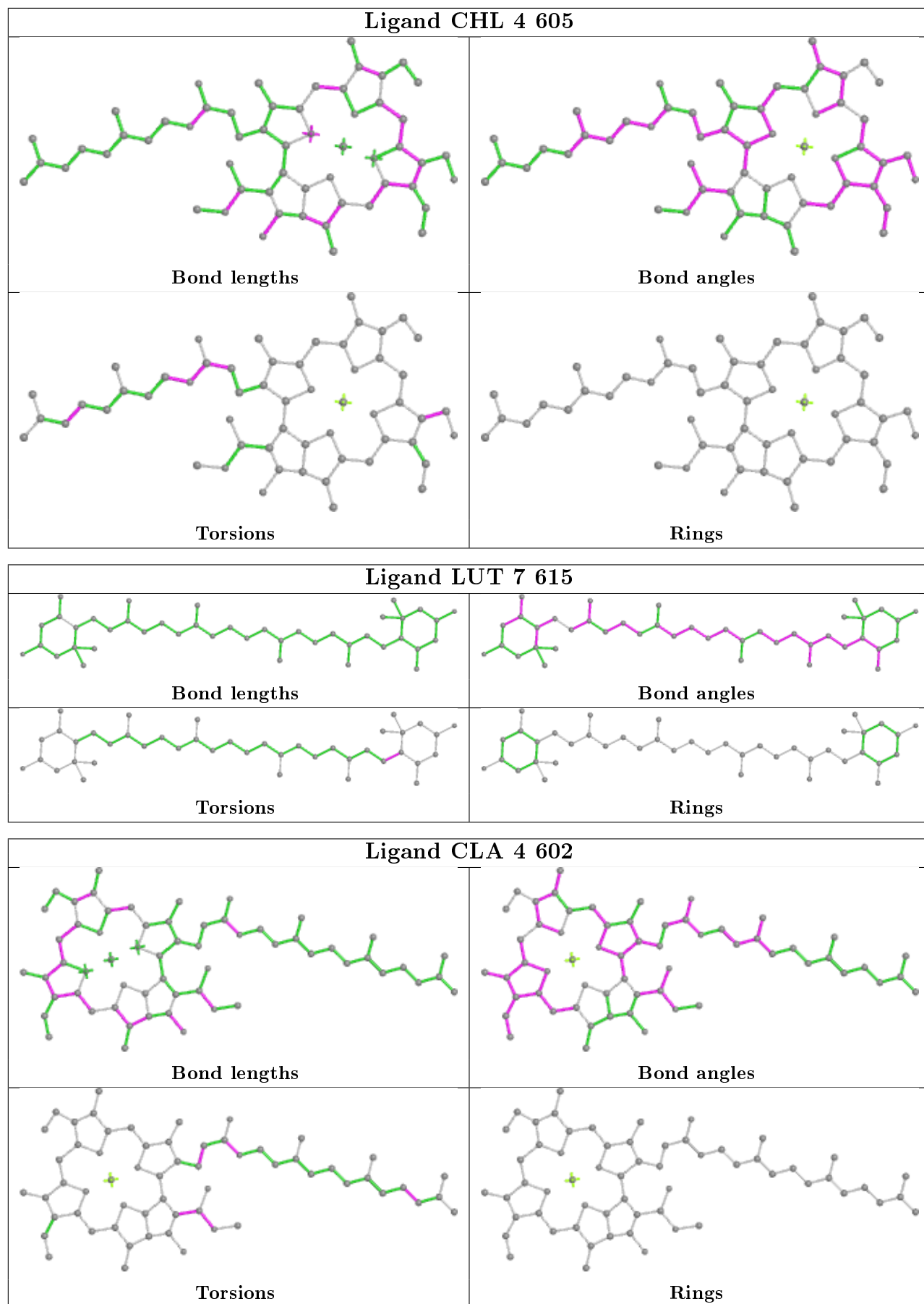


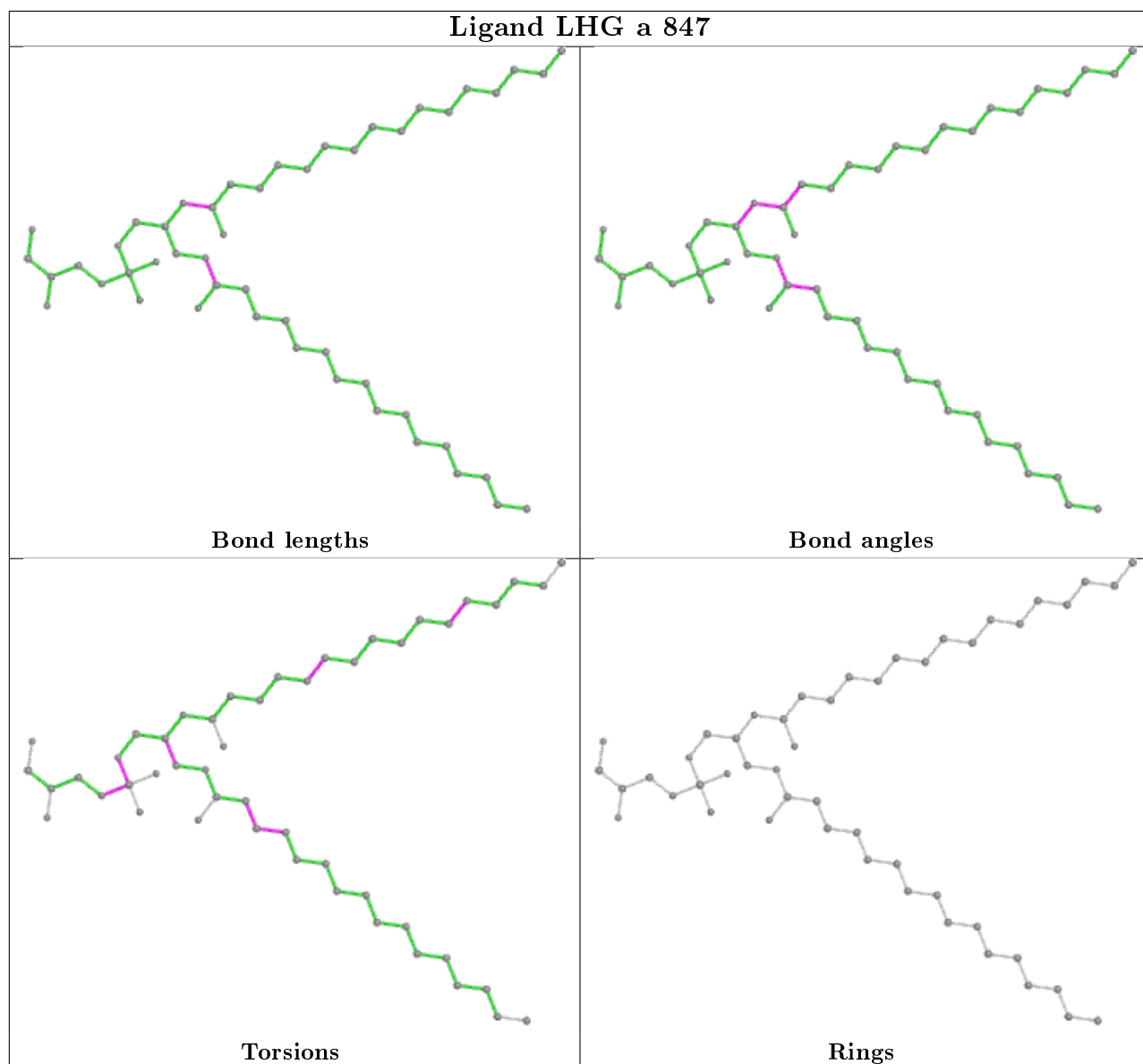
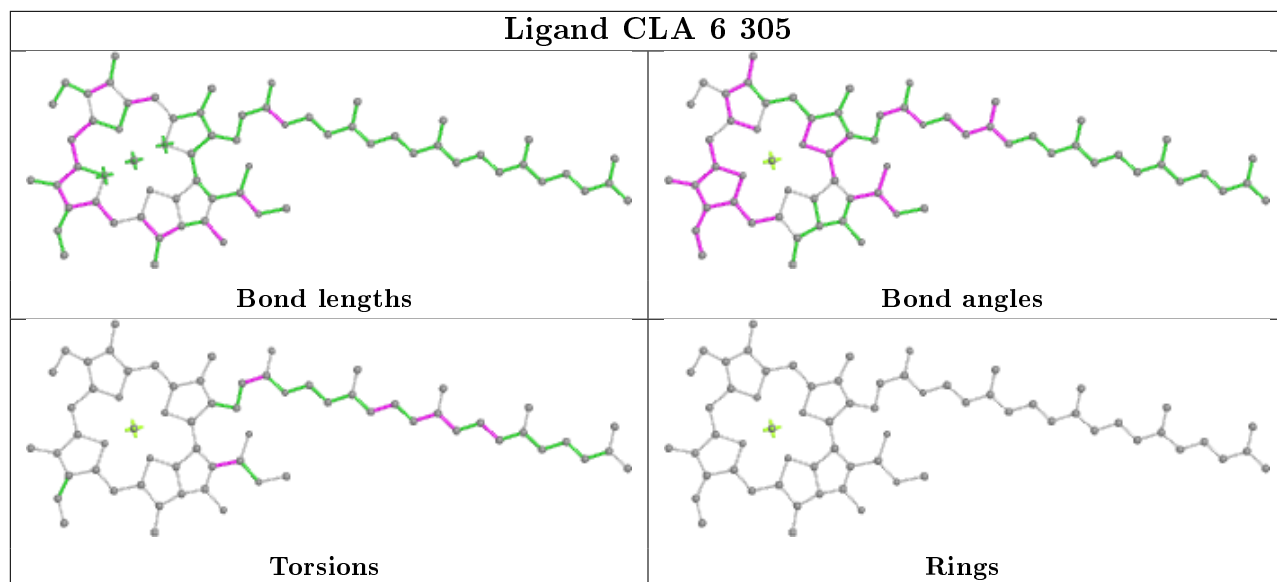


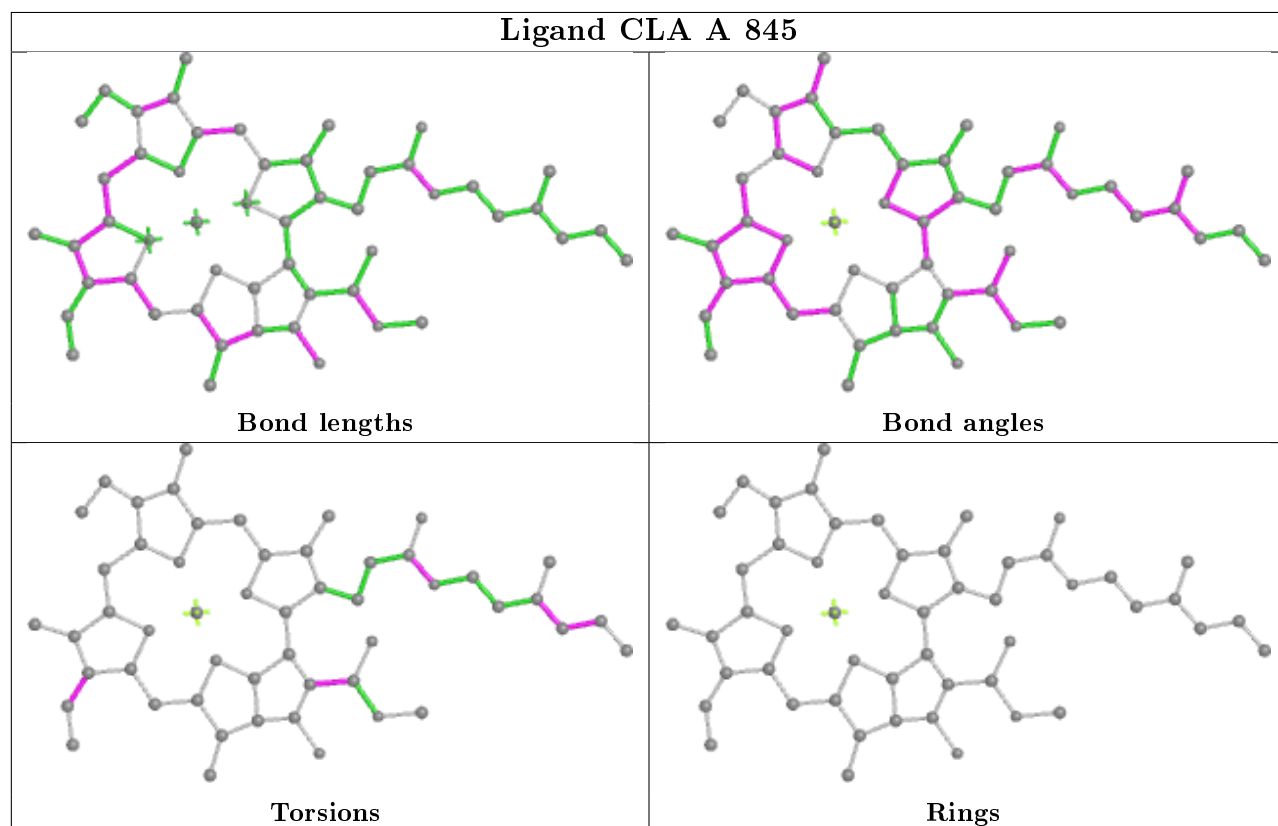
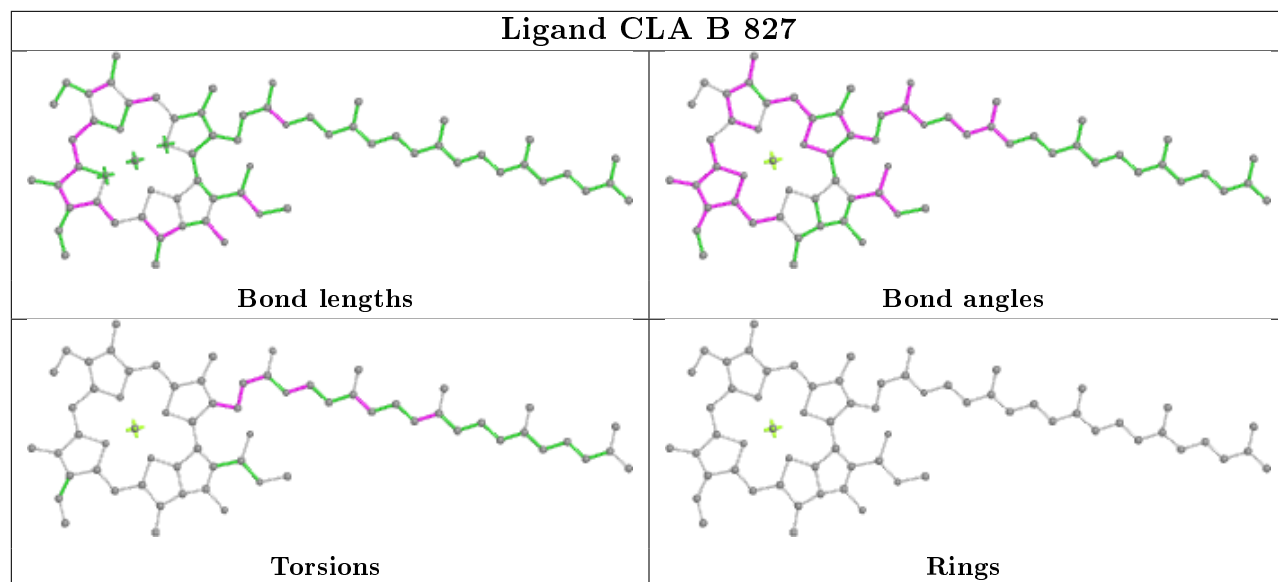


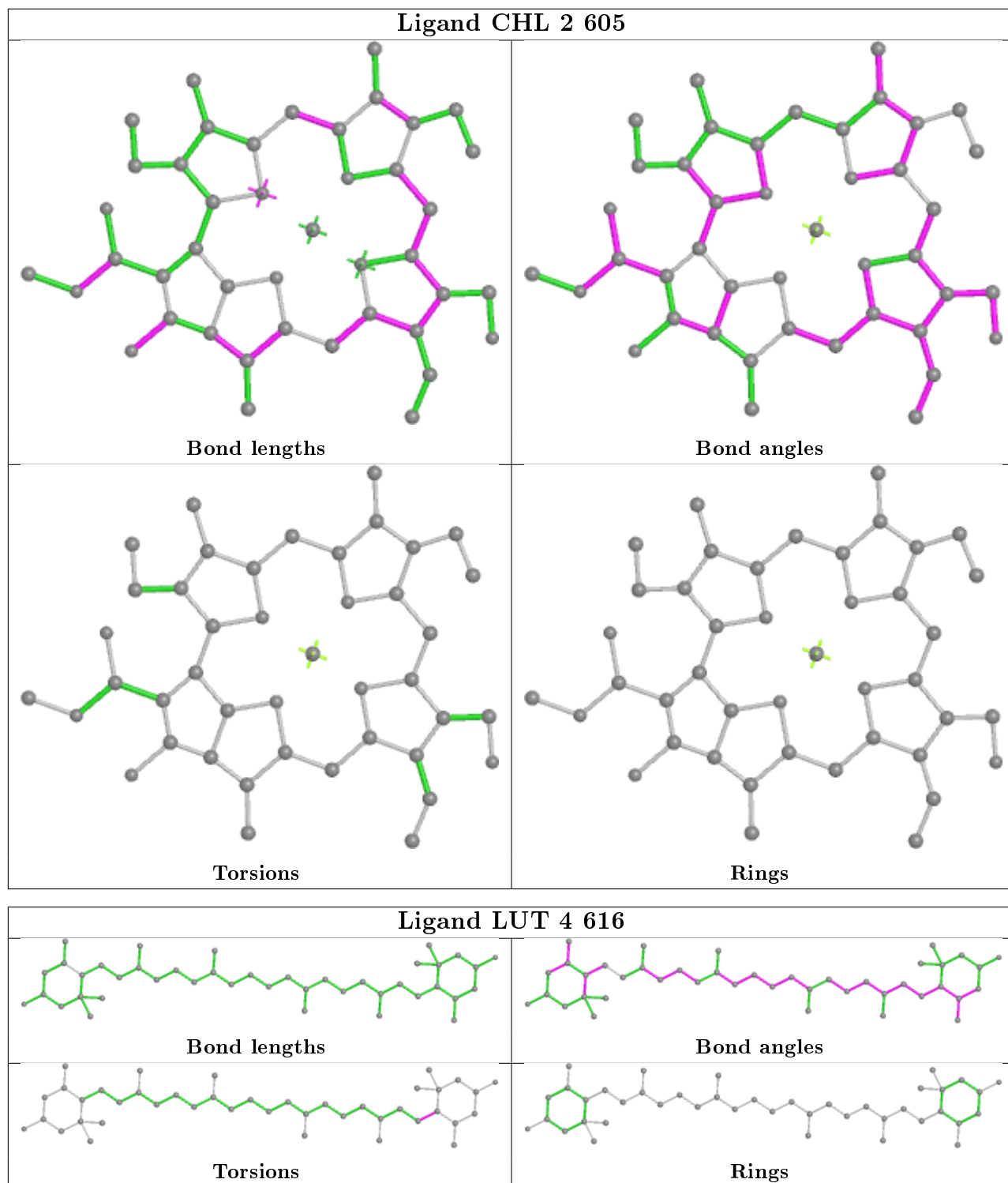


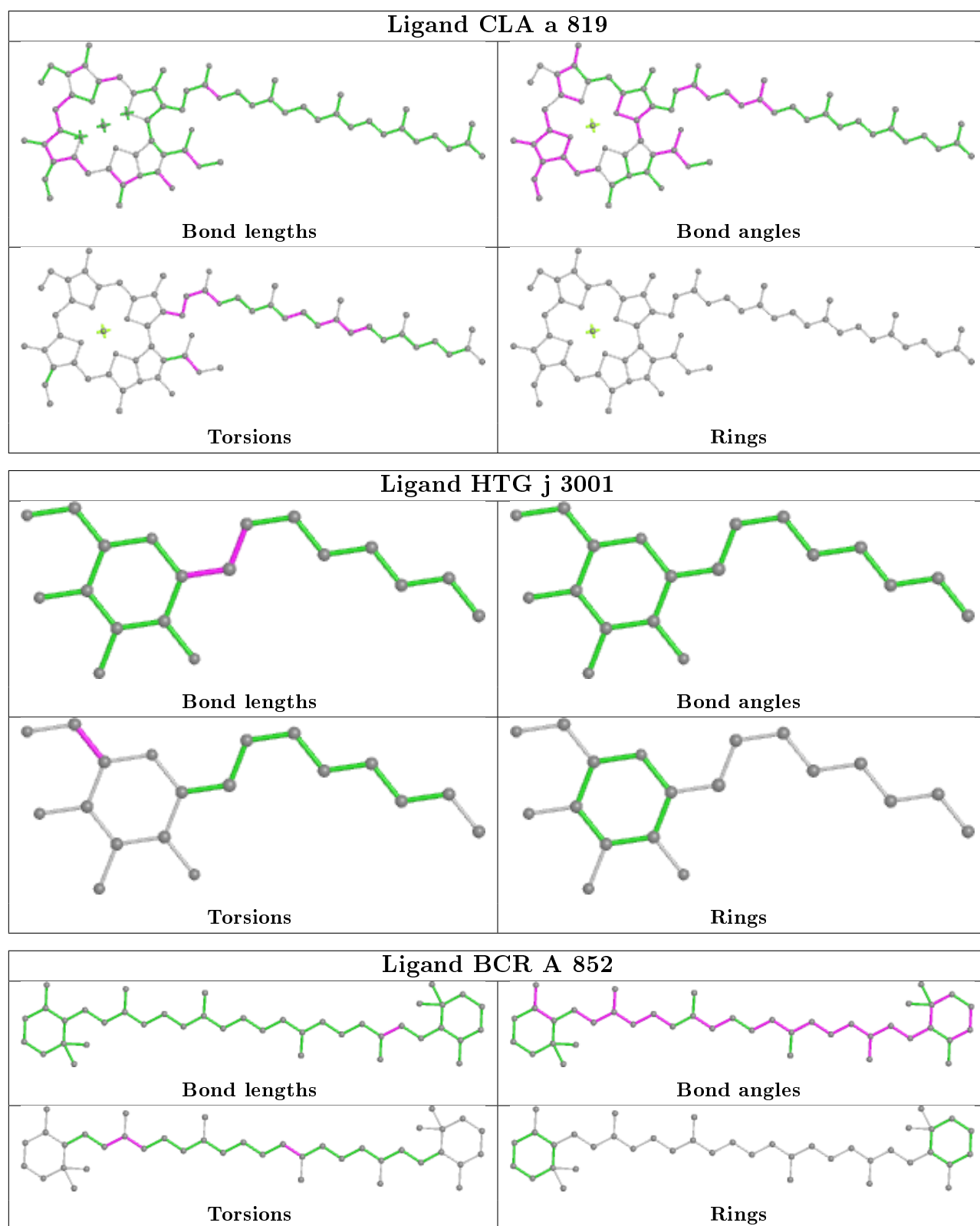


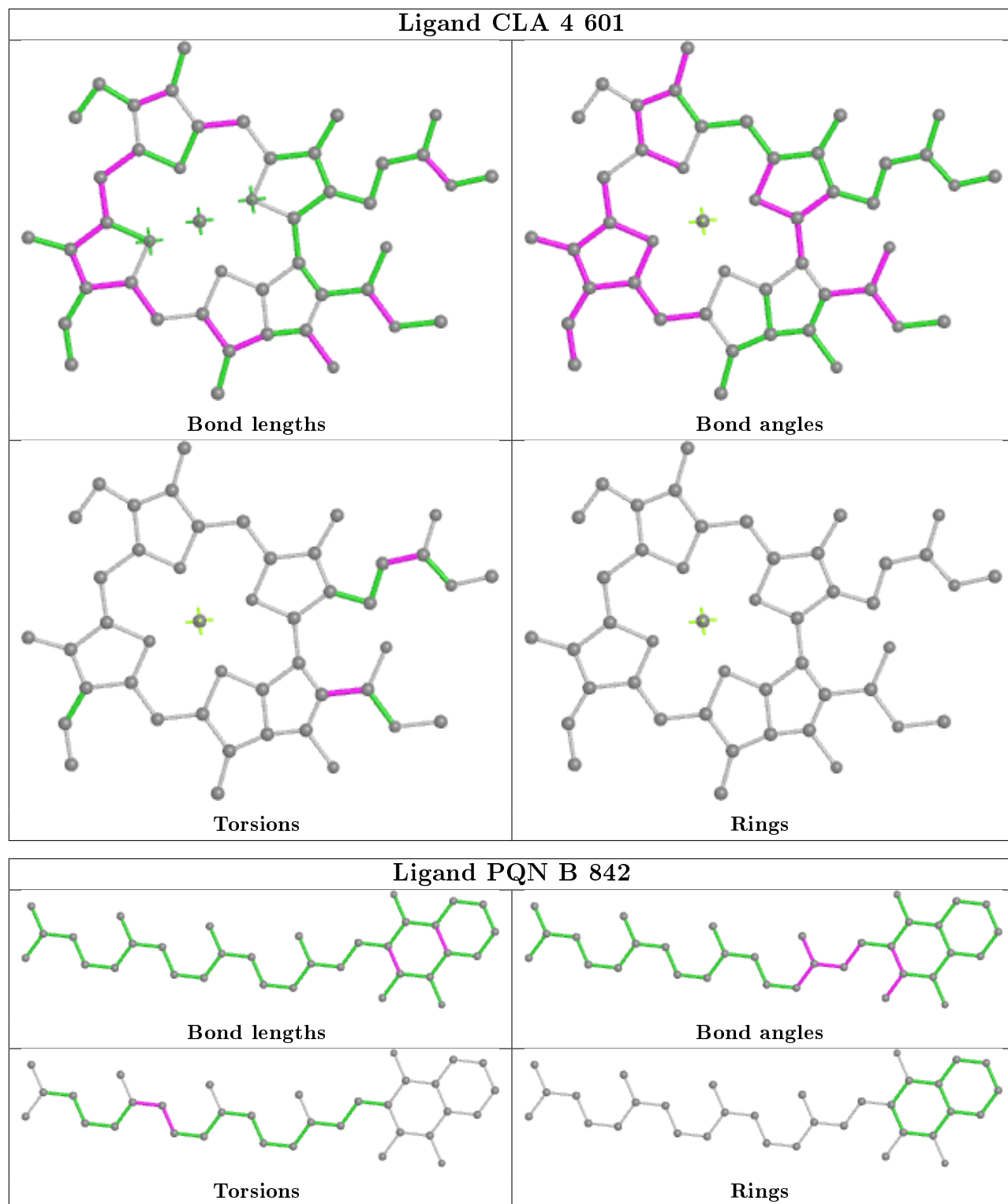


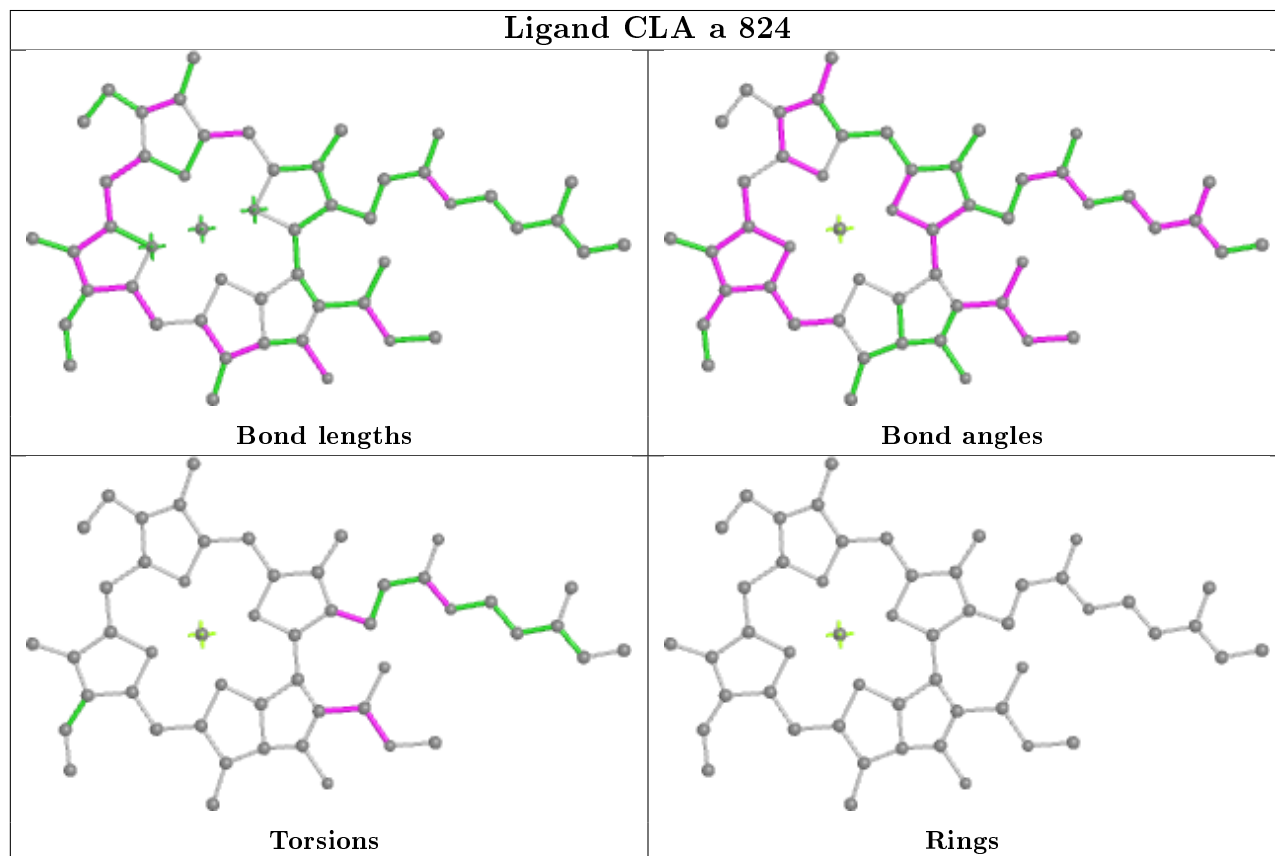
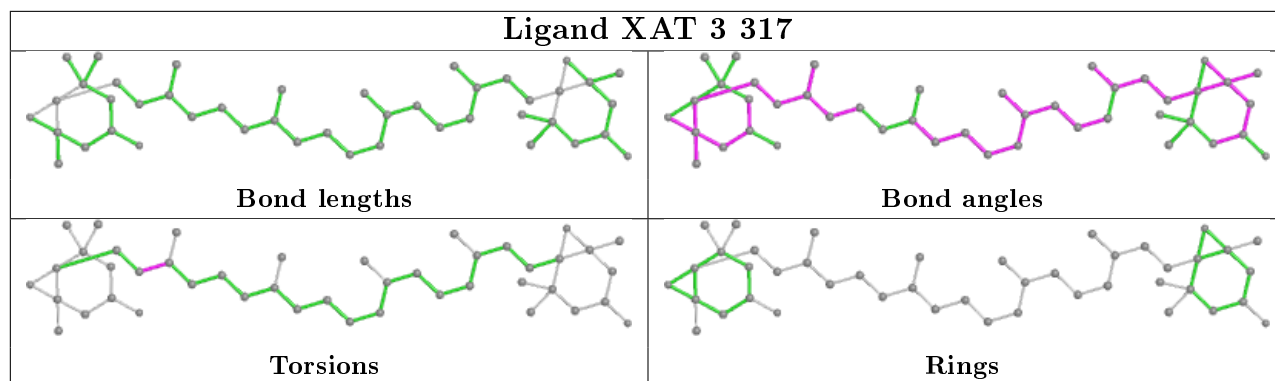


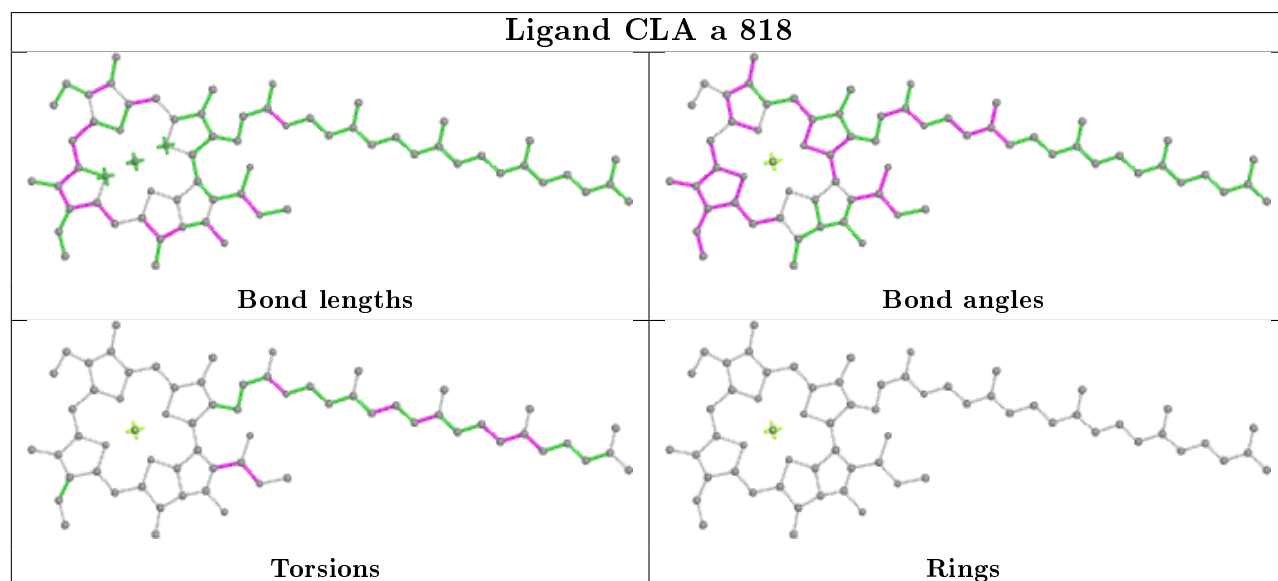
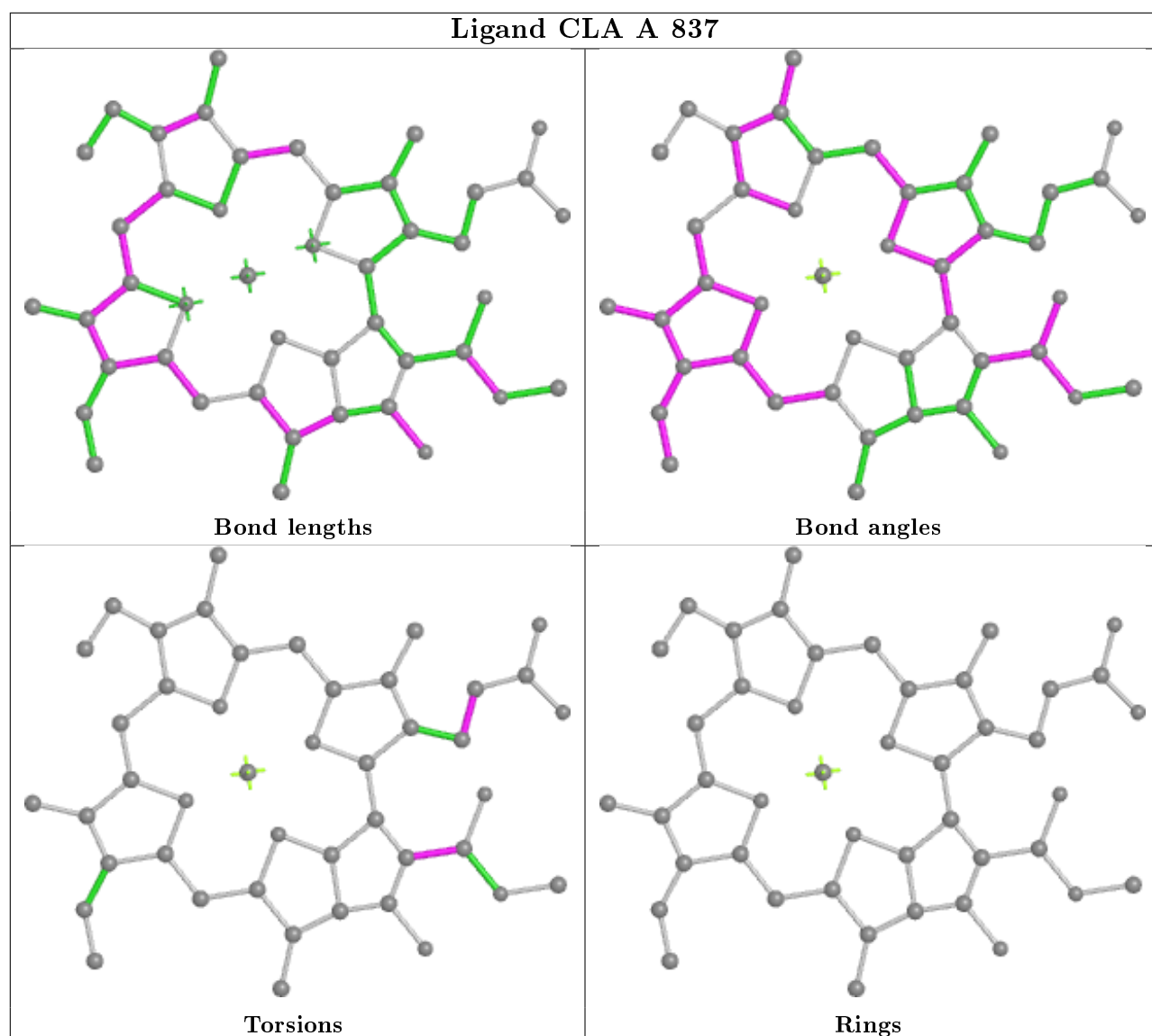


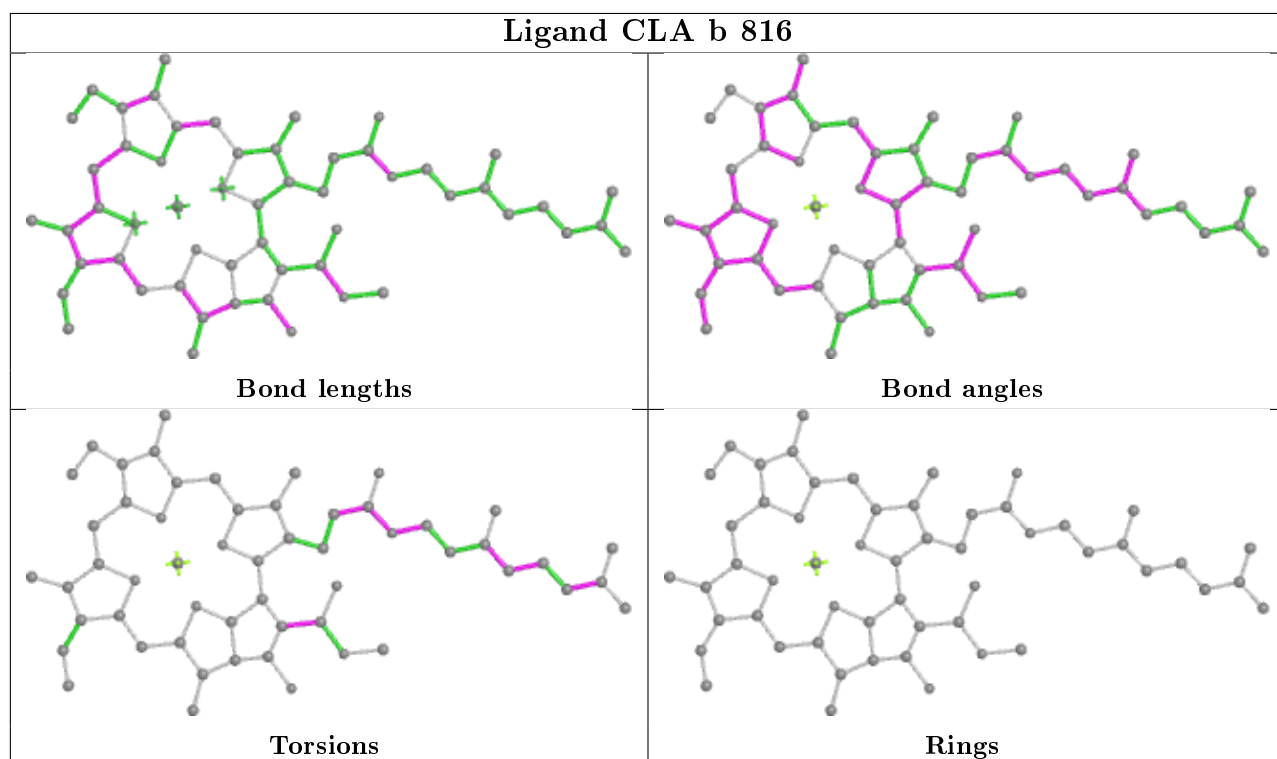
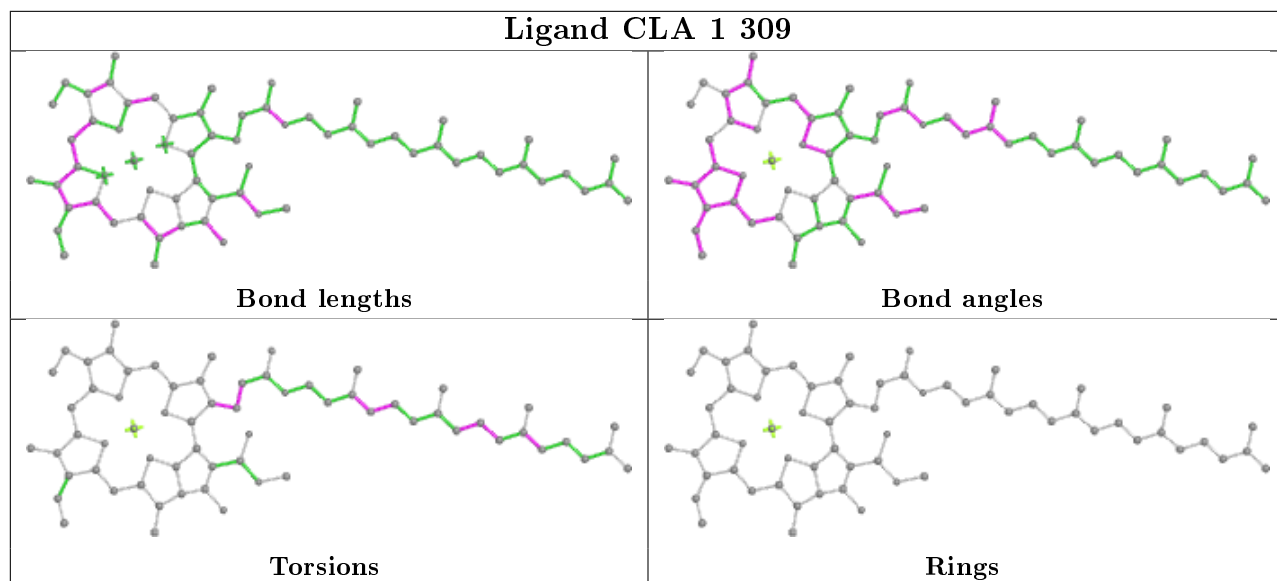
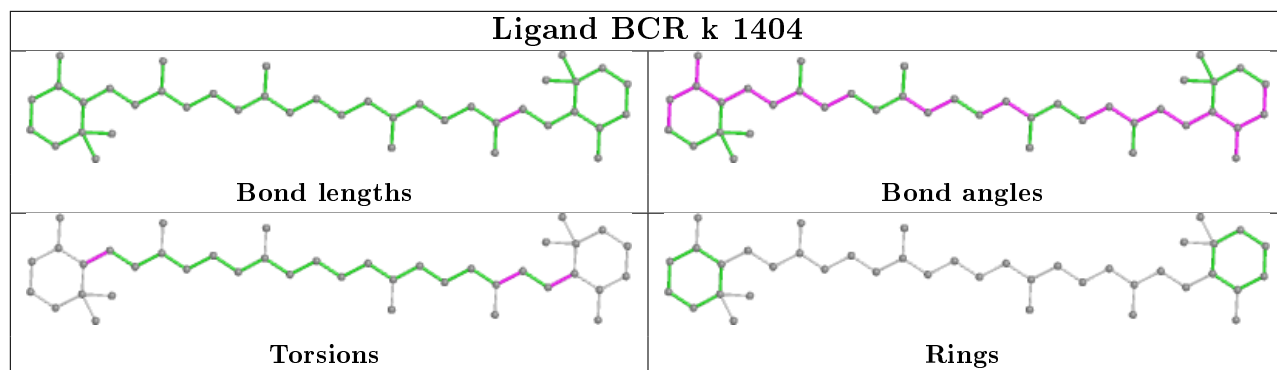


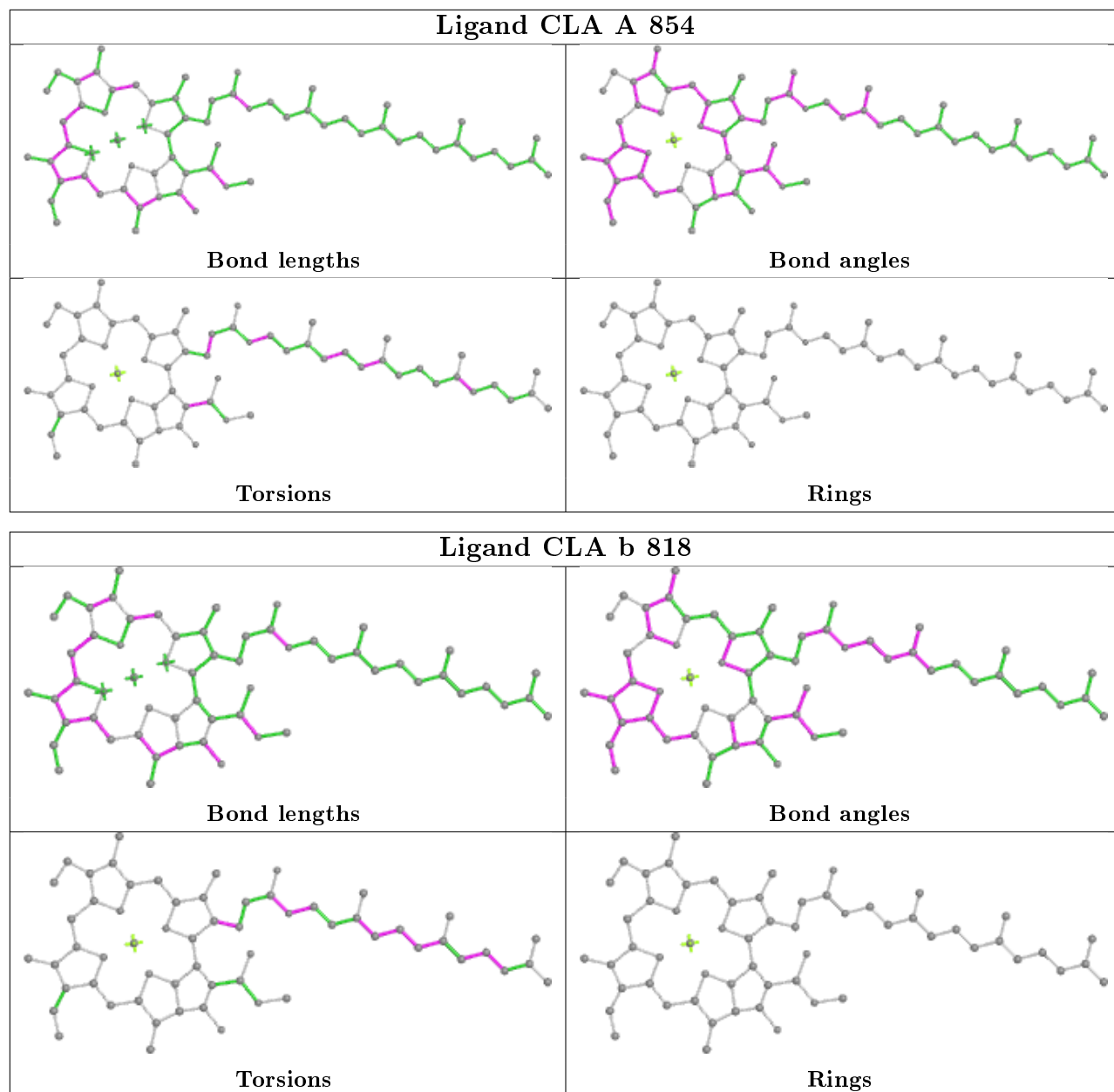


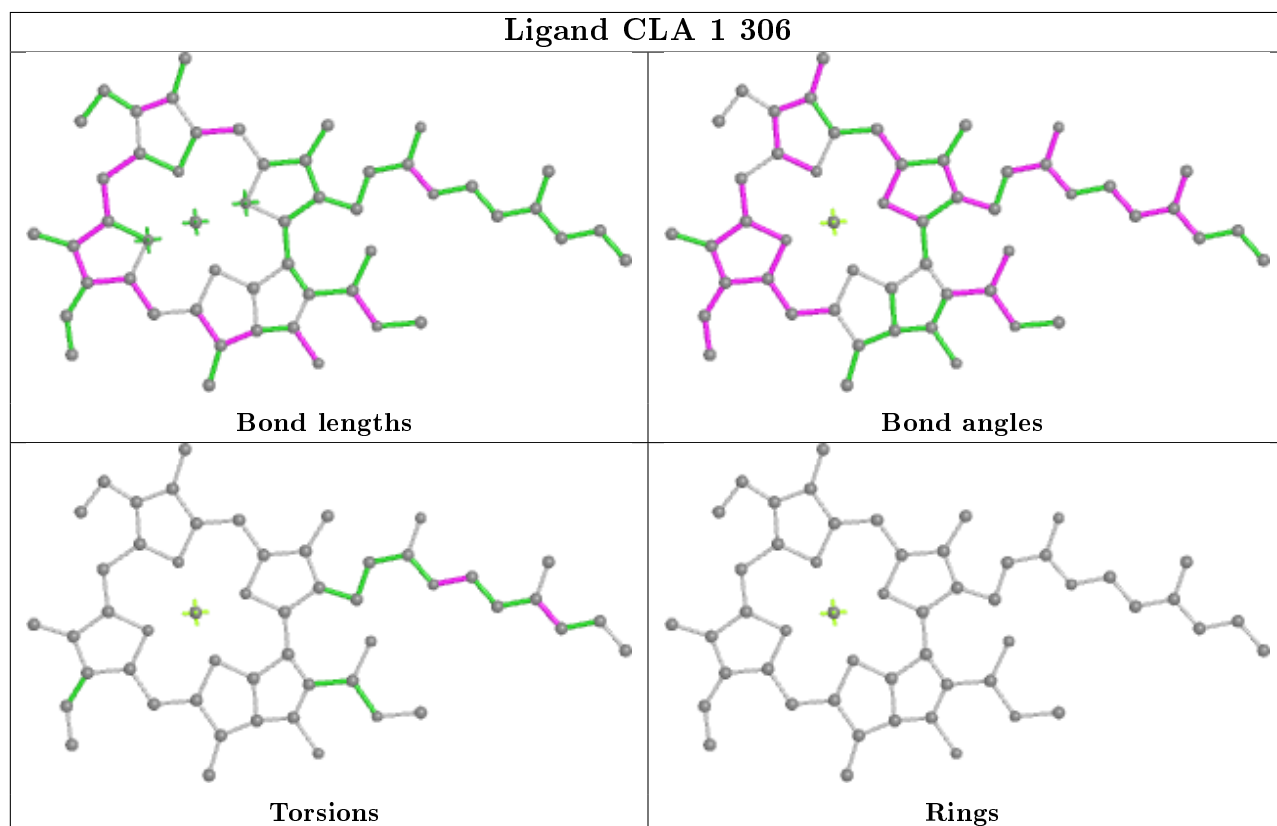
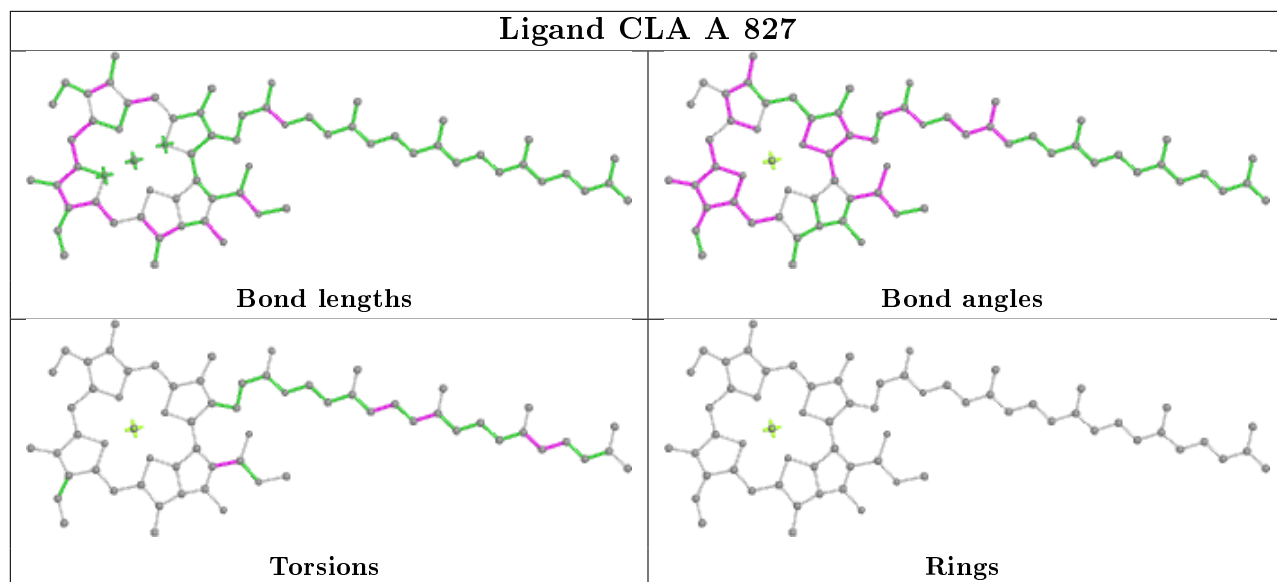


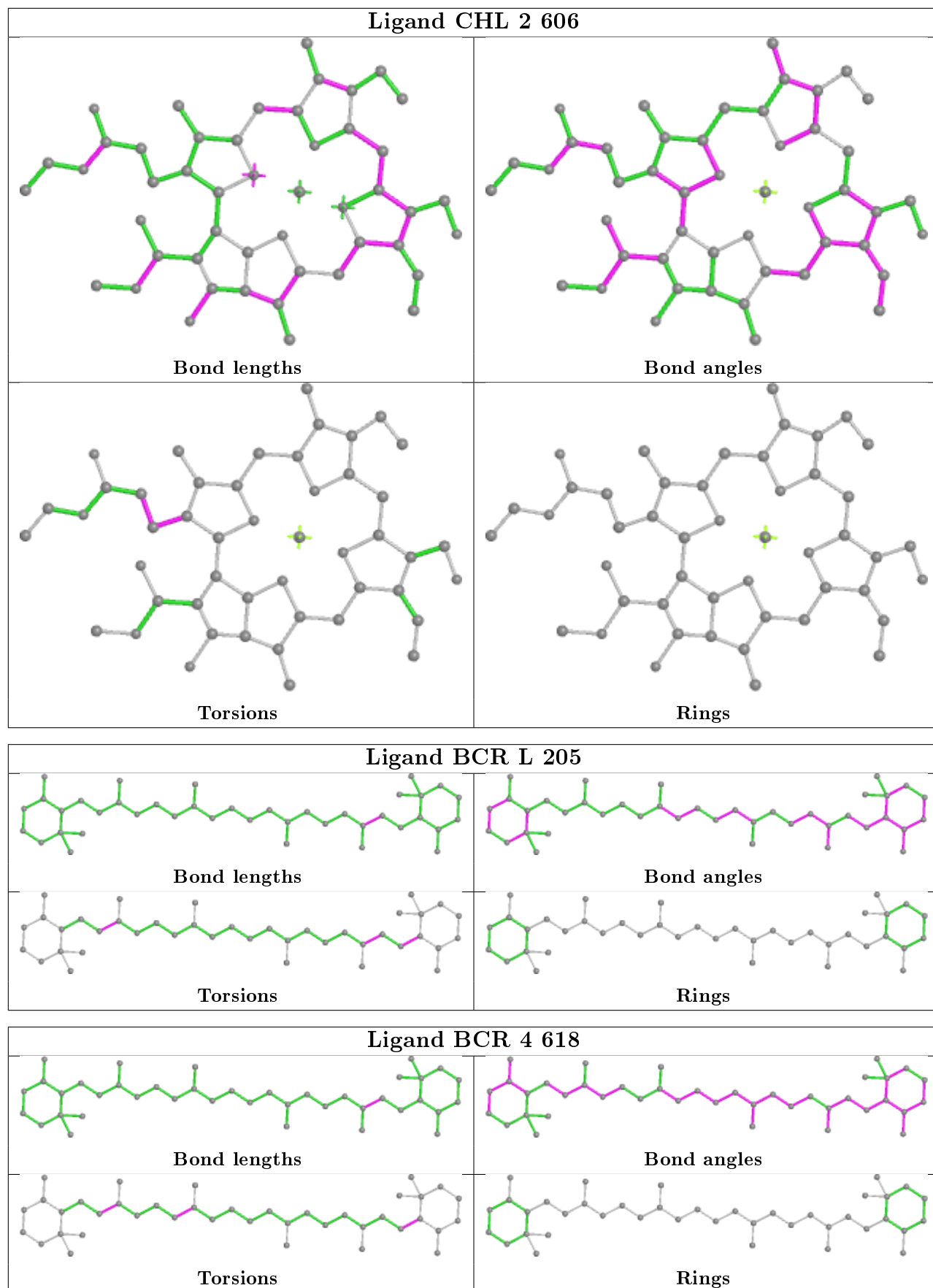


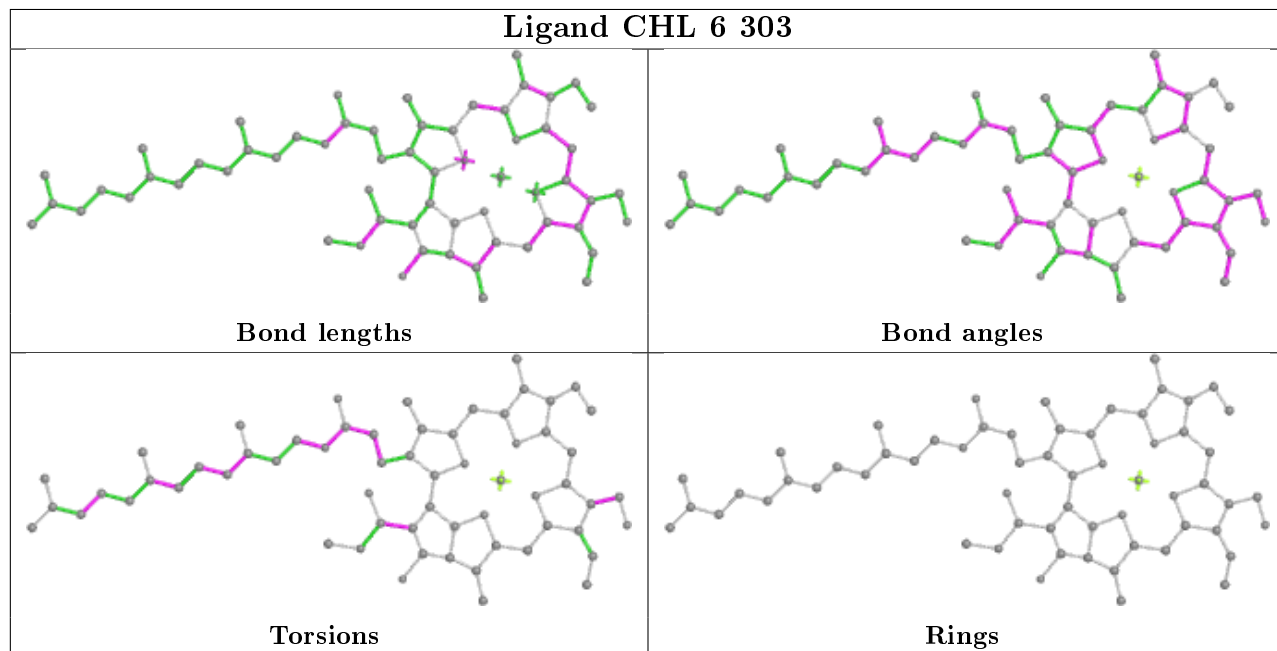
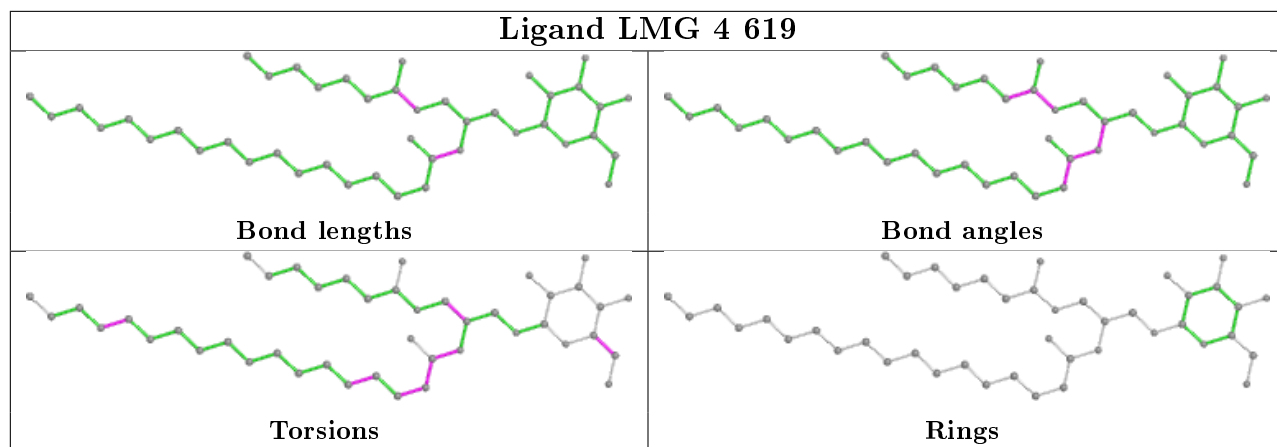


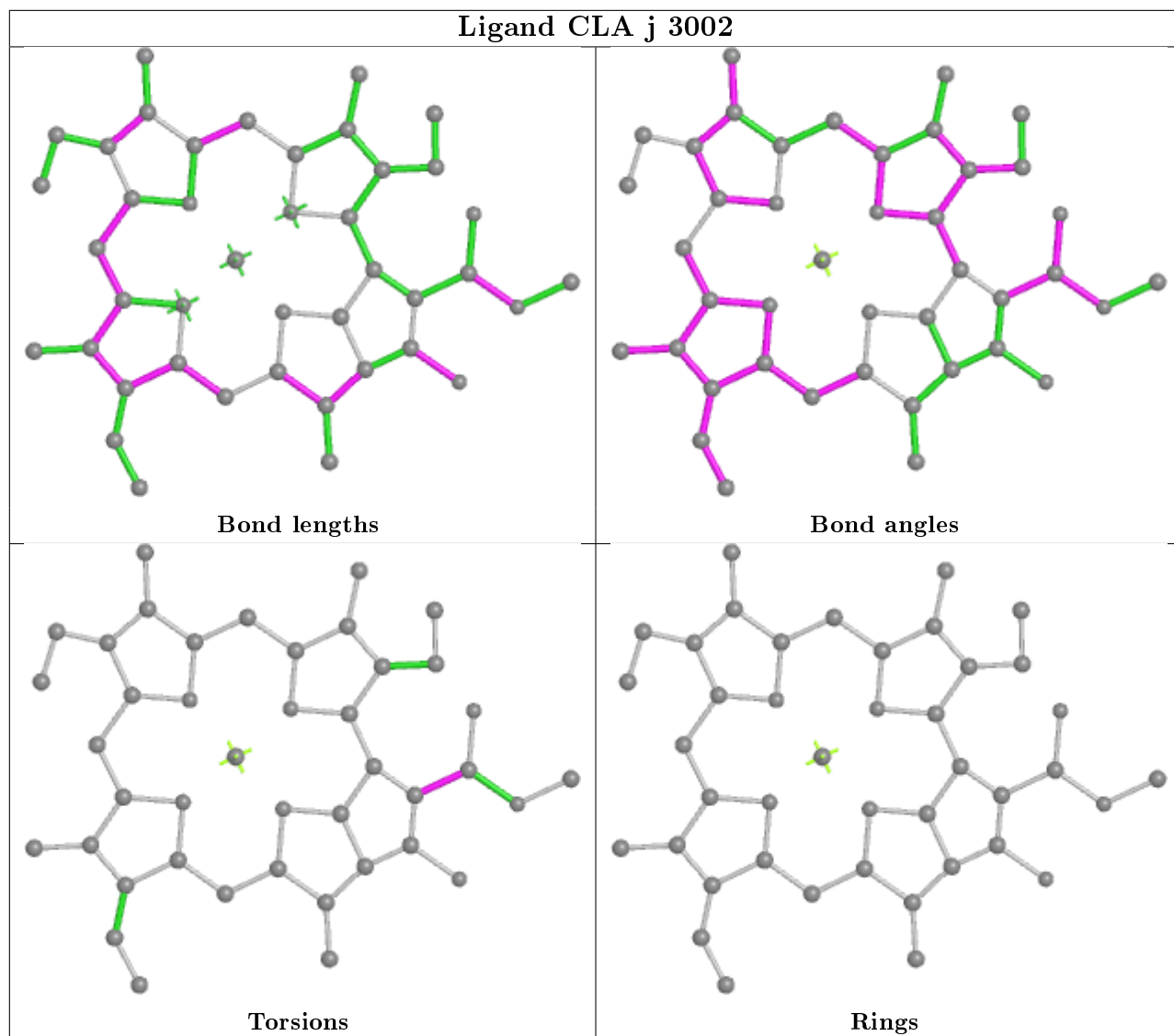


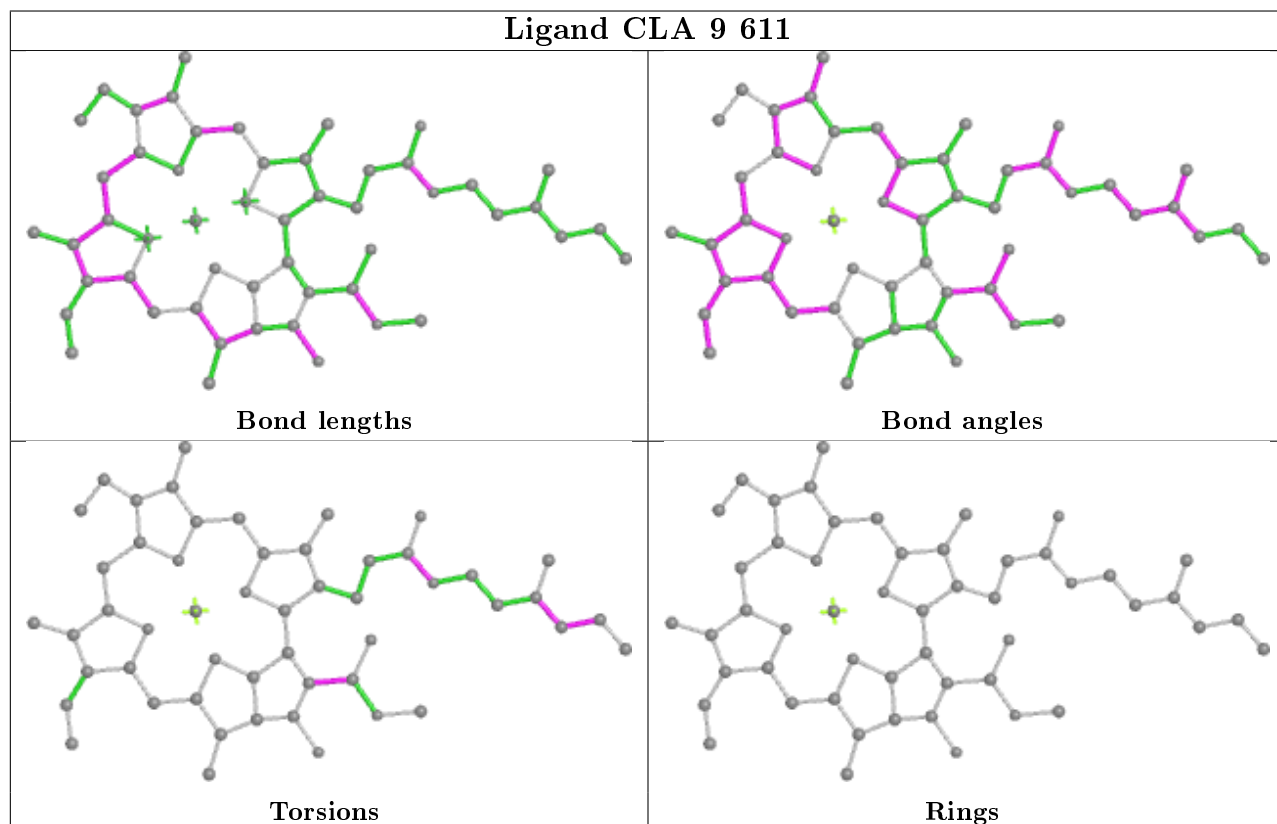
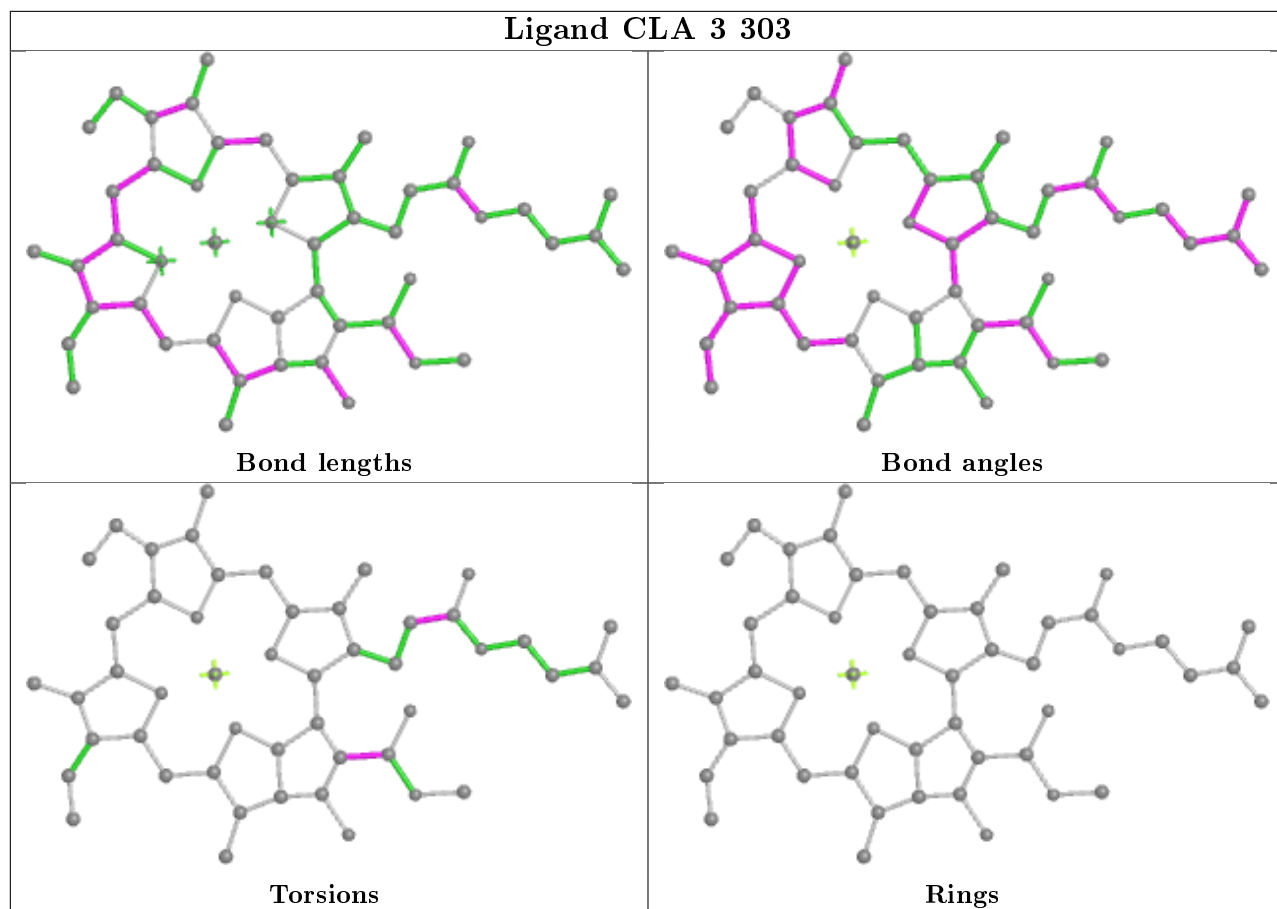


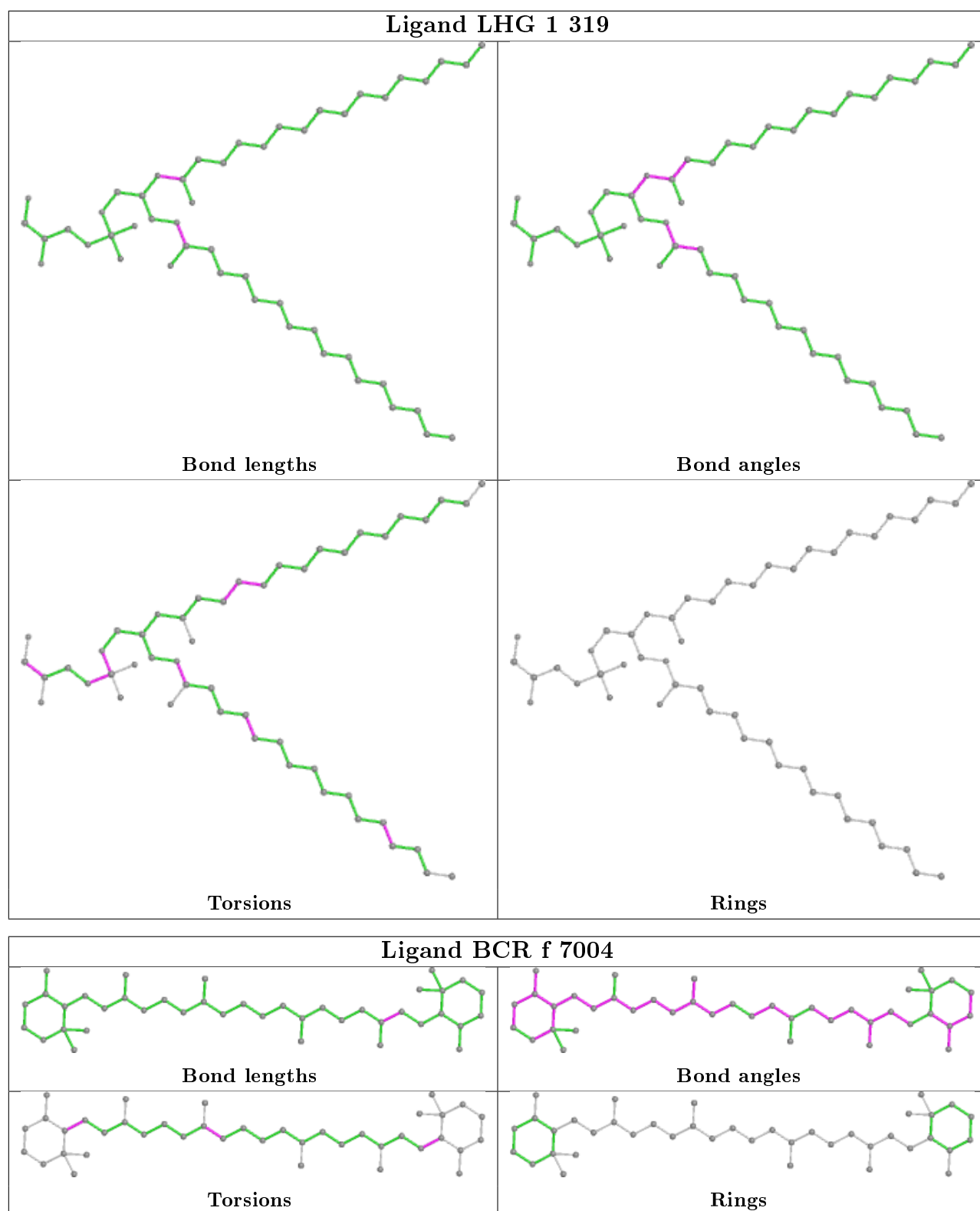


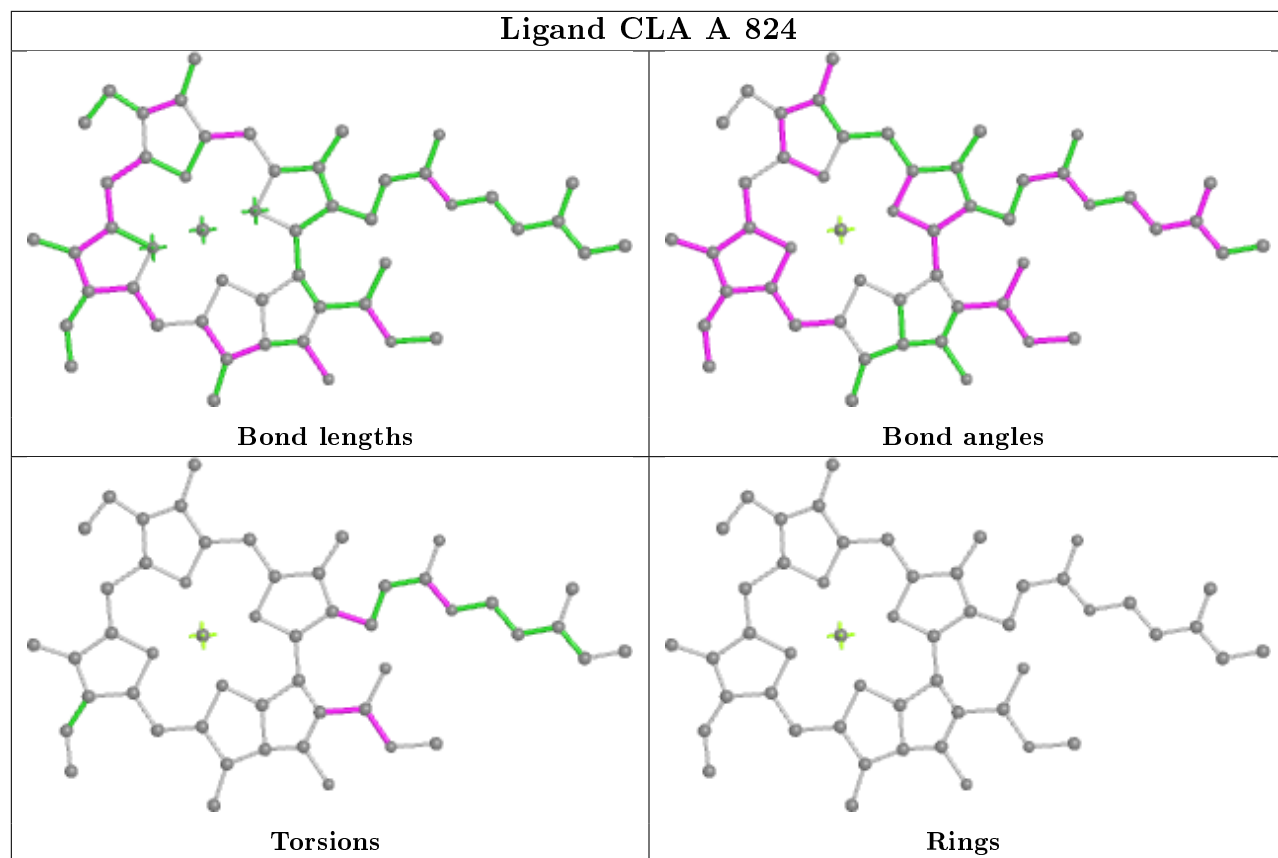


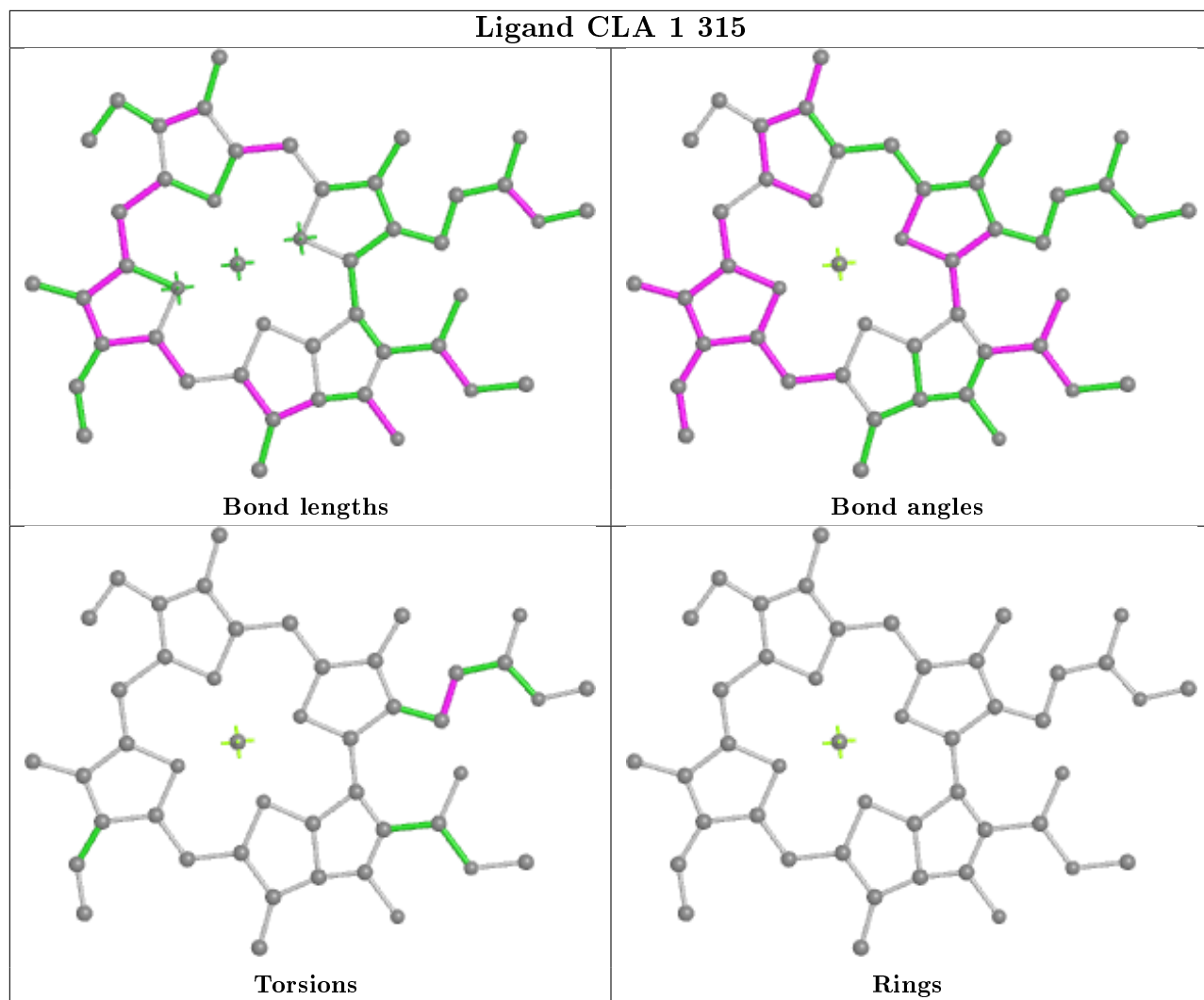


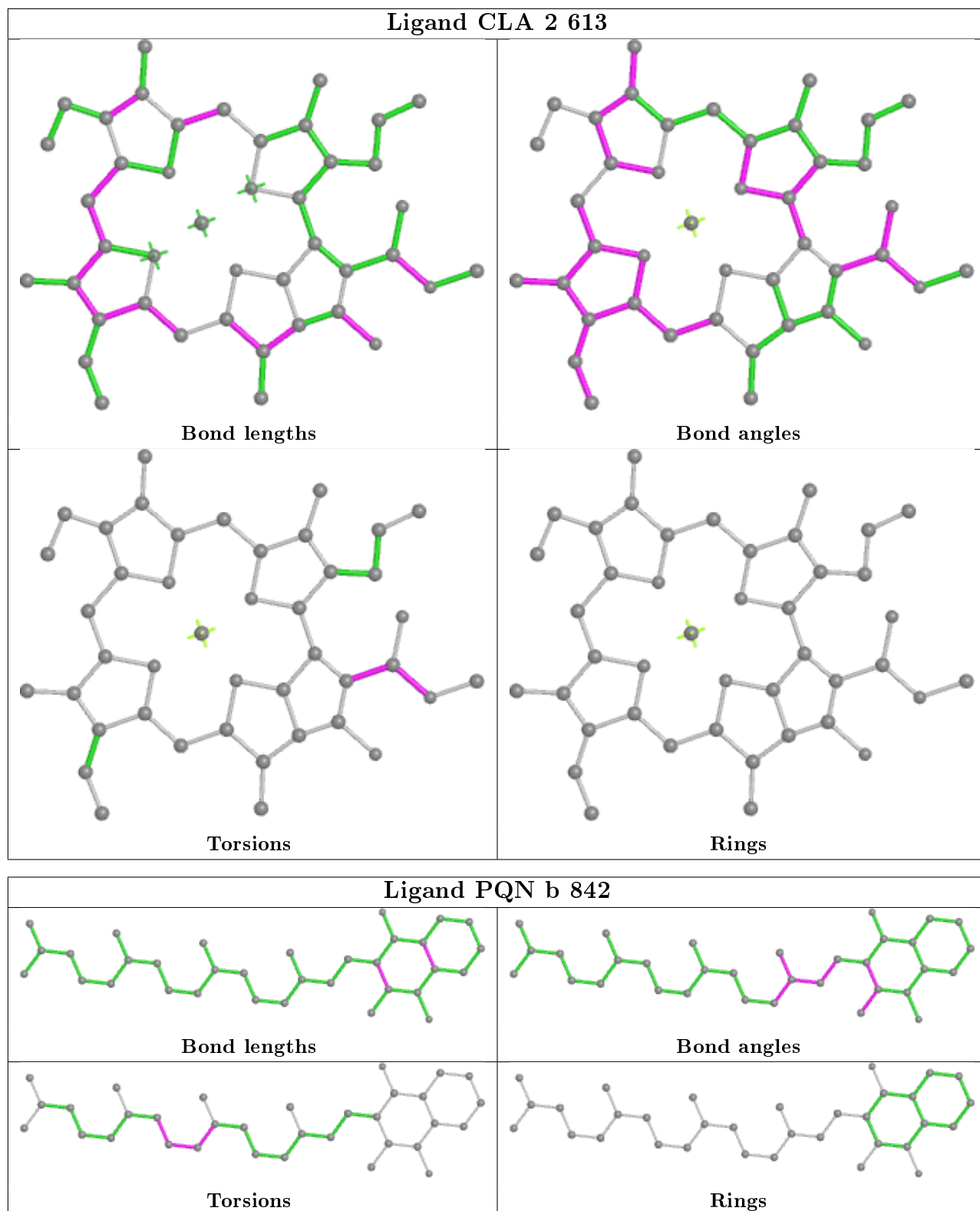


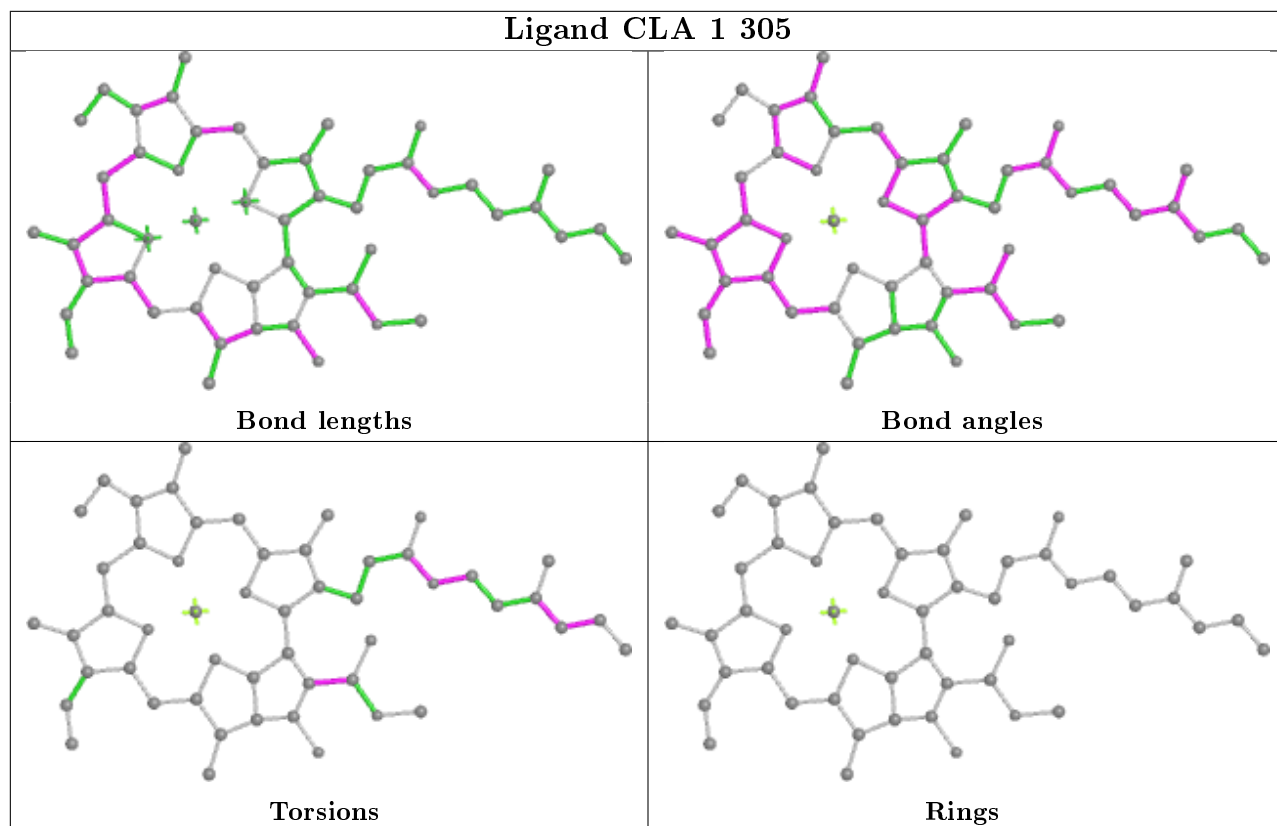
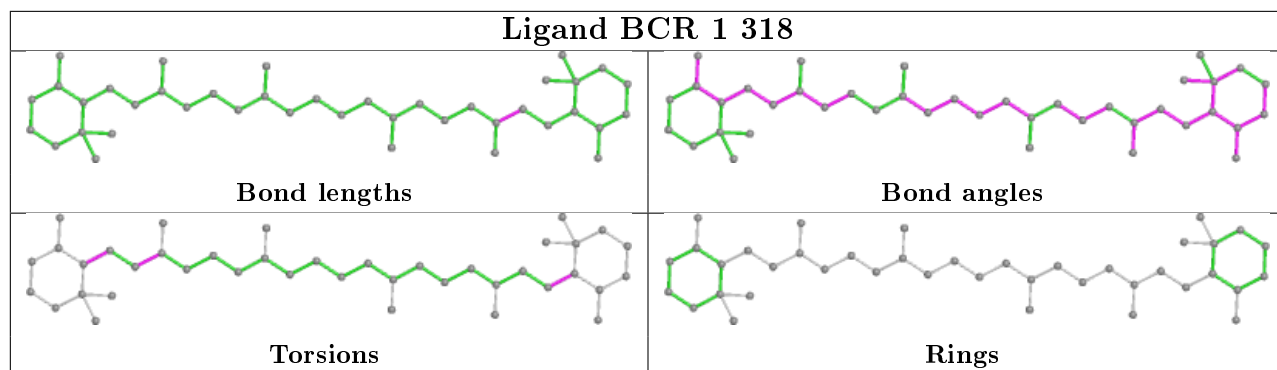


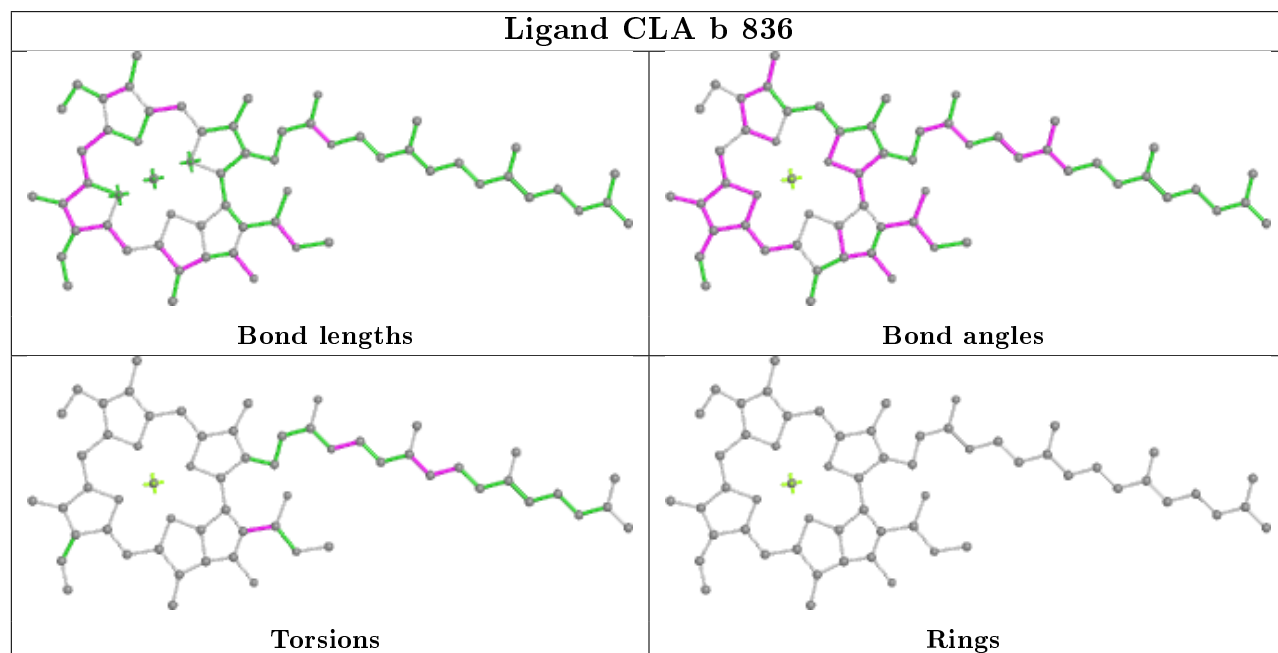
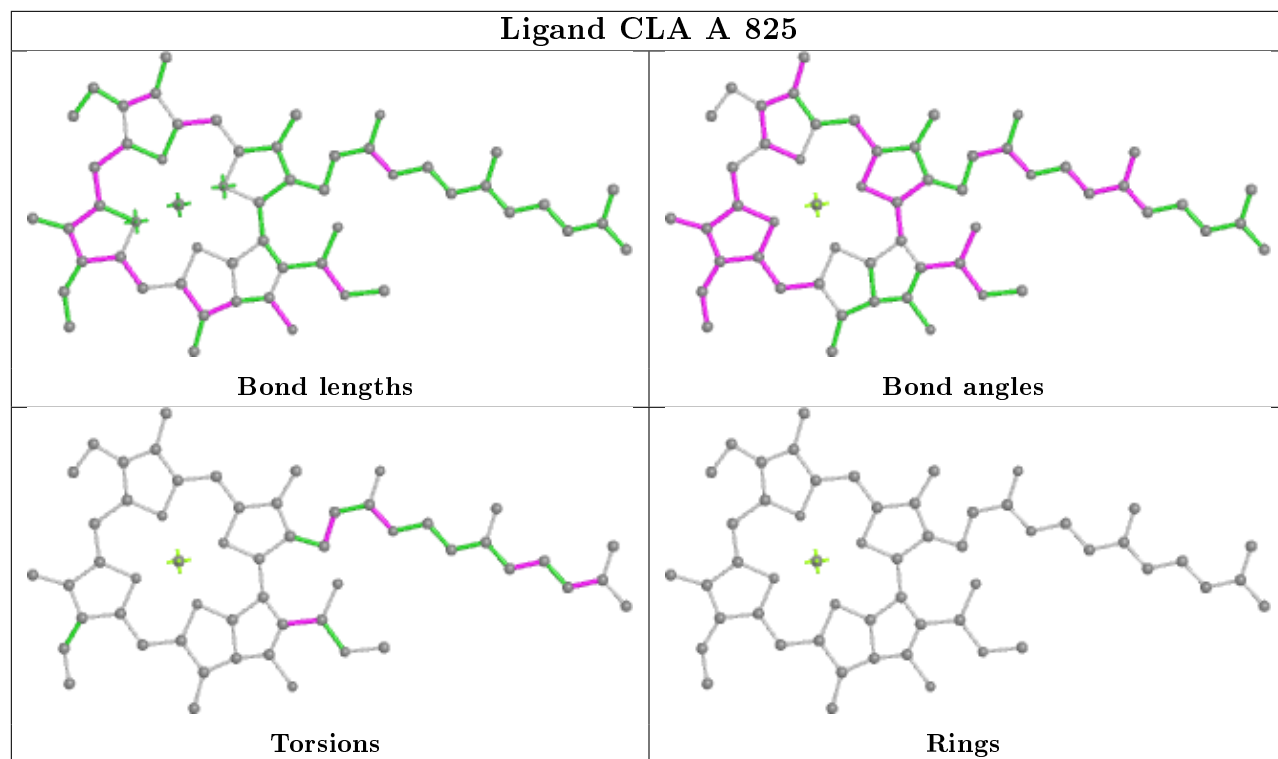


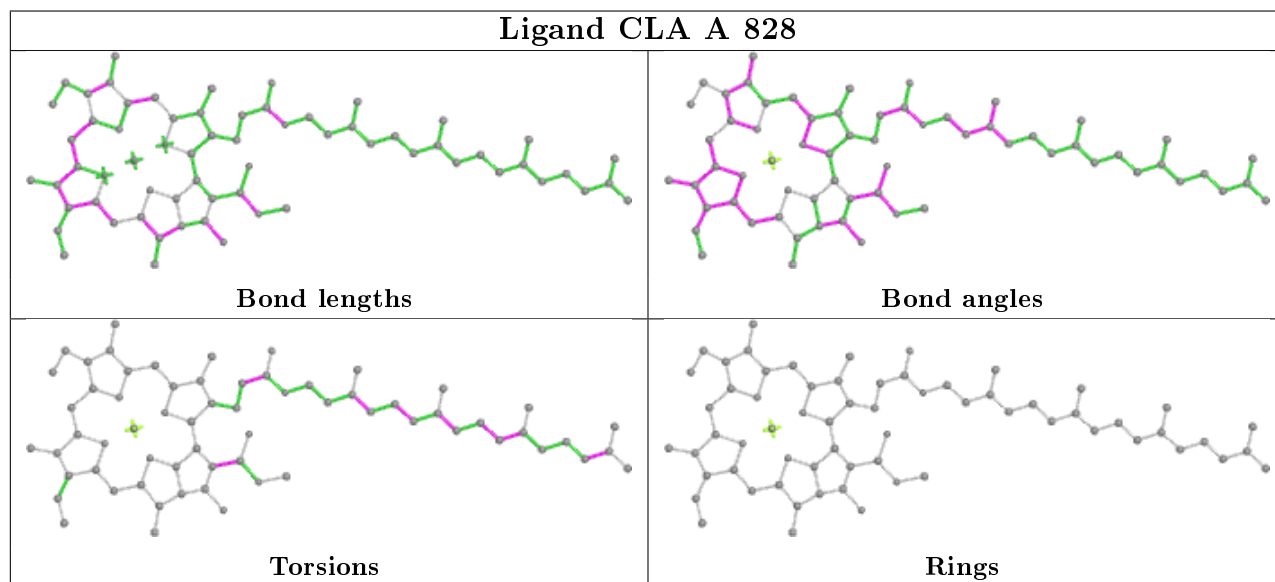
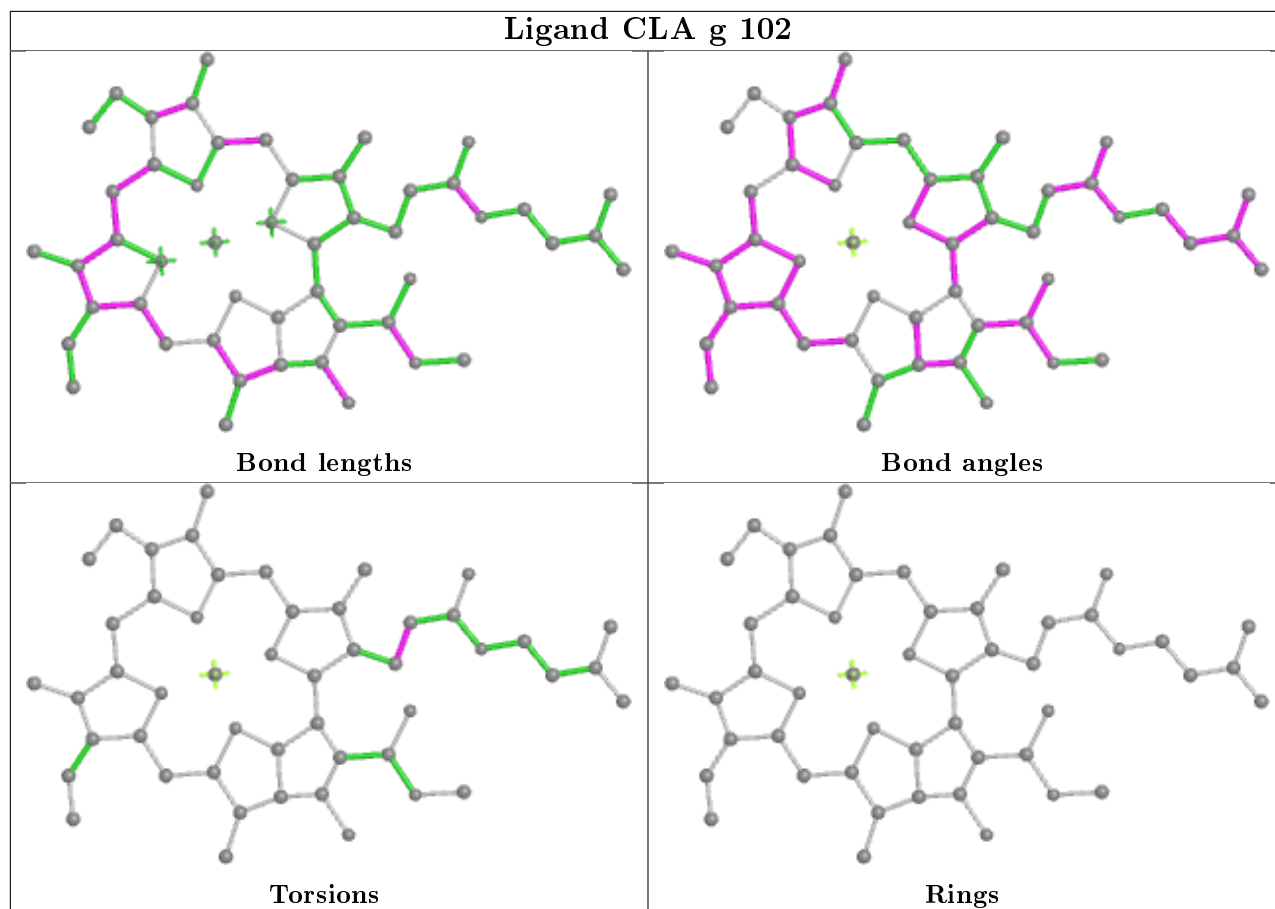


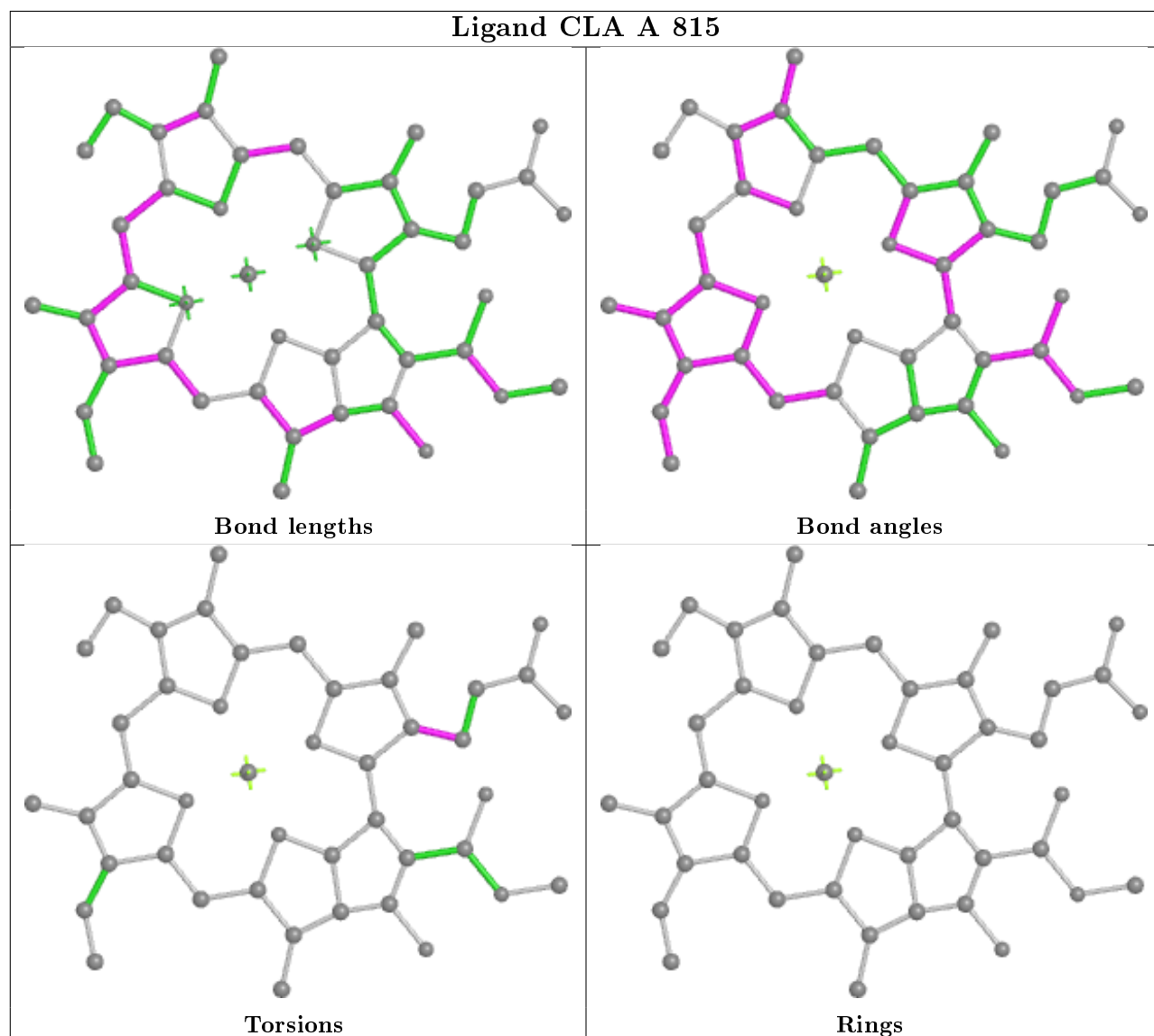
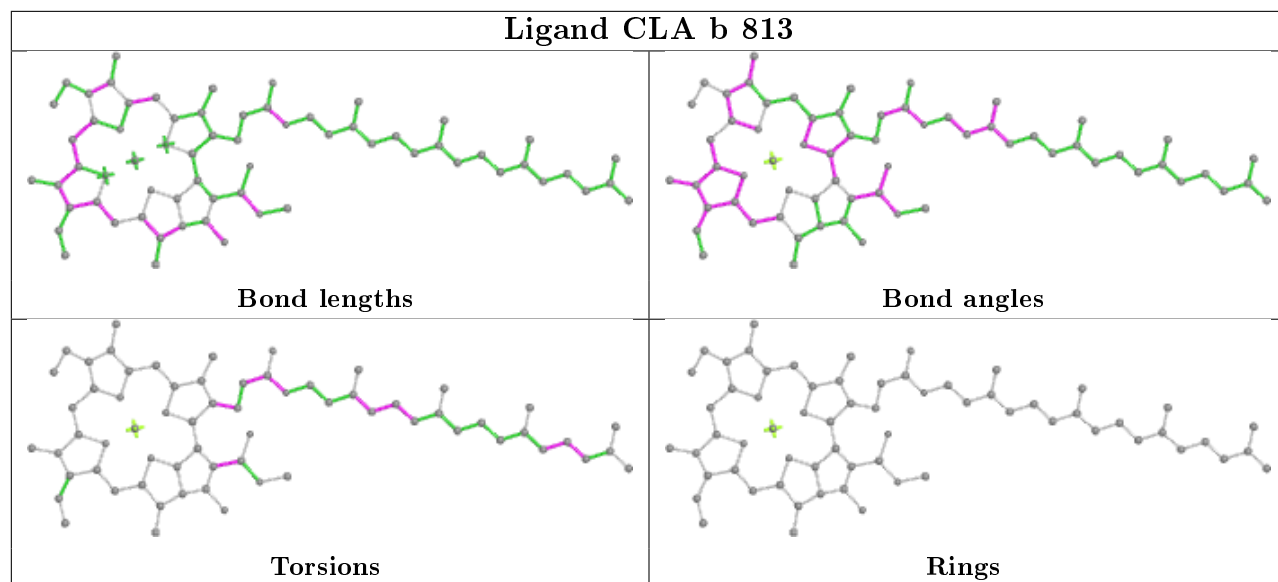


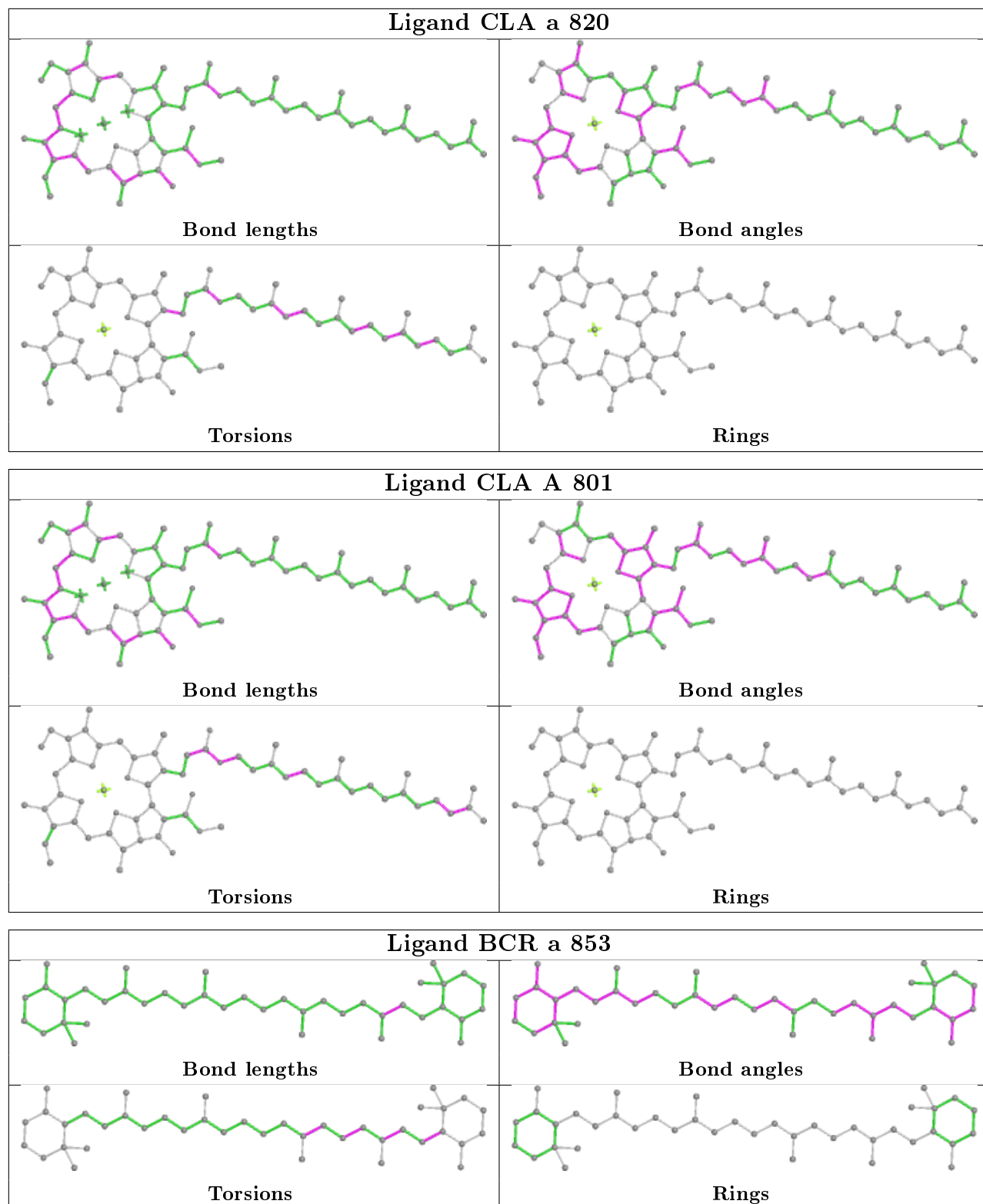


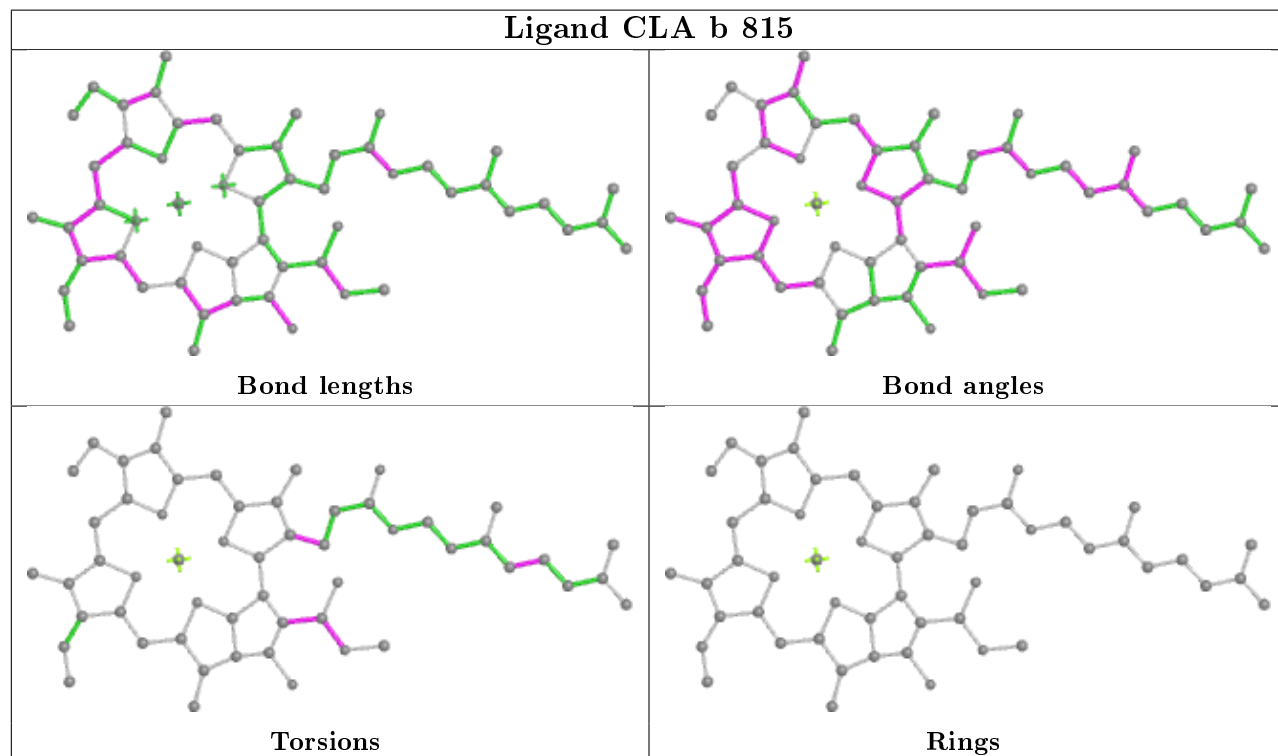
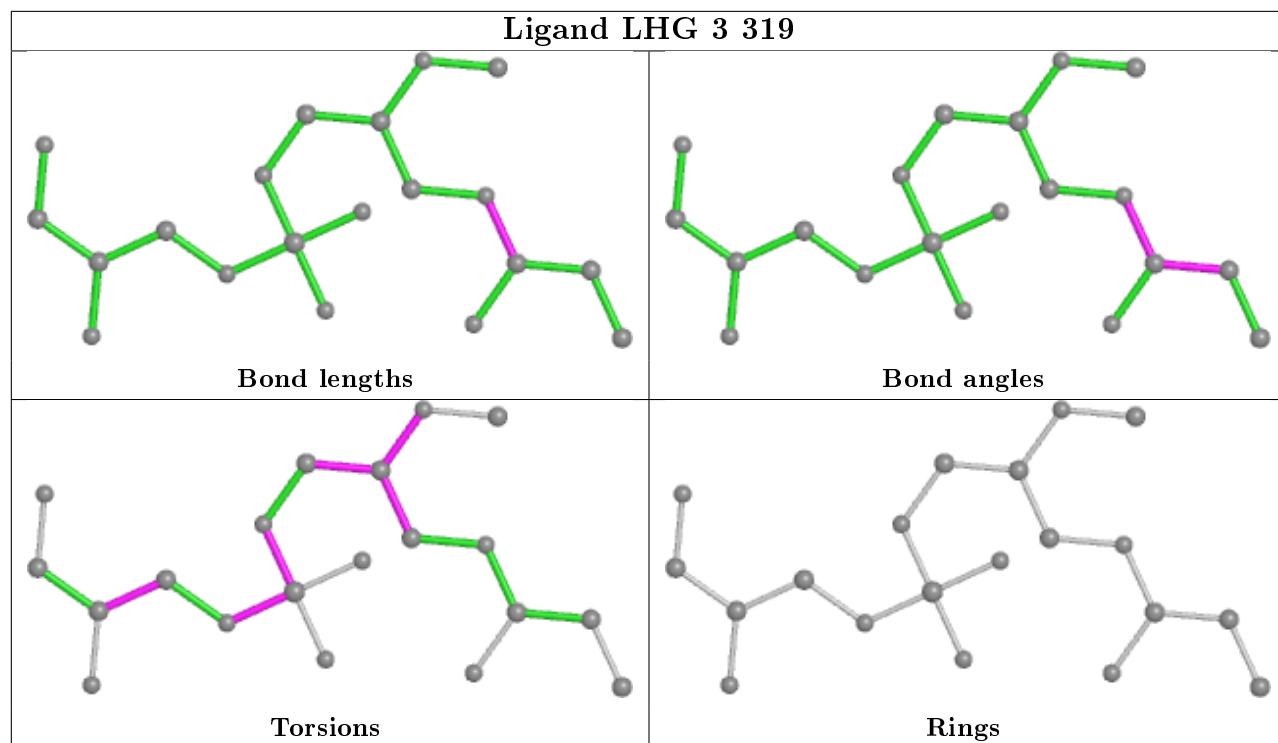


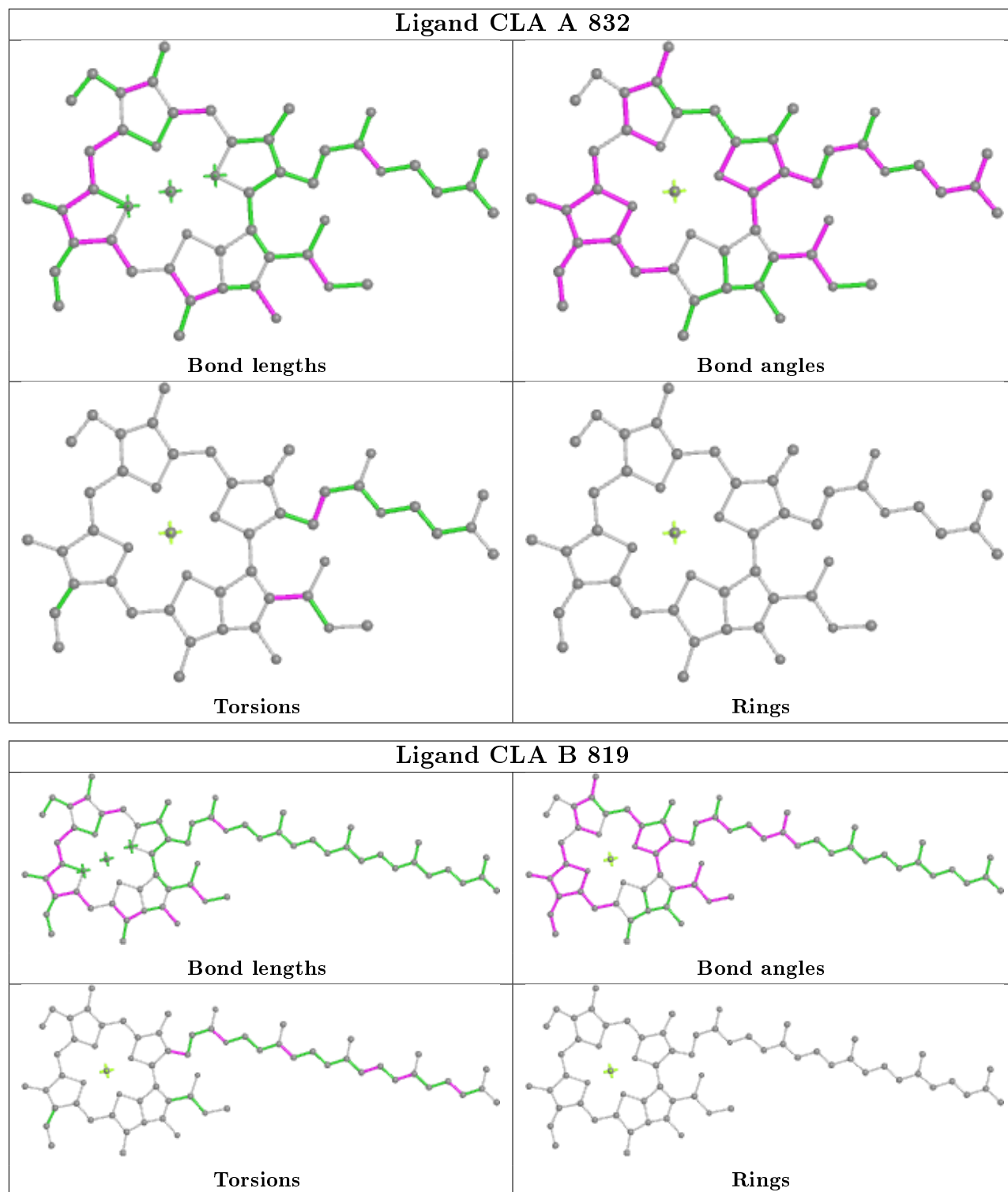


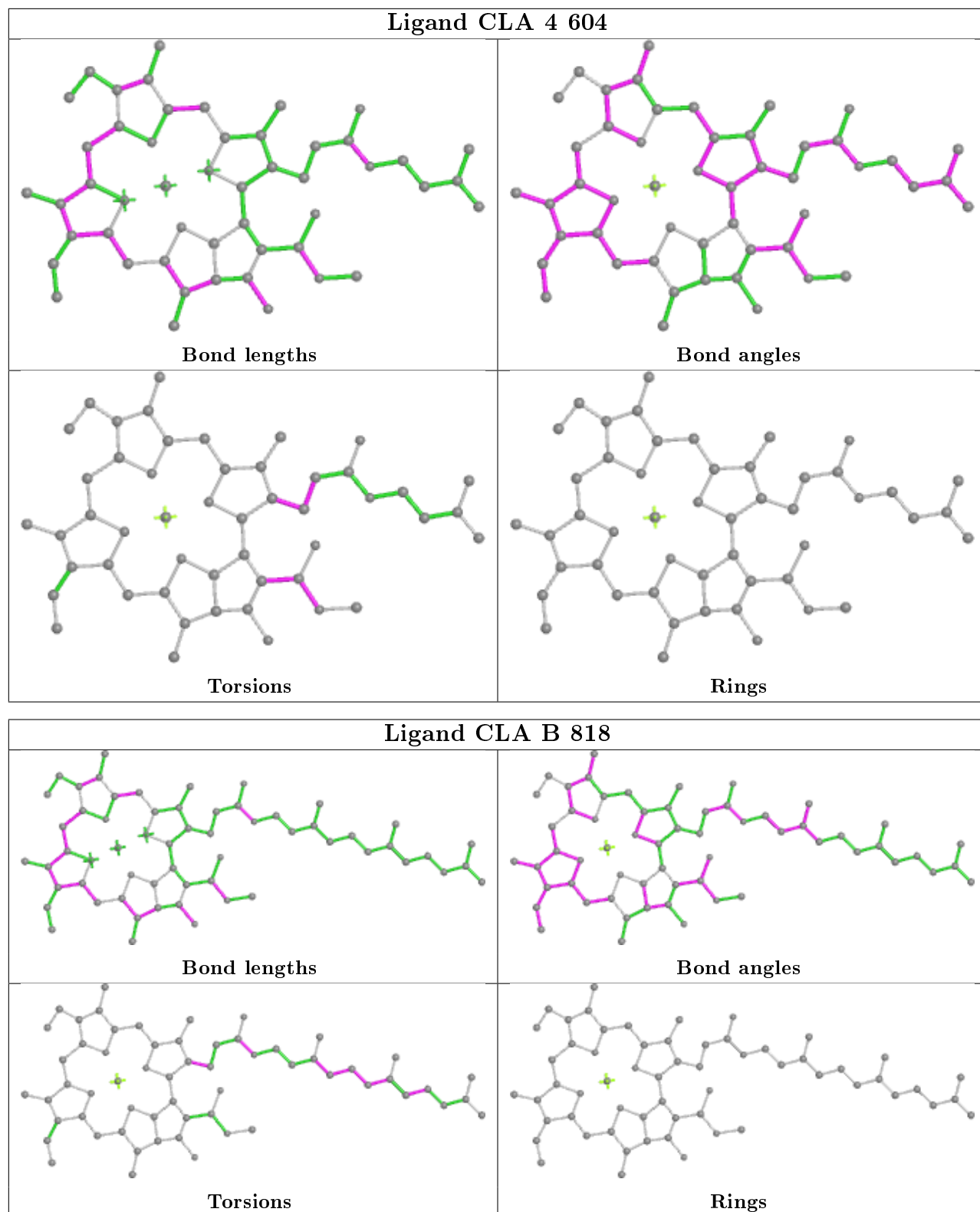


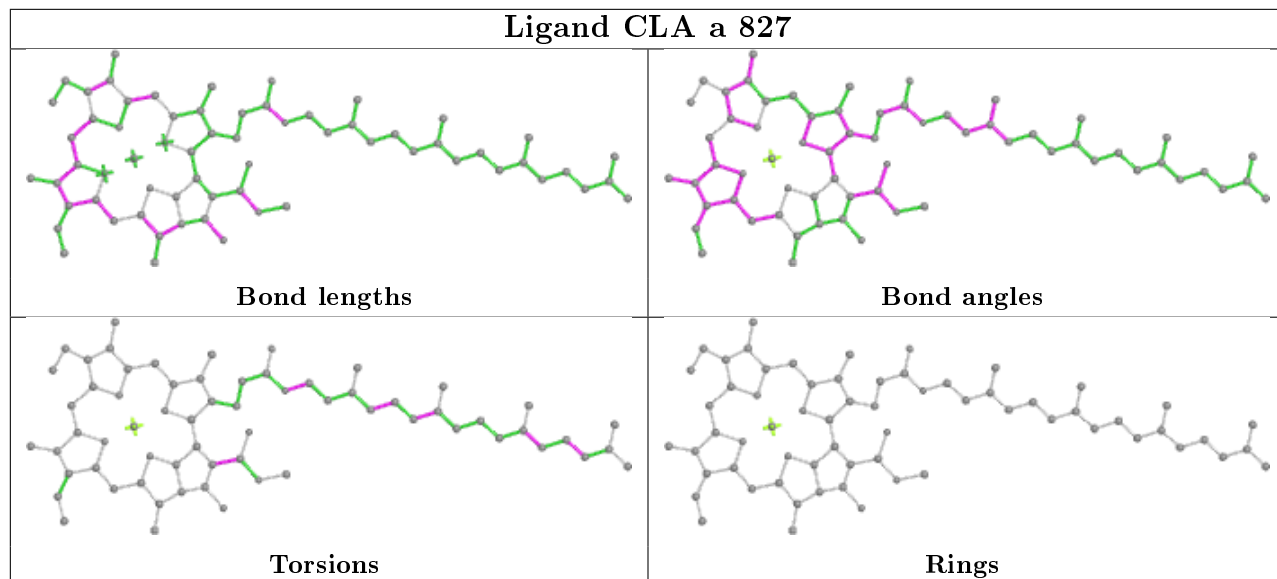
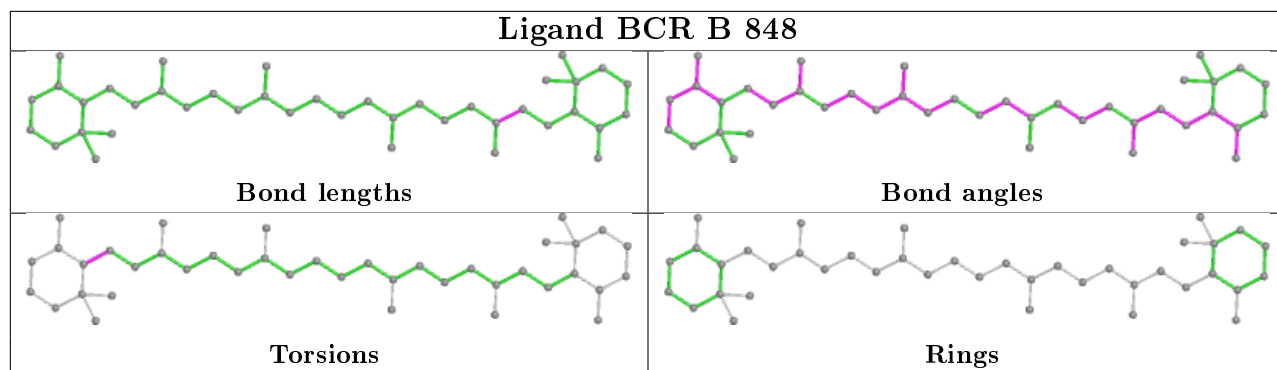


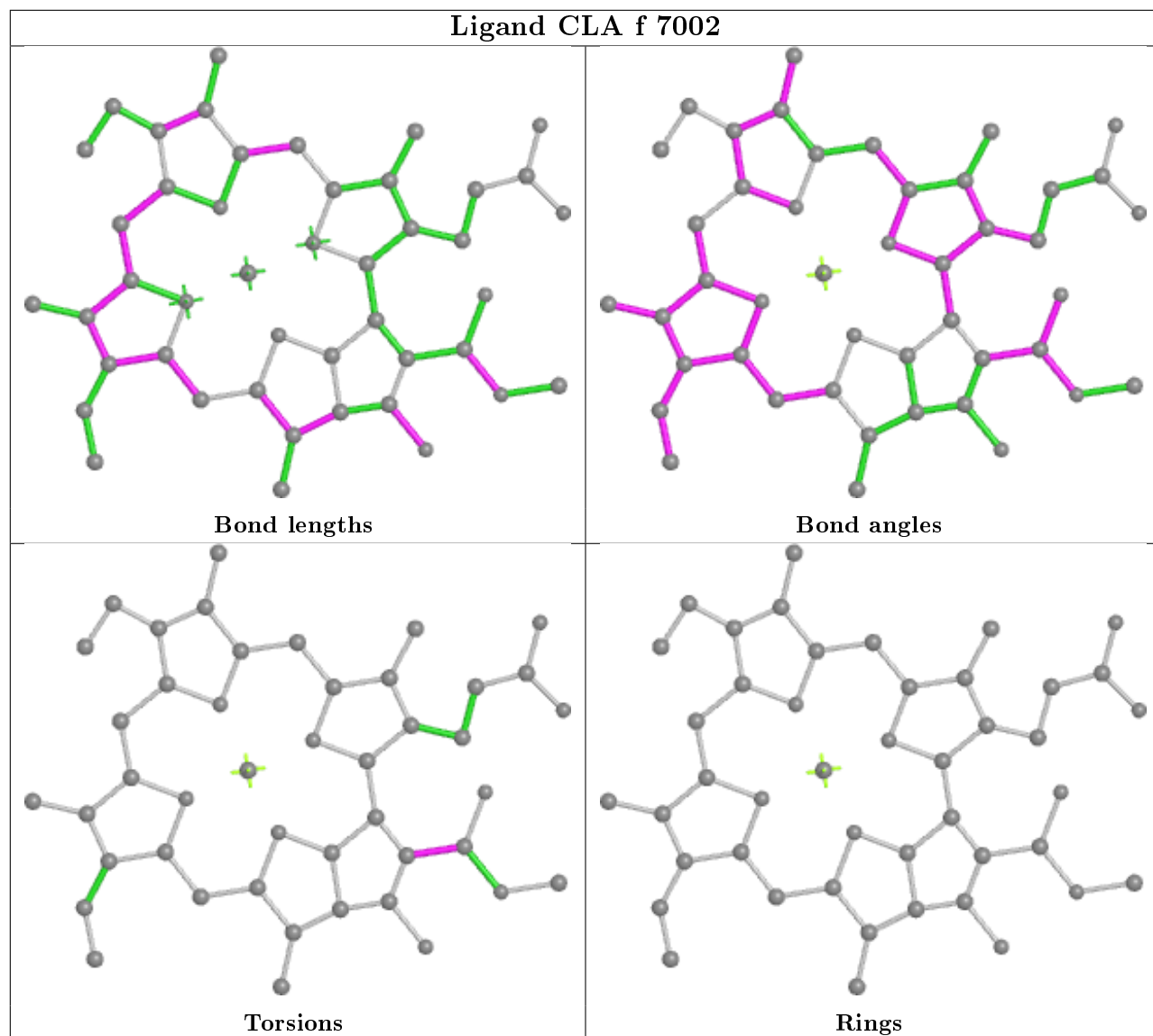


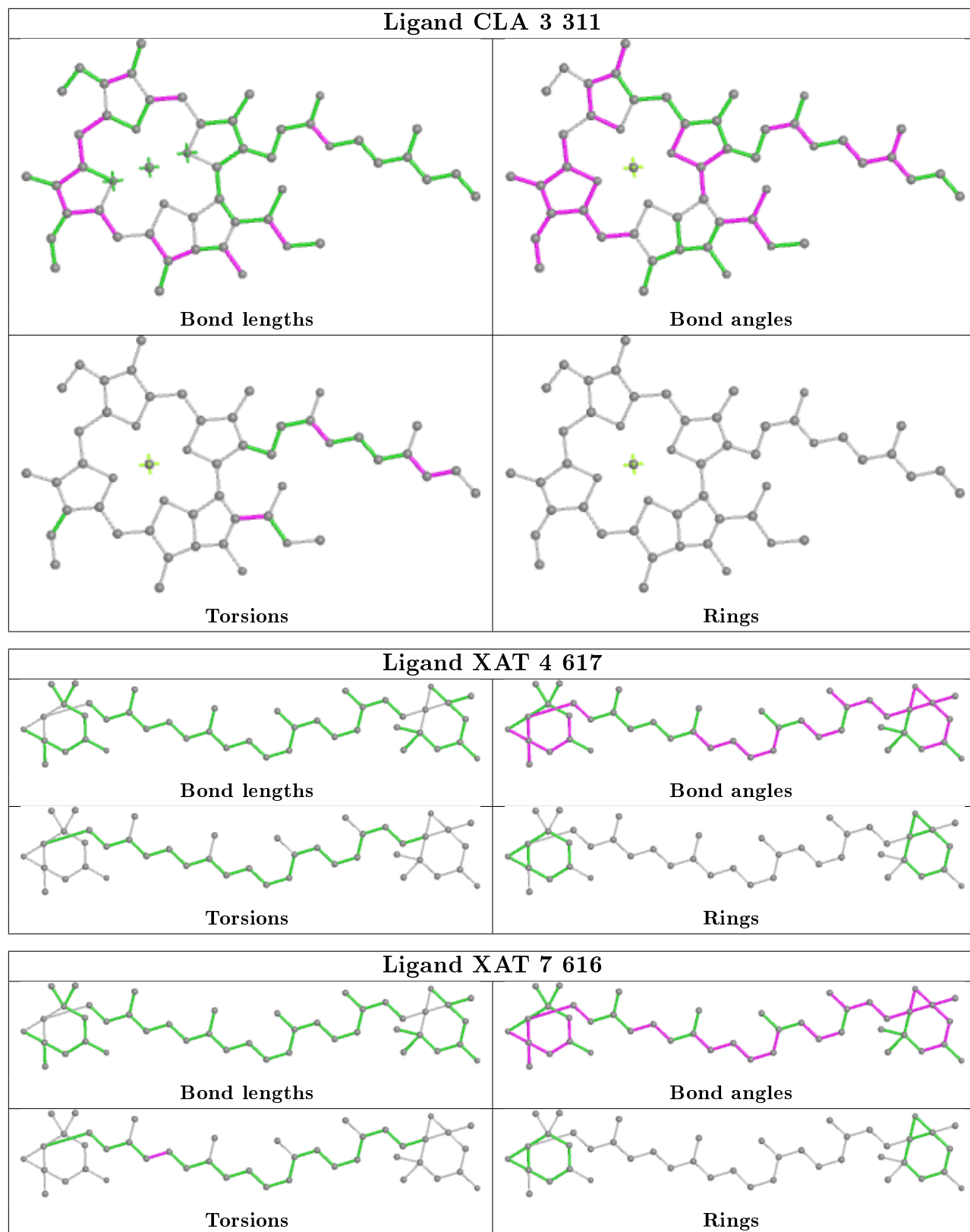


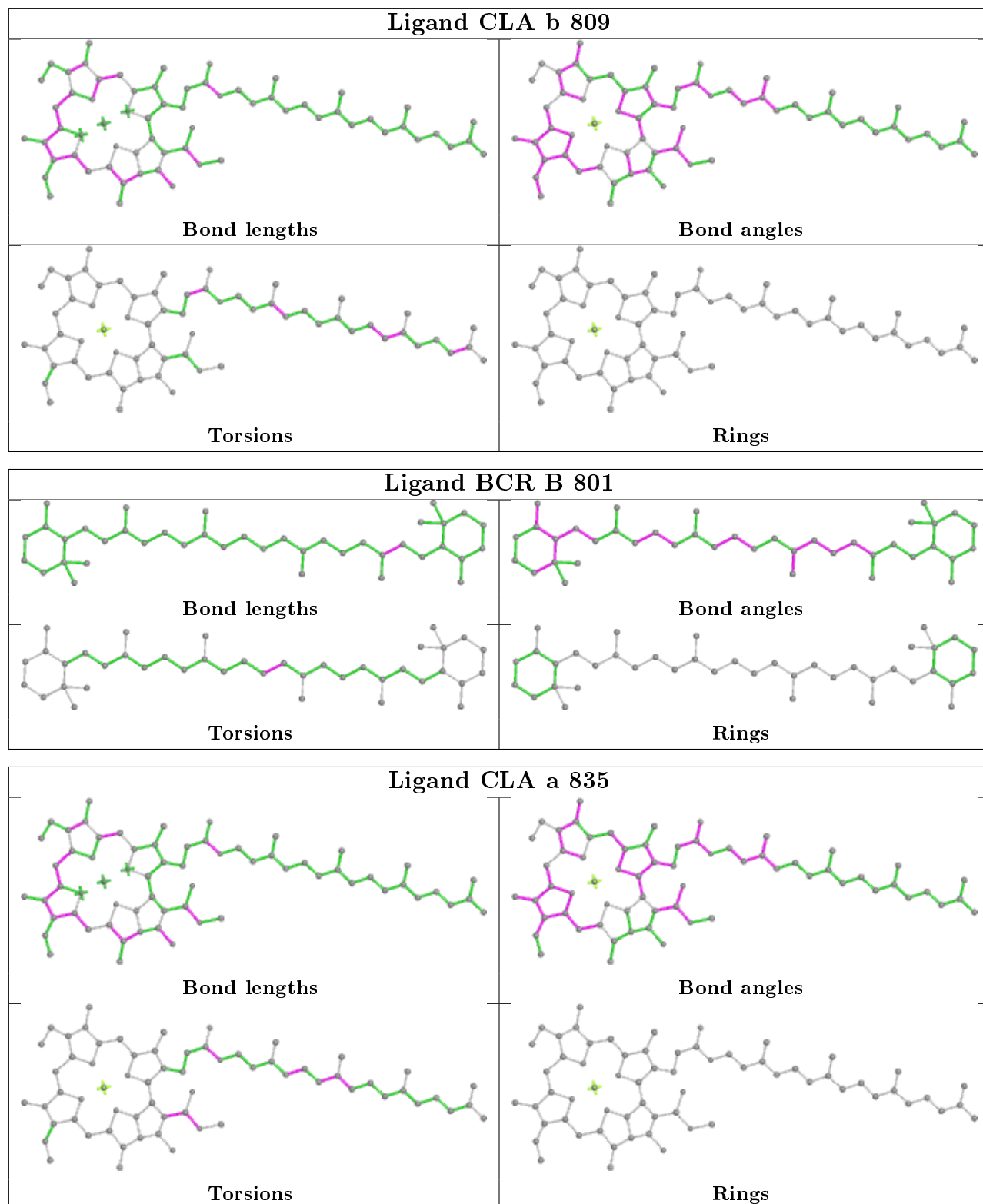


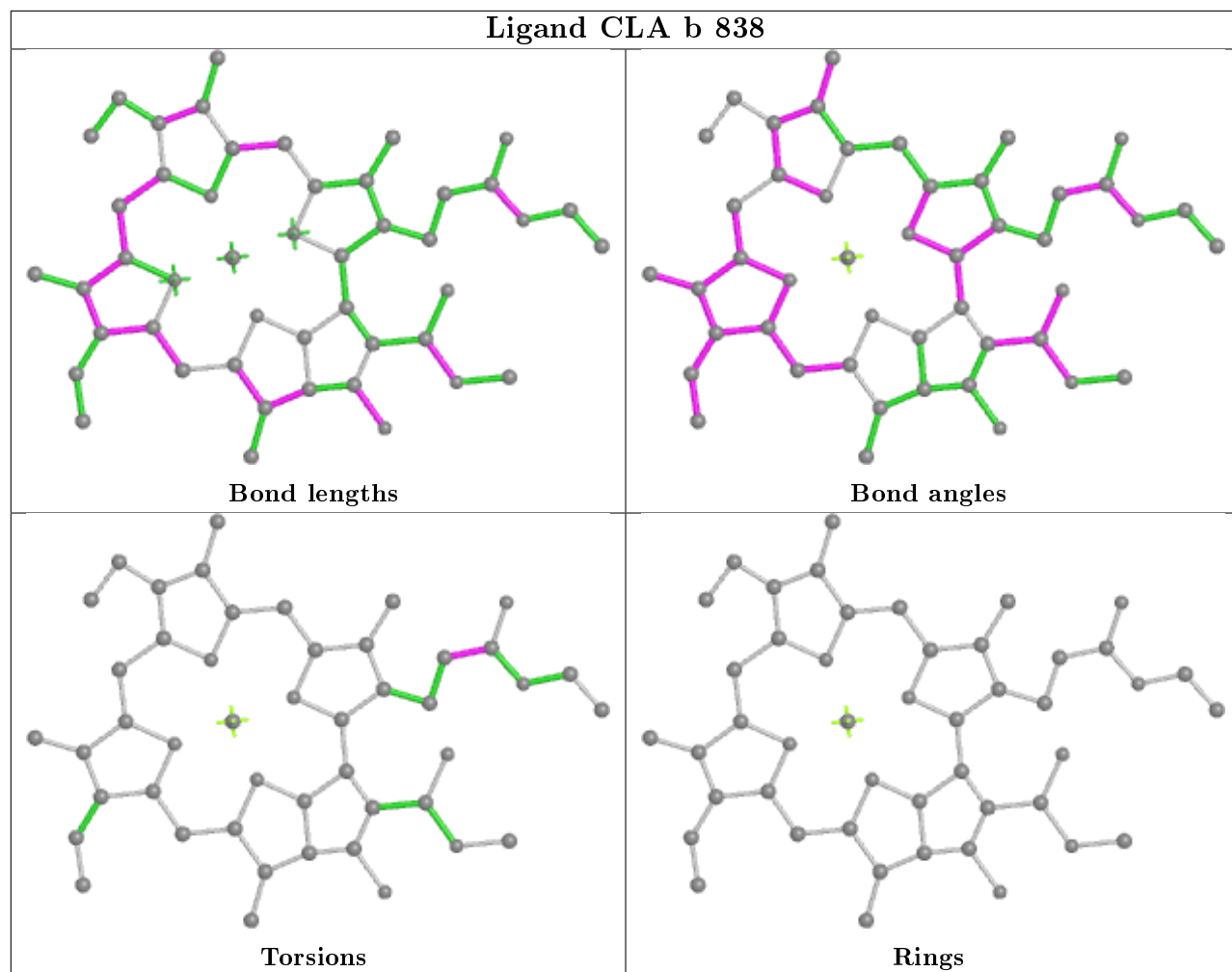


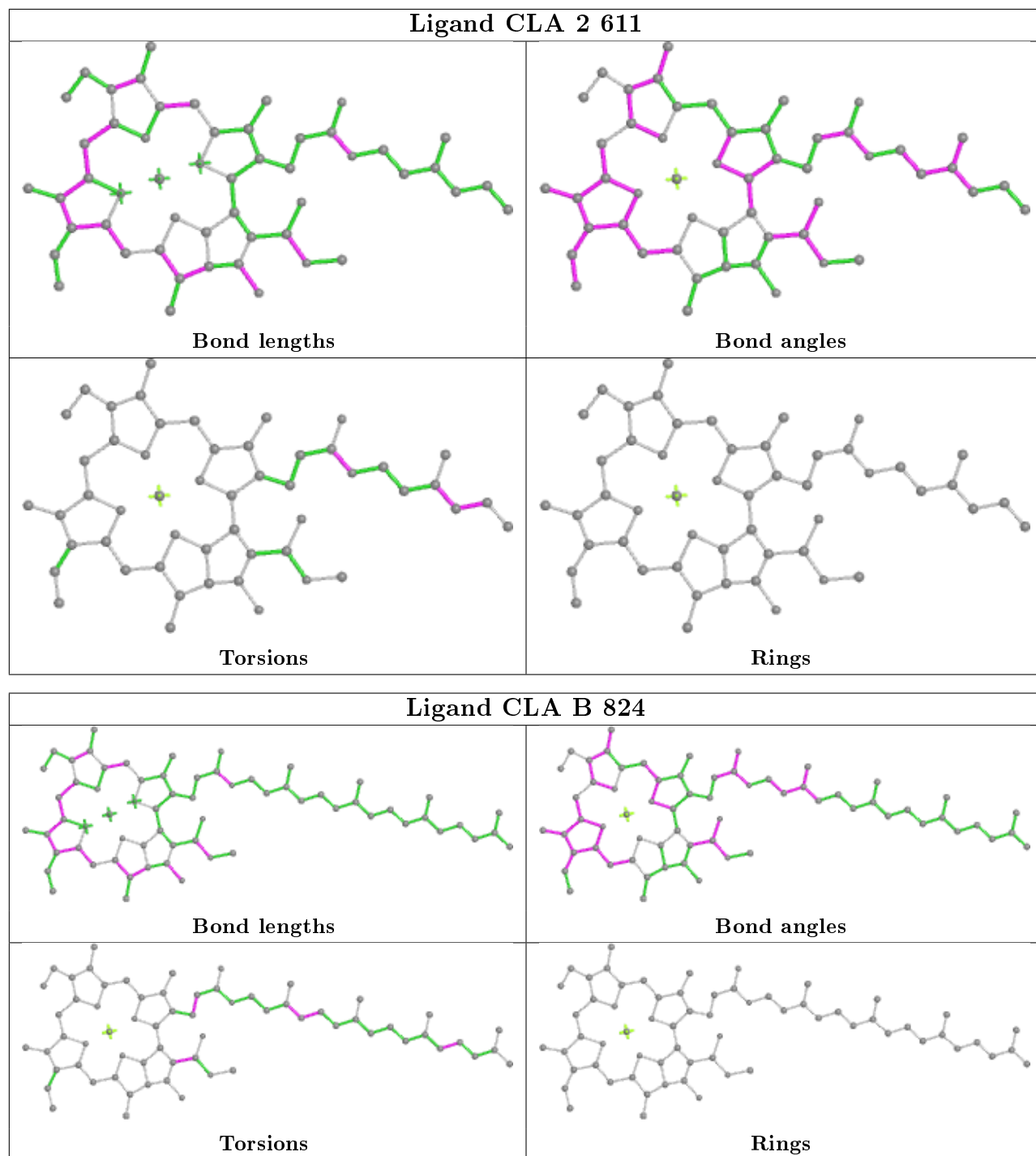


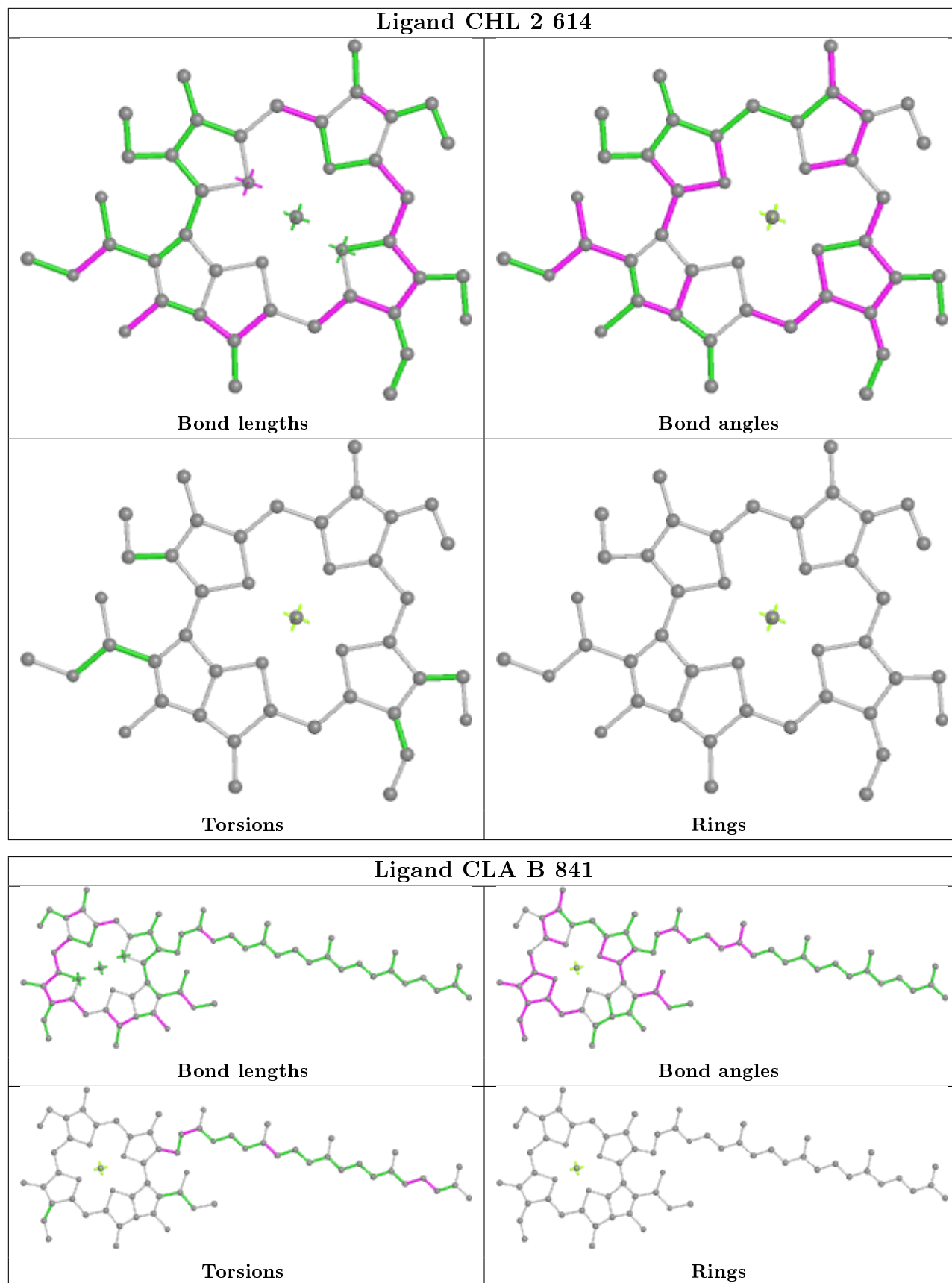


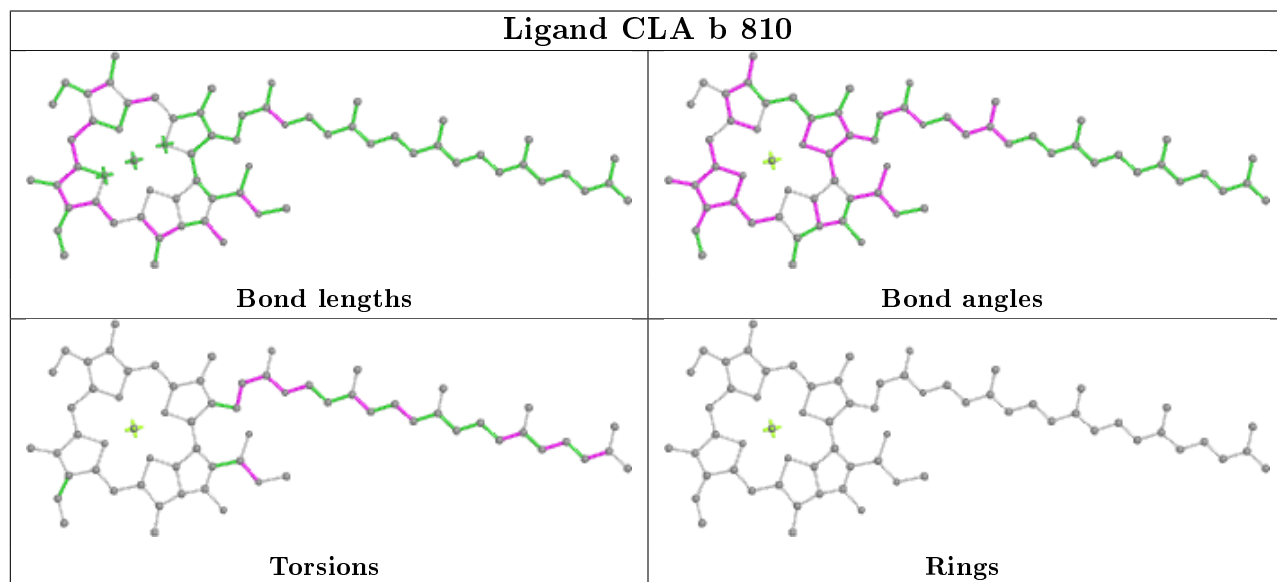
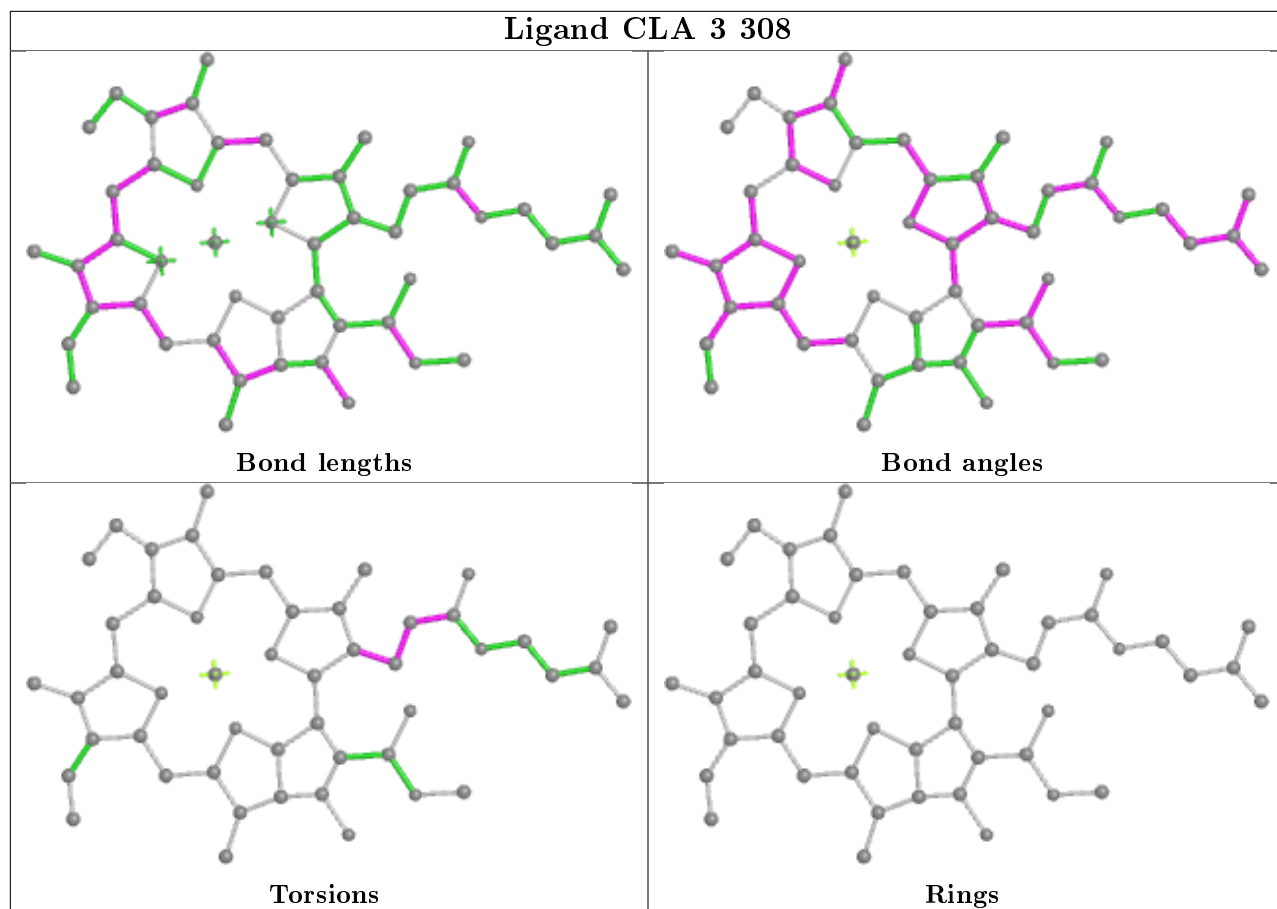


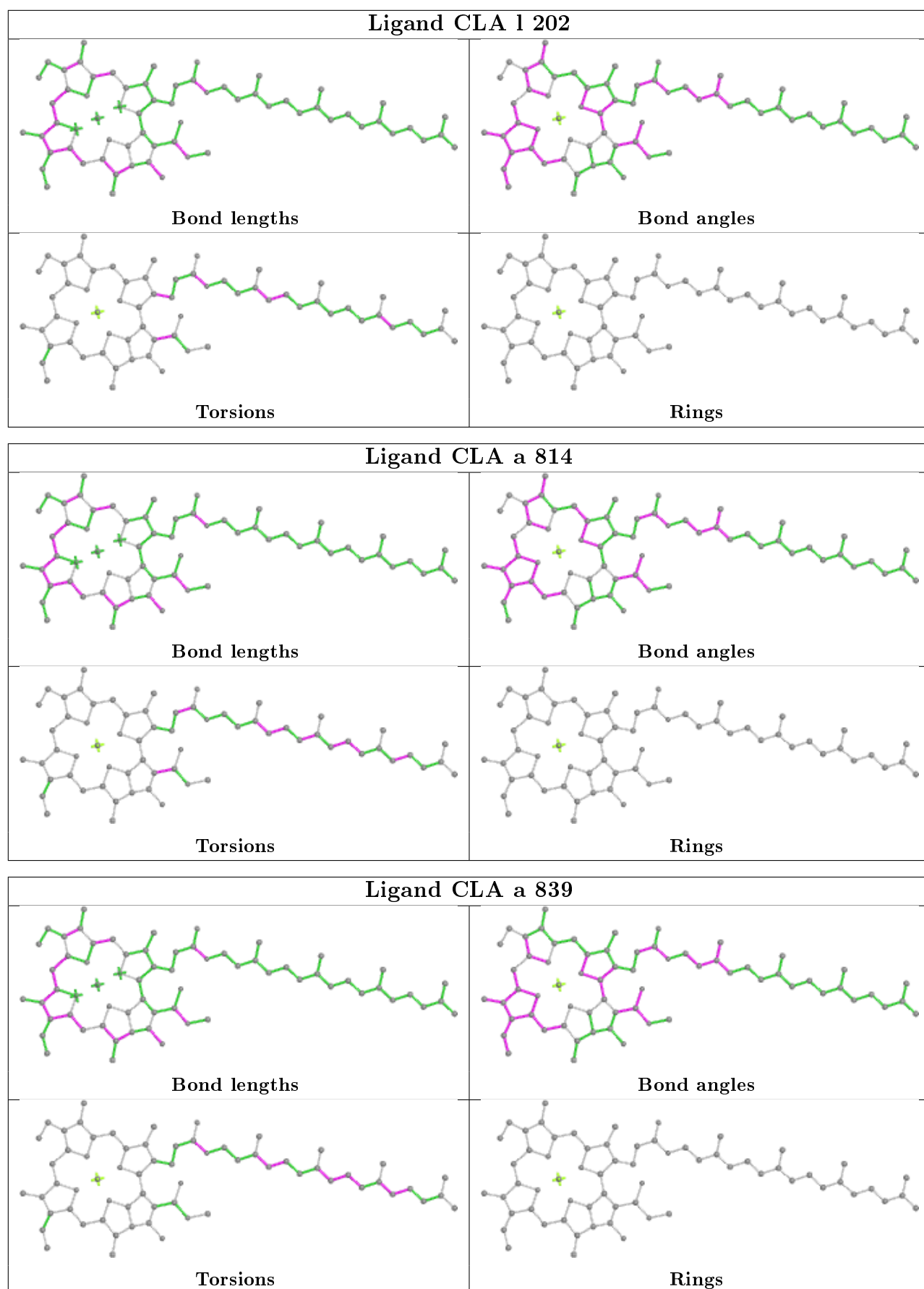


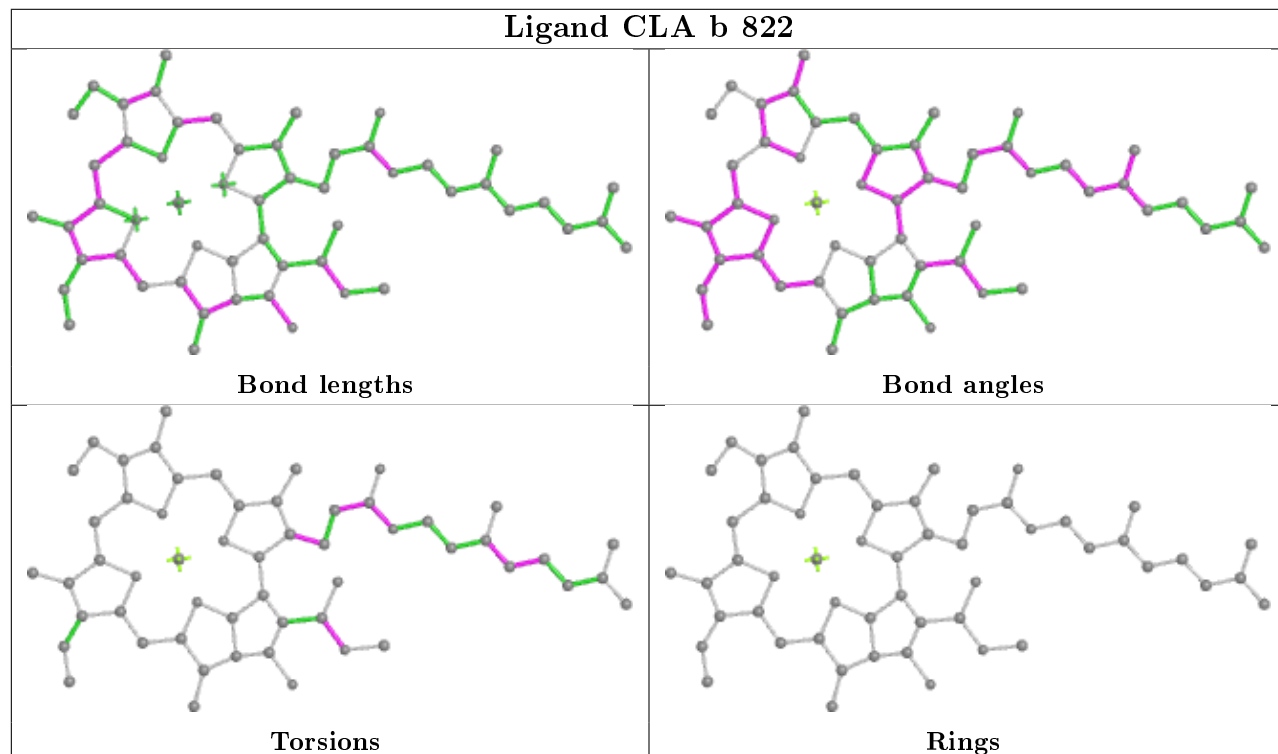
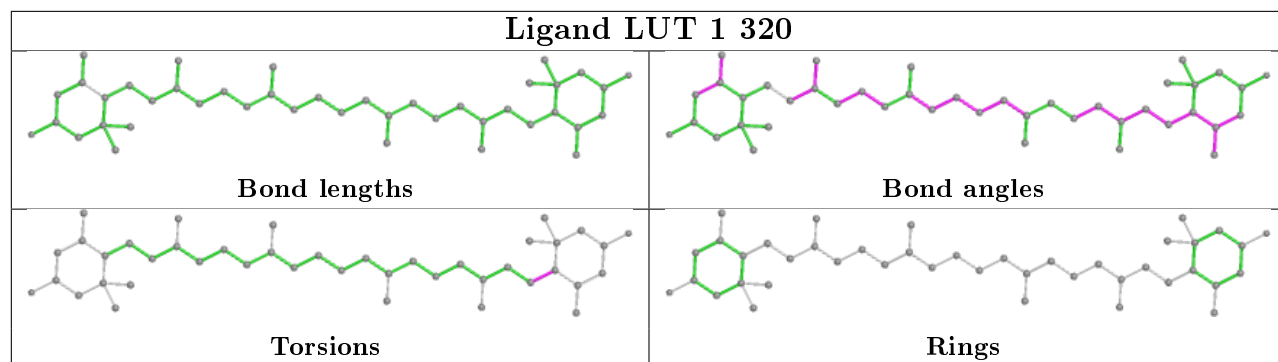


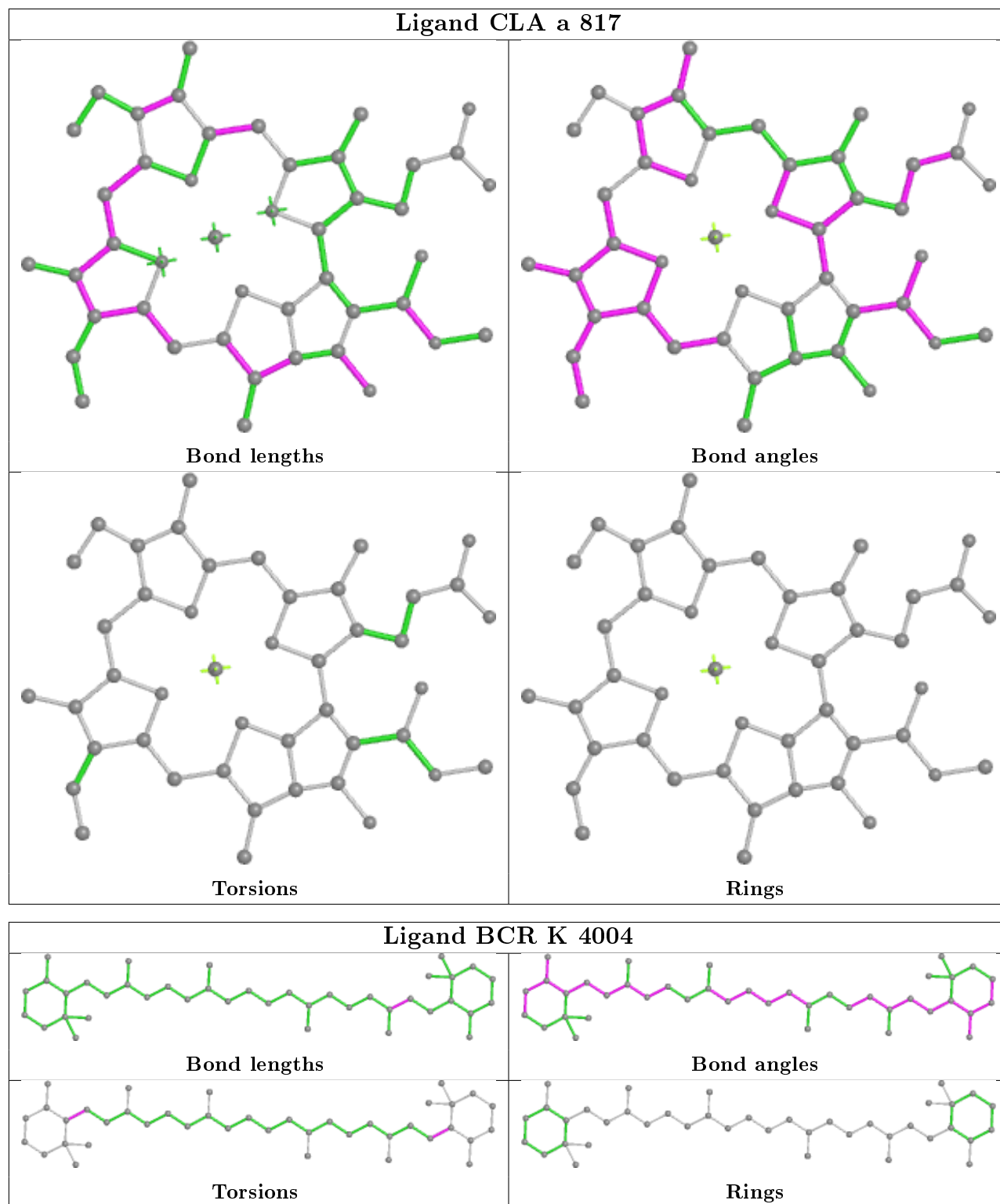


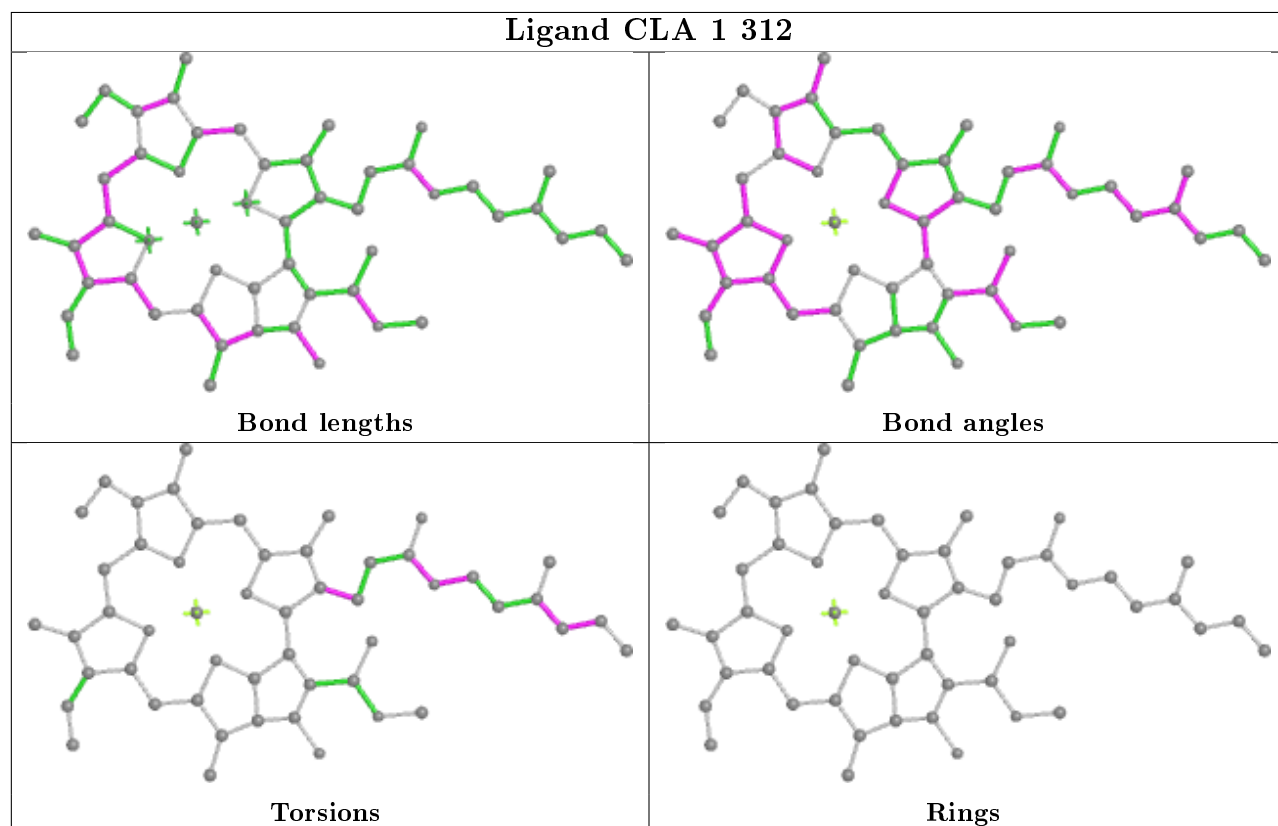
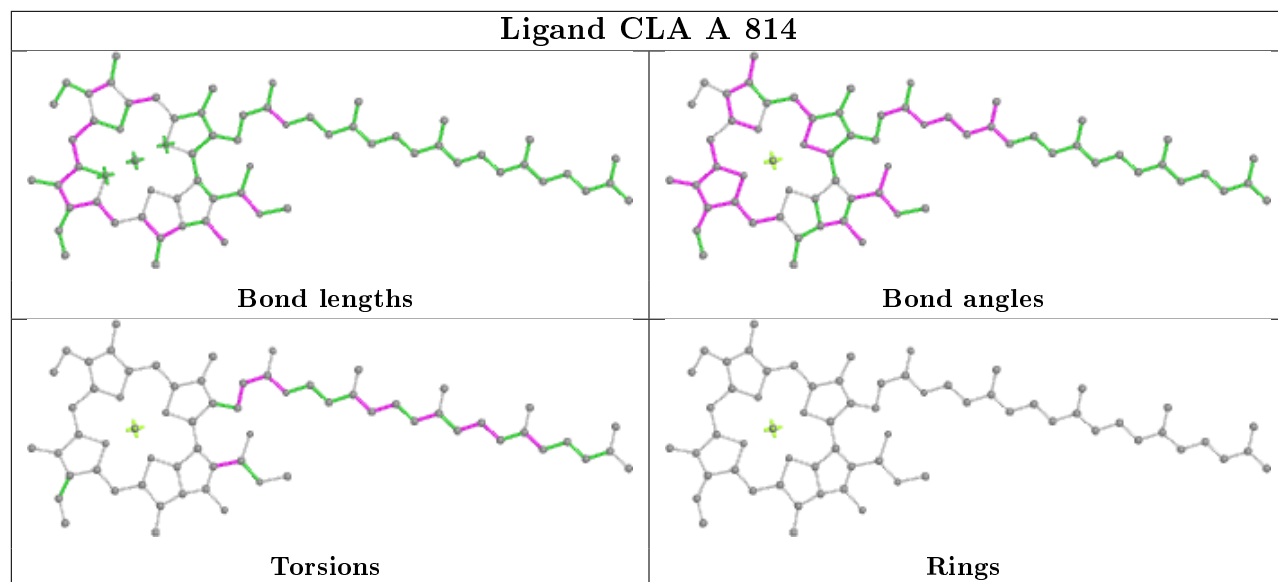


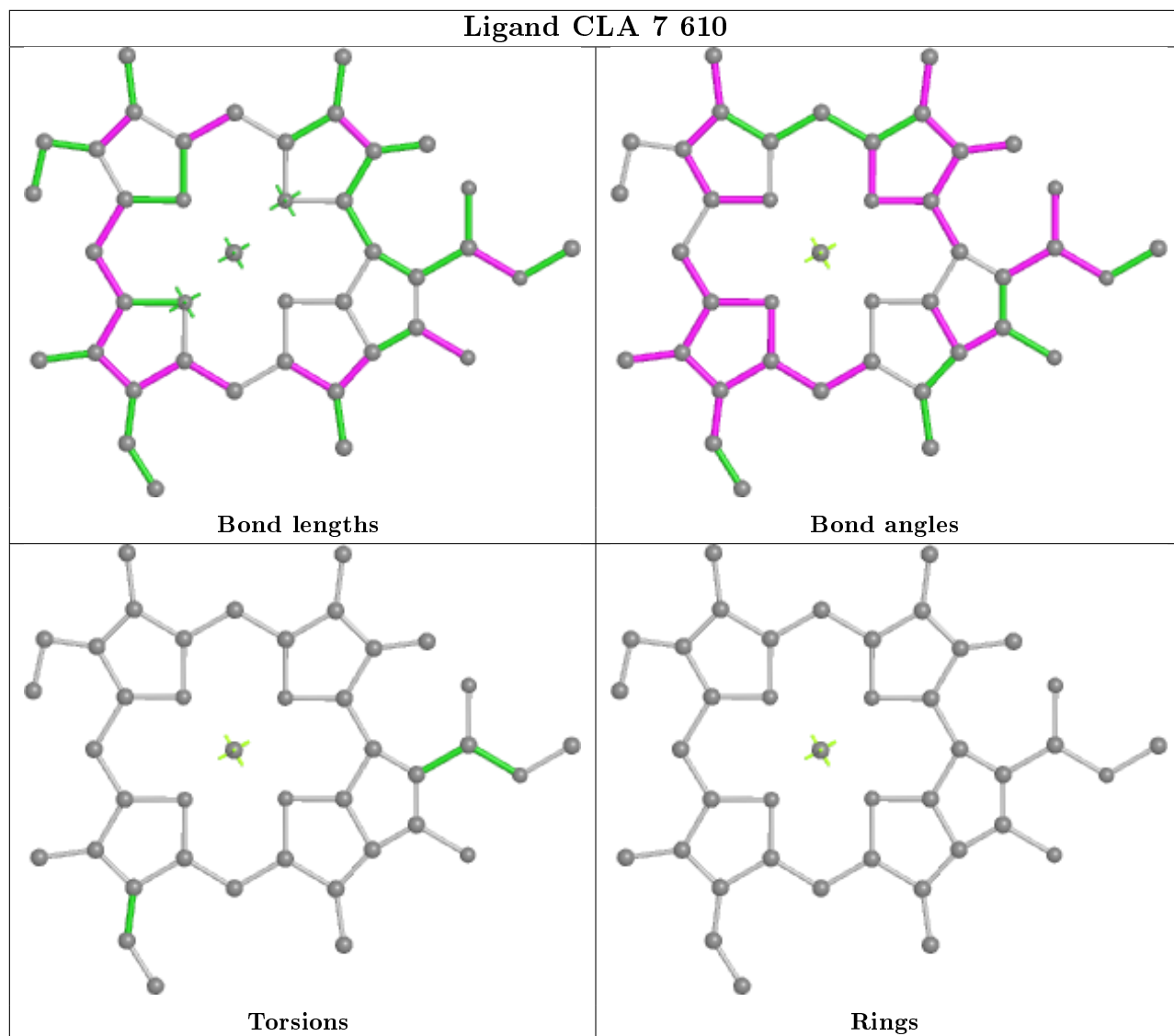


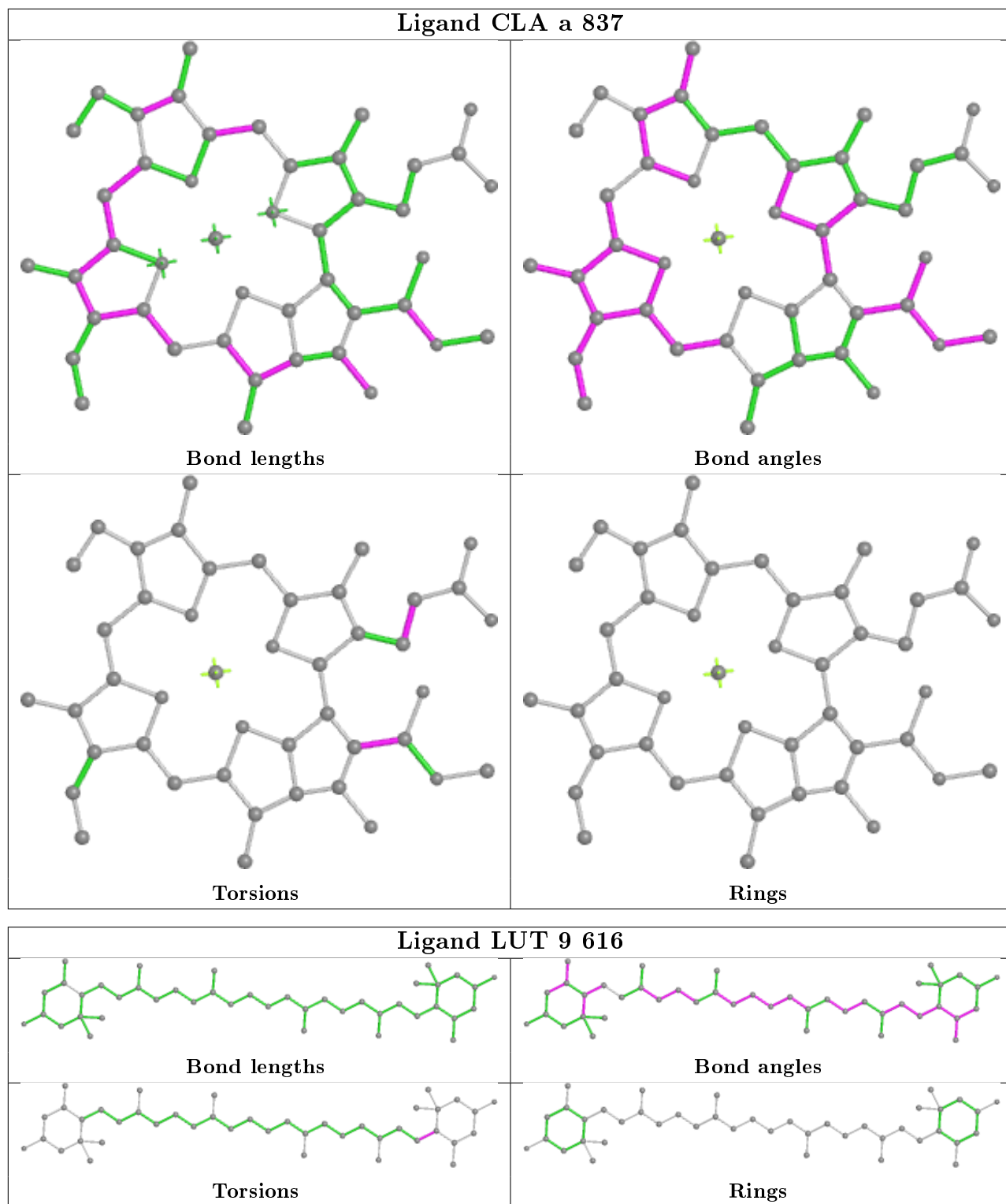


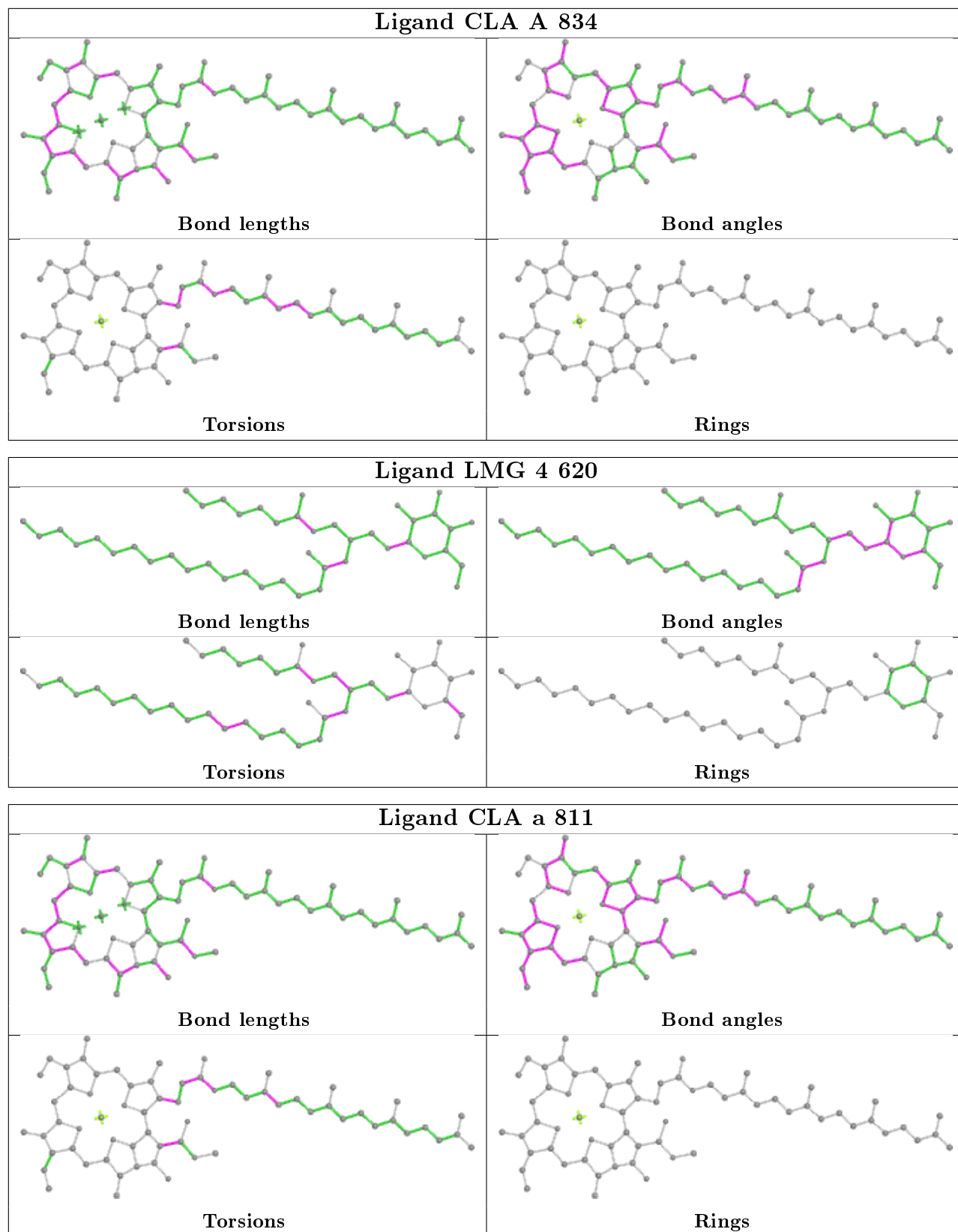


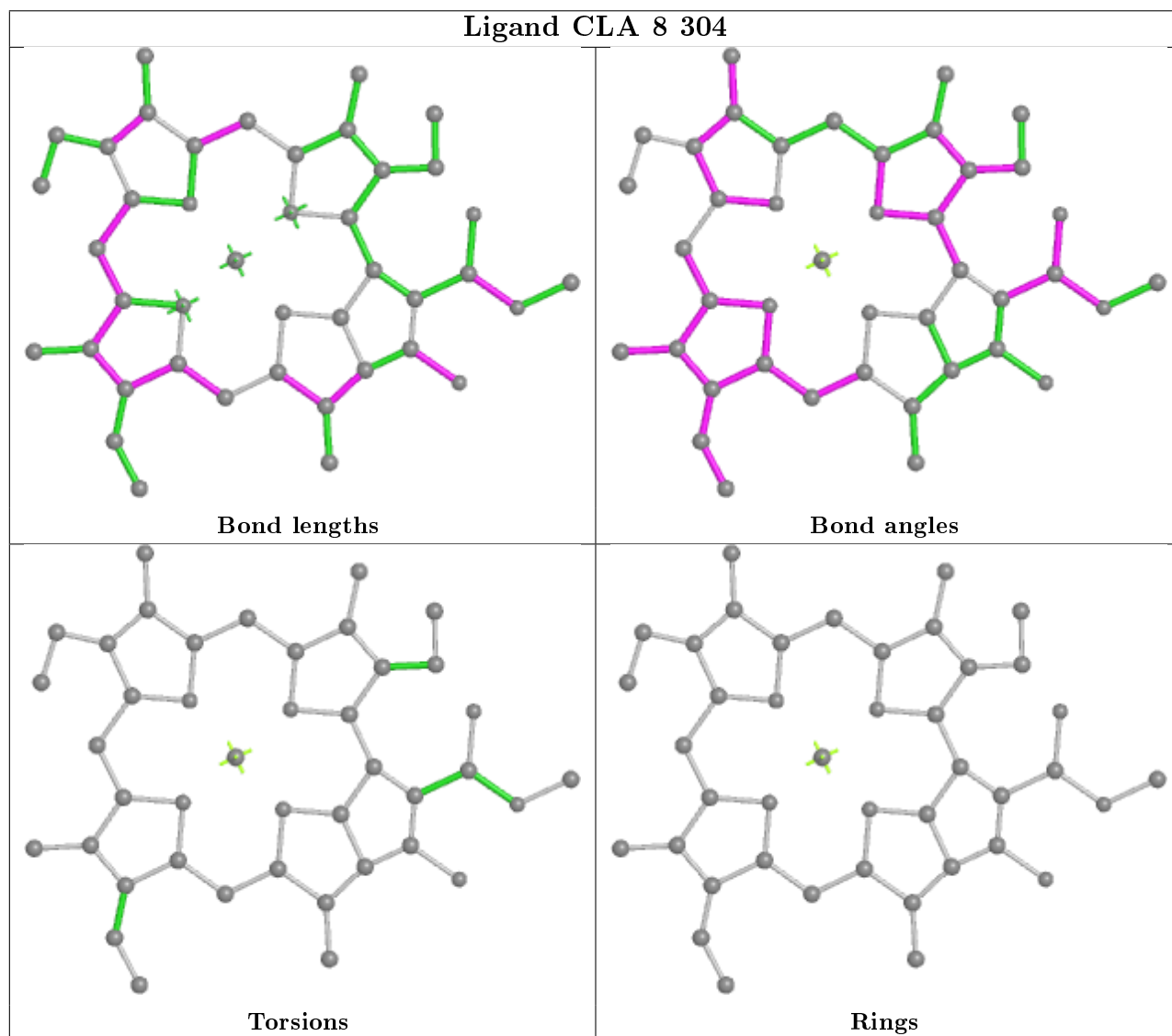
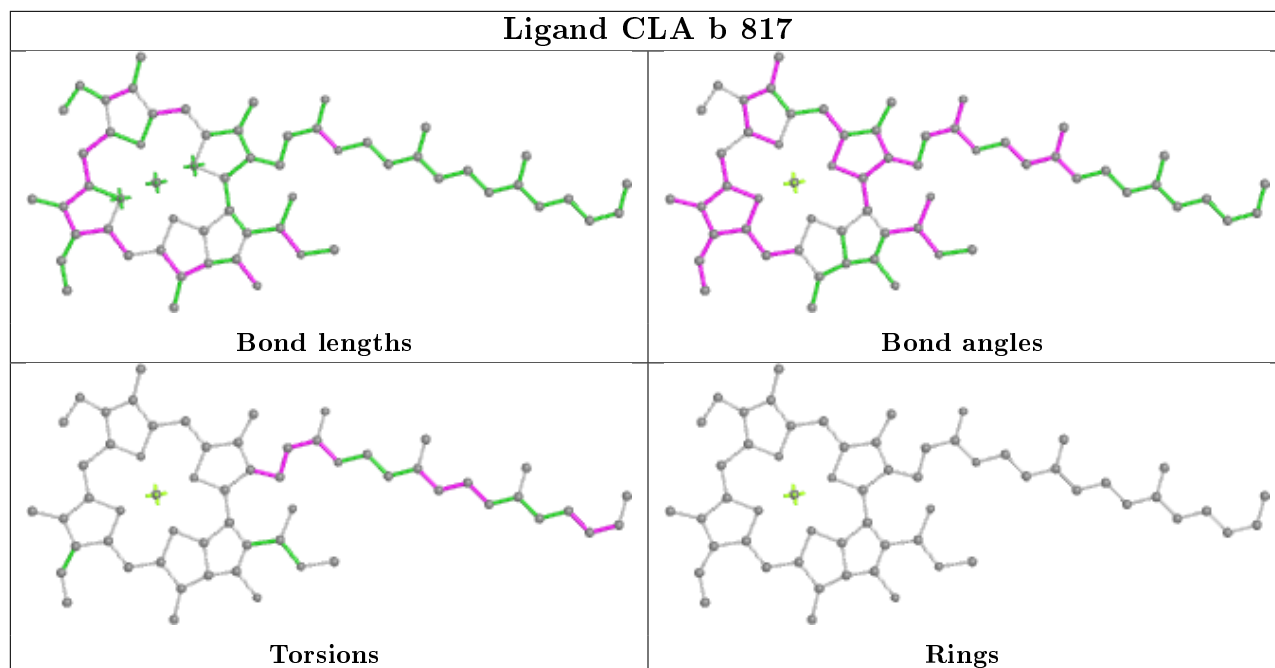


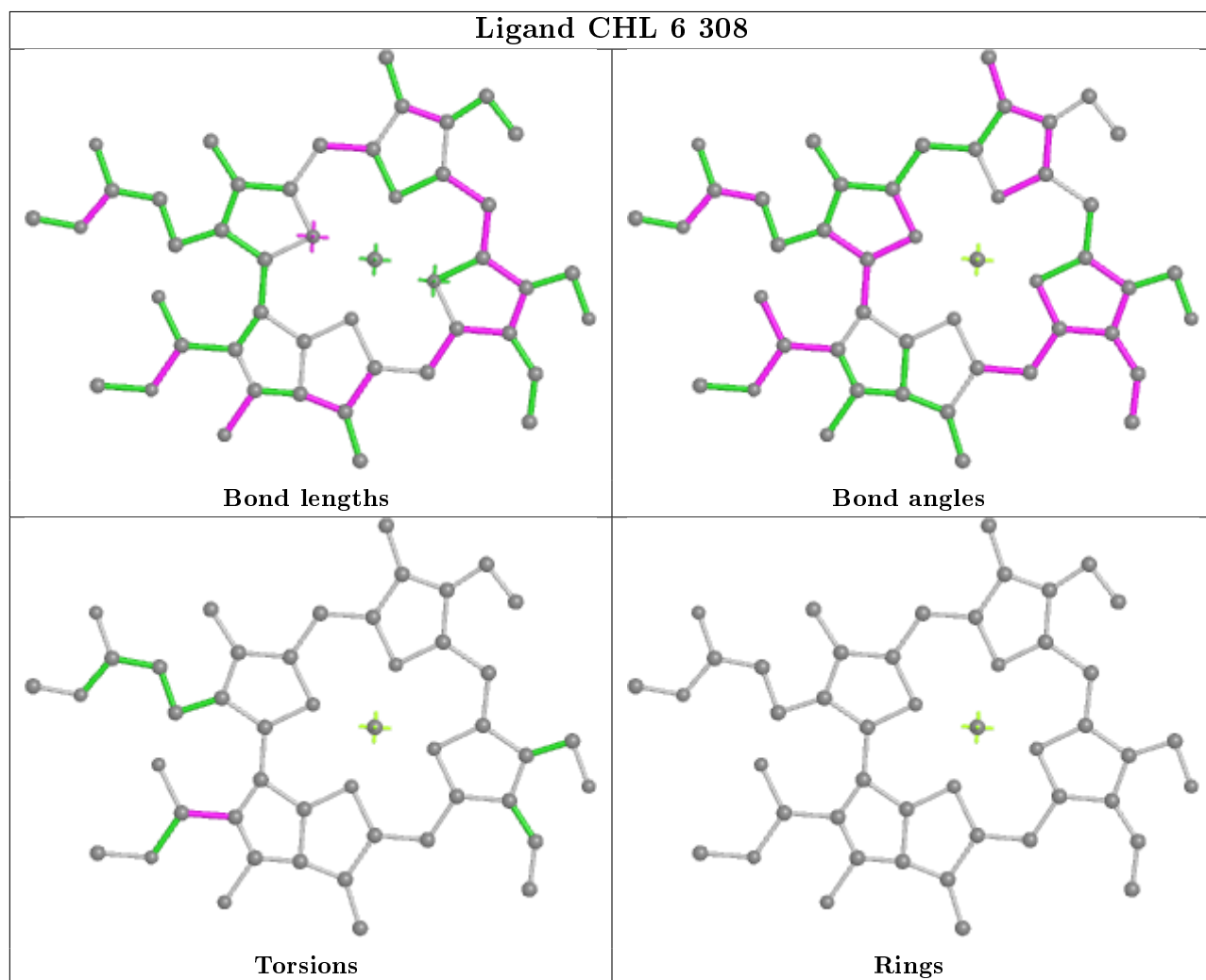
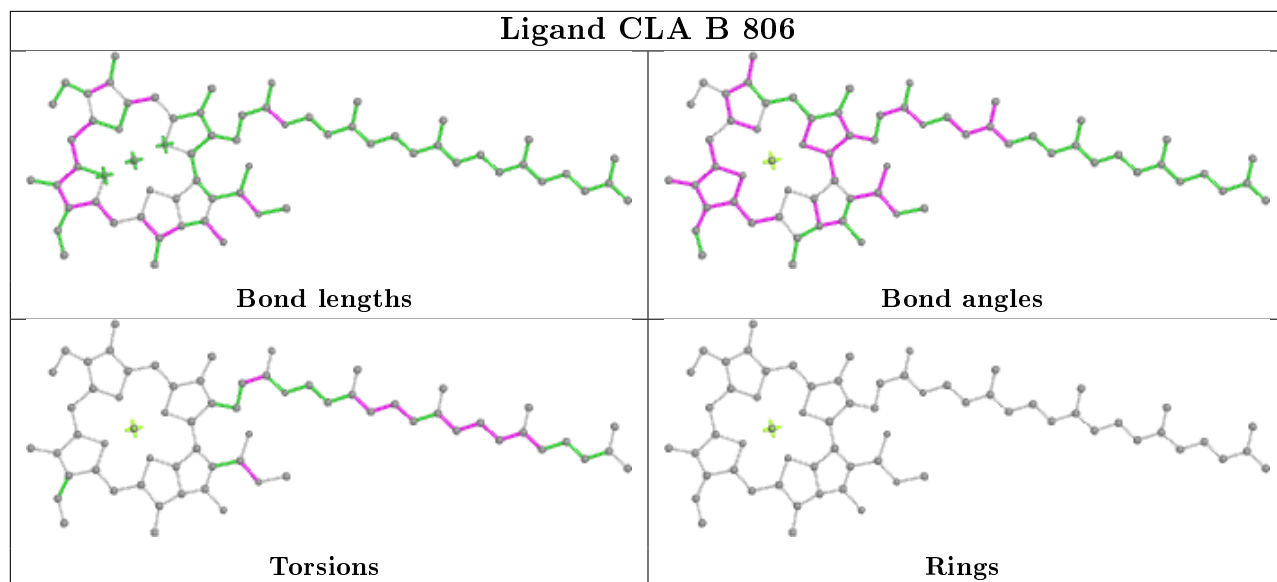


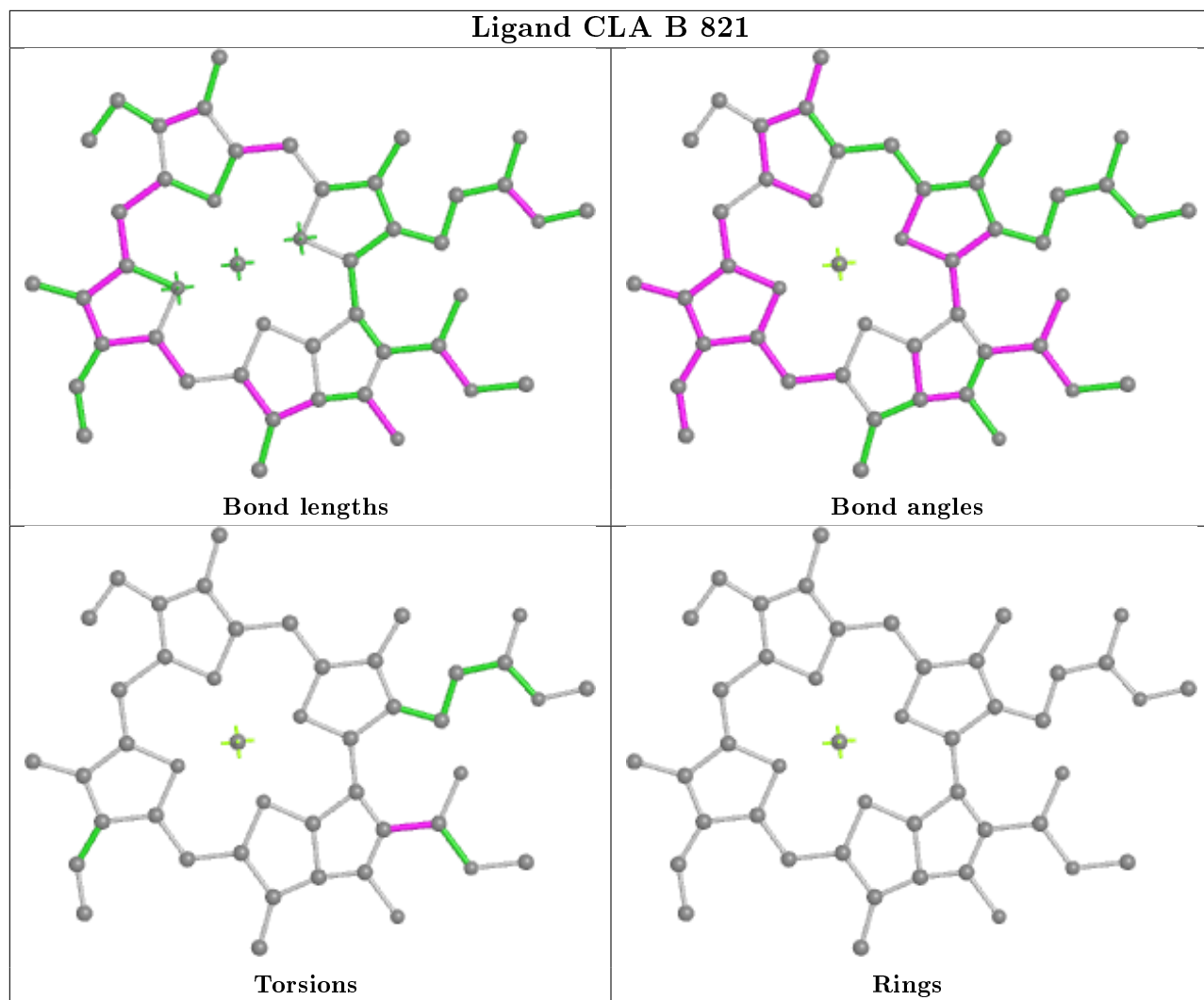


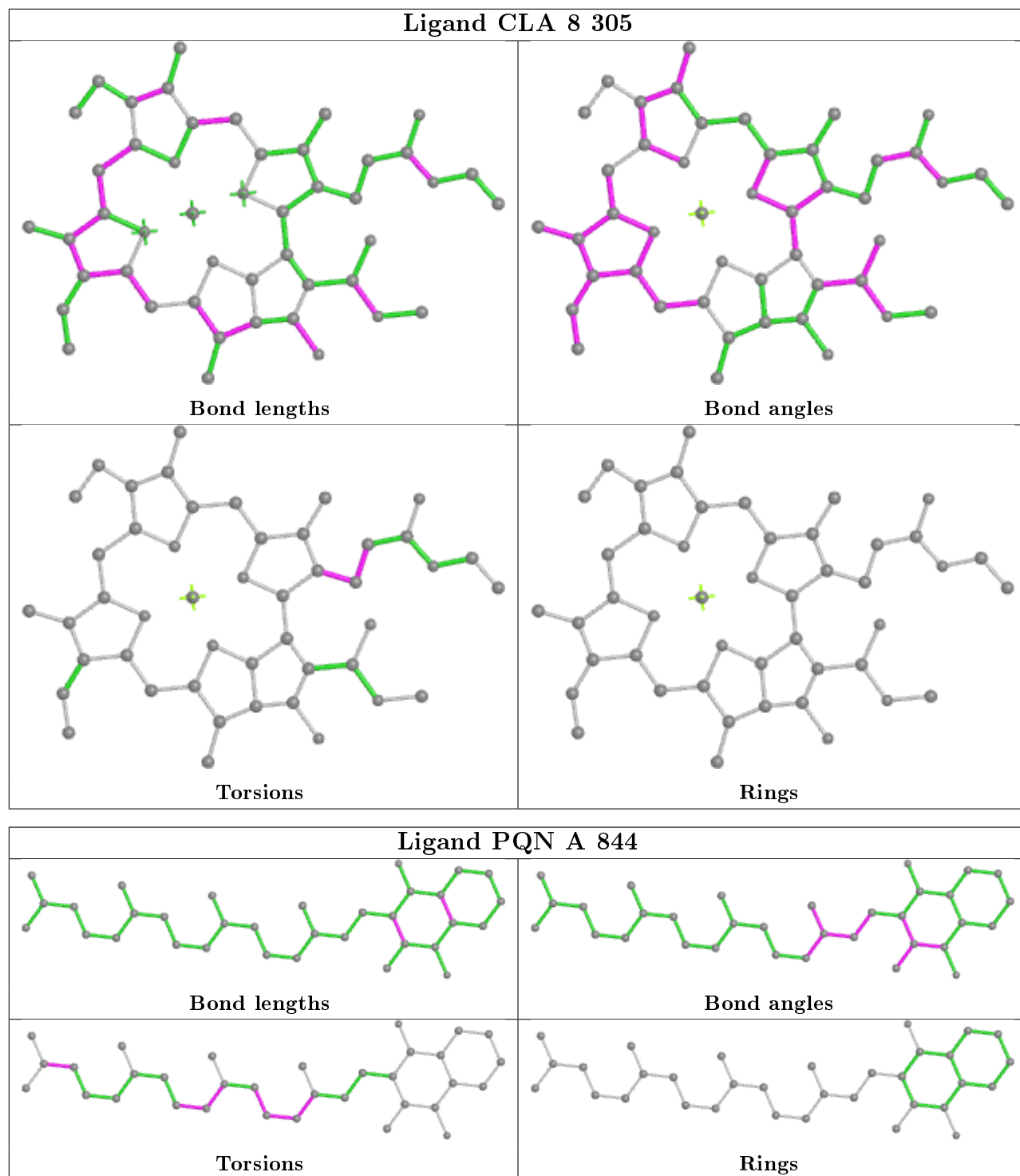


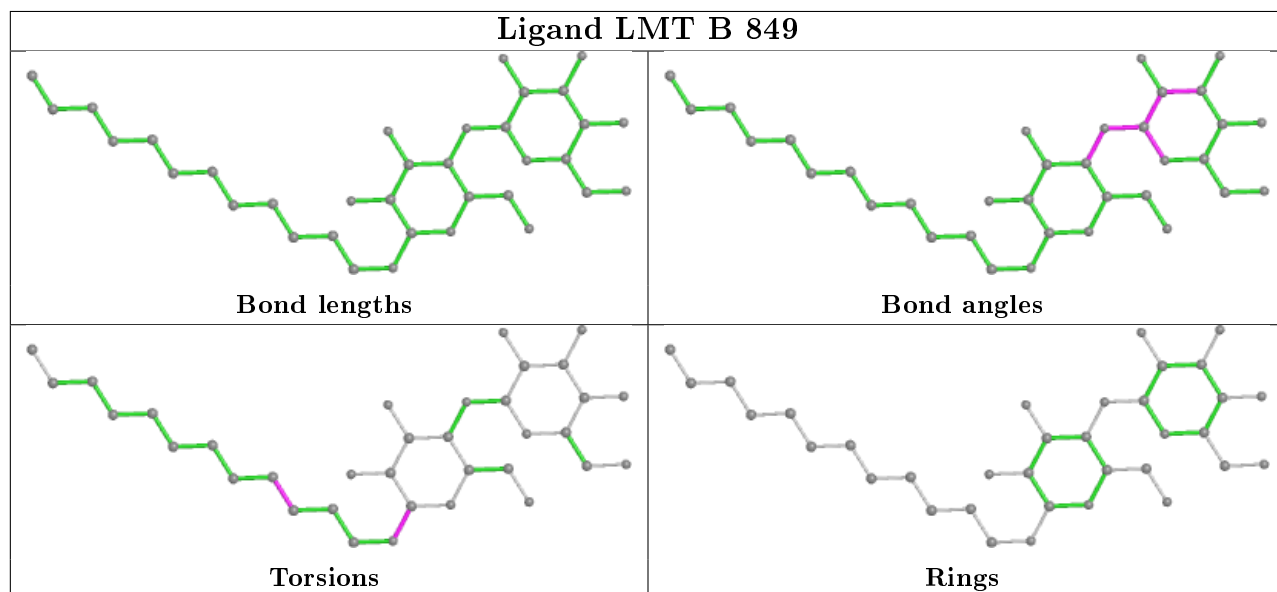
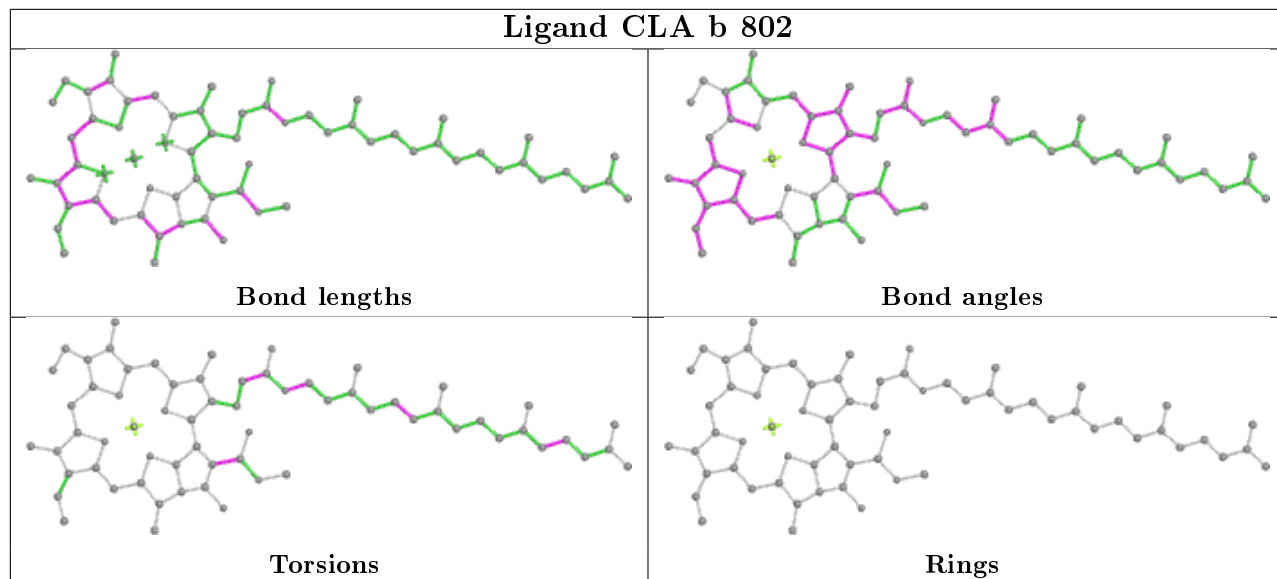
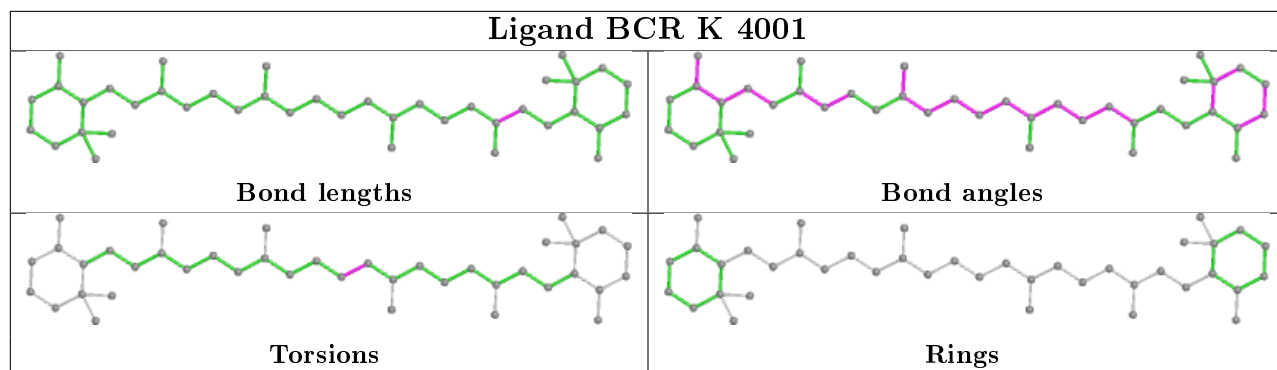


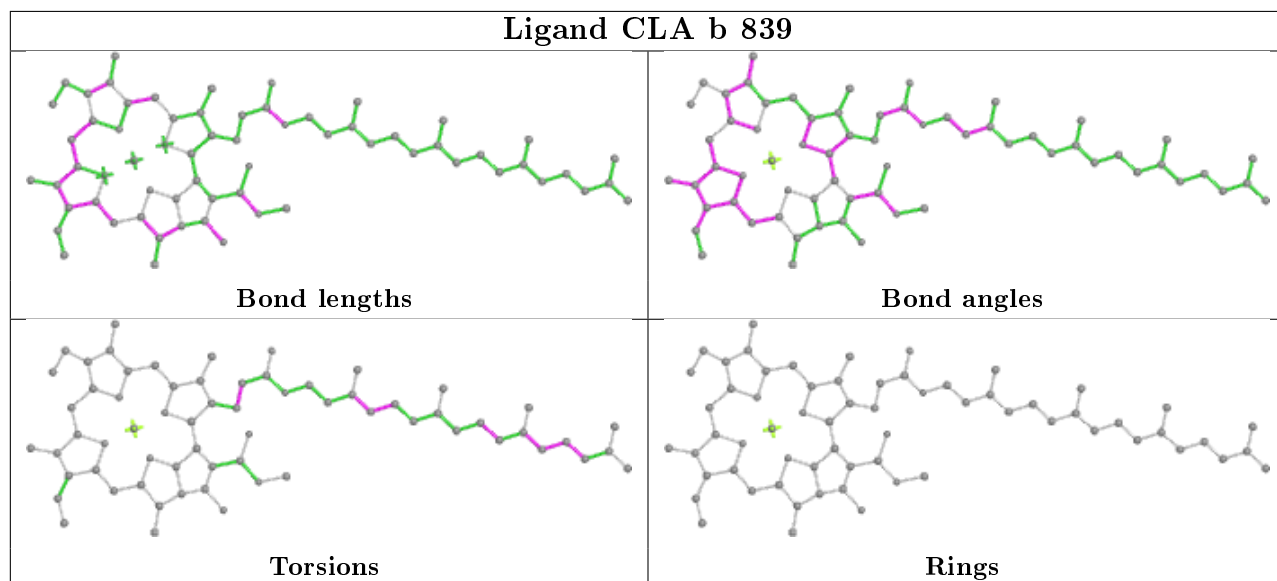
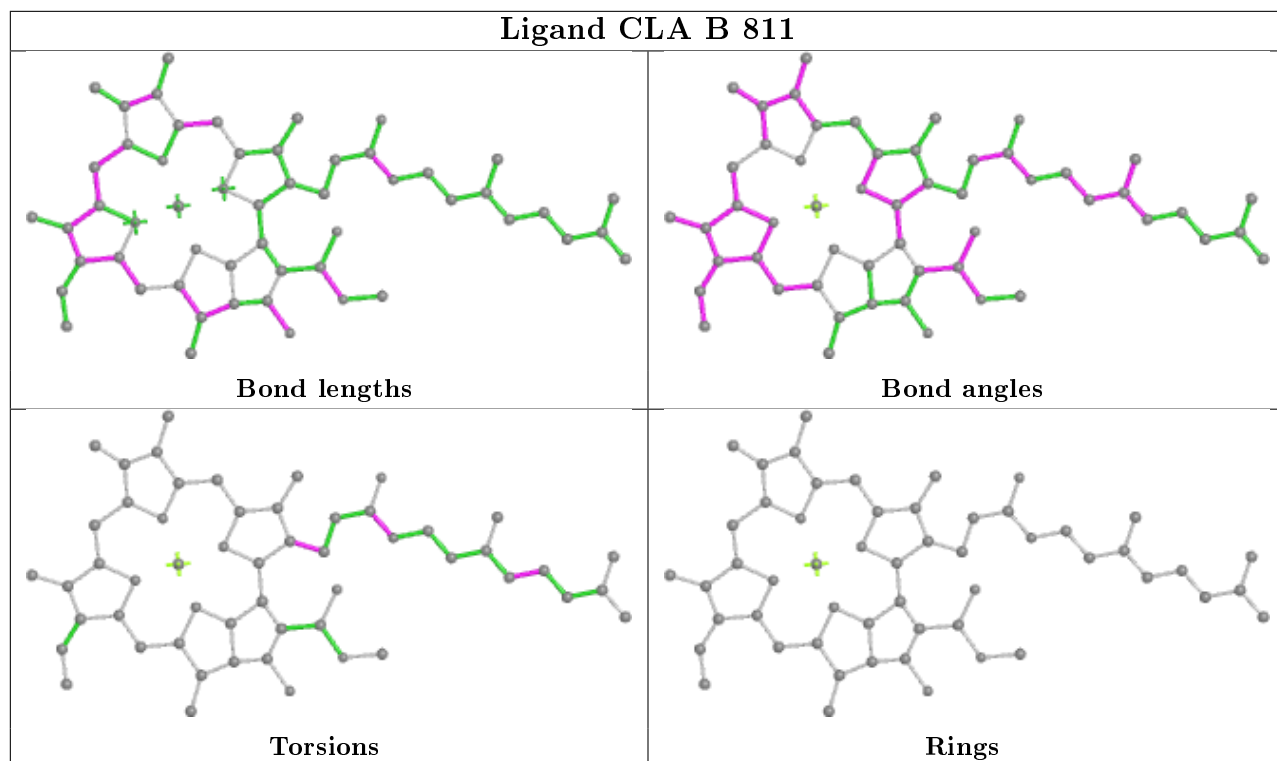
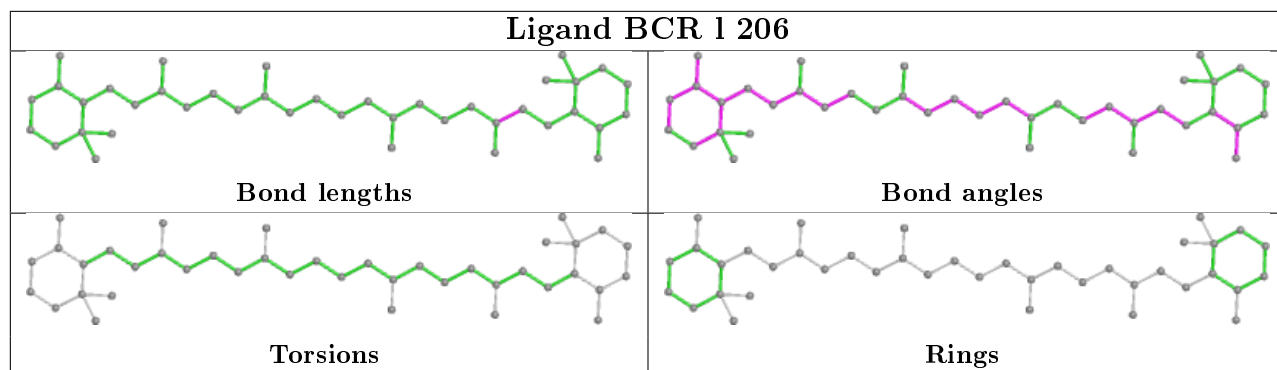




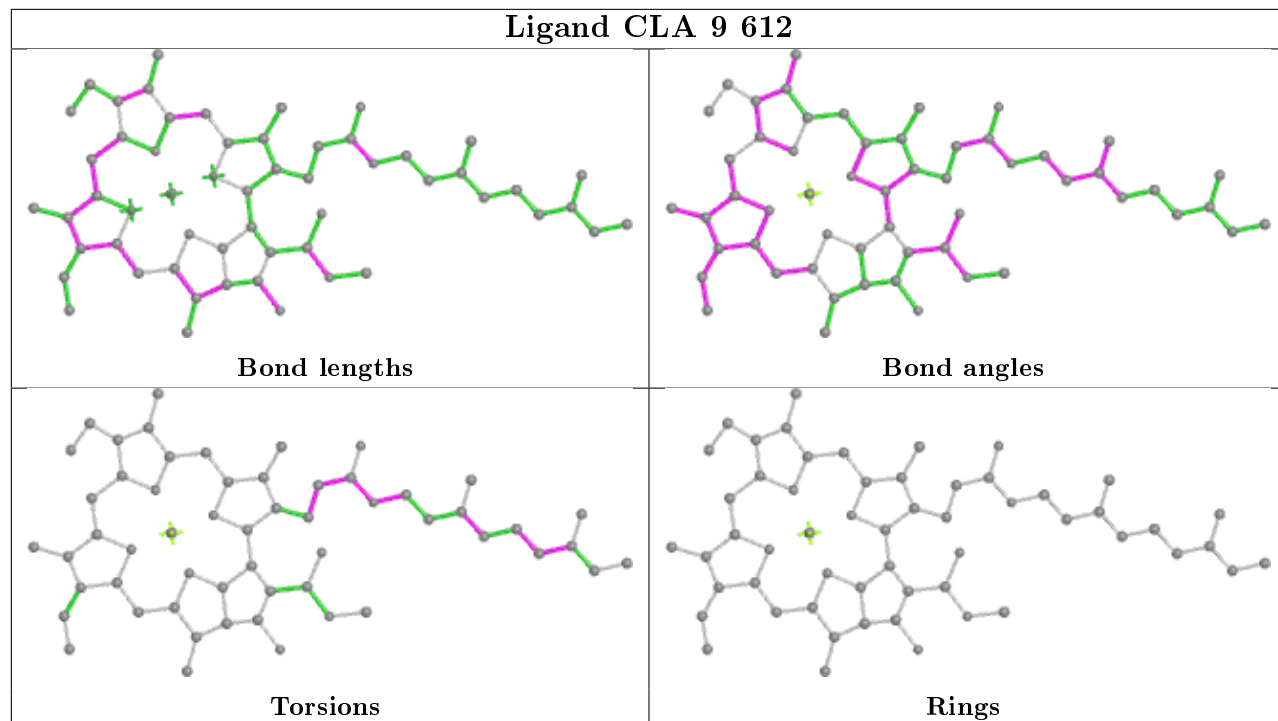




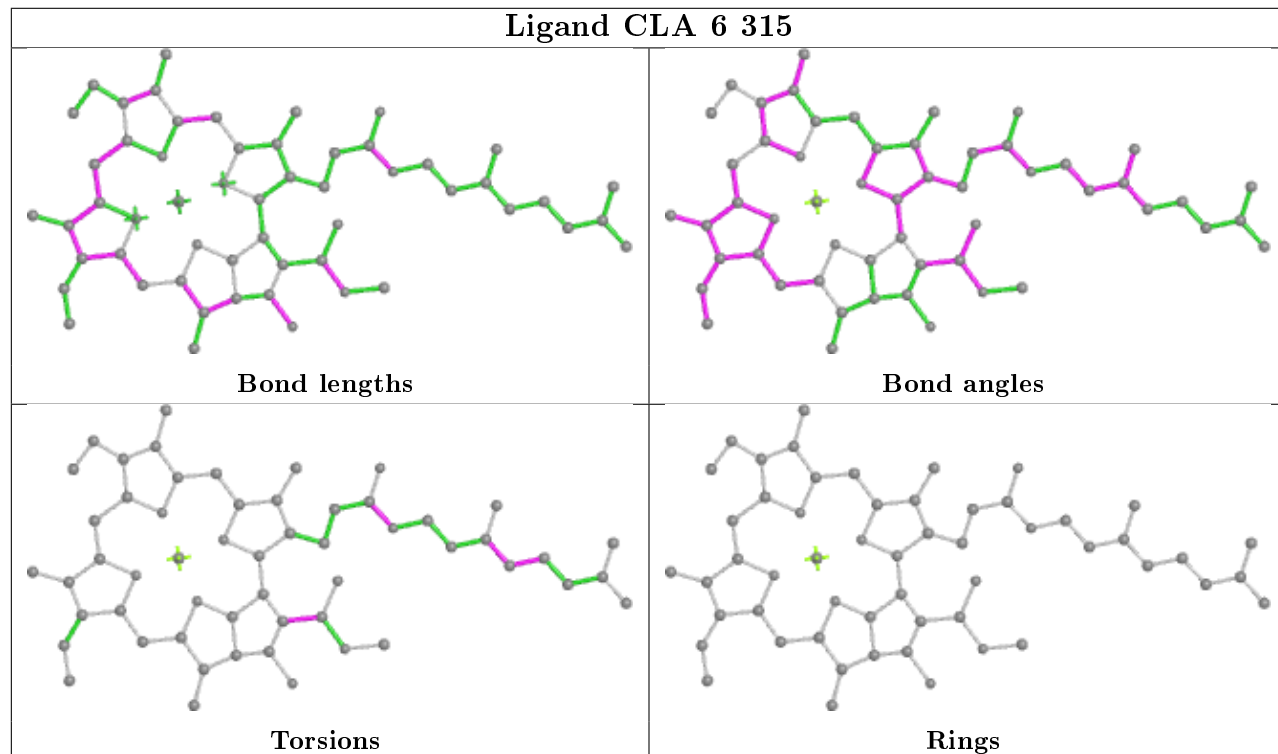


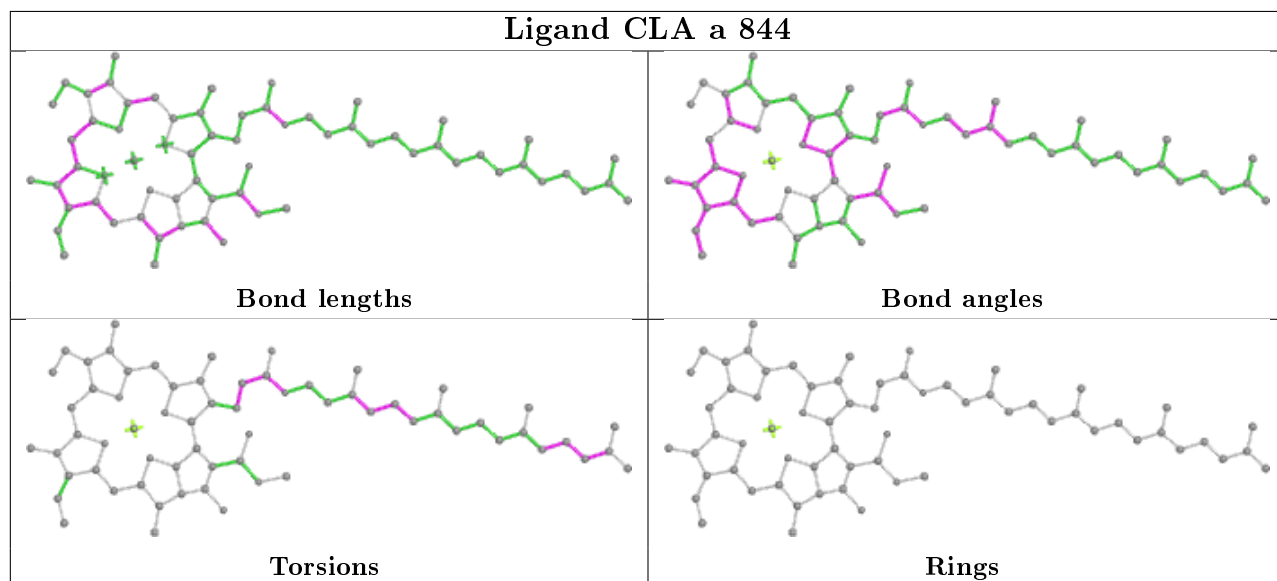
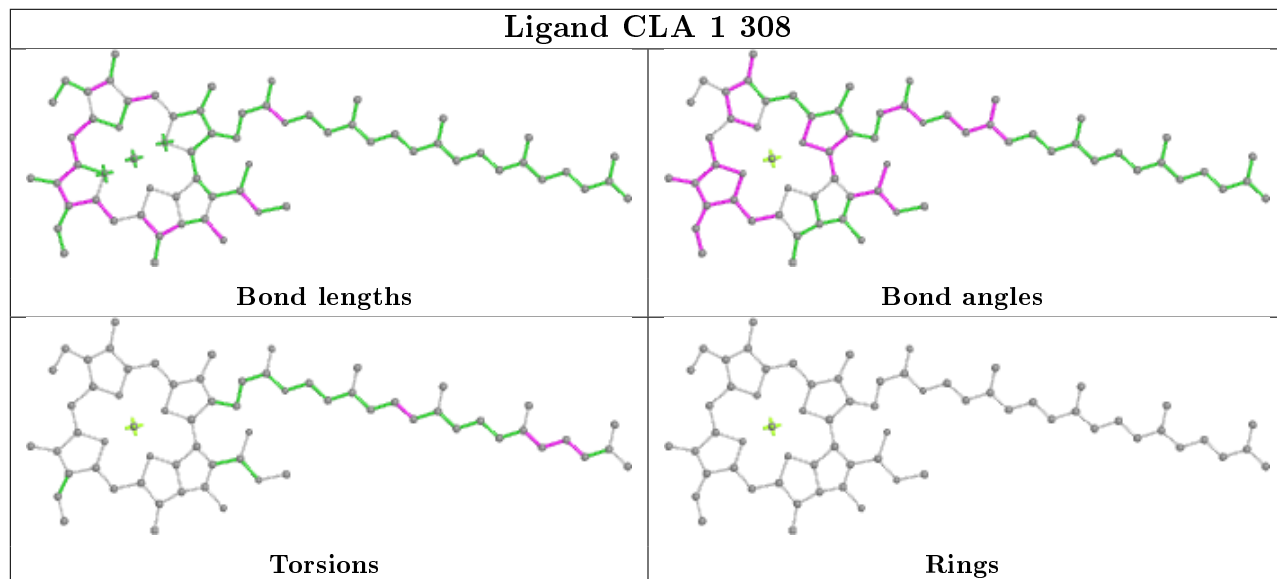
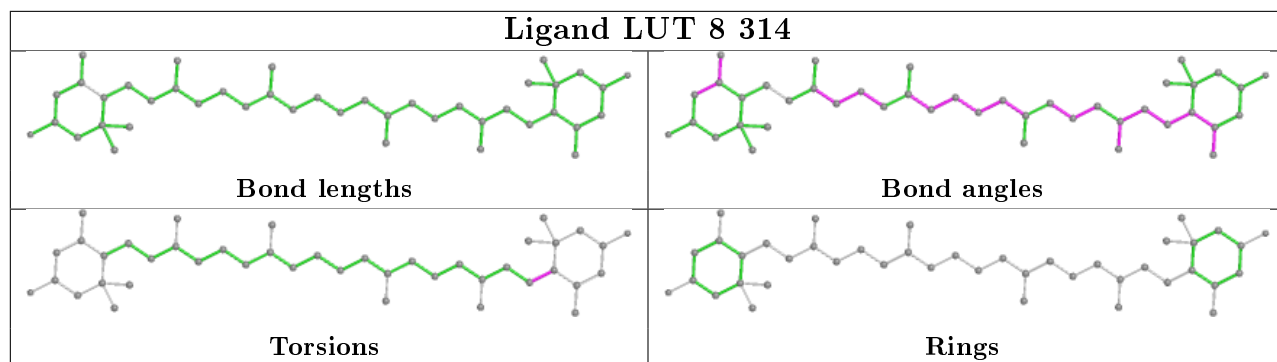


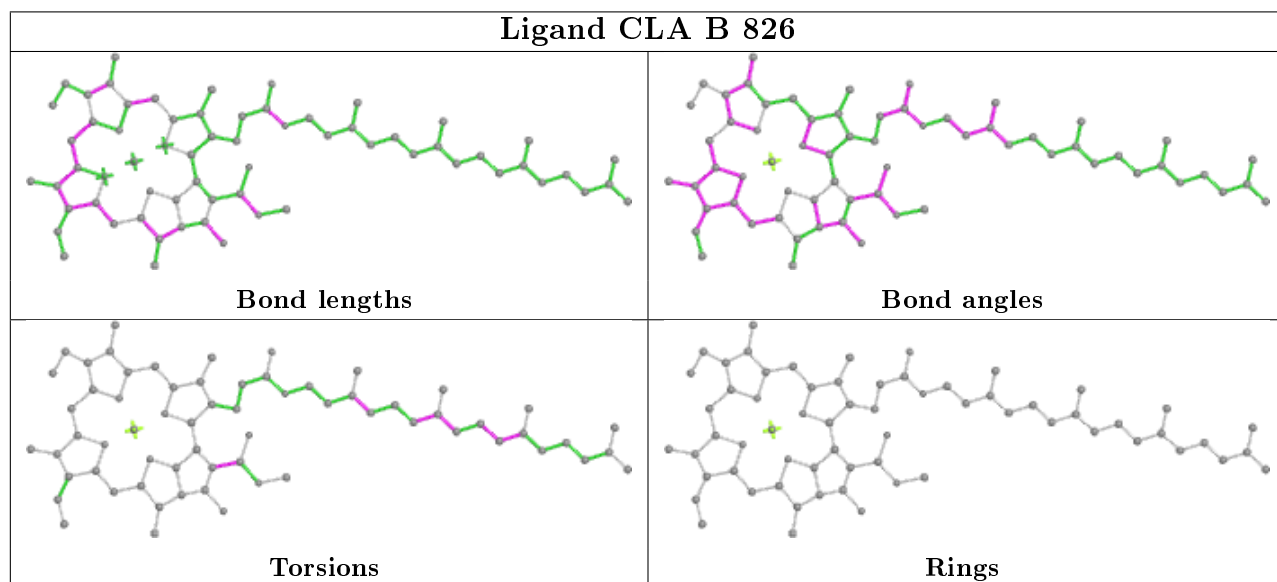
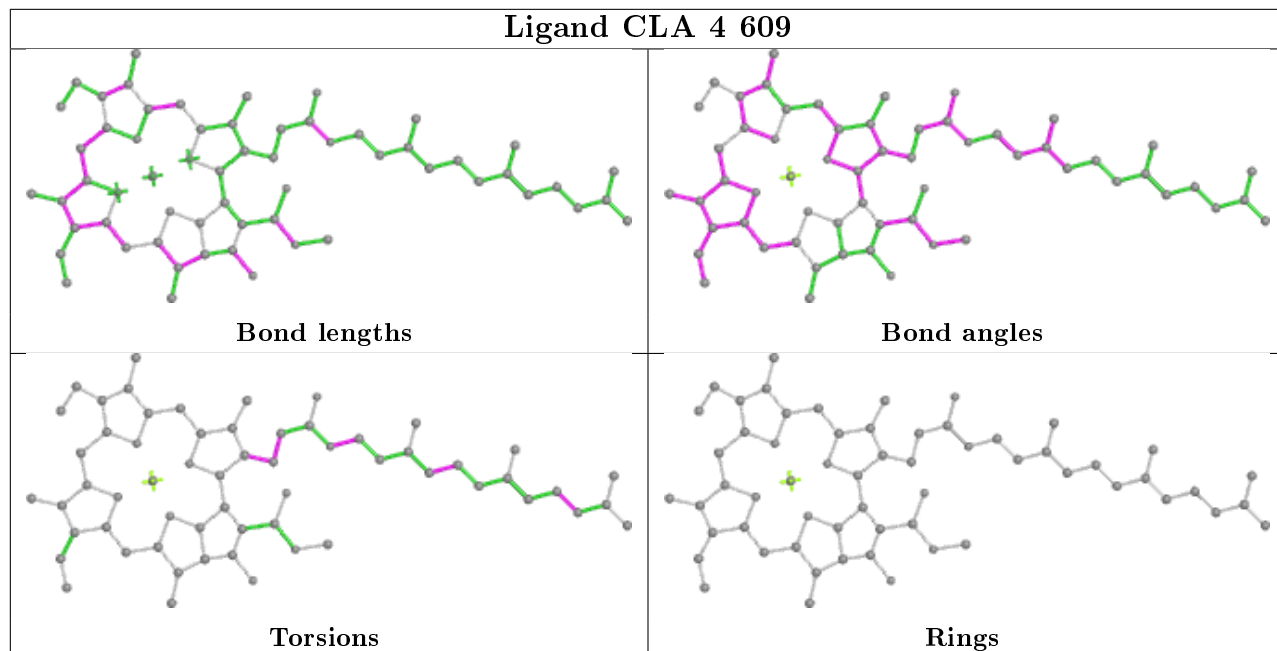
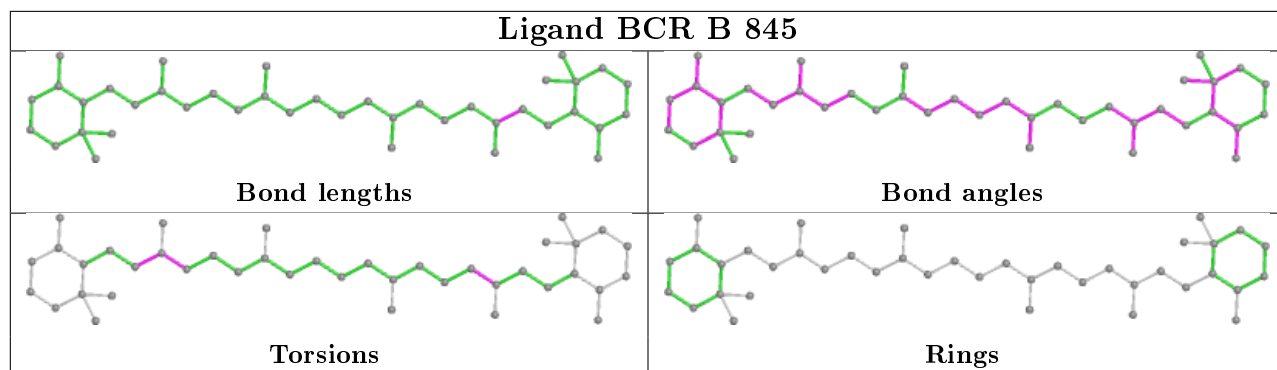
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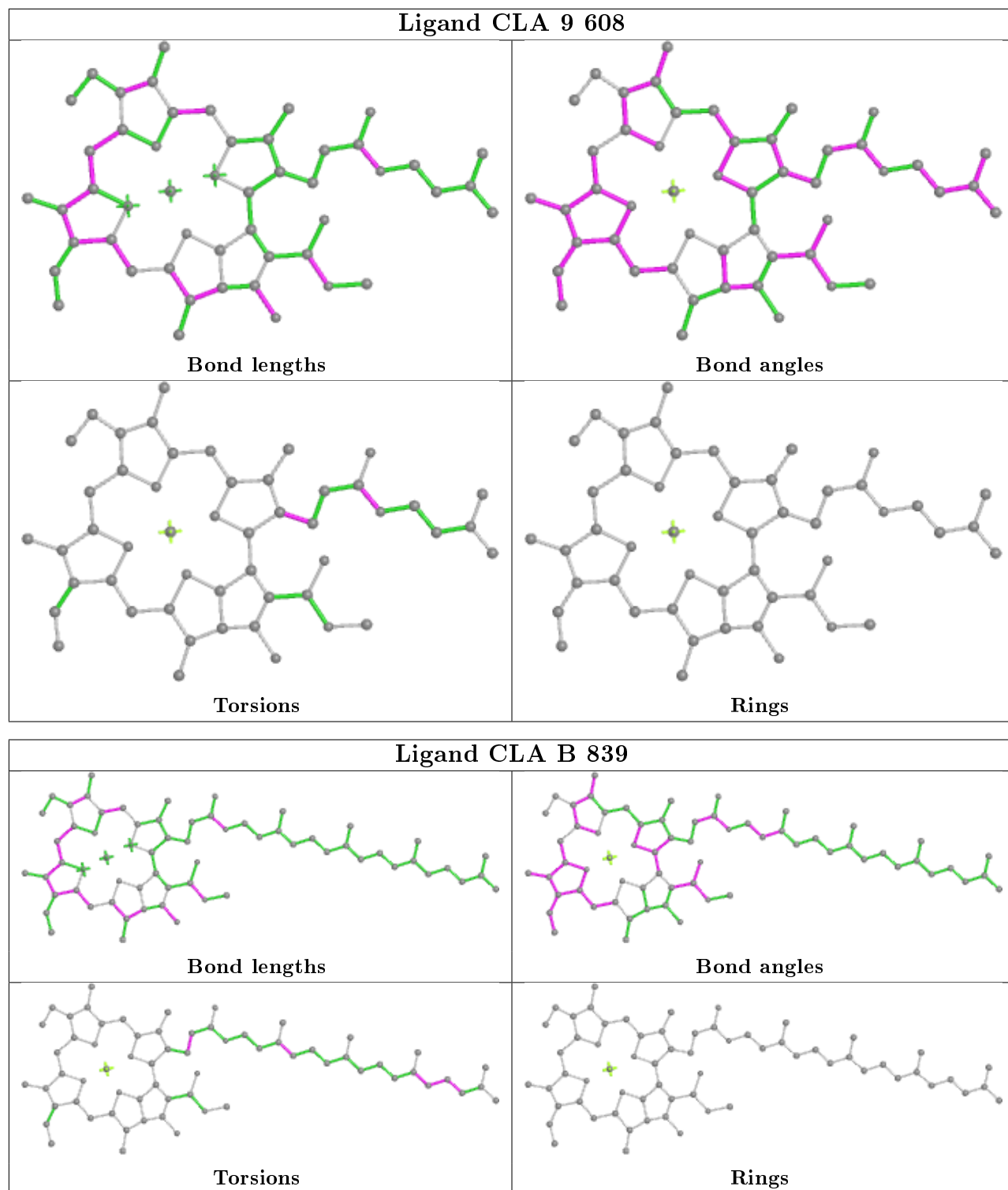


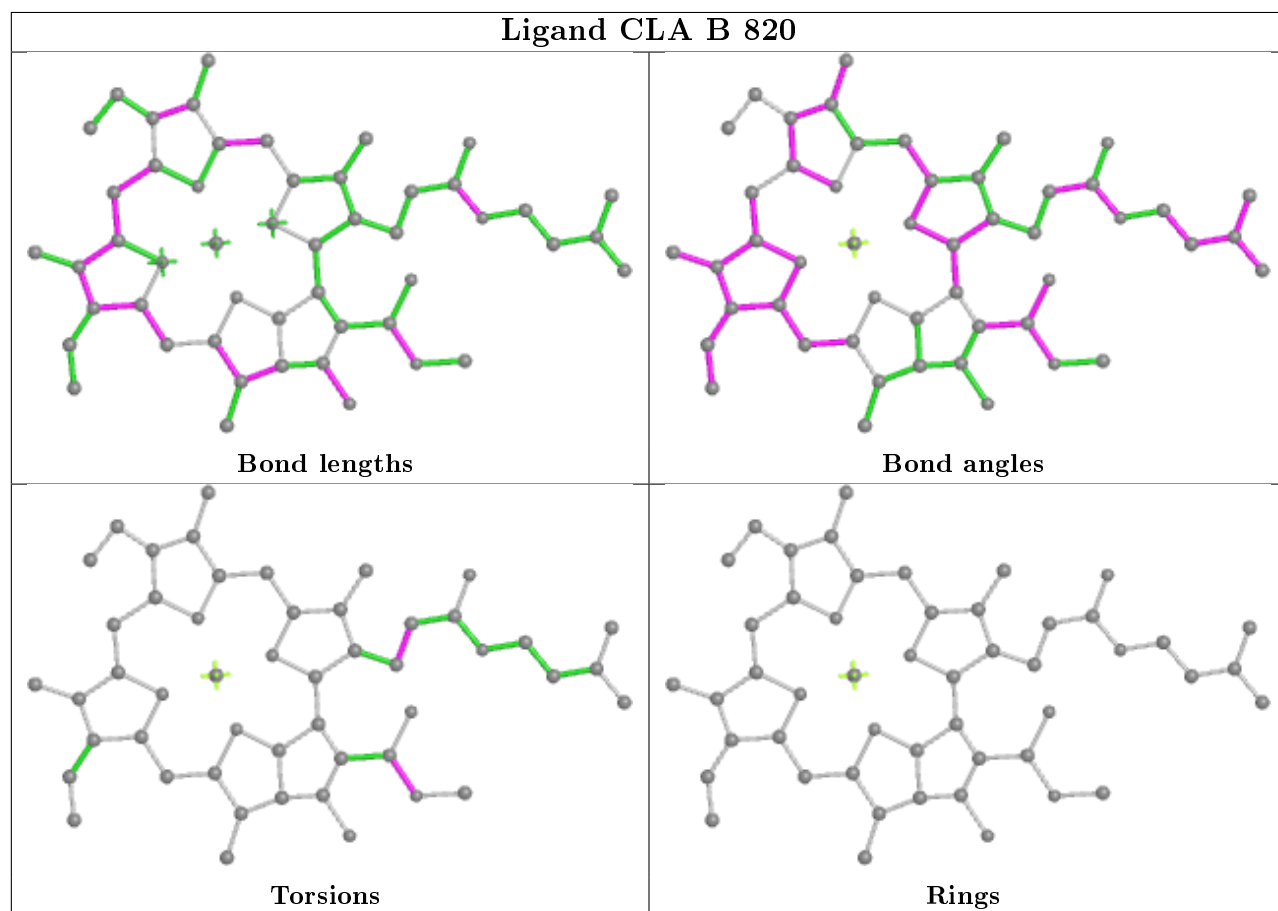
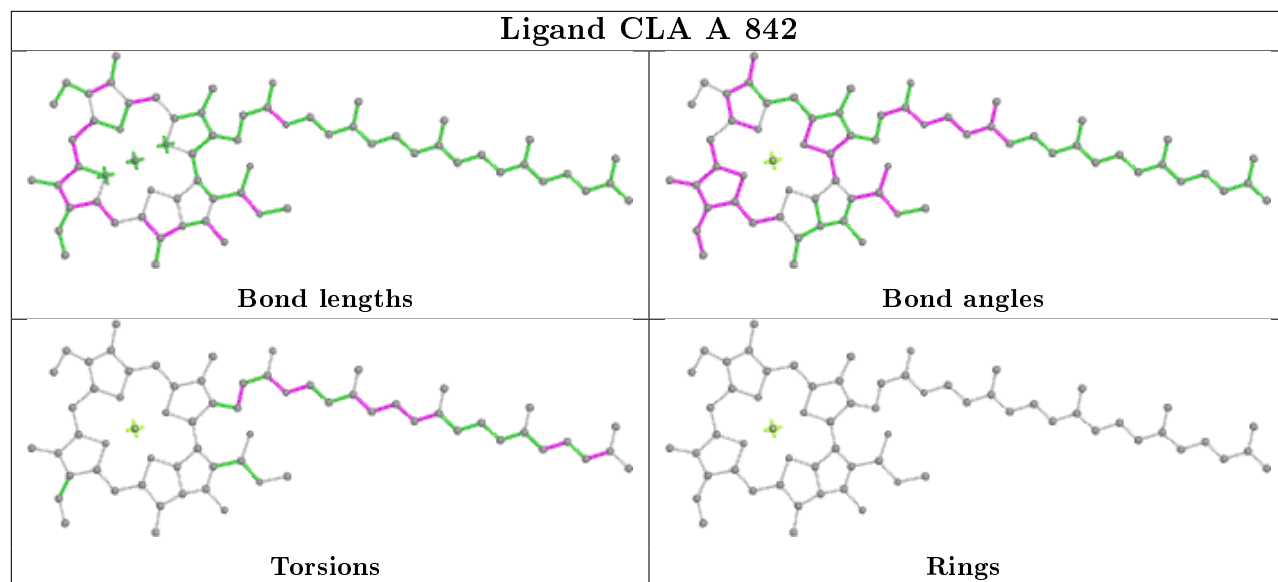
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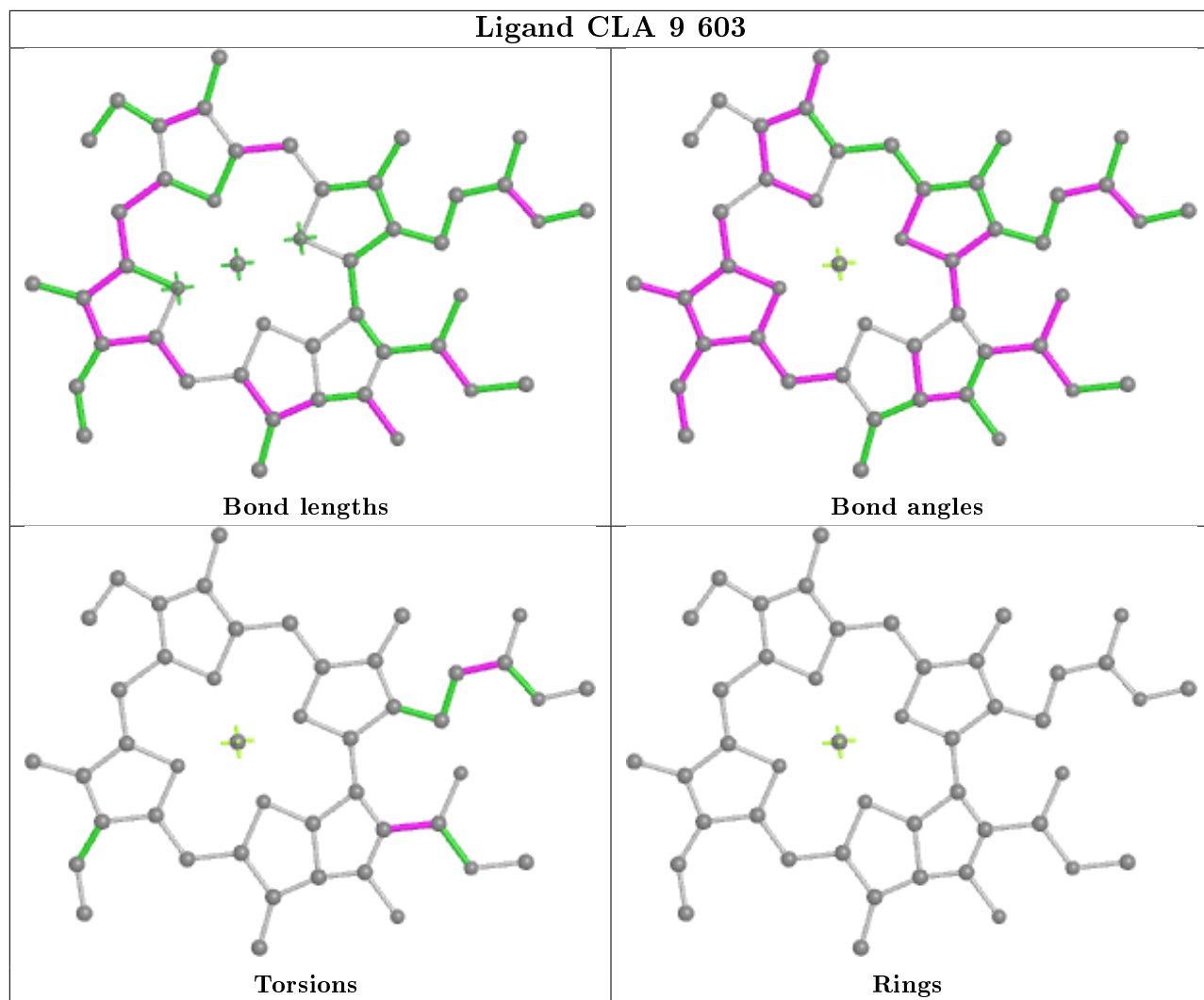


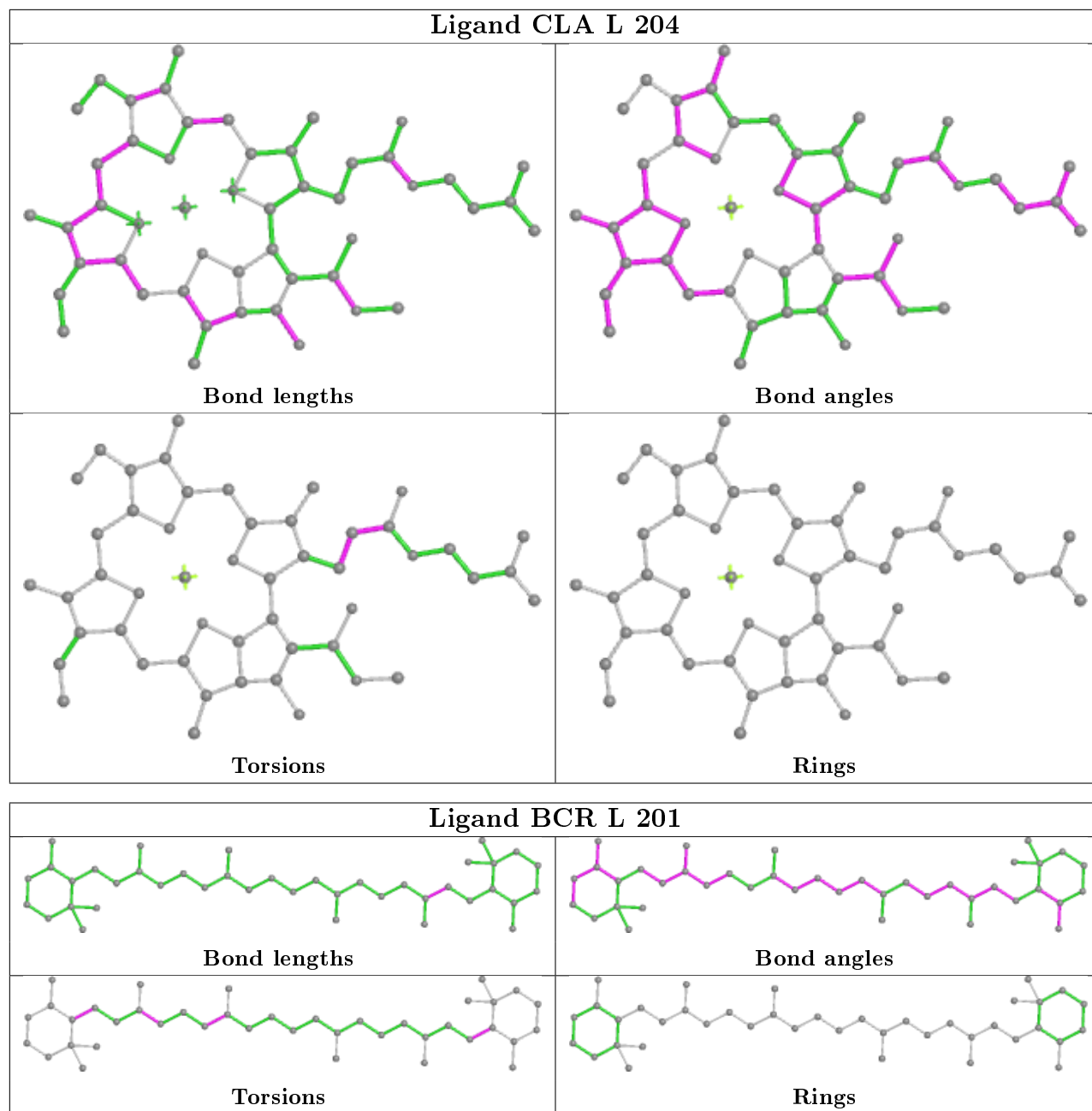


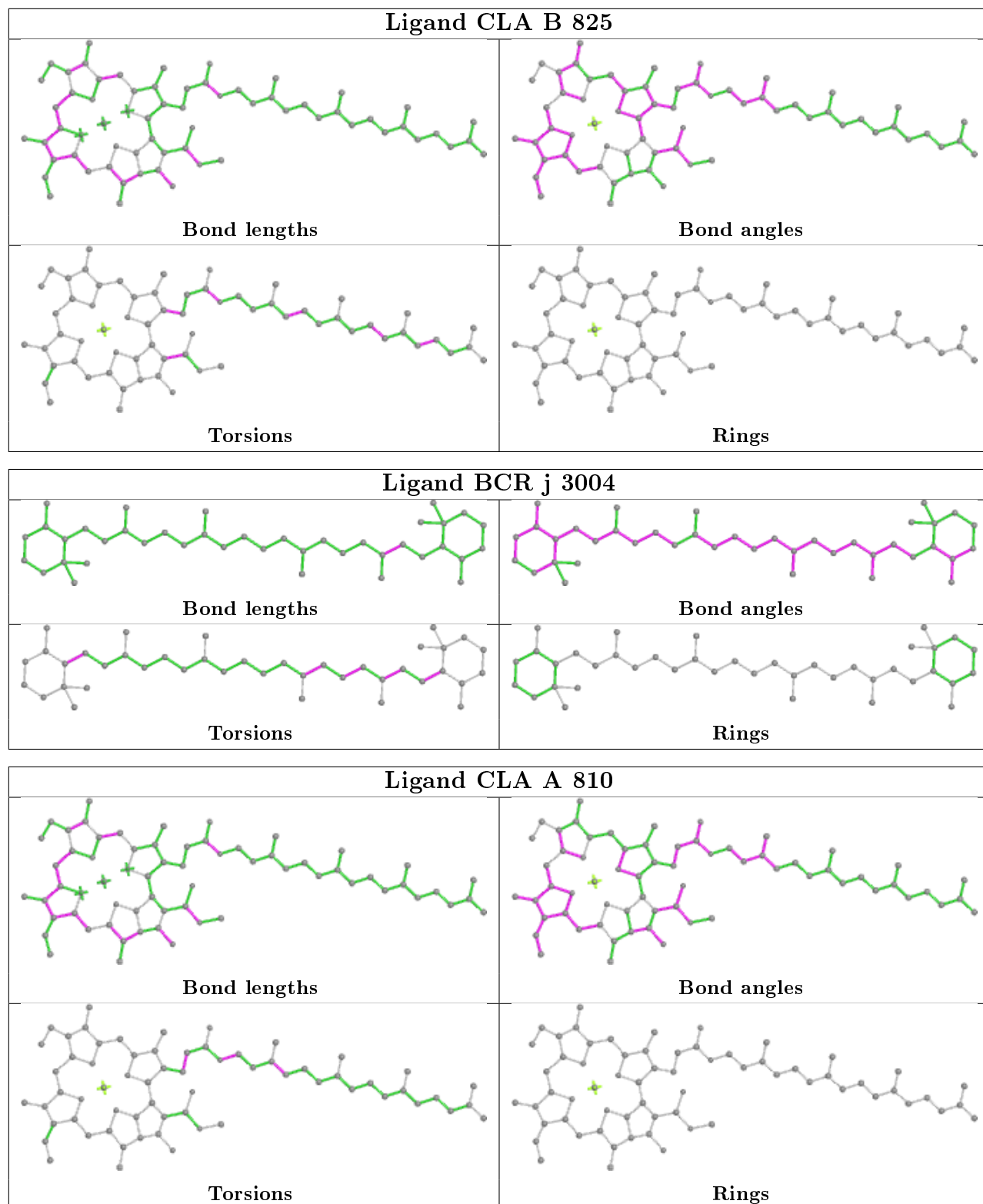


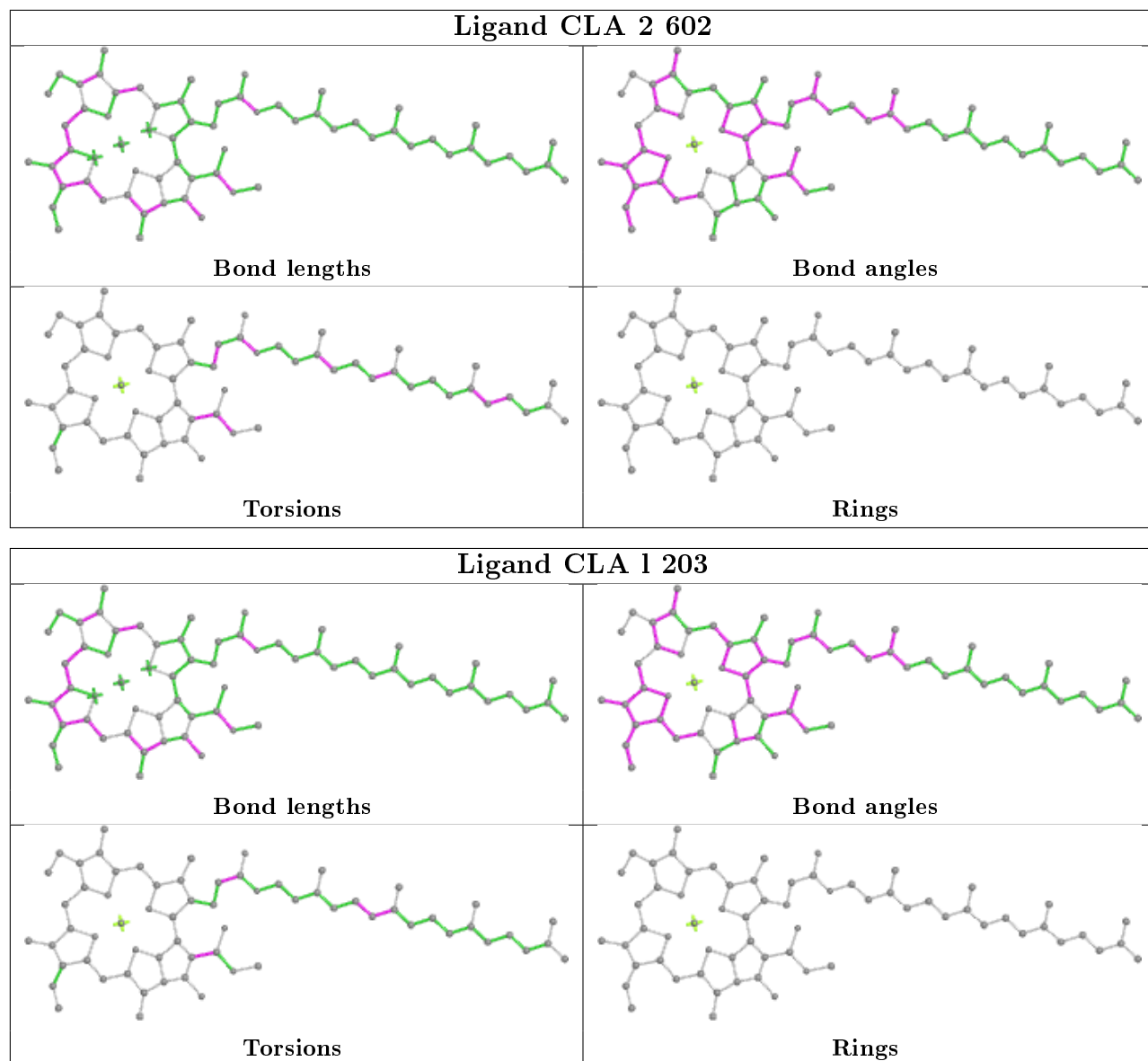


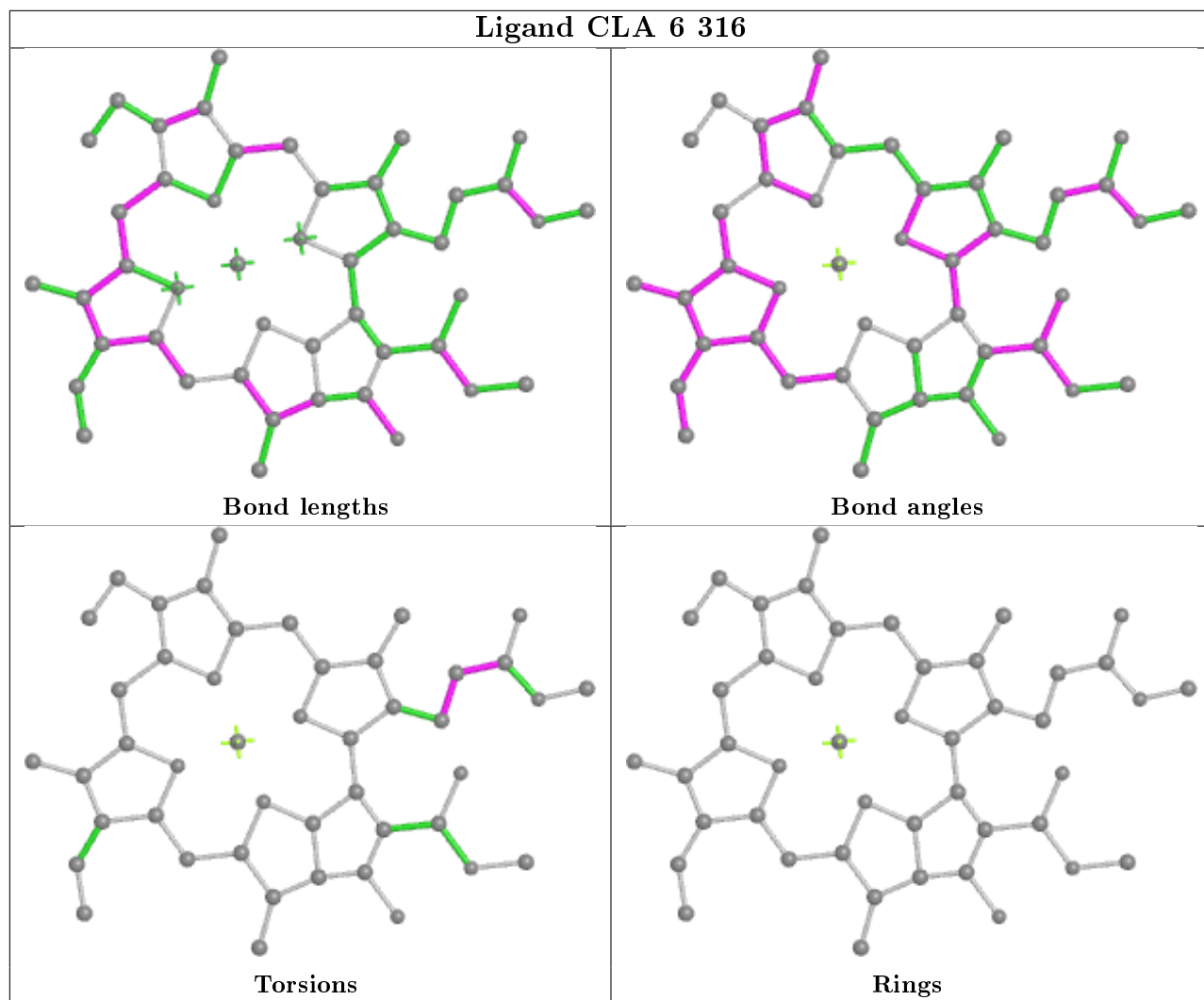


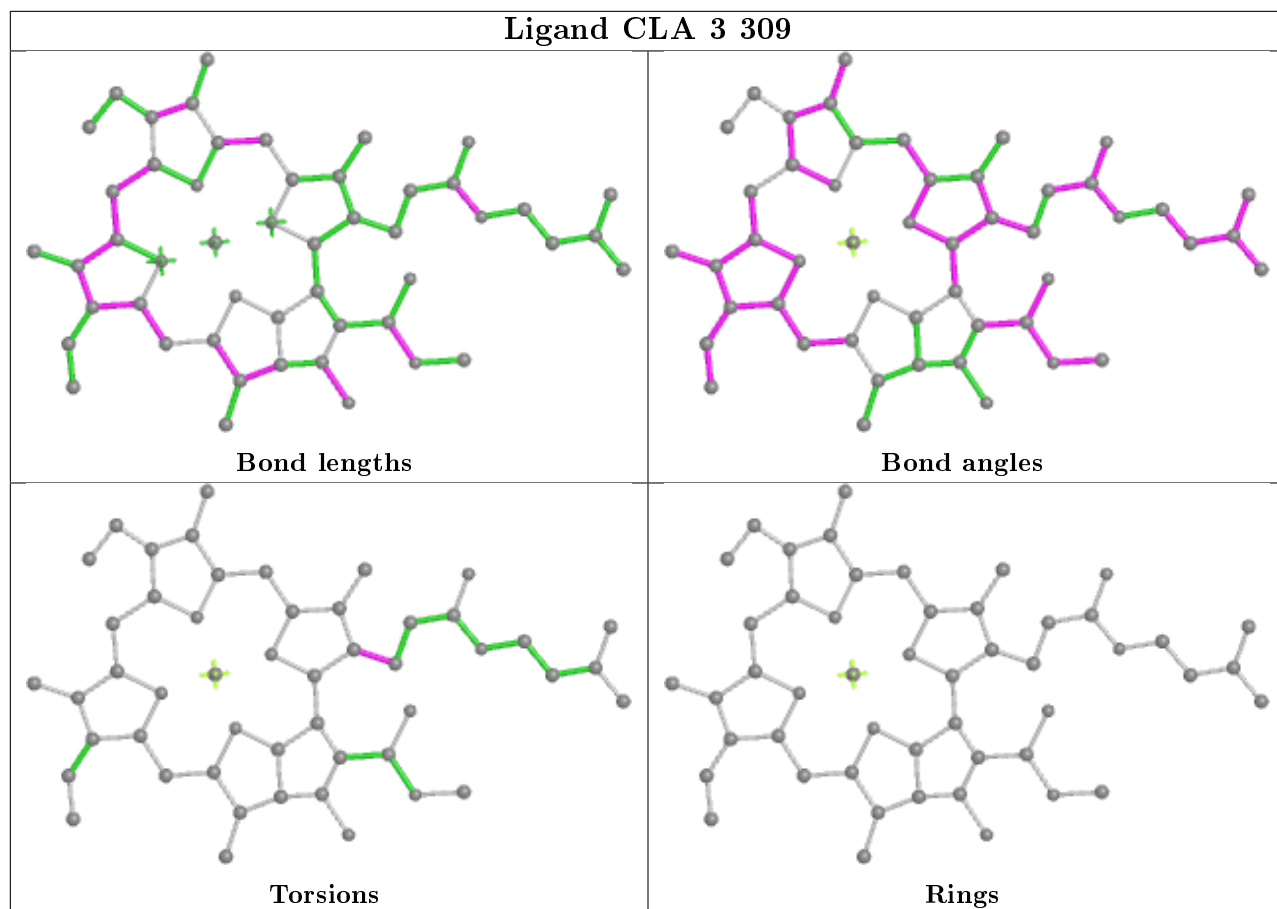
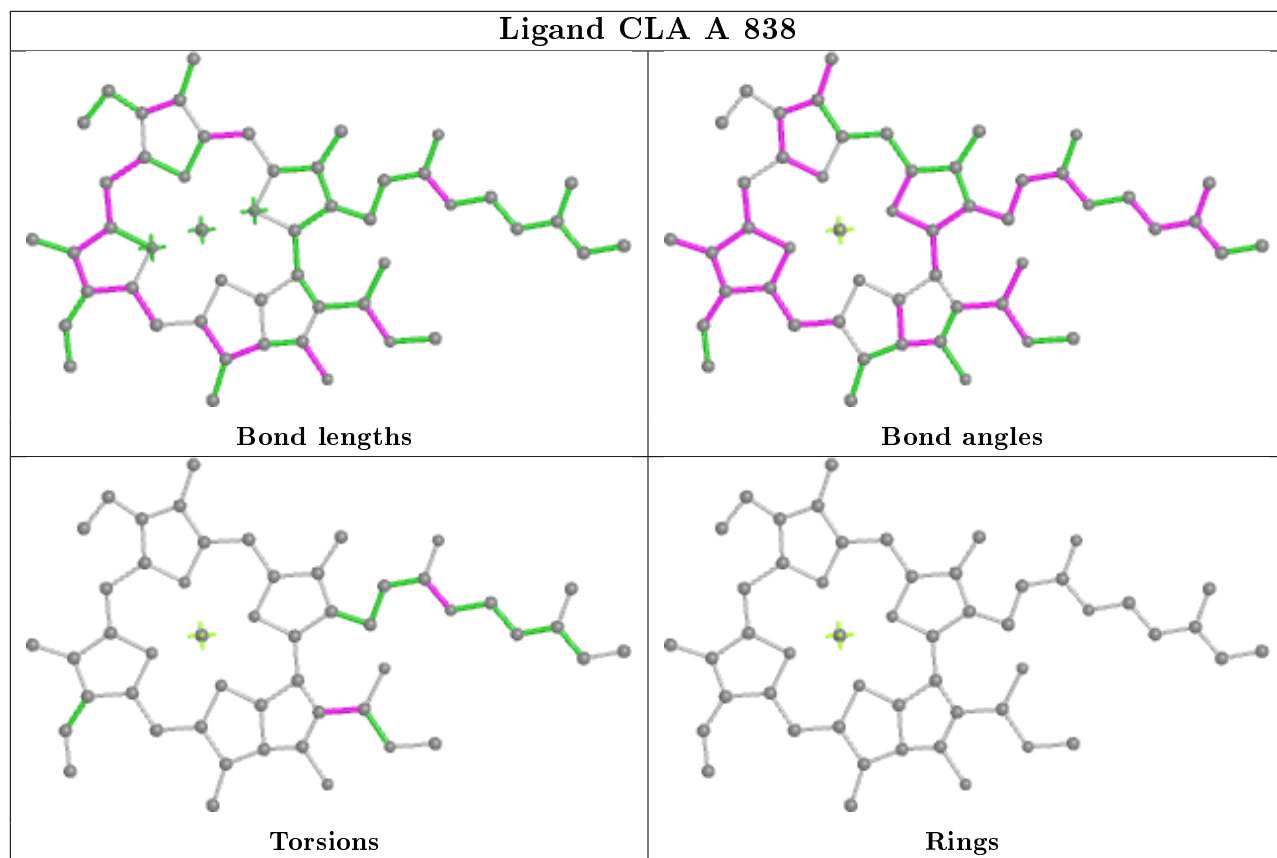


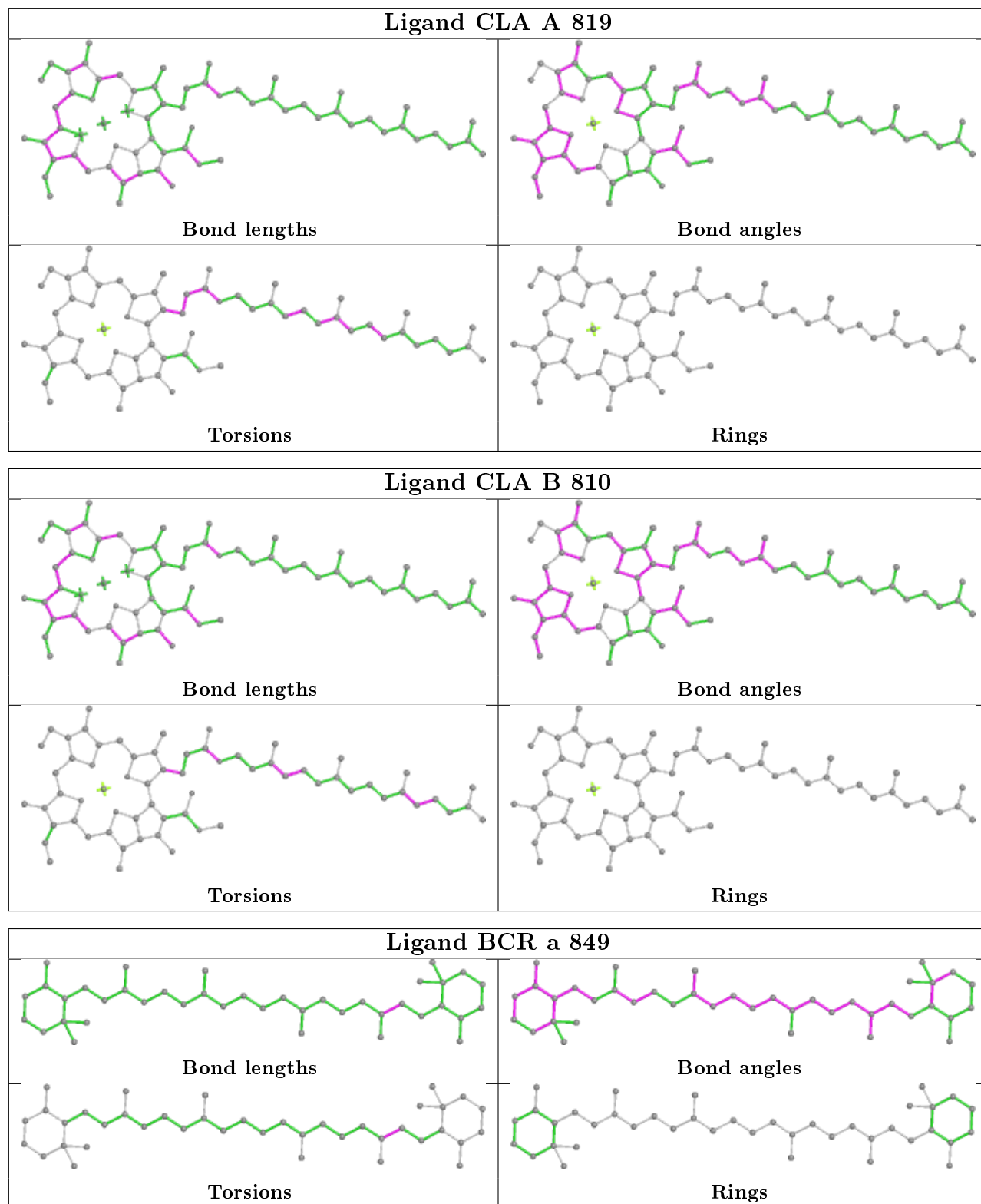


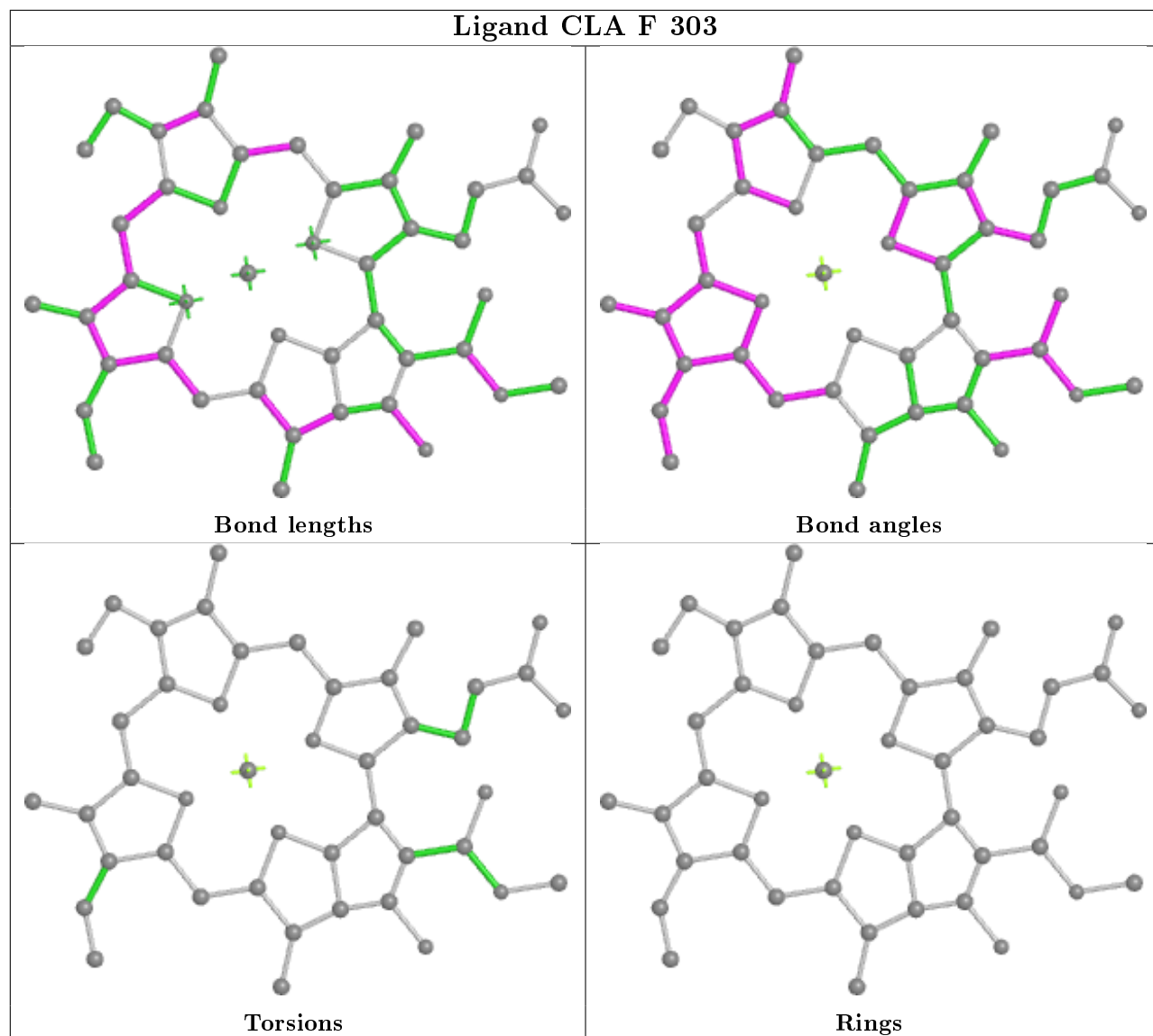


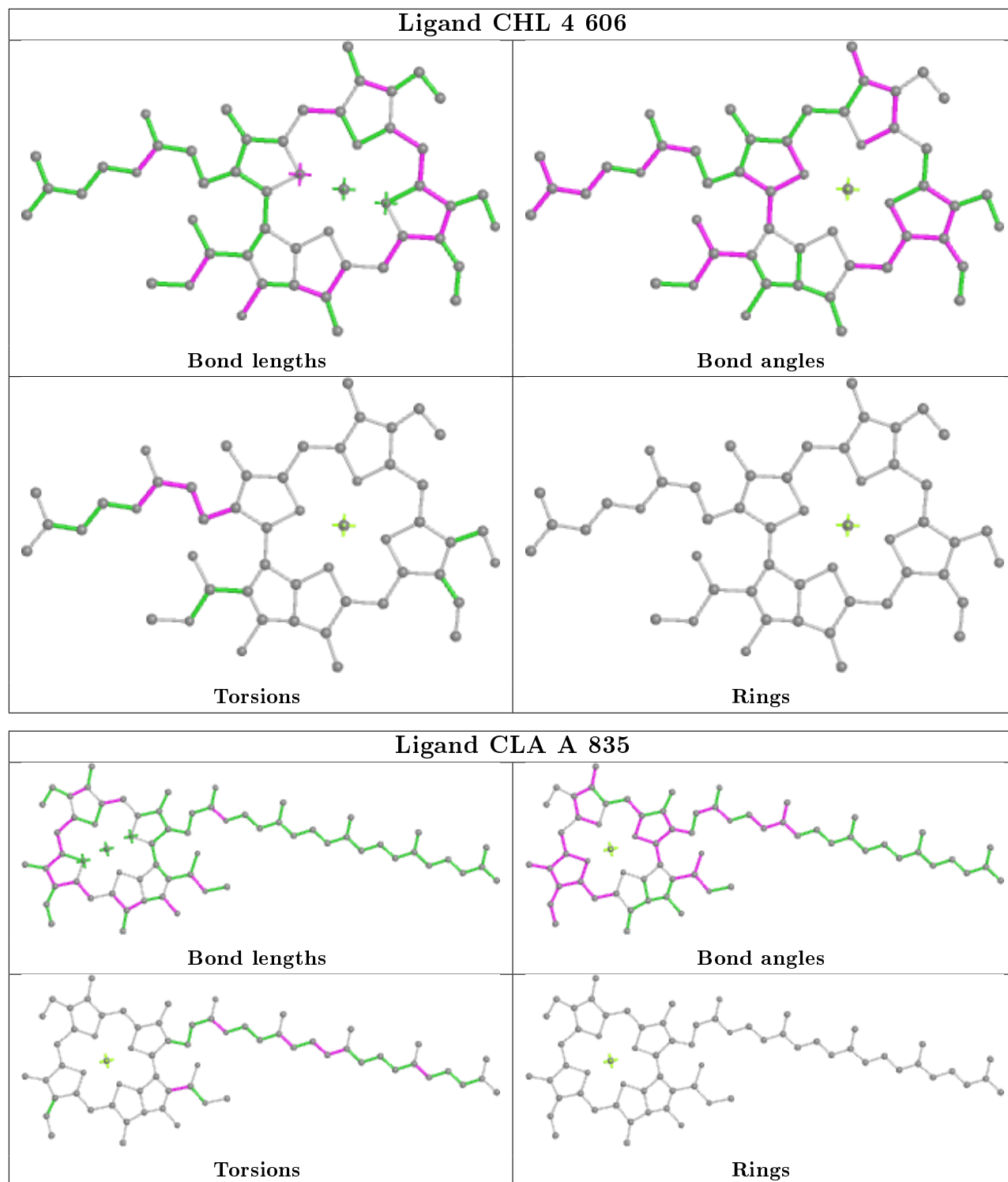


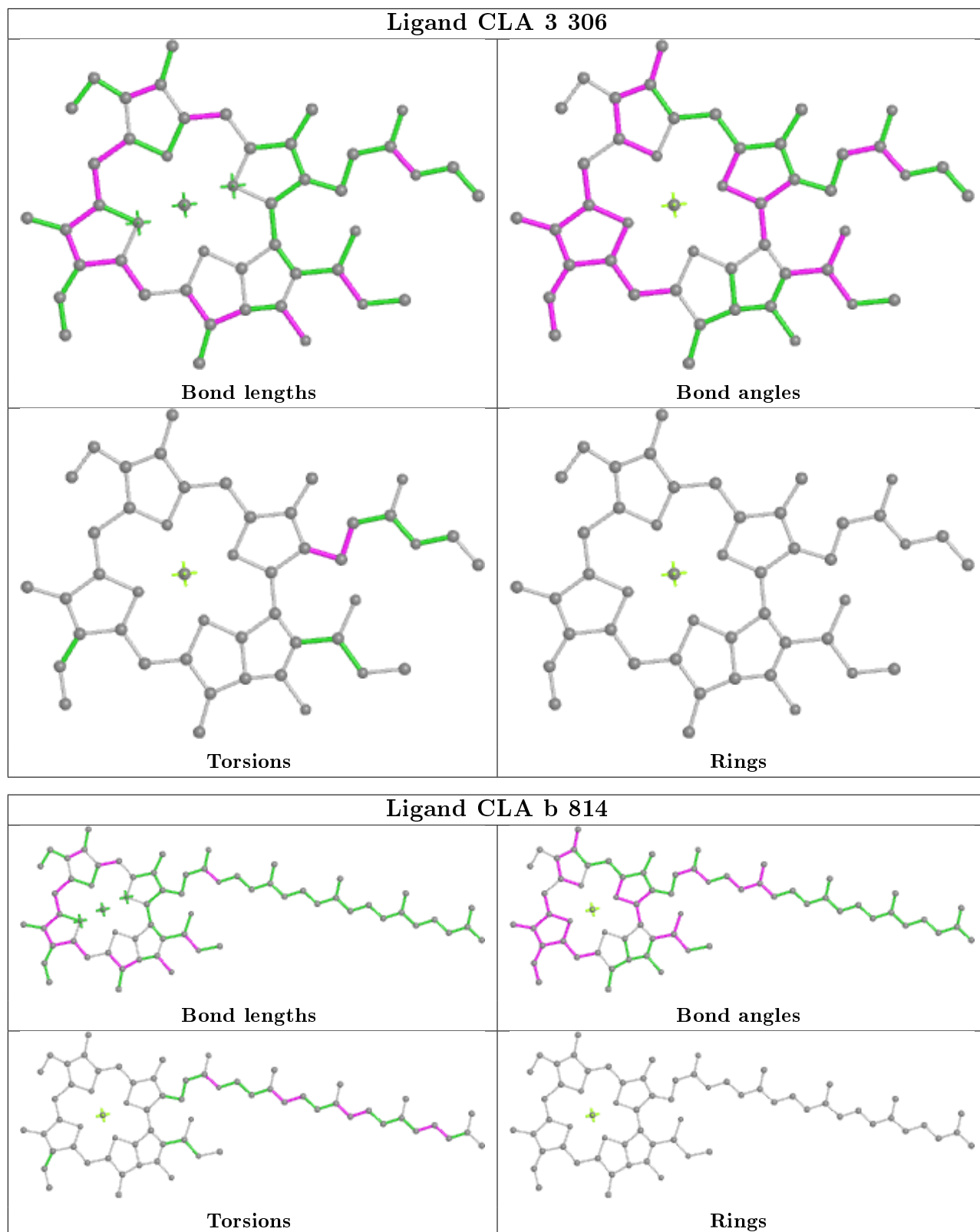


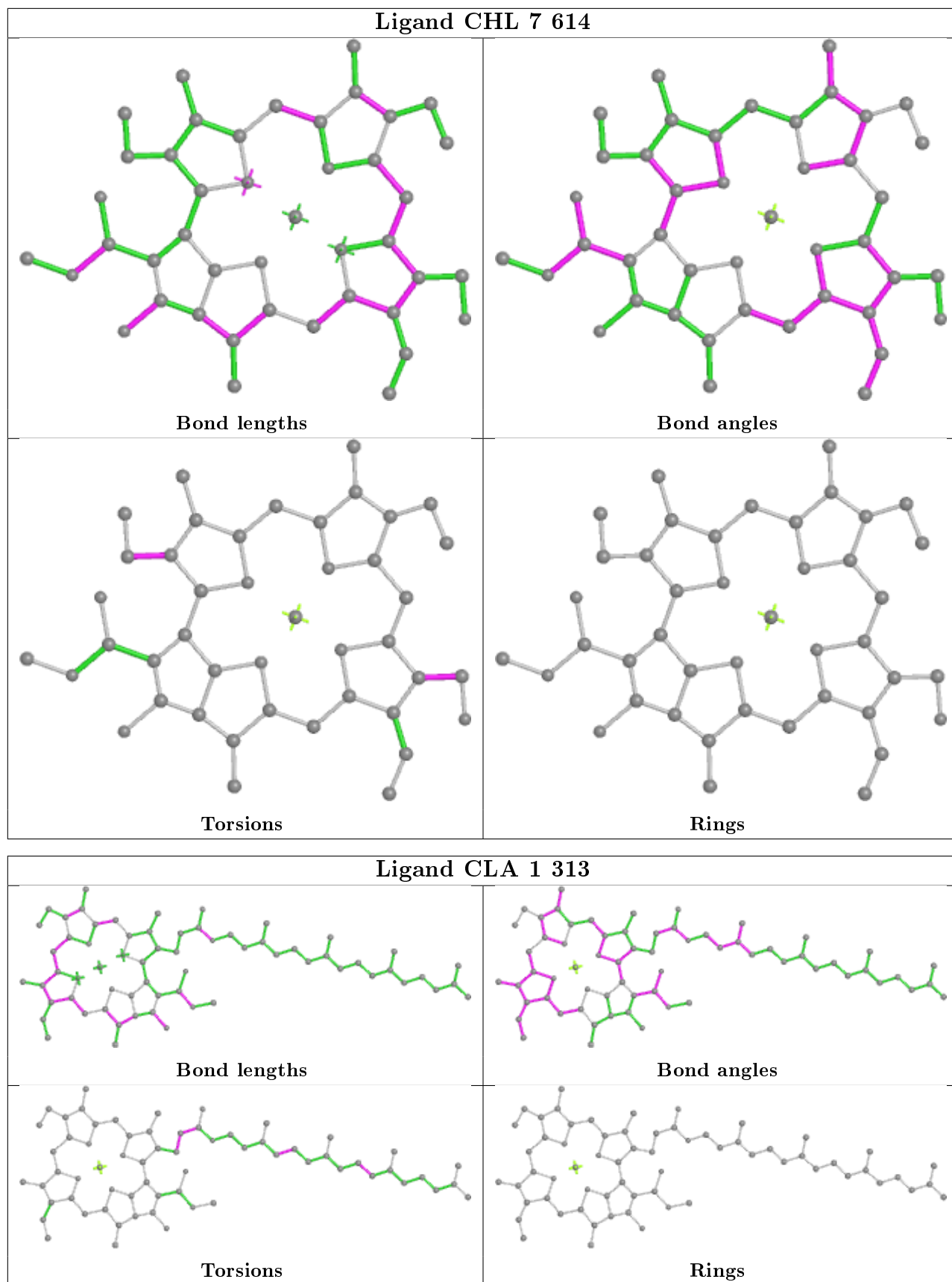


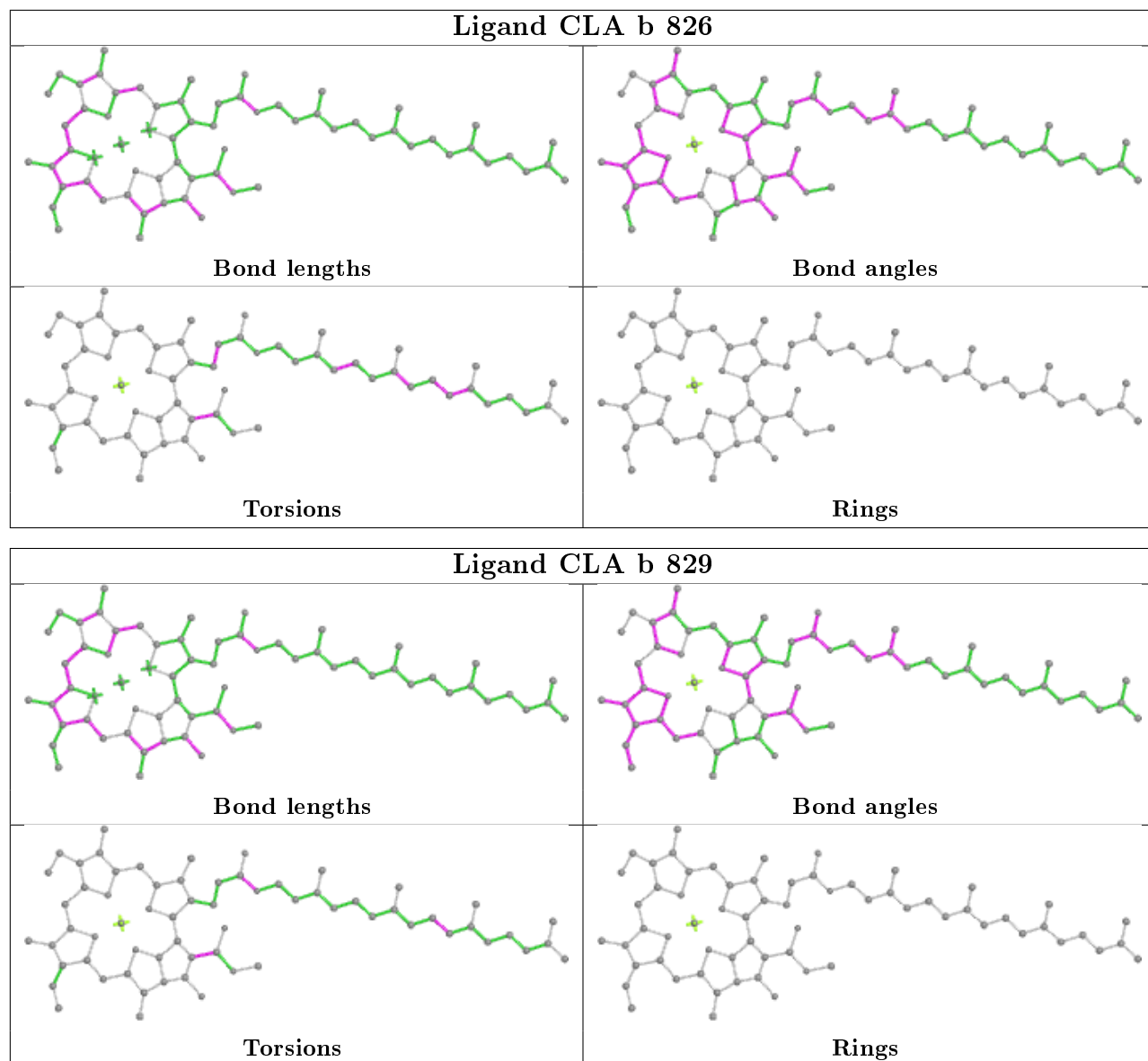


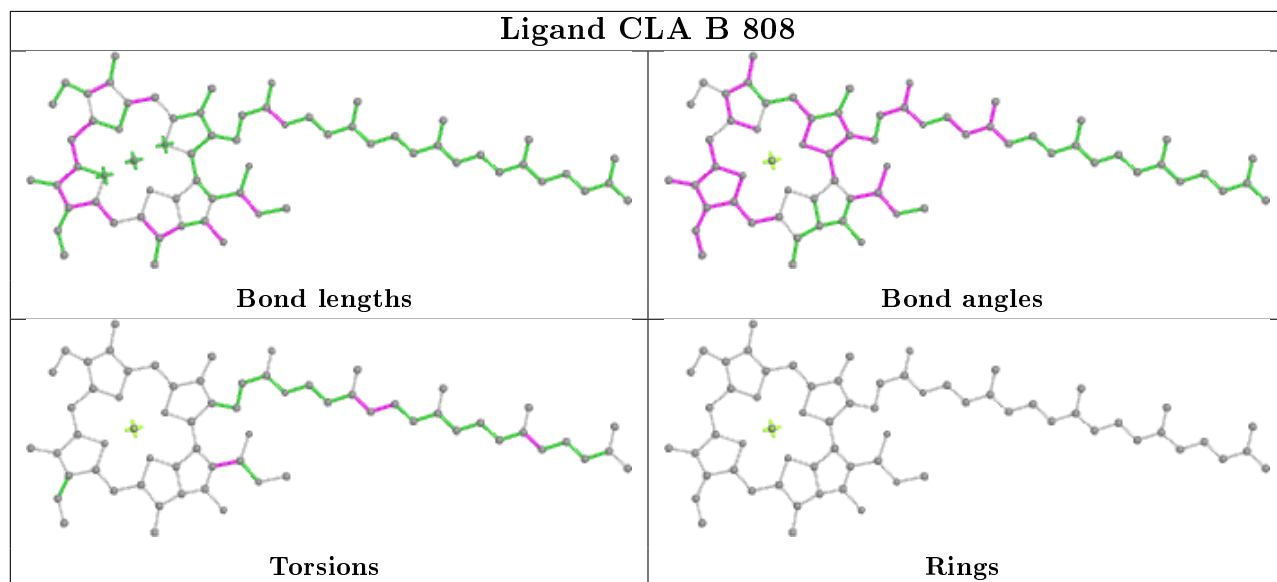
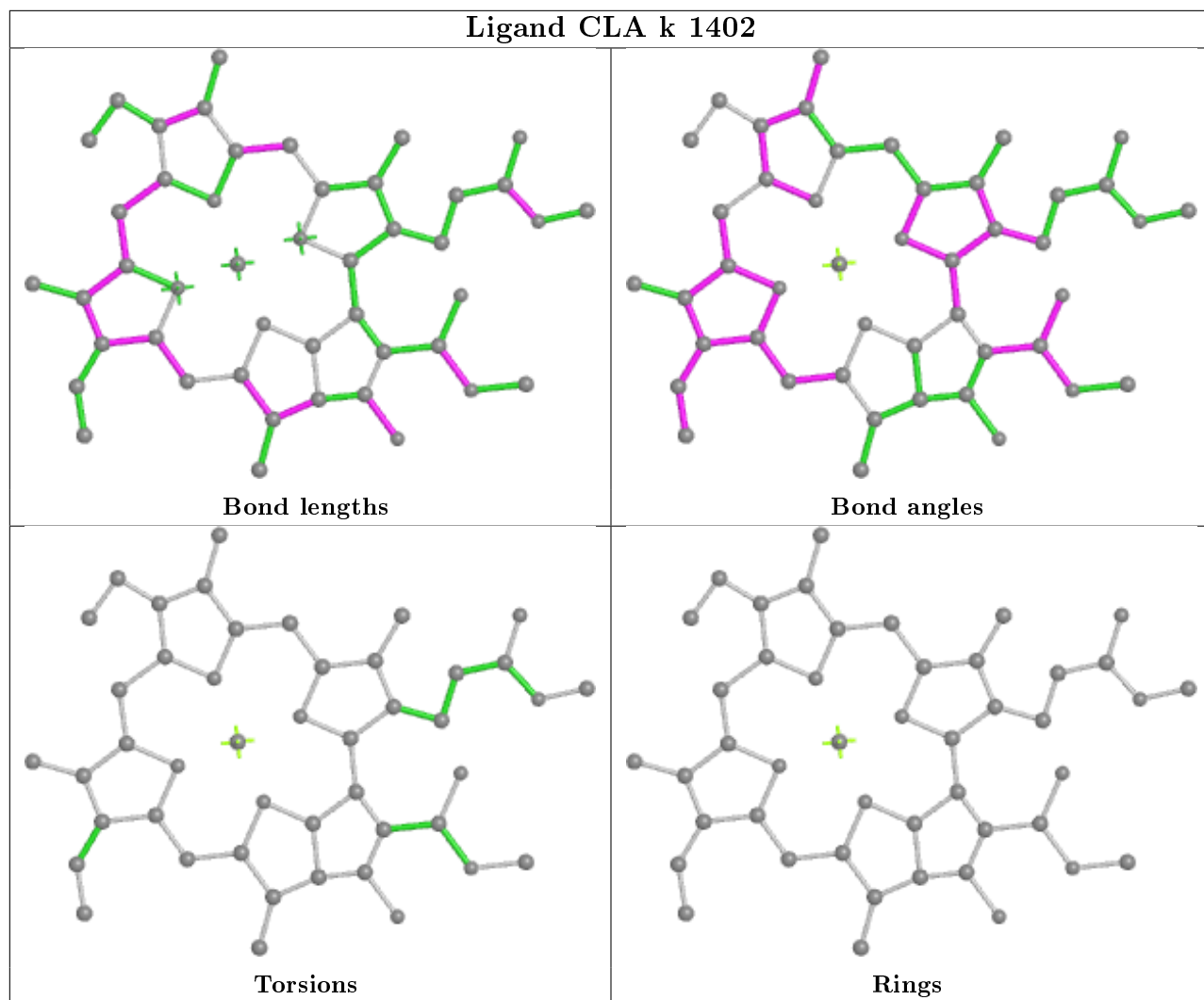




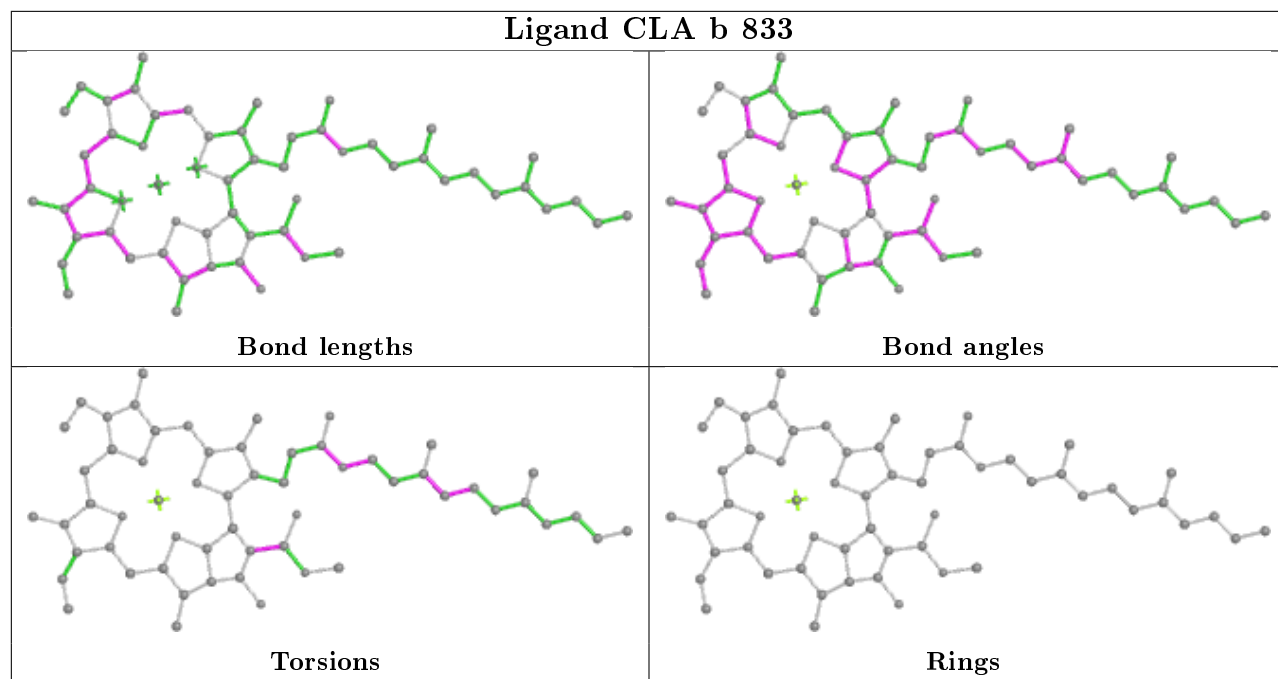




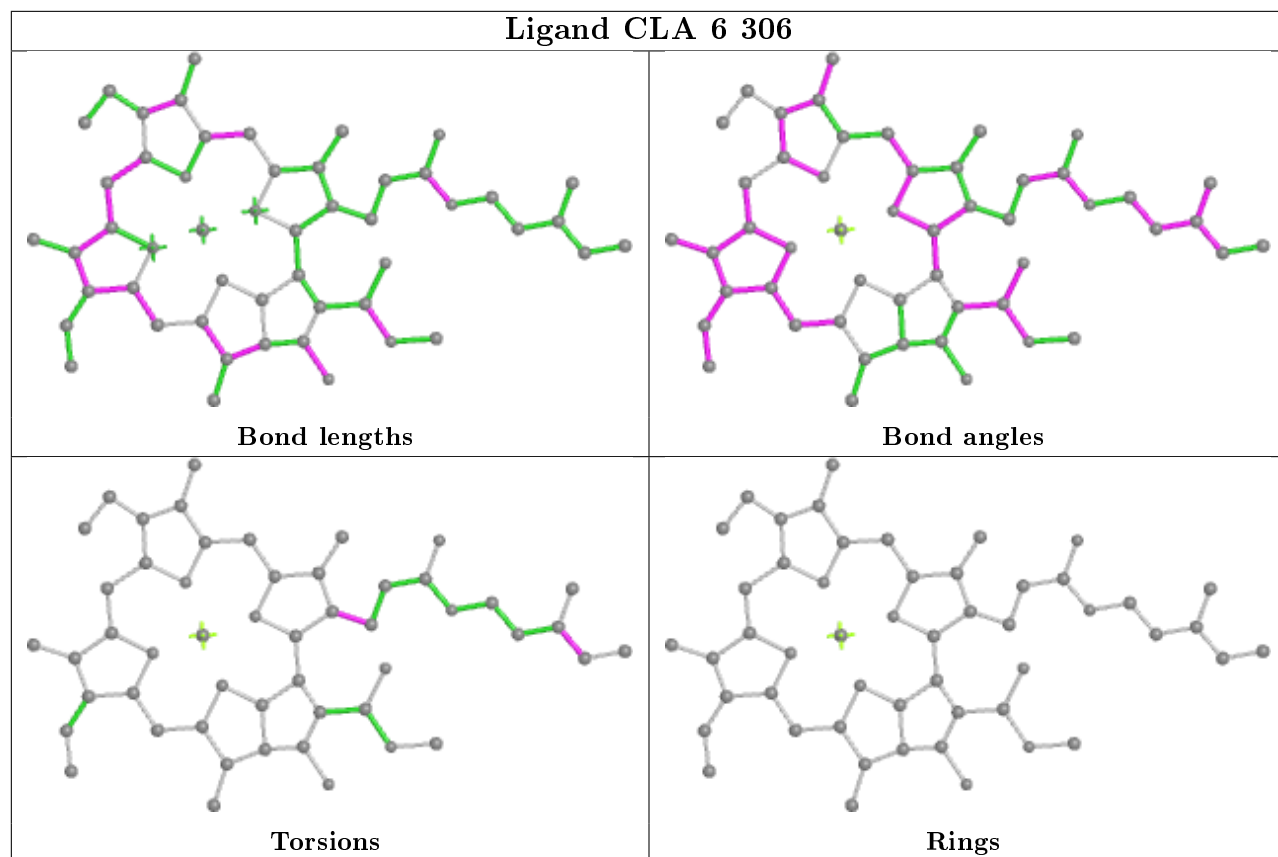


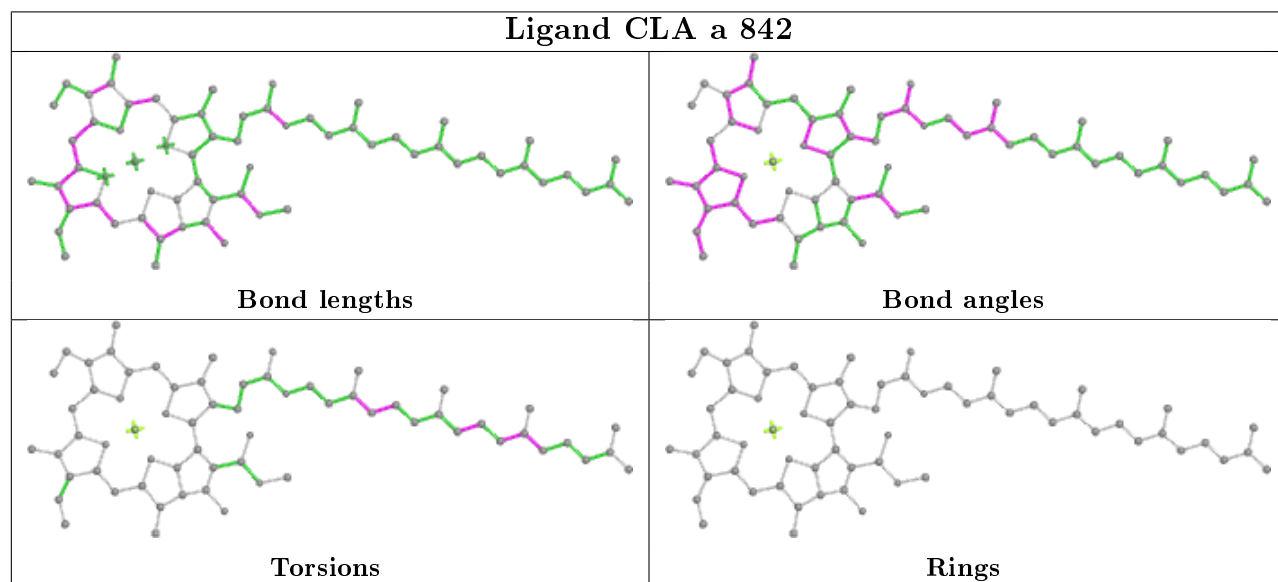
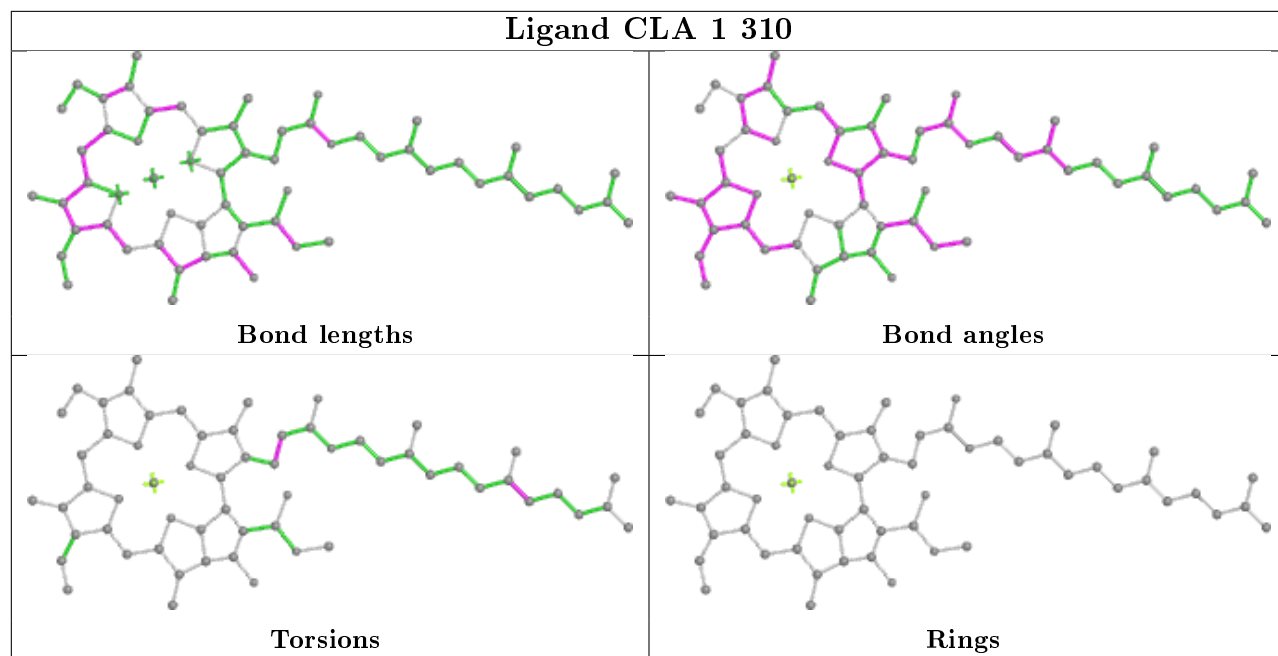


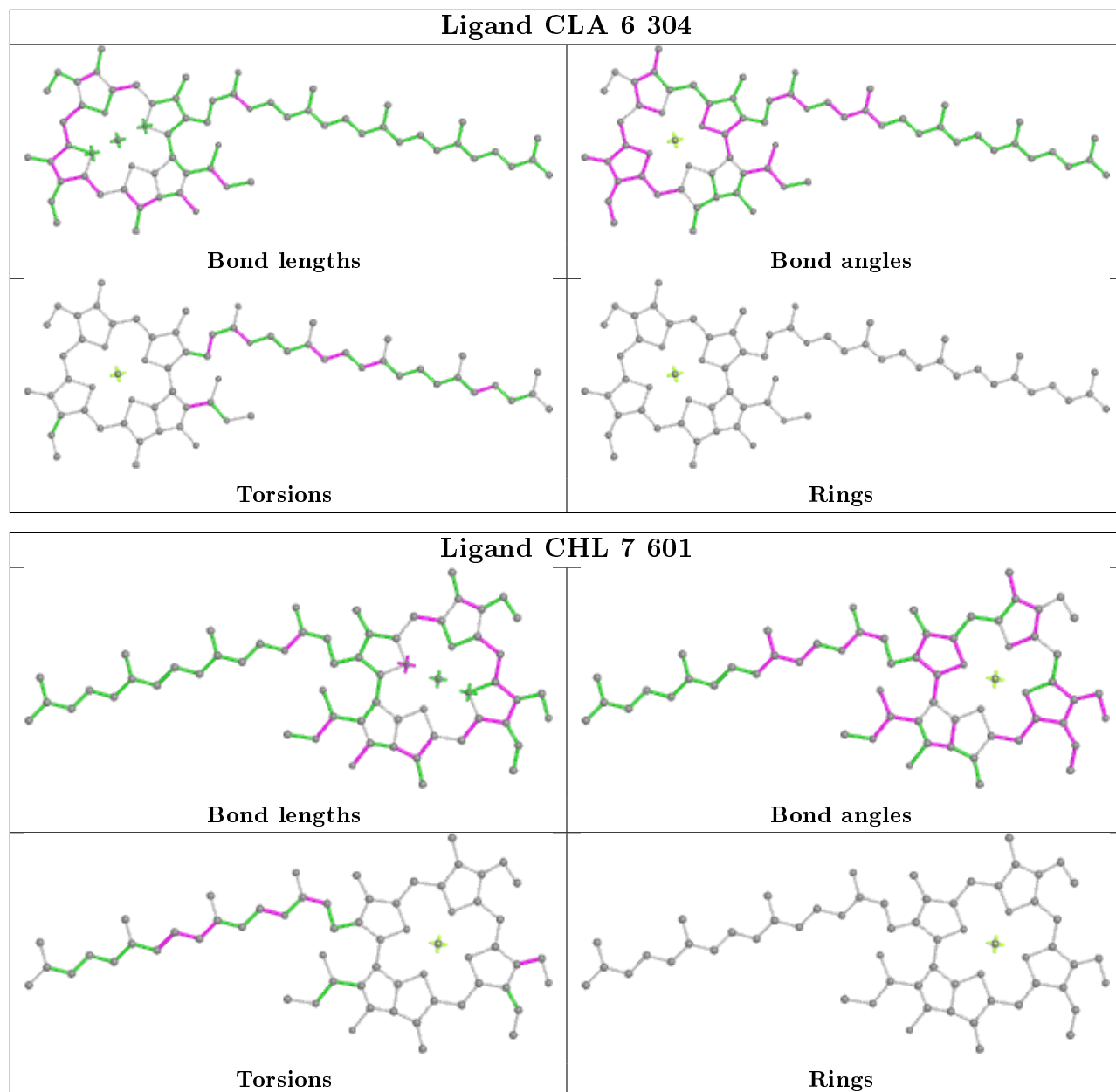
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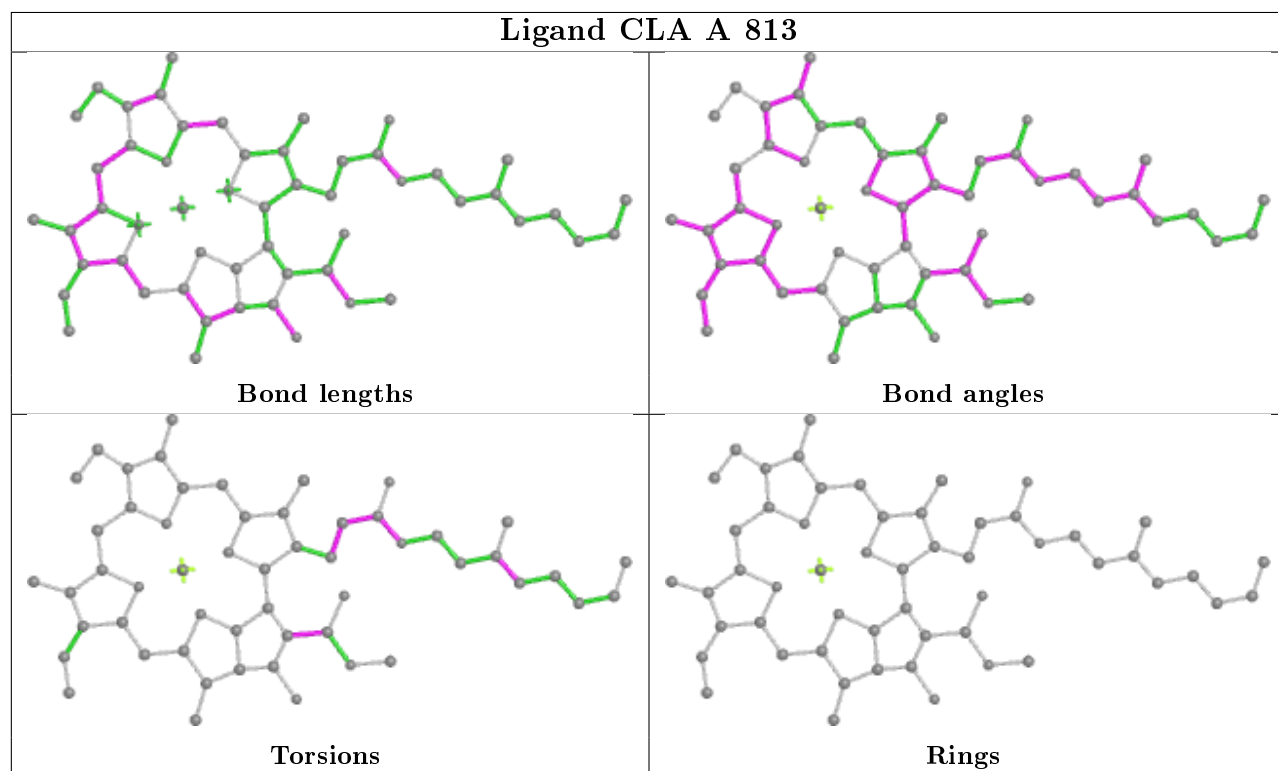
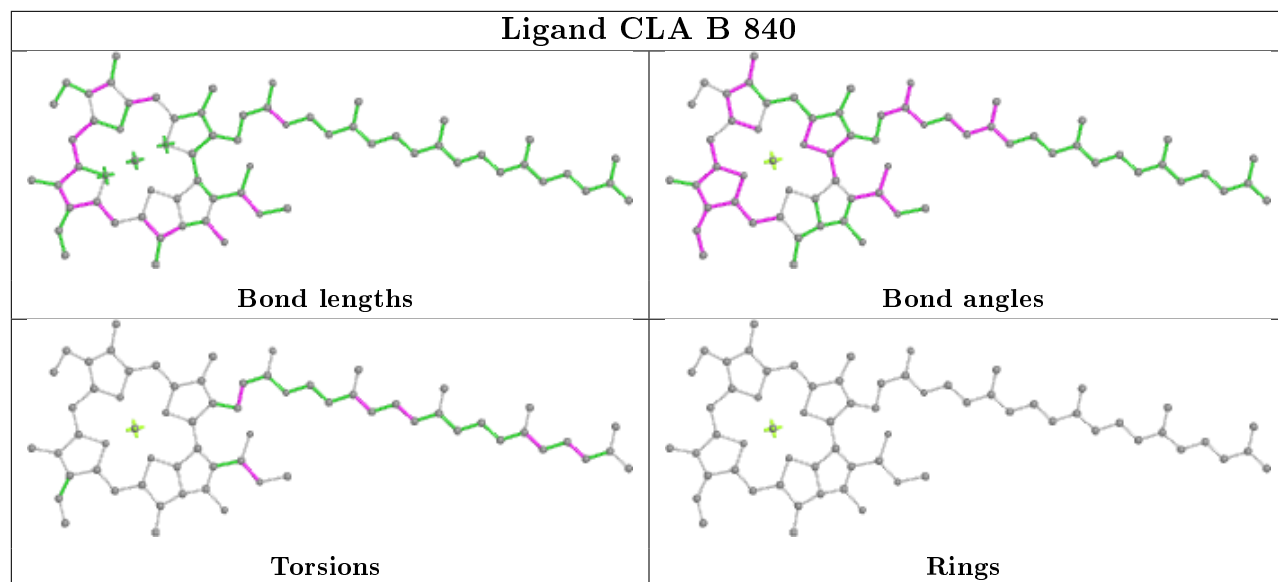


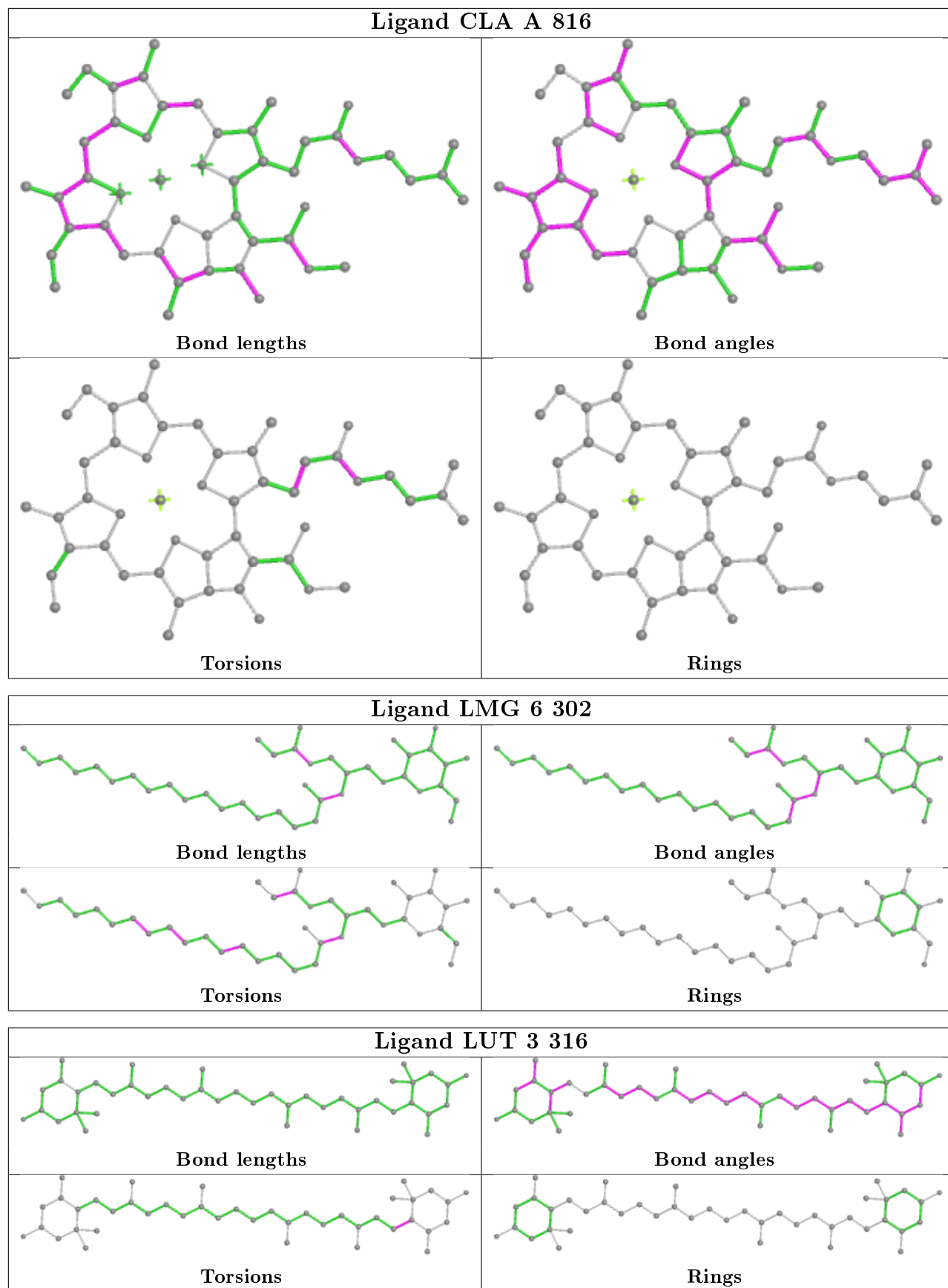
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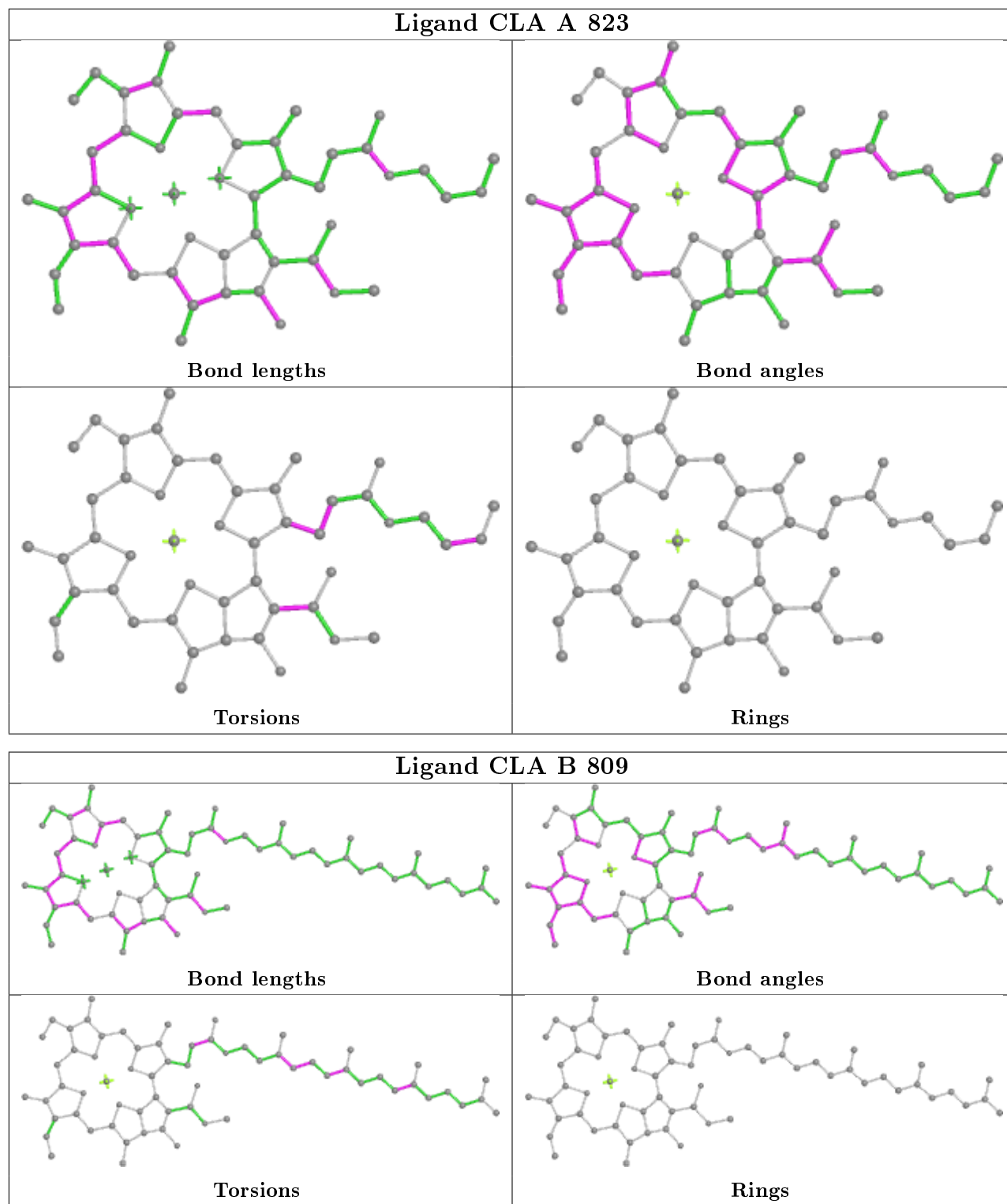


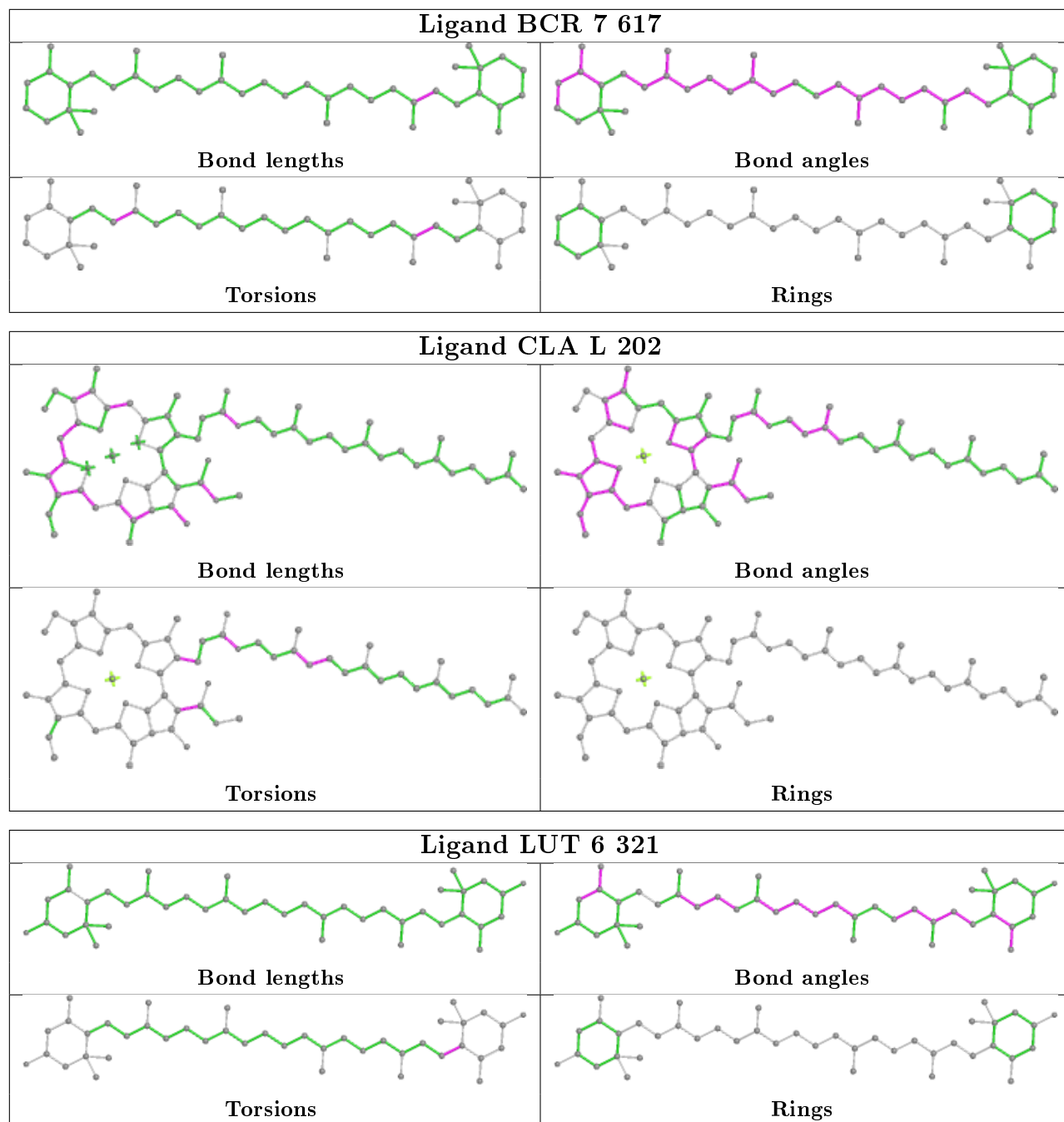


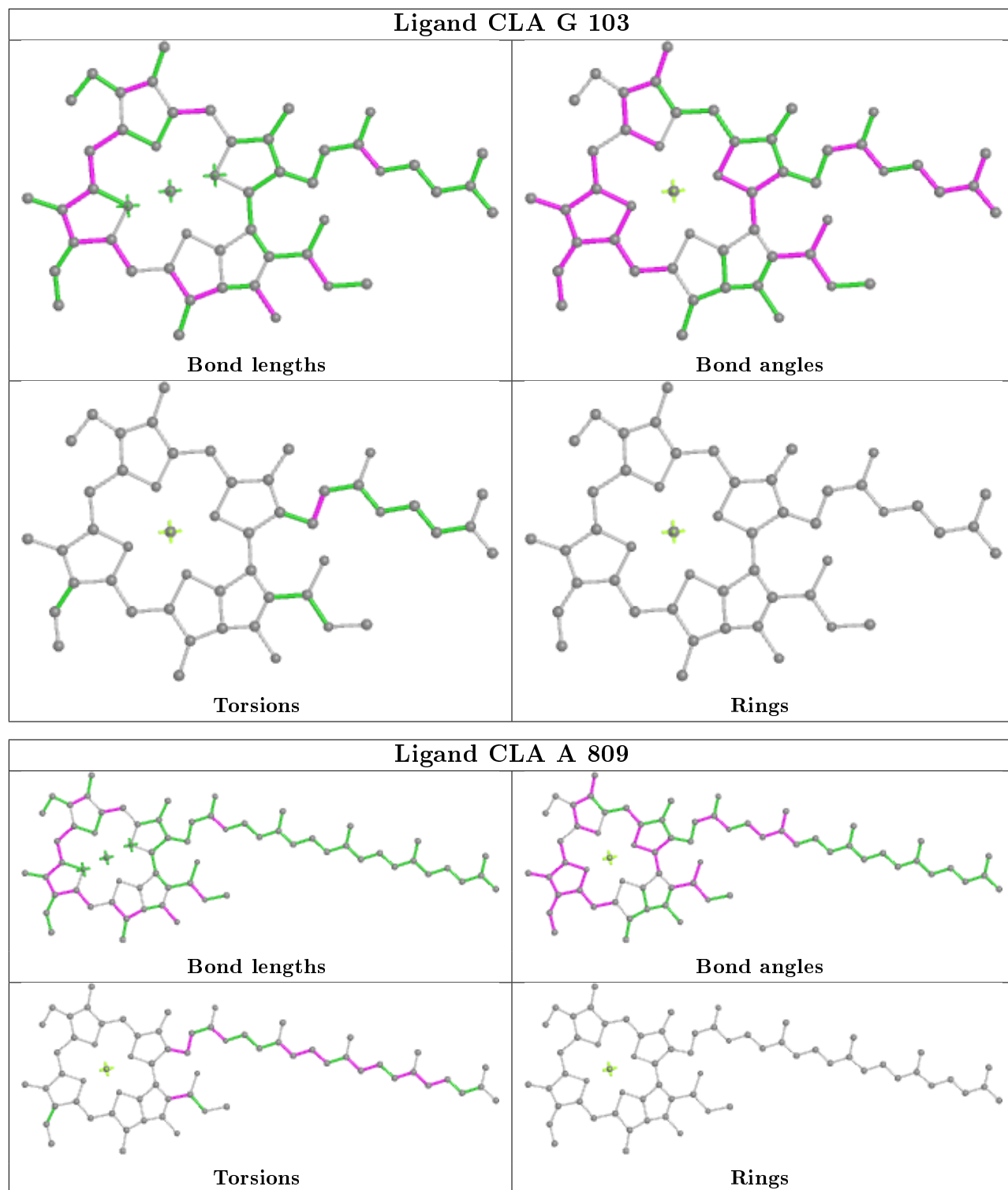


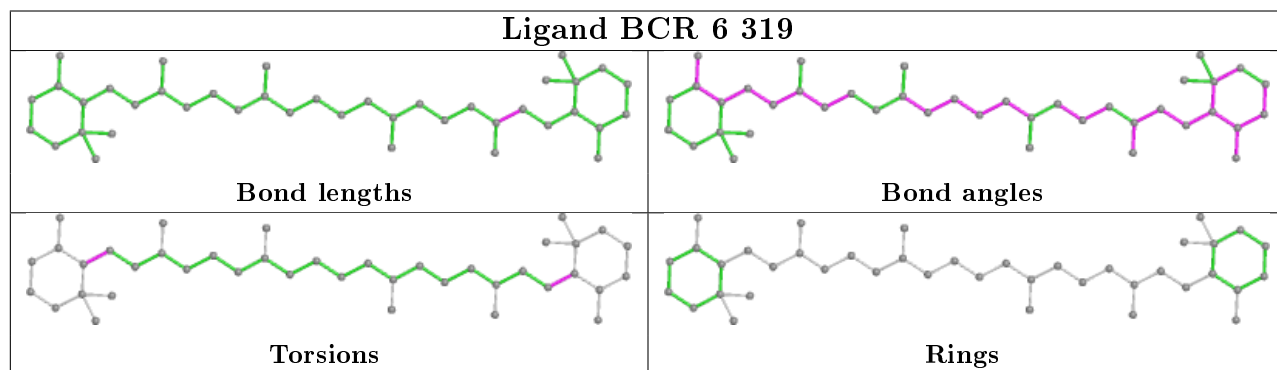
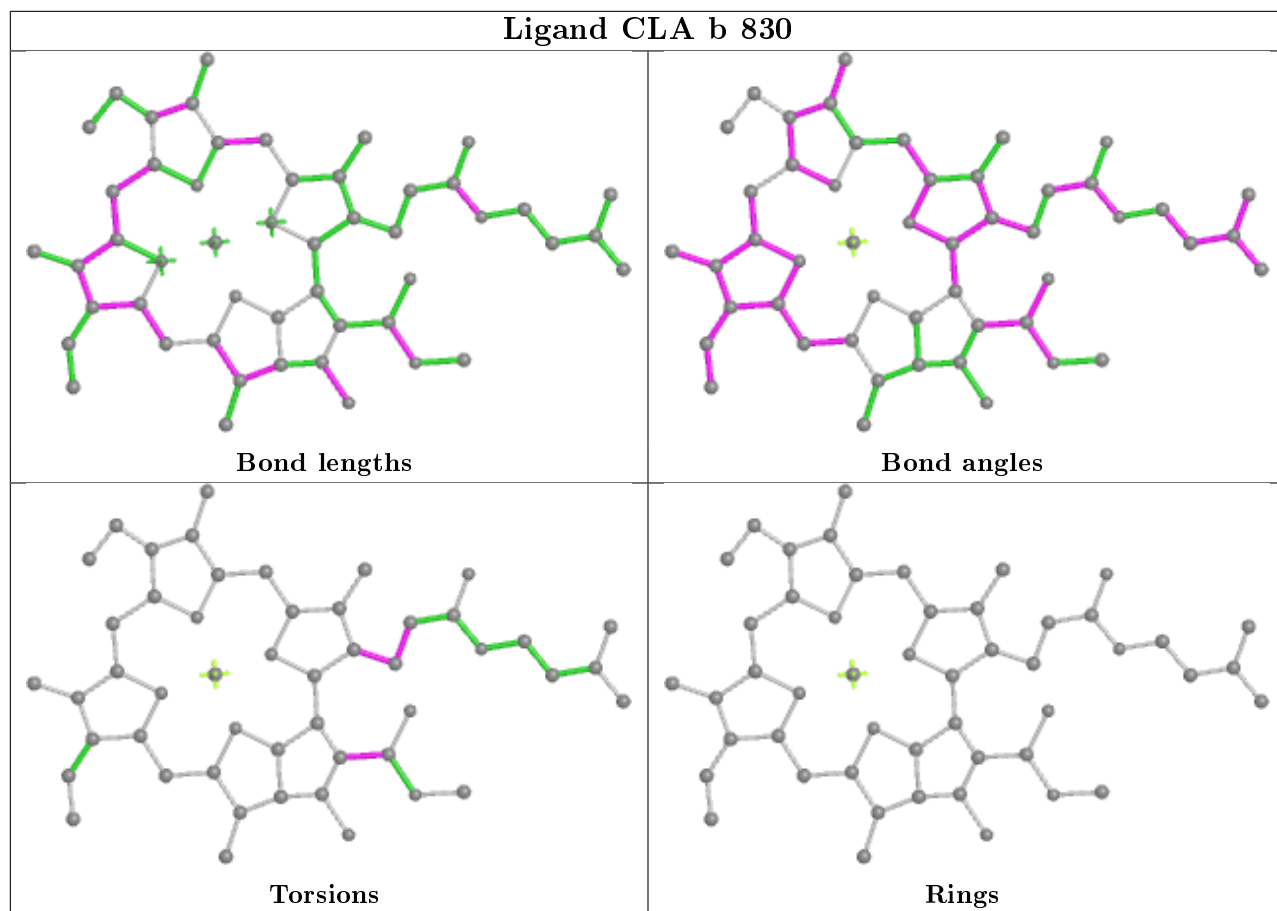
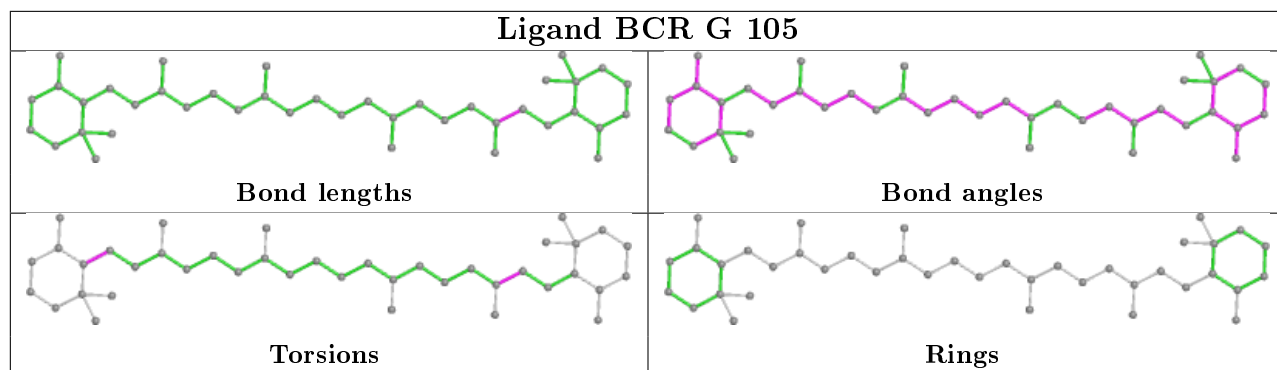


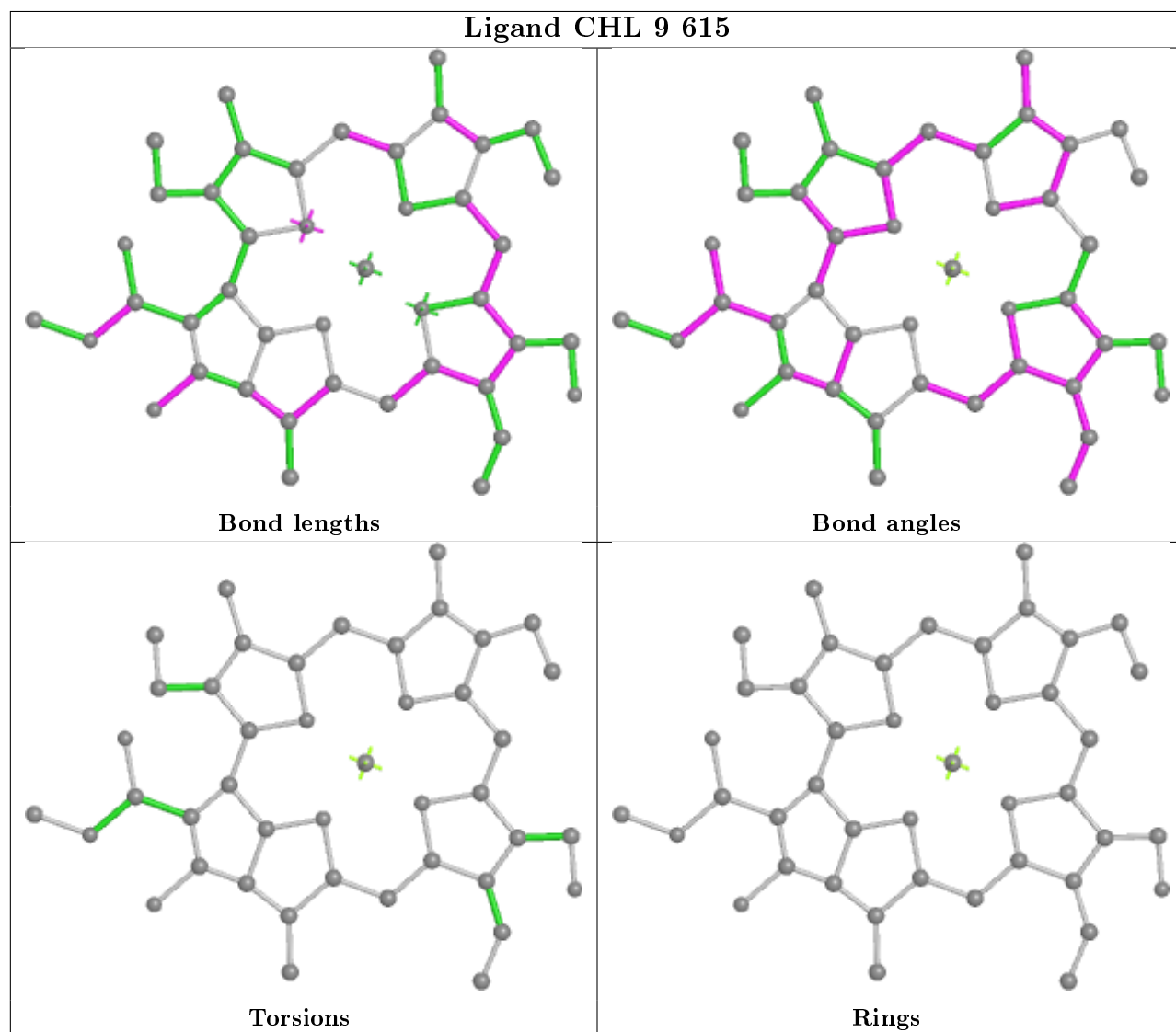
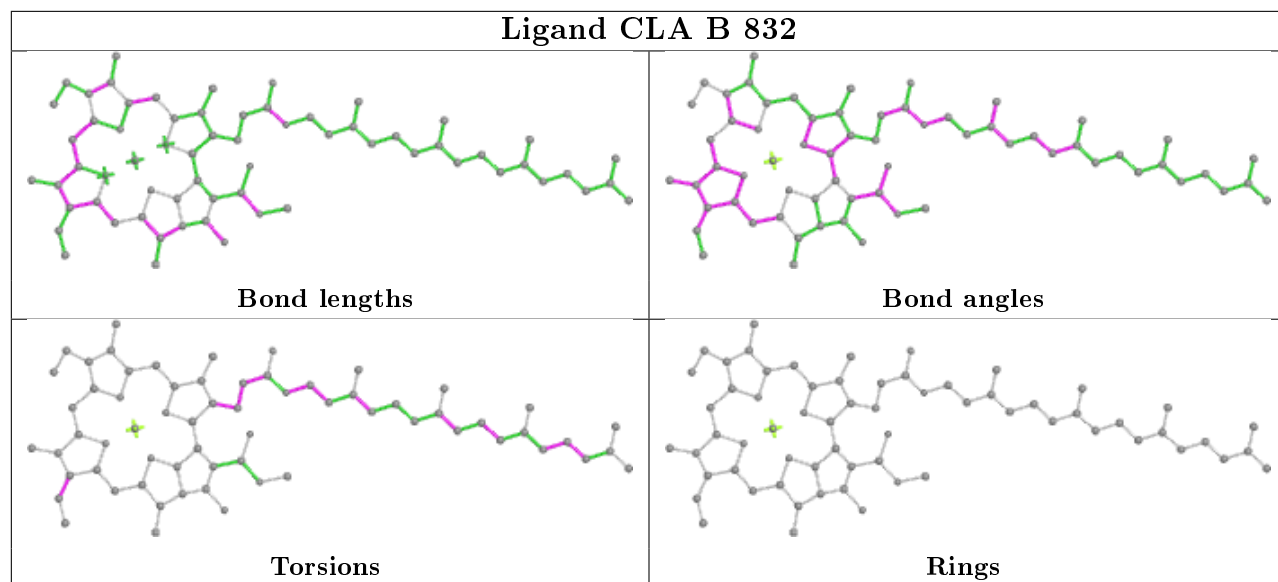


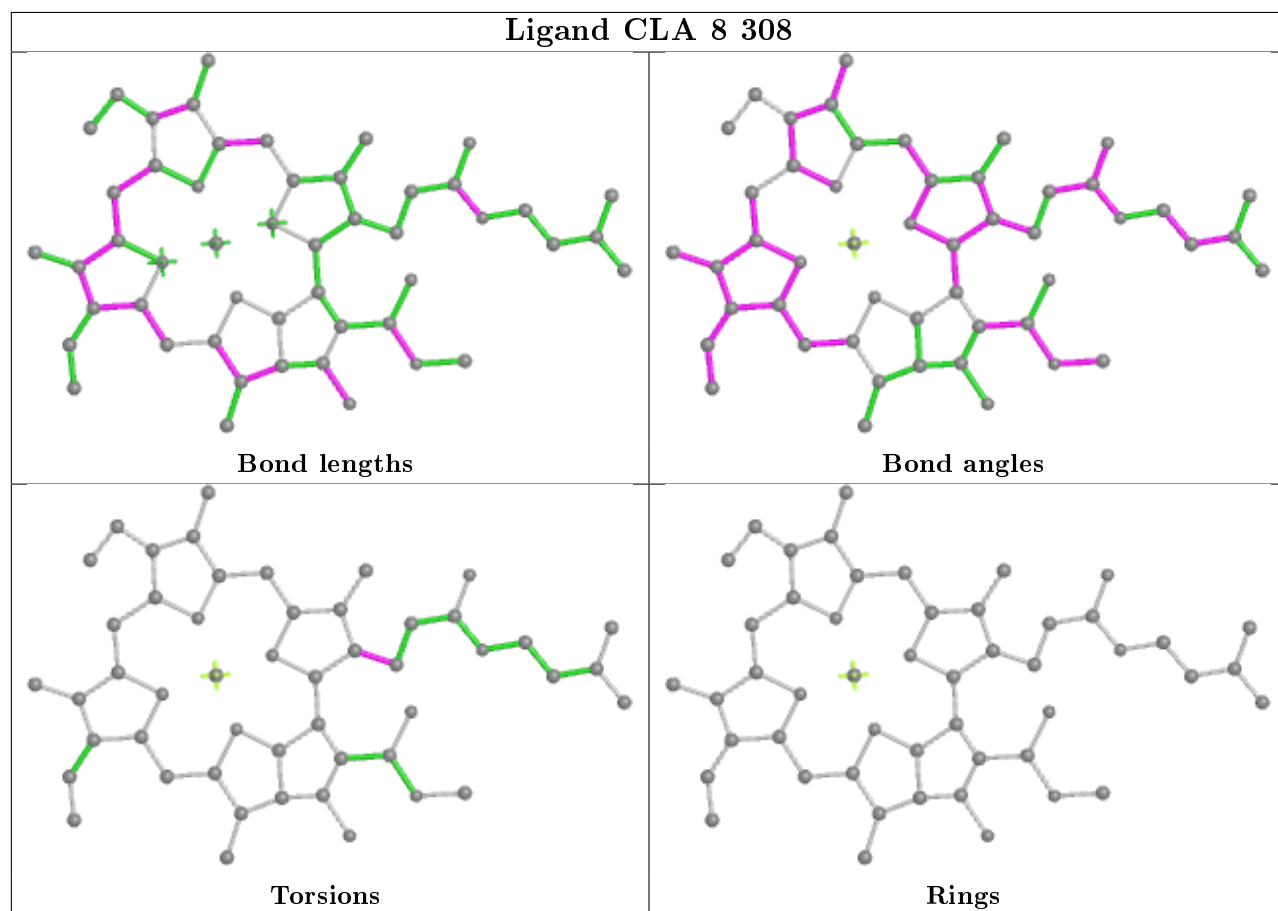
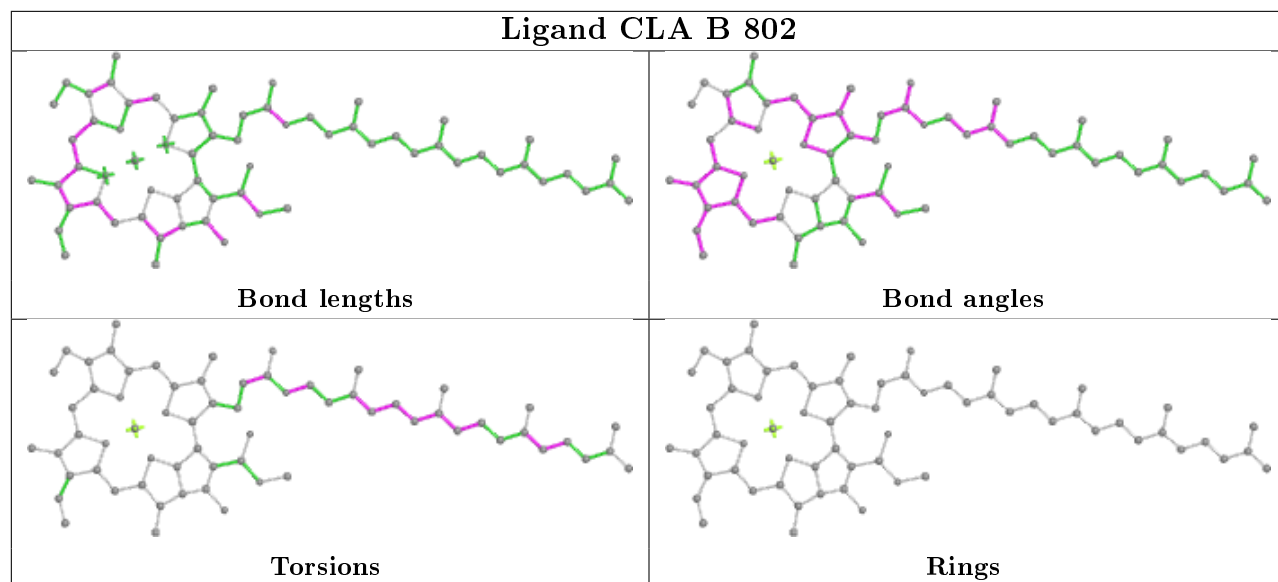


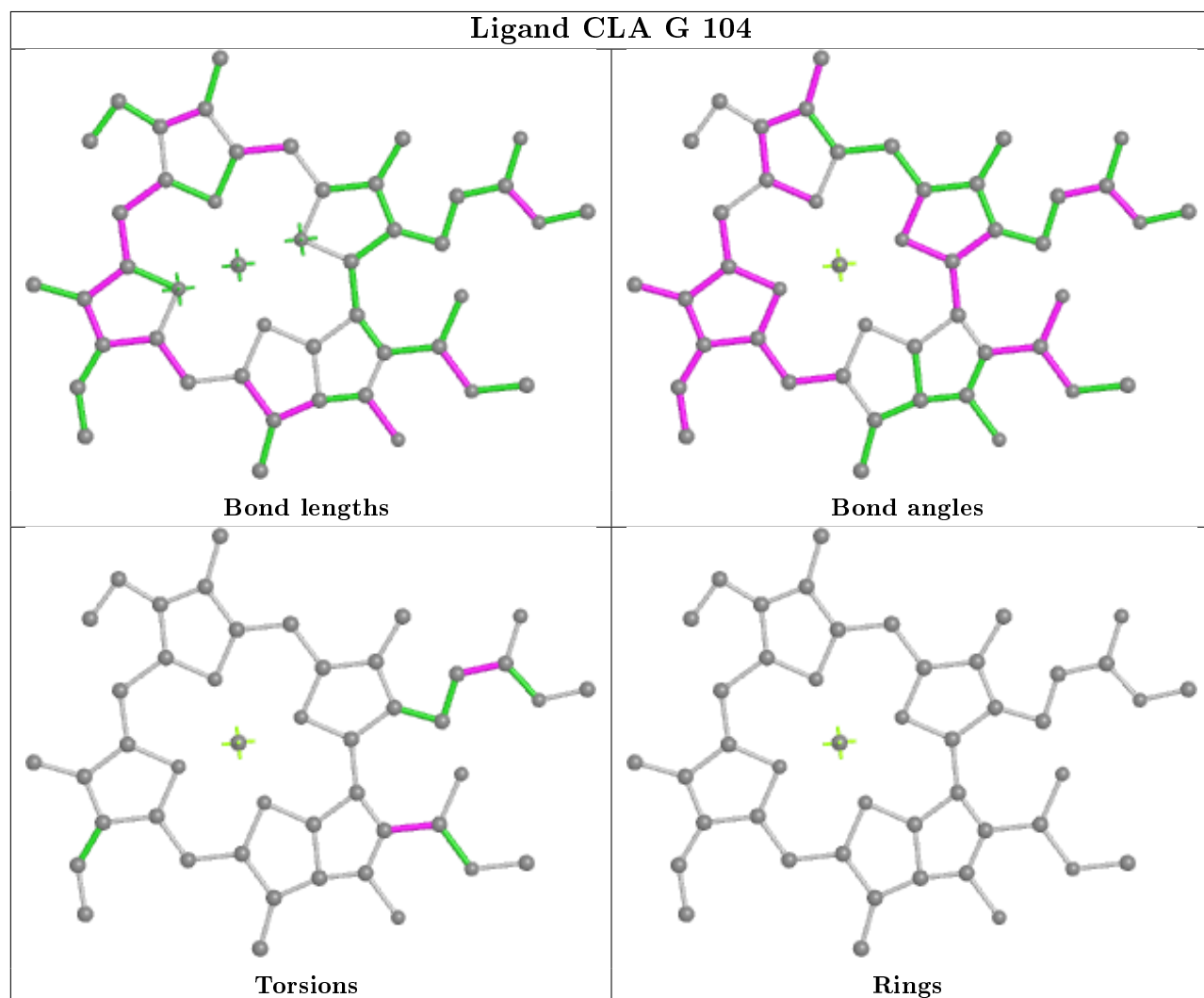
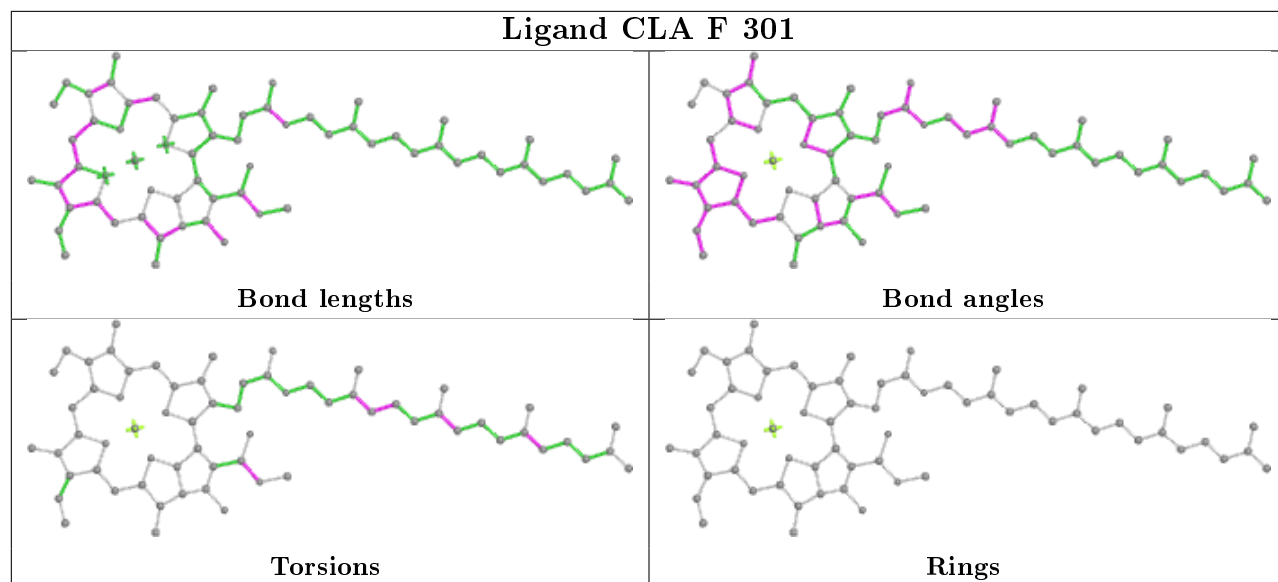


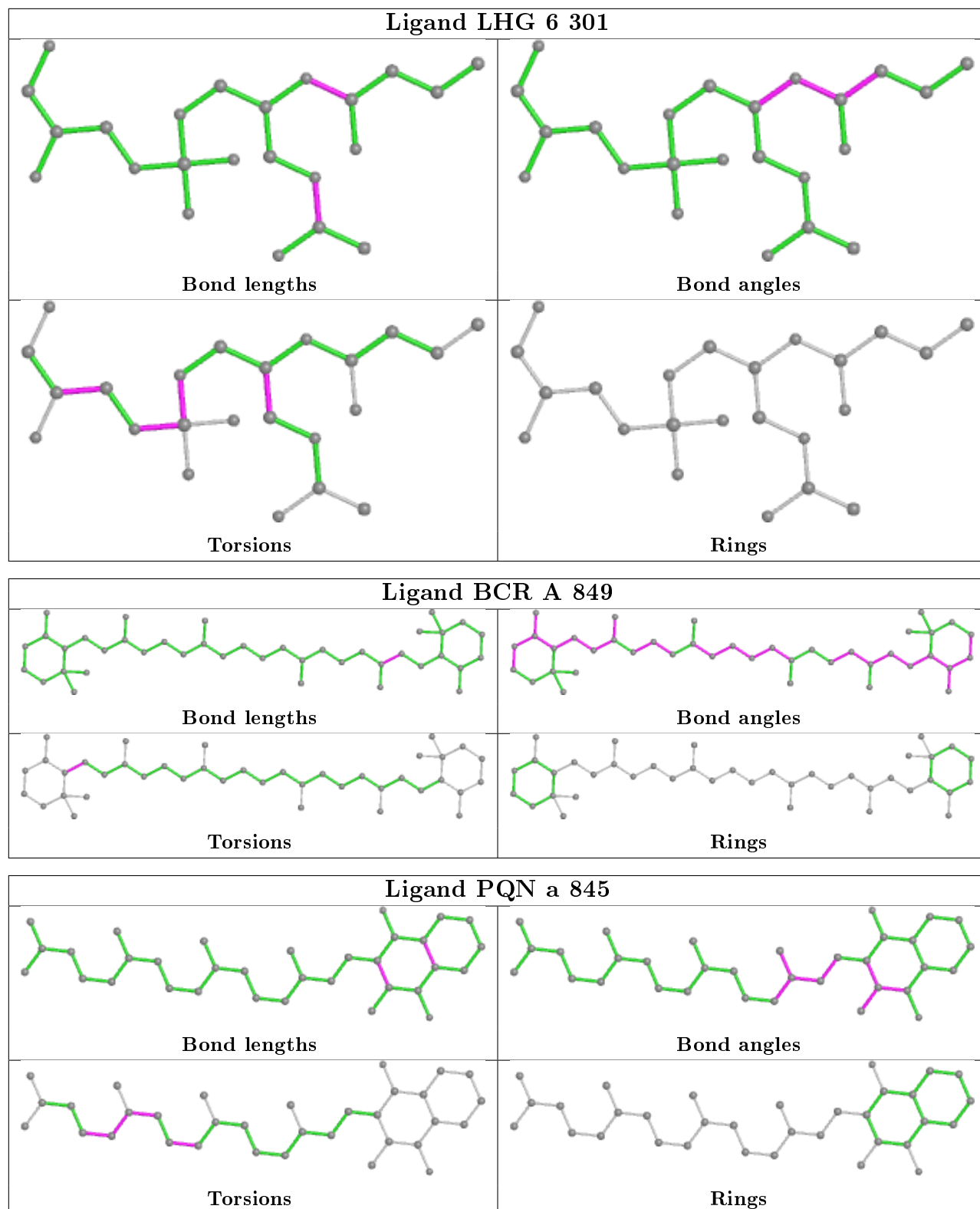


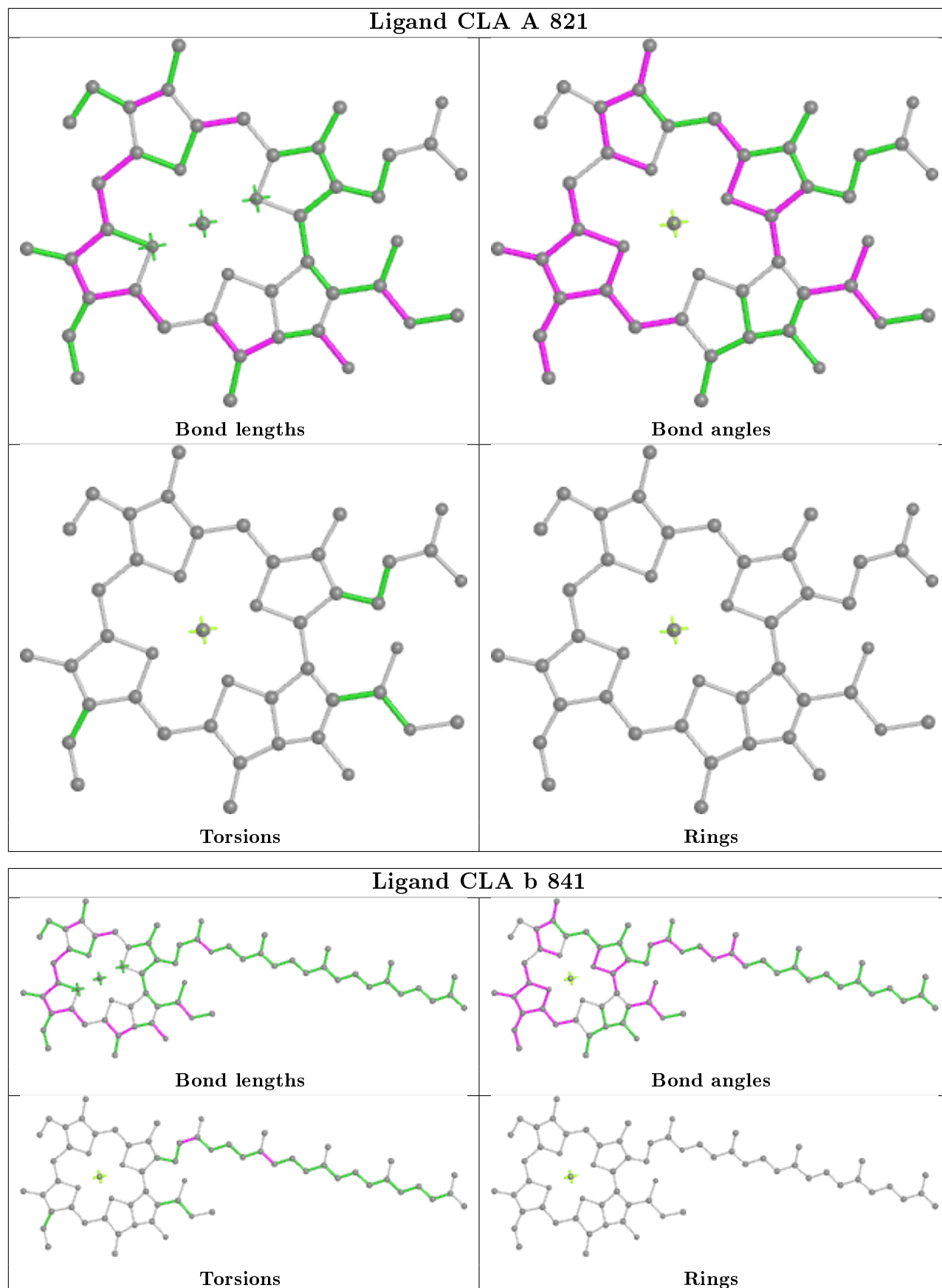


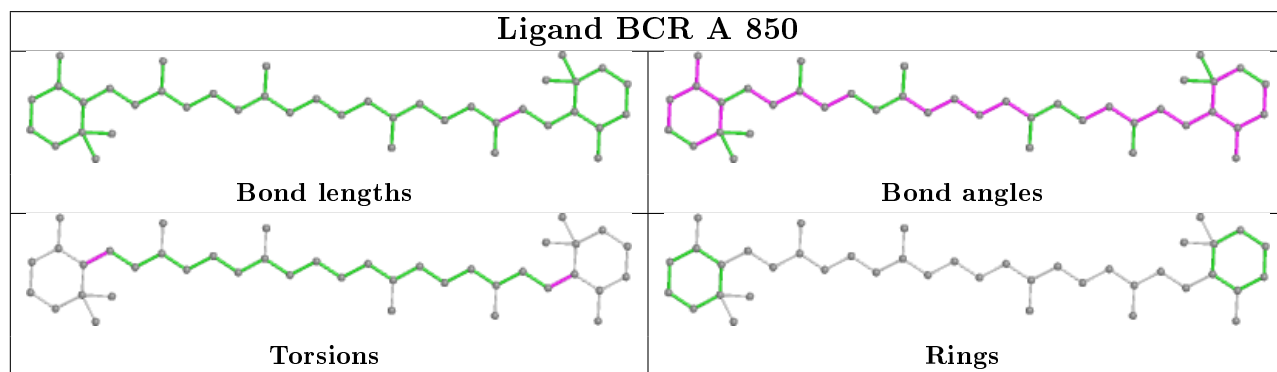
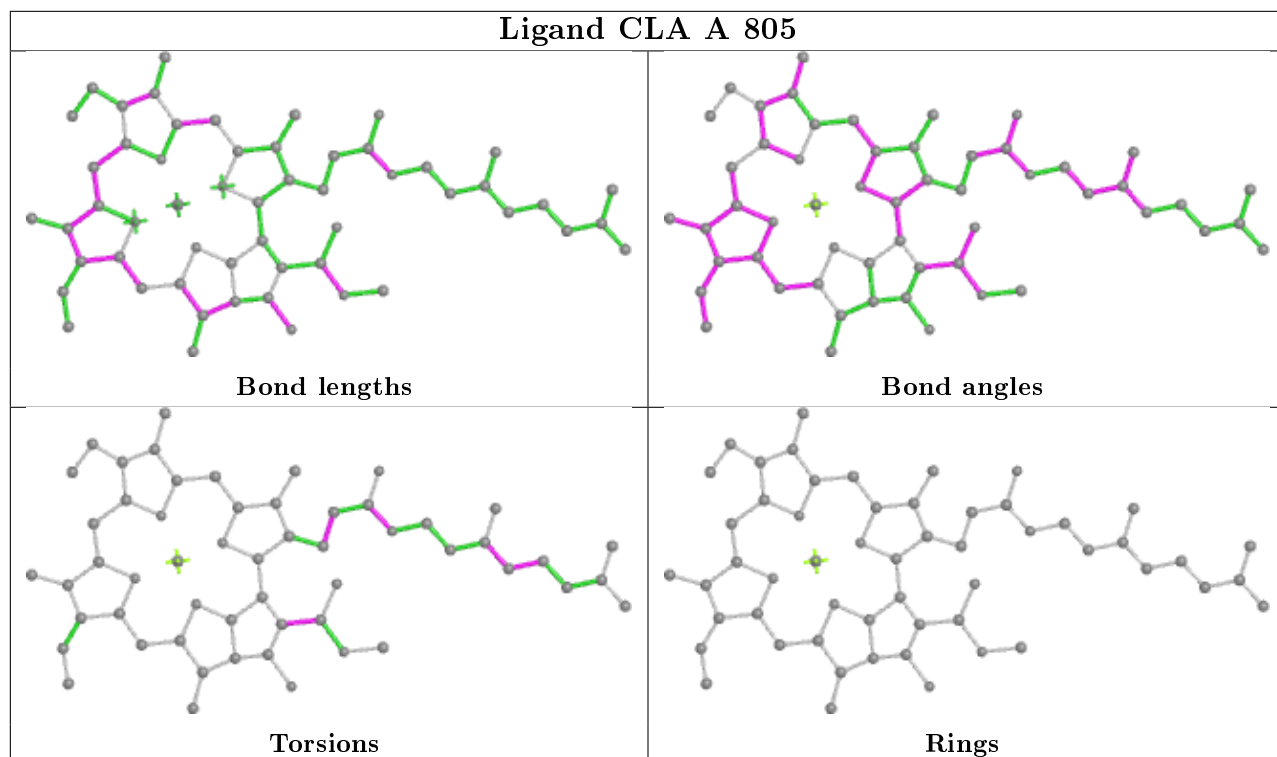
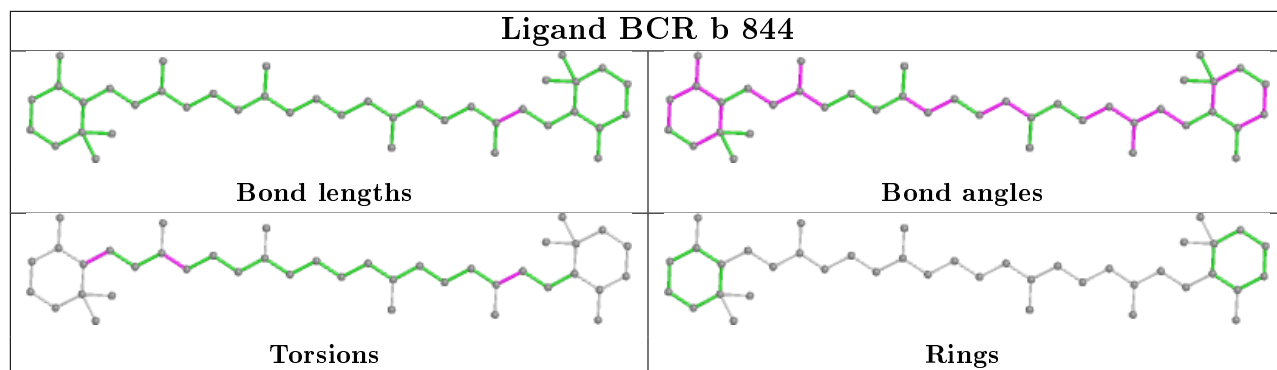


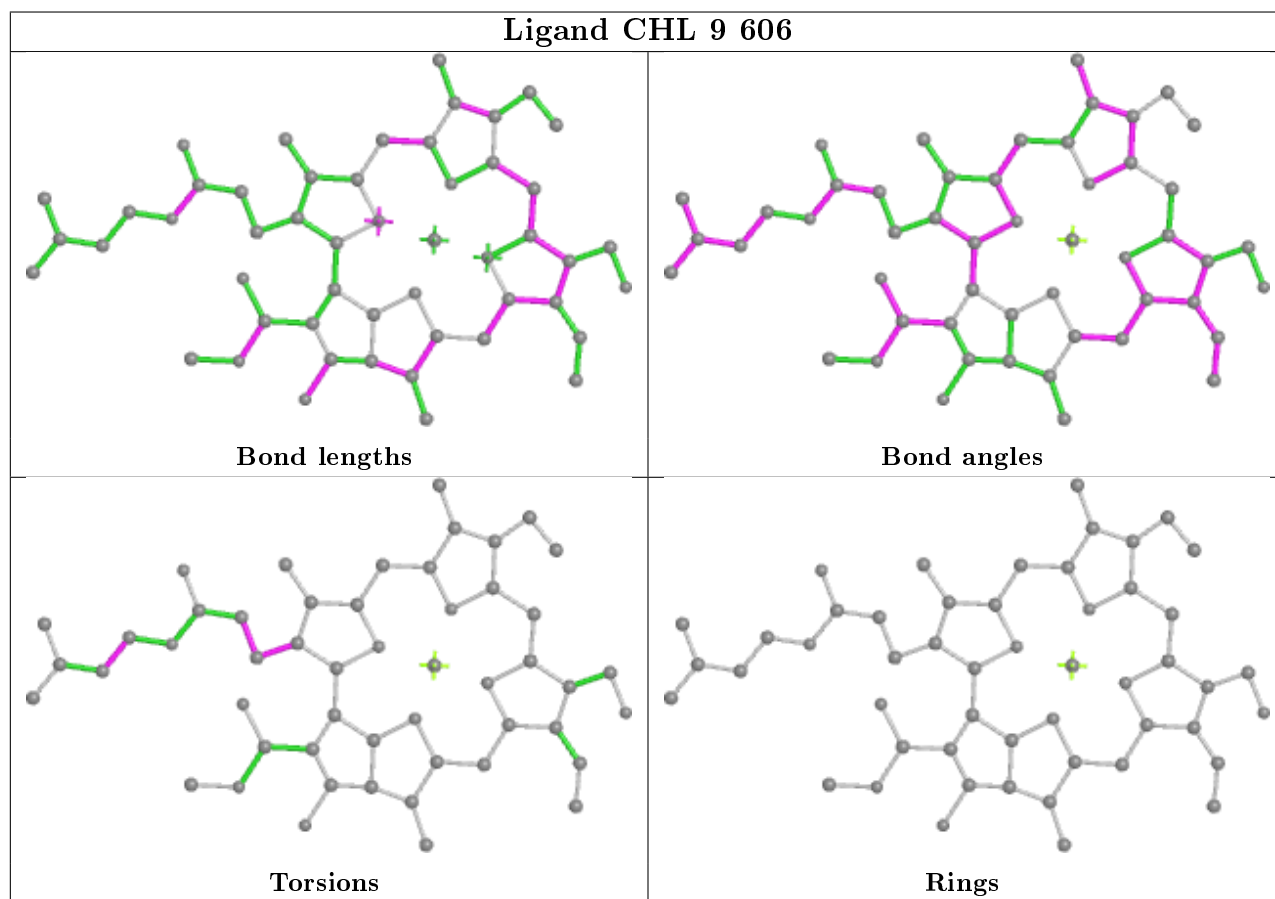
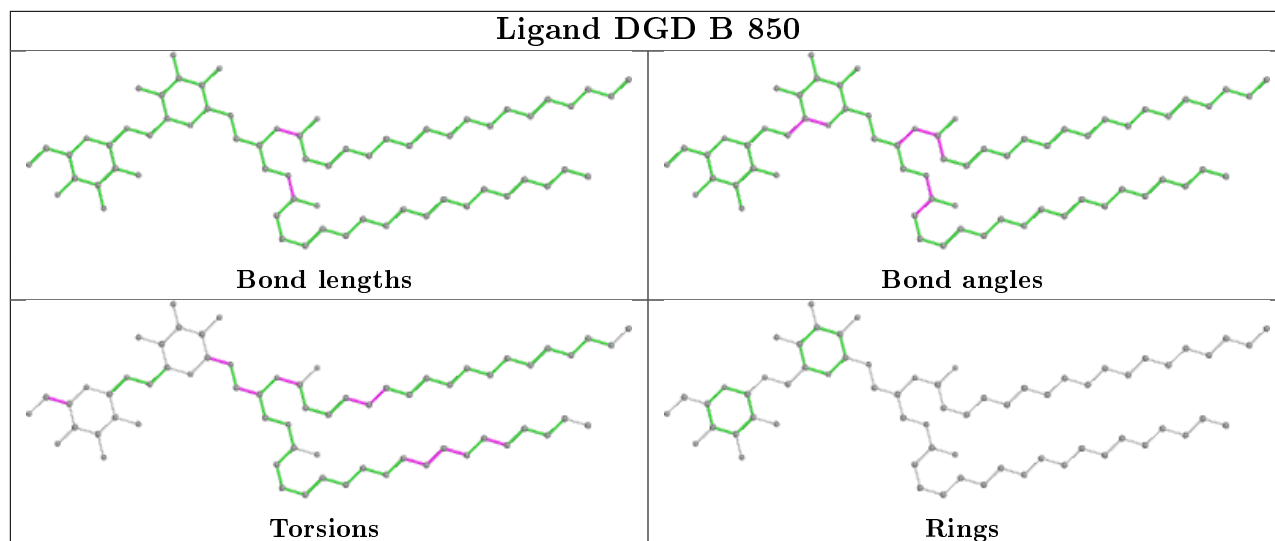


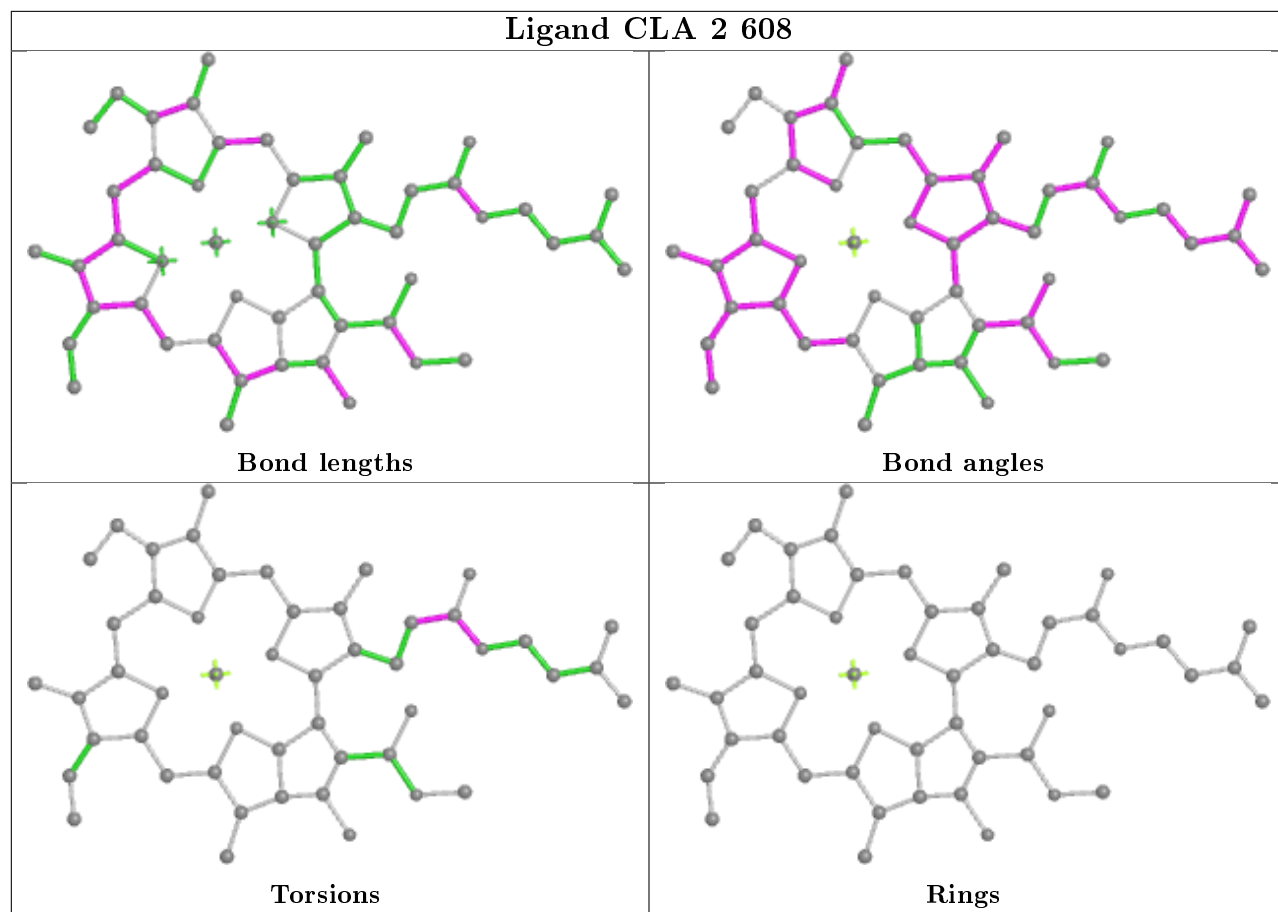


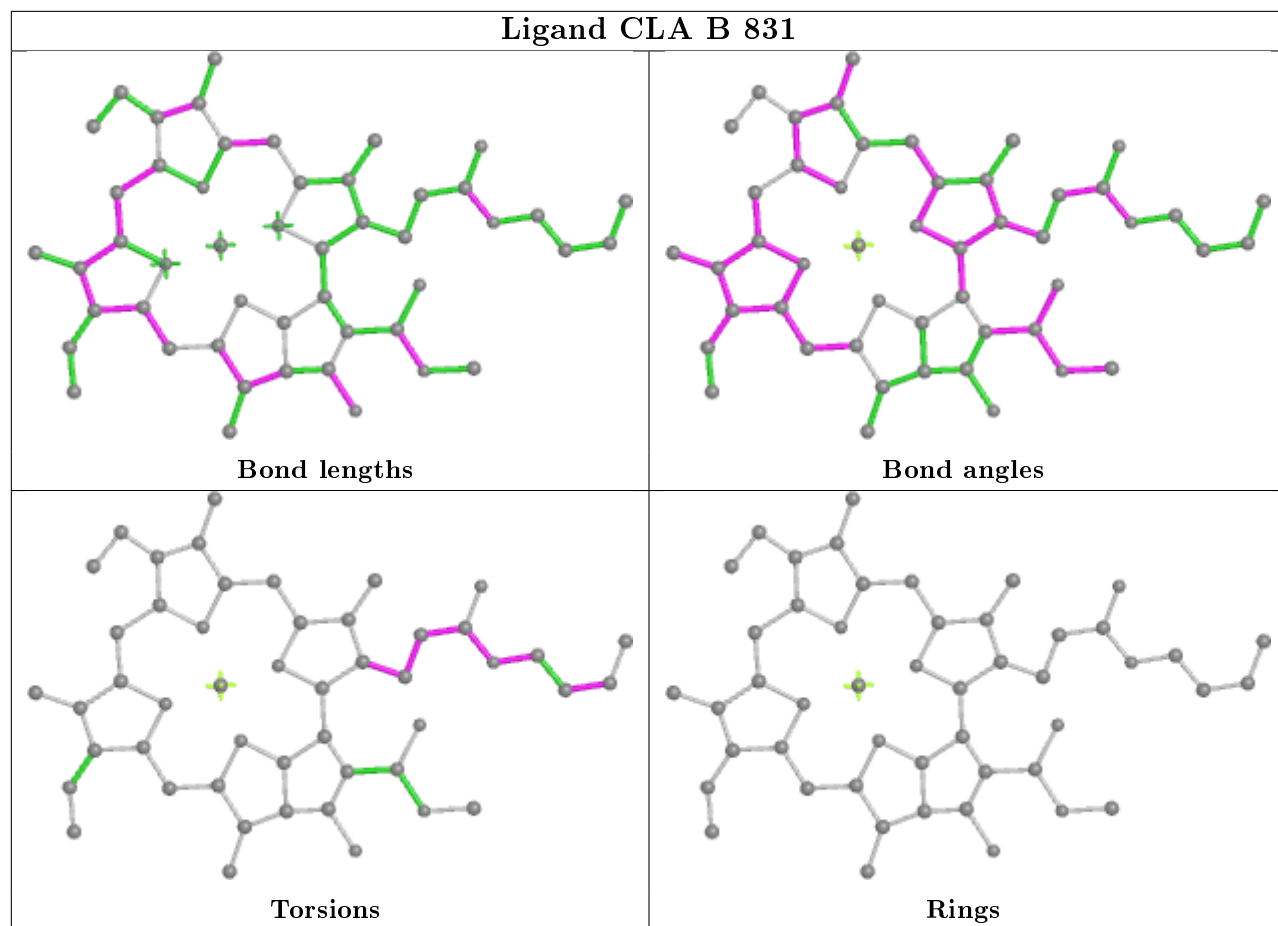


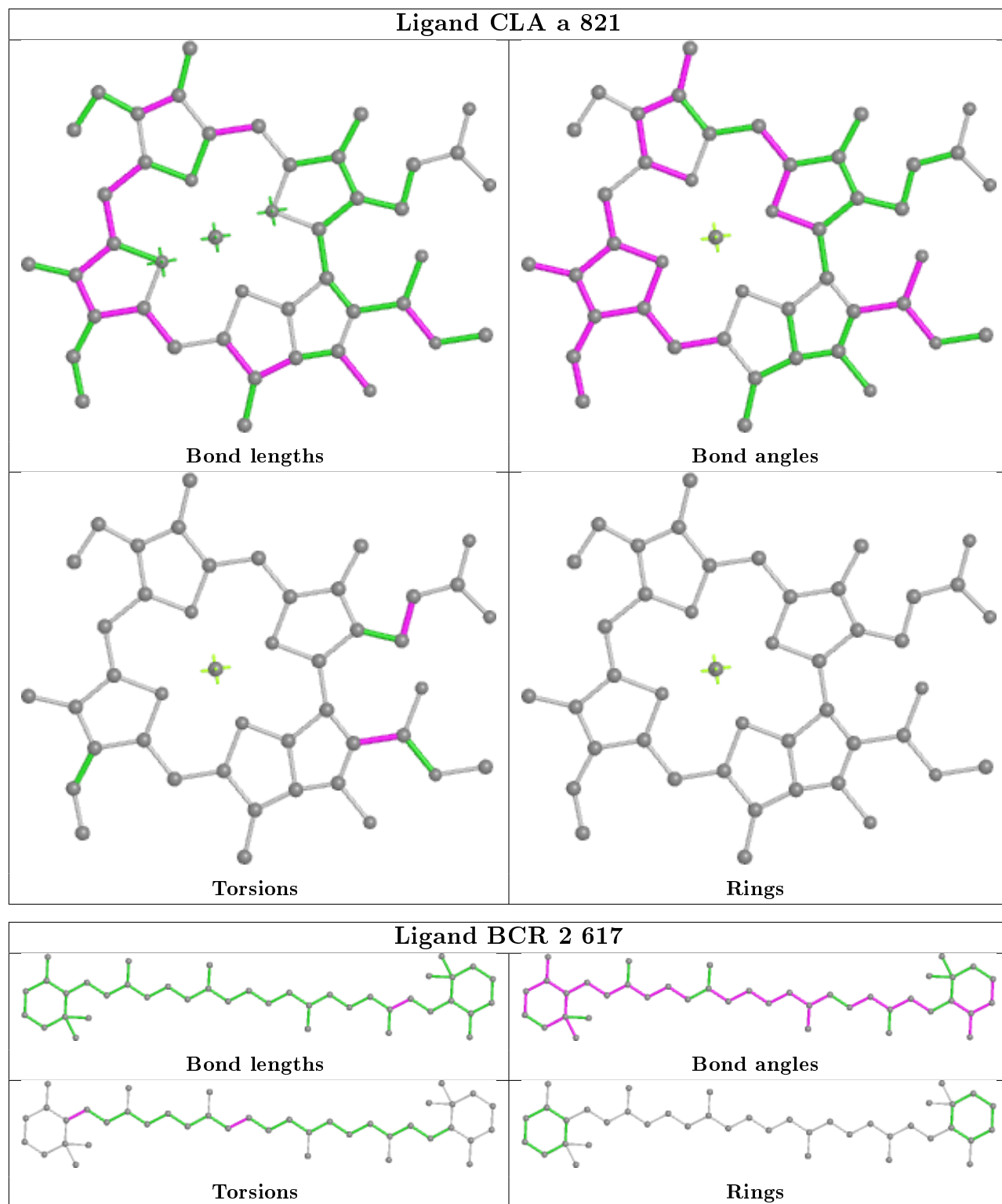


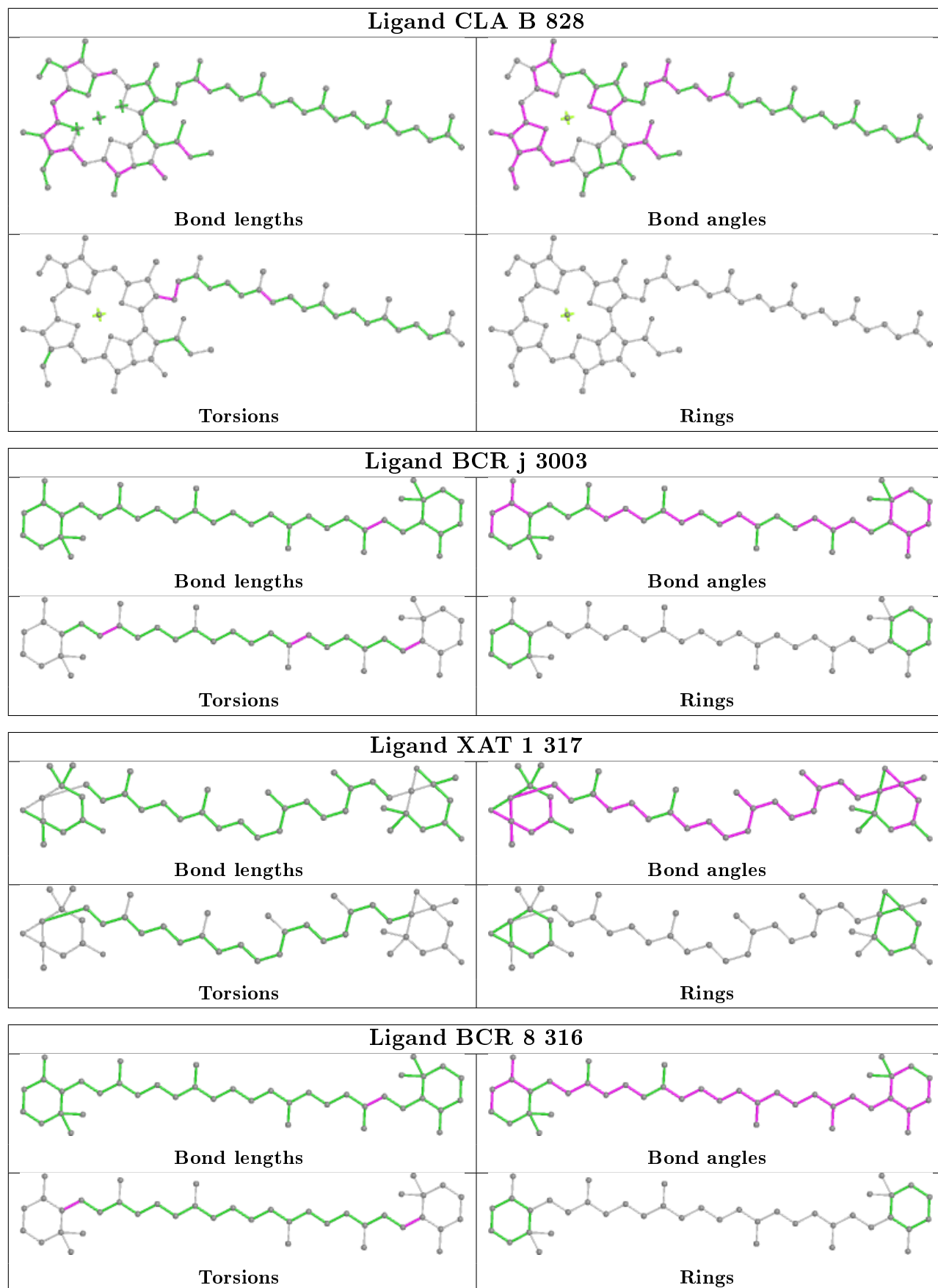


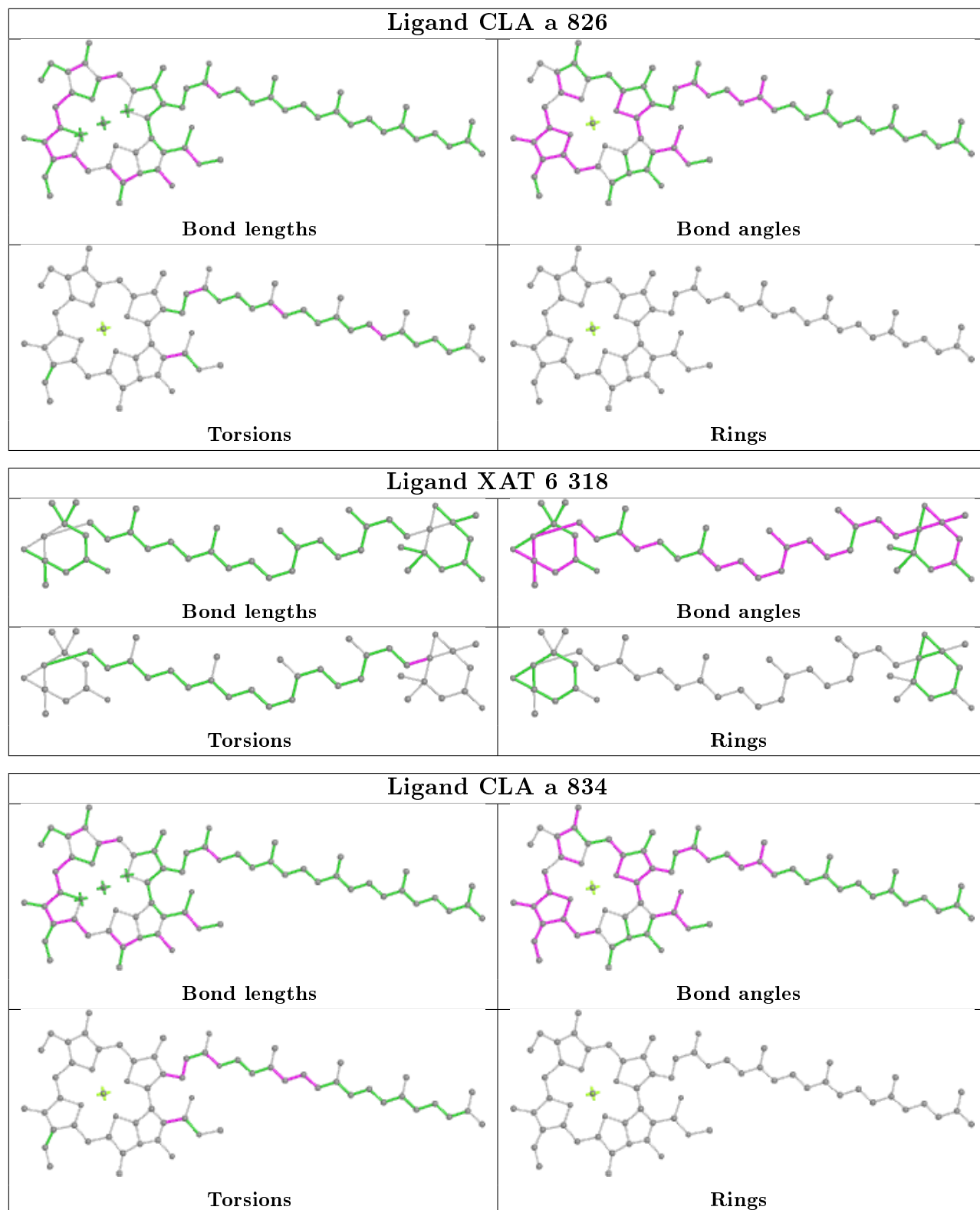


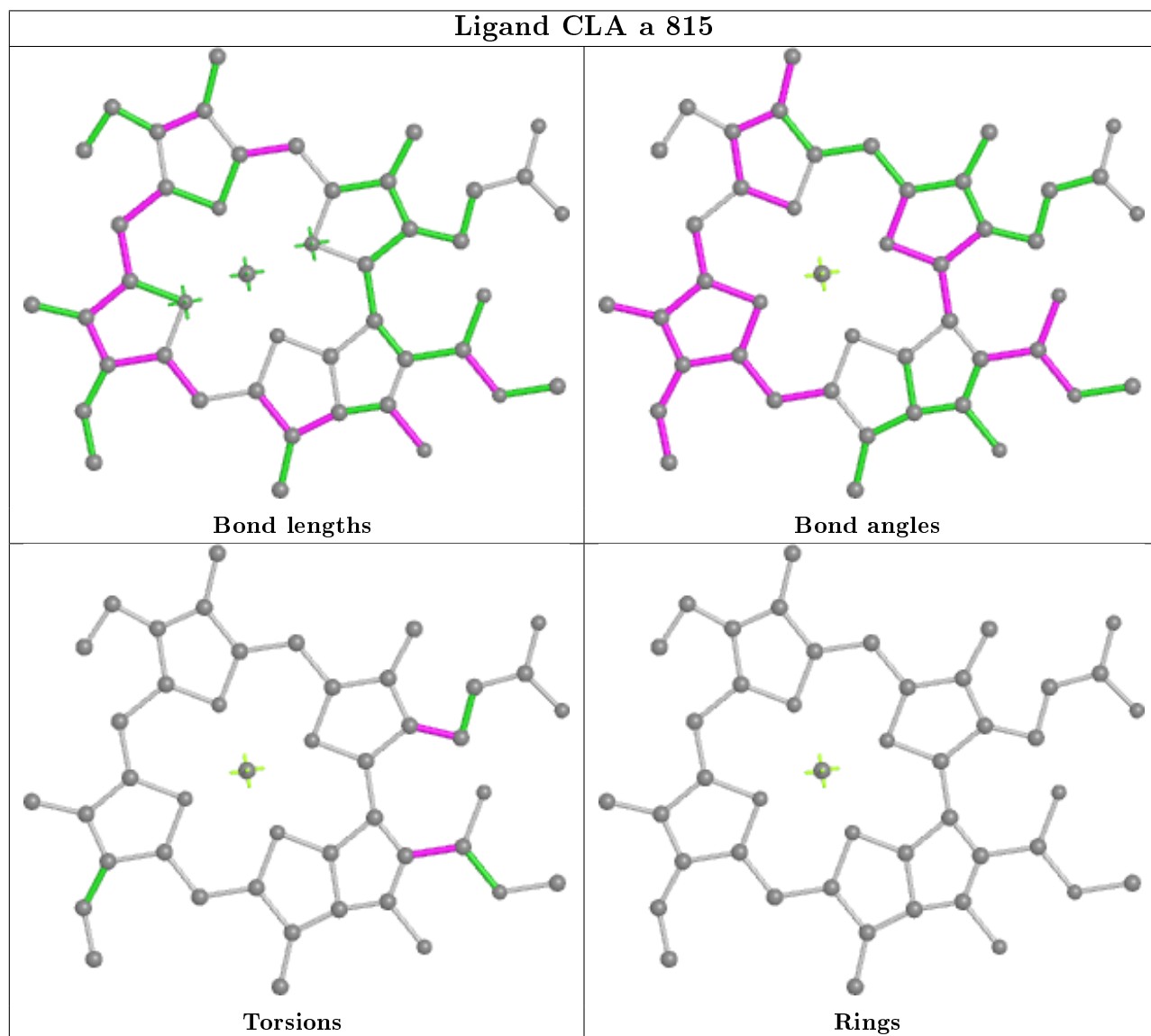
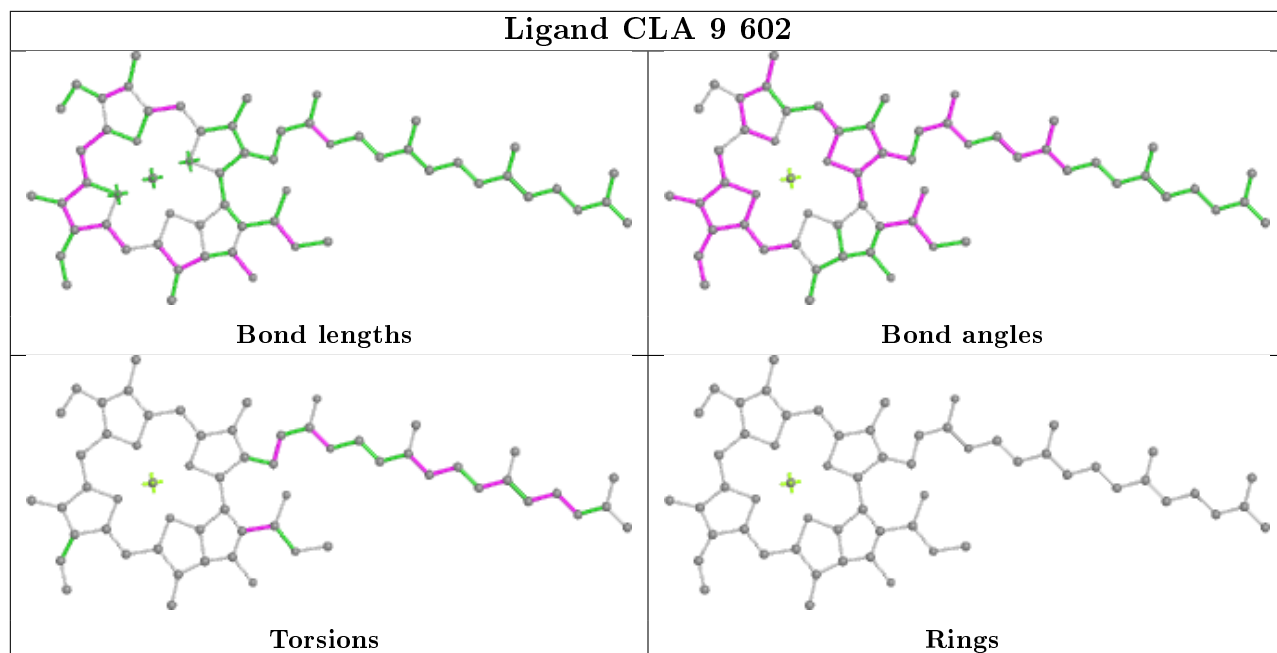


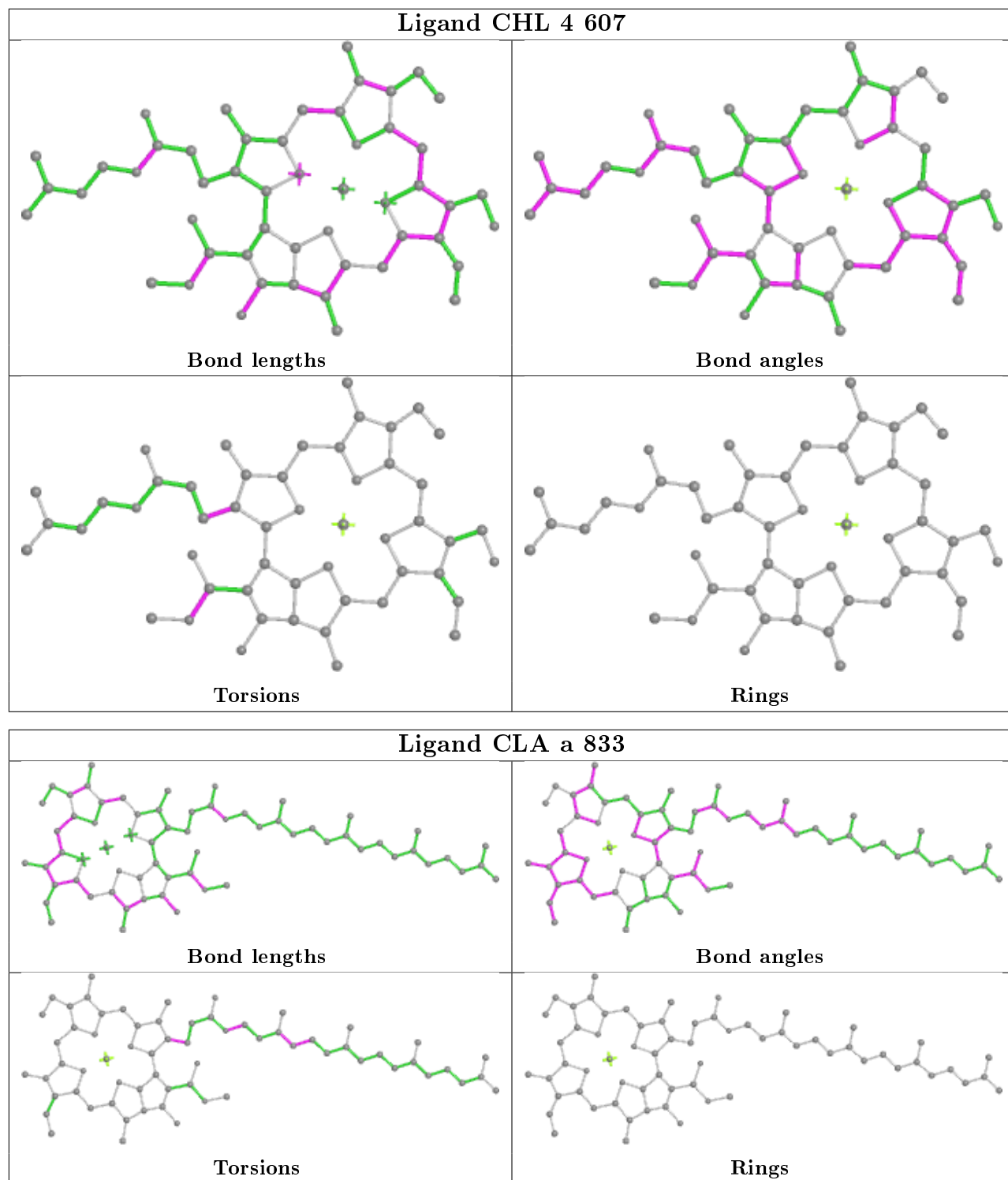


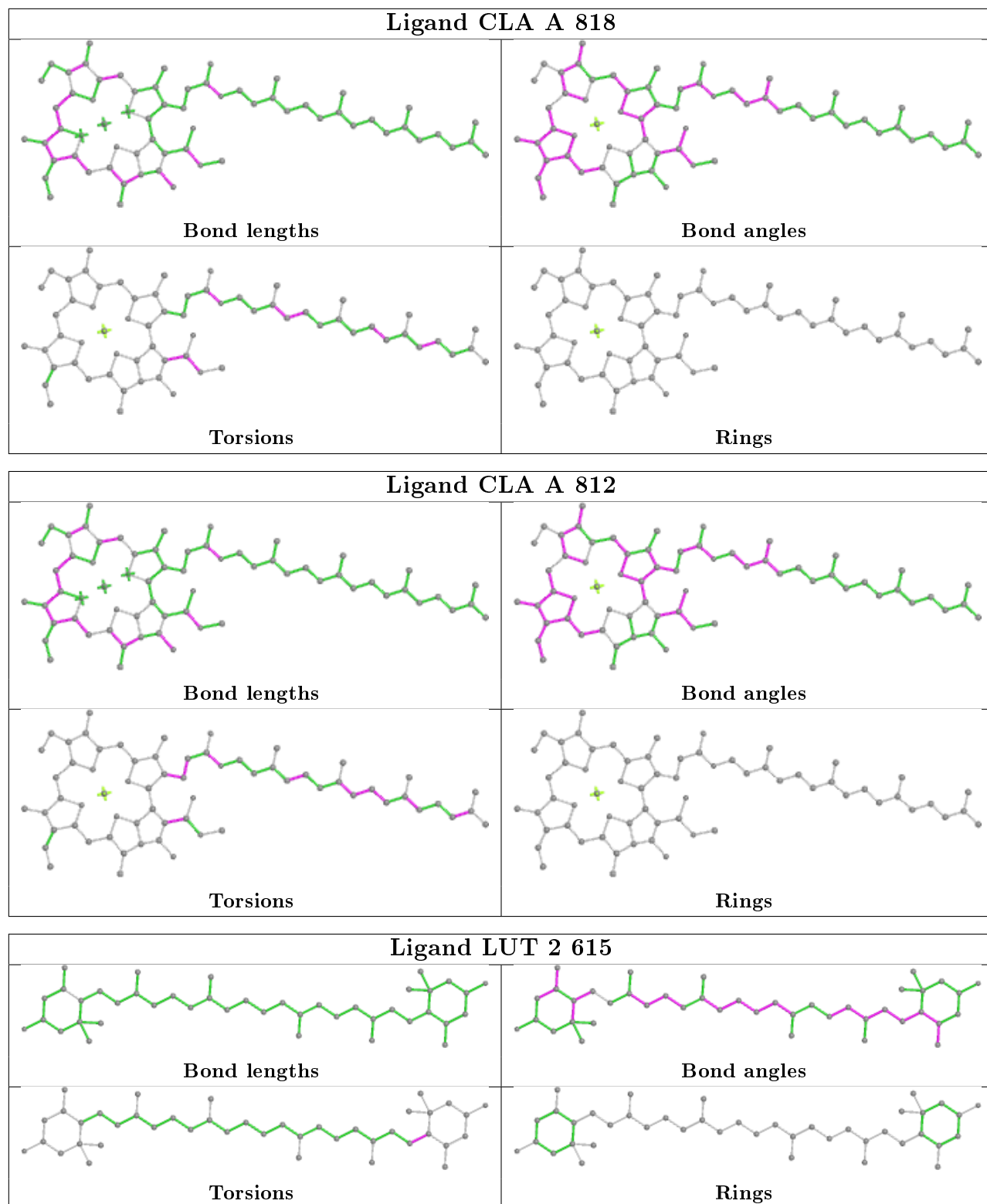


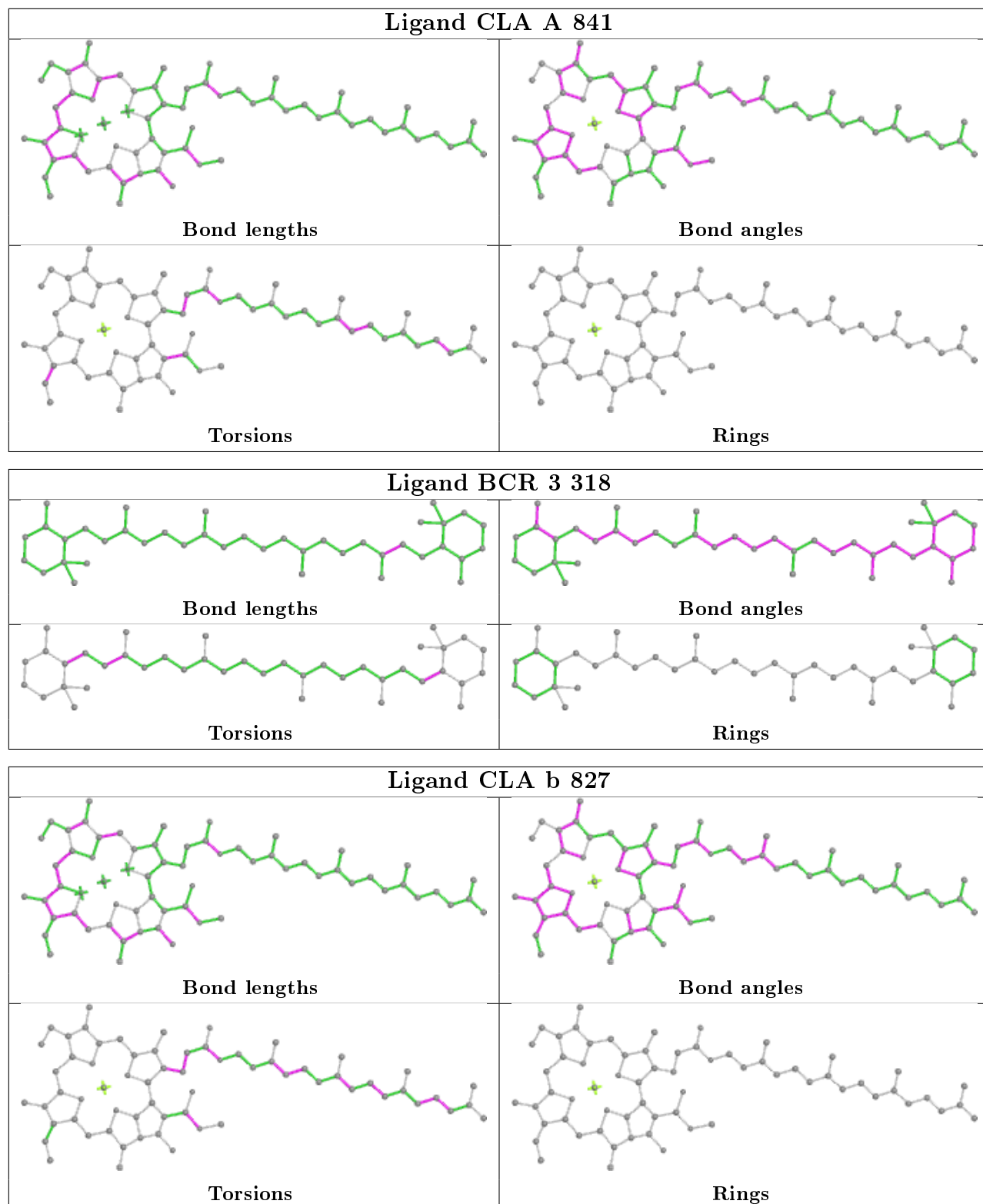


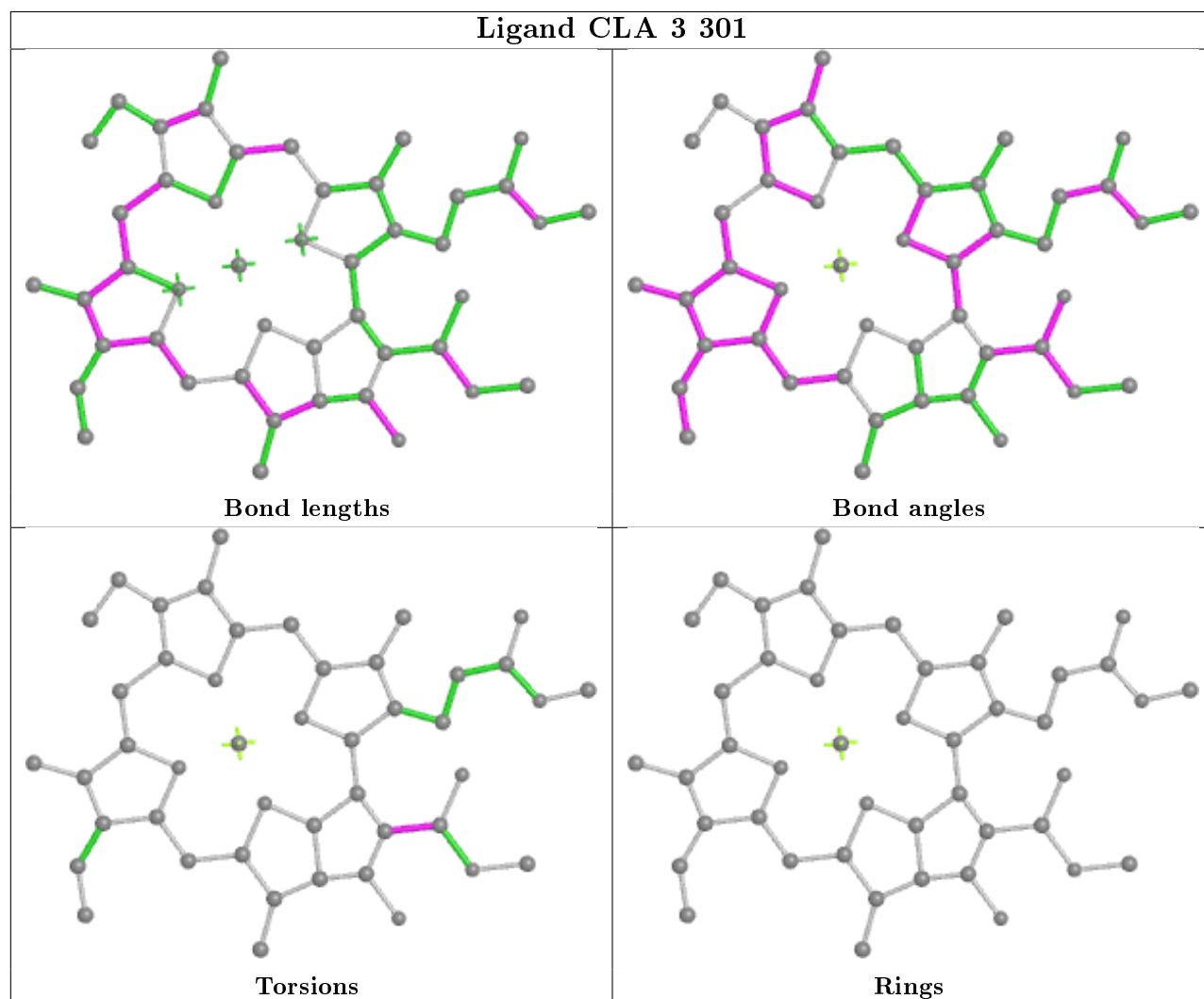
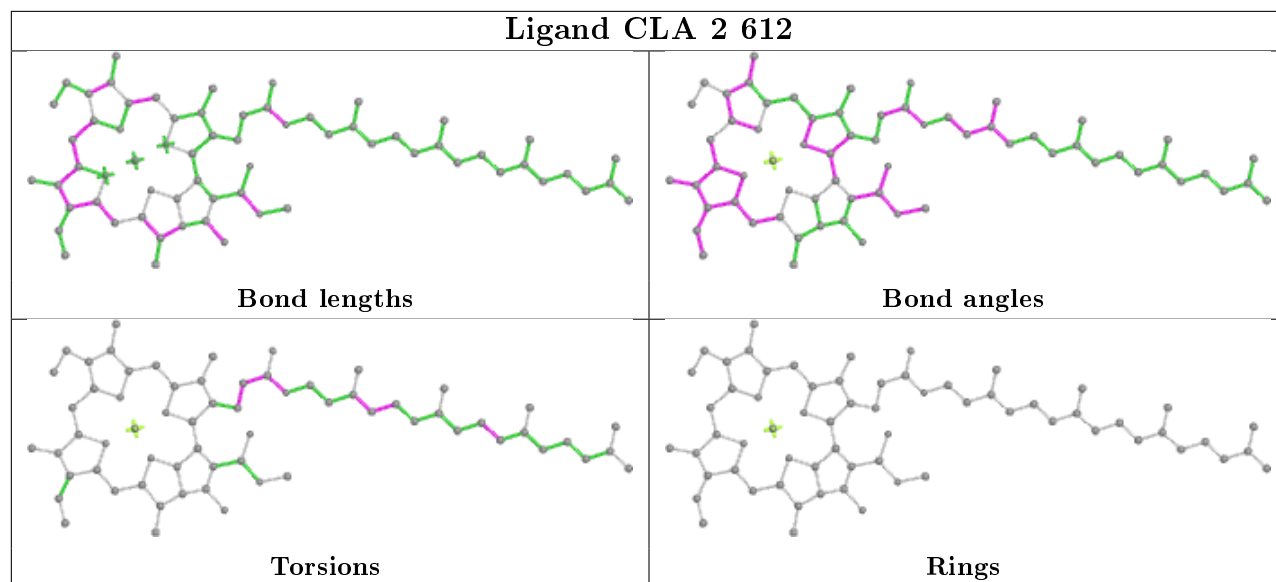


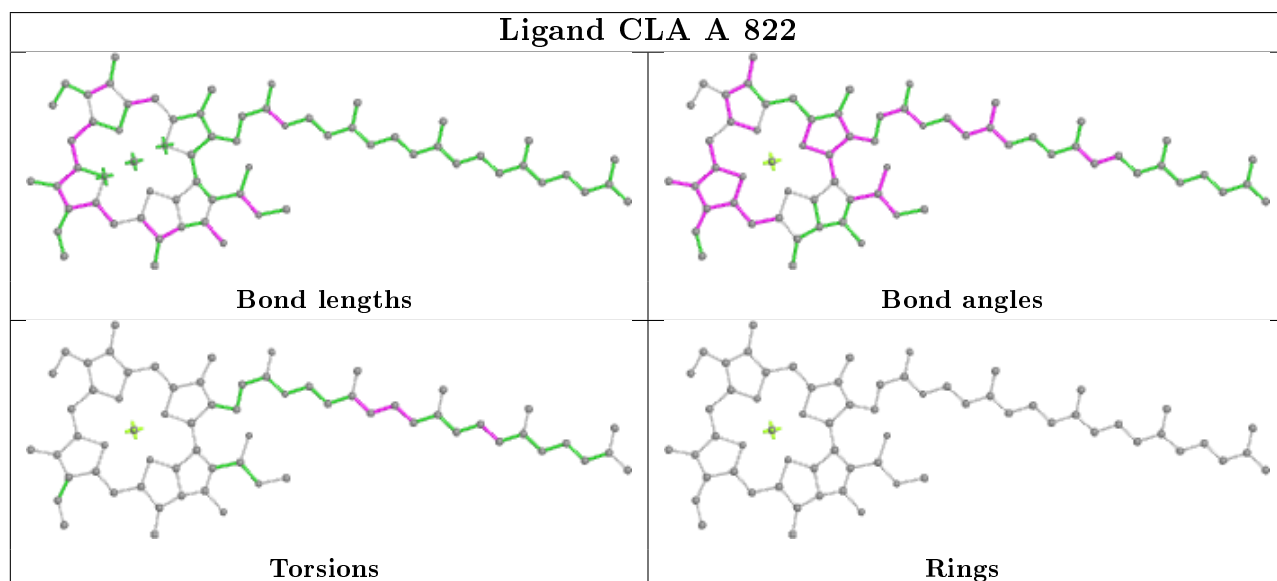
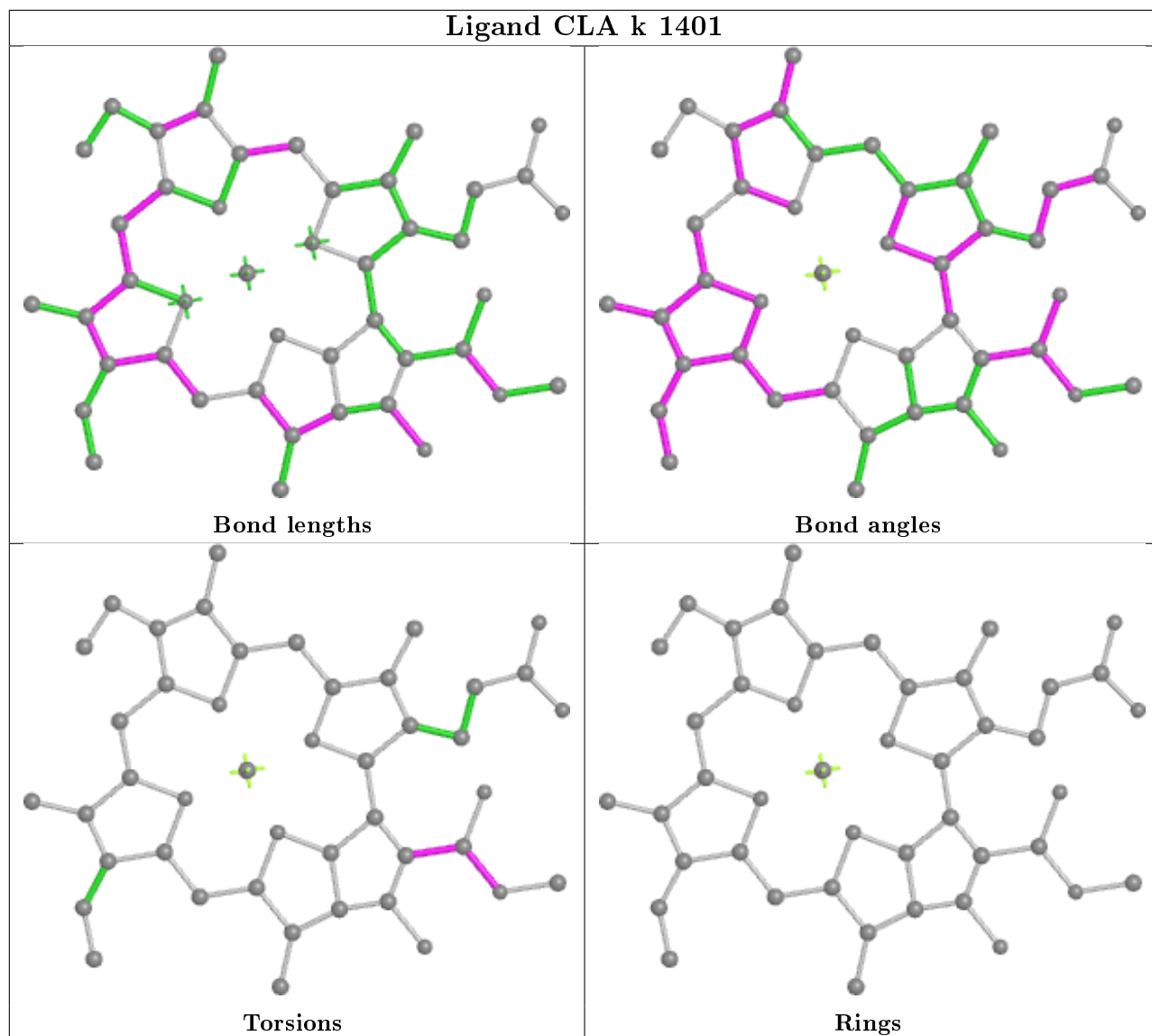


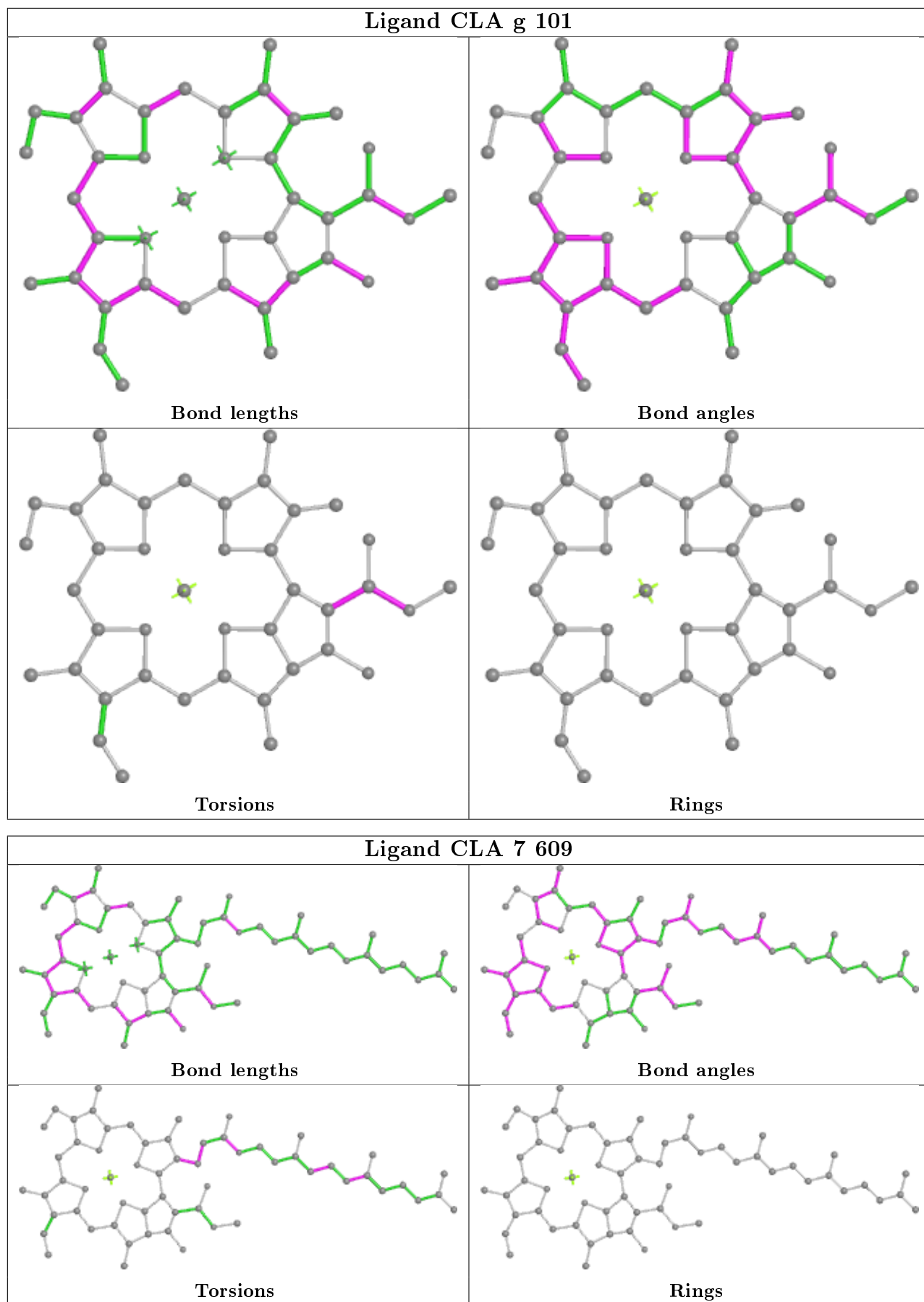


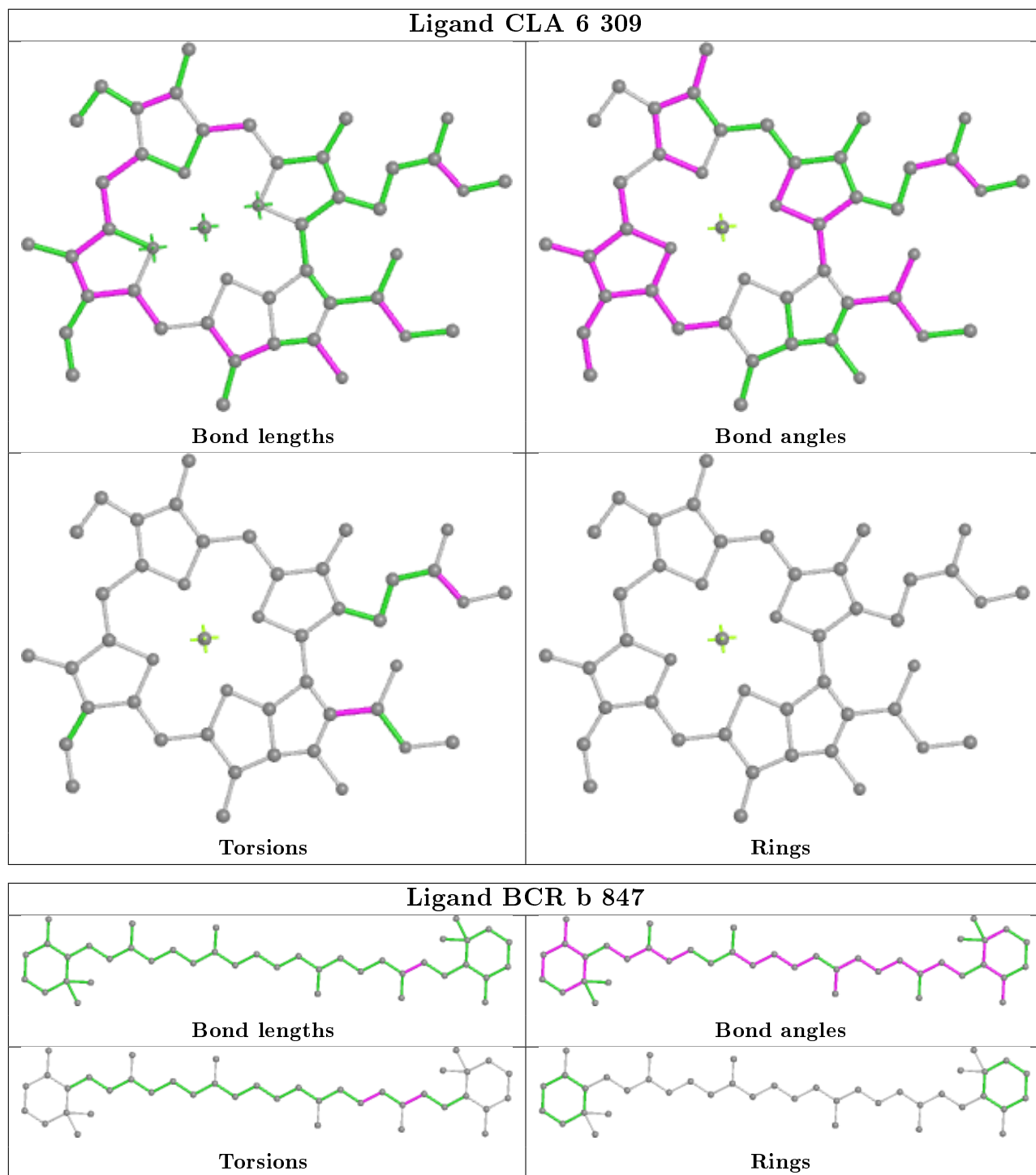


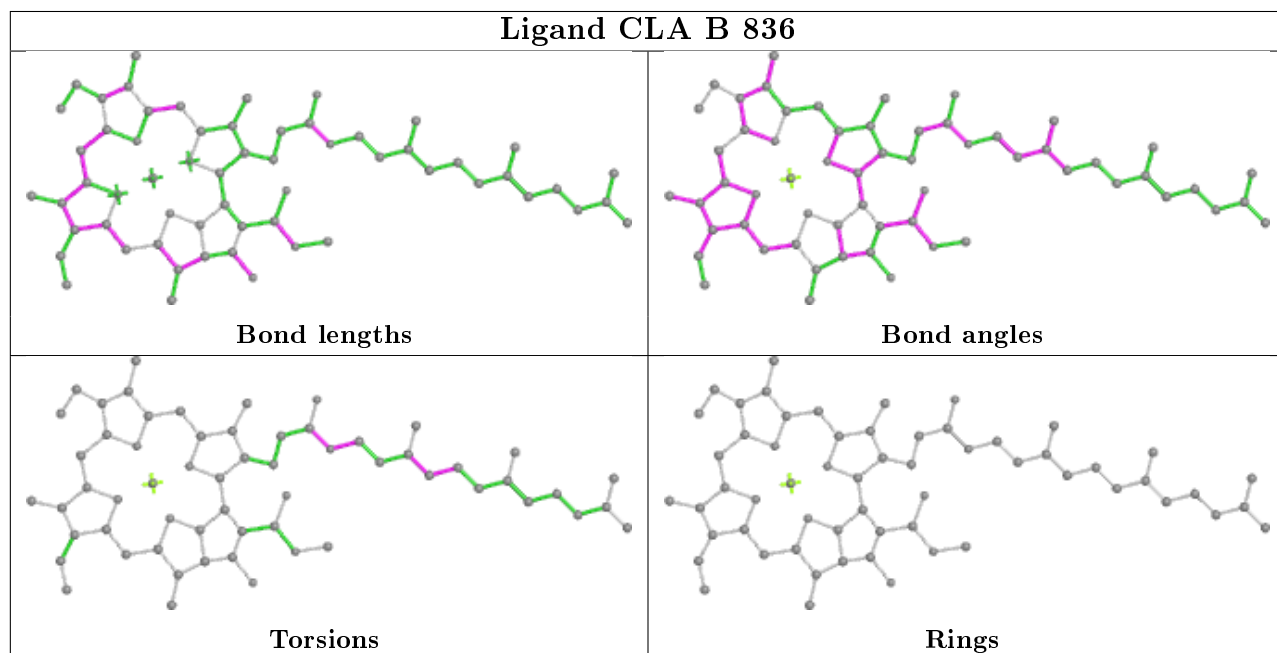
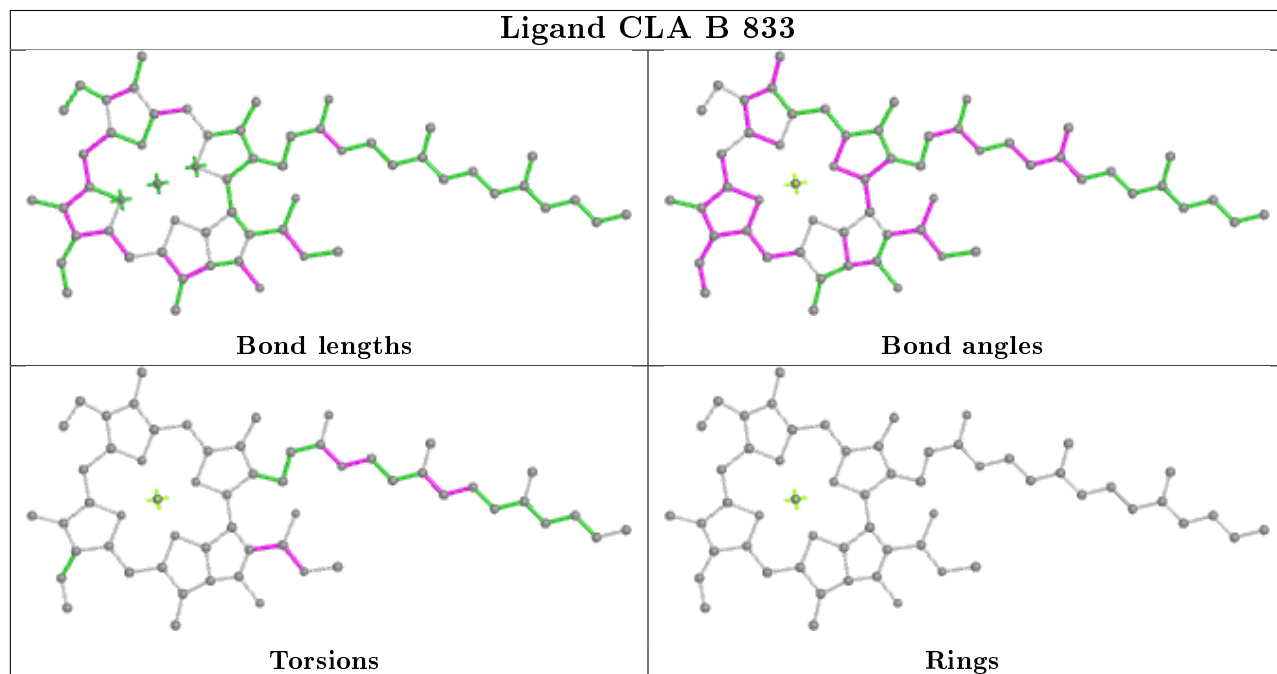
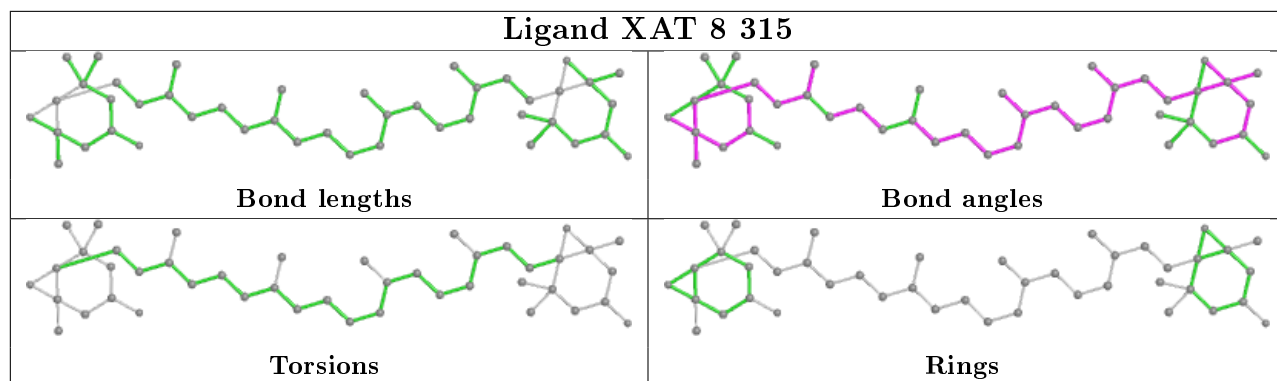


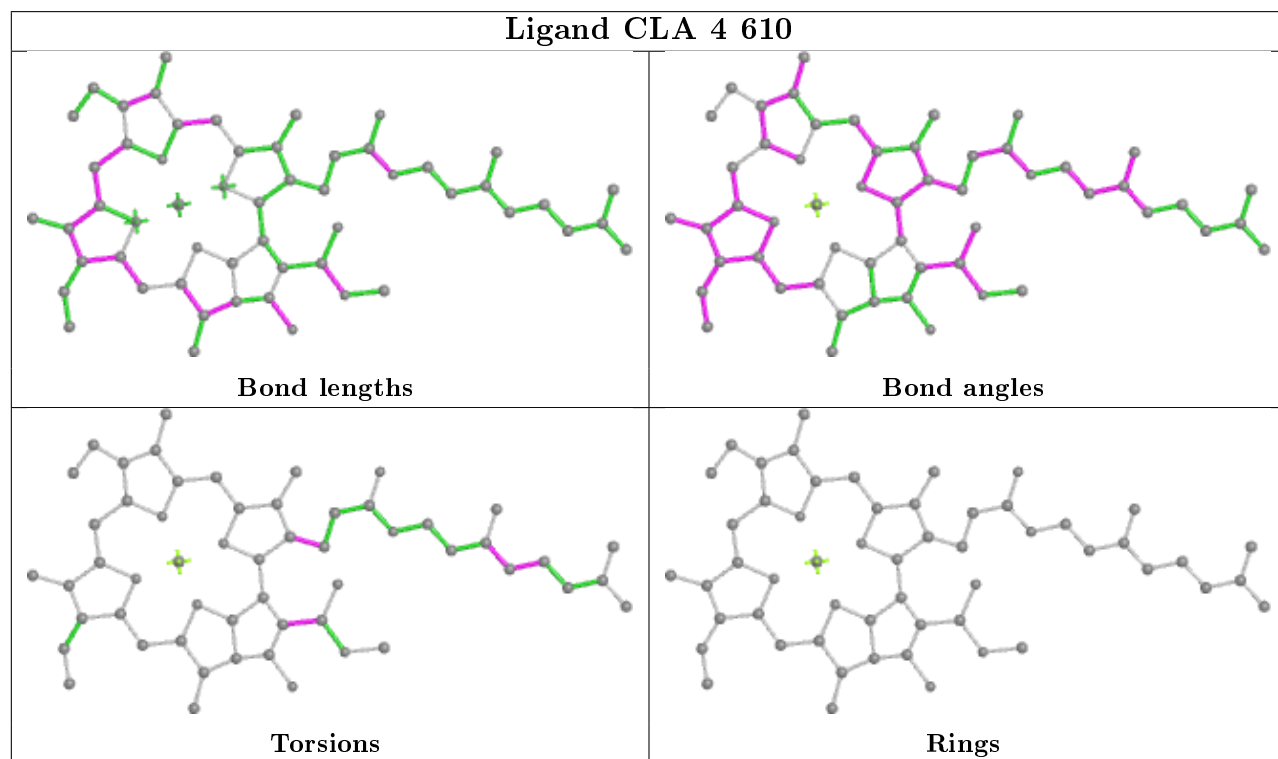
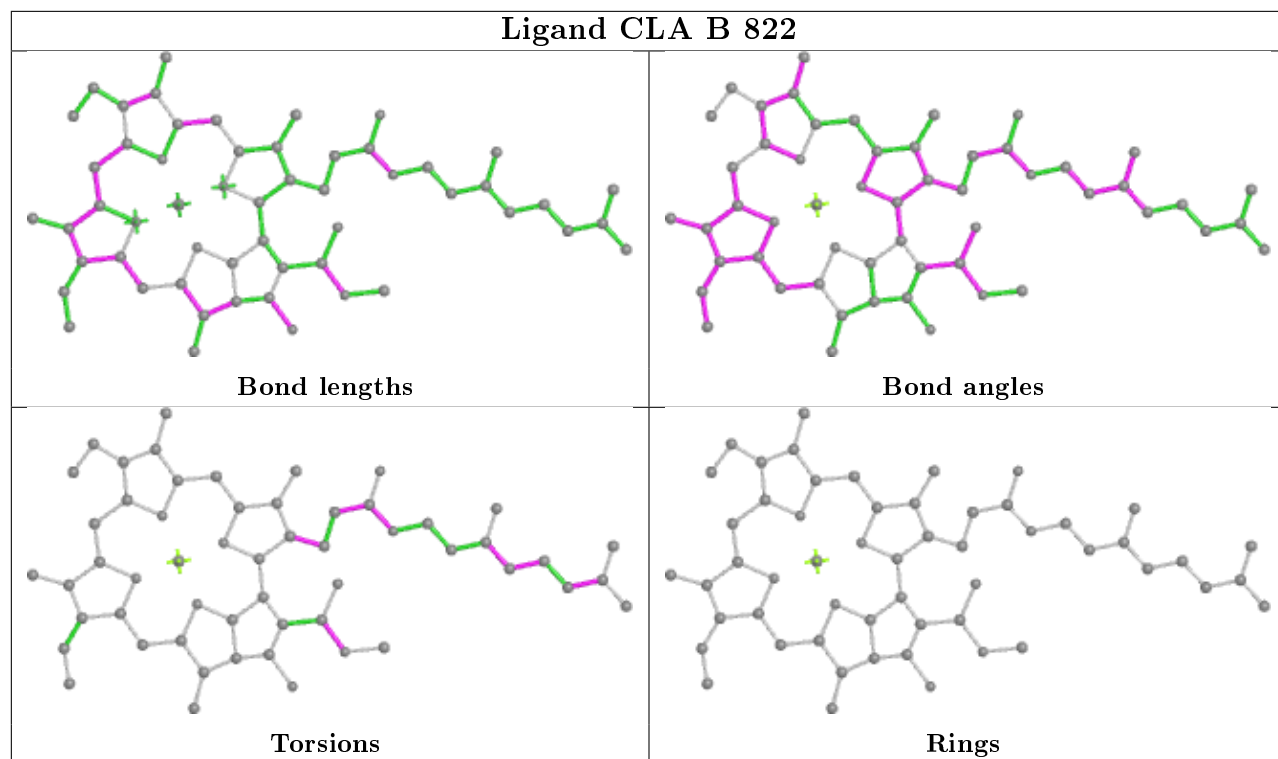


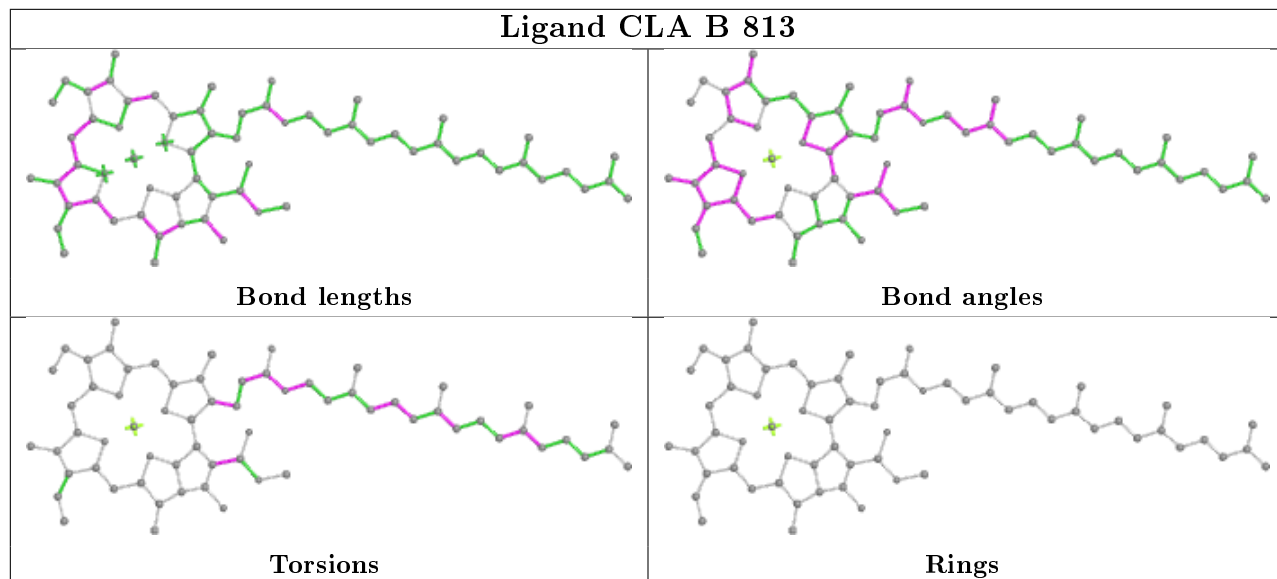
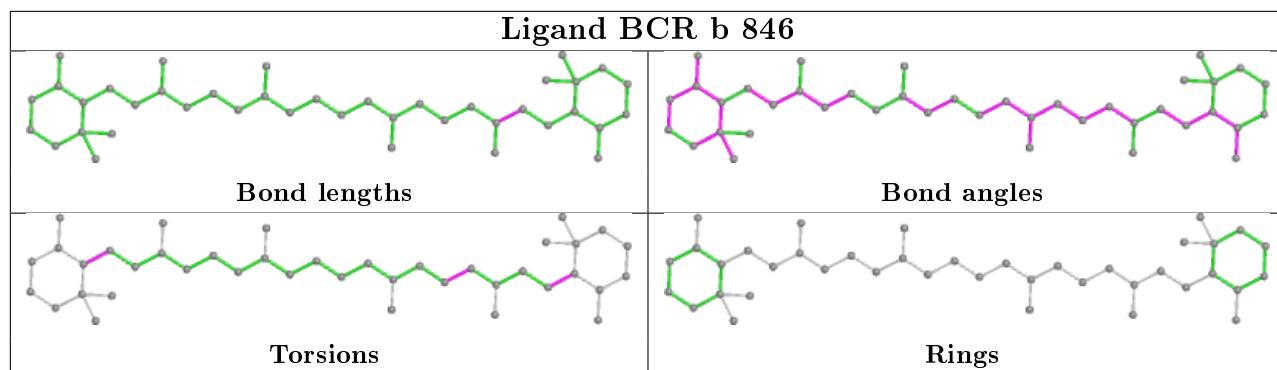


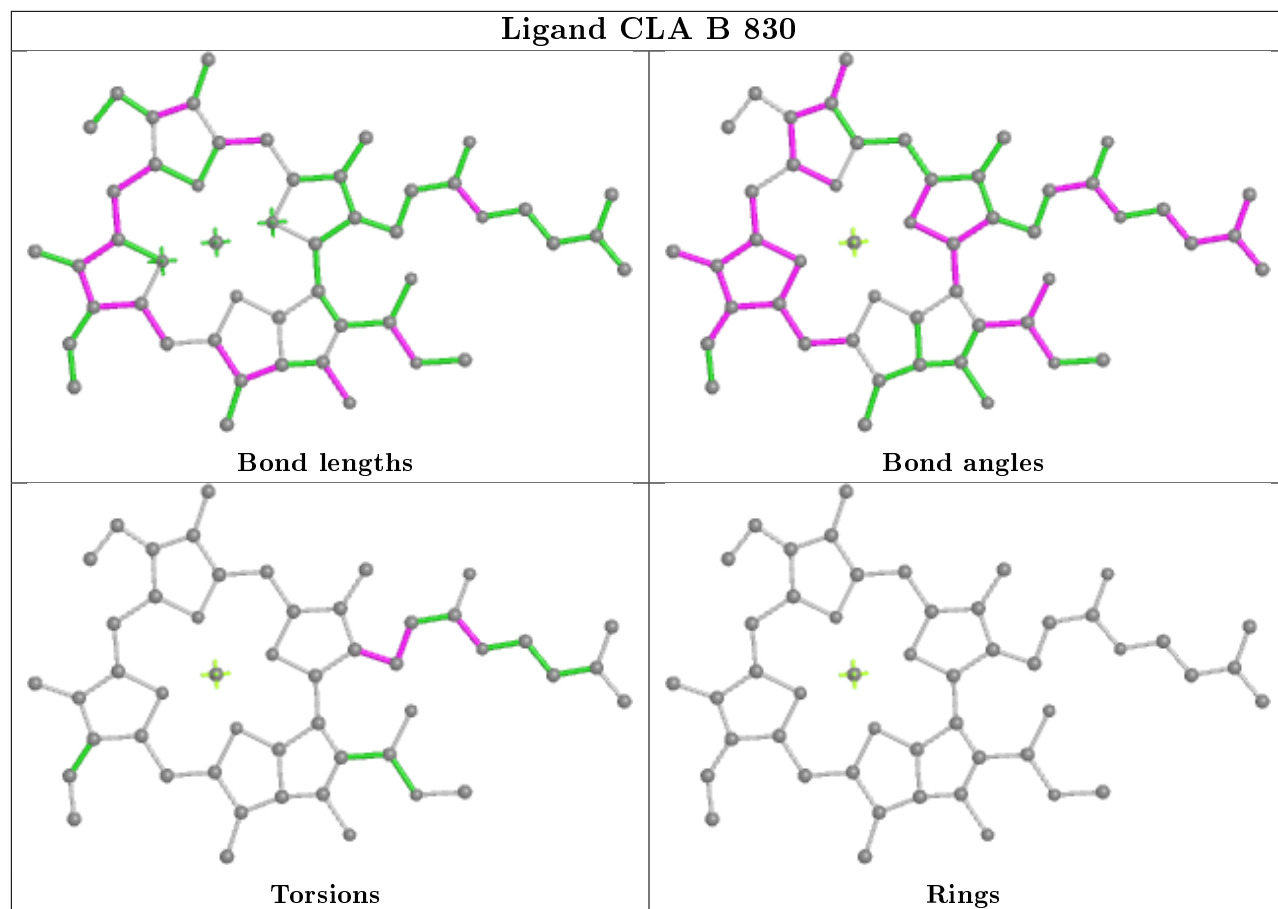


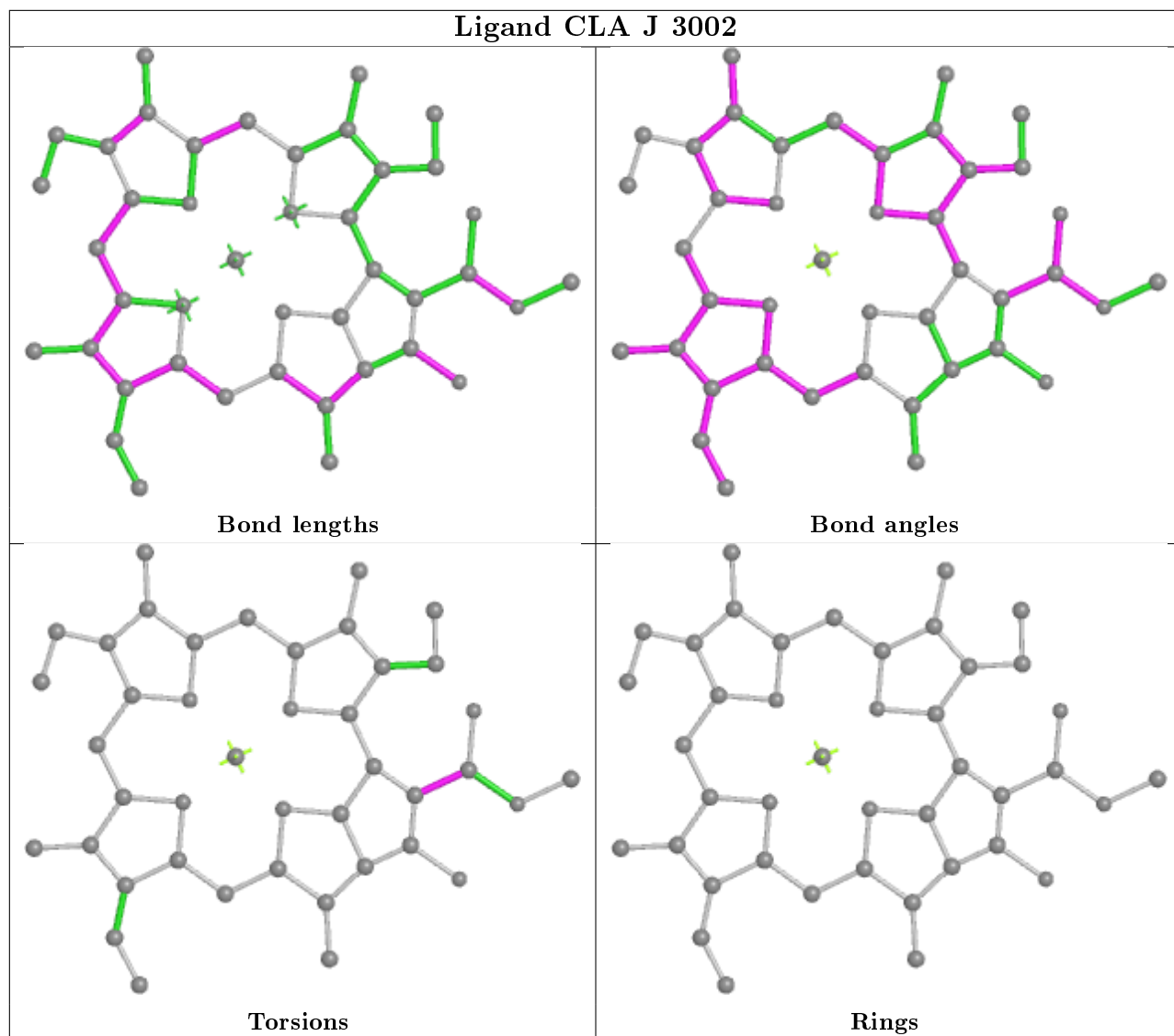


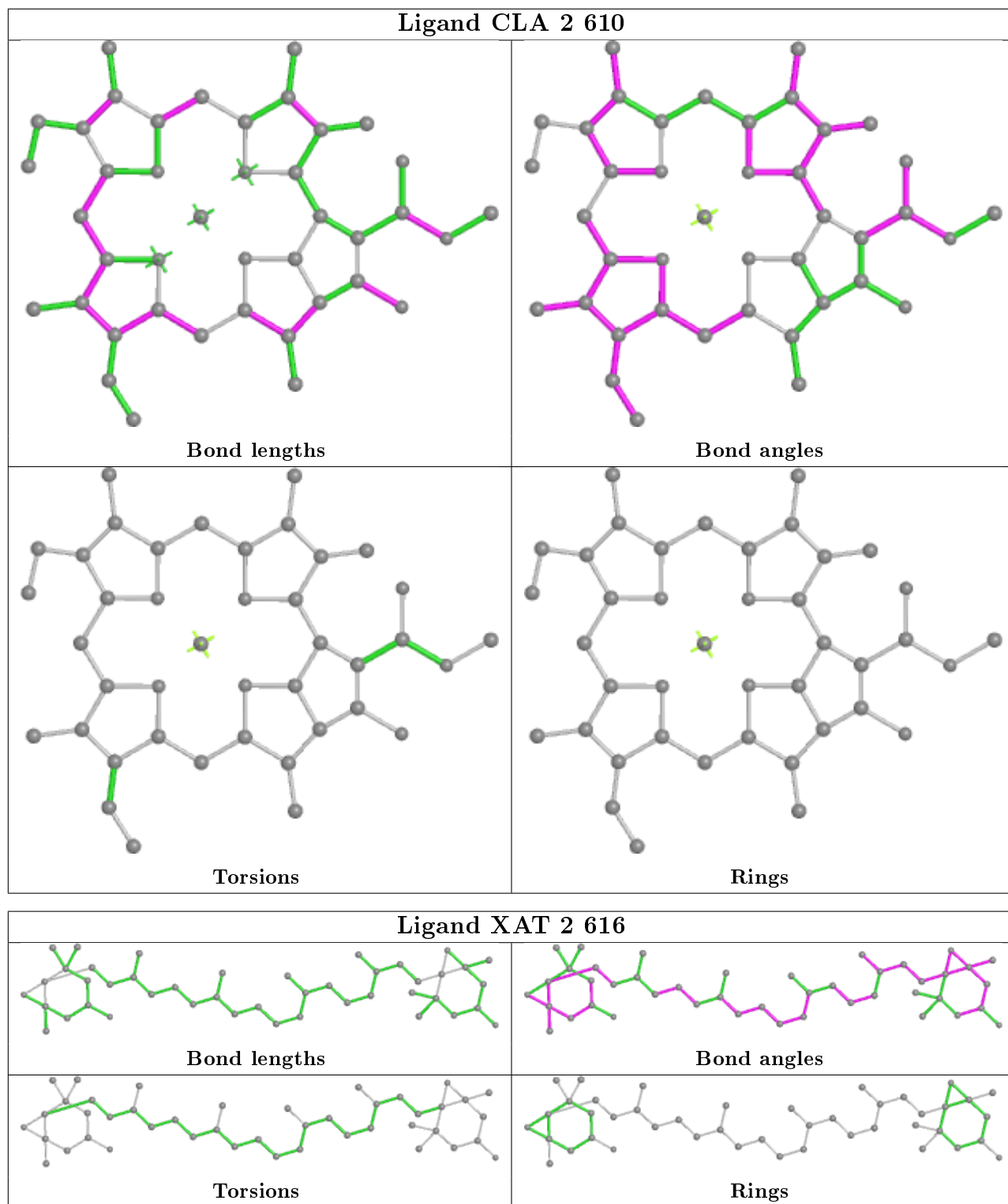


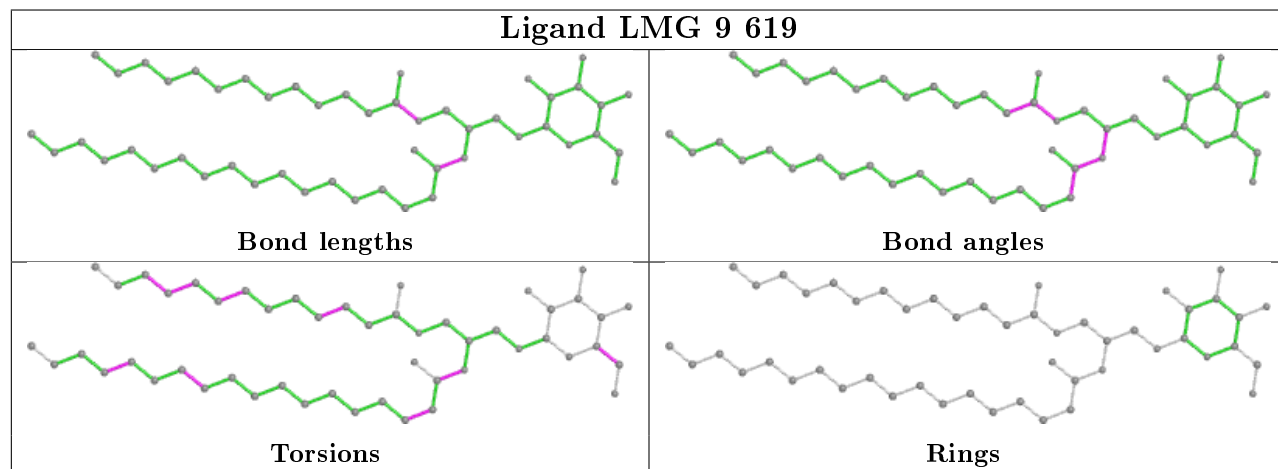
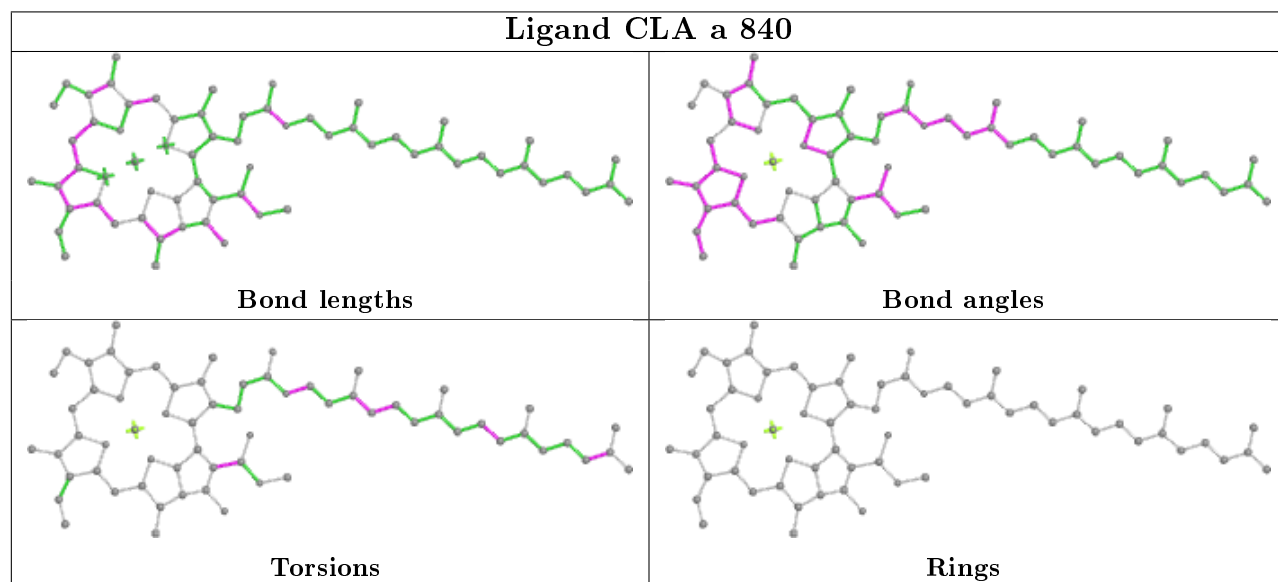
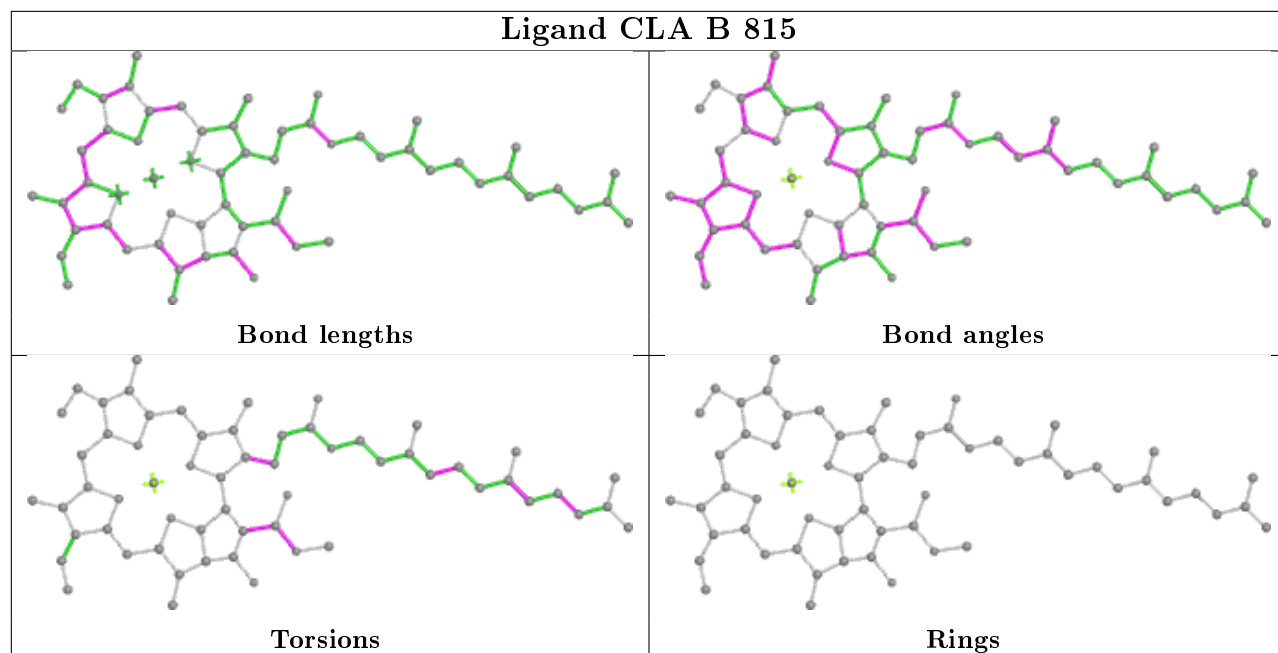


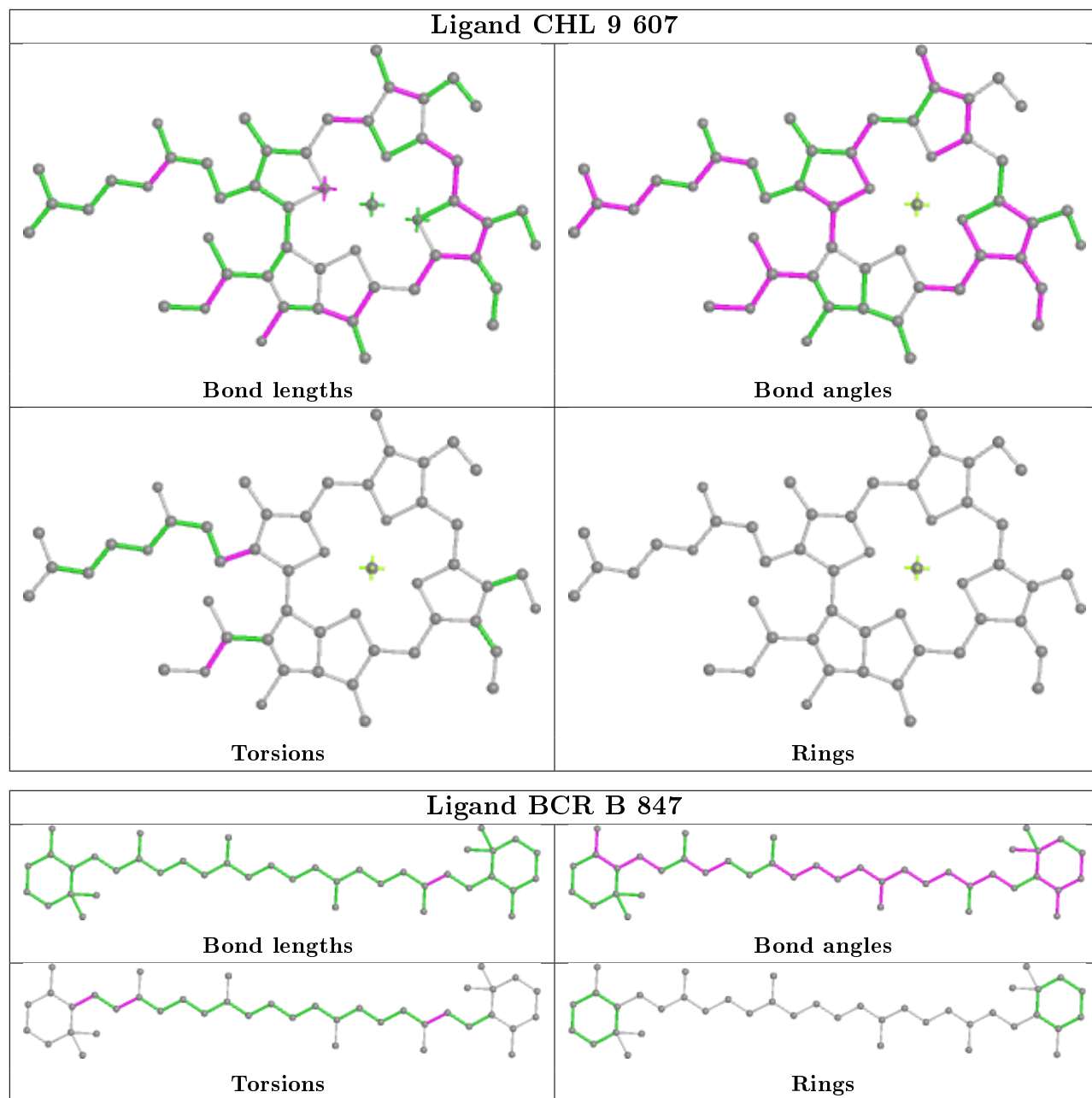


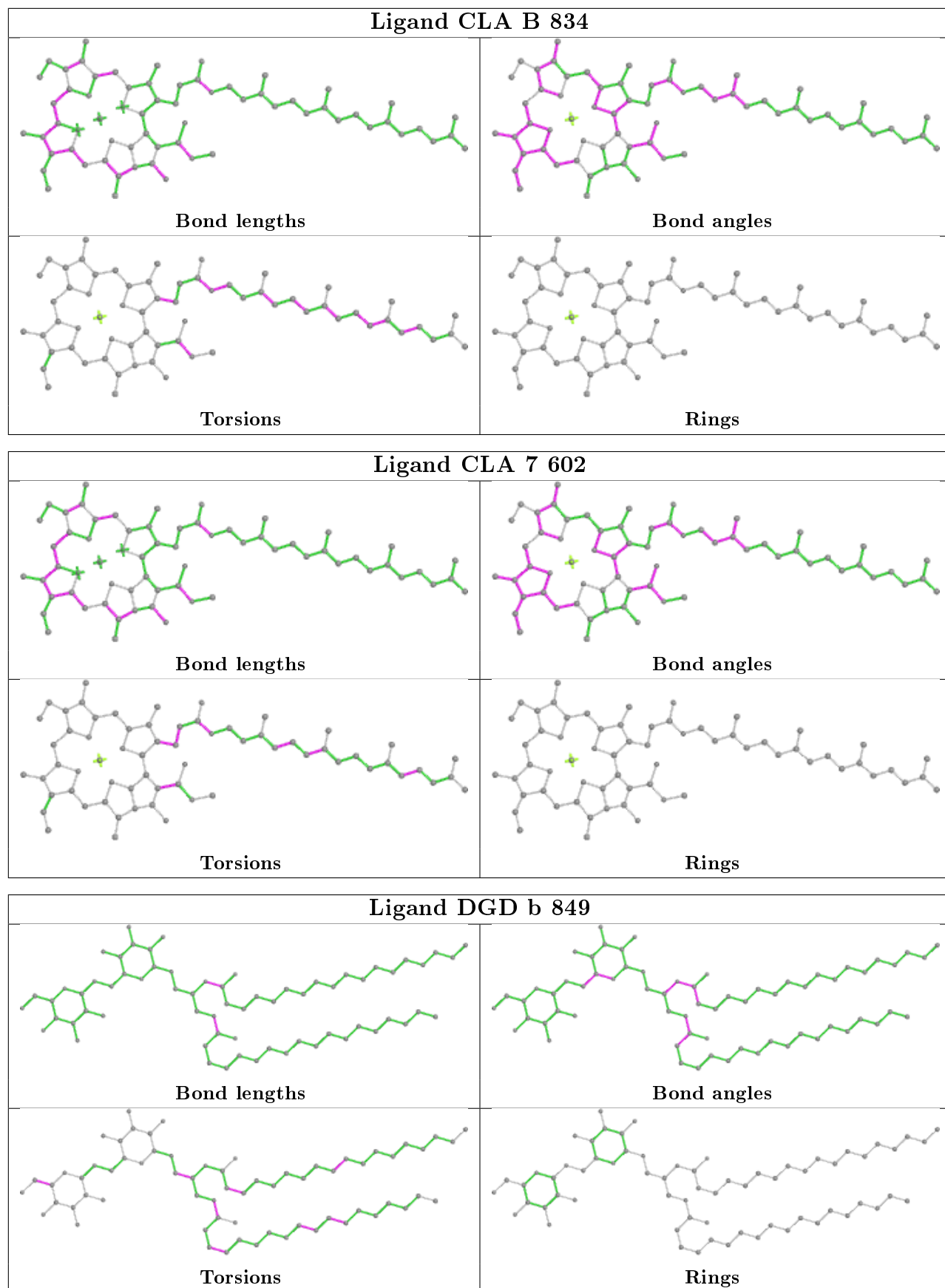


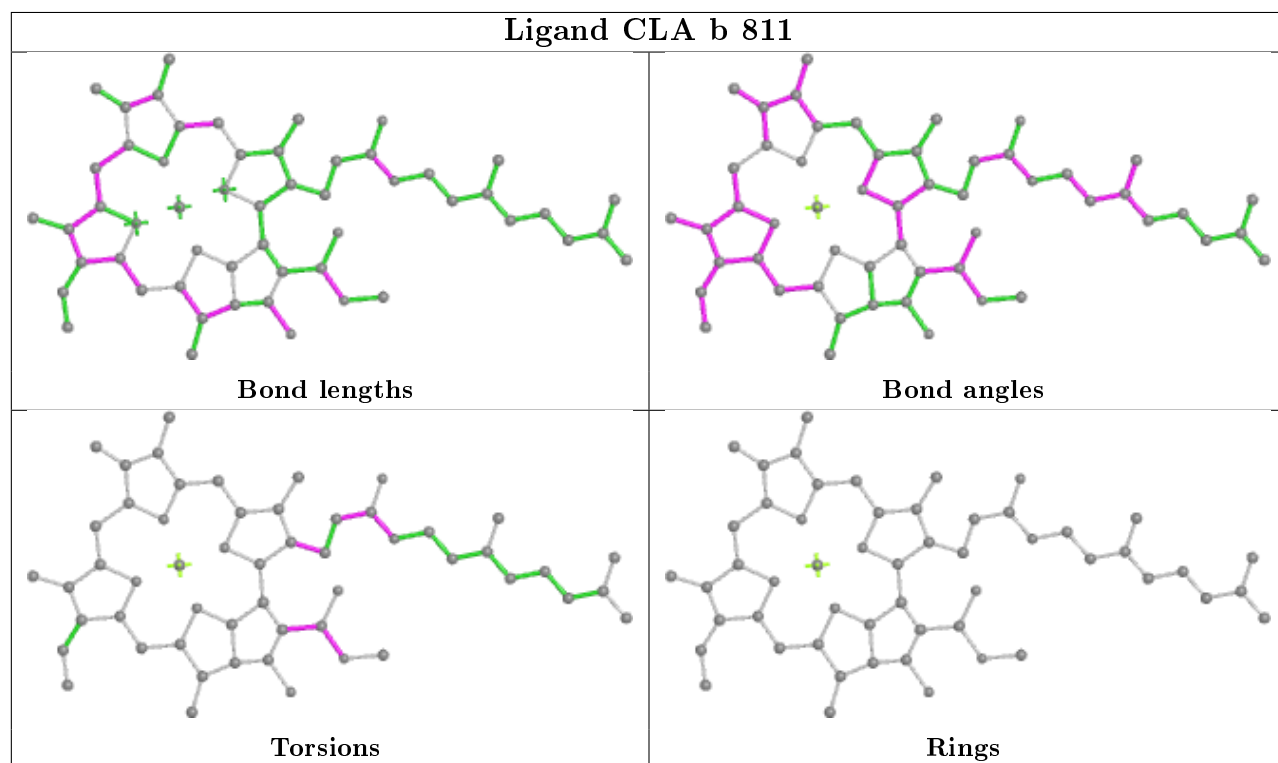
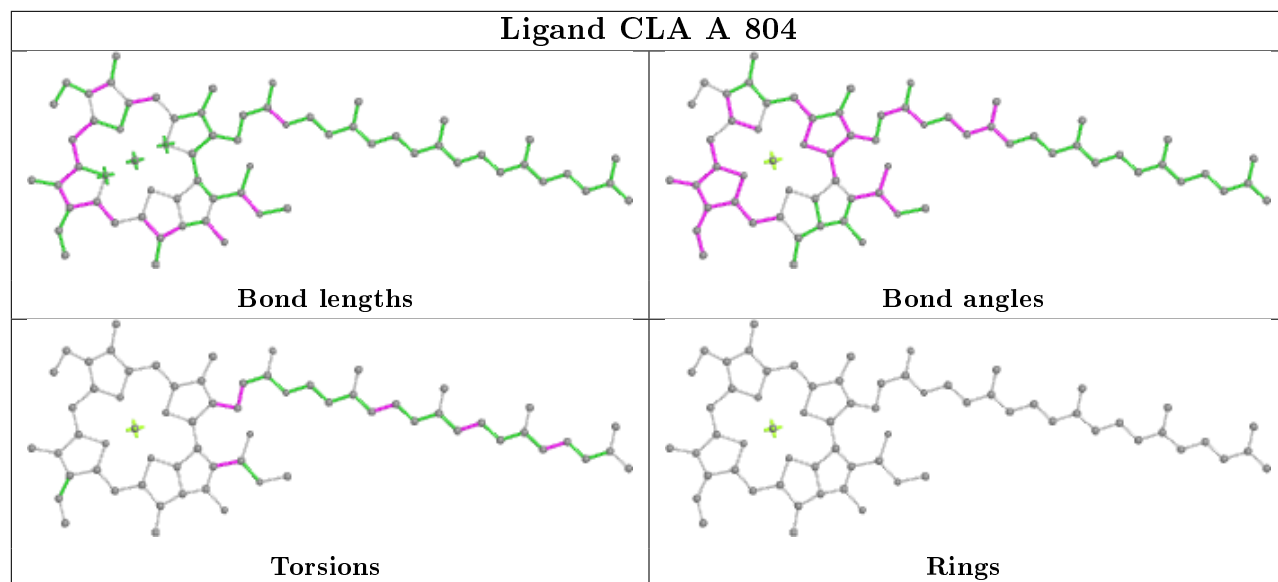


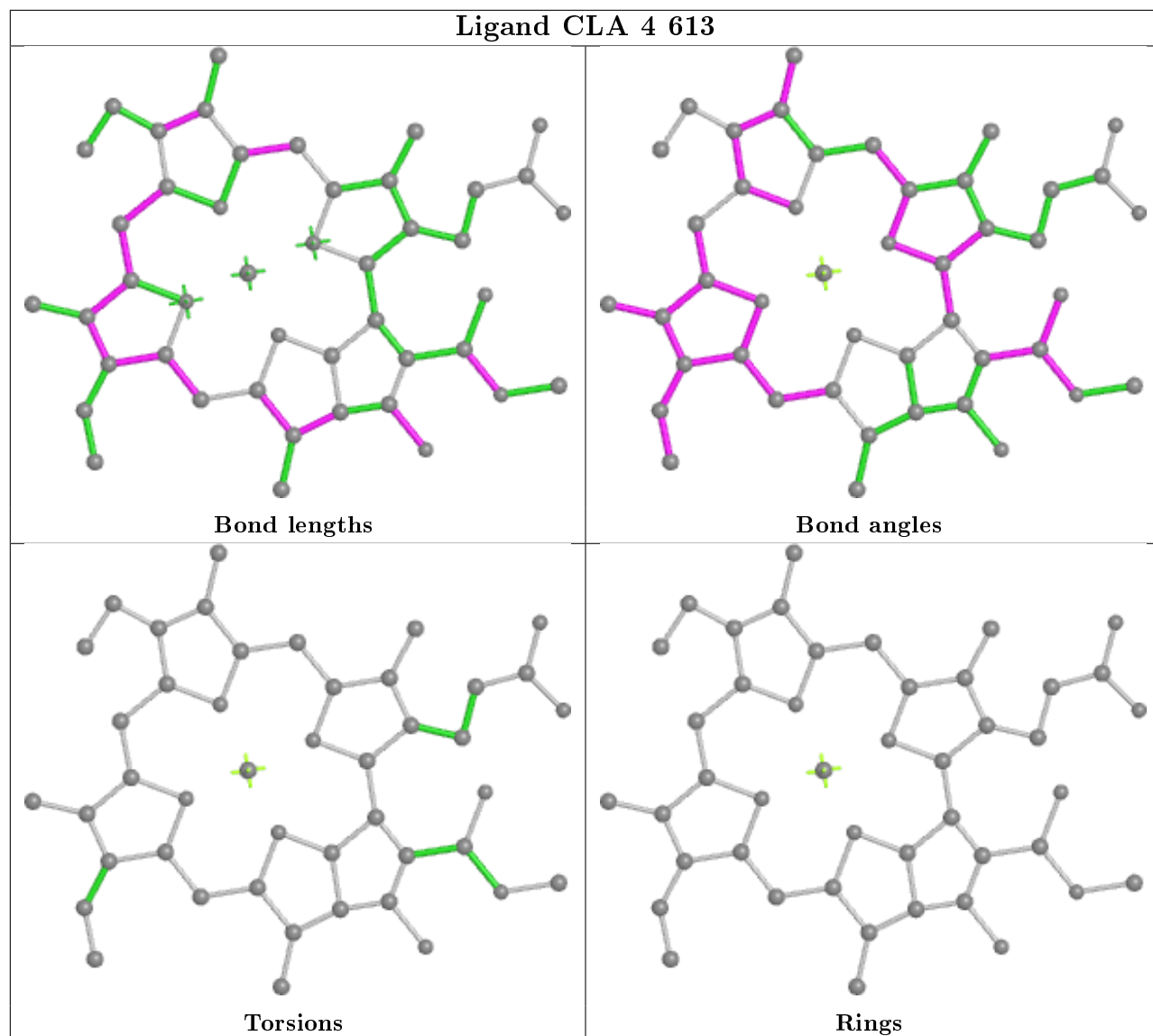


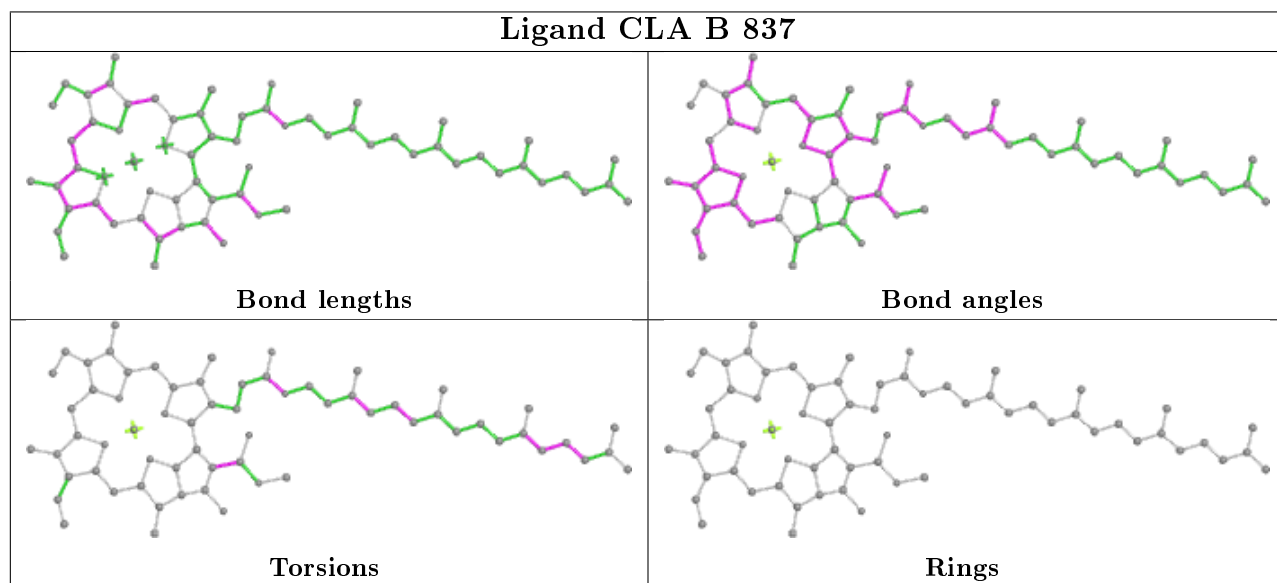
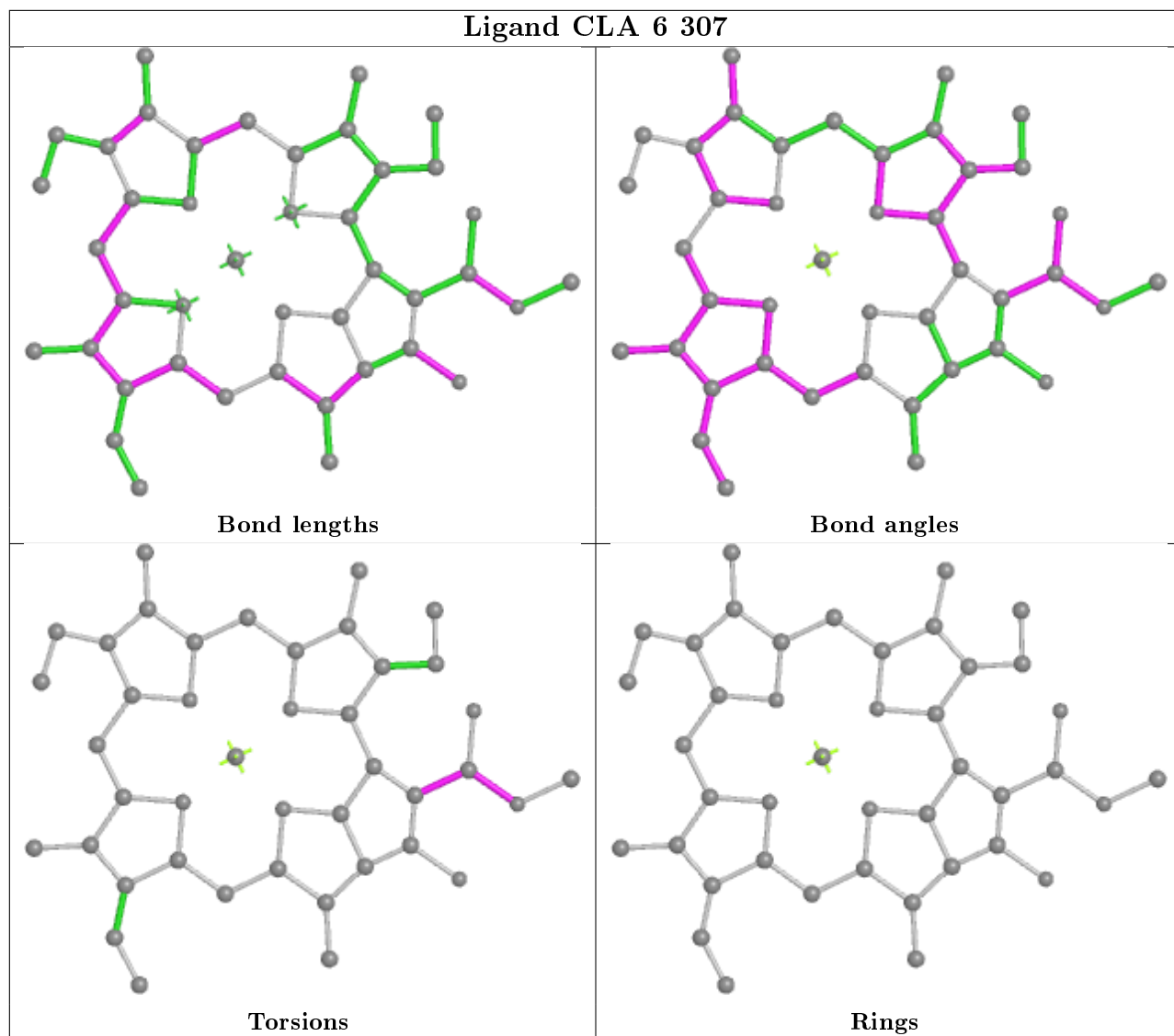


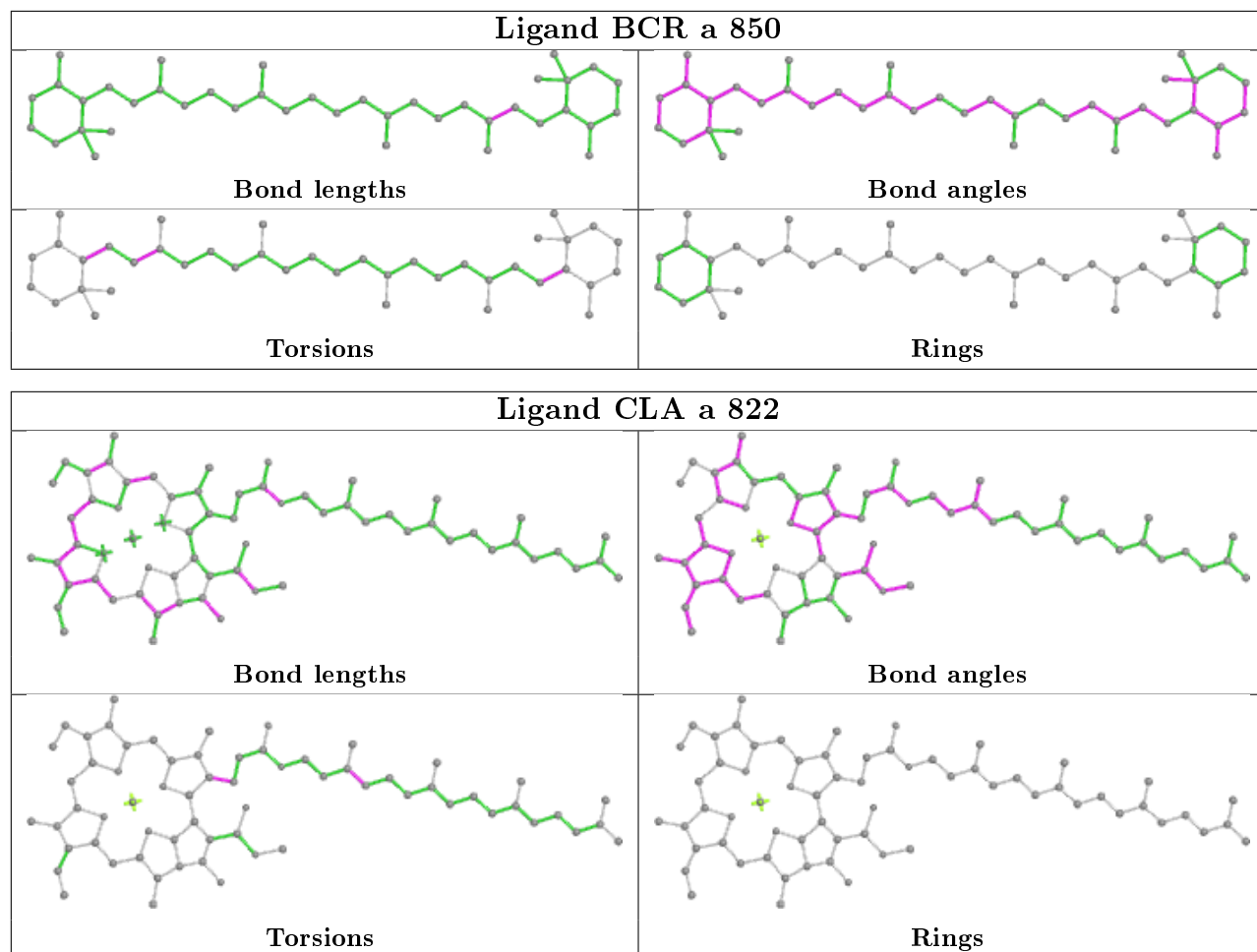


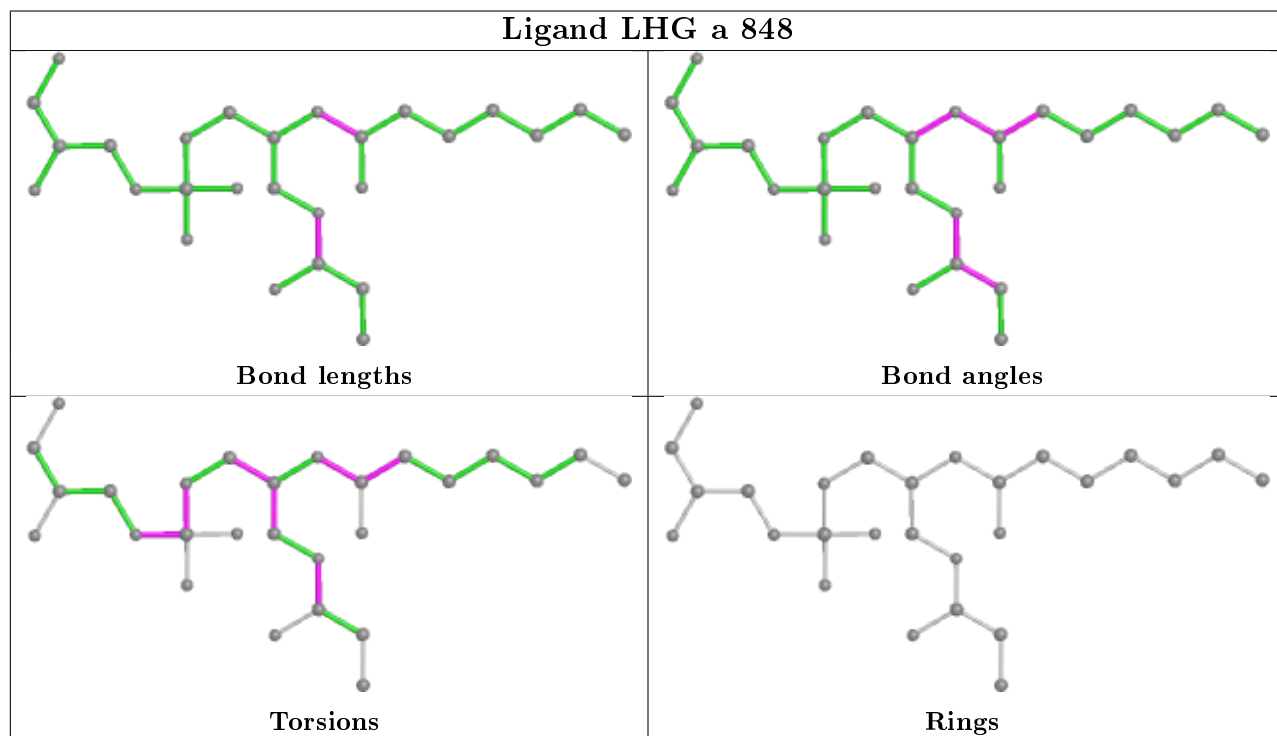
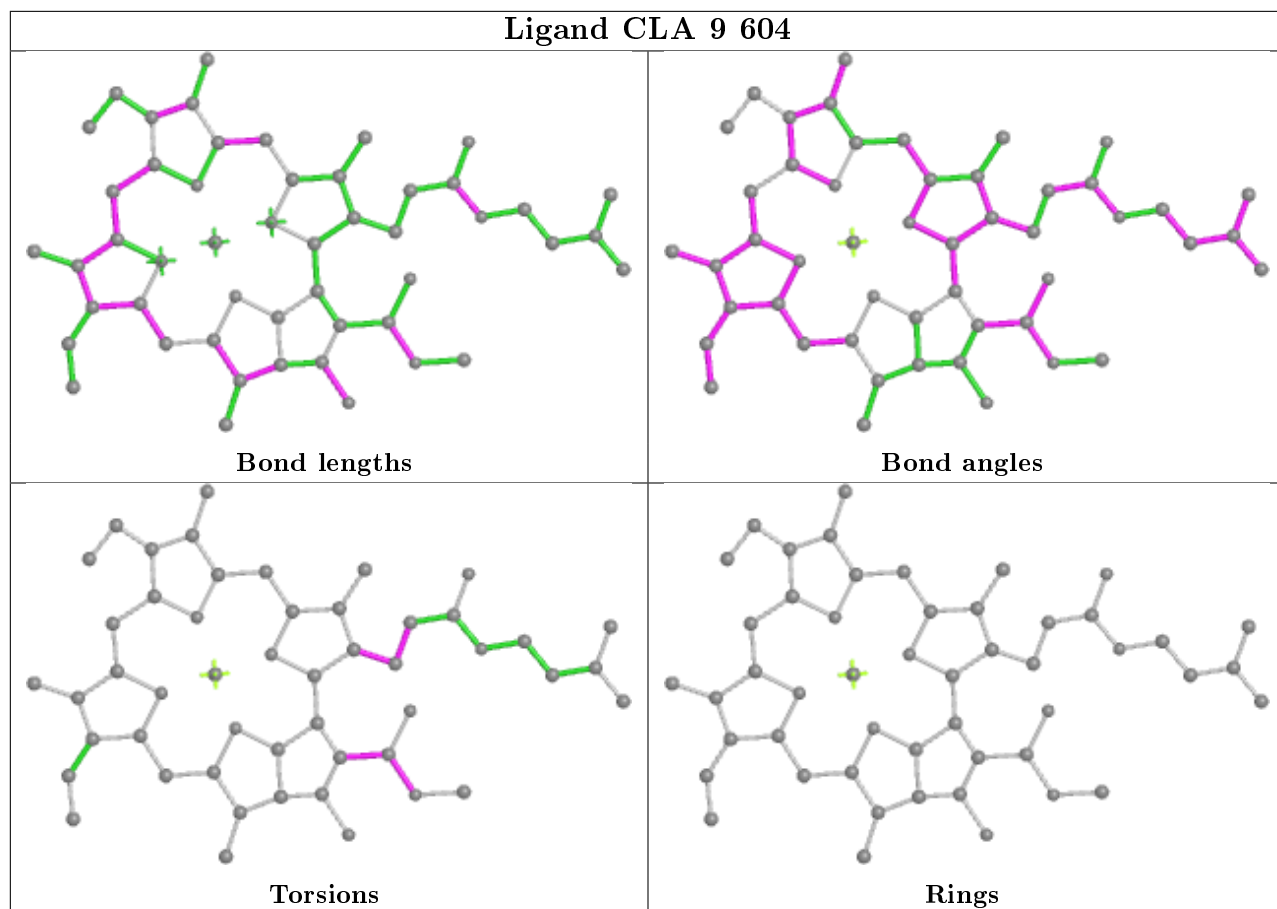


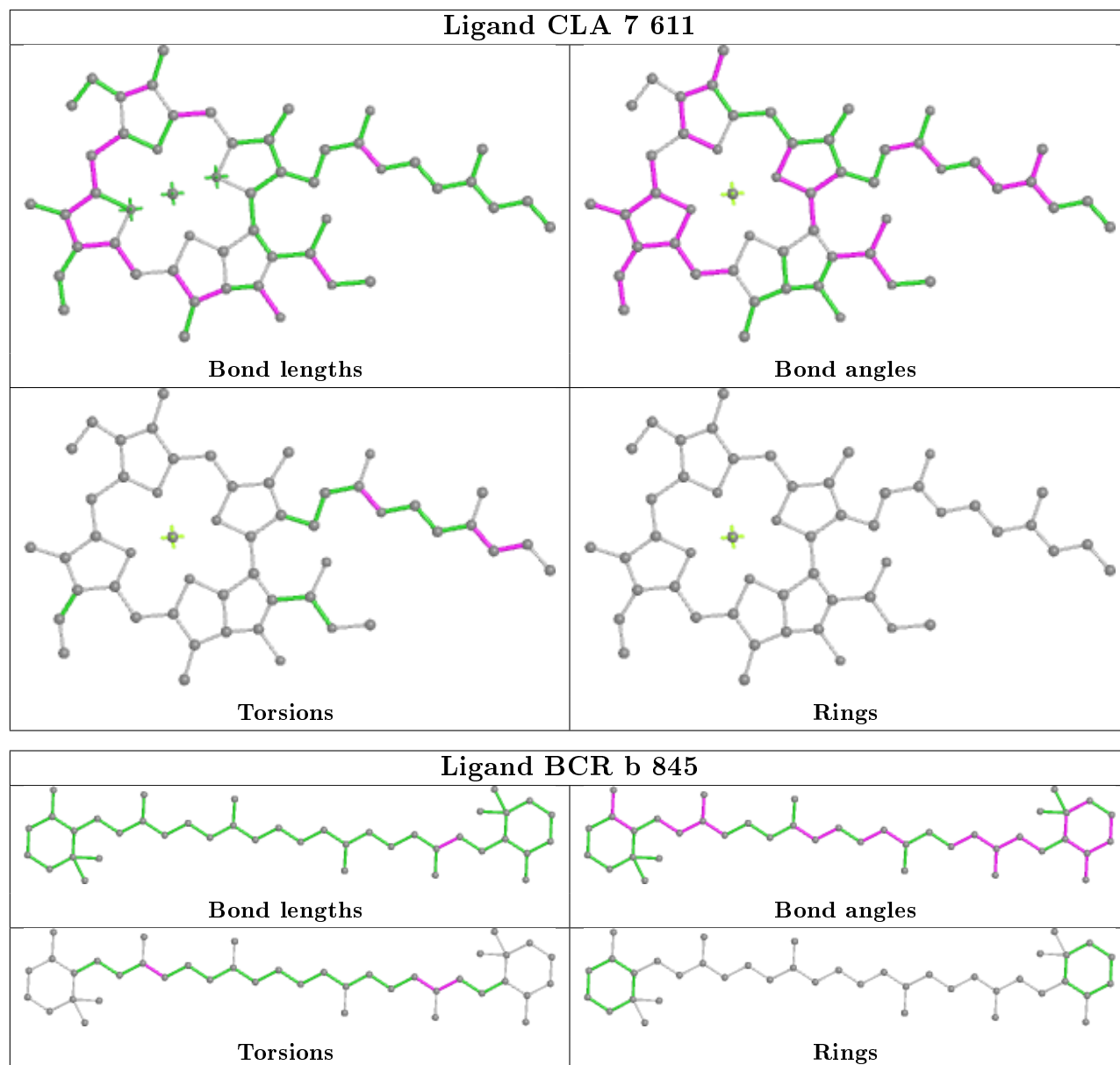


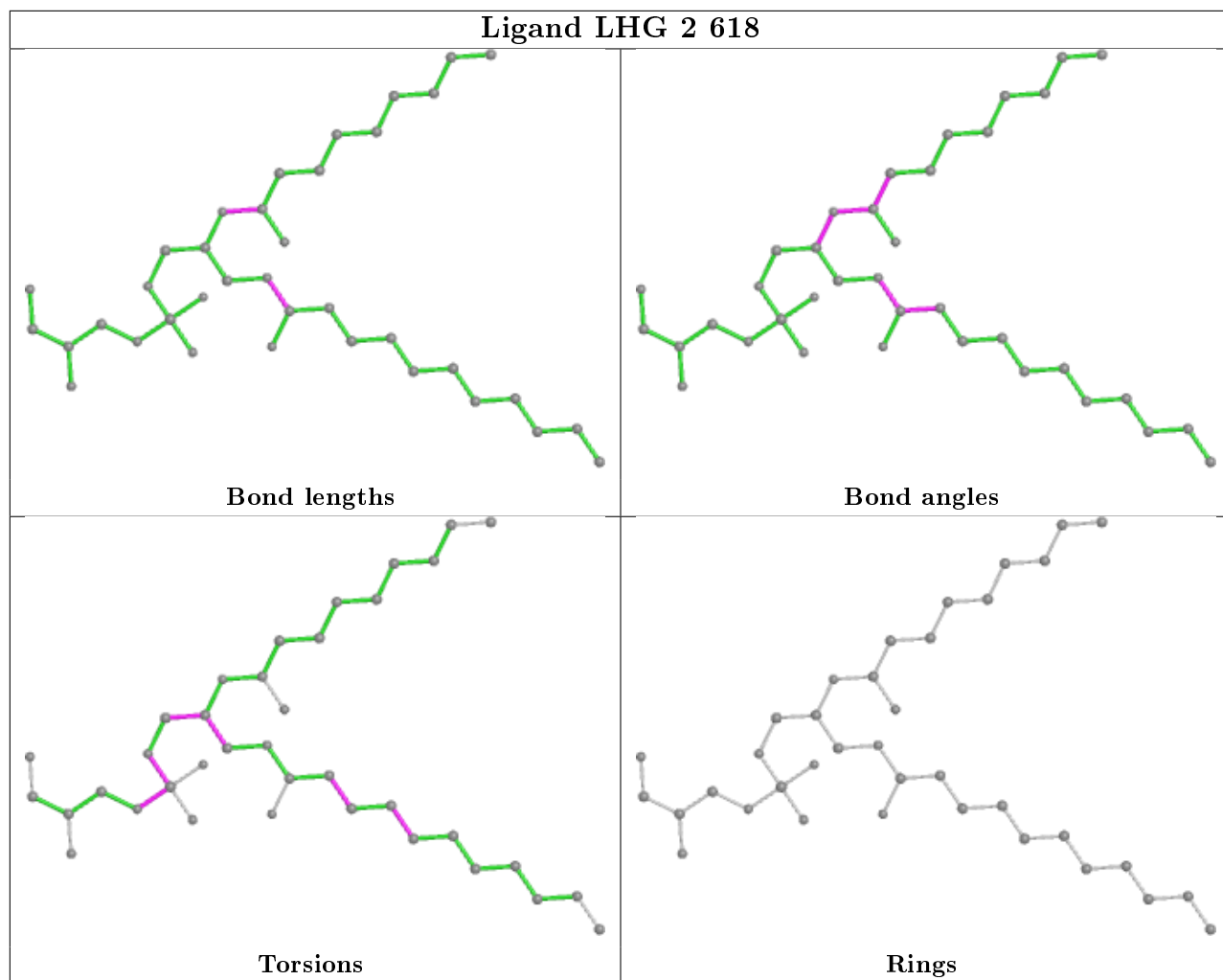


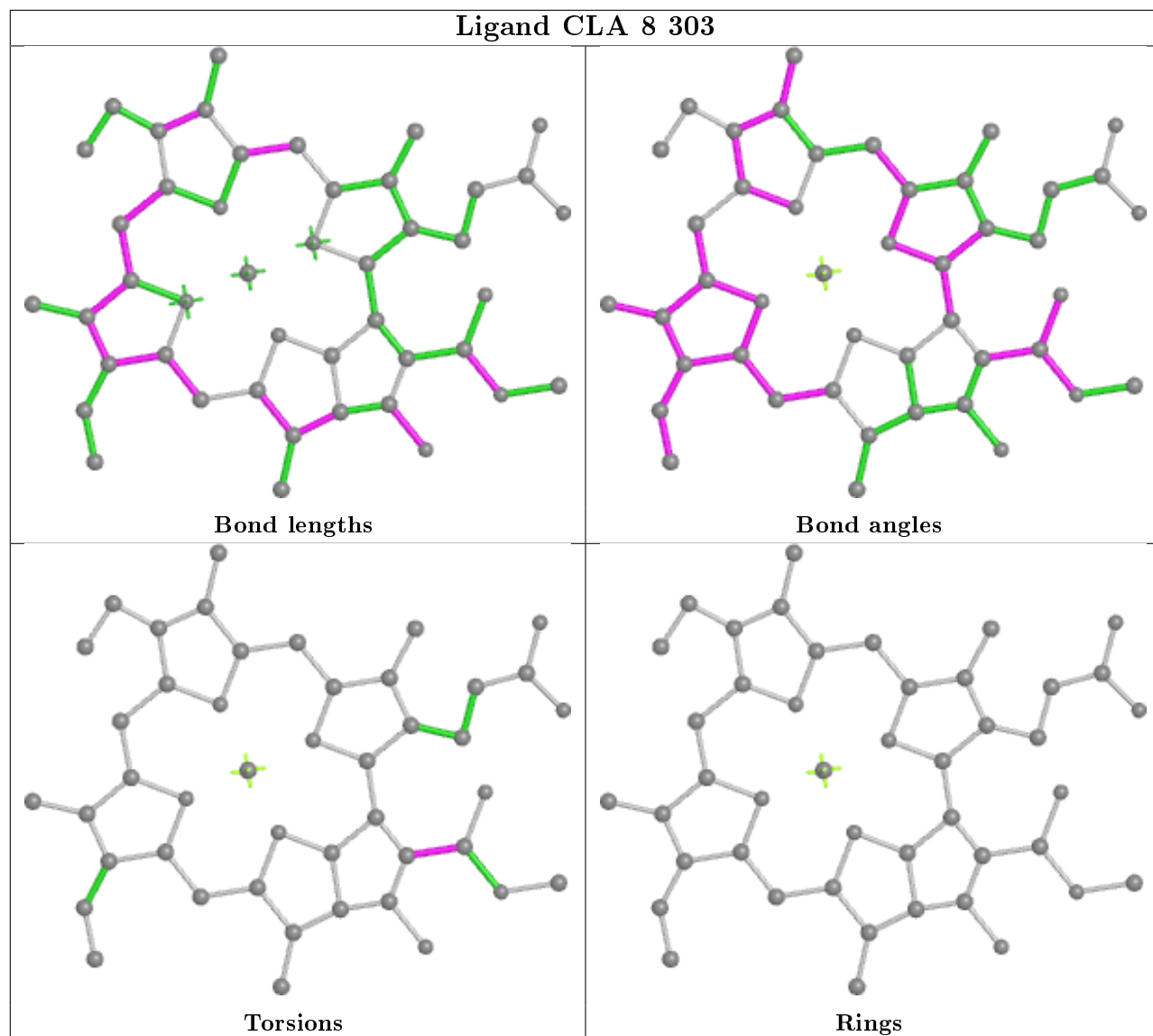


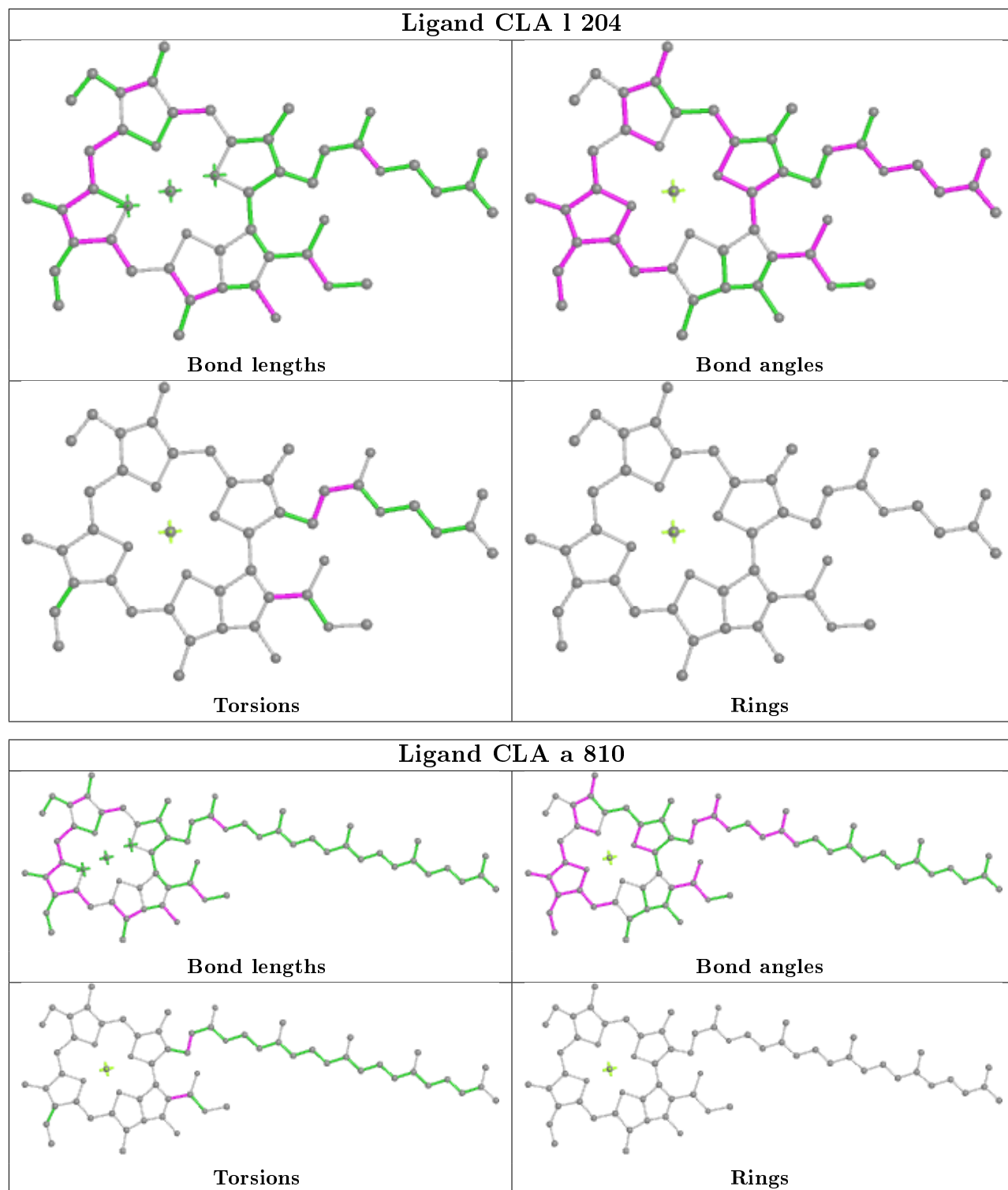


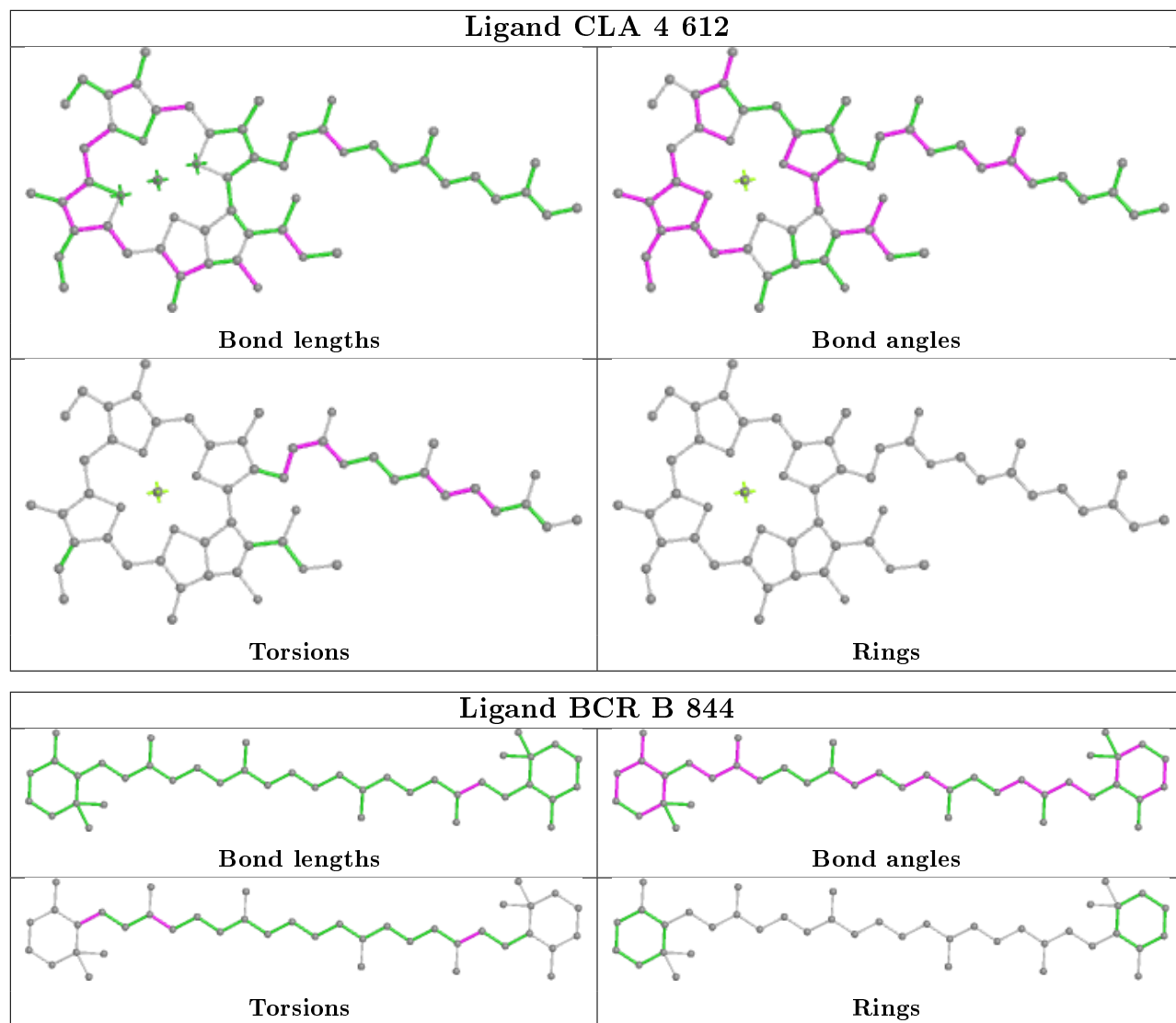


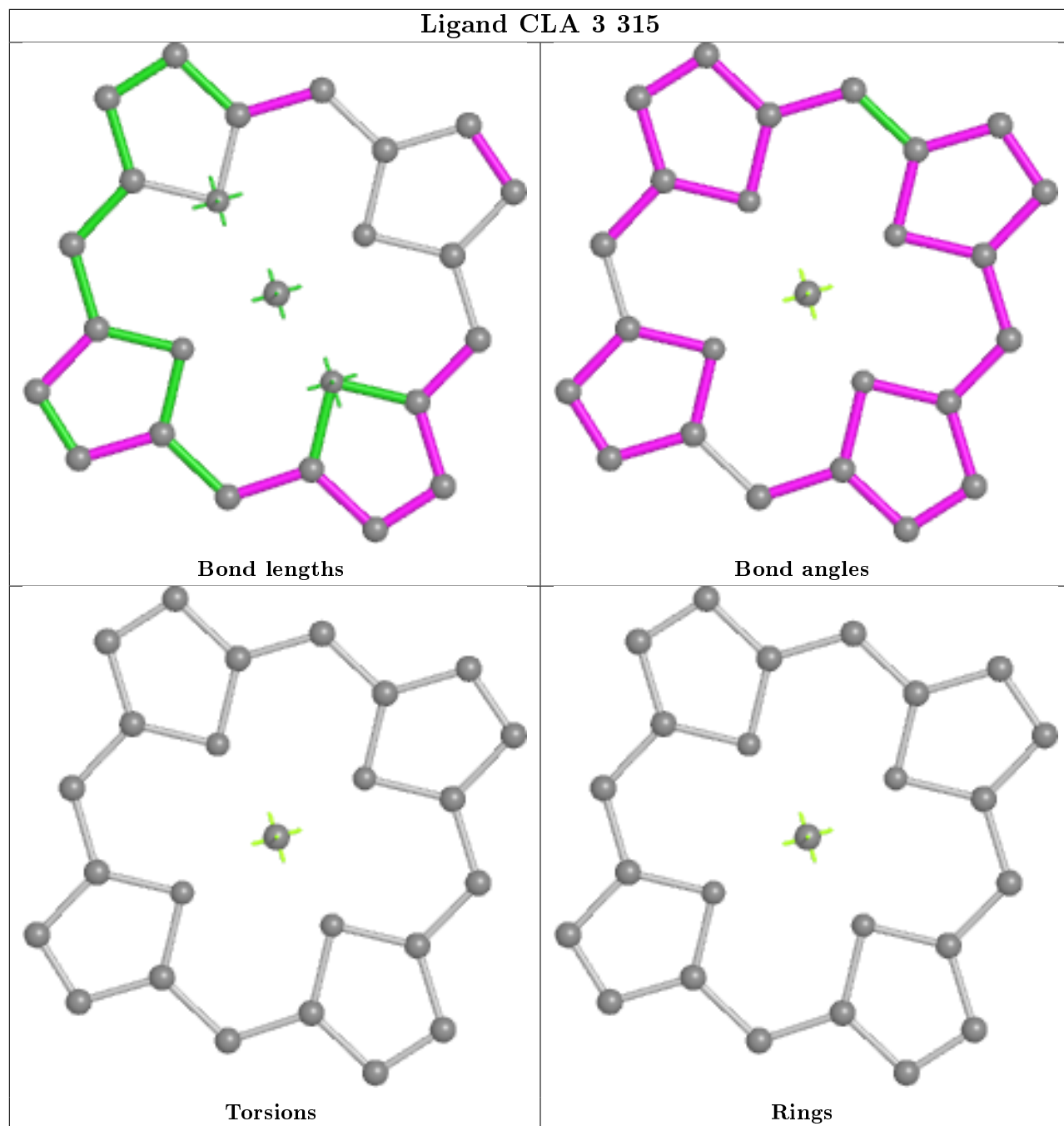


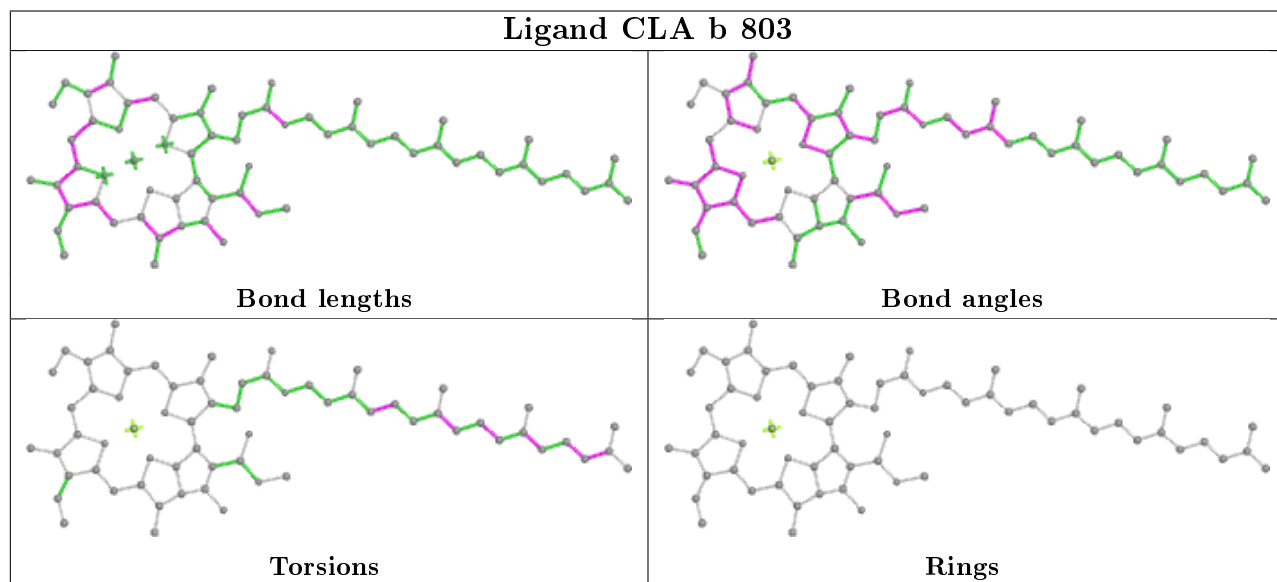
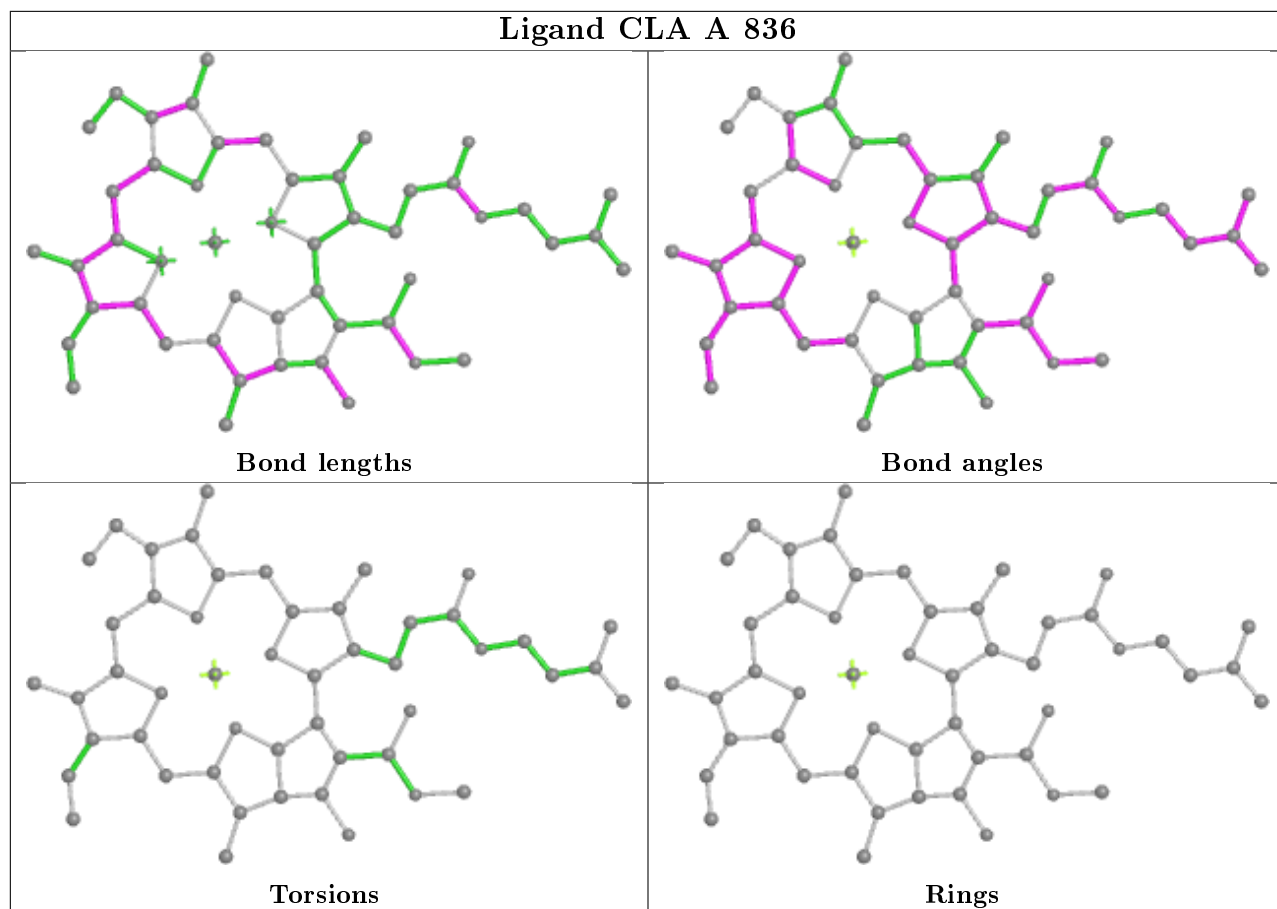


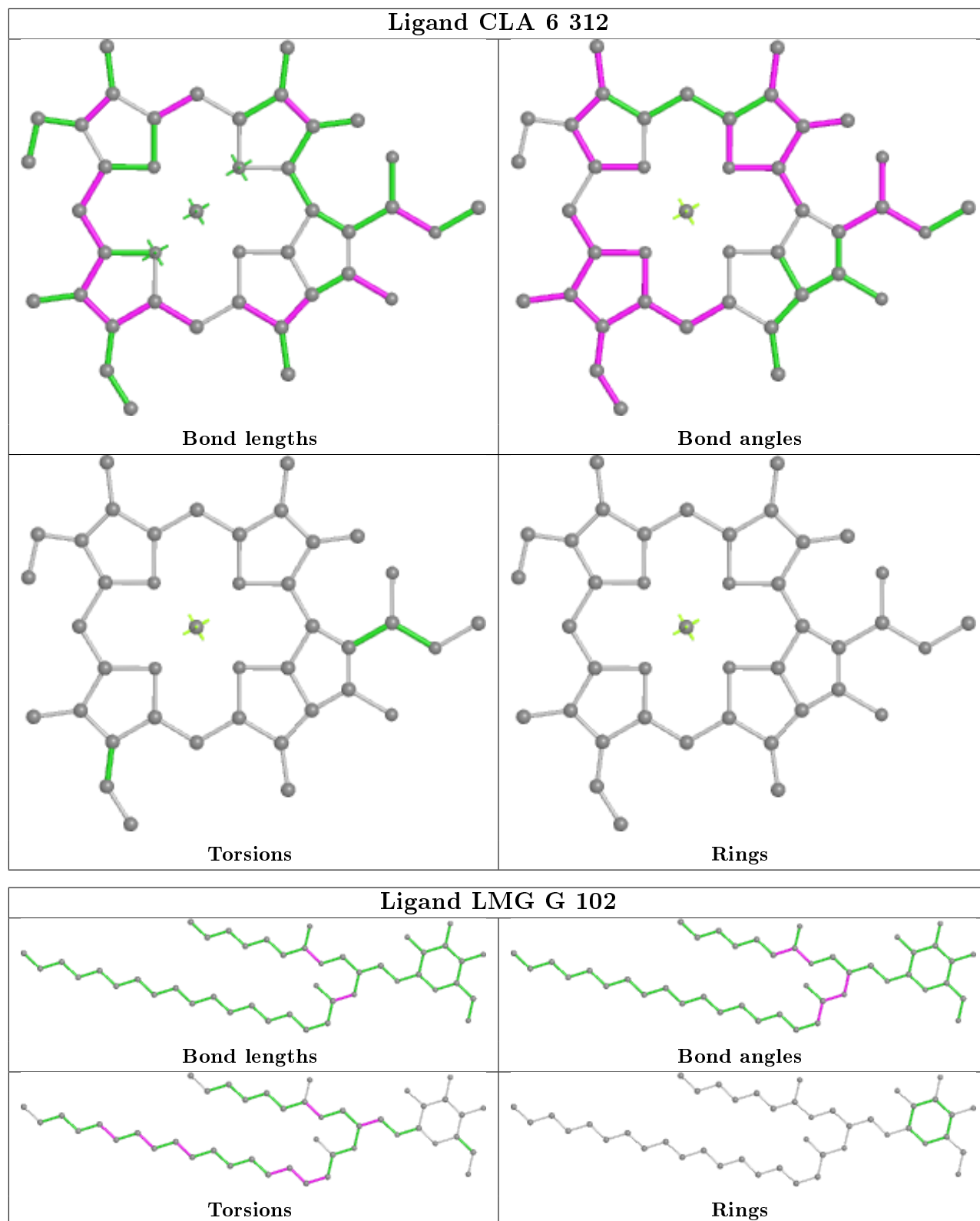


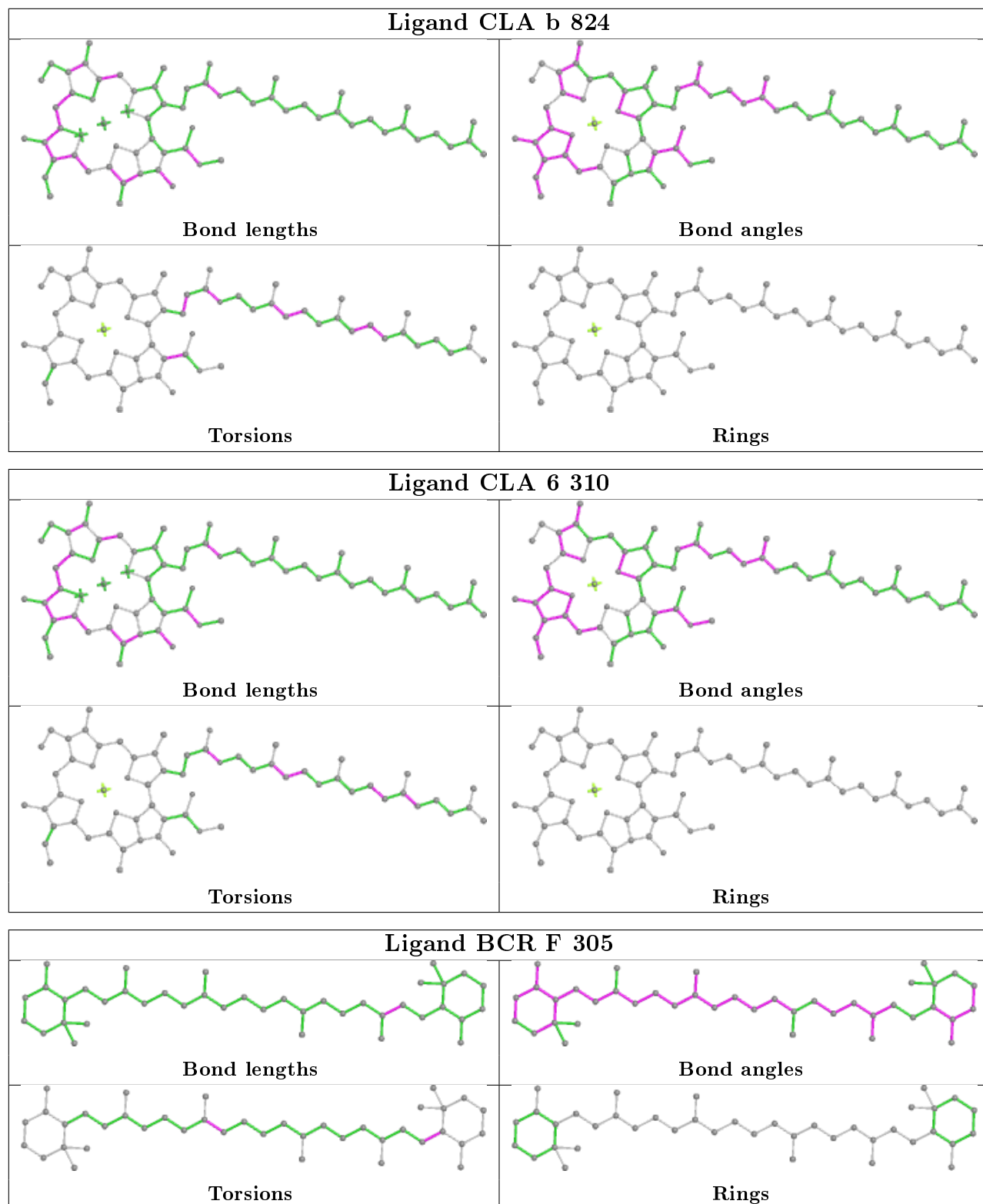


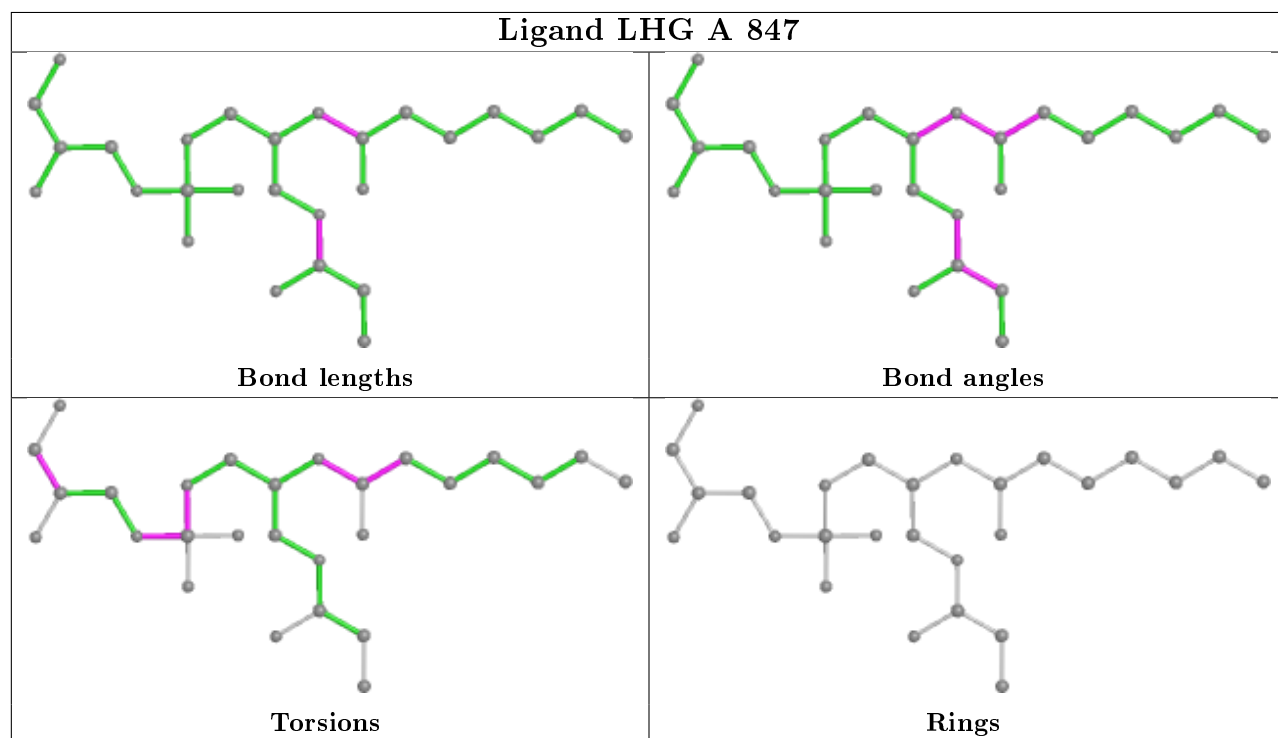
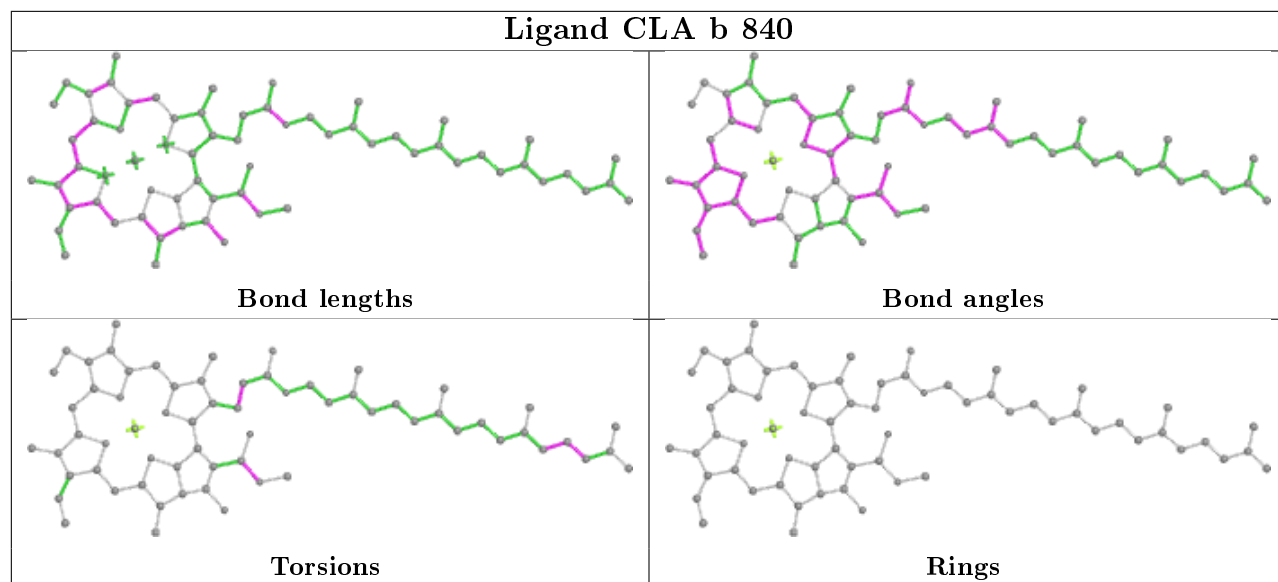


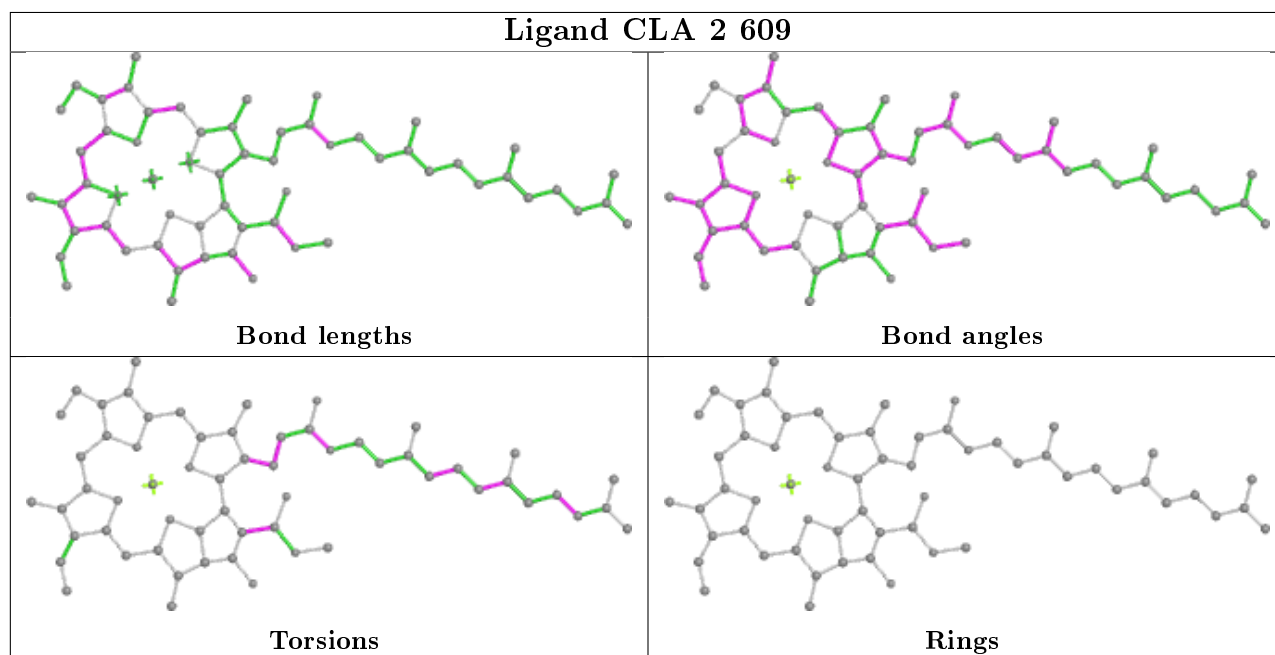
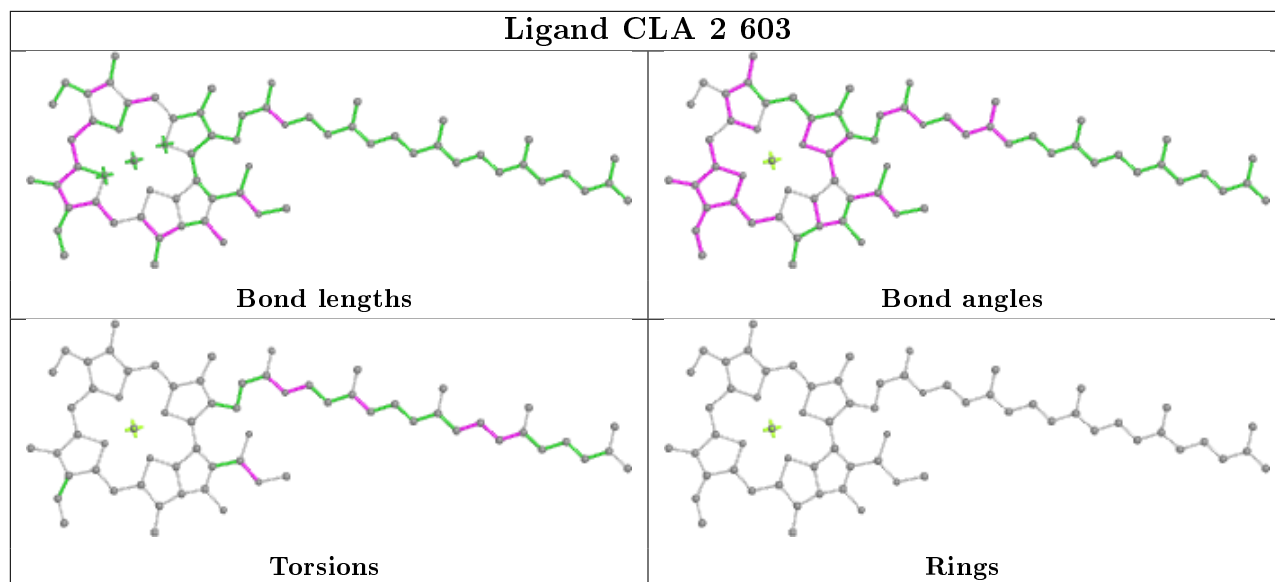


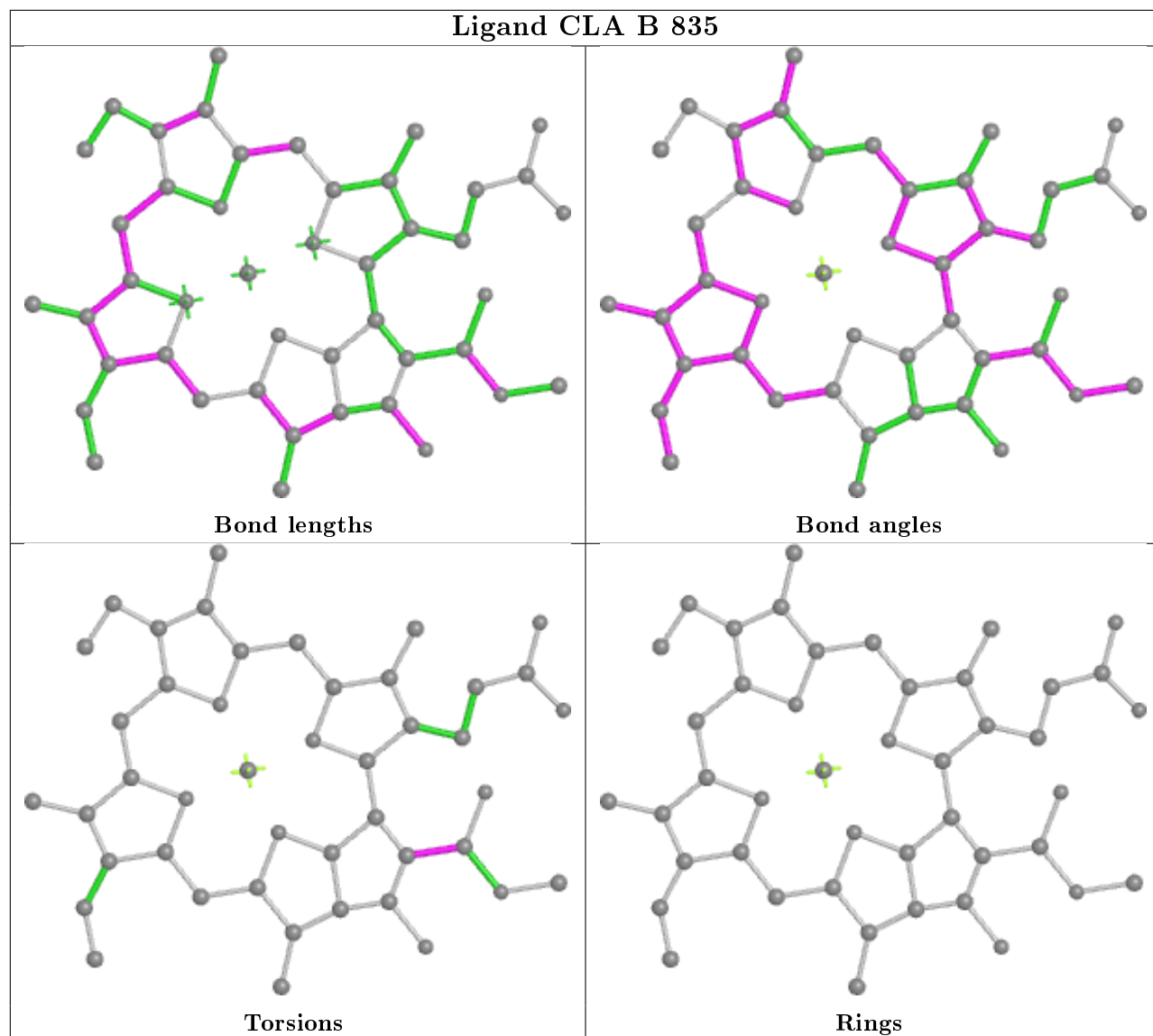


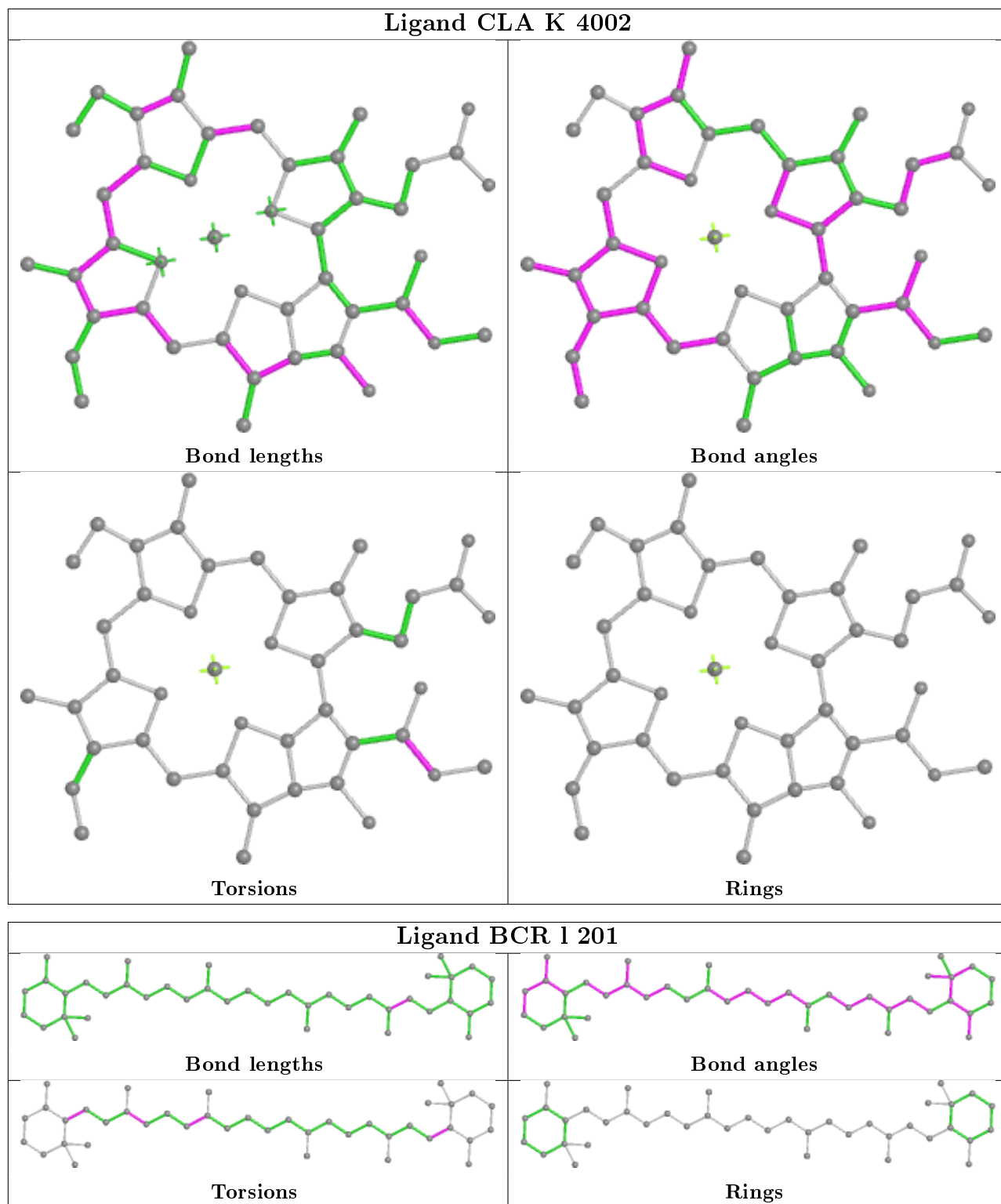


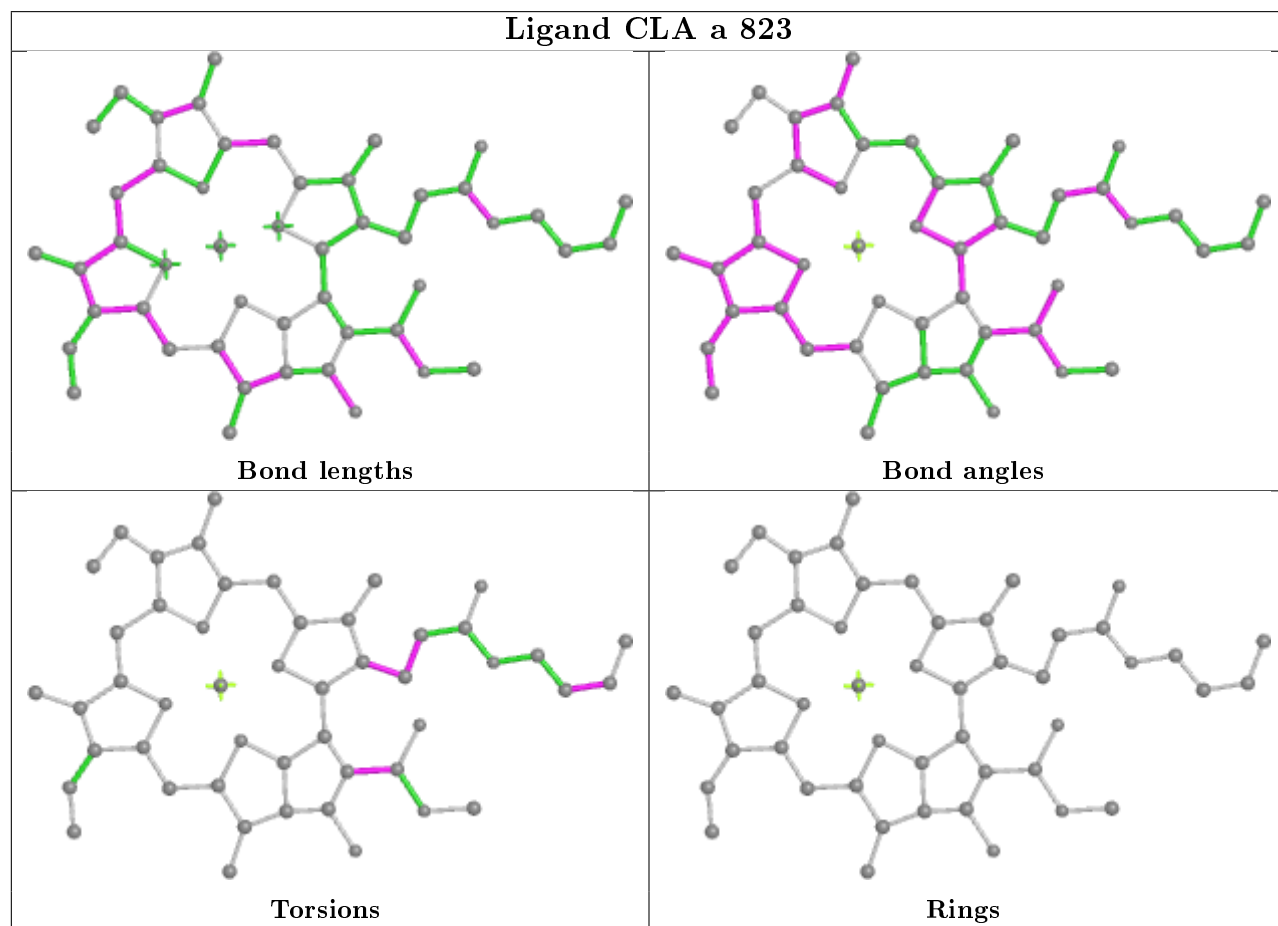
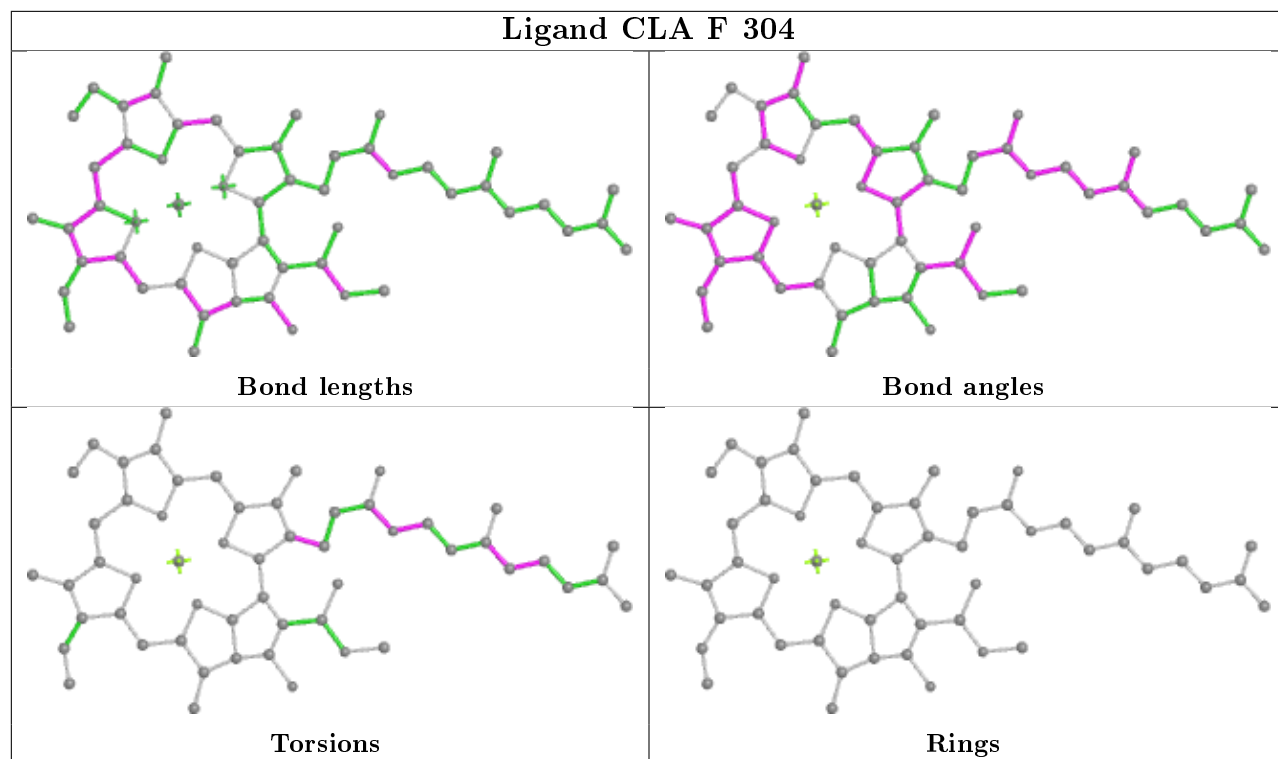


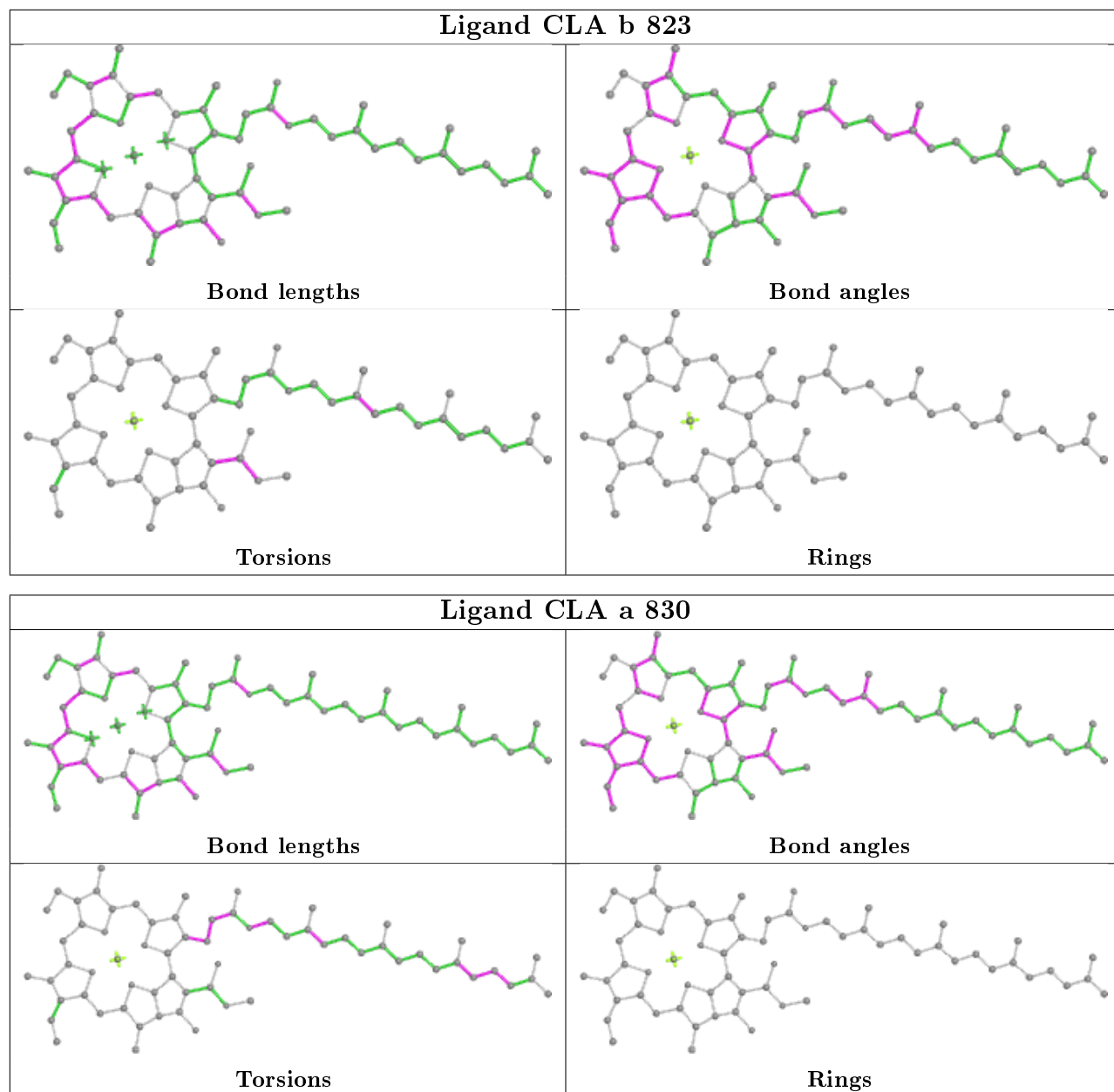


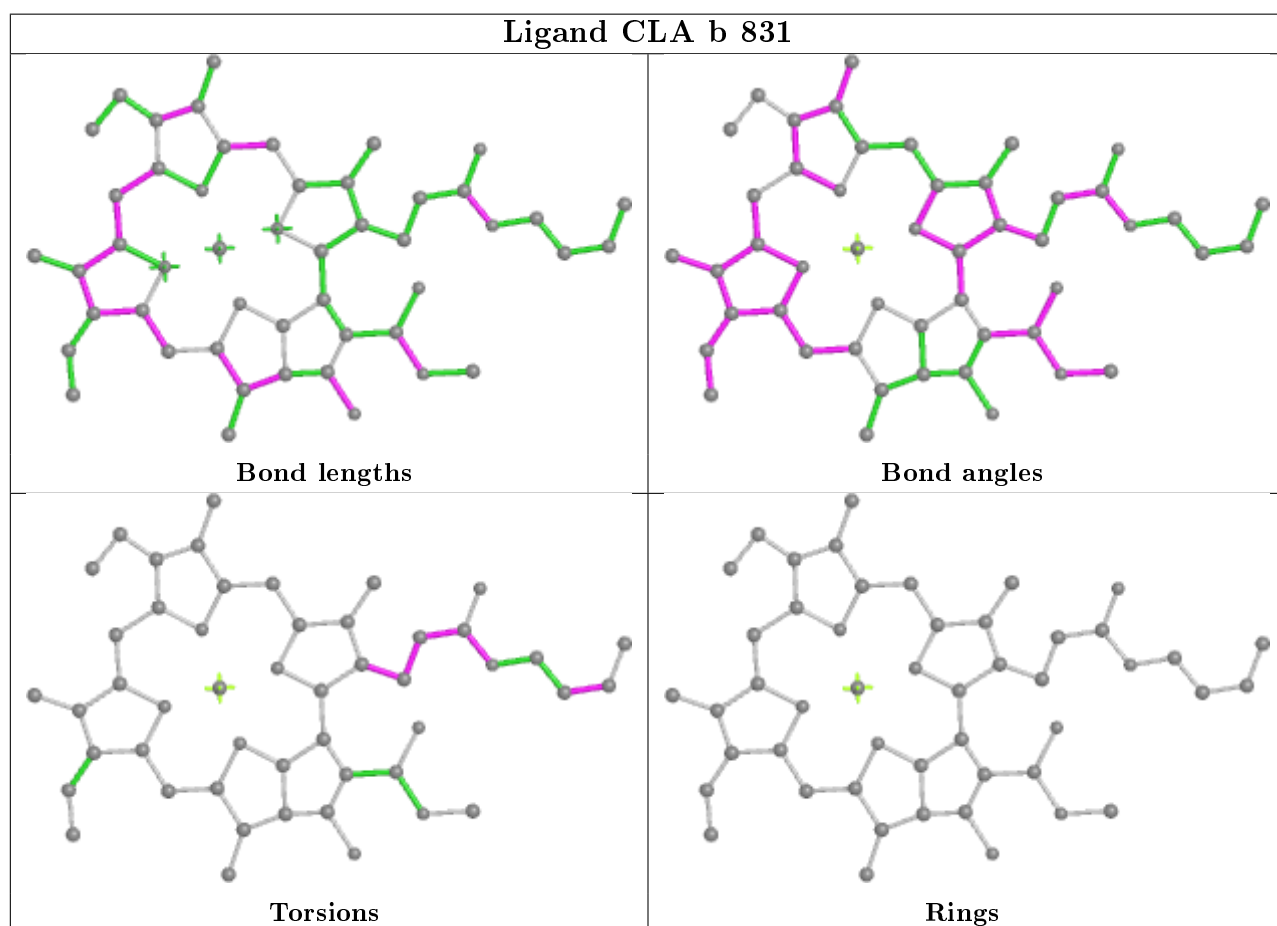
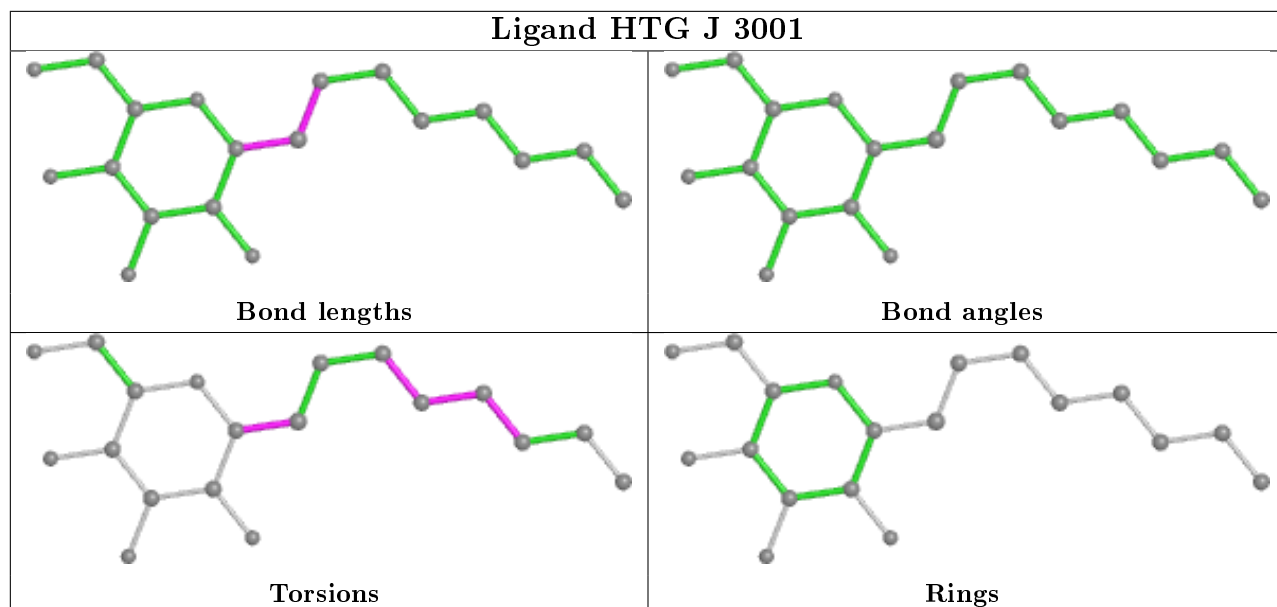


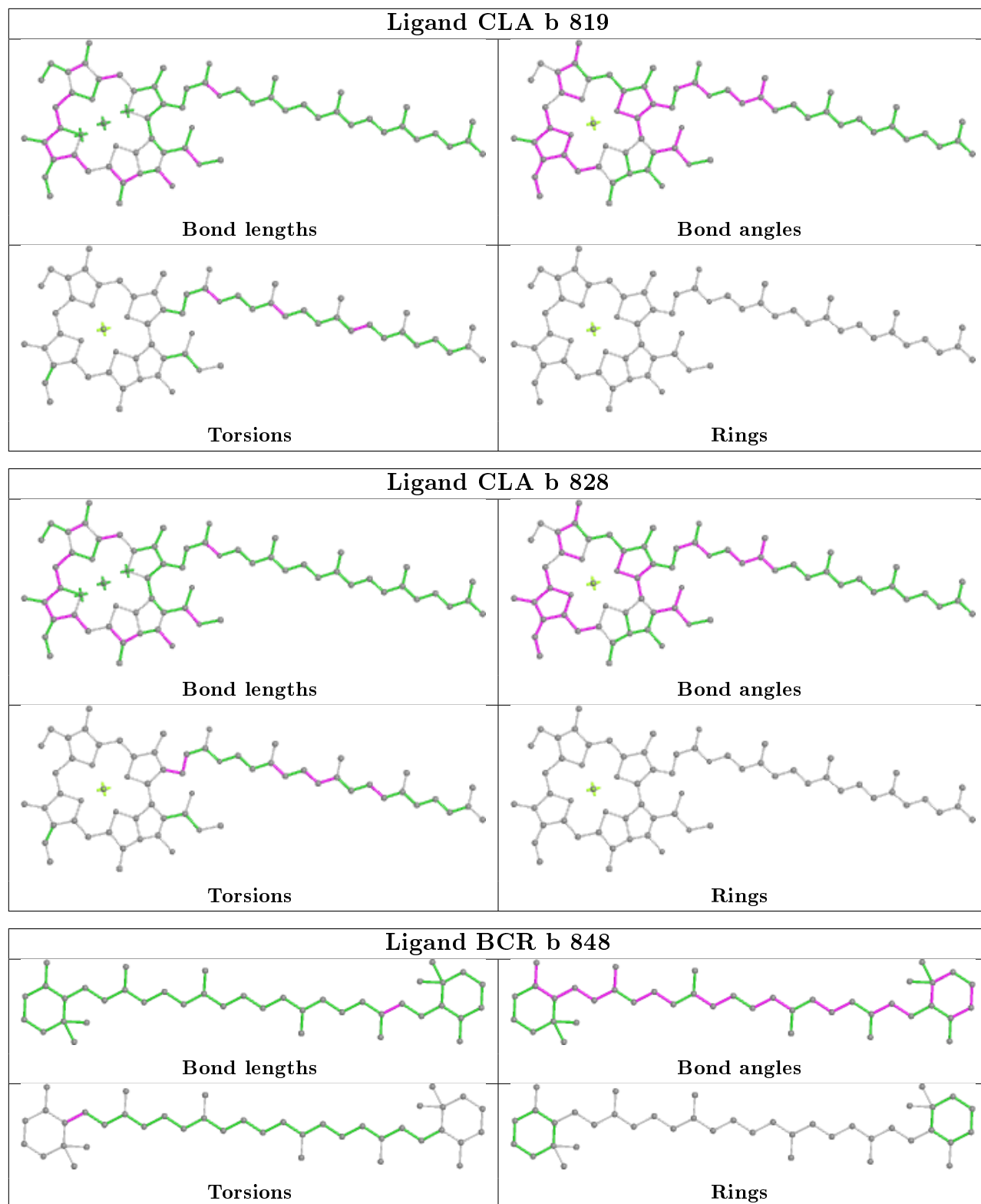


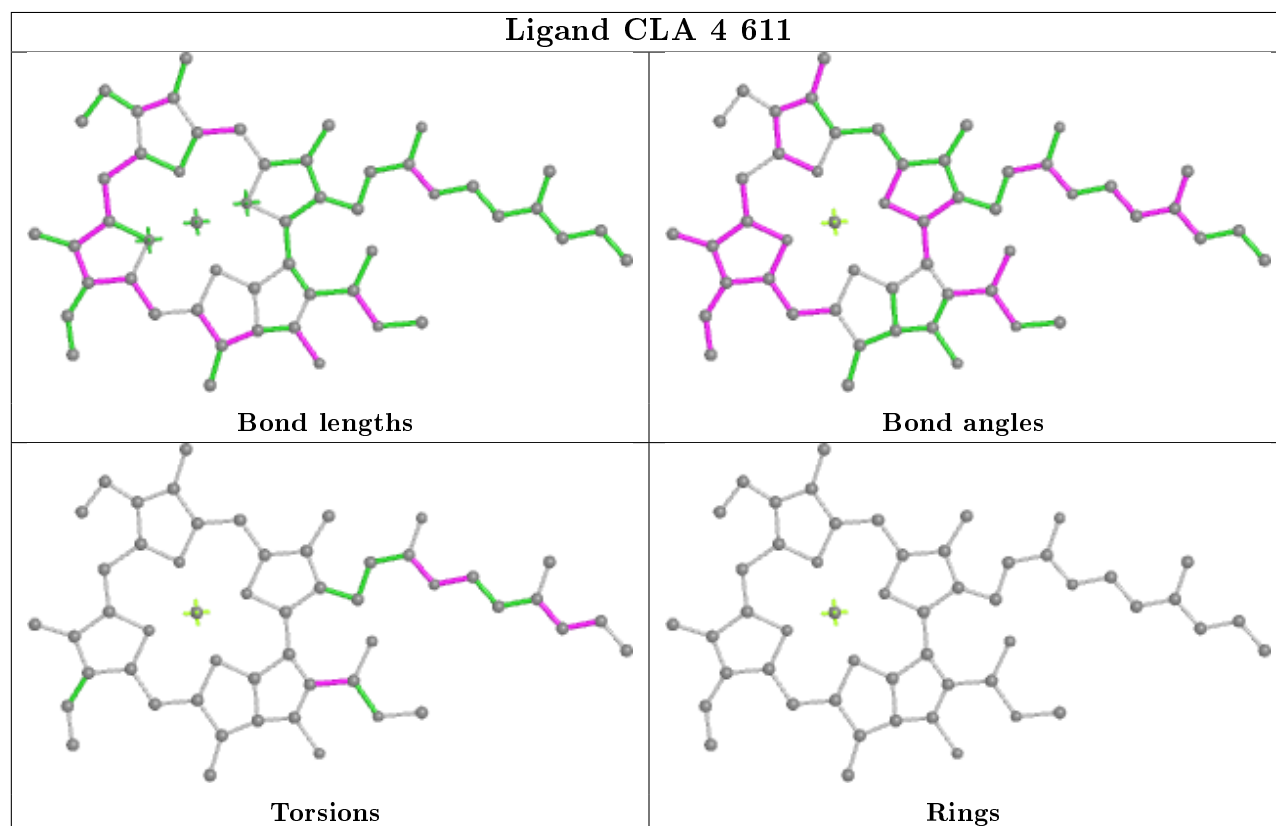
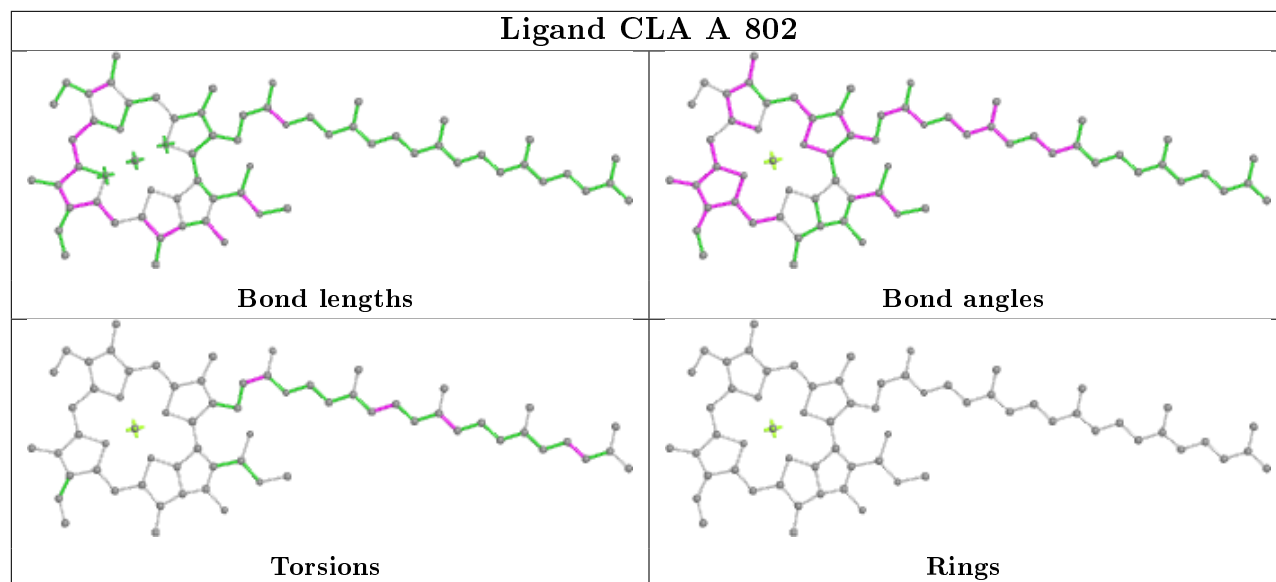


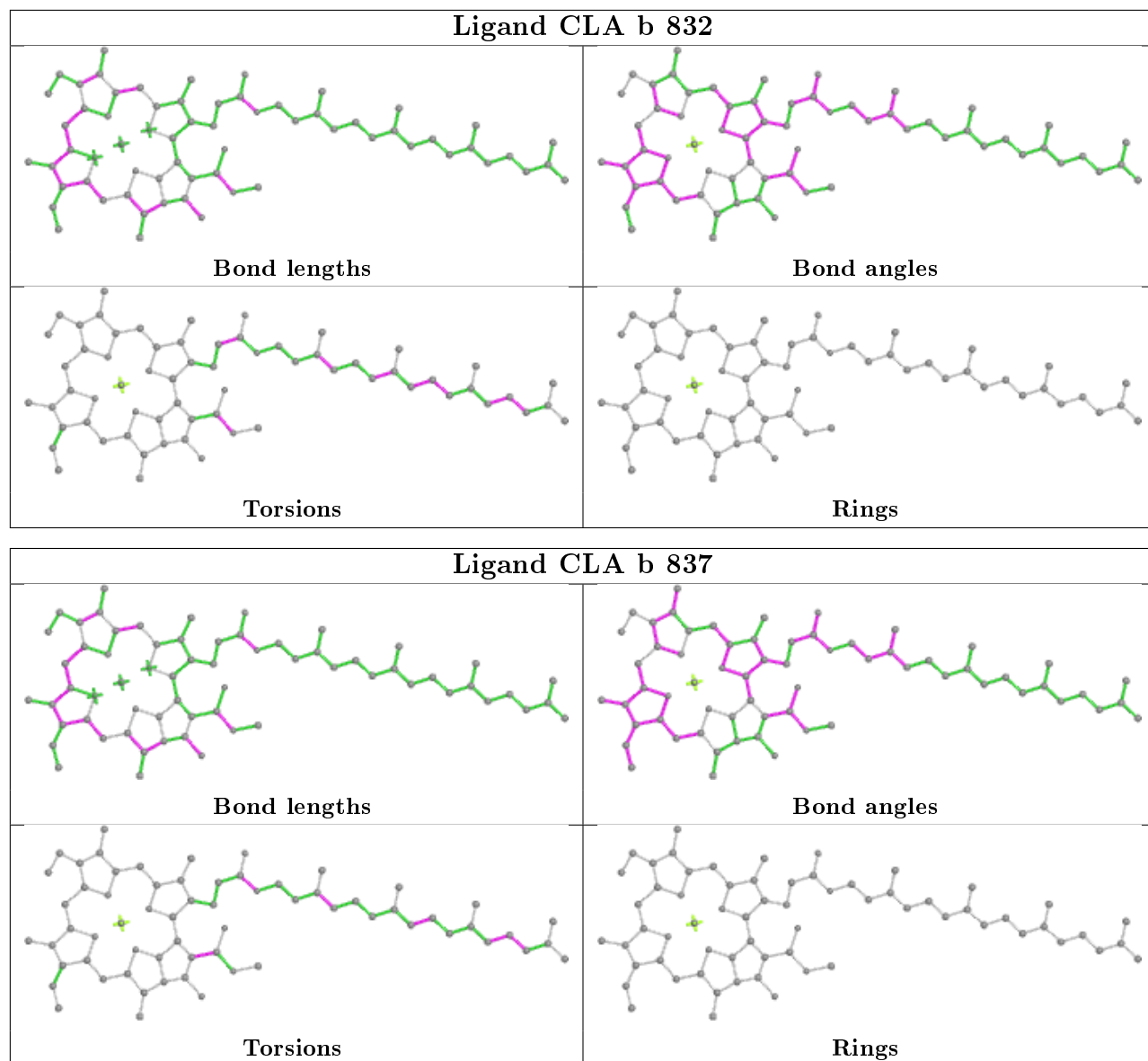


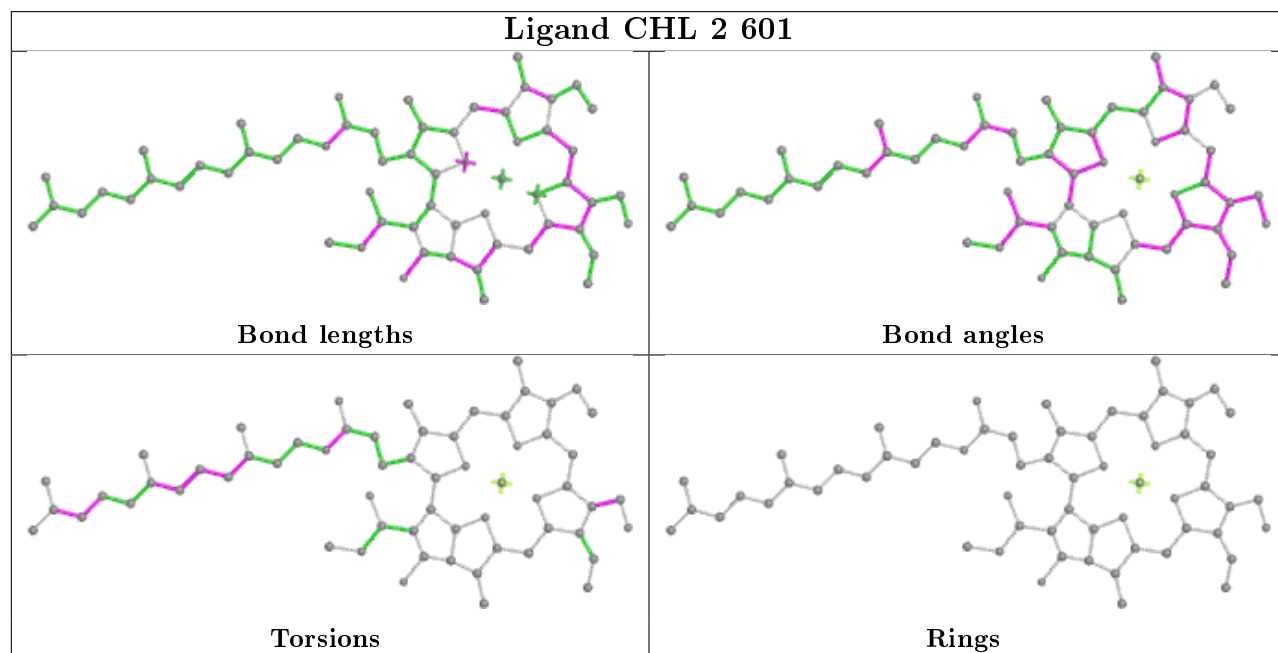
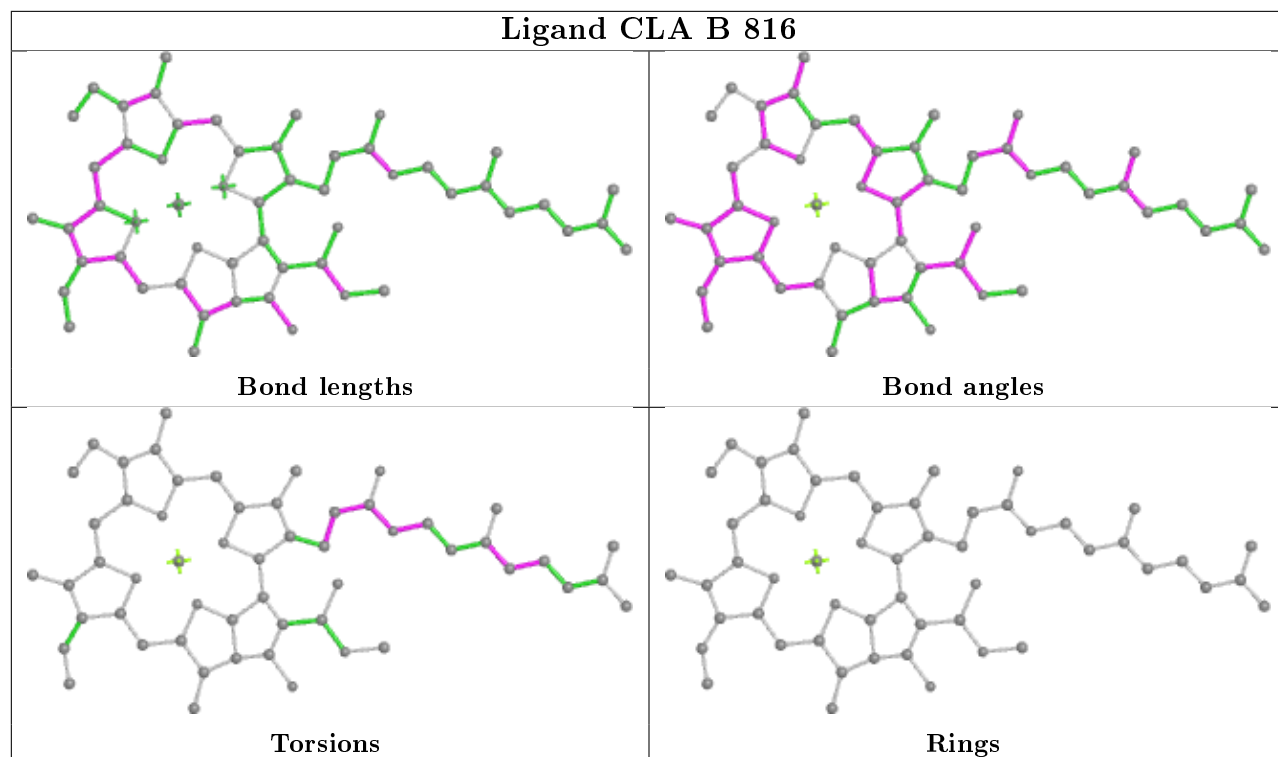


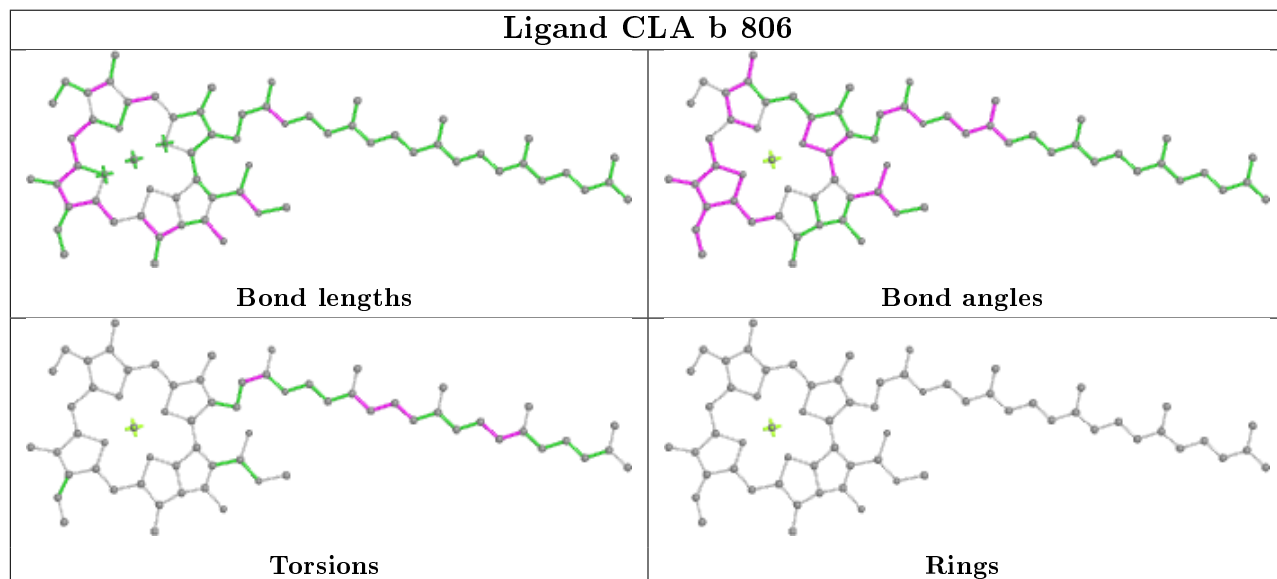
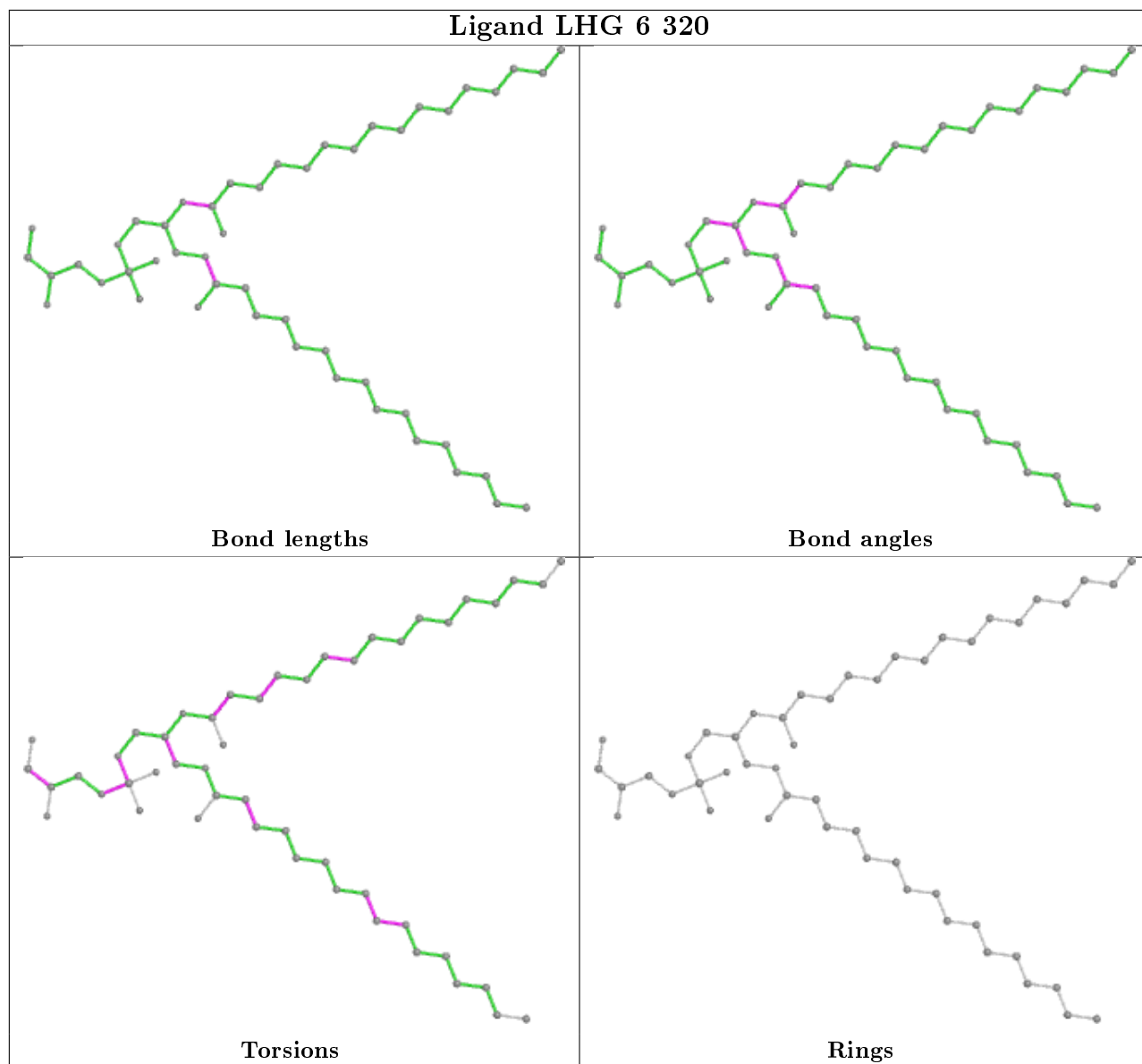


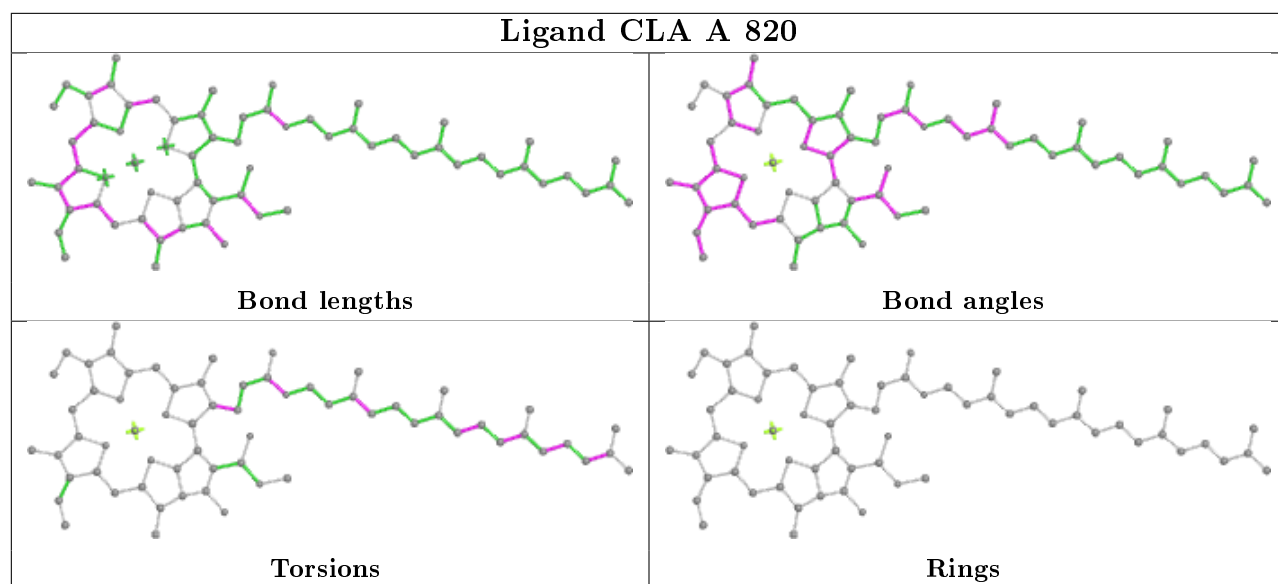
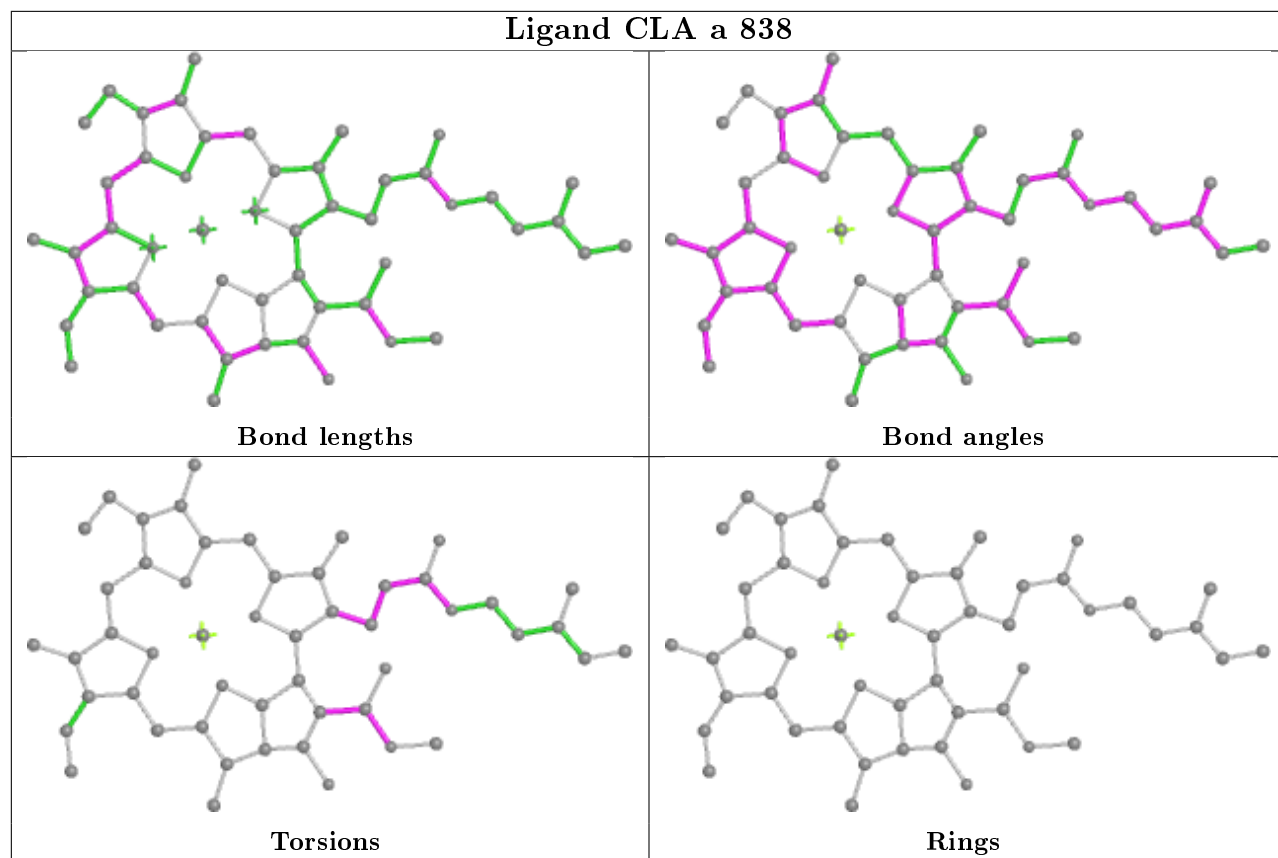


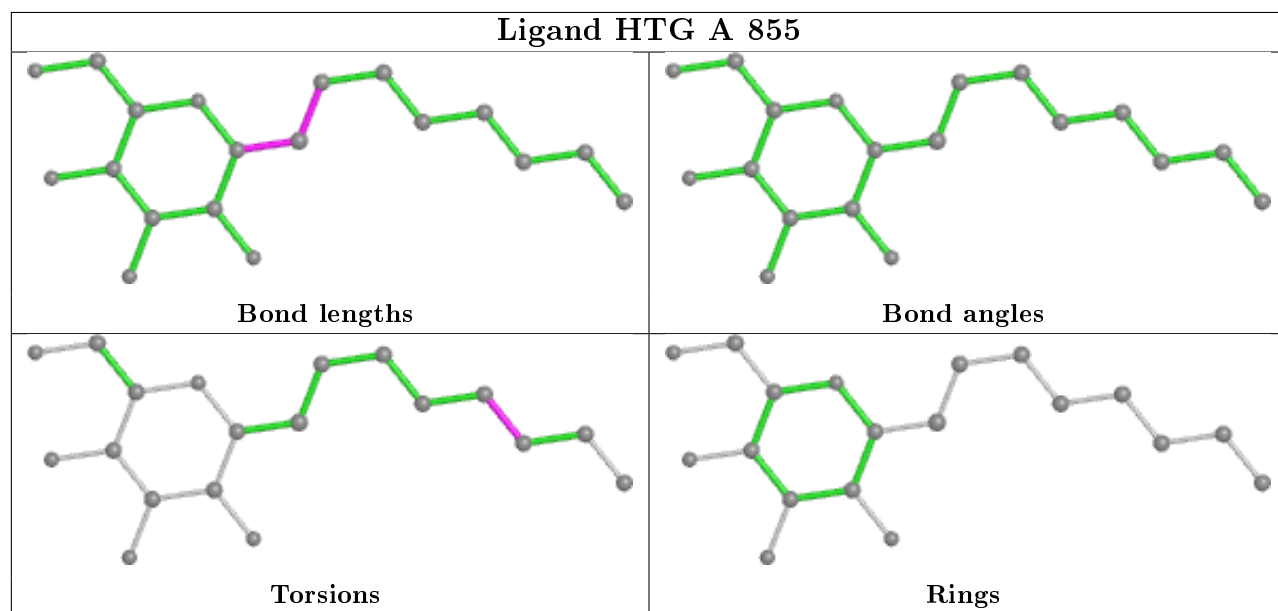
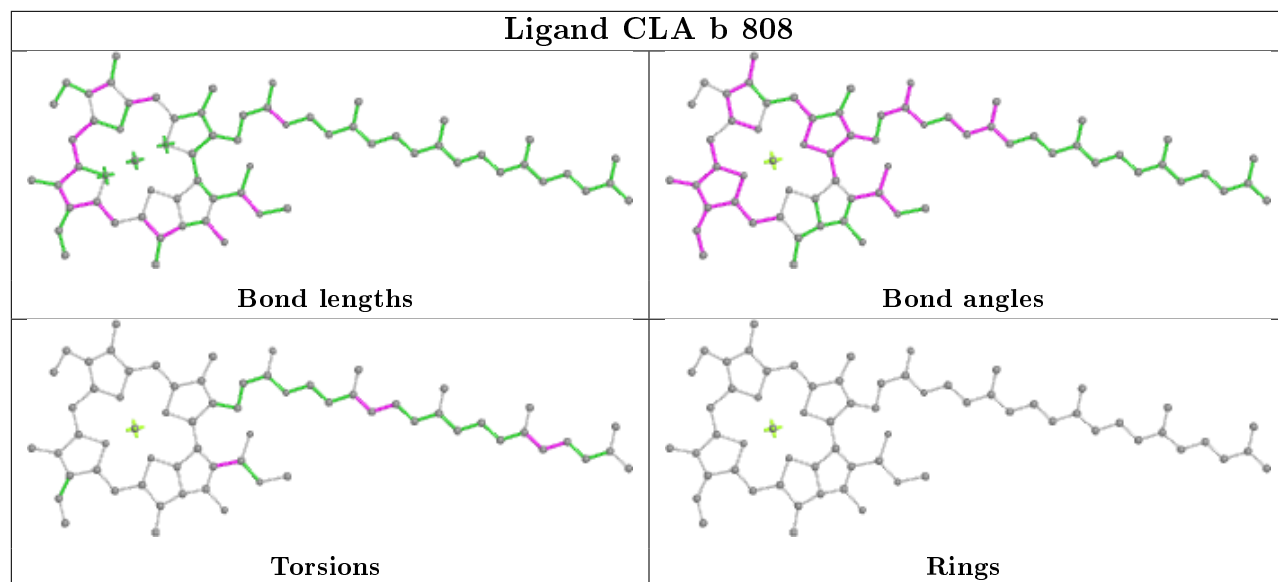


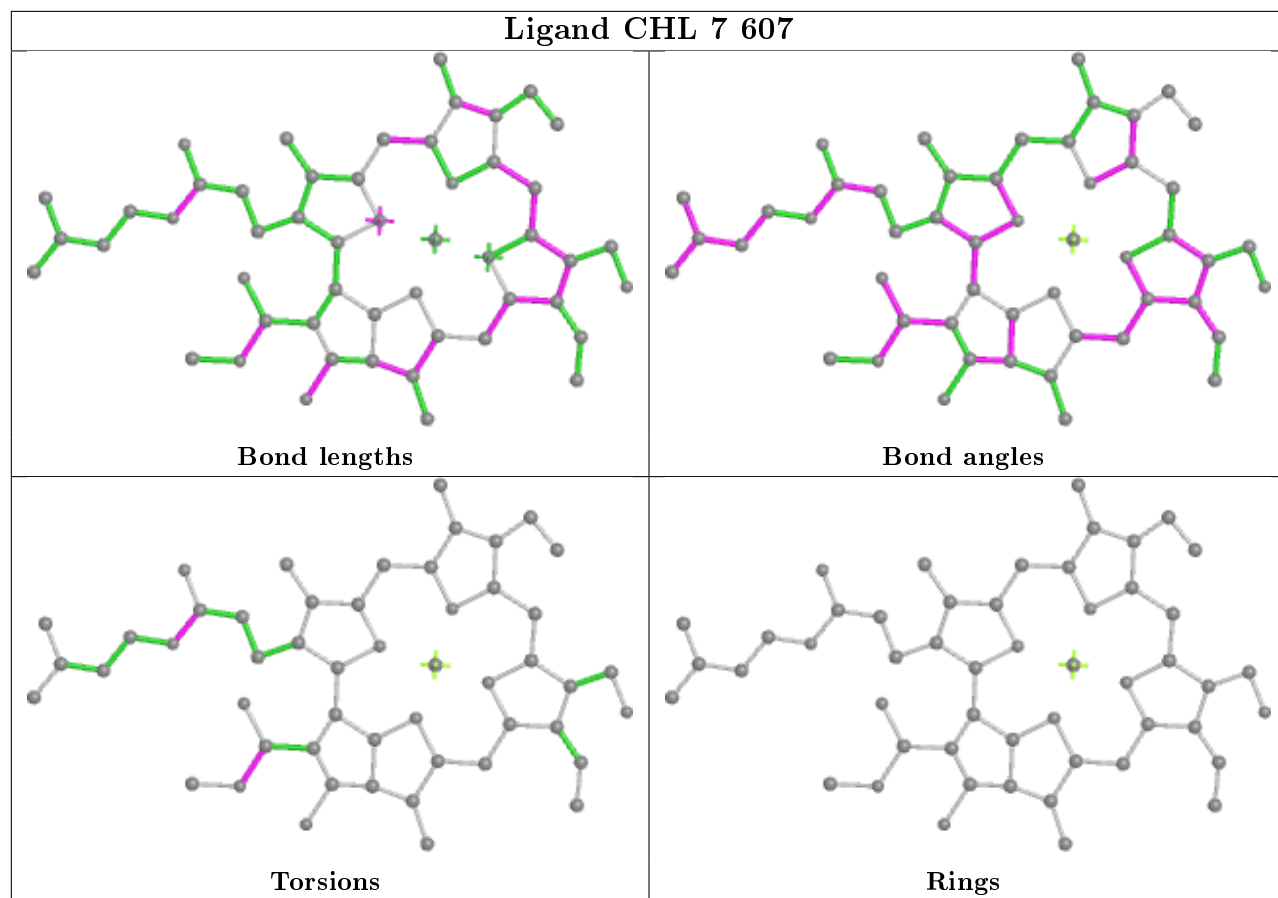


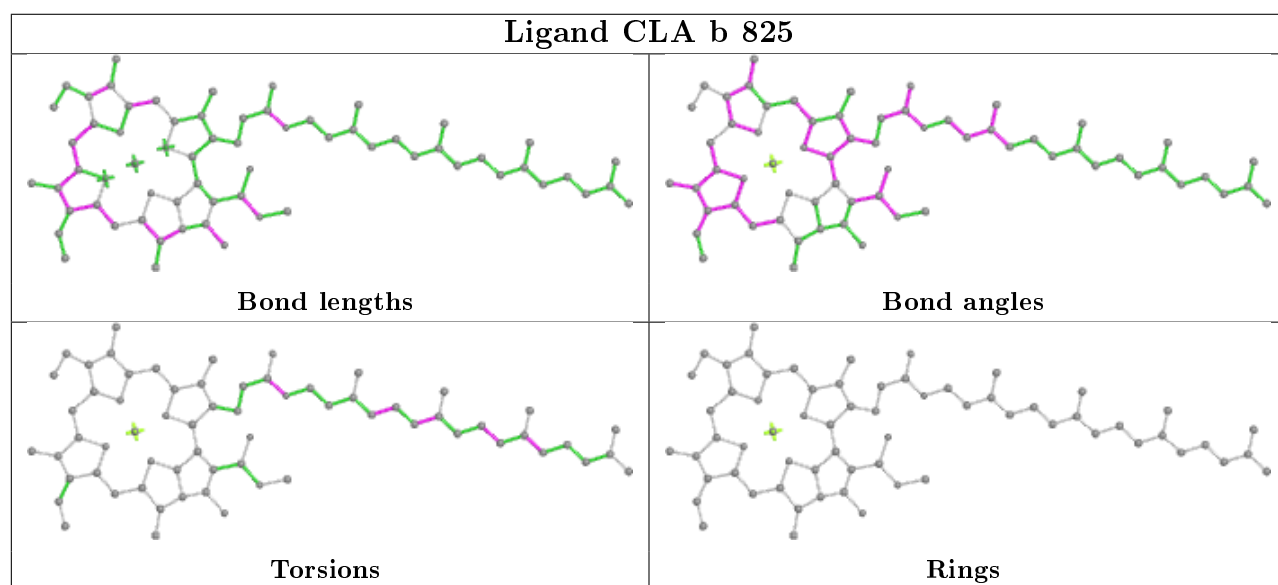
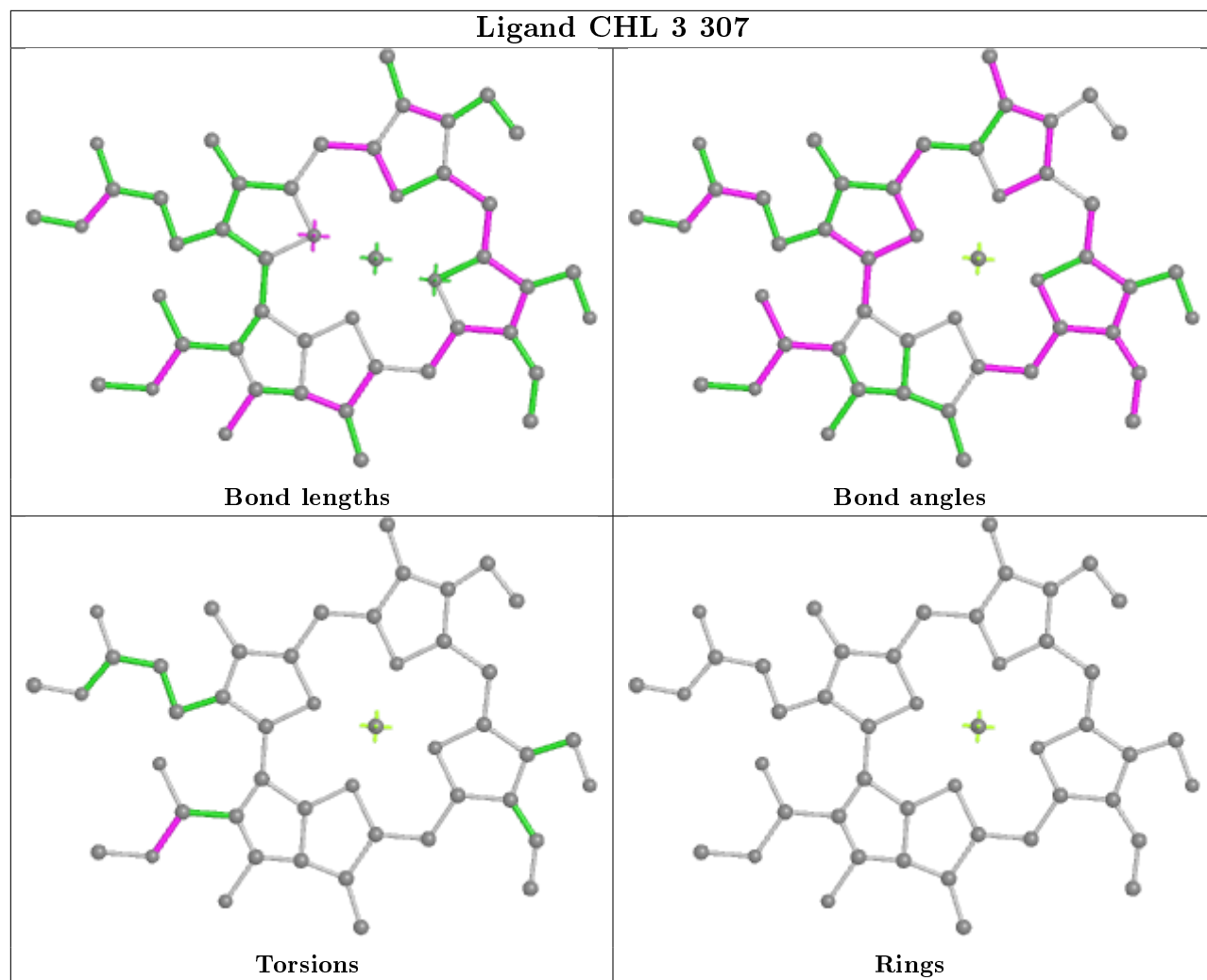


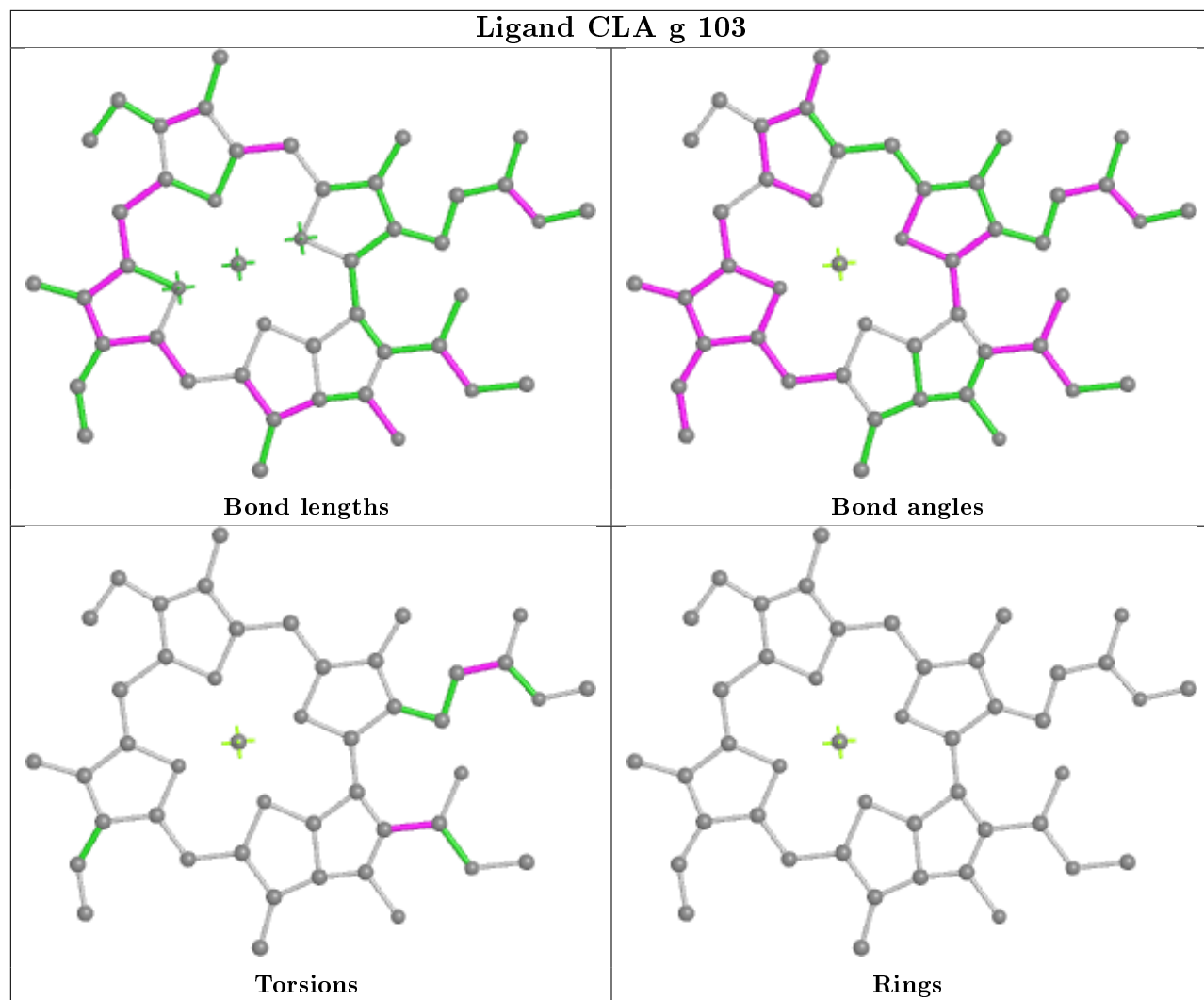


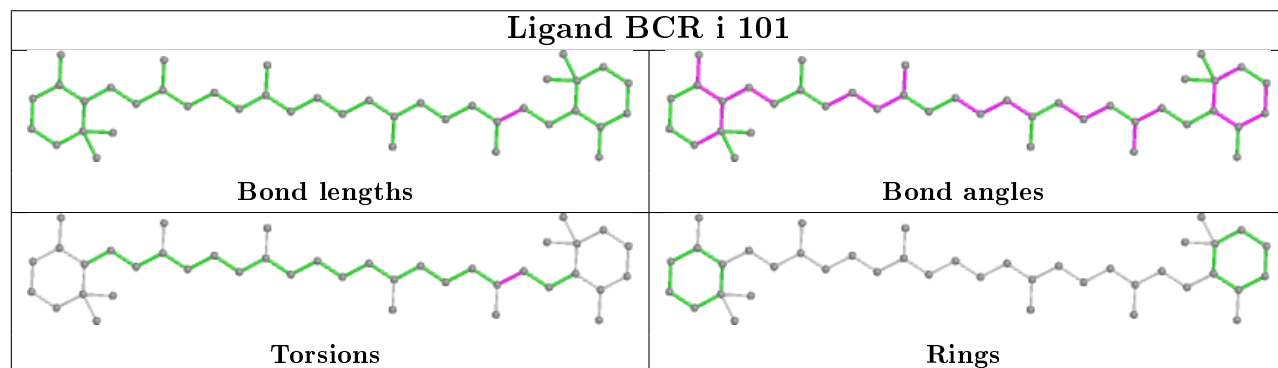
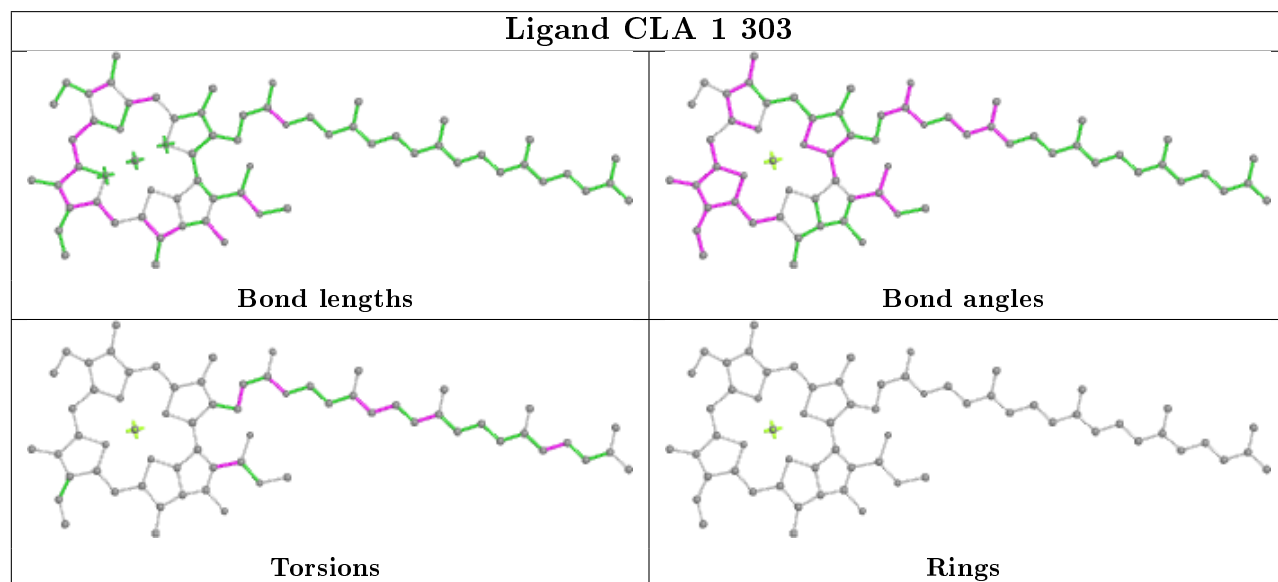
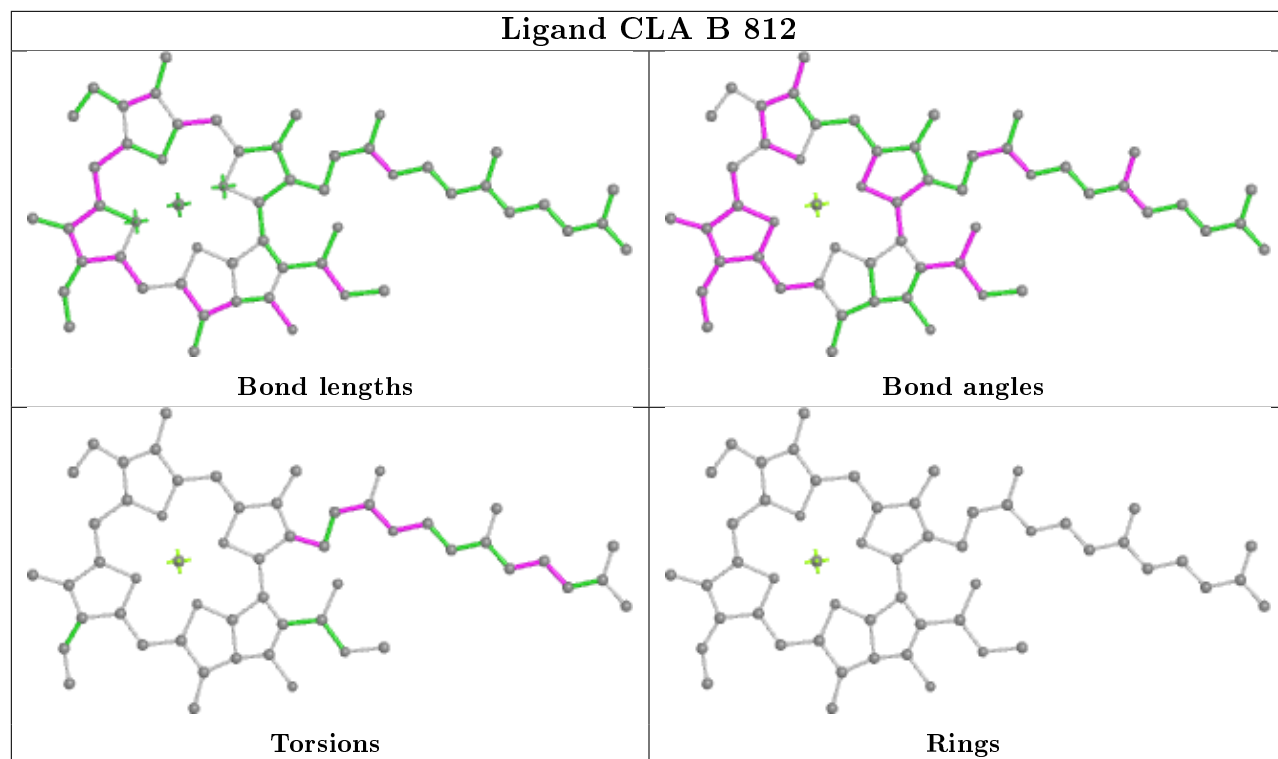


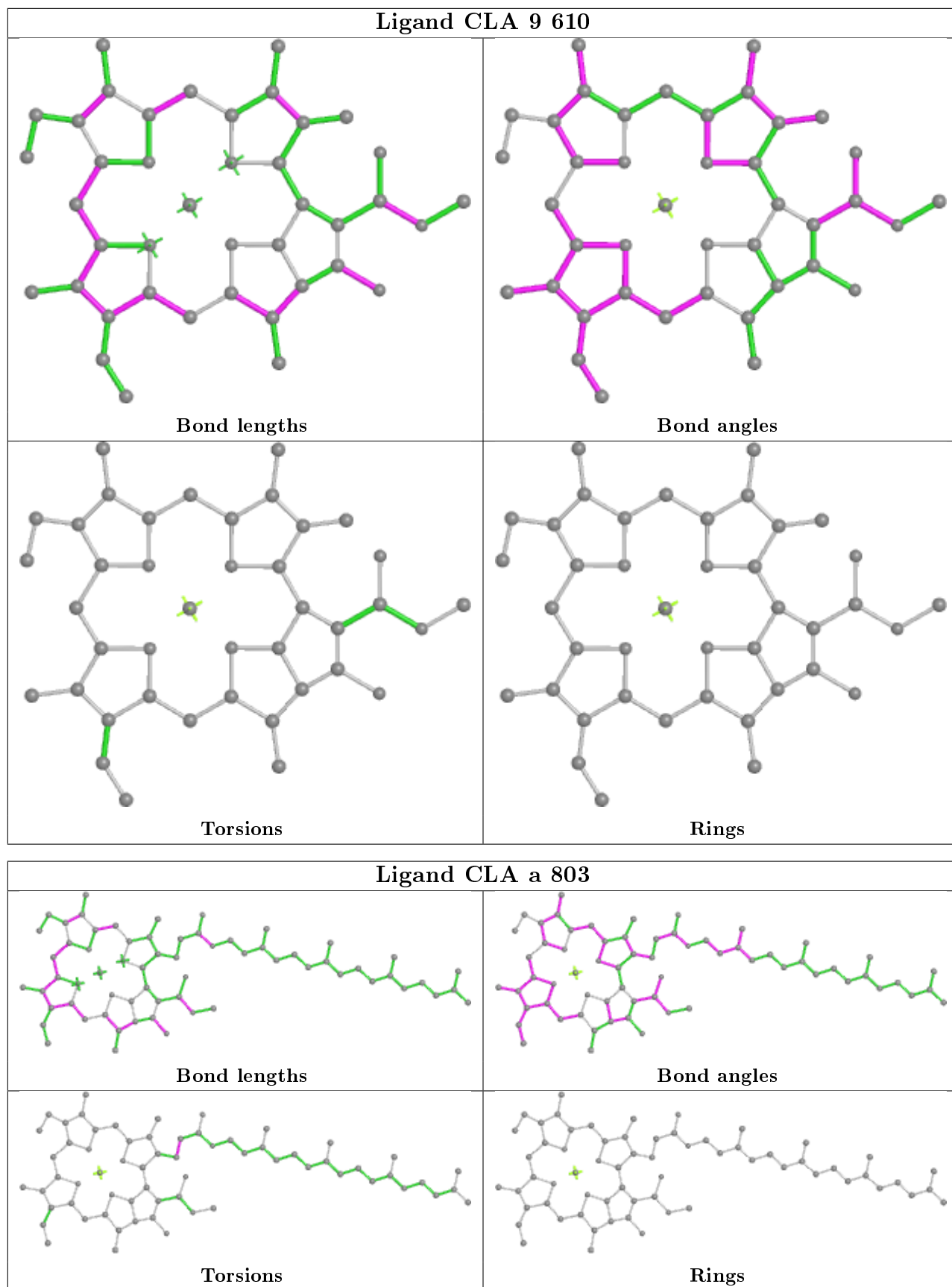


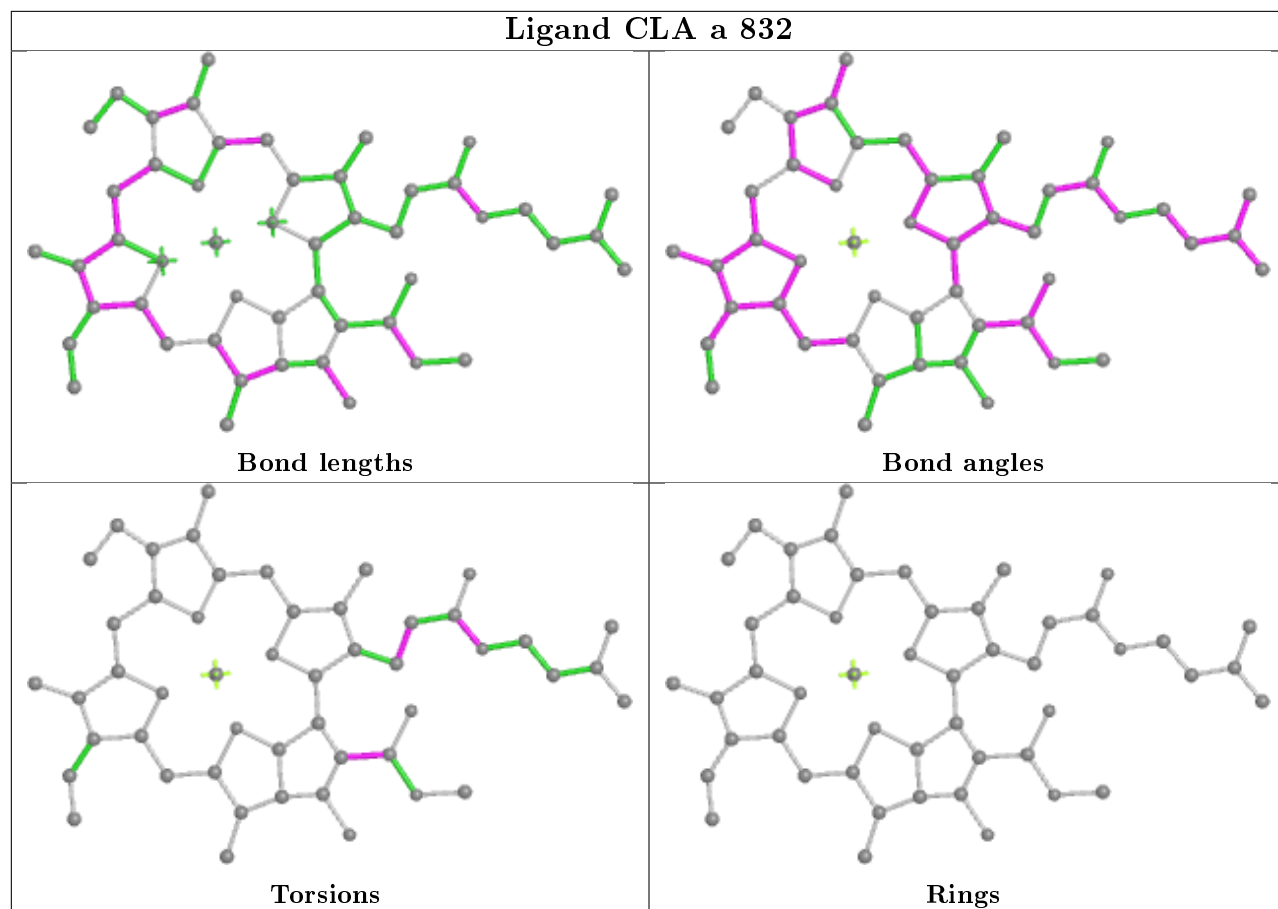


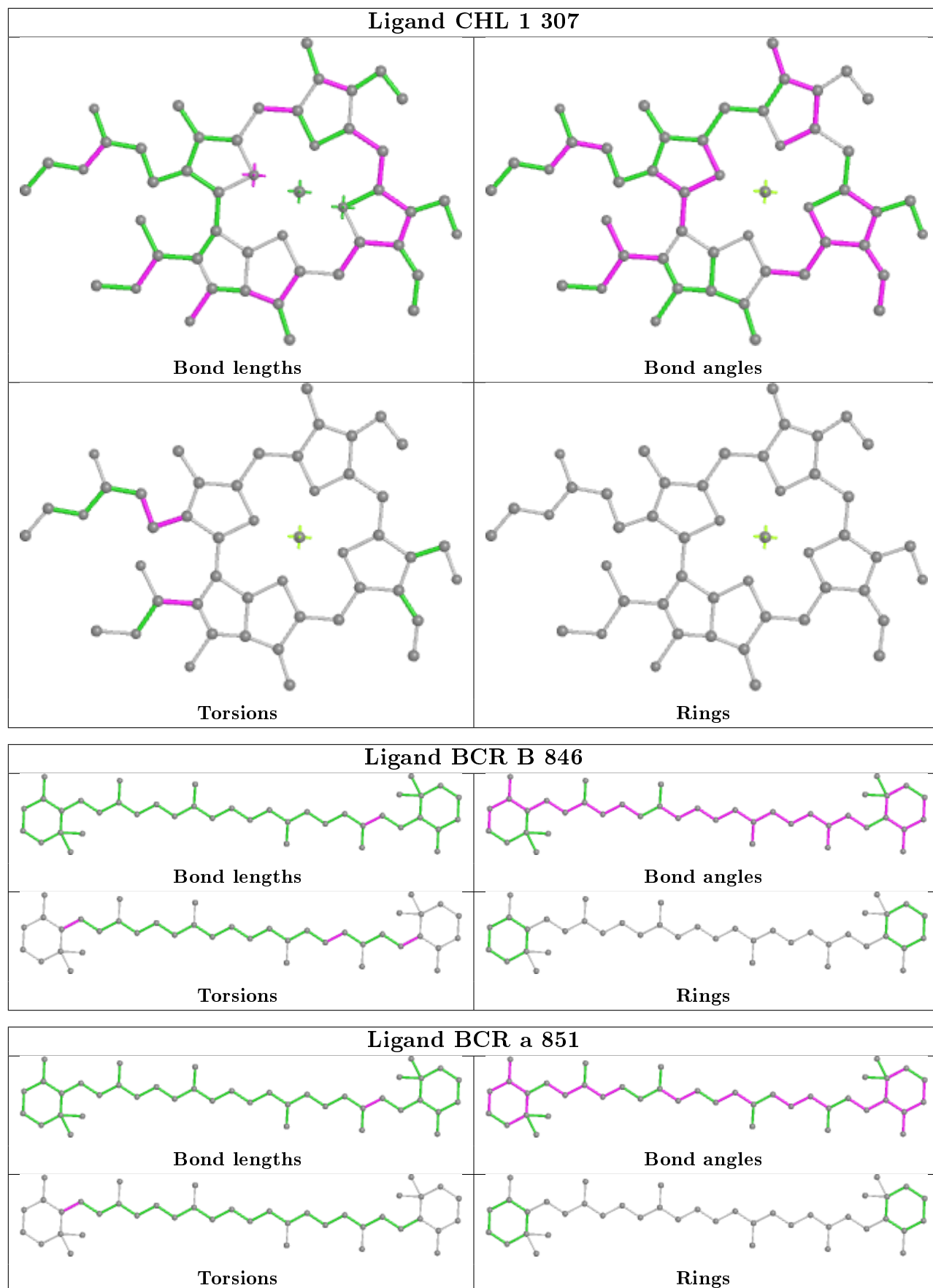


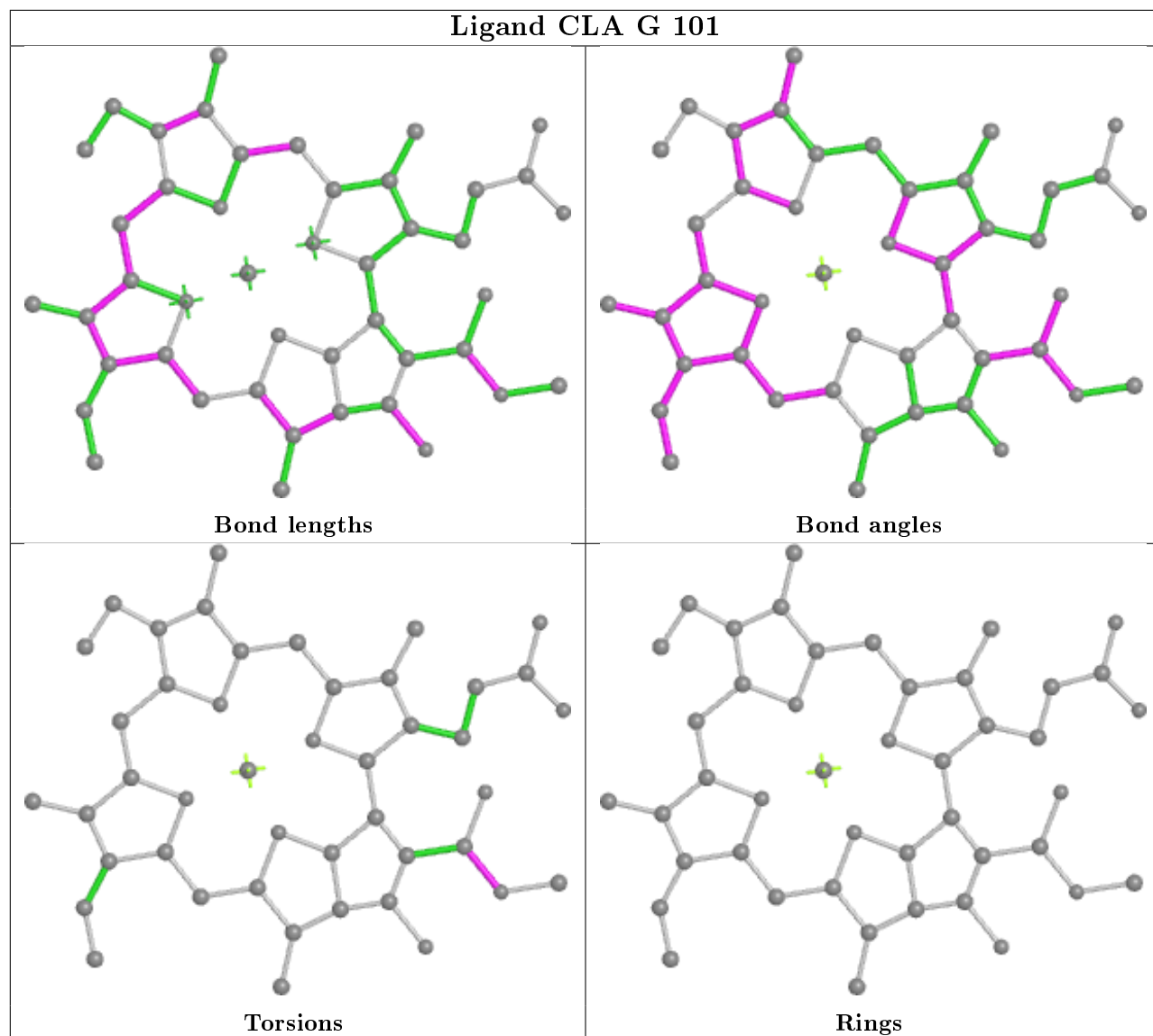


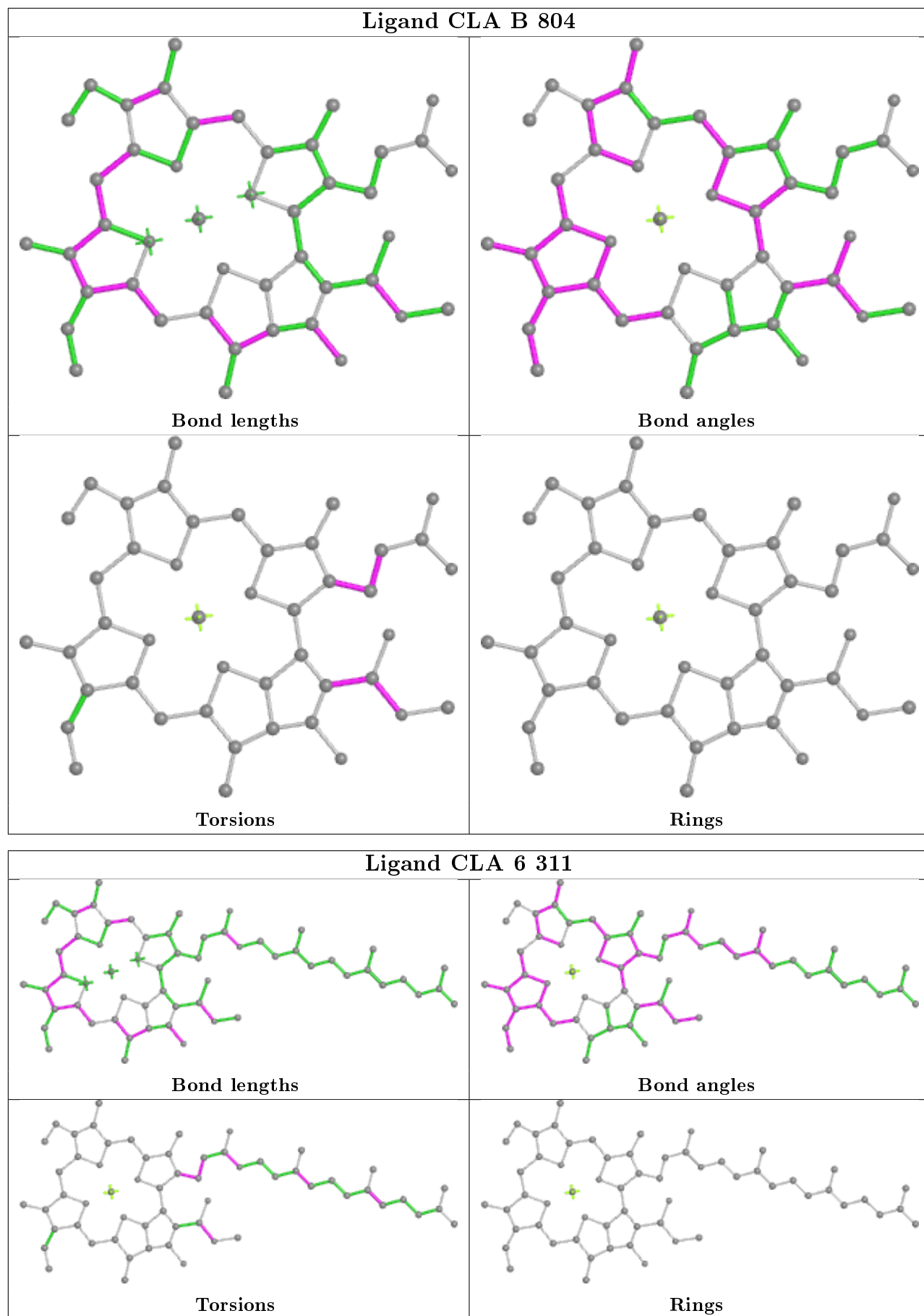


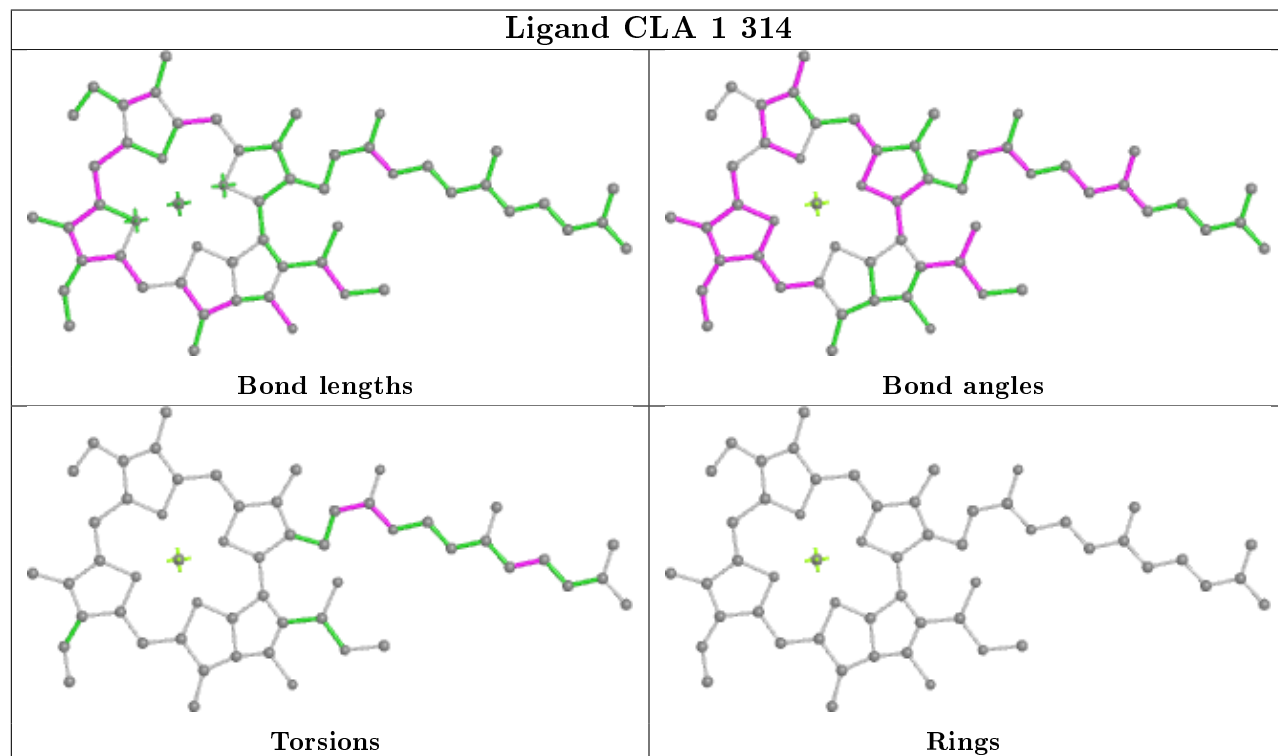
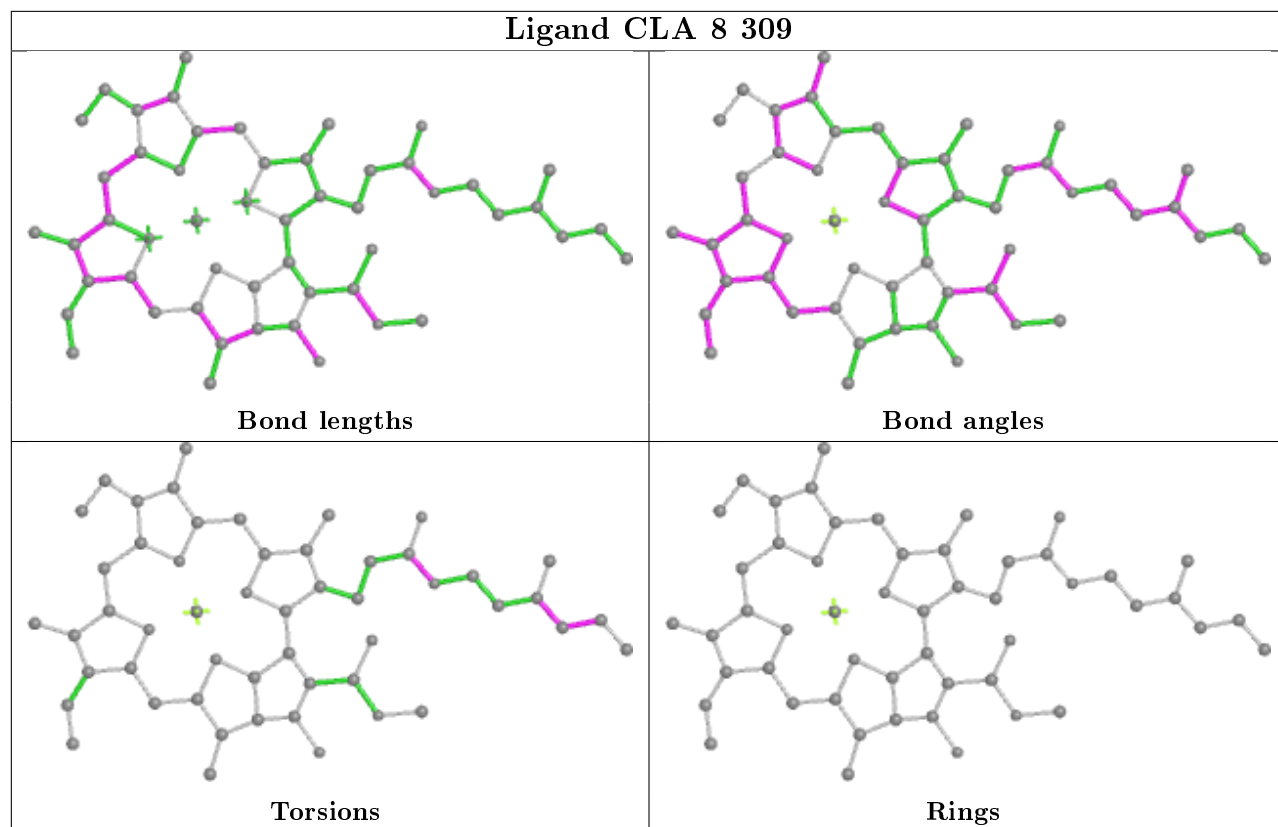


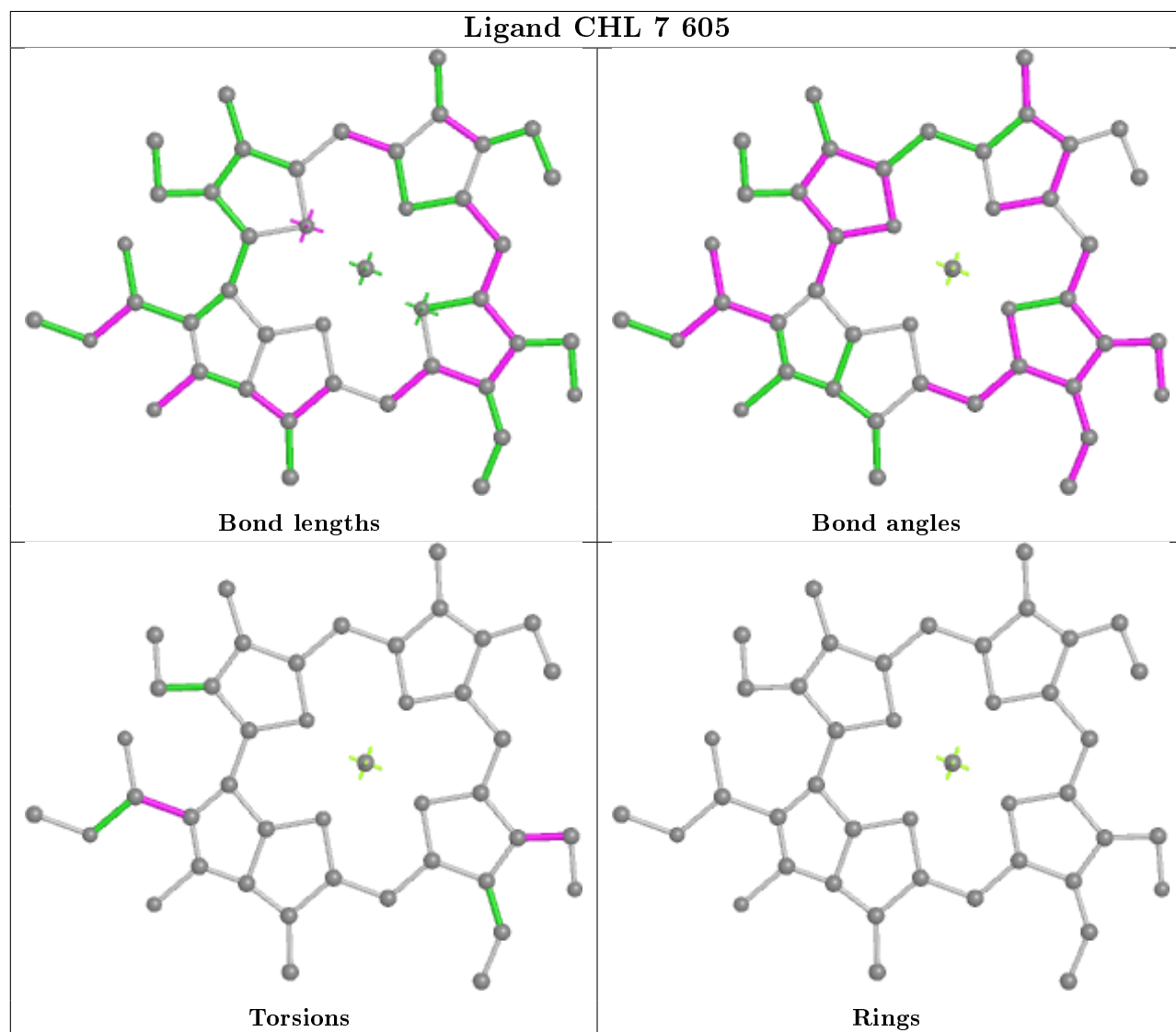
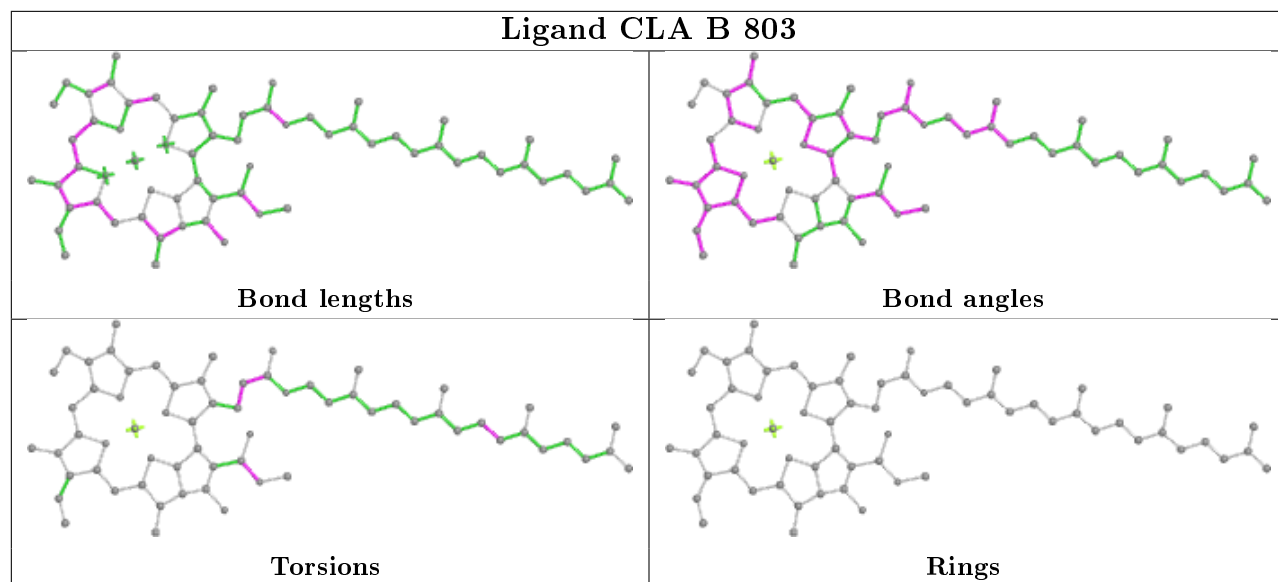


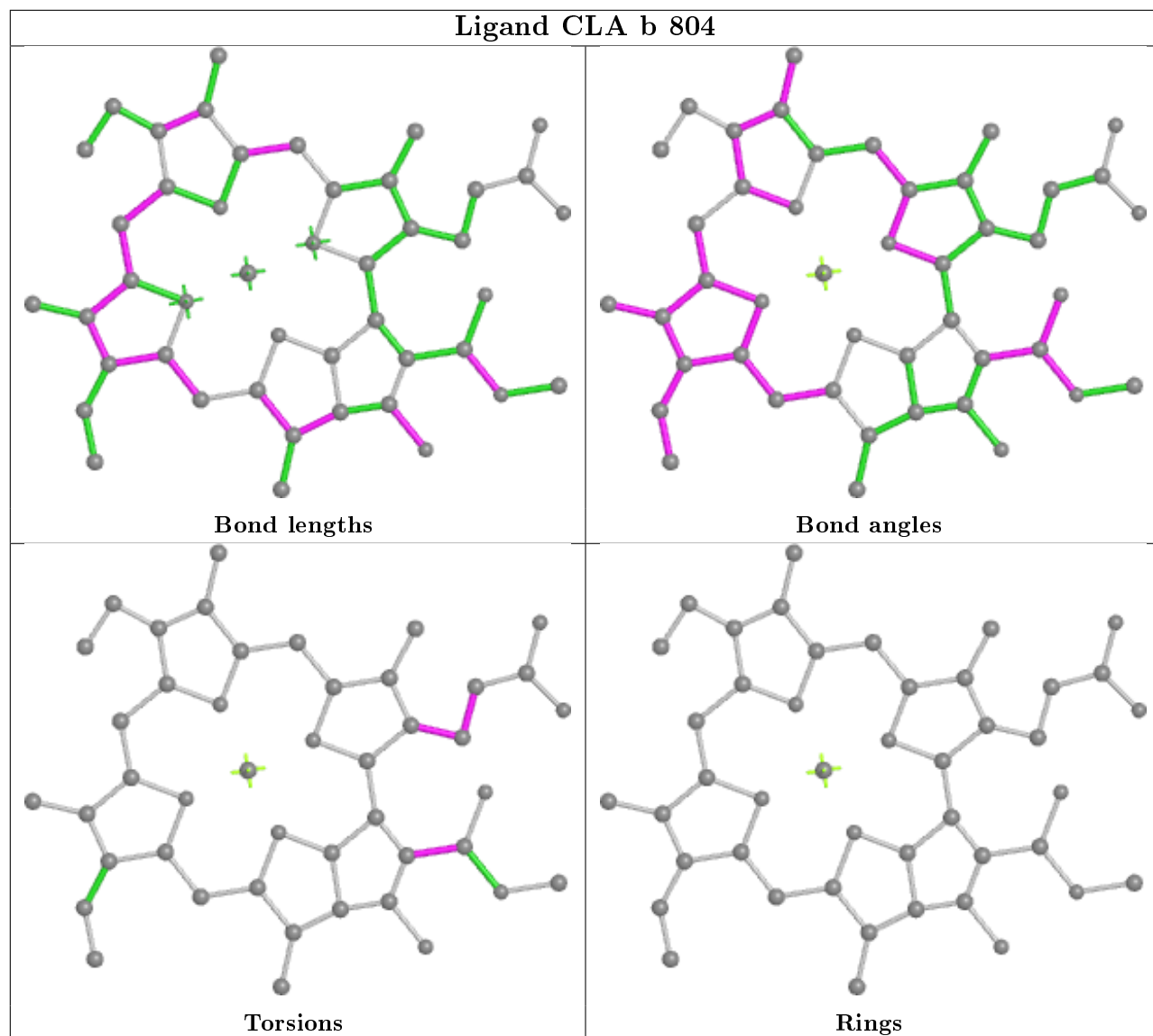




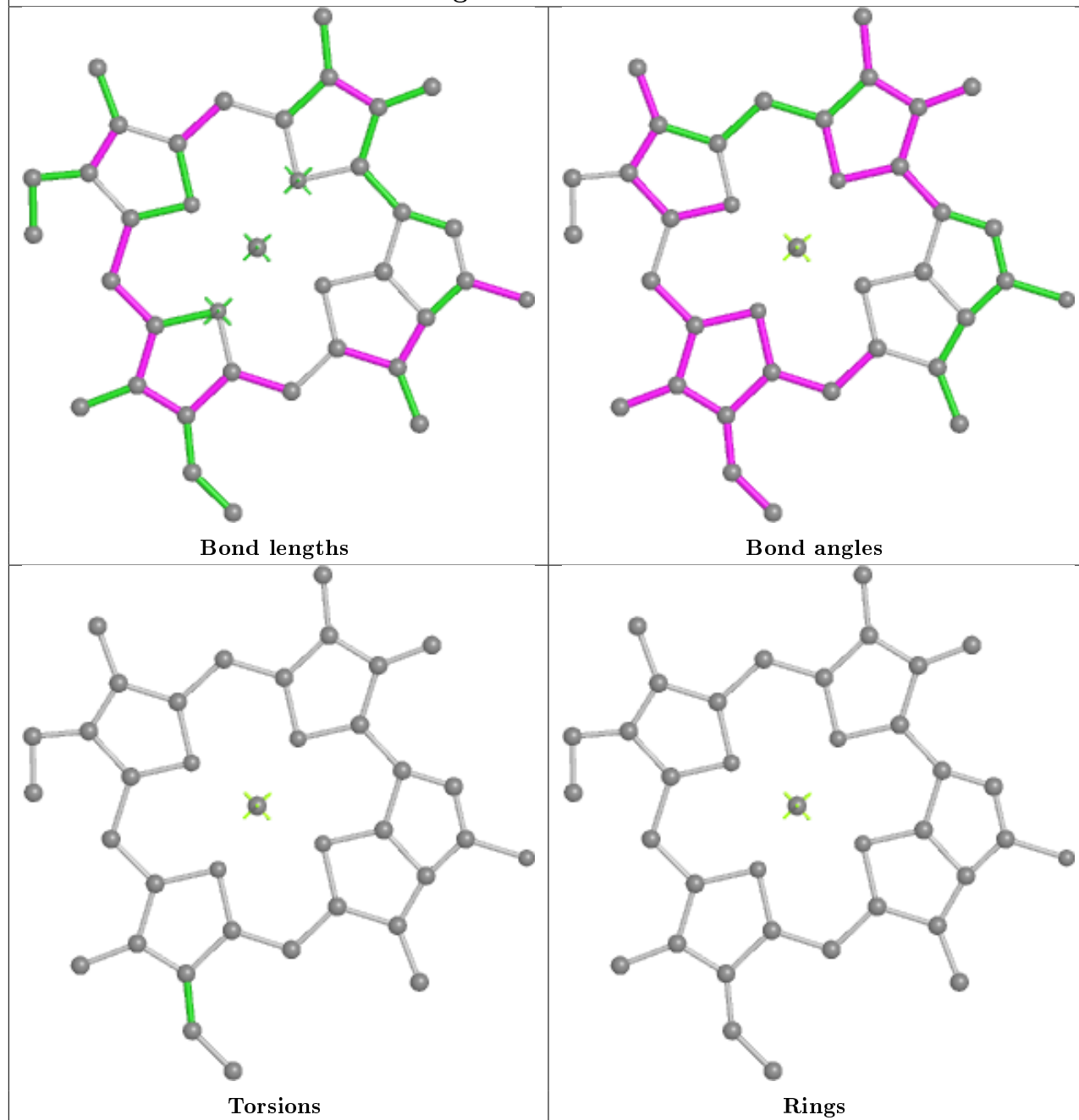


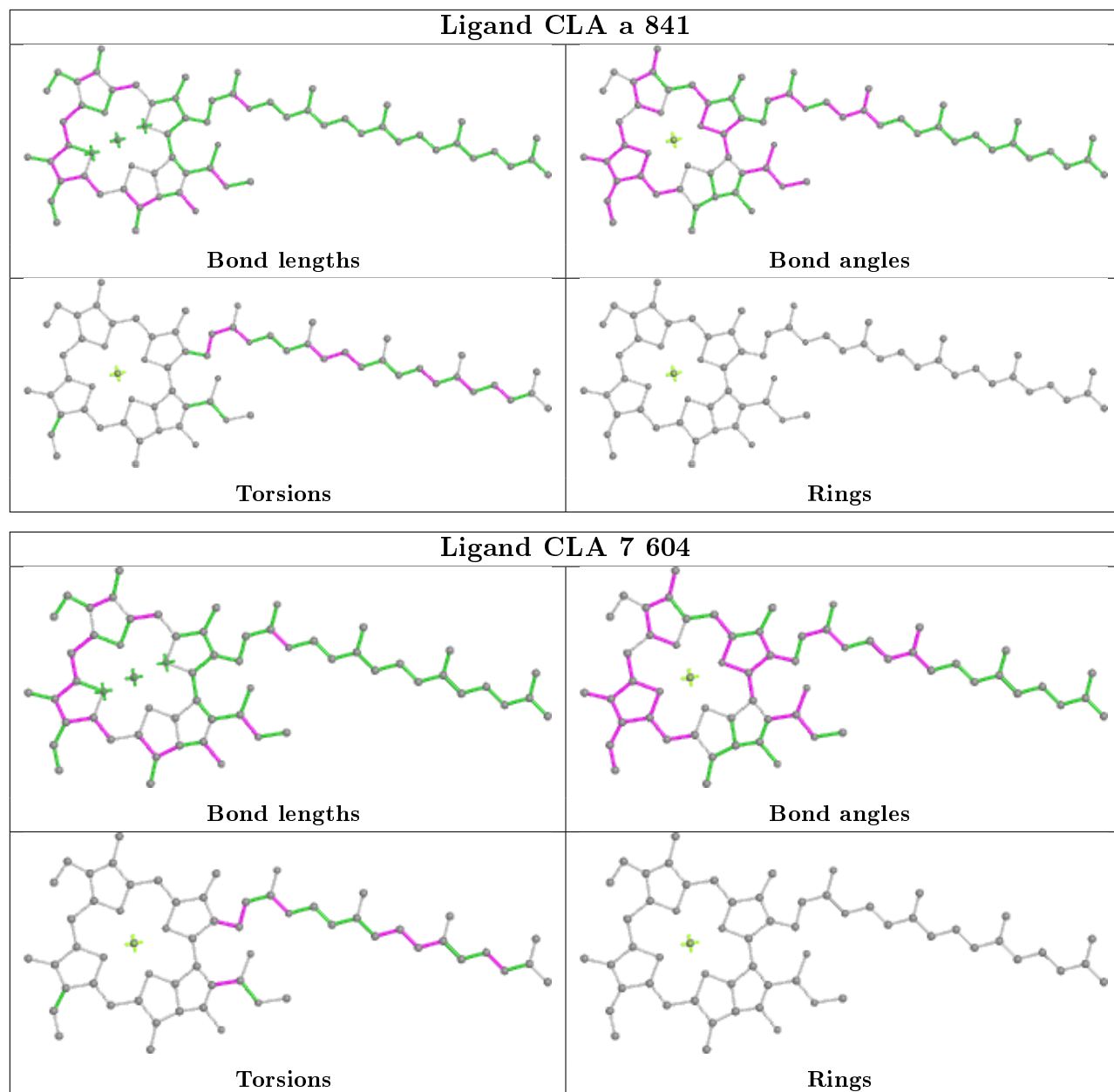


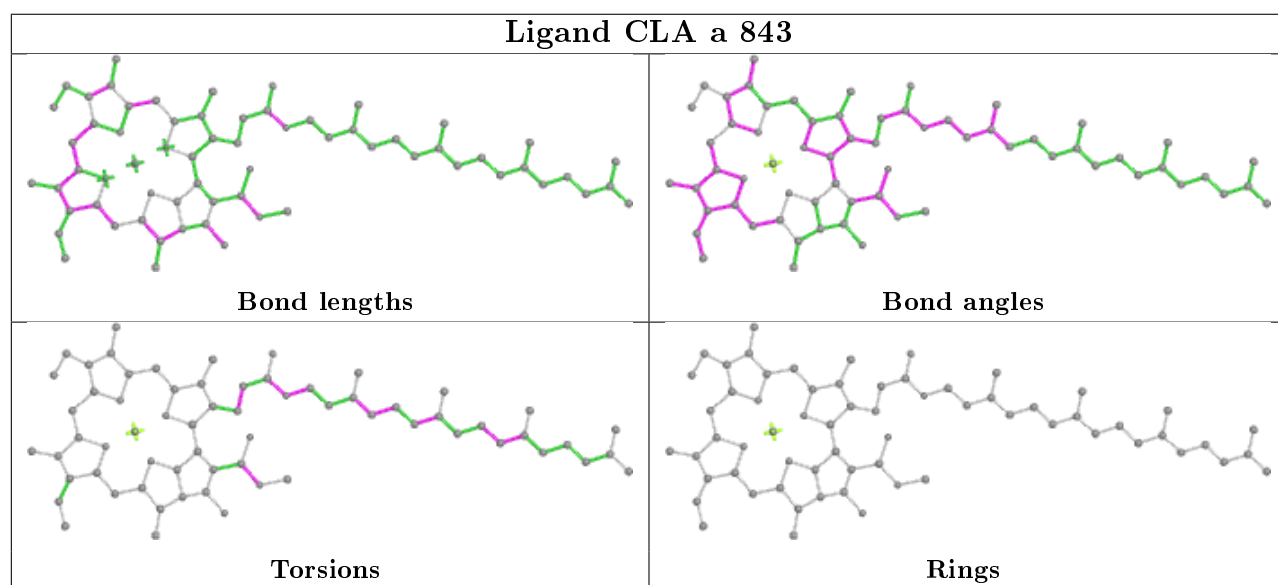
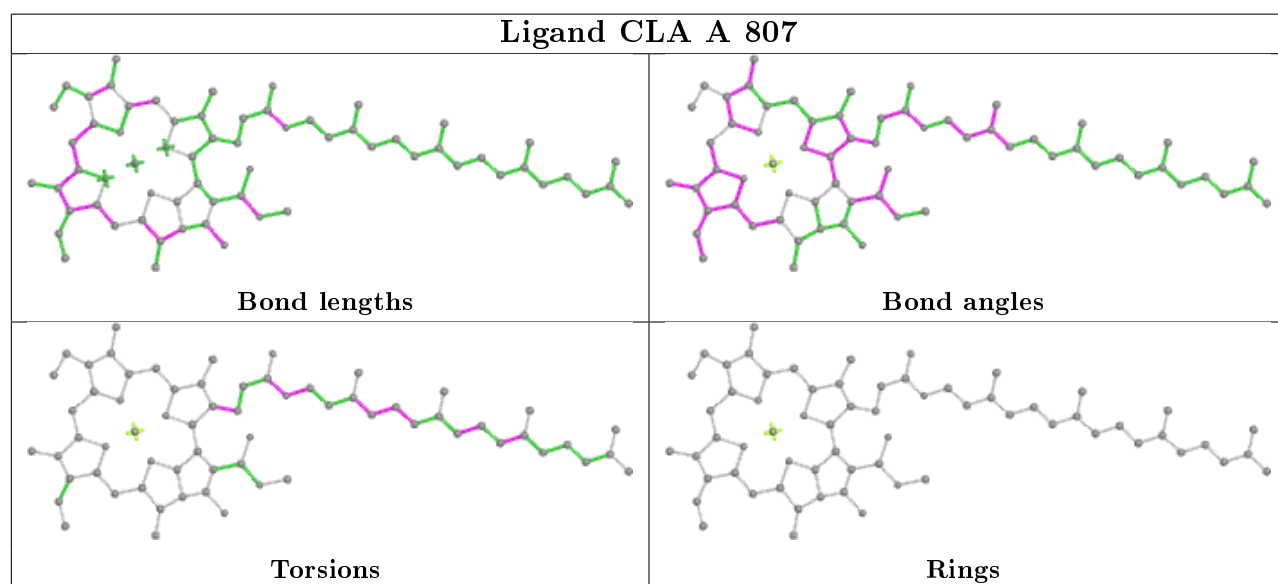
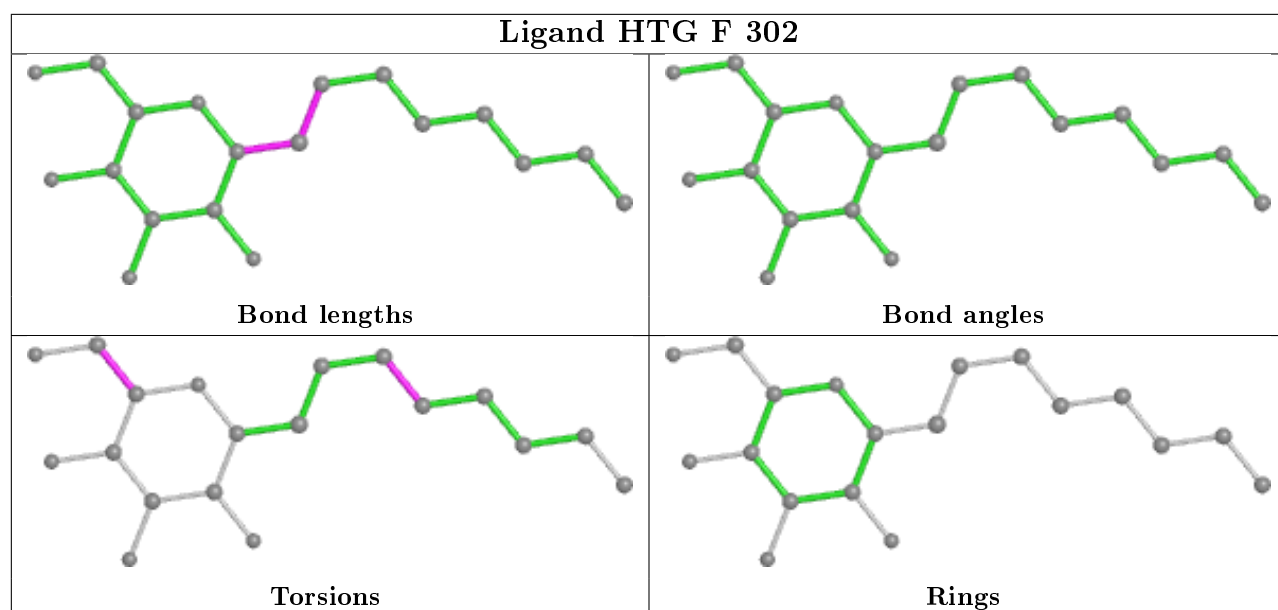


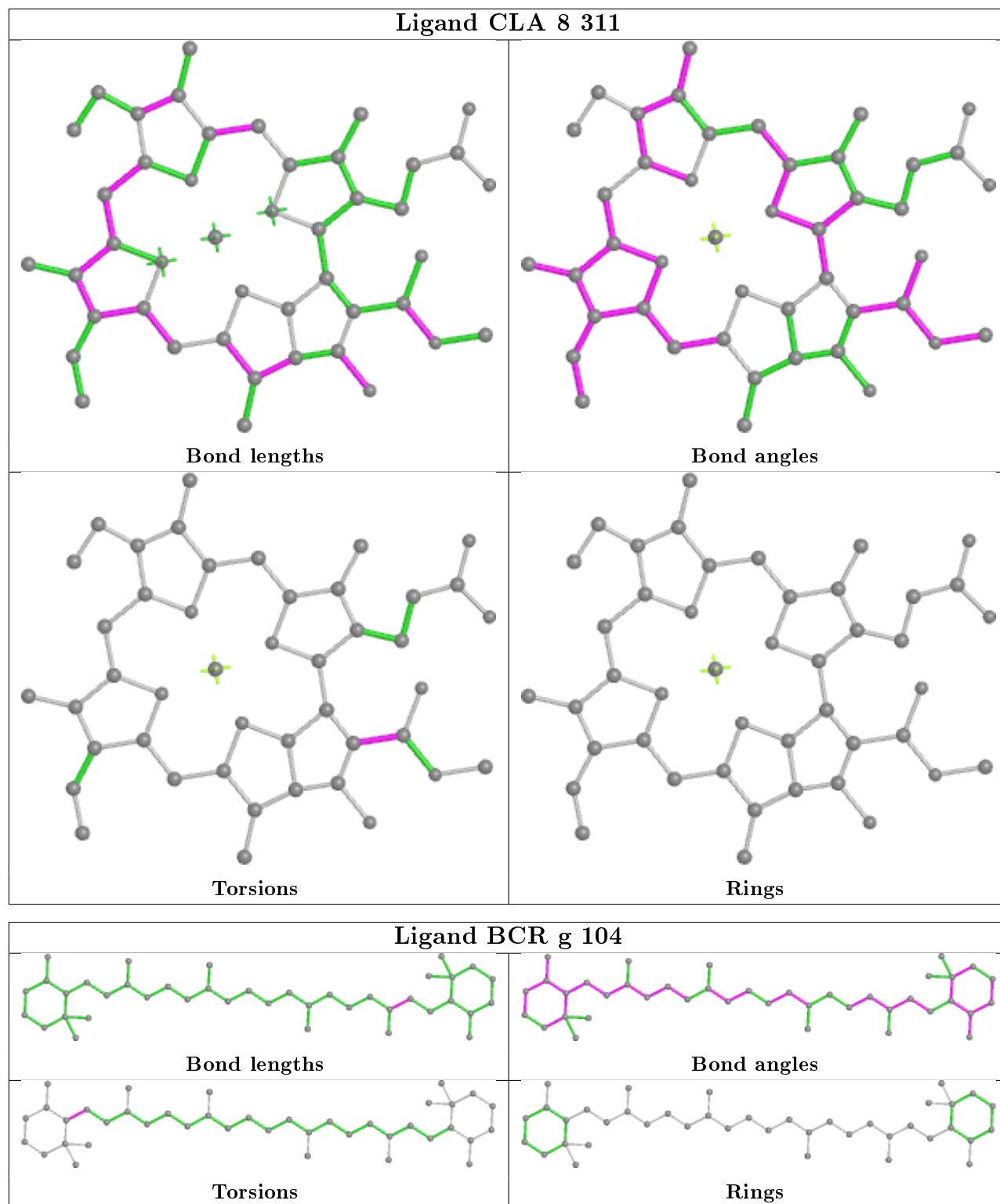


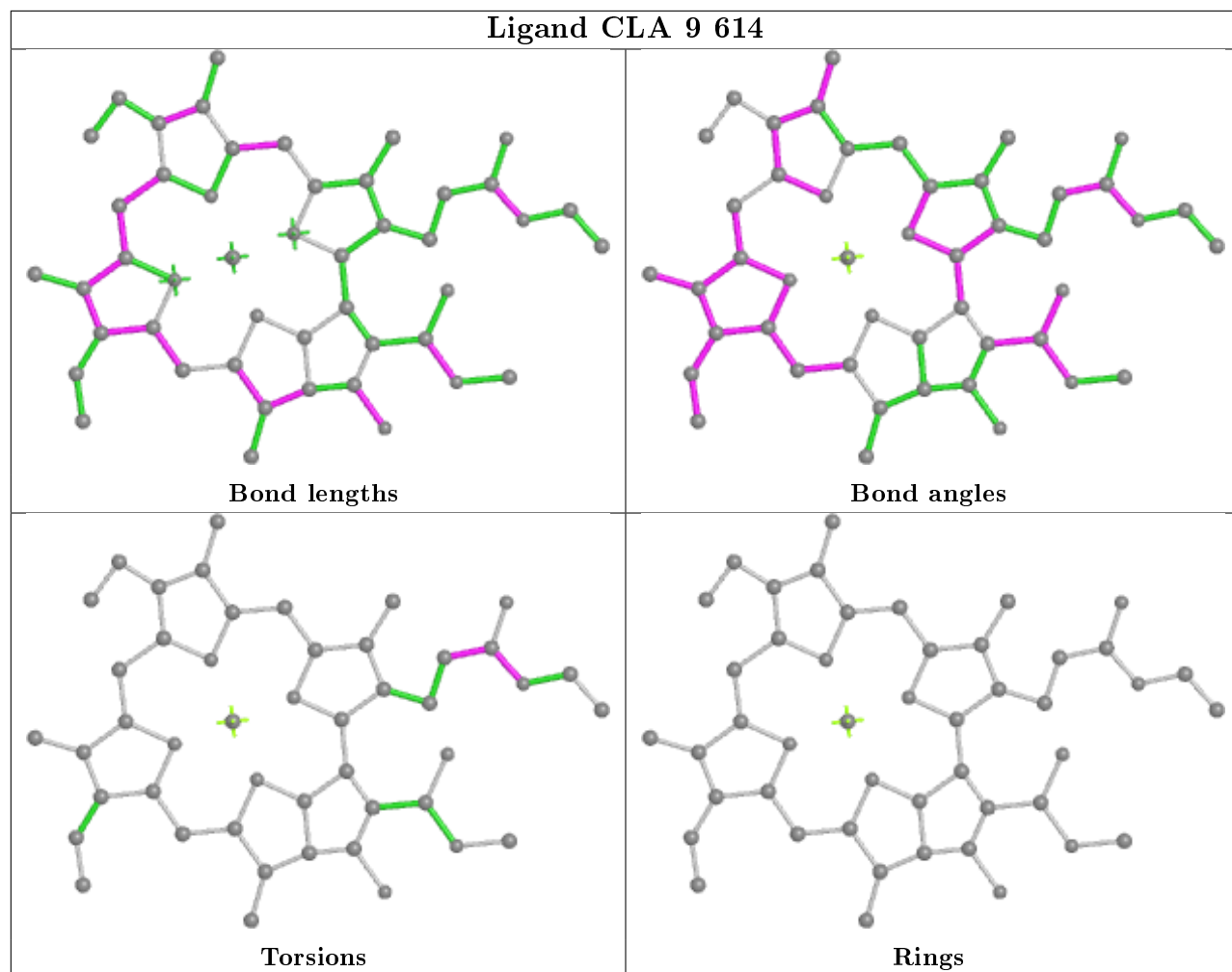
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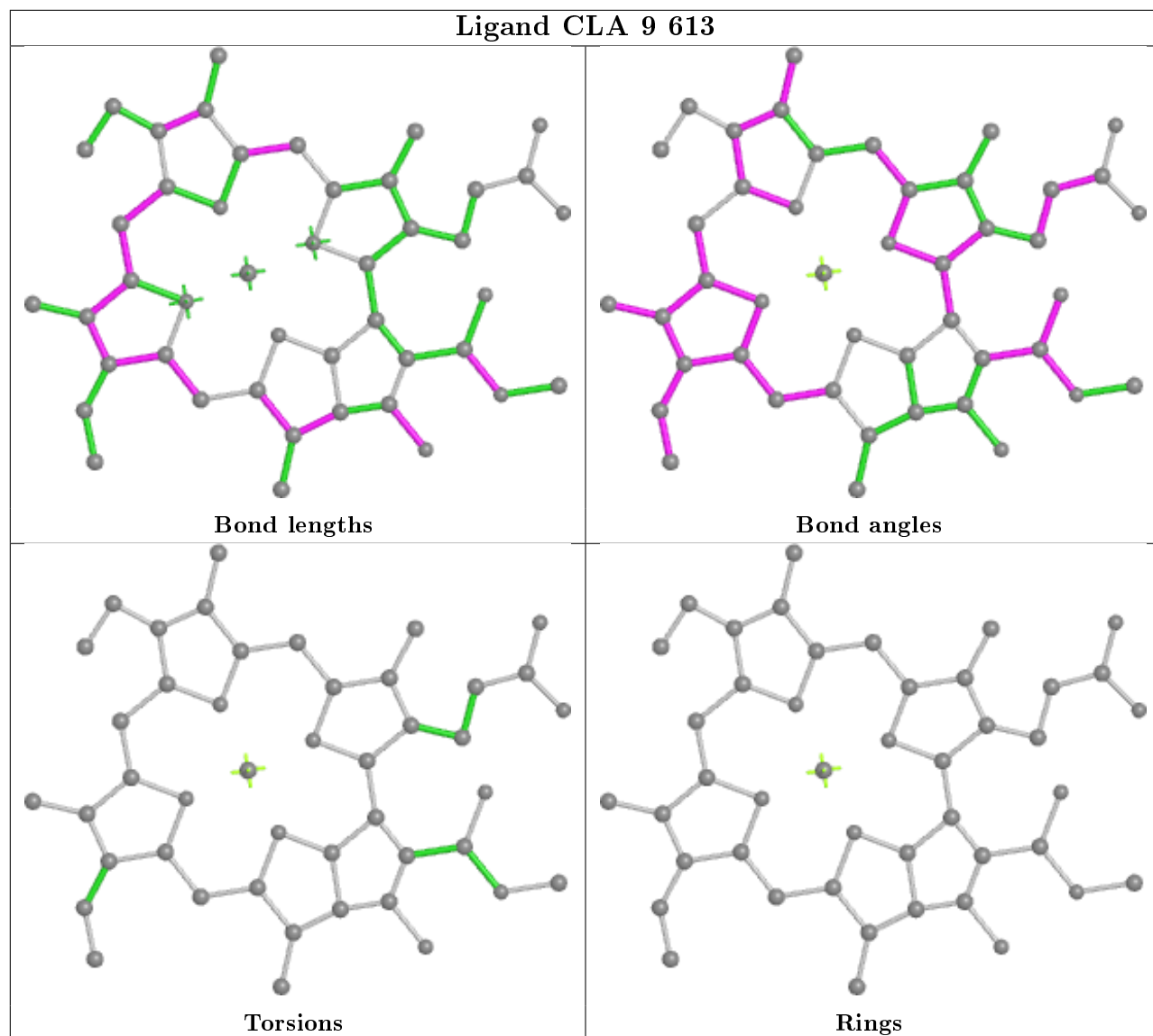


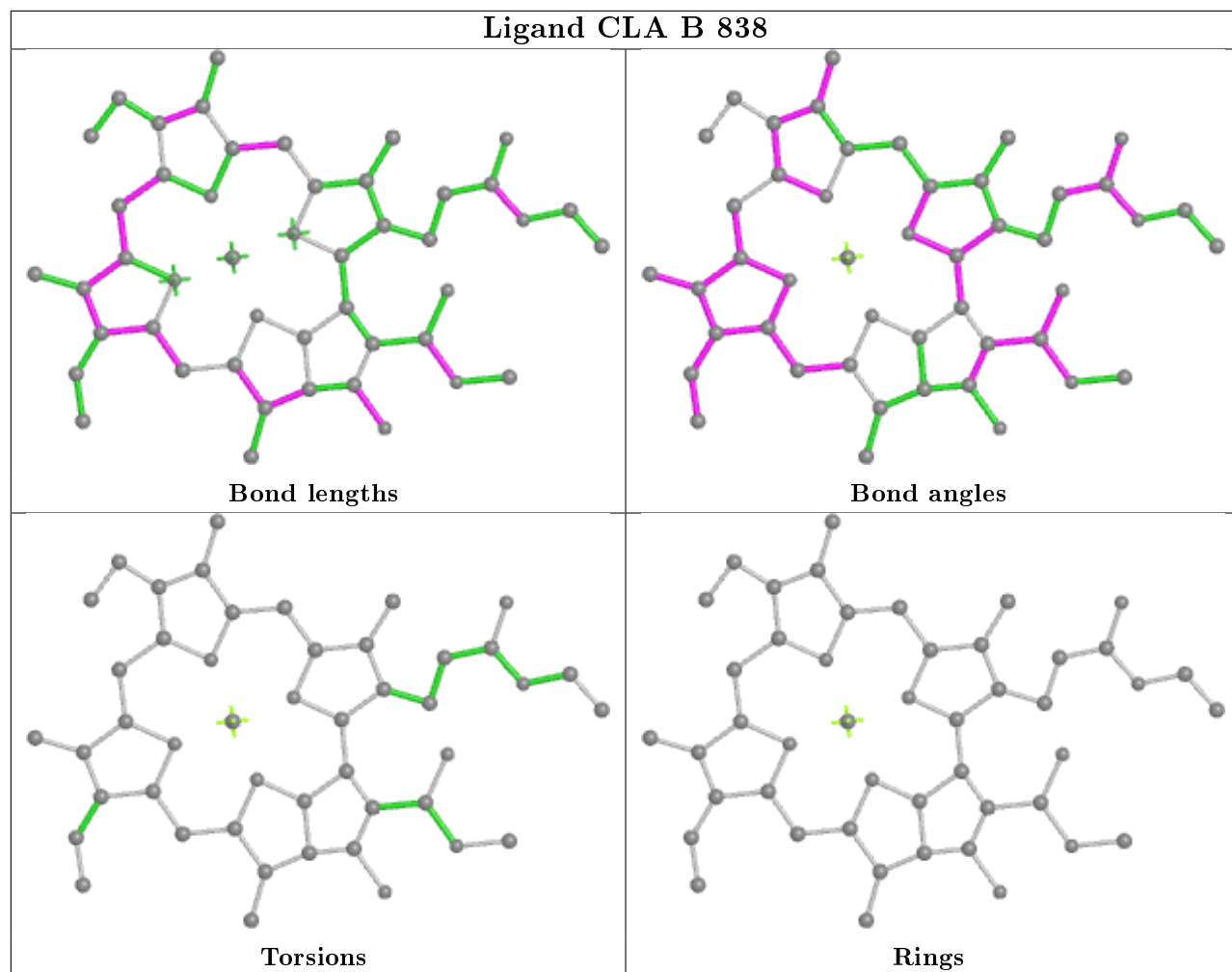


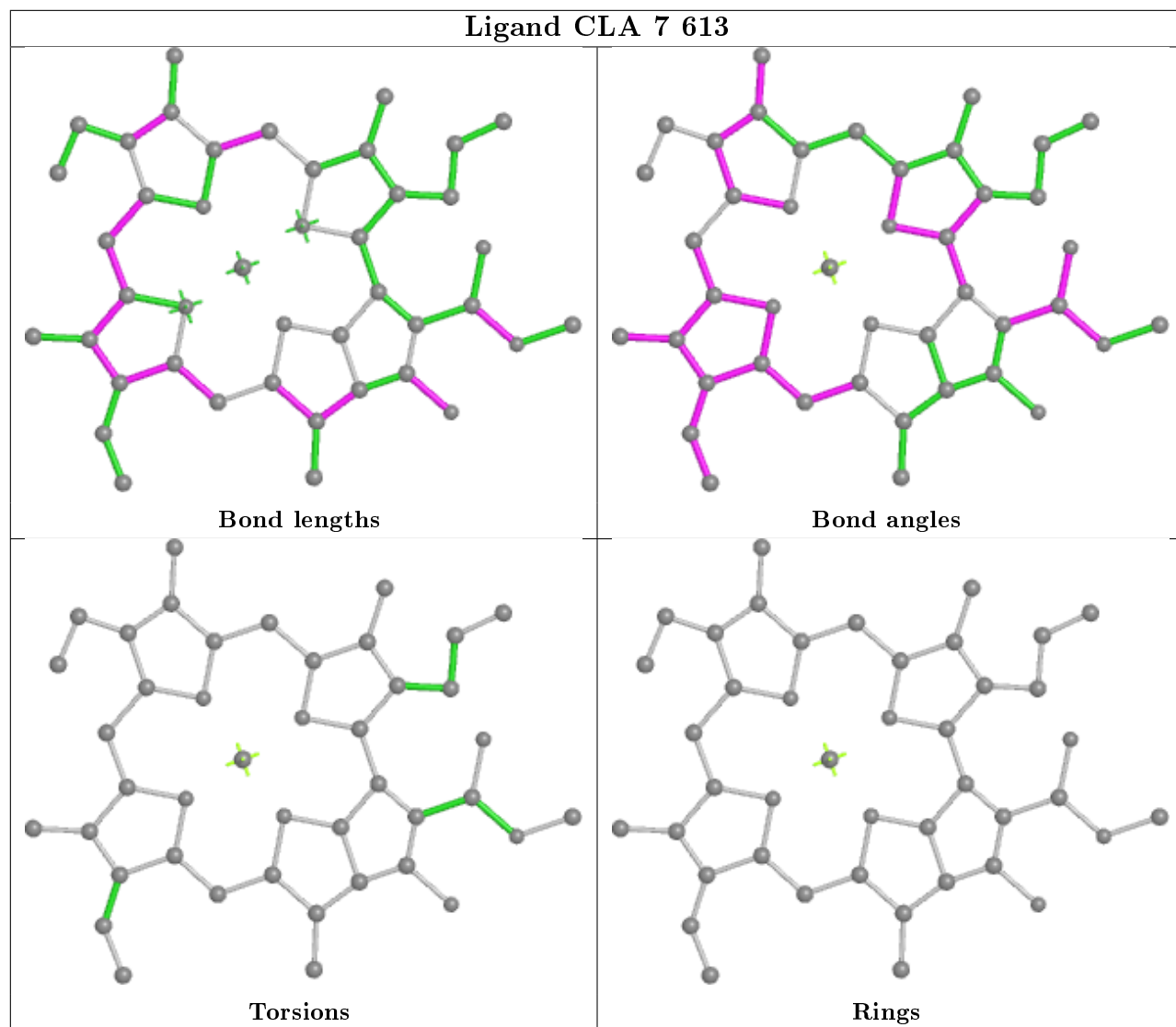


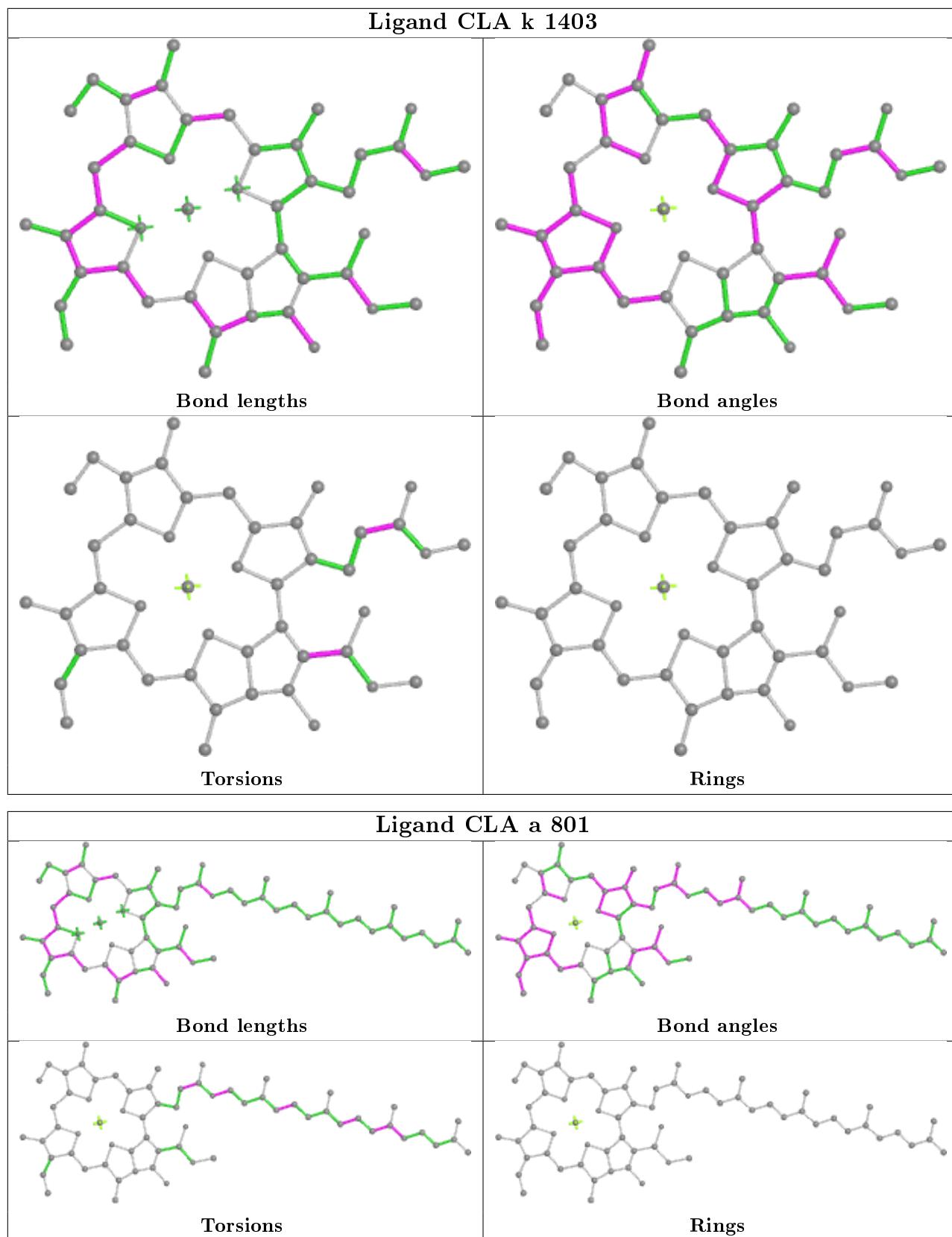


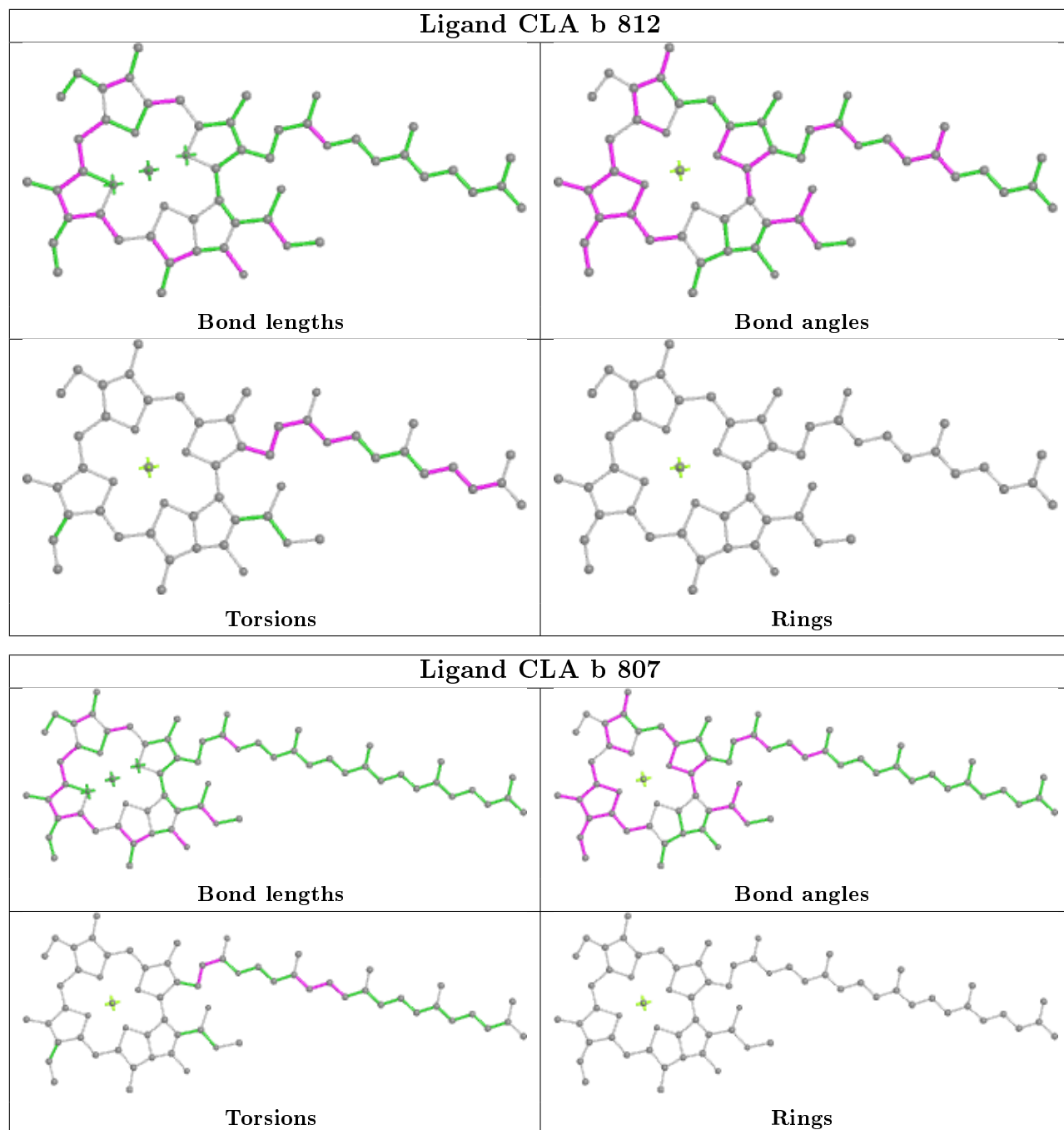


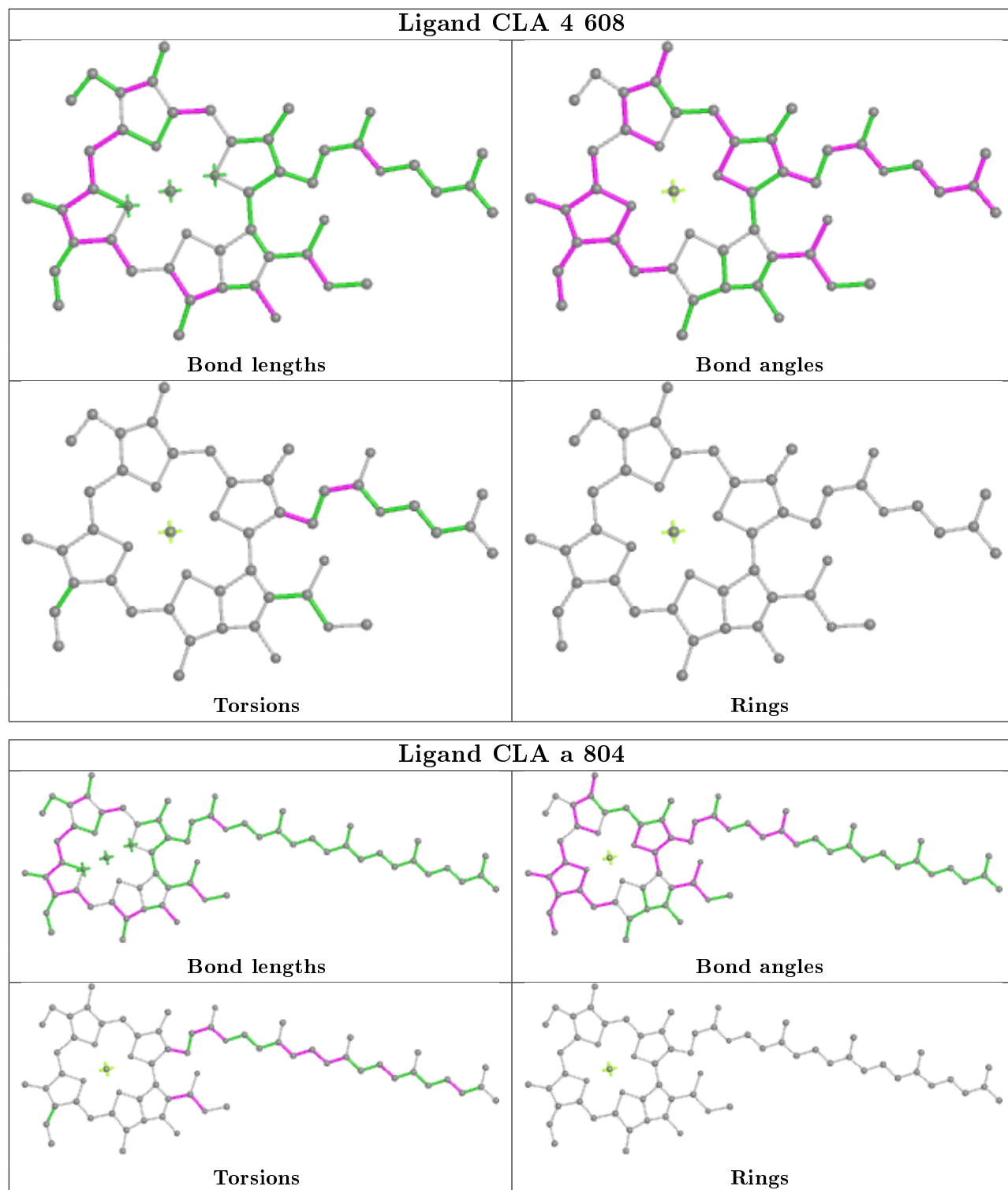


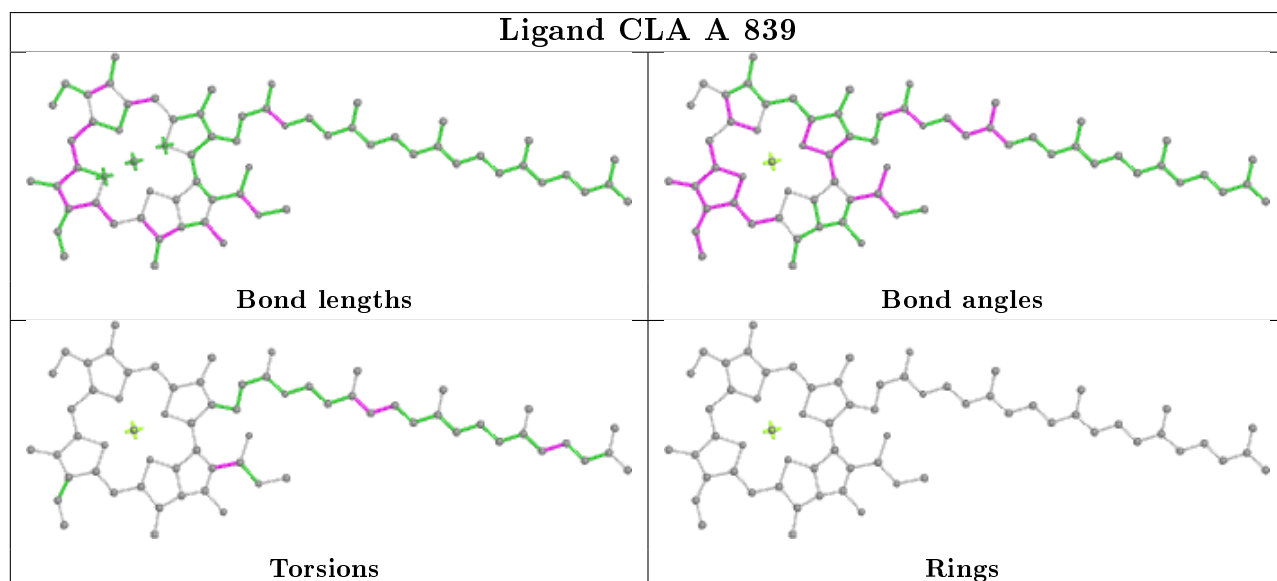
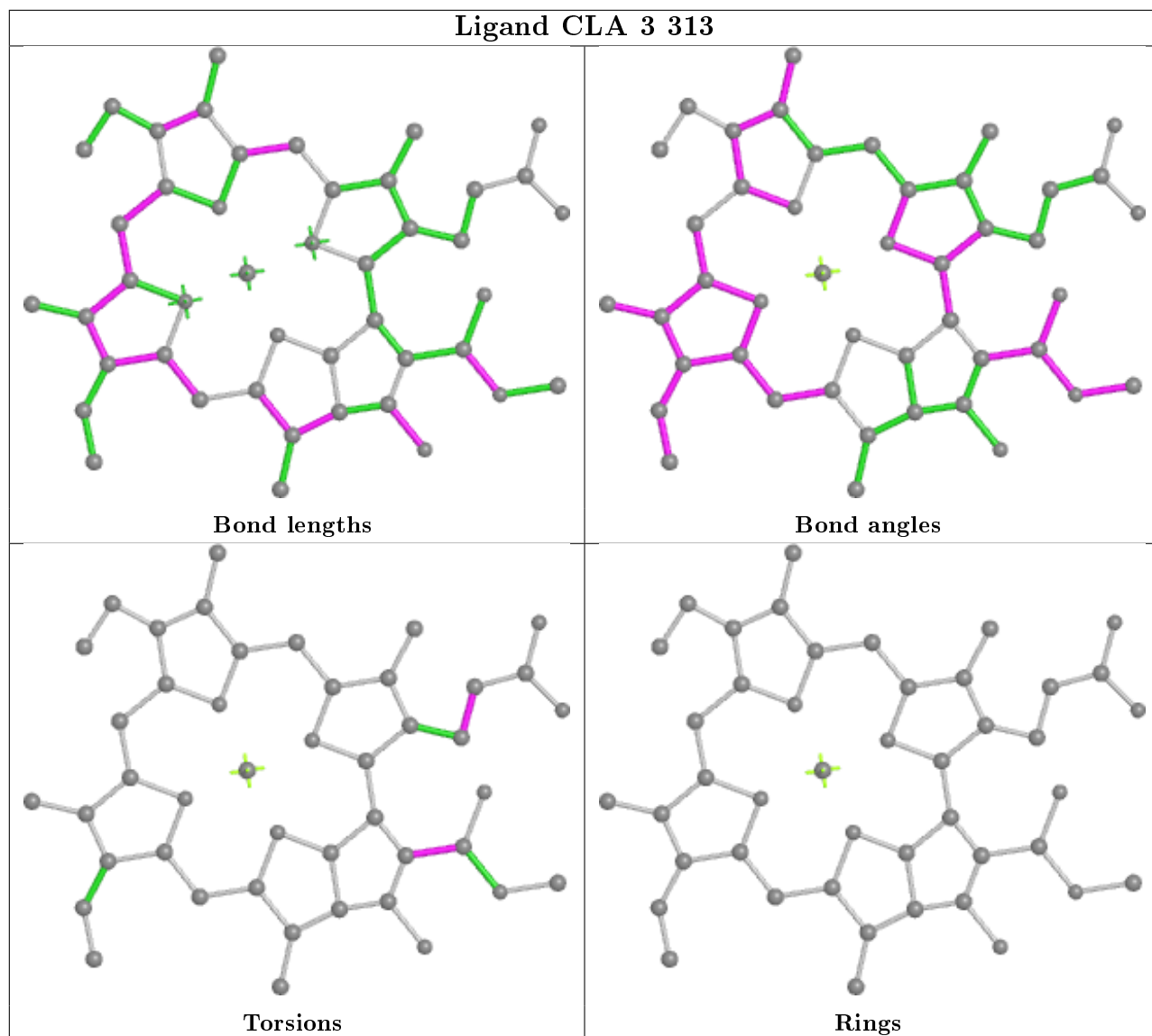


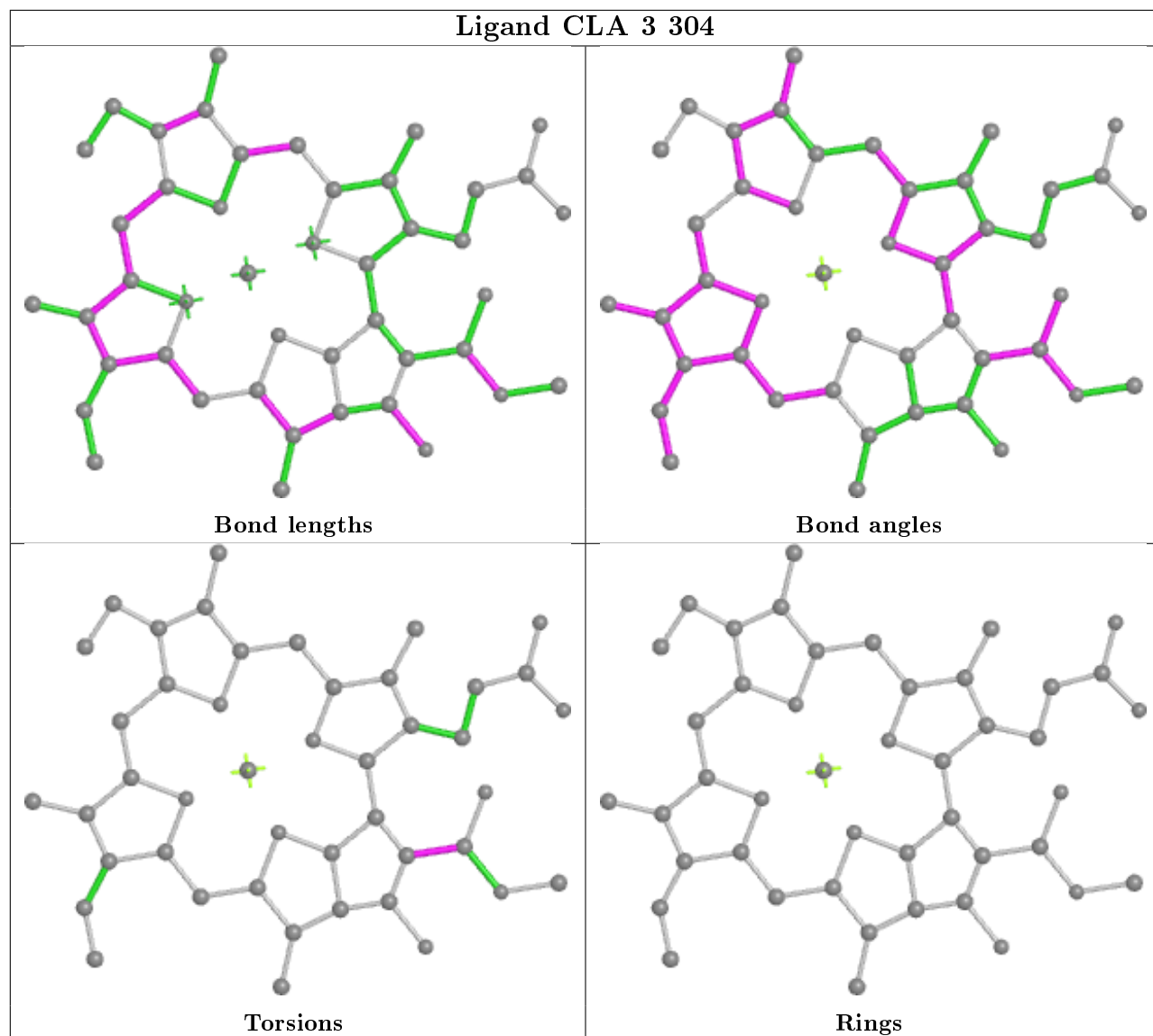


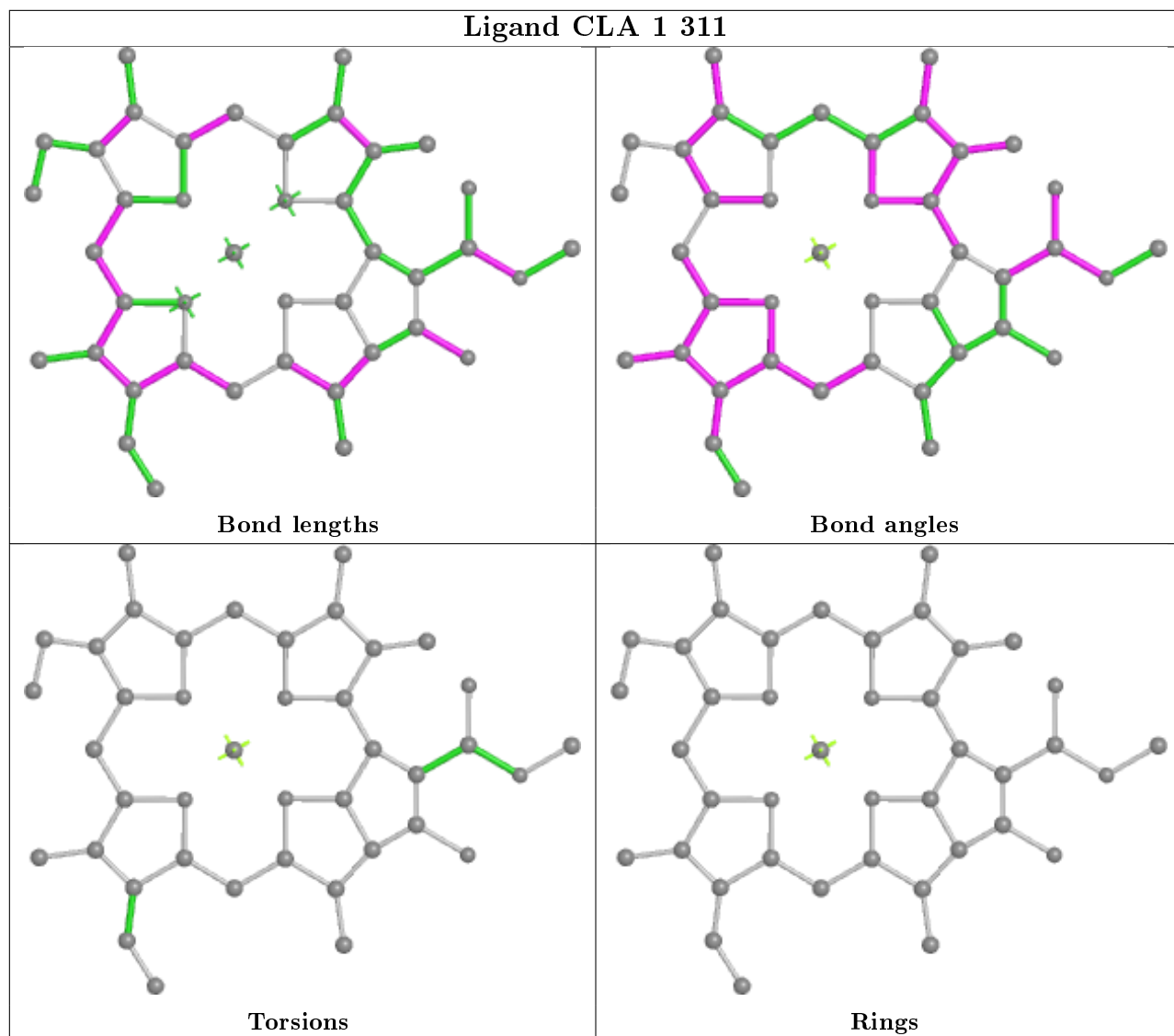


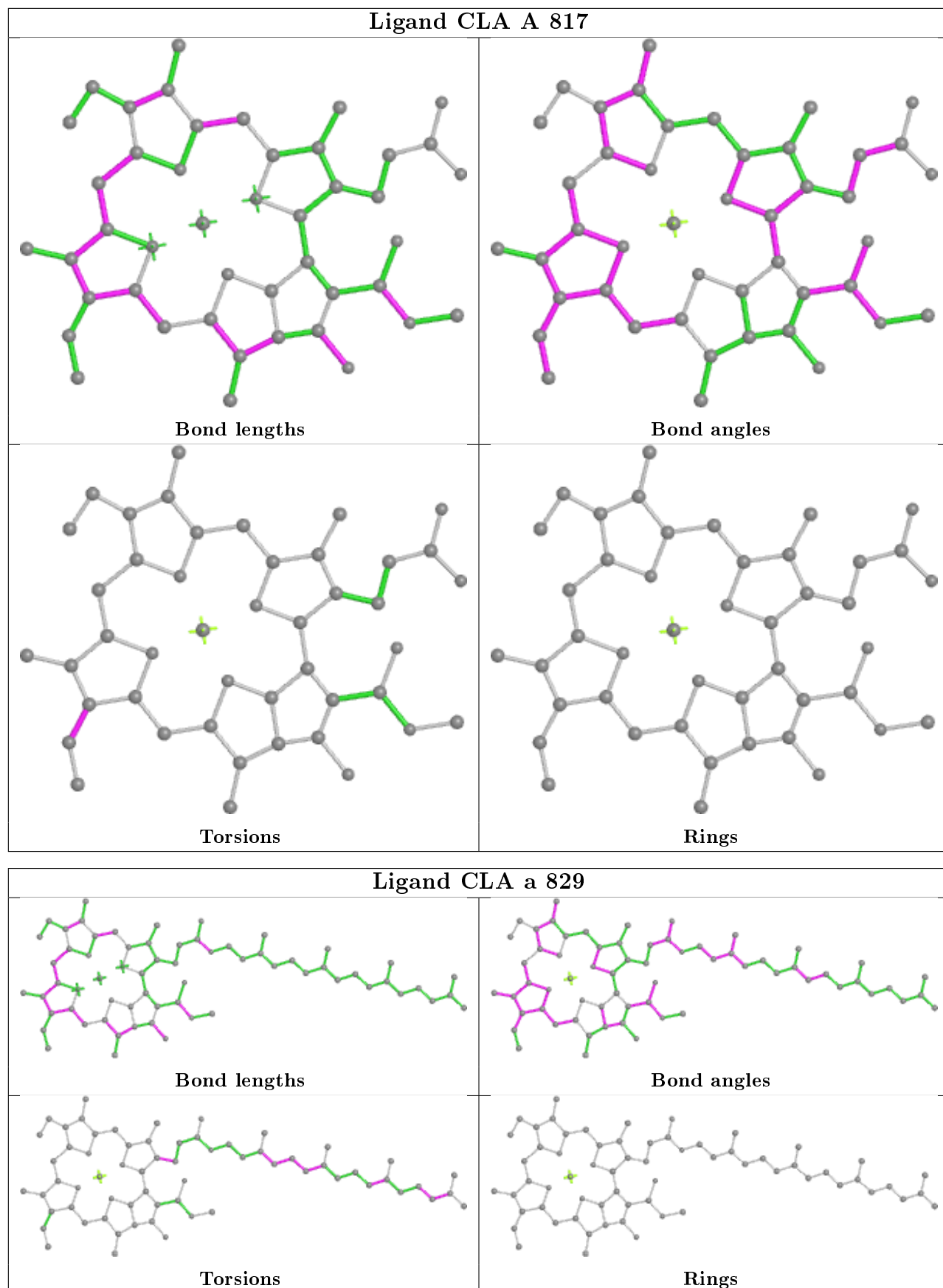


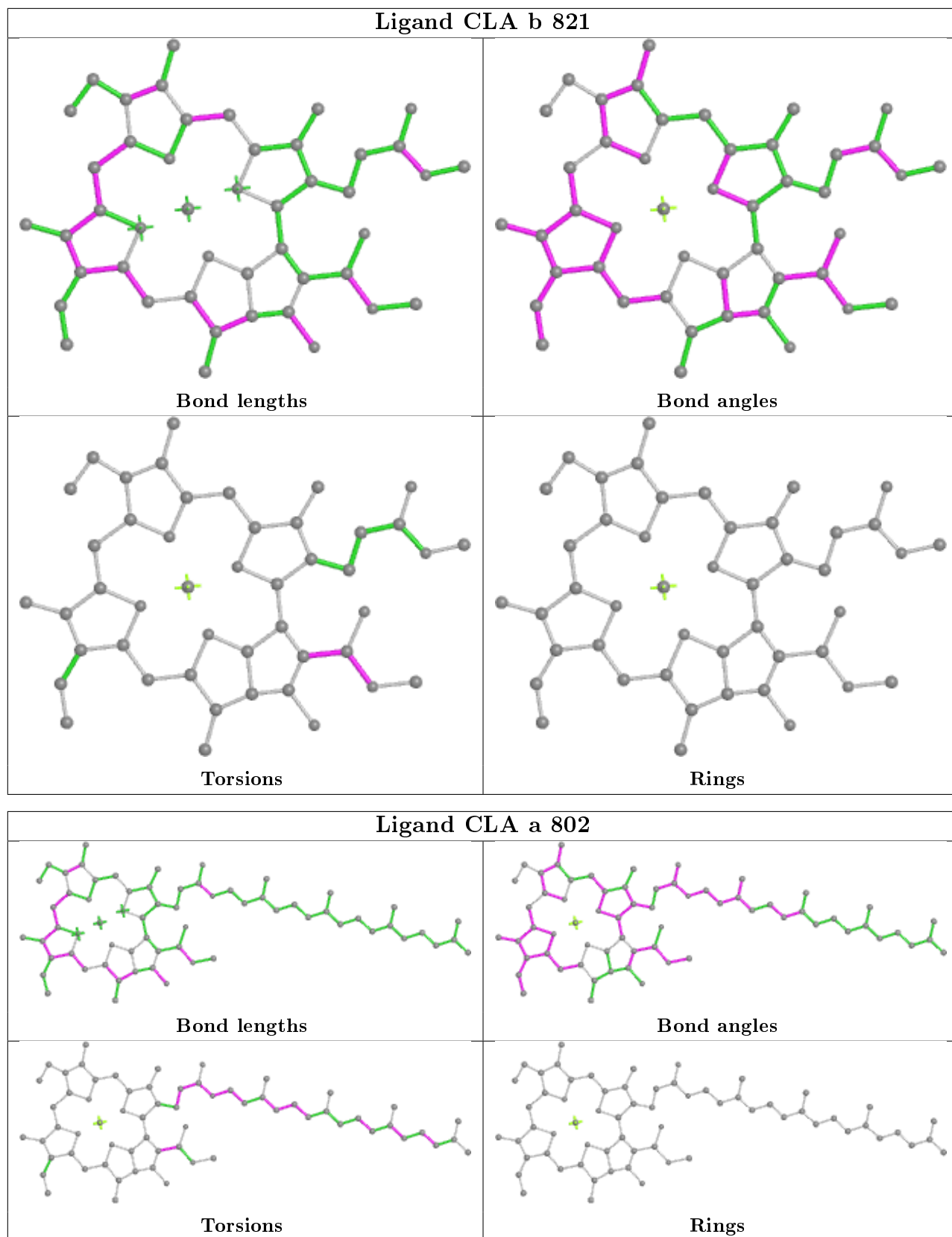


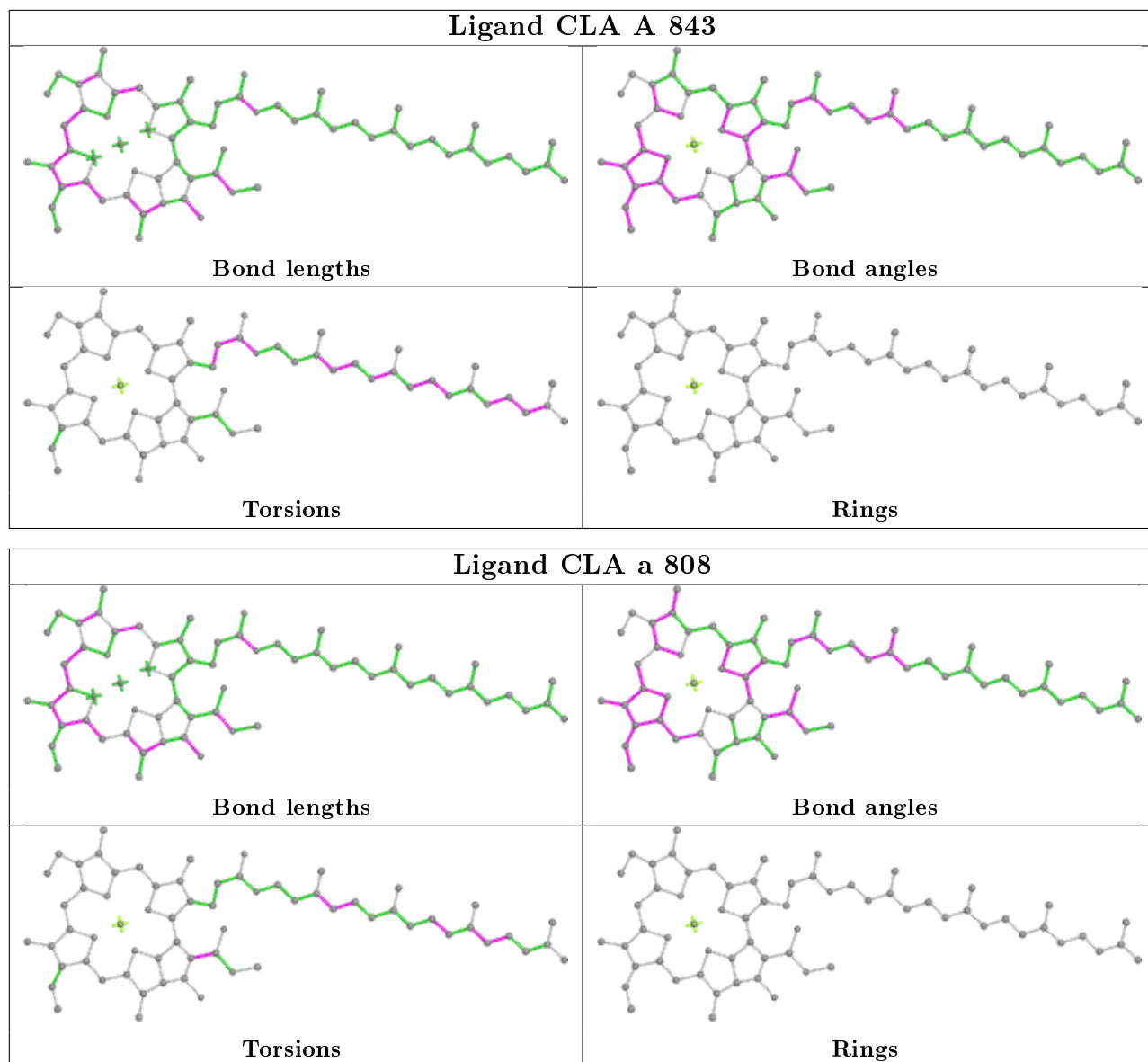


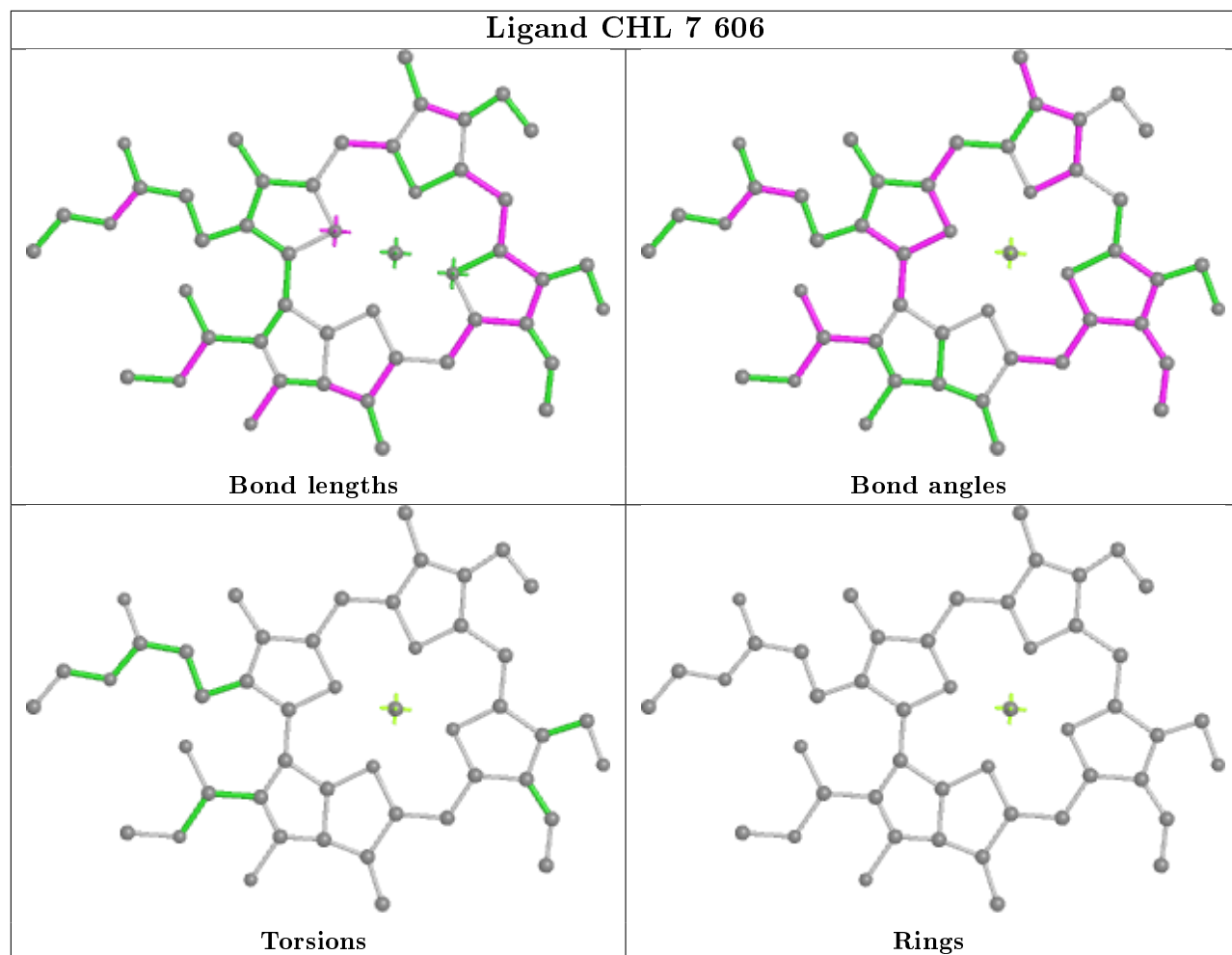


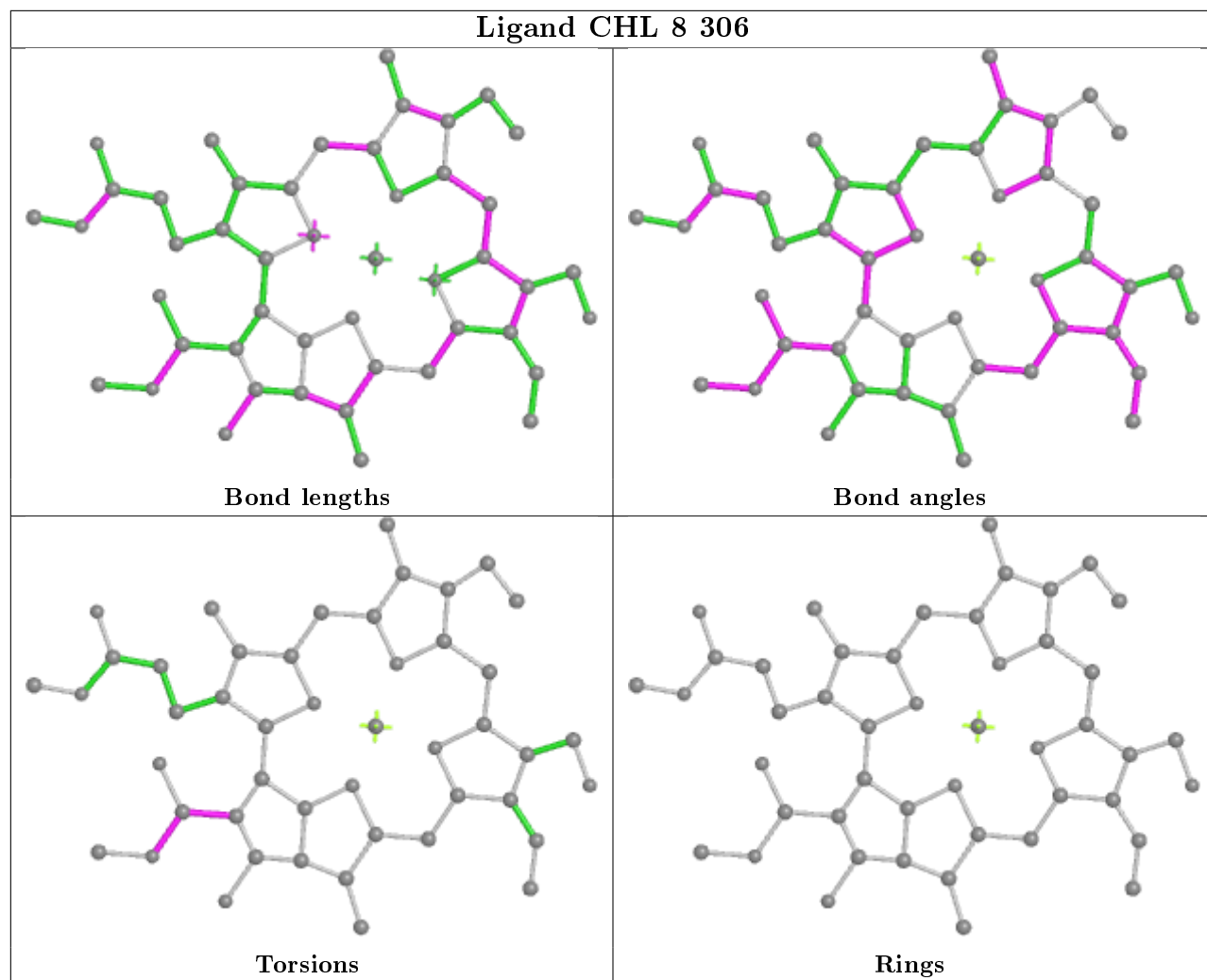


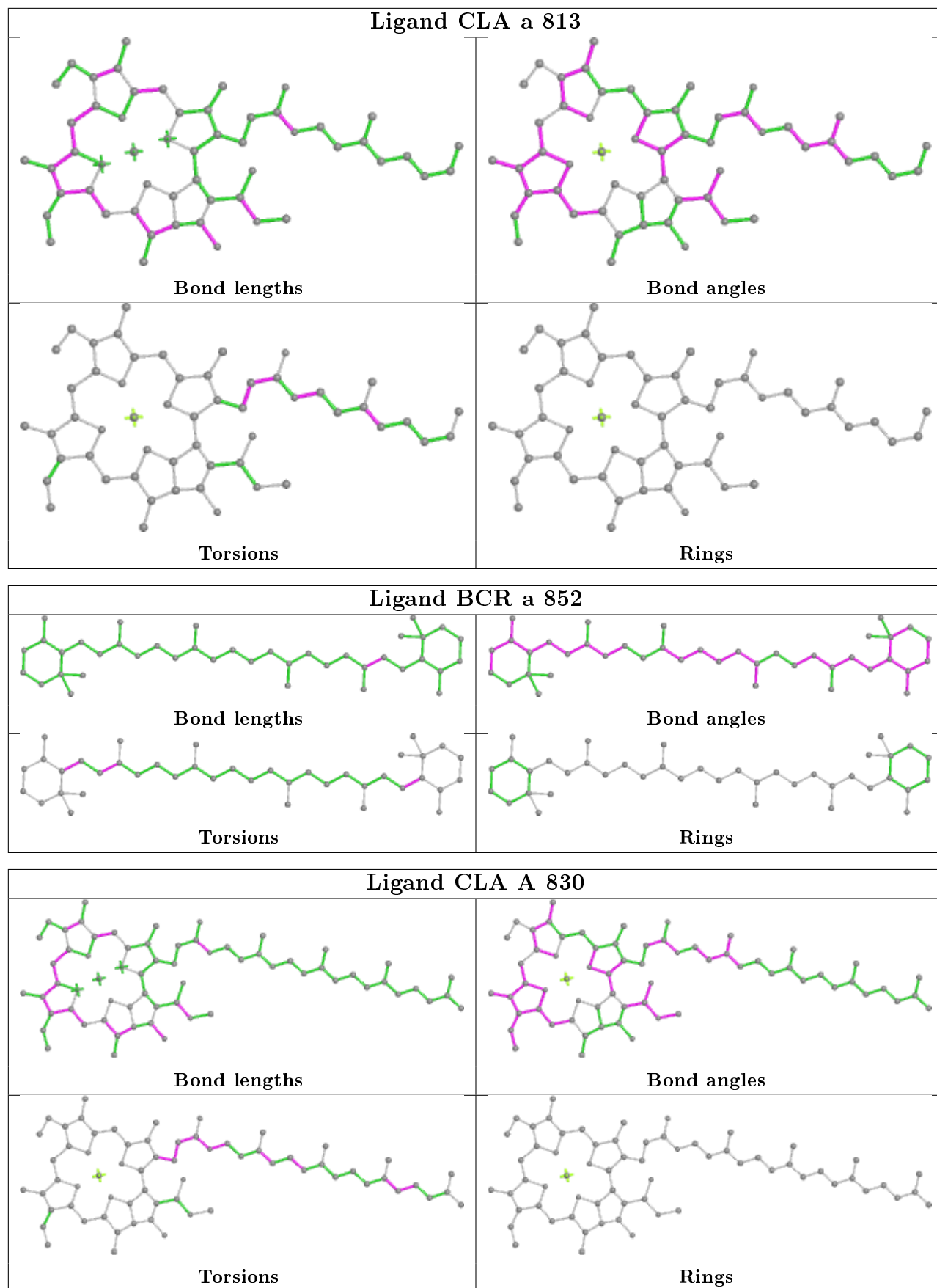


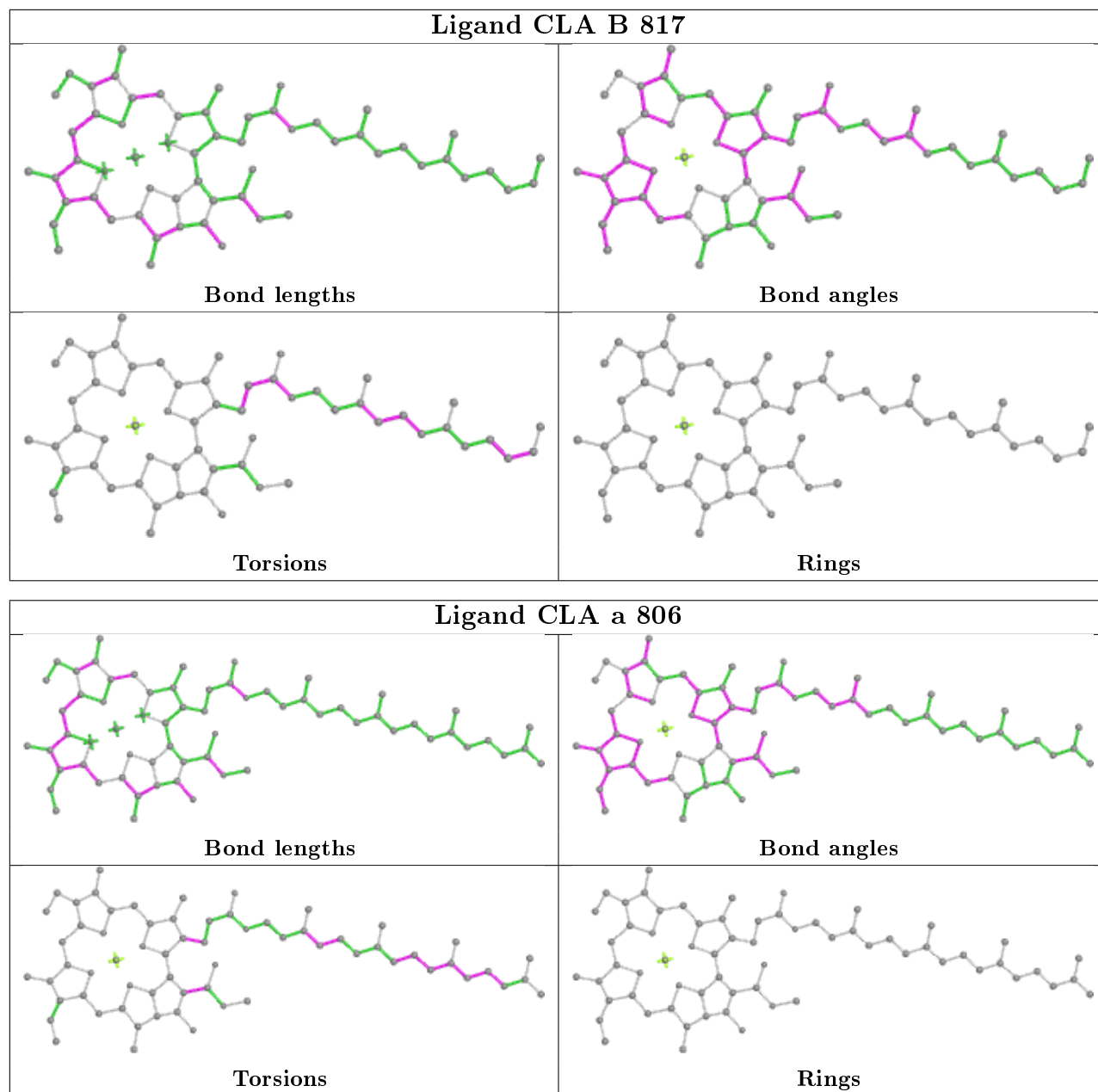


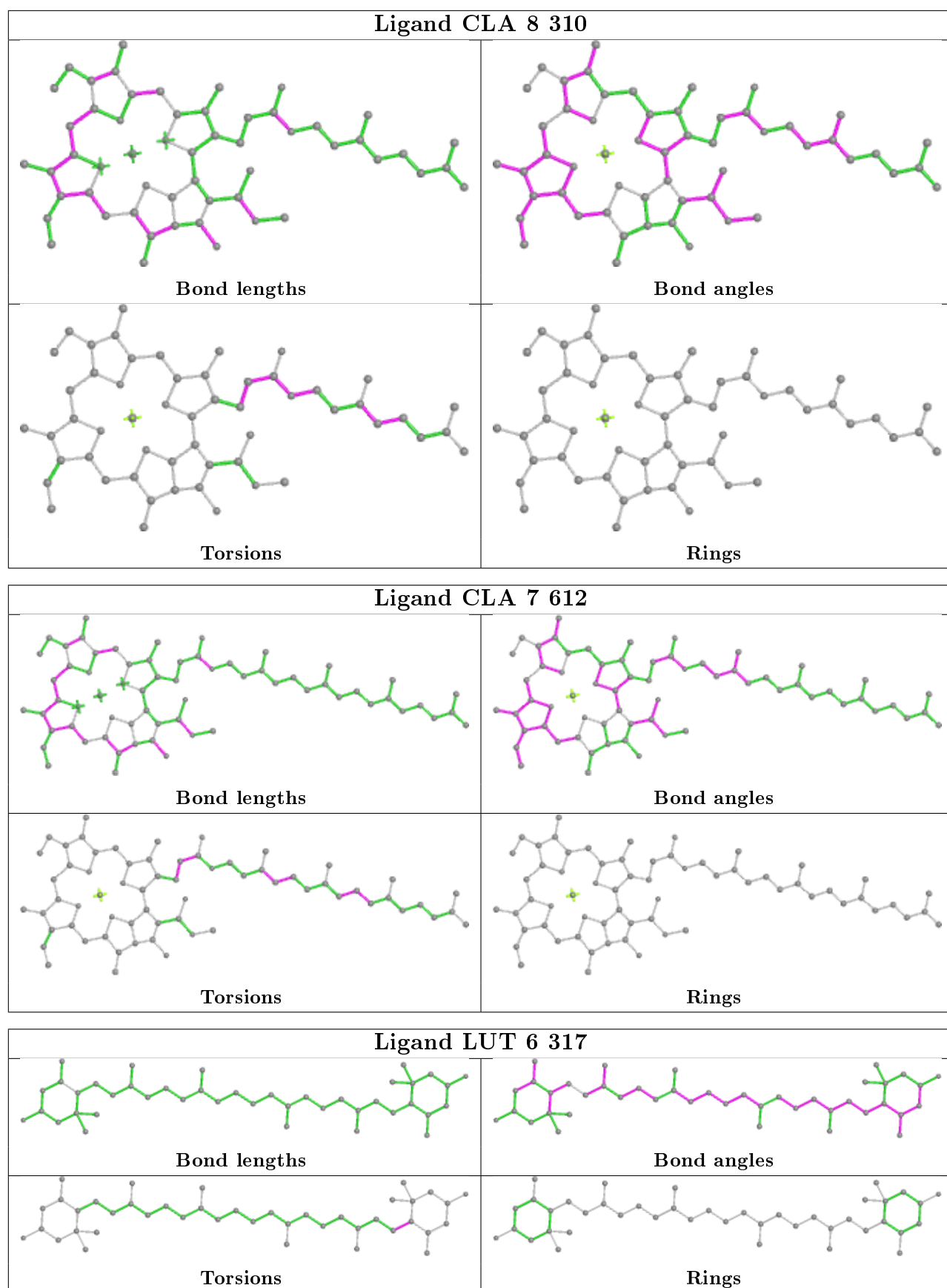


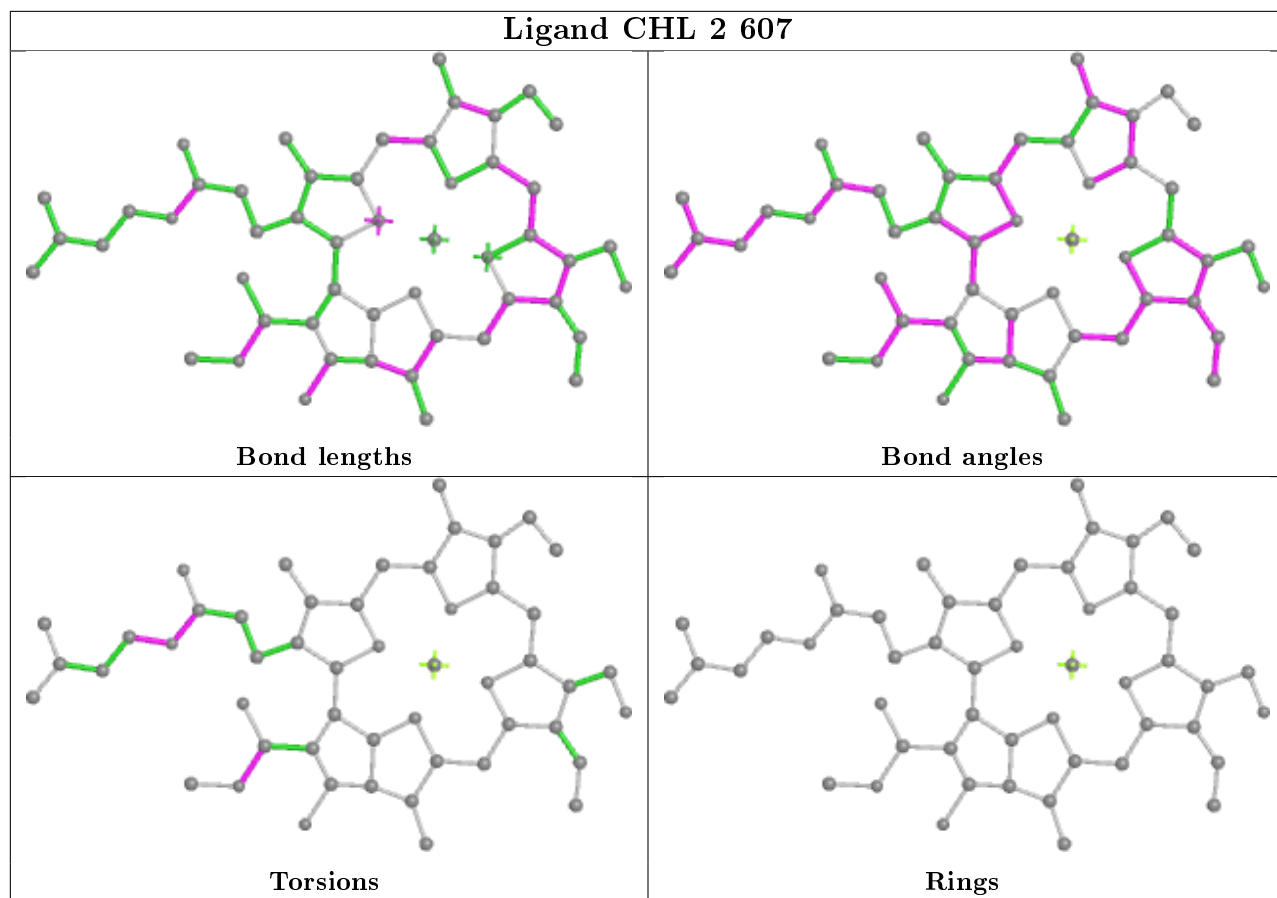


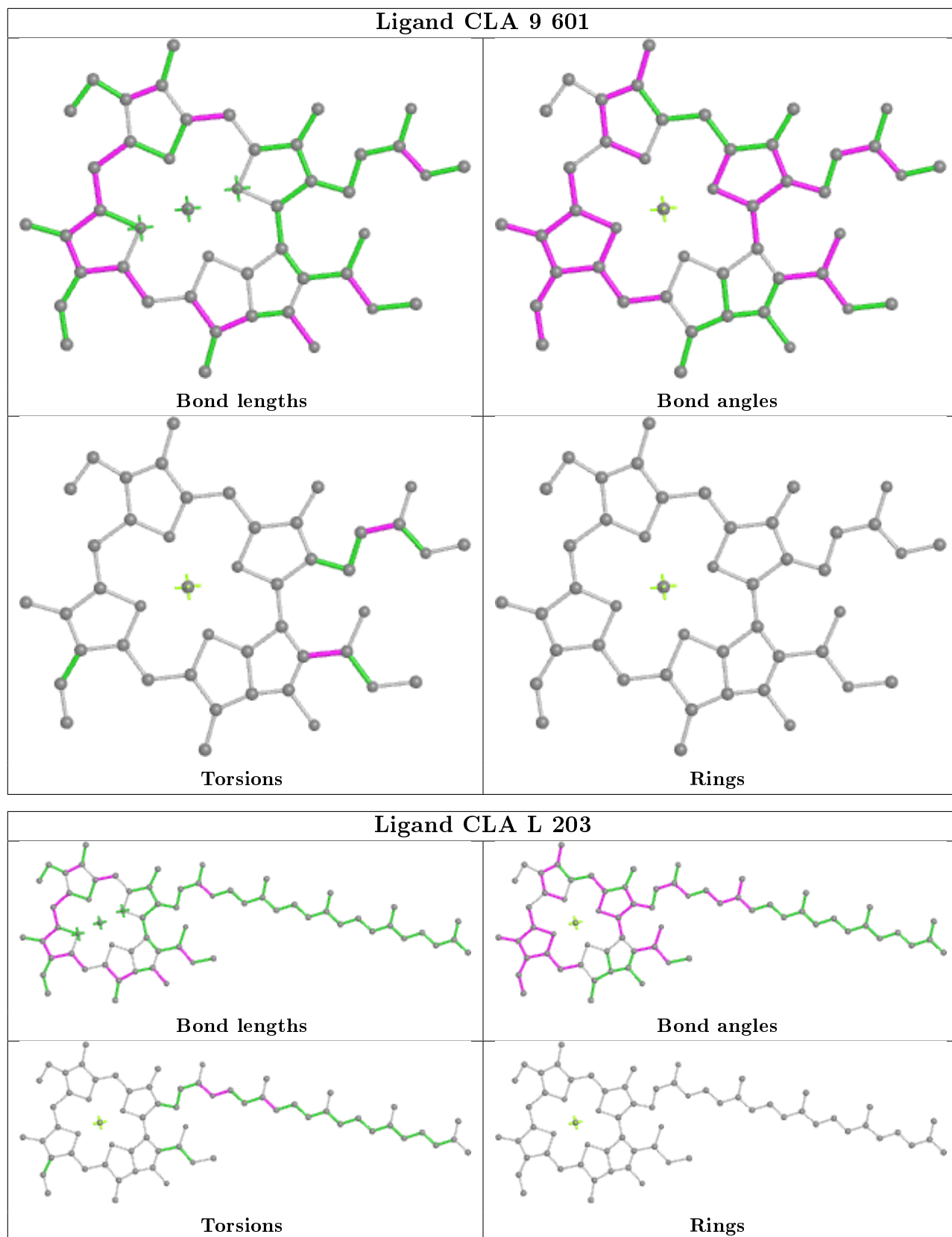


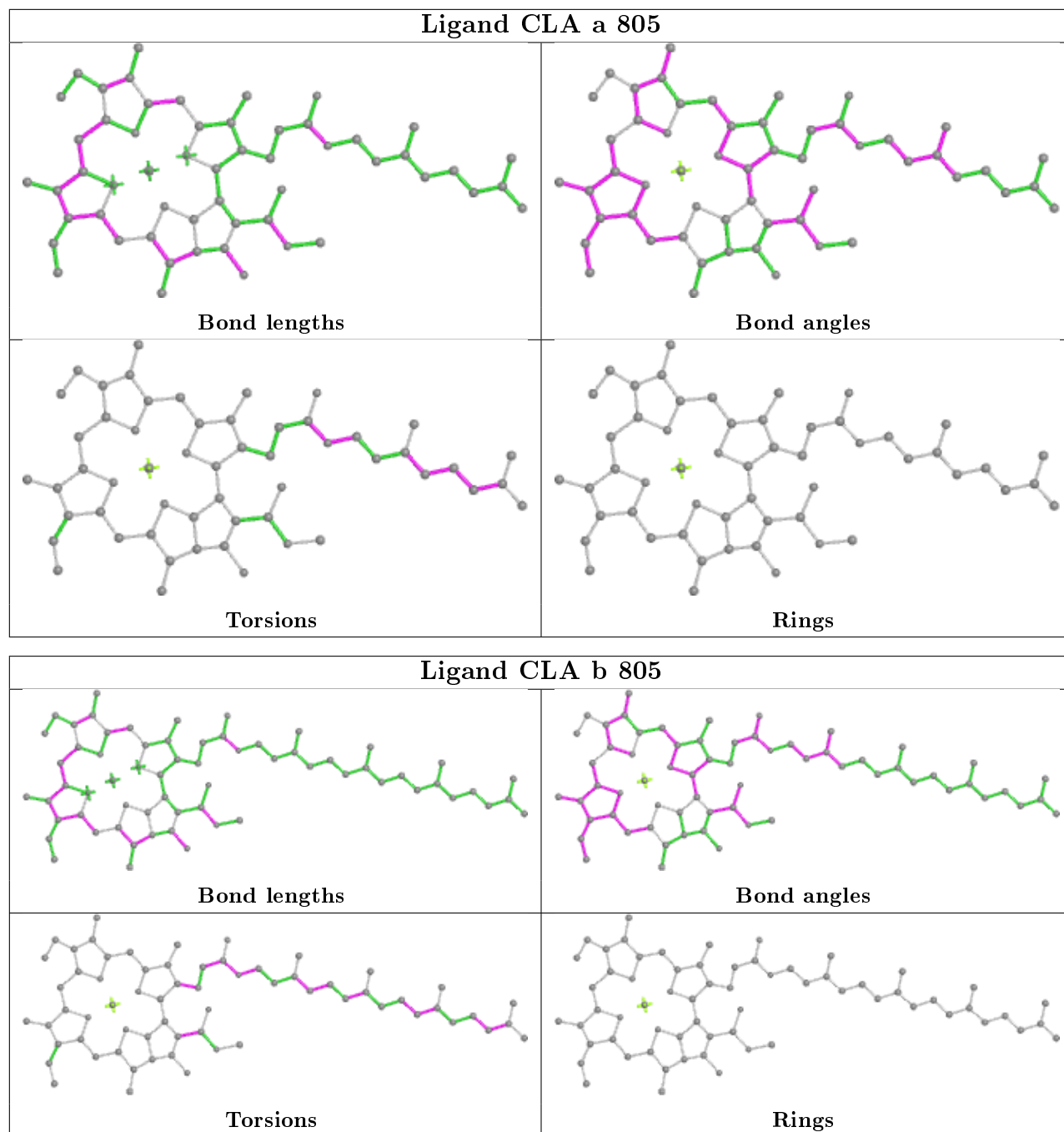


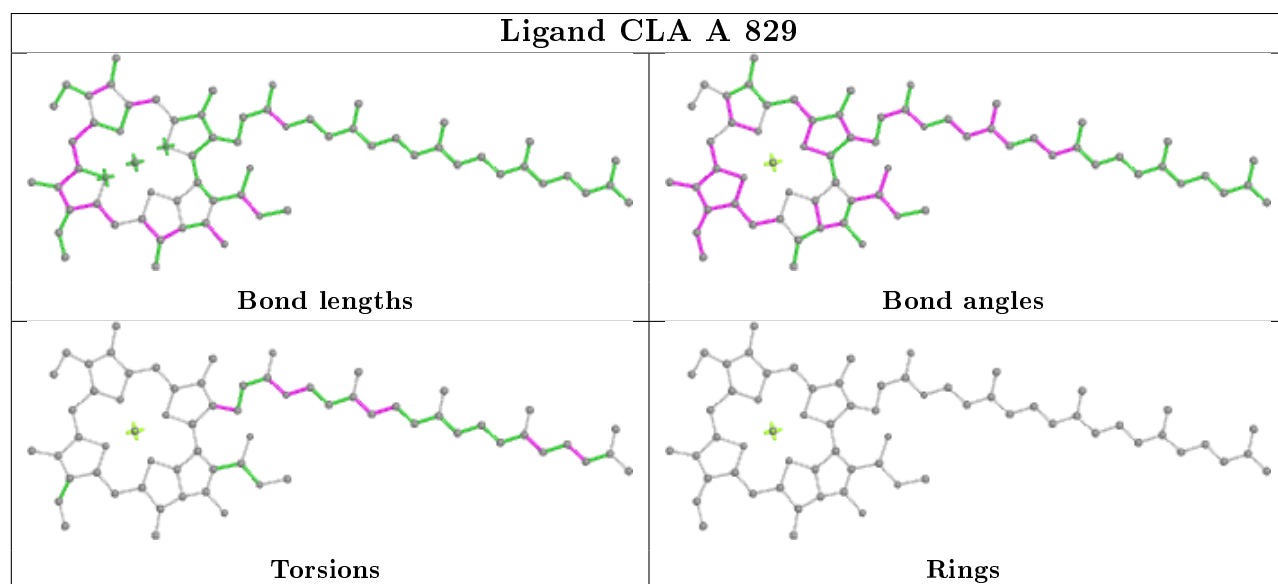
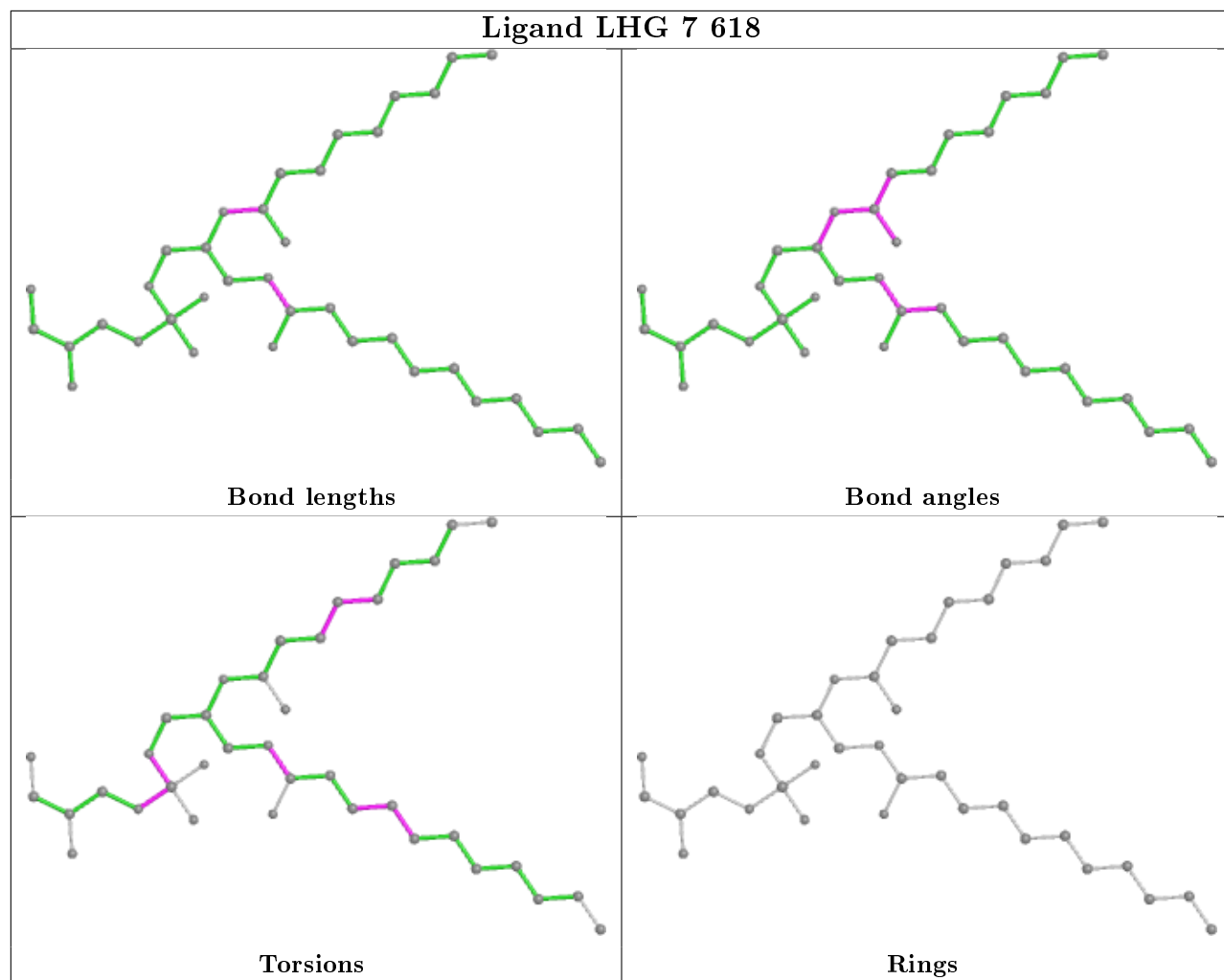


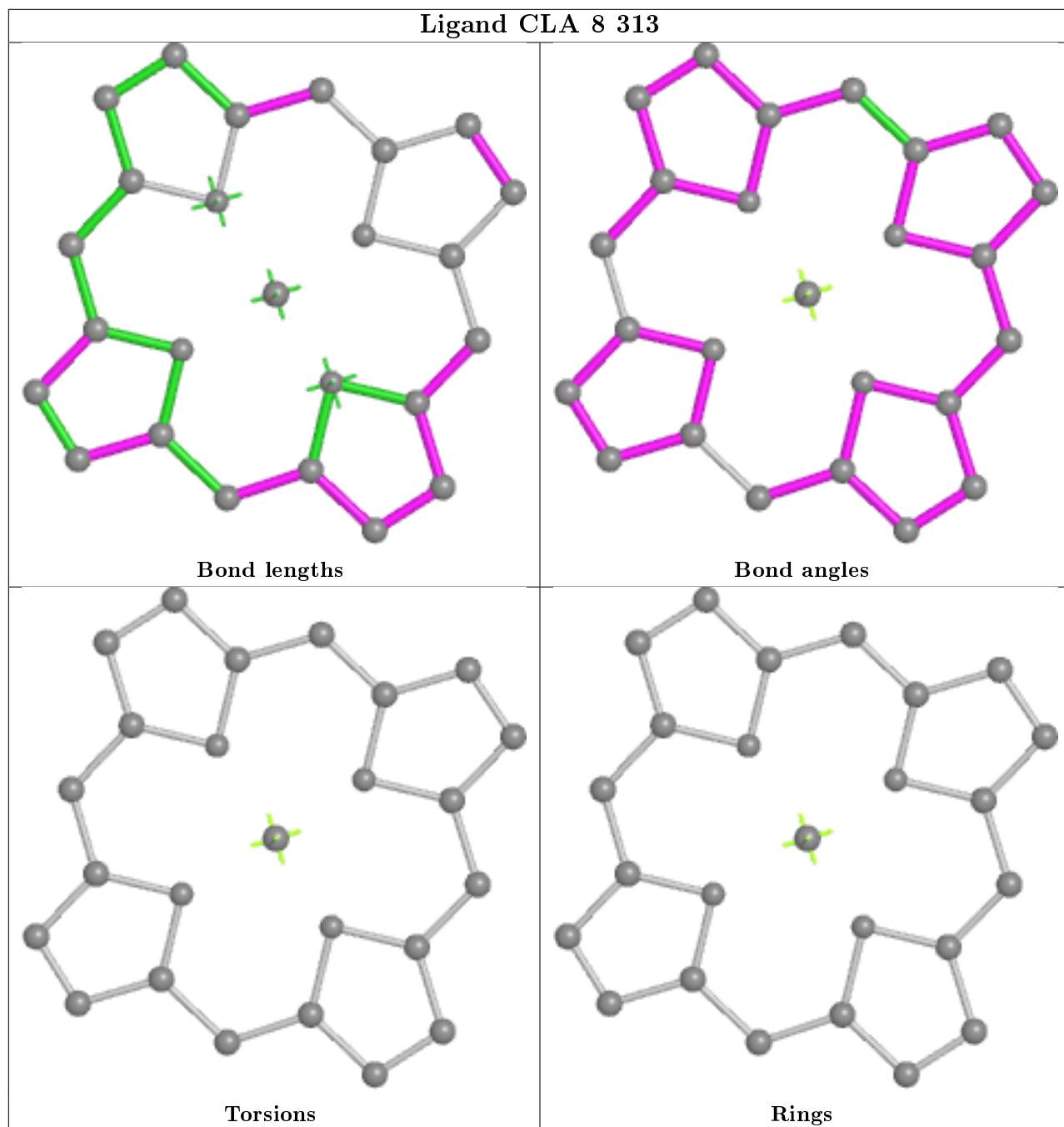
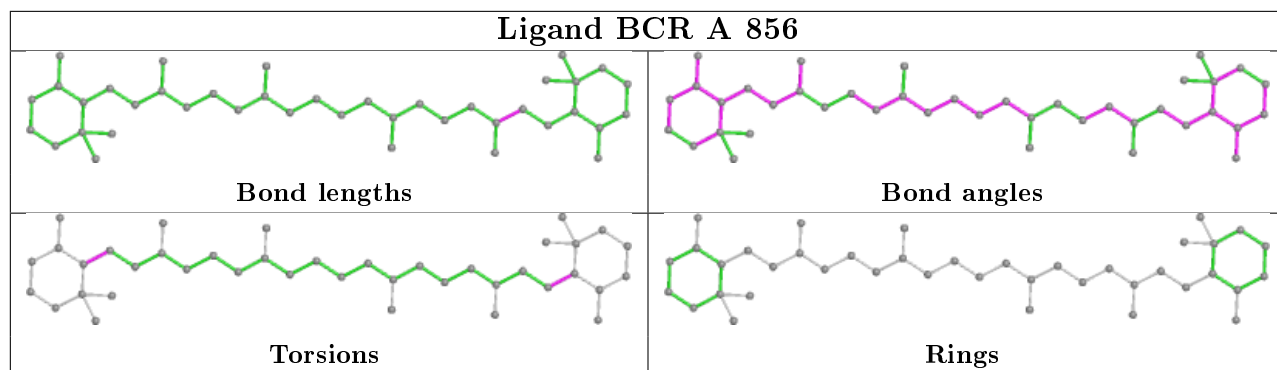


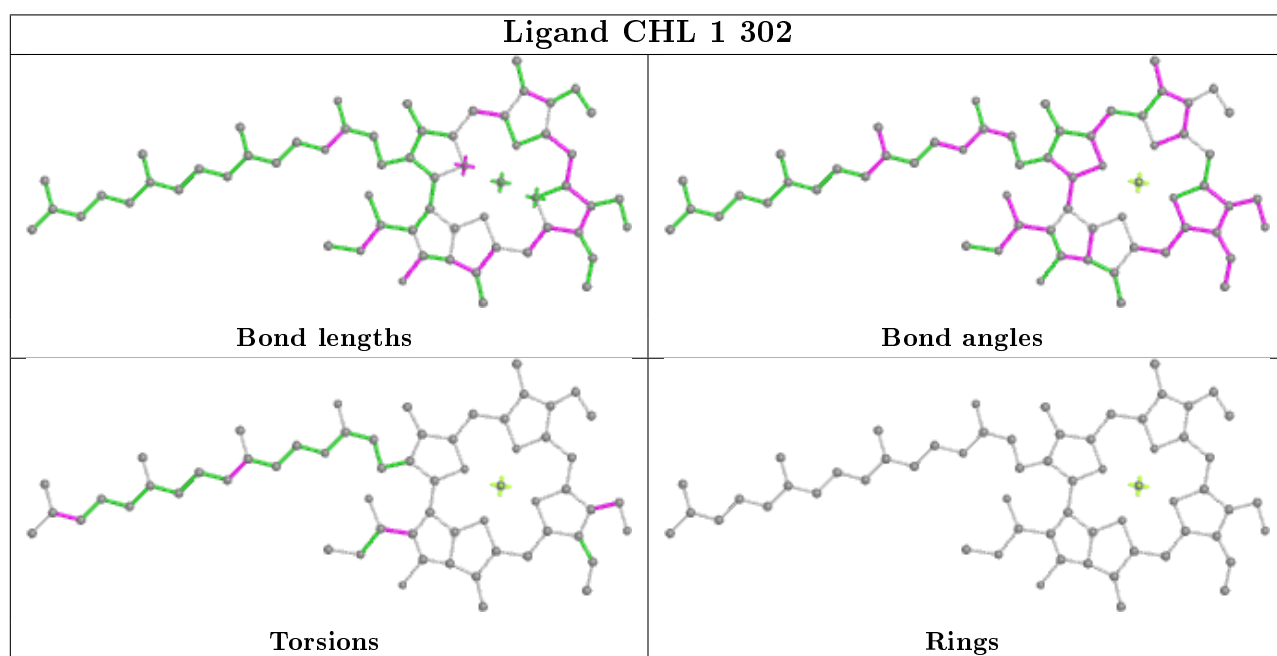
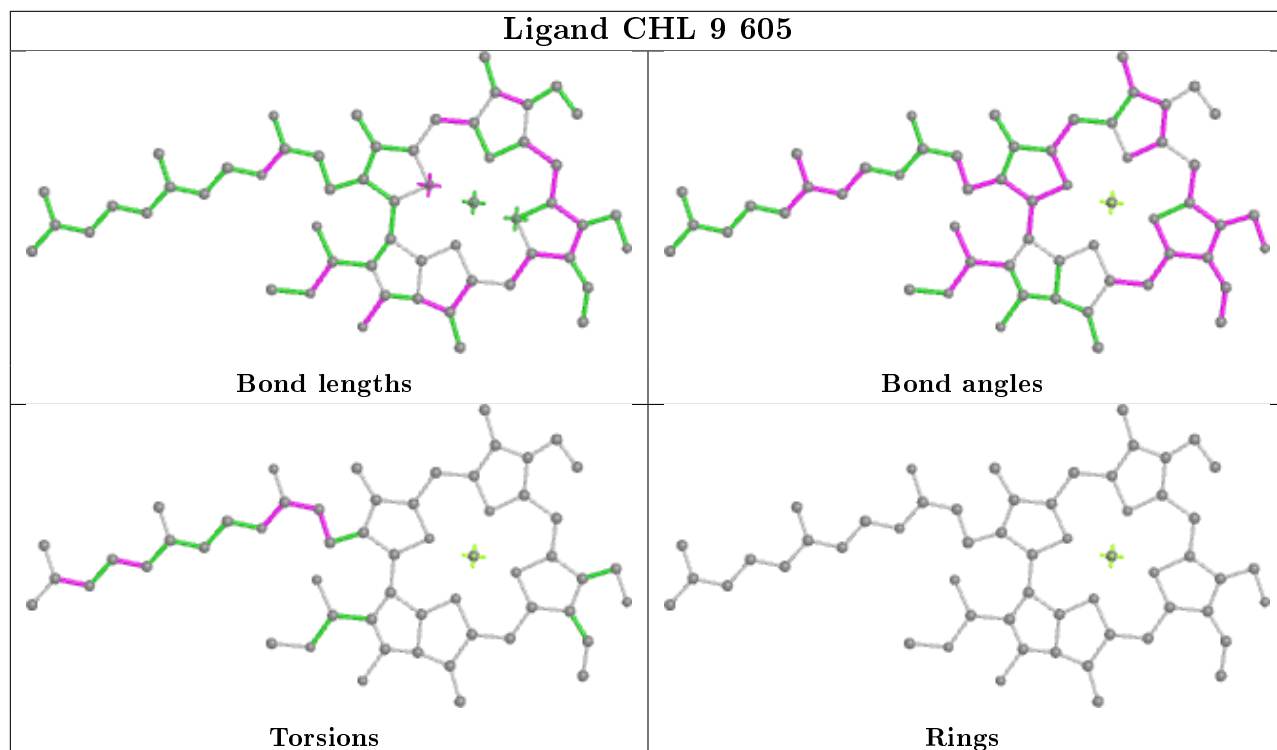
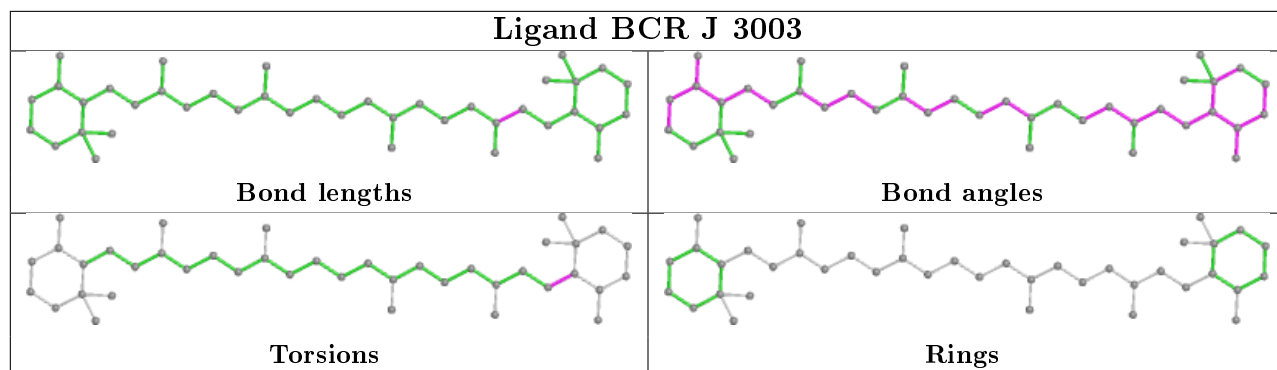


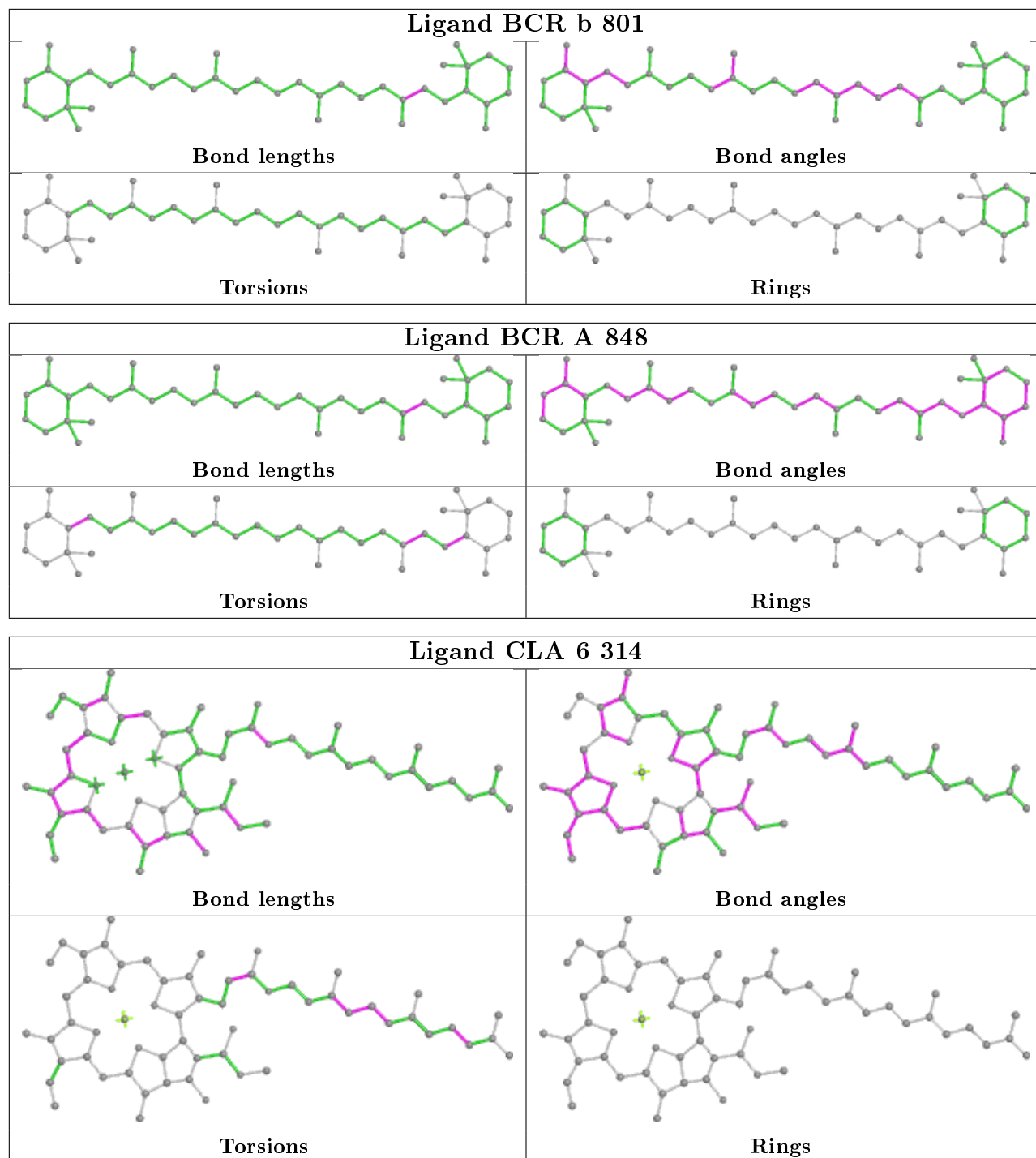


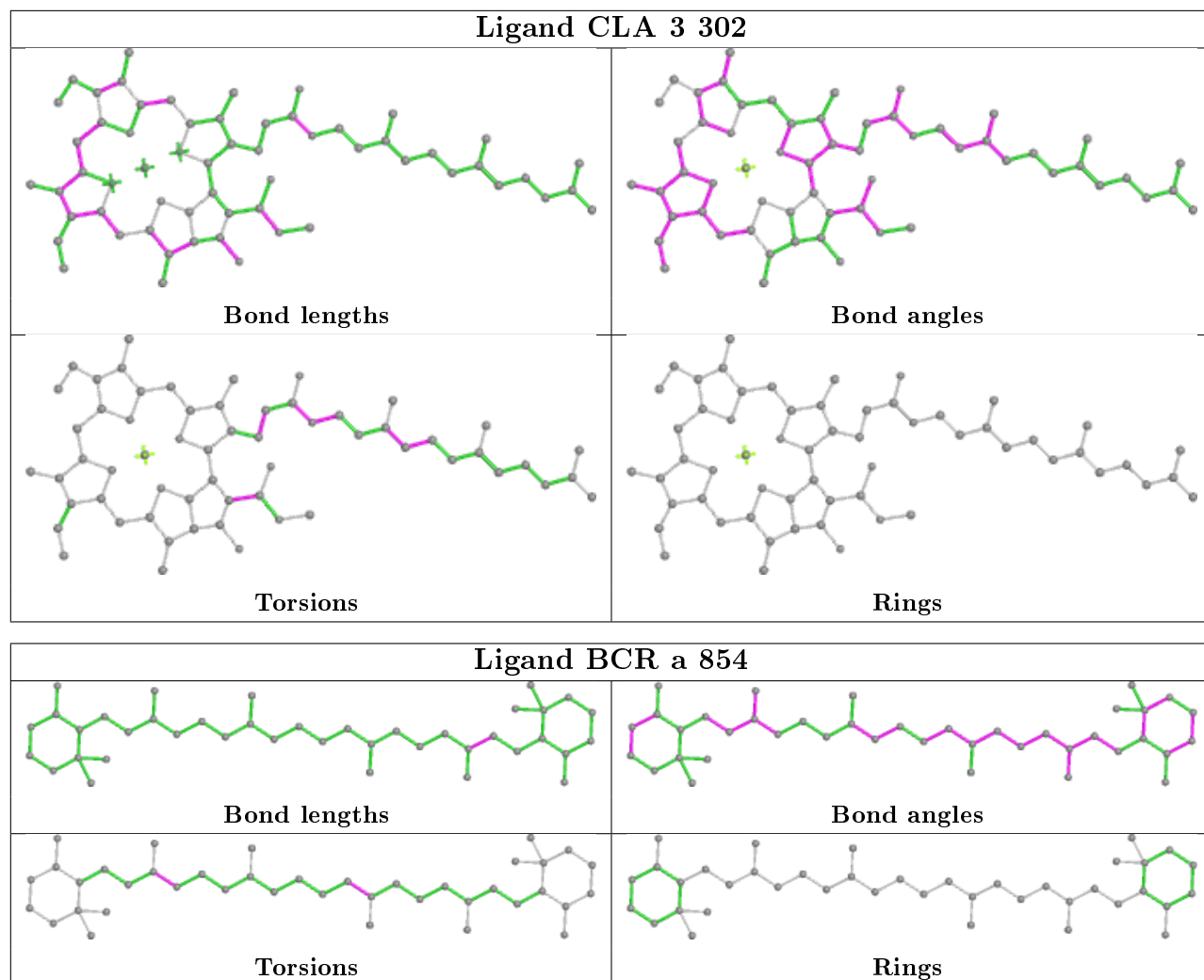


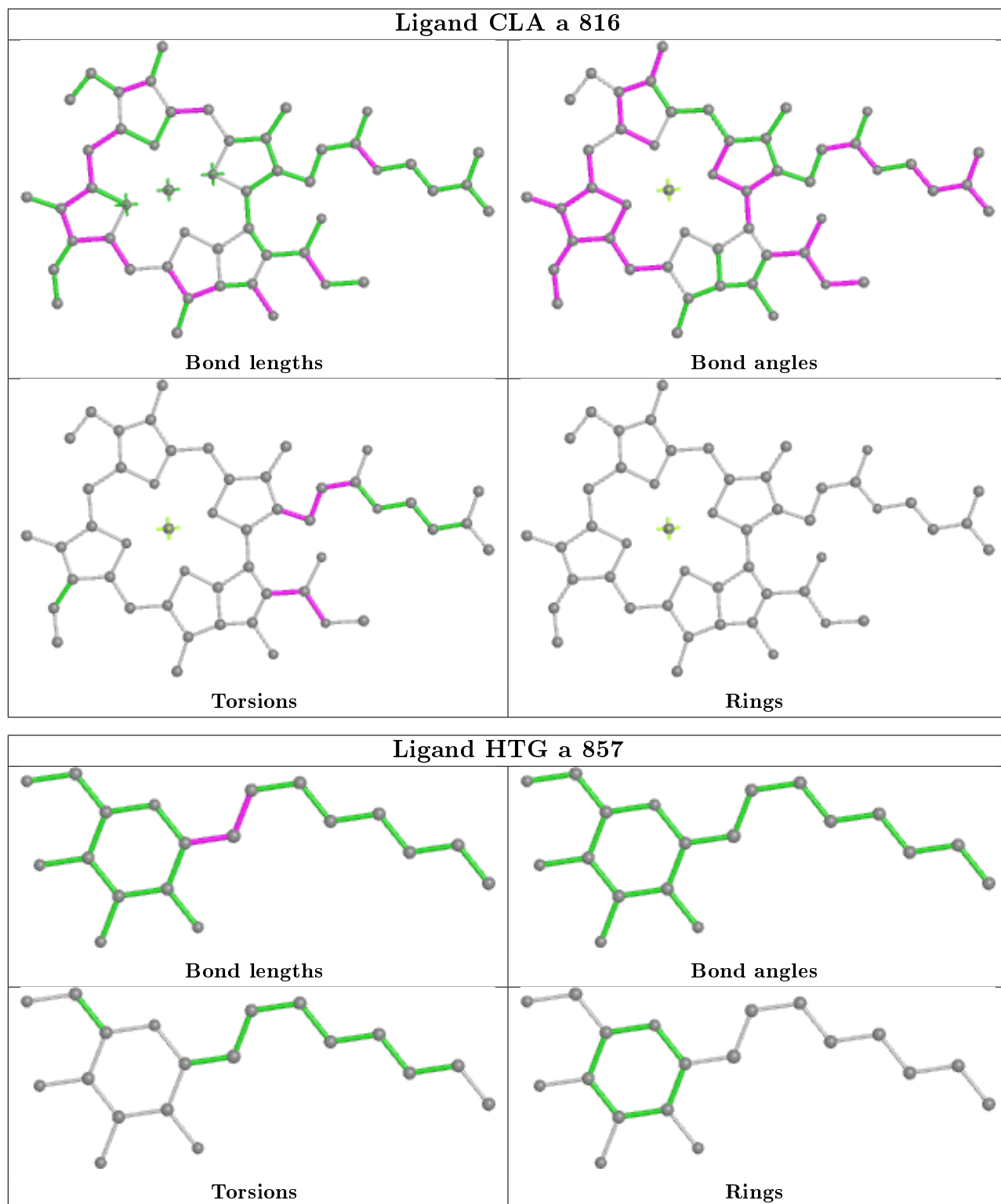


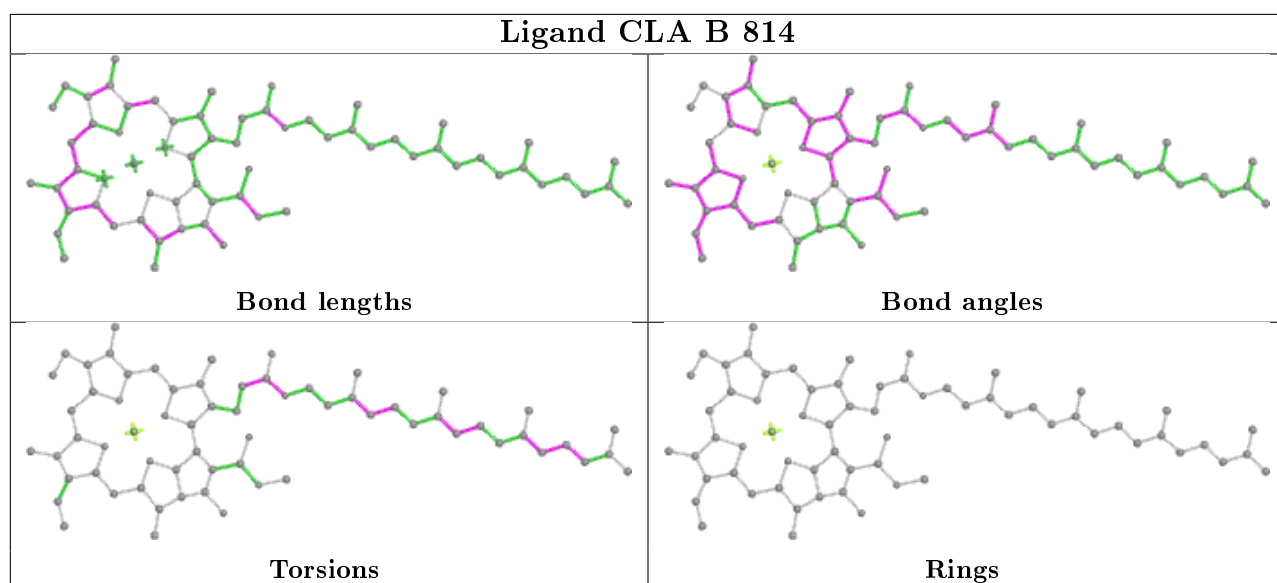
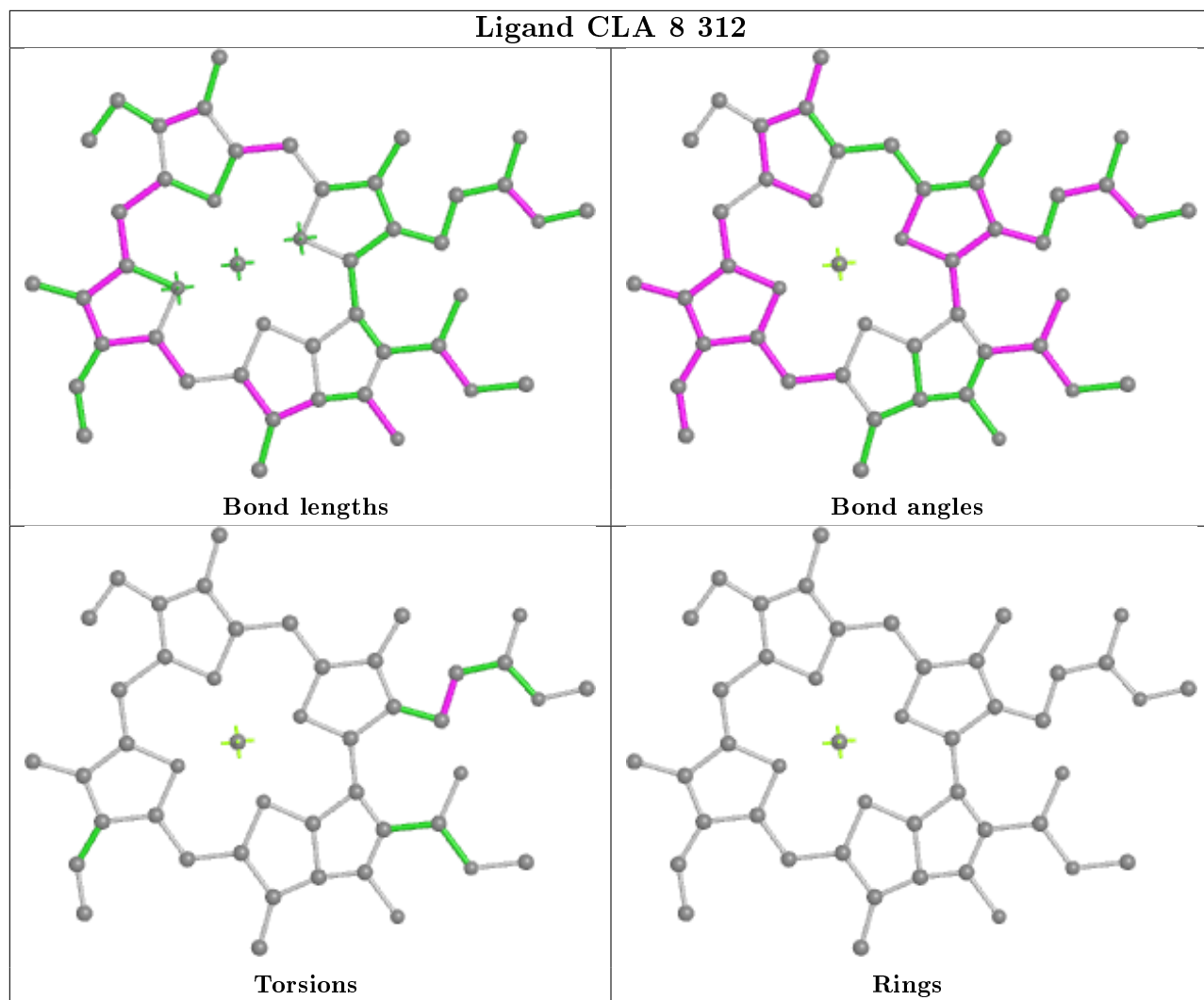


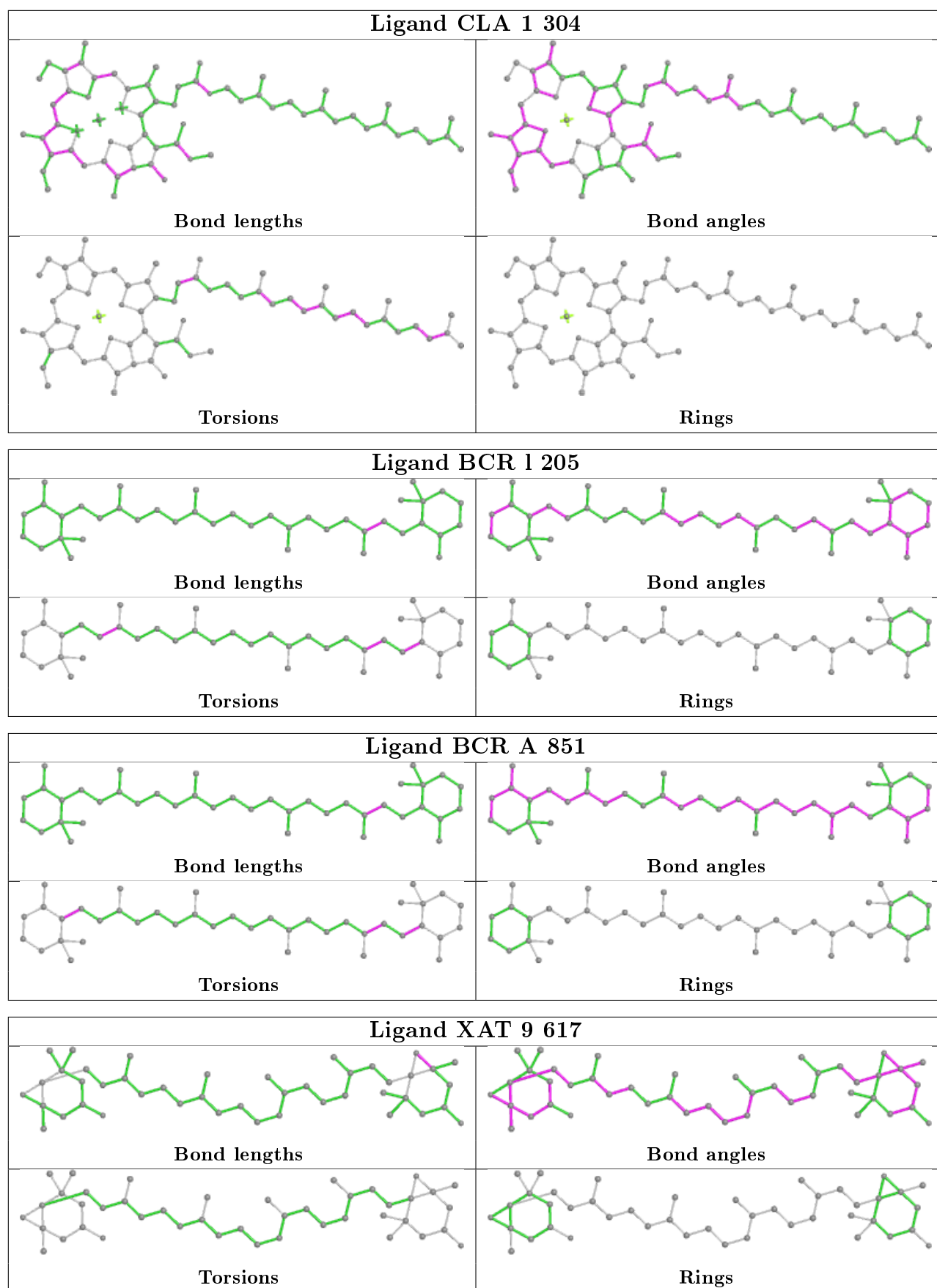


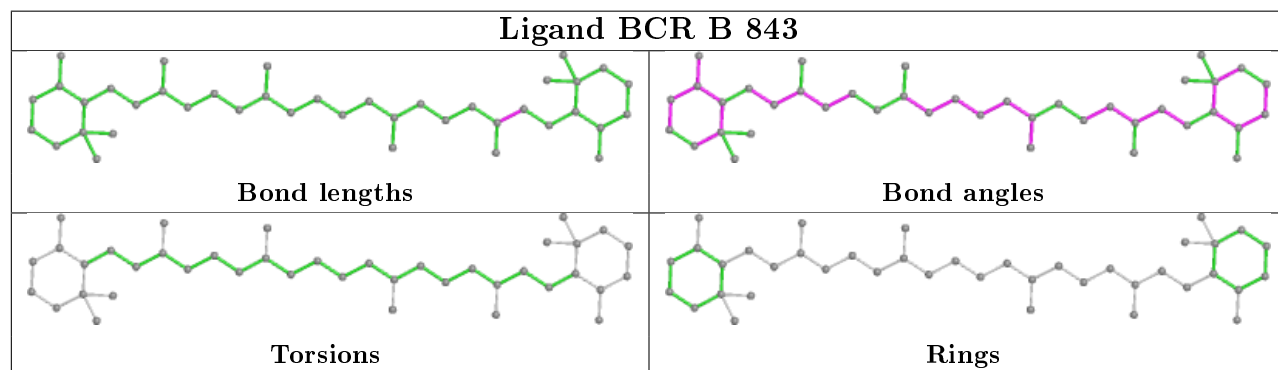
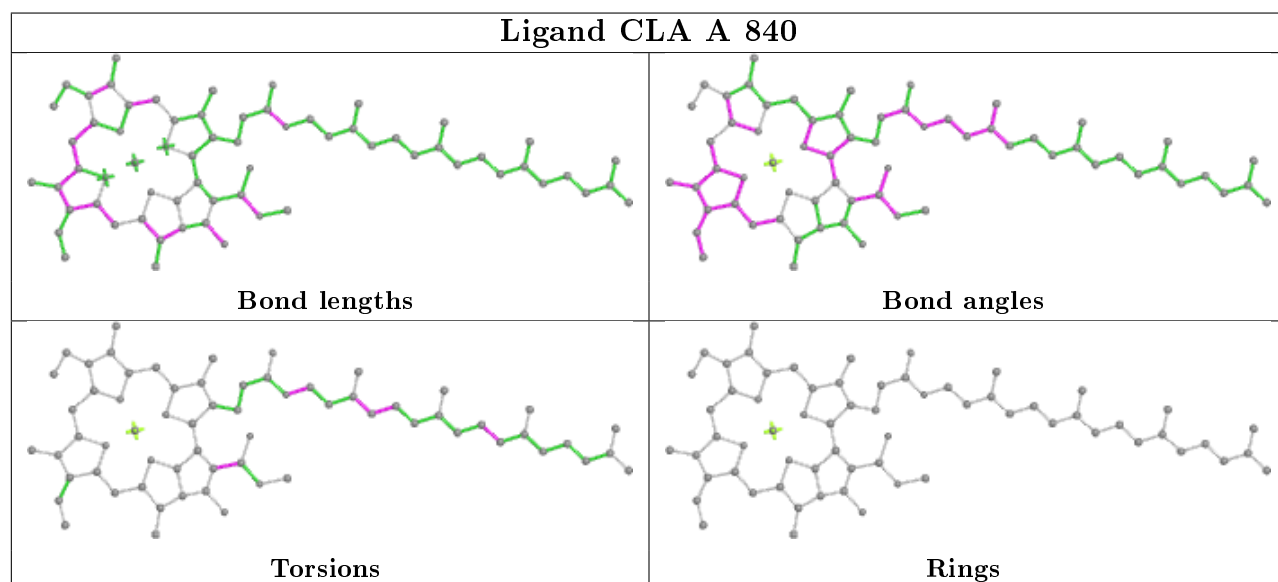
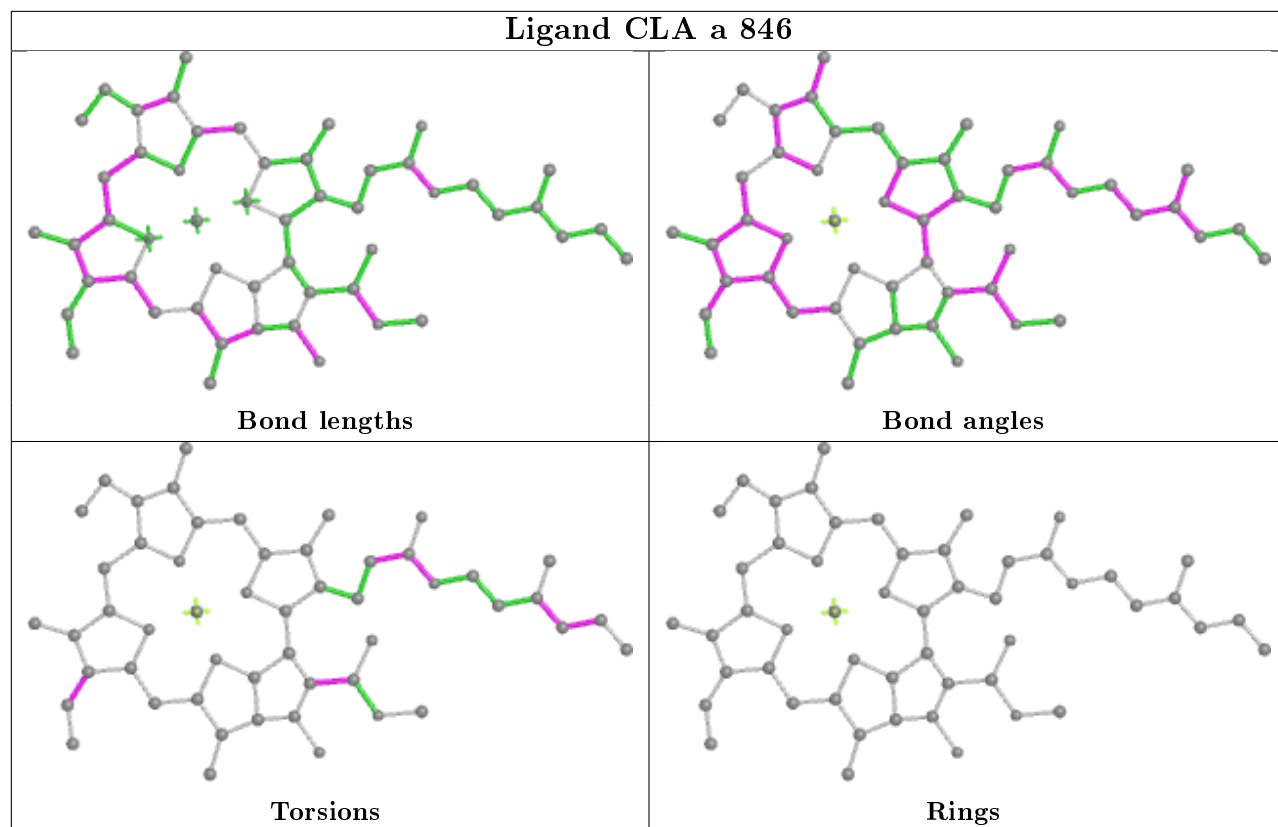


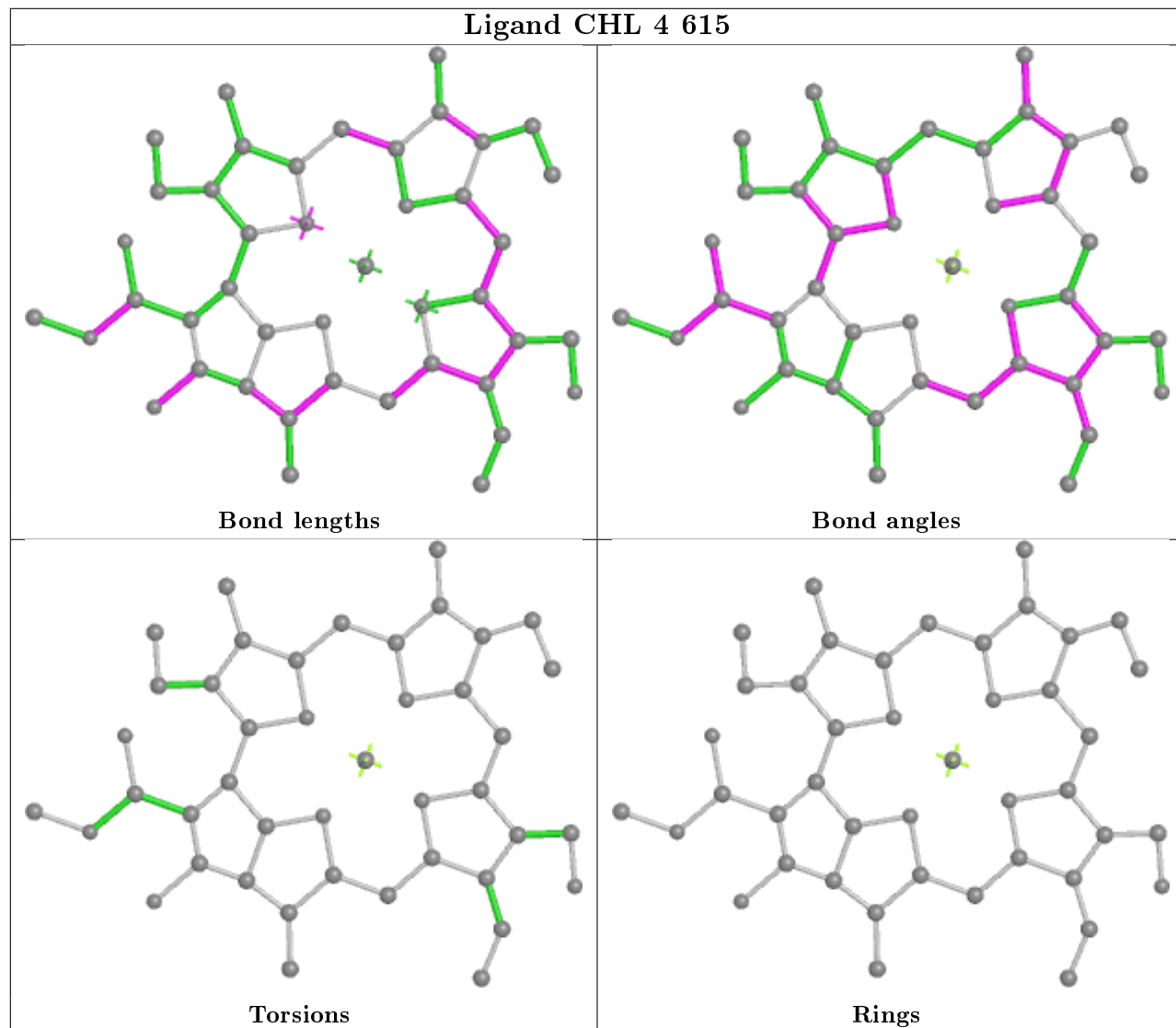
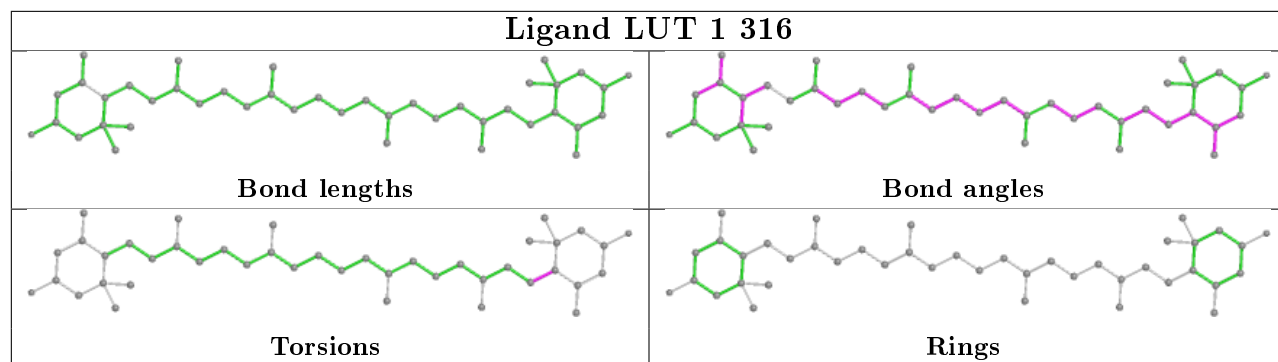


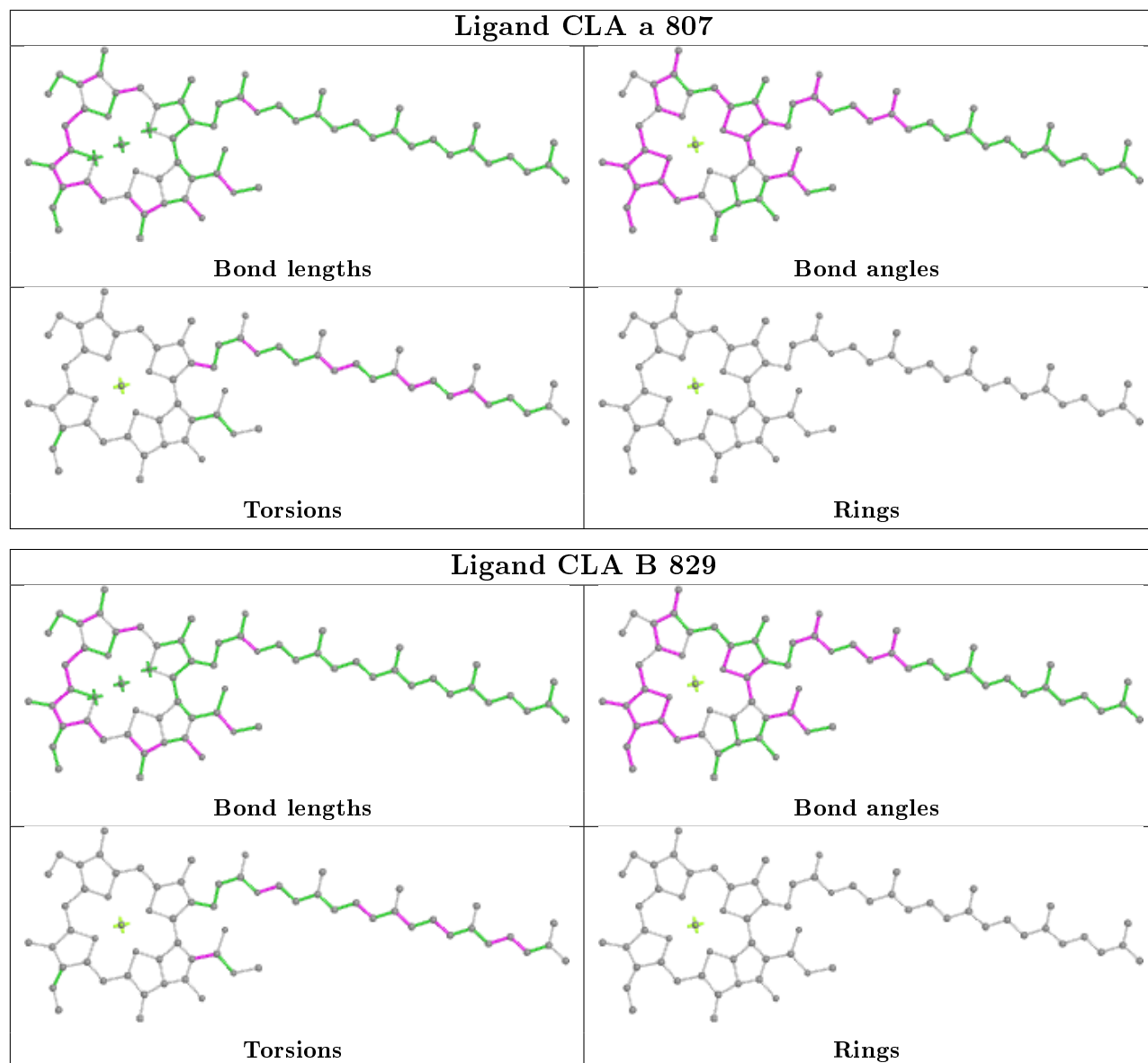


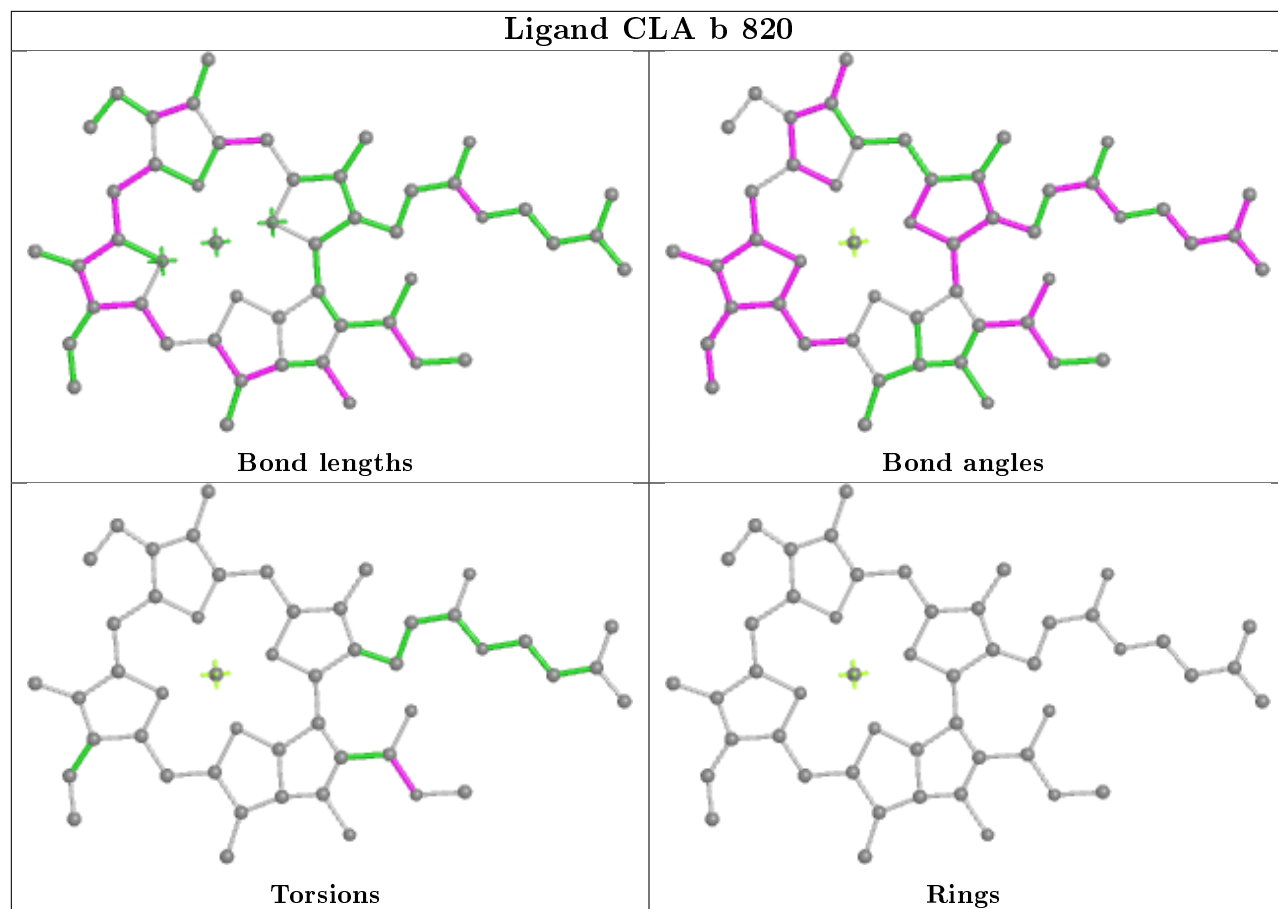


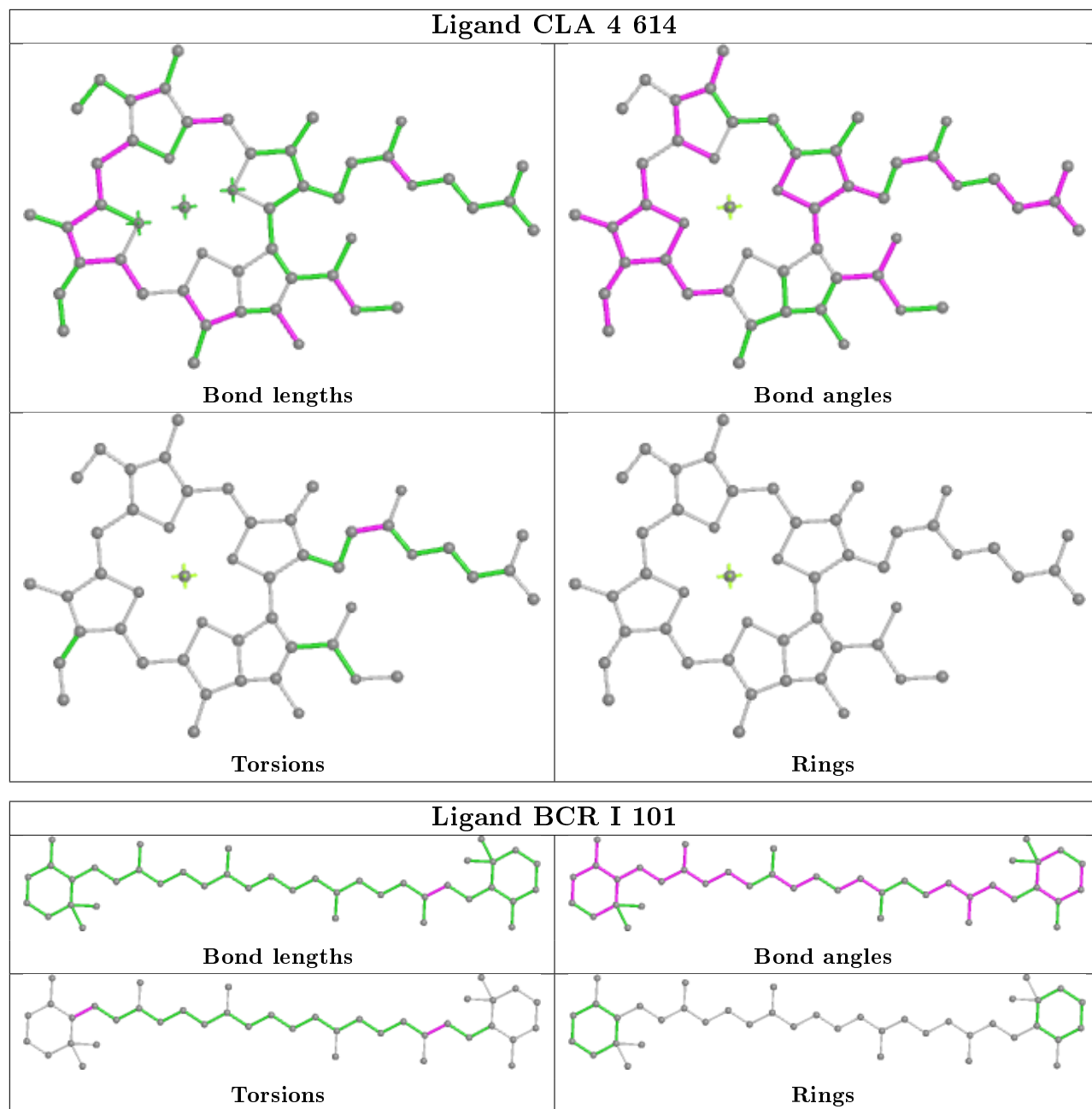




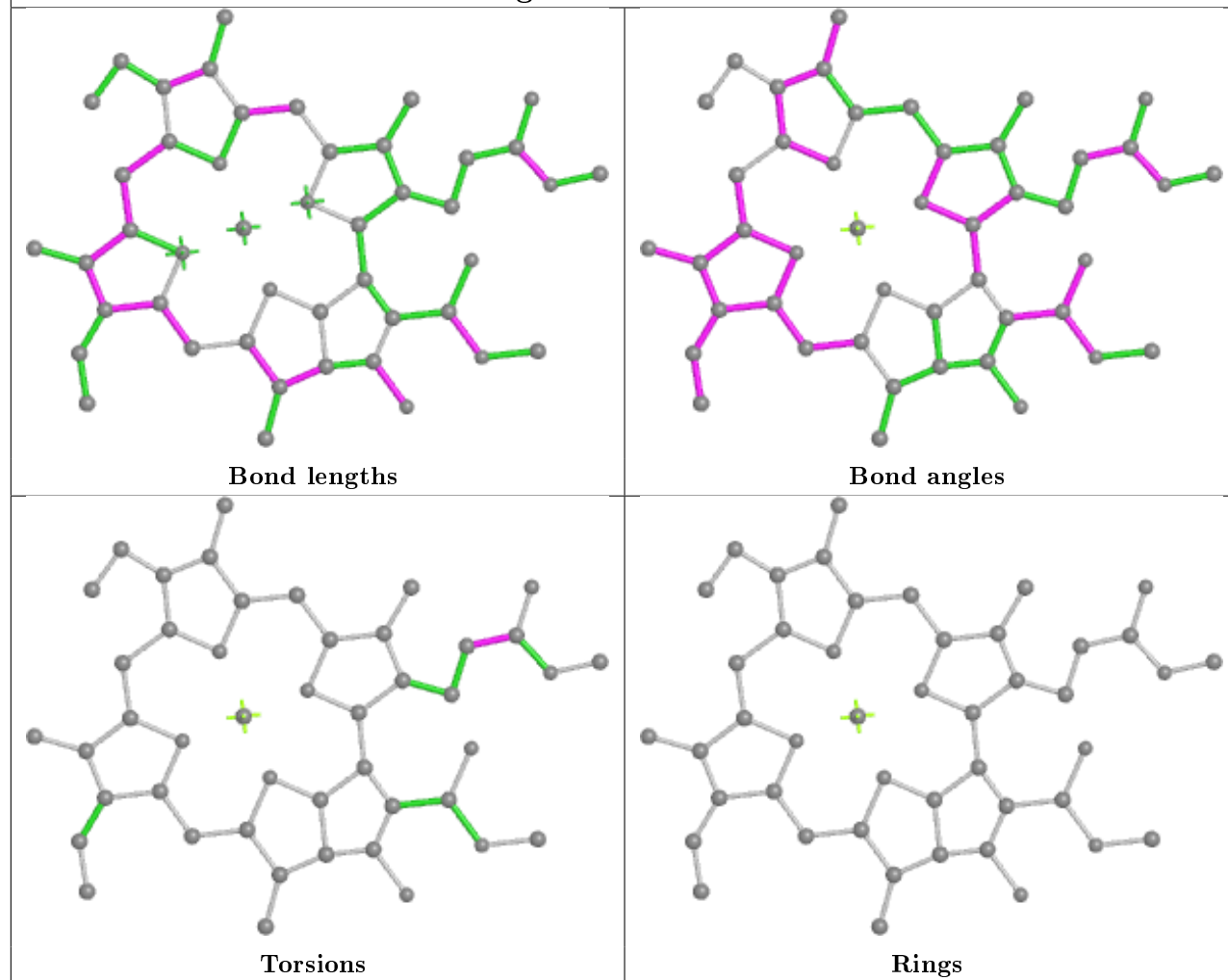




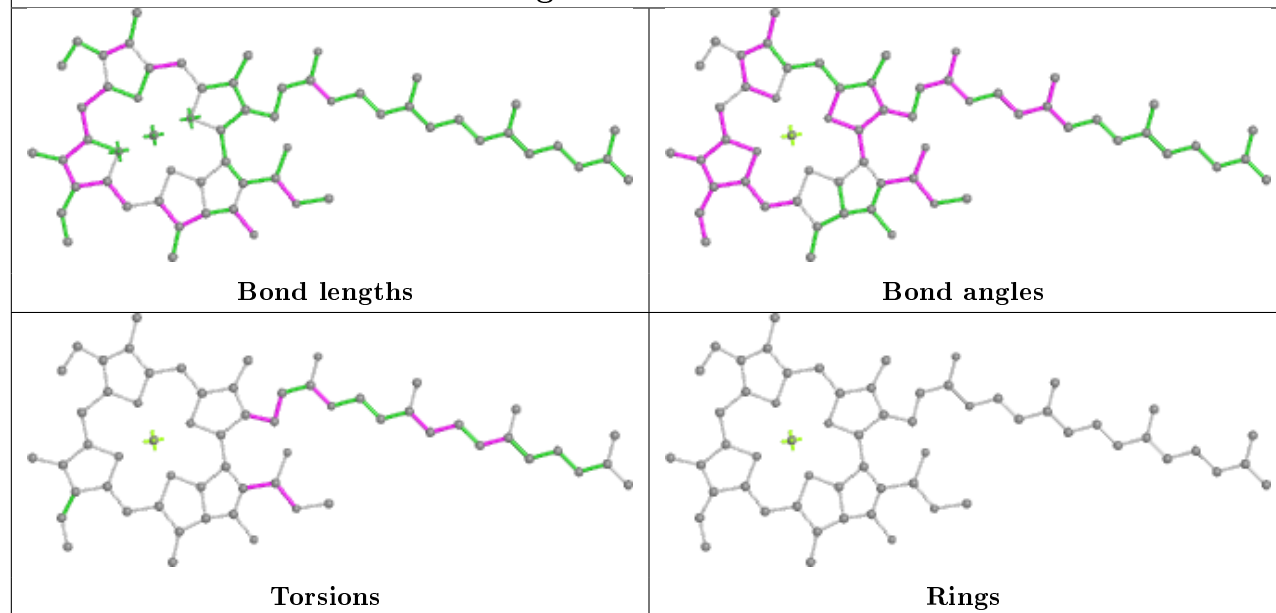


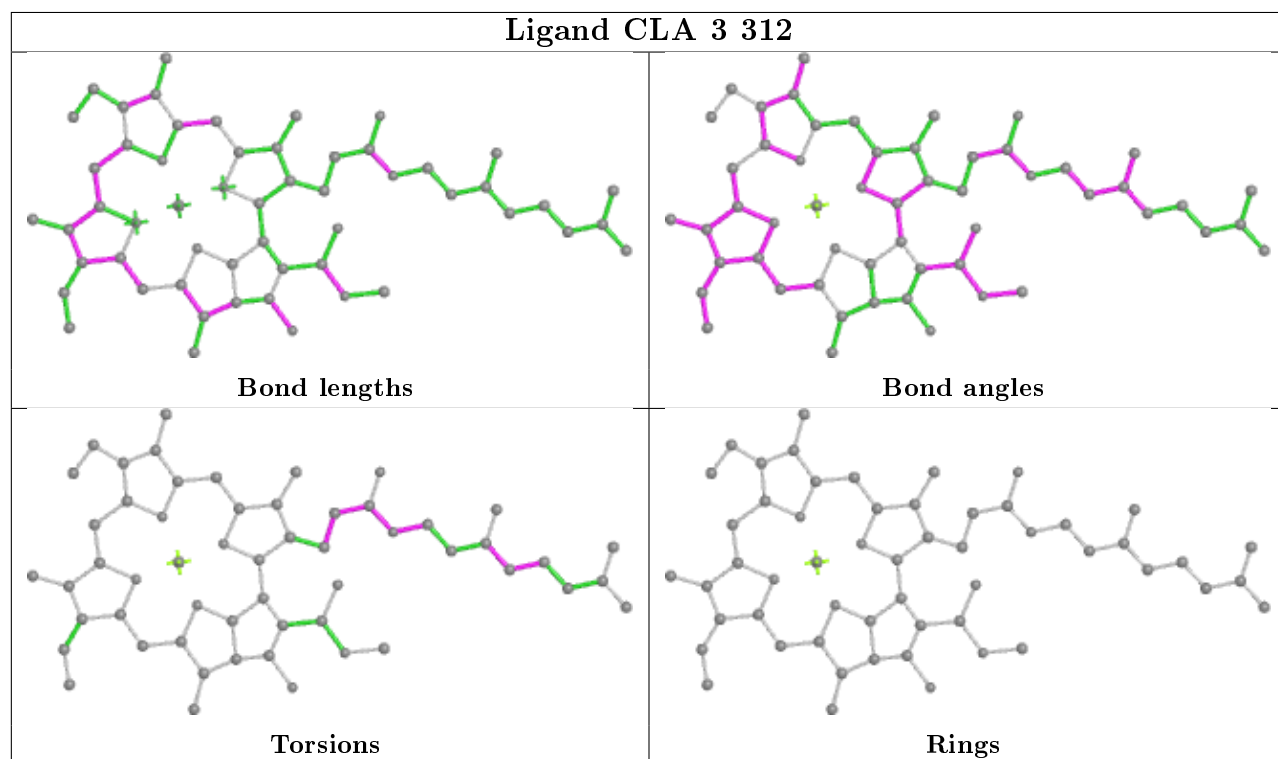
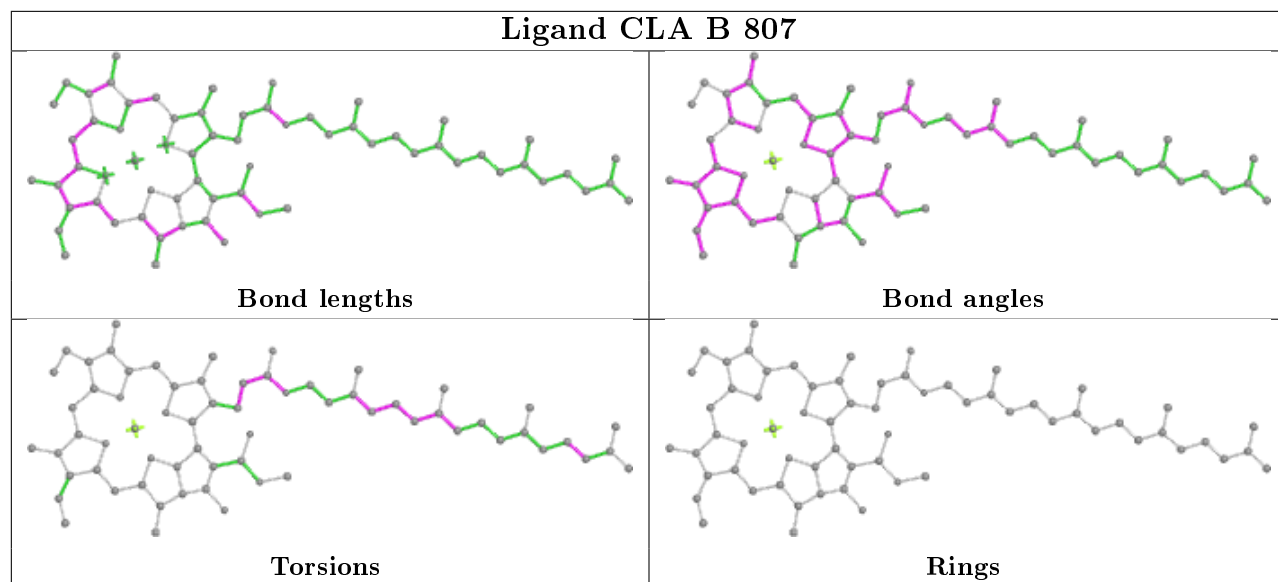


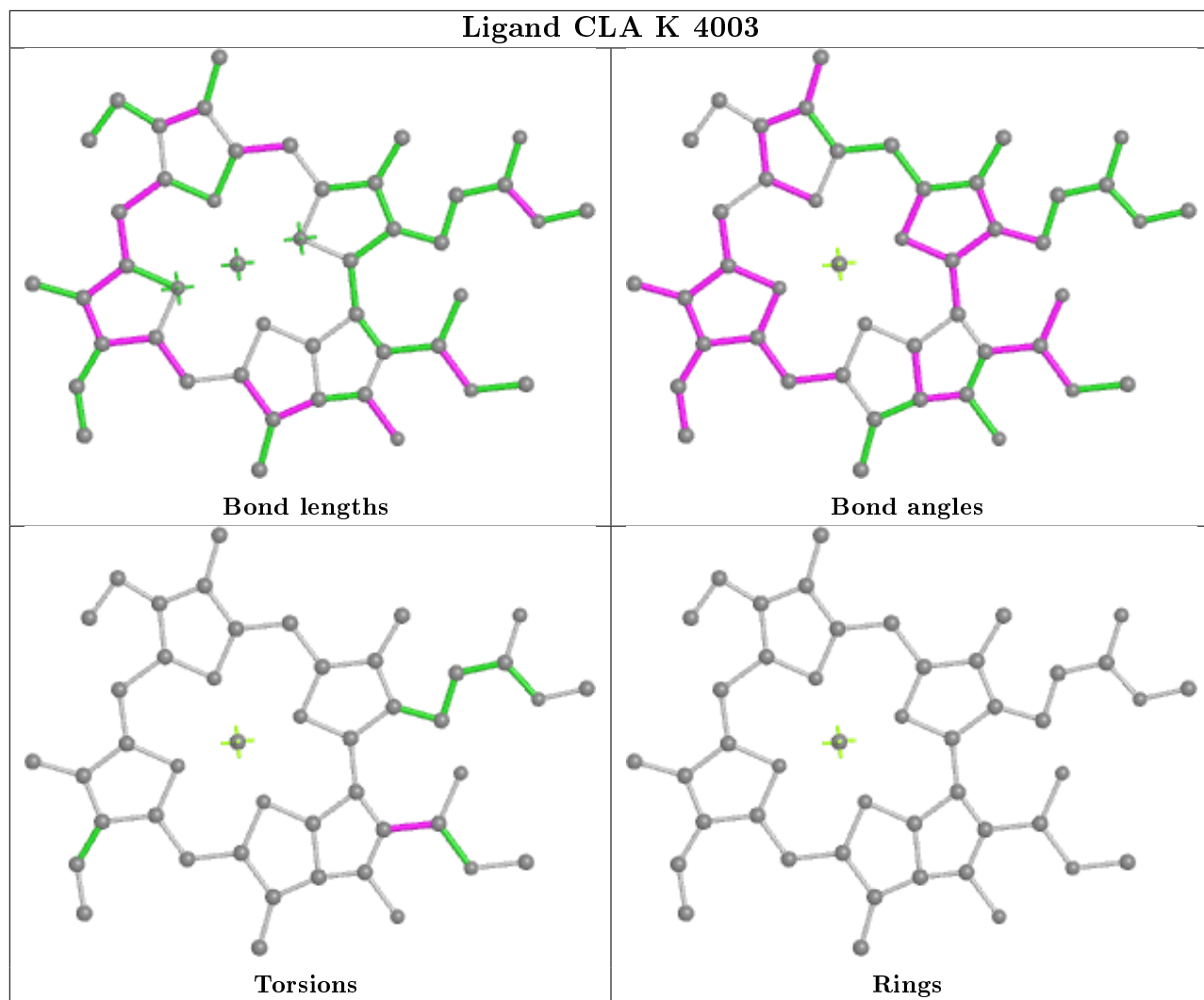
Ligand CLA 4 603

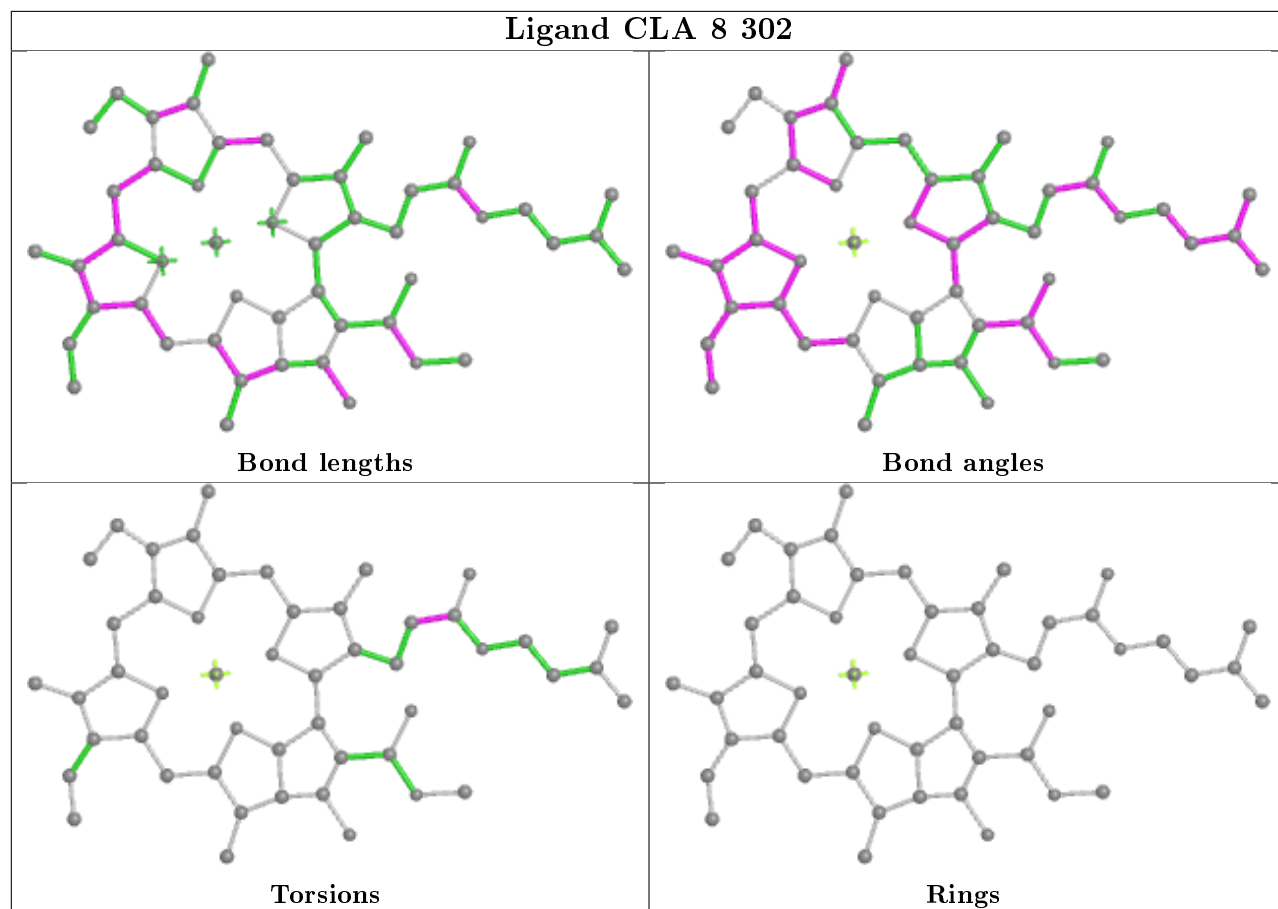


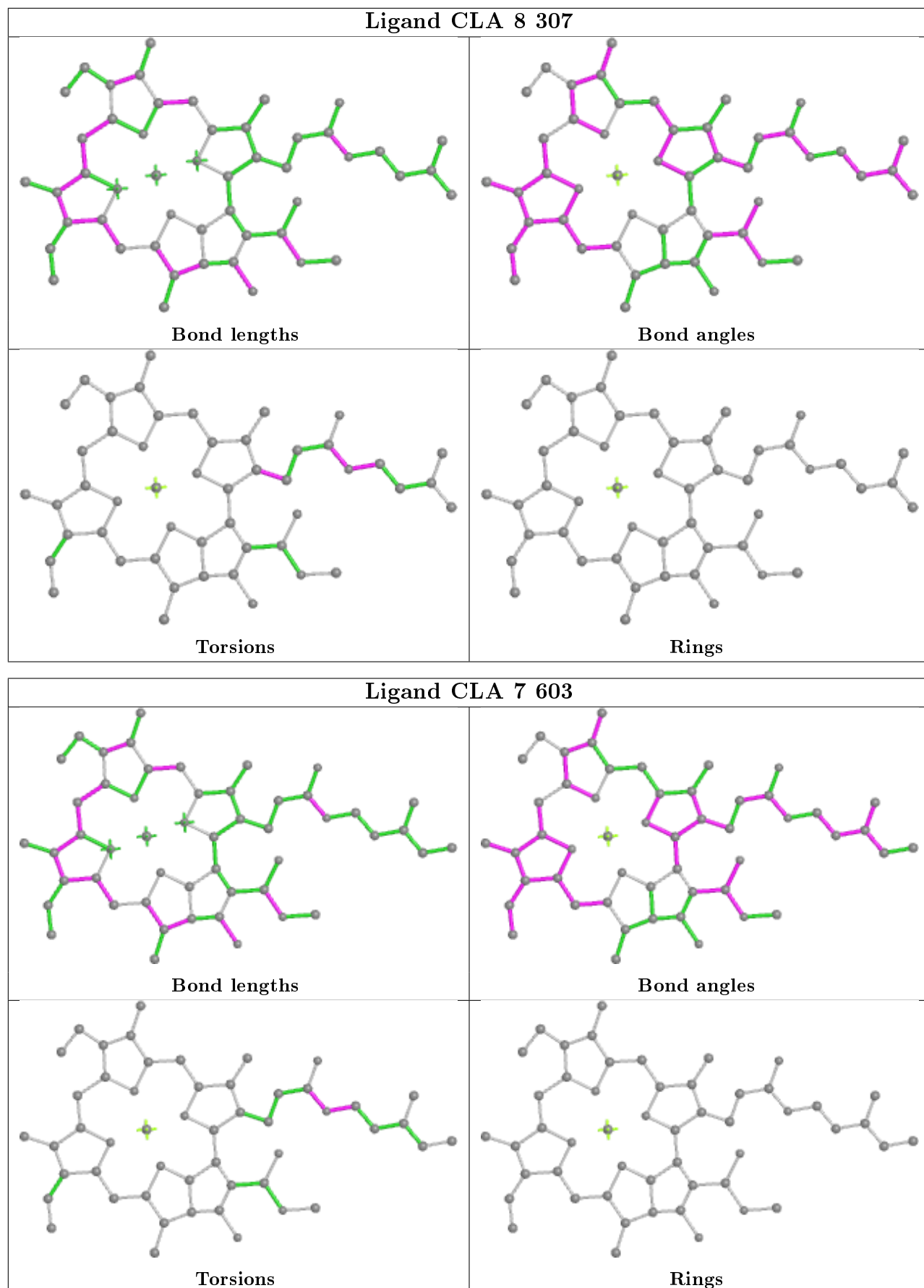
Ligand CLA 8 301











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 Fit of model and data i

6.1 Protein, DNA and RNA chains i

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	742/742 (100%)	0.17	32 (4%) 35 25	42, 58, 91, 169	0
1	a	742/742 (100%)	0.10	31 (4%) 36 26	36, 48, 81, 140	0
2	B	733/733 (100%)	0.34	66 (9%) 9 5	42, 56, 80, 121	0
2	b	733/733 (100%)	0.24	49 (6%) 17 10	36, 55, 86, 139	0
3	C	80/80 (100%)	0.15	5 (6%) 20 12	50, 62, 77, 96	0
3	c	80/80 (100%)	-0.18	0 100 100	44, 55, 72, 88	0
4	D	141/141 (100%)	0.38	11 (7%) 13 7	53, 71, 103, 163	0
4	d	140/141 (99%)	0.29	5 (3%) 42 32	45, 61, 92, 132	0
5	E	63/64 (98%)	0.96	14 (22%) 0 0	51, 77, 115, 127	0
5	e	63/64 (98%)	-0.09	1 (1%) 72 66	51, 78, 96, 119	0
6	F	151/151 (100%)	0.25	12 (7%) 12 7	50, 69, 98, 126	0
6	f	151/151 (100%)	0.15	8 (5%) 26 17	49, 73, 101, 132	0
7	G	95/95 (100%)	0.26	4 (4%) 36 26	60, 79, 103, 127	0
7	g	95/95 (100%)	0.45	12 (12%) 3 2	62, 83, 123, 171	0
8	H	90/90 (100%)	0.41	10 (11%) 5 3	61, 83, 116, 127	0
8	h	90/90 (100%)	-0.07	3 (3%) 46 36	51, 70, 100, 111	0
9	I	29/30 (96%)	-0.22	1 (3%) 45 35	53, 65, 87, 117	0
9	i	30/30 (100%)	-0.20	1 (3%) 46 36	48, 56, 80, 129	0
10	J	39/39 (100%)	0.00	2 (5%) 28 19	51, 62, 97, 100	0
10	j	39/39 (100%)	0.27	3 (7%) 13 7	48, 65, 95, 100	0
11	K	45/84 (53%)	1.76	16 (35%) 0 0	92, 111, 131, 143	0
11	k	46/84 (54%)	0.87	5 (10%) 5 3	68, 86, 126, 134	0
12	L	153/153 (100%)	0.23	15 (9%) 7 4	56, 80, 120, 143	0
12	l	151/153 (98%)	-0.32	0 100 100	42, 60, 87, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	1	195/195 (100%)	0.57	34 (17%)	1	1	61, 87, 119, 136	0
13	6	195/195 (100%)	0.60	30 (15%)	2	1	74, 114, 164, 176	0
14	2	206/206 (100%)	1.23	57 (27%)	0	0	67, 97, 133, 188	0
14	7	206/206 (100%)	0.63	30 (14%)	2	1	61, 89, 122, 158	0
15	3	218/218 (100%)	0.81	38 (17%)	1	1	62, 96, 133, 155	0
15	8	217/218 (99%)	0.38	24 (11%)	5	3	56, 81, 112, 142	0
16	4	196/196 (100%)	0.83	41 (20%)	1	0	61, 85, 115, 160	0
16	9	196/196 (100%)	0.46	22 (11%)	5	3	65, 97, 134, 155	0
All	All	6350/6434 (98%)	0.34	582 (9%)	9	5	36, 68, 116, 188	0

All (582) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	3	259	ASN	8.7
9	i	2	ILE	8.2
5	E	2	GLY	7.1
15	8	121	LEU	7.1
14	2	121	ILE	6.7
15	3	121	LEU	6.7
16	9	122	ASN	6.7
16	9	118	ILE	6.6
13	6	166	TYR	6.5
14	2	257	THR	6.2
7	g	63	PRO	6.1
15	8	120	GLY	6.1
13	6	163	PRO	6.0
14	2	256	PHE	5.9
14	7	256	PHE	5.6
14	2	139	THR	5.5
13	6	168	LYS	5.5
15	3	122	ILE	5.5
14	2	179	THR	5.3
14	2	177	LYS	5.3
13	1	98	TYR	5.2
15	3	219	LEU	5.2
5	E	4	LYS	5.1
14	2	189	LEU	5.1
5	E	3	PRO	5.1
6	F	188	LYS	5.1

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Mol	Chain	Res	Type	RSRZ
13	6	167	SER	5.0
14	7	53	ASP	5.0
15	3	128	LEU	4.9
16	4	138	SER	4.9
7	g	64	VAL	4.9
16	9	174	GLN	4.9
7	g	59	LYS	4.9
16	4	195	ALA	4.8
14	2	133	GLN	4.8
13	6	164	LEU	4.8
14	2	128	TYR	4.8
12	L	152	PHE	4.8
13	6	158	GLY	4.8
13	1	99	GLY	4.7
15	8	178	LYS	4.7
15	3	255	ALA	4.7
6	F	186	ASP	4.7
16	4	132	GLU	4.6
2	B	734	GLY	4.6
15	8	122	ILE	4.6
14	2	175	ASN	4.6
16	4	237	ILE	4.6
16	9	119	GLY	4.5
13	1	121	PRO	4.5
15	3	258	VAL	4.5
2	b	214	ASP	4.5
16	4	88	LEU	4.5
11	K	55	PHE	4.4
6	f	188	LYS	4.4
16	9	120	ILE	4.4
1	a	502	THR	4.4
13	6	161	PHE	4.4
16	9	132	GLU	4.3
16	9	133	GLU	4.2
1	a	516	GLY	4.2
14	7	202	GLN	4.2
2	b	110	LEU	4.2
2	B	377	TYR	4.2
16	4	134	TYR	4.2
2	B	714	SER	4.2
4	D	75	ASP	4.2
13	1	114	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
13	6	165	GLY	4.1
13	1	96	LEU	4.1
12	L	155	TYR	4.1
6	F	137	LEU	4.1
14	2	120	GLY	4.1
14	2	178	LEU	4.1
16	9	123	VAL	4.1
14	7	193	PRO	4.0
15	3	178	LYS	4.1
11	K	20	PHE	4.0
1	A	644	GLN	4.0
11	K	63	CYS	4.0
13	1	97	GLY	4.0
2	B	214	ASP	4.0
15	3	256	ASP	4.0
15	3	115	TYR	4.0
14	2	134	GLU	4.0
14	2	135	TYR	3.9
13	1	115	ALA	3.9
13	6	216	ASP	3.9
11	K	60	THR	3.9
11	K	62	ALA	3.9
13	6	219	HIS	3.9
14	2	68	ASP	3.8
14	7	70	SER	3.8
1	a	35	ALA	3.8
15	3	123	PRO	3.8
16	4	243	ASN	3.8
2	b	303	TYR	3.8
1	a	36	LYS	3.8
15	8	119	VAL	3.8
16	9	164	GLY	3.8
1	A	516	GLY	3.8
8	H	81	TYR	3.8
16	4	131	LYS	3.8
7	g	60	SER	3.7
16	4	235	GLN	3.7
13	1	147	MET	3.7
16	9	121	ILE	3.7
6	F	135	TYR	3.7
16	4	181	GLU	3.7
16	4	241	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
15	3	125	GLU	3.7
14	2	85	ASP	3.7
2	B	474	PHE	3.7
10	J	37	LEU	3.6
13	6	157	PRO	3.6
16	9	192	LEU	3.6
13	1	109	ALA	3.6
13	6	215	ALA	3.6
15	3	186	LYS	3.6
1	a	30	SER	3.6
2	b	346	SER	3.6
5	E	25	VAL	3.6
2	b	282	PHE	3.5
15	3	51	LEU	3.5
15	3	254	VAL	3.5
14	2	87	GLU	3.5
15	8	207	PHE	3.5
13	6	218	TRP	3.5
14	2	122	LEU	3.5
11	k	53	ALA	3.5
2	B	659	THR	3.5
2	b	474	PHE	3.5
4	D	188	PHE	3.5
2	B	379	ALA	3.5
11	K	17	LEU	3.5
7	G	1	GLU	3.5
2	b	583	MET	3.5
13	6	169	ASP	3.5
13	6	217	PRO	3.5
2	b	379	ALA	3.5
2	B	380	GLY	3.4
14	2	181	THR	3.4
8	H	75	SER	3.4
2	B	381	PHE	3.4
14	2	132	GLU	3.4
2	B	213	LEU	3.4
16	4	133	GLU	3.4
14	2	255	ALA	3.4
14	2	182	ASP	3.4
7	g	41	LEU	3.4
8	H	134	GLN	3.4
2	b	342	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
15	3	220	LYS	3.4
2	B	583	MET	3.4
16	4	205	ILE	3.4
15	3	207	PHE	3.4
5	E	57	LEU	3.3
6	F	189	LYS	3.3
2	B	580	VAL	3.3
15	3	174	GLY	3.3
2	b	344	ILE	3.3
2	b	584	LEU	3.3
2	B	713	PHE	3.3
2	b	580	VAL	3.3
1	a	517	GLY	3.3
2	b	345	THR	3.3
13	1	116	THR	3.3
2	b	482	ASN	3.3
2	b	317	ARG	3.3
6	f	224	GLU	3.3
10	j	2	ARG	3.3
14	2	231	TYR	3.3
8	h	58	PHE	3.3
11	K	57	LEU	3.3
12	L	47	LEU	3.3
16	4	242	HIS	3.3
11	k	2	PHE	3.2
14	7	125	PRO	3.2
1	a	519	ASP	3.2
14	2	131	GLY	3.2
16	4	199	GLU	3.2
5	E	37	PRO	3.2
15	3	257	PRO	3.2
16	9	165	SER	3.2
14	2	137	THR	3.2
2	B	585	ASN	3.2
14	2	198	SER	3.2
13	1	167	SER	3.2
13	6	156	TYR	3.2
2	B	588	GLY	3.2
2	B	709	GLY	3.2
14	2	136	PHE	3.2
2	B	587	ILE	3.2
2	B	206	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	a	501	GLY	3.2
11	K	77	GLY	3.2
6	f	189	LYS	3.2
16	9	206	ALA	3.2
6	F	147	LEU	3.2
8	H	140	PRO	3.2
13	6	111	PRO	3.1
2	B	584	LEU	3.1
15	3	260	ASN	3.1
5	E	23	GLY	3.1
14	7	221	ALA	3.1
1	a	627	THR	3.1
13	6	173	LEU	3.1
14	7	134	GLU	3.1
11	K	18	MET	3.1
1	a	551	VAL	3.1
2	B	664	LEU	3.1
2	b	213	LEU	3.1
14	7	175	ASN	3.1
11	K	78	LEU	3.1
16	4	236	HIS	3.1
15	8	115	TYR	3.1
2	B	378	ILE	3.1
14	2	168	ASN	3.1
6	F	158	GLU	3.0
16	4	83	GLU	3.0
14	7	110	ILE	3.0
14	2	176	ASN	3.0
5	E	60	ILE	3.0
15	3	126	THR	3.0
1	A	631	GLN	3.0
1	a	494	ASN	3.0
2	B	581	PHE	3.0
4	d	73	GLU	3.0
1	A	339	THR	3.0
16	4	123	VAL	3.0
16	9	125	LYS	3.0
5	E	28	VAL	3.0
2	B	717	TYR	3.0
6	F	141	SER	3.0
15	3	124	GLN	3.0
2	B	589	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	82	PHE	2.9
15	8	259	ASN	2.9
13	6	162	ASP	2.9
2	b	380	GLY	2.9
15	3	145	TRP	2.9
6	F	136	GLY	2.9
15	3	116	LEU	2.9
13	6	170	PRO	2.9
16	4	85	PRO	2.9
11	K	59	ASP	2.9
14	2	127	TRP	2.9
1	A	529	LEU	2.9
16	4	164	GLY	2.9
10	j	1	MET	2.9
13	6	66	PRO	2.9
12	L	29	ILE	2.9
15	3	59	LEU	2.9
1	A	111	ASN	2.9
1	A	607	ASN	2.9
16	4	230	PHE	2.9
1	a	208	ALA	2.9
2	B	662	MET	2.9
4	D	70	THR	2.9
2	B	712	HIS	2.9
12	L	149	TRP	2.9
15	3	138	PRO	2.8
14	2	76	GLY	2.8
2	B	454	LEU	2.8
13	1	160	ALA	2.8
15	3	142	TYR	2.8
13	6	159	GLY	2.8
2	B	591	THR	2.8
12	L	41	THR	2.8
15	3	247	TYR	2.8
15	8	247	TYR	2.8
6	f	222	ASN	2.8
2	b	586	THR	2.8
13	1	203	GLY	2.8
8	H	58	PHE	2.8
15	8	249	ASN	2.8
2	B	344	ILE	2.8
2	B	346	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	b	714	SER	2.8
3	C	39	ILE	2.8
8	h	79	SER	2.8
12	L	27	PRO	2.8
14	2	234	THR	2.8
16	4	177	LEU	2.8
13	1	52	PRO	2.8
2	b	340	SER	2.8
2	b	235	GLN	2.8
6	f	227	ASP	2.7
2	B	215	VAL	2.7
7	g	35	VAL	2.7
13	1	144	GLN	2.7
14	2	66	TRP	2.7
13	6	123	PRO	2.7
1	a	713	LYS	2.7
15	8	126	THR	2.7
7	g	92	GLY	2.7
13	1	120	ASN	2.7
16	4	86	GLU	2.7
14	2	52	PRO	2.7
2	B	374	HIS	2.7
14	7	249	HIS	2.7
6	f	135	TYR	2.7
11	k	54	GLY	2.7
14	7	124	THR	2.7
13	6	155	LYS	2.7
16	9	175	TYR	2.7
13	1	204	THR	2.7
1	A	110	LEU	2.7
5	E	38	VAL	2.7
1	A	28	LYS	2.7
16	4	115	PHE	2.7
15	3	111	ILE	2.7
1	a	498	LEU	2.7
12	L	156	VAL	2.7
2	B	577	TYR	2.7
2	B	343	VAL	2.7
8	H	137	LYS	2.7
1	A	734	GLY	2.7
13	1	56	GLY	2.7
5	E	5	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
12	L	78	GLN	2.6
2	B	345	THR	2.6
10	j	6	THR	2.6
11	K	15	THR	2.6
4	D	155	TYR	2.6
12	L	122	GLU	2.6
16	9	131	LYS	2.6
2	B	482	ASN	2.6
7	g	94	ASP	2.6
11	k	71	GLY	2.6
14	2	232	THR	2.6
16	4	167	ASN	2.6
4	D	126	PRO	2.6
6	F	154	ARG	2.6
14	7	255	ALA	2.6
14	7	128	TYR	2.6
15	8	128	LEU	2.6
15	8	179	GLN	2.6
8	H	79	SER	2.6
14	7	71	LEU	2.6
7	G	55	VAL	2.6
7	g	55	VAL	2.6
8	H	101	LEU	2.6
15	3	151	LEU	2.6
2	B	210	ASN	2.6
1	a	714	LEU	2.6
14	7	135	TYR	2.6
15	3	222	VAL	2.6
2	b	318	GLY	2.6
13	1	119	GLY	2.6
13	1	125	GLY	2.6
15	8	116	LEU	2.6
14	7	84	SER	2.6
2	B	458	ILE	2.6
11	K	56	THR	2.6
11	K	19	LEU	2.6
7	G	54	TYR	2.6
14	2	54	ARG	2.6
15	8	174	GLY	2.5
14	2	190	TRP	2.5
10	J	38	ILE	2.5
2	b	481	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	340	SER	2.5
14	2	201	PRO	2.5
8	h	60	LEU	2.5
14	2	226	TRP	2.5
16	4	202	GLU	2.5
9	I	2	ILE	2.5
14	2	188	GLY	2.5
16	9	96	LEU	2.5
13	6	194	PHE	2.5
15	3	118	LYS	2.5
1	A	689	SER	2.5
16	4	62	SER	2.5
1	A	365	LEU	2.5
13	1	122	VAL	2.5
13	6	149	LYS	2.5
6	f	77	ASP	2.5
2	B	579	ALA	2.5
1	a	715	LYS	2.5
2	b	157	LEU	2.5
2	b	527	LEU	2.5
7	g	58	LEU	2.5
12	L	31	TRP	2.5
13	6	67	ALA	2.5
14	7	66	TRP	2.5
1	A	210	LEU	2.5
2	b	305	LEU	2.5
16	4	239	ASP	2.4
15	8	124	GLN	2.4
2	b	384	THR	2.4
2	B	715	VAL	2.4
16	4	75	GLY	2.4
1	A	213	LEU	2.4
16	4	120	ILE	2.4
15	3	223	LYS	2.4
15	8	123	PRO	2.4
16	9	189	PHE	2.4
1	A	471	GLY	2.4
1	A	480	THR	2.4
2	b	343	VAL	2.4
1	a	450	CYS	2.4
14	7	123	ASN	2.4
1	A	604	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
7	G	26	PHE	2.4
1	A	517	GLY	2.4
4	D	105	ASP	2.4
1	a	367	SER	2.4
16	4	84	ASP	2.4
14	2	199	ALA	2.4
2	b	710	LEU	2.4
15	8	245	GLY	2.4
2	B	710	LEU	2.4
1	A	505	PRO	2.4
2	B	660	GLY	2.4
14	2	74	ASP	2.4
14	2	160	ASP	2.4
1	a	444	SER	2.4
4	d	82	ILE	2.4
12	L	28	LEU	2.4
2	b	375	HIS	2.3
2	b	186	SER	2.3
1	A	214	GLY	2.3
4	D	153	GLN	2.3
14	2	247	PRO	2.3
16	4	201	LYS	2.3
2	B	32	GLU	2.3
14	7	127	TRP	2.3
7	g	40	GLY	2.3
8	H	78	PRO	2.3
1	a	27	ILE	2.3
2	B	718	ILE	2.3
14	2	67	LEU	2.3
3	C	41	SER	2.3
2	B	282	PHE	2.3
4	d	112	PHE	2.3
15	8	189	GLY	2.3
12	L	151	TYR	2.3
1	a	548	THR	2.3
2	B	663	PHE	2.3
5	e	5	ARG	2.3
2	B	711	VAL	2.3
15	3	250	LEU	2.3
2	B	384	THR	2.3
14	2	129	THR	2.3
15	3	120	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
16	4	67	THR	2.3
16	4	165	SER	2.3
3	C	27	GLU	2.3
14	7	201	PRO	2.3
2	b	525	LEU	2.3
15	3	127	ALA	2.3
1	A	681	GLY	2.3
1	a	366	GLY	2.3
2	B	342	GLY	2.3
1	a	28	LYS	2.3
14	7	52	PRO	2.3
1	A	738	TYR	2.3
13	6	46	TYR	2.3
16	9	191	PRO	2.3
1	a	210	LEU	2.3
13	1	159	GLY	2.3
14	2	245	ALA	2.3
2	B	453	ILE	2.3
15	8	180	TYR	2.3
15	3	132	GLN	2.3
2	b	585	ASN	2.2
7	g	50	ARG	2.2
1	A	212	GLY	2.2
1	a	209	GLY	2.2
2	B	347	LEU	2.2
13	1	211	ALA	2.2
13	6	117	TYR	2.2
2	b	187	SER	2.2
2	b	313	GLY	2.2
14	7	130	ALA	2.2
2	b	320	LYS	2.2
11	k	7	THR	2.2
2	B	339	ALA	2.2
4	D	169	LYS	2.2
2	B	529	THR	2.2
2	B	586	THR	2.2
15	8	177	GLY	2.2
2	b	579	ALA	2.2
2	b	587	ILE	2.2
2	B	582	TRP	2.2
2	b	377	TYR	2.2
2	B	487	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
13	1	118	LEU	2.2
13	1	152	GLU	2.2
1	A	87	SER	2.2
2	b	281	ALA	2.2
16	4	238	SER	2.2
2	b	475	ASP	2.2
11	K	61	LEU	2.2
16	4	233	LEU	2.2
2	b	300	SER	2.2
15	3	139	ALA	2.2
15	8	138	PRO	2.2
1	A	519	ASP	2.2
2	b	341	LEU	2.2
14	7	68	ASP	2.2
14	2	250	ALA	2.2
2	B	530	THR	2.2
1	a	46	LYS	2.2
14	2	248	GLY	2.2
3	C	26	LEU	2.2
8	H	55	SER	2.2
16	9	225	THR	2.2
1	A	384	TYR	2.2
2	b	526	GLY	2.1
2	B	525	LEU	2.1
2	b	347	LEU	2.1
2	b	109	ALA	2.1
13	6	114	GLN	2.1
14	7	237	ILE	2.1
14	2	203	LYS	2.1
14	2	251	THR	2.1
1	a	690	LEU	2.1
14	2	239	ASN	2.1
11	K	11	MET	2.1
5	E	29	ASP	2.1
14	7	111	PHE	2.1
4	d	182	GLN	2.1
14	2	55	PRO	2.1
4	d	151	LYS	2.1
12	L	154	LEU	2.1
13	1	181	ILE	2.1
16	4	136	ALA	2.1
1	a	447	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
14	7	198	SER	2.1
13	1	117	TYR	2.1
13	1	127	LEU	2.1
2	B	382	ILE	2.1
3	C	38	GLN	2.1
6	F	111	ASP	2.1
12	L	5	GLN	2.1
1	A	404	GLY	2.1
16	4	64	GLY	2.1
2	B	375	HIS	2.1
14	2	119	LEU	2.1
2	b	382	ILE	2.1
5	E	7	ALA	2.1
14	2	254	ALA	2.1
14	7	203	LYS	2.1
2	B	634	GLY	2.1
2	B	716	GLY	2.1
4	D	76	PRO	2.1
13	1	218	TRP	2.1
15	8	205	LEU	2.1
16	4	65	TYR	2.1
4	D	185	GLY	2.1
13	1	123	PRO	2.1
14	7	126	SER	2.1
16	4	234	LEU	2.1
14	2	53	ASP	2.1
2	b	184	GLY	2.1
1	a	135	ASP	2.0
2	b	530	THR	2.0
5	E	27	ALA	2.0
16	9	228	GLY	2.0
4	D	168	PRO	2.0
1	A	174	PHE	2.0
13	1	194	PHE	2.0
6	F	155	HIS	2.0
13	1	165	GLY	2.0
2	B	504	ASN	2.0
14	2	115	PHE	2.0
16	4	66	LEU	2.0
1	A	175	ALA	2.0
1	a	214	GLY	2.0
16	9	241	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	685	VAL	2.0
6	f	107	LEU	2.0
13	1	128	PRO	2.0
15	8	217	LEU	2.0
1	A	176	GLY	2.0
2	B	526	GLY	2.0
14	7	85	ASP	2.0
1	A	90	PHE	2.0
1	a	520	LEU	2.0
13	1	47	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
20	BCR	L	206	40/40	0.48	0.79	146,151,156,156	0
20	BCR	K	4004	40/40	0.49	0.62	94,115,138,138	0
20	BCR	K	4001	40/40	0.59	0.41	91,94,96,96	0
17	CLA	8	309	52/65	0.60	0.51	155,164,169,259	0
20	BCR	2	617	40/40	0.67	0.77	125,133,163,164	0
27	LUT	6	317	42/42	0.67	0.43	86,93,118,120	0
20	BCR	7	617	40/40	0.69	0.63	112,119,127,128	0
25	LMG	4	620	44/55	0.69	0.42	89,97,111,113	0
19	LHG	a	848	27/49	0.73	0.33	74,95,125,127	0
25	LMG	6	302	40/55	0.75	0.34	116,148,163,164	0
27	LUT	6	321	42/42	0.75	0.49	107,113,133,134	0
17	CLA	K	4002	45/65	0.76	0.46	115,123,125,154	0
20	BCR	l	206	40/40	0.77	0.52	77,82,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
20	BCR	1	318	40/40	0.77	0.50	94,105,126,127	0
19	LHG	3	319	20/49	0.79	0.50	152,157,193,194	0
25	LMG	4	619	44/55	0.80	0.35	82,92,103,104	0
24	DGD	B	850	66/66	0.80	0.33	52,71,93,102	0
23	LMT	B	849	35/35	0.80	0.33	80,97,102,103	0
17	CLA	3	301	46/65	0.80	0.78	142,149,154,175	0
20	BCR	A	856	40/40	0.81	0.25	65,71,85,85	0
17	CLA	3	310	37/65	0.82	0.63	179,186,191,221	0
17	CLA	6	316	46/65	0.82	0.30	152,162,171,203	0
20	BCR	6	319	40/40	0.82	0.47	104,124,138,140	0
19	LHG	A	847	27/49	0.83	0.26	68,88,113,113	0
20	BCR	b	844	40/40	0.83	0.32	52,67,91,93	0
25	LMG	G	102	44/55	0.83	0.21	72,95,110,113	0
17	CLA	8	313	25/65	0.83	0.28	102,110,116,146	0
17	CLA	K	4003	46/65	0.83	0.29	81,119,128,130	0
22	HTG	F	302	19/19	0.84	0.31	43,98,105,107	0
20	BCR	A	850	40/40	0.84	0.30	53,72,112,112	0
25	LMG	9	619	50/55	0.84	0.29	68,88,96,98	0
17	CLA	L	202	65/65	0.84	0.37	83,111,131,132	0
17	CLA	A	824	51/65	0.84	0.38	77,89,118,118	0
17	CLA	k	1403	46/65	0.85	0.21	89,95,103,110	0
22	HTG	J	3001	19/19	0.85	0.19	73,76,78,82	0
20	BCR	G	105	40/40	0.85	0.30	63,71,83,83	0
17	CLA	A	845	52/65	0.85	0.41	90,115,146,149	0
28	XAT	9	617	44/44	0.85	0.23	72,81,97,98	0
20	BCR	4	618	40/40	0.85	0.30	79,86,89,90	0
27	LUT	4	616	42/42	0.85	0.31	71,90,94,95	0
20	BCR	g	104	40/40	0.86	0.40	57,102,117,118	0
26	CHL	2	606	48/66	0.86	0.46	89,97,105,107	0
20	BCR	a	852	40/40	0.86	0.33	40,62,120,120	0
26	CHL	2	605	43/66	0.86	0.27	77,89,100,106	0
17	CLA	g	101	41/65	0.86	0.21	146,164,166,167	0
17	CLA	A	837	45/65	0.86	0.28	84,95,103,165	0
17	CLA	1	309	65/65	0.86	0.25	71,79,106,108	0
24	DGD	b	849	66/66	0.86	0.27	41,64,90,91	0
22	HTG	f	7001	19/19	0.86	0.33	49,104,107,108	0
28	XAT	3	317	44/44	0.87	0.26	61,74,100,101	0
17	CLA	7	604	60/65	0.87	0.34	92,101,106,109	0
20	BCR	a	849	40/40	0.87	0.25	56,63,75,76	0
20	BCR	k	1404	40/40	0.87	0.26	49,89,103,104	0
20	BCR	B	844	40/40	0.87	0.28	50,53,85,87	0
17	CLA	3	313	45/65	0.87	0.41	85,97,102,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	CLA	3	315	25/65	0.87	0.26	112,115,121,157	0
20	BCR	8	316	40/40	0.87	0.36	66,71,88,90	0
17	CLA	l	202	65/65	0.87	0.40	57,88,111,113	0
27	LUT	1	320	42/42	0.87	0.22	71,79,90,91	0
26	CHL	9	615	43/66	0.87	0.34	90,144,147,148	0
27	LUT	7	615	42/42	0.87	0.47	72,83,97,98	0
26	CHL	7	605	43/66	0.87	0.27	85,89,93,99	0
20	BCR	b	845	40/40	0.88	0.24	46,67,106,106	0
17	CLA	2	613	43/65	0.88	0.23	80,88,94,95	0
17	CLA	b	841	65/65	0.88	0.20	64,80,92,94	0
17	CLA	k	1401	45/65	0.88	0.34	75,83,94,96	0
17	CLA	b	824	65/65	0.88	0.28	45,51,69,72	0
17	CLA	2	604	60/65	0.88	0.35	100,111,118,119	0
17	CLA	2	609	60/65	0.88	0.23	73,87,98,101	0
20	BCR	j	3004	40/40	0.88	0.24	56,71,82,84	0
17	CLA	6	313	52/65	0.88	0.24	83,94,119,120	0
17	CLA	3	302	60/65	0.88	0.20	67,79,85,95	0
20	BCR	A	851	40/40	0.88	0.28	43,66,78,79	0
26	CHL	2	614	43/66	0.88	0.33	116,134,143,145	0
17	CLA	a	846	52/65	0.88	0.32	86,102,115,140	0
17	CLA	b	811	54/65	0.88	0.29	50,74,114,114	0
17	CLA	B	821	46/65	0.88	0.23	51,60,72,80	0
17	CLA	8	311	45/65	0.89	0.34	100,110,122,161	0
17	CLA	B	815	60/65	0.89	0.22	60,72,100,102	0
17	CLA	6	310	65/65	0.89	0.25	80,90,121,126	0
17	CLA	4	609	60/65	0.89	0.31	69,86,106,111	0
17	CLA	3	311	52/65	0.89	0.40	129,142,154,157	0
17	CLA	A	832	50/65	0.89	0.24	52,70,98,99	0
17	CLA	9	604	50/65	0.89	0.23	105,116,125,126	0
19	LHG	6	320	49/49	0.89	0.32	90,100,111,113	0
20	BCR	A	848	40/40	0.89	0.32	50,59,95,95	0
28	XAT	7	616	44/44	0.89	0.33	57,64,73,74	0
17	CLA	1	314	55/65	0.89	0.23	78,93,105,110	0
27	LUT	9	616	42/42	0.89	0.38	68,79,103,104	0
17	CLA	6	305	65/65	0.89	0.23	83,87,104,110	0
17	CLA	A	823	49/65	0.89	0.25	66,79,104,105	0
17	CLA	B	829	65/65	0.89	0.26	42,50,76,77	0
17	CLA	4	610	55/65	0.89	0.28	72,88,94,122	0
17	CLA	g	103	46/65	0.90	0.28	87,99,103,116	0
17	CLA	1	303	65/65	0.90	0.24	60,67,83,90	0
17	CLA	k	1402	46/65	0.90	0.26	62,78,100,106	0
17	CLA	2	610	41/65	0.90	0.21	80,94,108,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
17	CLA	1	310	60/65	0.90	0.25	63,80,90,92	0
17	CLA	A	805	55/65	0.90	0.23	45,54,89,89	0
20	BCR	B	847	40/40	0.90	0.31	44,49,52,53	0
17	CLA	B	834	65/65	0.90	0.21	46,58,90,90	0
17	CLA	A	834	65/65	0.90	0.24	49,60,71,75	0
17	CLA	B	811	54/65	0.90	0.21	58,74,103,104	0
20	BCR	B	845	40/40	0.90	0.18	47,63,102,102	0
20	BCR	9	618	40/40	0.90	0.30	86,92,100,101	0
17	CLA	3	304	45/65	0.90	0.21	109,122,133,162	0
26	CHL	7	606	48/66	0.90	0.29	71,87,104,105	0
17	CLA	4	604	50/65	0.90	0.30	75,84,111,114	0
17	CLA	A	812	65/65	0.90	0.21	49,63,74,82	0
19	LHG	7	618	37/49	0.90	0.25	83,95,102,104	0
27	LUT	2	615	42/42	0.90	0.27	77,84,89,89	0
17	CLA	2	612	65/65	0.90	0.32	70,93,113,118	0
17	CLA	9	611	52/65	0.90	0.37	76,89,102,103	0
19	LHG	1	319	49/49	0.90	0.27	77,84,109,109	0
17	CLA	b	830	50/65	0.90	0.21	46,59,70,74	0
26	CHL	4	606	51/66	0.90	0.22	71,81,109,110	0
17	CLA	6	309	46/65	0.90	0.30	92,99,106,137	0
17	CLA	F	304	55/65	0.90	0.21	52,69,95,95	0
28	XAT	8	315	44/44	0.90	0.23	64,69,80,83	0
17	CLA	b	814	65/65	0.90	0.19	47,55,69,71	0
17	CLA	j	3002	42/65	0.91	0.15	91,94,96,97	0
17	CLA	a	836	50/65	0.91	0.17	42,54,73,74	0
17	CLA	2	608	50/65	0.91	0.18	65,69,108,111	0
26	CHL	1	307	48/66	0.91	0.19	75,95,109,110	0
20	BCR	B	846	40/40	0.91	0.23	49,53,70,70	0
17	CLA	6	311	60/65	0.91	0.46	81,99,115,116	0
17	CLA	L	203	65/65	0.91	0.23	64,74,87,89	0
17	CLA	B	824	65/65	0.91	0.27	48,53,70,74	0
17	CLA	7	602	65/65	0.91	0.20	62,70,88,93	0
17	CLA	9	612	56/65	0.91	0.24	68,77,89,92	0
17	CLA	a	824	51/65	0.91	0.23	61,74,91,93	0
17	CLA	4	613	45/65	0.91	0.25	92,103,108,160	0
17	CLA	6	307	42/65	0.91	0.27	112,126,137,139	0
20	BCR	I	101	40/40	0.91	0.23	54,60,65,65	0
17	CLA	9	613	45/65	0.91	0.20	87,105,115,137	0
17	CLA	A	806	65/65	0.91	0.29	46,51,59,59	0
17	CLA	b	812	55/65	0.91	0.22	59,70,103,104	0
17	CLA	b	807	65/65	0.91	0.22	42,51,102,104	0
17	CLA	a	804	65/65	0.91	0.21	36,52,71,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
17	CLA	G	103	50/65	0.91	0.23	61,80,91,93	0
17	CLA	7	611	52/65	0.91	0.33	87,104,123,126	0
17	CLA	9	609	60/65	0.91	0.37	72,93,107,108	0
17	CLA	4	612	56/65	0.91	0.19	63,78,87,88	0
17	CLA	B	817	59/65	0.91	0.22	46,53,59,64	0
17	CLA	7	608	50/65	0.91	0.20	60,65,93,96	0
17	CLA	3	309	50/65	0.91	0.23	76,95,104,107	0
17	CLA	1	305	52/65	0.91	0.23	76,101,105,108	0
17	CLA	8	308	50/65	0.91	0.33	75,81,87,88	0
20	BCR	b	847	40/40	0.91	0.24	40,49,69,70	0
20	BCR	B	843	40/40	0.91	0.23	54,64,72,72	0
17	CLA	B	814	65/65	0.91	0.20	50,57,80,82	0
26	CHL	4	605	56/66	0.91	0.26	69,88,96,102	0
17	CLA	B	818	60/65	0.91	0.26	45,50,57,61	0
17	CLA	B	813	65/65	0.91	0.23	47,51,54,55	0
17	CLA	J	3002	42/65	0.91	0.18	92,105,119,148	0
17	CLA	b	831	49/65	0.91	0.23	51,55,71,71	0
17	CLA	b	820	50/65	0.91	0.21	65,72,77,82	0
17	CLA	4	611	52/65	0.91	0.28	71,88,123,125	0
17	CLA	A	836	50/65	0.92	0.17	60,73,80,86	0
17	CLA	a	823	49/65	0.92	0.17	60,67,102,104	0
17	CLA	b	823	60/65	0.92	0.23	50,60,92,94	0
17	CLA	3	314	46/65	0.92	0.18	73,78,101,103	0
27	LUT	3	316	42/42	0.92	0.25	74,78,97,99	0
26	CHL	6	308	47/66	0.92	0.23	103,135,146,149	0
26	CHL	2	601	61/66	0.92	0.32	68,99,113,115	0
17	CLA	b	815	55/65	0.92	0.28	62,78,93,94	0
17	CLA	b	825	65/65	0.92	0.32	38,55,82,83	0
17	CLA	b	817	59/65	0.92	0.24	56,59,67,68	0
17	CLA	B	836	60/65	0.92	0.22	43,46,97,97	0
20	BCR	L	205	40/40	0.92	0.21	51,61,70,71	0
17	CLA	f	7003	55/65	0.92	0.24	68,87,121,122	0
20	BCR	b	846	40/40	0.92	0.22	48,56,76,77	0
22	HTG	j	3001	19/19	0.92	0.37	61,71,80,84	0
17	CLA	4	601	46/65	0.92	0.20	84,92,95,111	0
17	CLA	4	602	60/65	0.92	0.19	54,67,73,74	0
28	XAT	2	616	44/44	0.92	0.25	69,79,86,87	0
17	CLA	B	823	60/65	0.92	0.20	46,57,84,84	0
17	CLA	a	840	65/65	0.92	0.32	36,41,87,89	0
17	CLA	1	308	65/65	0.92	0.37	57,92,120,121	0
26	CHL	9	607	51/66	0.92	0.27	67,77,98,99	0
27	LUT	8	314	42/42	0.92	0.39	57,73,82,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
17	CLA	B	802	65/65	0.92	0.30	40,44,50,52	0
17	CLA	B	827	65/65	0.92	0.40	49,61,78,80	0
17	CLA	L	204	50/65	0.92	0.19	76,84,109,109	0
17	CLA	A	804	65/65	0.92	0.23	46,58,70,71	0
17	CLA	B	825	65/65	0.92	0.35	42,50,83,88	0
17	CLA	a	817	45/65	0.92	0.19	64,73,78,79	0
17	CLA	A	839	65/65	0.92	0.19	54,60,80,83	0
17	CLA	A	808	65/65	0.92	0.18	52,61,113,115	0
17	CLA	A	817	45/65	0.92	0.22	66,75,86,92	0
17	CLA	A	814	65/65	0.92	0.31	50,59,67,68	0
26	CHL	9	606	51/66	0.92	0.19	86,106,118,119	0
28	XAT	6	318	44/44	0.92	0.24	71,81,94,95	0
17	CLA	8	310	55/65	0.92	0.33	74,88,99,104	0
17	CLA	B	810	65/65	0.92	0.22	59,77,84,86	0
20	BCR	j	3003	40/40	0.92	0.22	42,52,59,61	0
17	CLA	8	303	45/65	0.92	0.26	75,92,99,133	0
17	CLA	A	827	65/65	0.92	0.27	40,60,97,98	0
20	BCR	J	3003	40/40	0.92	0.21	45,54,67,68	0
26	CHL	9	605	56/66	0.92	0.18	80,94,97,126	0
20	BCR	b	801	40/40	0.92	0.20	36,43,52,55	0
17	CLA	A	835	65/65	0.92	0.23	58,67,75,81	0
17	CLA	A	818	65/65	0.92	0.22	58,71,95,97	0
17	CLA	6	312	41/65	0.92	0.20	90,102,109,129	0
17	CLA	1	306	52/65	0.92	0.17	90,99,109,111	0
26	CHL	7	614	43/66	0.92	0.29	105,120,127,139	0
20	BCR	3	318	40/40	0.92	0.23	77,83,105,108	0
17	CLA	1	313	65/65	0.92	0.21	81,88,108,112	0
27	LUT	1	316	42/42	0.92	0.19	69,74,100,101	0
26	CHL	4	615	43/66	0.92	0.19	61,74,87,89	0
17	CLA	g	102	50/65	0.92	0.33	92,107,123,124	0
17	CLA	B	835	45/65	0.92	0.17	57,66,70,72	0
17	CLA	6	306	51/65	0.92	0.24	118,123,130,131	0
28	XAT	4	617	44/44	0.93	0.19	63,72,87,88	0
17	CLA	B	822	55/65	0.93	0.22	48,58,82,83	0
17	CLA	b	816	55/65	0.93	0.19	57,65,72,75	0
17	CLA	6	315	55/65	0.93	0.28	105,114,131,131	0
20	BCR	f	7004	40/40	0.93	0.20	55,62,66,66	0
20	BCR	i	101	40/40	0.93	0.18	36,45,49,50	0
17	CLA	a	839	65/65	0.93	0.24	36,43,65,69	0
17	CLA	a	812	65/65	0.93	0.23	47,59,70,77	0
17	CLA	G	101	45/65	0.93	0.21	74,79,85,89	0
17	CLA	b	822	55/65	0.93	0.16	46,60,80,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	CLA	B	839	65/65	0.93	0.25	53,60,69,72	0
17	CLA	1	315	46/65	0.93	0.15	76,87,93,132	0
17	CLA	b	835	45/65	0.93	0.16	86,92,94,96	0
17	CLA	3	305	42/65	0.93	0.20	67,78,84,90	0
17	CLA	G	104	46/65	0.93	0.31	70,93,100,111	0
19	LHG	6	301	23/49	0.93	0.15	67,101,110,111	0
20	BCR	A	849	40/40	0.93	0.44	54,62,83,84	0
17	CLA	A	821	45/65	0.93	0.21	69,74,88,109	0
17	CLA	A	810	65/65	0.93	0.19	43,51,85,89	0
17	CLA	7	613	43/65	0.93	0.23	73,78,82,86	0
17	CLA	2	602	65/65	0.93	0.21	66,73,80,83	0
17	CLA	l	203	65/65	0.93	0.20	40,51,71,73	0
17	CLA	1	312	52/65	0.93	0.20	70,76,99,100	0
17	CLA	A	826	65/65	0.93	0.23	47,57,65,66	0
17	CLA	a	837	45/65	0.93	0.17	57,65,74,77	0
17	CLA	A	825	55/65	0.93	0.16	58,67,74,78	0
17	CLA	A	833	65/65	0.93	0.22	54,61,101,102	0
17	CLA	b	834	65/65	0.93	0.22	61,74,105,106	0
28	XAT	1	317	44/44	0.93	0.21	63,68,93,96	0
17	CLA	a	813	54/65	0.93	0.19	43,51,60,70	0
17	CLA	l	204	50/65	0.93	0.18	46,59,100,104	0
17	CLA	a	811	65/65	0.93	0.20	42,59,94,96	0
20	BCR	a	853	40/40	0.93	0.26	44,48,66,67	0
26	CHL	4	607	51/66	0.93	0.20	57,73,82,85	0
26	CHL	2	607	51/66	0.93	0.21	66,75,117,118	0
17	CLA	9	601	46/65	0.93	0.18	81,91,95,110	0
17	CLA	8	304	42/65	0.93	0.18	59,72,78,80	0
17	CLA	b	829	65/65	0.93	0.23	39,54,67,69	0
17	CLA	a	819	65/65	0.93	0.22	38,54,96,99	0
17	CLA	b	833	58/65	0.93	0.20	48,63,77,78	0
17	CLA	B	805	65/65	0.93	0.25	45,47,53,60	0
17	CLA	A	831	65/65	0.93	0.21	43,52,59,61	0
26	CHL	7	601	61/66	0.93	0.20	62,74,93,95	0
17	CLA	6	314	60/65	0.93	0.23	66,109,124,125	0
17	CLA	B	840	65/65	0.93	0.33	41,50,72,78	0
17	CLA	a	816	50/65	0.93	0.23	43,52,94,96	0
22	HTG	a	857	19/19	0.93	0.24	53,70,79,81	0
20	BCR	l	201	40/40	0.93	0.21	38,46,54,54	0
20	BCR	l	205	40/40	0.93	0.24	39,46,52,54	0
17	CLA	A	813	54/65	0.93	0.21	60,68,77,95	0
17	CLA	7	609	60/65	0.93	0.27	64,86,97,97	0
26	CHL	6	303	61/66	0.93	0.20	78,91,102,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	BCR	b	843	40/40	0.93	0.20	54,60,68,69	0
17	CLA	b	821	46/65	0.93	0.18	58,69,90,118	0
17	CLA	B	833	58/65	0.93	0.18	43,52,79,80	0
17	CLA	b	832	65/65	0.93	0.22	36,55,70,79	0
17	CLA	B	816	55/65	0.93	0.20	60,67,73,91	0
17	CLA	B	807	65/65	0.93	0.21	51,66,113,117	0
17	CLA	3	312	55/65	0.93	0.15	86,107,114,117	0
17	CLA	B	809	65/65	0.93	0.23	41,50,81,82	0
17	CLA	b	813	65/65	0.94	0.23	44,57,67,69	0
19	LHG	A	846	49/49	0.94	0.21	44,49,58,59	0
17	CLA	a	826	65/65	0.94	0.22	39,43,48,56	0
17	CLA	4	608	50/65	0.94	0.17	56,66,76,86	0
17	CLA	3	306	47/65	0.94	0.18	67,79,90,91	0
17	CLA	9	602	60/65	0.94	0.18	60,67,74,86	0
17	CLA	a	815	45/65	0.94	0.19	41,54,63,63	0
17	CLA	A	809	65/65	0.94	0.19	44,51,63,65	0
17	CLA	a	833	65/65	0.94	0.25	39,46,98,102	0
17	CLA	A	843	65/65	0.94	0.26	48,64,79,81	0
17	CLA	b	819	65/65	0.94	0.24	50,57,92,95	0
26	CHL	8	306	47/66	0.94	0.21	60,64,79,84	0
20	BCR	b	848	40/40	0.94	0.20	37,42,45,47	0
17	CLA	b	809	65/65	0.94	0.20	39,50,72,75	0
17	CLA	A	830	65/65	0.94	0.28	45,53,58,61	0
17	CLA	2	611	52/65	0.94	0.17	68,83,119,128	0
17	CLA	A	801	65/65	0.94	0.27	40,44,49,53	0
17	CLA	7	612	65/65	0.94	0.24	56,66,87,89	0
18	PQN	B	842	33/33	0.94	0.44	46,56,63,63	0
17	CLA	9	608	50/65	0.94	0.18	72,78,103,105	0
17	CLA	A	820	65/65	0.94	0.22	46,50,57,58	0
17	CLA	a	805	55/65	0.94	0.18	38,43,76,78	0
17	CLA	b	805	65/65	0.94	0.21	42,45,52,58	0
26	CHL	7	607	51/66	0.94	0.20	64,70,92,98	0
17	CLA	A	829	65/65	0.94	0.23	42,46,55,58	0
17	CLA	B	841	65/65	0.94	0.19	49,56,63,68	0
17	CLA	F	301	65/65	0.94	0.19	48,55,83,87	0
17	CLA	3	308	50/65	0.94	0.20	76,86,93,104	0
20	BCR	L	201	40/40	0.94	0.18	51,59,72,73	0
26	CHL	1	302	61/66	0.94	0.21	64,74,101,105	0
17	CLA	a	842	65/65	0.94	0.21	47,59,96,98	0
17	CLA	a	832	50/65	0.94	0.20	41,54,78,83	0
17	CLA	6	304	65/65	0.94	0.20	66,79,104,106	0
19	LHG	2	618	37/49	0.94	0.30	80,91,127,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
17	CLA	a	834	65/65	0.94	0.24	37,44,48,50	0
17	CLA	B	804	45/65	0.94	0.18	44,50,68,77	0
17	CLA	a	814	65/65	0.94	0.24	39,47,64,67	0
17	CLA	1	304	65/65	0.94	0.21	63,70,95,97	0
17	CLA	B	806	65/65	0.94	0.27	43,52,60,64	0
17	CLA	b	840	65/65	0.94	0.23	36,41,59,67	0
17	CLA	B	803	65/65	0.94	0.33	39,50,61,68	0
17	CLA	A	811	65/65	0.94	0.26	54,69,89,90	0
17	CLA	b	836	60/65	0.94	0.24	43,53,106,107	0
17	CLA	a	856	65/65	0.94	0.26	36,41,56,59	0
17	CLA	a	821	45/65	0.94	0.19	51,62,70,87	0
20	BCR	B	848	40/40	0.94	0.33	40,45,51,52	0
17	CLA	B	830	50/65	0.94	0.17	45,56,75,75	0
17	CLA	4	614	50/65	0.94	0.20	60,68,90,91	0
17	CLA	B	837	65/65	0.94	0.23	49,55,61,65	0
17	CLA	9	614	47/65	0.94	0.22	62,75,97,99	0
17	CLA	2	603	65/65	0.94	0.16	64,72,106,108	0
17	CLA	A	828	65/65	0.94	0.22	49,61,79,84	0
17	CLA	b	827	65/65	0.95	0.28	40,53,83,83	0
17	CLA	B	808	65/65	0.95	0.25	41,45,70,73	0
17	CLA	1	311	41/65	0.95	0.17	67,74,81,82	0
17	CLA	b	837	65/65	0.95	0.21	46,57,69,70	0
17	CLA	a	829	65/65	0.95	0.23	35,41,56,58	0
17	CLA	A	840	65/65	0.95	0.23	48,55,95,96	0
17	CLA	a	802	65/65	0.95	0.27	35,42,56,62	0
17	CLA	9	603	46/65	0.95	0.17	62,64,77,78	0
17	CLA	a	808	65/65	0.95	0.20	54,63,86,87	0
17	CLA	b	838	47/65	0.95	0.22	38,44,54,64	0
17	CLA	a	822	65/65	0.95	0.17	42,46,53,57	0
17	CLA	b	806	65/65	0.95	0.26	39,43,52,65	0
17	CLA	a	838	51/65	0.95	0.19	36,40,63,68	0
17	CLA	b	818	60/65	0.95	0.28	44,47,53,56	0
17	CLA	b	808	65/65	0.95	0.18	39,47,53,59	0
17	CLA	a	806	65/65	0.95	0.21	37,39,49,51	0
17	CLA	A	822	65/65	0.95	0.20	49,67,76,79	0
26	CHL	3	307	47/66	0.95	0.17	72,77,94,97	0
17	CLA	8	305	47/65	0.95	0.15	61,71,78,79	0
17	CLA	3	303	50/65	0.95	0.21	60,67,75,76	0
17	CLA	b	802	65/65	0.95	0.24	36,41,45,52	0
17	CLA	B	812	55/65	0.95	0.21	53,62,106,107	0
20	BCR	B	801	40/40	0.95	0.21	43,46,54,55	0
17	CLA	7	610	41/65	0.95	0.19	74,82,94,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	CLA	9	610	41/65	0.95	0.26	99,103,113,114	0
17	CLA	a	810	65/65	0.95	0.19	44,59,94,95	0
17	CLA	A	816	50/65	0.95	0.20	52,70,108,108	0
19	LHG	1	301	23/49	0.95	0.20	63,84,93,94	0
17	CLA	A	838	51/65	0.95	0.17	45,60,67,68	0
20	BCR	a	851	40/40	0.95	0.32	37,53,66,67	0
17	CLA	a	809	65/65	0.95	0.20	36,39,53,57	0
17	CLA	A	819	65/65	0.95	0.21	54,65,117,120	0
17	CLA	B	828	65/65	0.95	0.29	43,48,58,61	0
17	CLA	b	810	65/65	0.95	0.17	39,49,59,62	0
20	BCR	F	305	40/40	0.95	0.20	46,51,58,60	0
17	CLA	F	303	45/65	0.95	0.20	51,60,71,76	0
17	CLA	8	312	46/65	0.95	0.15	57,66,99,103	0
17	CLA	a	841	65/65	0.95	0.21	55,62,65,67	0
17	CLA	A	815	45/65	0.95	0.19	54,59,65,70	0
17	CLA	a	827	65/65	0.95	0.27	35,41,82,85	0
17	CLA	a	843	65/65	0.95	0.24	35,39,60,65	0
17	CLA	a	818	65/65	0.95	0.21	45,53,81,83	0
17	CLA	a	828	65/65	0.95	0.22	37,44,67,72	0
17	CLA	B	826	65/65	0.95	0.28	44,50,56,64	0
17	CLA	A	803	65/65	0.95	0.27	39,44,54,59	0
17	CLA	B	838	47/65	0.95	0.30	43,48,65,68	0
17	CLA	a	807	65/65	0.95	0.22	35,41,50,54	0
17	CLA	A	854	65/65	0.95	0.31	40,44,57,59	0
17	CLA	B	832	65/65	0.95	0.23	43,48,73,76	0
17	CLA	b	826	65/65	0.95	0.27	48,55,59,62	0
17	CLA	A	842	65/65	0.95	0.23	42,45,56,65	0
17	CLA	4	603	46/65	0.95	0.19	54,62,69,72	0
17	CLA	A	841	65/65	0.95	0.19	44,50,55,60	0
17	CLA	B	820	50/65	0.95	0.20	53,69,95,100	0
17	CLA	A	802	65/65	0.95	0.29	41,45,51,53	0
17	CLA	8	302	50/65	0.95	0.16	46,54,73,74	0
17	CLA	7	603	51/65	0.95	0.19	52,60,97,98	0
20	BCR	A	852	40/40	0.96	0.23	42,44,49,50	0
18	PQN	a	845	33/33	0.96	0.22	35,48,54,58	0
17	CLA	b	828	65/65	0.96	0.29	41,47,56,56	0
17	CLA	b	804	45/65	0.96	0.14	42,52,68,75	0
17	CLA	a	831	65/65	0.96	0.19	36,43,54,56	0
17	CLA	a	835	65/65	0.96	0.19	36,43,48,49	0
17	CLA	b	839	65/65	0.96	0.18	38,44,50,53	0
17	CLA	a	825	55/65	0.96	0.18	39,44,58,68	0
17	CLA	A	807	65/65	0.96	0.27	44,47,58,69	0

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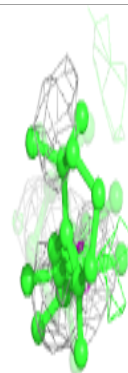
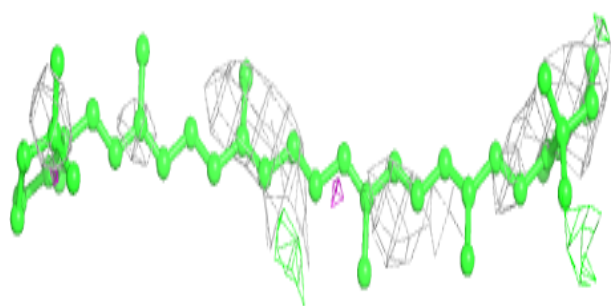
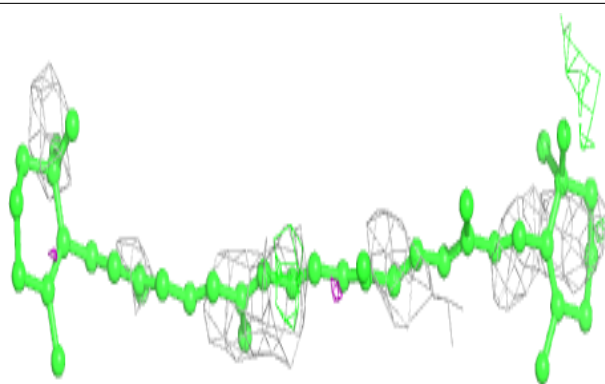
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
18	PQN	b	842	33/33	0.96	0.22	36,41,49,50	0
17	CLA	f	7002	45/65	0.96	0.16	54,59,76,77	0
17	CLA	a	803	65/65	0.96	0.23	35,38,50,53	0
18	PQN	A	844	33/33	0.96	0.24	42,45,57,58	0
17	CLA	B	819	65/65	0.96	0.23	46,53,80,83	0
17	CLA	a	844	65/65	0.96	0.23	38,49,59,64	0
17	CLA	8	301	60/65	0.96	0.17	56,64,68,72	0
17	CLA	B	831	49/65	0.96	0.18	45,53,62,65	0
19	LHG	a	847	49/49	0.96	0.21	35,41,47,48	0
17	CLA	a	801	65/65	0.96	0.21	35,39,44,46	0
20	BCR	a	850	40/40	0.96	0.23	39,48,79,81	0
17	CLA	8	307	50/65	0.96	0.18	52,65,91,93	0
22	HTG	A	855	19/19	0.96	0.16	68,72,74,75	0
17	CLA	b	803	65/65	0.97	0.27	35,40,47,49	0
20	BCR	a	854	40/40	0.97	0.19	35,40,47,47	0
17	CLA	a	830	65/65	0.97	0.21	36,40,47,49	0
17	CLA	a	820	65/65	0.98	0.20	38,43,48,50	0
21	SF4	a	855	8/8	0.98	0.20	37,37,43,43	0
21	SF4	A	853	8/8	0.99	0.18	43,44,48,51	0
21	SF4	c	102	8/8	0.99	0.12	41,50,62,77	0
21	SF4	c	101	8/8	0.99	0.16	41,46,54,56	0
21	SF4	C	101	8/8	0.99	0.14	47,49,53,57	0
21	SF4	C	102	8/8	0.99	0.09	51,62,72,84	0

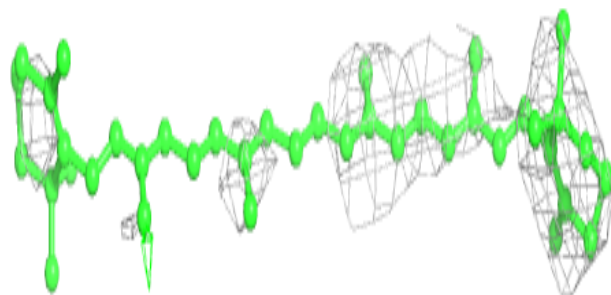
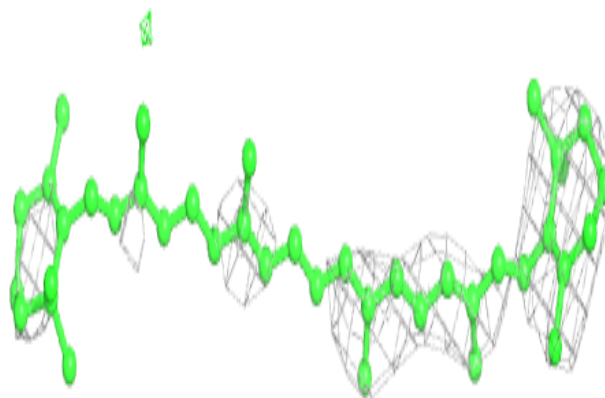
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

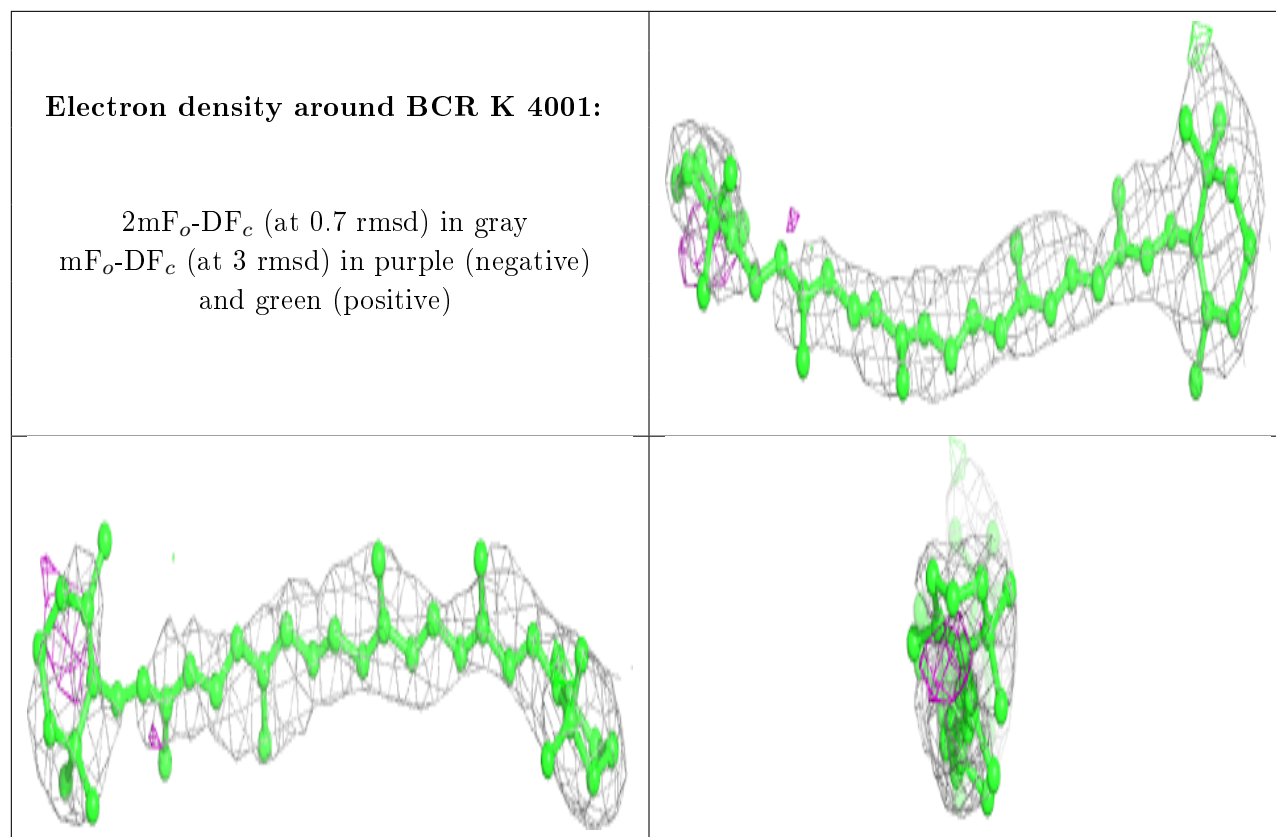
Electron density around BCR L 206:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around BCR K 4004:**

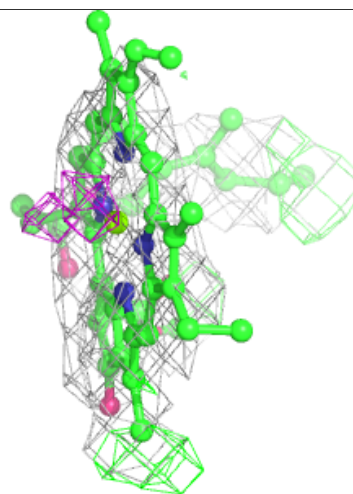
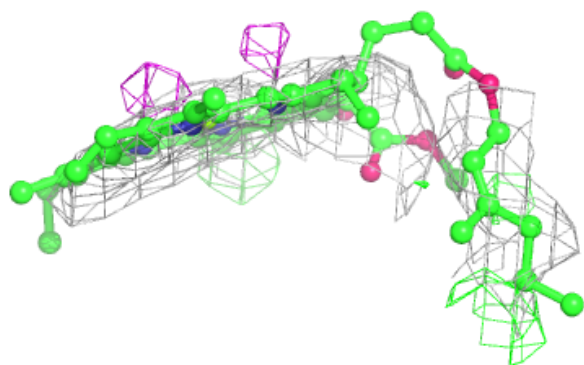
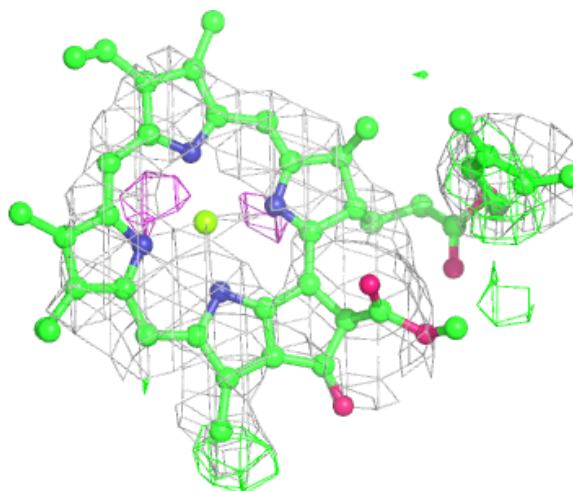
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





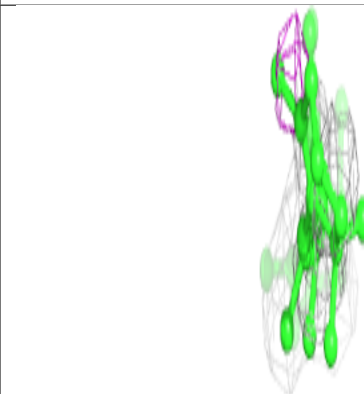
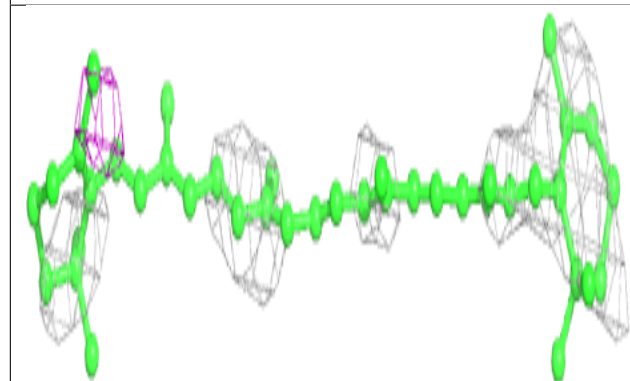
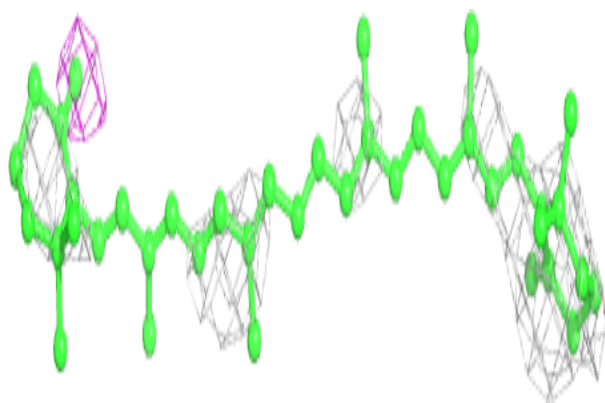
Electron density around CLA 8 309:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

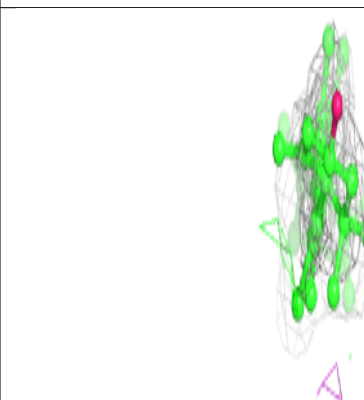
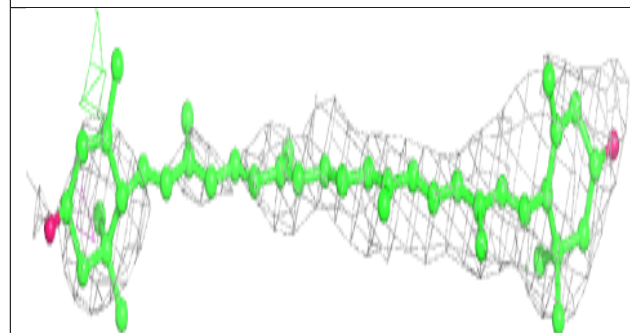
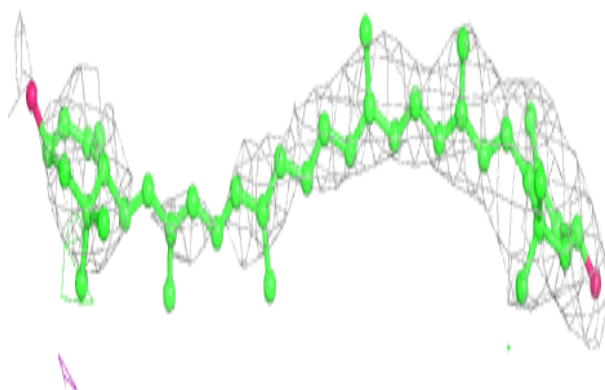


Electron density around BCR 2 617:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

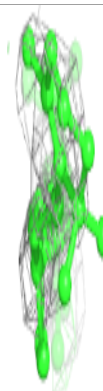
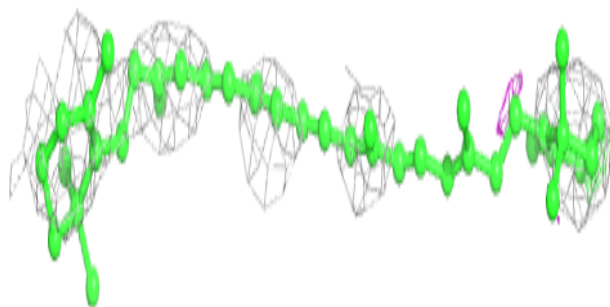
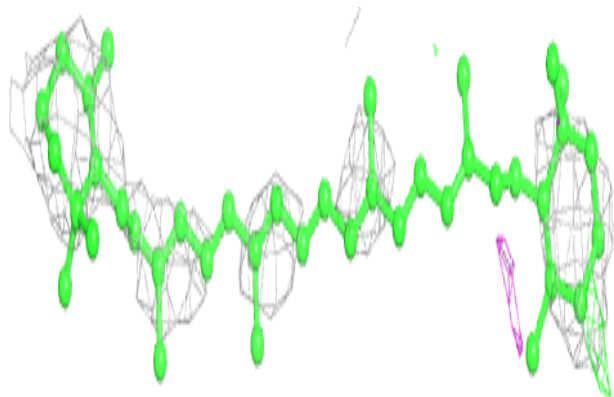
**Electron density around LUT 6 317:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

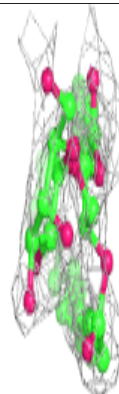
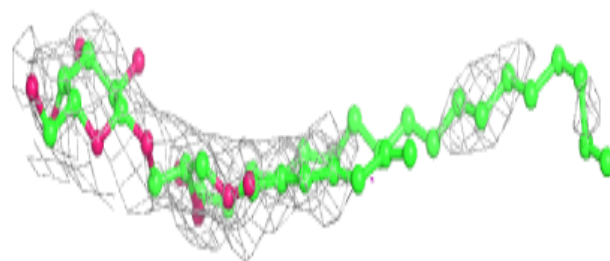
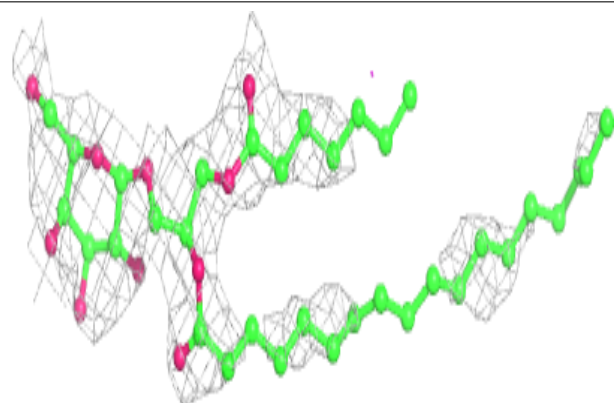


Electron density around BCR 7 617:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

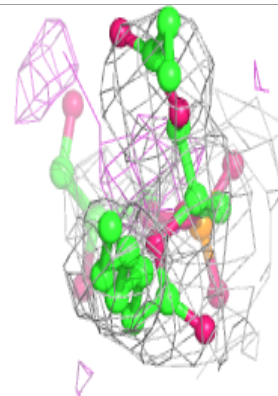
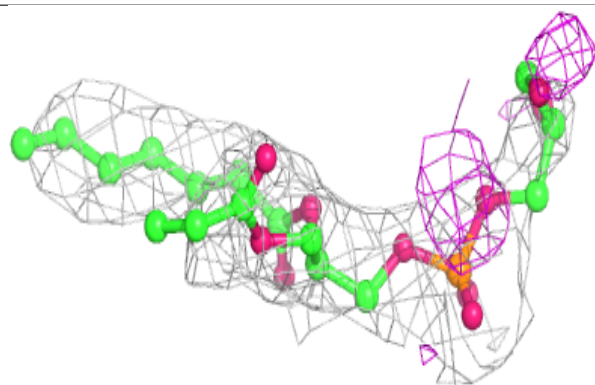
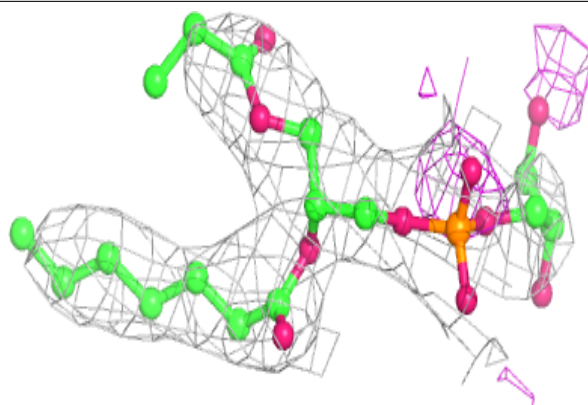
**Electron density around LMG 4 620:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

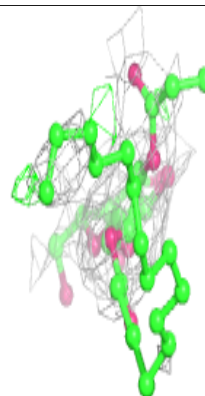
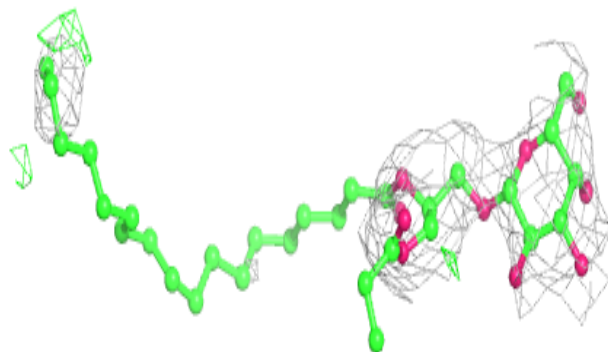
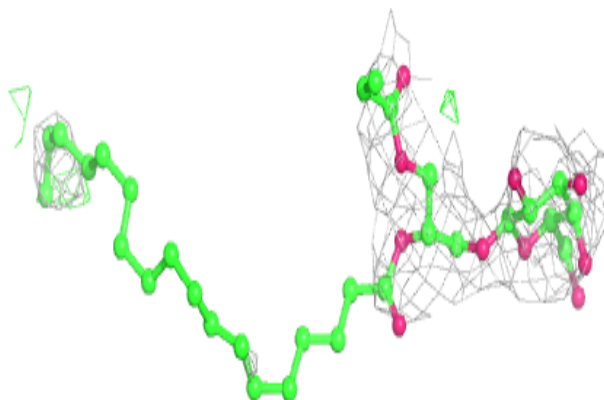


Electron density around LHG a 848:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

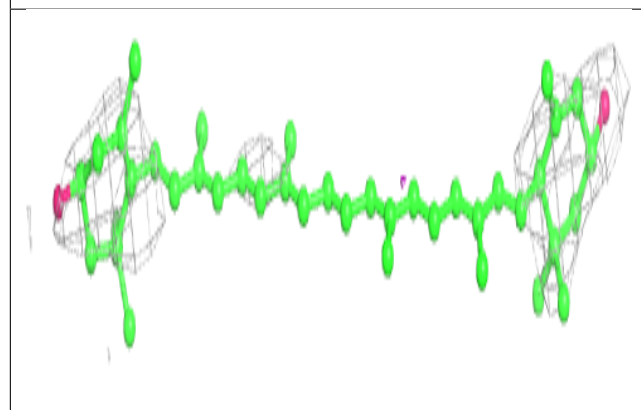
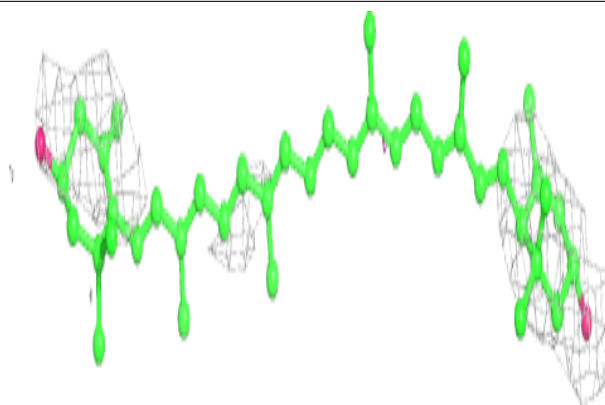
**Electron density around LMG 6 302:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



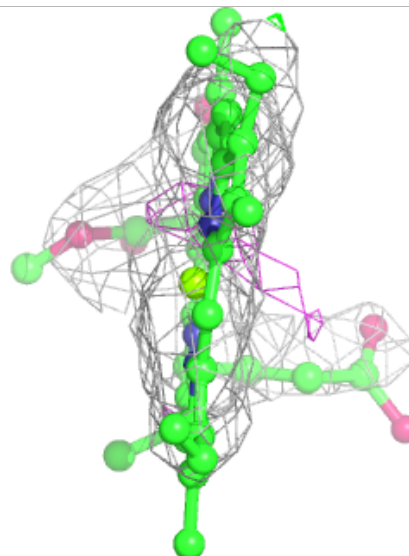
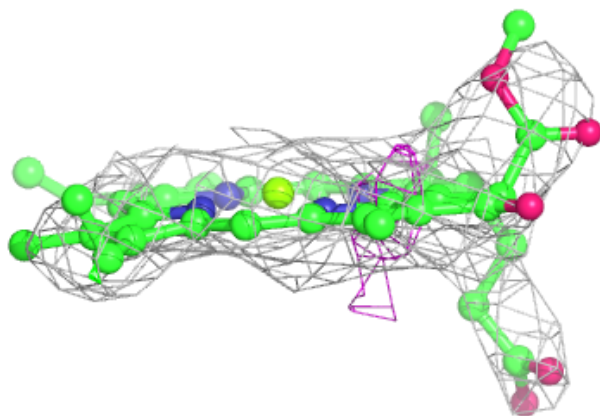
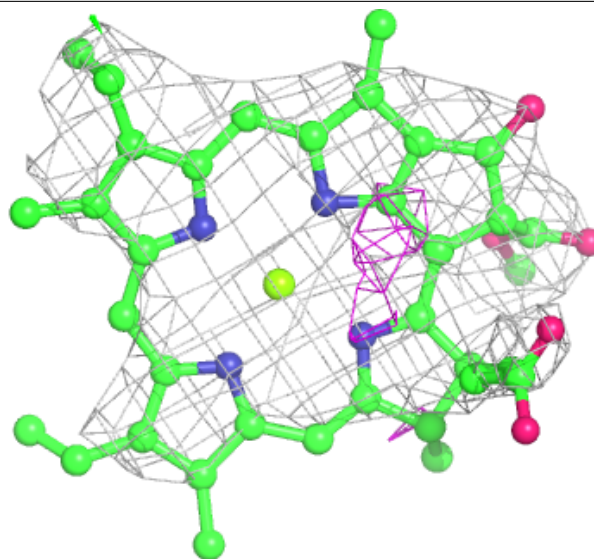
Electron density around LUT 6 321:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



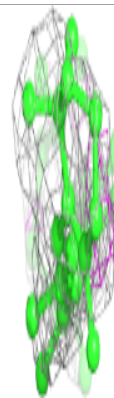
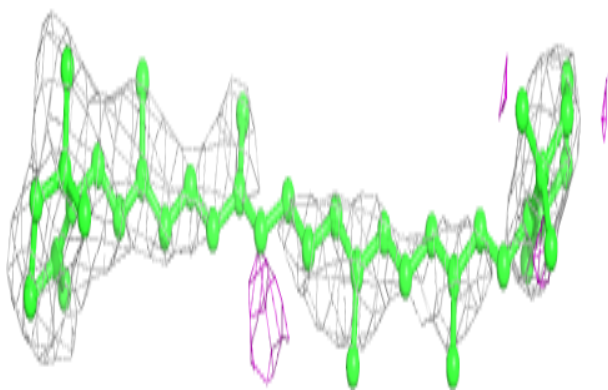
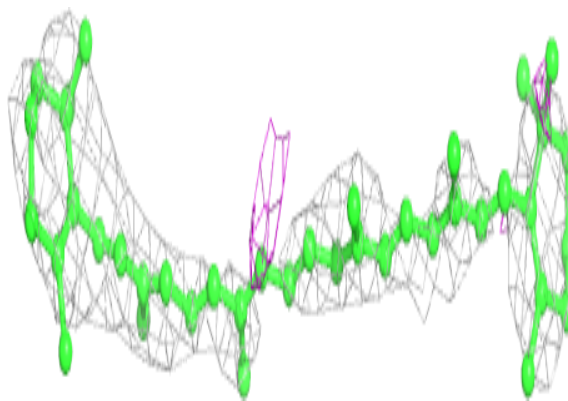
Electron density around CLA K 4002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

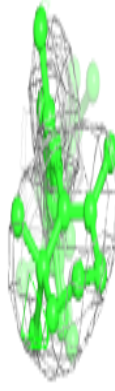
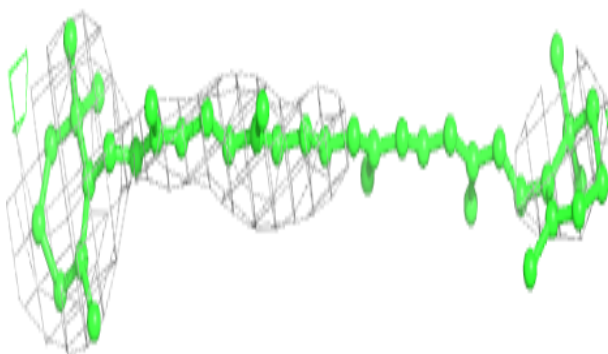
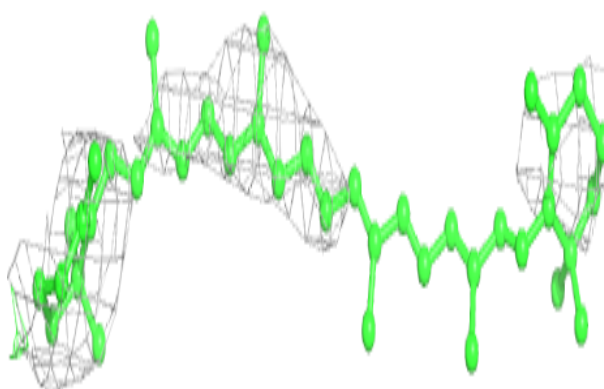


Electron density around BCR 1 206:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

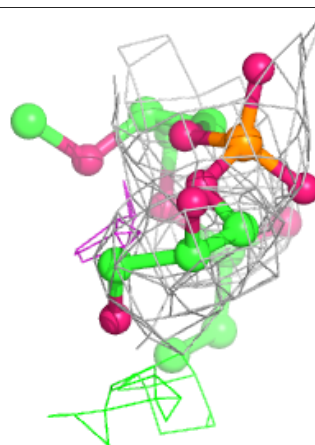
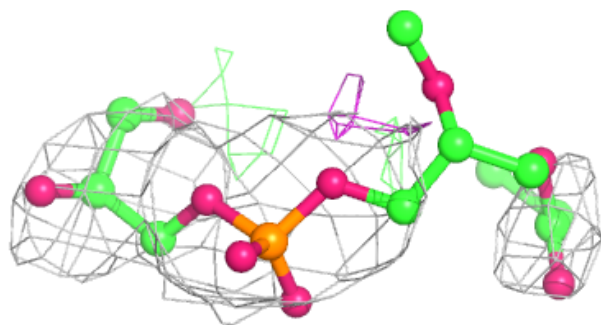
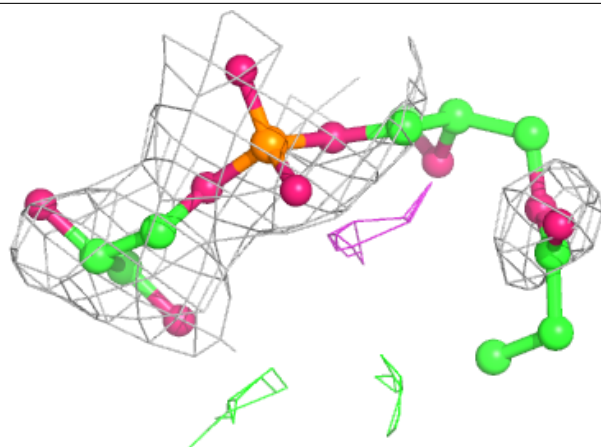
**Electron density around BCR 1 318:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

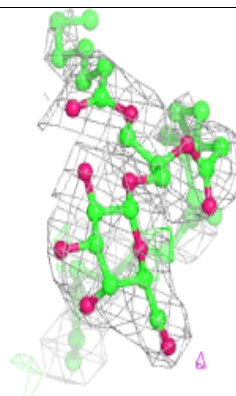
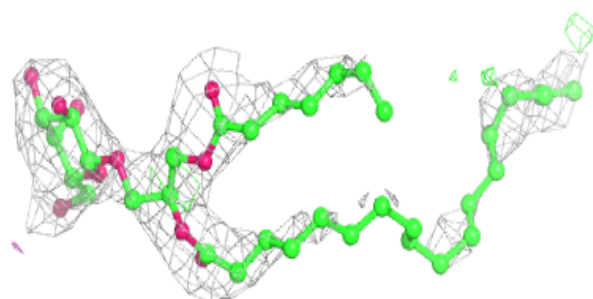
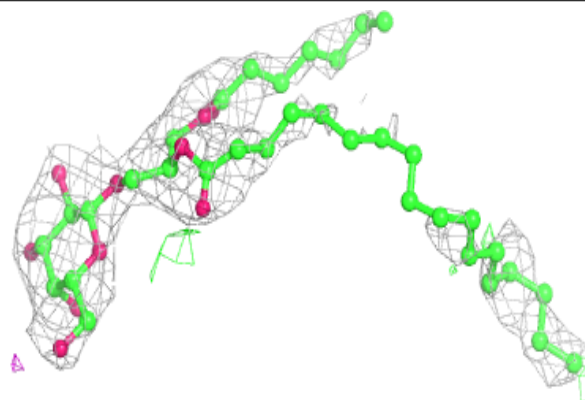


Electron density around LHG 3 319:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

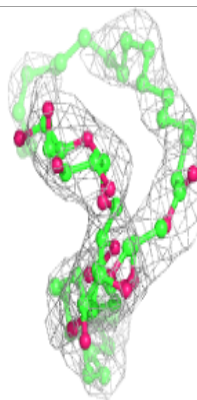
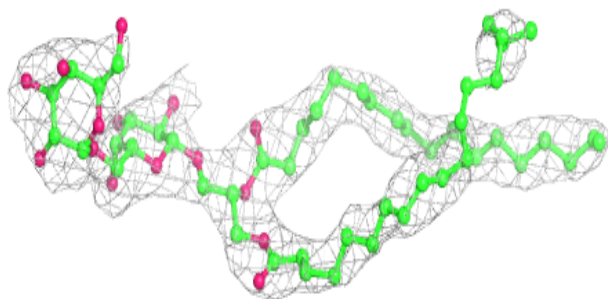
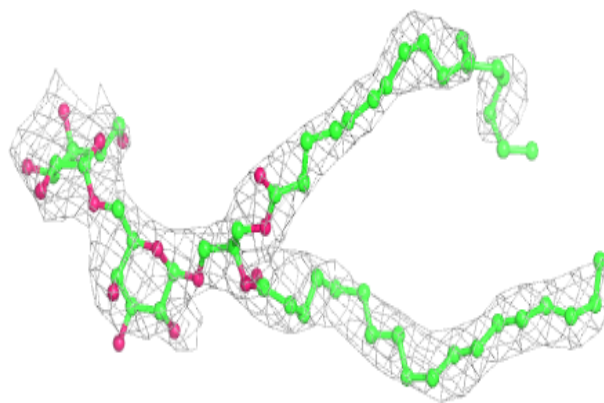
**Electron density around LMG 4 619:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

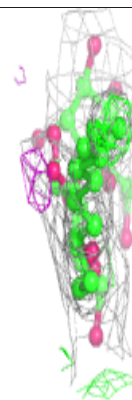
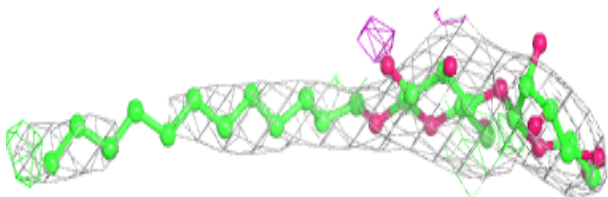
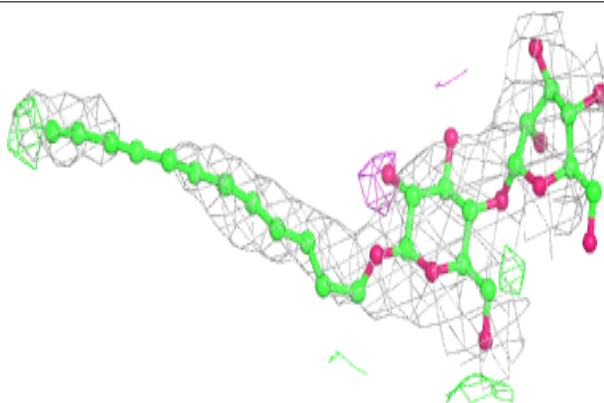


Electron density around DGD B 850:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

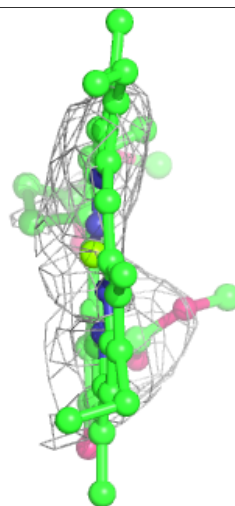
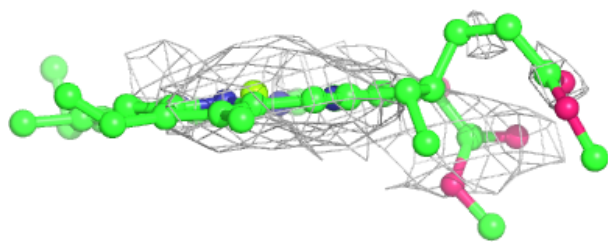
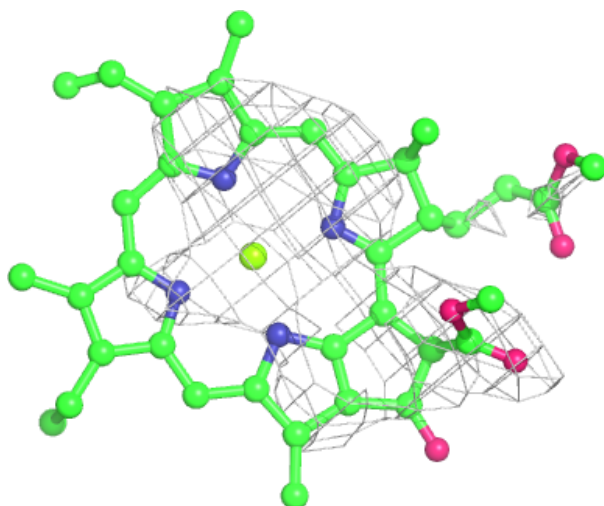
**Electron density around LMT B 849:**

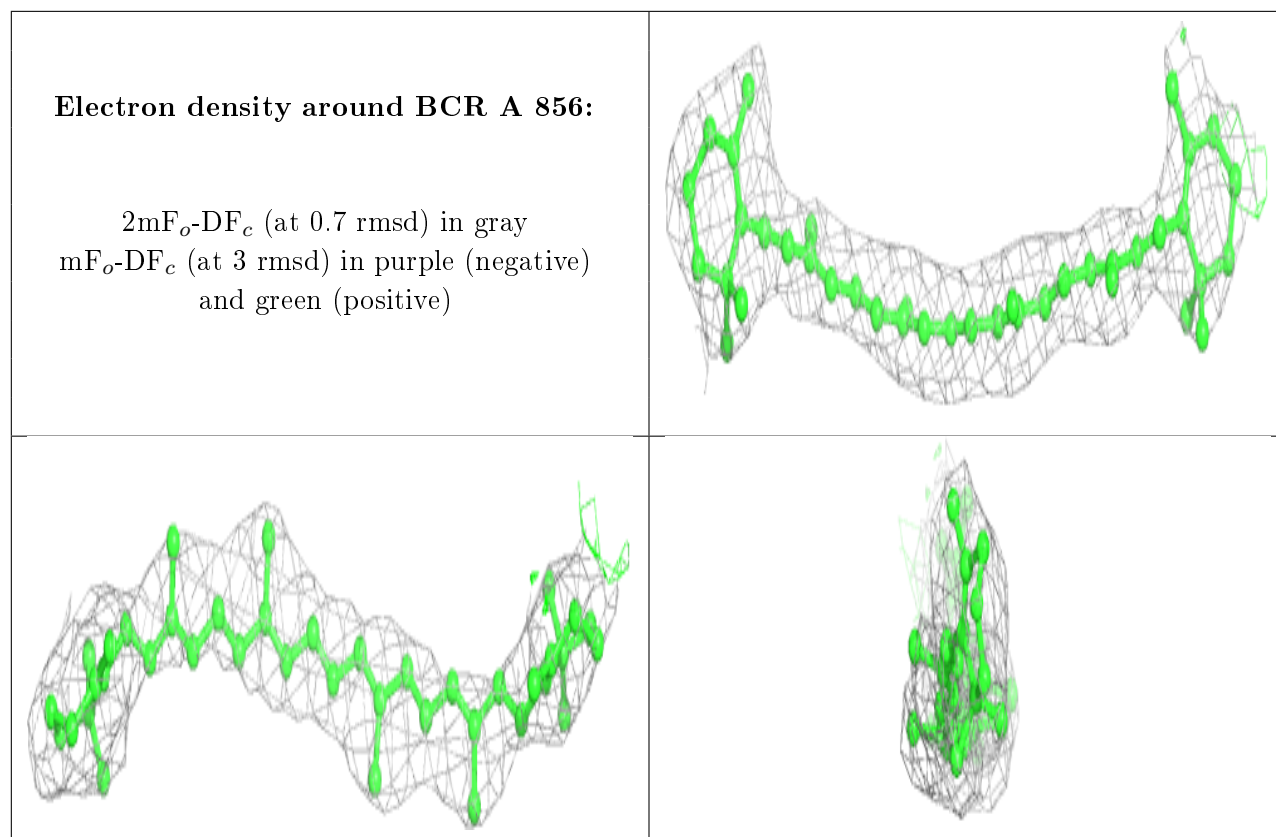
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 3 301:

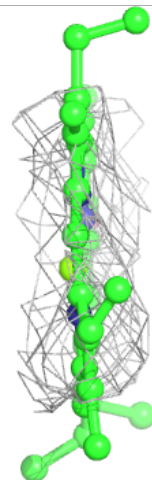
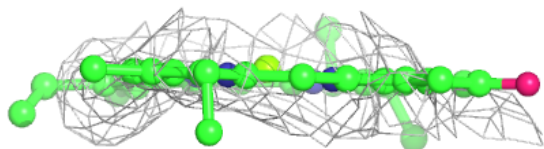
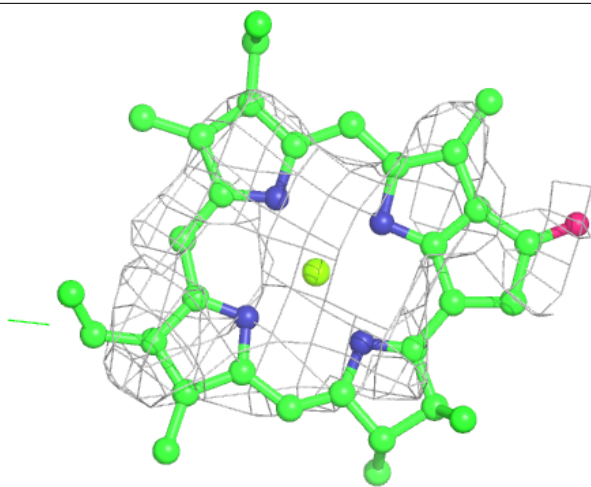
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





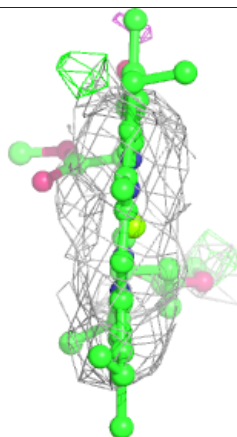
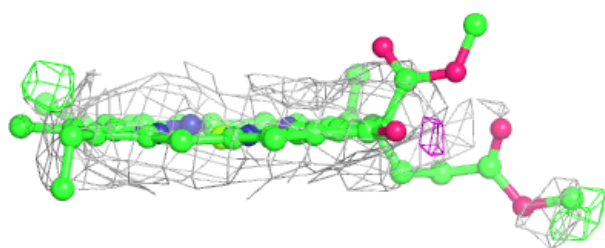
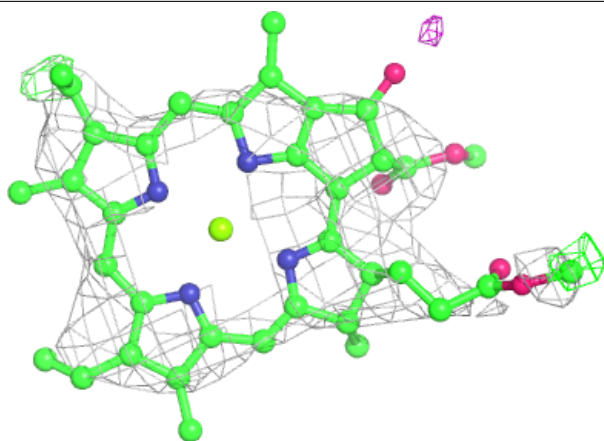
Electron density around CLA 3 310:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

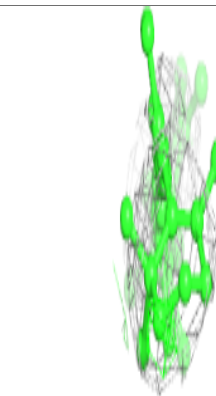
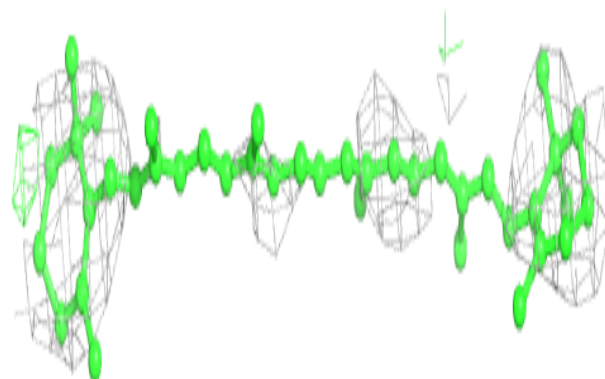
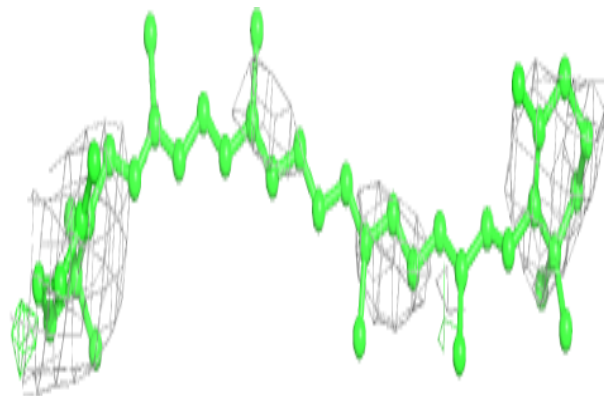


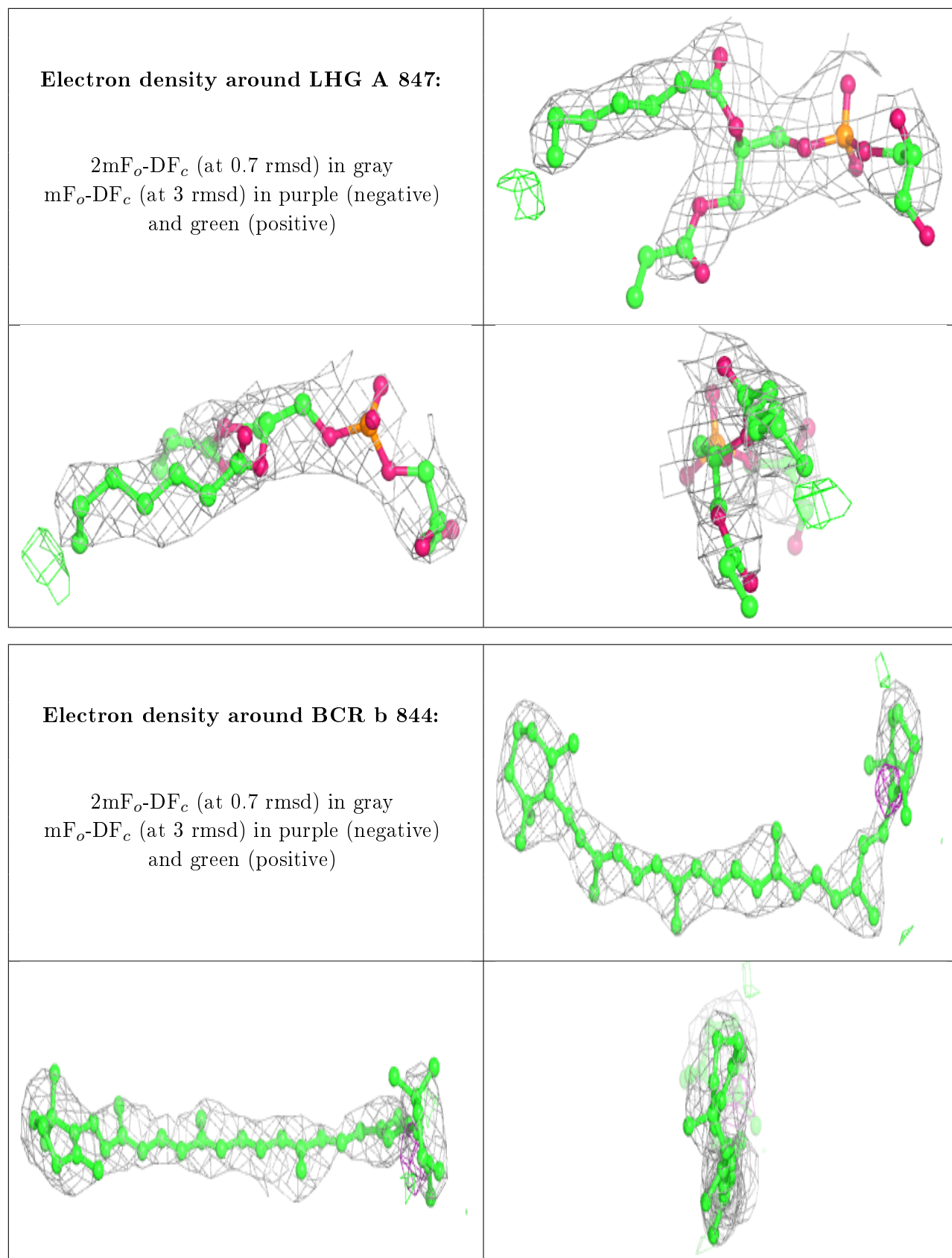
Electron density around CLA 6 316:

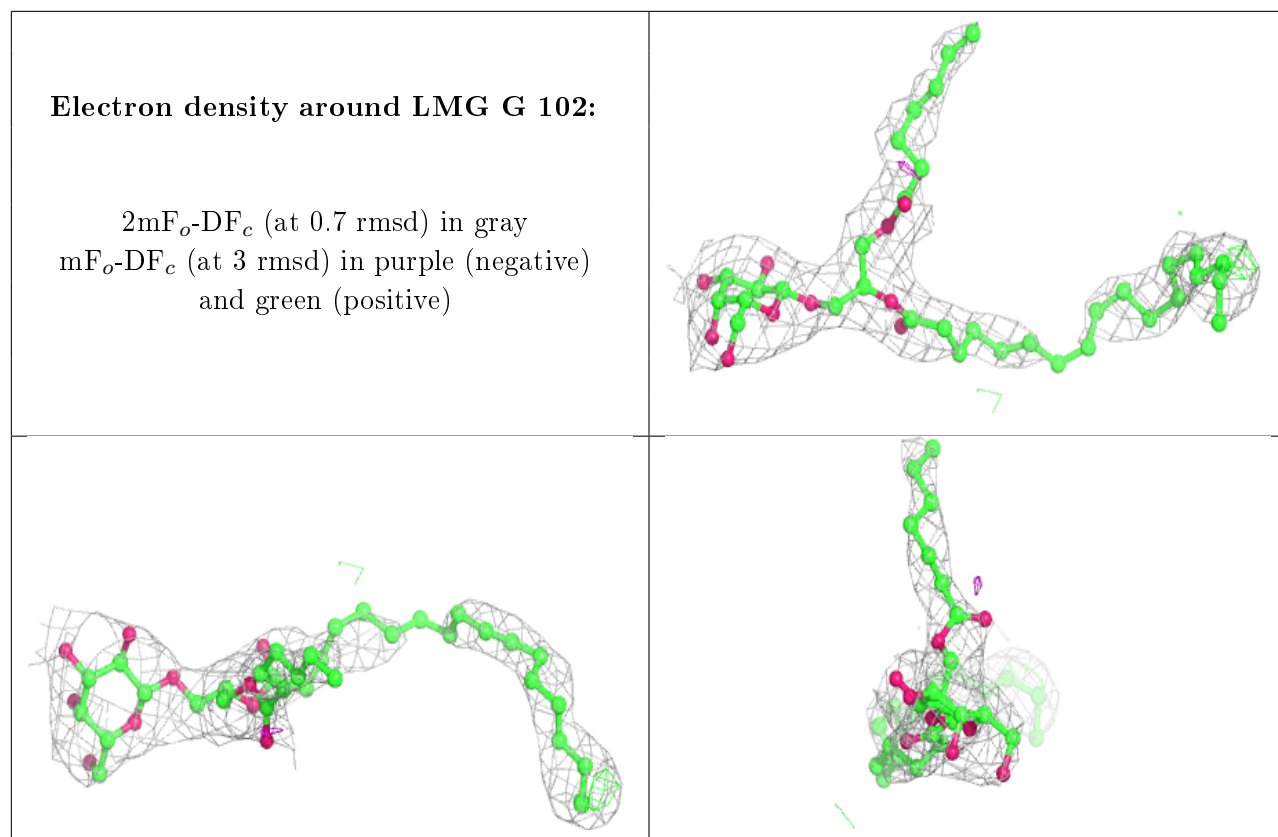
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around BCR 6 319:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

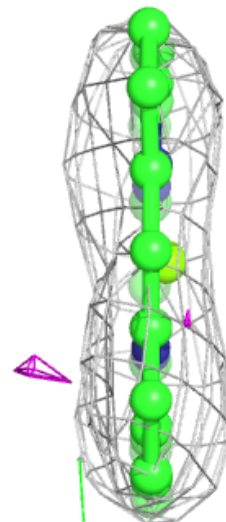
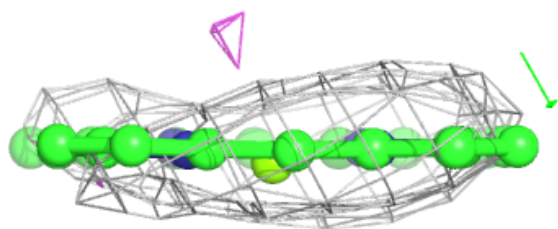
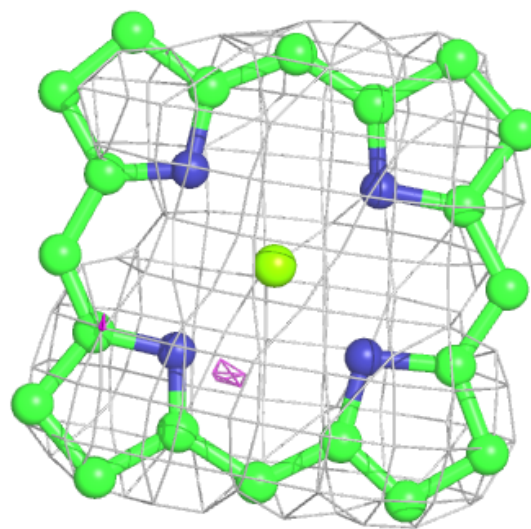






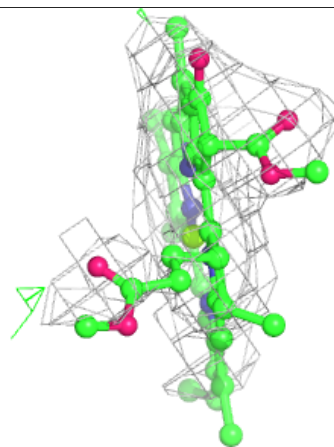
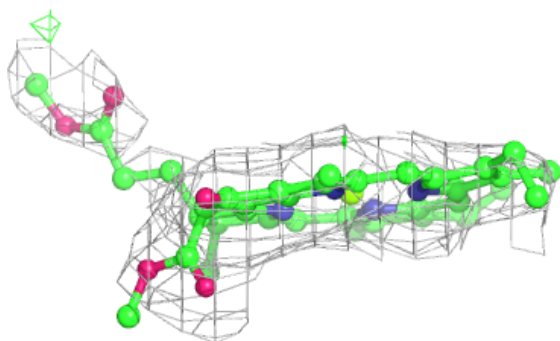
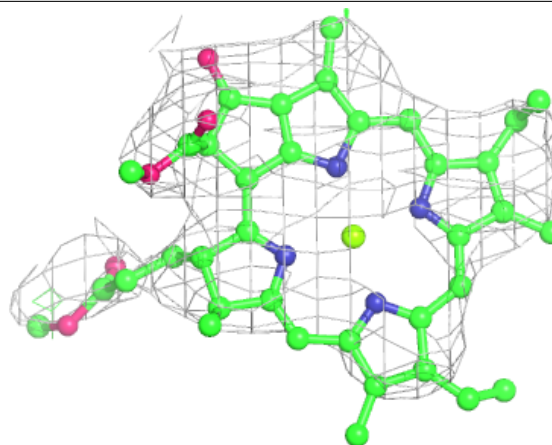
Electron density around CLA 8 313:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

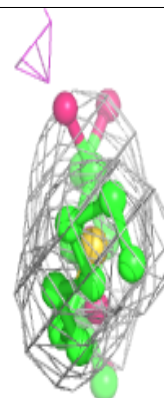
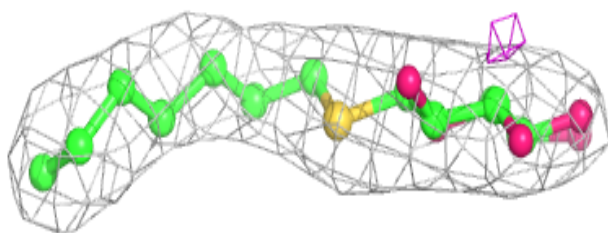
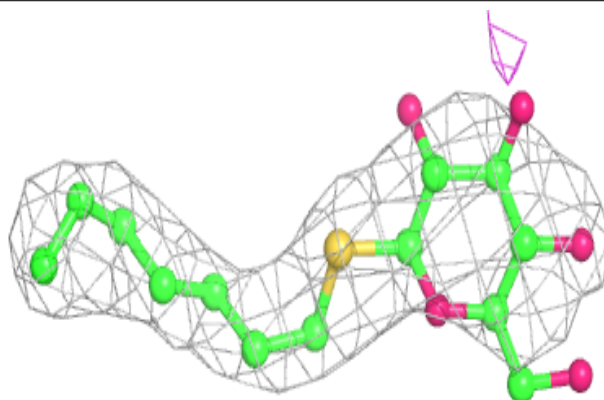


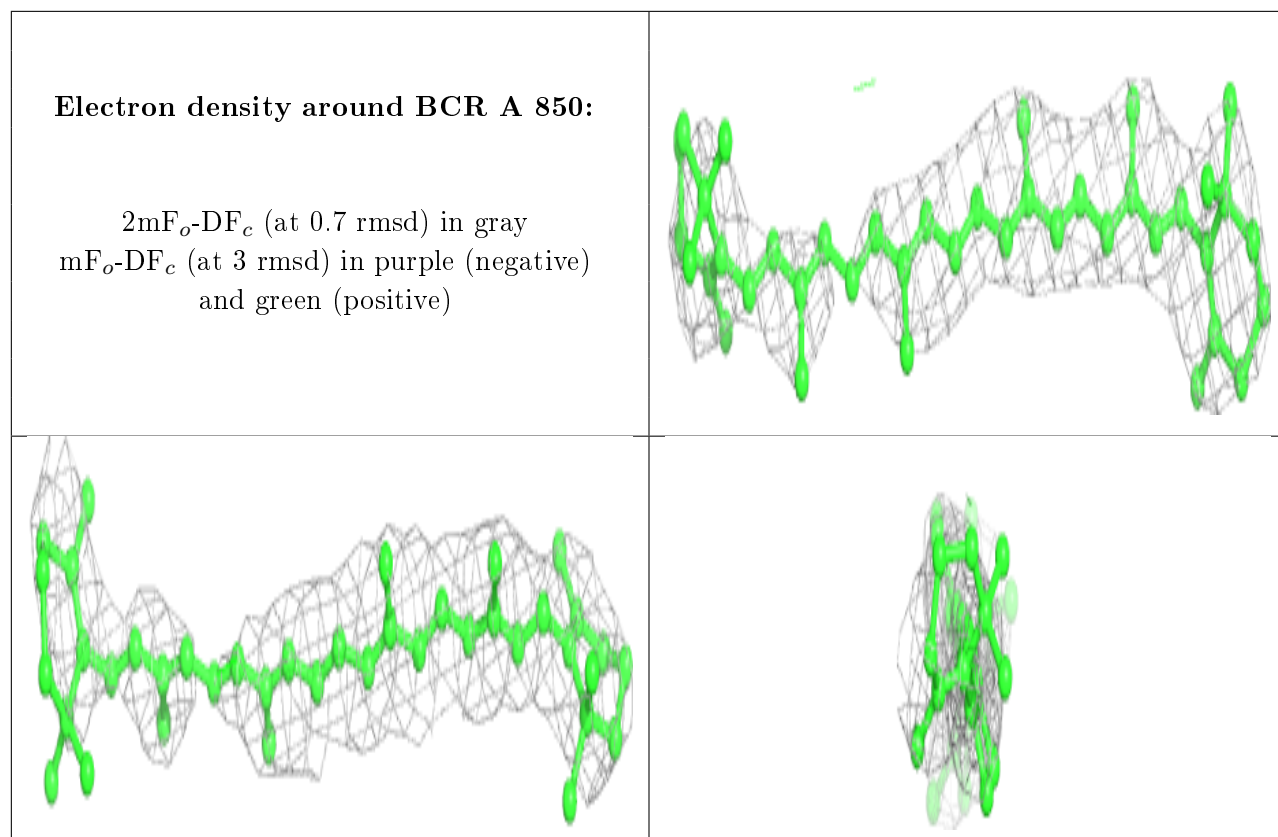
Electron density around CLA K 4003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around HTG F 302:**

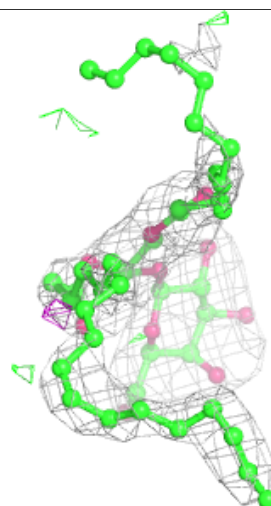
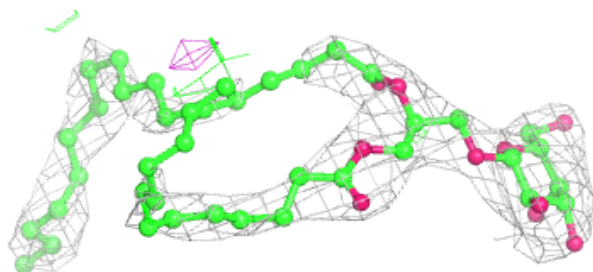
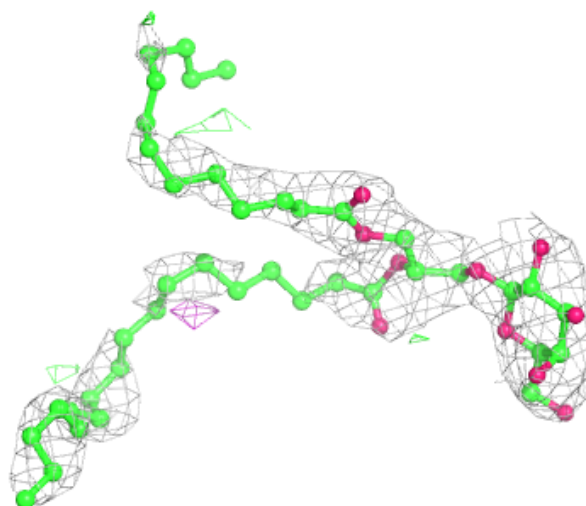
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





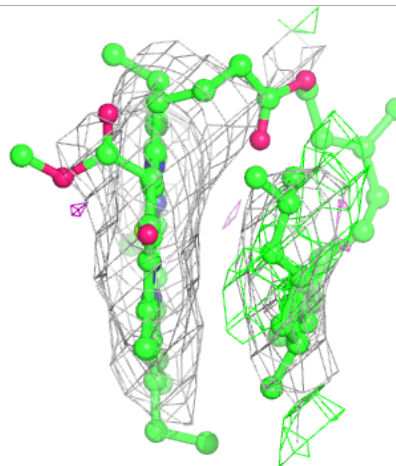
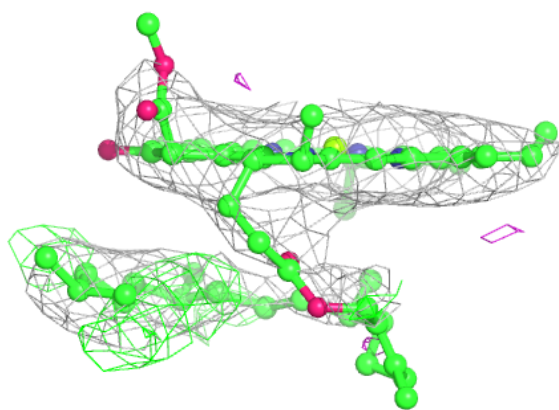
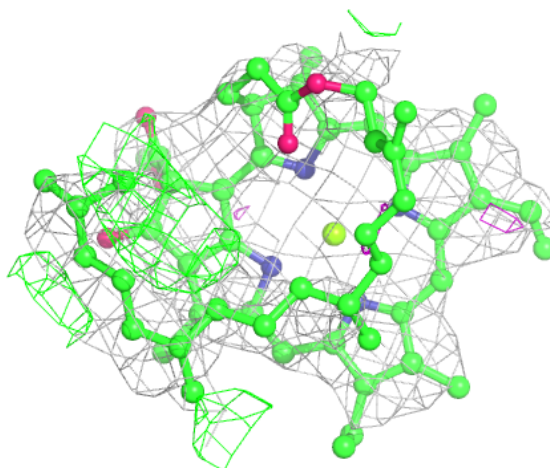
Electron density around LMG 9 619:

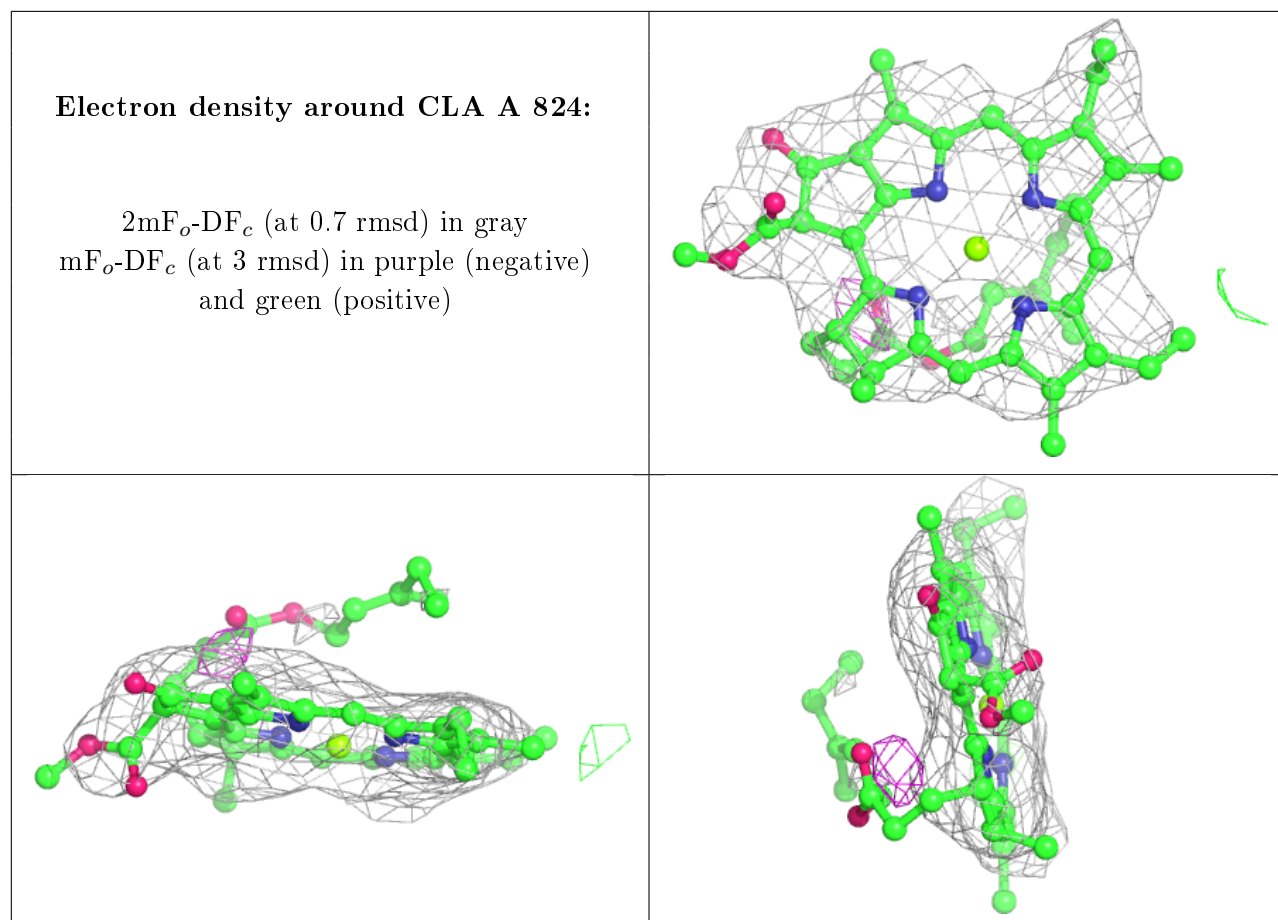
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA L 202:

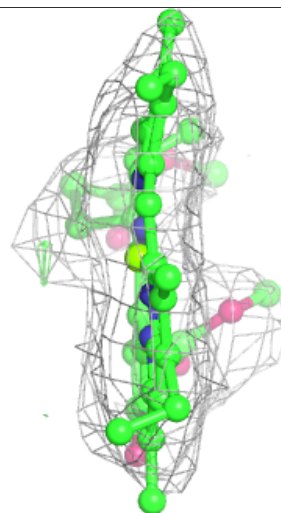
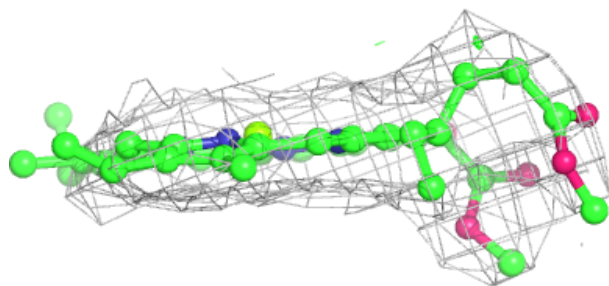
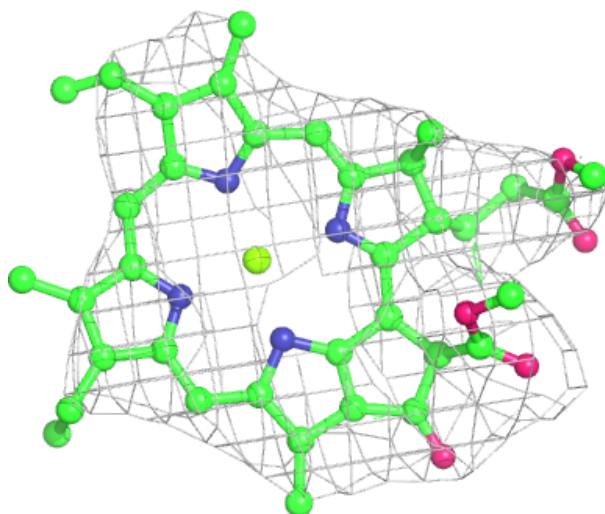
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





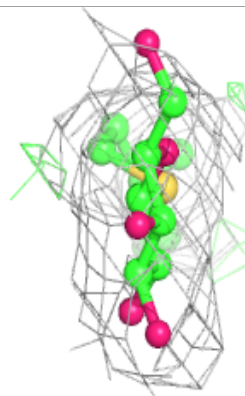
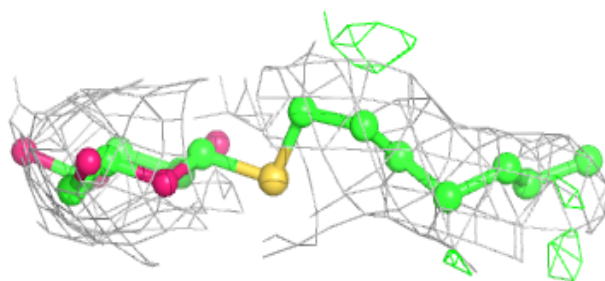
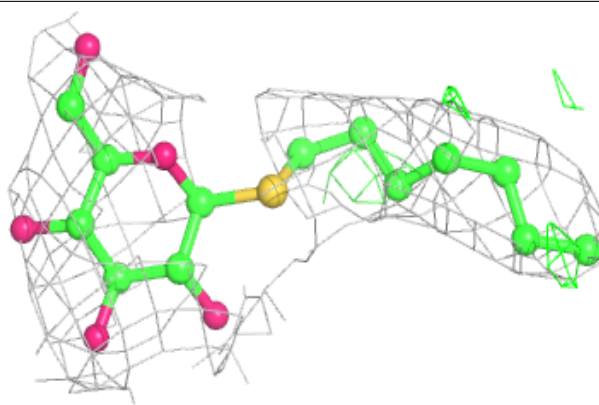
Electron density around CLA k 1403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

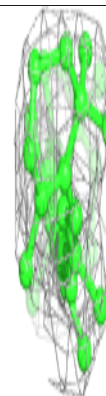
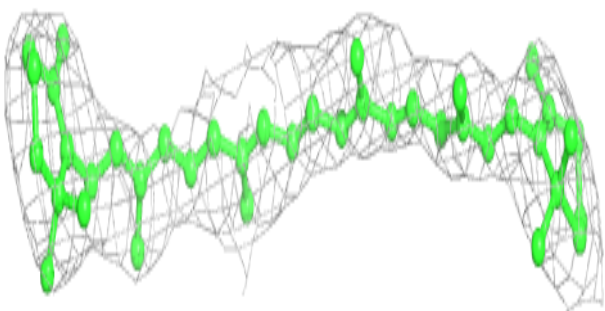
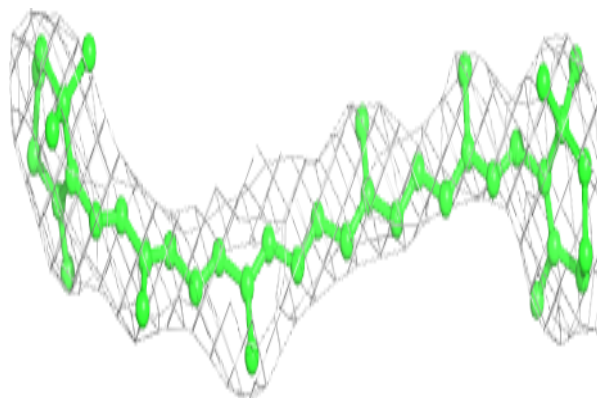


Electron density around HTG J 3001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

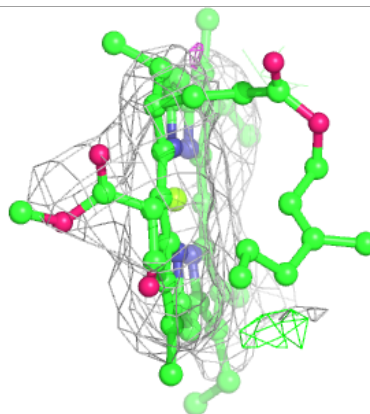
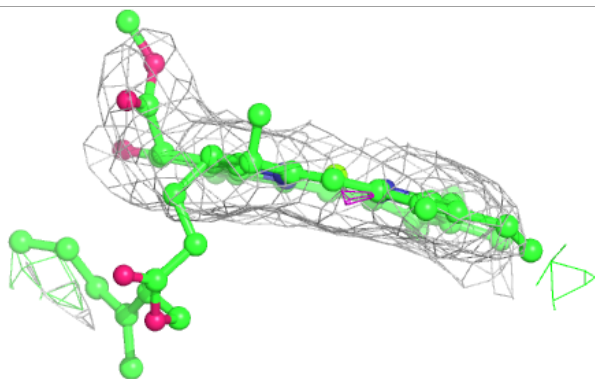
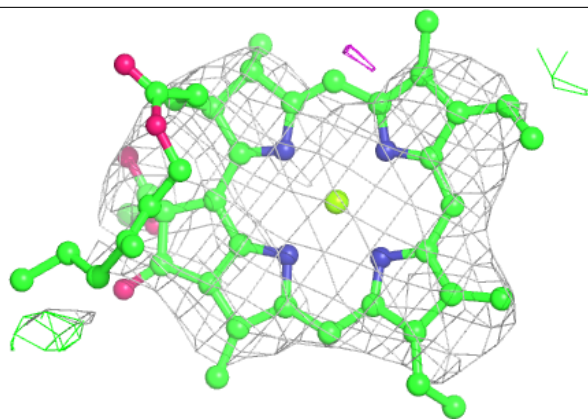
**Electron density around BCR G 105:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

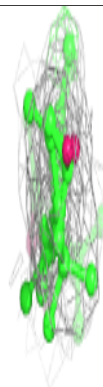
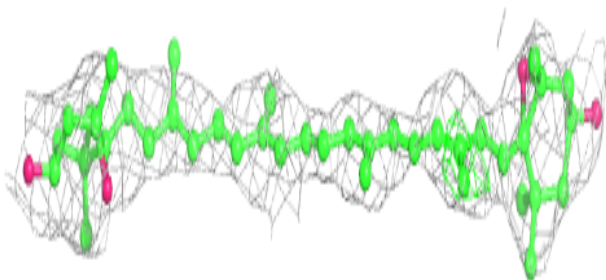
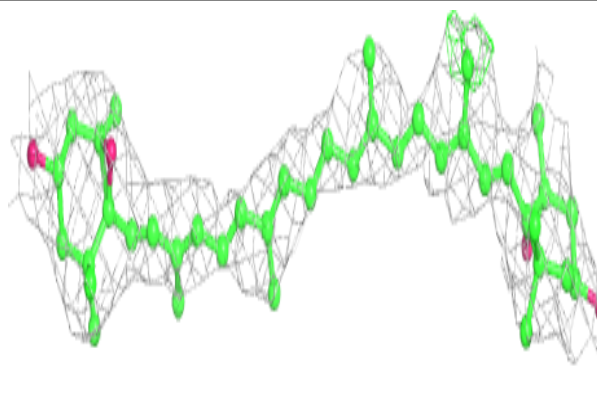


Electron density around CLA A 845:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

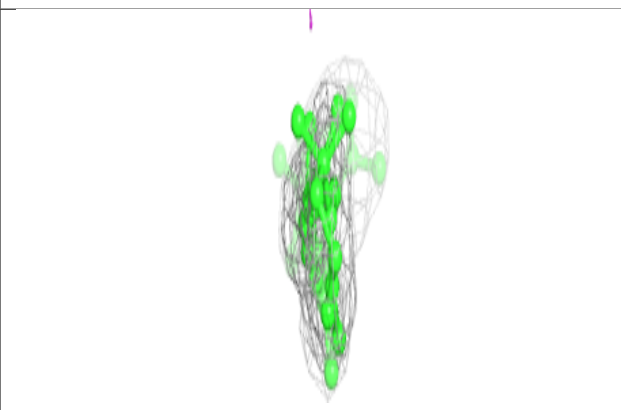
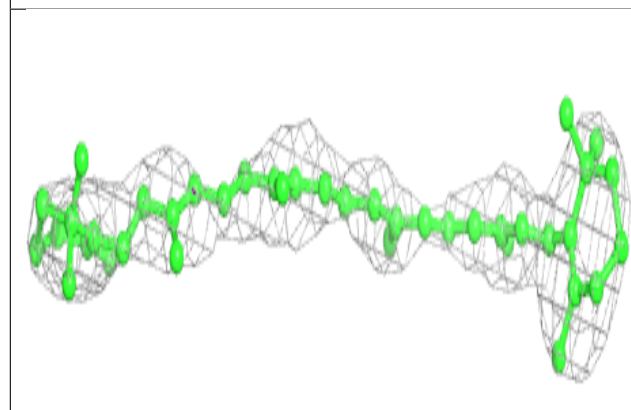
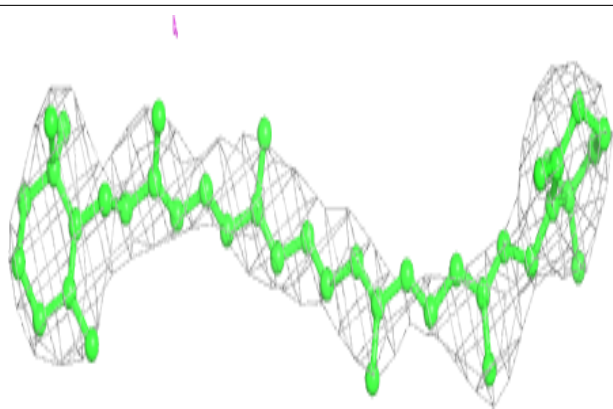
**Electron density around XAT 9 617:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

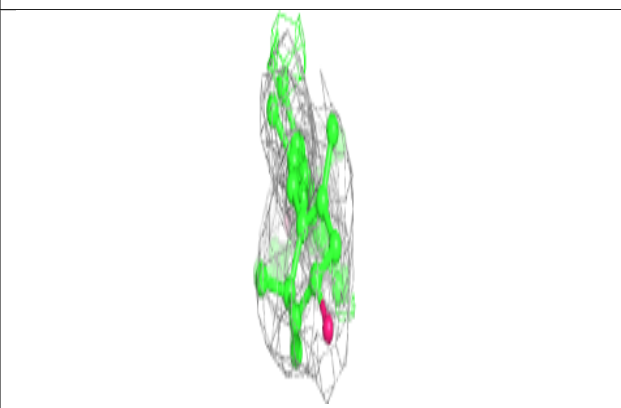
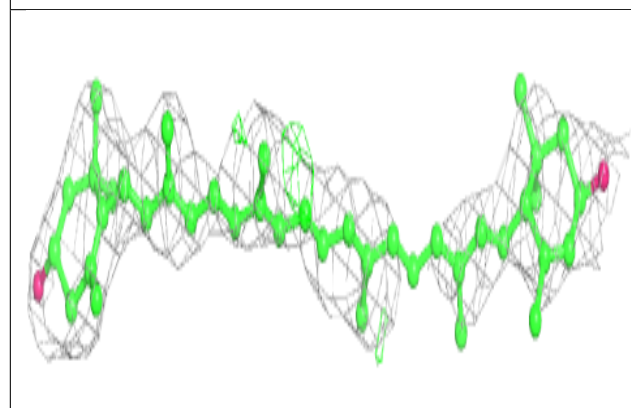
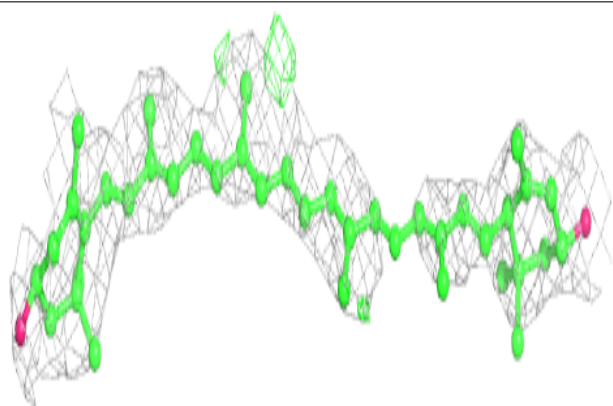


Electron density around BCR 4 618:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

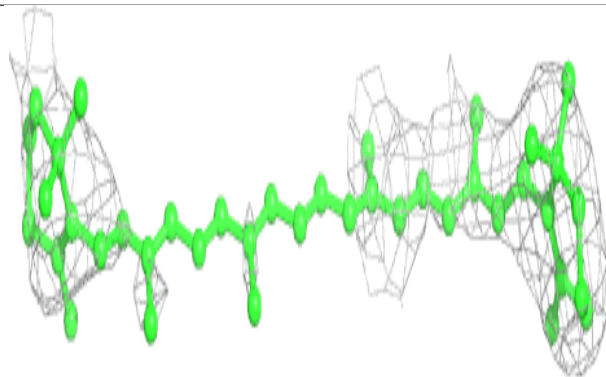
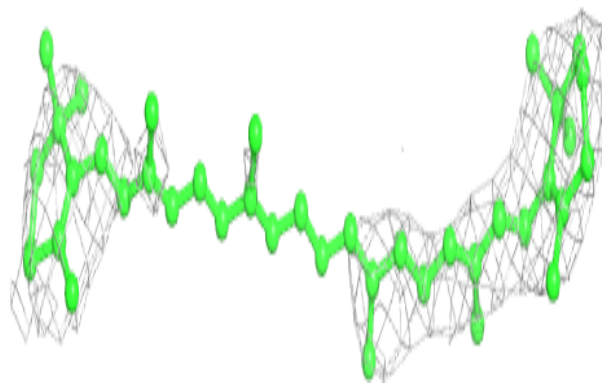
**Electron density around LUT 4 616:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



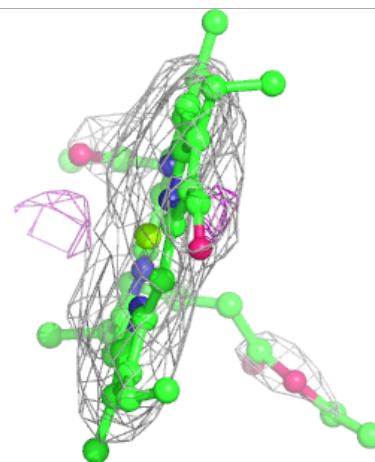
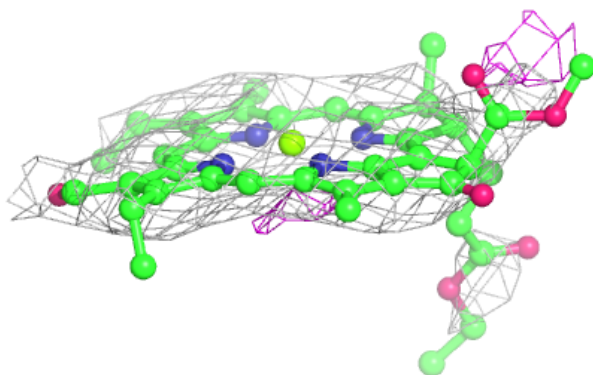
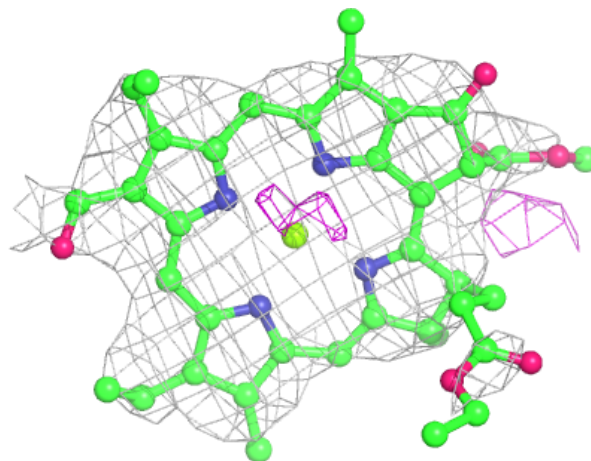
Electron density around BCR g 104:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



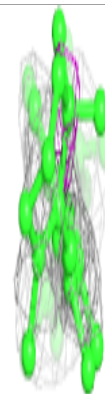
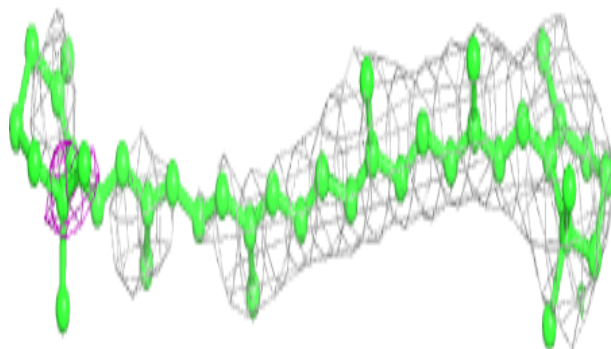
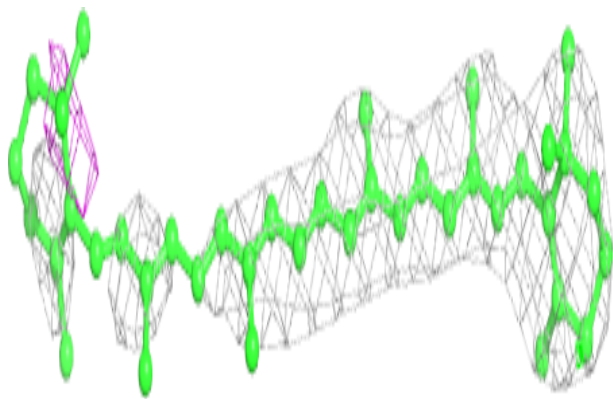
Electron density around CHL 2 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



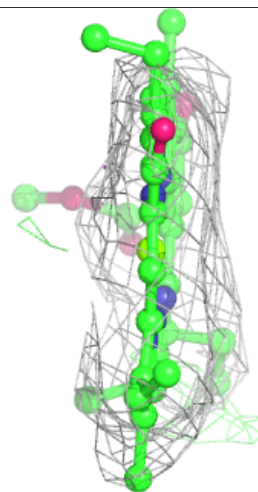
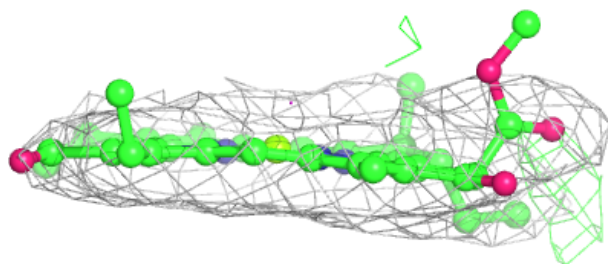
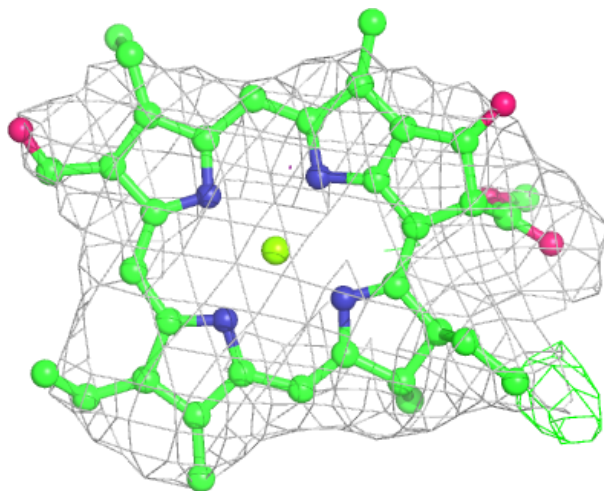
Electron density around BCR a 852:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



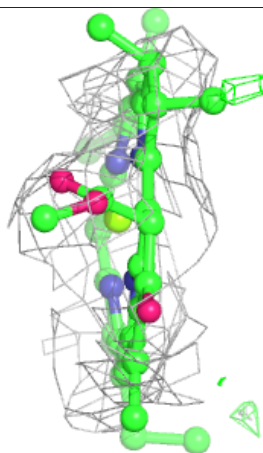
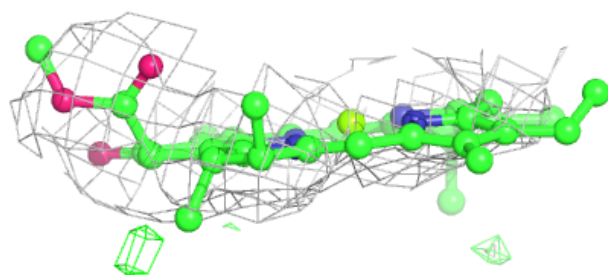
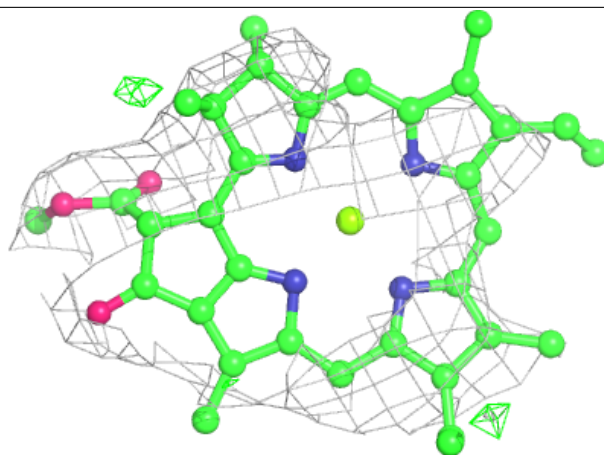
Electron density around CHL 2 605:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



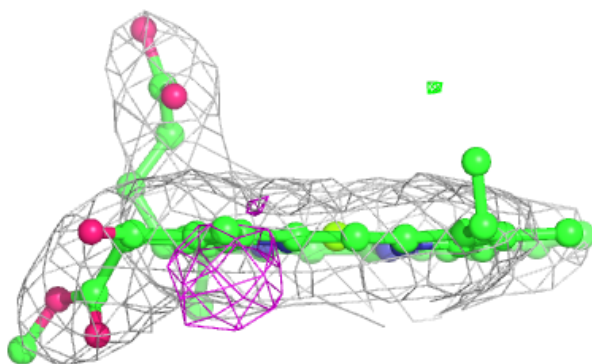
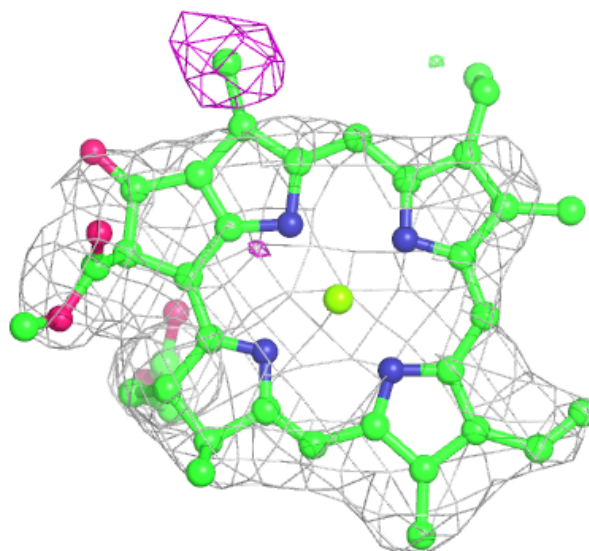
Electron density around CLA g 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



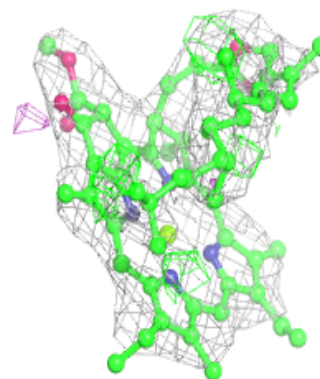
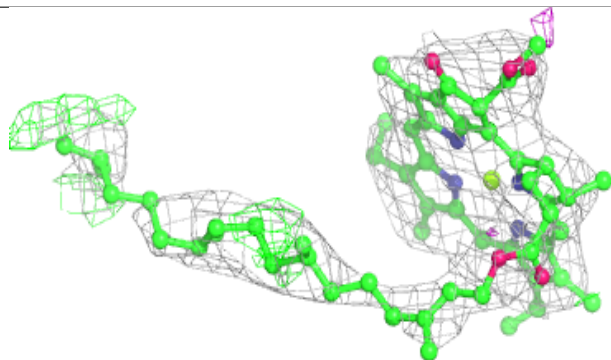
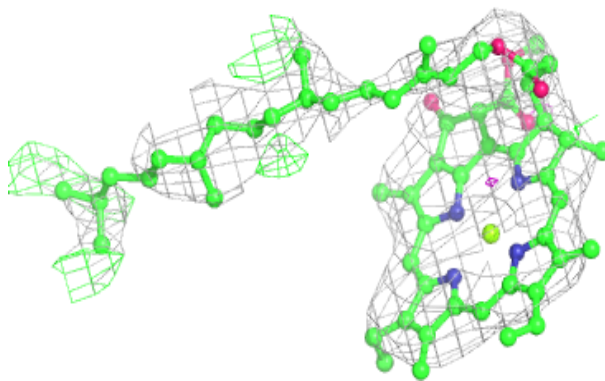
Electron density around CLA A 837:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

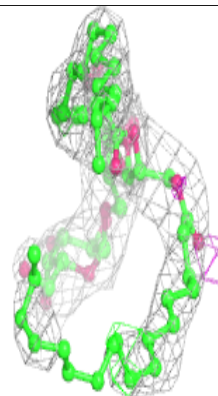
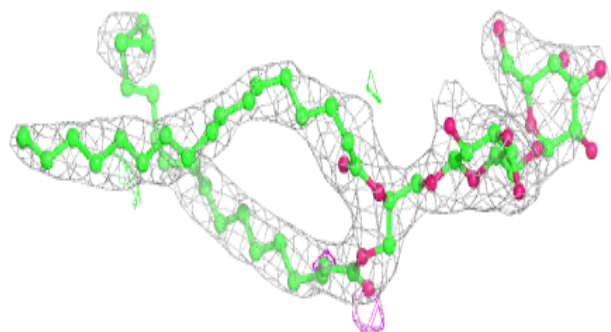
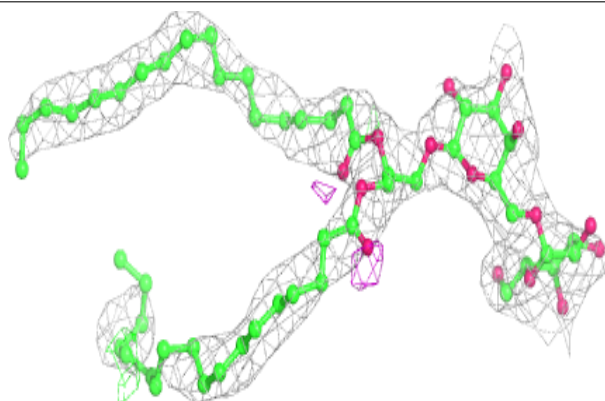


Electron density around CLA 1 309:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

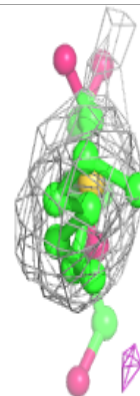
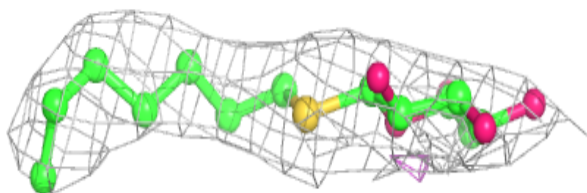
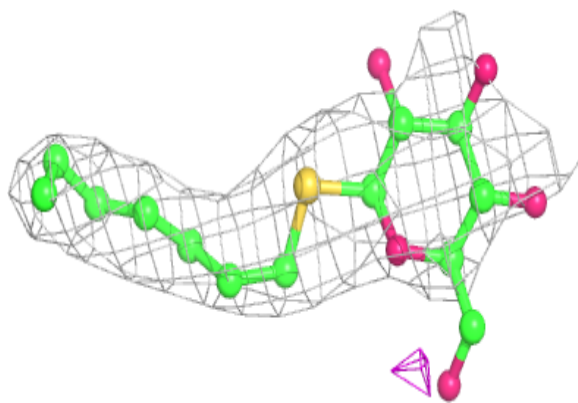
**Electron density around DGD b 849:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

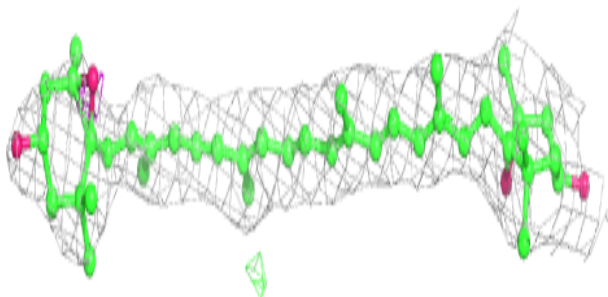
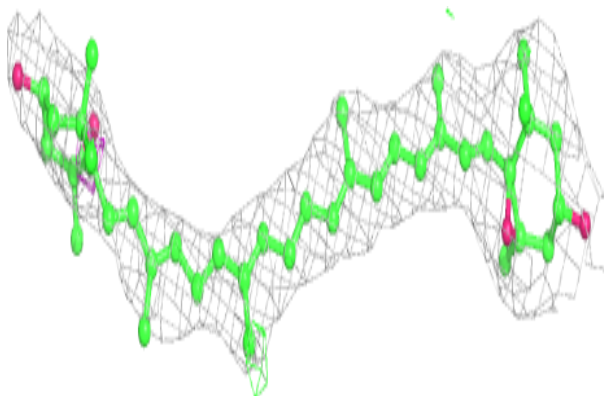


Electron density around HTG f 7001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

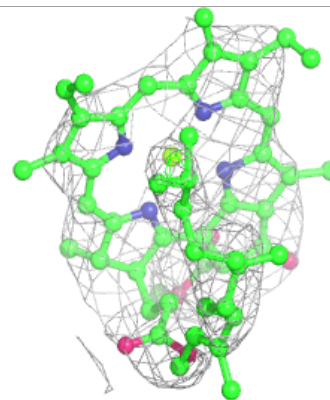
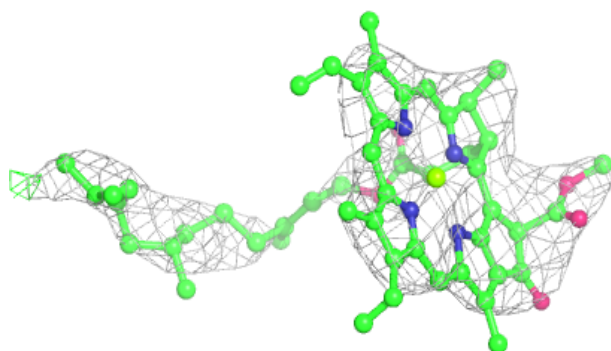
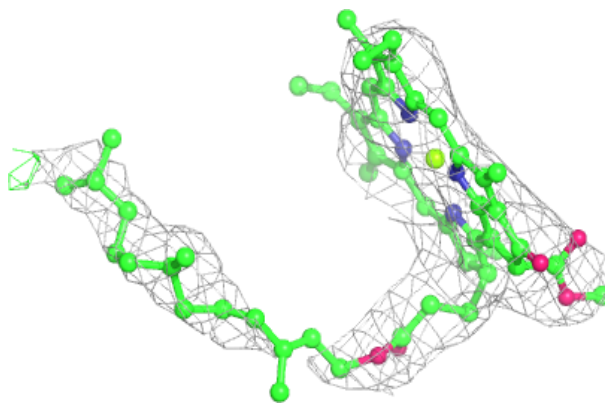
**Electron density around XAT 3 317:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

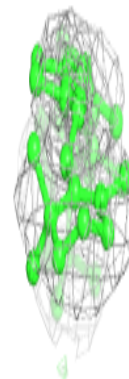
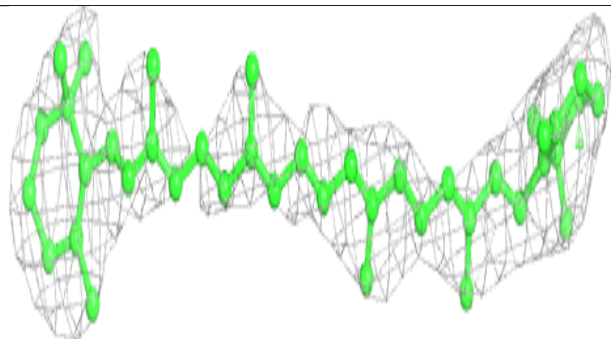
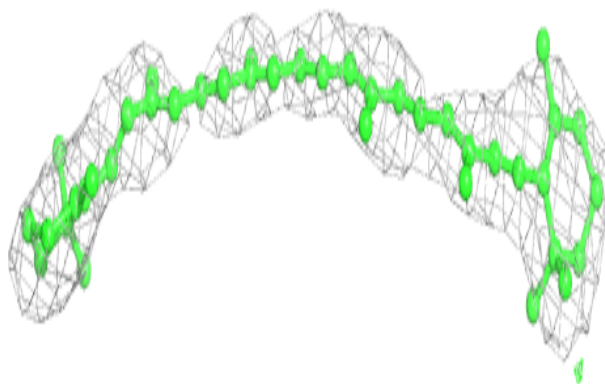


Electron density around CLA 7 604:

$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)

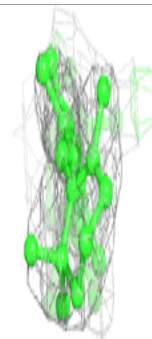
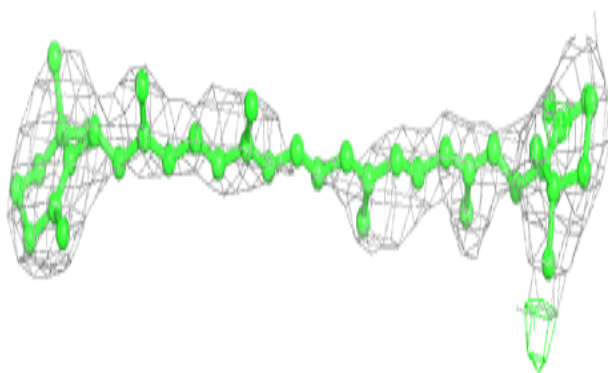
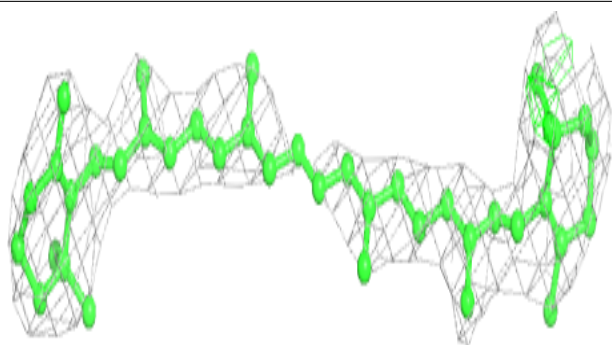
**Electron density around BCR a 849:**

$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)

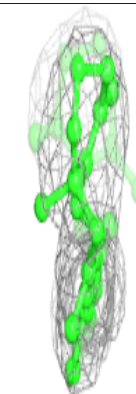
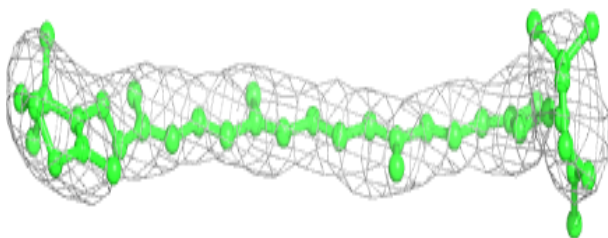
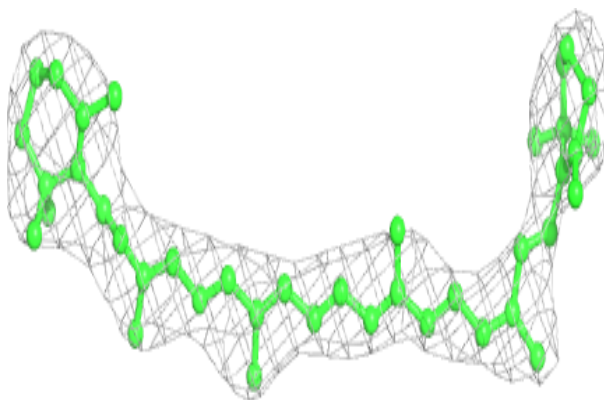


Electron density around BCR k 1404:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

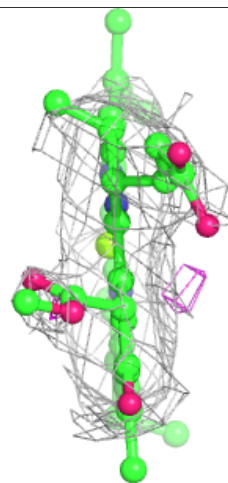
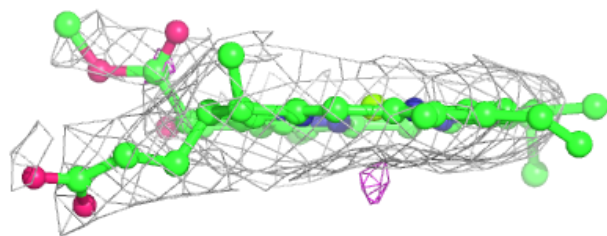
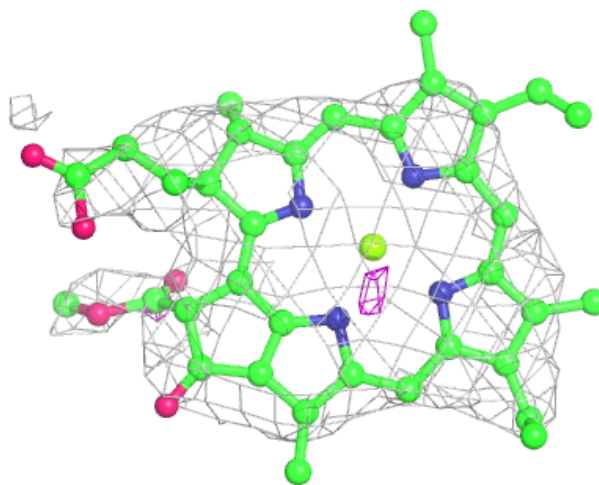
**Electron density around BCR B 844:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



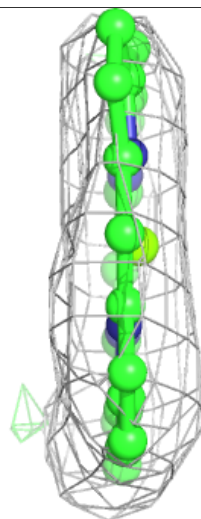
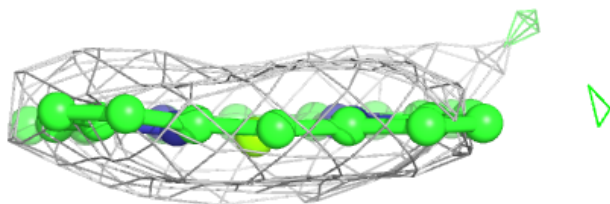
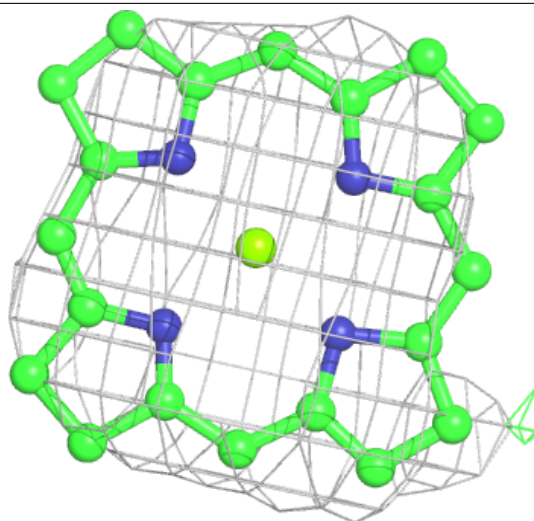
Electron density around CLA 3 313:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



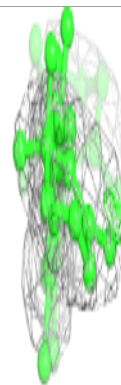
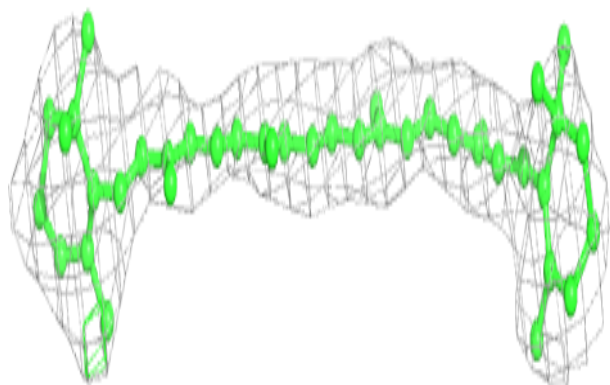
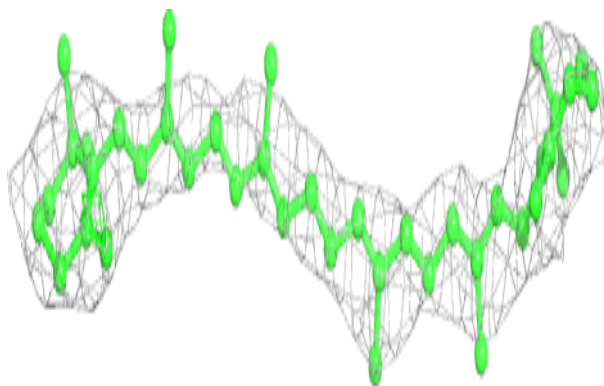
Electron density around CLA 3 315:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



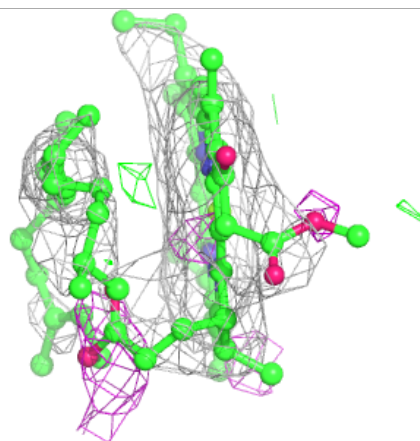
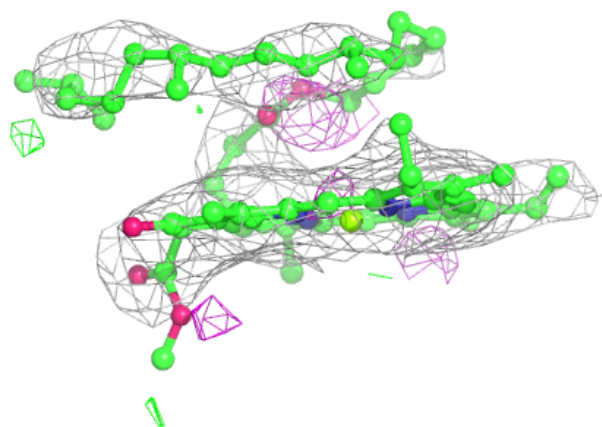
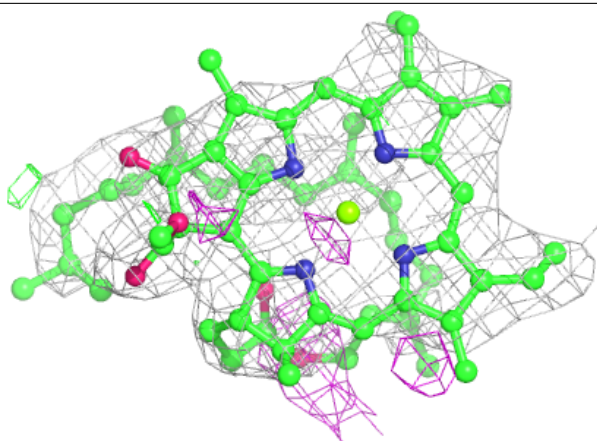
Electron density around BCR 8 316:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



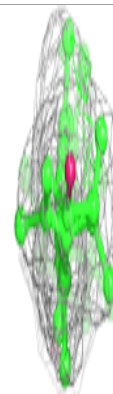
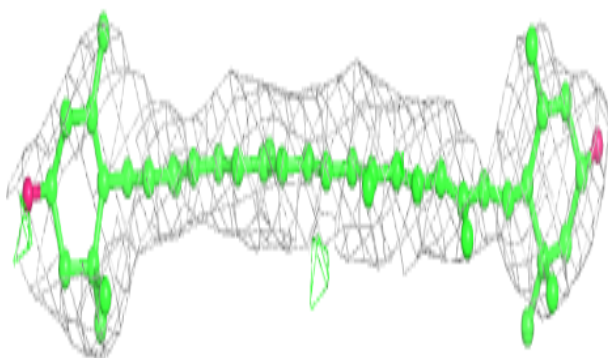
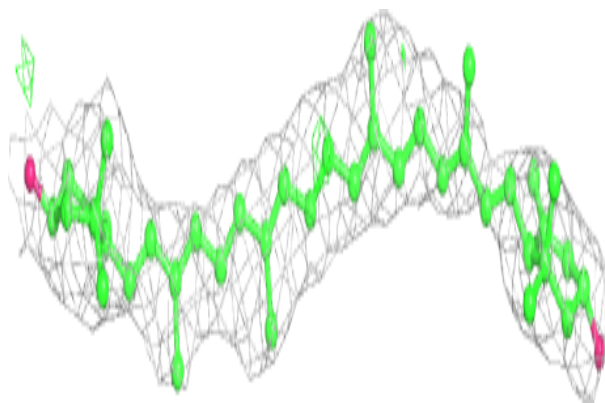
Electron density around CLA 1 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



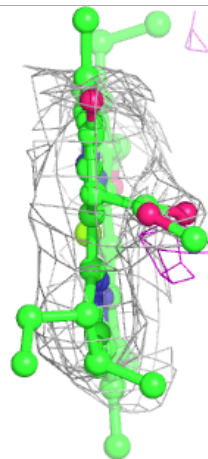
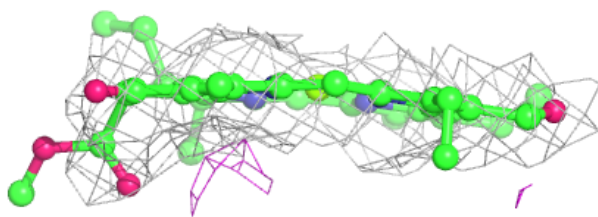
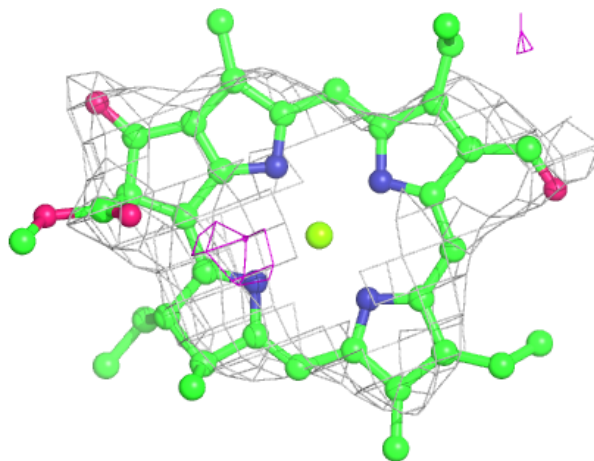
Electron density around LUT 1 320:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



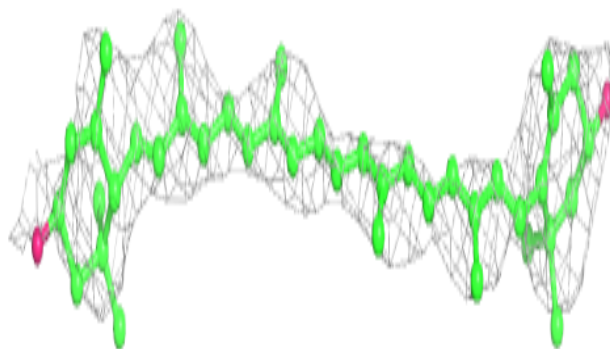
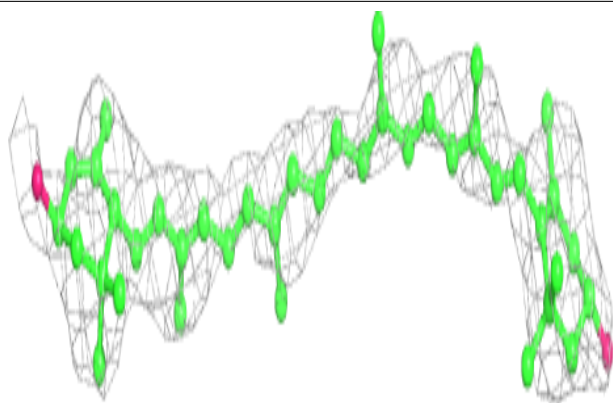
Electron density around CHL 9 615:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

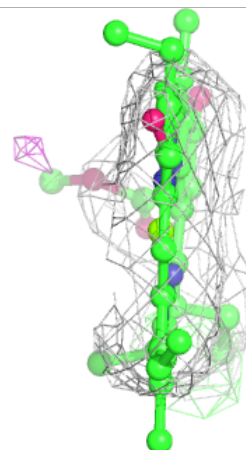
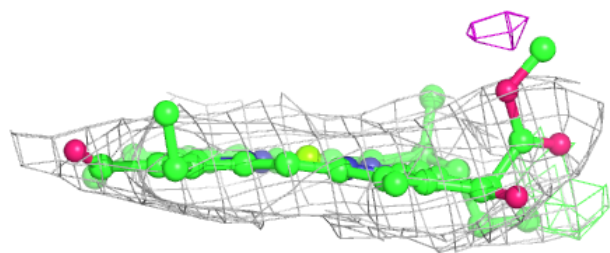
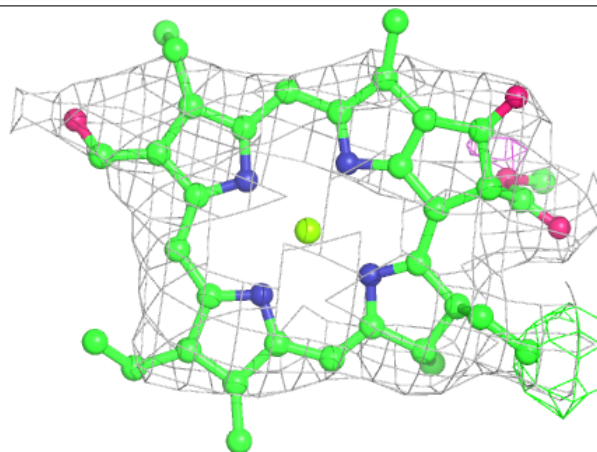


Electron density around LUT 7 615:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

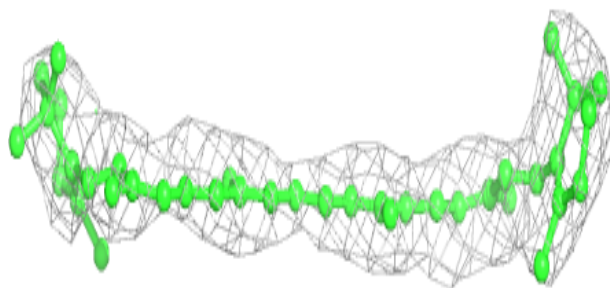
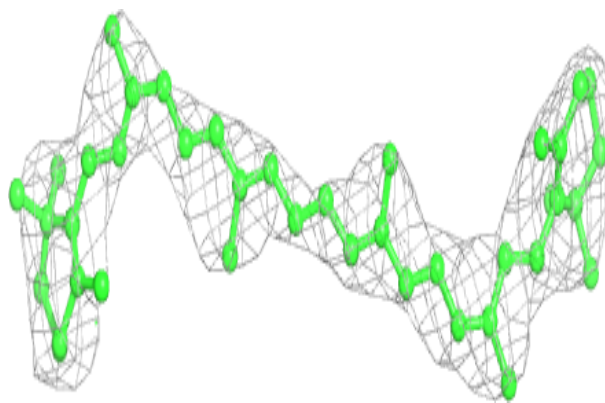
**Electron density around CHL 7 605:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



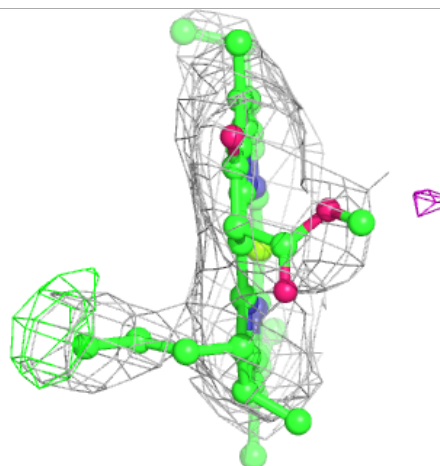
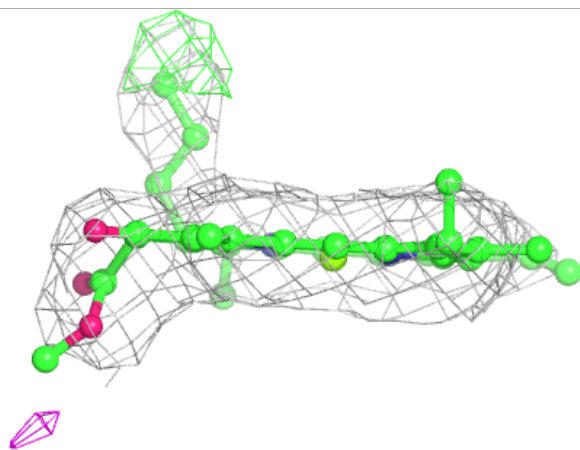
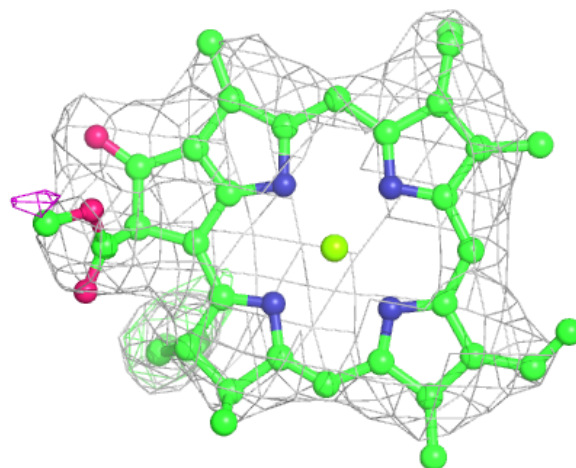
Electron density around BCR b 845:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



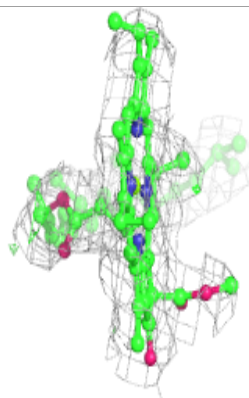
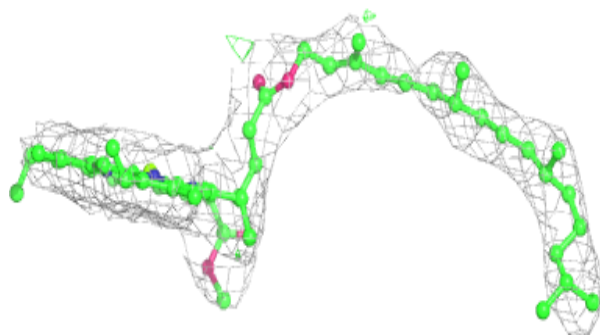
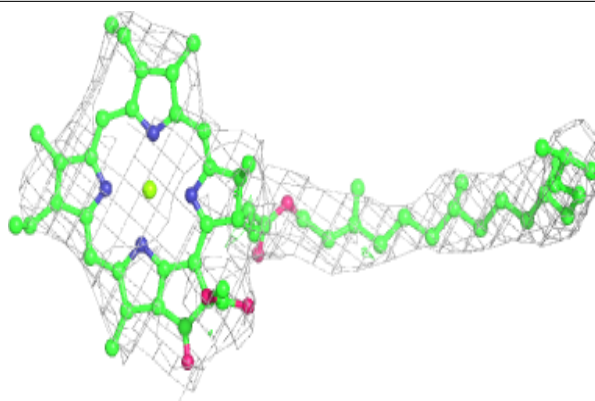
Electron density around CLA 2 613:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



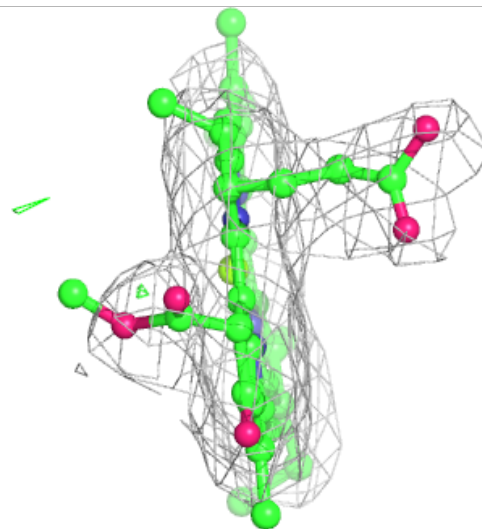
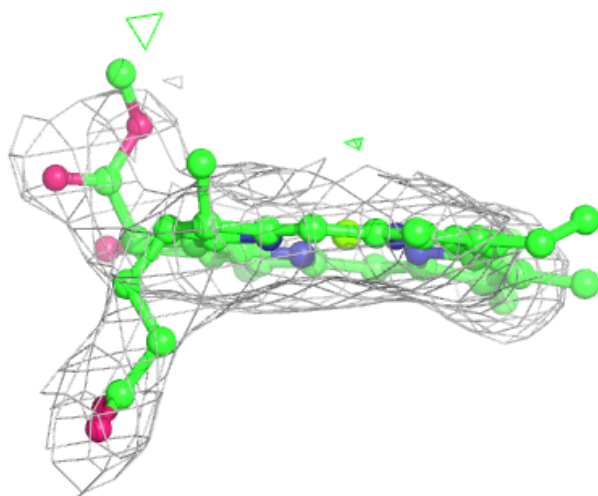
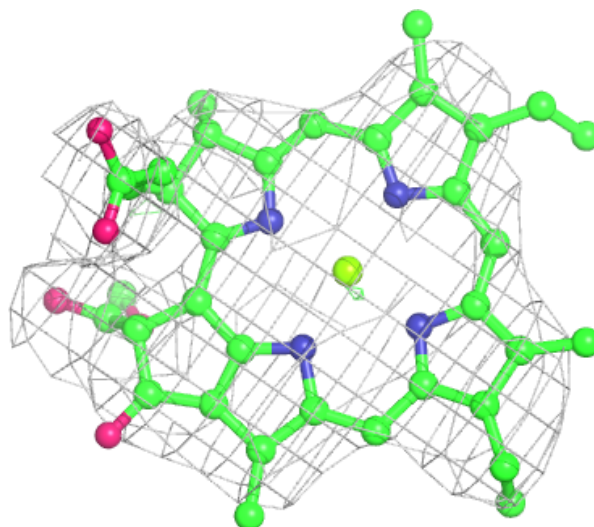
Electron density around CLA b 841:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



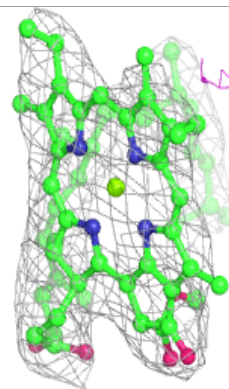
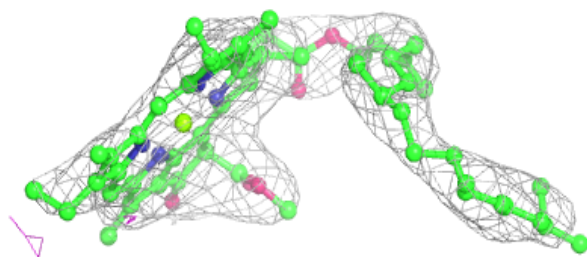
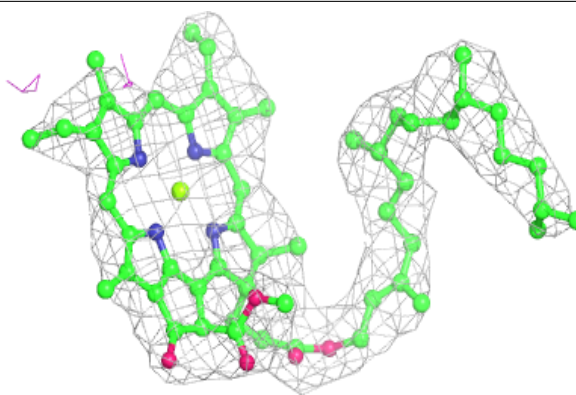
Electron density around CLA k 1401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

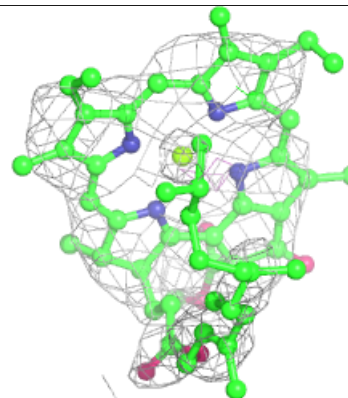
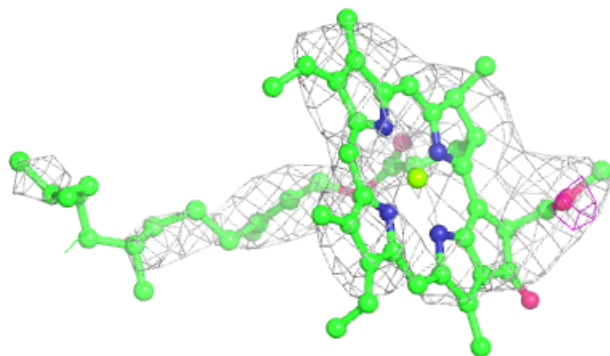
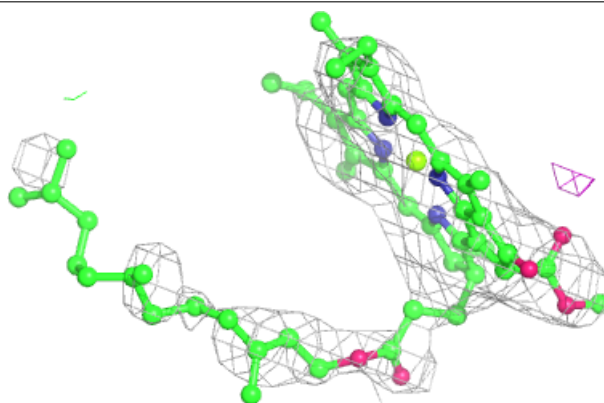


Electron density around CLA b 824:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

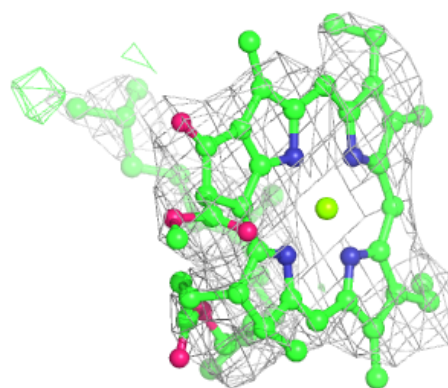
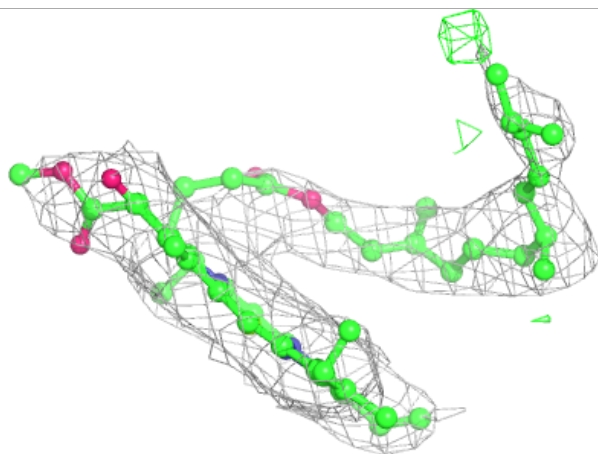
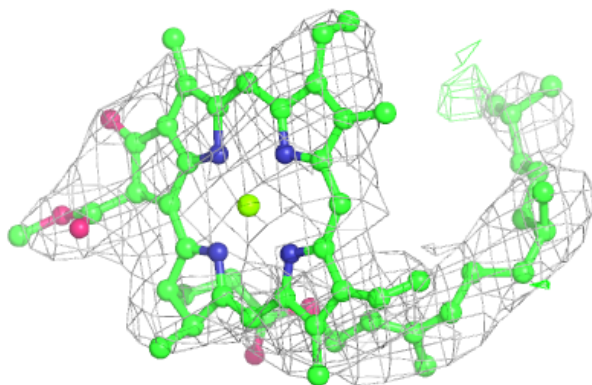
**Electron density around CLA 2 604:**

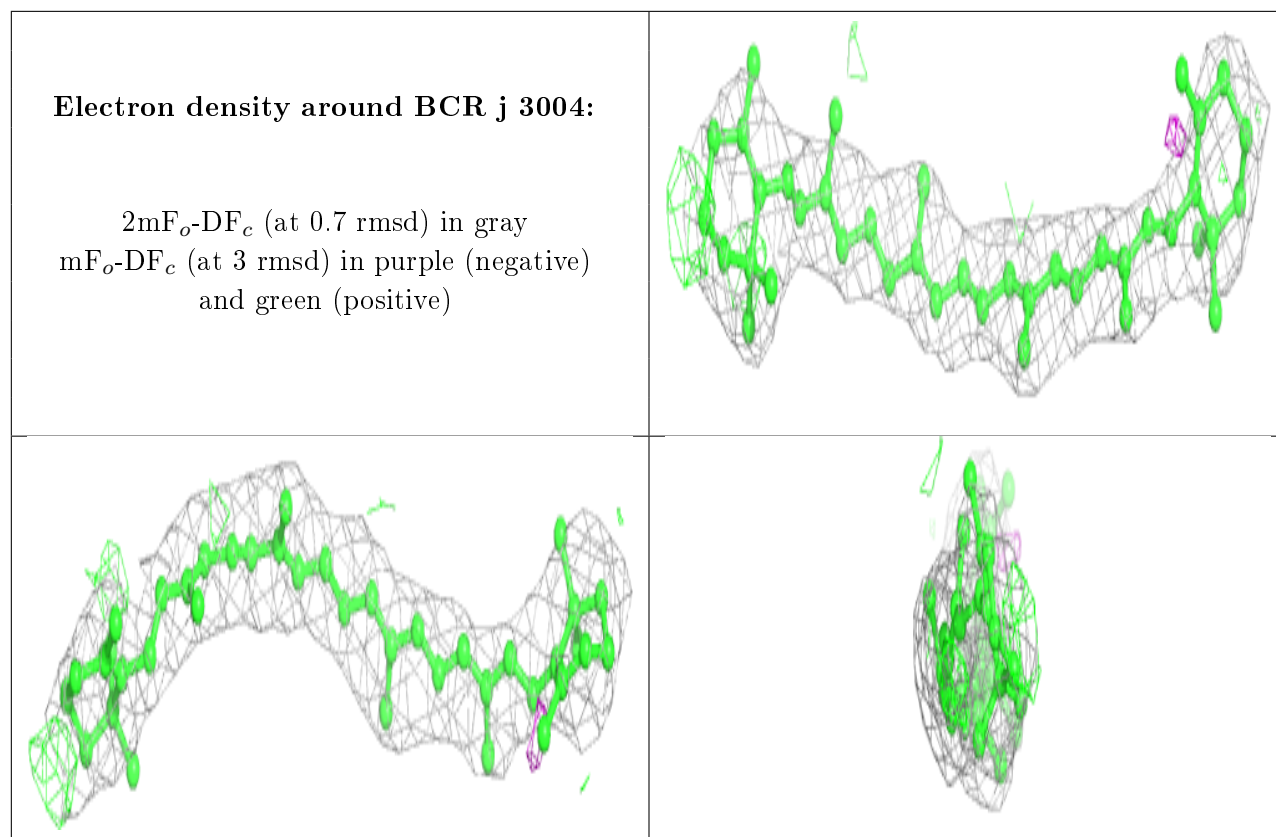
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 2 609:

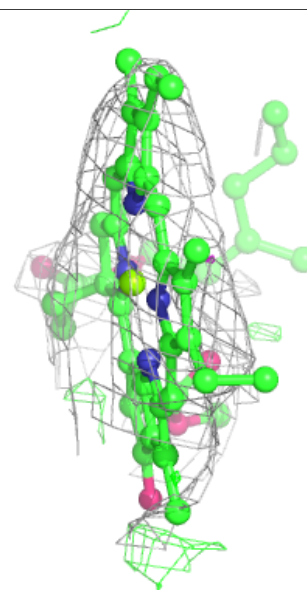
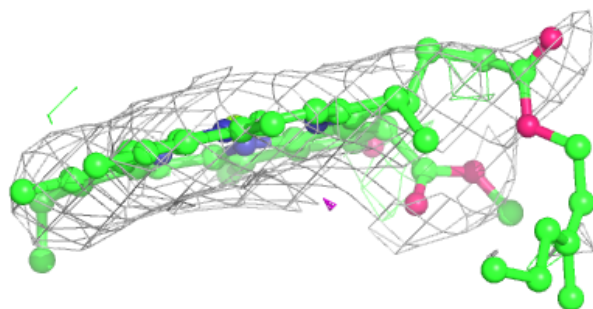
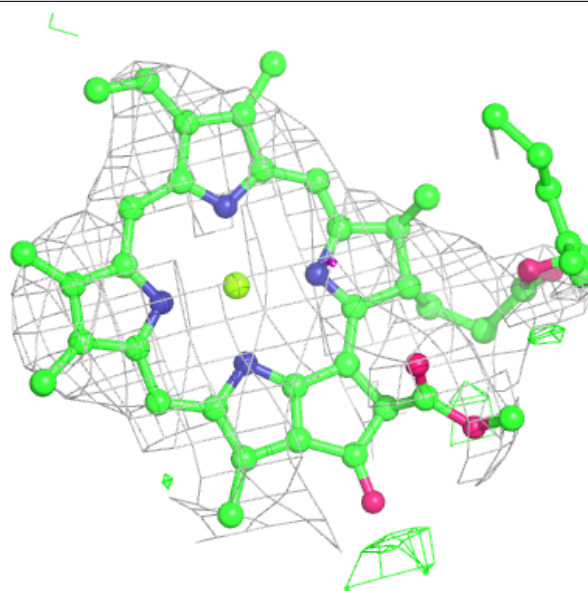
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





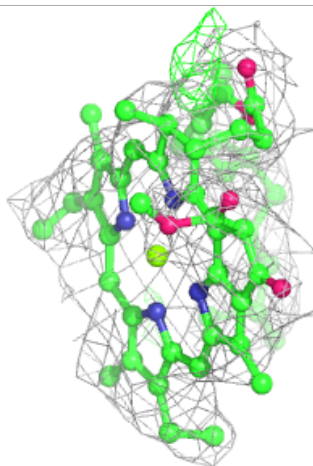
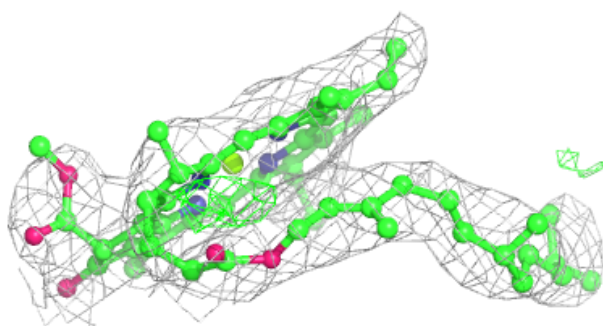
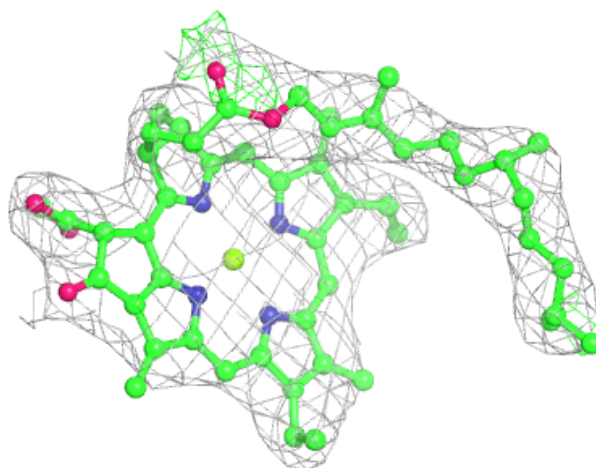
Electron density around CLA 6 313:

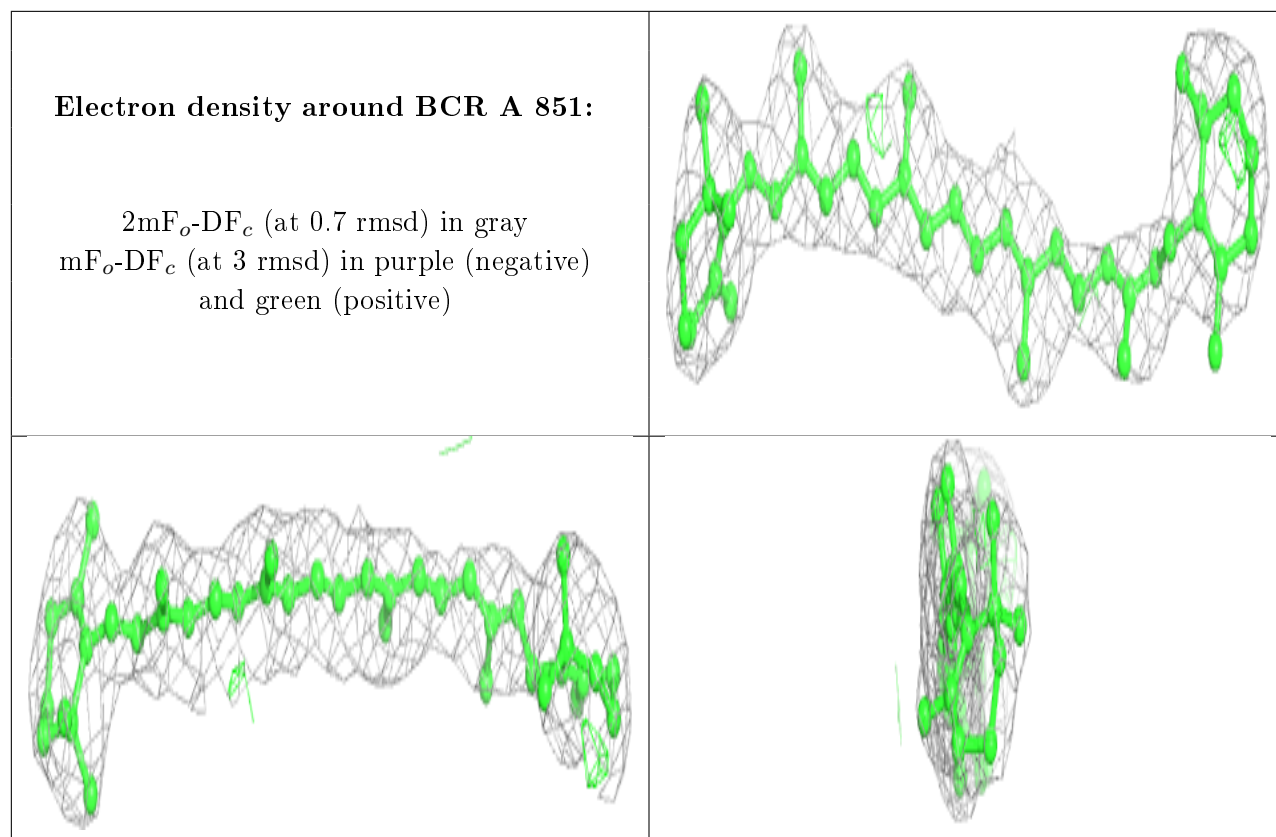
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 3 302:

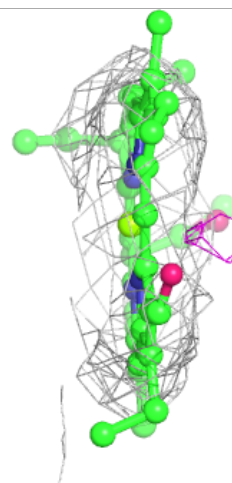
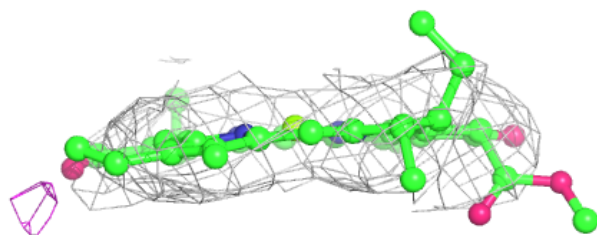
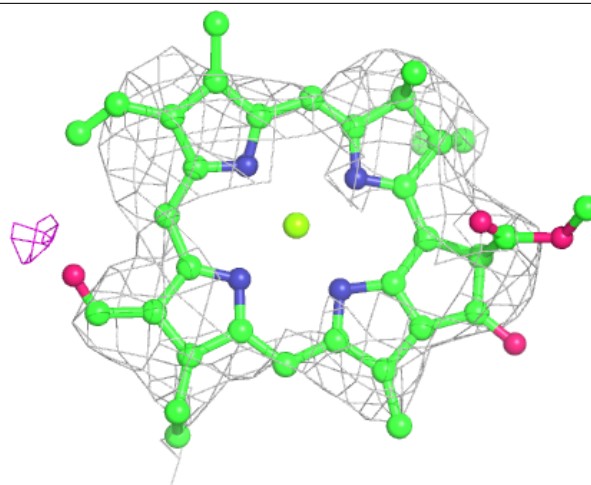
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





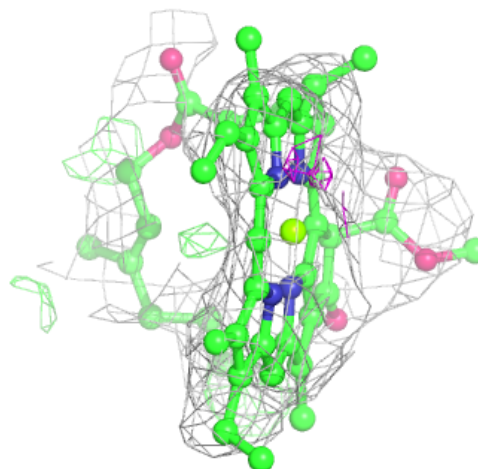
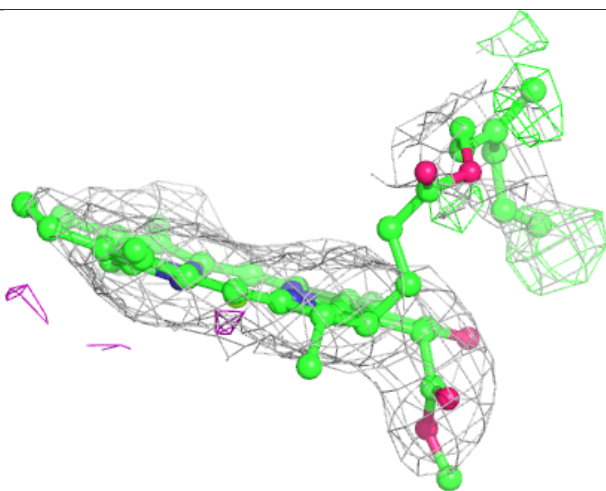
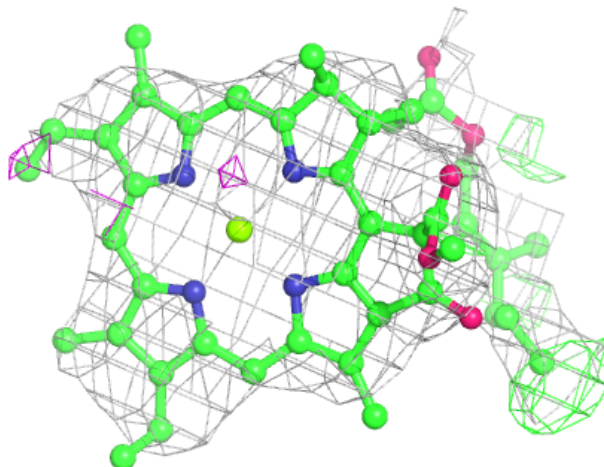
Electron density around CHL 2 614:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



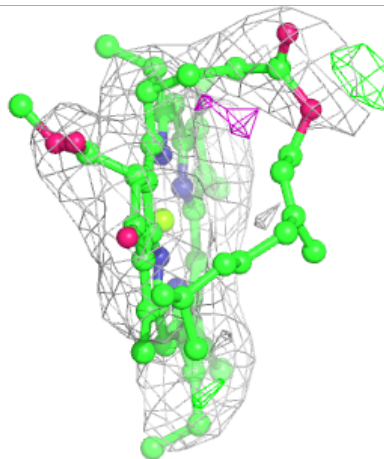
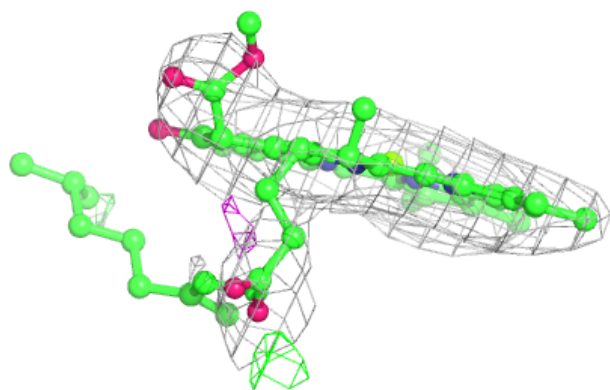
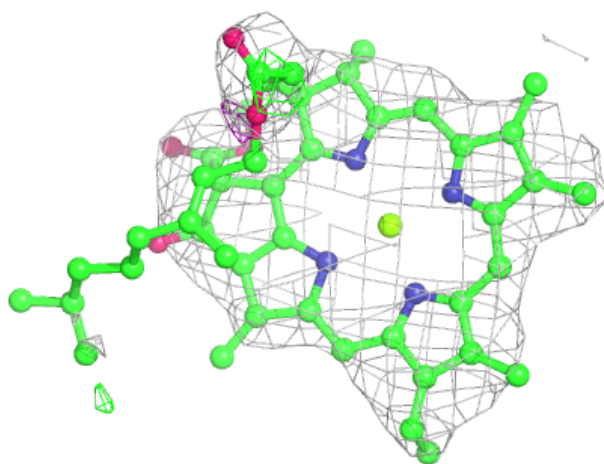
Electron density around CLA a 846:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



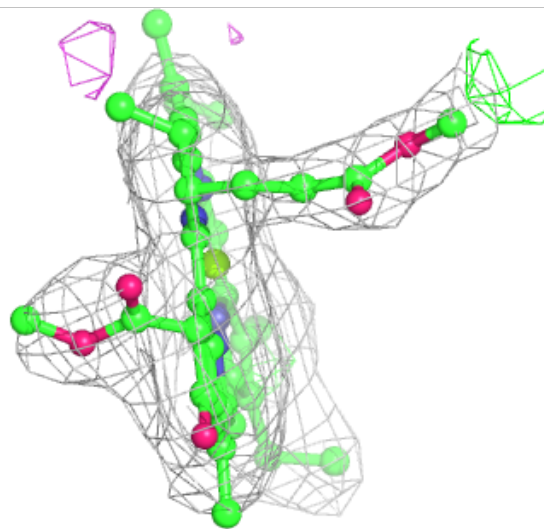
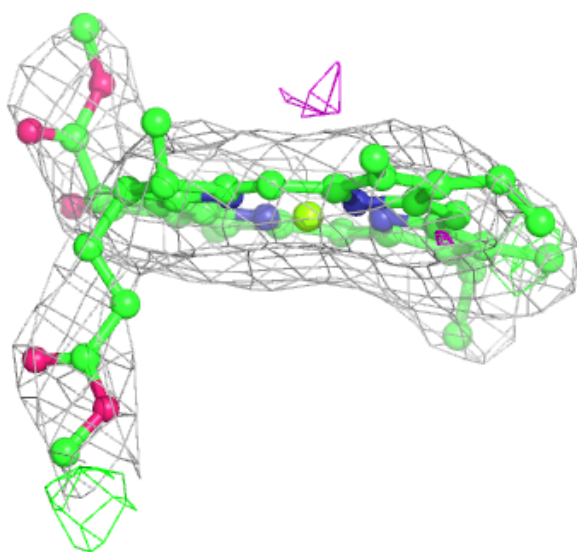
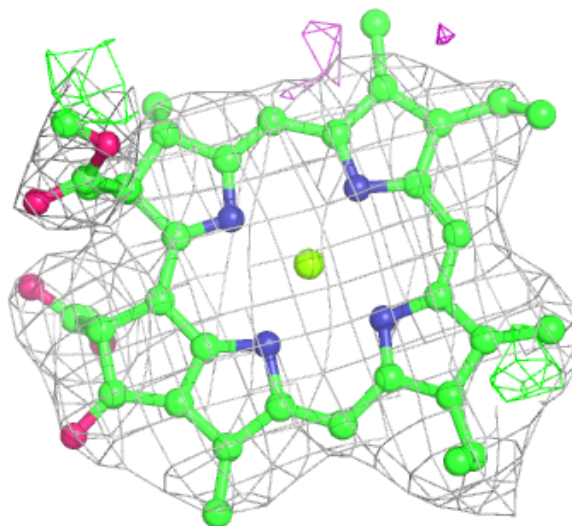
Electron density around CLA b 811:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



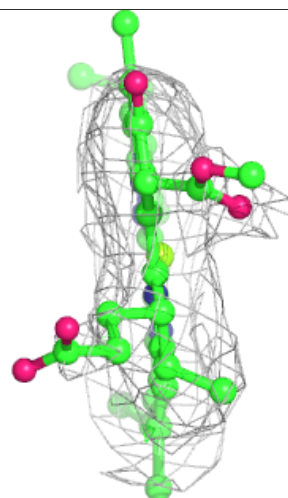
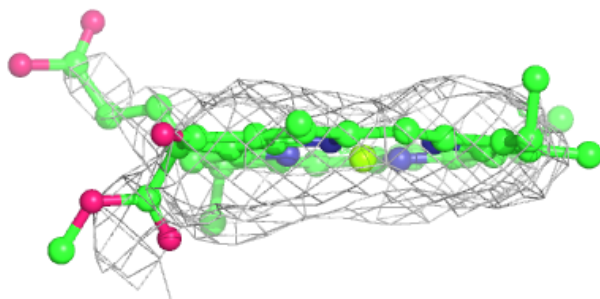
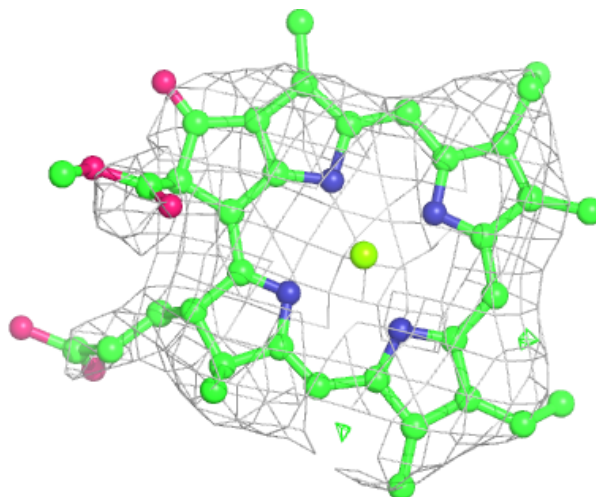
Electron density around CLA B 821:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



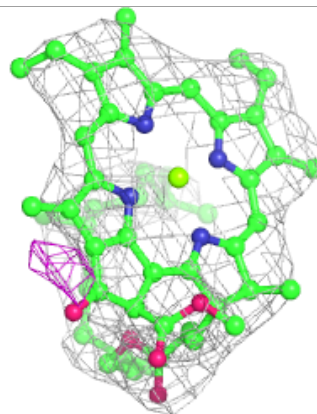
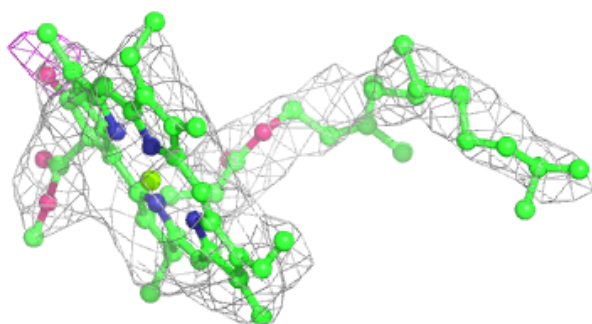
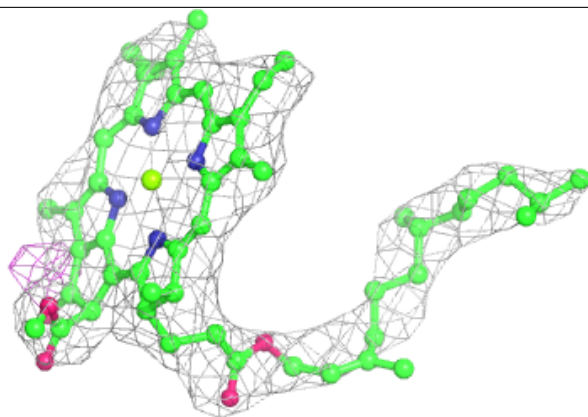
Electron density around CLA 8 311:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

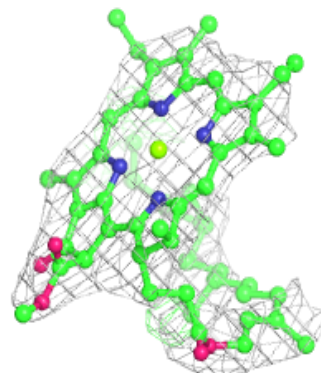
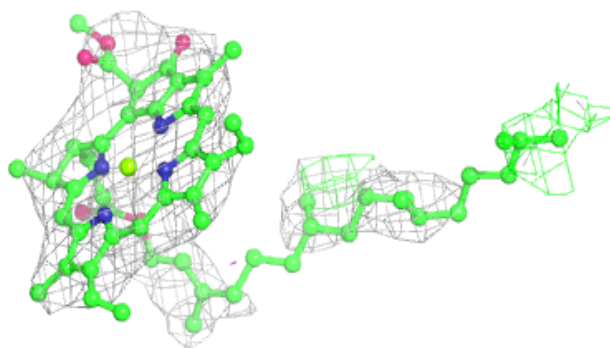
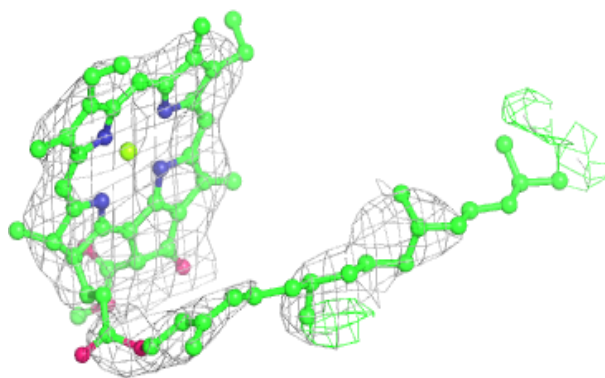


Electron density around CLA B 815:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

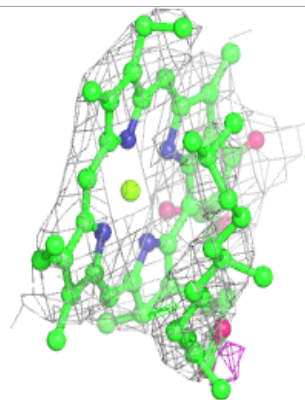
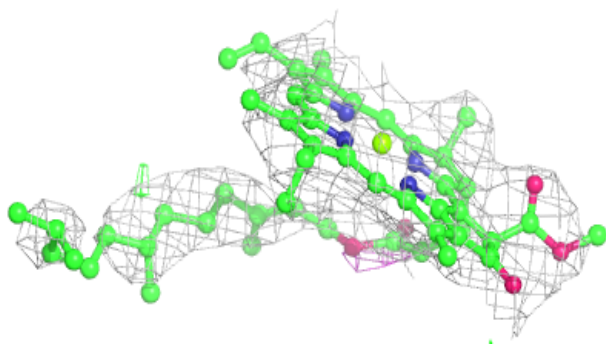
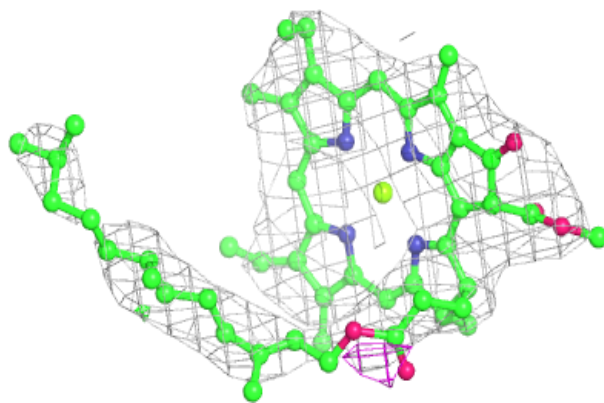
**Electron density around CLA 6 310:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

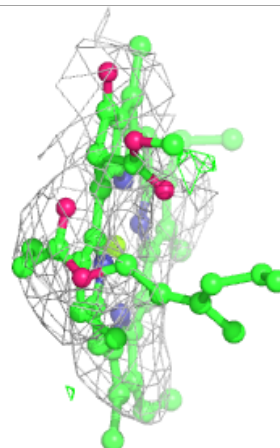
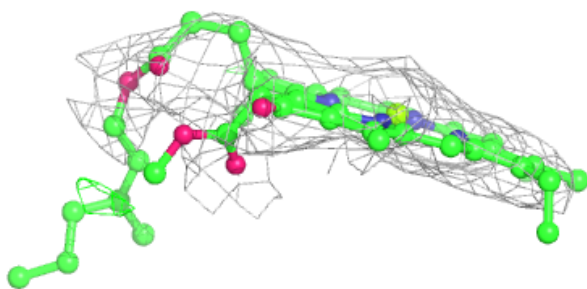
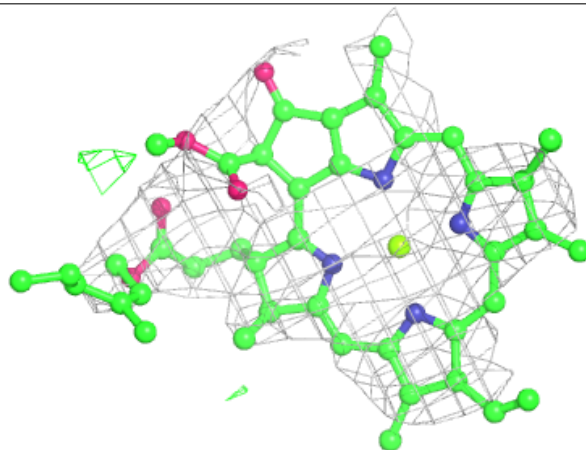


Electron density around CLA 4 609:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

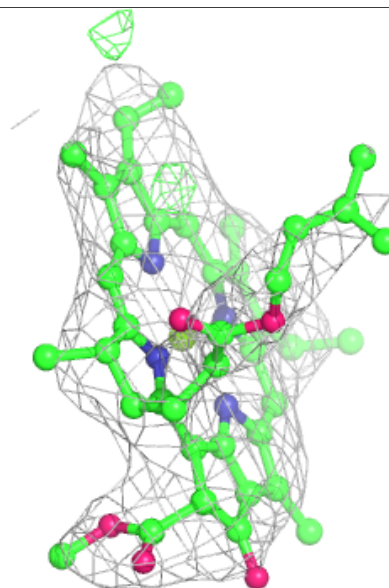
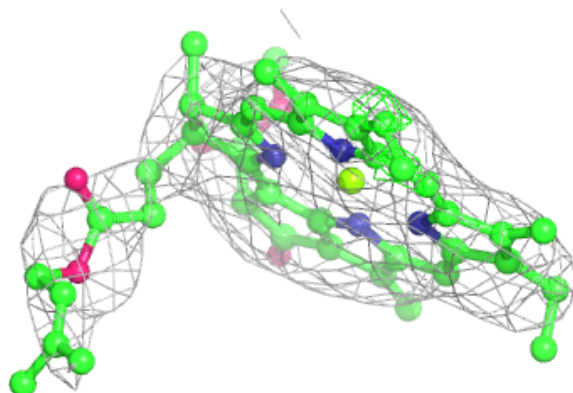
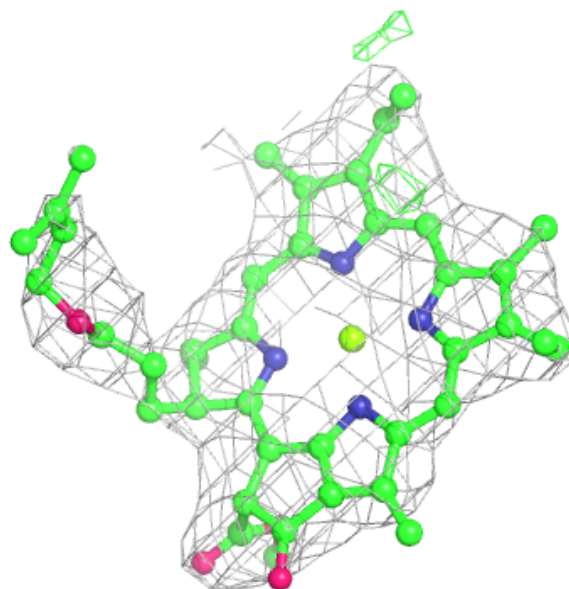
**Electron density around CLA 3 311:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



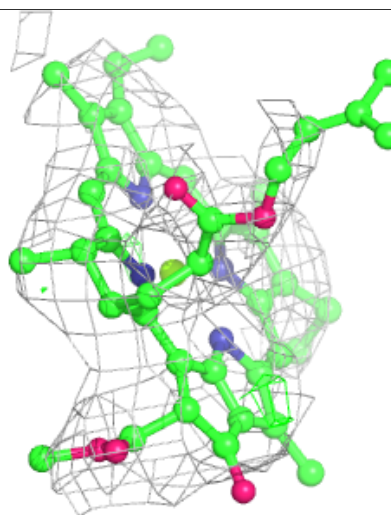
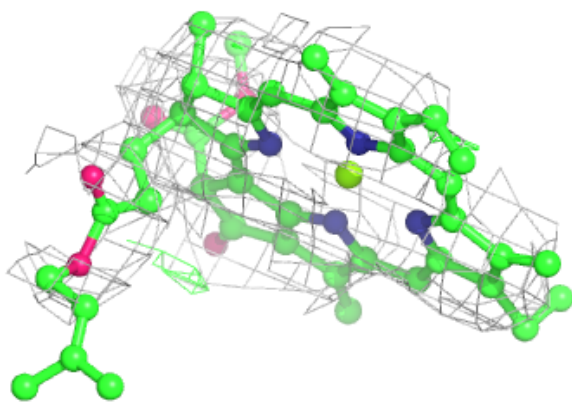
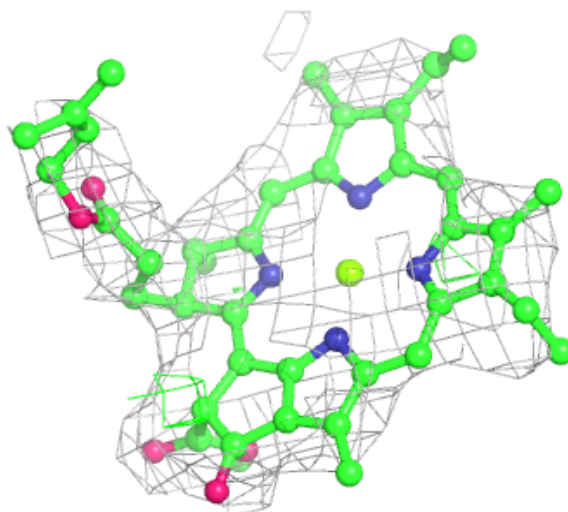
Electron density around CLA A 832:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



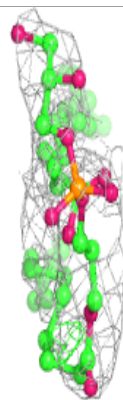
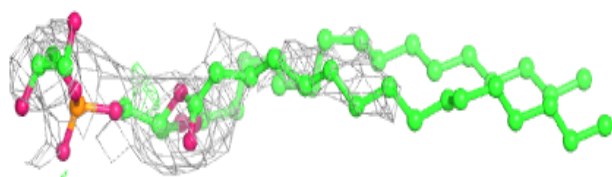
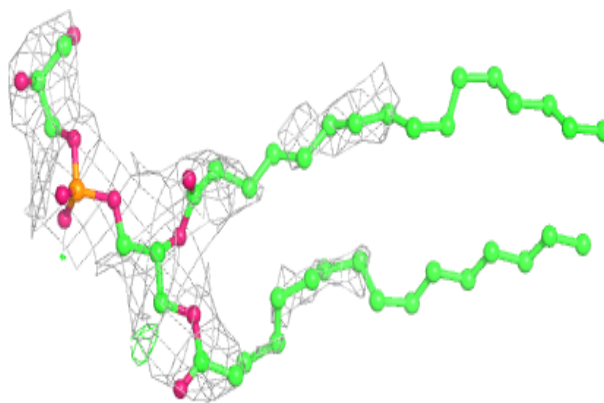
Electron density around CLA 9 604:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

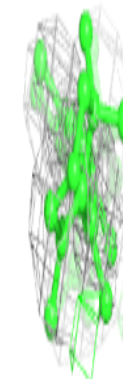
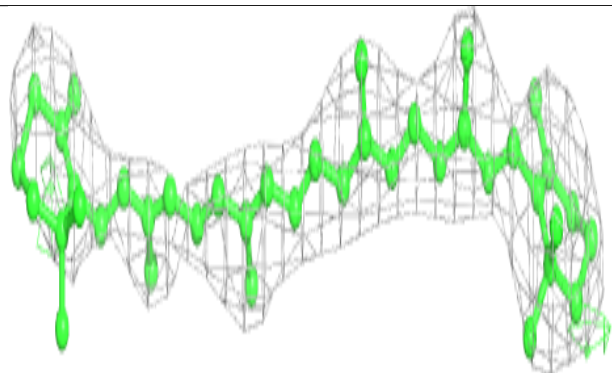
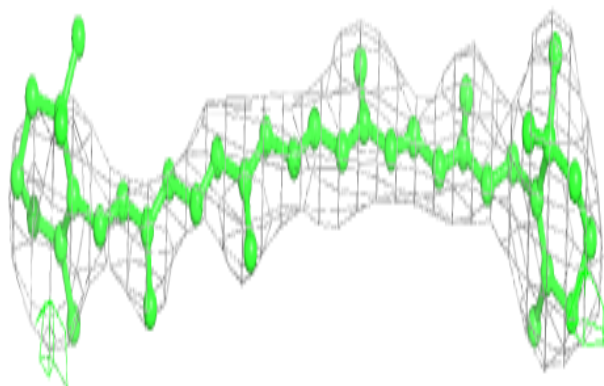


Electron density around LHG 6 320:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

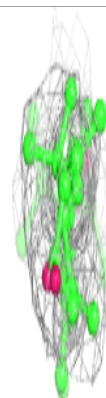
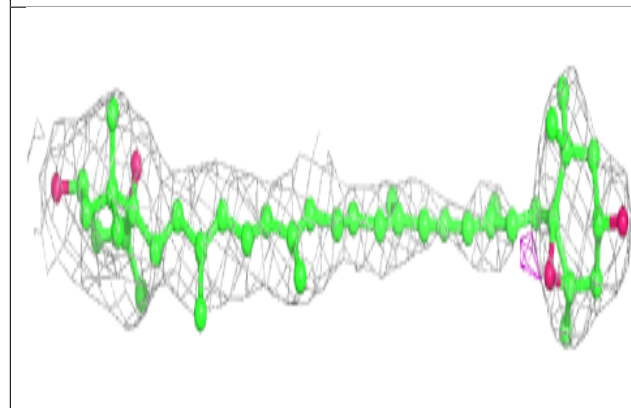
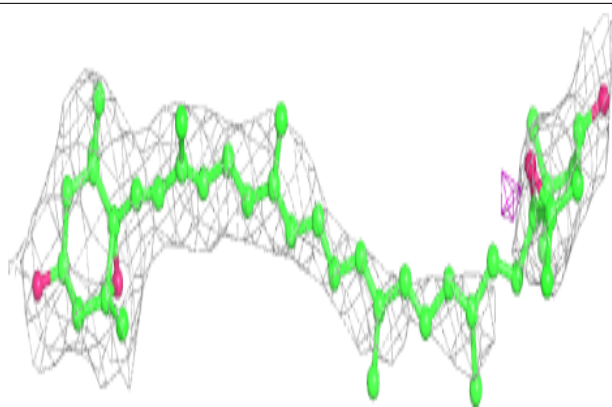
**Electron density around BCR A 848:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



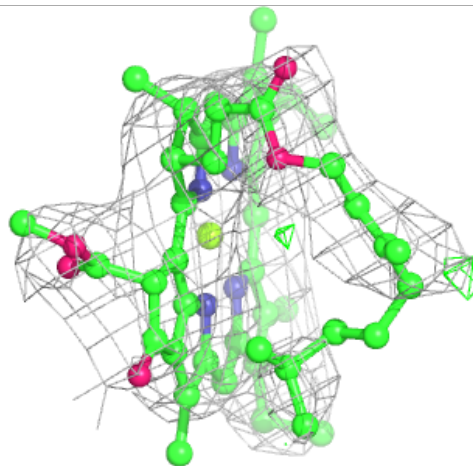
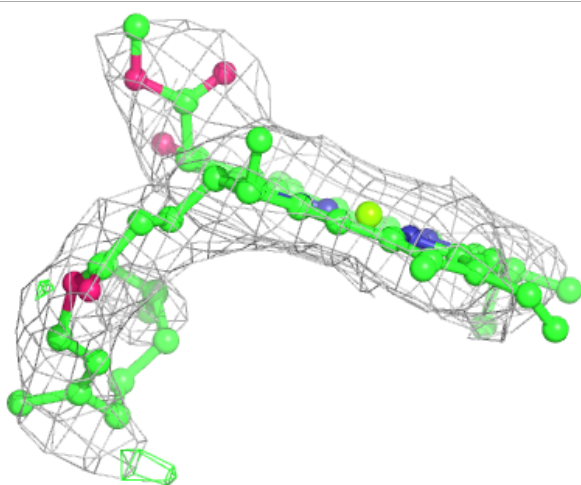
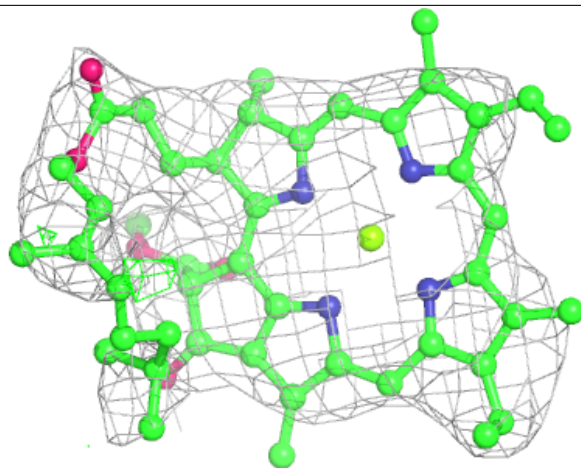
Electron density around XAT 7 616:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



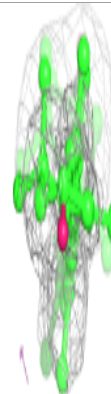
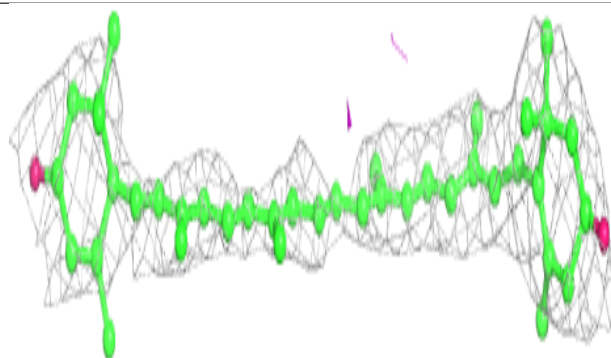
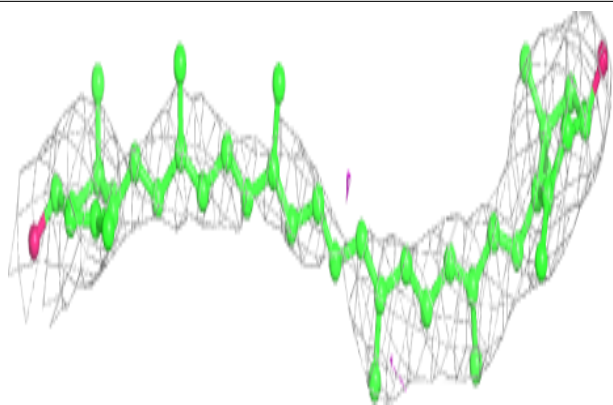
Electron density around CLA 1 314:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



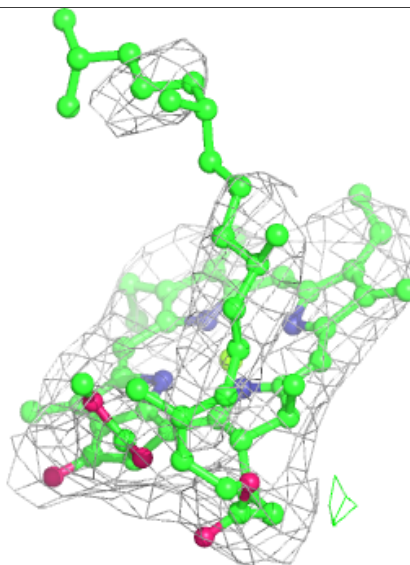
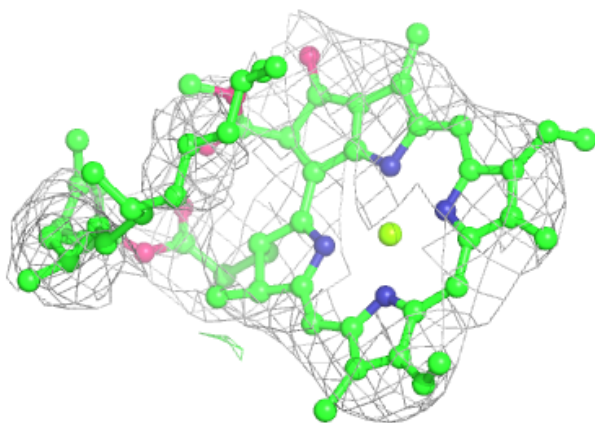
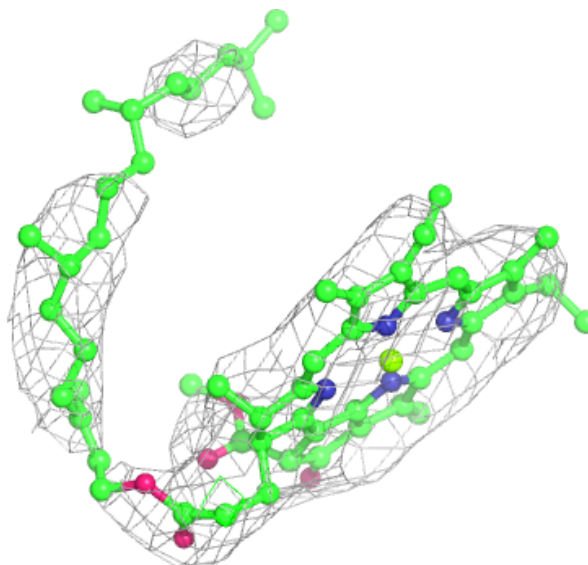
Electron density around LUT 9 616:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



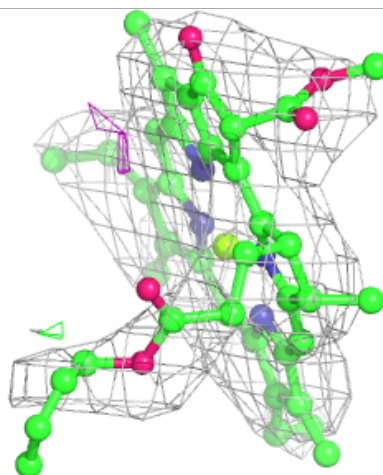
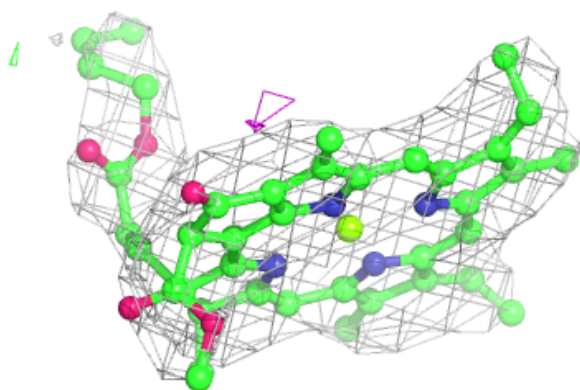
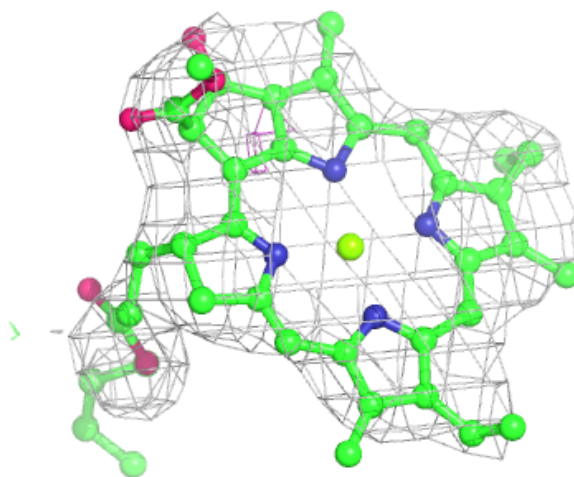
Electron density around CLA 6 305:

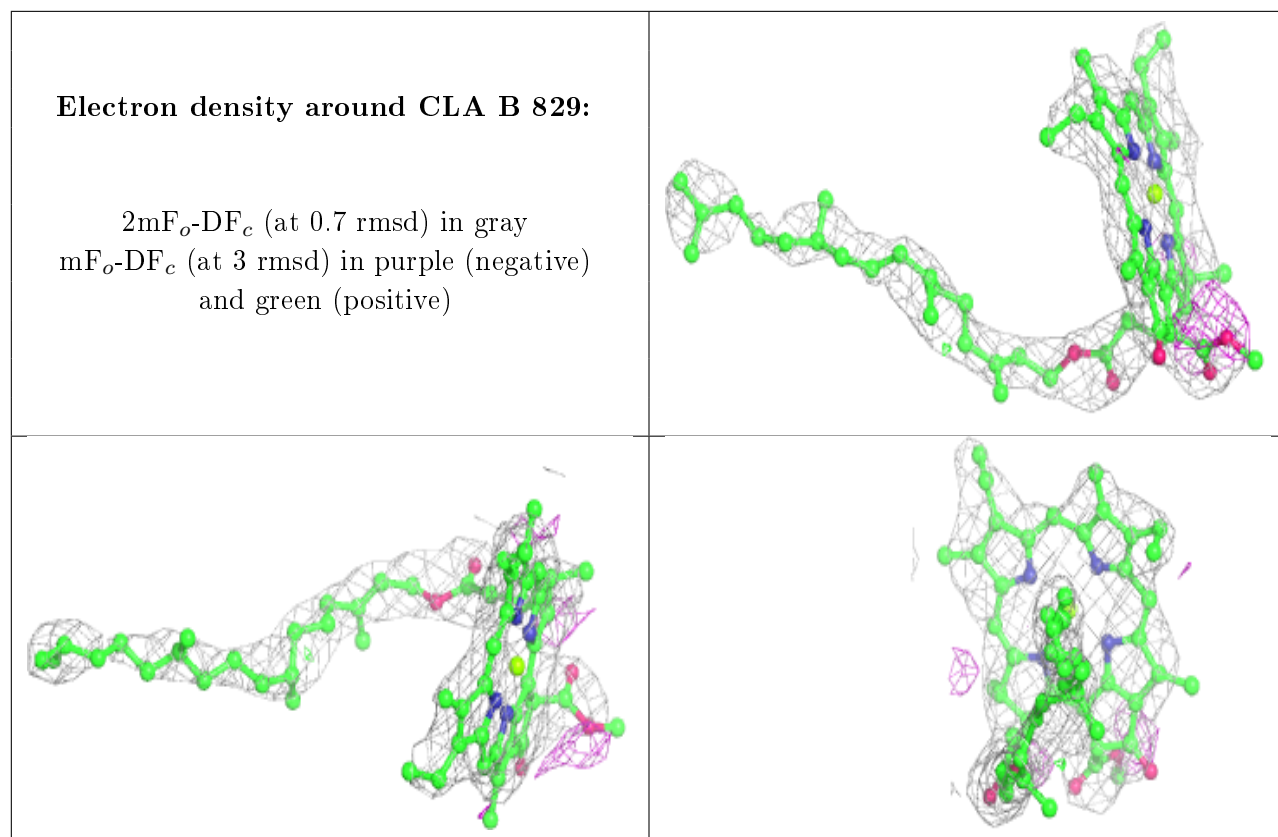
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA A 823:

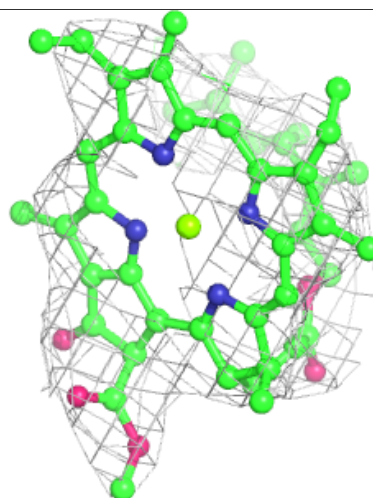
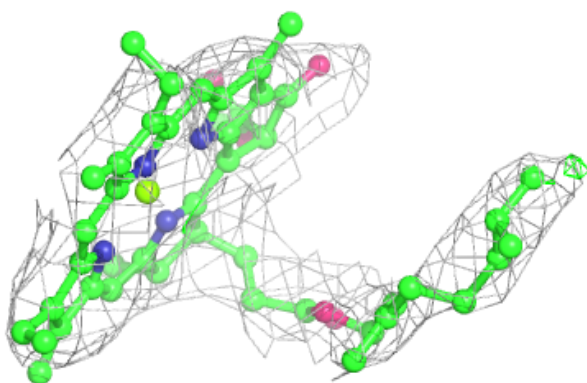
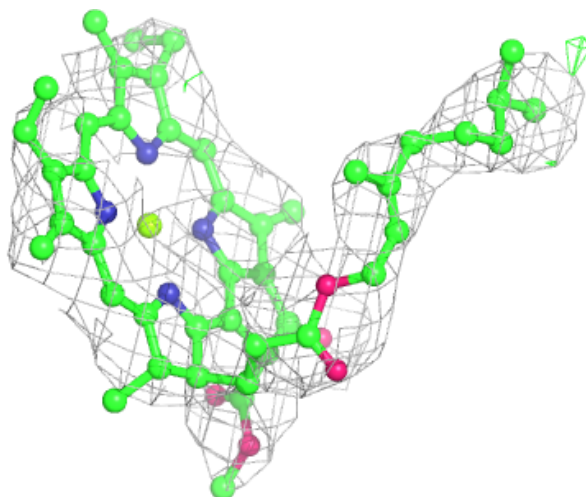
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





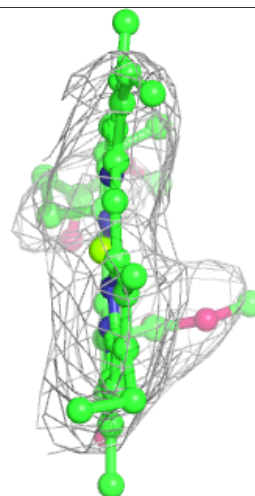
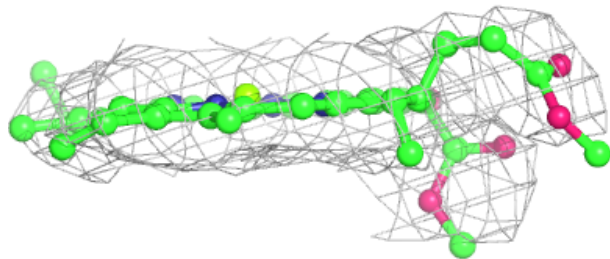
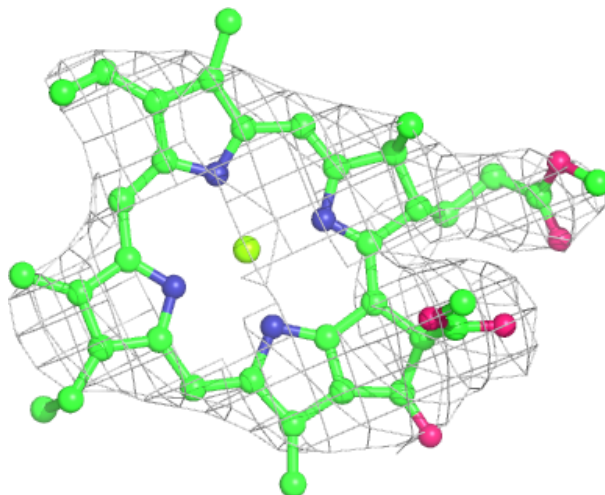
Electron density around CLA 4 610:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



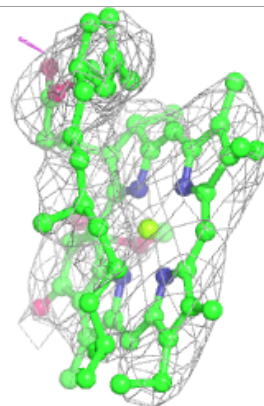
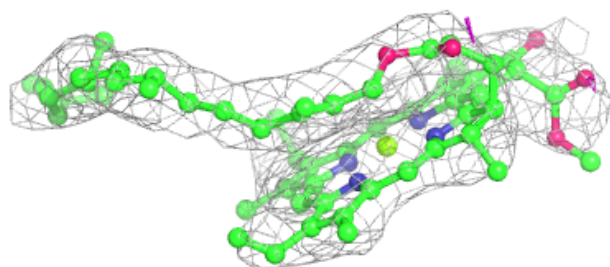
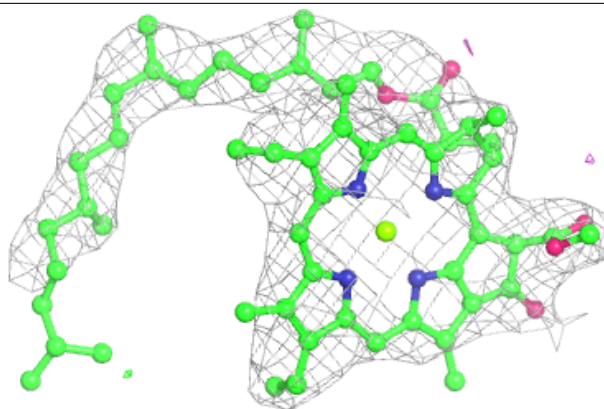
Electron density around CLA g 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



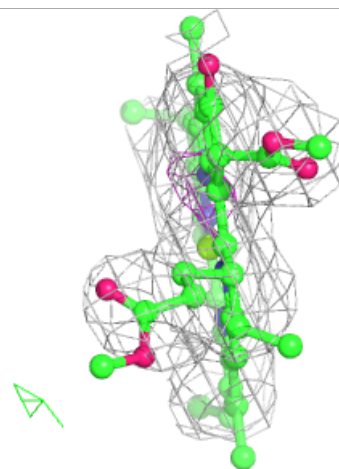
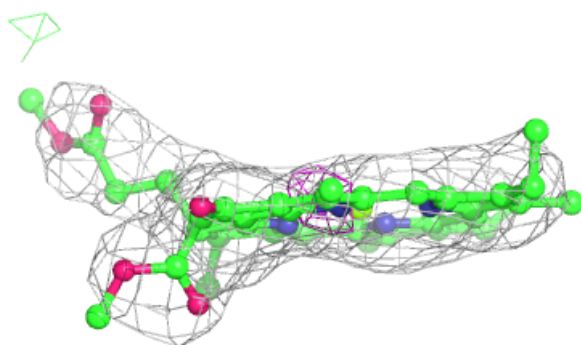
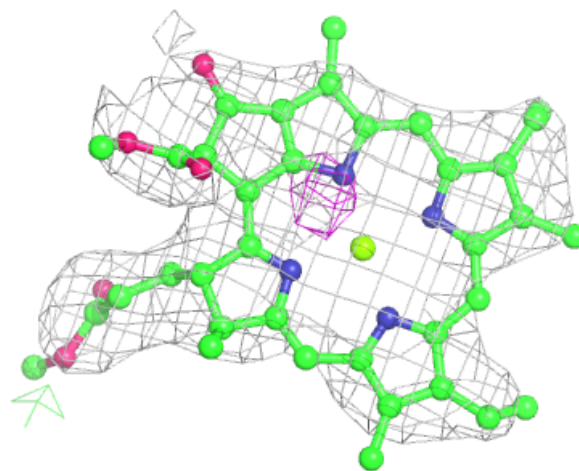
Electron density around CLA 1 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



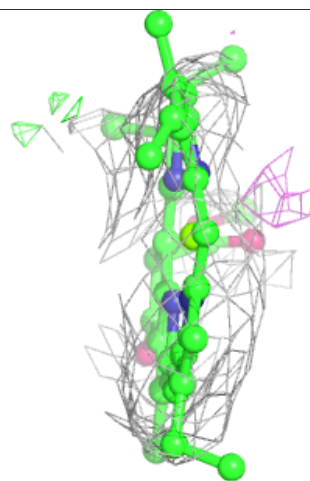
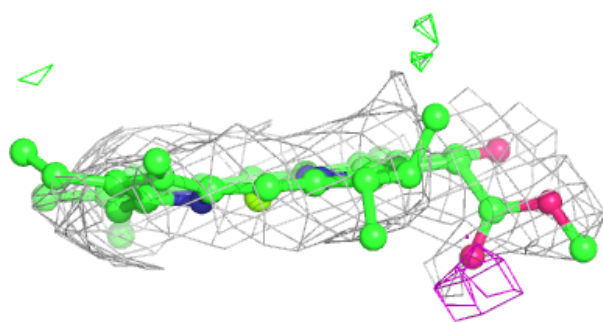
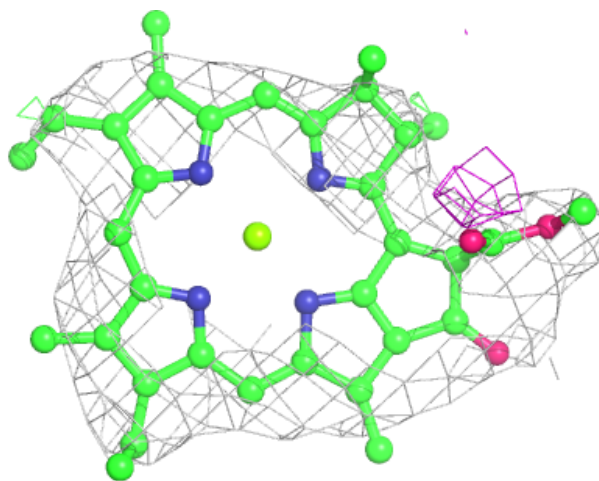
Electron density around CLA k 1402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



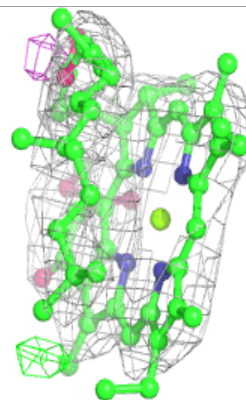
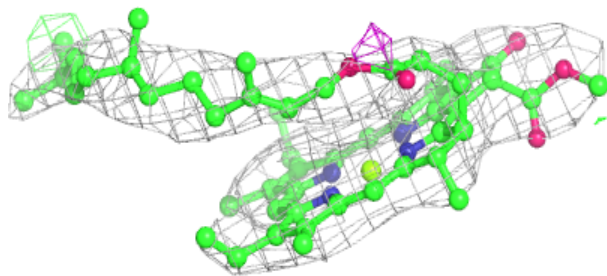
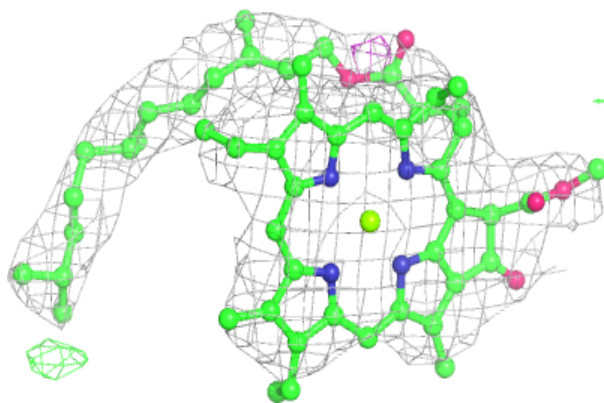
Electron density around CLA 2 610:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



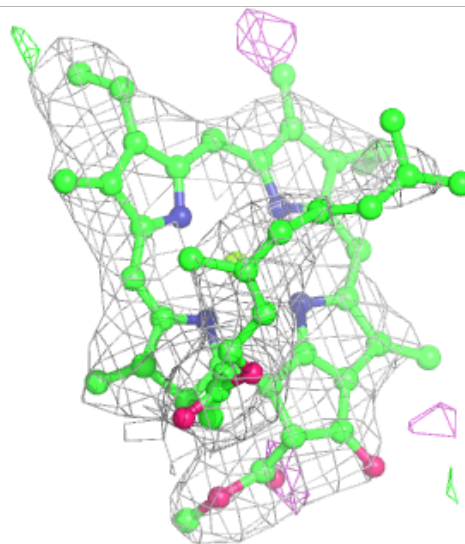
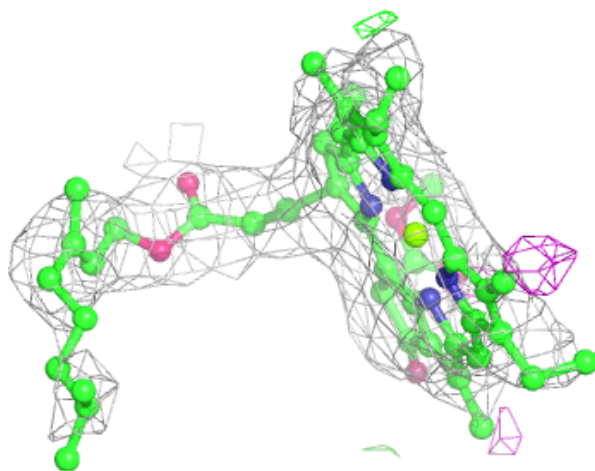
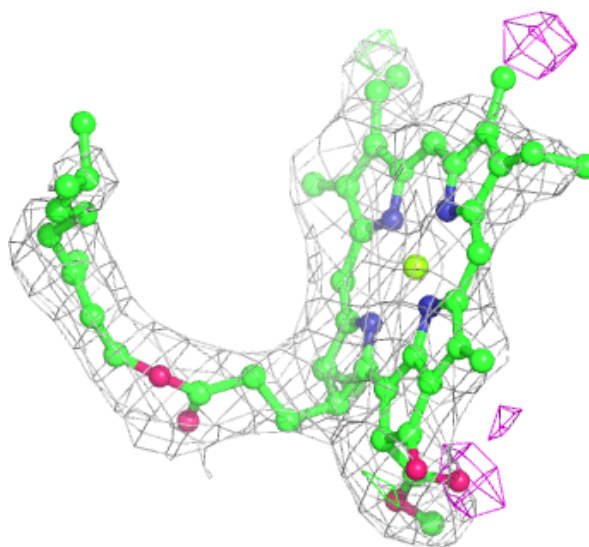
Electron density around CLA 1 310:

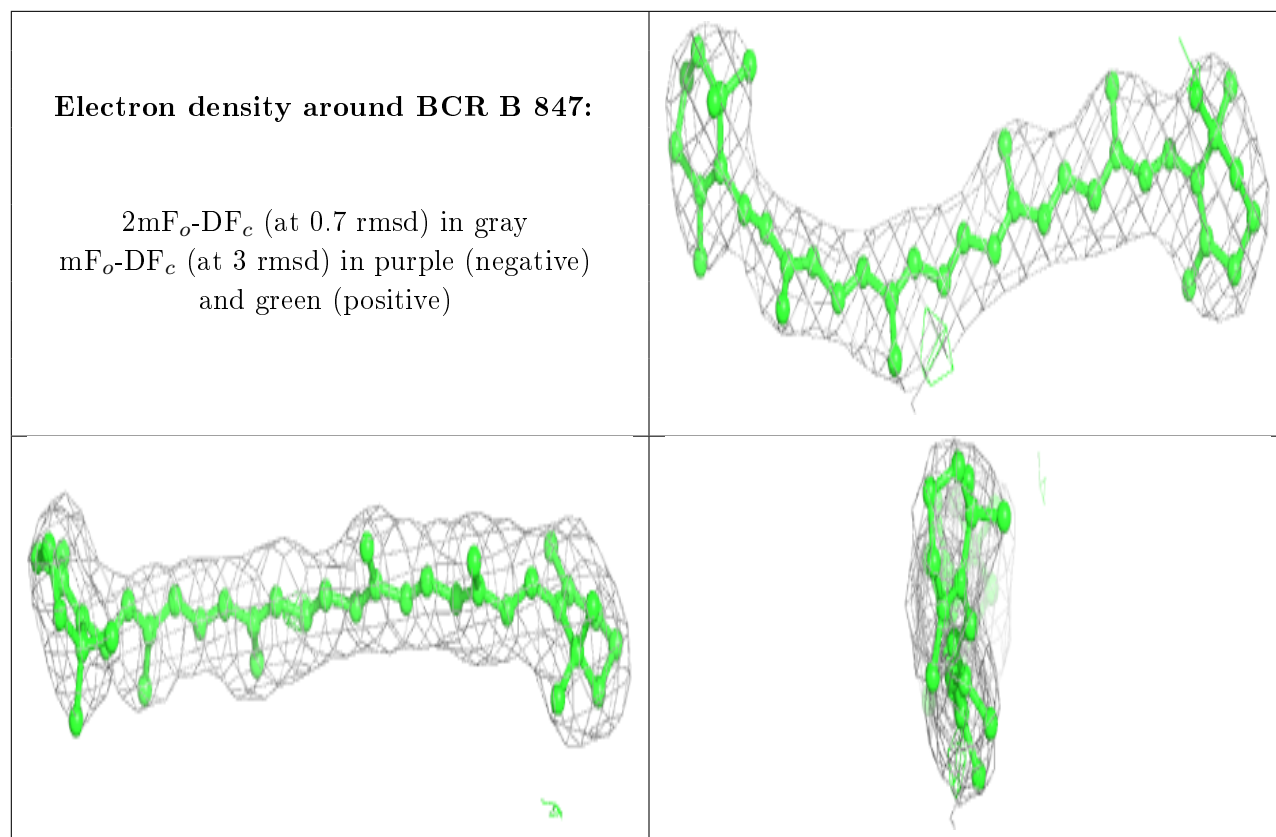
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA A 805:

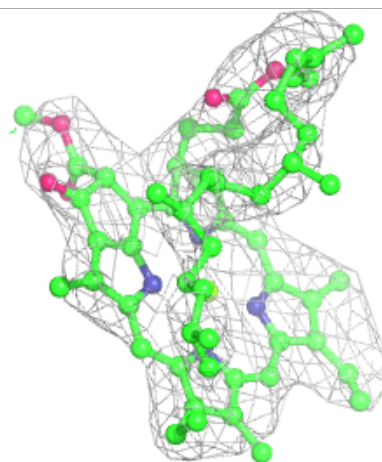
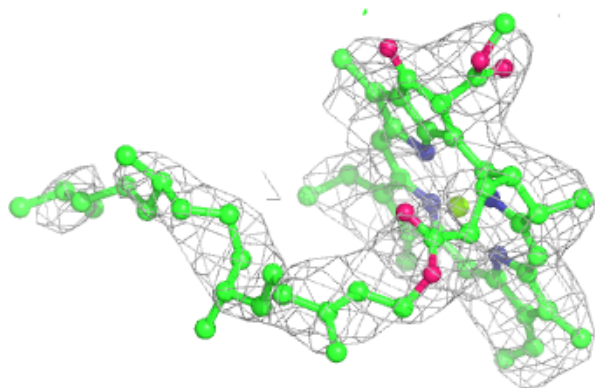
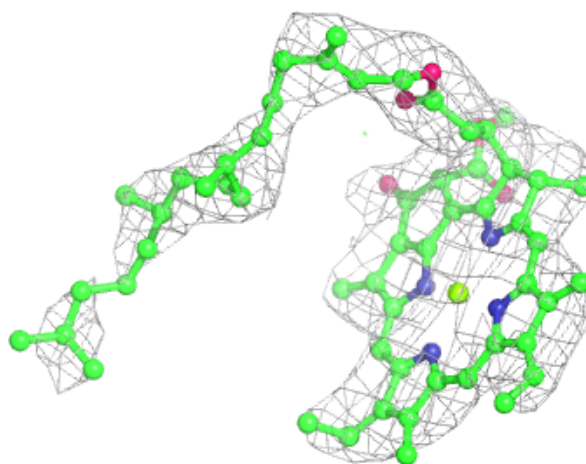
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

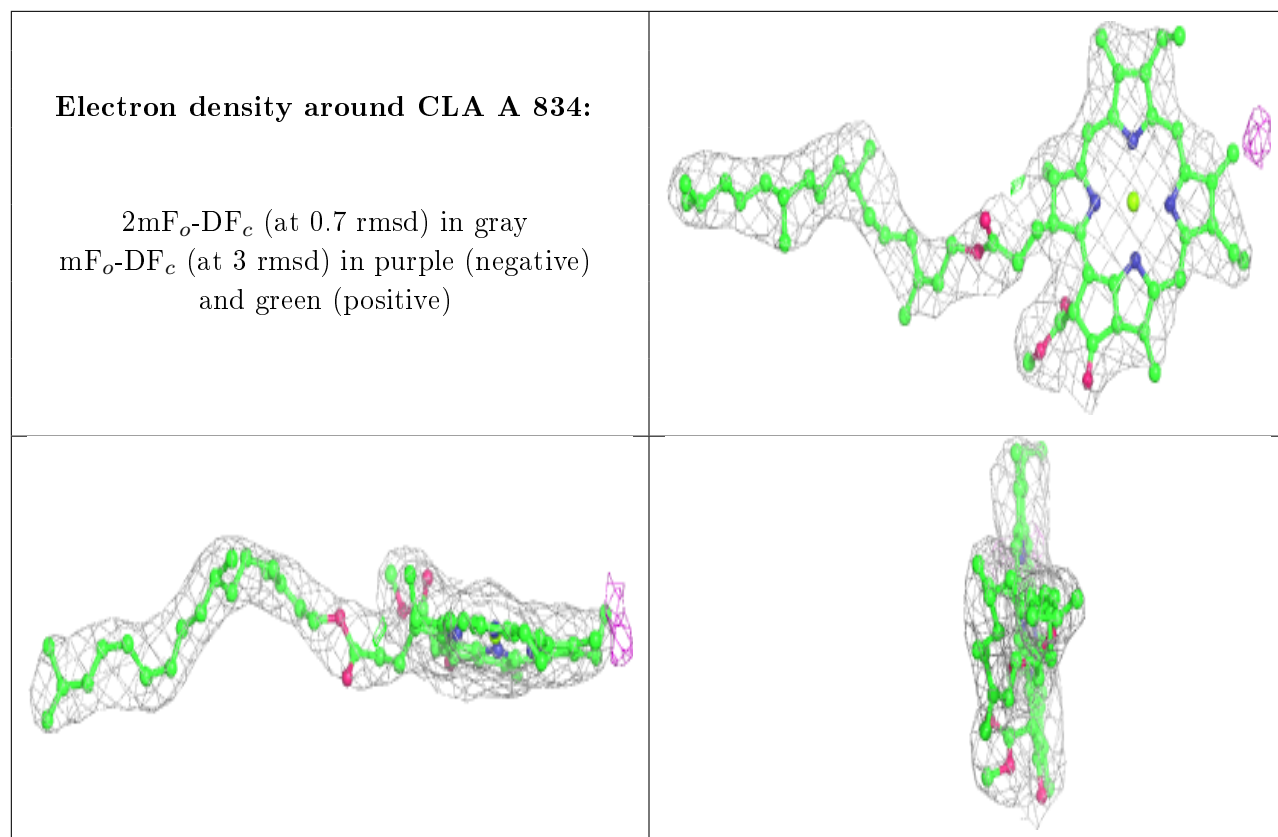




Electron density around CLA B 834:

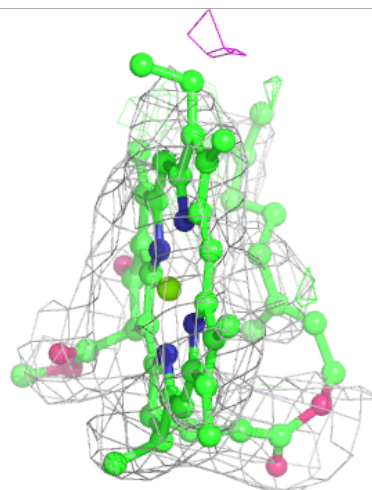
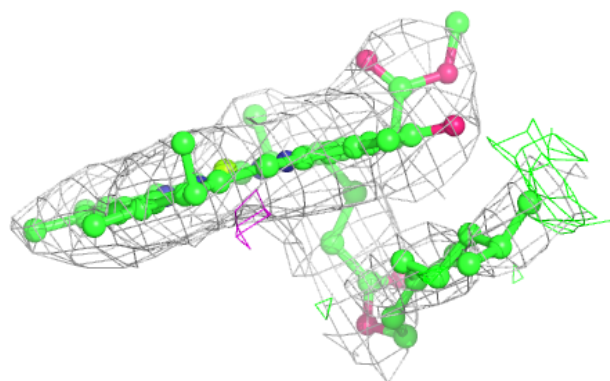
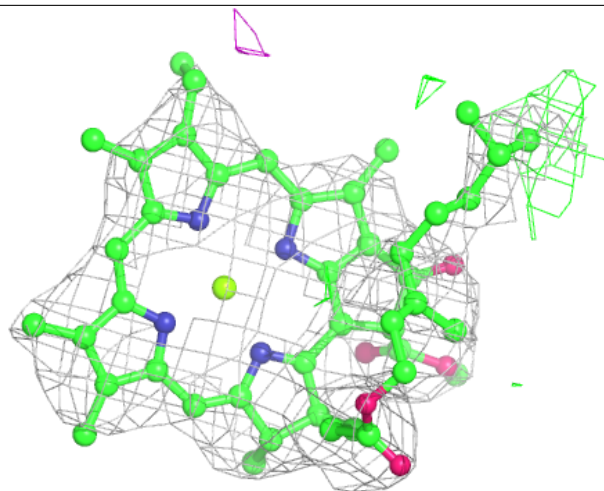
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

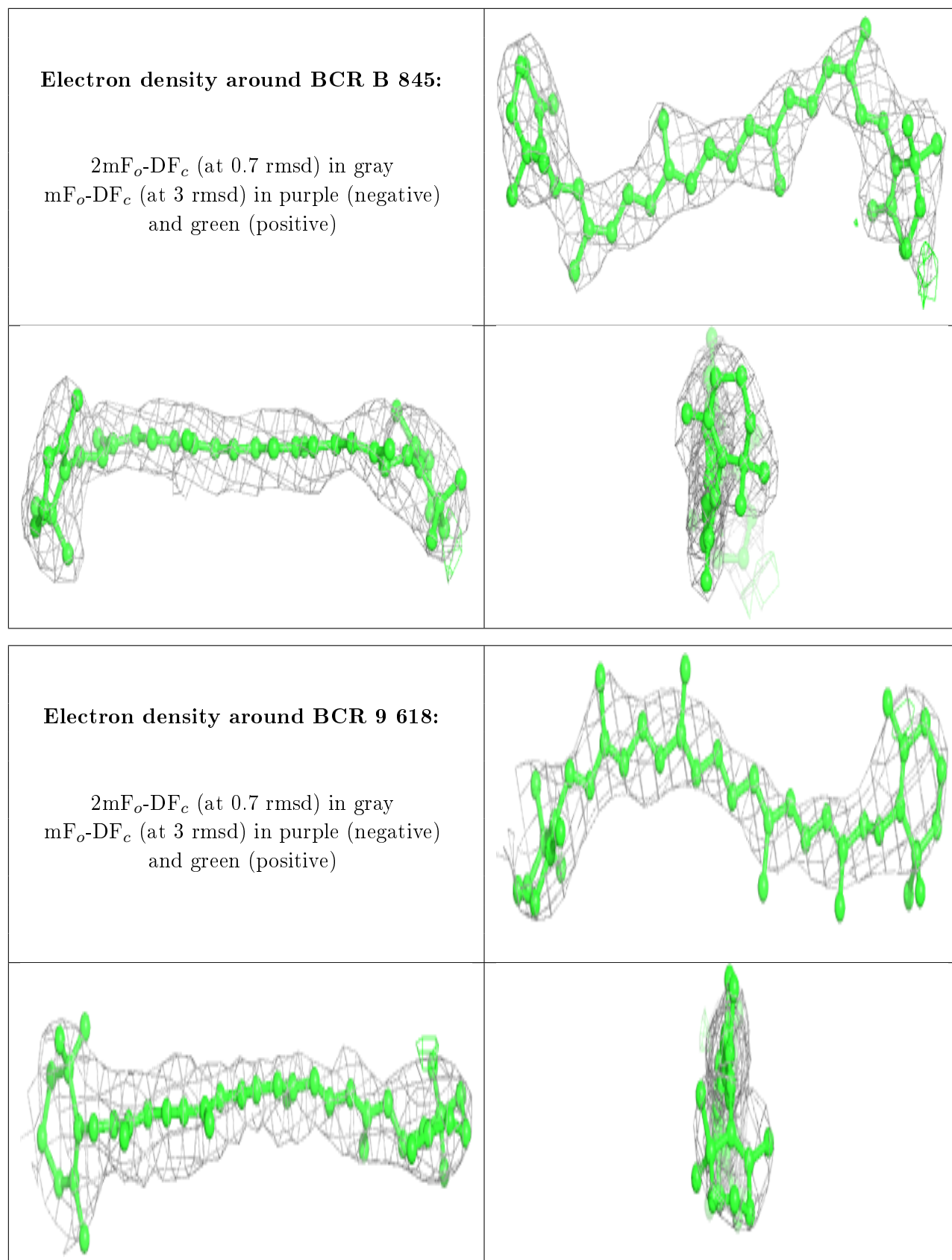




Electron density around CLA B 811:

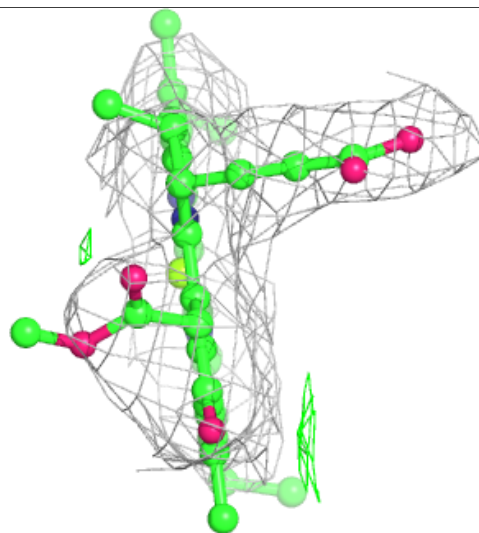
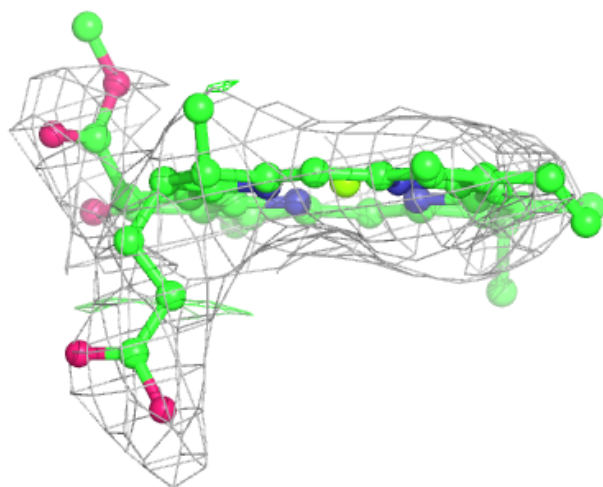
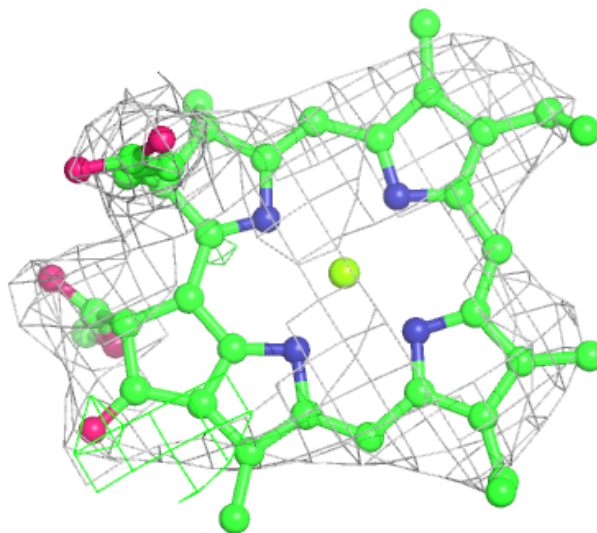
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





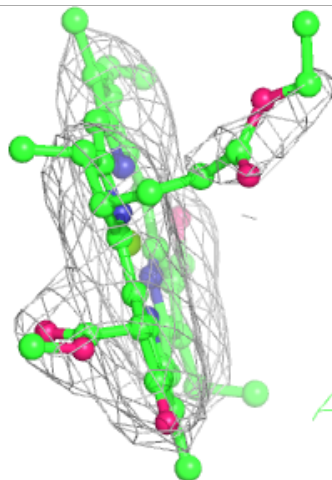
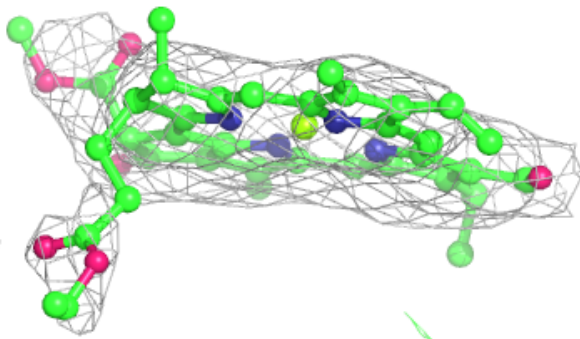
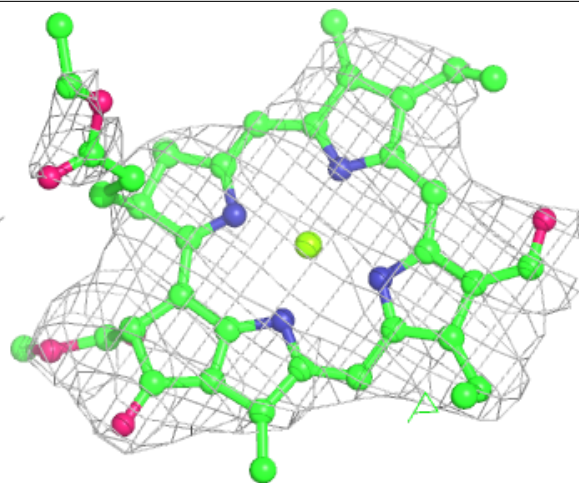
Electron density around CLA 3 304:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



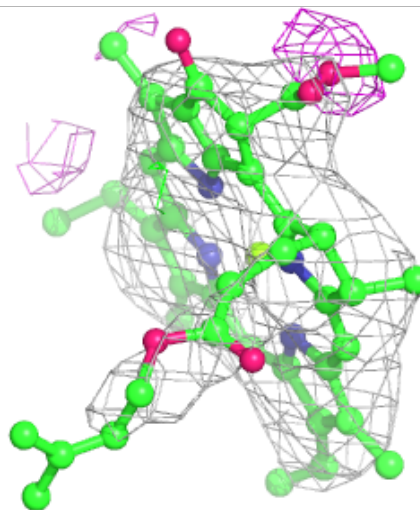
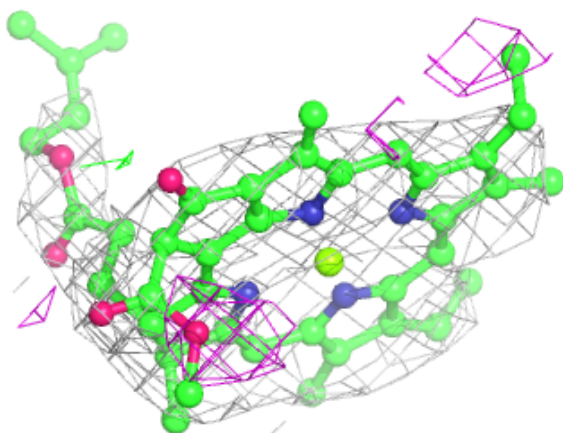
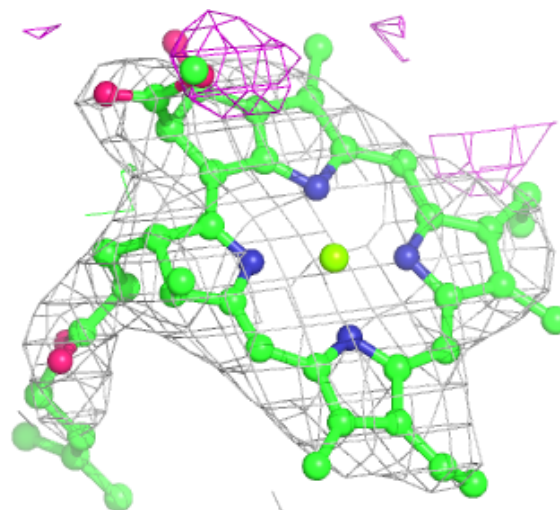
Electron density around CHL 7 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



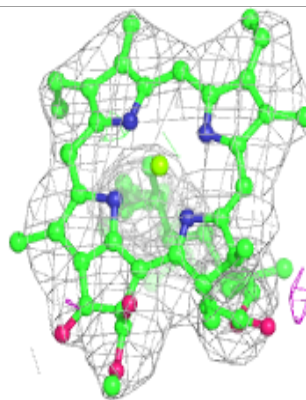
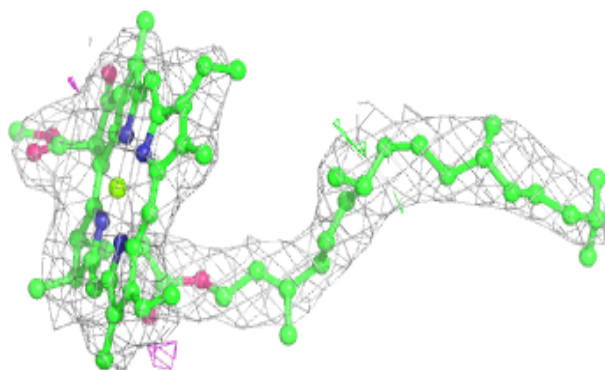
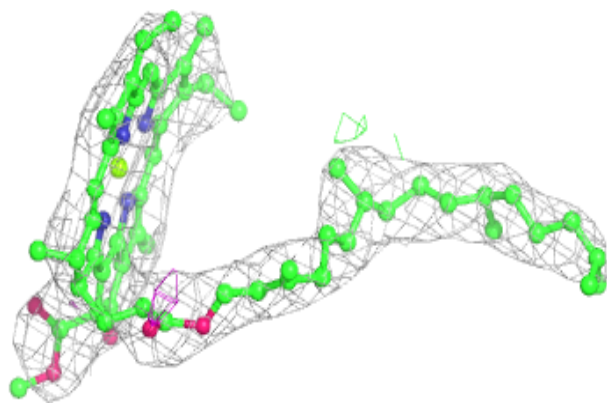
Electron density around CLA 4 604:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

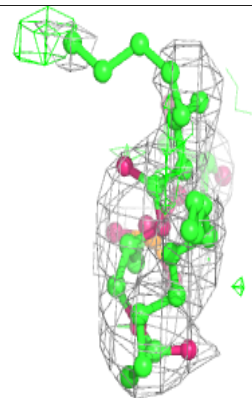
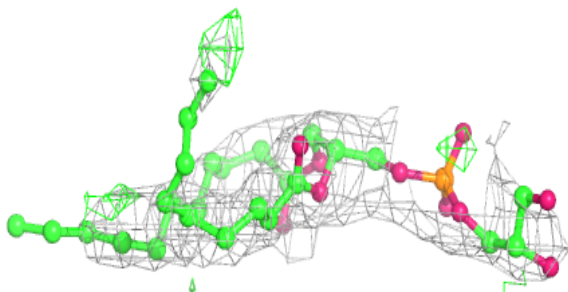
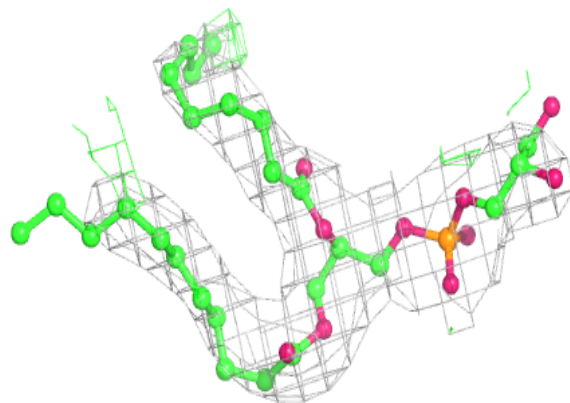


Electron density around CLA A 812:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

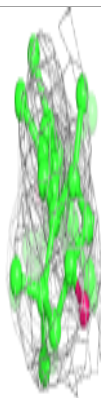
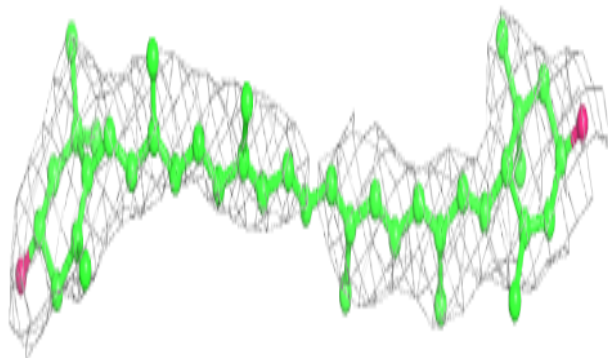
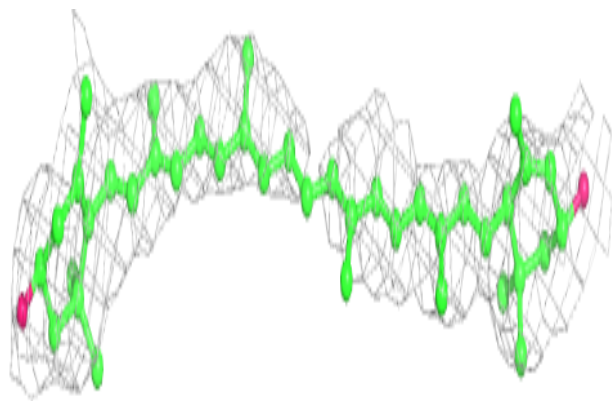
**Electron density around LHG 7 618:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

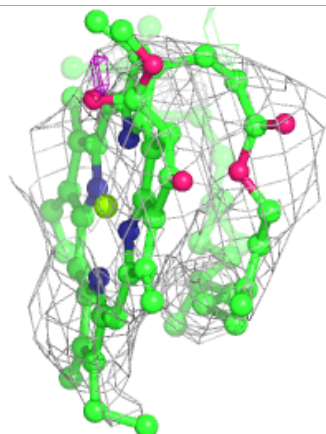
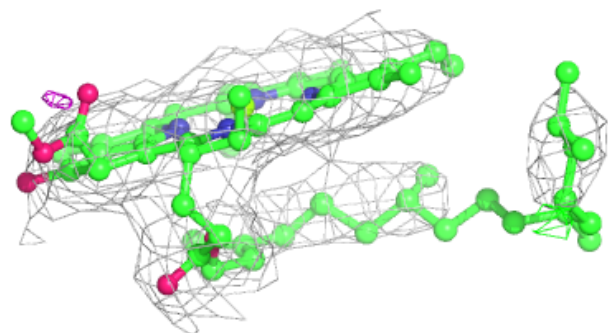
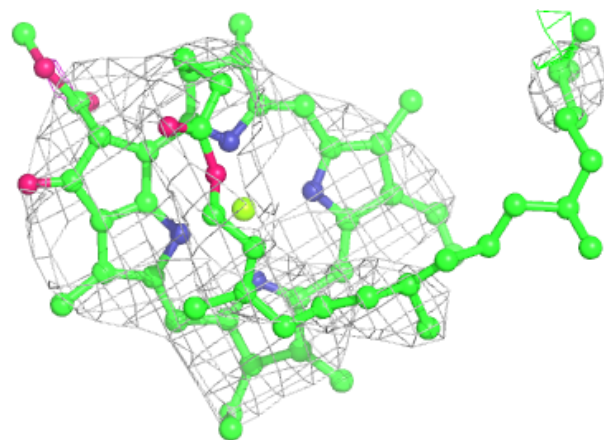


Electron density around LUT 2 615:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

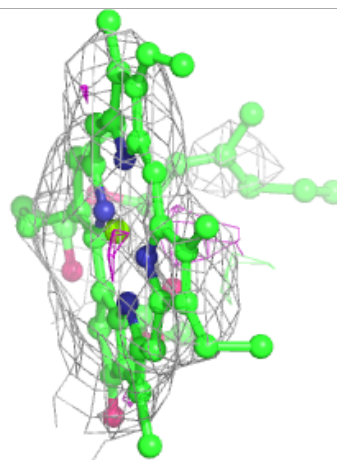
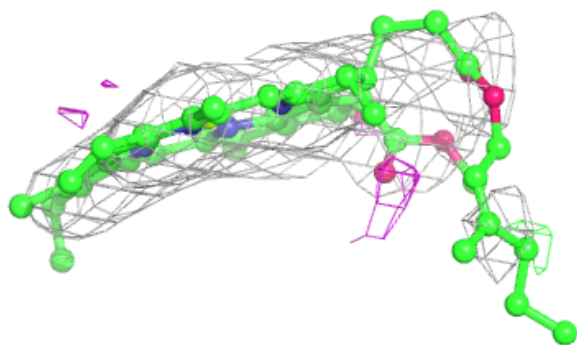
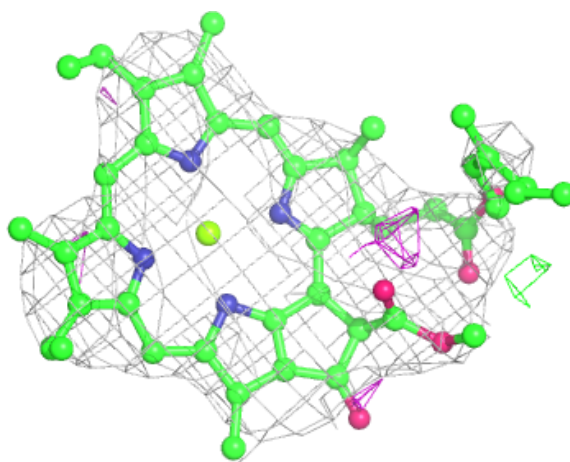
**Electron density around CLA 2 612:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



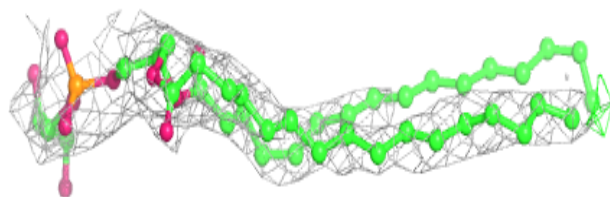
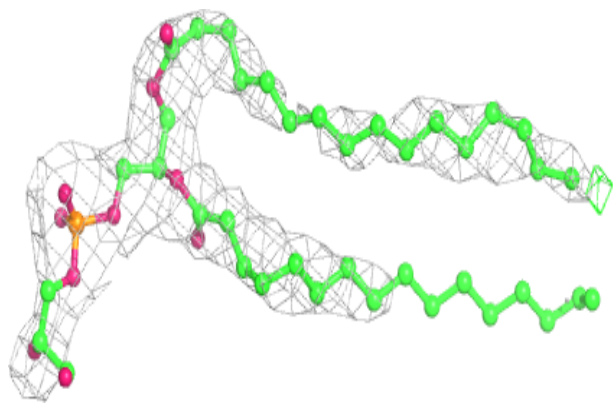
Electron density around CLA 9 611:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



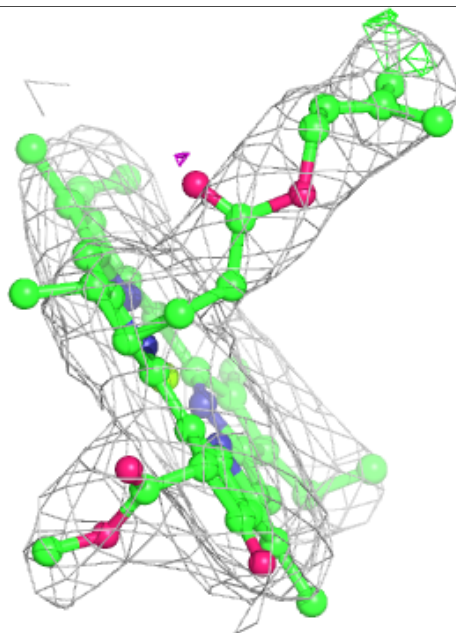
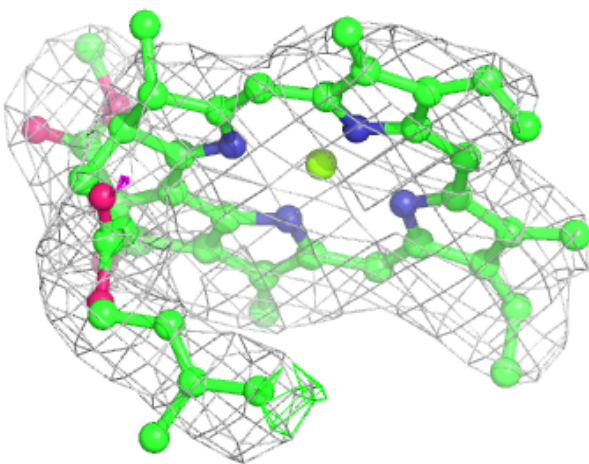
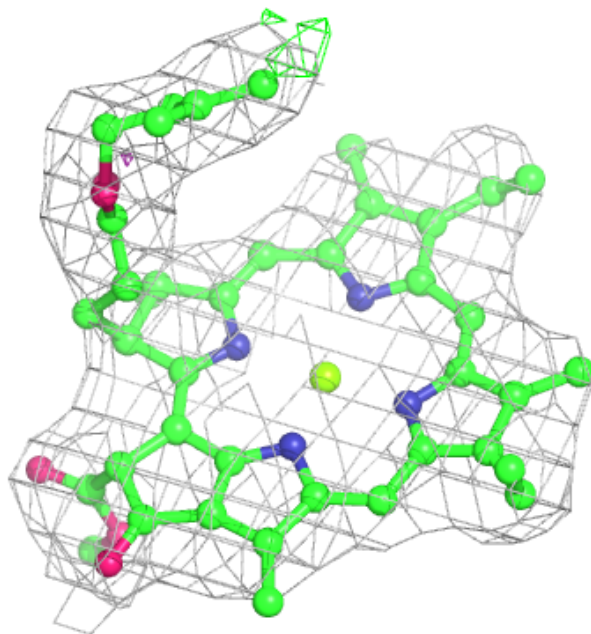
Electron density around LHG 1 319:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



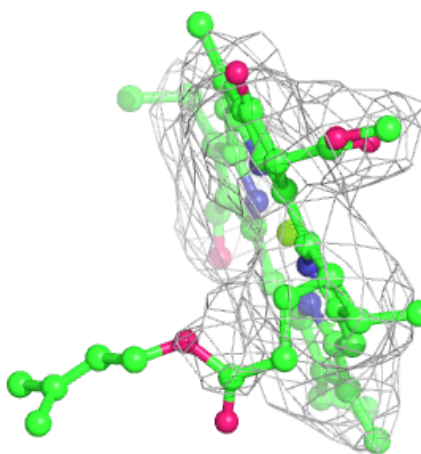
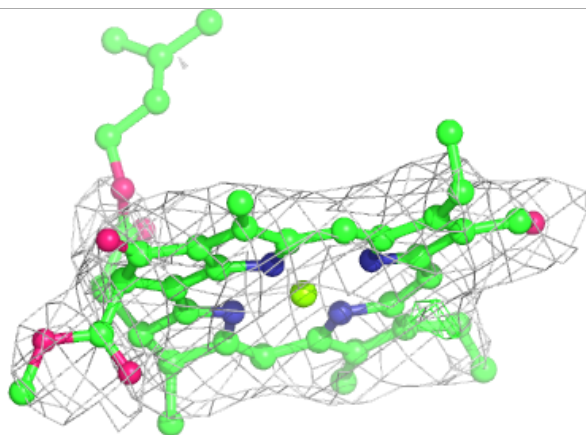
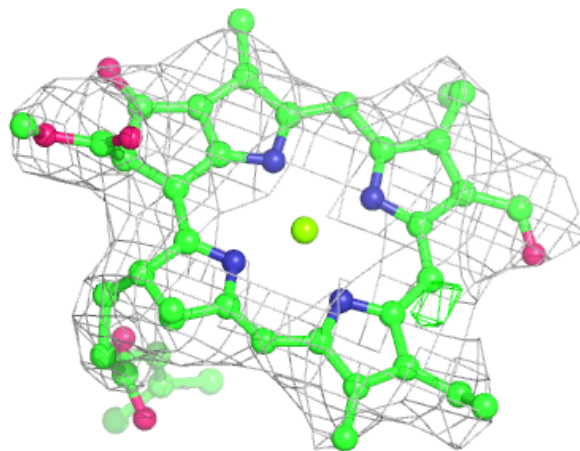
Electron density around CLA b 830:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



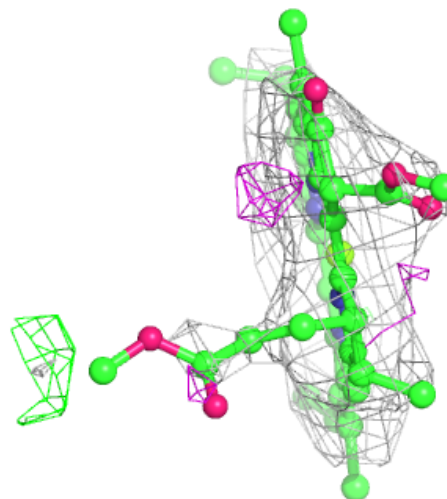
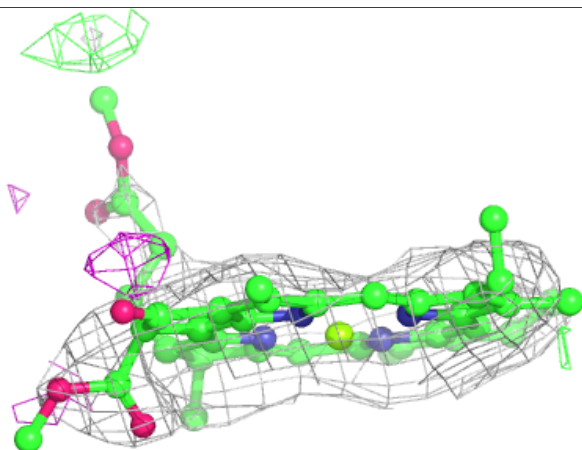
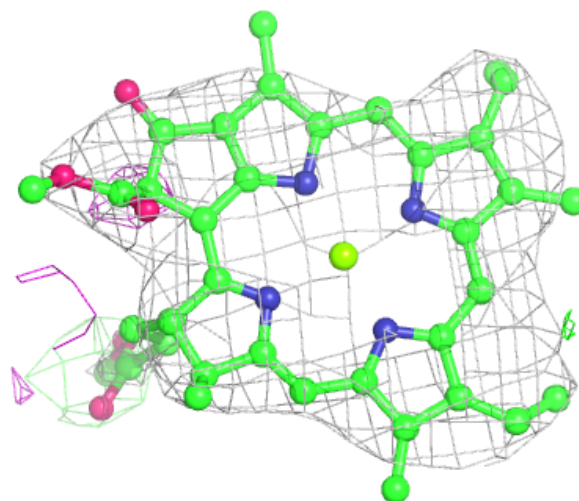
Electron density around CHL 4 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



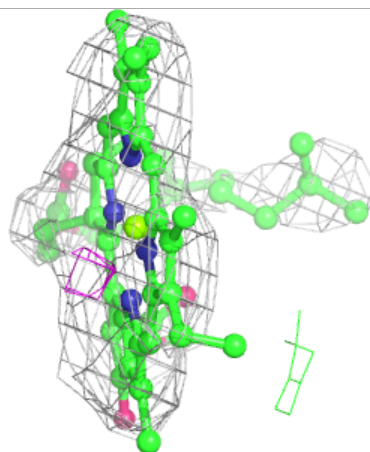
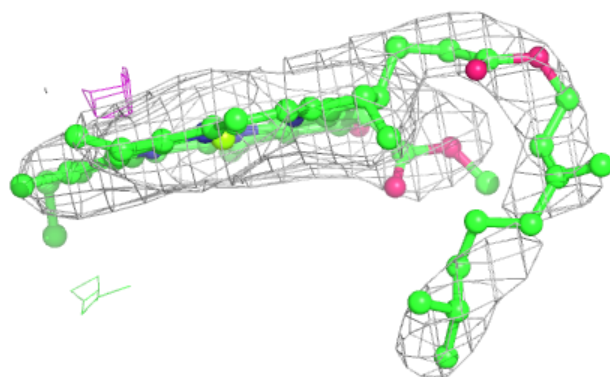
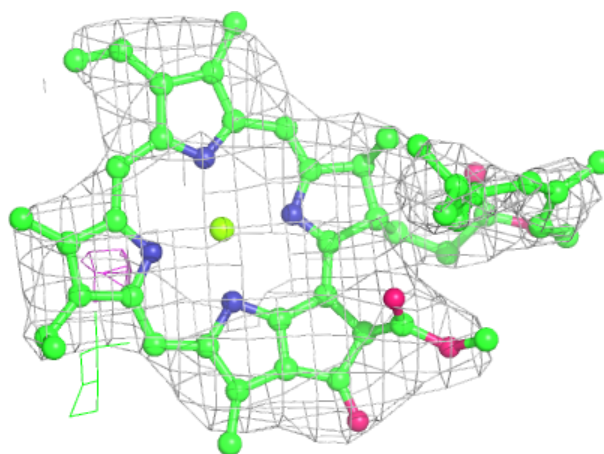
Electron density around CLA 6 309:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



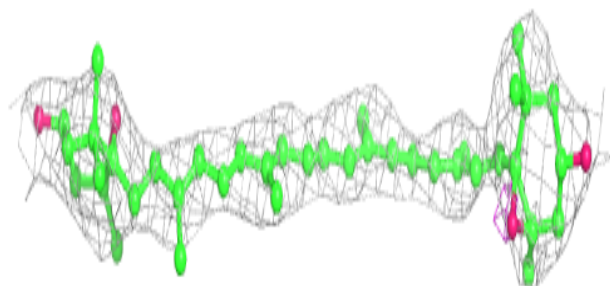
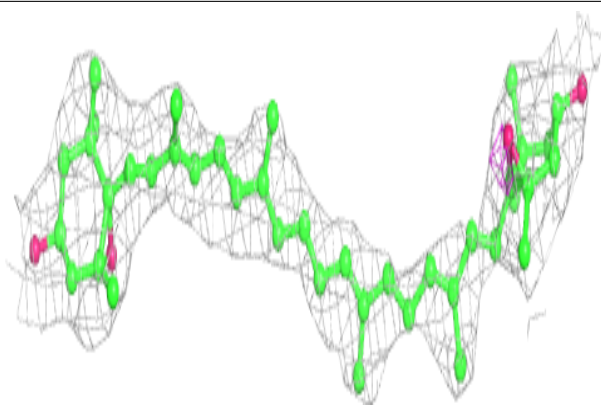
Electron density around CLA F 304:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

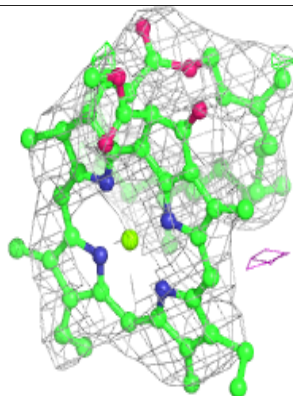
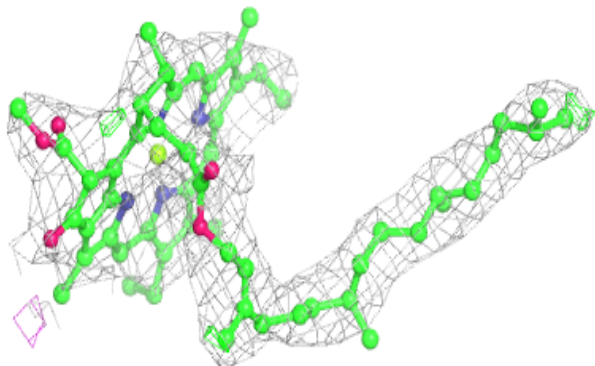
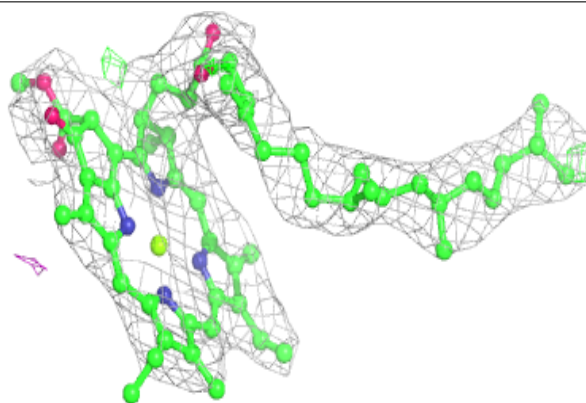


Electron density around XAT 8 315:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

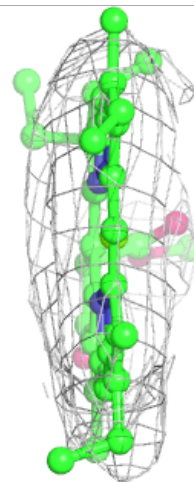
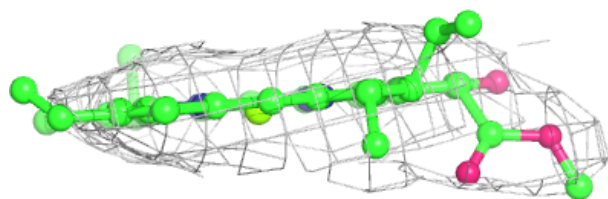
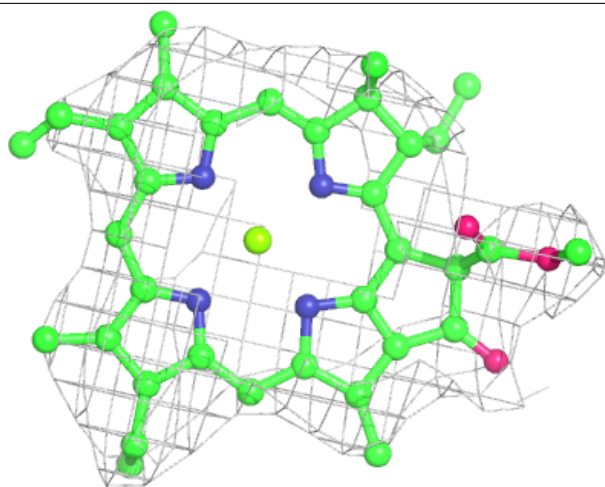
**Electron density around CLA b 814:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



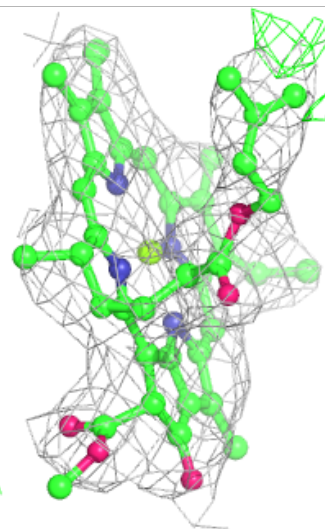
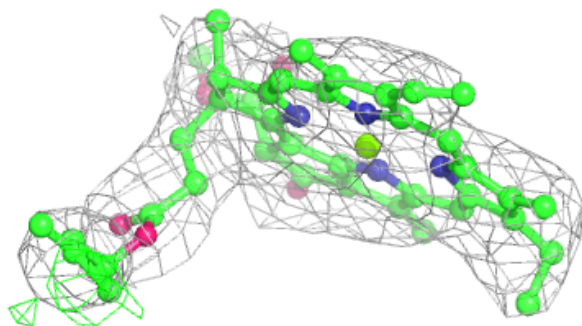
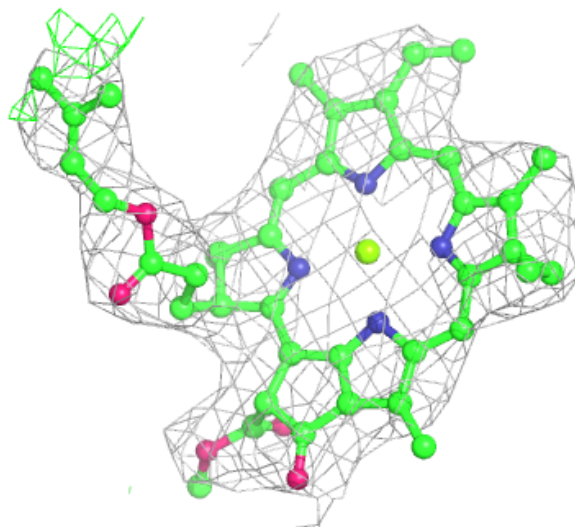
Electron density around CLA j 3002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



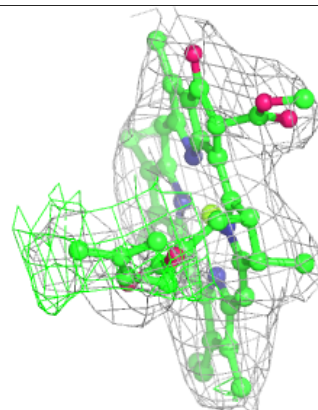
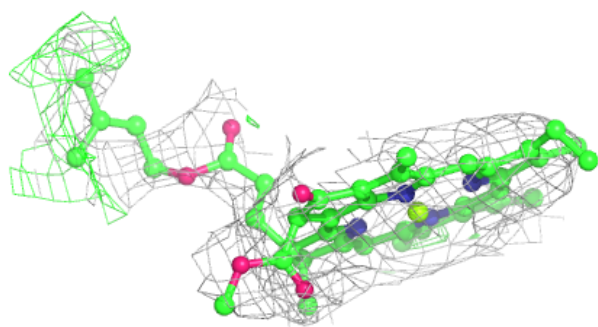
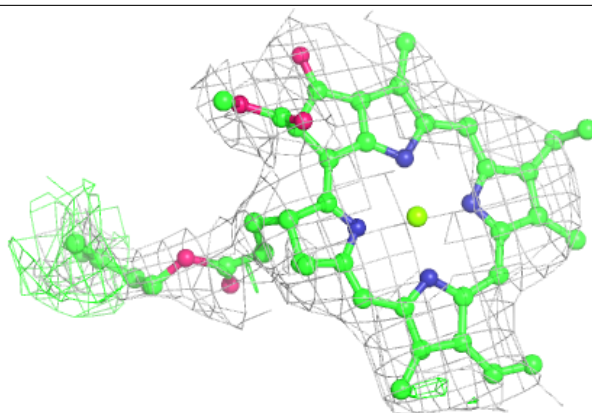
Electron density around CLA a 836:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



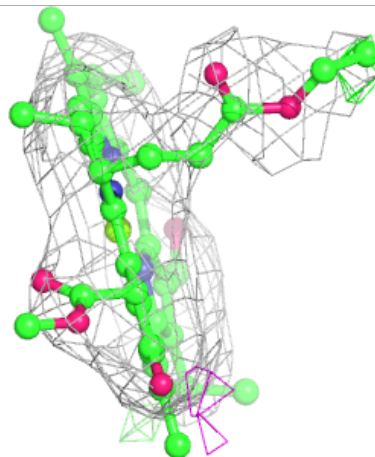
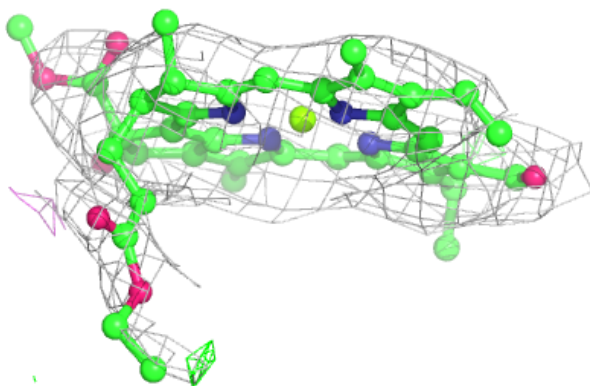
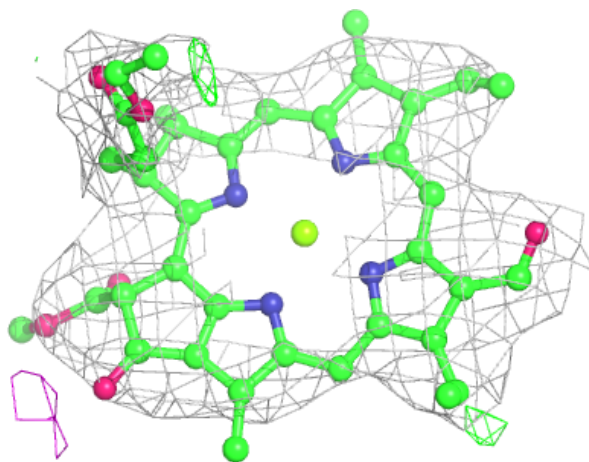
Electron density around CLA 2 608:

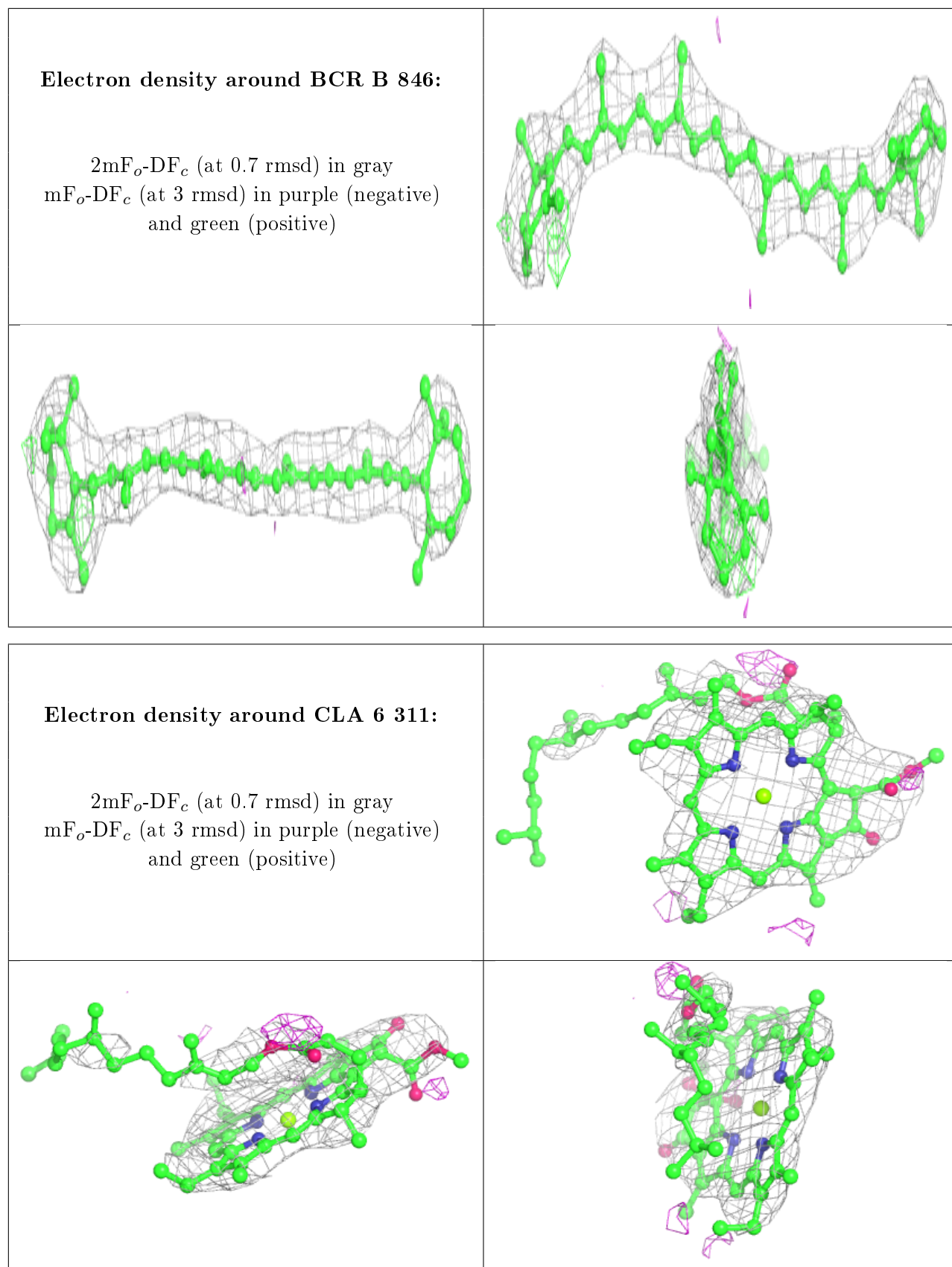
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CHL 1 307:

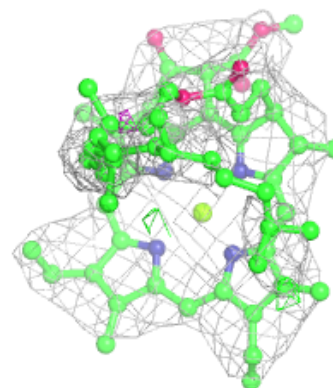
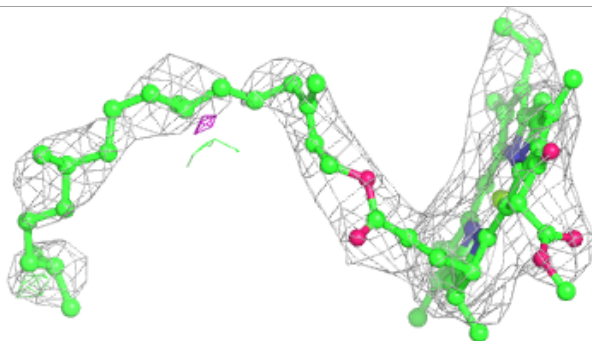
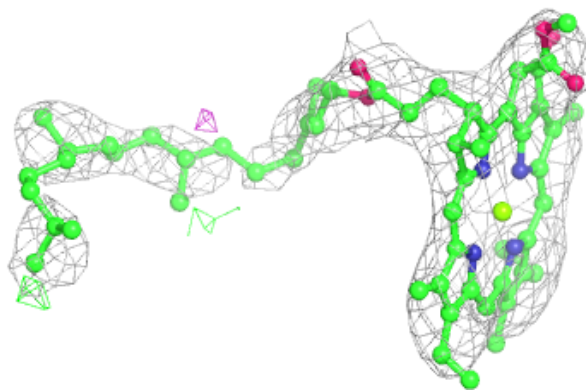
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



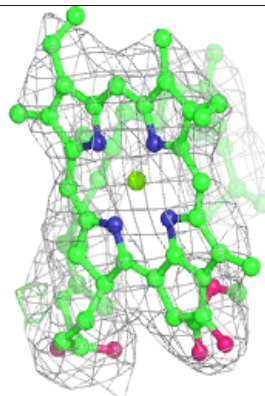
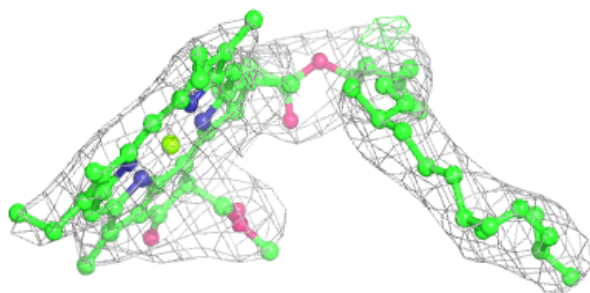
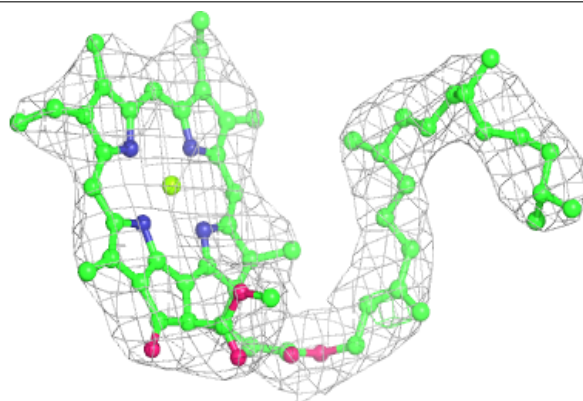


Electron density around CLA L 203:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

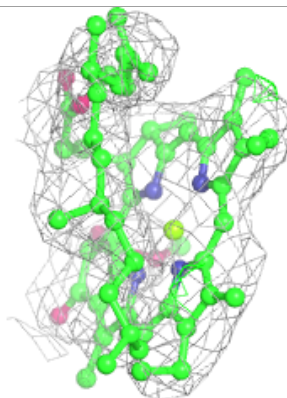
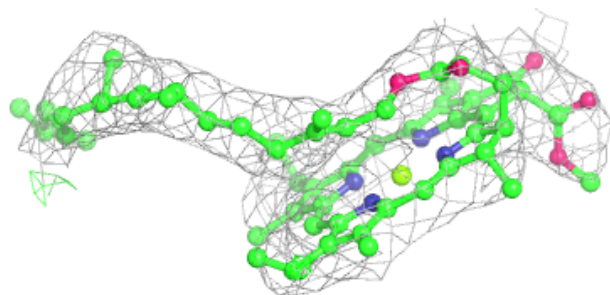
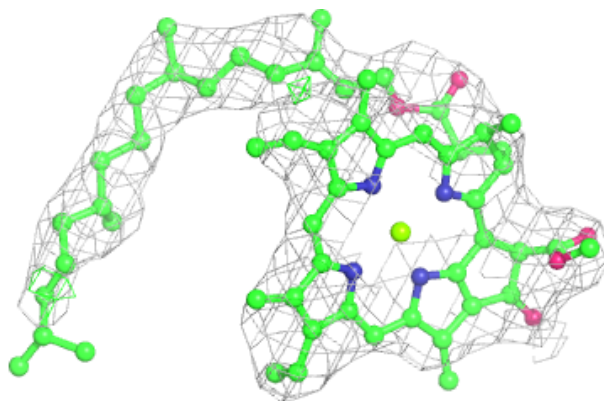
**Electron density around CLA B 824:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

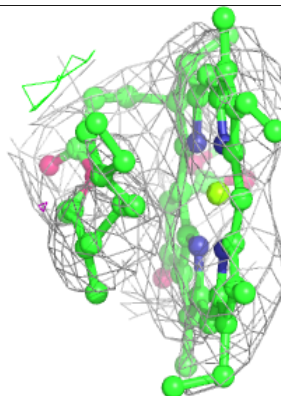
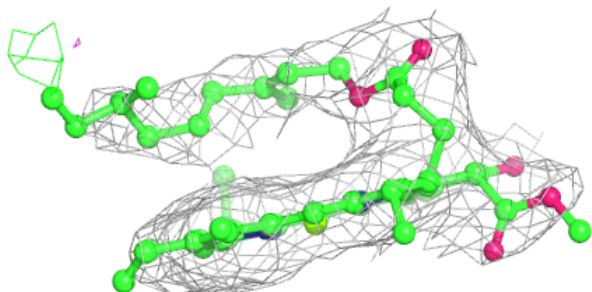
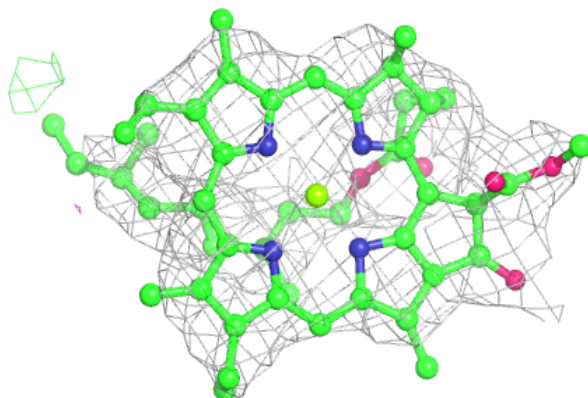


Electron density around CLA 7 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

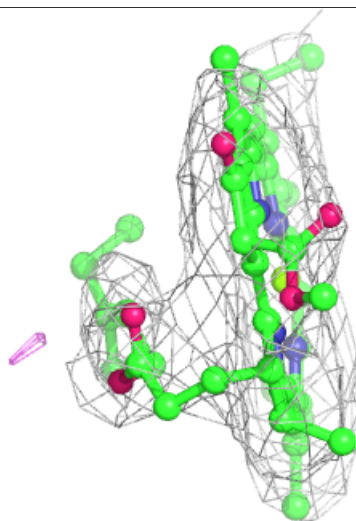
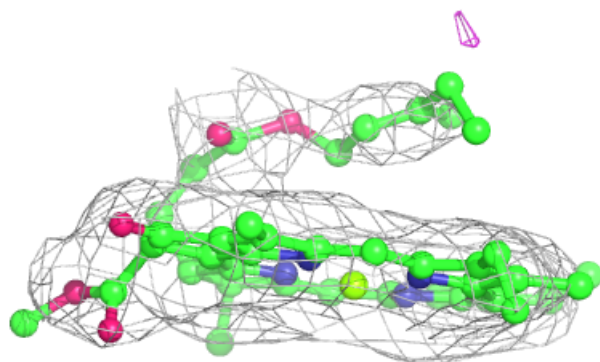
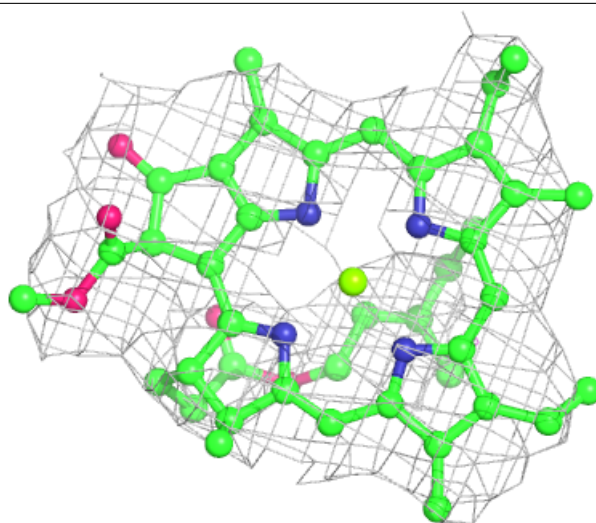
**Electron density around CLA 9 612:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



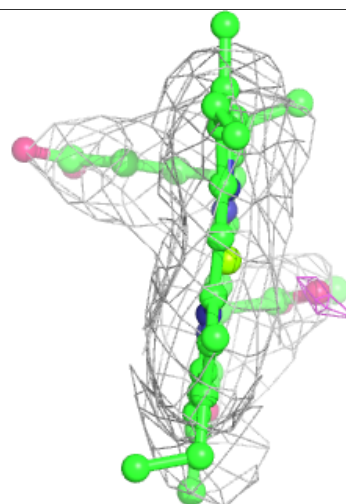
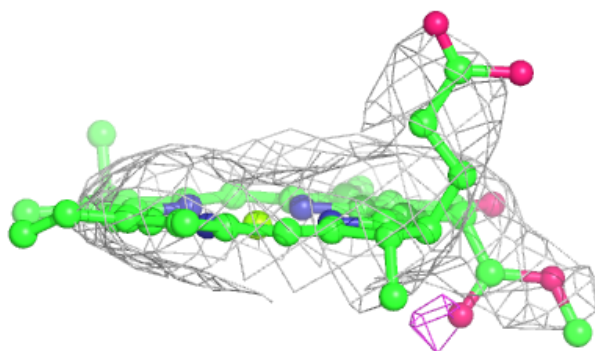
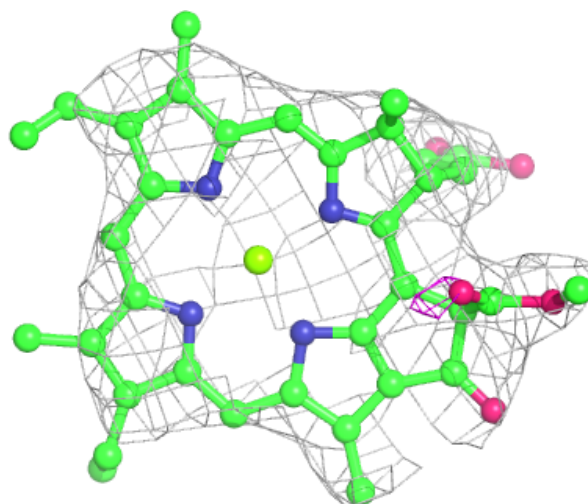
Electron density around CLA a 824:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



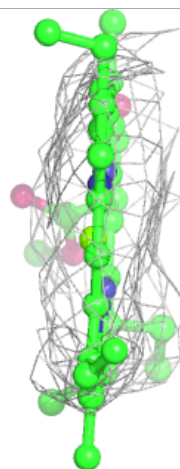
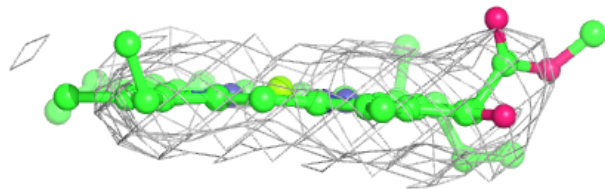
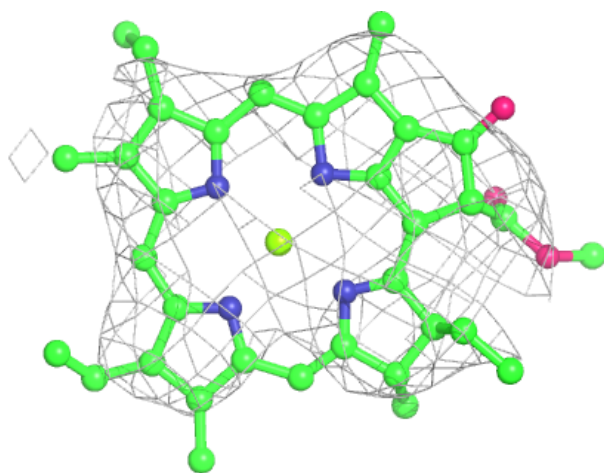
Electron density around CLA 4 613:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



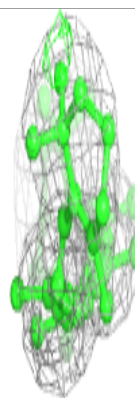
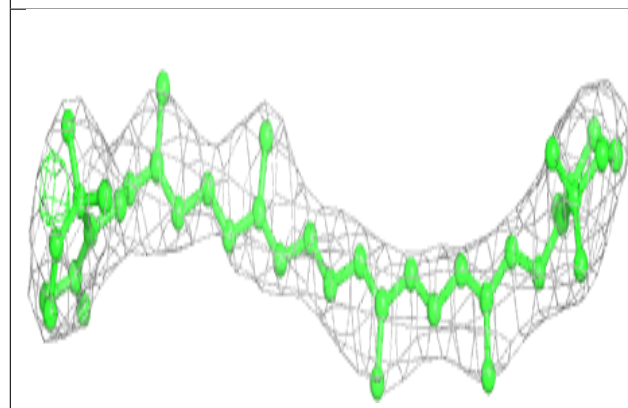
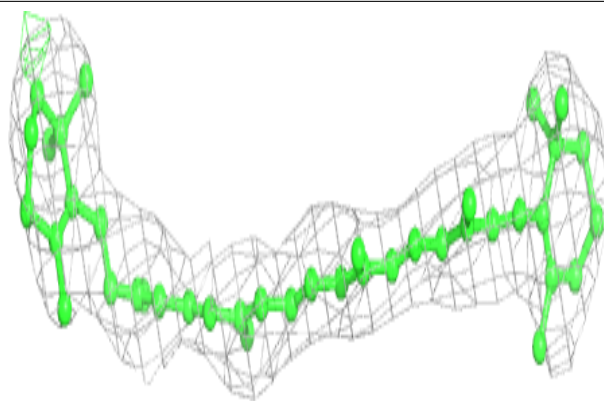
Electron density around CLA 6 307:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



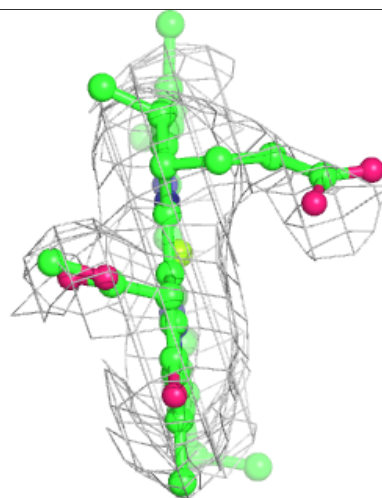
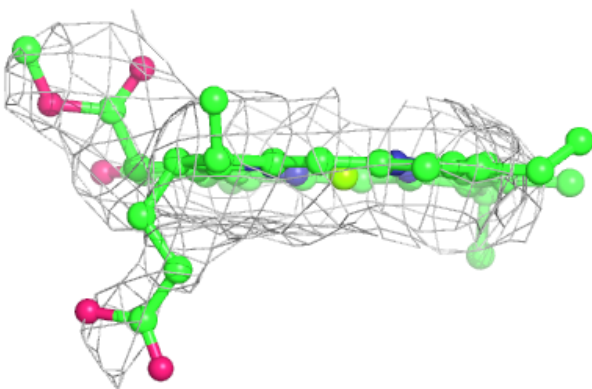
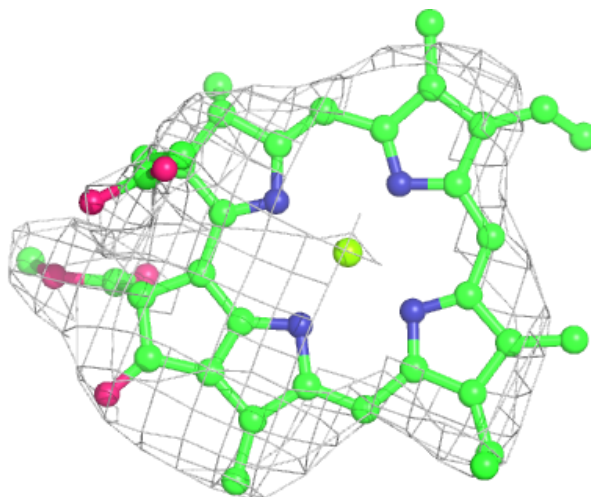
Electron density around BCR I 101:

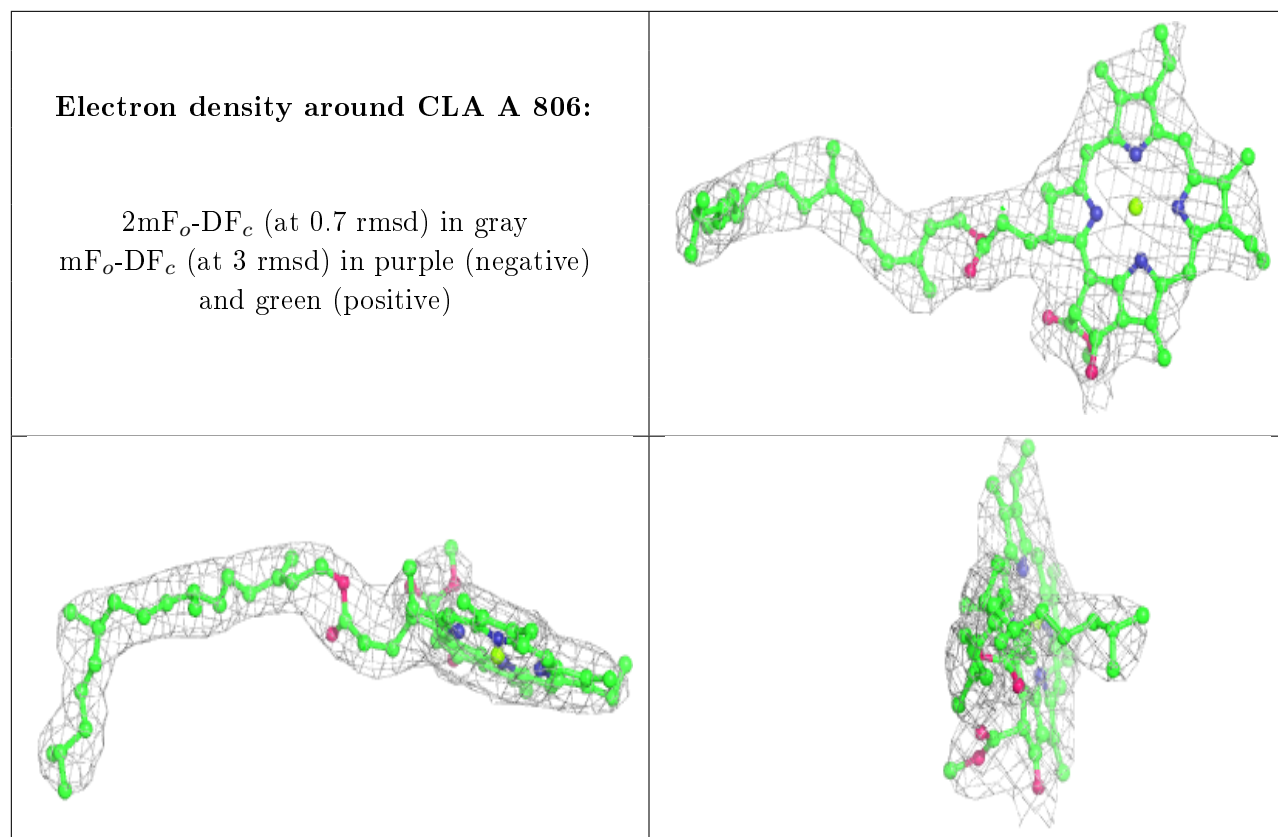
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 9 613:

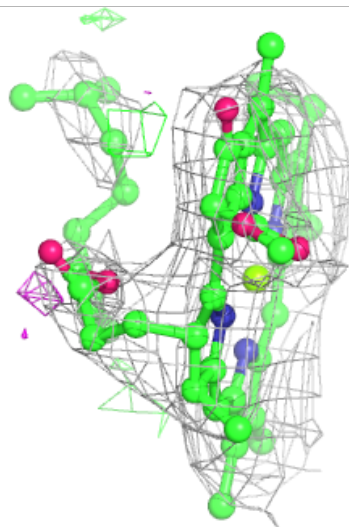
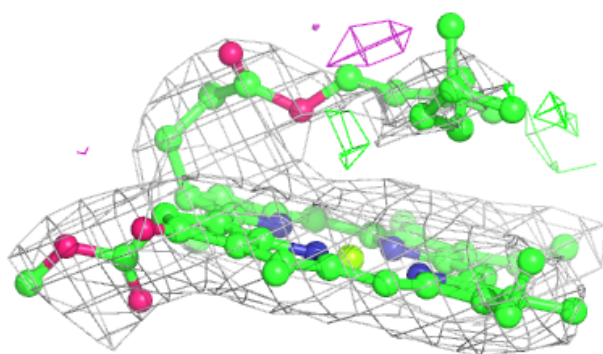
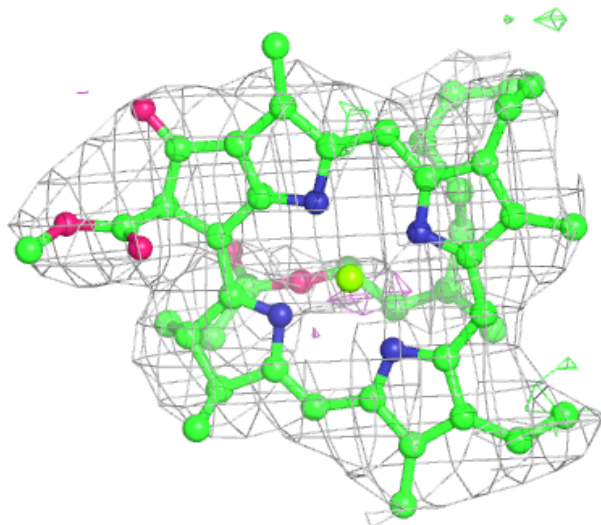
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





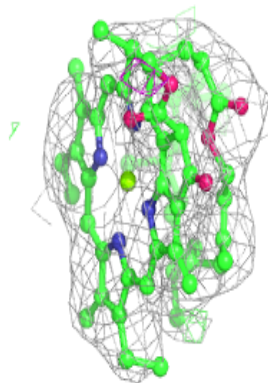
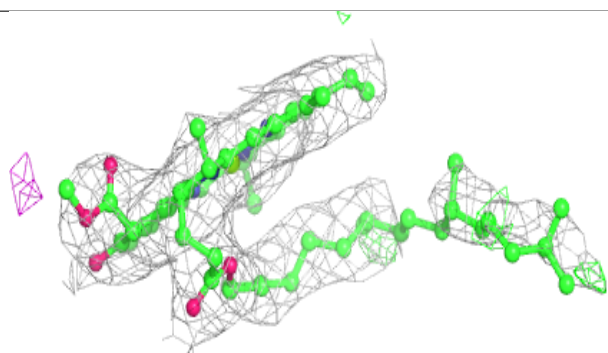
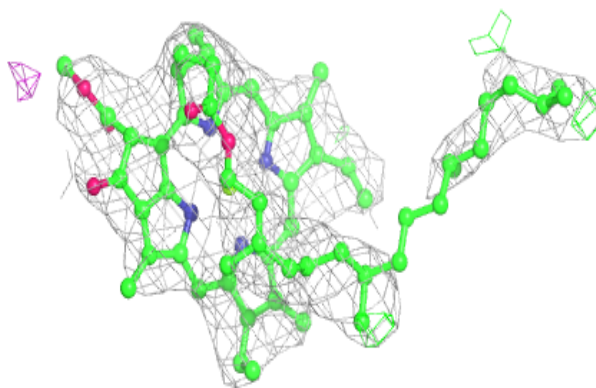
Electron density around CLA b 812:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

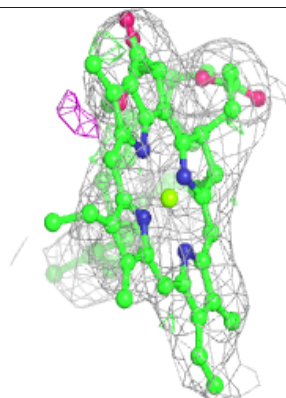
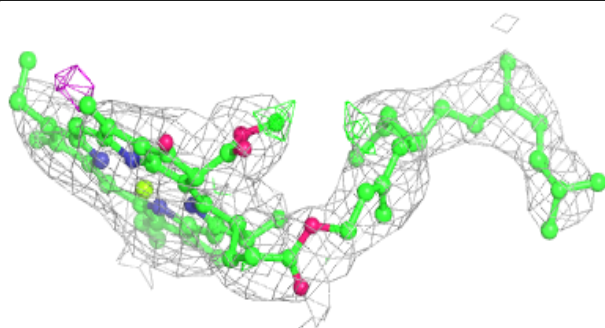
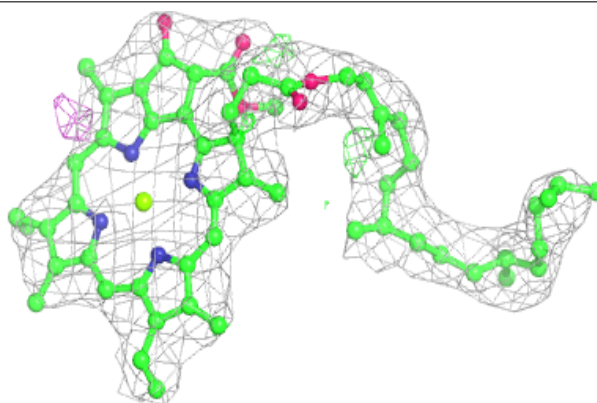


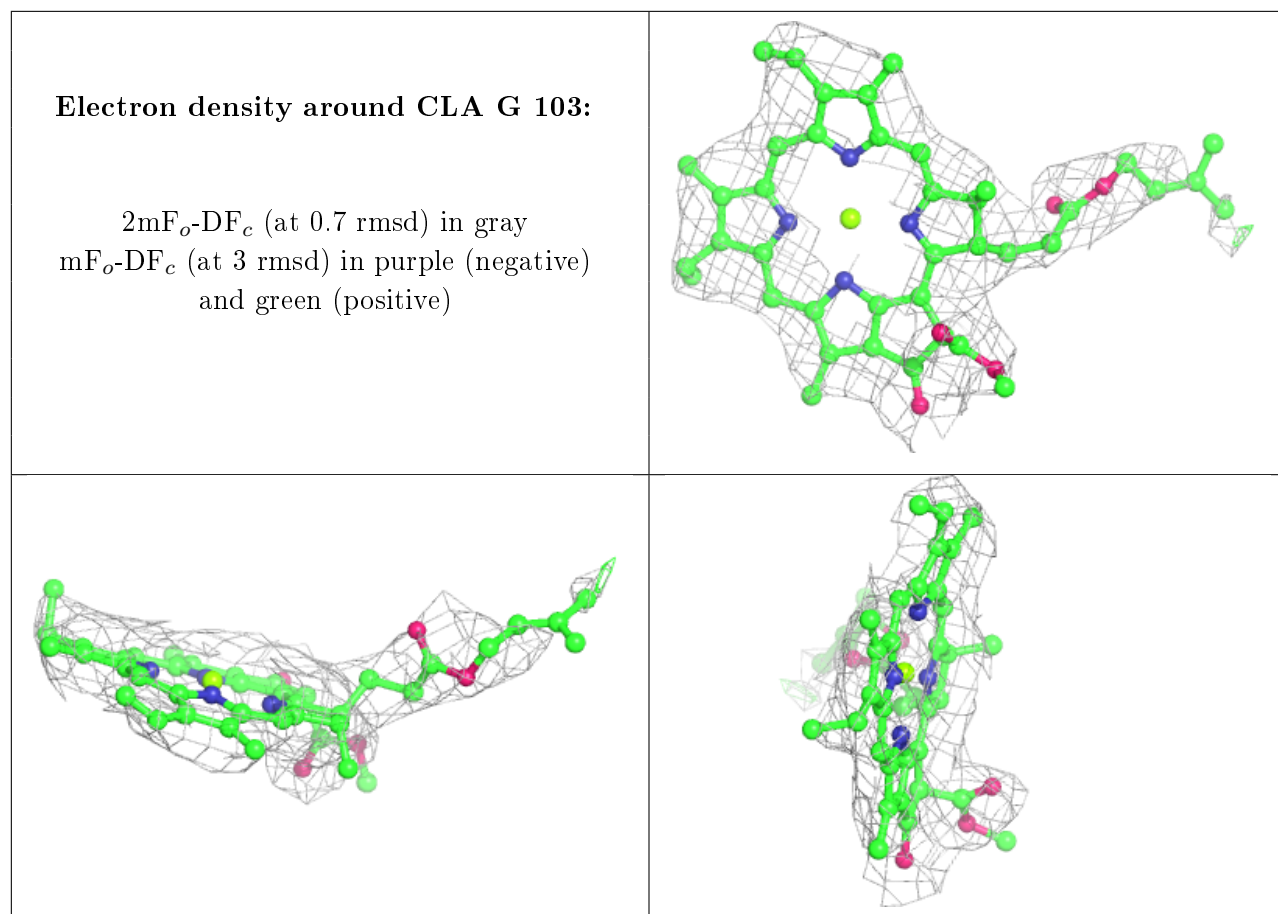
Electron density around CLA b 807:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CLA a 804:**

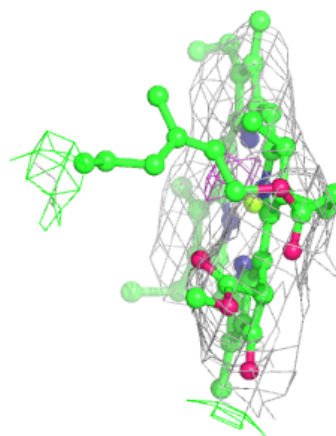
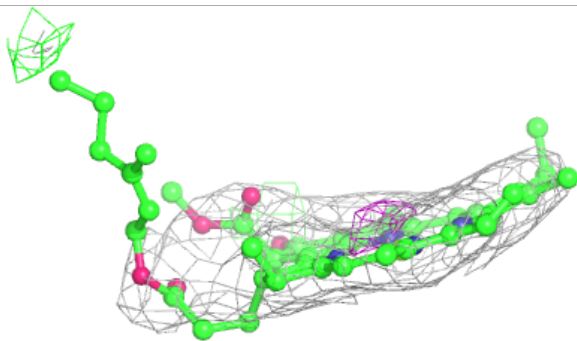
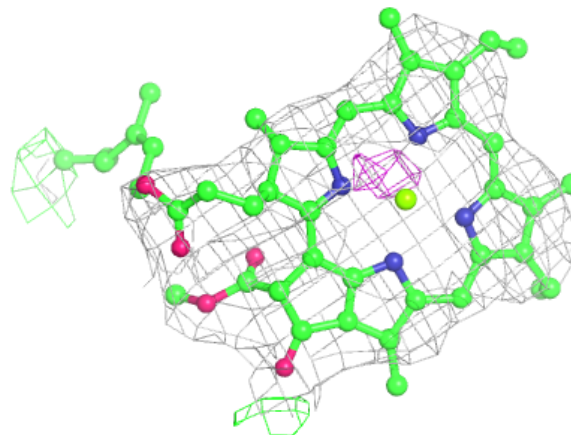
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





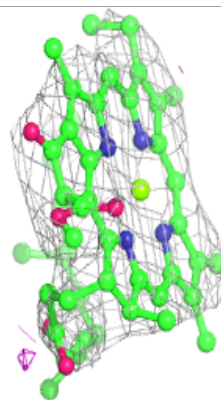
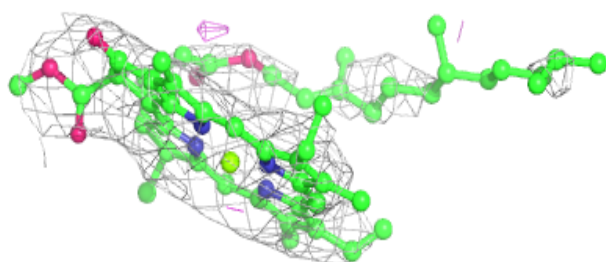
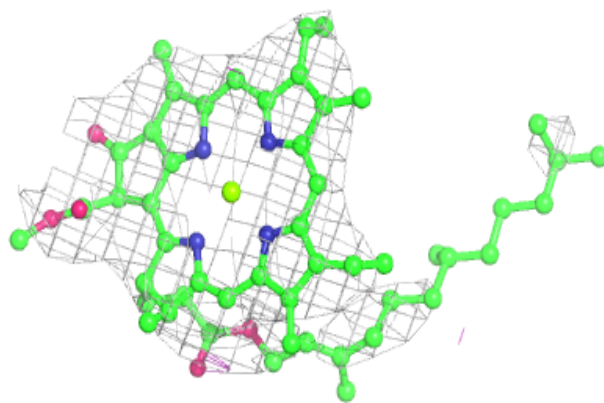
Electron density around CLA 7 611:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

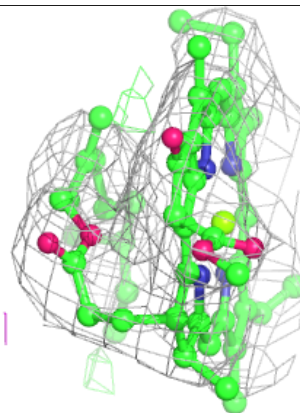
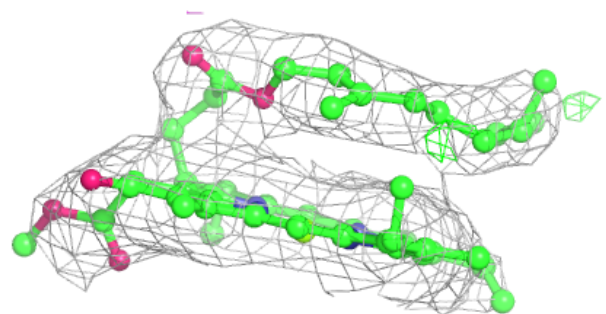
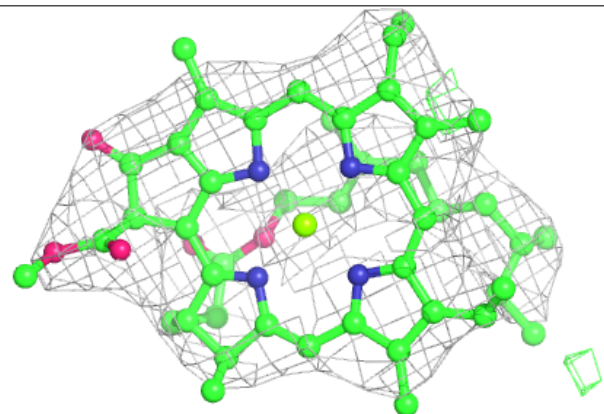


Electron density around CLA 9 609:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

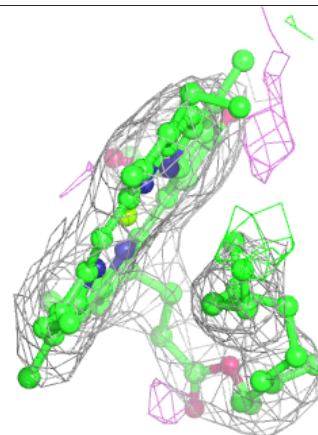
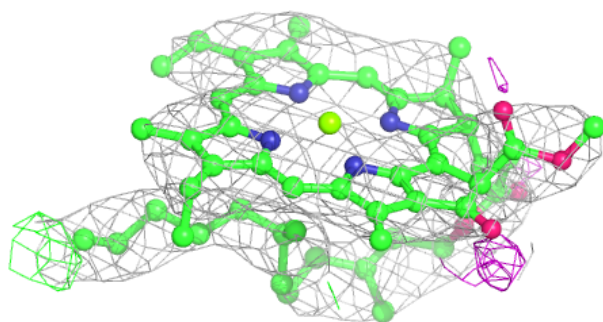
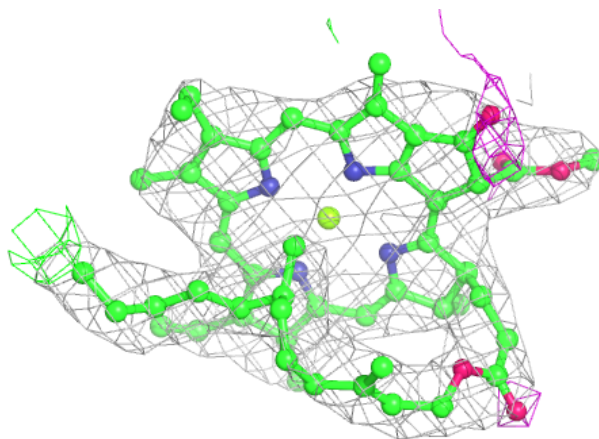
**Electron density around CLA 4 612:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



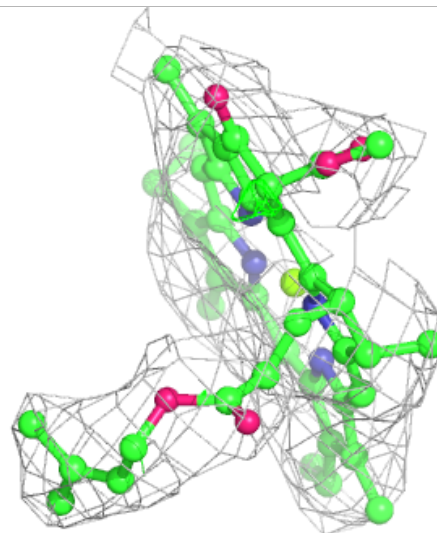
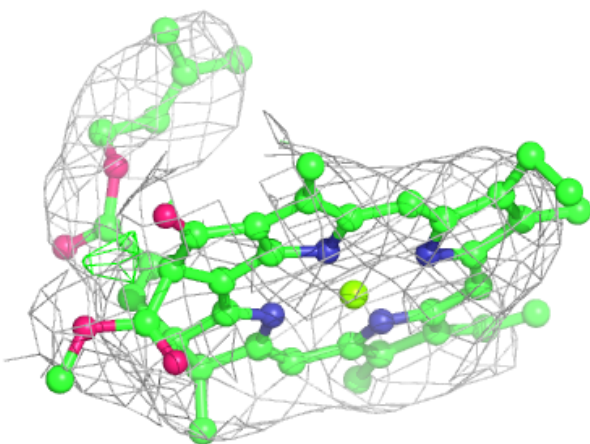
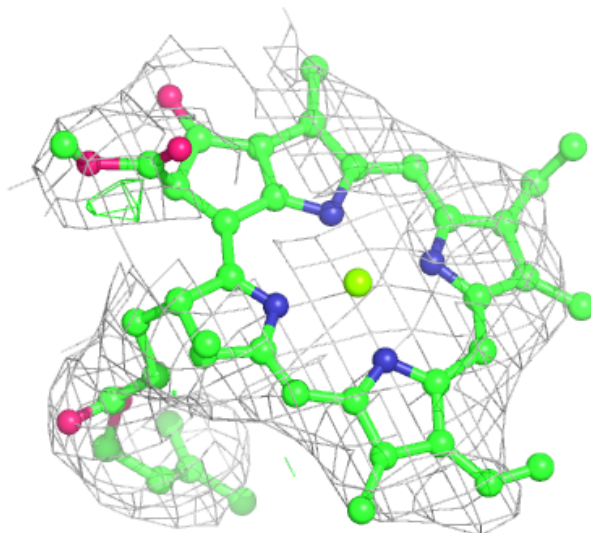
Electron density around CLA B 817:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



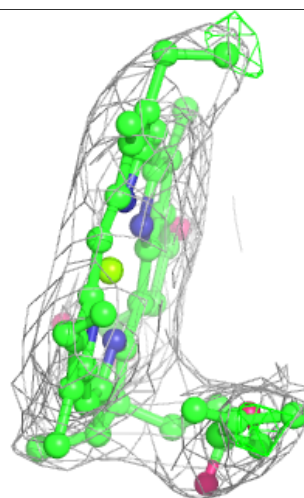
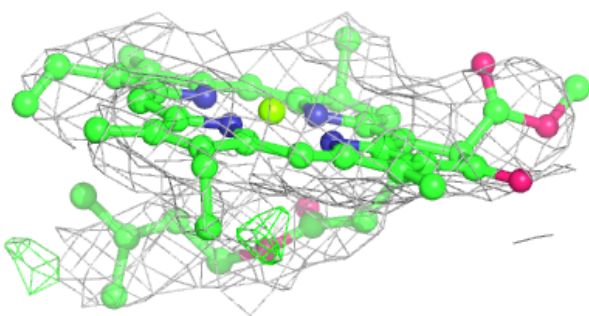
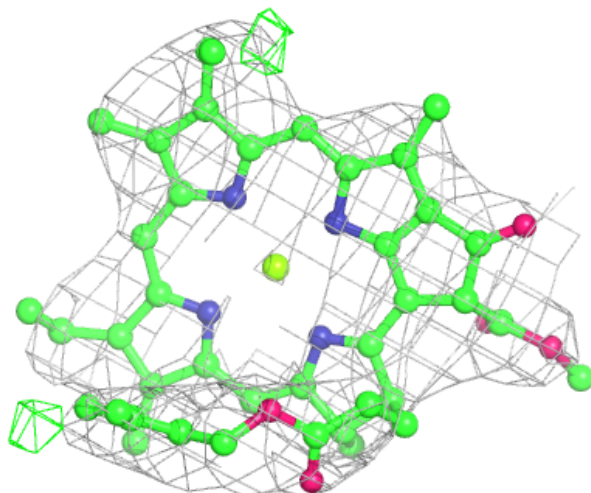
Electron density around CLA 7 608:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



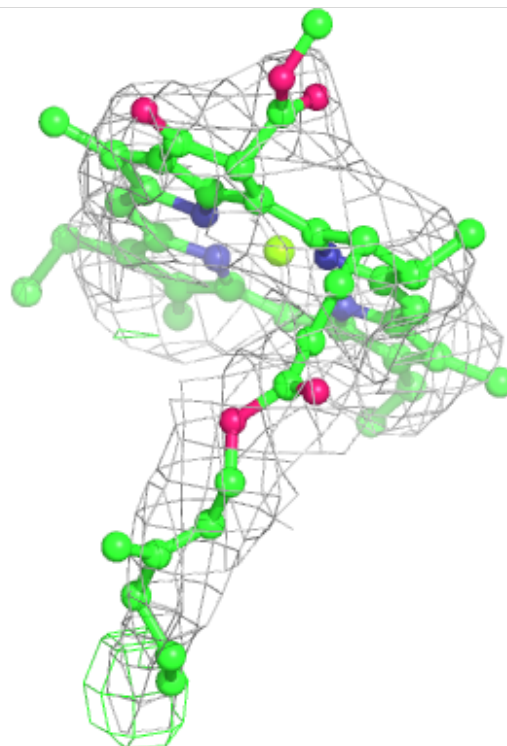
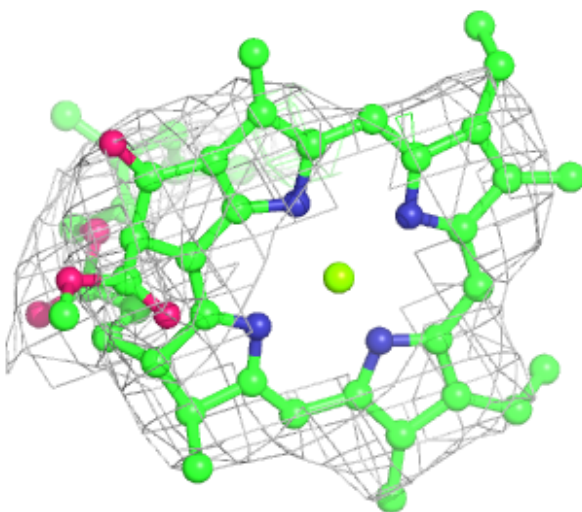
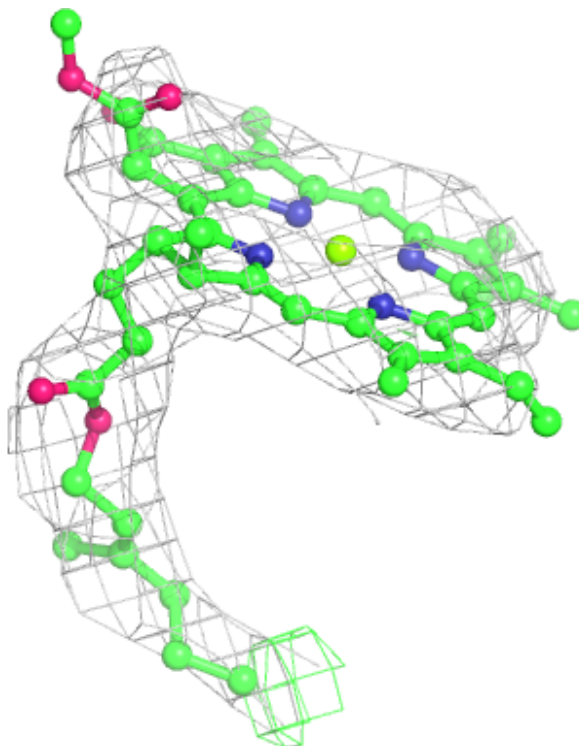
Electron density around CLA 3 309:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



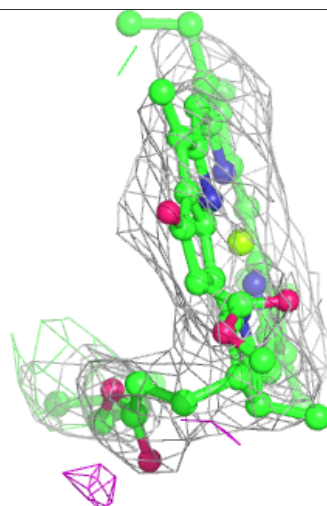
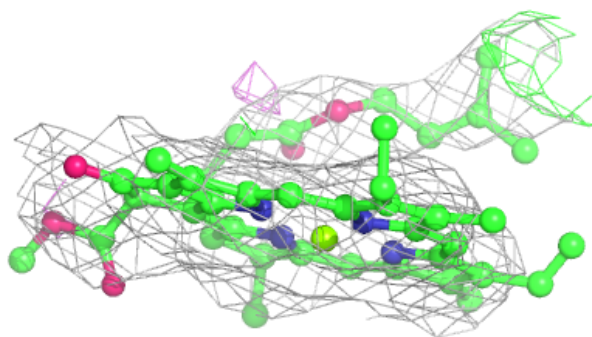
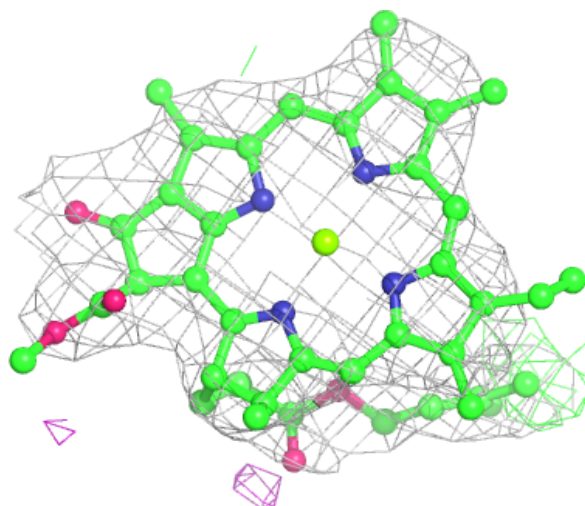
Electron density around CLA 1 305:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



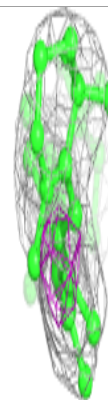
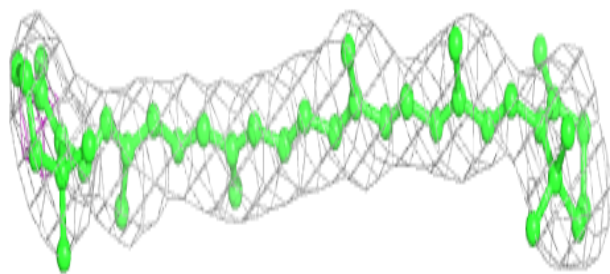
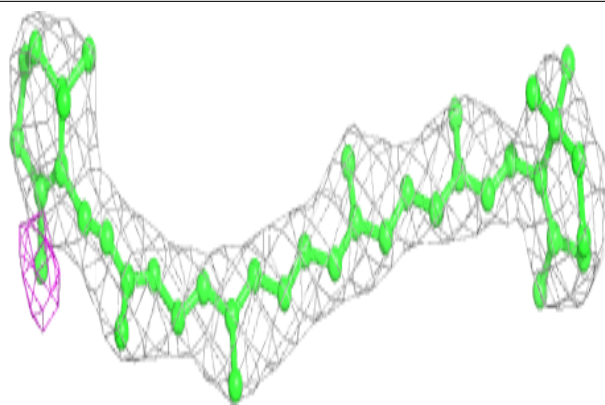
Electron density around CLA 8 308:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

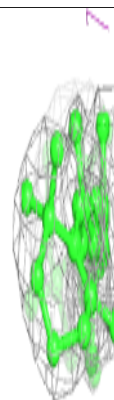
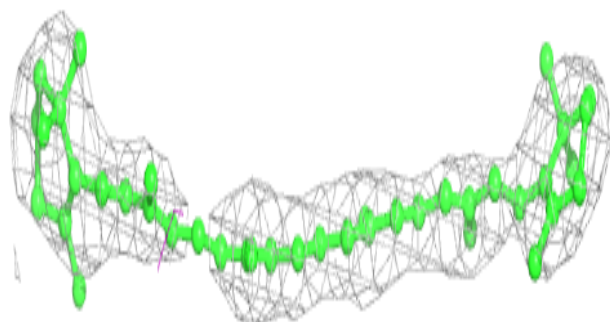
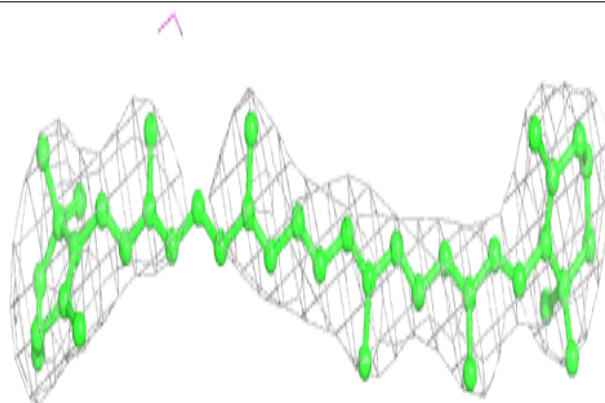


Electron density around BCR b 847:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

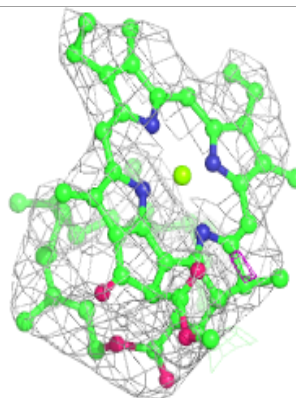
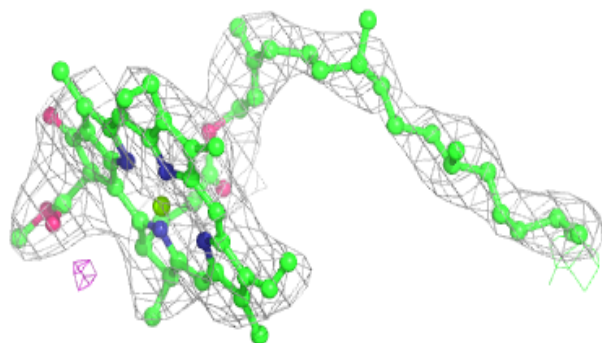
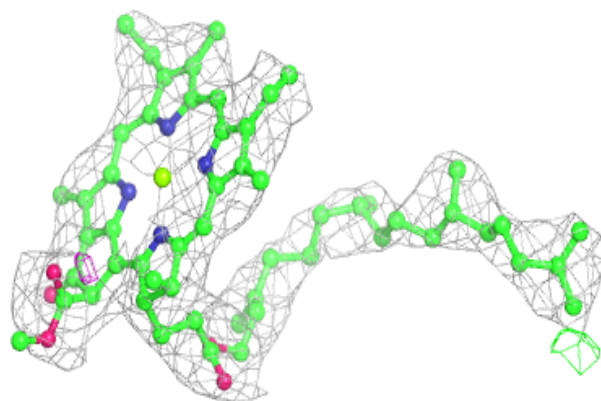
**Electron density around BCR B 843:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

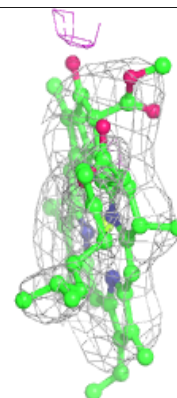
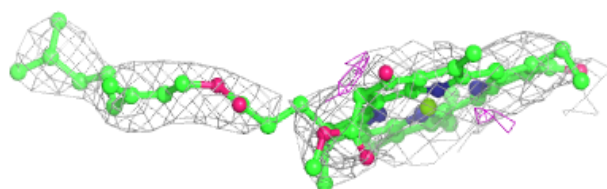
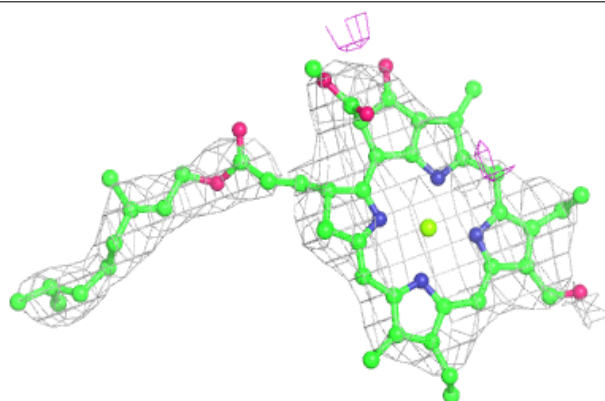


Electron density around CLA B 814:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

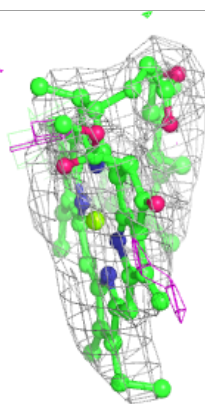
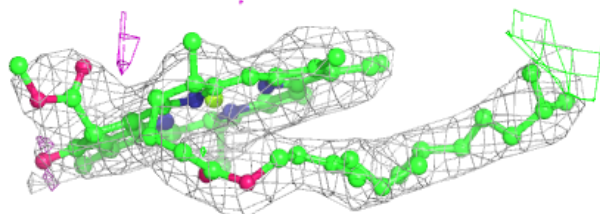
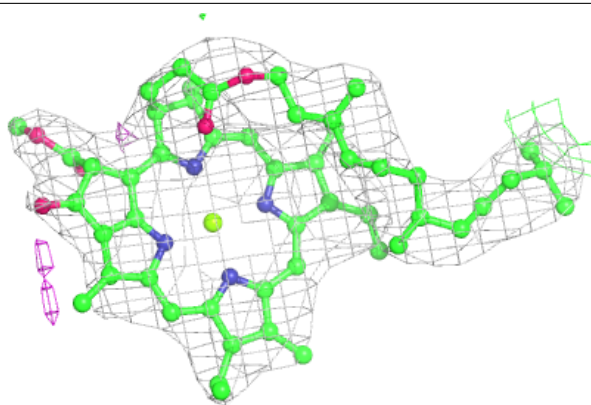
**Electron density around CHL 4 605:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

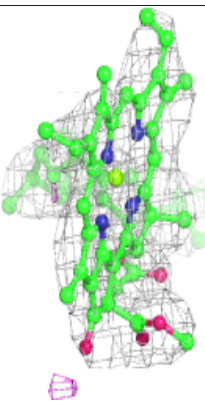
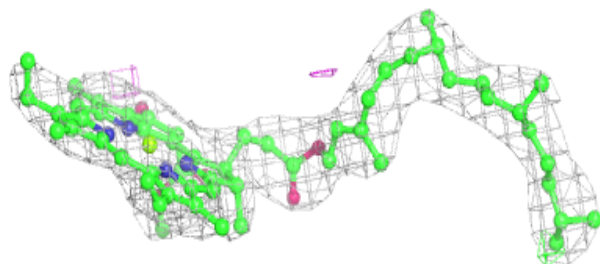
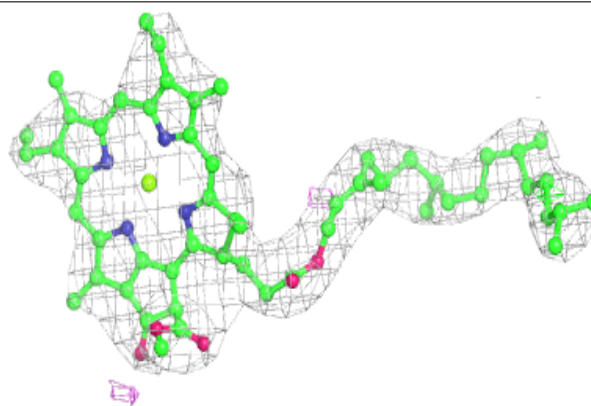


Electron density around CLA B 818:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

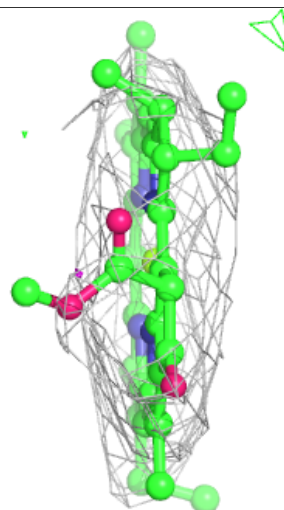
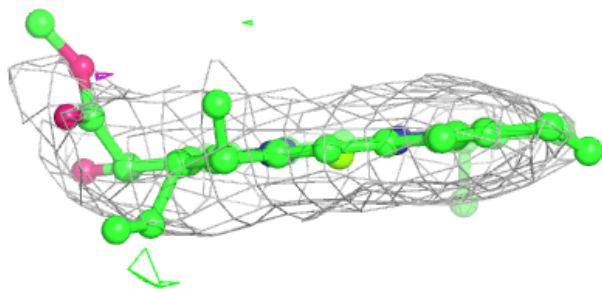
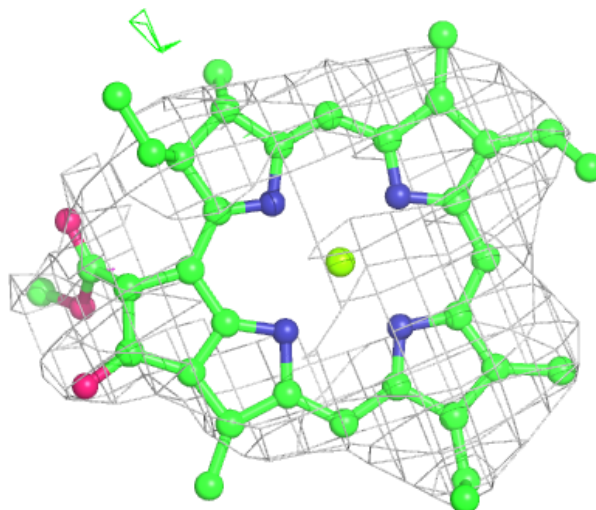
**Electron density around CLA B 813:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



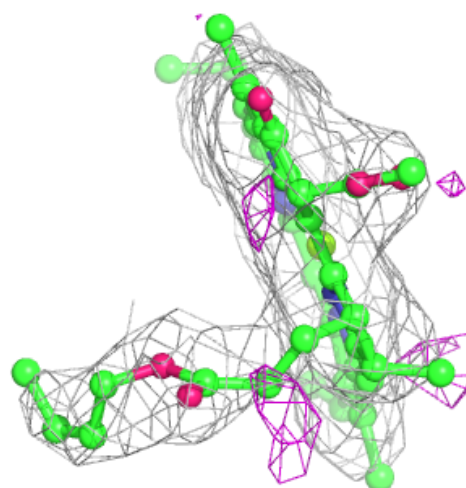
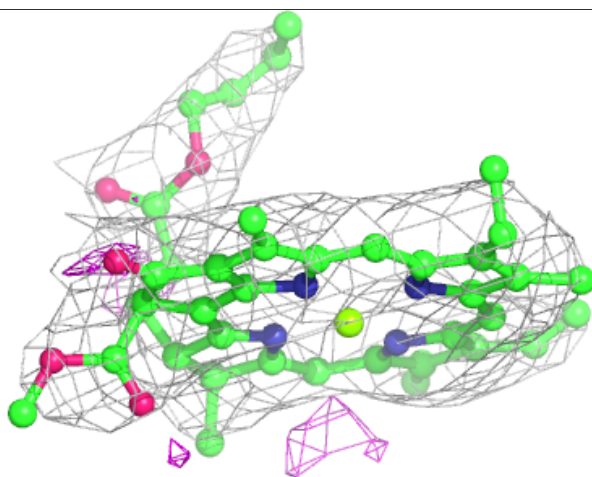
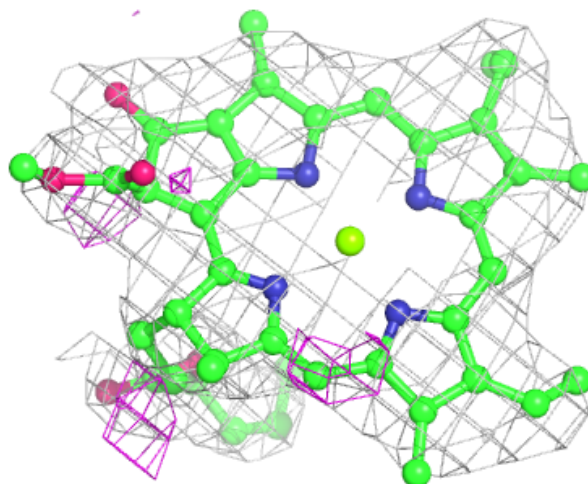
Electron density around CLA J 3002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



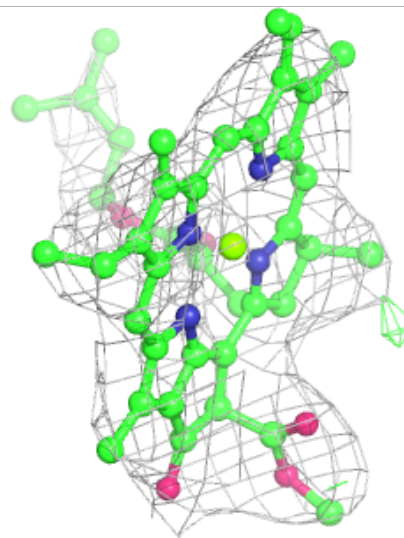
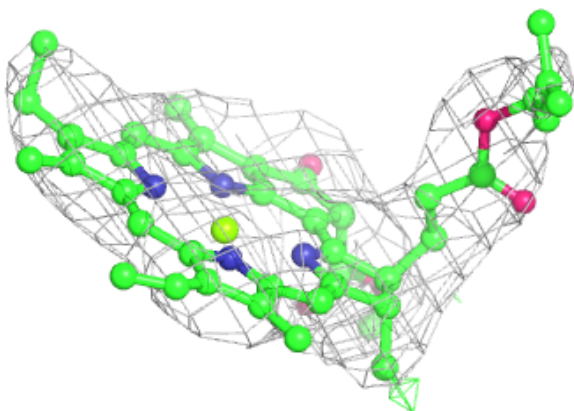
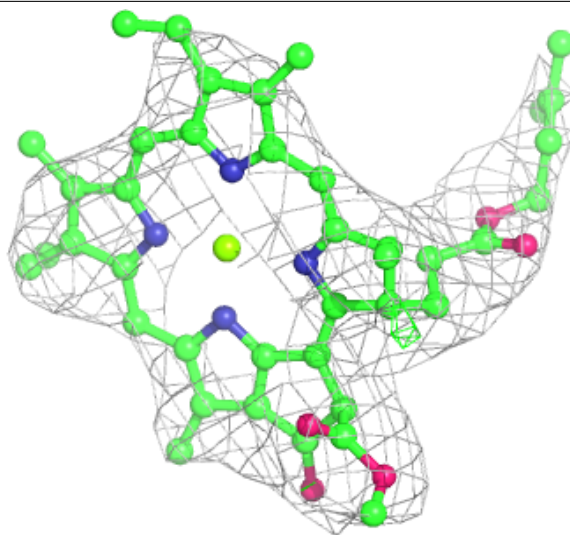
Electron density around CLA b 831:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



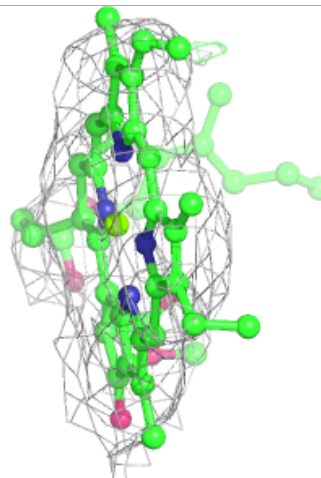
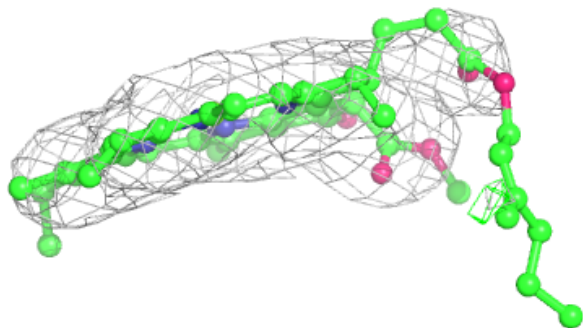
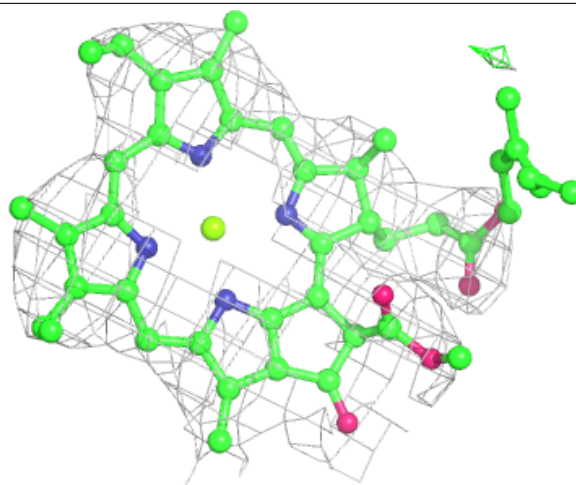
Electron density around CLA b 820:

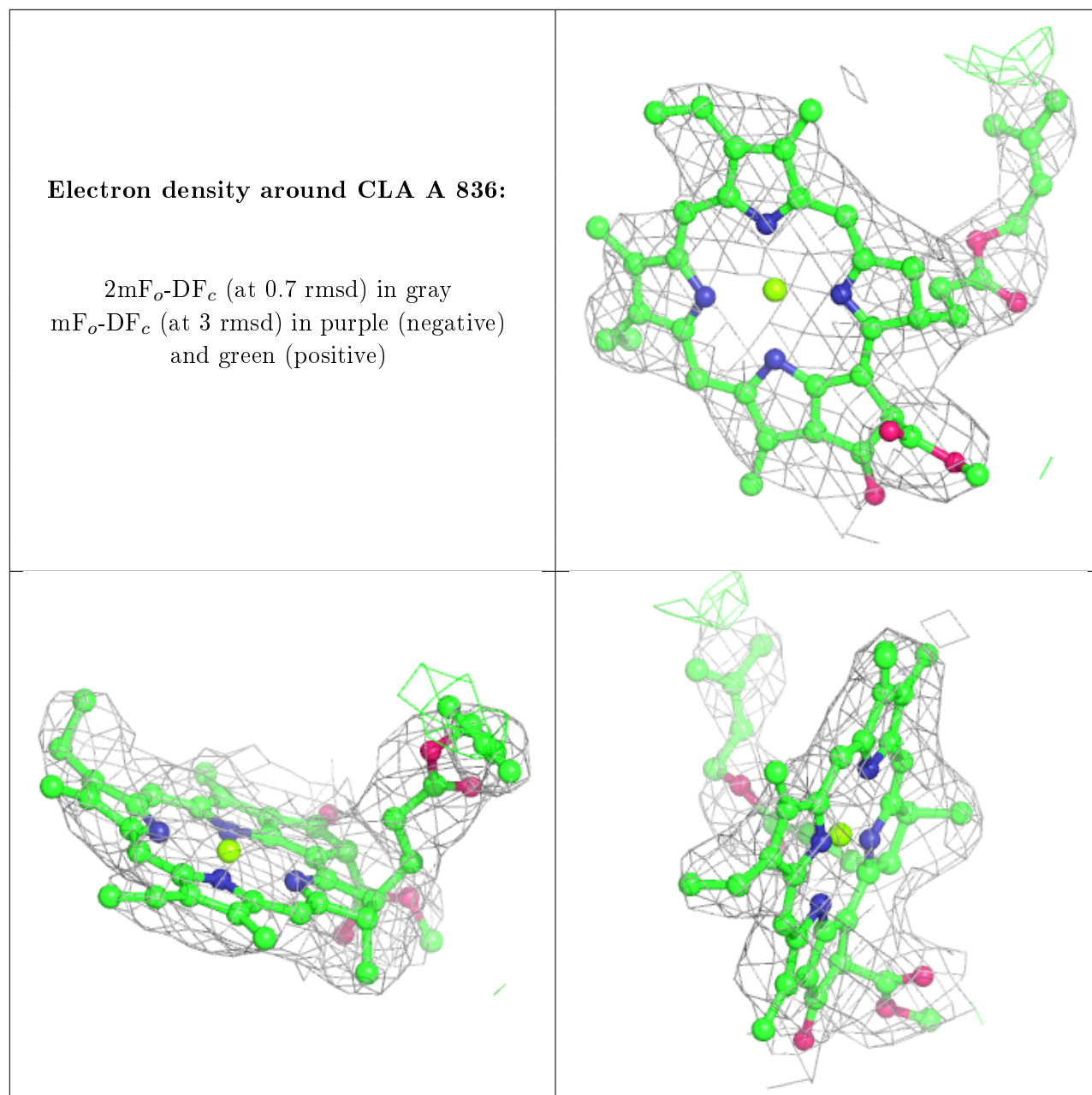
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 4 611:

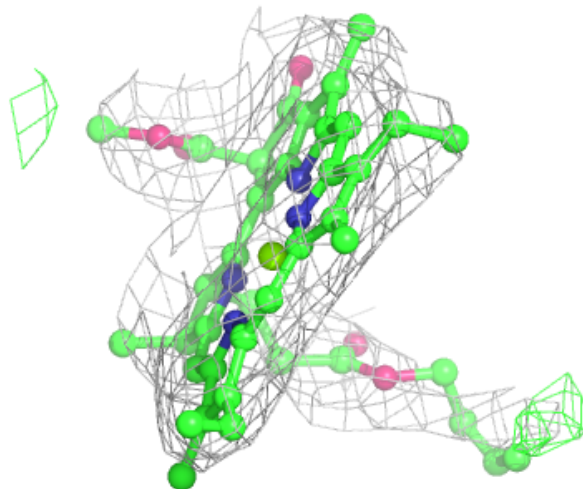
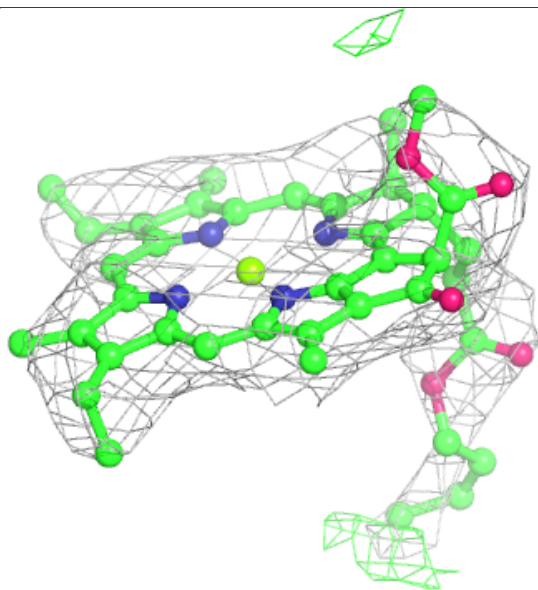
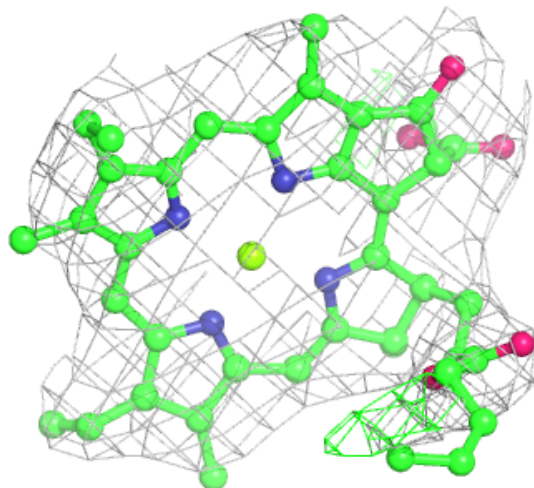
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





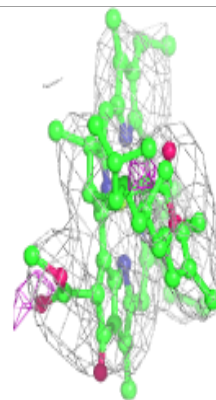
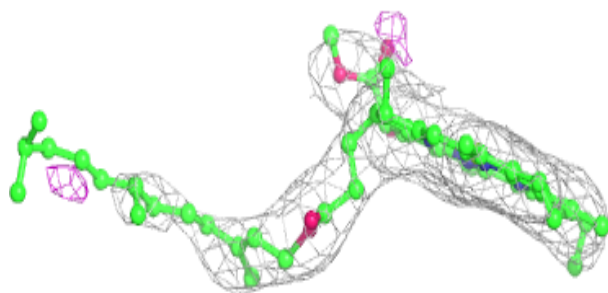
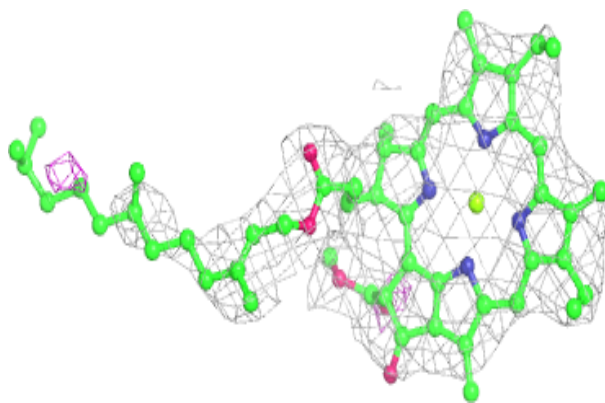
Electron density around CLA a 823:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

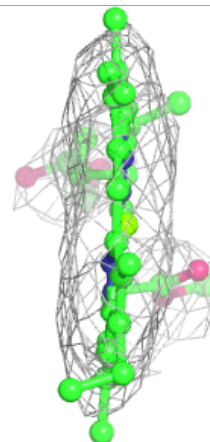
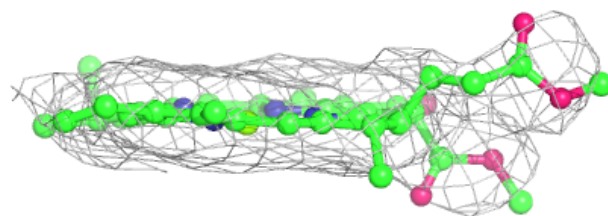
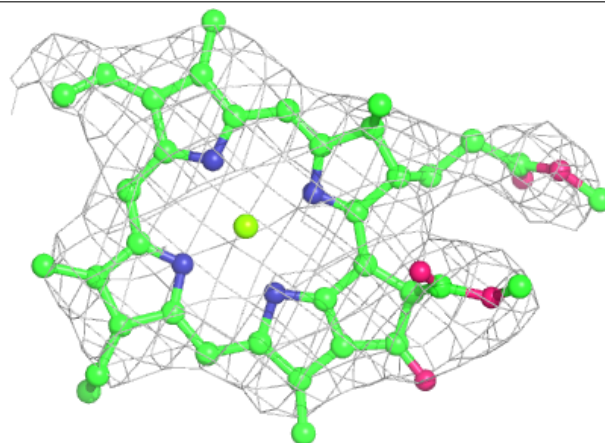


Electron density around CLA b 823:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

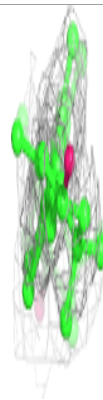
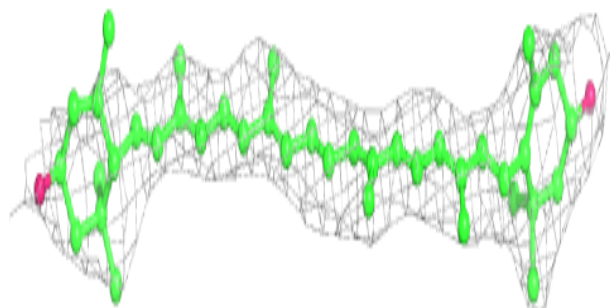
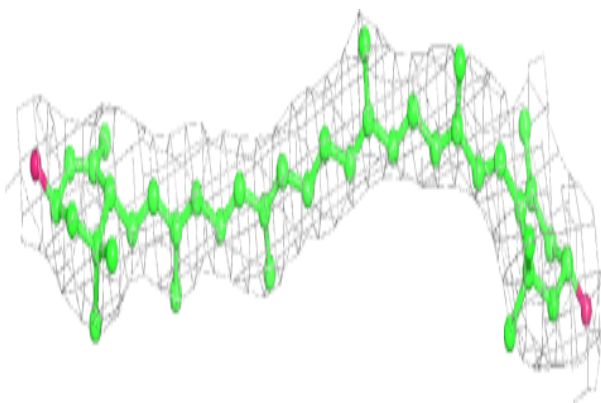
**Electron density around CLA 3 314:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

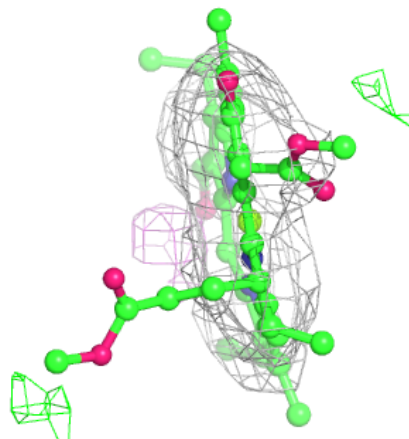
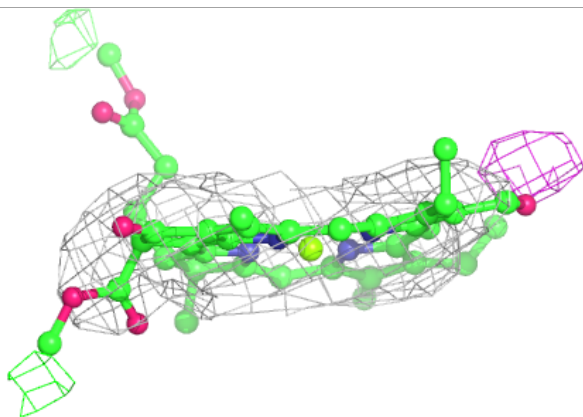
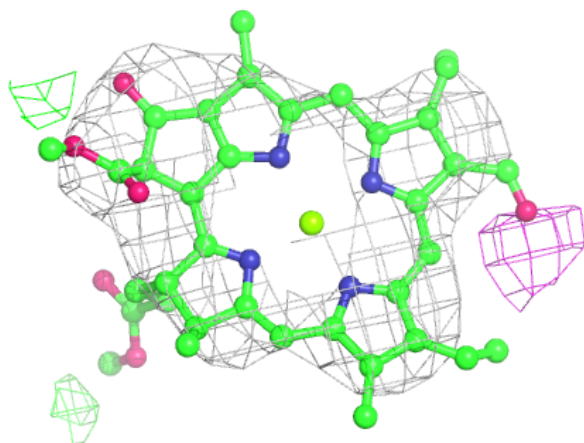


Electron density around LUT 3 316:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

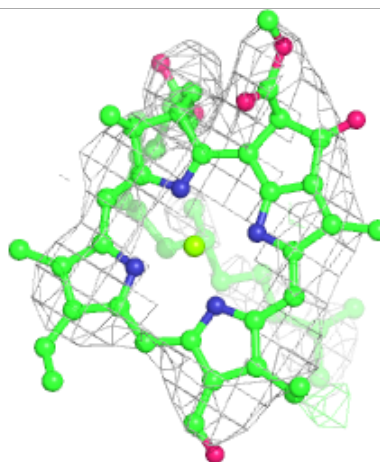
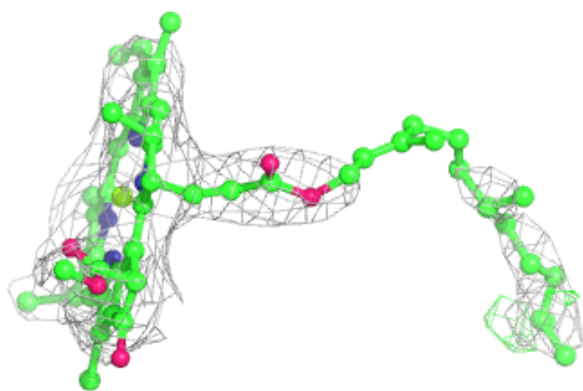
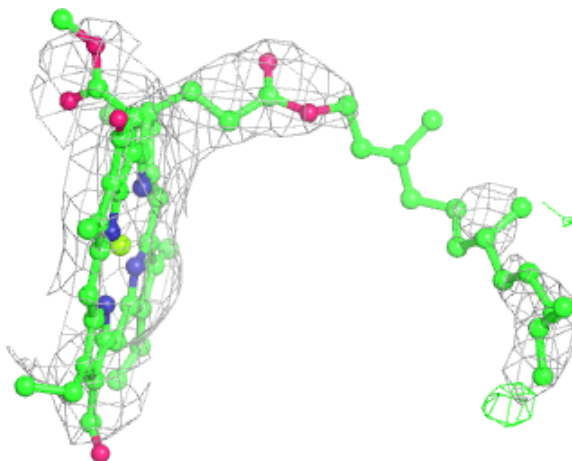
**Electron density around CHL 6 308:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



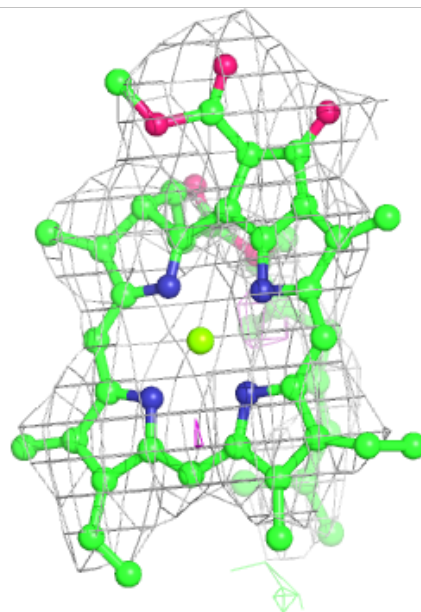
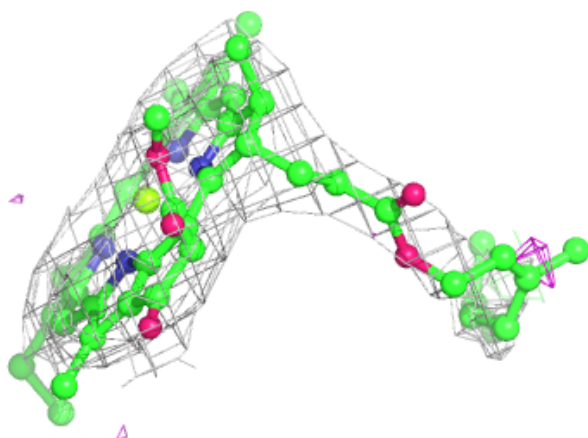
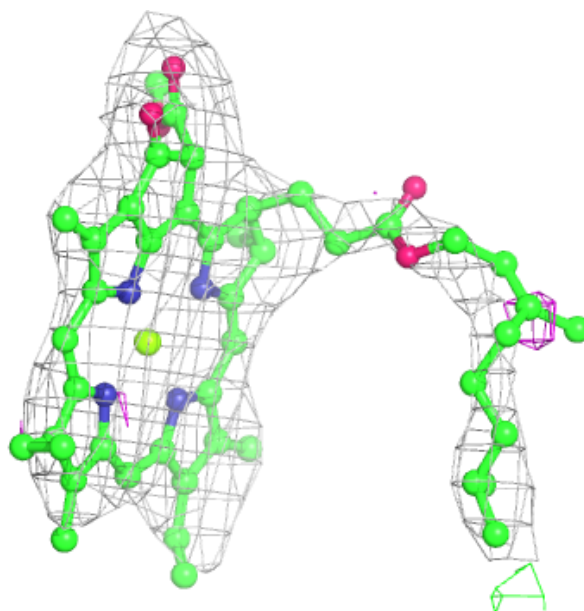
Electron density around CHL 2 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



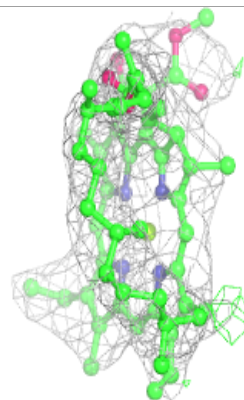
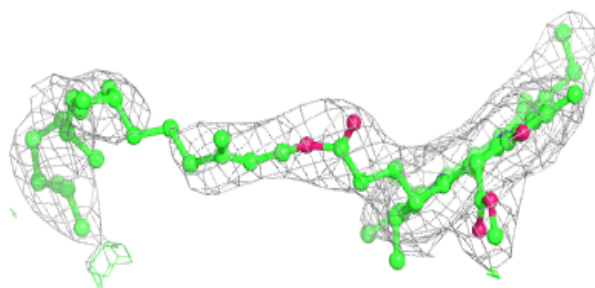
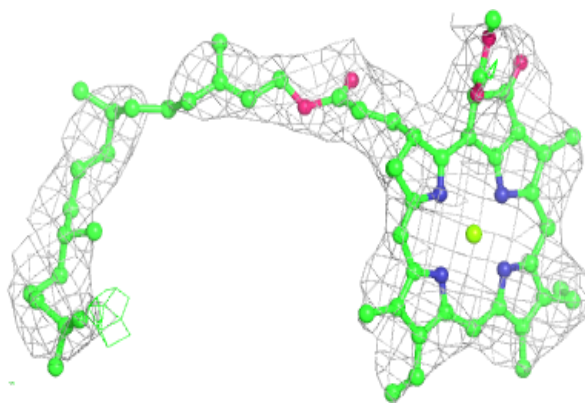
Electron density around CLA b 815:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

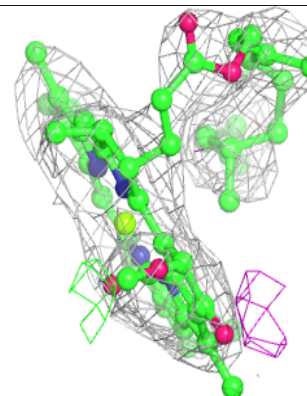
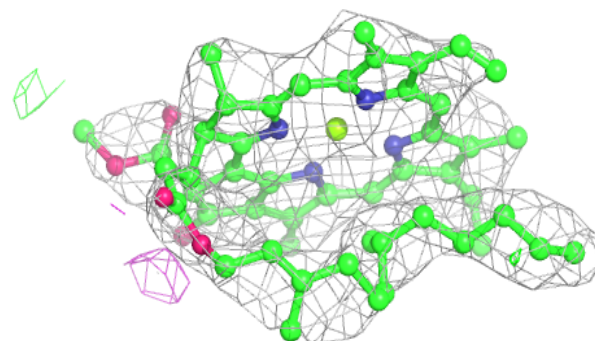
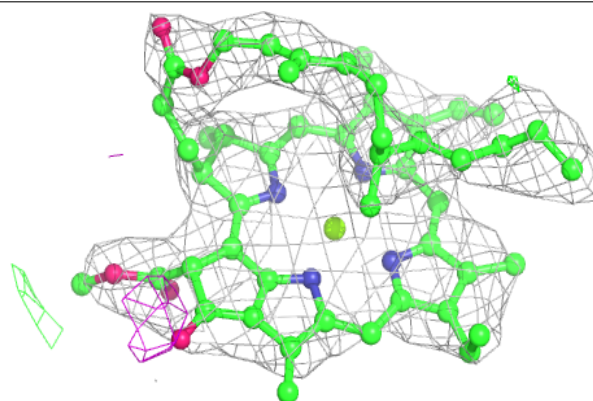


Electron density around CLA b 825:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

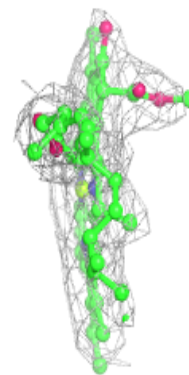
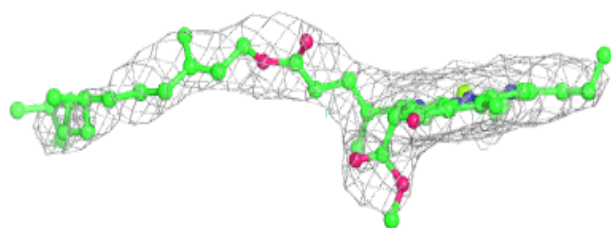
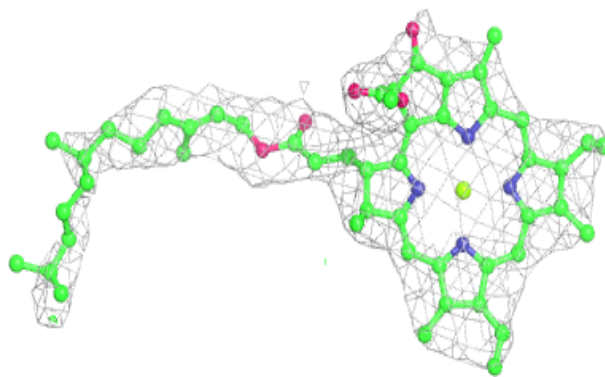
**Electron density around CLA b 817:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

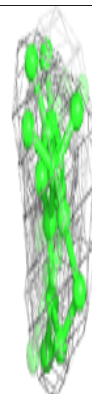
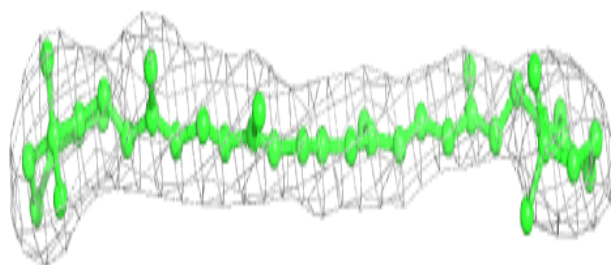
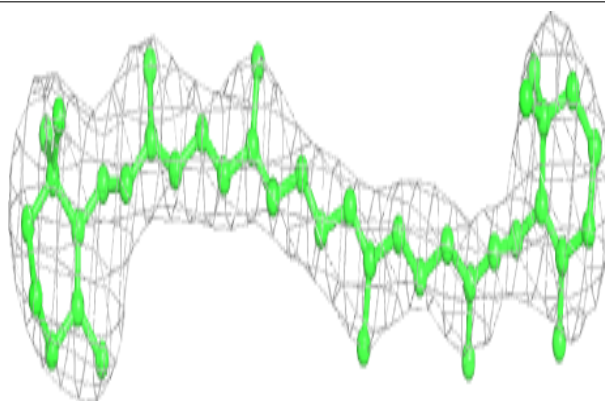


Electron density around CLA B 836:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

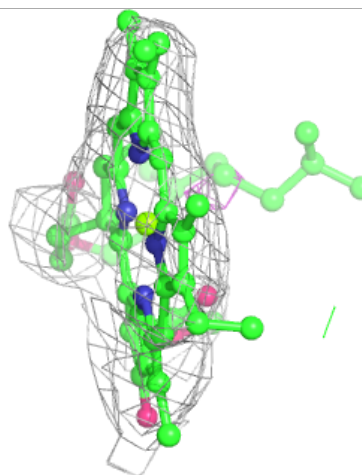
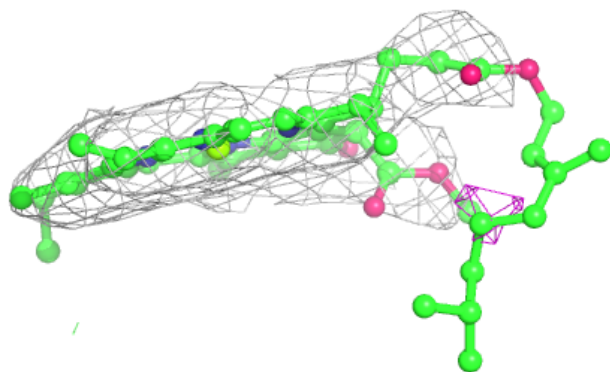
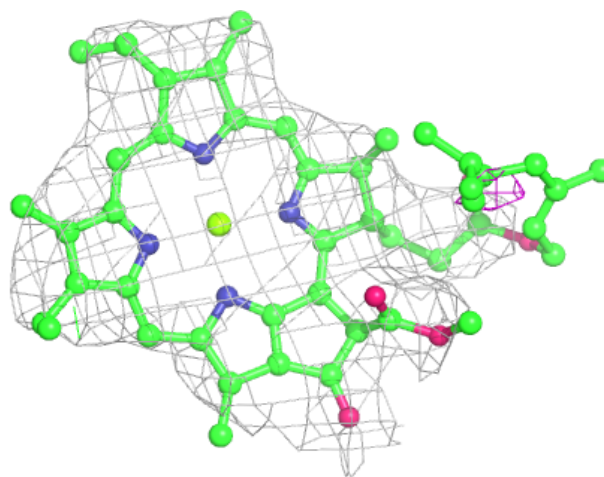
**Electron density around BCR L 205:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



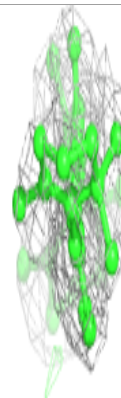
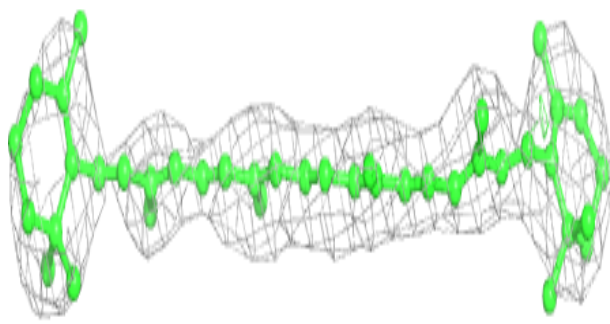
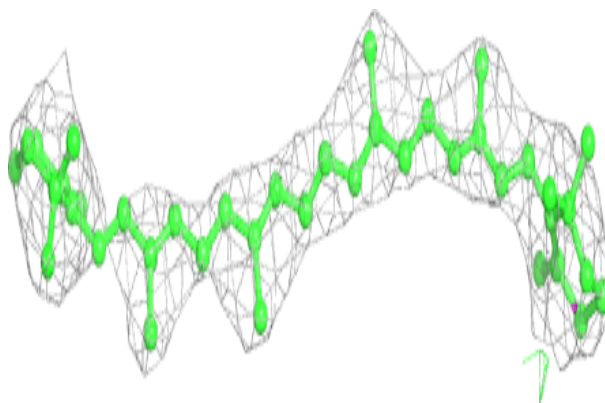
Electron density around CLA f 7003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

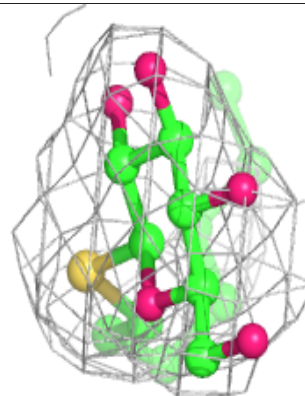
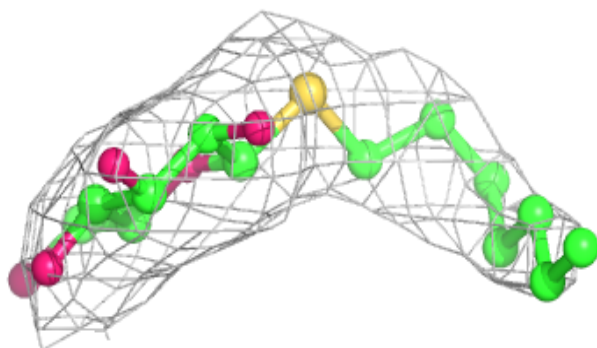
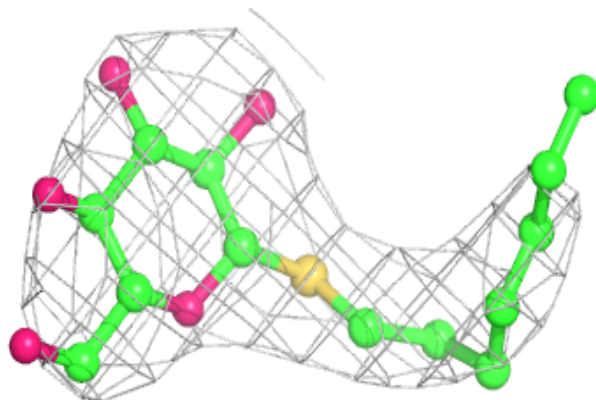


Electron density around BCR b 846:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

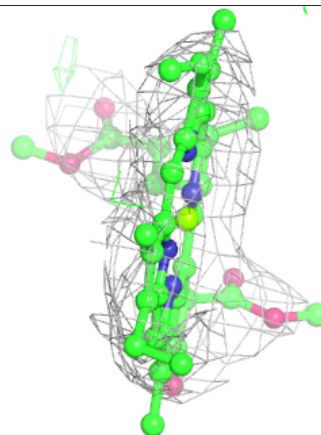
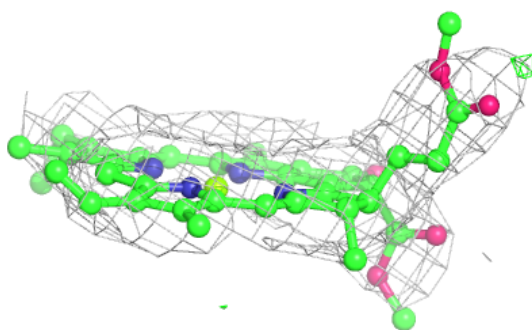
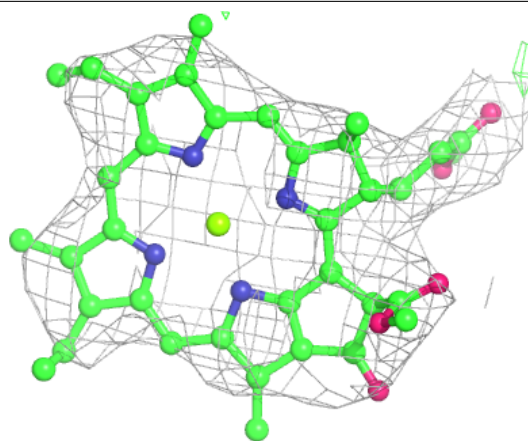
**Electron density around HTG j 3001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

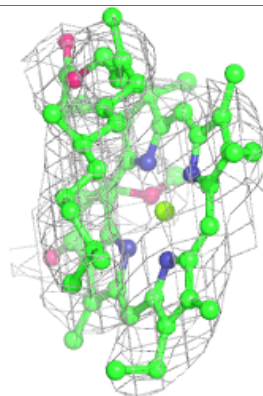
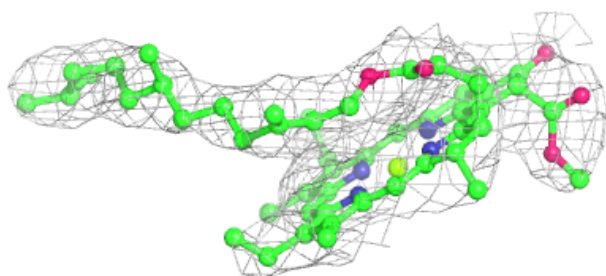
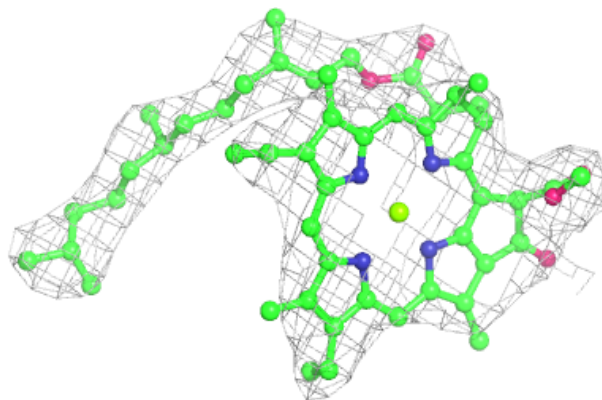


Electron density around CLA 4 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

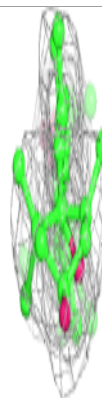
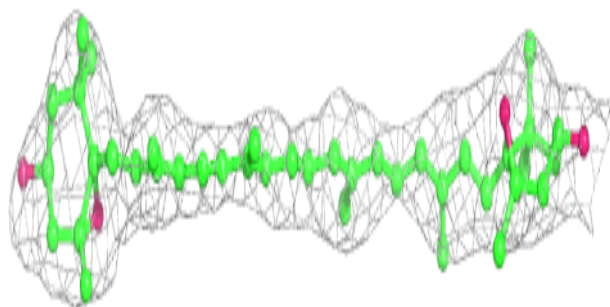
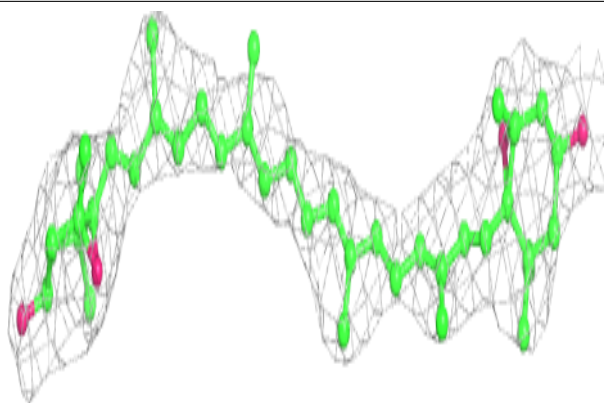
**Electron density around CLA 4 602:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

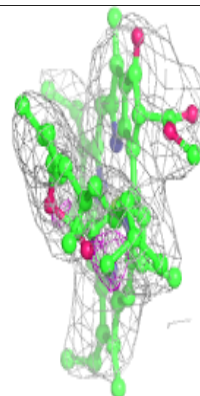
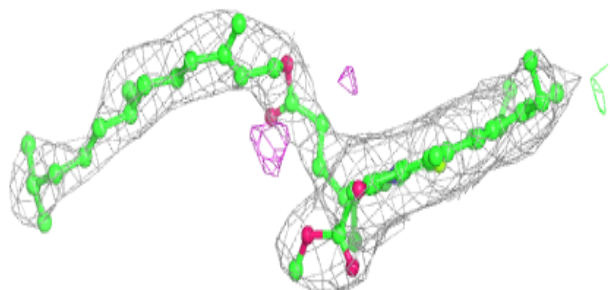
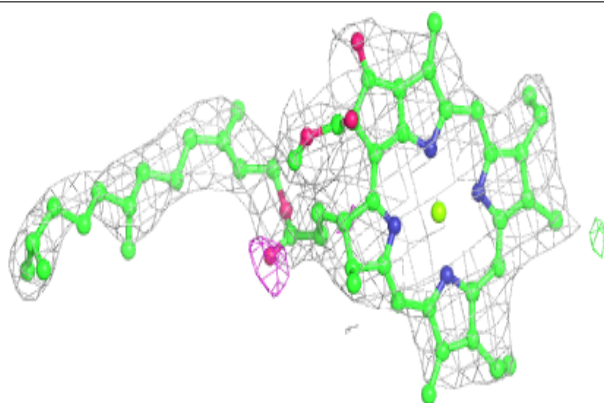


Electron density around XAT 2 616:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

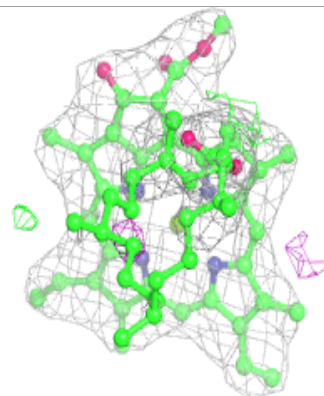
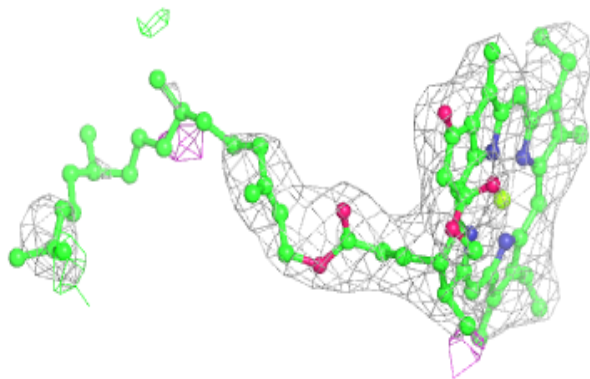
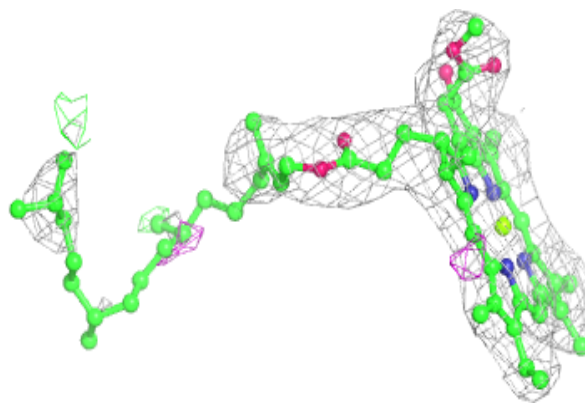
**Electron density around CLA B 823:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



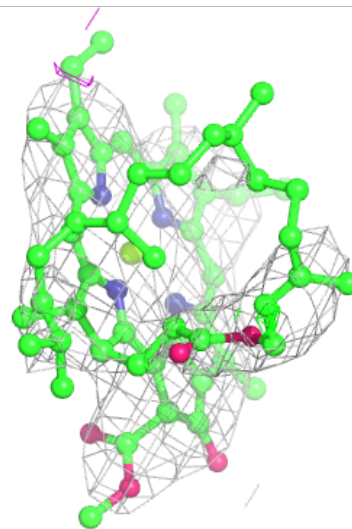
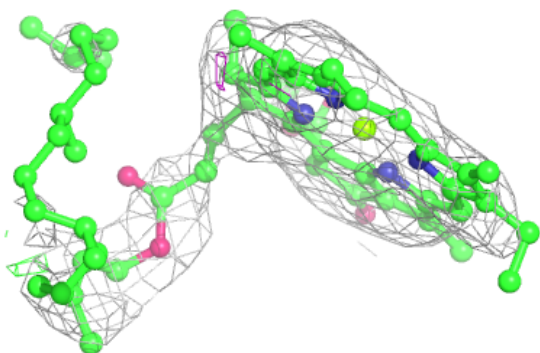
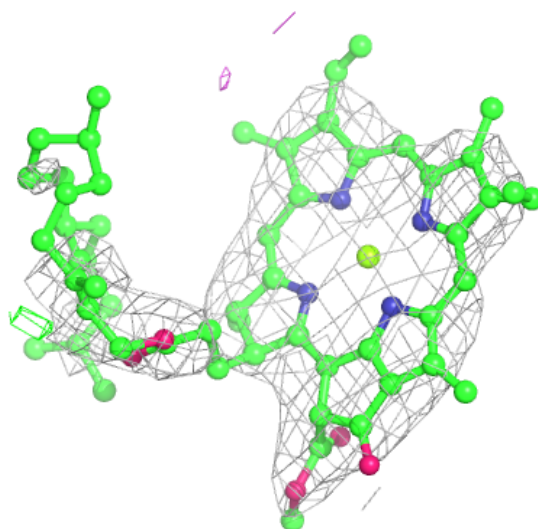
Electron density around CLA a 840:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



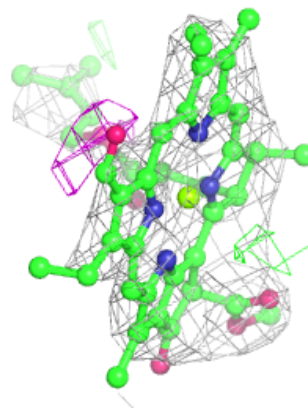
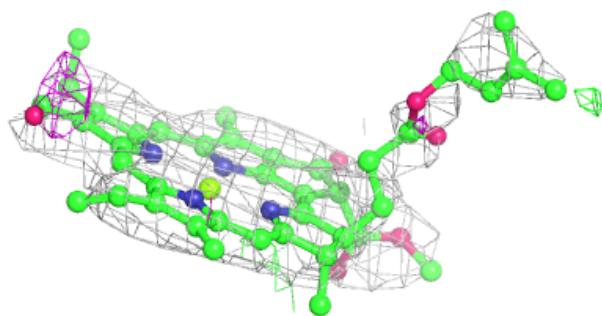
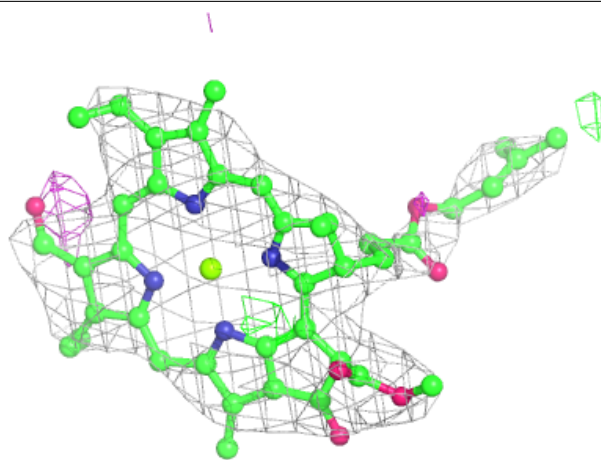
Electron density around CLA 1 308:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



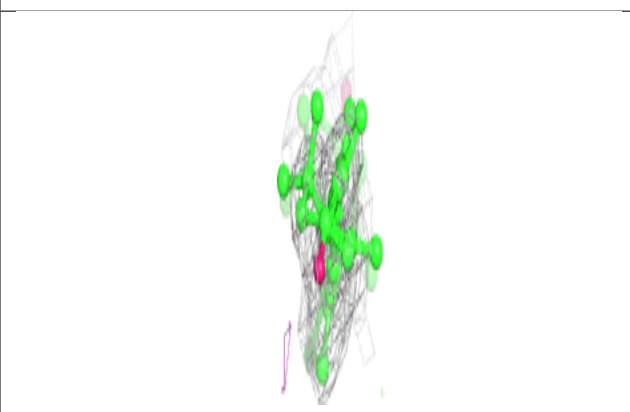
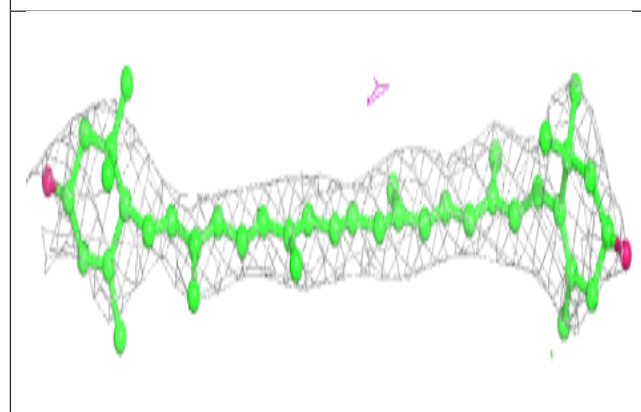
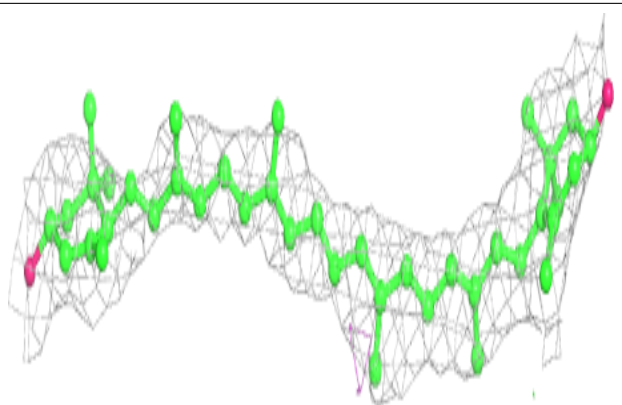
Electron density around CHL 9 607:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

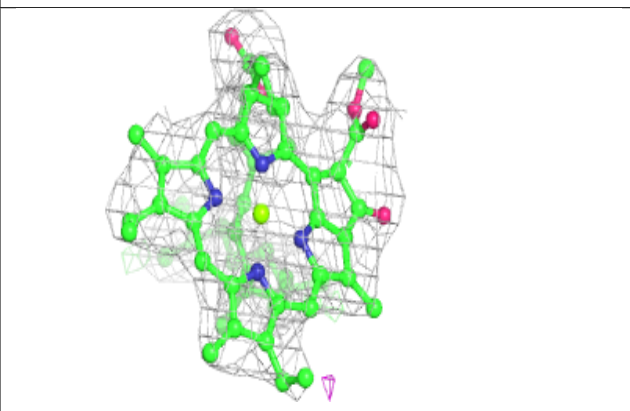
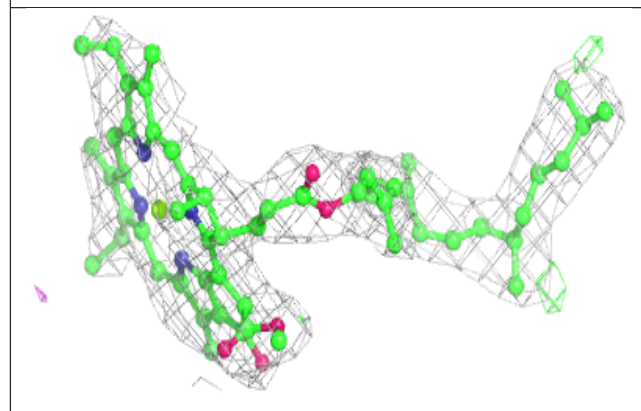
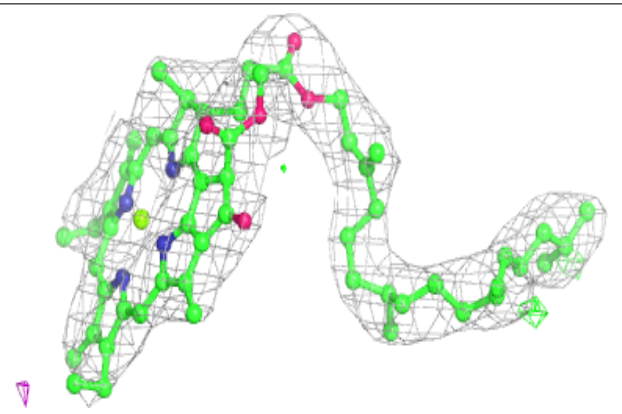


Electron density around LUT 8 314:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

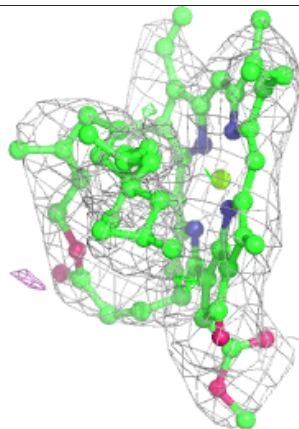
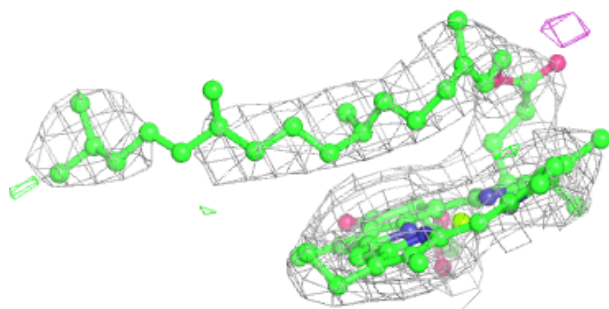
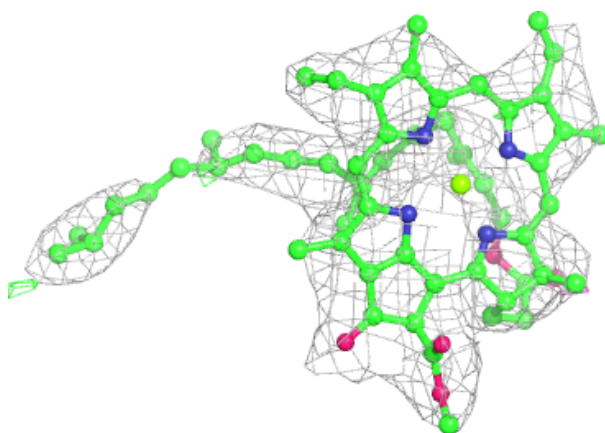
**Electron density around CLA B 802:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



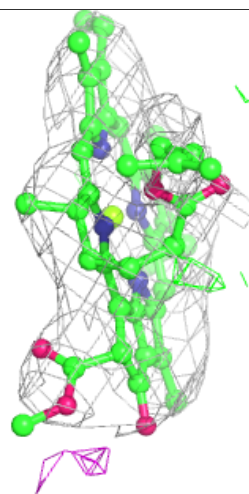
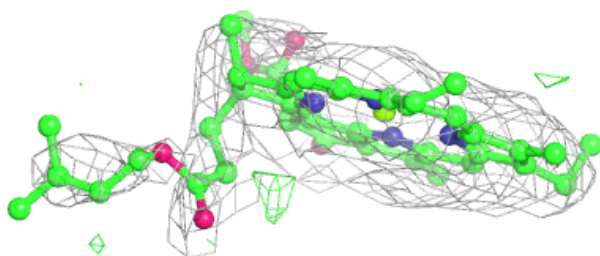
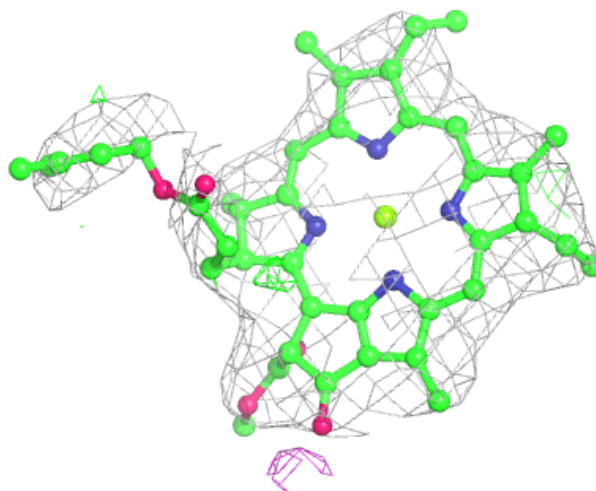
Electron density around CLA B 827:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



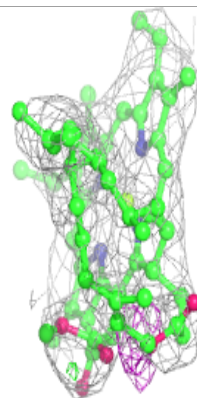
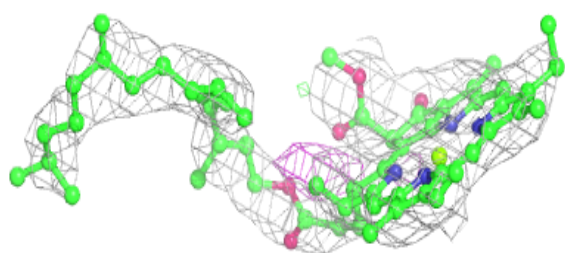
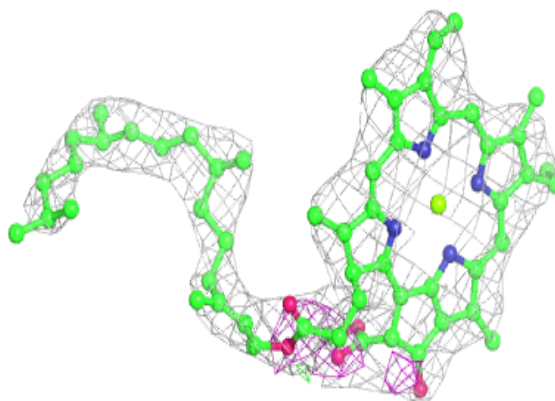
Electron density around CLA L 204:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

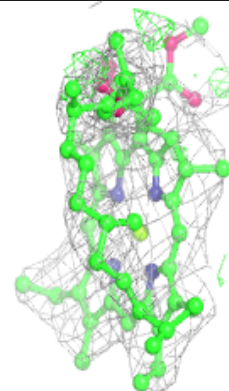
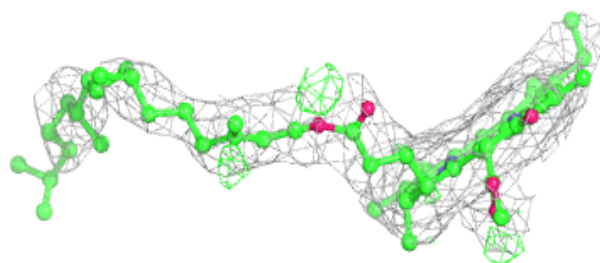
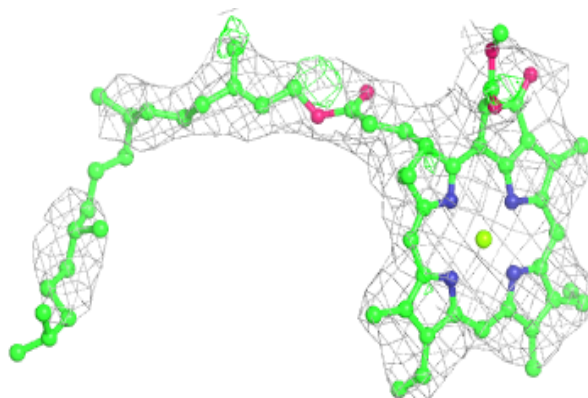


Electron density around CLA A 804:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

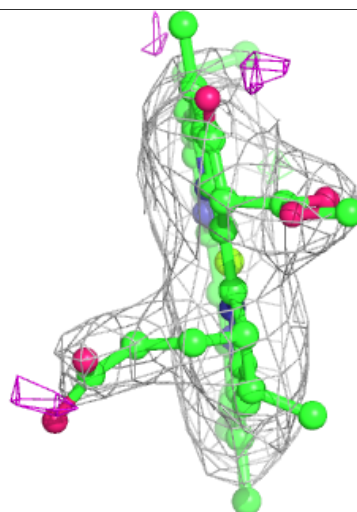
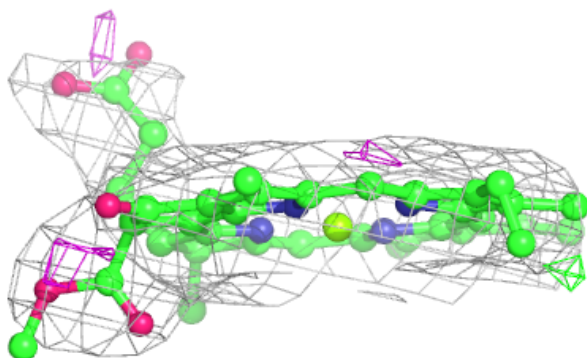
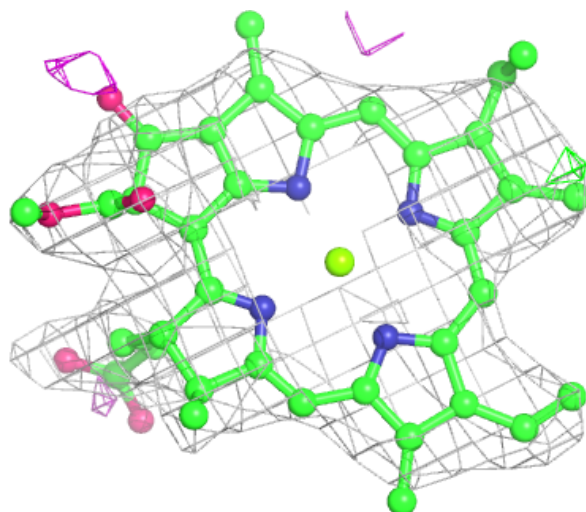
**Electron density around CLA B 825:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



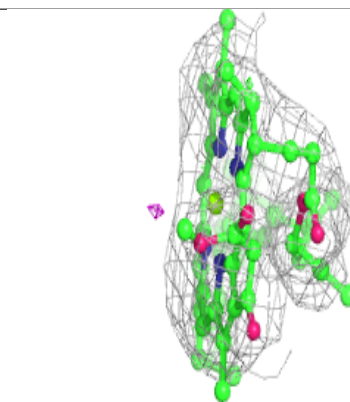
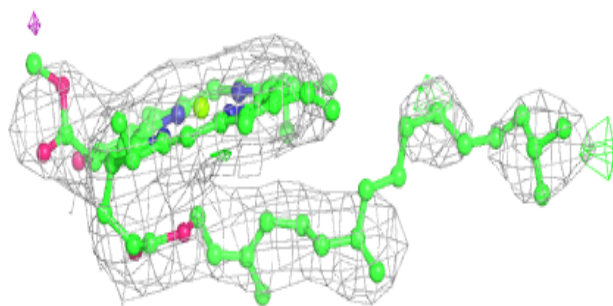
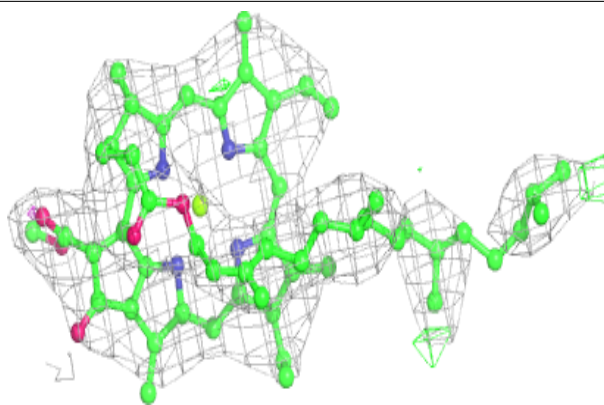
Electron density around CLA a 817:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

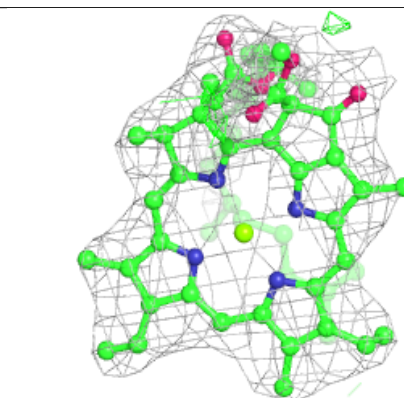
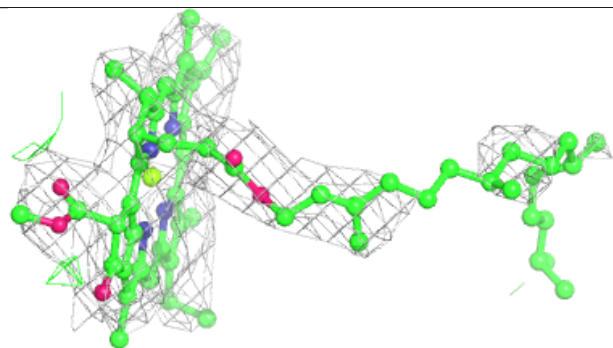
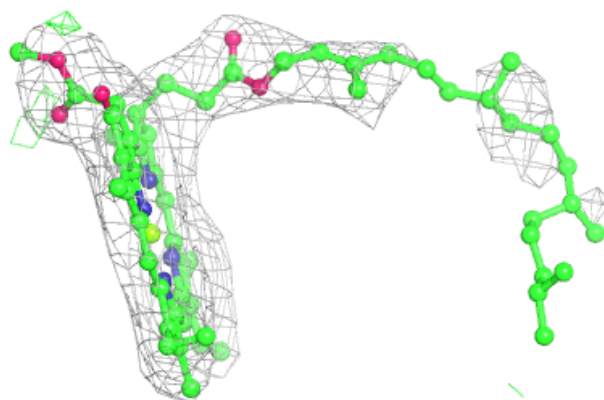


Electron density around CLA A 839:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

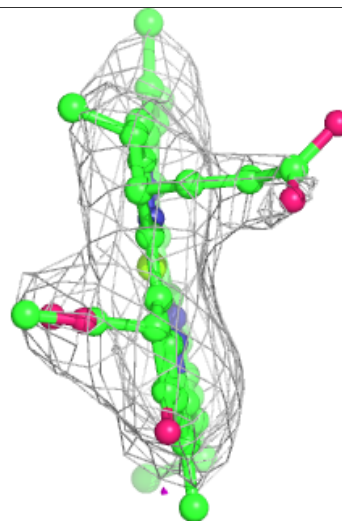
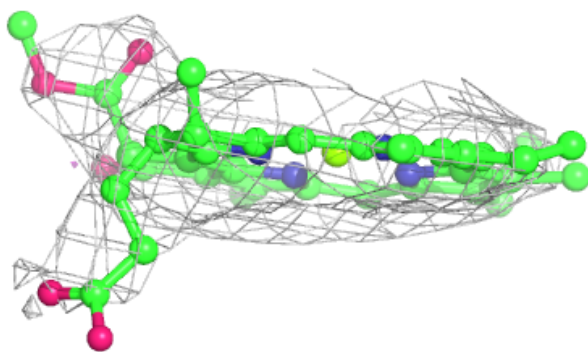
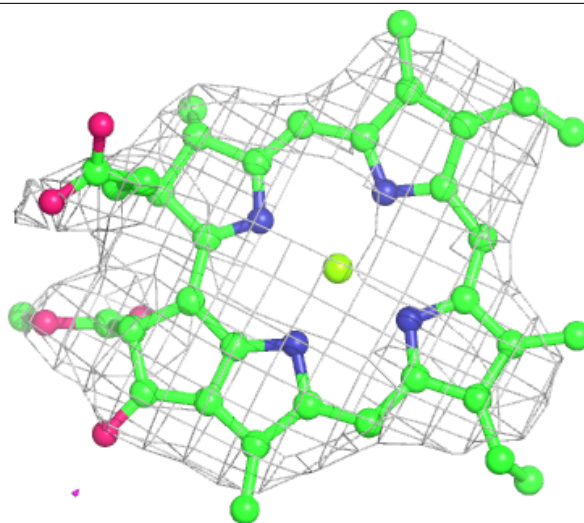
**Electron density around CLA A 808:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



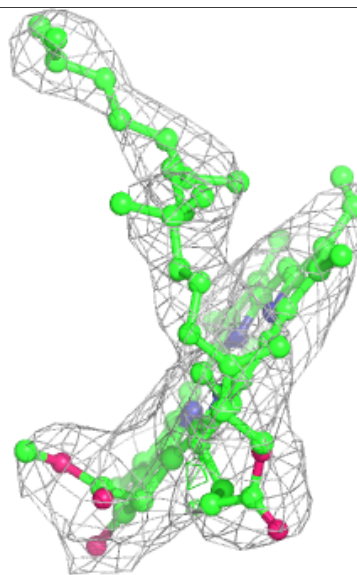
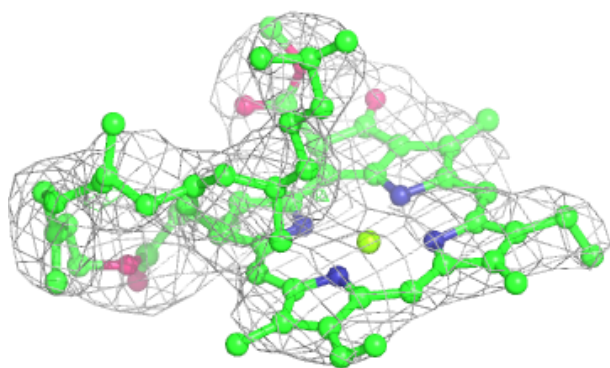
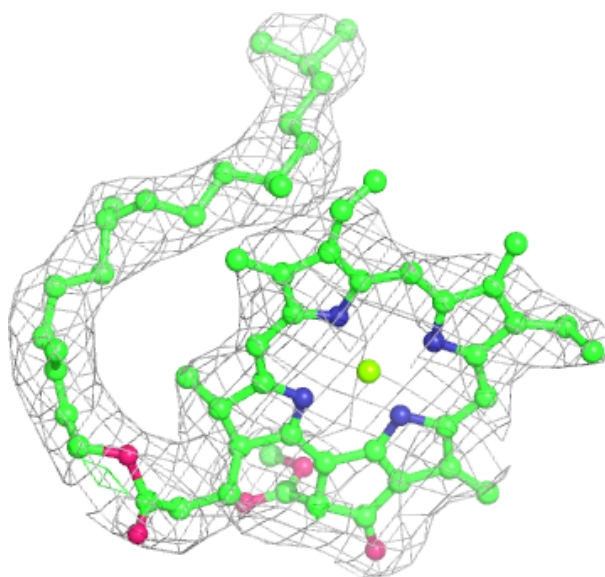
Electron density around CLA A 817:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



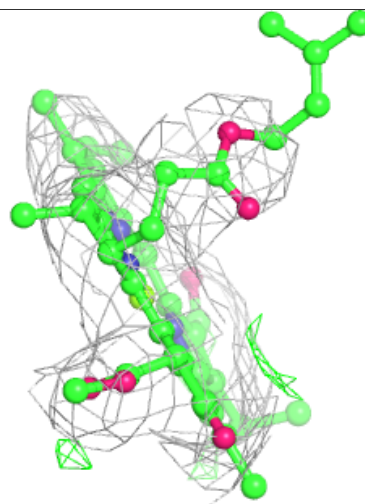
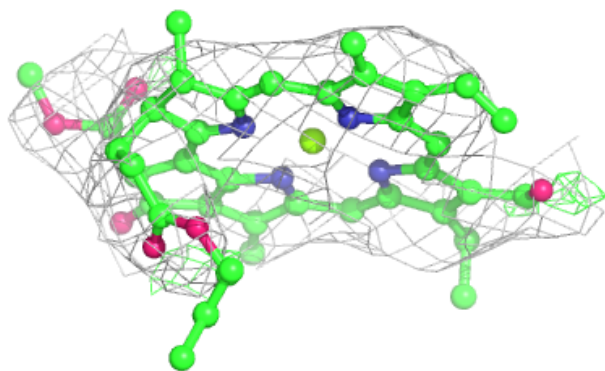
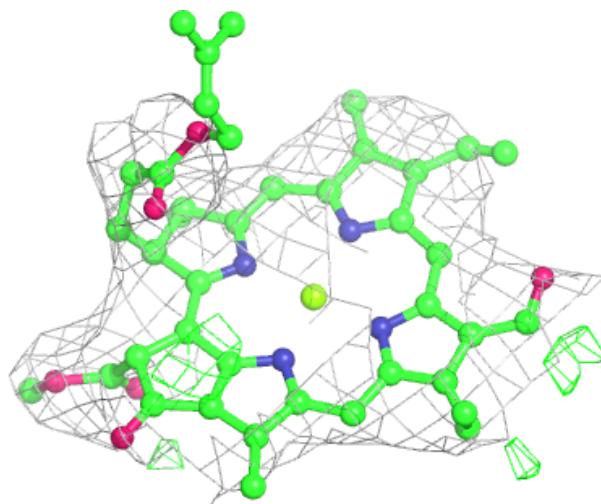
Electron density around CLA A 814:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



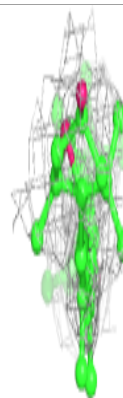
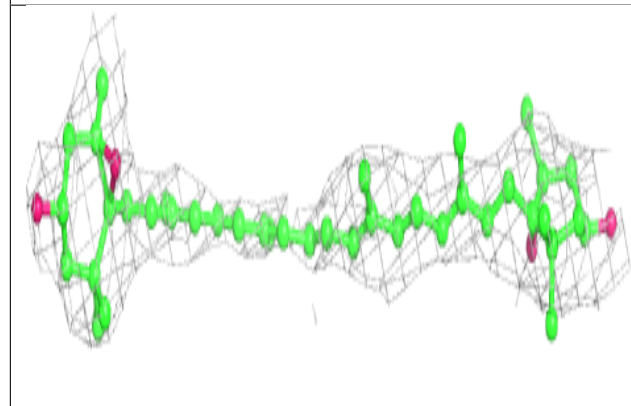
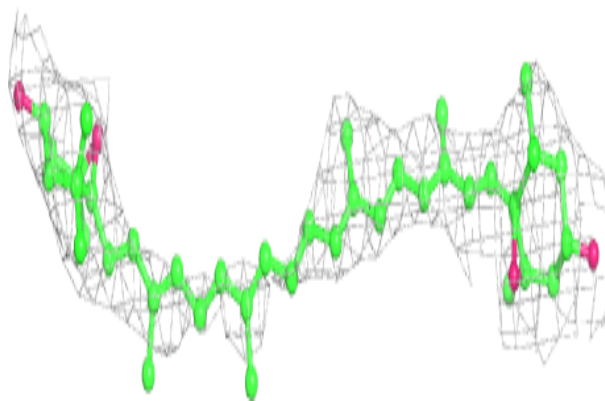
Electron density around CHL 9 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



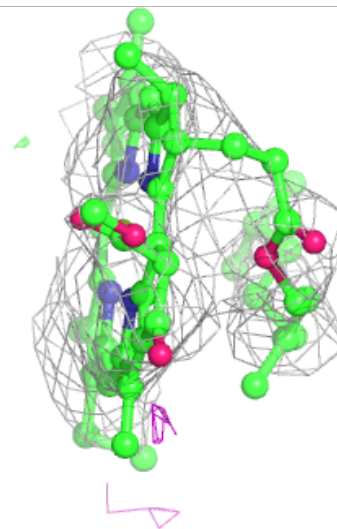
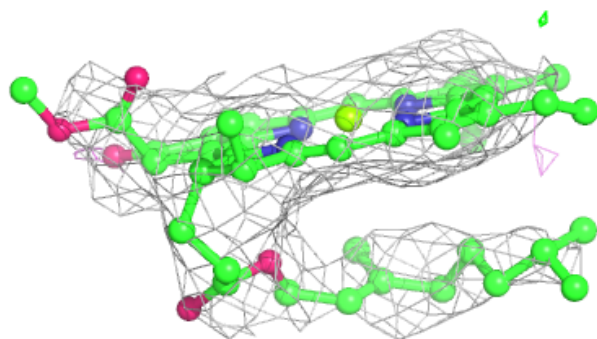
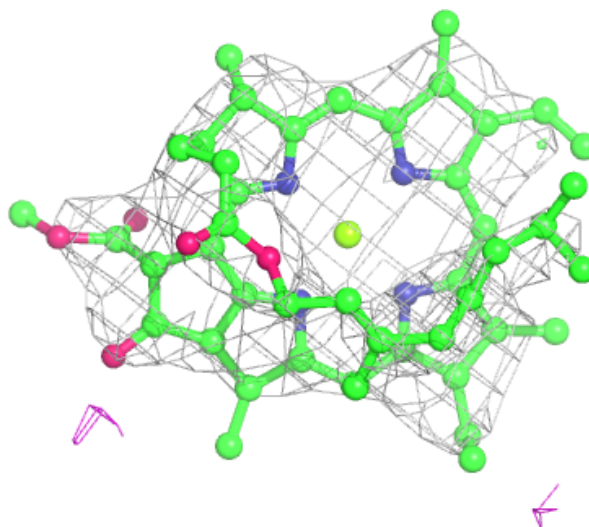
Electron density around XAT 6 318:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



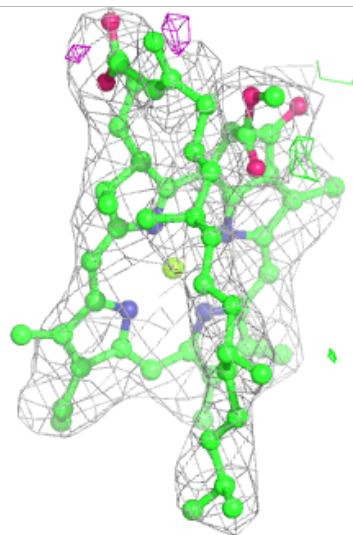
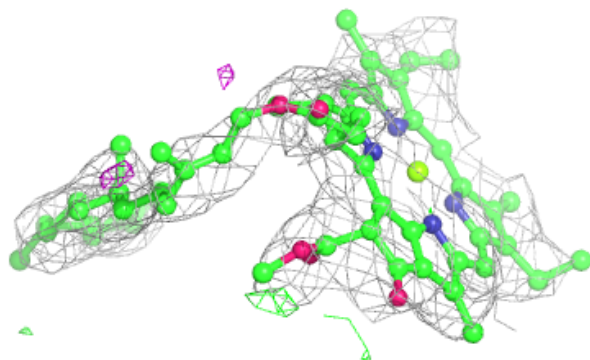
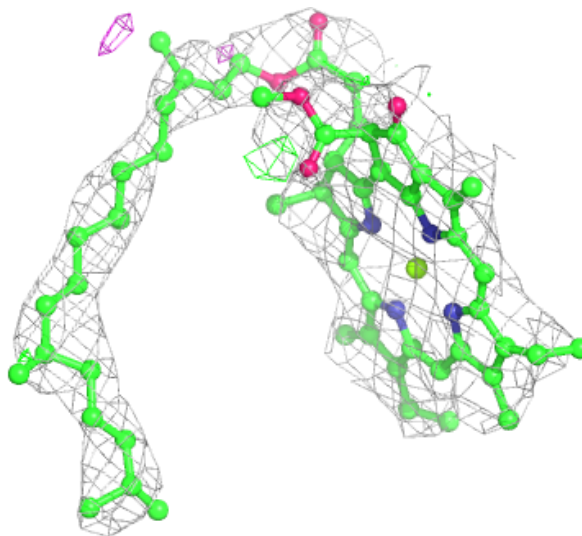
Electron density around CLA 8 310:

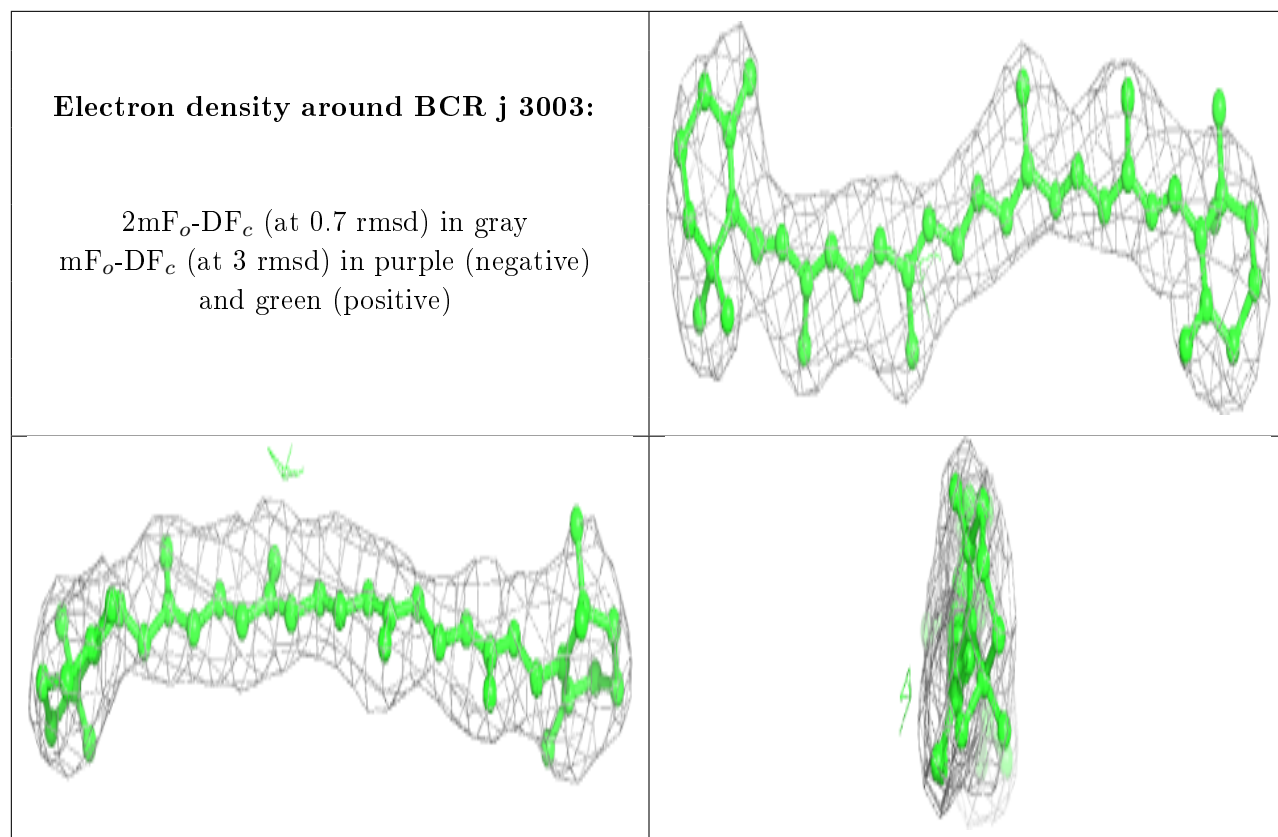
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 810:

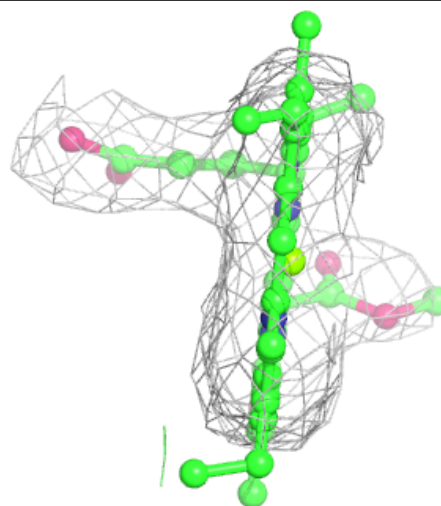
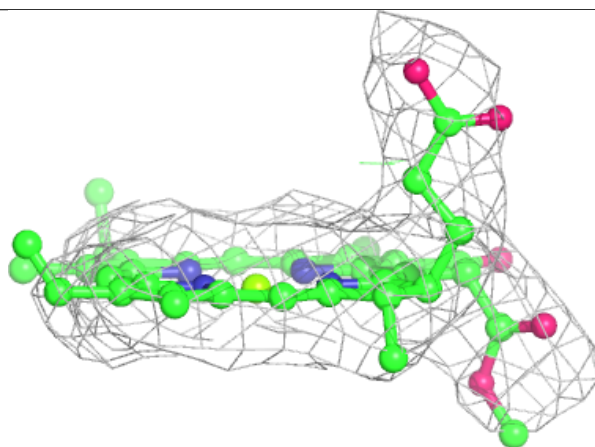
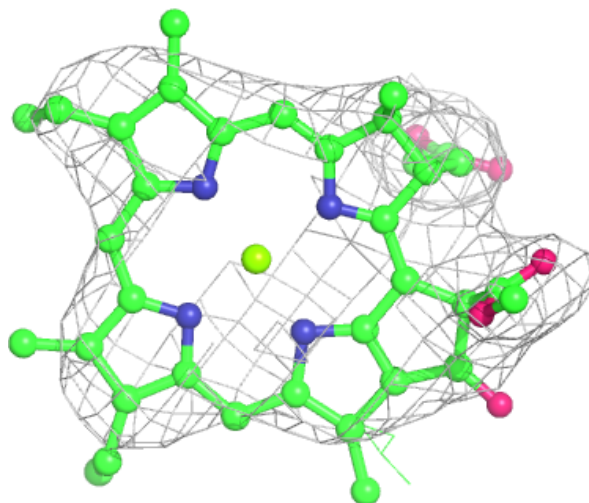
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





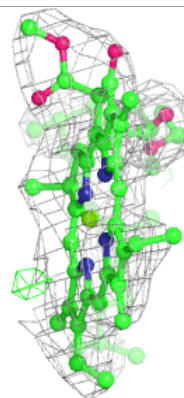
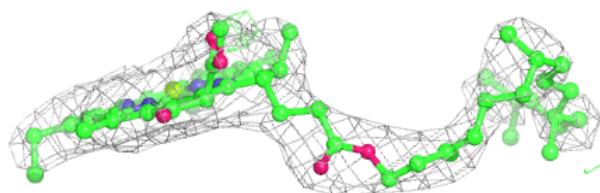
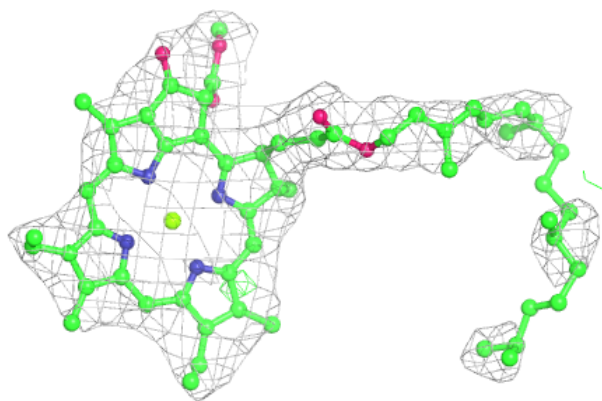
Electron density around CLA 8 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

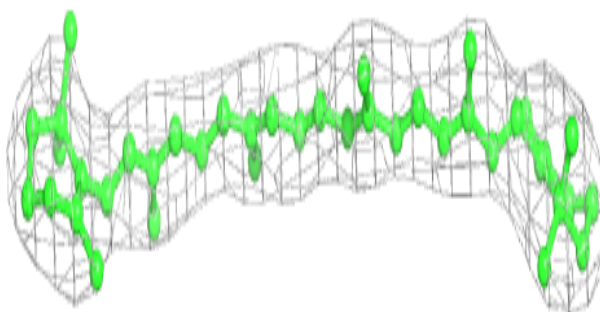
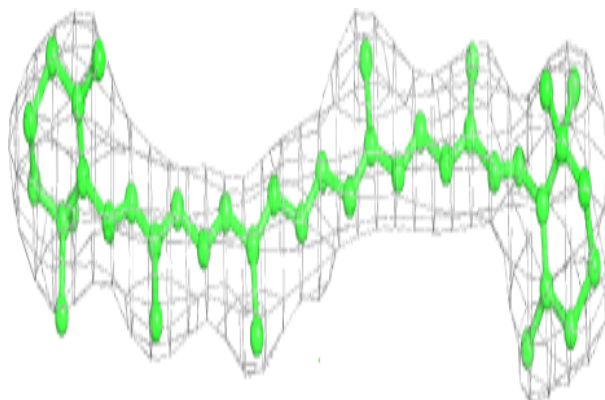


Electron density around CLA A 827:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

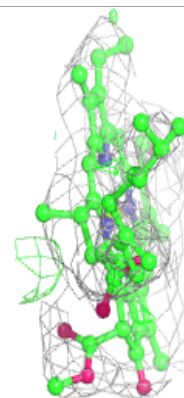
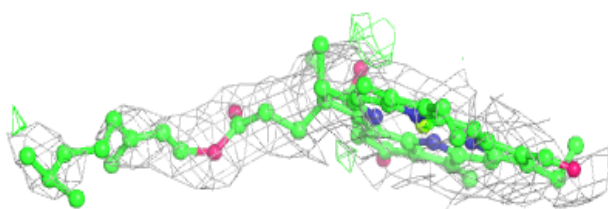
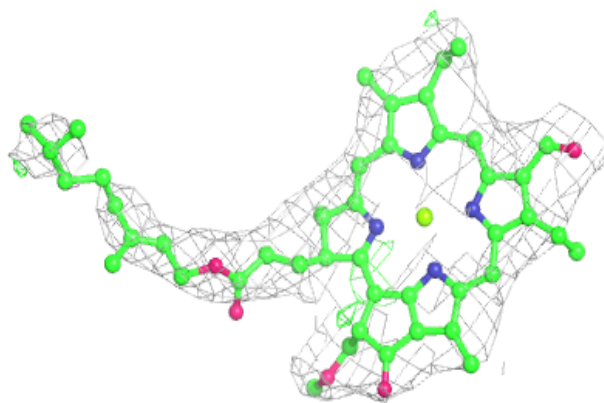
**Electron density around BCR J 3003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

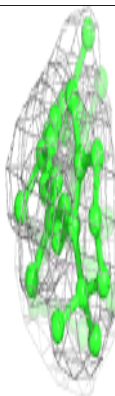
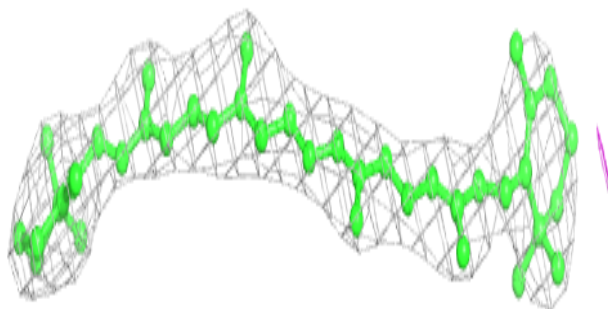
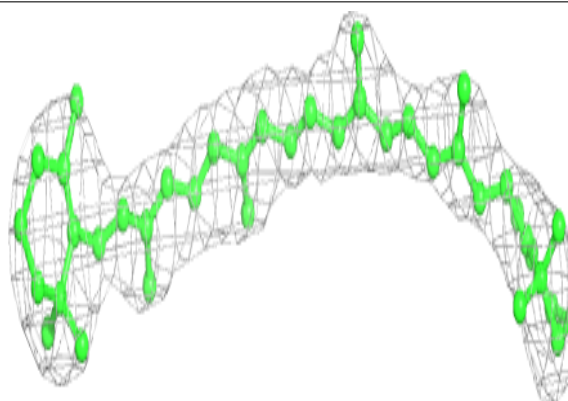


Electron density around CHL 9 605:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

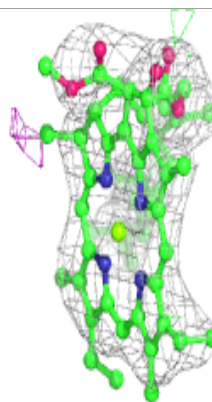
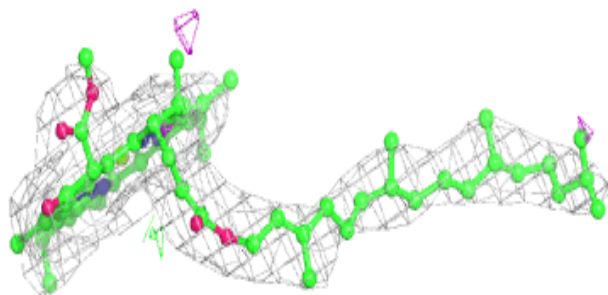
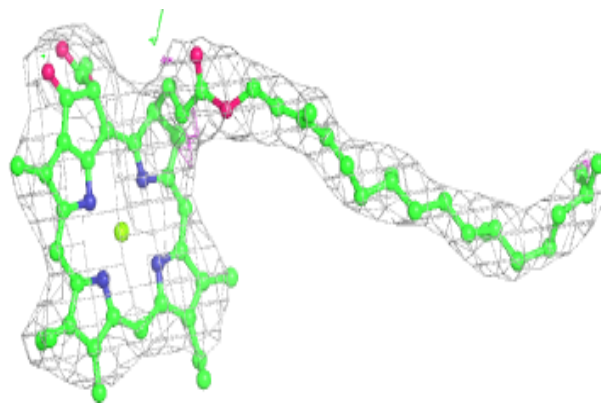
**Electron density around BCR b 801:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

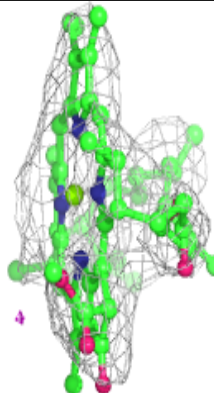
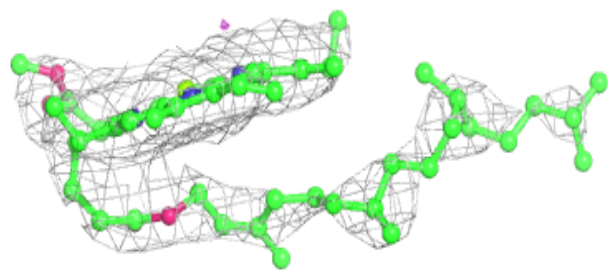
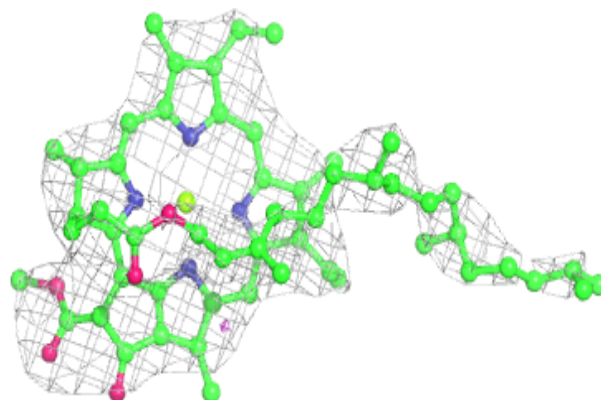


Electron density around CLA A 835:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

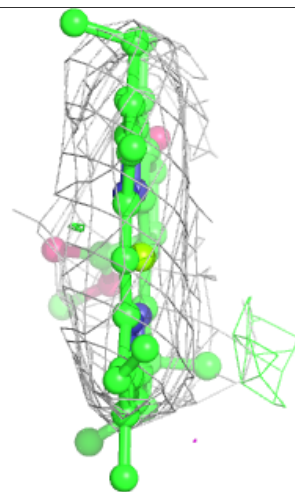
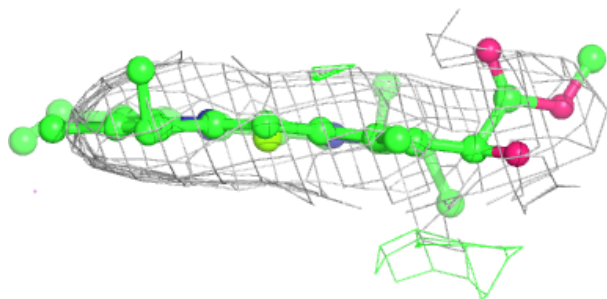
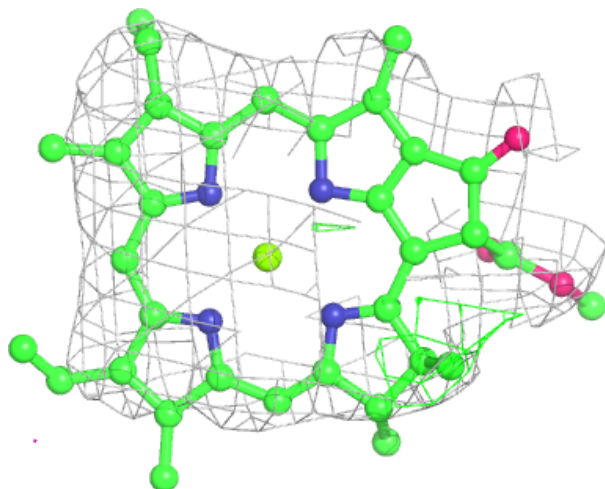
**Electron density around CLA A 818:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



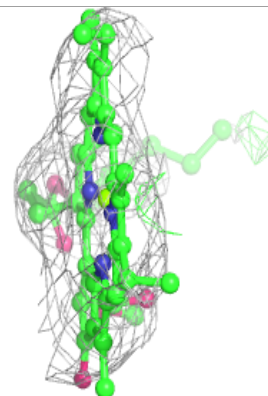
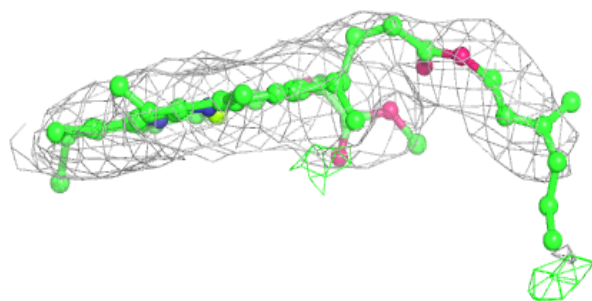
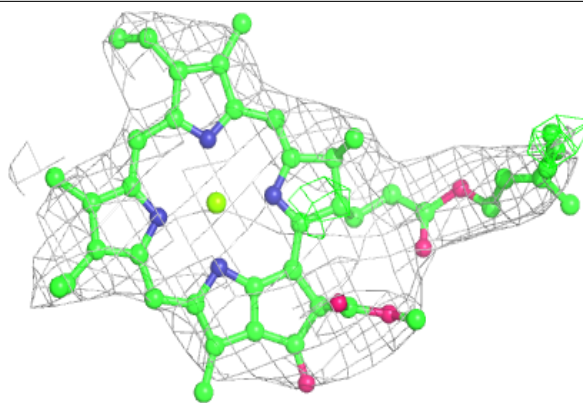
Electron density around CLA 6 312:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



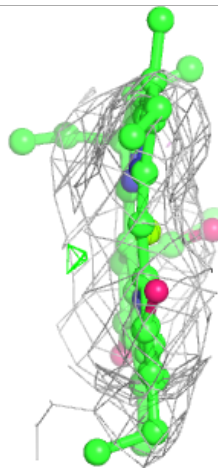
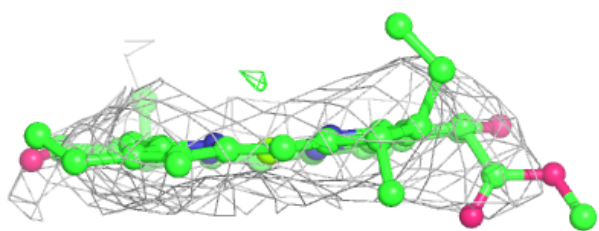
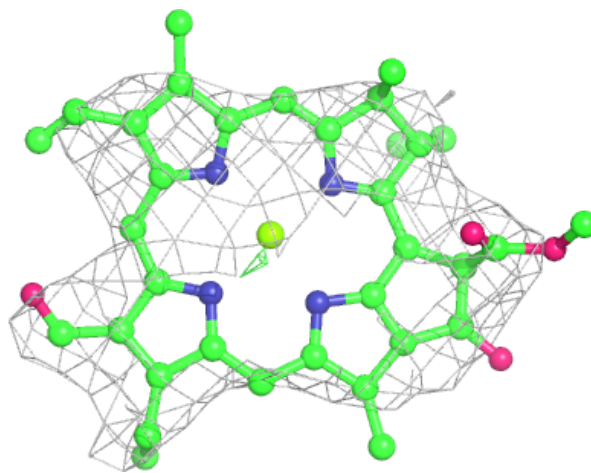
Electron density around CLA 1 306:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



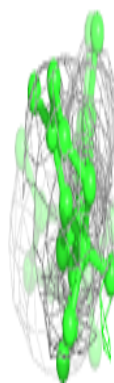
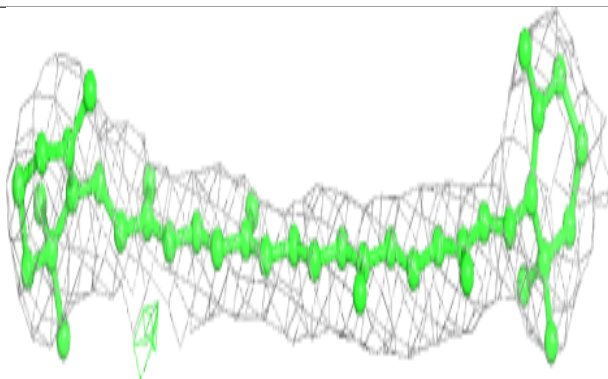
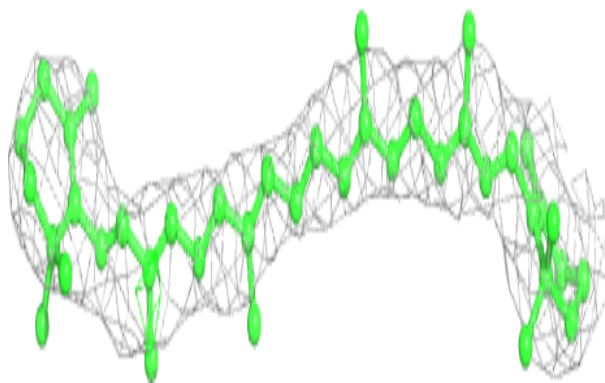
Electron density around CHL 7 614:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

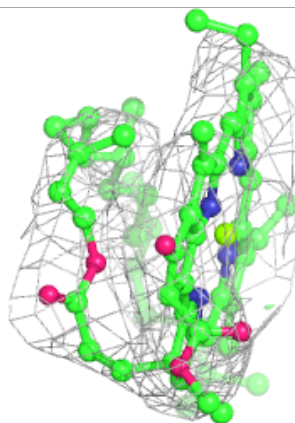
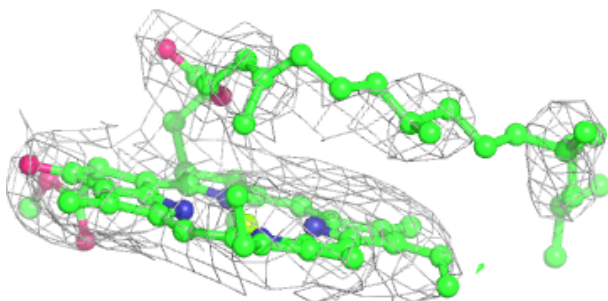
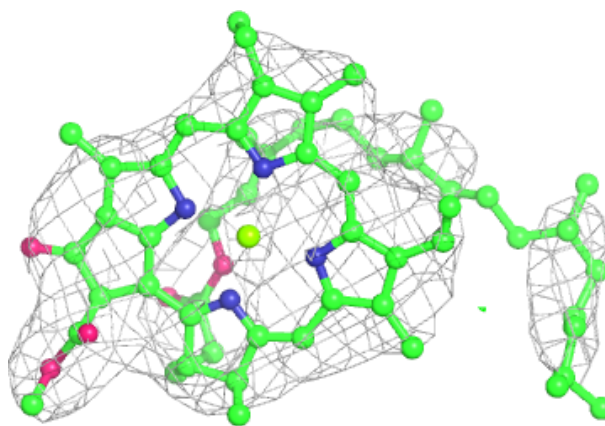


Electron density around BCR 3 318:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

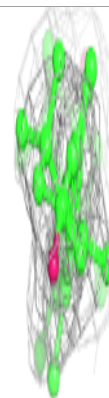
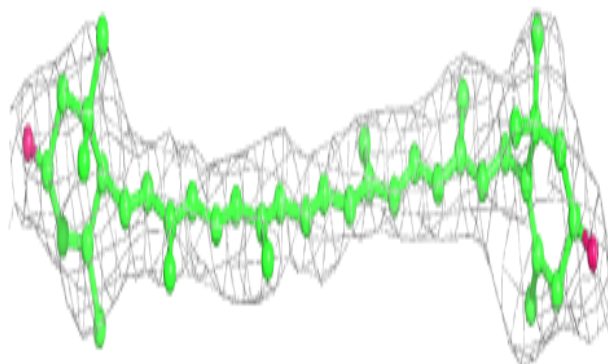
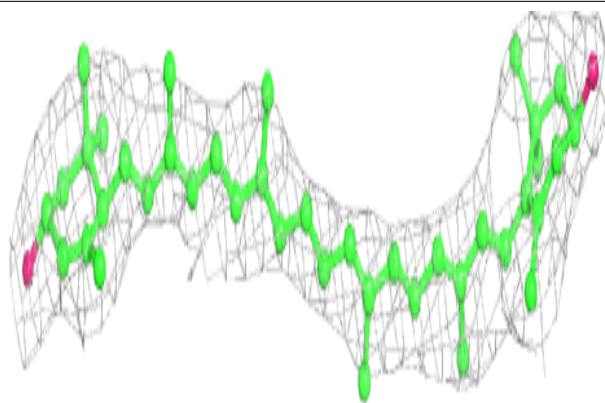
**Electron density around CLA 1 313:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



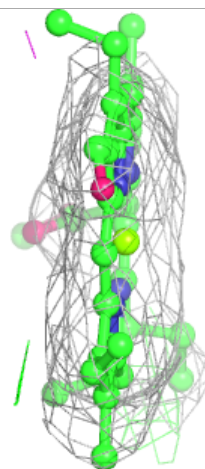
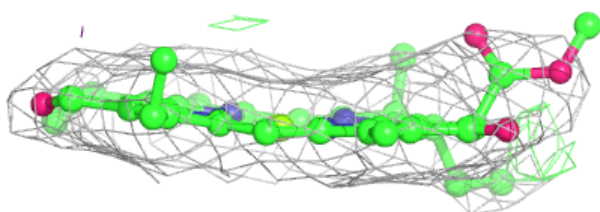
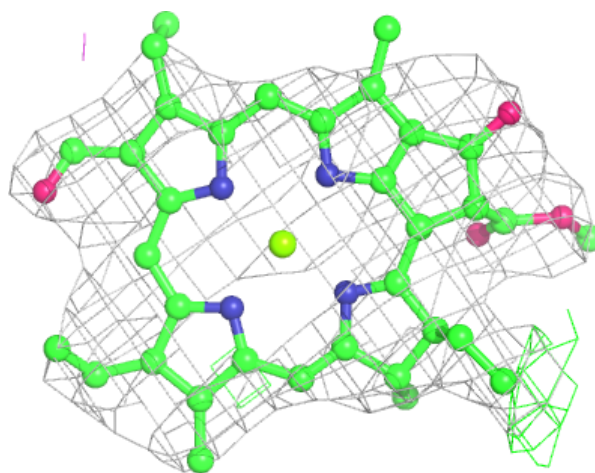
Electron density around LUT 1 316:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



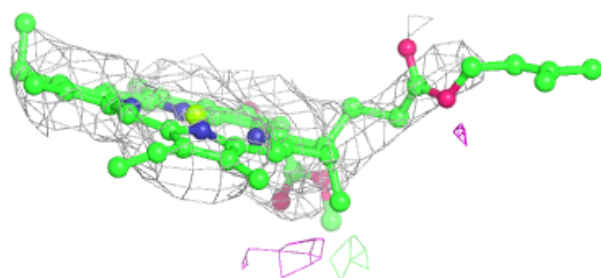
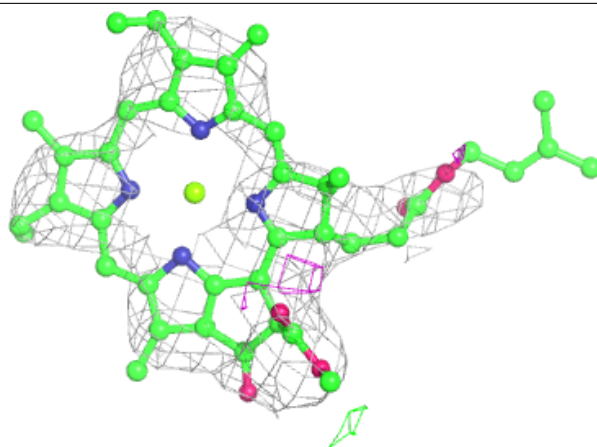
Electron density around CHL 4 615:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



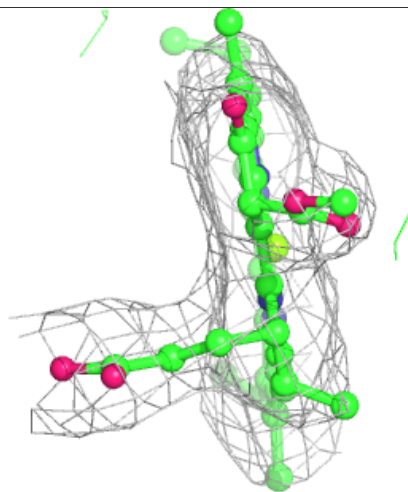
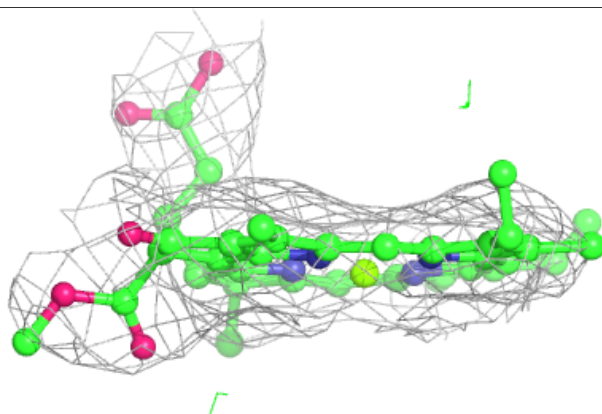
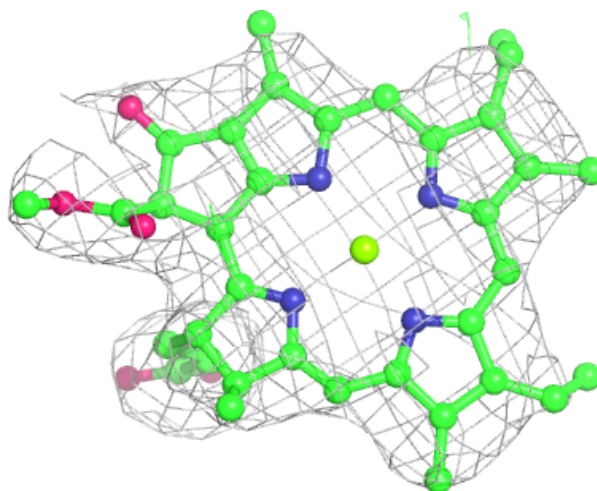
Electron density around CLA g 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



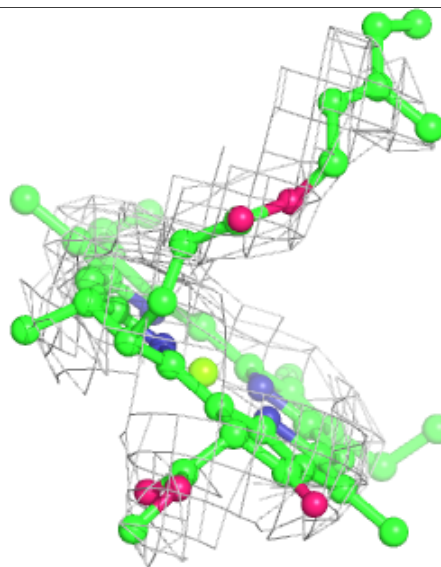
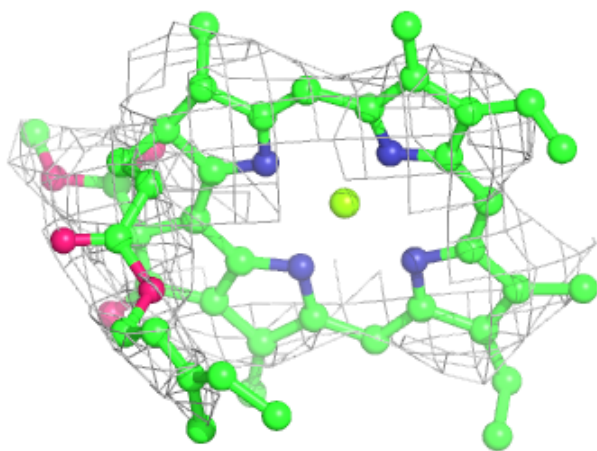
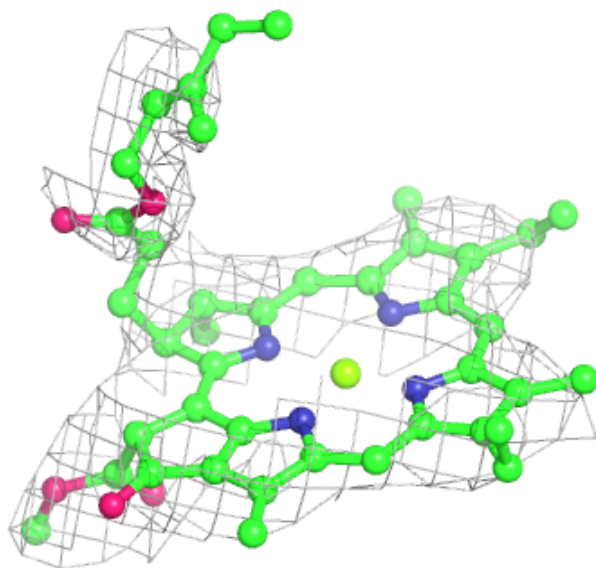
Electron density around CLA B 835:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



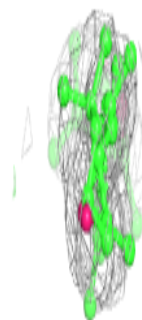
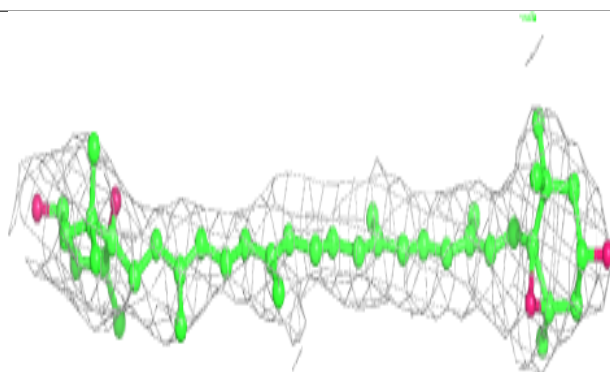
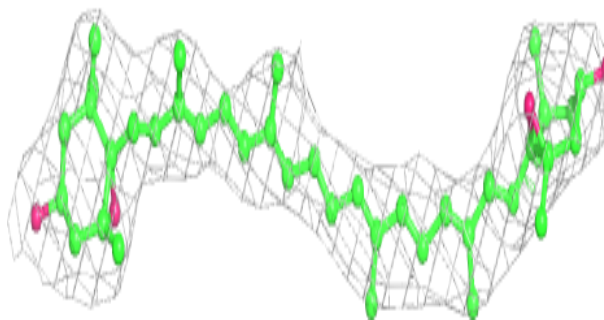
Electron density around CLA 6 306:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



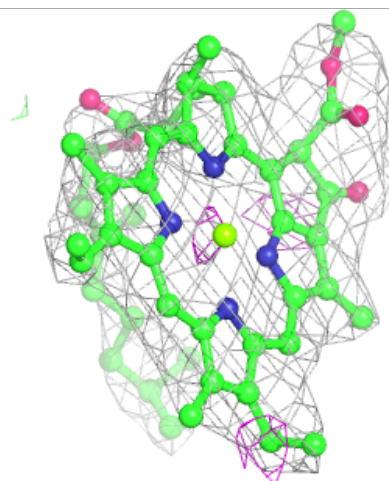
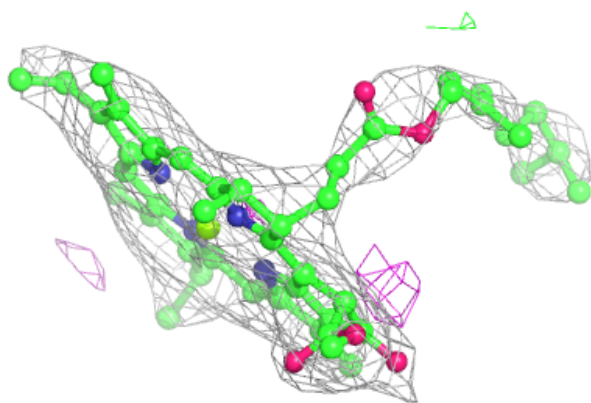
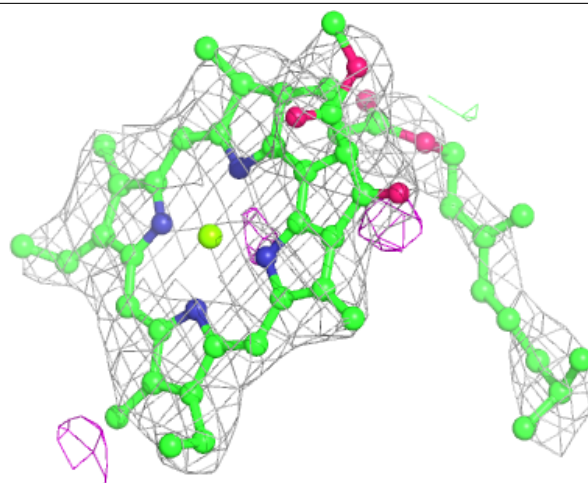
Electron density around XAT 4 617:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



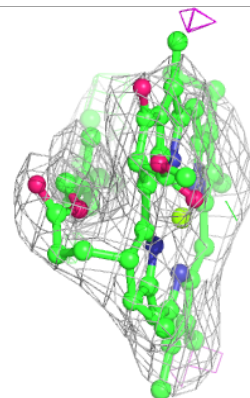
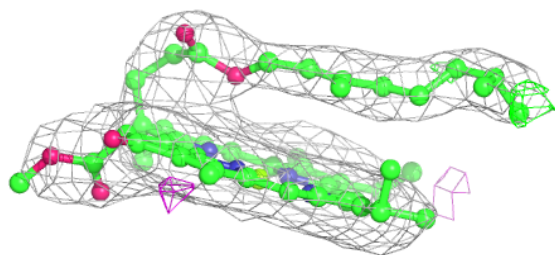
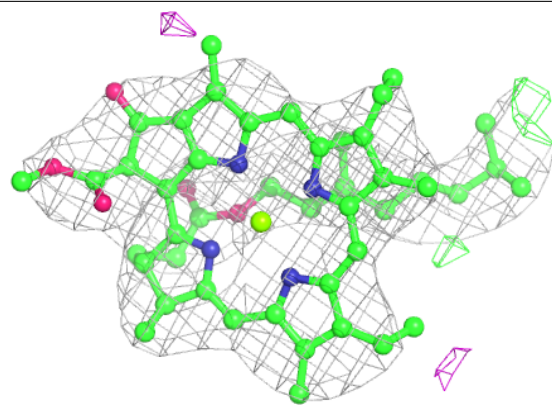
Electron density around CLA B 822:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



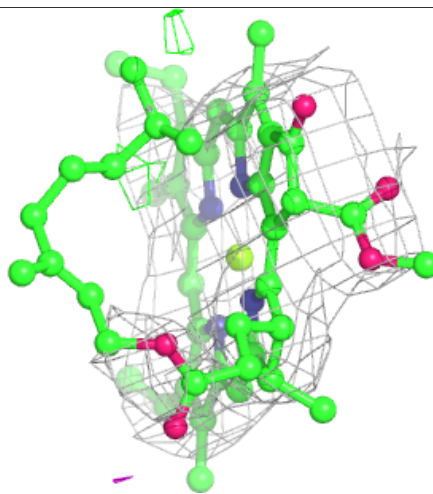
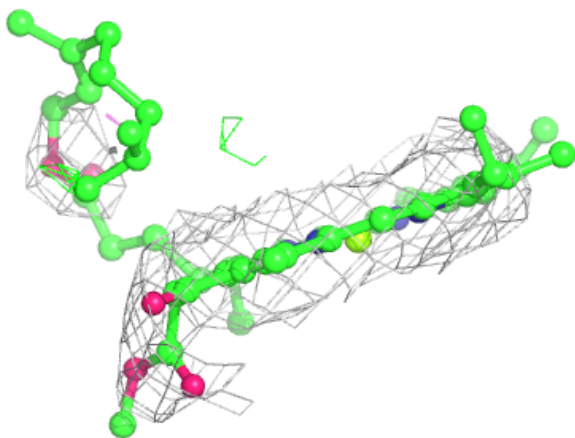
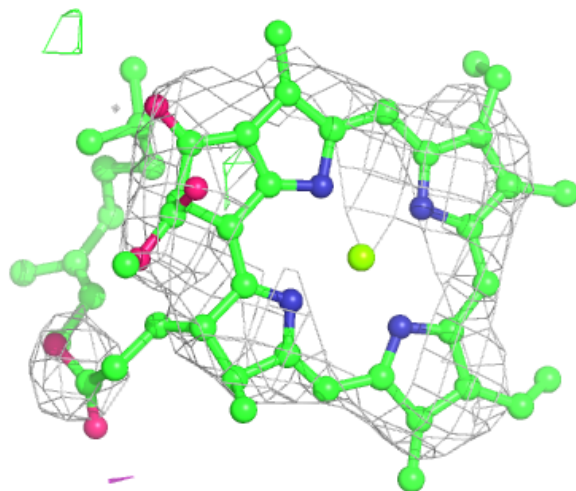
Electron density around CLA b 816:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



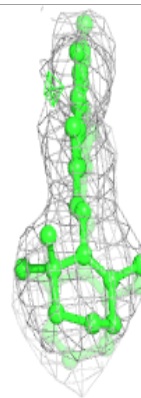
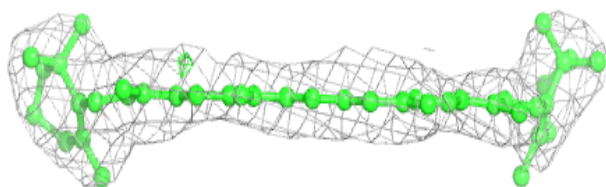
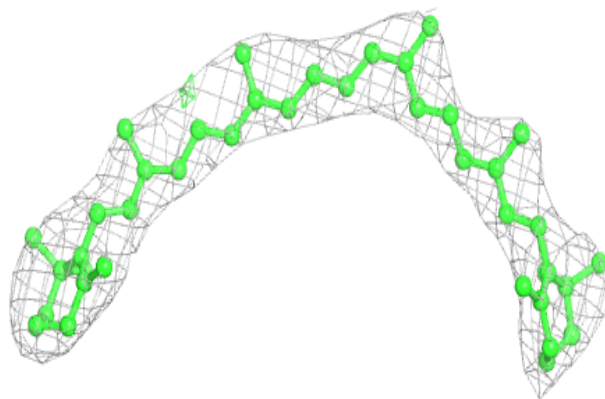
Electron density around CLA 6 315:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

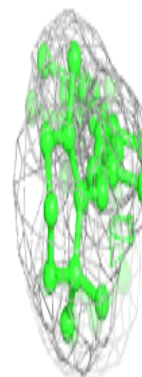
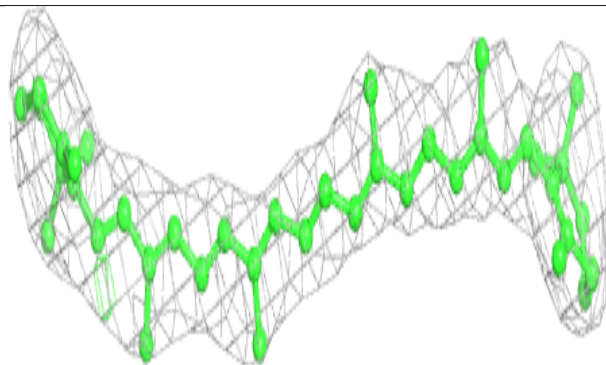
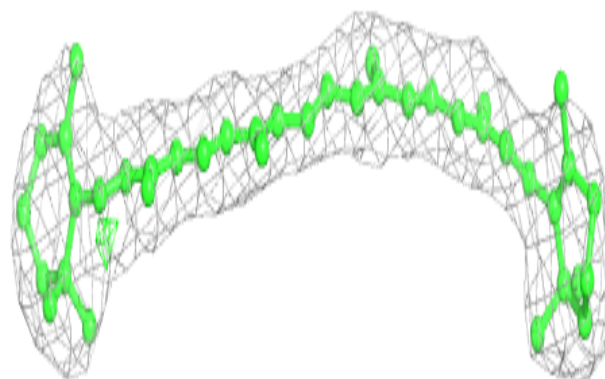


Electron density around BCR f 7004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

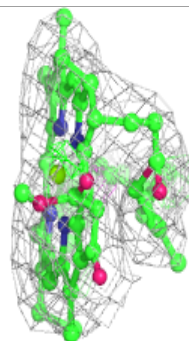
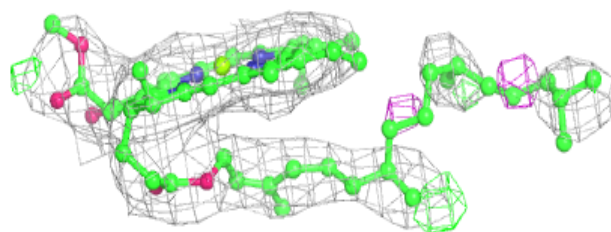
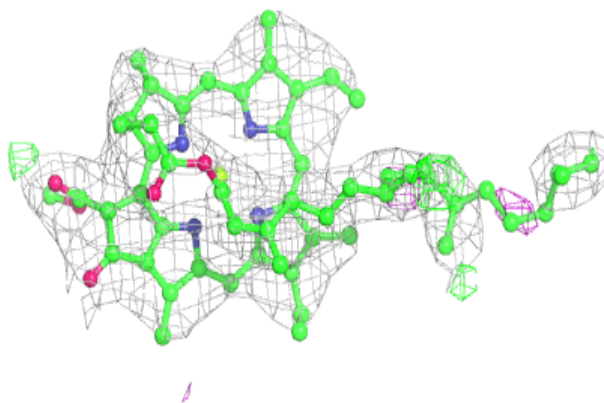
**Electron density around BCR i 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

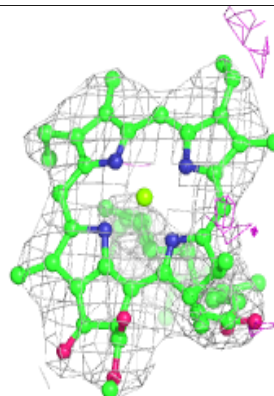
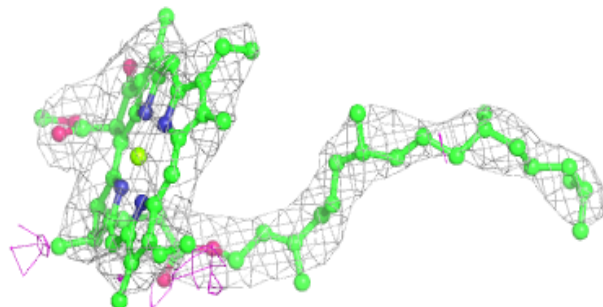
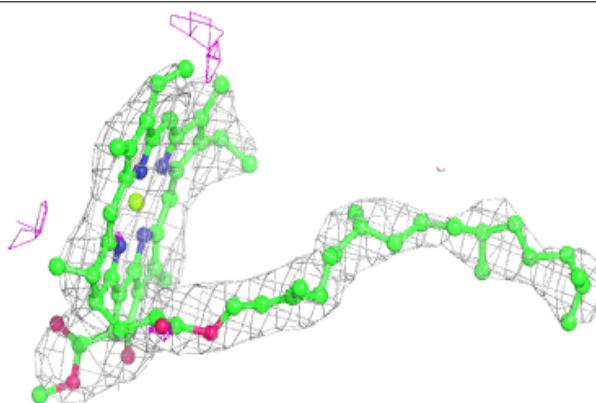


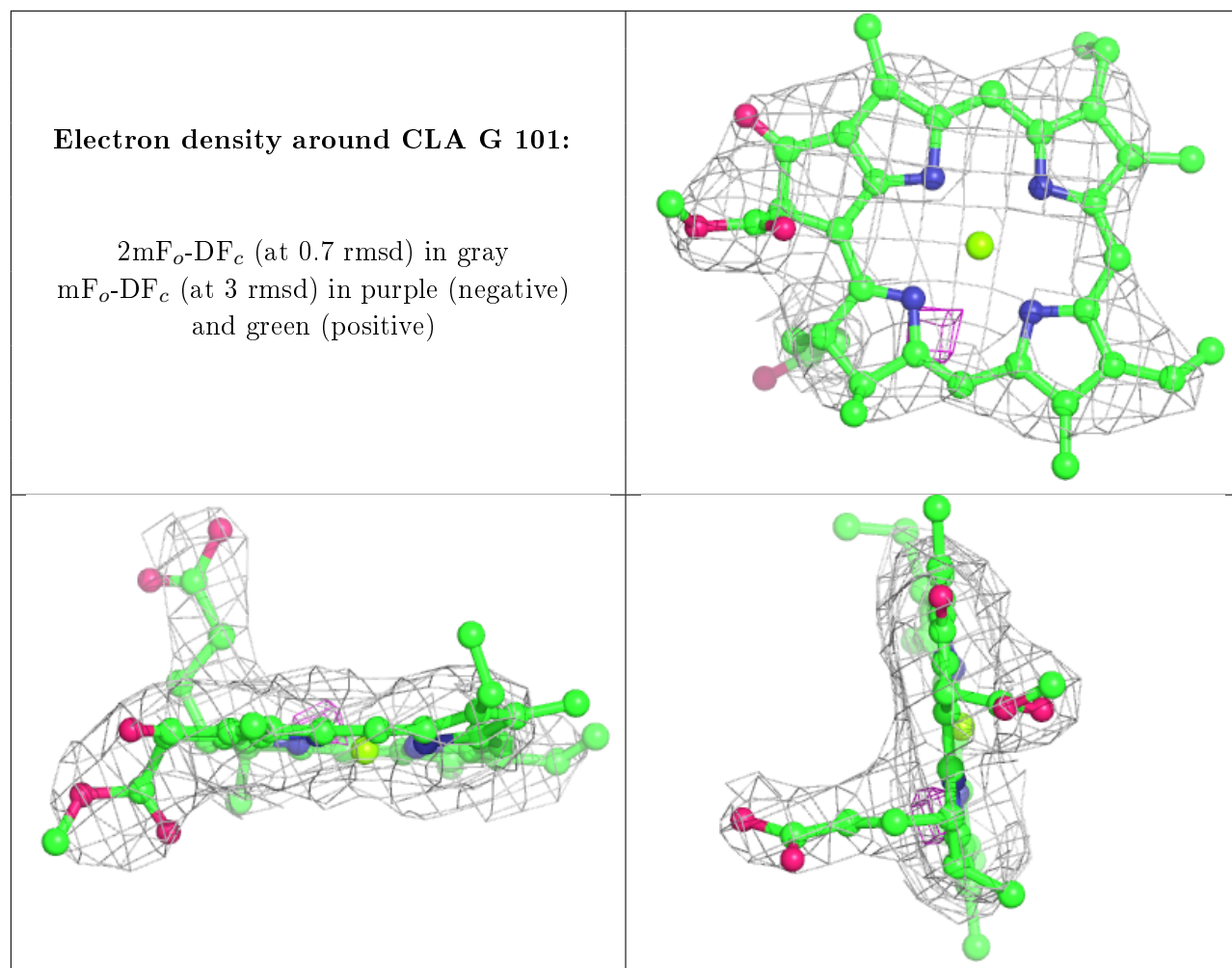
Electron density around CLA a 839:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CLA a 812:**

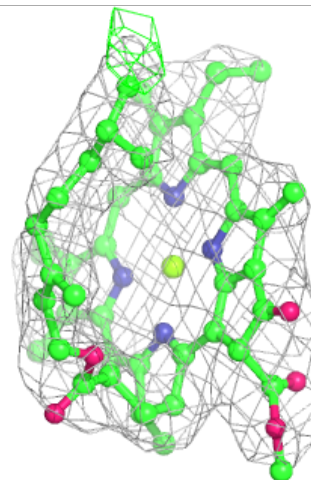
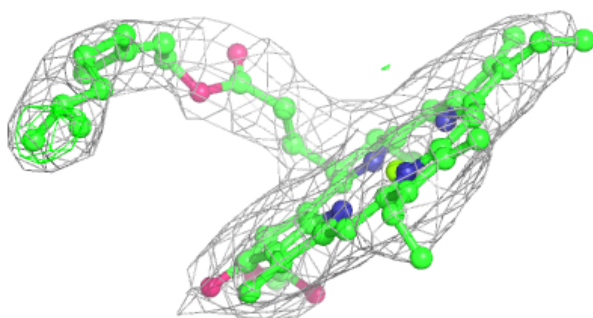
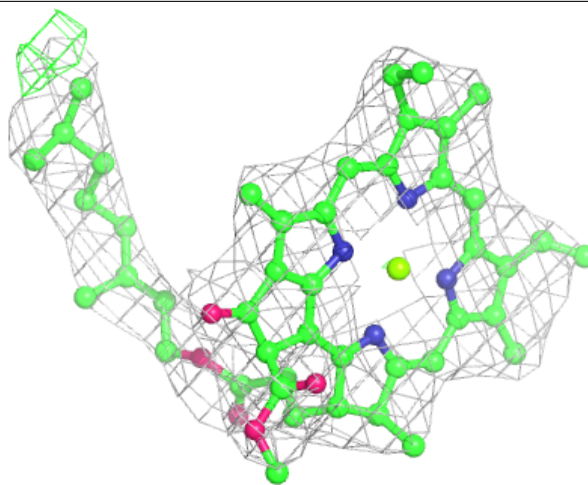
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





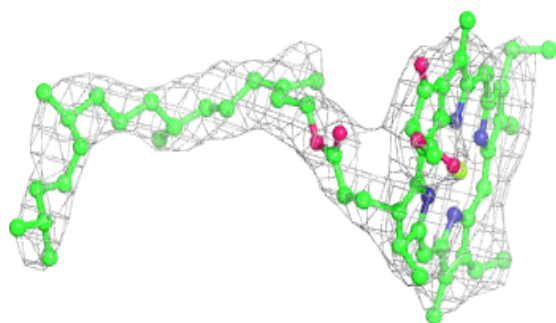
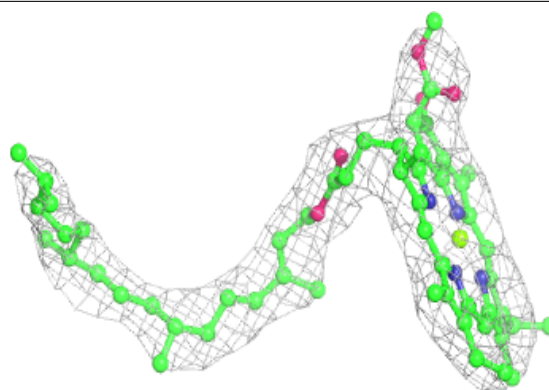
Electron density around CLA b 822:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

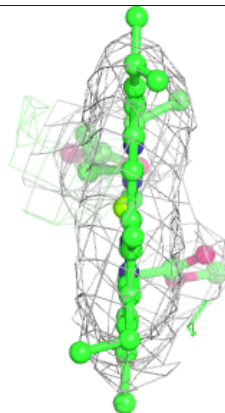
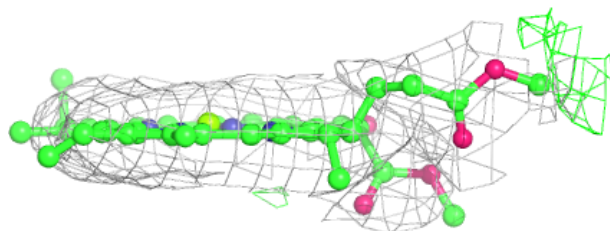
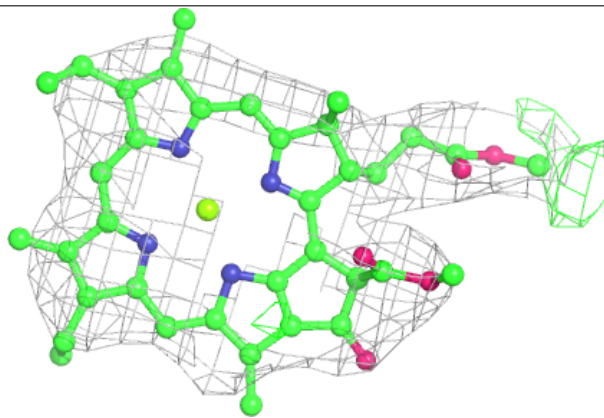


Electron density around CLA B 839:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

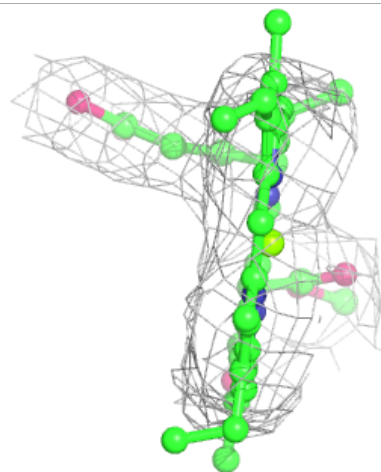
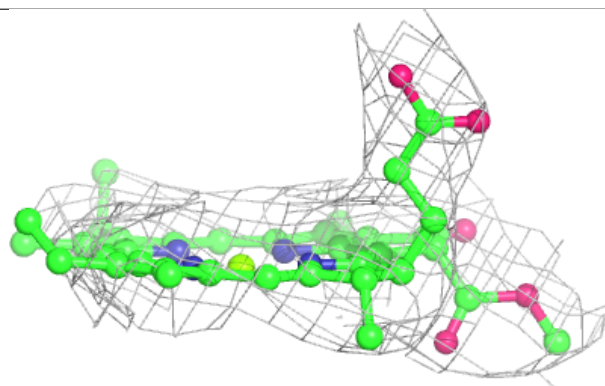
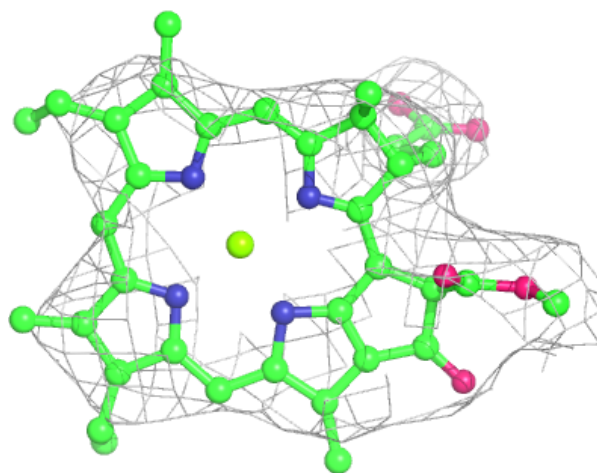
**Electron density around CLA 1 315:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



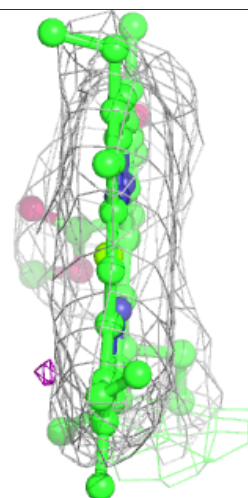
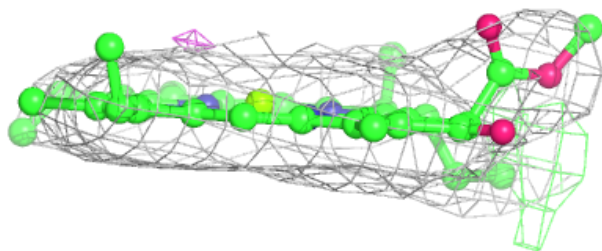
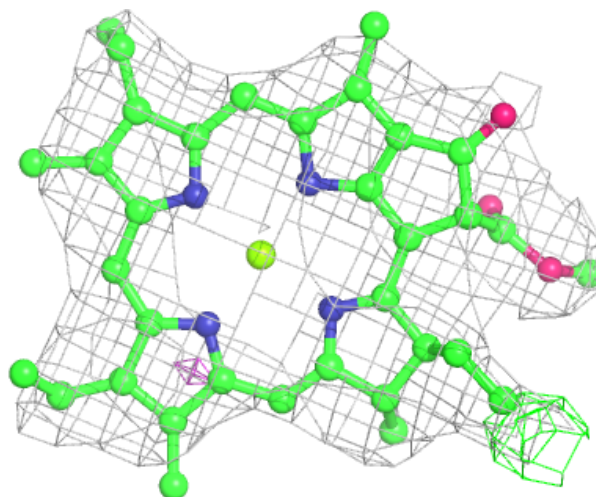
Electron density around CLA b 835:

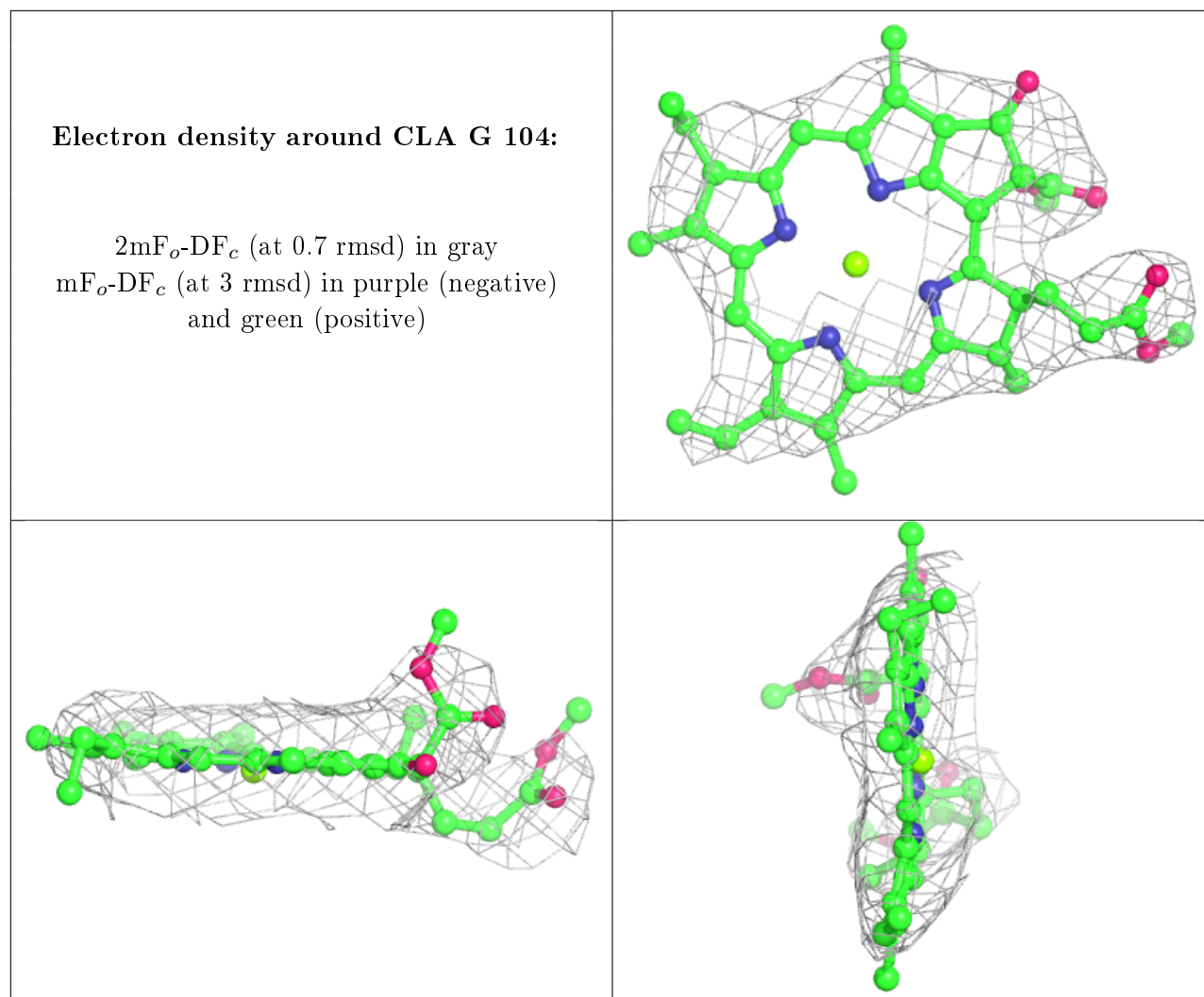
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 3 305:

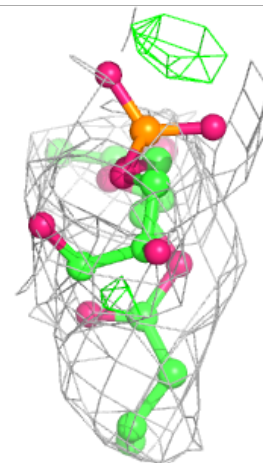
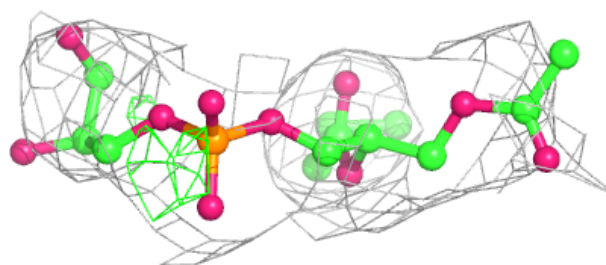
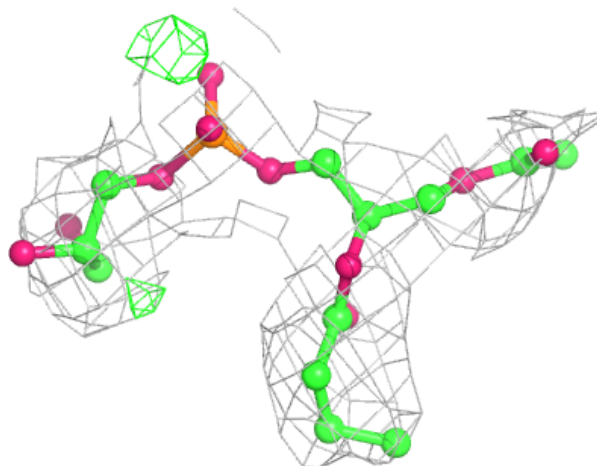
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

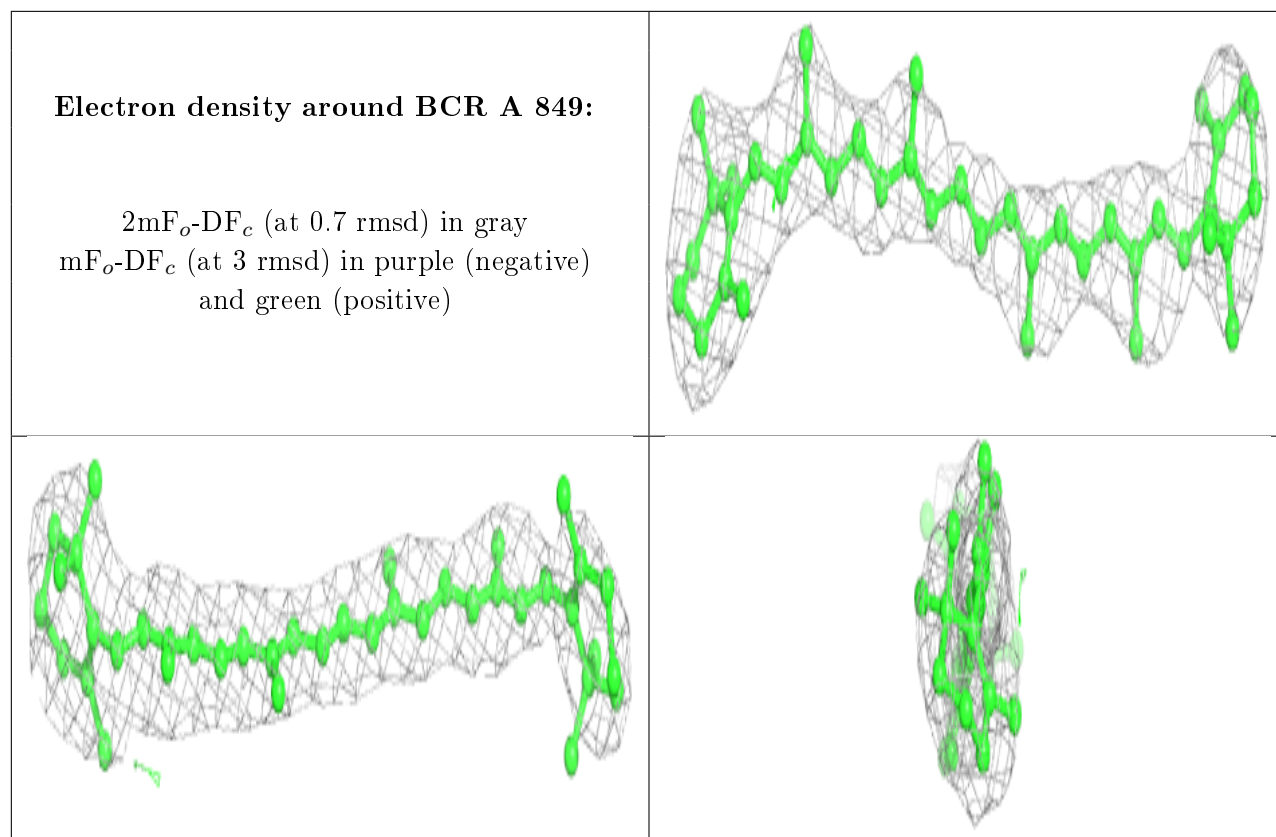




Electron density around LHG 6 301:

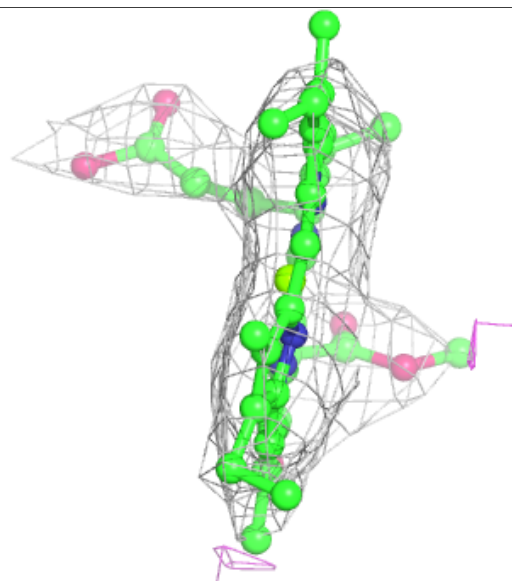
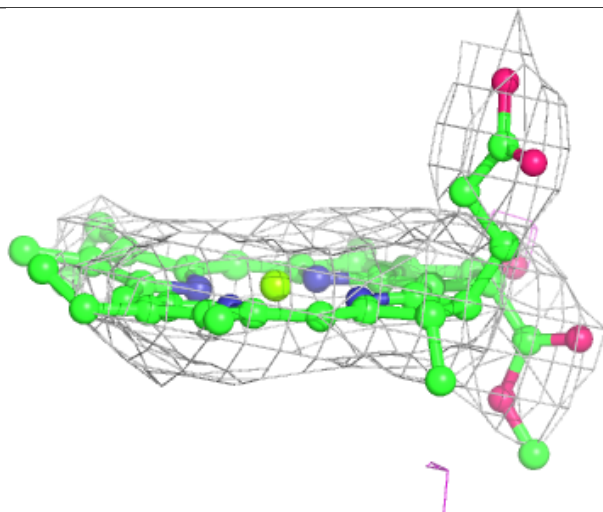
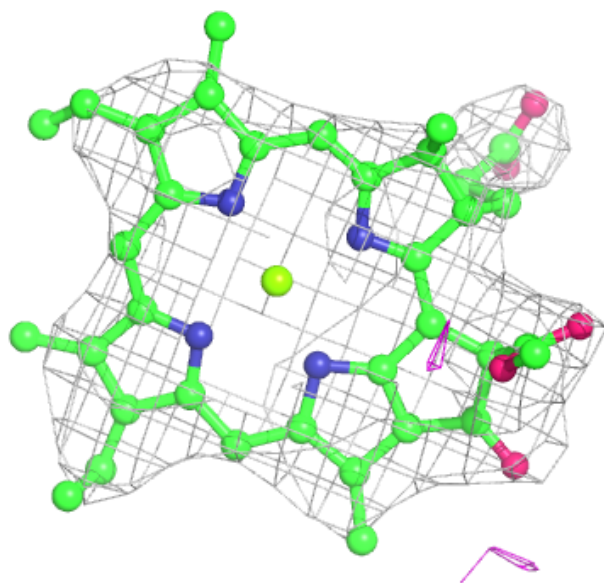
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

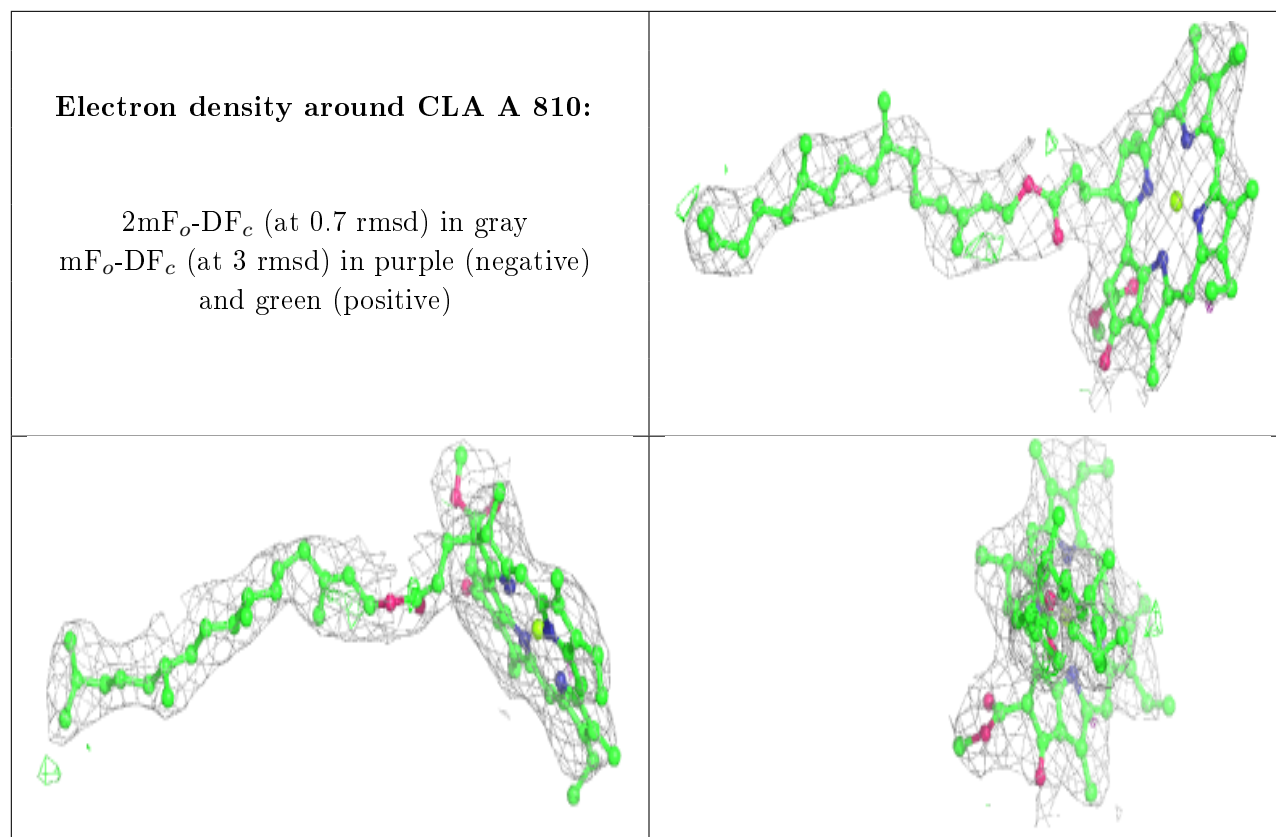




Electron density around CLA A 821:

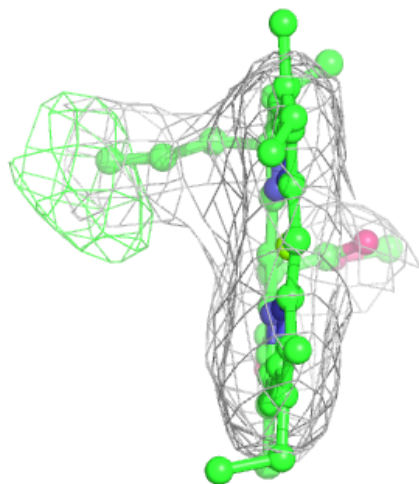
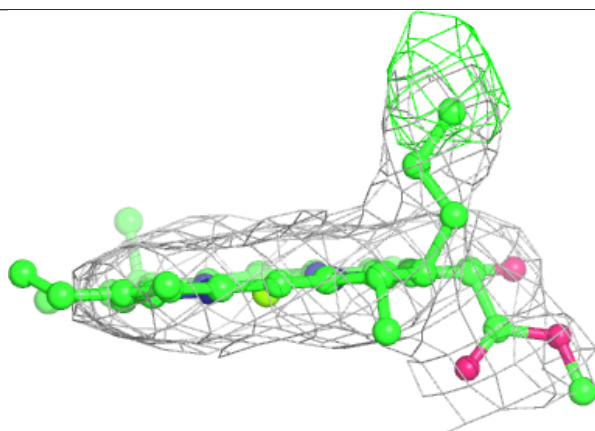
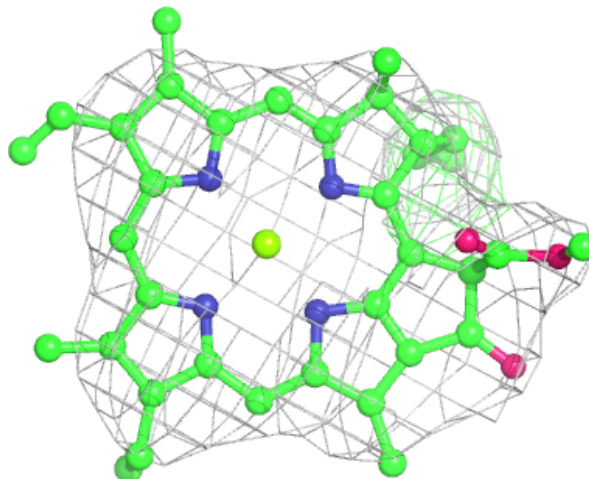
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





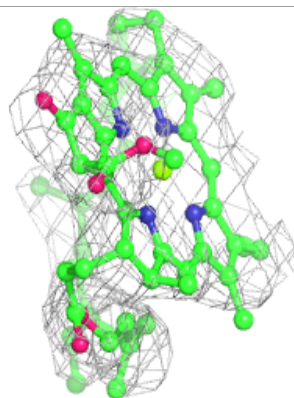
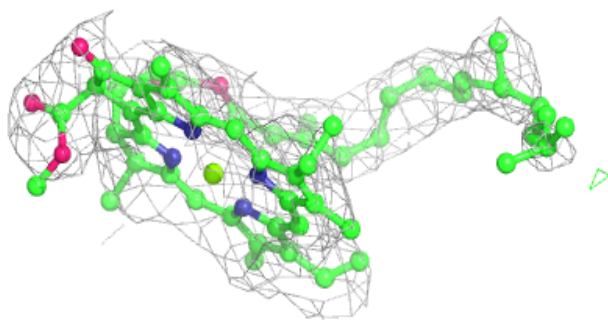
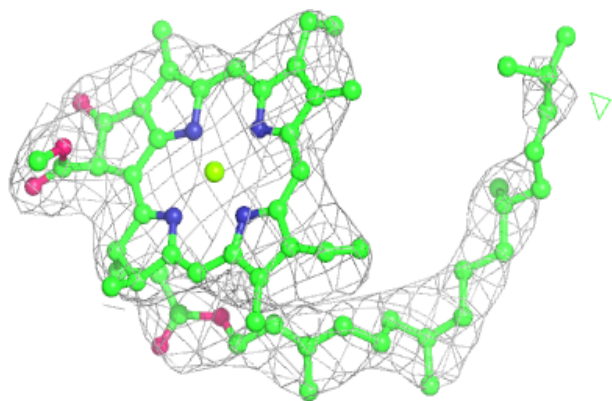
Electron density around CLA 7 613:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

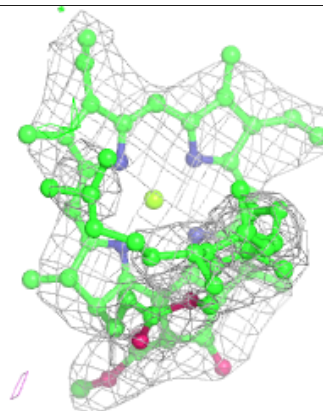
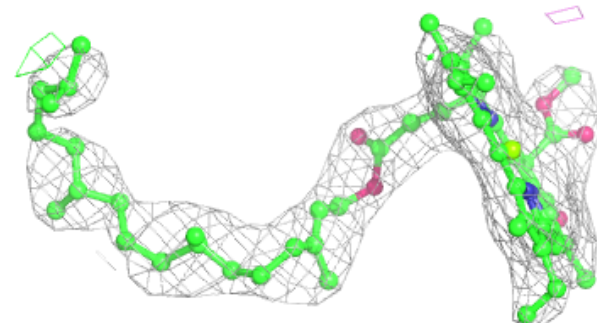
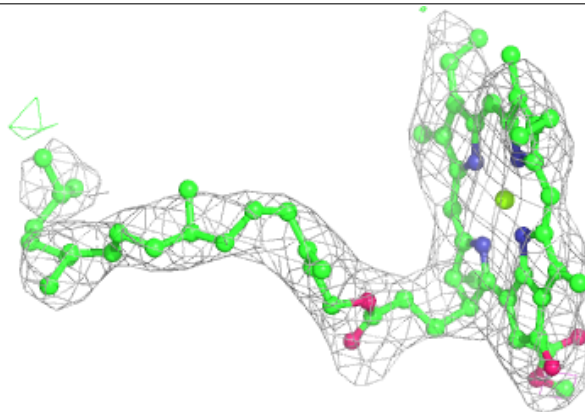


Electron density around CLA 2 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

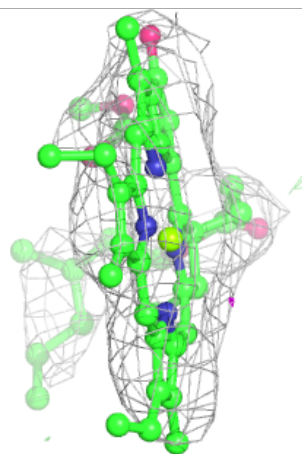
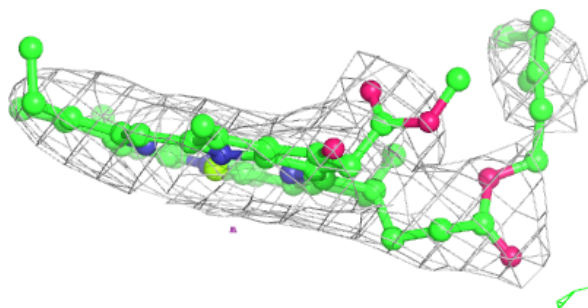
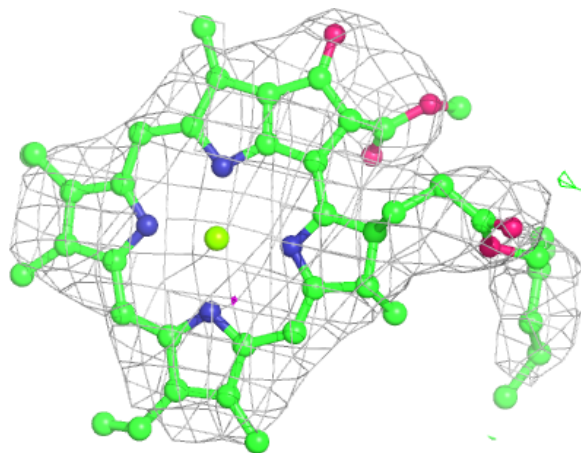
**Electron density around CLA 1 203:**

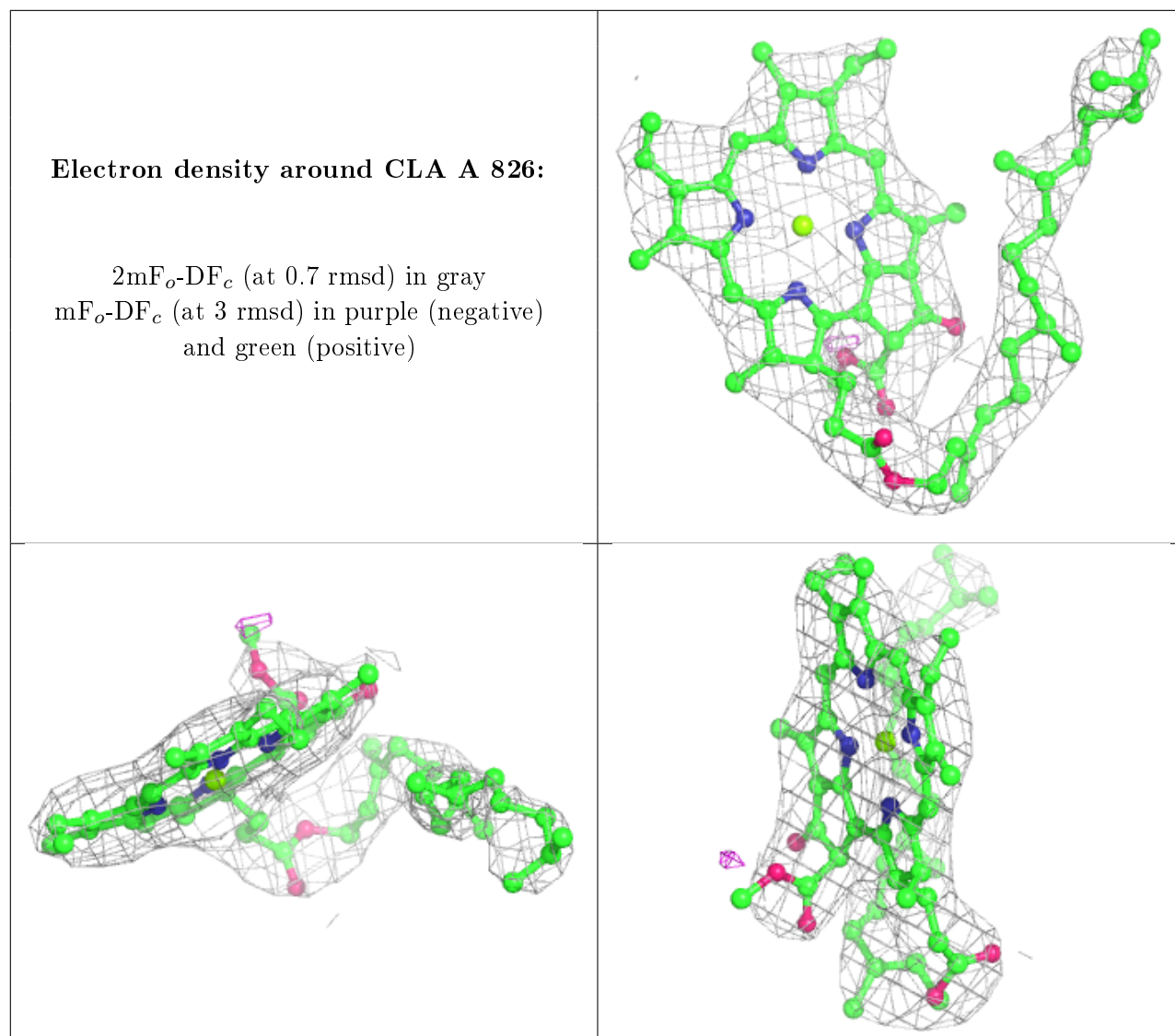
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 1 312:

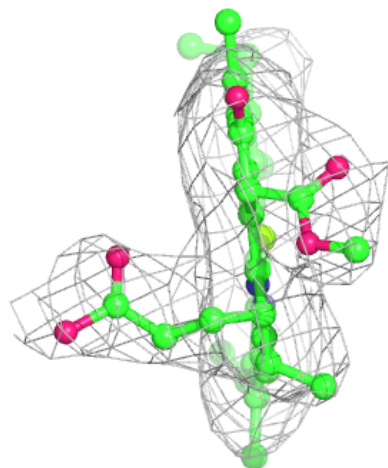
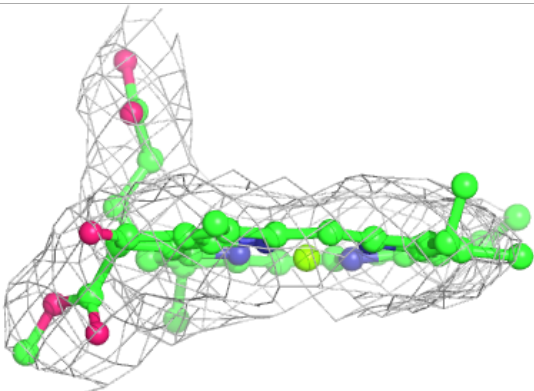
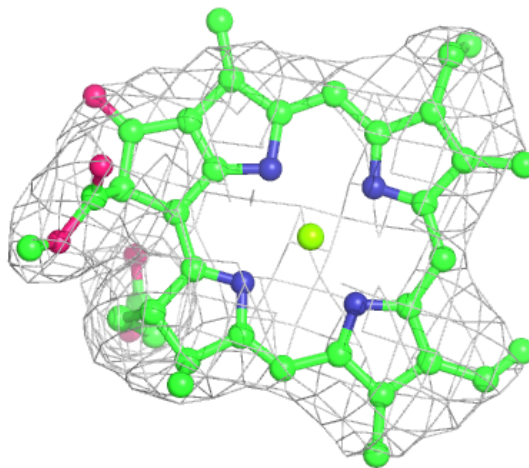
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

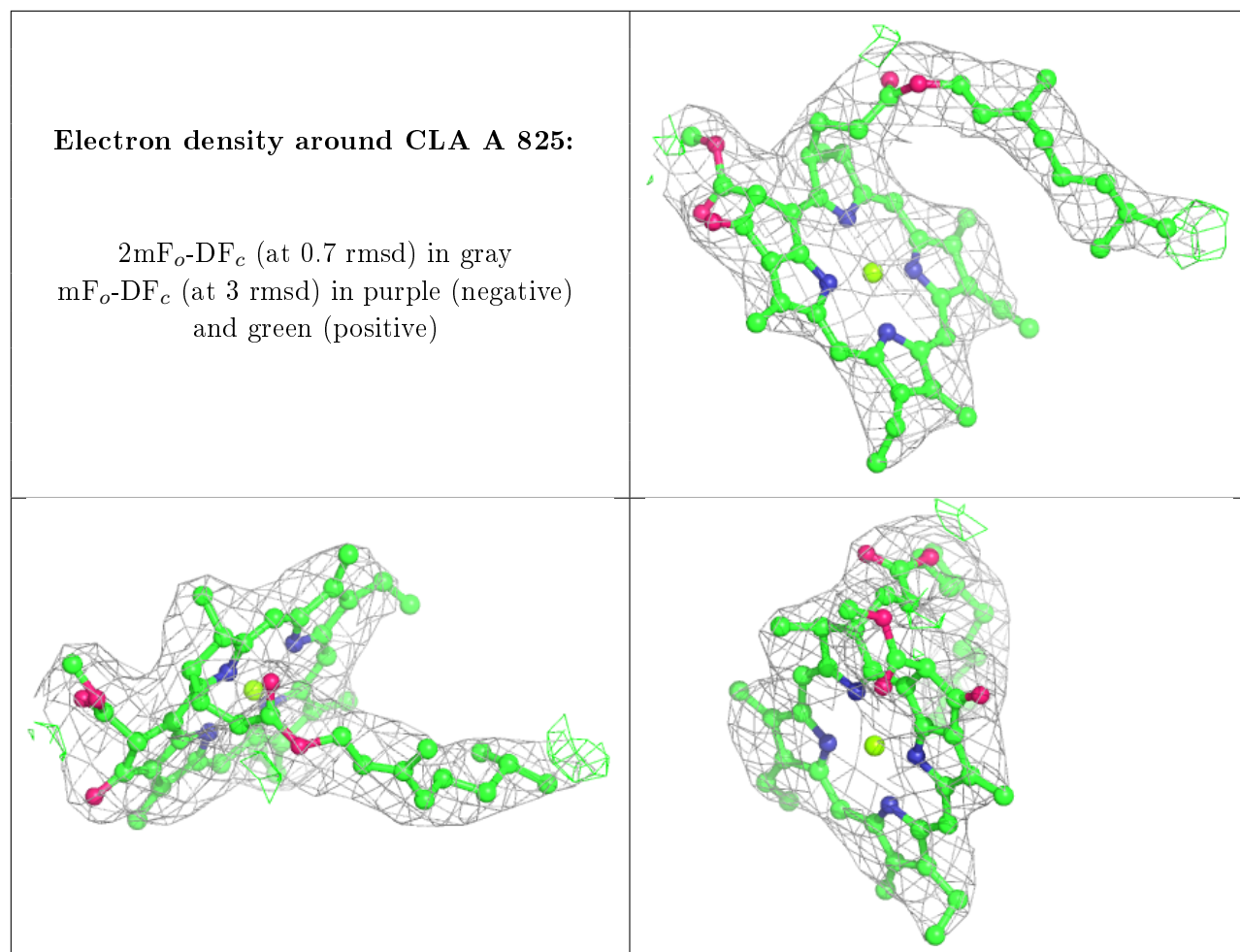


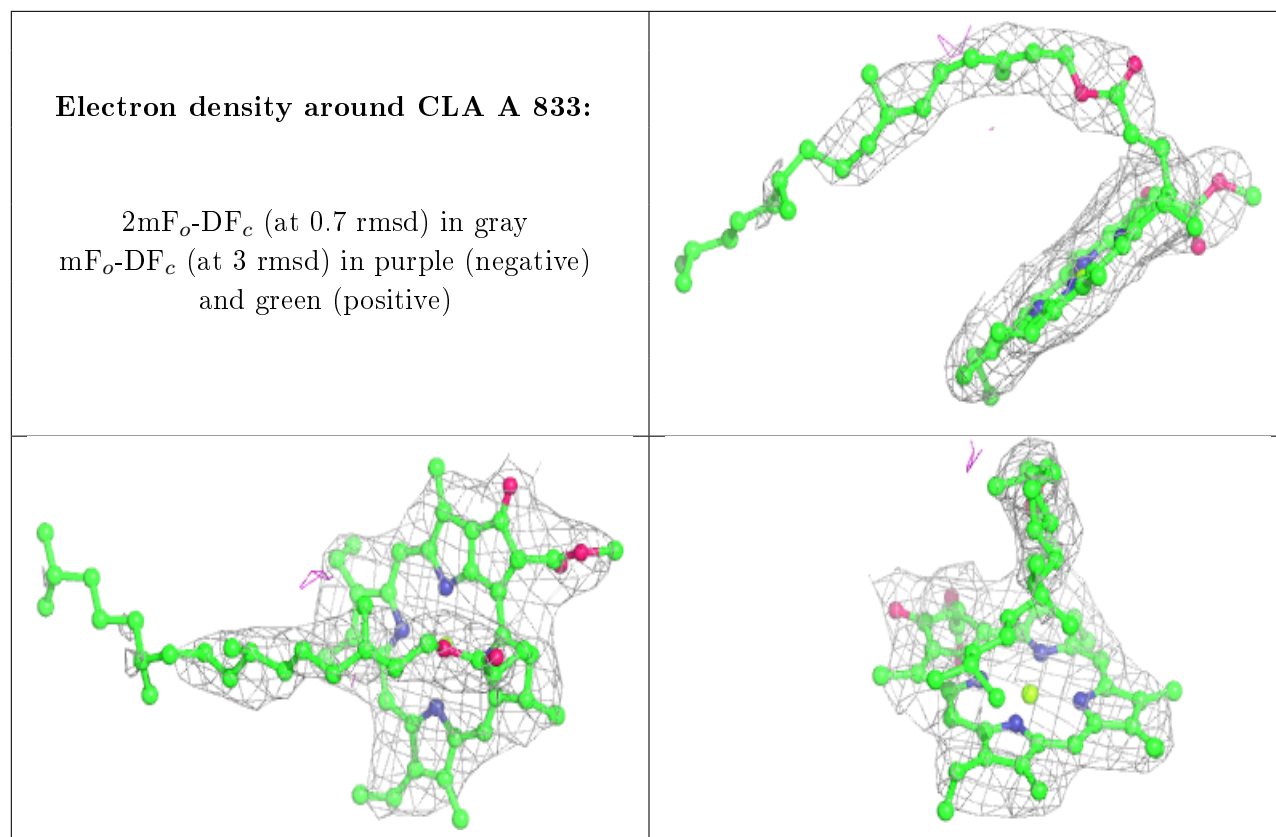


Electron density around CLA a 837:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

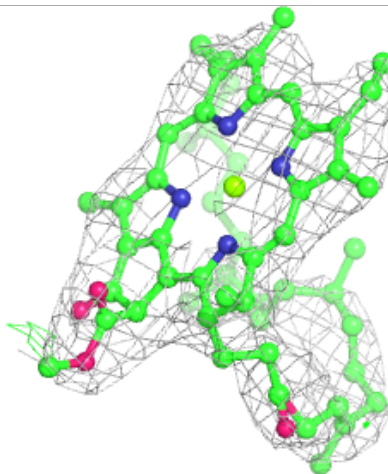
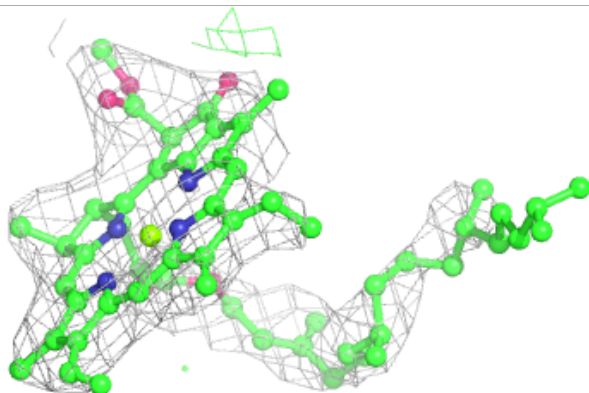
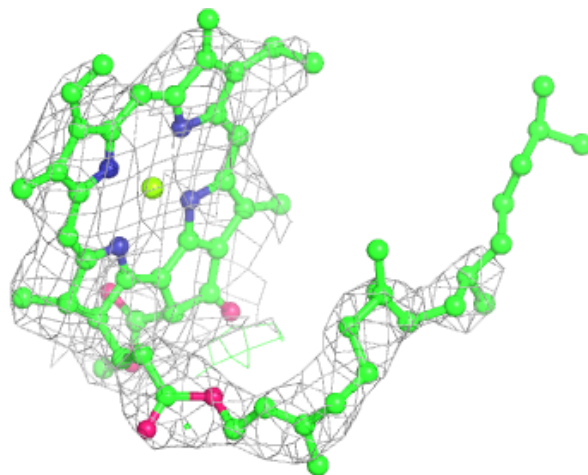






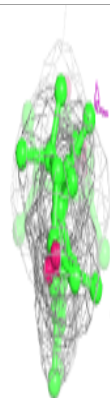
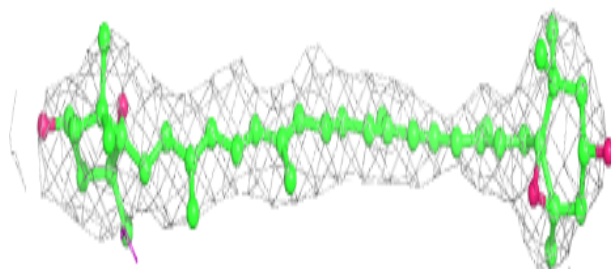
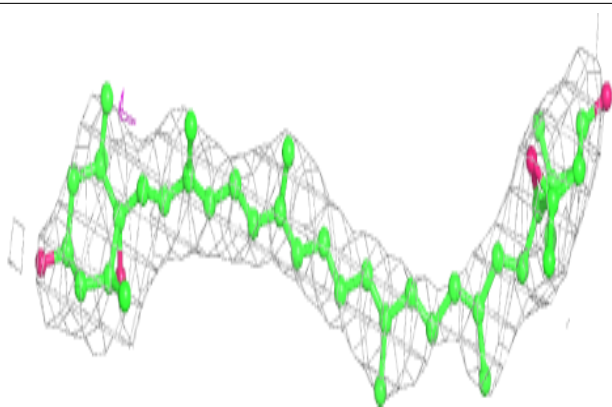
Electron density around CLA b 834:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

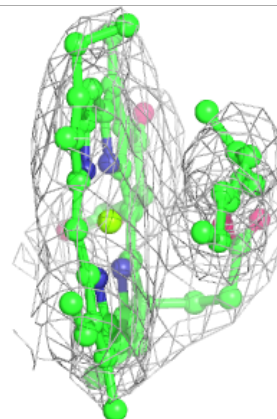
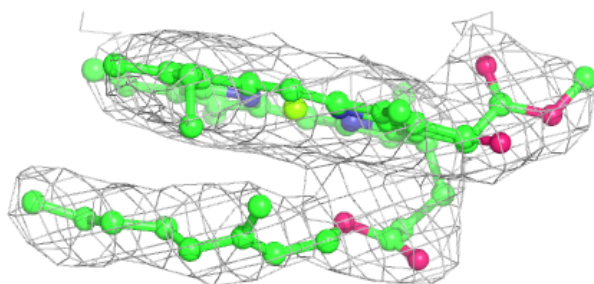
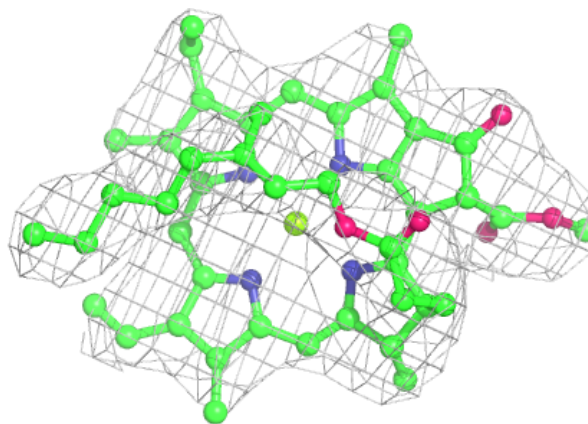


Electron density around XAT 1 317:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

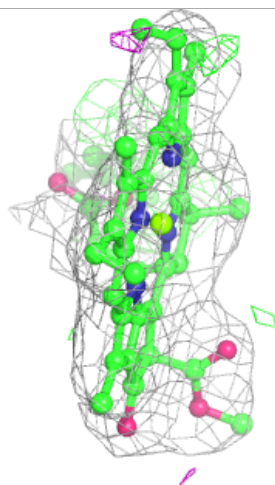
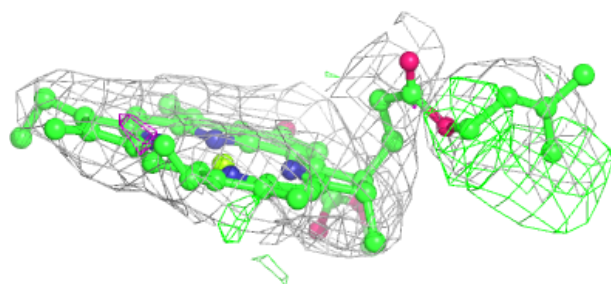
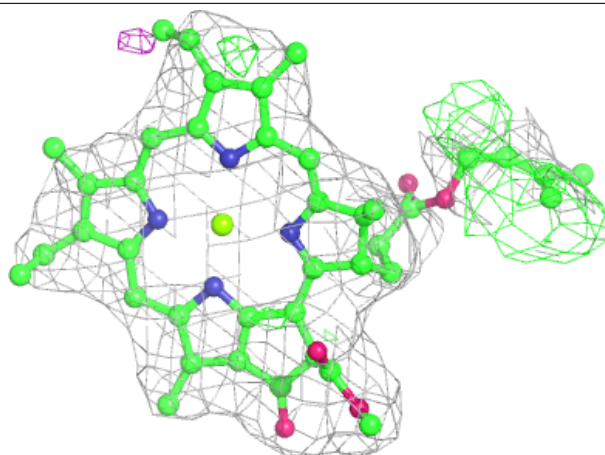
**Electron density around CLA a 813:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



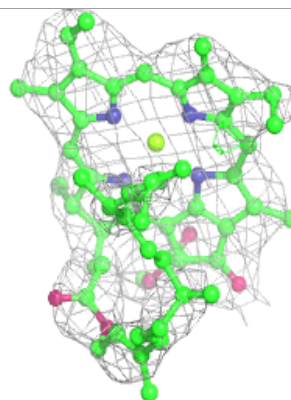
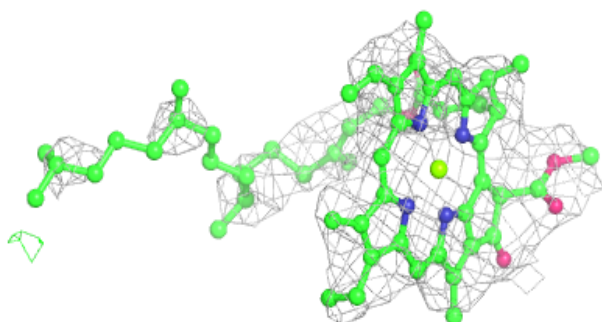
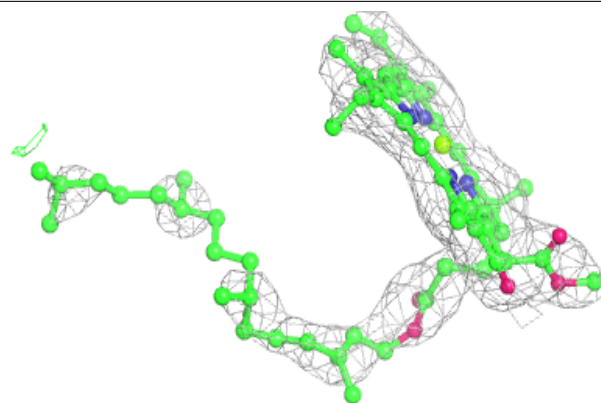
Electron density around CLA 1 204:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

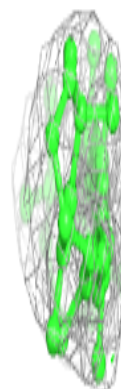
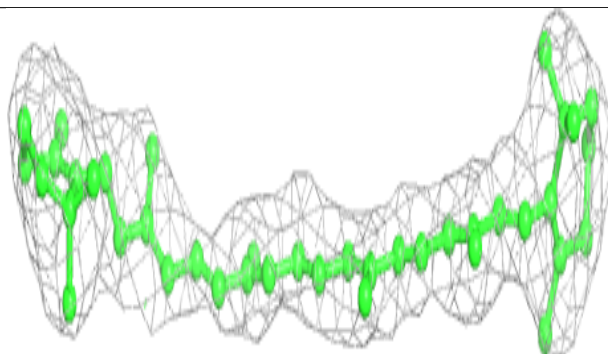
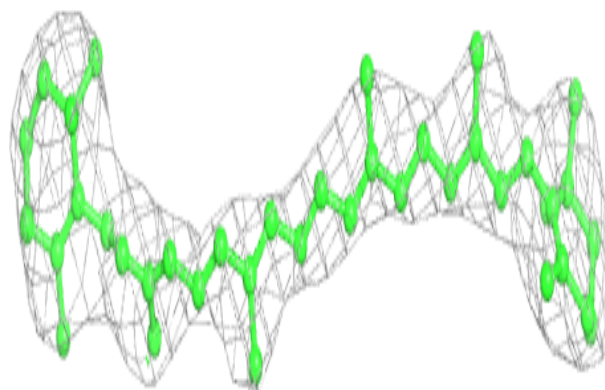


Electron density around CLA a 811:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

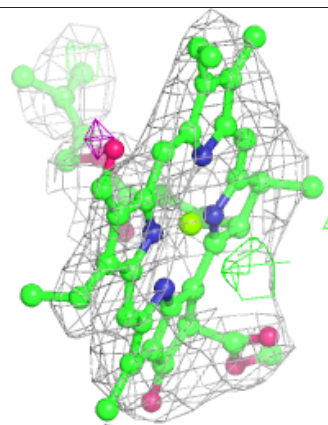
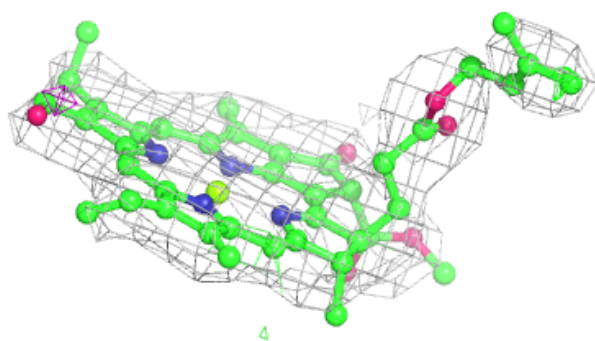
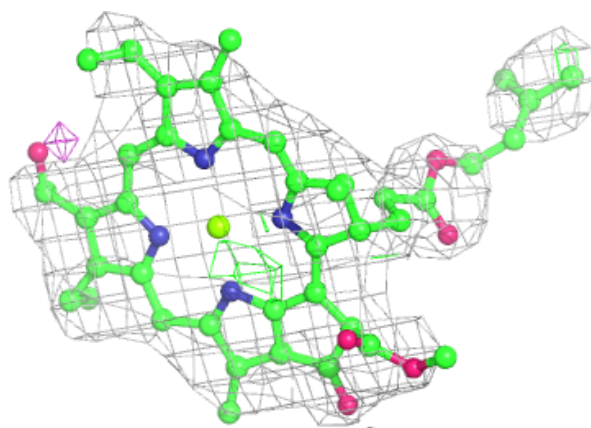
**Electron density around BCR a 853:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

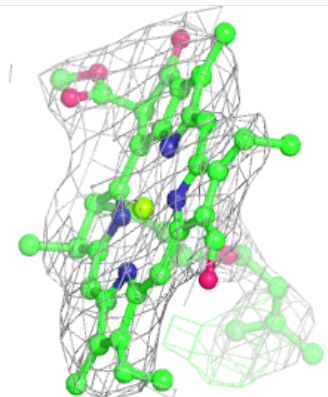
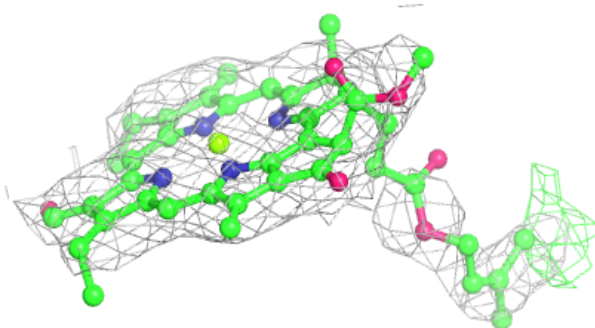
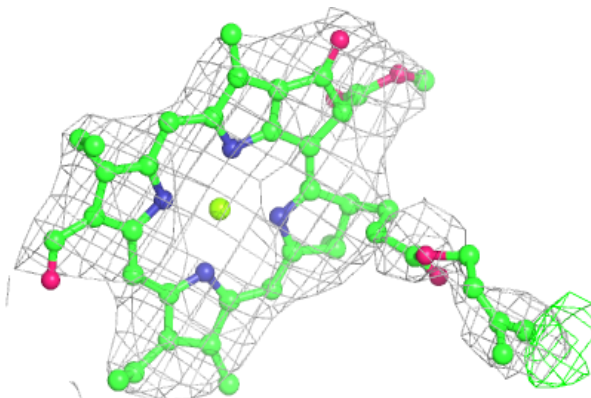


Electron density around CHL 4 607:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

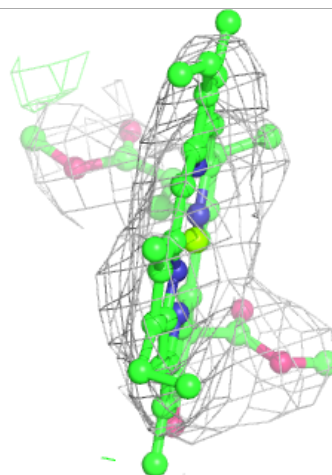
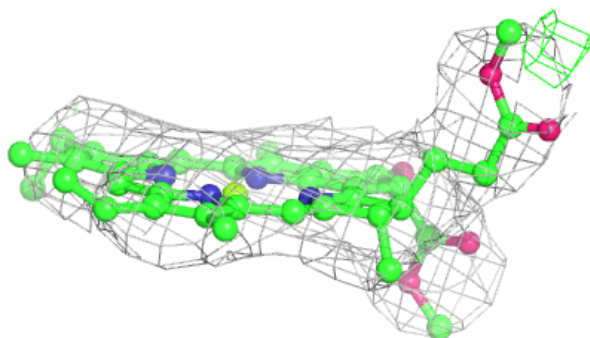
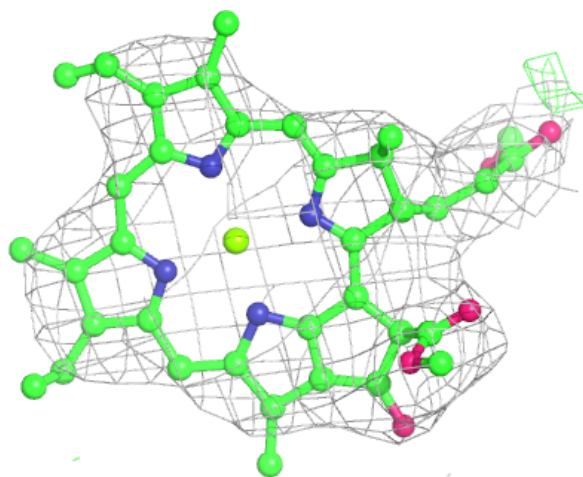
**Electron density around CHL 2 607:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



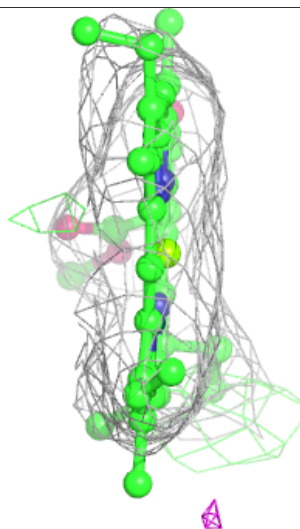
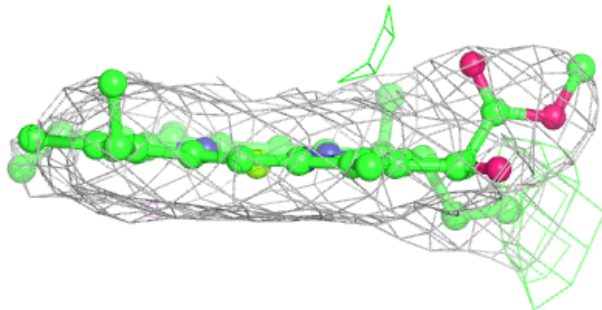
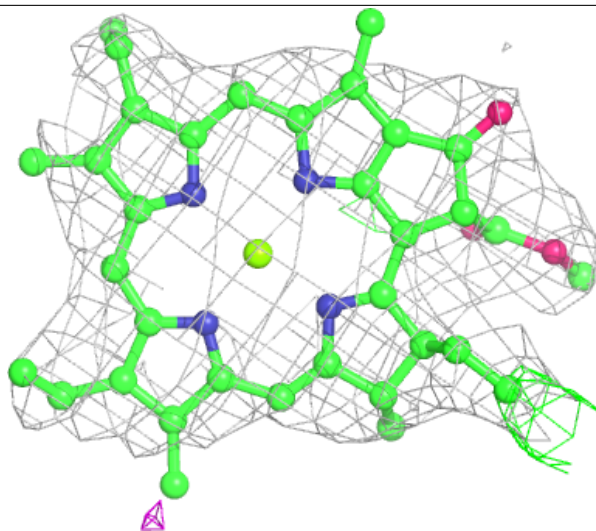
Electron density around CLA 9 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



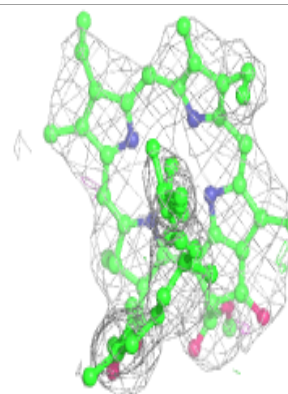
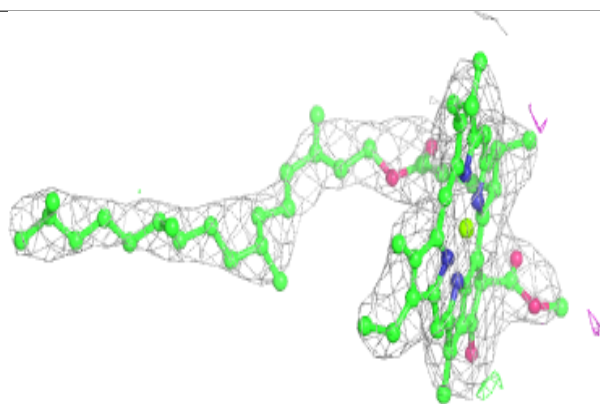
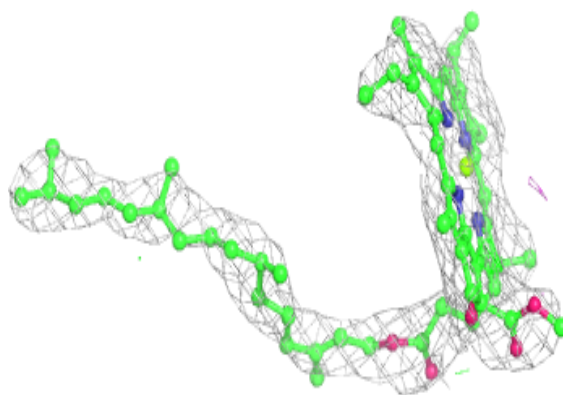
Electron density around CLA 8 304:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

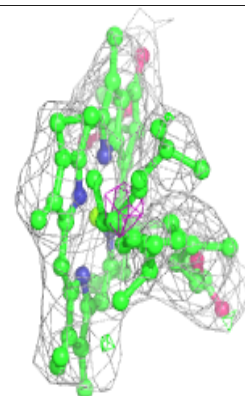
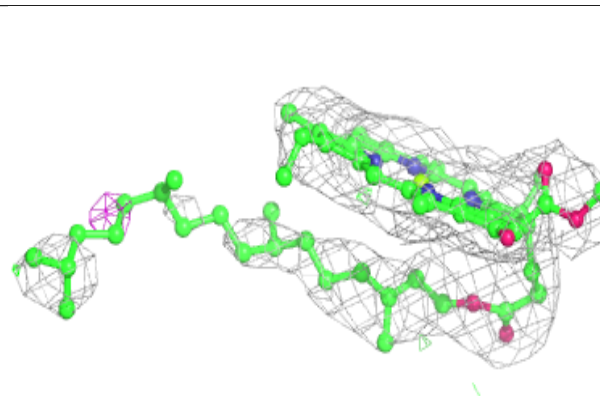
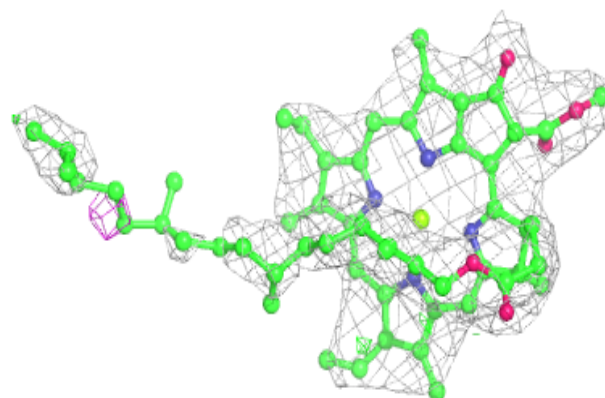


Electron density around CLA b 829:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

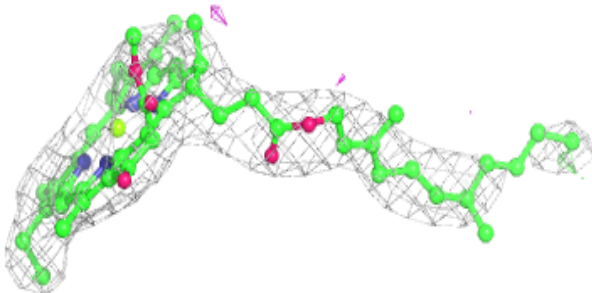
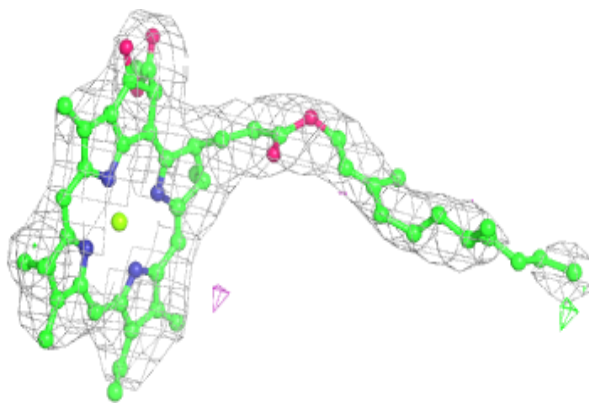
**Electron density around CLA a 819:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

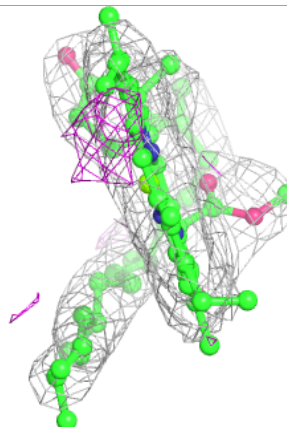
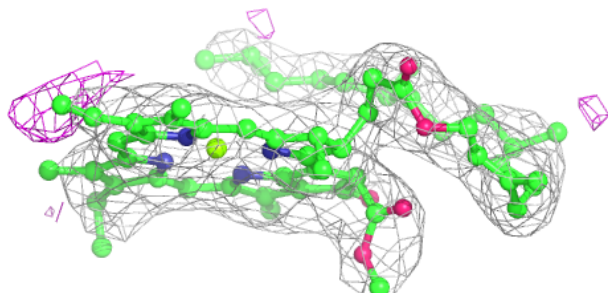
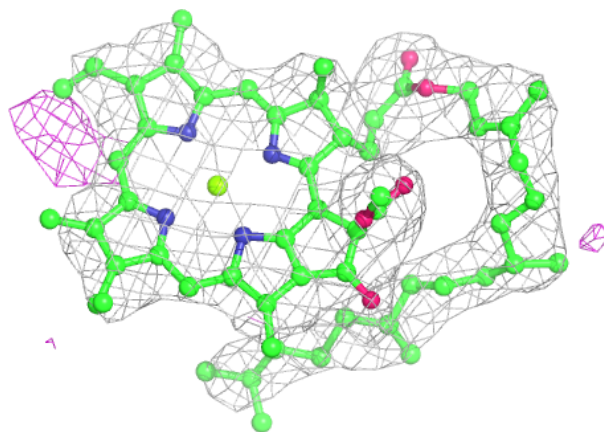


Electron density around CLA b 833:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

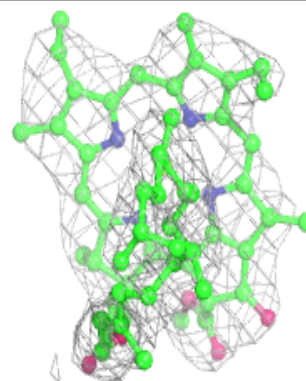
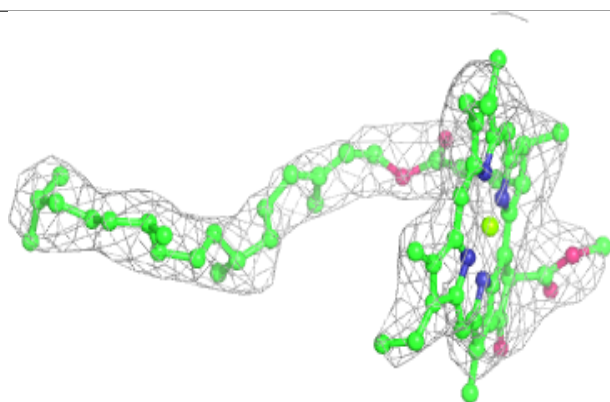
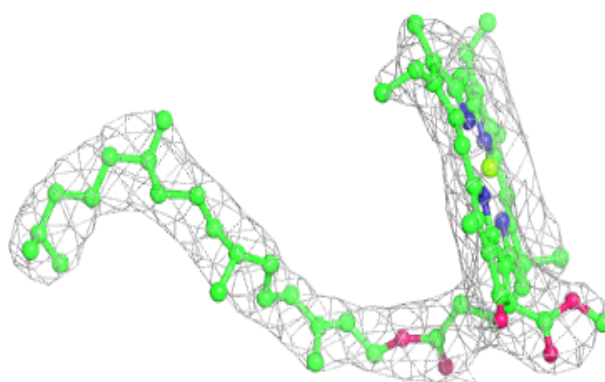
**Electron density around CLA B 805:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

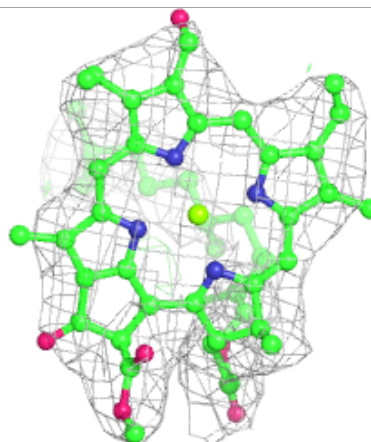
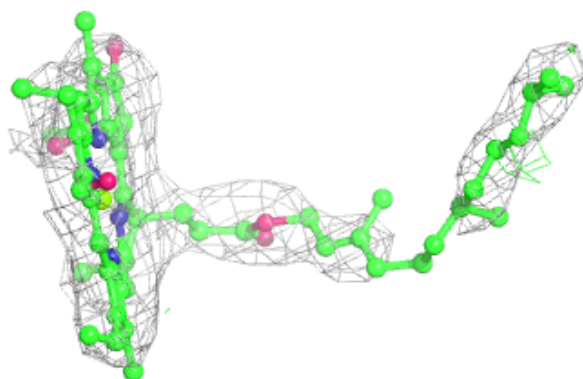
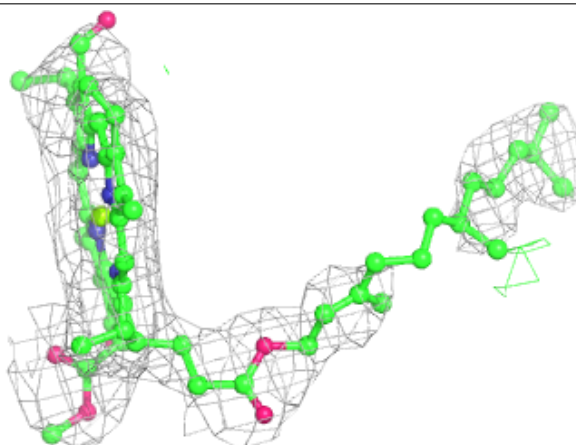


Electron density around CLA A 831:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

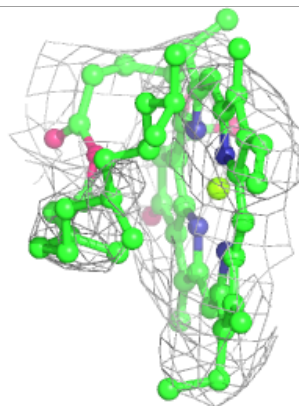
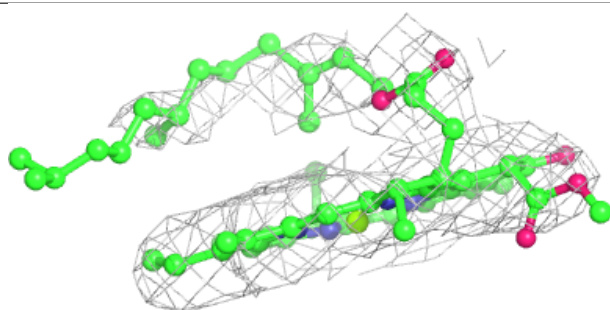
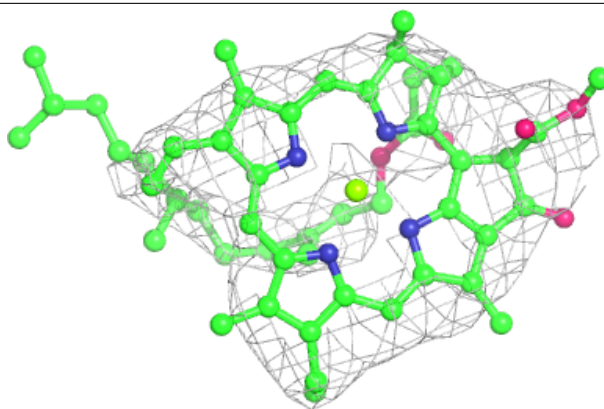
**Electron density around CHL 7 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

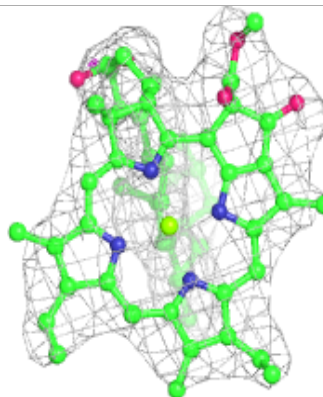
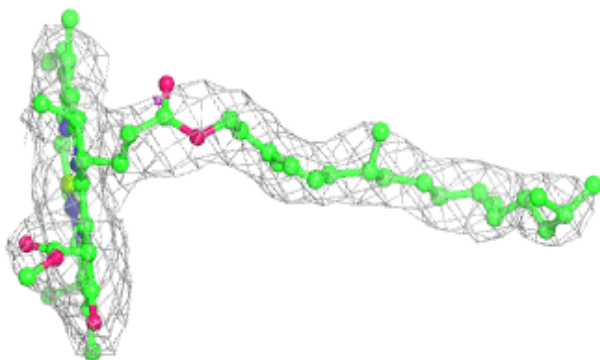
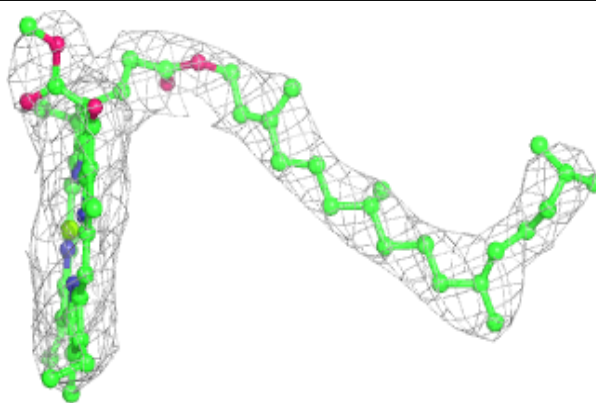


Electron density around CLA 6 314:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

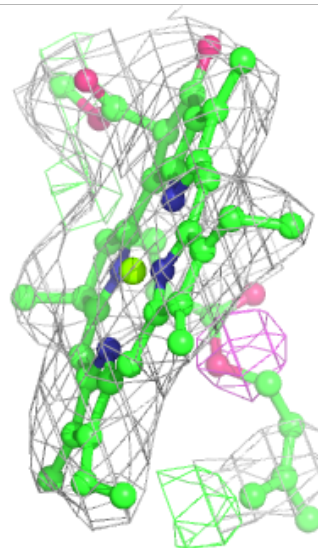
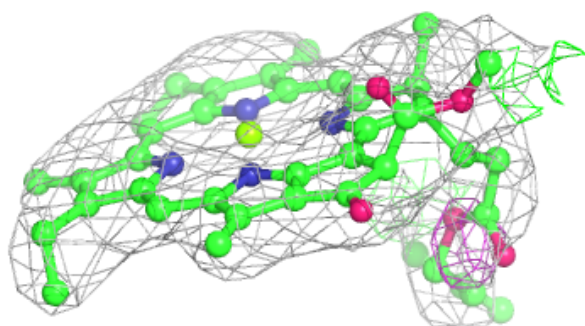
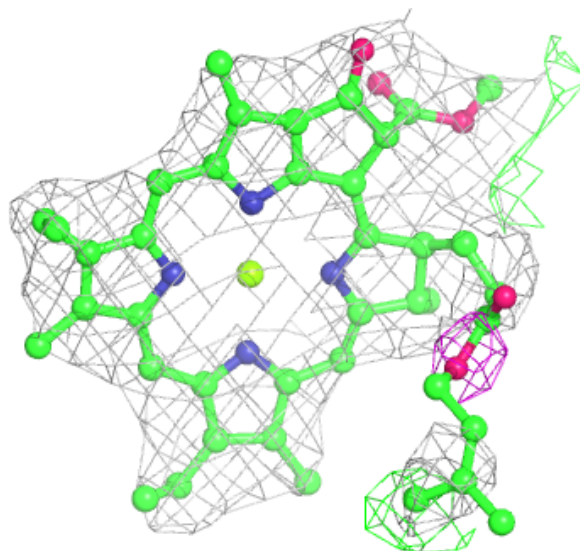
**Electron density around CLA B 840:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



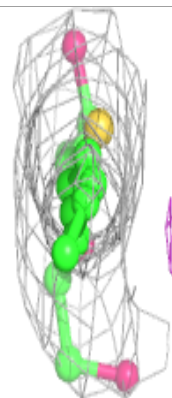
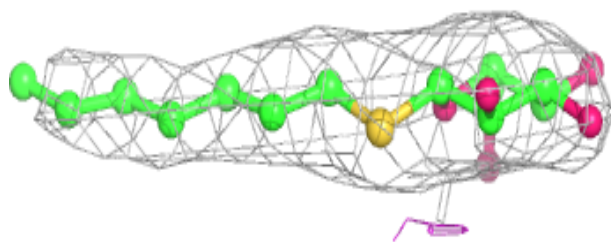
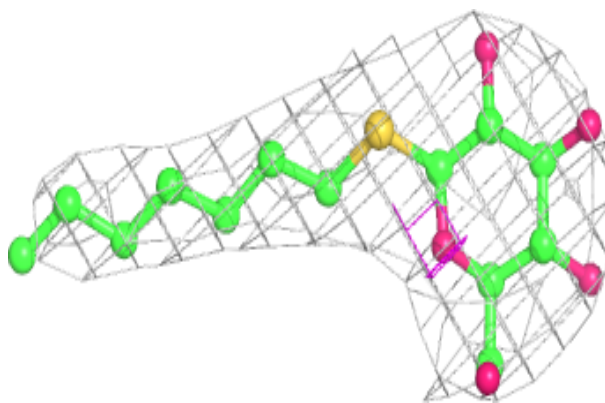
Electron density around CLA a 816:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

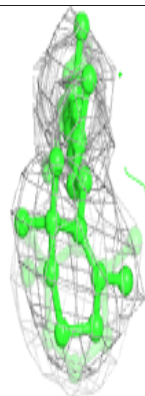
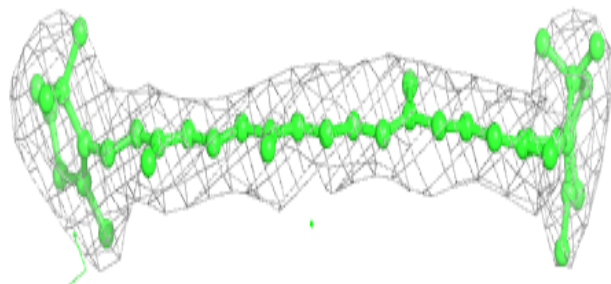
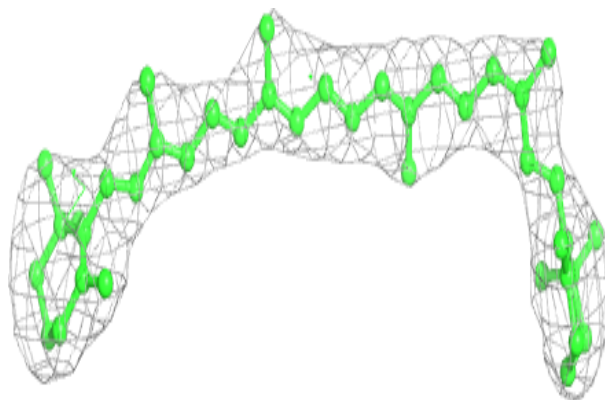


Electron density around HTG a 857:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

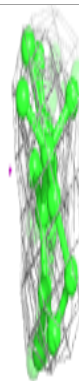
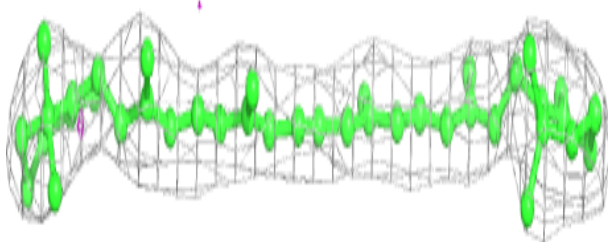
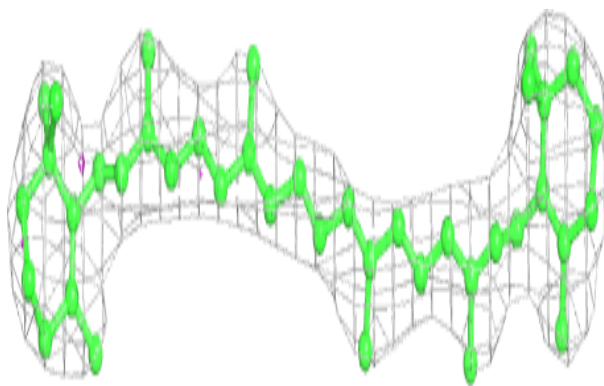
**Electron density around BCR 1 201:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

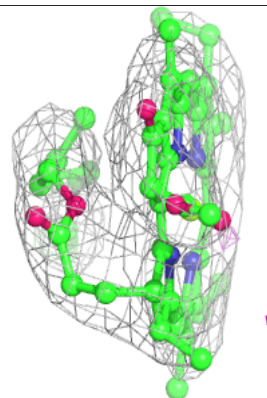
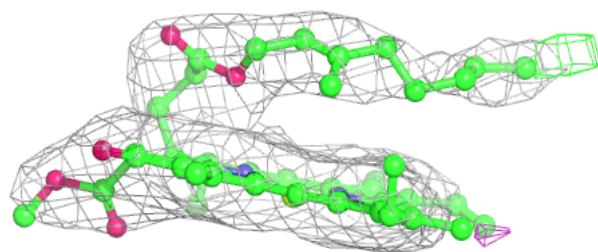
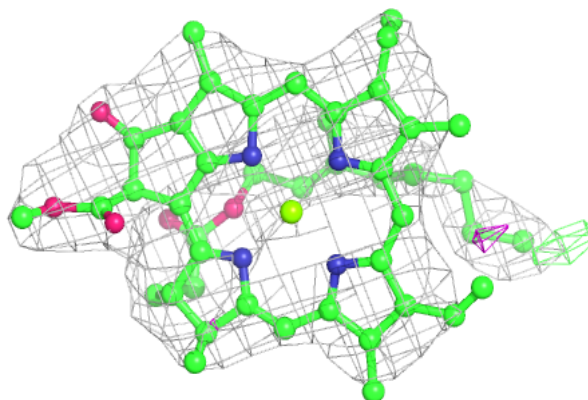


Electron density around BCR I 205:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

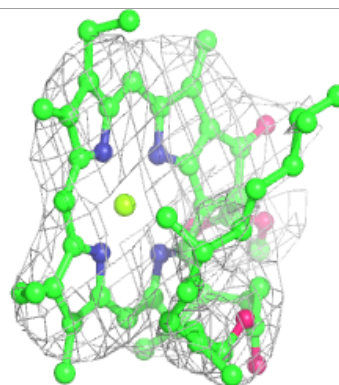
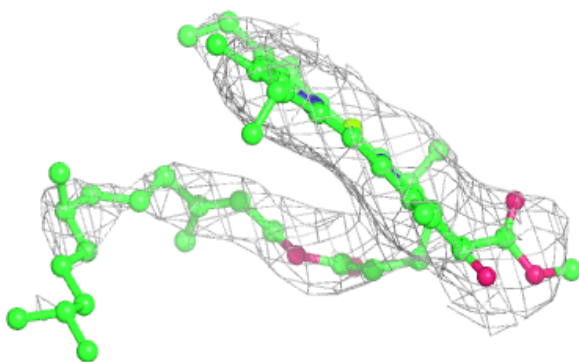
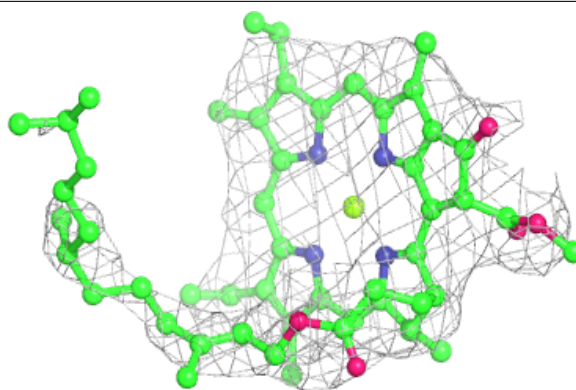
**Electron density around CLA A 813:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



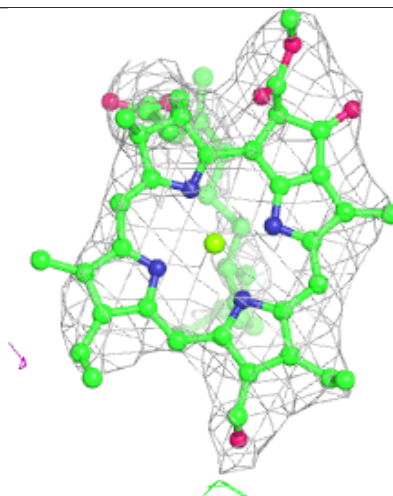
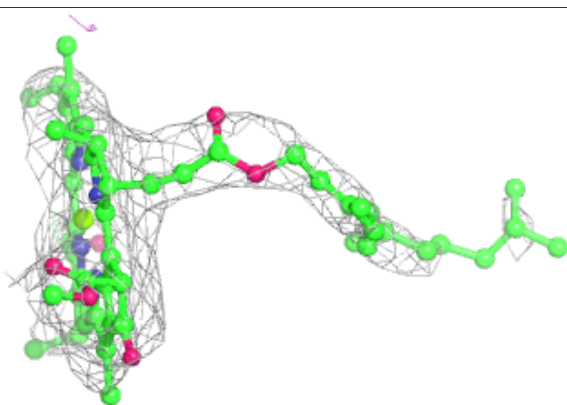
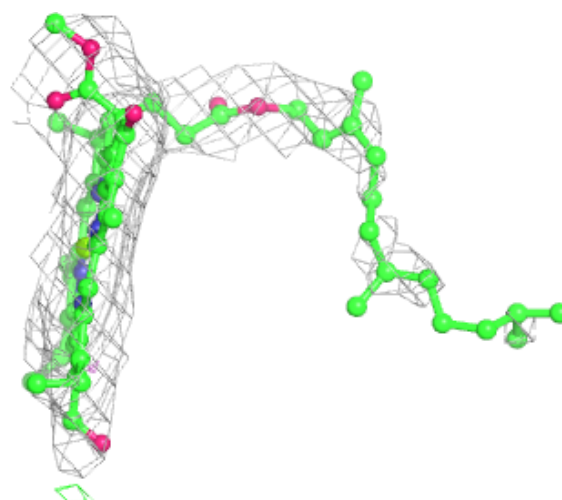
Electron density around CLA 7 609:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



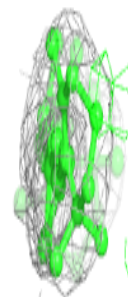
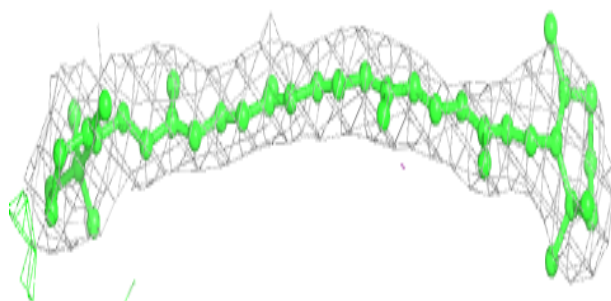
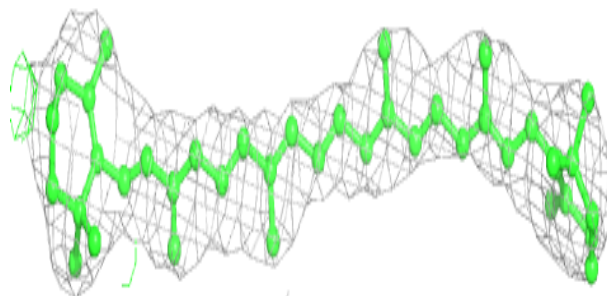
Electron density around CHL 6 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



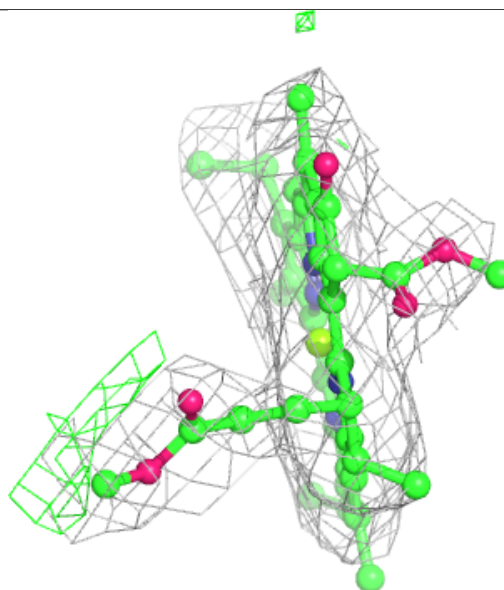
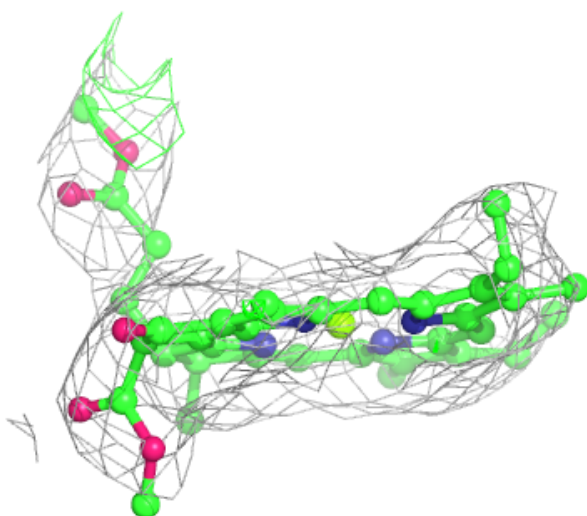
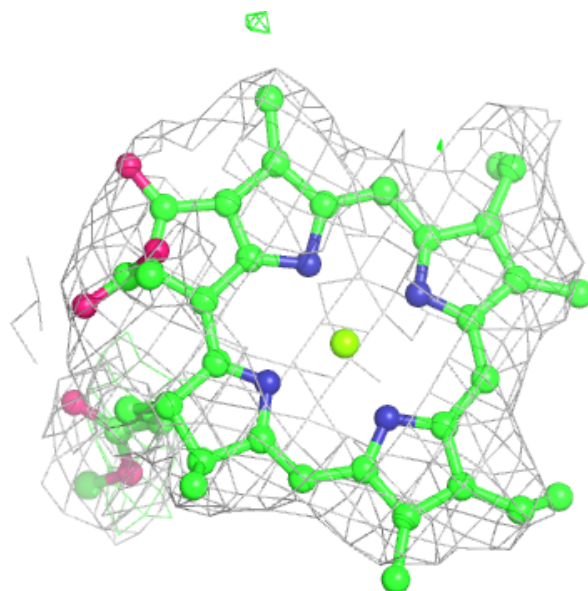
Electron density around BCR b 843:

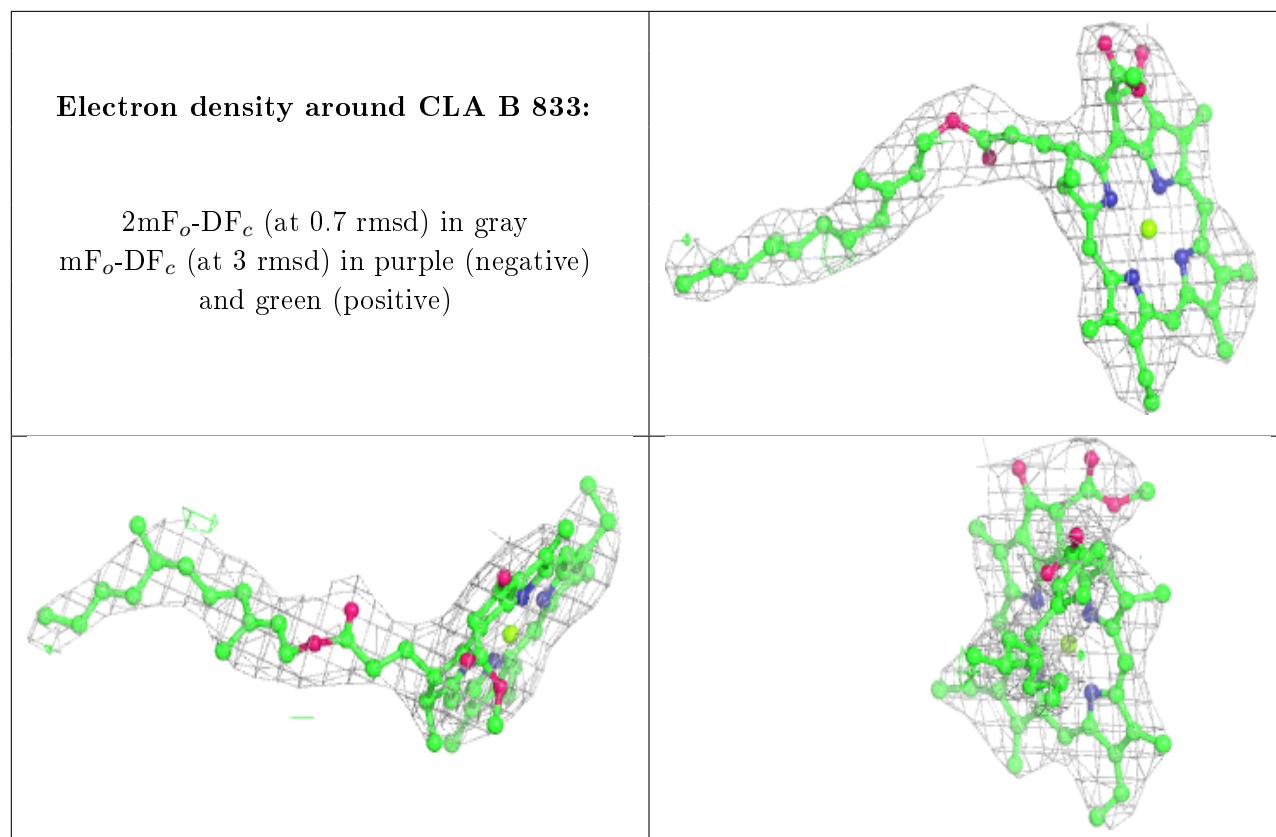
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 821:

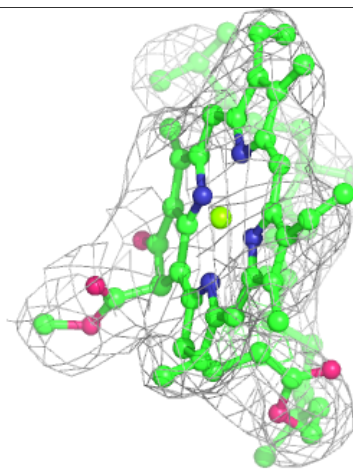
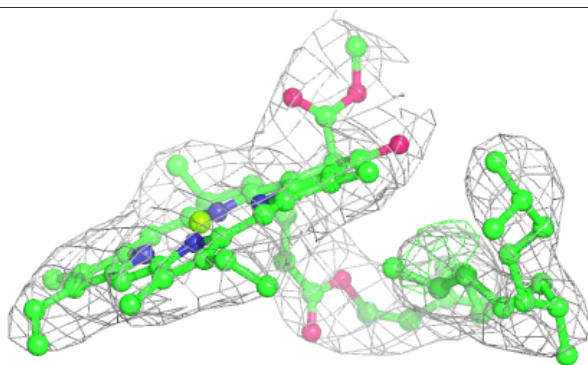
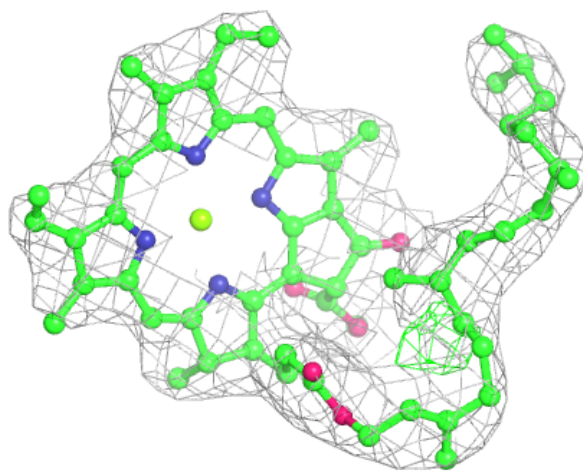
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





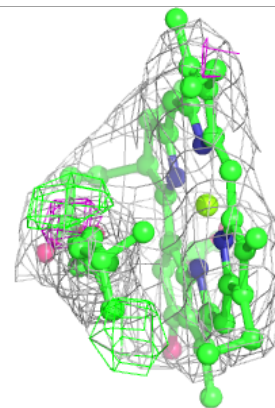
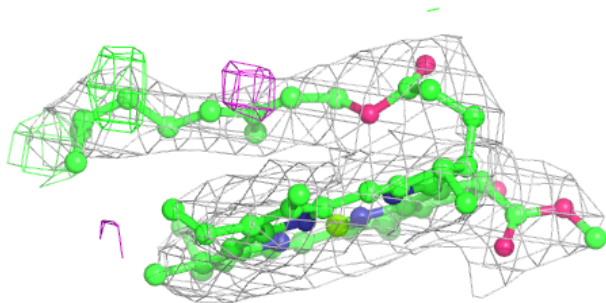
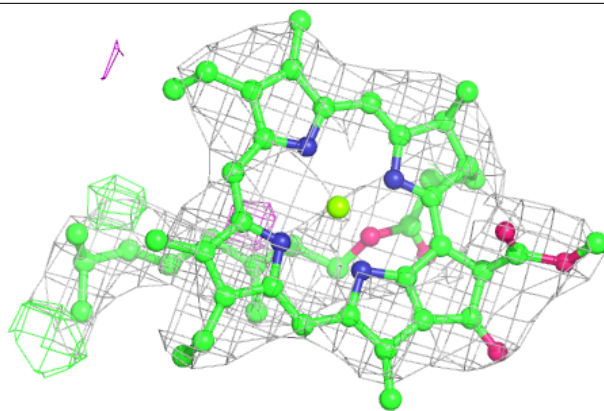
Electron density around CLA b 832:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

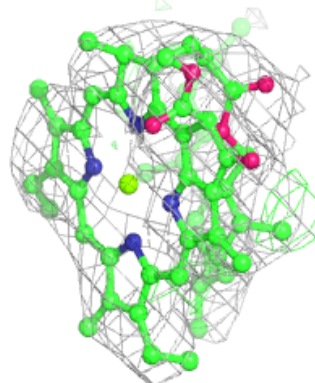
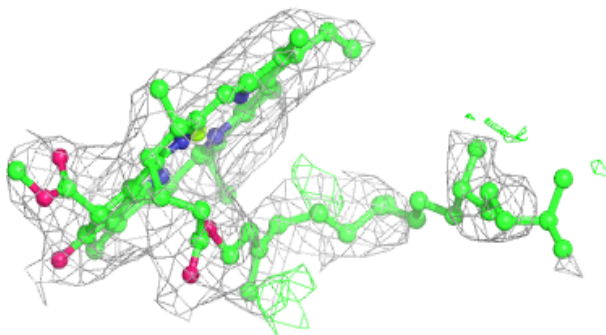
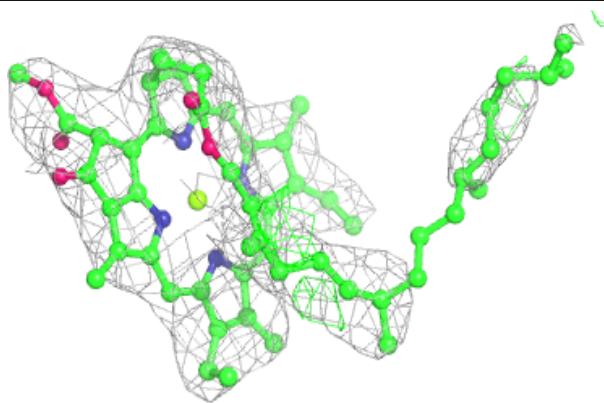


Electron density around CLA B 816:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

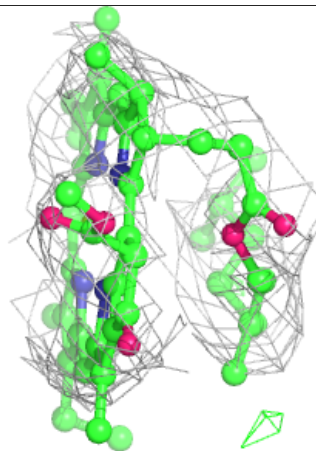
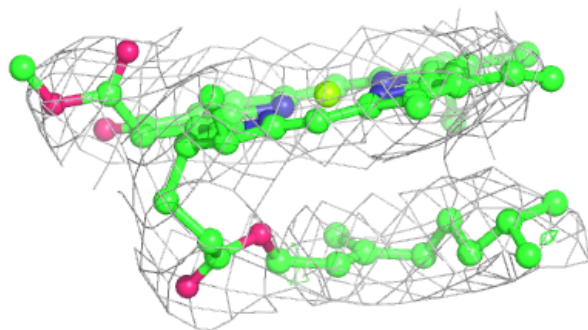
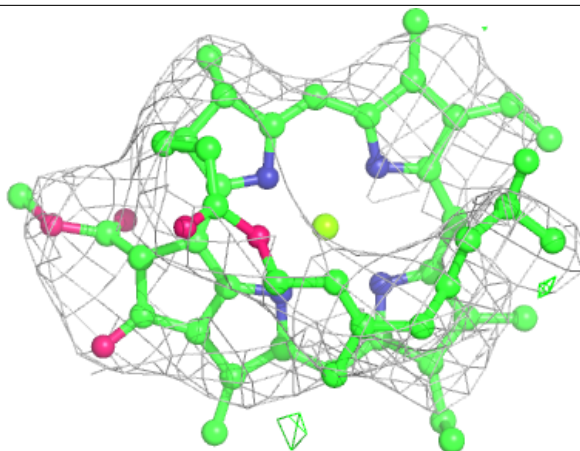
**Electron density around CLA B 807:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

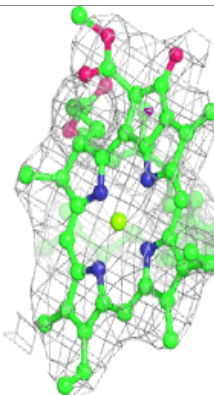
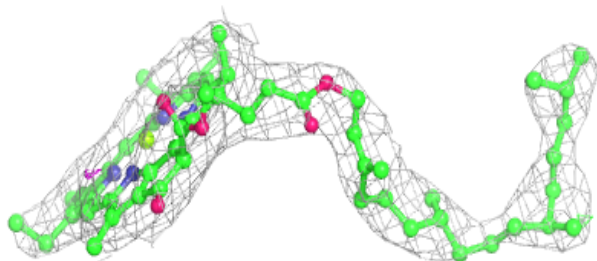
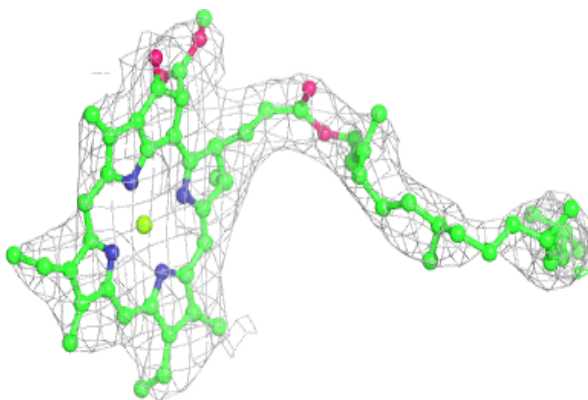


Electron density around CLA 3 312:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

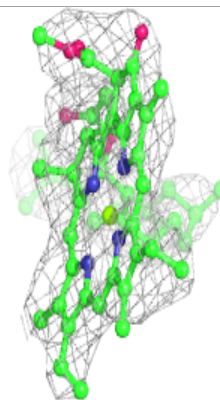
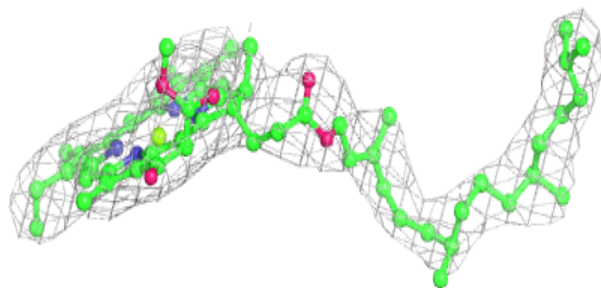
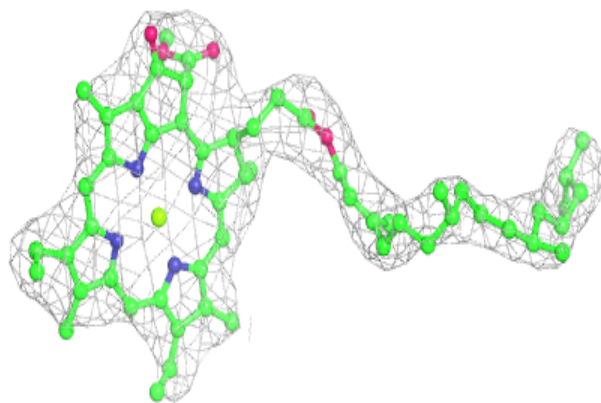
**Electron density around CLA B 809:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

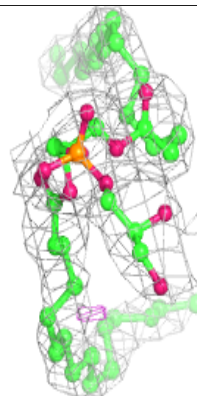
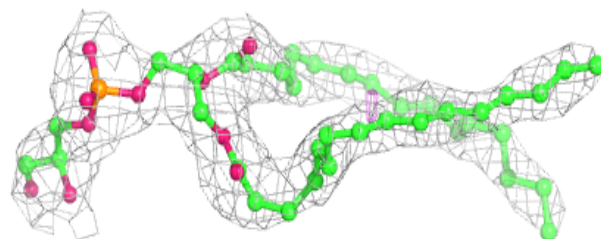
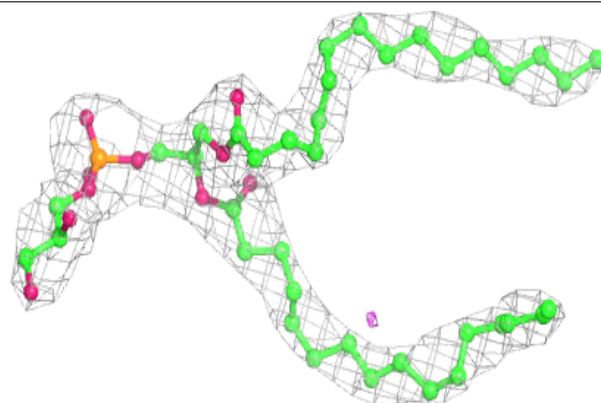


Electron density around CLA b 813:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

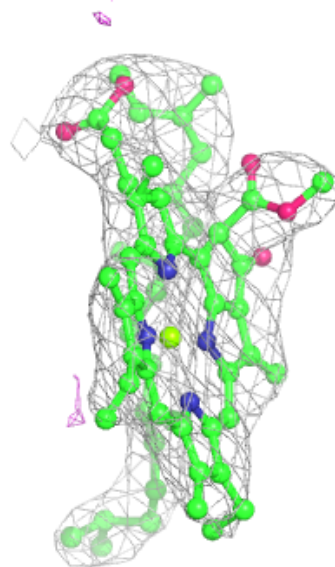
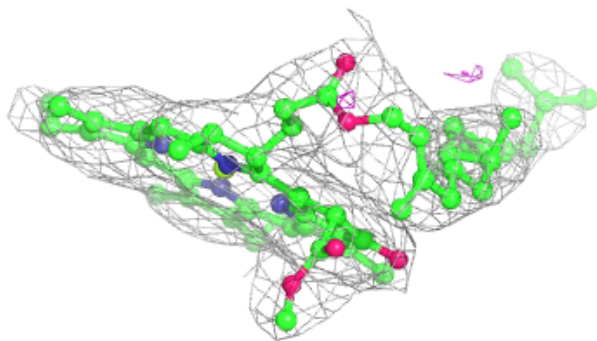
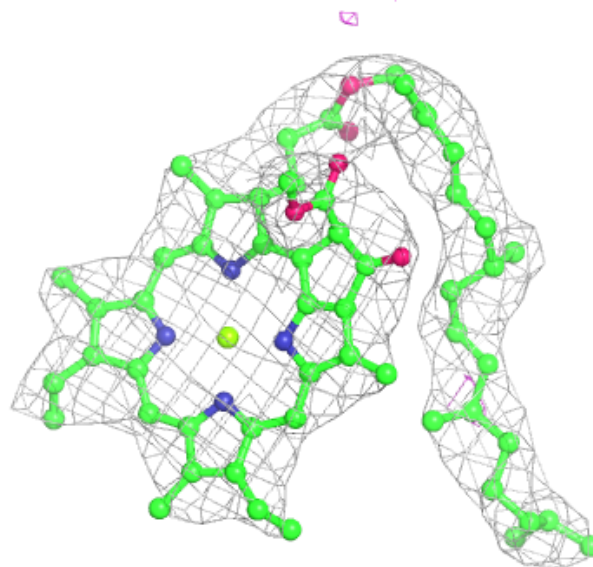
**Electron density around LHG A 846:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



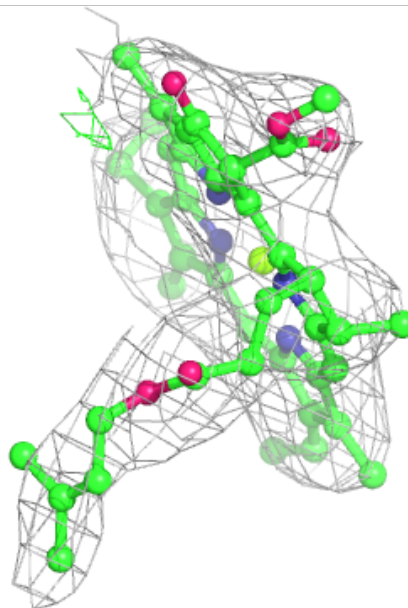
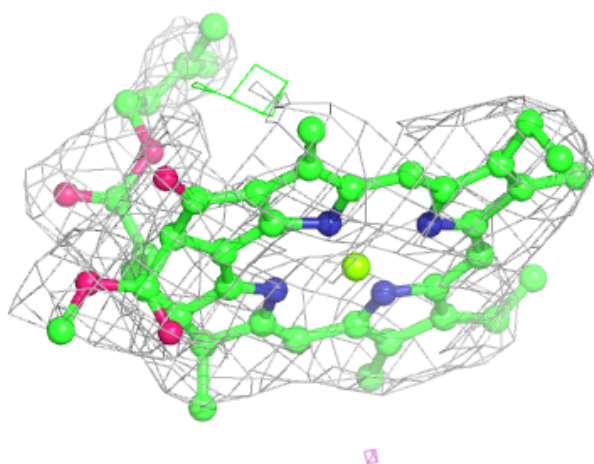
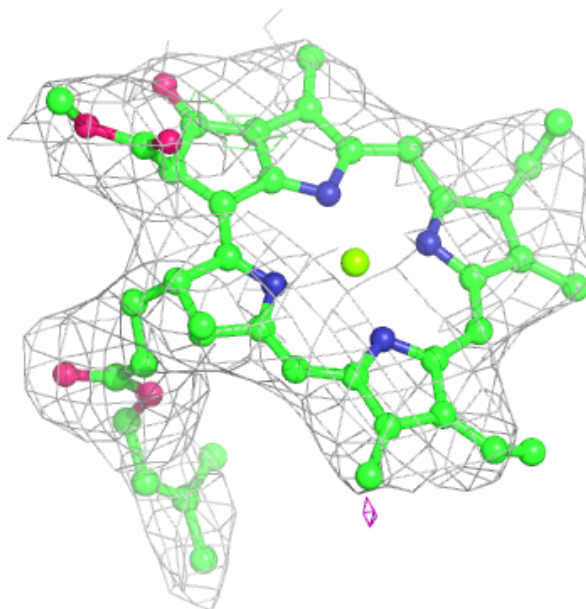
Electron density around CLA a 826:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



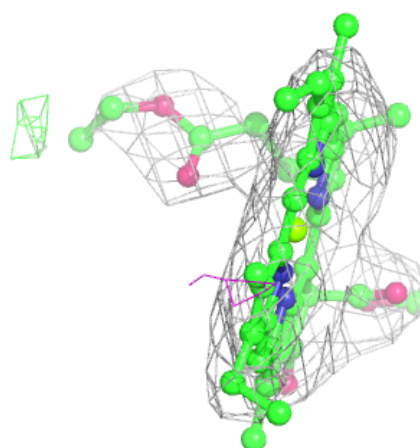
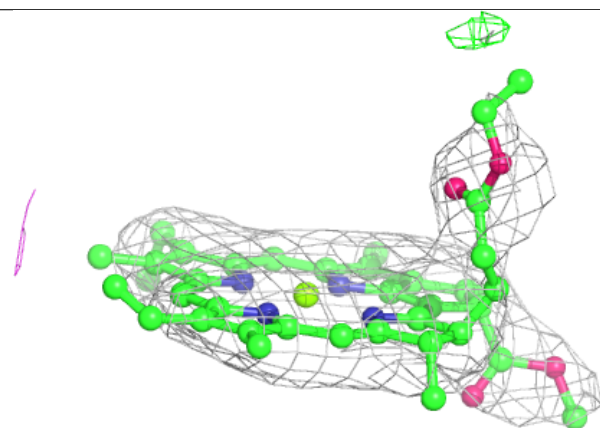
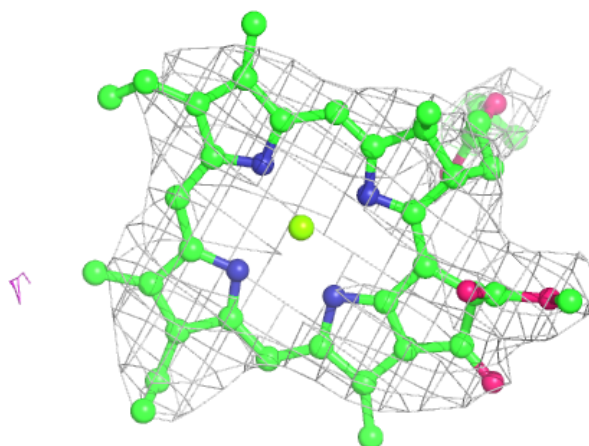
Electron density around CLA 4 608:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



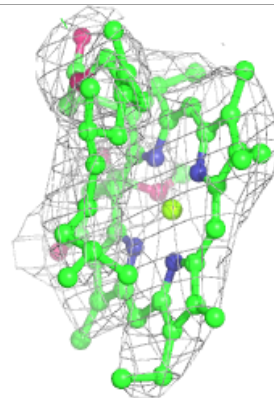
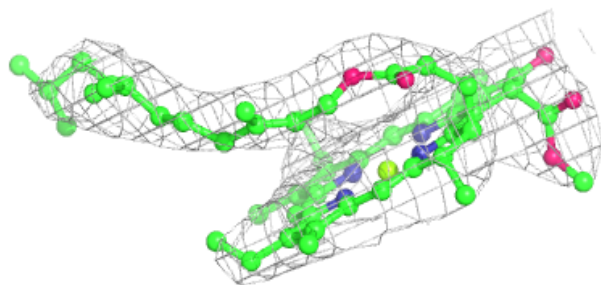
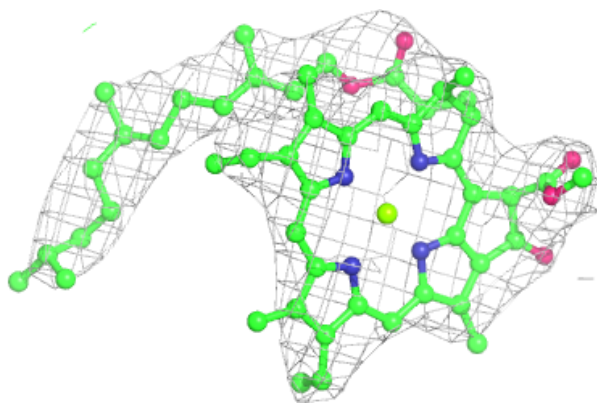
Electron density around CLA 3 306:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



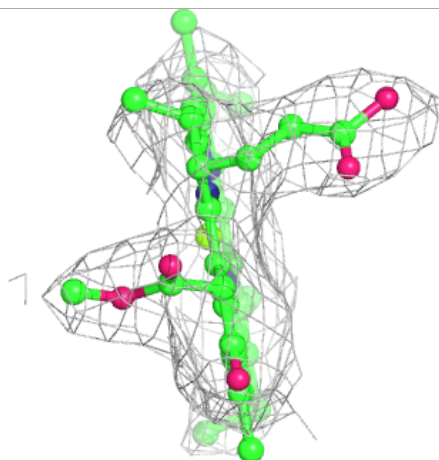
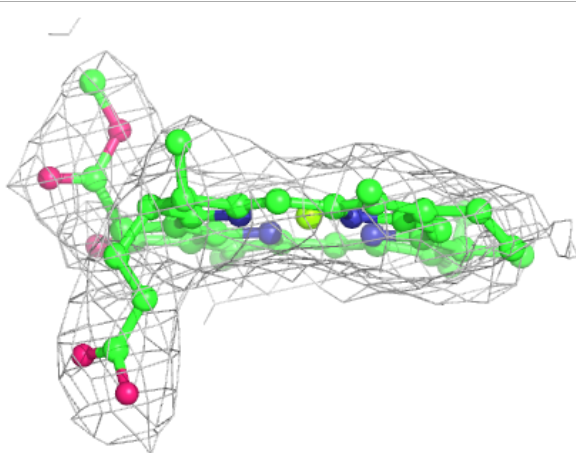
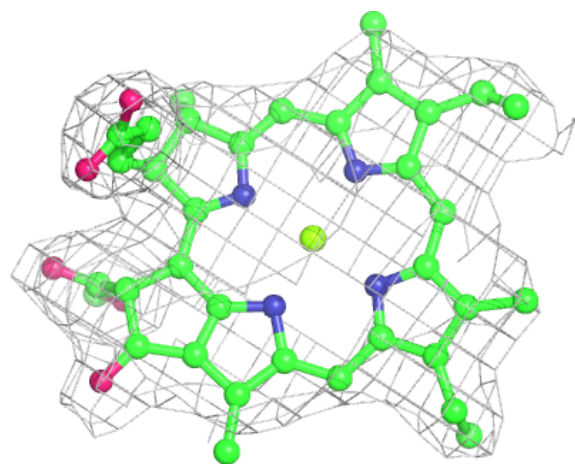
Electron density around CLA 9 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



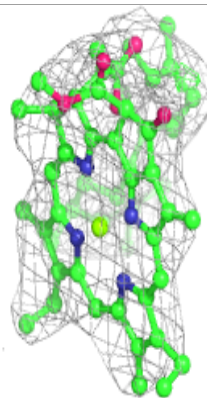
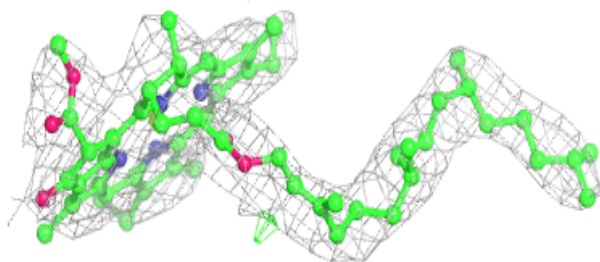
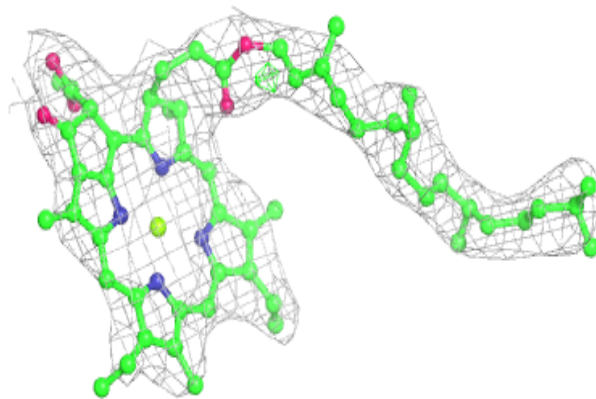
Electron density around CLA a 815:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

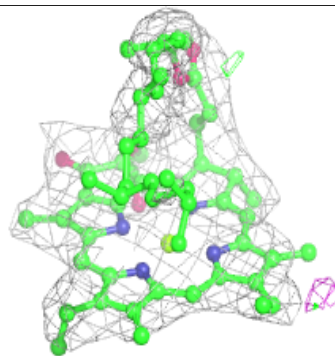
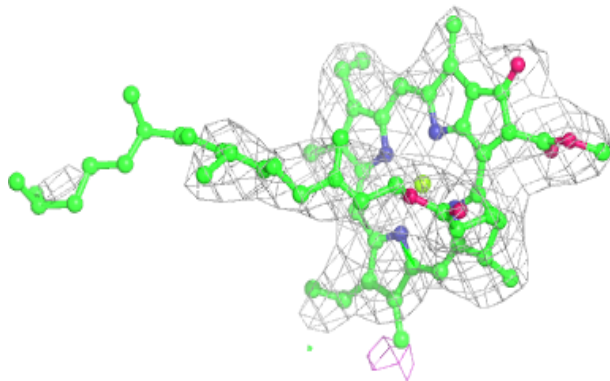
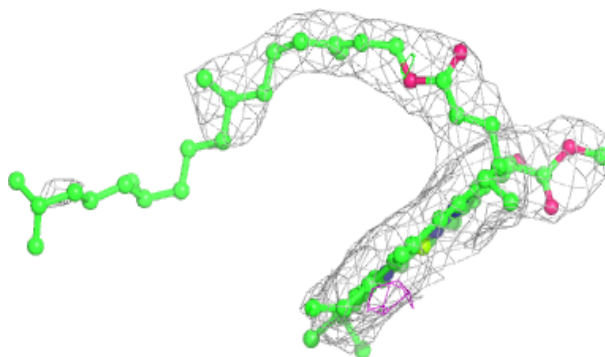


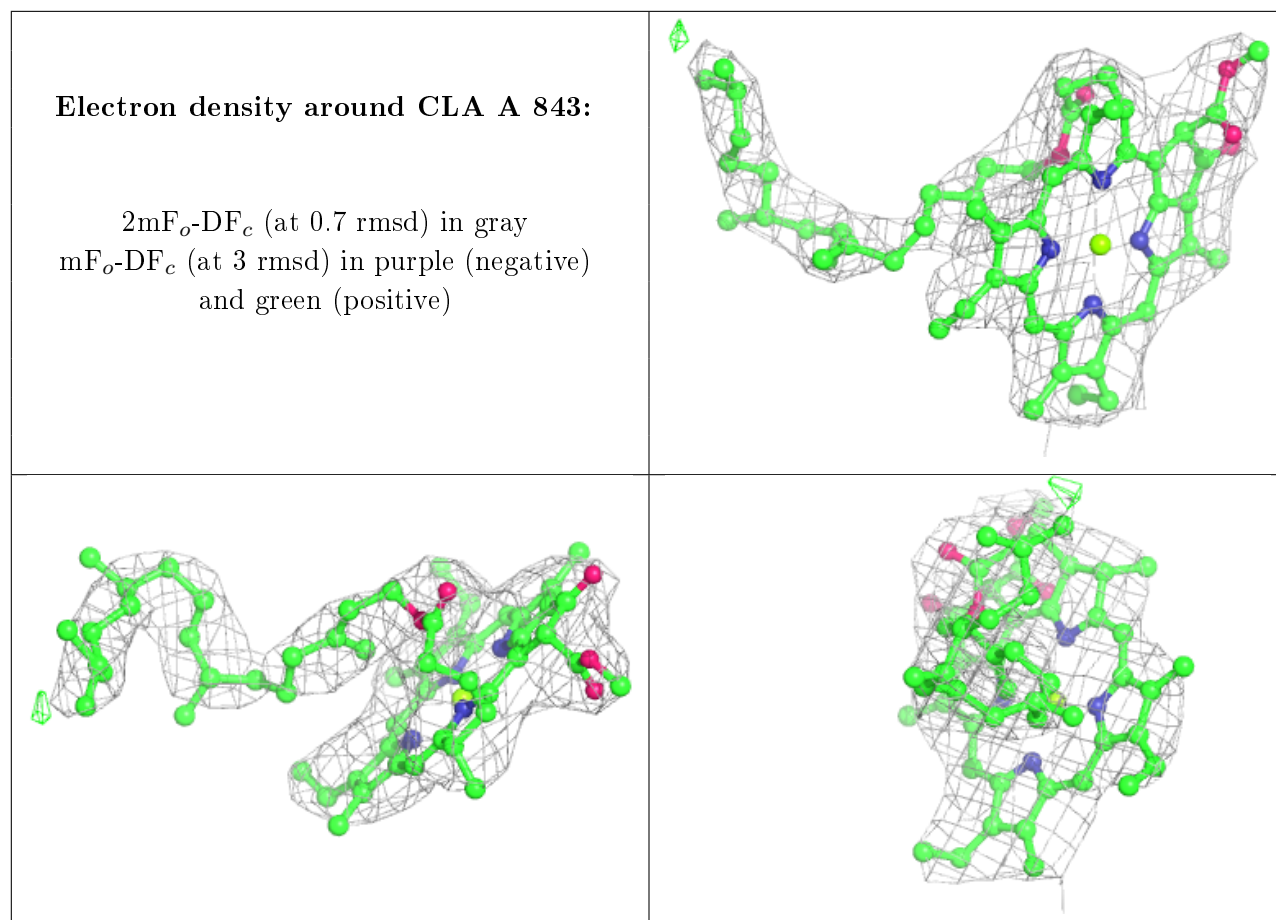
Electron density around CLA A 809:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CLA a 833:**

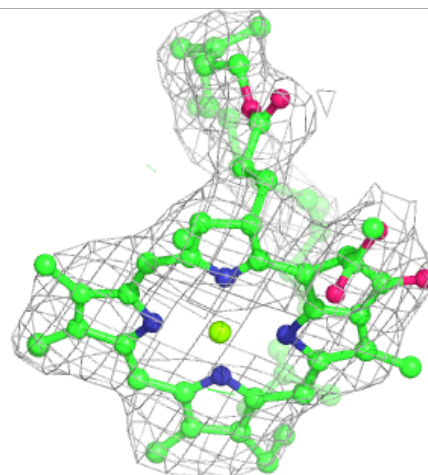
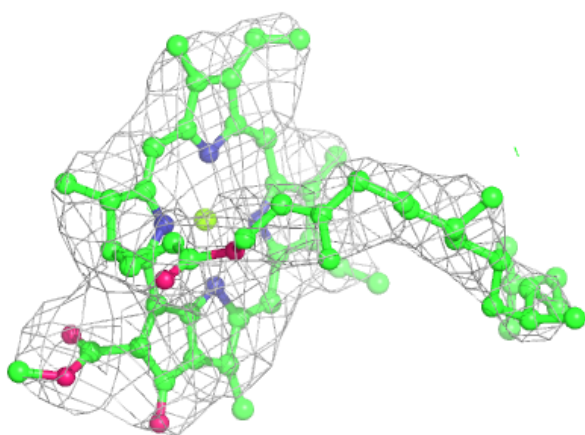
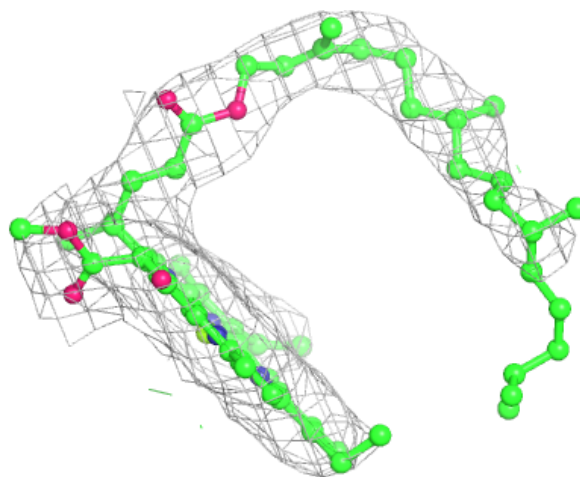
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





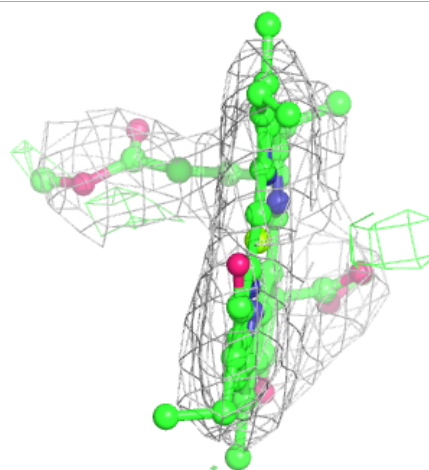
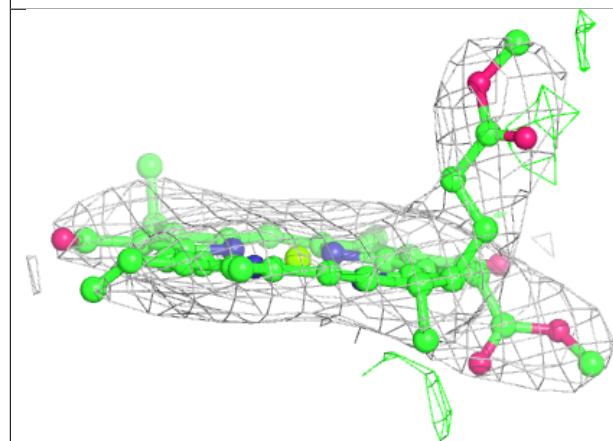
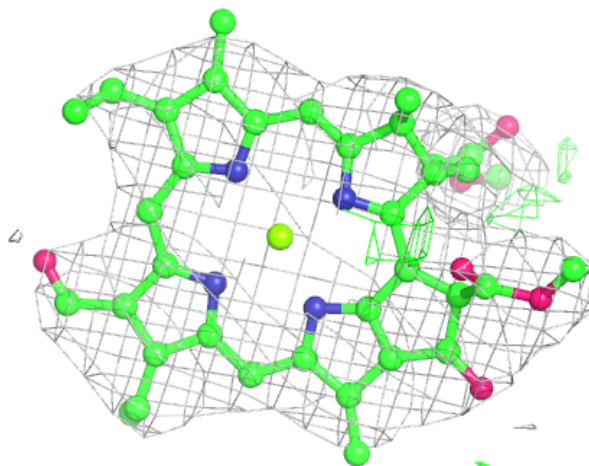
Electron density around CLA b 819:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



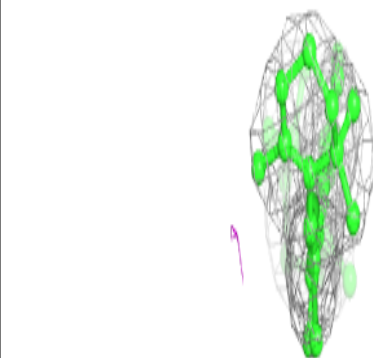
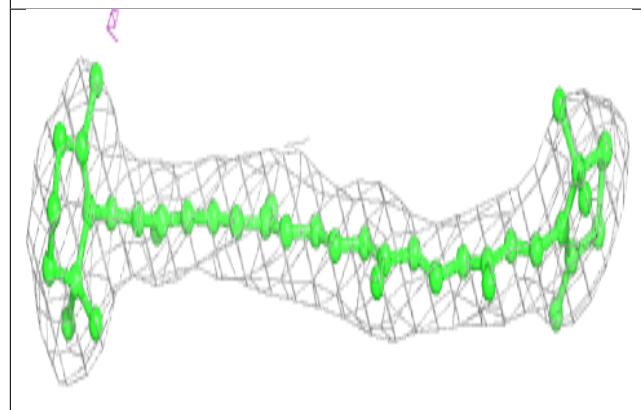
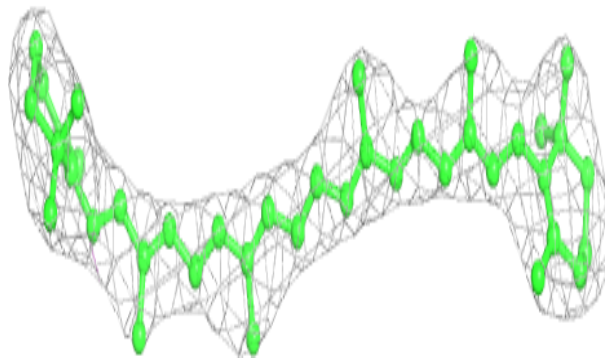
Electron density around CHL 8 306:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

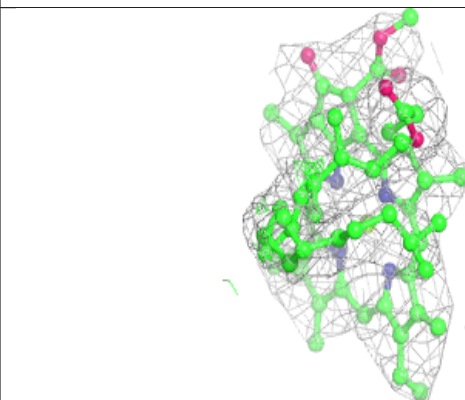
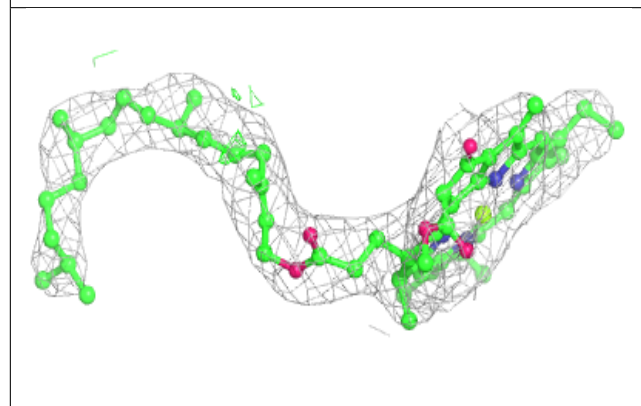
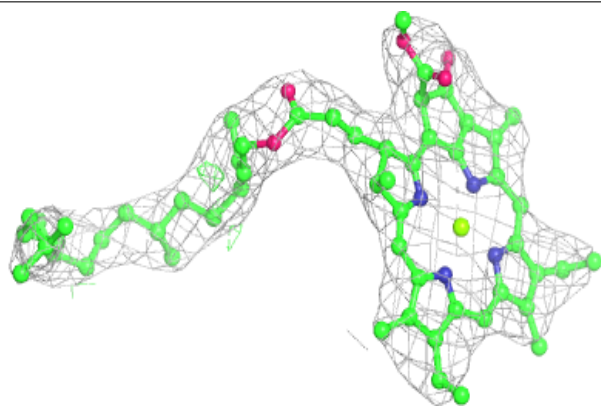


Electron density around BCR b 848:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

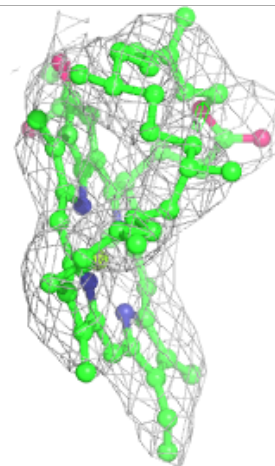
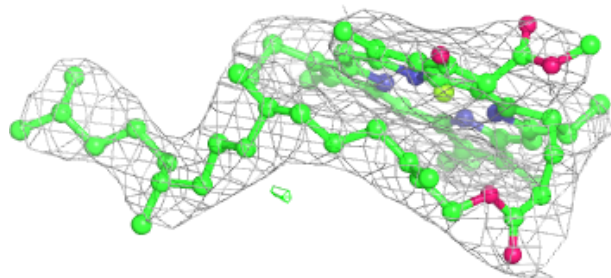
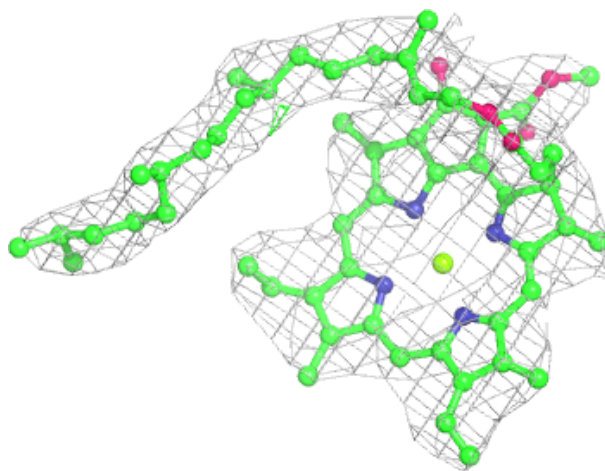
**Electron density around CLA b 809:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



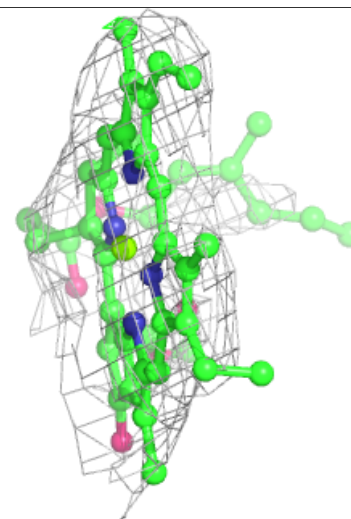
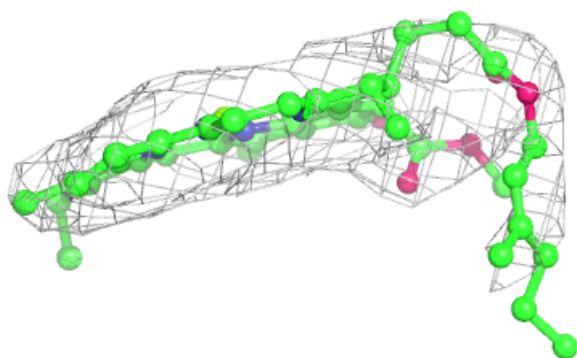
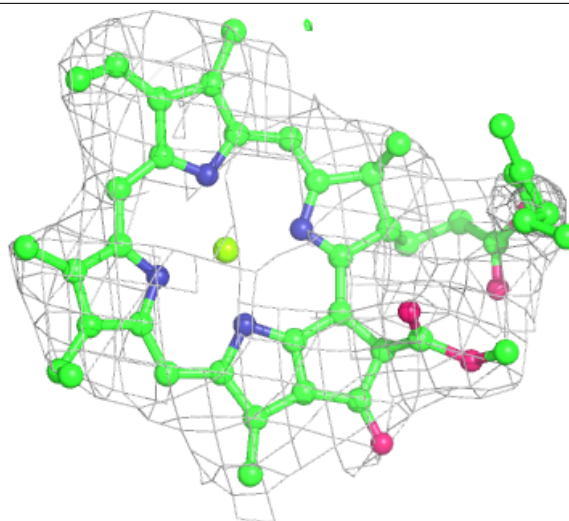
Electron density around CLA A 830:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



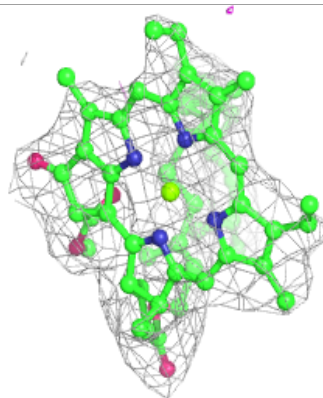
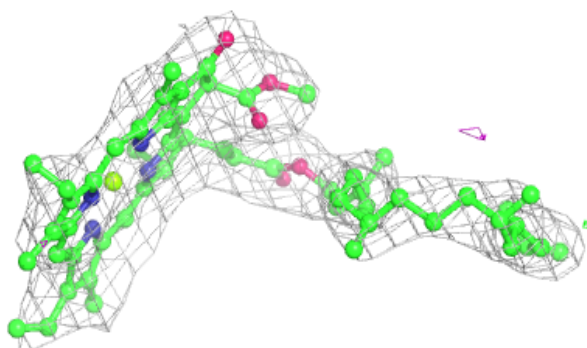
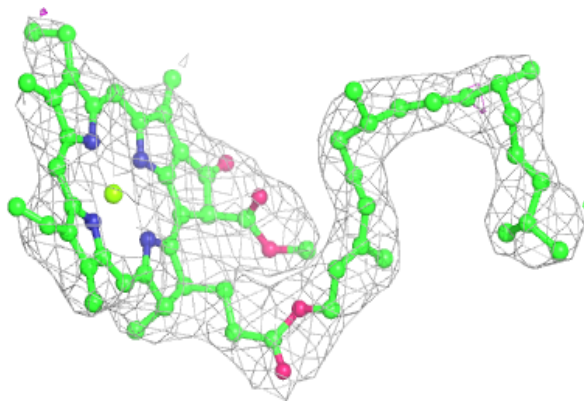
Electron density around CLA 2 611:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

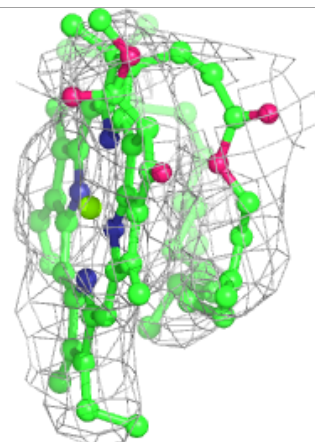
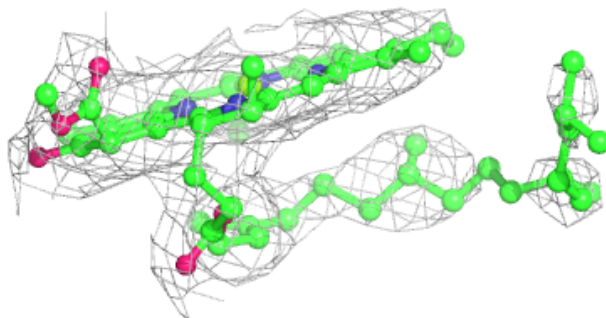
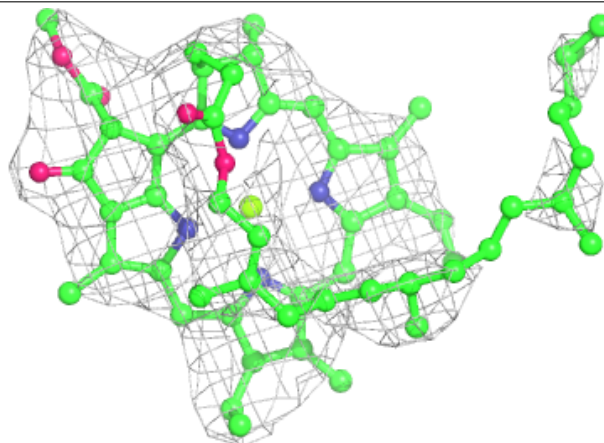


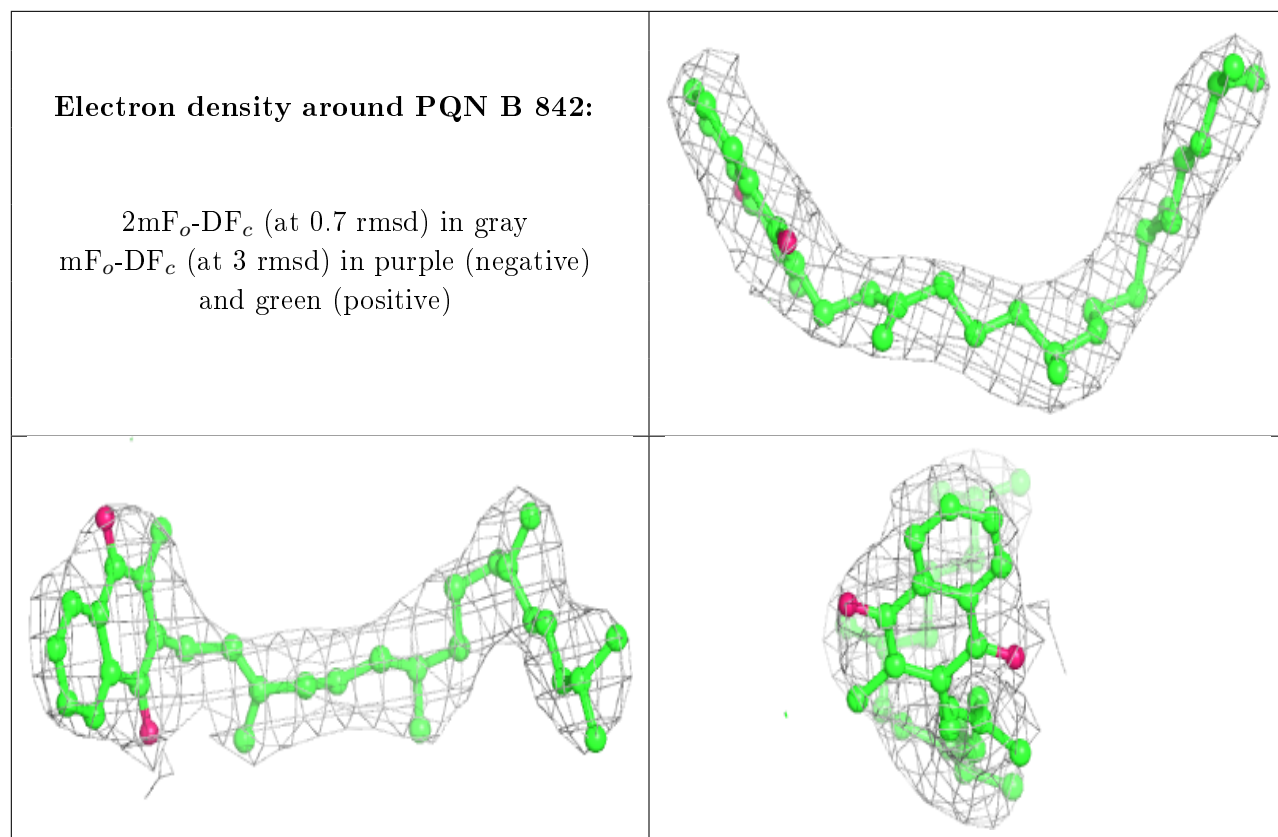
Electron density around CLA A 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CLA 7 612:**

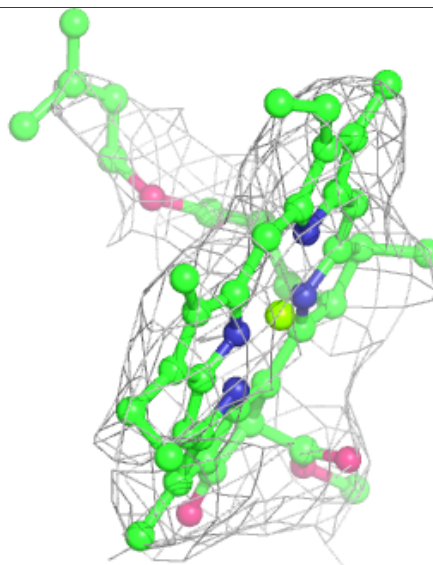
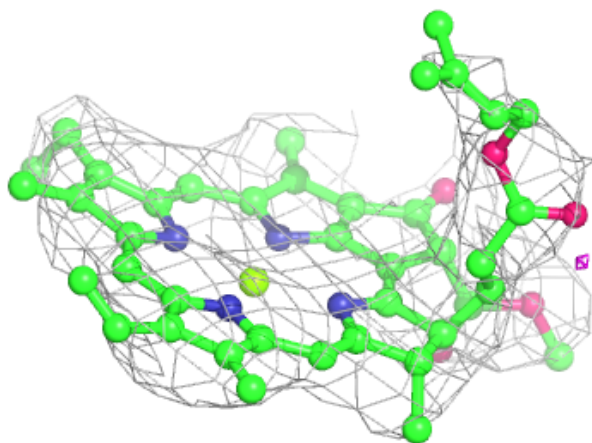
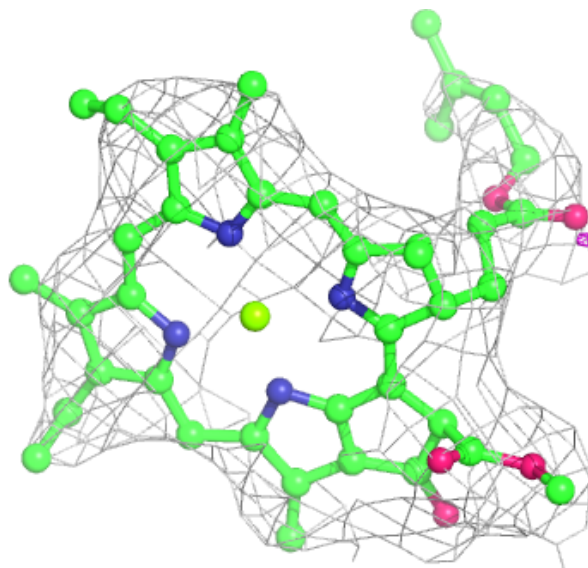
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

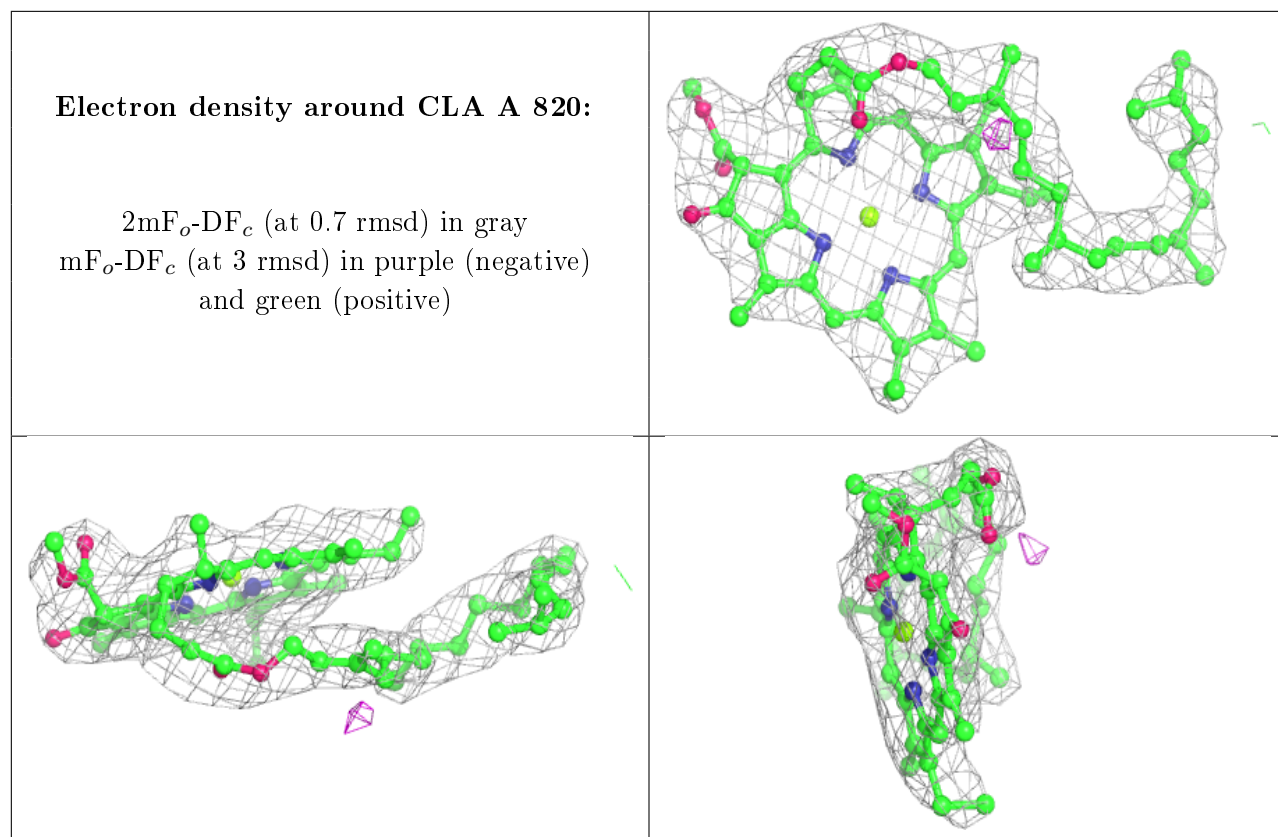




Electron density around CLA 9 608:

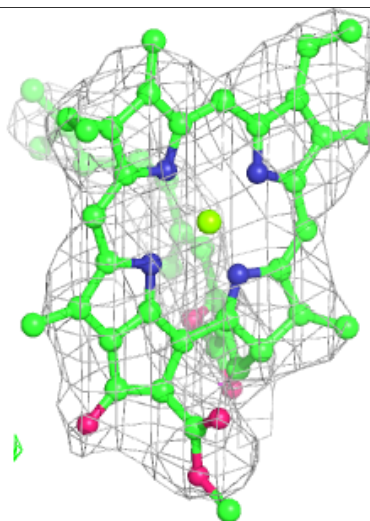
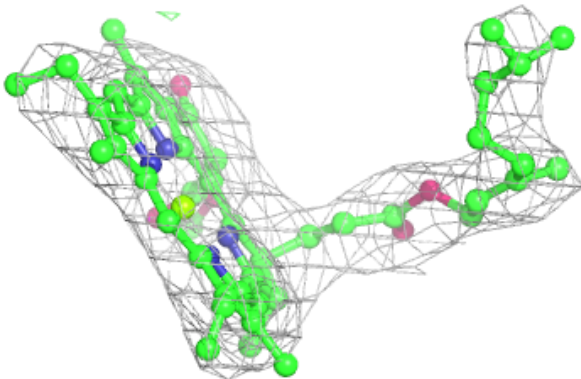
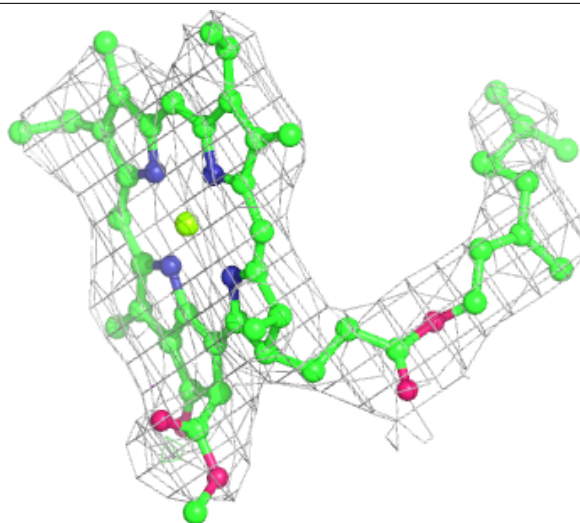
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





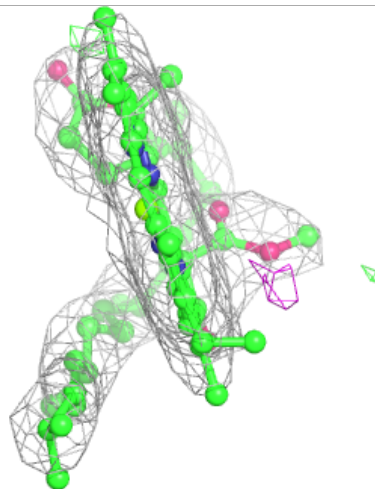
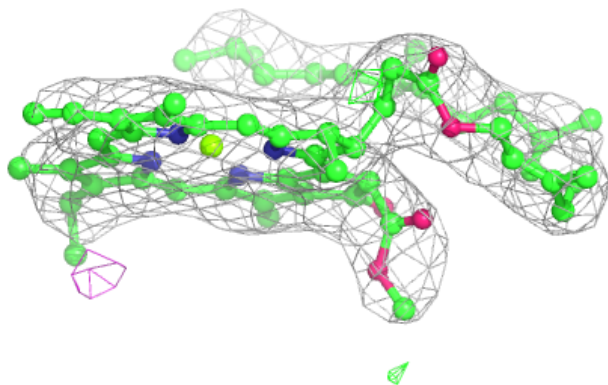
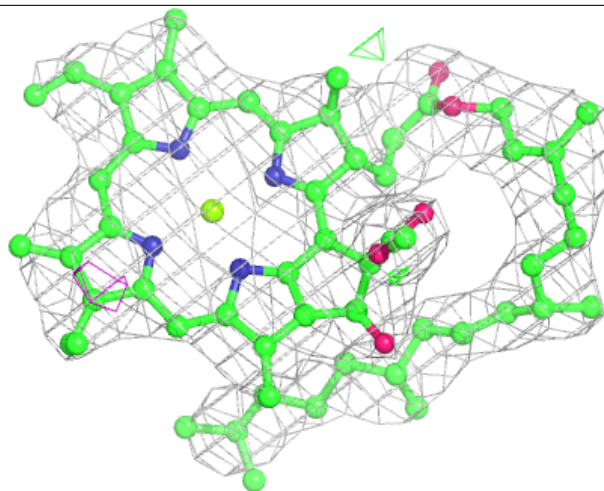
Electron density around CLA a 805:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



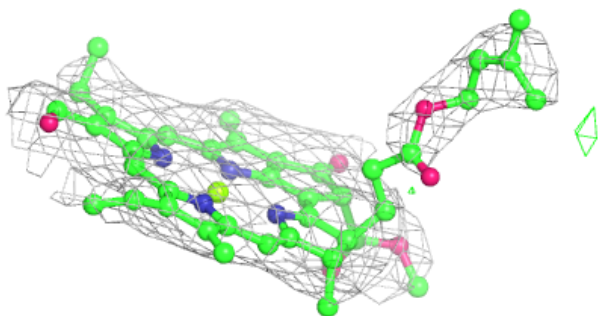
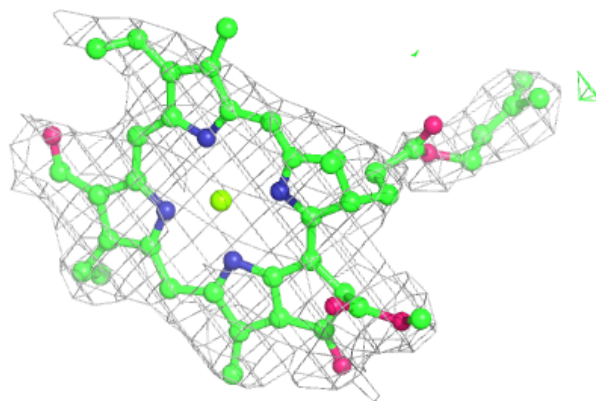
Electron density around CLA b 805:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

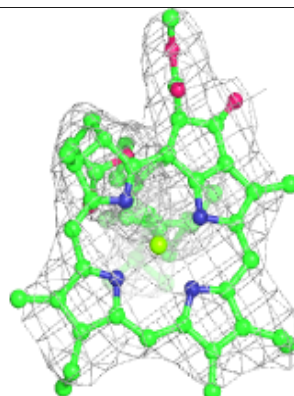
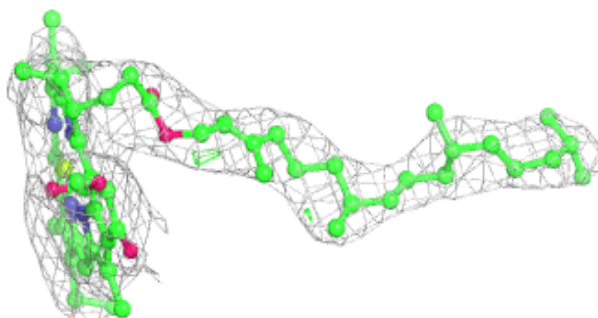
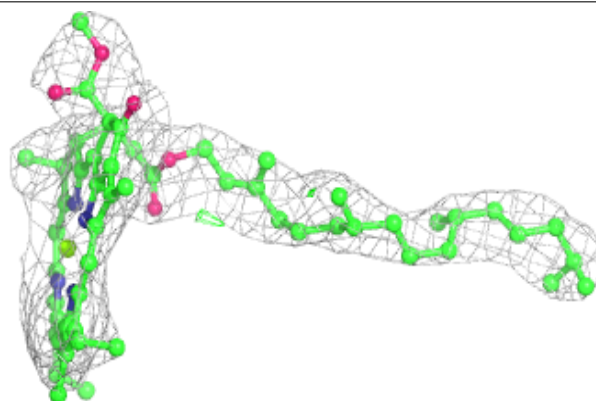


Electron density around CHL 7 607:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

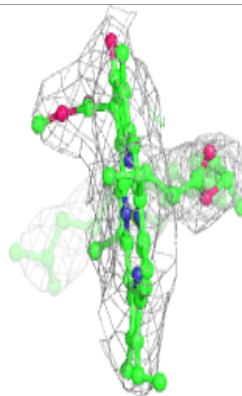
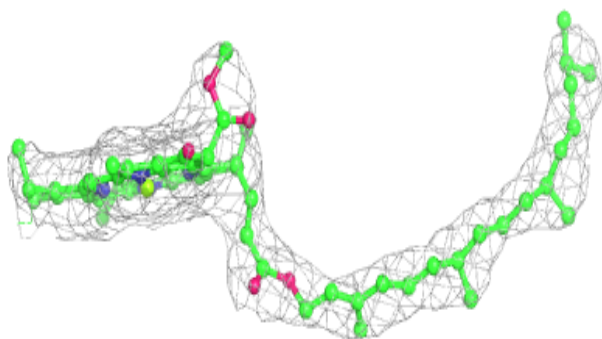
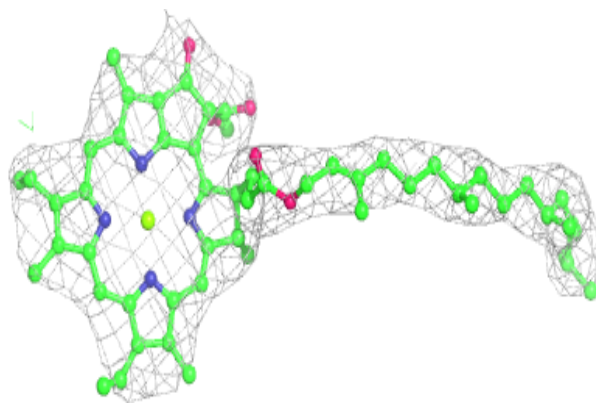
**Electron density around CLA A 829:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

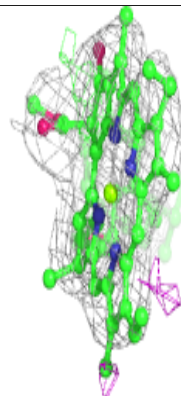
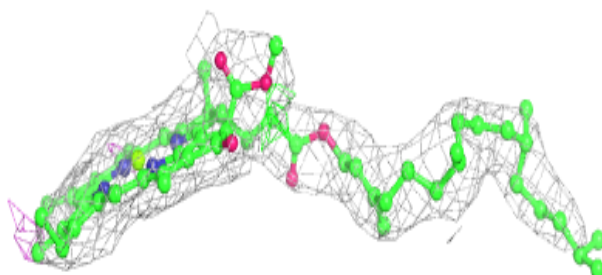
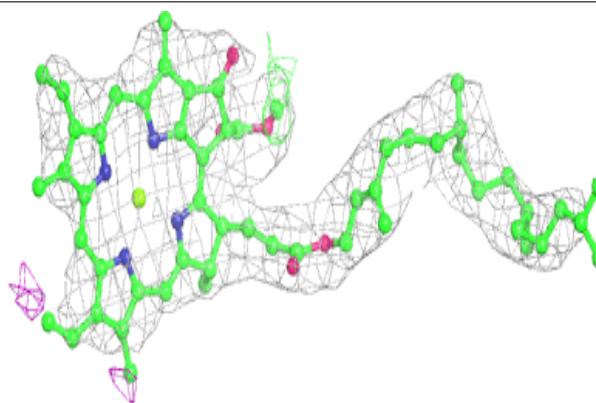


Electron density around CLA B 841:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

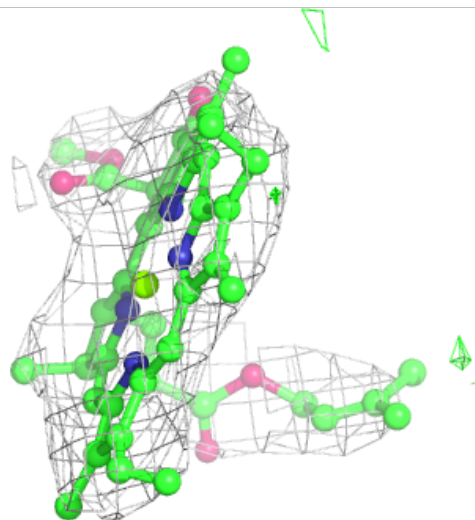
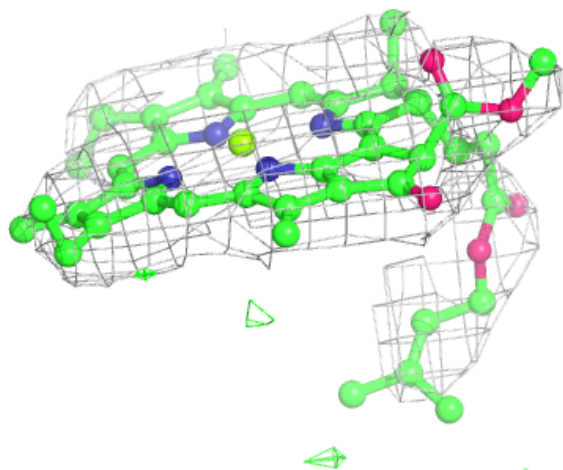
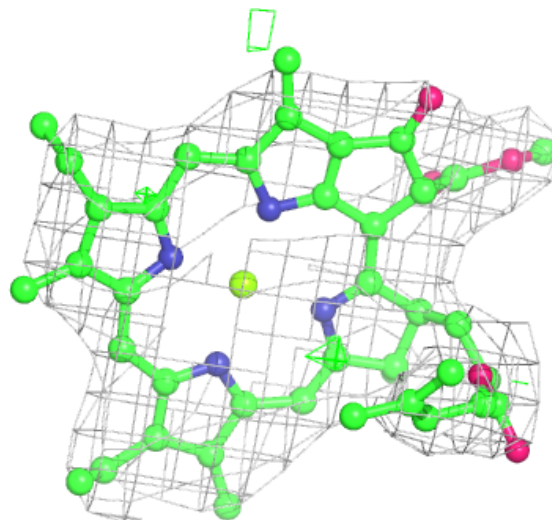
**Electron density around CLA F 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



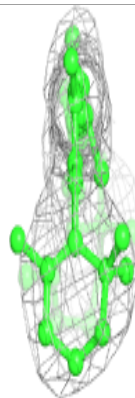
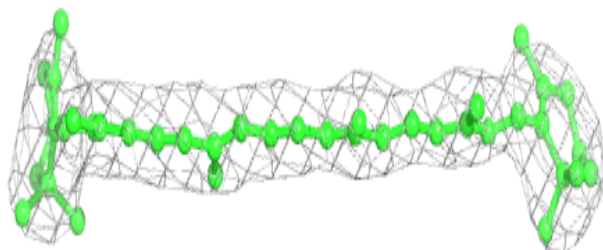
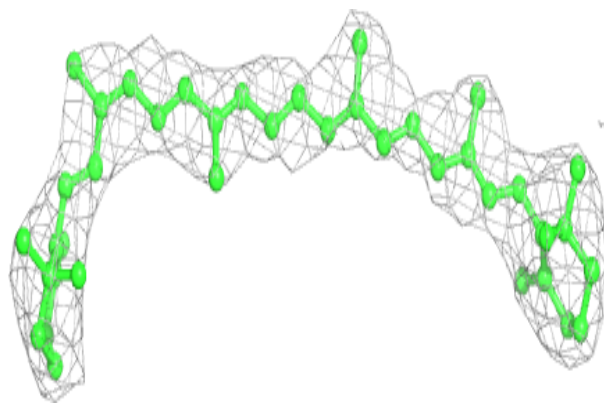
Electron density around CLA 3 308:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



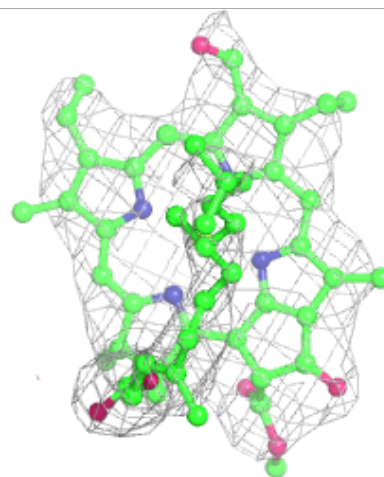
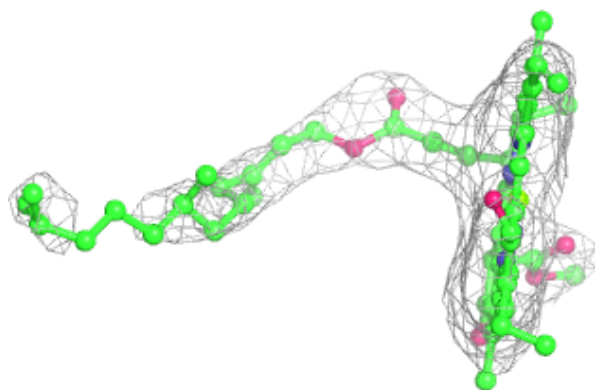
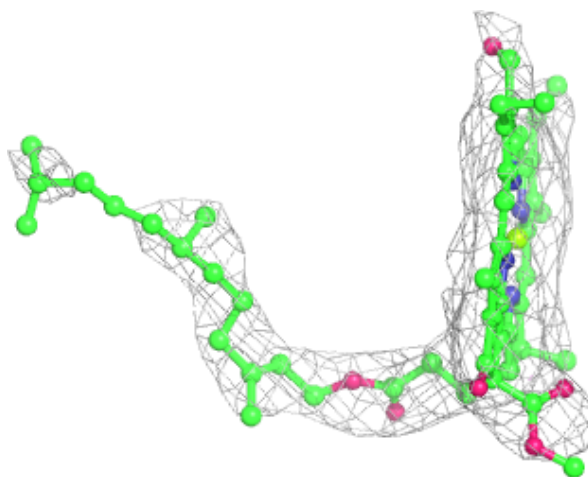
Electron density around BCR L 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



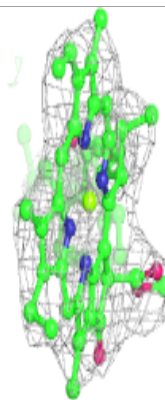
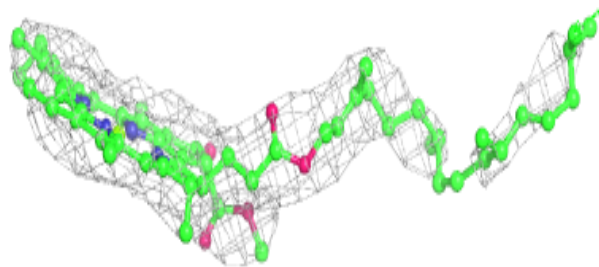
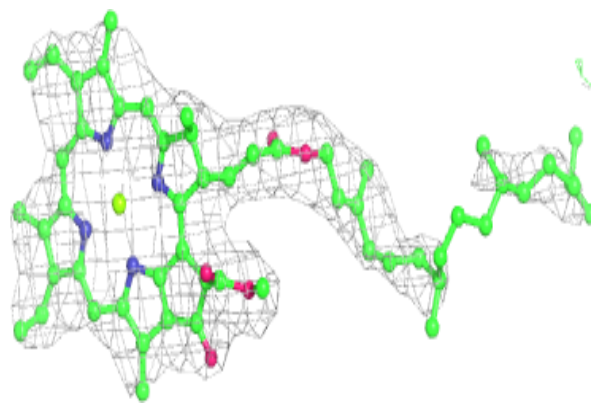
Electron density around CHL 1 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



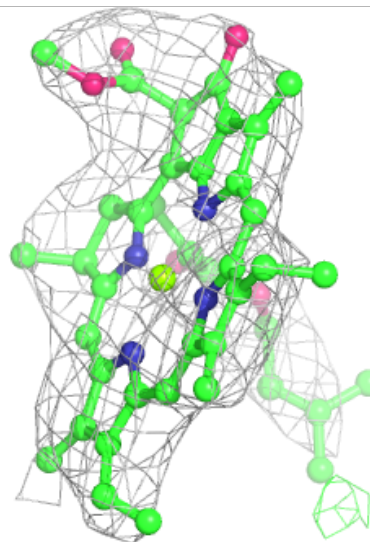
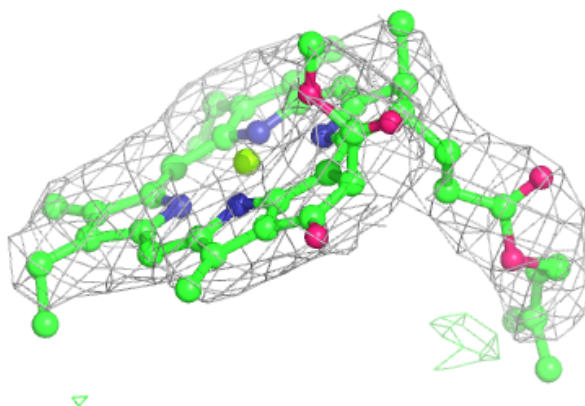
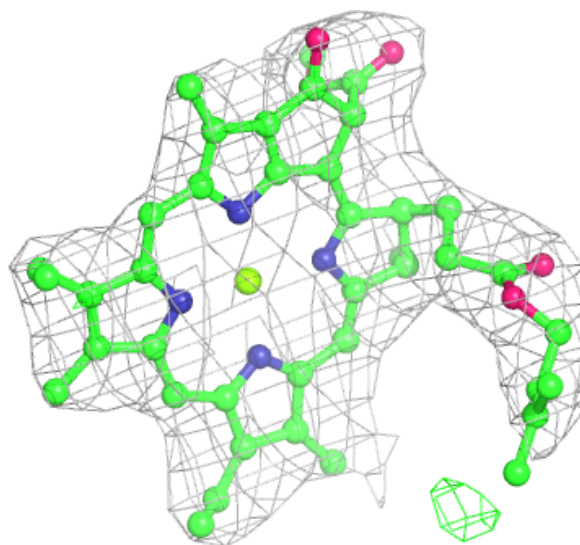
Electron density around CLA a 842:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



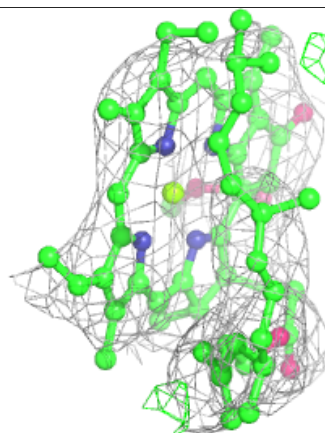
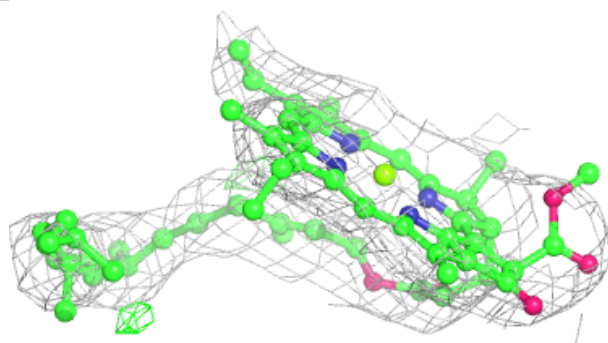
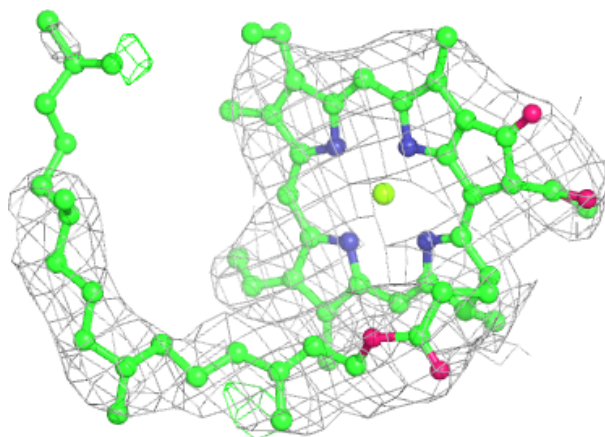
Electron density around CLA a 832:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

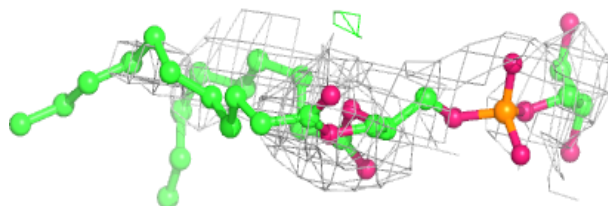


Electron density around CLA 6 304:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

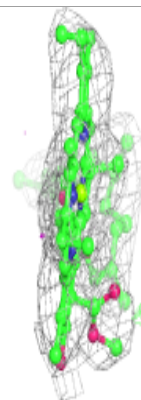
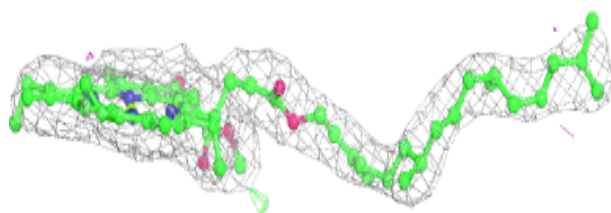
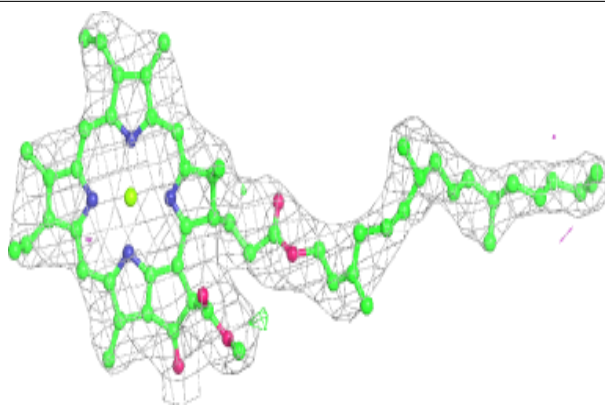
**Electron density around LHG 2 618:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



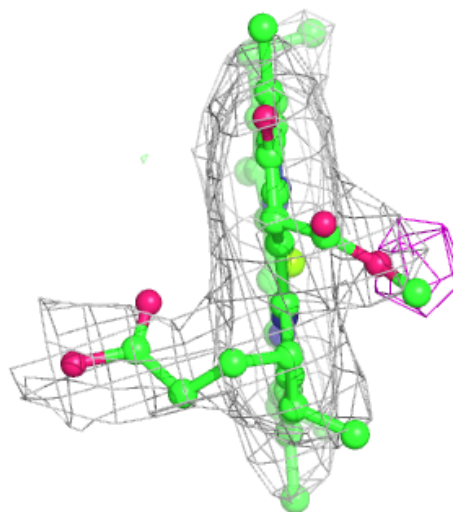
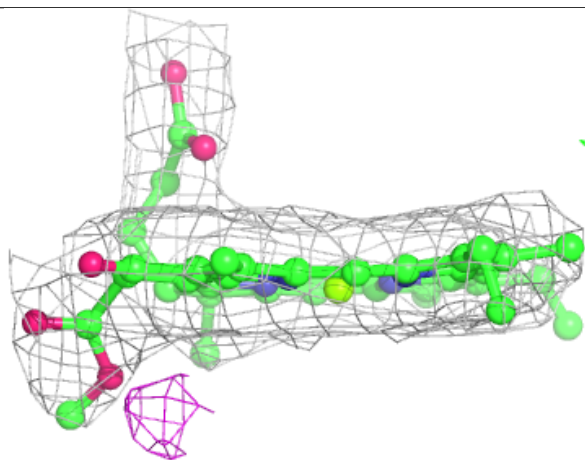
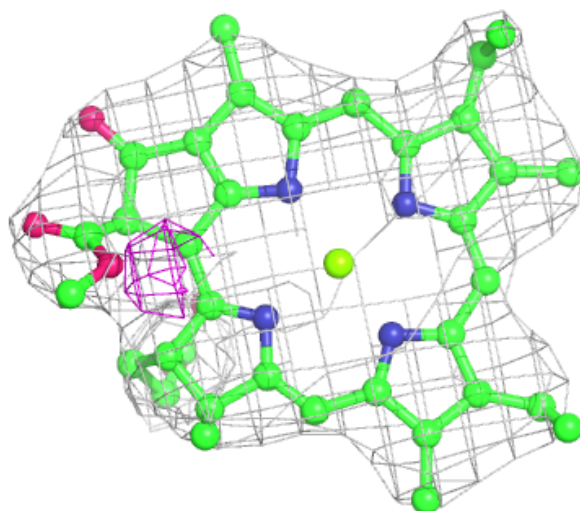
Electron density around CLA a 834:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



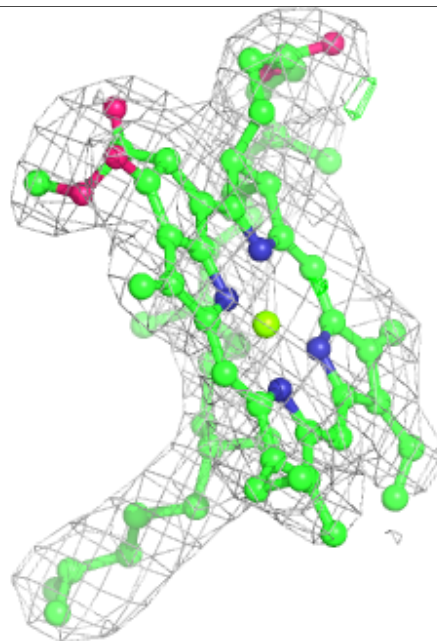
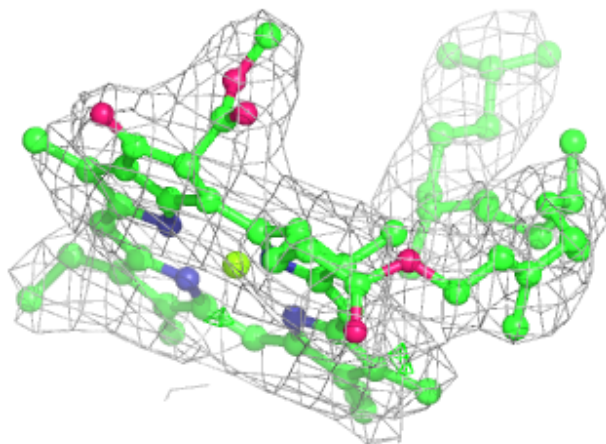
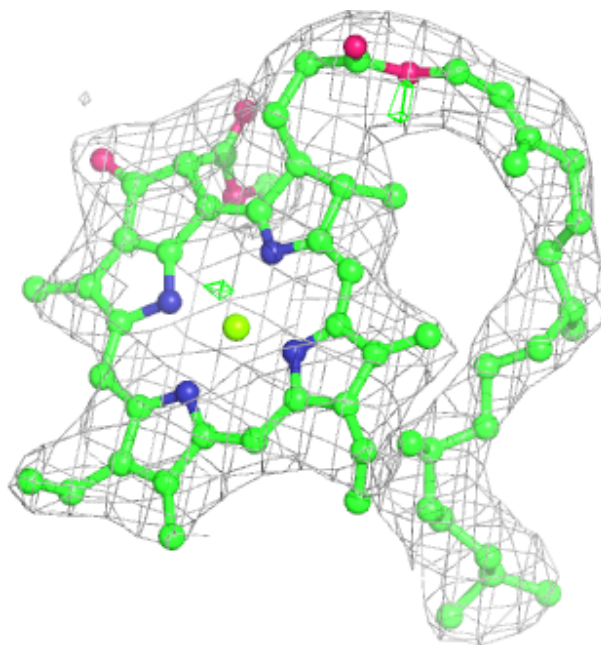
Electron density around CLA B 804:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



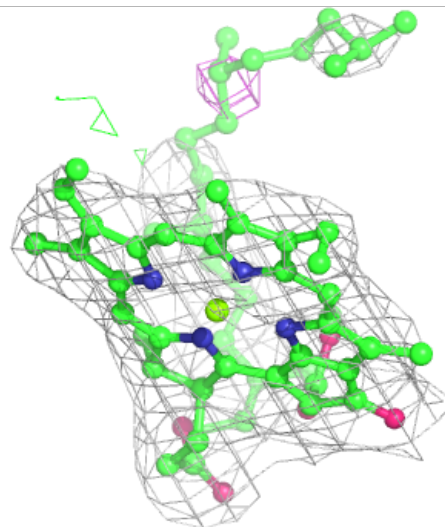
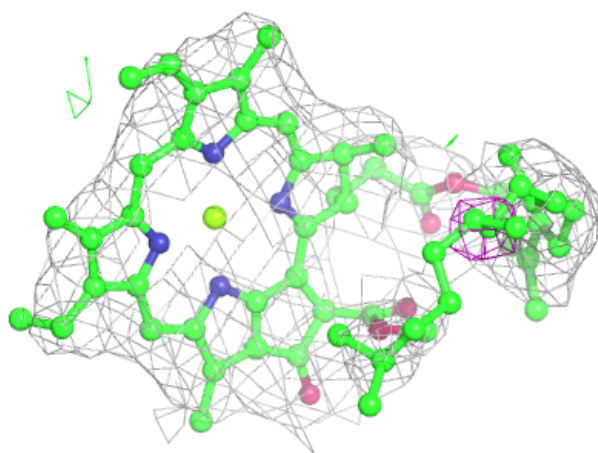
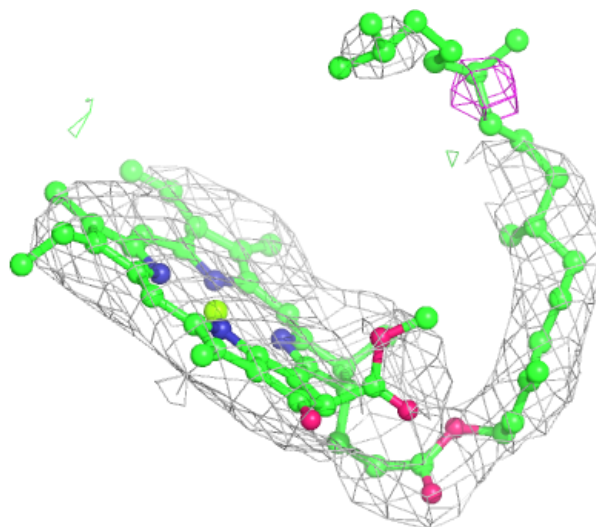
Electron density around CLA a 814:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



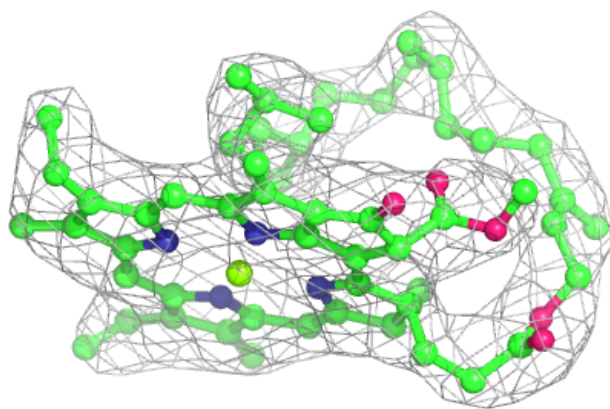
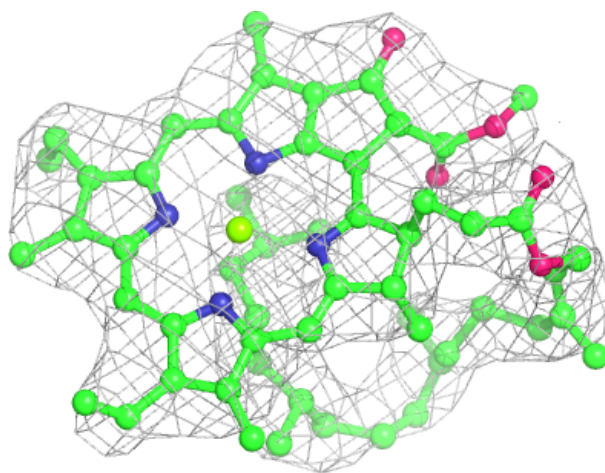
Electron density around CLA 1 304:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



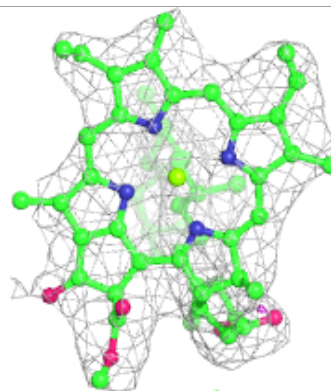
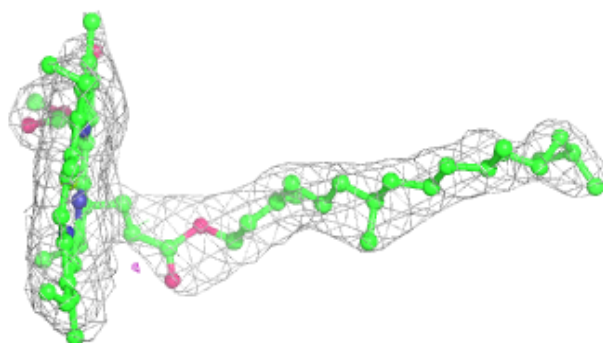
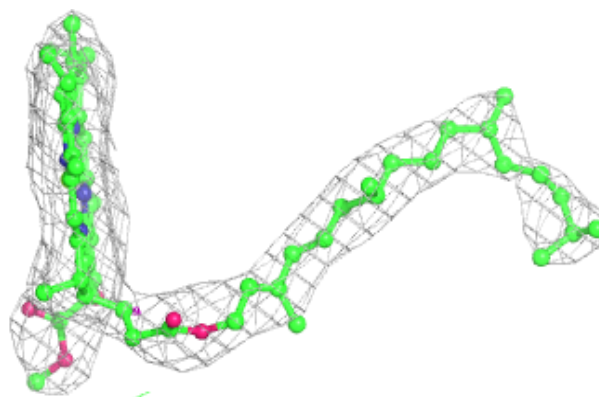
Electron density around CLA B 806:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

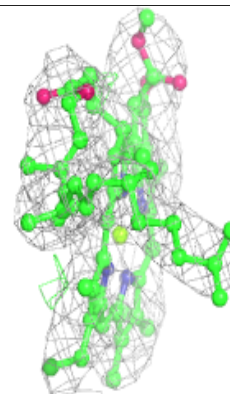
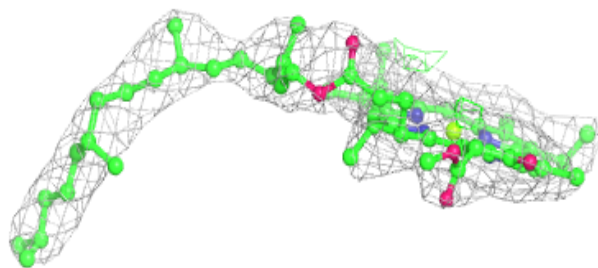
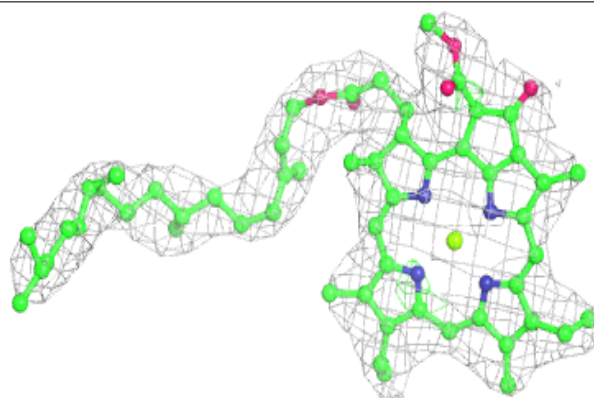


Electron density around CLA b 840:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

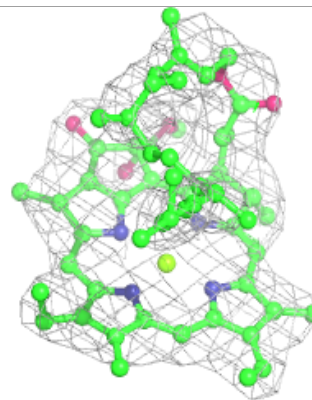
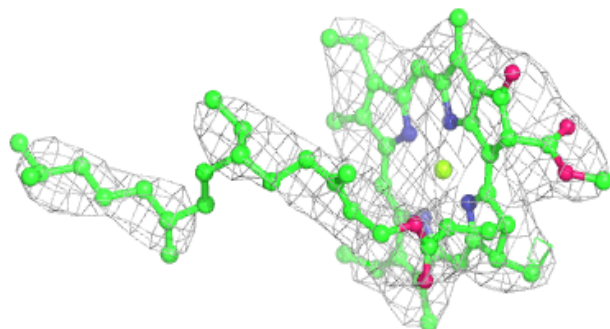
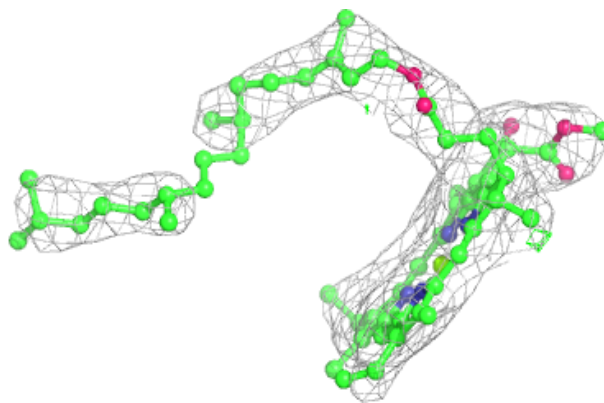
**Electron density around CLA B 803:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

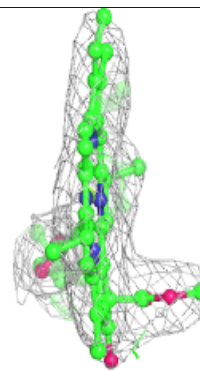
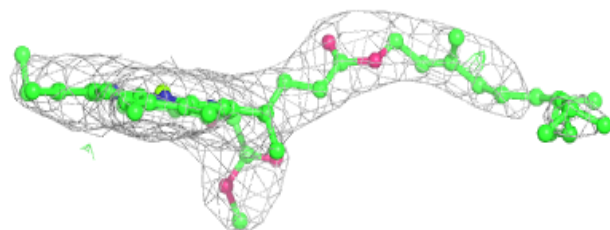
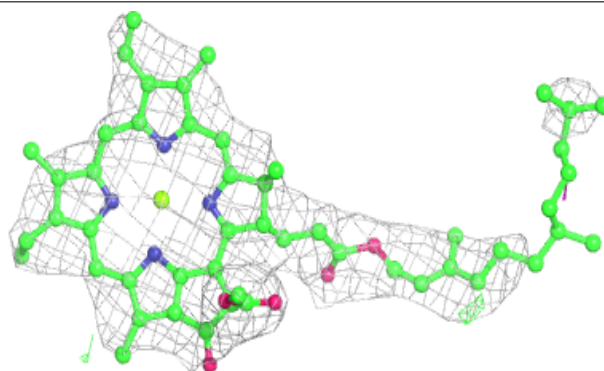


Electron density around CLA A 811:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

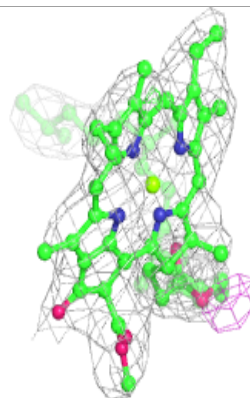
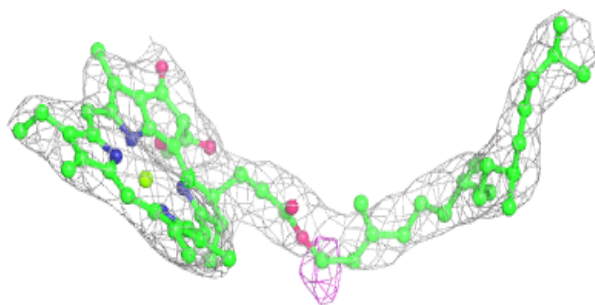
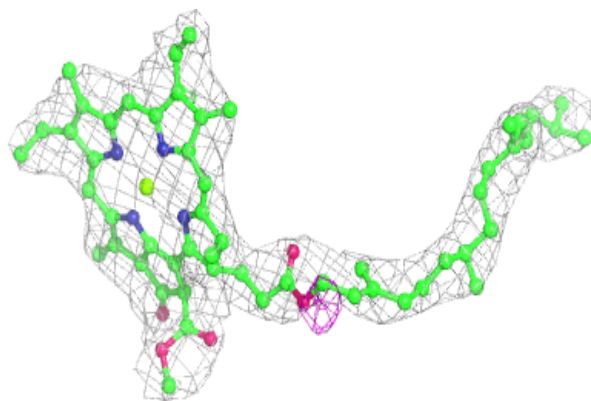
**Electron density around CLA b 836:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



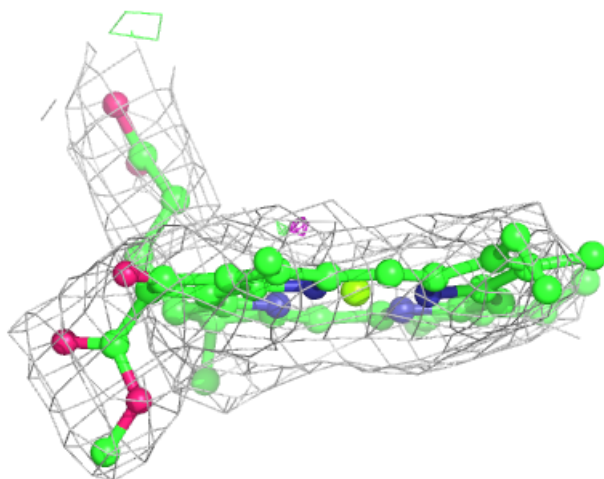
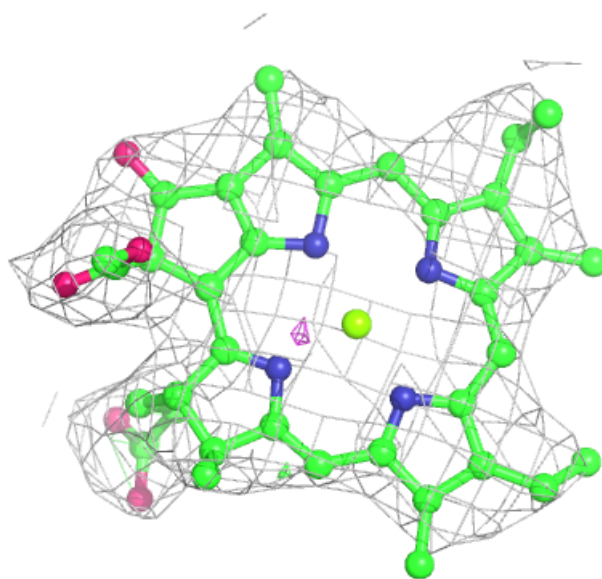
Electron density around CLA a 856:

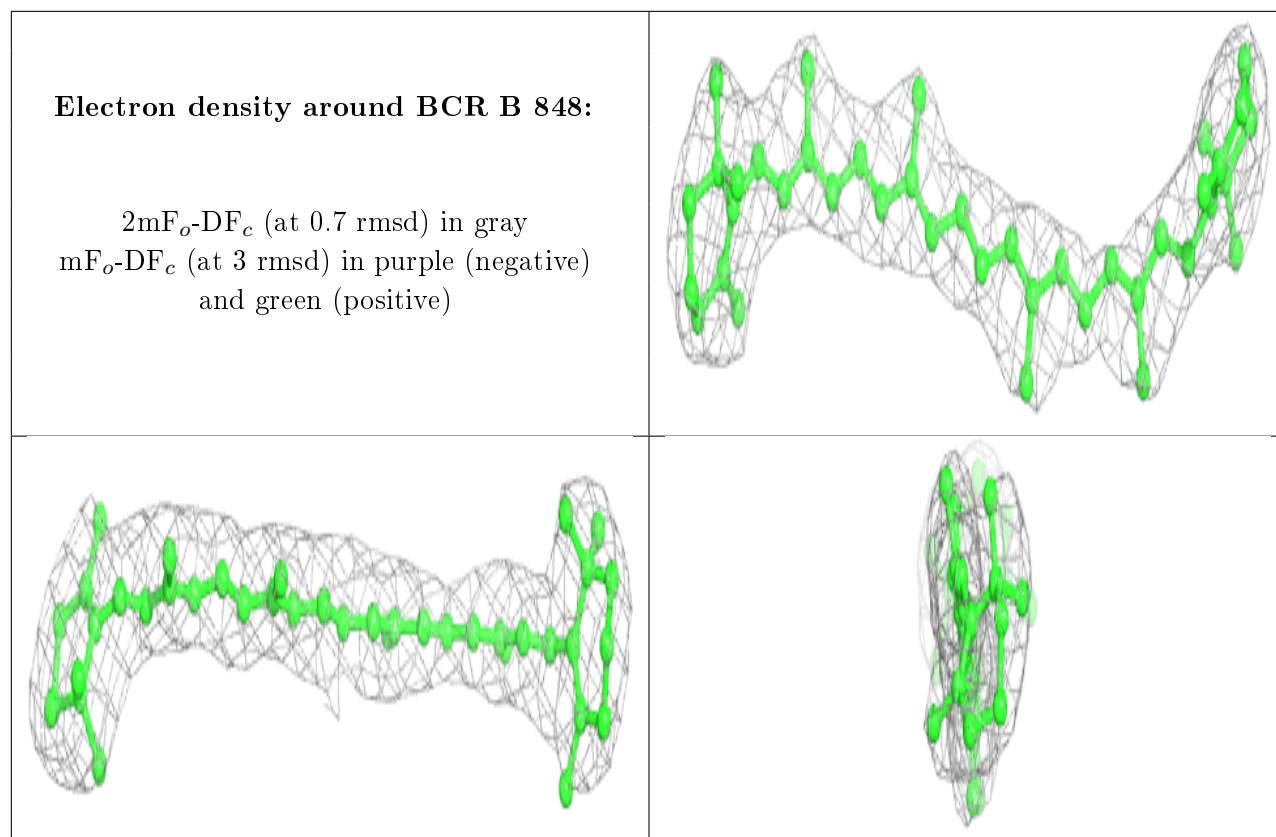
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA a 821:

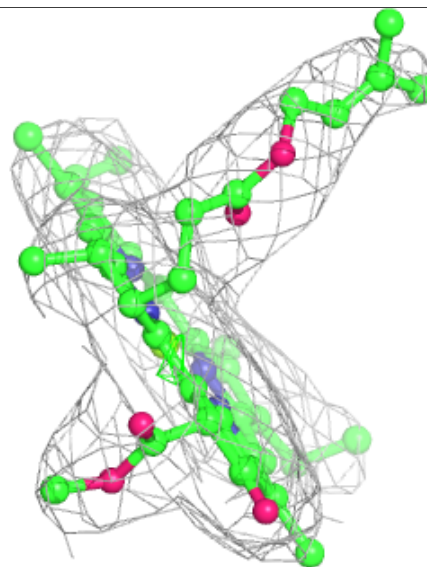
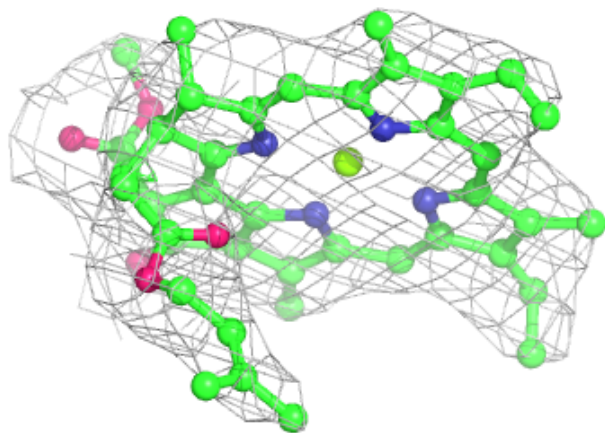
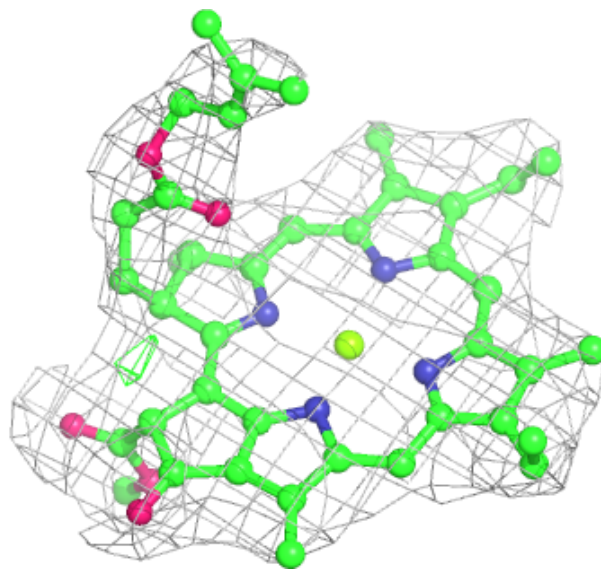
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





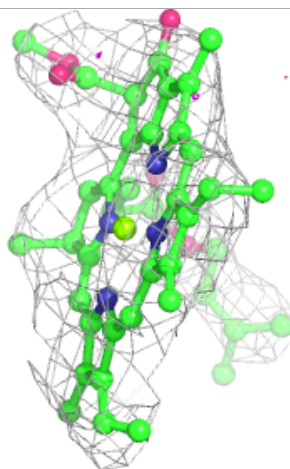
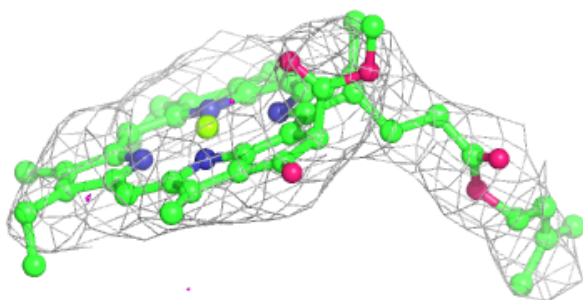
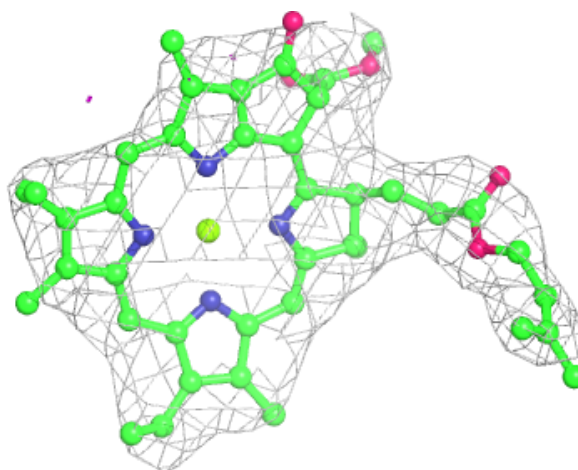
Electron density around CLA B 830:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



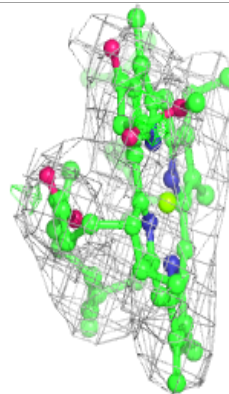
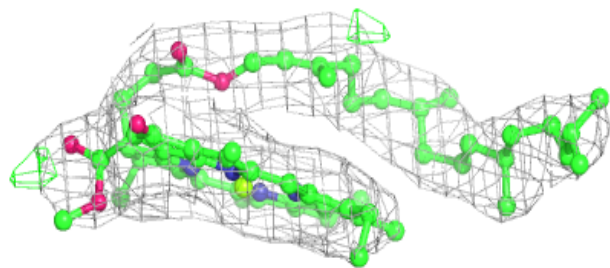
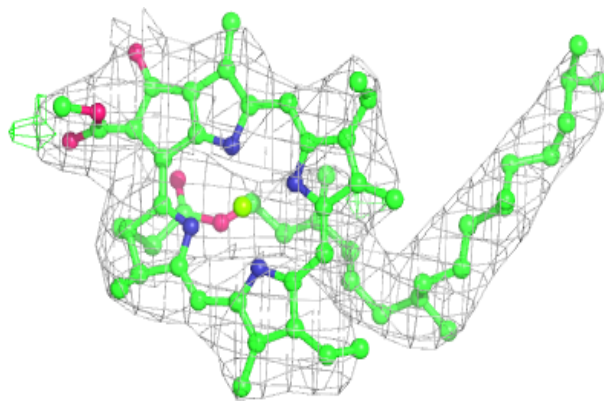
Electron density around CLA 4 614:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



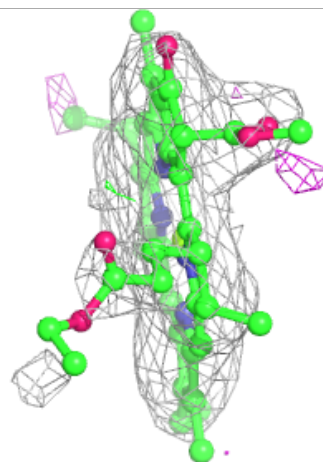
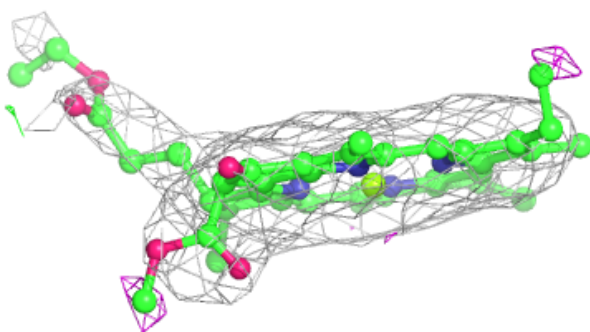
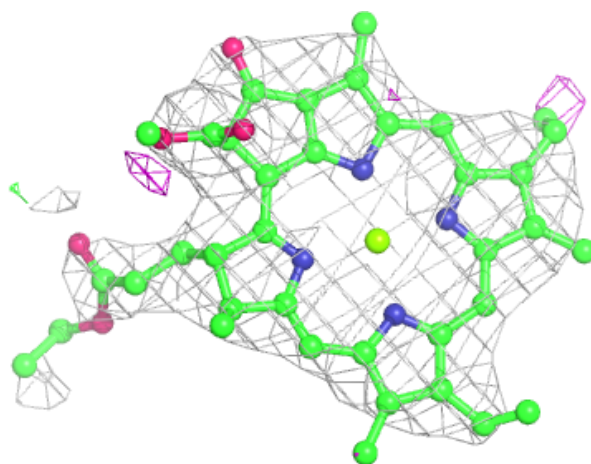
Electron density around CLA B 837:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



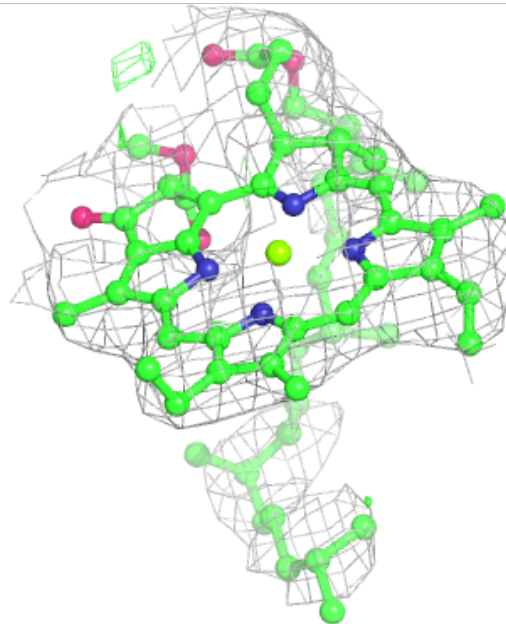
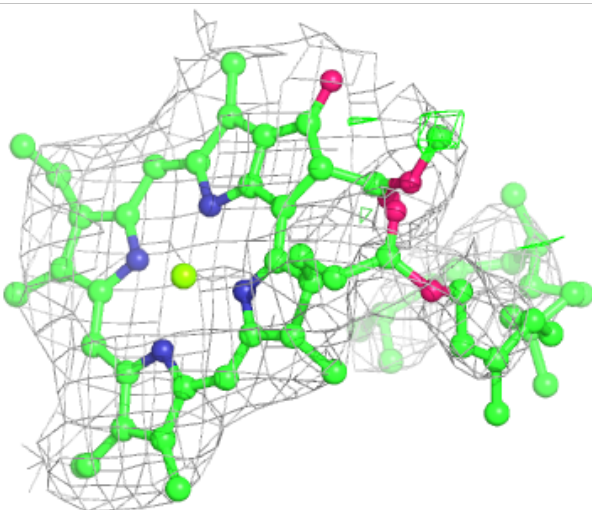
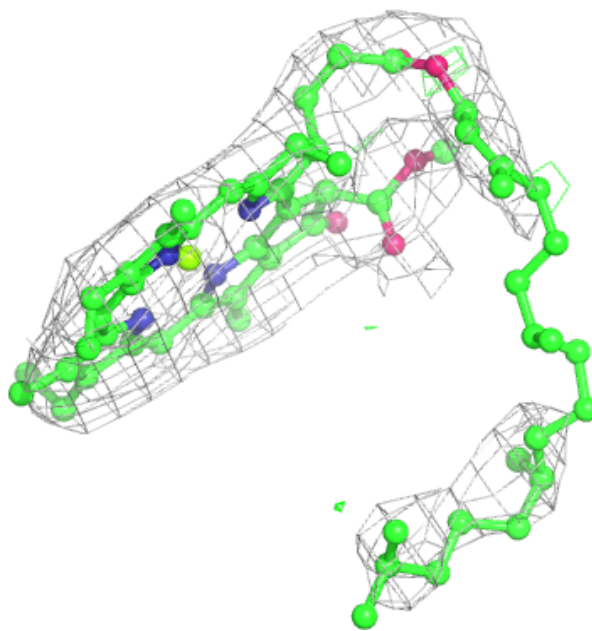
Electron density around CLA 9 614:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



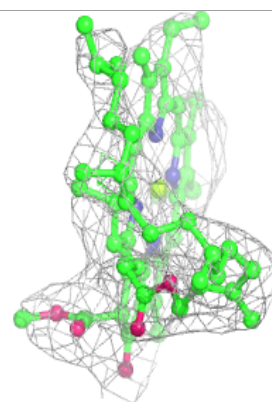
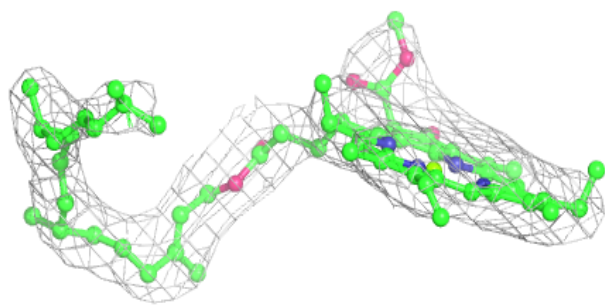
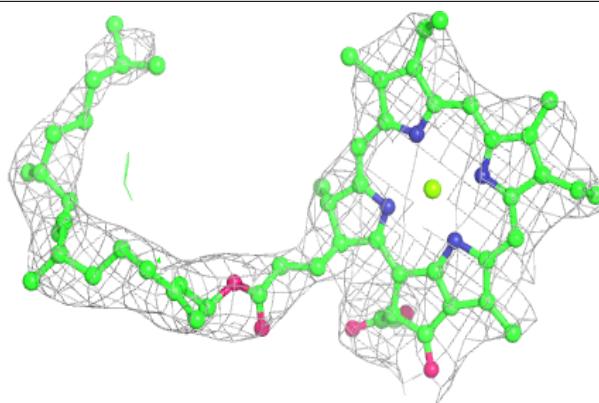
Electron density around CLA 2 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

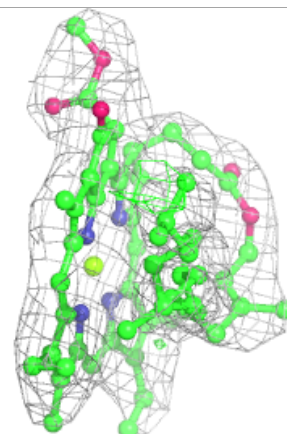
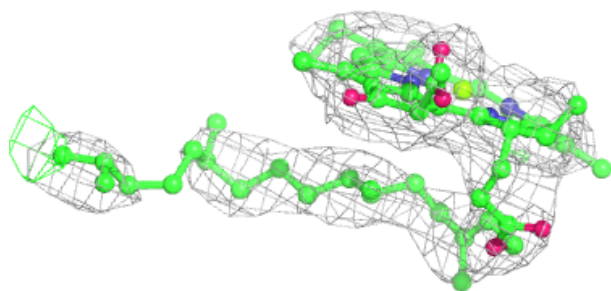
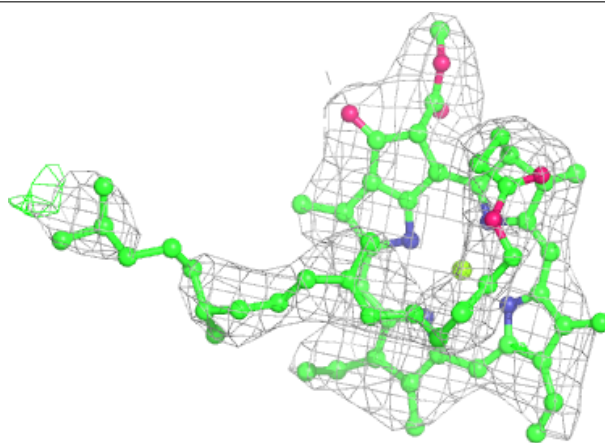


Electron density around CLA A 828:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

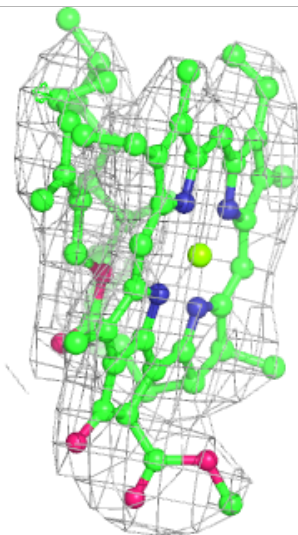
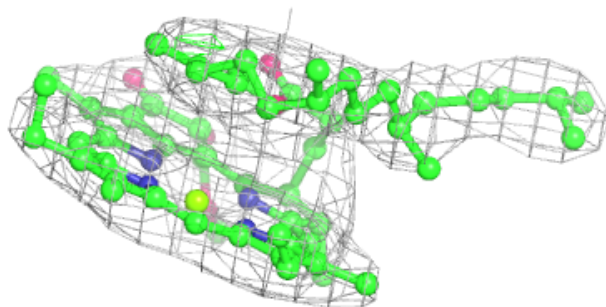
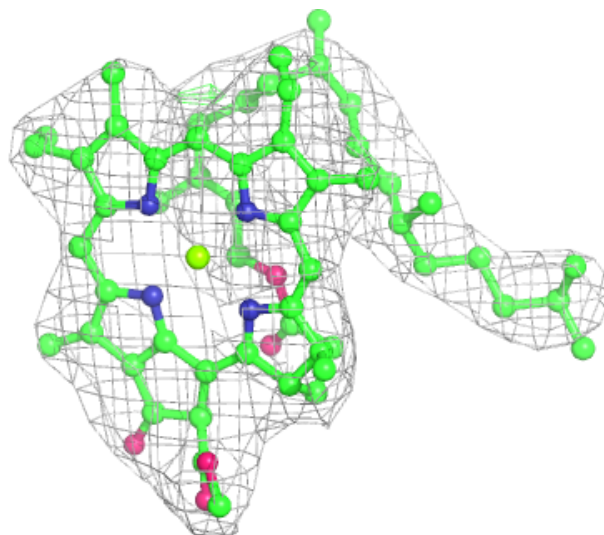
**Electron density around CLA b 827:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



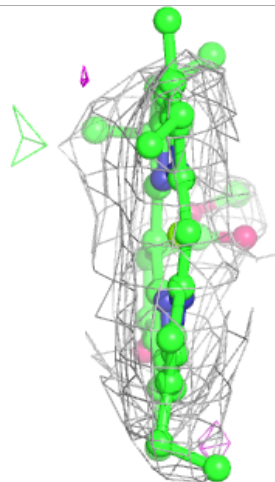
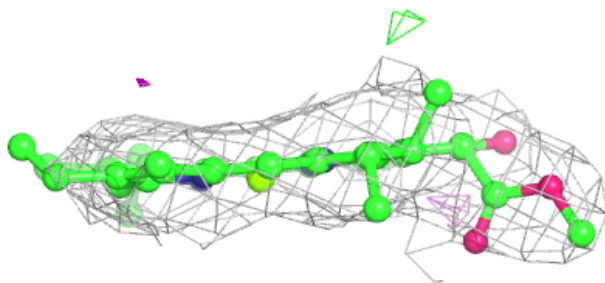
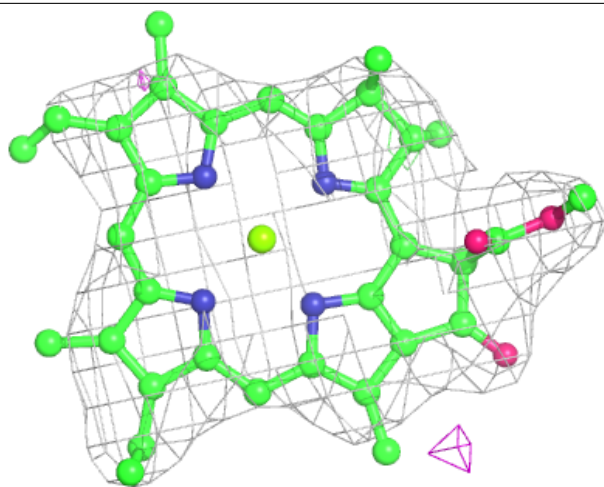
Electron density around CLA B 808:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



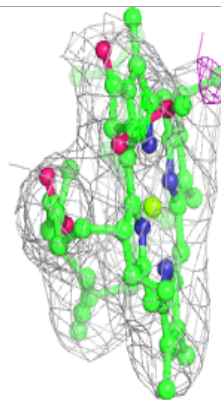
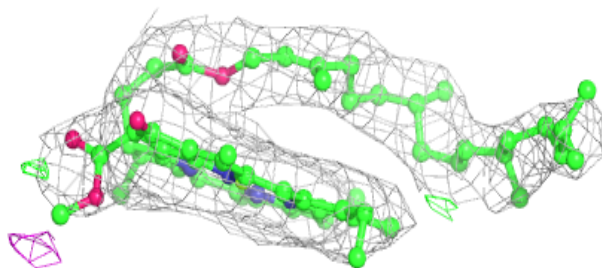
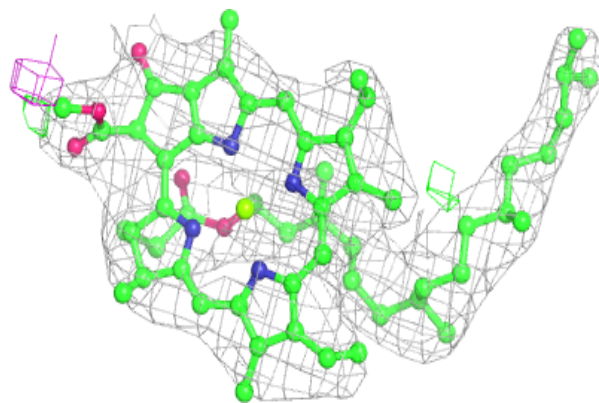
Electron density around CLA 1 311:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

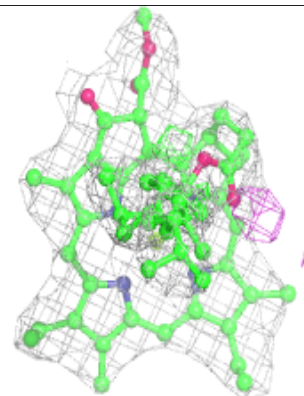
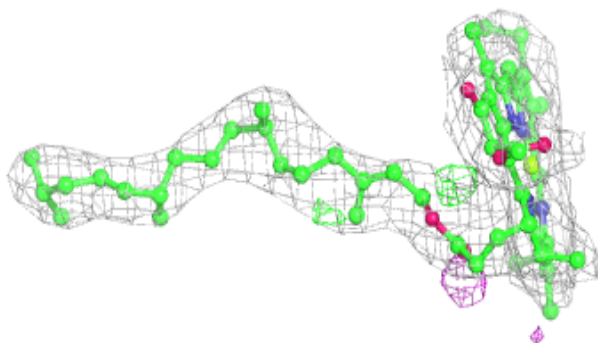
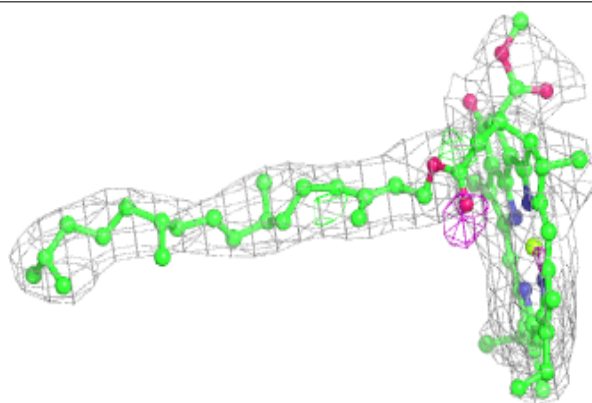


Electron density around CLA b 837:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

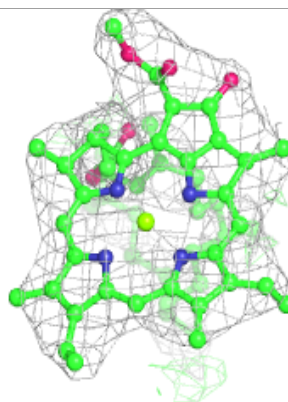
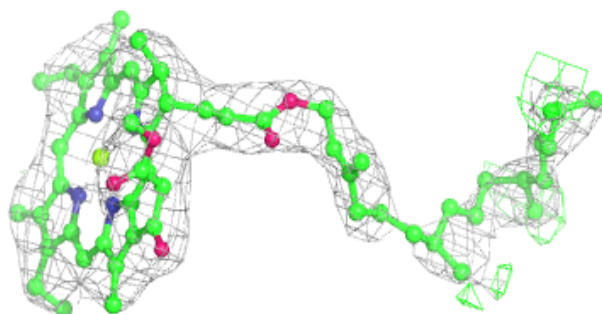
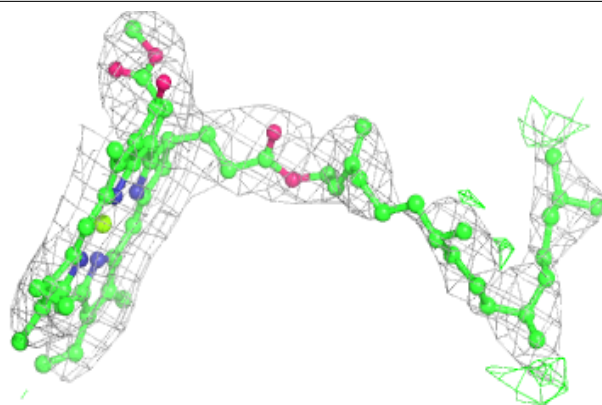
**Electron density around CLA a 829:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

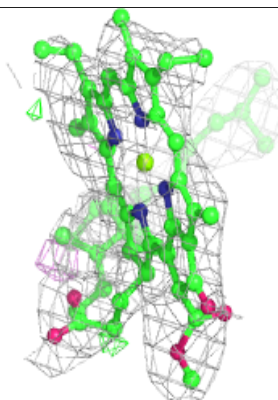
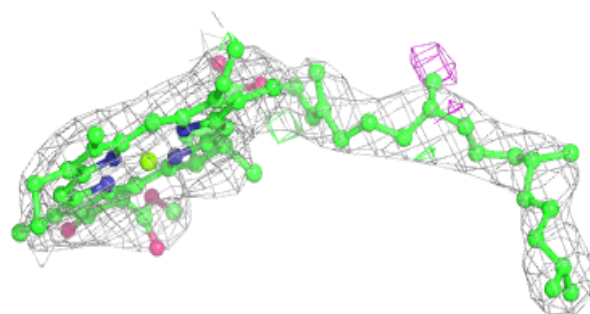
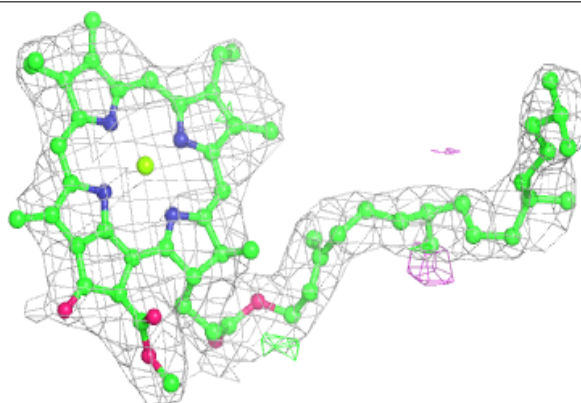


Electron density around CLA A 840:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

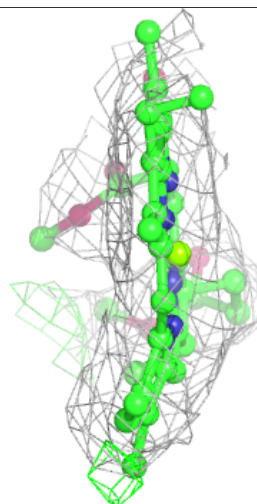
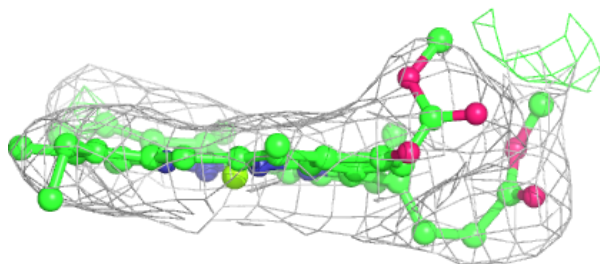
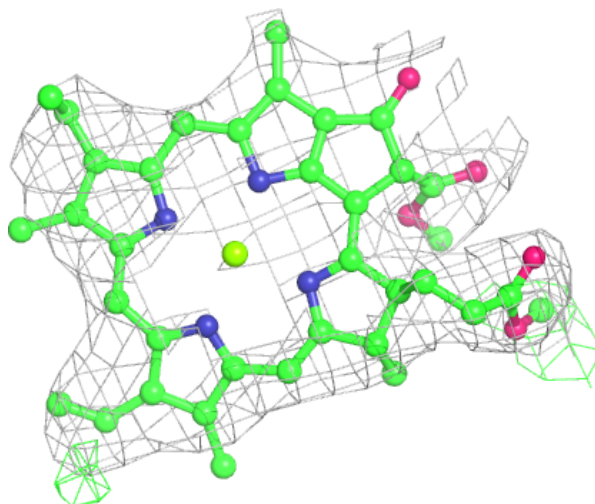
**Electron density around CLA a 802:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



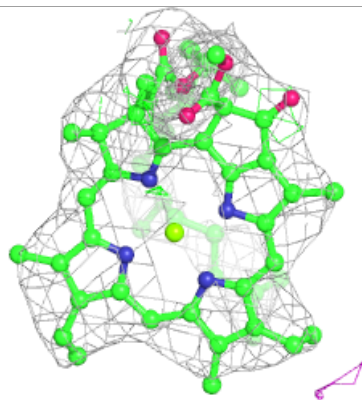
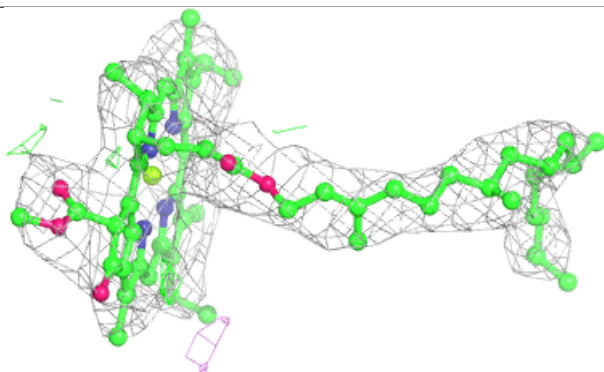
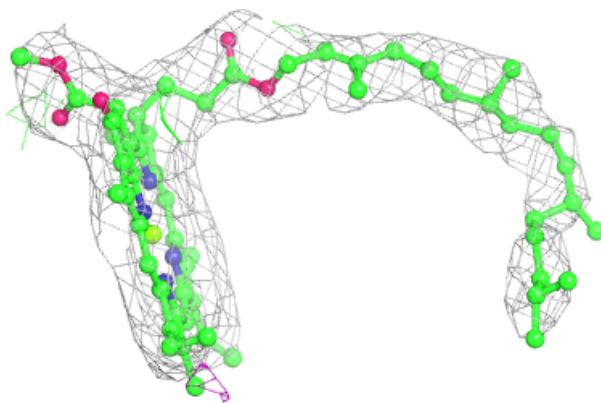
Electron density around CLA 9 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



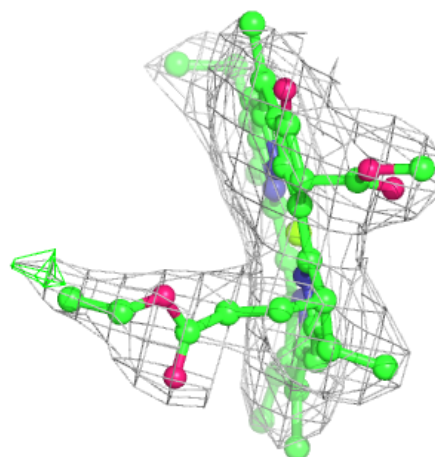
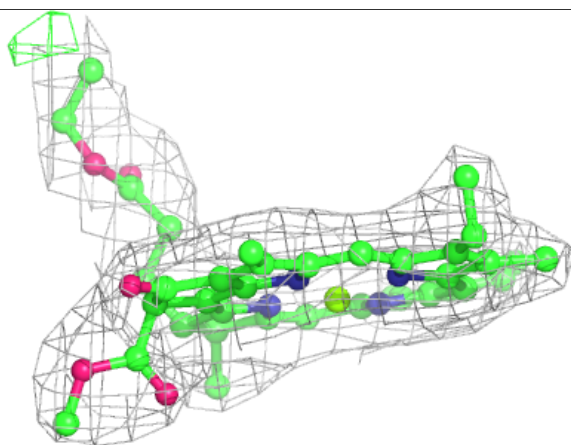
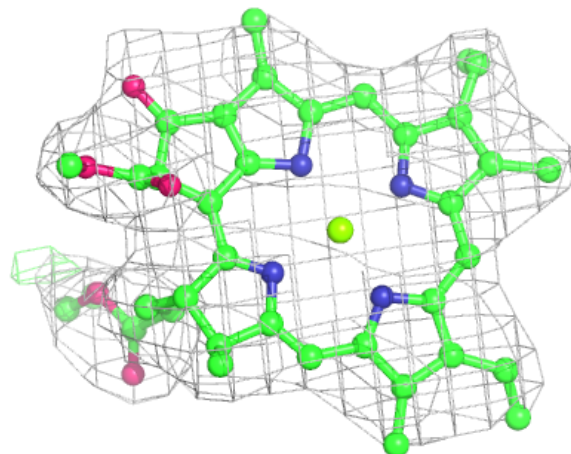
Electron density around CLA a 808:

$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)



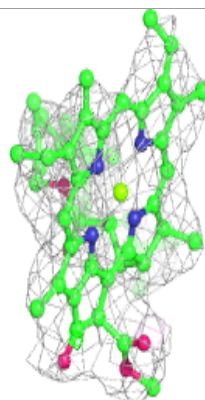
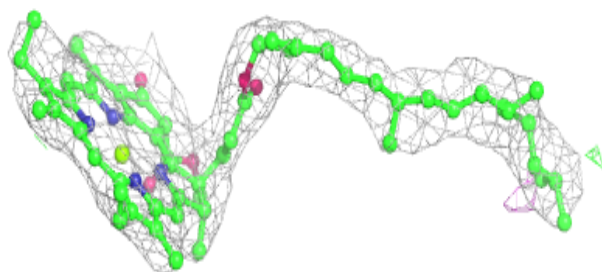
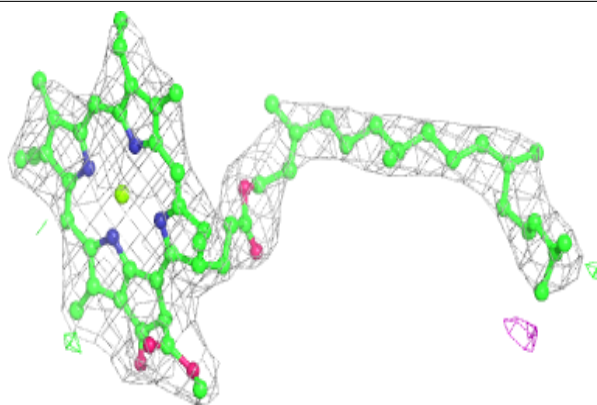
Electron density around CLA b 838:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



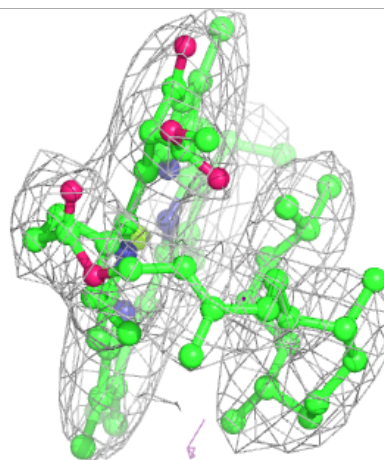
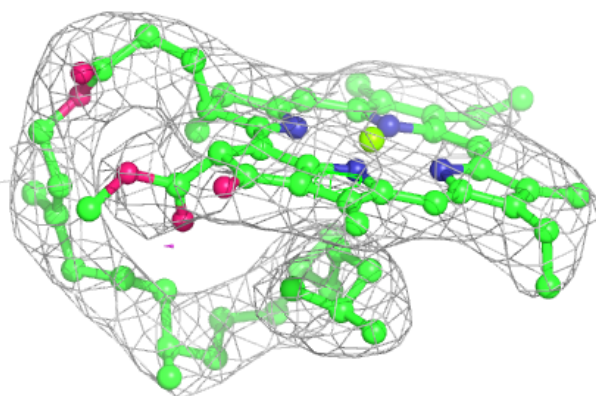
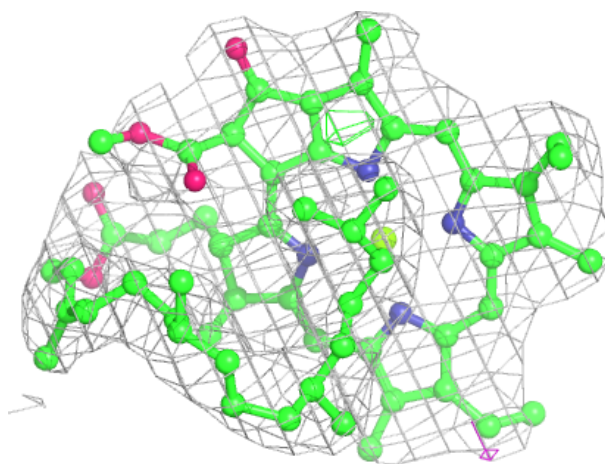
Electron density around CLA a 822:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



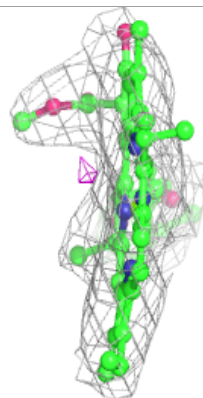
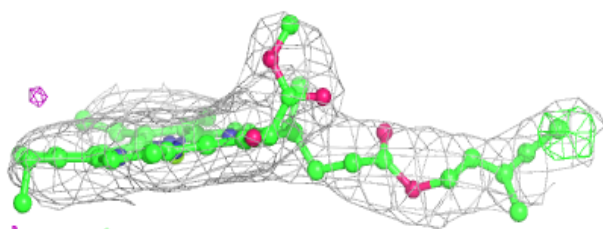
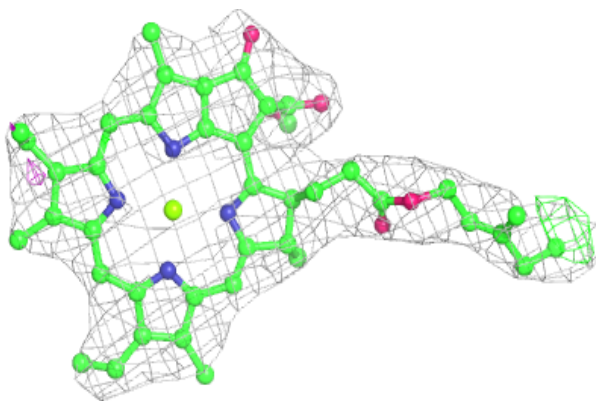
Electron density around CLA b 806:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

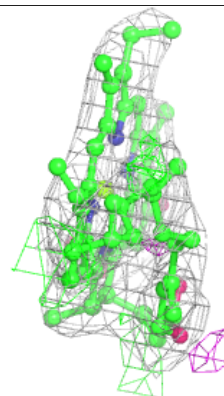
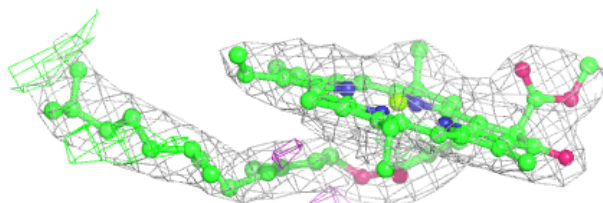
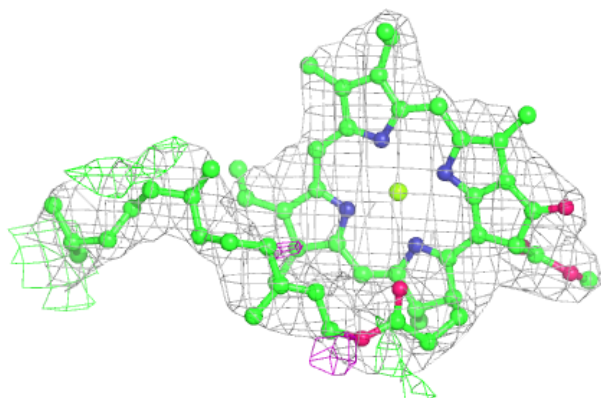


Electron density around CLA a 838:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

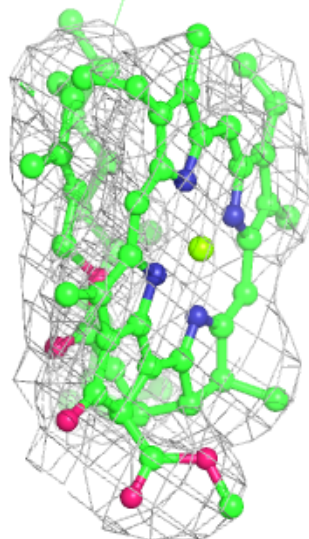
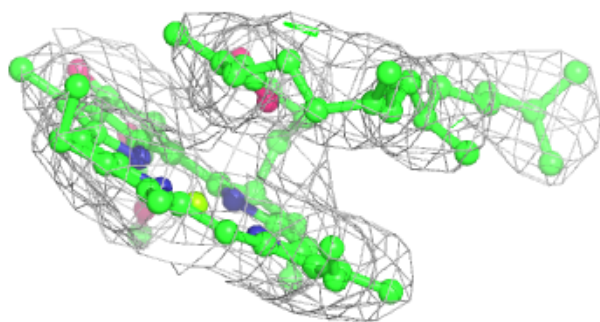
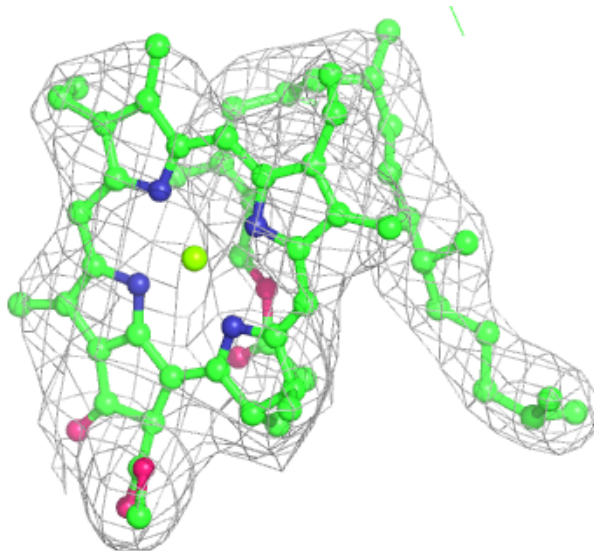
**Electron density around CLA b 818:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



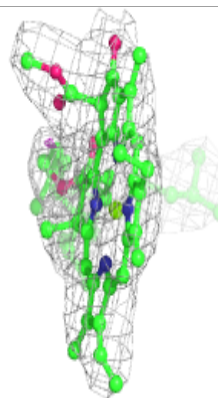
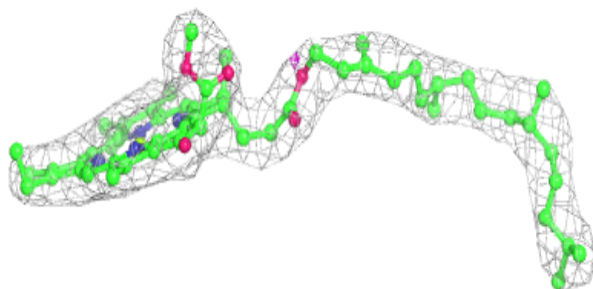
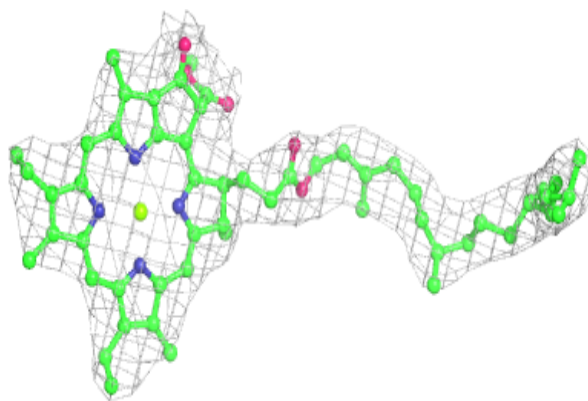
Electron density around CLA b 808:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

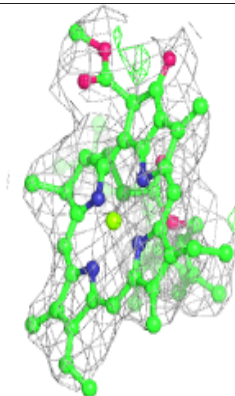
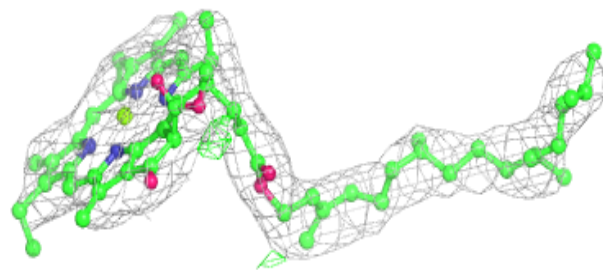
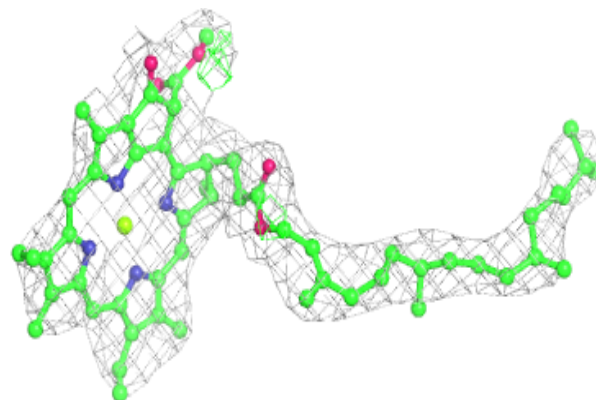


Electron density around CLA a 806:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

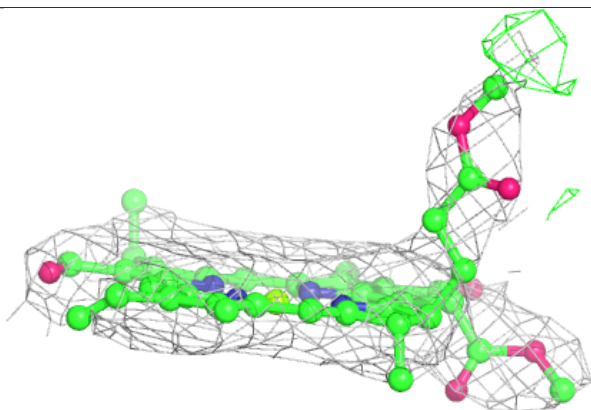
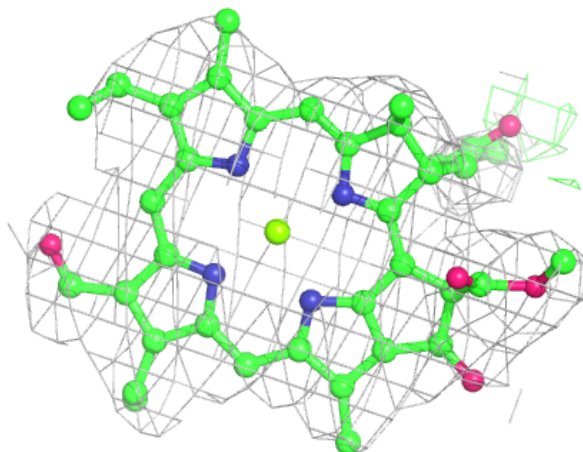
**Electron density around CLA A 822:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



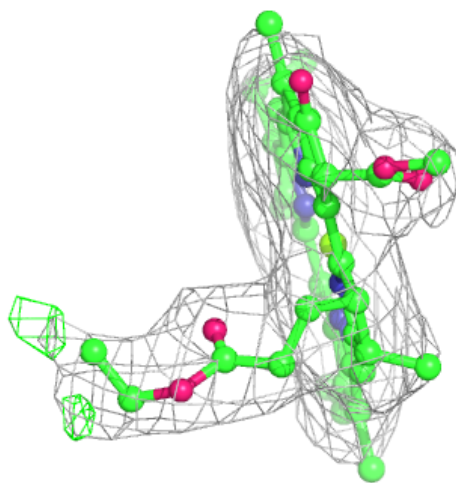
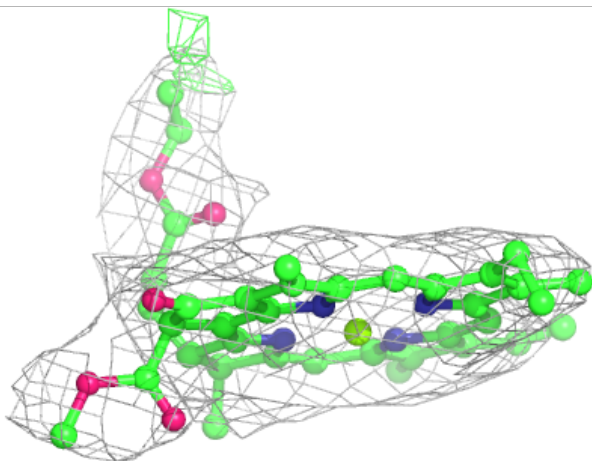
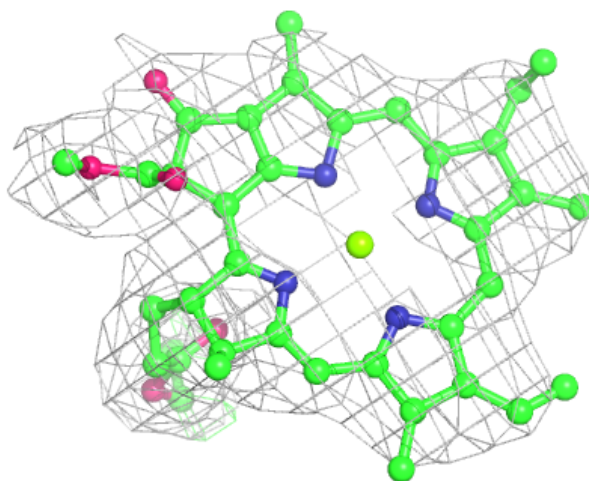
Electron density around CHL 3 307:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



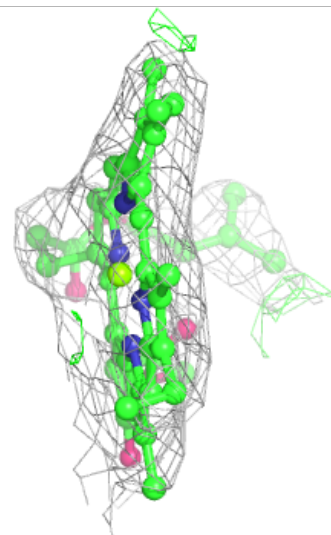
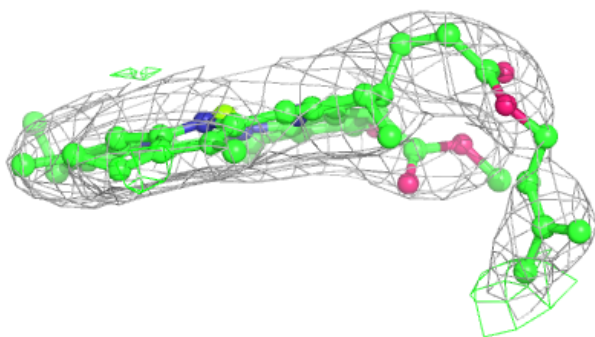
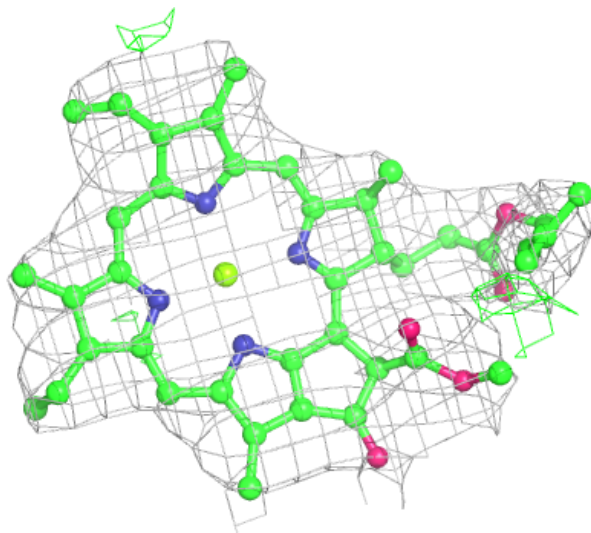
Electron density around CLA 8 305:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



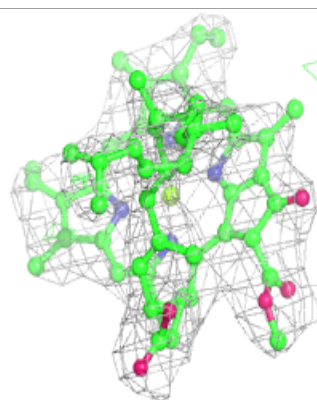
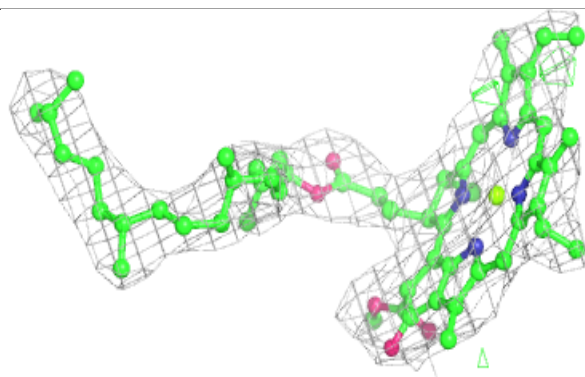
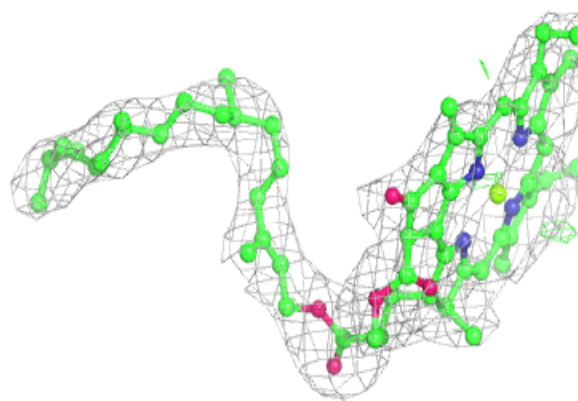
Electron density around CLA 3 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



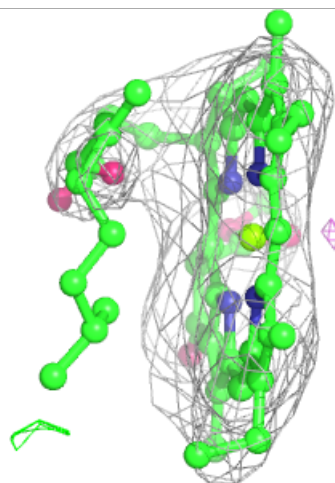
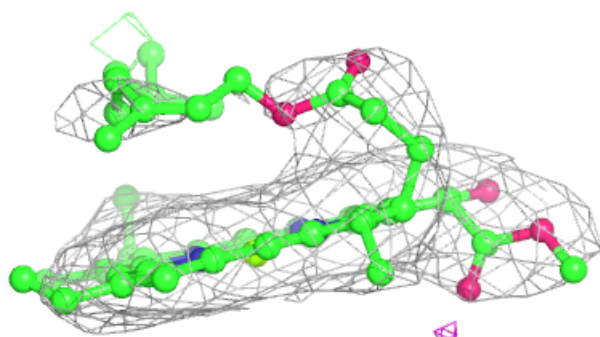
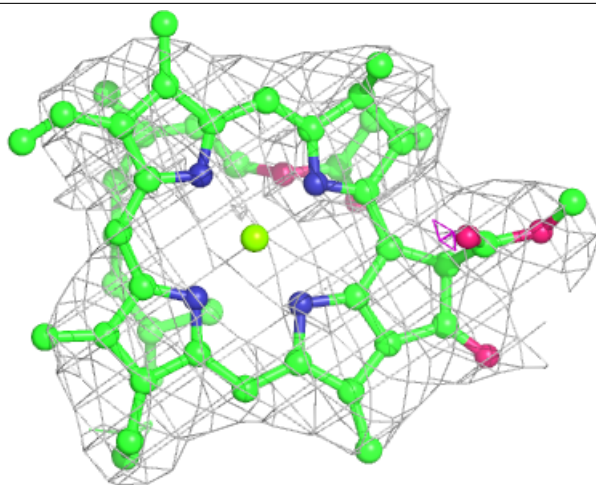
Electron density around CLA b 802:

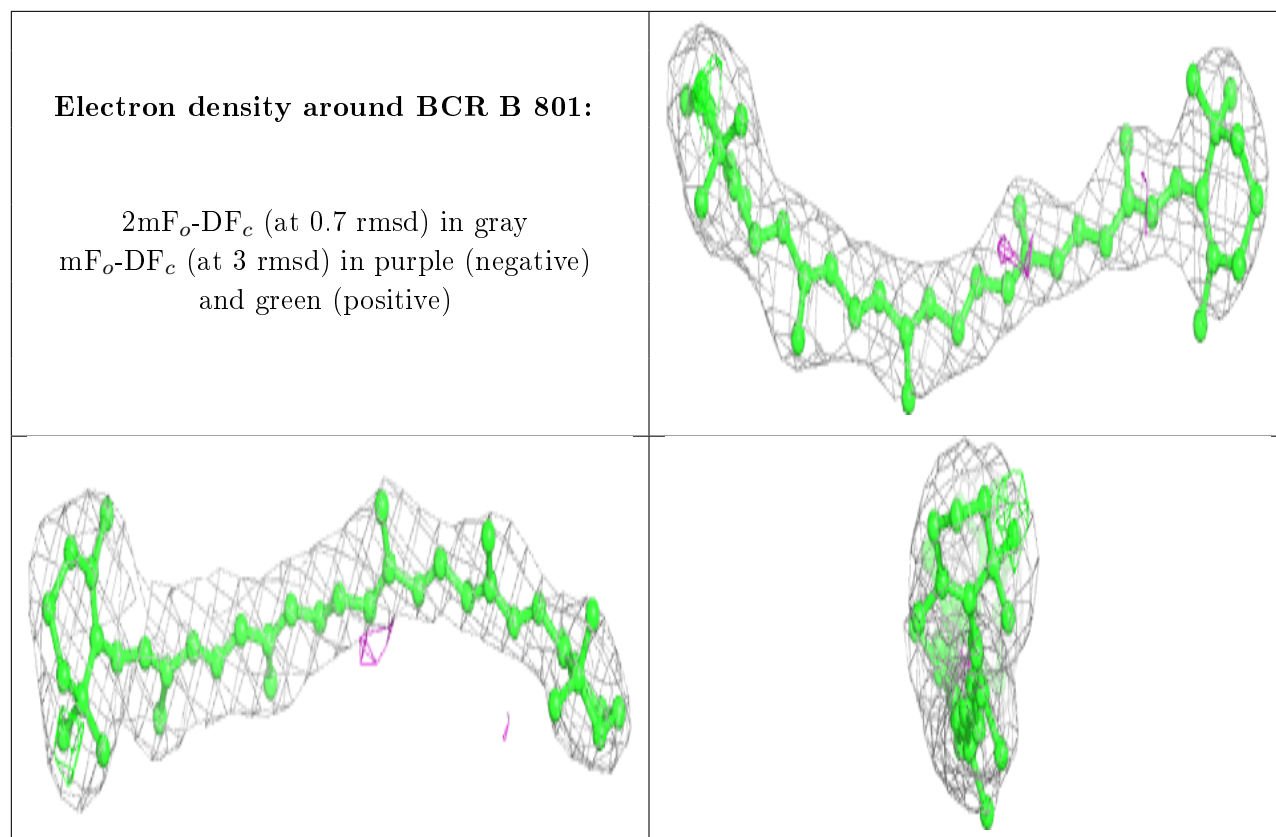
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 812:

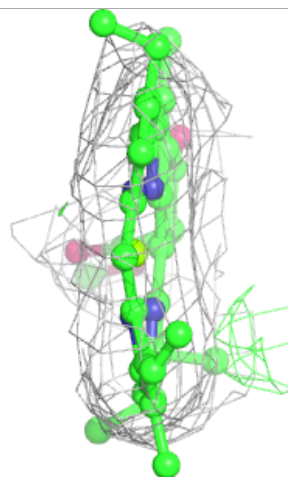
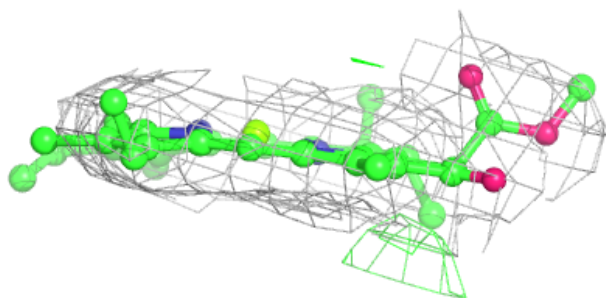
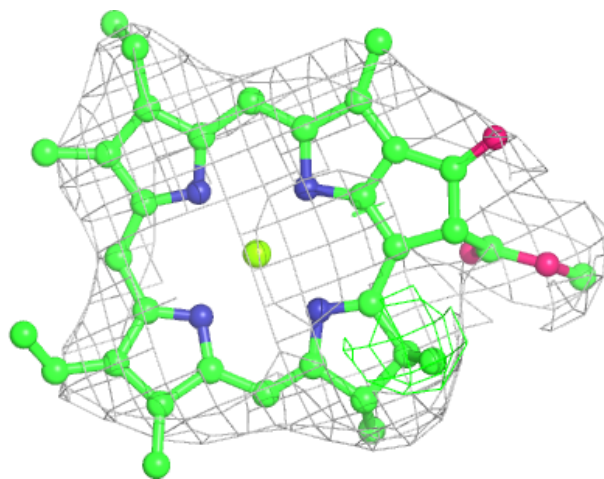
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





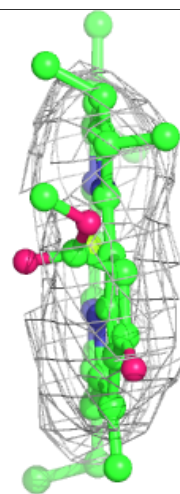
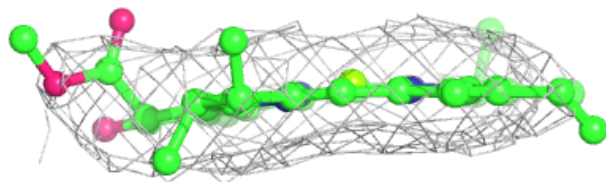
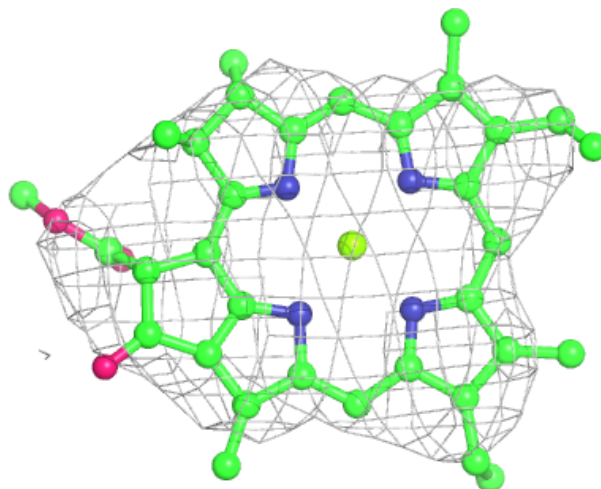
Electron density around CLA 7 610:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



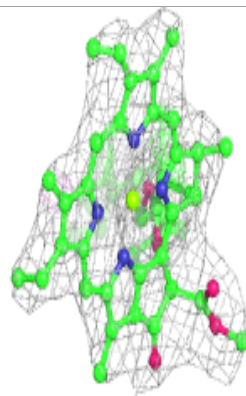
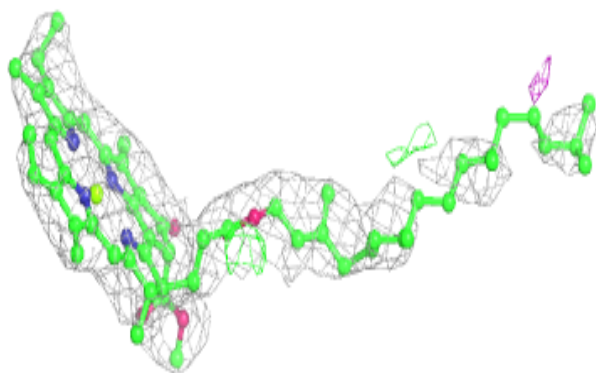
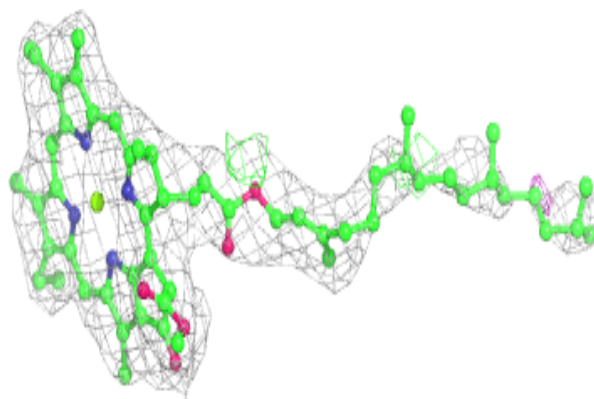
Electron density around CLA 9 610:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



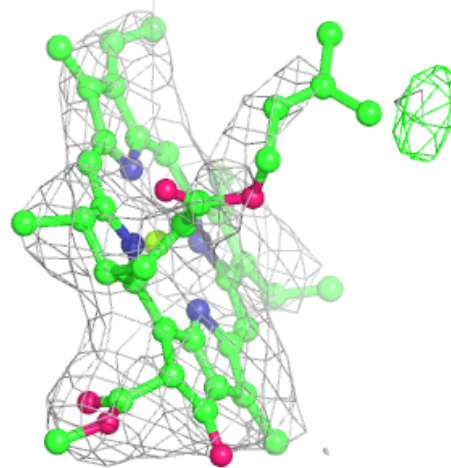
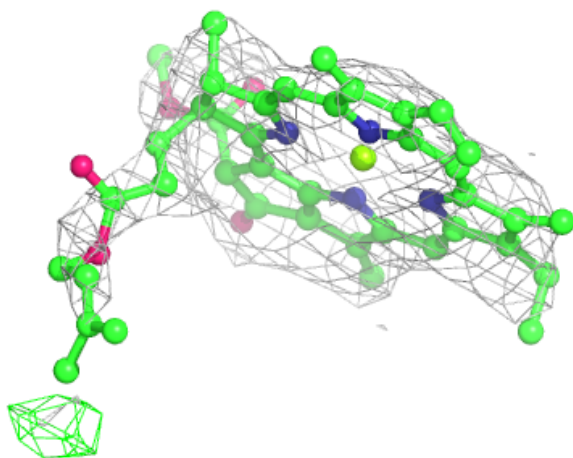
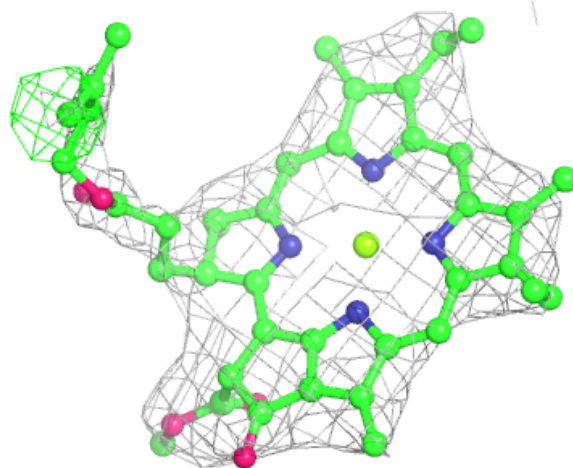
Electron density around CLA a 810:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



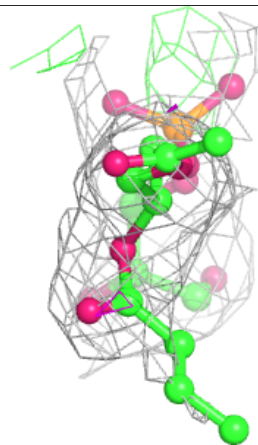
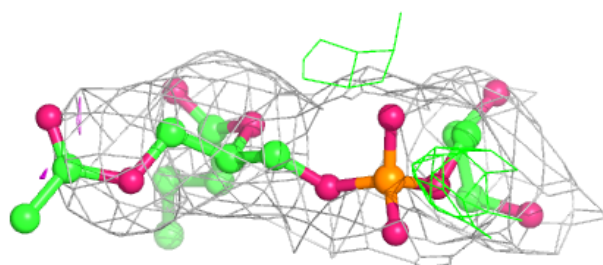
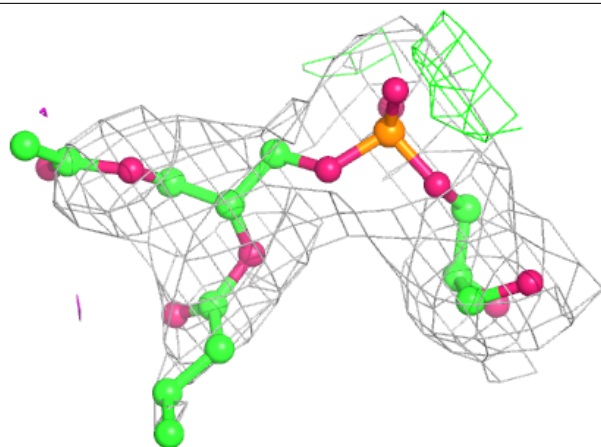
Electron density around CLA A 816:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

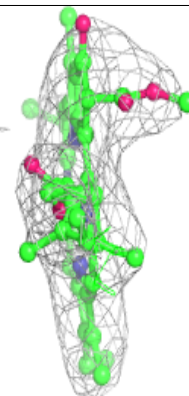
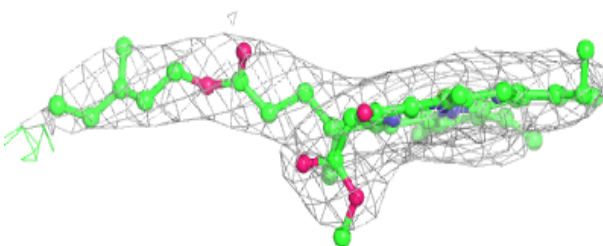
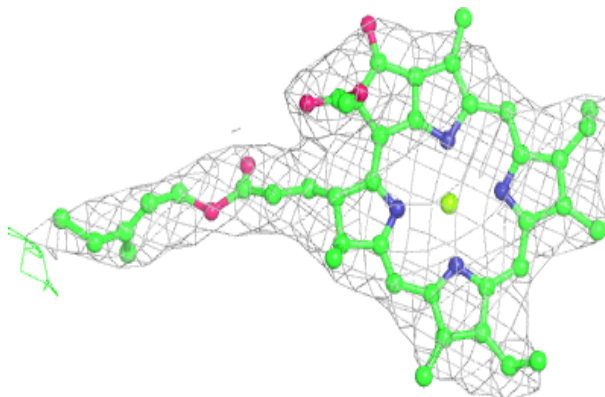


Electron density around LHG 1 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

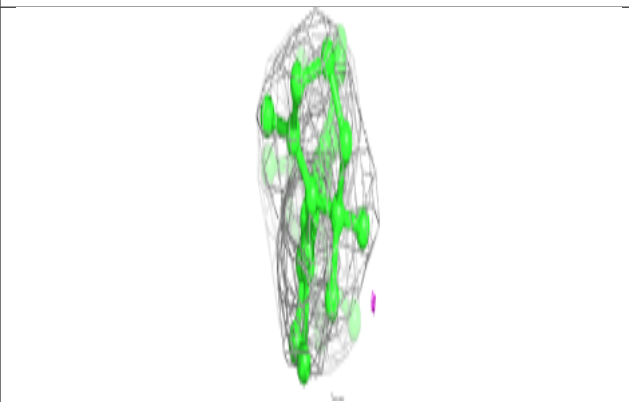
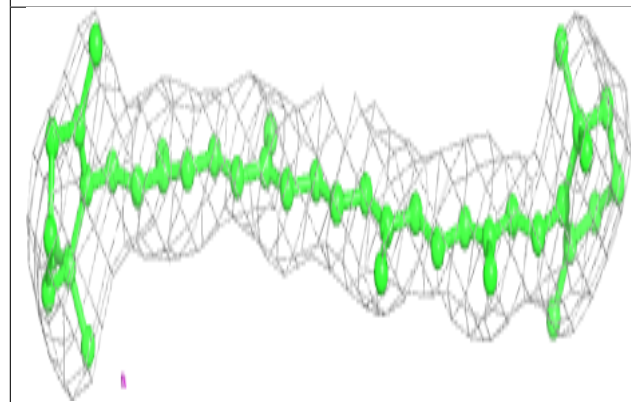
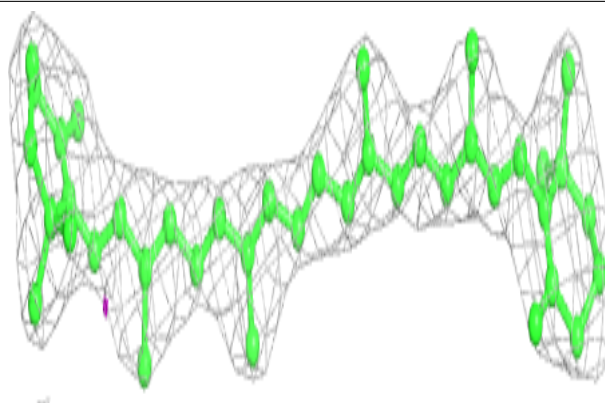
**Electron density around CLA A 838:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

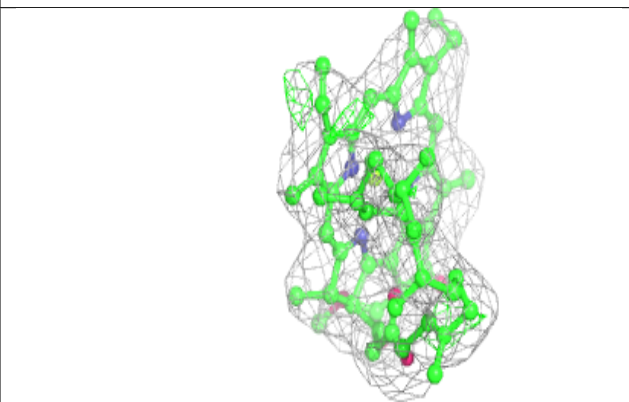
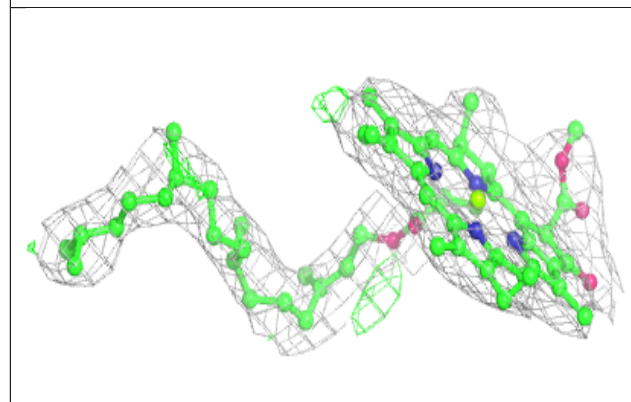
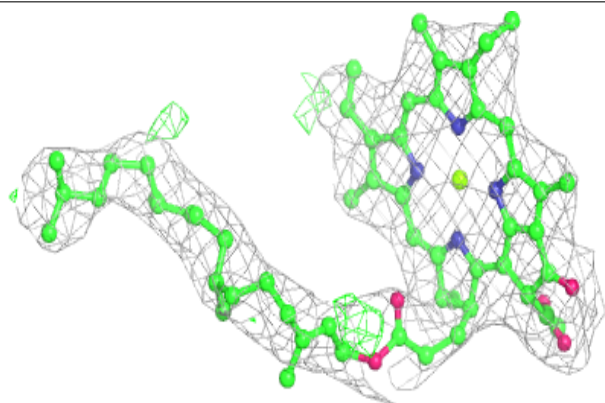


Electron density around BCR a 851:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

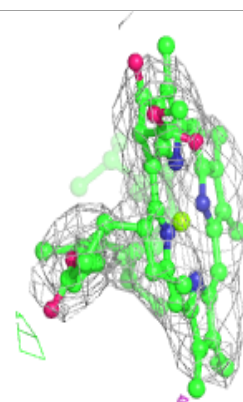
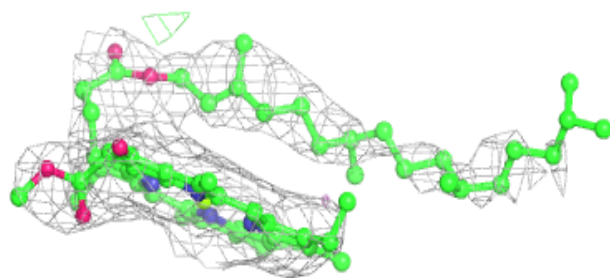
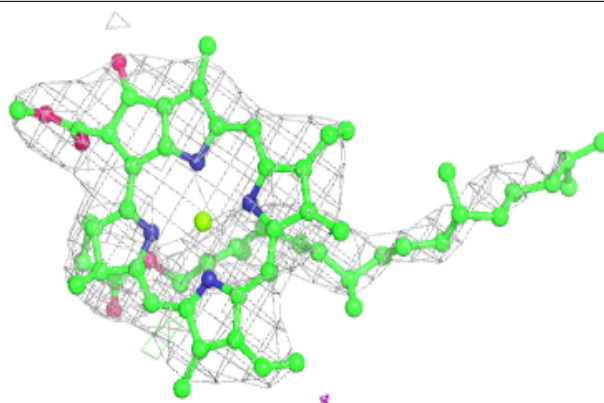
**Electron density around CLA a 809:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

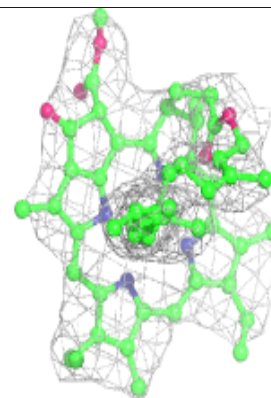
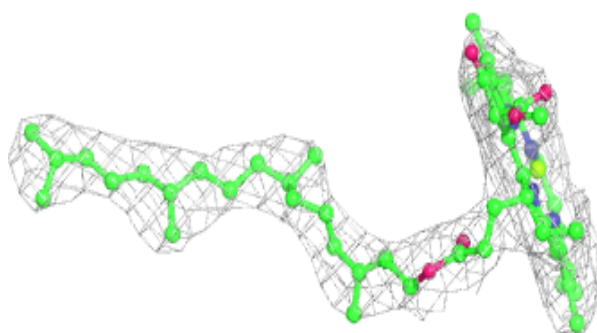
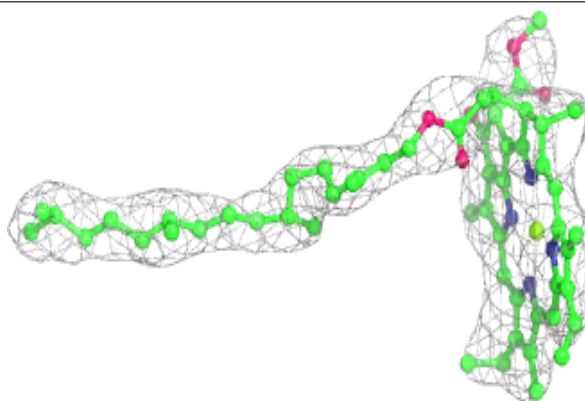


Electron density around CLA A 819:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

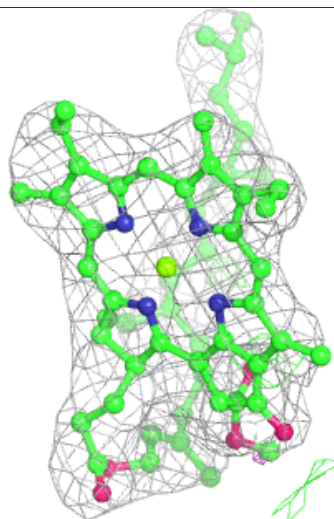
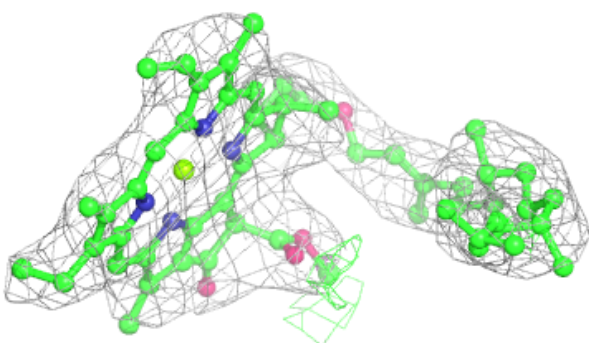
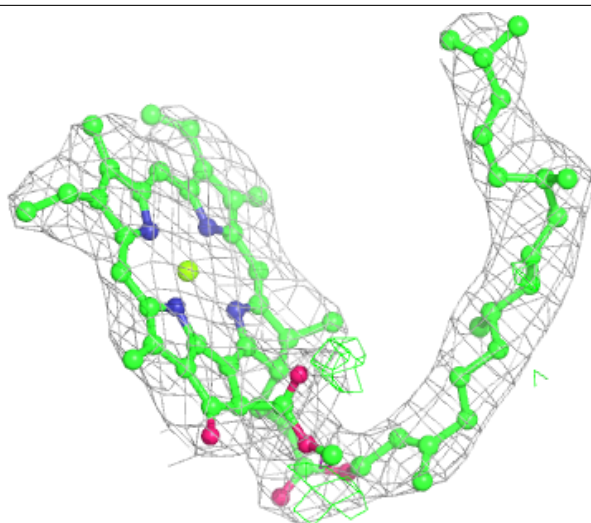
**Electron density around CLA B 828:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



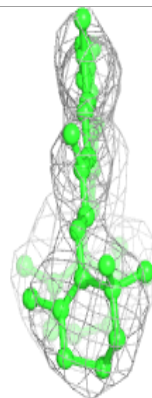
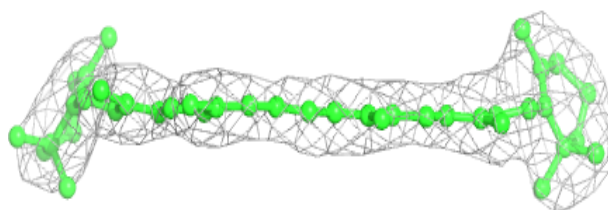
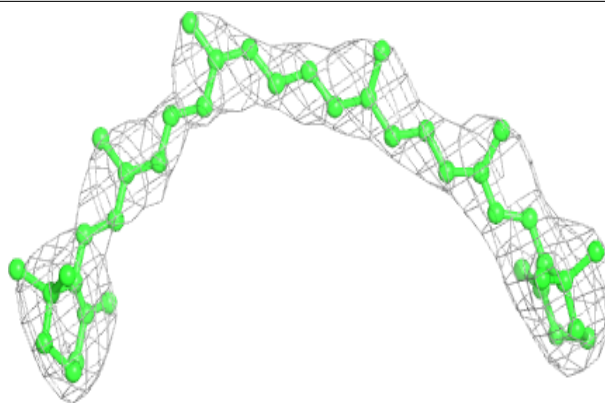
Electron density around CLA b 810:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



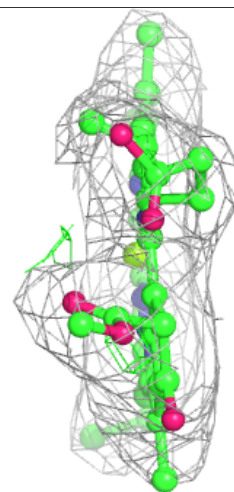
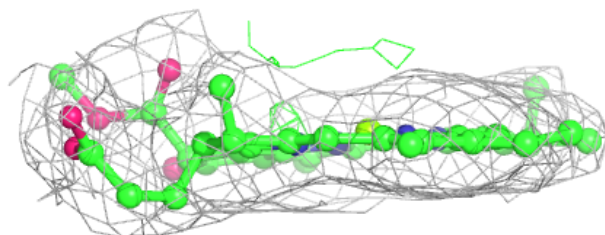
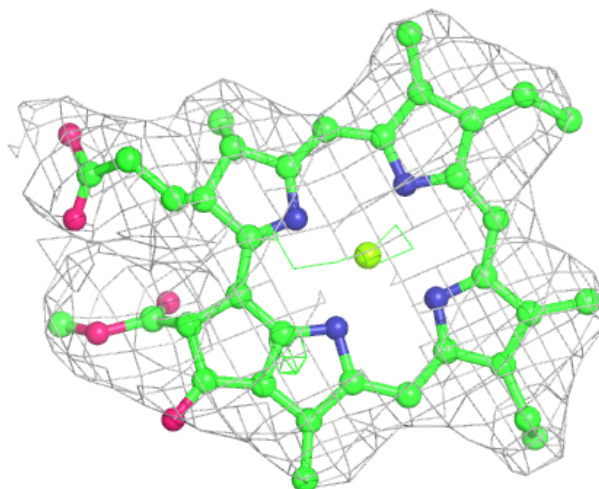
Electron density around BCR F 305:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



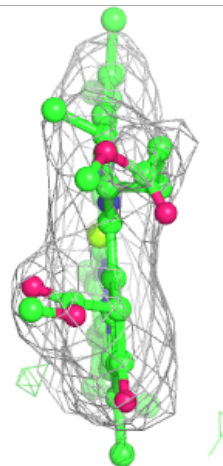
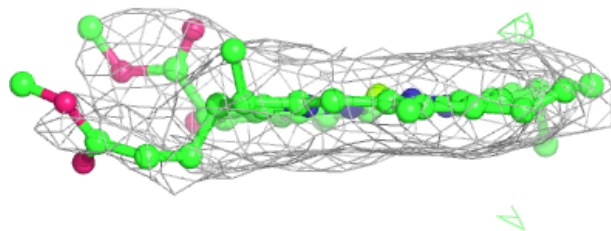
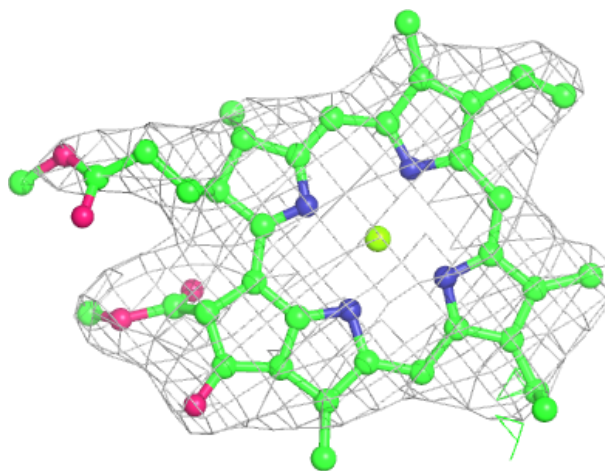
Electron density around CLA F 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



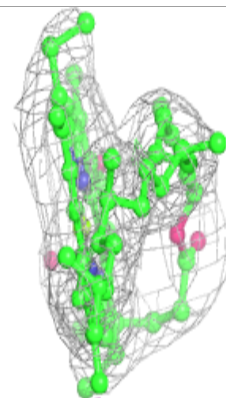
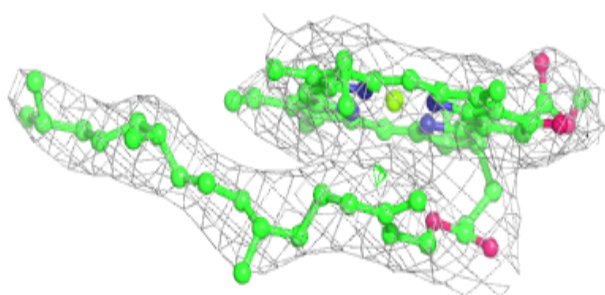
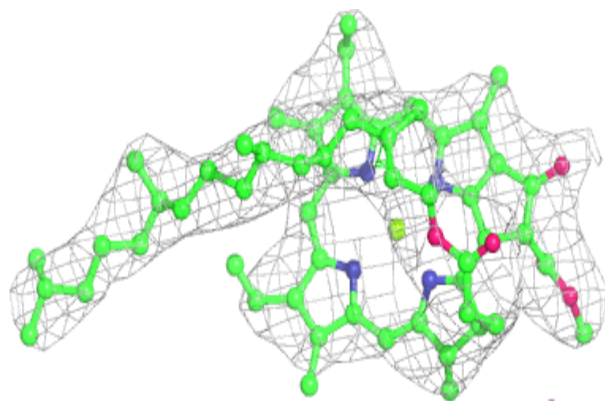
Electron density around CLA 8 312:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



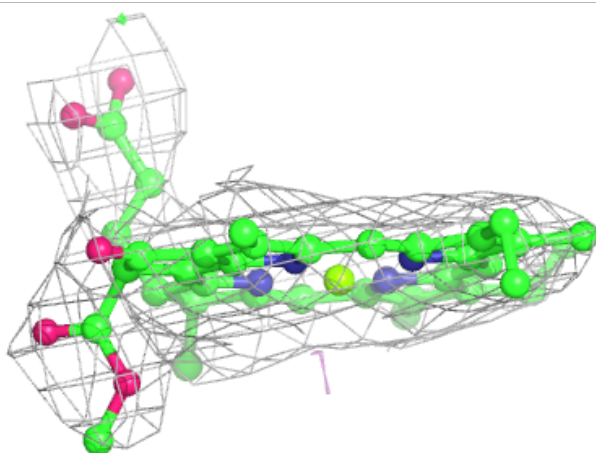
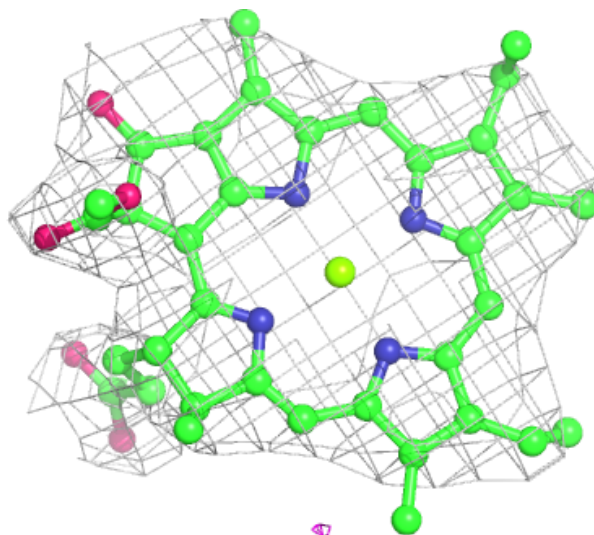
Electron density around CLA a 841:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



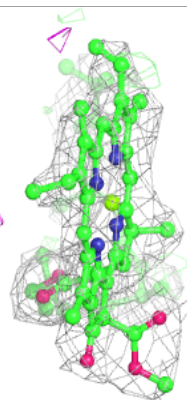
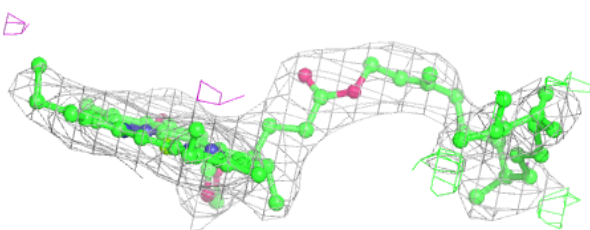
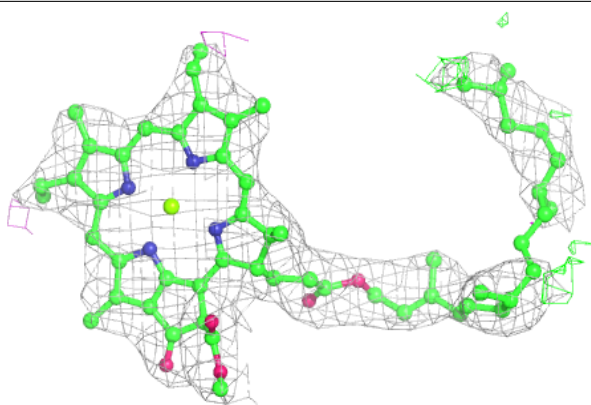
Electron density around CLA A 815:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

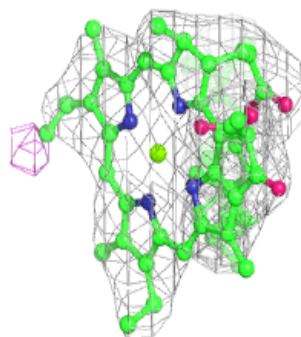
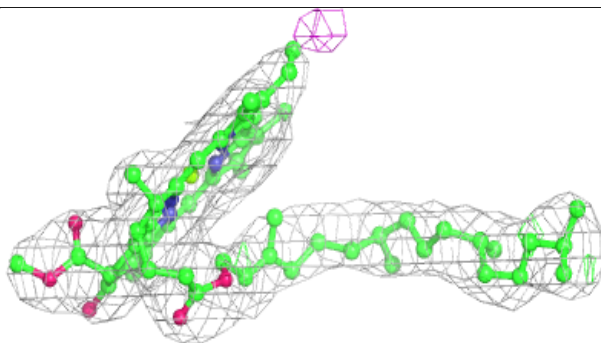
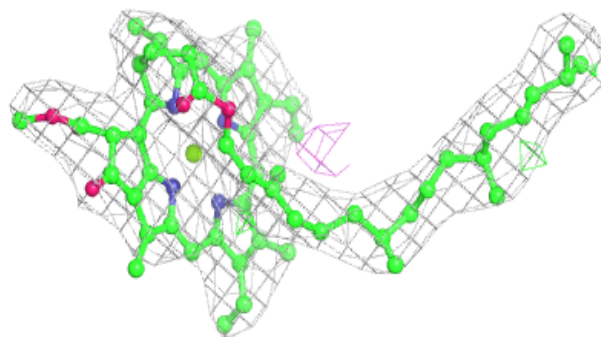


Electron density around CLA a 827:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

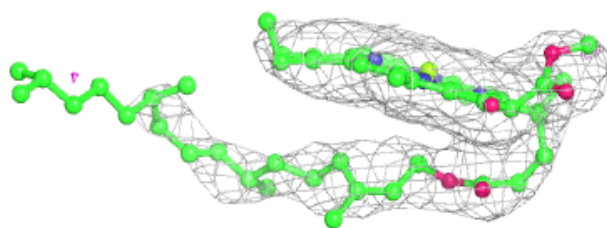
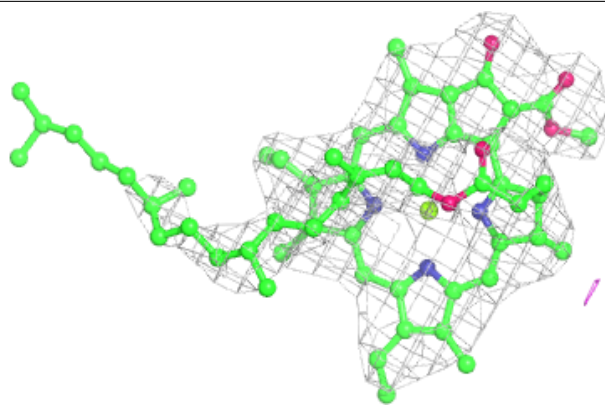
**Electron density around CLA a 843:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

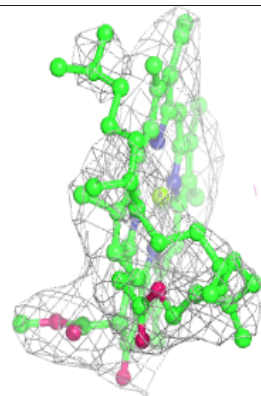
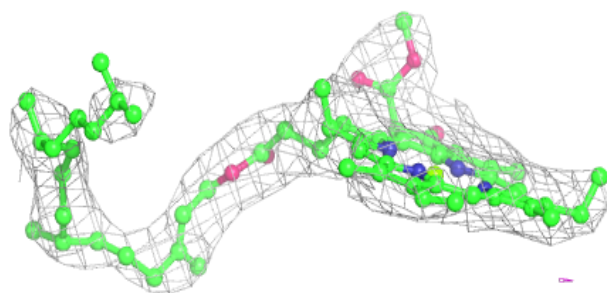
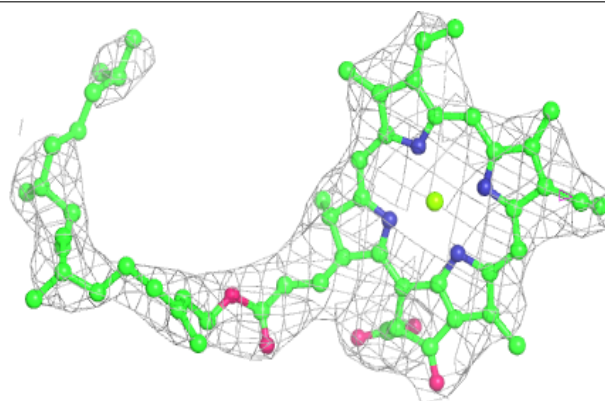


Electron density around CLA a 818:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

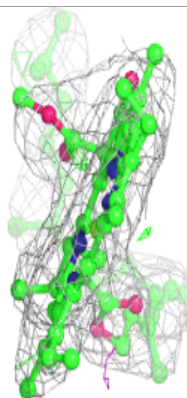
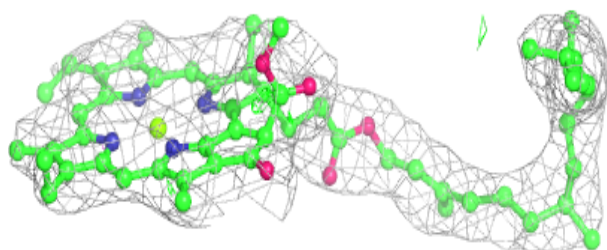
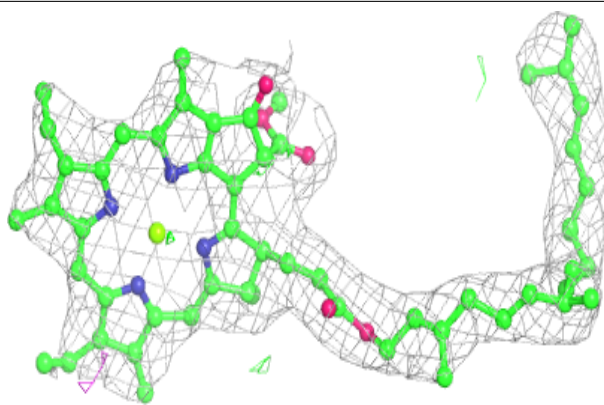
**Electron density around CLA a 828:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

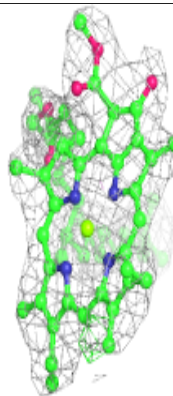
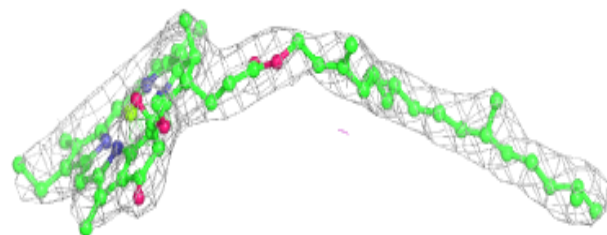
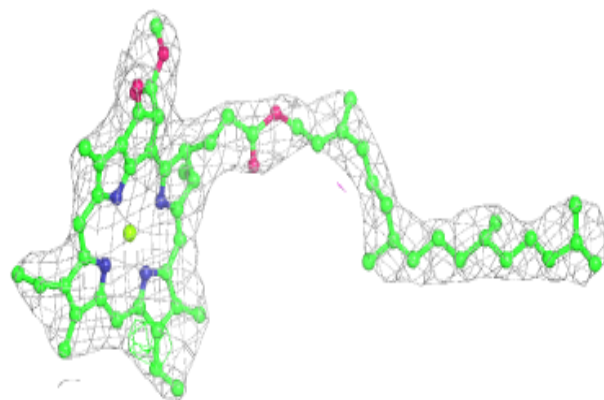


Electron density around CLA B 826:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

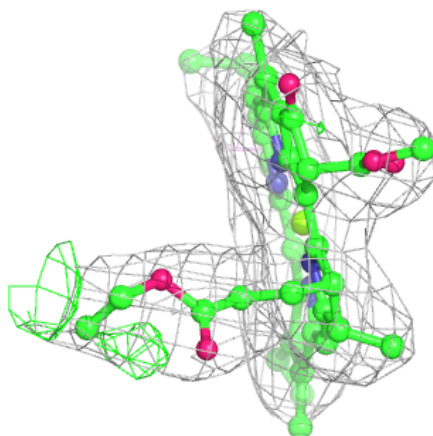
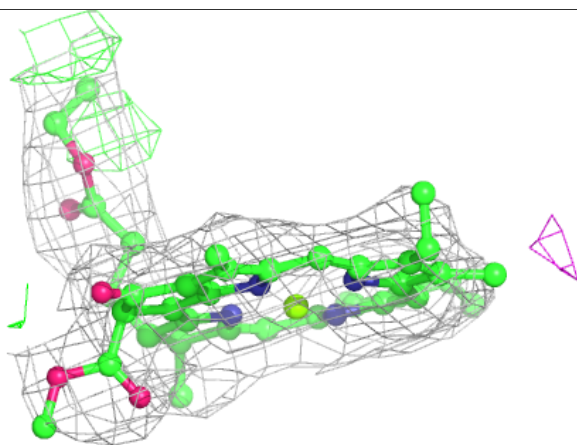
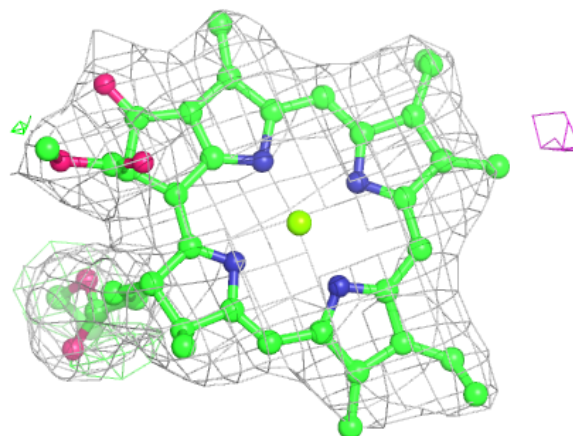
**Electron density around CLA A 803:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



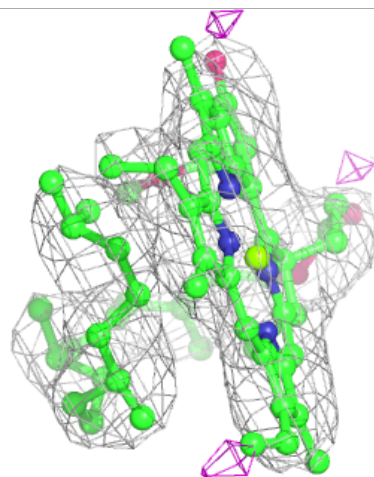
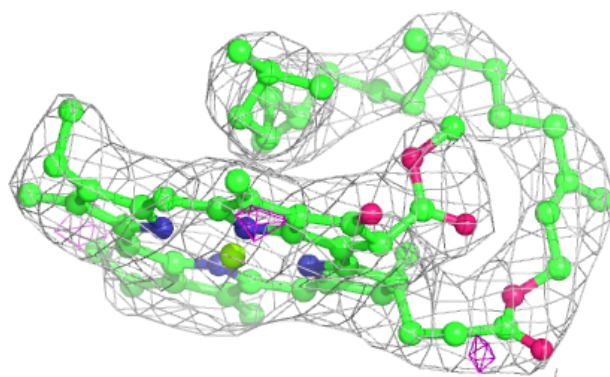
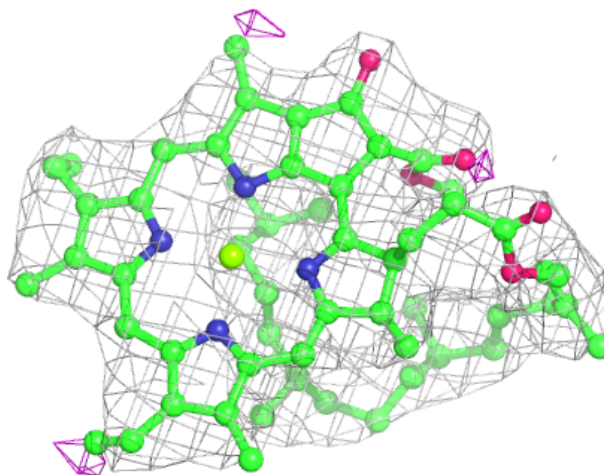
Electron density around CLA B 838:

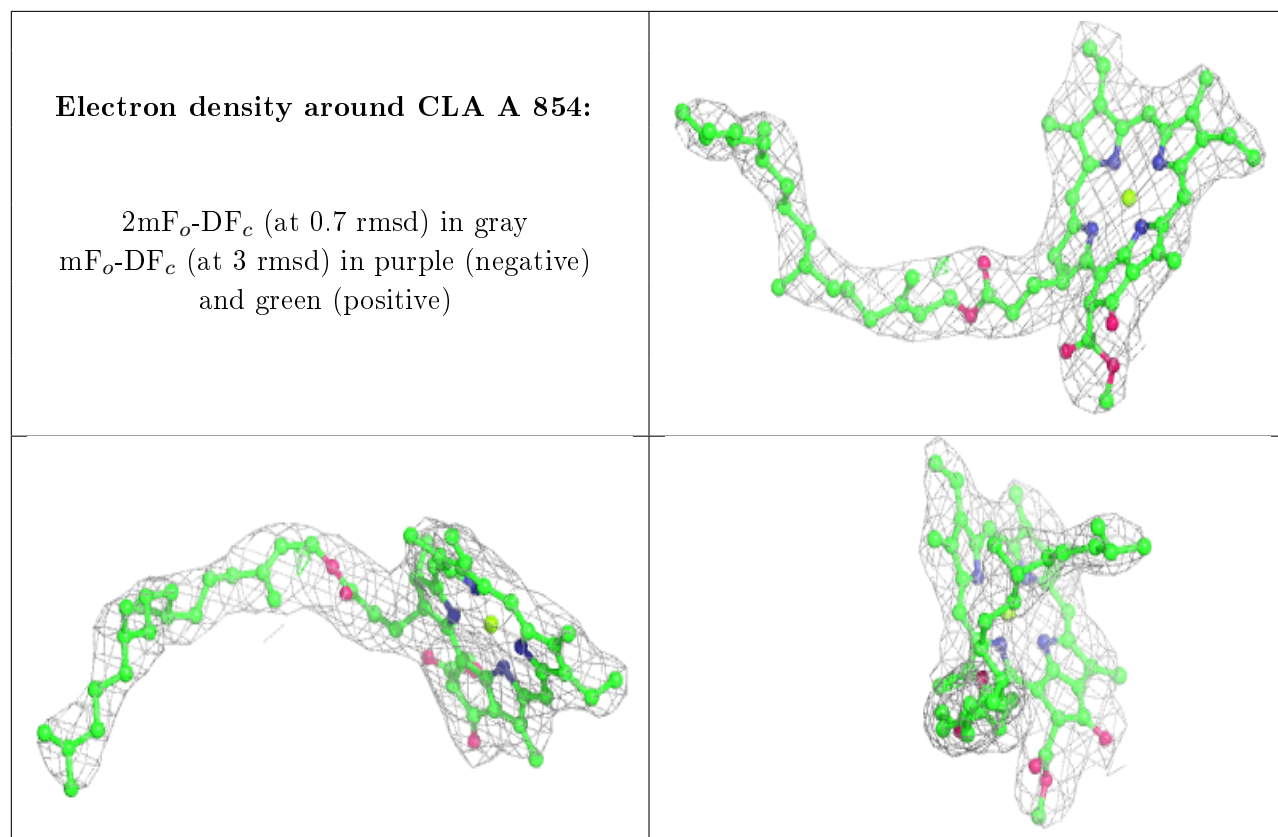
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA a 807:

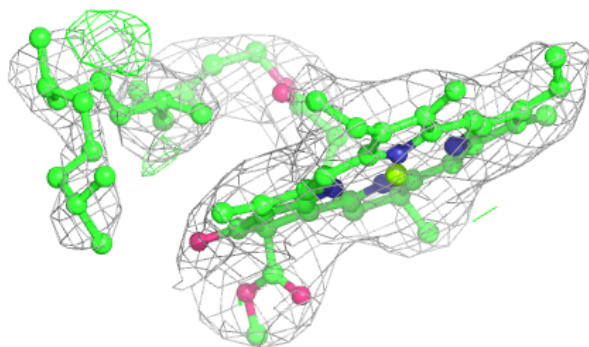
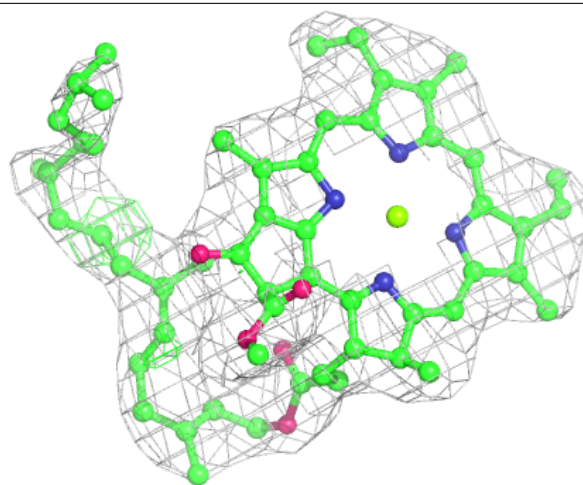
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





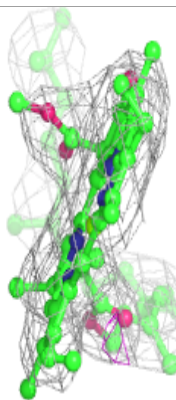
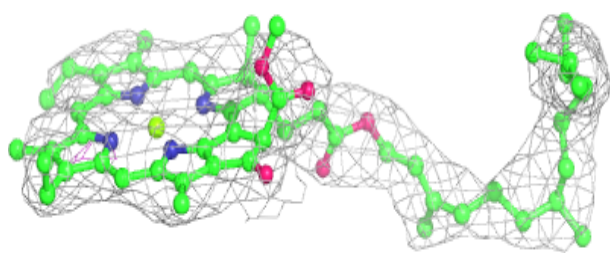
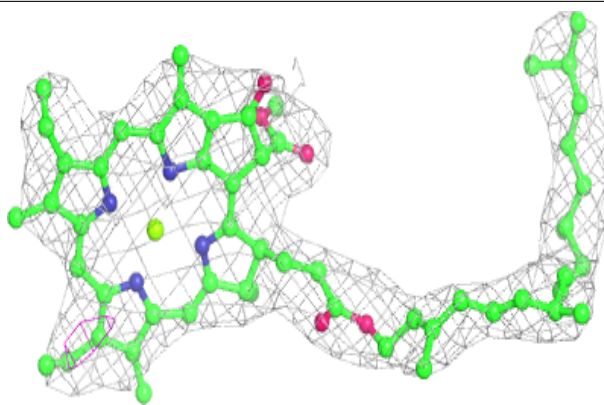
Electron density around CLA B 832:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

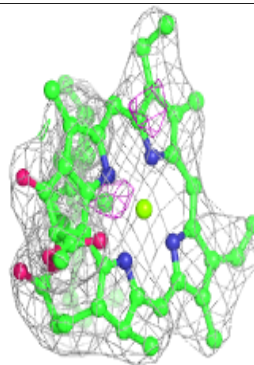
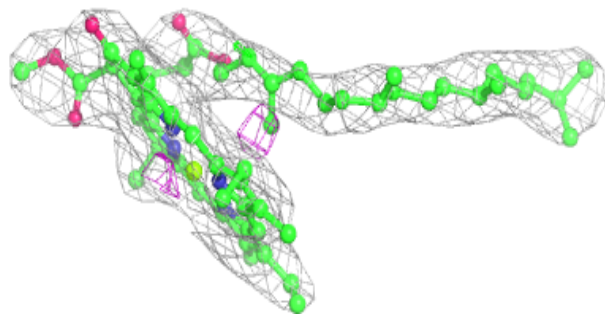
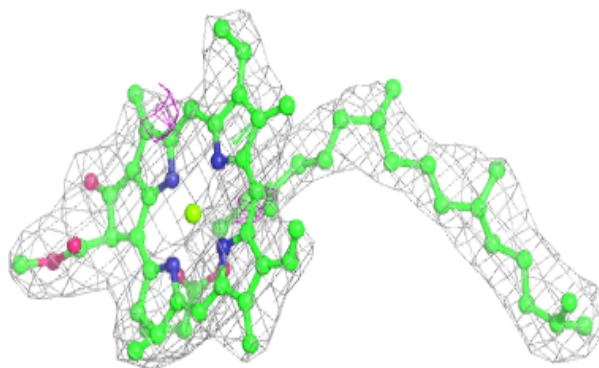


Electron density around CLA b 826:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

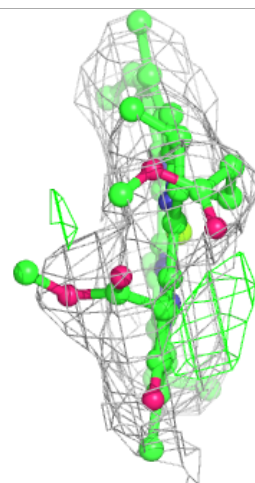
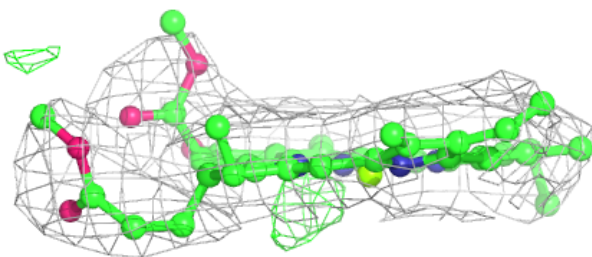
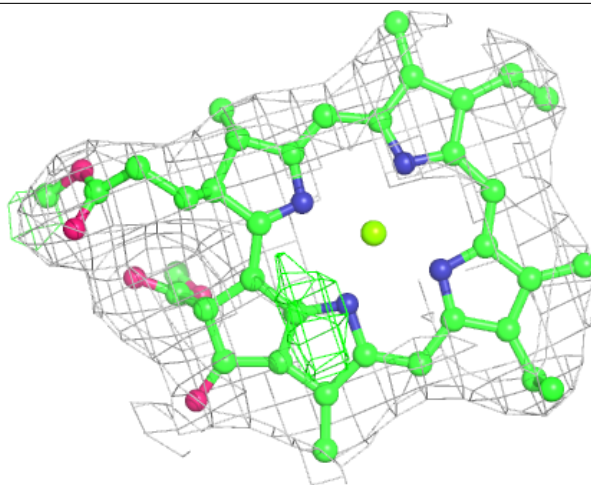
**Electron density around CLA A 842:**

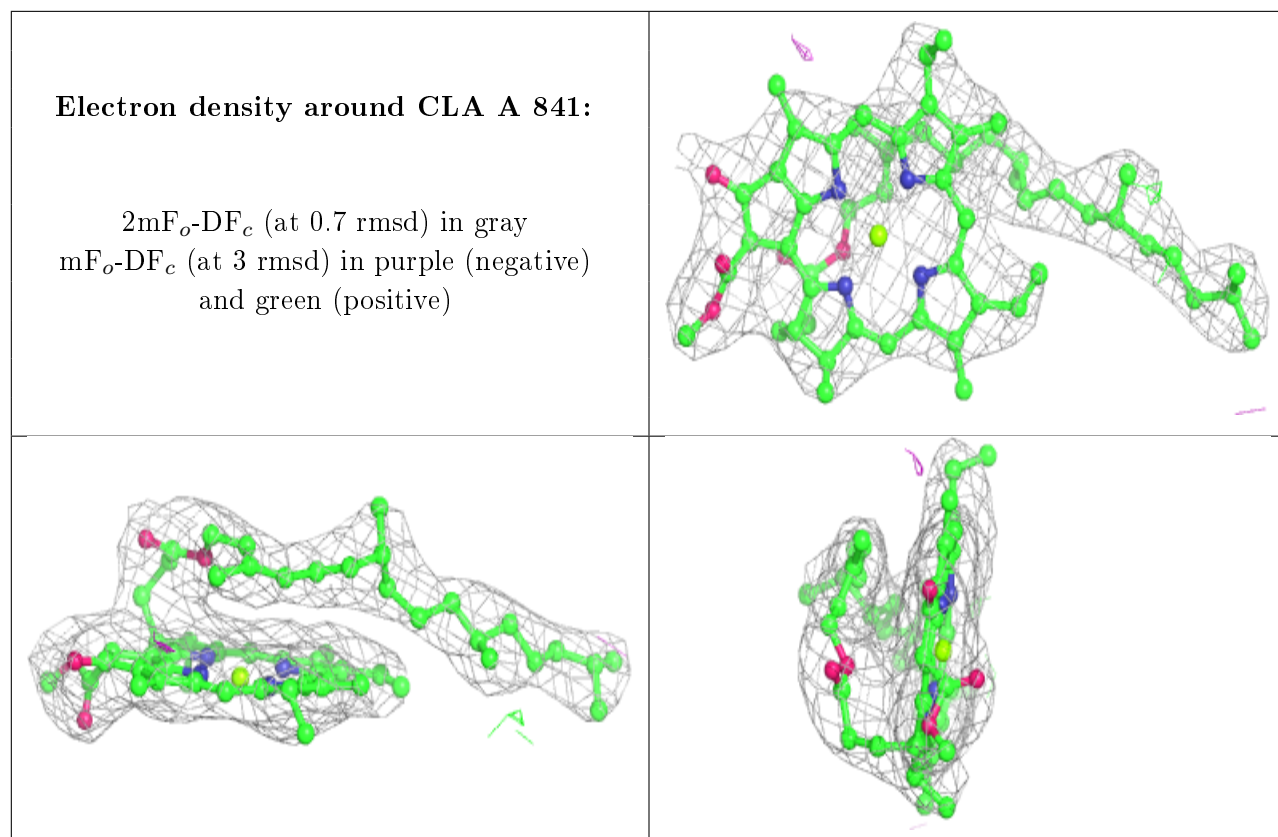
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 4 603:

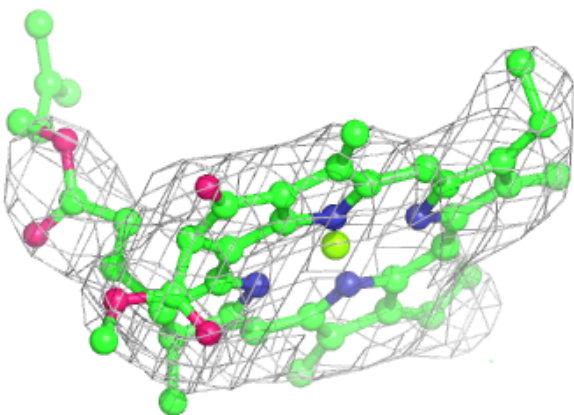
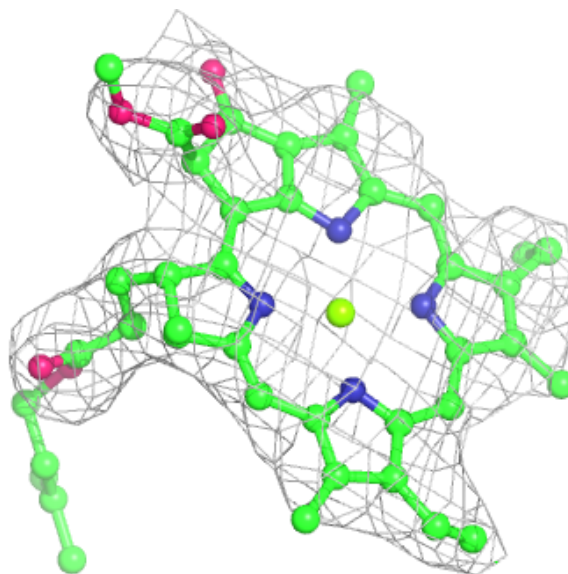
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

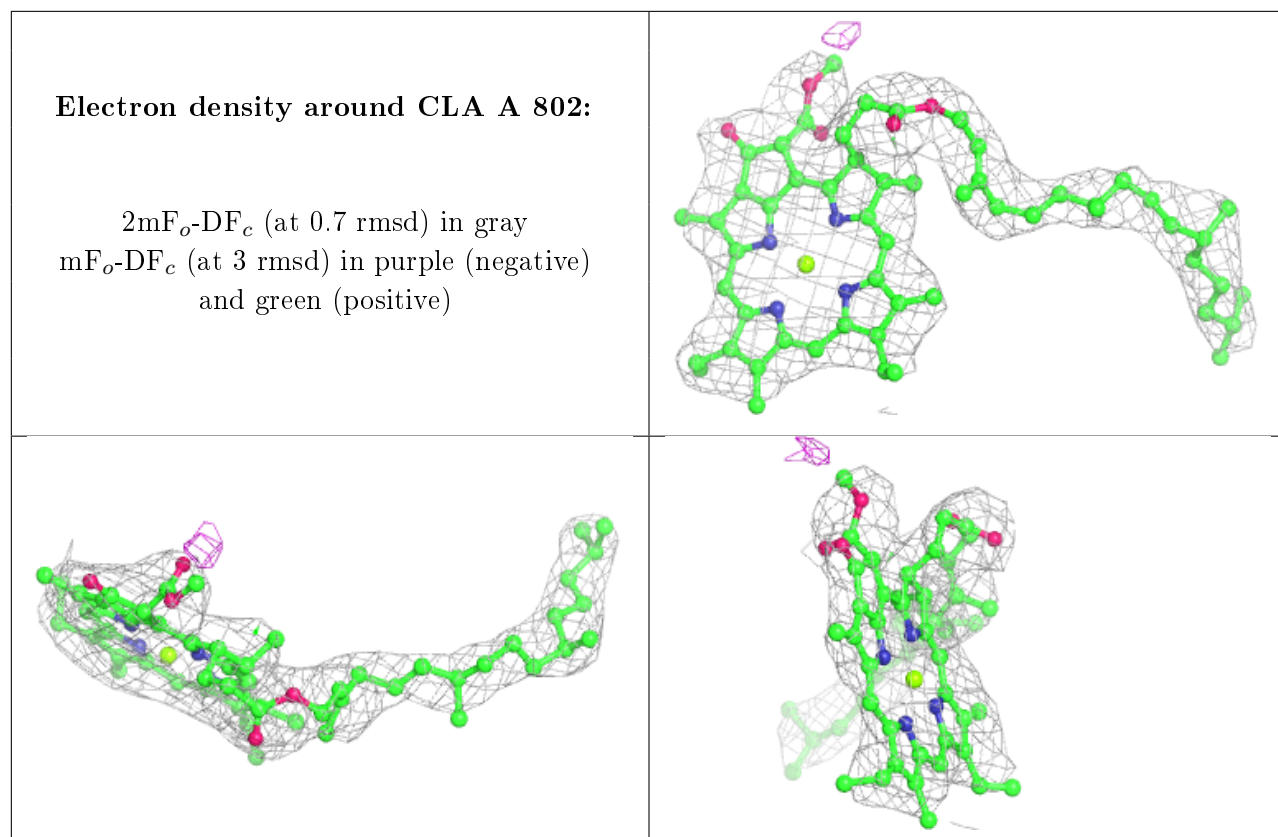




Electron density around CLA B 820:

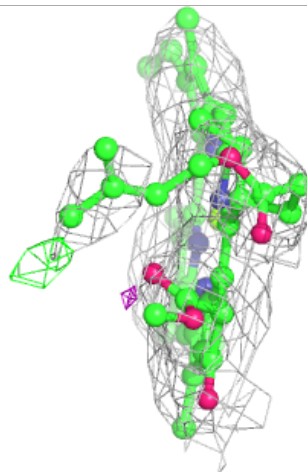
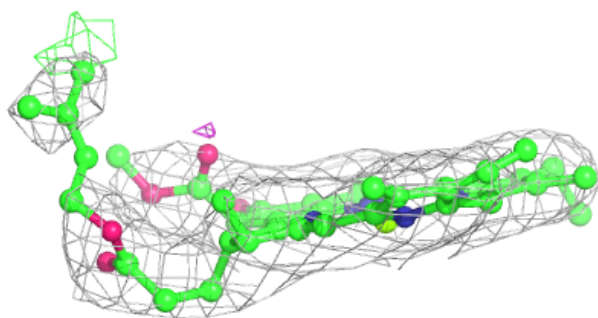
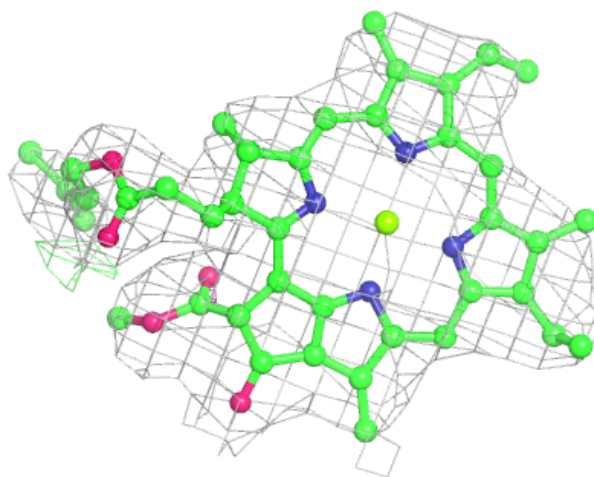
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





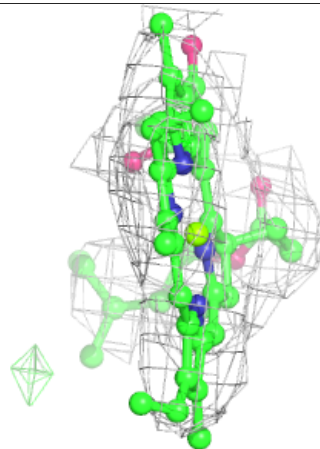
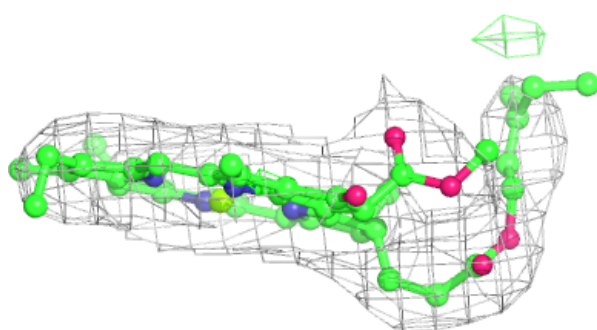
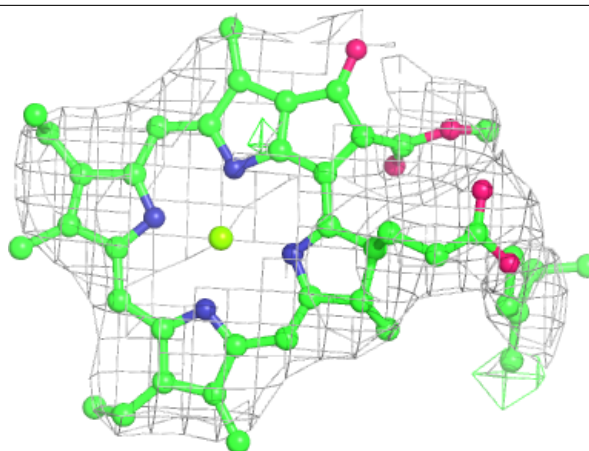
Electron density around CLA 8 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

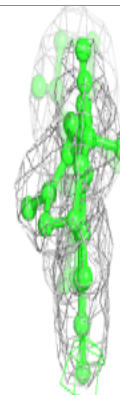
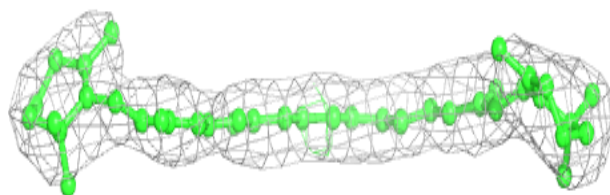
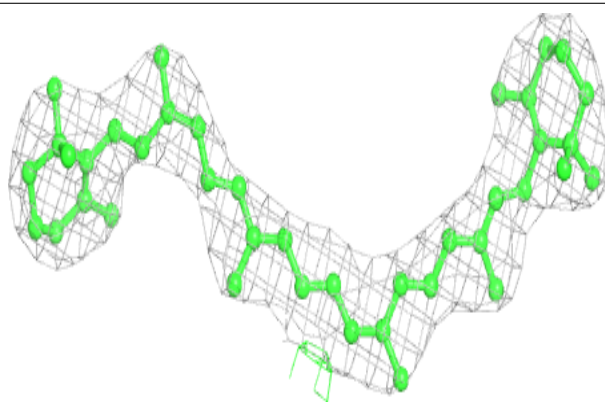


Electron density around CLA 7 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

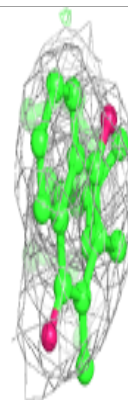
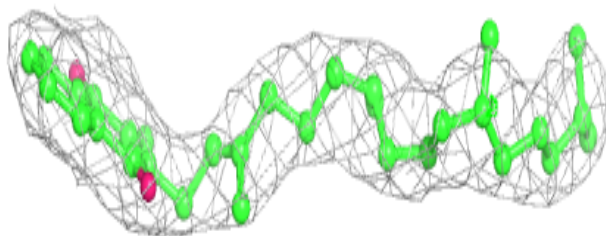
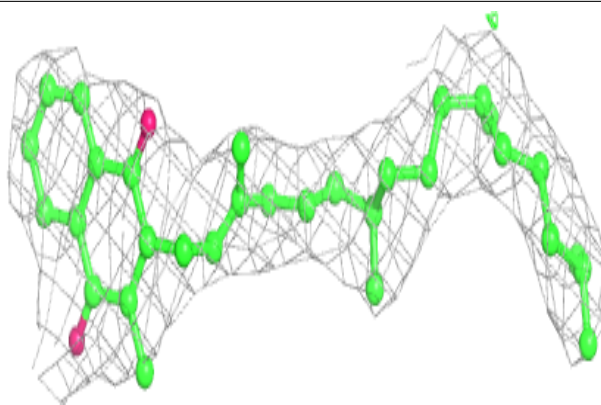
**Electron density around BCR A 852:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

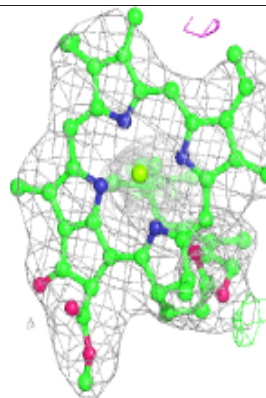
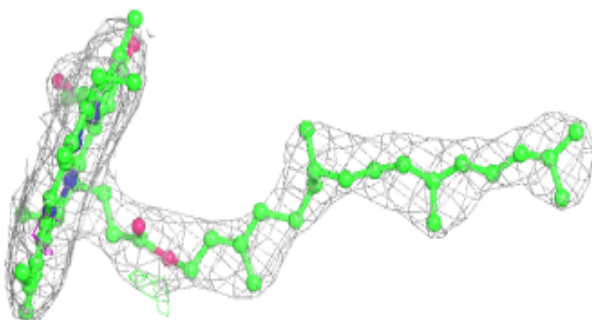
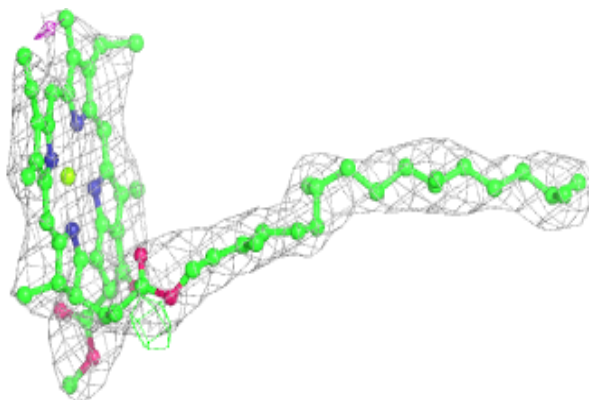


Electron density around PQN a 845:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

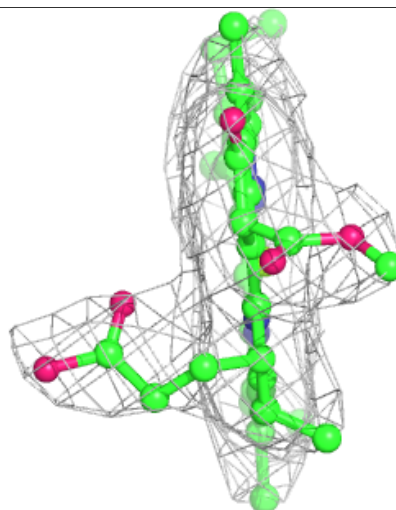
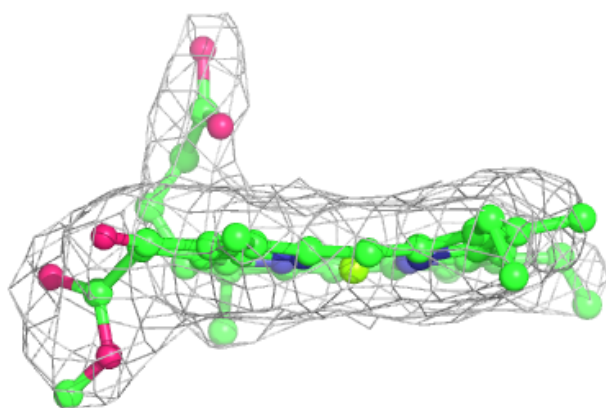
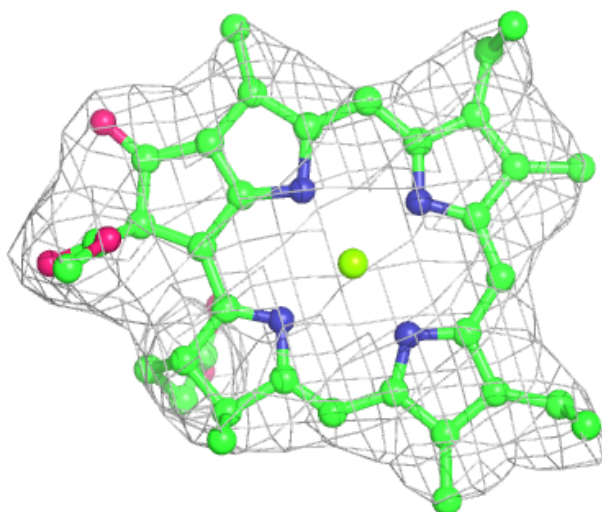
**Electron density around CLA b 828:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



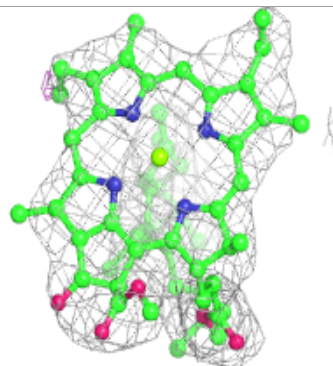
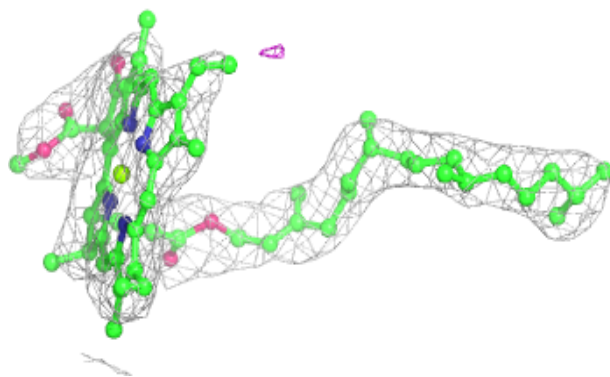
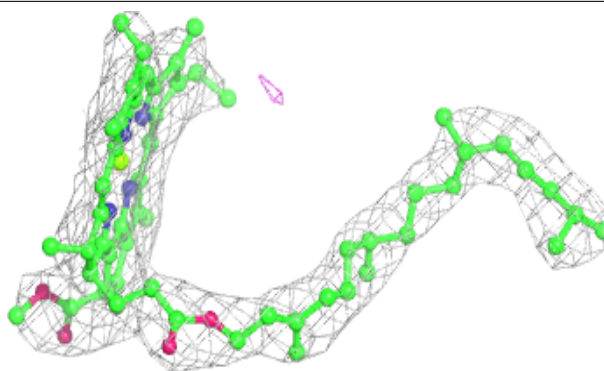
Electron density around CLA b 804:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

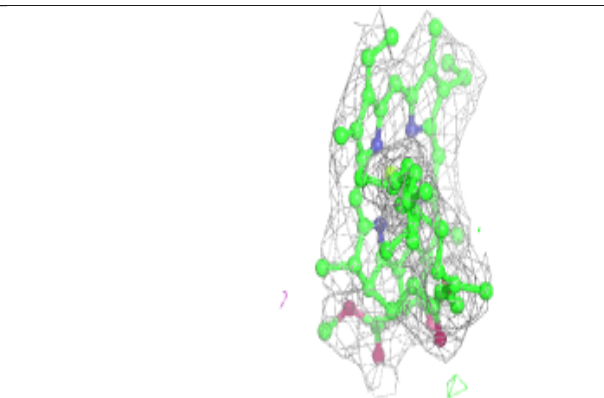
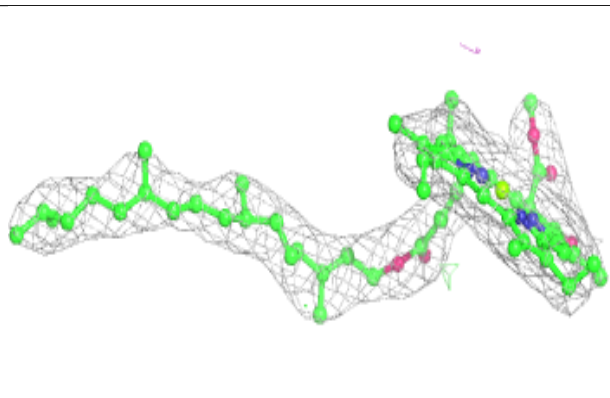
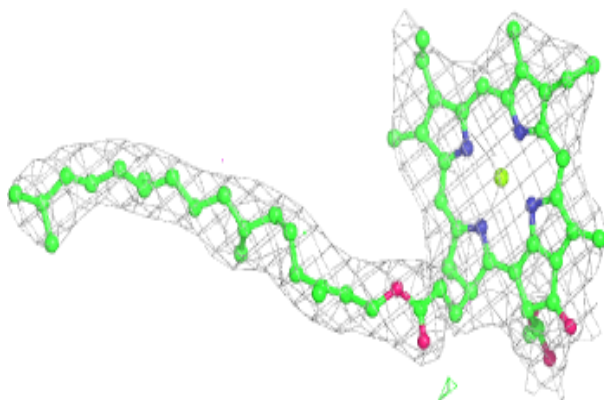


Electron density around CLA a 831:

$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)

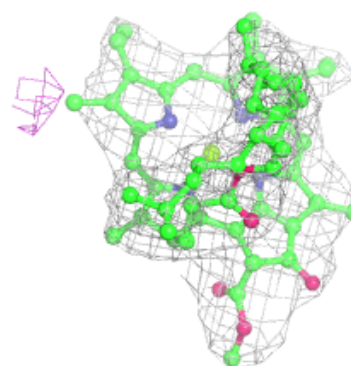
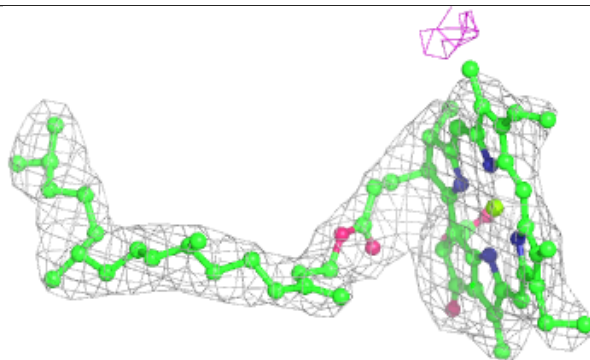
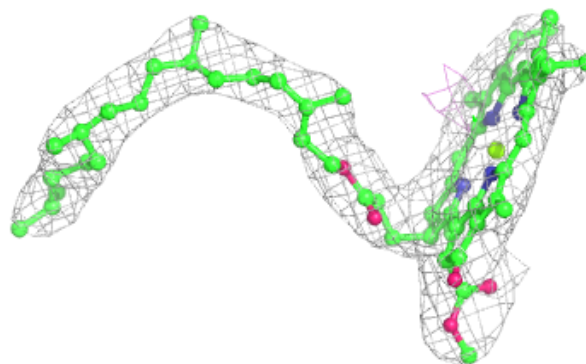
**Electron density around CLA a 835:**

$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)



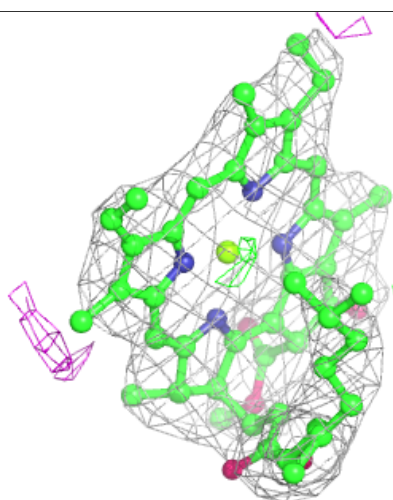
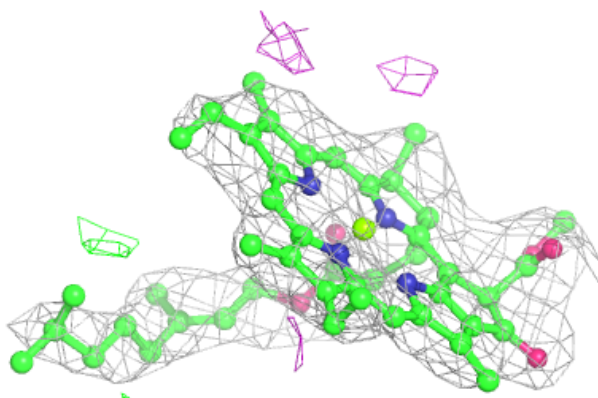
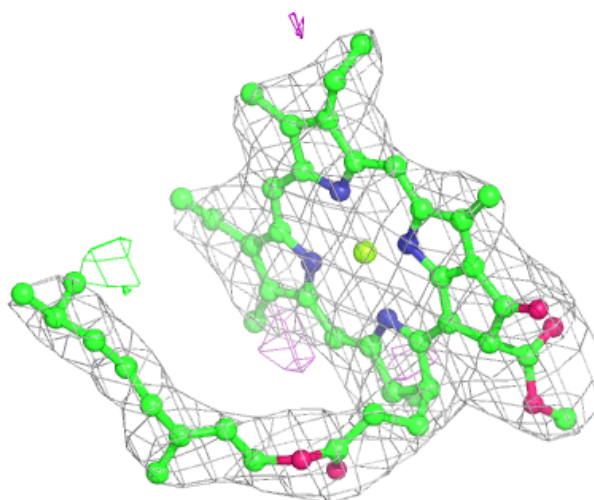
Electron density around CLA b 839:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



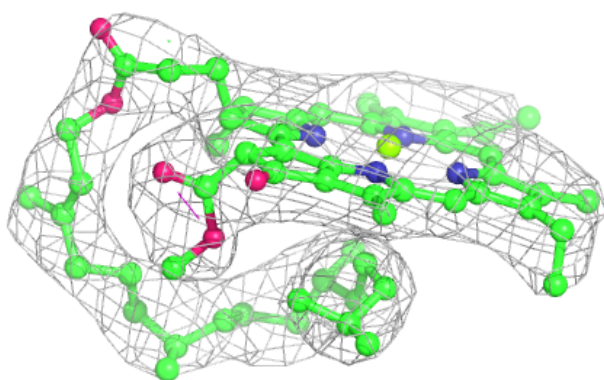
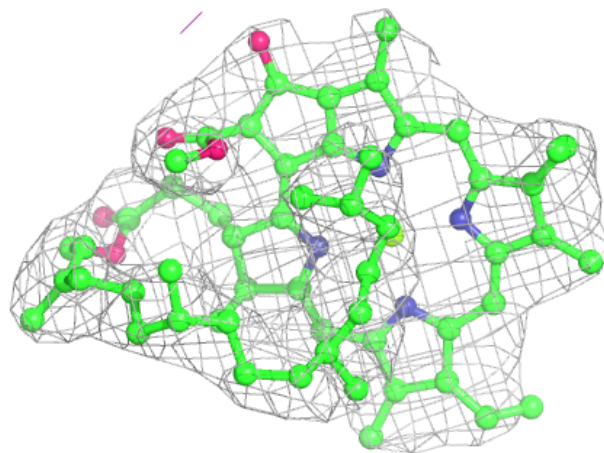
Electron density around CLA a 825:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



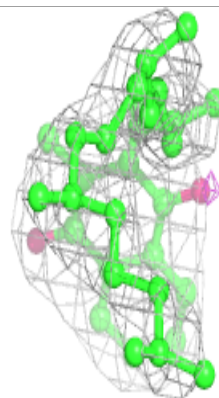
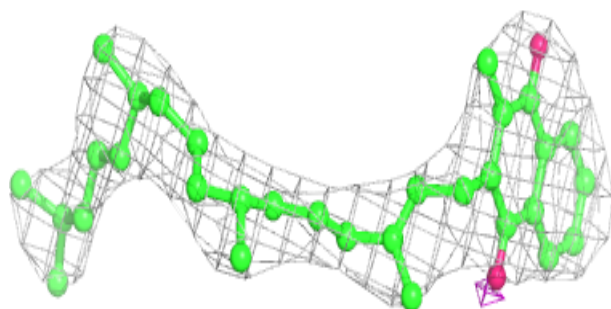
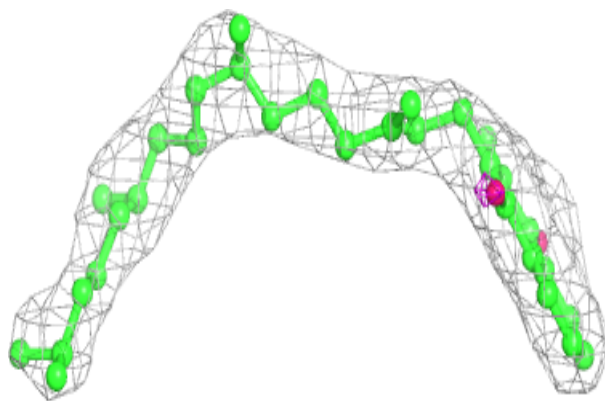
Electron density around CLA A 807:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



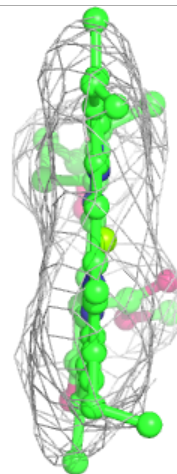
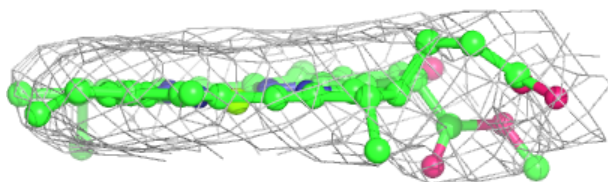
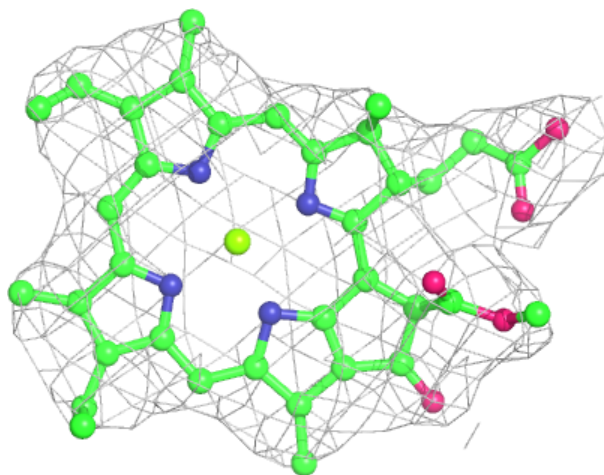
Electron density around PQN b 842:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



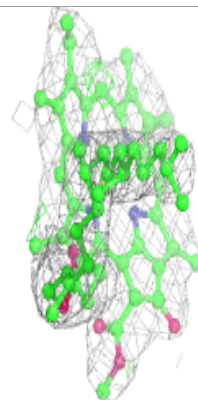
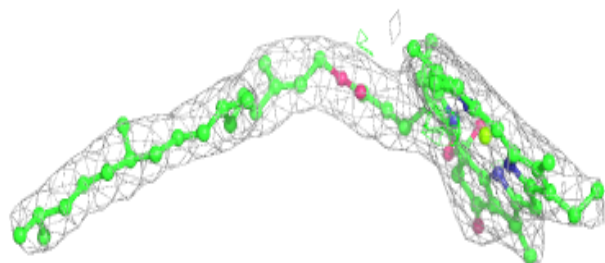
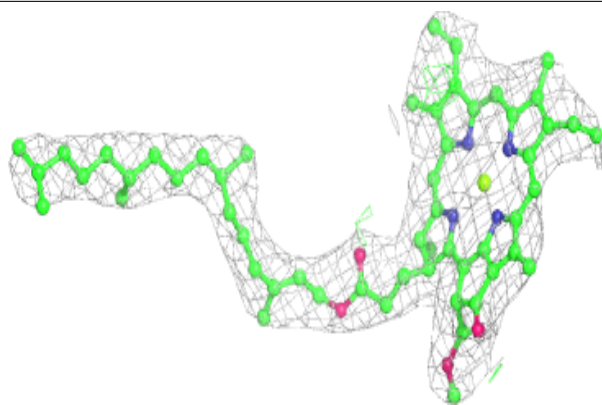
Electron density around CLA f 7002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

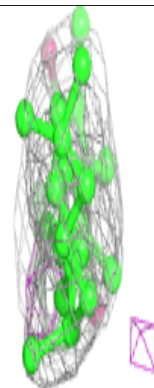
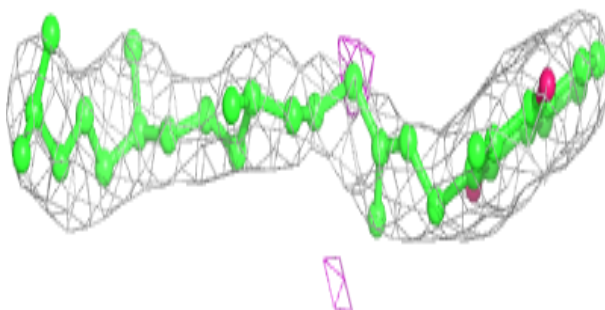
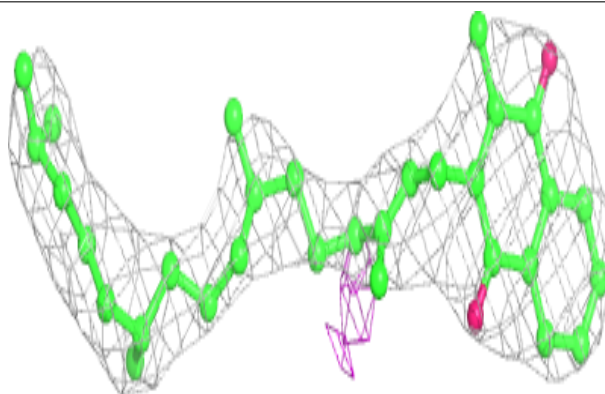


Electron density around CLA a 803:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

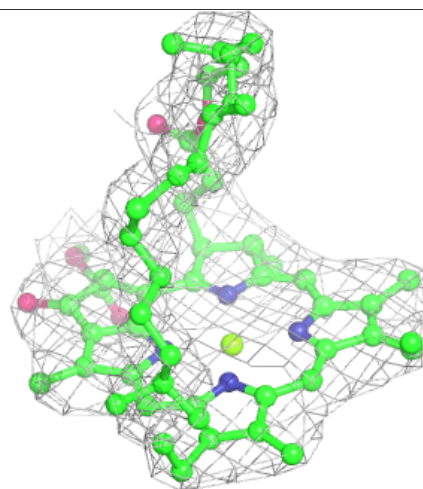
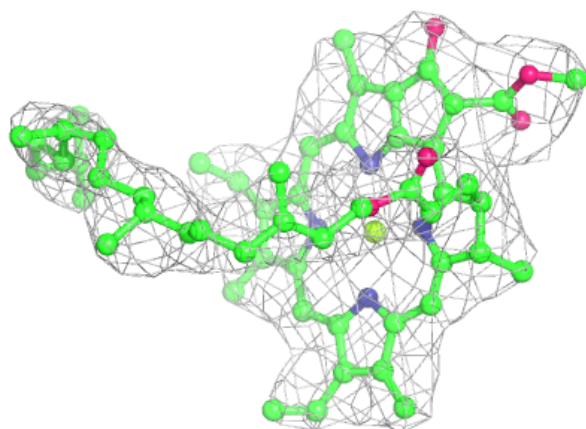
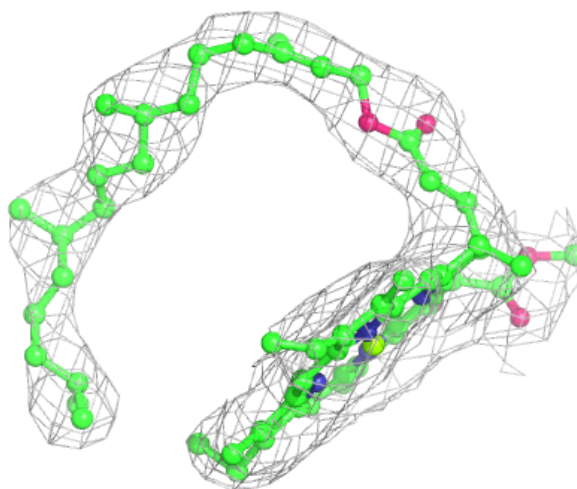
**Electron density around PQN A 844:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



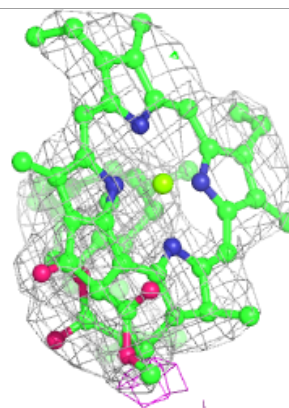
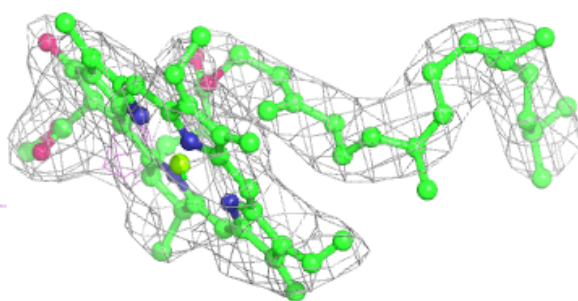
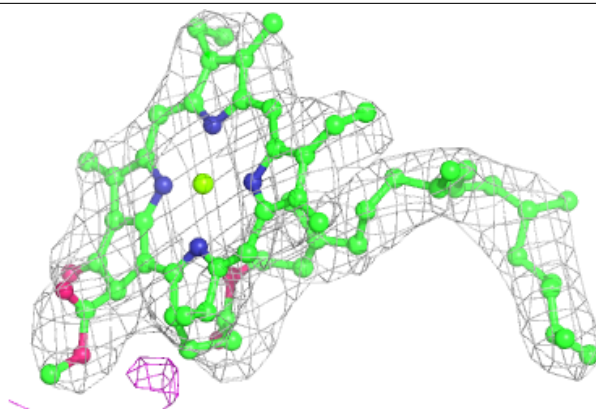
Electron density around CLA B 819:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

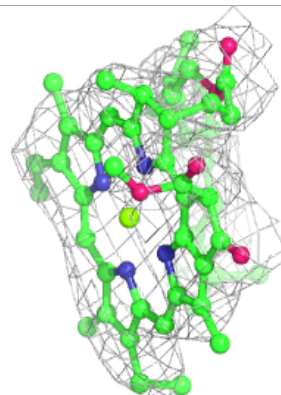
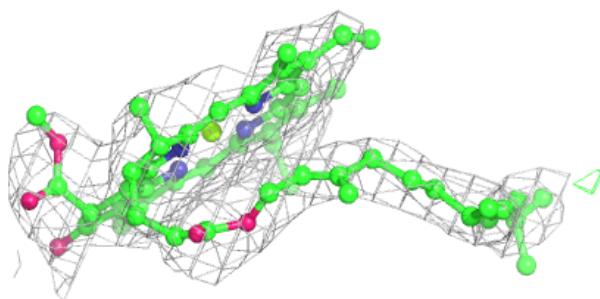
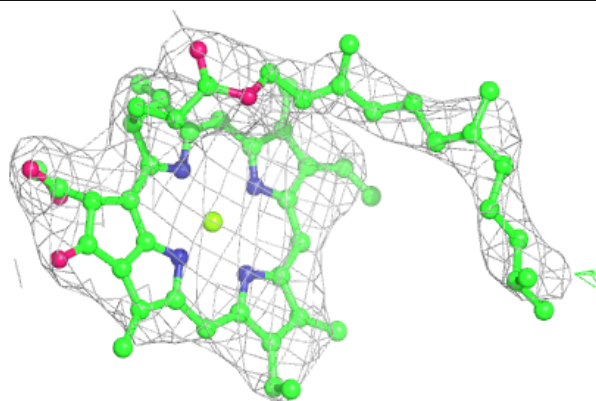


Electron density around CLA a 844:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

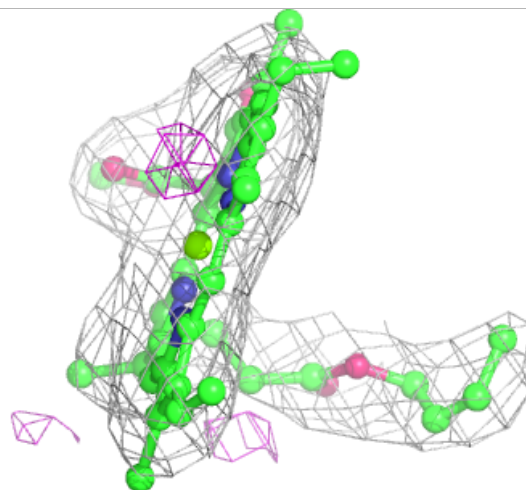
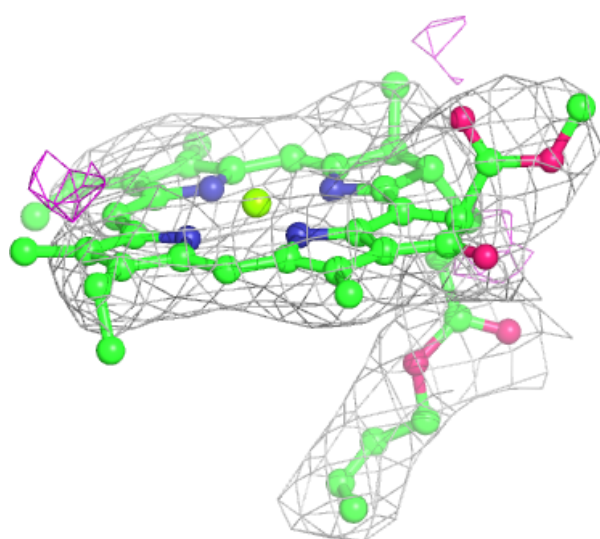
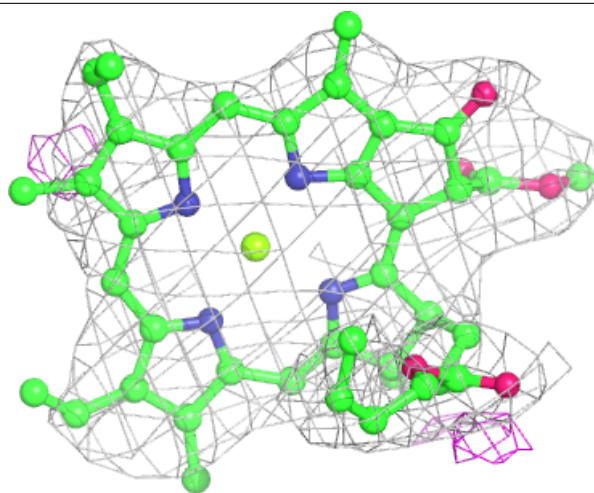
**Electron density around CLA 8 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



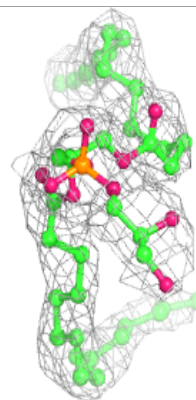
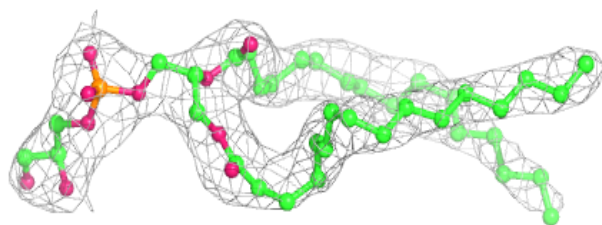
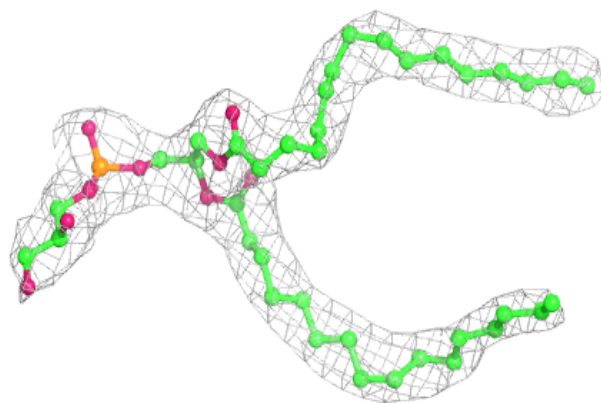
Electron density around CLA B 831:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

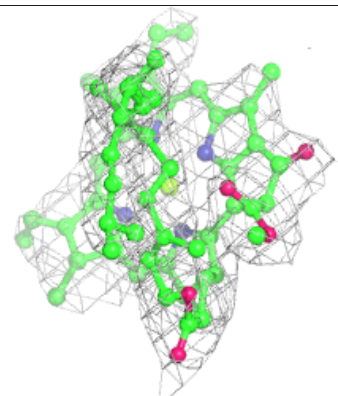
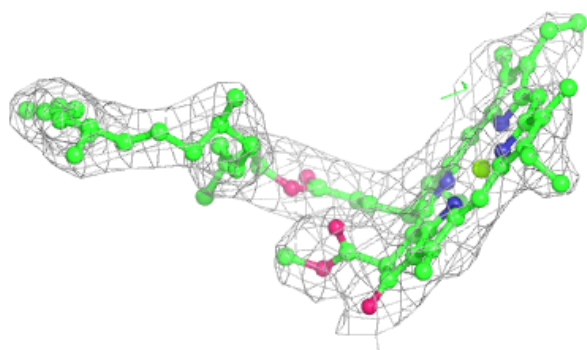
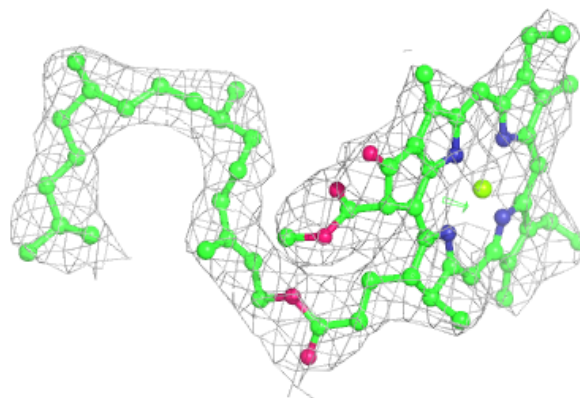


Electron density around LHG a 847:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

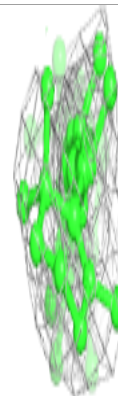
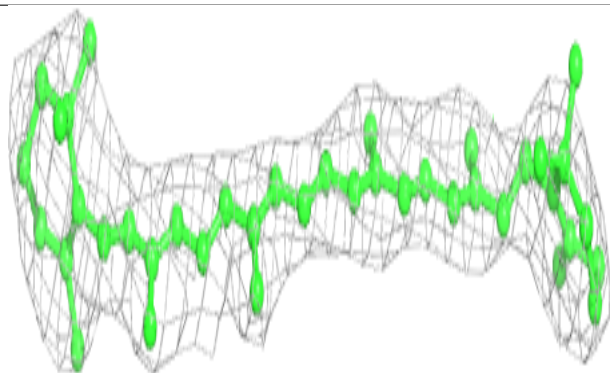
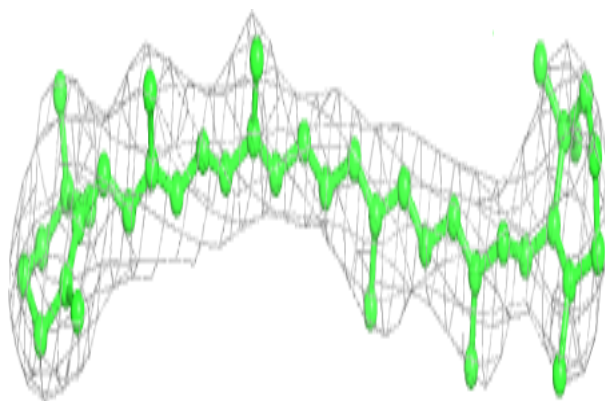
**Electron density around CLA a 801:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



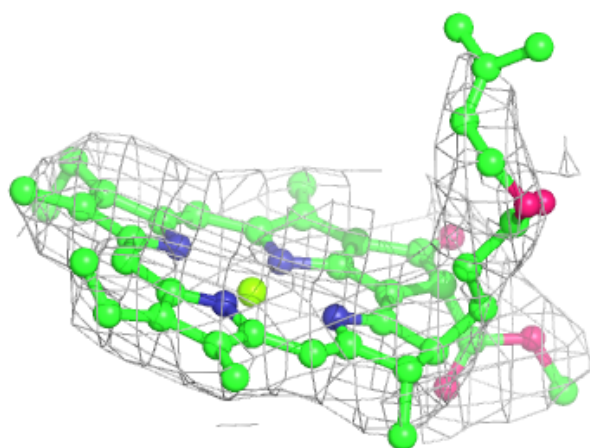
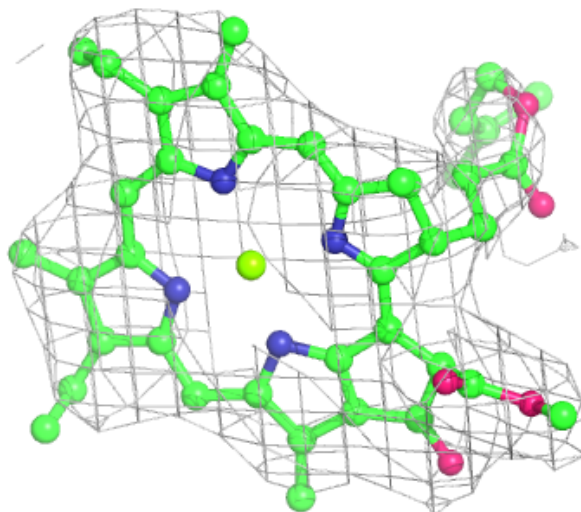
Electron density around BCR a 850:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



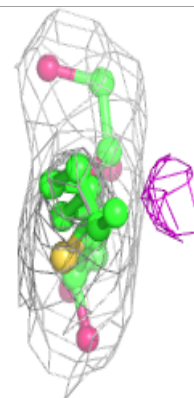
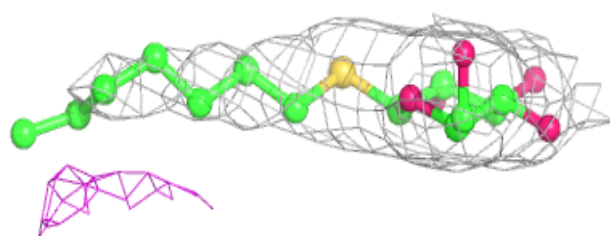
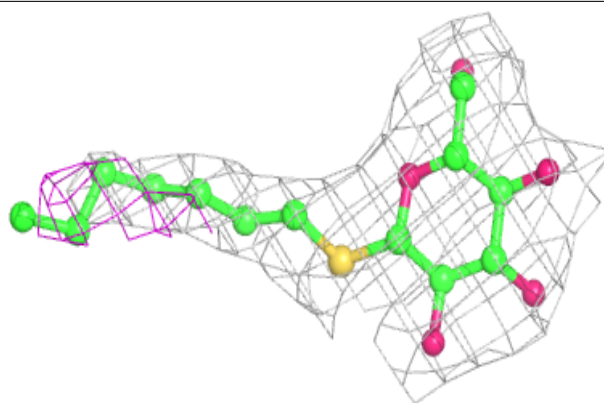
Electron density around CLA 8 307:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

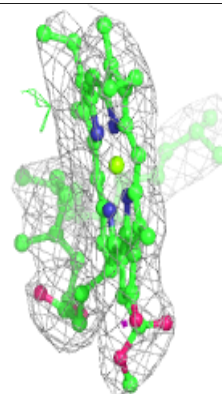
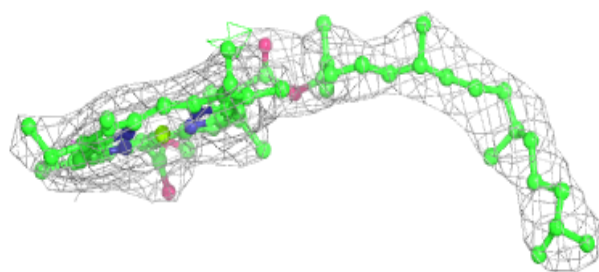
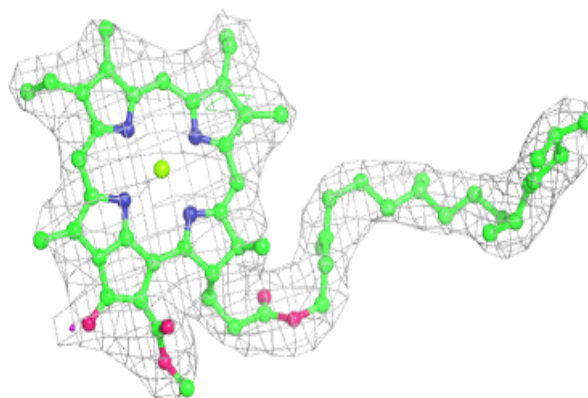


Electron density around HTG A 855:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

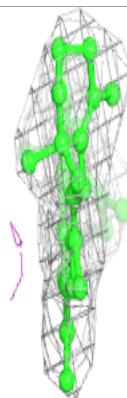
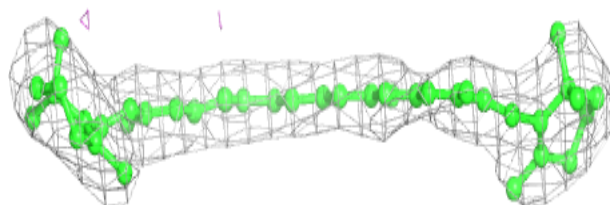
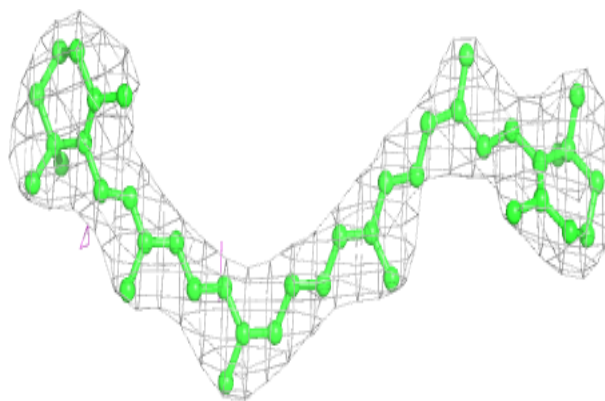
**Electron density around CLA b 803:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



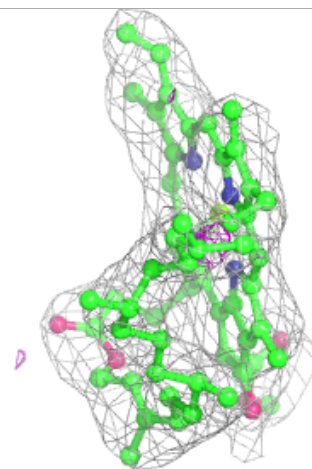
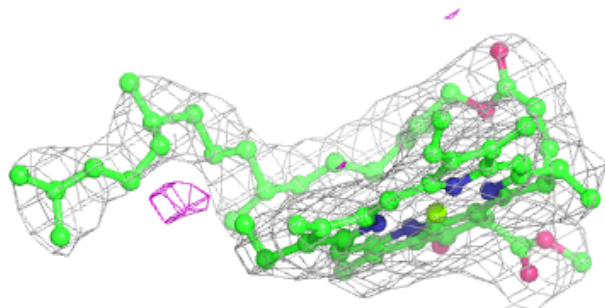
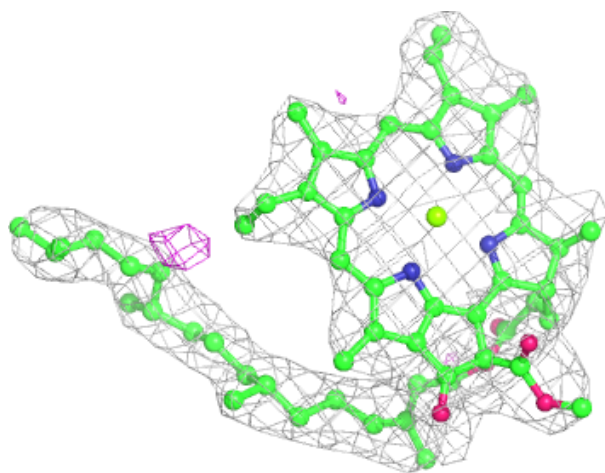
Electron density around BCR a 854:

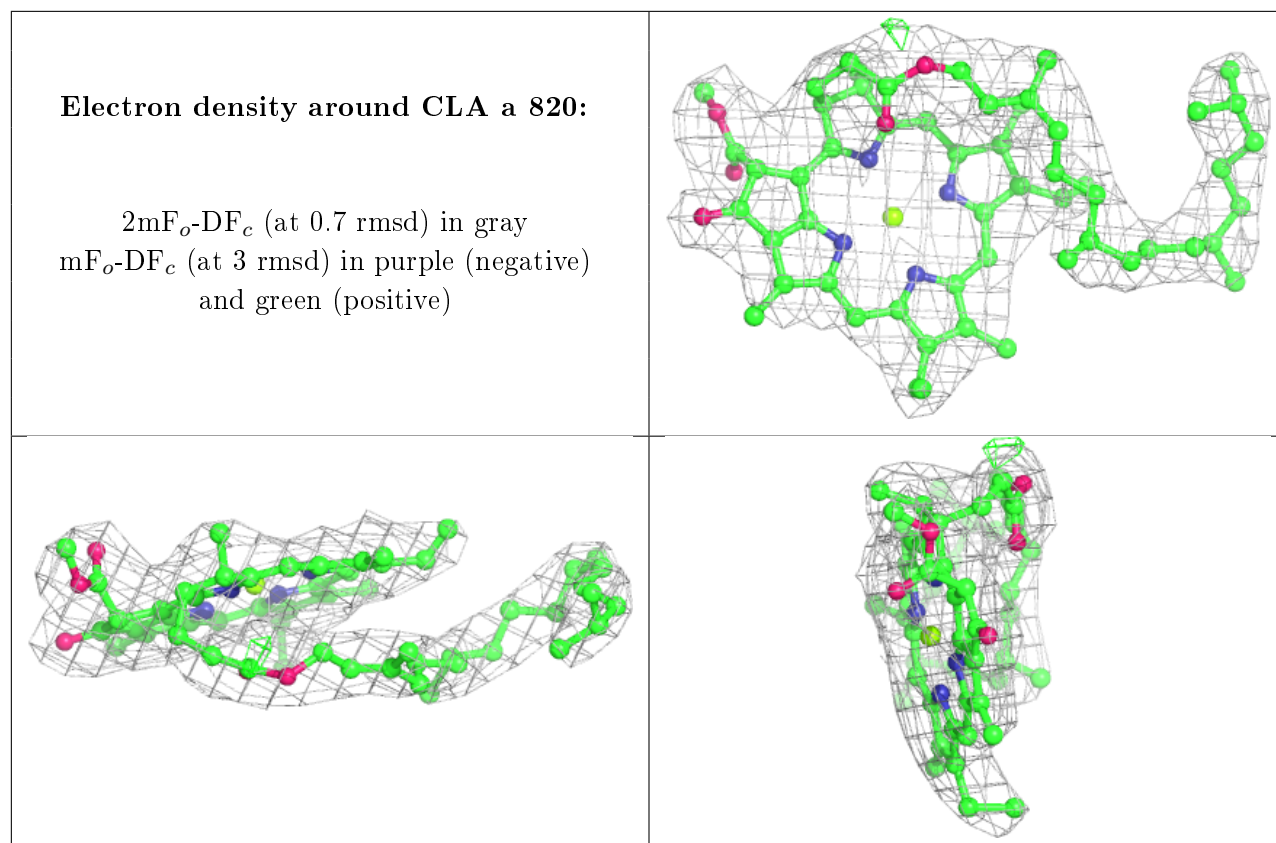
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA a 830:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.