



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2021 – 12:45 PM EST

PDB ID : 7M76
Title : Room Temperature XFEL Crystallography reveals asymmetry in the vicinity of the two phylloquinones in Photosystem I
Authors : Keable, S.M.; Simon, P.S.; Kolsch, A.; Kern, J.; Yachandra, V.K.; Zouni, A.; Yano, J.
Deposited on : 2021-03-26
Resolution : 3.00 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 : 2.23.2
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) : 2.23.2

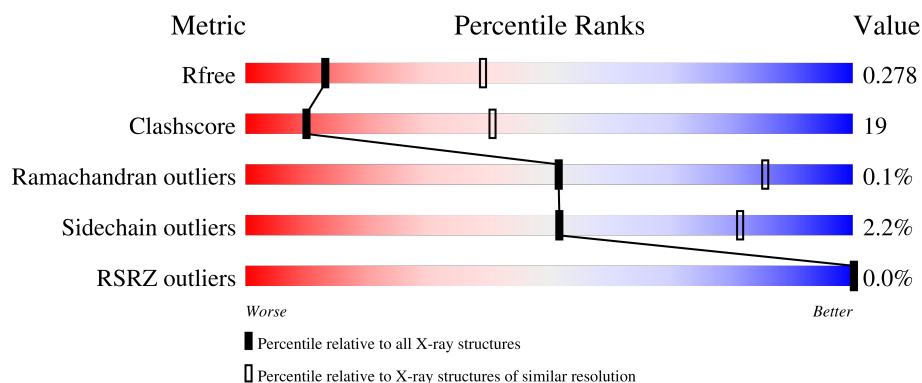
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



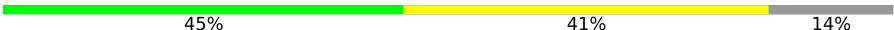


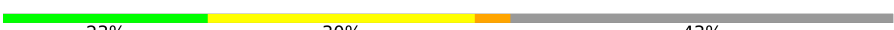



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 of 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	755	<div> <div>59%</div> <div>38%</div> <div>..</div> </div>
2	B	740	<div> <div>66%</div> <div>34%</div> <div>.</div> </div>
3	C	80	<div> <div>62%</div> <div>36%</div> <div>.</div> </div>
4	D	138	<div> <div>68%</div> <div>32%</div> </div>
5	E	75	<div> <div>67%</div> <div>23%</div> <div>.. 8%</div> </div>

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Mol	Chain	Length	Quality of chain
6	F	164	
7	I	38	
8	J	41	
9	K	83	
10	L	154	
11	M	31	
12	X	35	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CL0	A	801	X	-	-	-
14	CLA	A	802	X	-	-	-
14	CLA	A	803	X	-	-	-
14	CLA	A	804	X	-	-	-
14	CLA	A	805	X	-	-	-
14	CLA	A	806	X	-	-	-
14	CLA	A	807	X	-	-	-
14	CLA	A	808	X	-	-	-
14	CLA	A	809	X	-	-	-
14	CLA	A	810	X	-	-	-
14	CLA	A	811	X	-	-	-
14	CLA	A	812	X	-	-	-
14	CLA	A	813	X	-	-	-
14	CLA	A	814	X	-	-	-
14	CLA	A	815	X	-	-	-
14	CLA	A	816	X	-	-	-
14	CLA	A	817	X	-	-	-
14	CLA	A	818	X	-	-	-
14	CLA	A	819	X	-	-	-
14	CLA	A	820	X	-	-	-
14	CLA	A	821	X	-	-	-
14	CLA	A	822	X	-	-	-
14	CLA	A	823	X	-	-	-
14	CLA	A	824	X	-	-	-
14	CLA	A	825	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	826	X	-	-	-
14	CLA	A	827	X	-	-	-
14	CLA	A	828	X	-	-	-
14	CLA	A	829	X	-	-	-
14	CLA	A	830	X	-	-	-
14	CLA	A	831	X	-	-	-
14	CLA	A	832	X	-	-	-
14	CLA	A	833	X	-	-	-
14	CLA	A	834	X	-	-	-
14	CLA	A	835	X	-	-	-
14	CLA	A	836	X	-	-	-
14	CLA	A	837	X	-	-	-
14	CLA	A	838	X	-	-	-
14	CLA	A	839	X	-	-	-
14	CLA	A	840	X	-	-	-
14	CLA	A	841	X	-	-	-
14	CLA	A	842	X	-	-	-
14	CLA	A	843	X	-	-	-
14	CLA	A	844	X	-	-	-
14	CLA	A	845	X	-	-	-
14	CLA	A	856	X	-	-	-
14	CLA	B	3003	X	-	-	-
14	CLA	B	3004	X	-	-	-
14	CLA	B	3005	X	-	-	-
14	CLA	B	3006	X	-	-	-
14	CLA	B	3007	X	-	-	-
14	CLA	B	3008	X	-	-	-
14	CLA	B	3009	X	-	-	-
14	CLA	B	3010	X	-	-	-
14	CLA	B	3011	X	-	-	-
14	CLA	B	3012	X	-	-	-
14	CLA	B	3013	X	-	-	-
14	CLA	B	3014	X	-	-	-
14	CLA	B	3015	X	-	-	-
14	CLA	B	3016	X	-	-	-
14	CLA	B	3017	X	-	-	-
14	CLA	B	3018	X	-	-	-
14	CLA	B	3019	X	-	-	-
14	CLA	B	3020	X	-	-	-
14	CLA	B	3021	X	-	-	-
14	CLA	B	3022	X	-	-	-
14	CLA	B	3023	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	3024	X	-	-	-
14	CLA	B	3026	X	-	-	-
14	CLA	B	3027	X	-	-	-
14	CLA	B	3028	X	-	-	-
14	CLA	B	3029	X	-	-	-
14	CLA	B	3030	X	-	-	-
14	CLA	B	3031	X	-	-	-
14	CLA	B	3032	X	-	-	-
14	CLA	B	3033	X	-	-	-
14	CLA	B	3034	X	-	-	-
14	CLA	B	3035	X	-	-	-
14	CLA	B	3036	X	-	-	-
14	CLA	B	3037	X	-	-	-
14	CLA	B	3039	X	-	-	-
14	CLA	B	3041	X	-	-	-
14	CLA	B	3042	X	-	-	-
14	CLA	F	202	X	-	-	-
14	CLA	J	101	X	-	-	-
14	CLA	J	102	X	-	-	-
14	CLA	K	101	X	-	-	-
14	CLA	K	103	X	-	-	-
14	CLA	L	204	X	-	-	-
14	CLA	L	205	X	-	-	-
14	CLA	L	206	X	-	-	-
14	CLA	M	102	X	-	-	-
14	CLA	X	1701	X	-	-	-

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 48797 atoms, of which 24384 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
1	A	740	Total	C	H	N	O	S	0	0	0
			11422	3794	5638	988	976	26			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	739	Total	C	H	N	O	S	0	0	0
			11507	3876	5618	987	1005	21			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	80	Total	C	H	N	O	S	0	0	0
			1174	367	576	103	117	11			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	138	Total	C	H	N	O	S	0	0	0
			2152	682	1077	186	204	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	69	Total	C	H	N	O	0	0	0
			1067	342	528	93	104			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	F	141	Total	C	H	N	O	S	0	0	0
			2141	680	1076	184	197	4			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	I	38	Total	C	H	N	O	S	0	0	0
			607	208	306	40	48	5			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
8	J	41	Total	C	H	N	O	S	0	0	0
			685	231	347	51	54	2			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
9	K	47	Total	C	H	N	O	S	0	0	0
			687	217	354	58	57	1			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
10	L	151	Total	C	H	N	O	S	0	0	0
			2244	735	1125	179	201	4			

There is a discrepancy between the modelled and reference sequences:

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

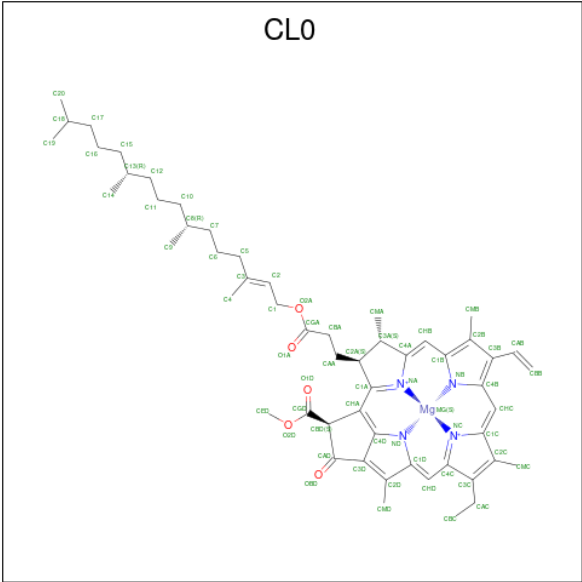
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
11	M	31	Total	C	H	N	O	S	0	0	0
			505	161	264	36	43	1			

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

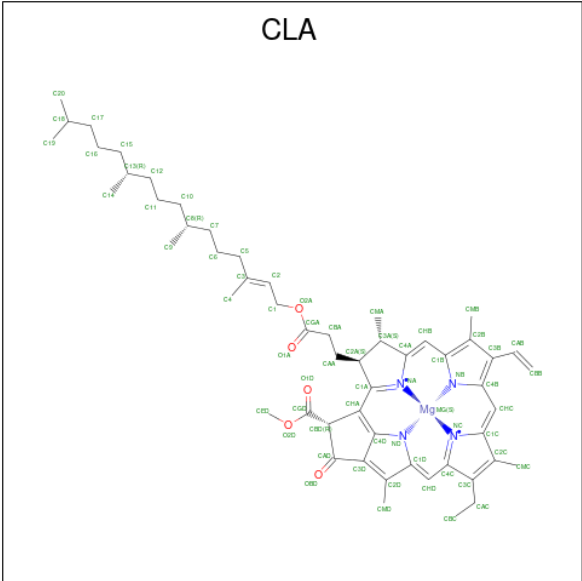
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	X	29	Total	C	H	N	O	0	0	0
			459	172	217	35	35			

- Molecule 13 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			92	41	41	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			88	39	39	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			72	35	29	1	4	3		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			88	39	39	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			92	41	41	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	A	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			89	40	39	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			92	41	41	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			82	37	35	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			92	41	41	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			95	42	43	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			104	45	49	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			82	37	35	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		

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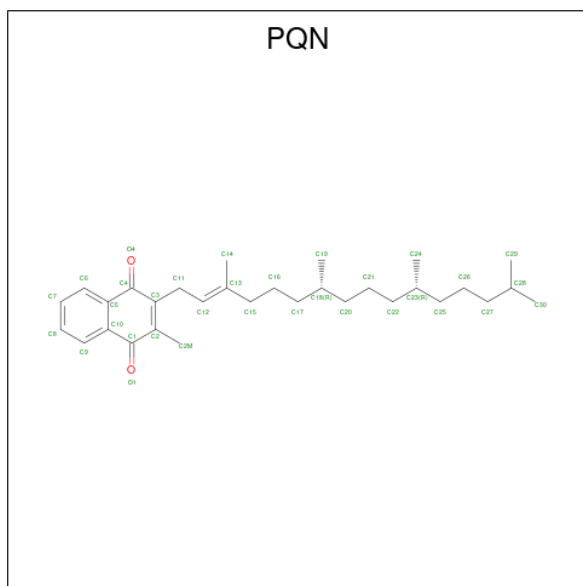
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
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			104	45	49	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			79	36	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			88	39	39	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			113	48	55	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			82	37	35	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	F	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		

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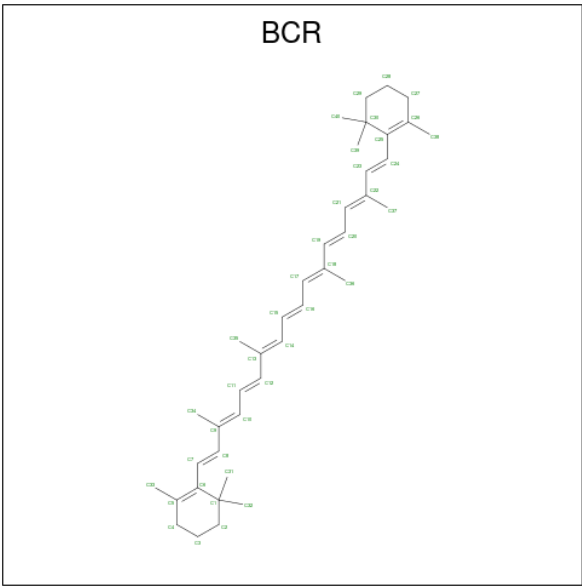
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	J	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	J	1	Total	C	H	Mg	N	O	0	0
			62	31	25	1	4	1		
14	K	1	Total	C	H	Mg	N	O	0	0
			70	33	29	1	4	3		
14	K	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	L	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	L	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	L	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	M	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	X	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		

- Molecule 15 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	A	1	Total	C	H	O	0	0
			79	31	46	2		
15	B	1	Total	C	H	O	0	0
			79	31	46	2		

- Molecule 16 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



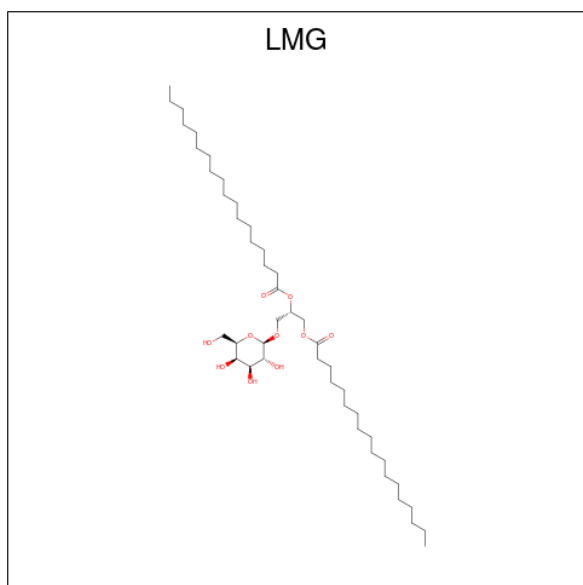
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	A	1	Total	C	H	0	0
			96	40	56		
16	A	1	Total	C	H	0	0
			96	40	56		
16	A	1	Total	C	H	0	0
			96	40	56		
16	A	1	Total	C	H	0	0
			96	40	56		
16	A	1	Total	C	H	0	0
			96	40	56		
16	B	1	Total	C	H	0	0
			96	40	56		
16	B	1	Total	C	H	0	0
			96	40	56		
16	B	1	Total	C	H	0	0
			96	40	56		
16	B	1	Total	C	H	0	0
			96	40	56		
16	B	1	Total	C	H	0	0
			96	40	56		
16	F	1	Total	C	H	0	0
			96	40	56		
16	F	1	Total	C	H	0	0
			96	40	56		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	I	1	Total	C	H	0	0
			96	40	56		
16	J	1	Total	C	H	0	0
			96	40	56		
16	J	1	Total	C	H	0	0
			96	40	56		
16	J	1	Total	C	H	0	0
			96	40	56		
16	K	1	Total	C	H	0	0
			96	40	56		
16	L	1	Total	C	H	0	0
			96	40	56		
16	L	1	Total	C	H	0	0
			96	40	56		
16	L	1	Total	C	H	0	0
			96	40	56		
16	M	1	Total	C	H	0	0
			96	40	56		

- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



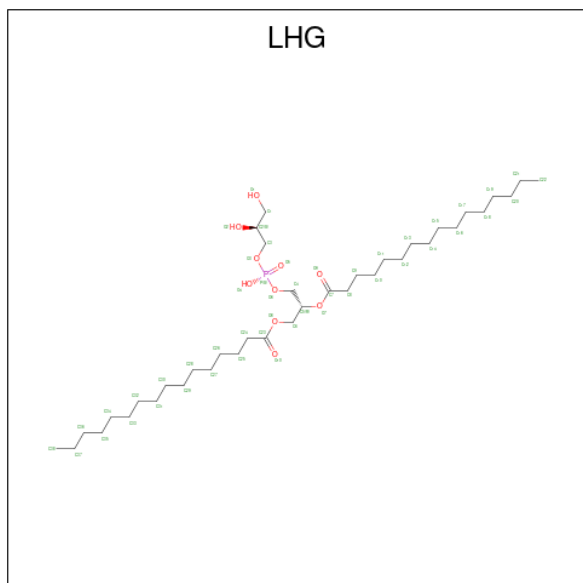
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	H	O	0	0
			118	38	70	10		
17	A	1	Total	C	H	O	0	0
			67	22	37	8		

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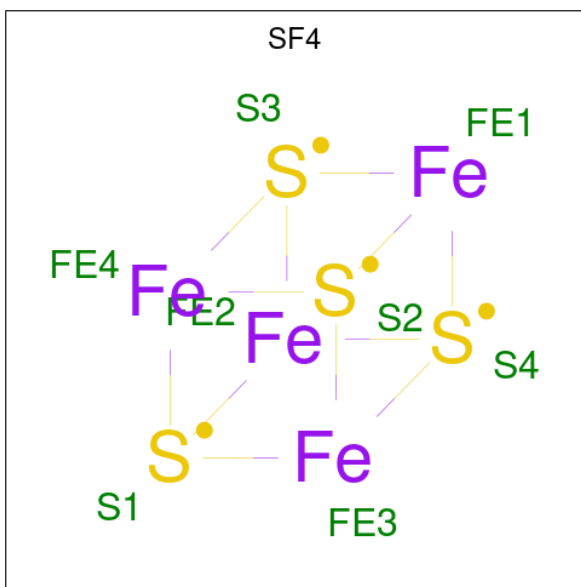
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	B	1	Total	C	H	O	0	0
			141	45	86	10		
17	I	1	Total	C	H	O	0	0
			91	30	51	10		

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
18	A	1	Total	C	H	O	P	0	0
			53	16	26	10	1		
18	B	1	Total	C	H	O	P	0	0
			43	12	20	10	1		
18	M	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

- Molecule 19 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

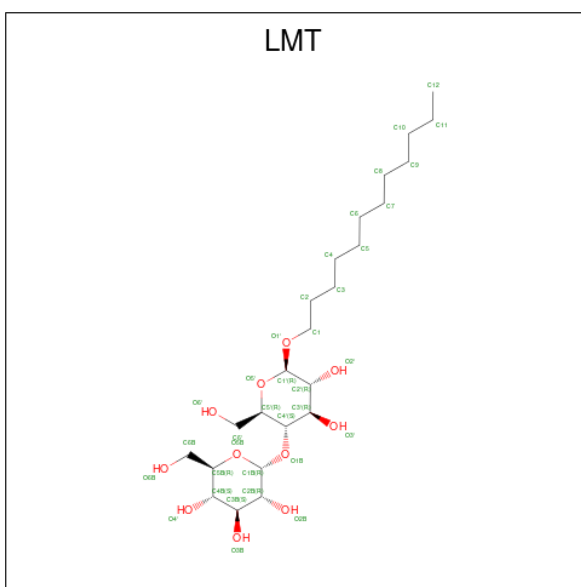


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	B	1	Total	Fe	S	0	0
			8	4	4		
19	C	1	Total	Fe	S	0	0
			8	4	4		
19	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 20 is CALCIUM ION (three-letter code: CA) (formula: Ca).

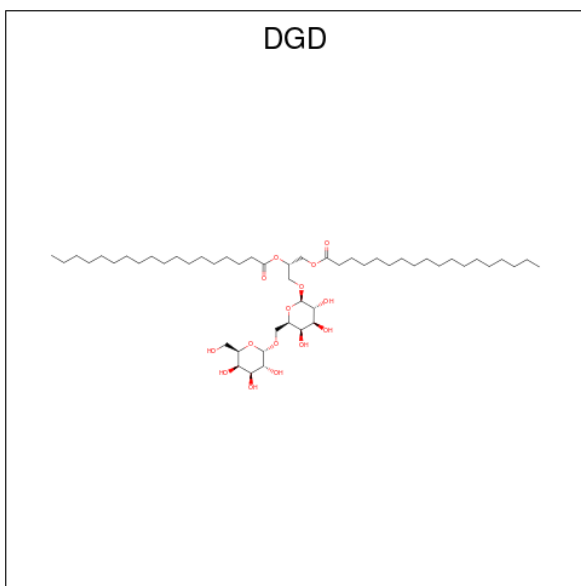
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	B	1	Total	Ca	0	0
			1	1		
20	L	1	Total	Ca	0	0
			1	1		

- Molecule 21 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	L	1	Total	C	H	O	0	0
			81	24	46	11		

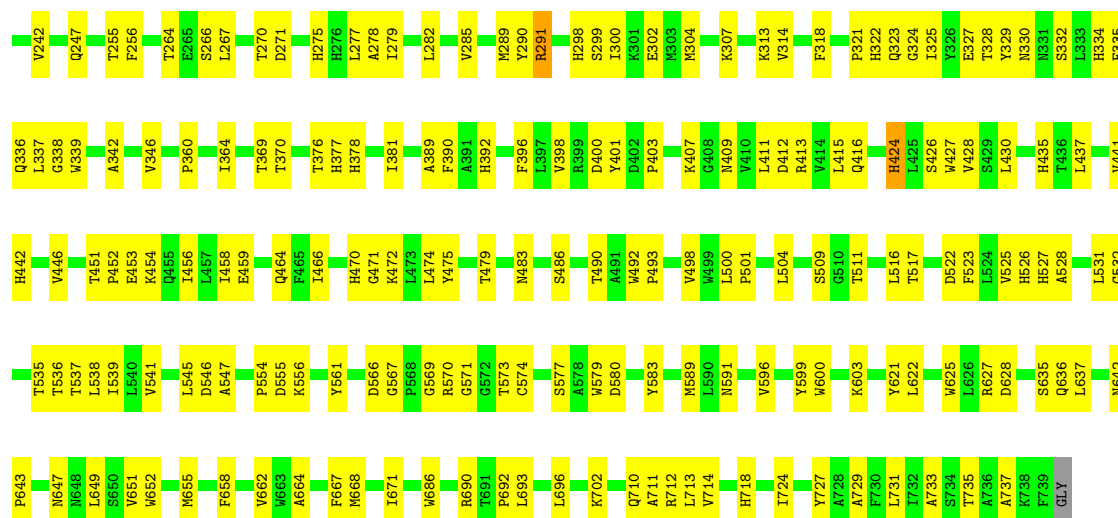
- Molecule 22 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	L	1	Total	C	H	O	0	0
			162	51	96	15		

- Molecule 23 is water.

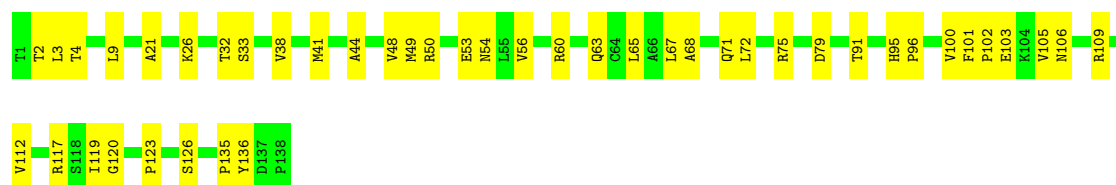
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	8	Total 8	O 8	0	0
23	B	8	Total 8	O 8	0	0
23	J	1	Total 1	O 1	0	0
23	L	2	Total 2	O 2	0	0
23	M	1	Total 1	O 1	0	0



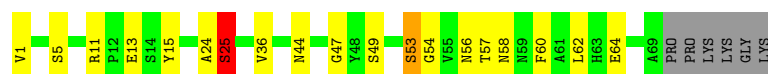
• Molecule 3: Photosystem I iron-sulfur center



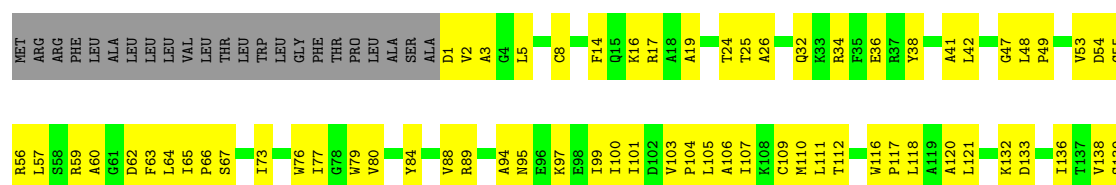
• Molecule 4: Photosystem I reaction center subunit II



• Molecule 5: Photosystem I reaction center subunit IV



• Molecule 6: Photosystem I reaction center subunit III





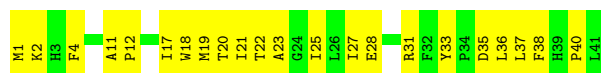
- Molecule 7: Photosystem I reaction center subunit VIII

Chain I: 58% 42%



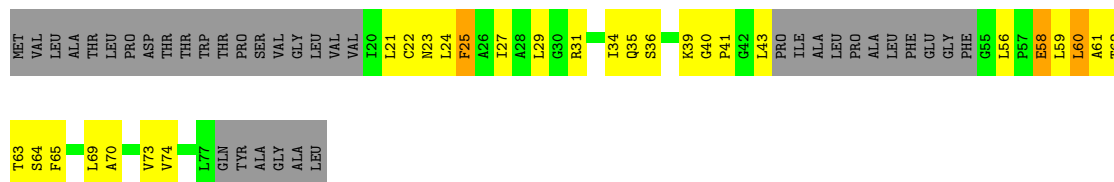
- Molecule 8: Photosystem I reaction center subunit IX

Chain J: 46% 54%



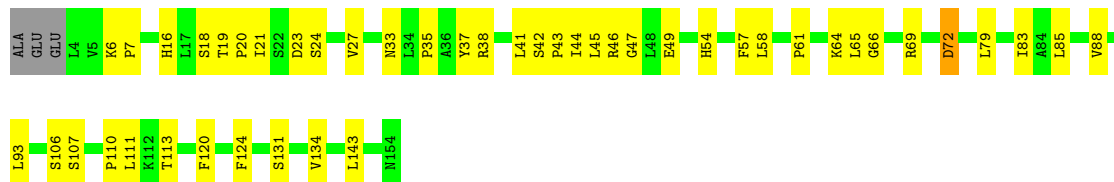
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain K: 23% 30% 43%



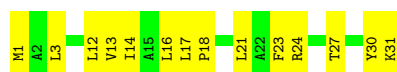
- Molecule 10: Photosystem I reaction center subunit XI

Chain L: 68% 29% ..



- Molecule 11: Photosystem I reaction center subunit XII

Chain M: 55% 45%



- Molecule 12: Photosystem I 4.8K protein

Chain X: 40% 37% 6% 17%

ALA	THR	LYS	SER	ALA	LYS	P7	T8	Y9		R12	T13	F14	W15	A16	V17	L18	L19	L20		N23	F24	L25		Y29	Y30	F31		L34	K35
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4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	284.27 Å 284.27 Å 165.75 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.23 – 3.00 25.23 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (25.23-3.00) 83.1 (25.23-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.23 (at 2.99 Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.268 , 0.278 0.268 , 0.278	Depositor DCC
R_{free} test set	1997 reflections (1.32%)	wwPDB-VP
Wilson B-factor (Å ²)	60.8	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , -11.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.045 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	48797	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: LMG, SF4, CA, LMT, BCR, DGD, CL0, CLA, LHG, PQN

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	0.33	0/5983	0.60	3/8158 (0.0%)
2	B	0.33	0/6107	0.56	0/8345
3	C	0.37	0/608	0.60	0/824
4	D	0.33	0/1101	0.60	0/1492
5	E	0.33	0/551	0.59	0/750
6	F	0.35	0/1087	0.64	0/1476
7	I	0.32	0/312	0.61	0/425
8	J	0.34	0/350	0.59	0/477
9	K	0.32	0/337	0.75	0/454
10	L	0.34	0/1148	0.59	0/1558
11	M	0.39	0/244	0.59	0/332
12	X	0.37	0/251	0.59	0/342
All	All	0.33	0/18079	0.59	3/24633 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
3	C	0	1
9	K	0	1
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	LEU	CA-CB-CG	5.48	127.90	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	493	LEU	CA-CB-CG	5.16	127.16	115.30
1	A	171	LEU	CA-CB-CG	5.13	127.10	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	521	GLY	Peptide
1	A	617	MET	Peptide
3	C	60	ASP	Peptide
9	K	58	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5784	5638	5639	290	0
2	B	5889	5618	5649	222	0
3	C	598	576	580	27	0
4	D	1075	1077	1077	33	0
5	E	539	528	528	14	0
6	F	1065	1076	1077	70	0
7	I	301	306	306	18	0
8	J	338	347	347	27	0
9	K	333	354	354	38	0
10	L	1119	1125	1125	32	0
11	M	241	264	264	15	0
12	X	242	217	249	16	0
13	A	65	72	72	3	0
14	A	2628	2615	2615	157	0
14	B	2284	2232	2232	108	0
14	F	45	33	33	8	0
14	J	82	58	58	4	0
14	K	86	62	62	5	0
14	L	195	216	216	5	0
14	M	45	33	33	4	0
14	X	45	33	33	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	A	33	46	46	9	0
15	B	33	46	46	2	0
16	A	200	280	280	20	0
16	B	240	336	336	18	0
16	F	80	112	112	8	0
16	I	40	56	56	4	0
16	J	120	168	168	20	0
16	K	40	56	56	5	0
16	L	120	168	168	7	0
16	M	40	56	56	2	0
17	A	78	107	105	1	0
17	B	55	86	86	0	0
17	I	40	51	50	3	0
18	A	76	100	98	7	0
18	B	23	20	16	2	0
18	M	49	74	74	3	0
19	B	8	0	0	0	0
19	C	16	0	0	1	0
20	B	1	0	0	0	0
20	L	1	0	0	0	0
21	L	35	46	45	0	0
22	L	66	96	96	2	0
23	A	8	0	0	4	0
23	B	8	0	0	0	0
23	J	1	0	0	0	0
23	L	2	0	0	0	0
23	M	1	0	0	0	0
All	All	24413	24384	24443	928	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (928) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:60:LEU:O	9:K:63:THR:N	1.88	1.04
1:A:454:HIS:O	1:A:458:LEU:HD13	1.61	0.98
1:A:661:VAL:HG22	1:A:749:ALA:HB3	1.47	0.97
1:A:661:VAL:HG21	1:A:746:PHE:HA	1.46	0.97
4:D:3:LEU:HD21	4:D:91:THR:HG21	1.52	0.91
8:J:21:ILE:O	8:J:25:ILE:HD12	1.70	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:HD12	1:A:69:SER:N	1.88	0.86
3:C:9:THR:HG1	3:C:63:SER:HG	1.04	0.86
6:F:1:ASP:N	6:F:5:LEU:O	2.08	0.84
14:A:826:CLA:MG	23:A:902:HOH:O	1.21	0.83
2:B:479:THR:HG21	12:X:29:TYR:O	1.80	0.82
14:A:834:CLA:HMD2	14:A:835:CLA:H143	1.62	0.82
1:A:65:LEU:HD12	1:A:68:ILE:HD11	1.61	0.81
1:A:336:PHE:O	1:A:432:ARG:NH1	2.14	0.81
16:A:851:BCR:H362	14:A:856:CLA:C4	2.12	0.80
2:B:181:LEU:HD21	14:B:3014:CLA:H43	1.64	0.79
10:L:20:PRO:O	10:L:24:SER:OG	2.01	0.78
4:D:32:THR:OG1	4:D:79:ASP:OD2	2.00	0.78
10:L:110:PRO:O	10:L:113:THR:HG22	1.83	0.78
14:B:3005:CLA:HED2	14:B:3005:CLA:H2A	1.65	0.78
1:A:243:ILE:HD12	14:A:817:CLA:HBC2	1.66	0.77
6:F:53:VAL:HG13	6:F:63:PHE:CD2	2.19	0.76
14:A:822:CLA:HMB2	14:A:826:CLA:HMA3	1.68	0.75
1:A:513:PHE:HE1	14:A:828:CLA:HBC2	1.51	0.75
6:F:88:VAL:HG12	6:F:94:ALA:HA	1.68	0.75
2:B:546:ASP:O	2:B:556:LYS:NZ	2.16	0.74
14:B:3008:CLA:H192	18:M:101:LHG:H383	1.68	0.74
14:A:802:CLA:OBD	14:B:3003:CLA:HMB3	1.87	0.74
1:A:376:ALA:O	1:A:510:SER:OG	2.06	0.74
2:B:114:ILE:HD11	2:B:116:TYR:CZ	2.22	0.73
2:B:184:VAL:HG23	16:B:3045:BCR:H352	1.70	0.73
10:L:33:ASN:O	10:L:38:ARG:NE	2.21	0.73
9:K:21:LEU:HD12	14:K:101:CLA:C3D	2.18	0.72
1:A:361:ALA:HB1	16:A:850:BCR:H343	1.71	0.72
15:A:846:PQN:H193	16:F:201:BCR:H382	1.69	0.72
2:B:307:LYS:O	2:B:314:VAL:HG23	1.90	0.72
1:A:120:ILE:HD13	16:J:104:BCR:H322	1.72	0.71
2:B:304:MET:HE1	2:B:325:ILE:HD11	1.72	0.71
2:B:561:TYR:O	2:B:577:SER:OG	2.06	0.71
2:B:555:ASP:OD1	3:C:65:ARG:NH1	2.24	0.71
16:A:851:BCR:H362	14:A:856:CLA:H42	1.72	0.70
14:A:811:CLA:HBC3	14:A:811:CLA:HHD	1.73	0.70
8:J:33:TYR:CE2	16:J:105:BCR:H401	2.27	0.70
2:B:441:VAL:HG13	14:B:3034:CLA:HMC3	1.71	0.70
6:F:53:VAL:HG22	6:F:63:PHE:HB2	1.74	0.70
1:A:473:ASP:OD2	23:A:901:HOH:O	2.10	0.69
14:M:102:CLA:H2A	14:M:102:CLA:HED2	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:710:GLN:O	2:B:714:VAL:HG23	1.93	0.69
2:B:569:GLY:HA3	3:C:55:THR:HG22	1.75	0.69
2:B:168:LYS:O	2:B:330:ASN:ND2	2.23	0.68
11:M:23:PHE:O	11:M:27:THR:HG23	1.94	0.68
2:B:74:GLU:OE2	11:M:1:MET:N	2.27	0.68
1:A:66:GLU:OE1	1:A:186:LYS:HE2	1.95	0.67
1:A:140:THR:HG22	14:A:809:CLA:HMD1	1.77	0.67
1:A:722:LEU:HD23	1:A:726:GLN:OE1	1.95	0.67
14:A:826:CLA:ND	23:A:902:HOH:O	2.27	0.67
1:A:523:LYS:NZ	1:A:755:GLY:O	2.21	0.67
2:B:537:THR:HG22	14:B:3026:CLA:HMC2	1.75	0.67
6:F:139:SER:O	6:F:141:ARG:NH1	2.27	0.67
8:J:33:TYR:HD2	16:J:105:BCR:H391	1.58	0.67
2:B:528:ALA:HB1	14:B:3003:CLA:H192	1.77	0.66
1:A:215:HIS:O	1:A:219:VAL:N	2.27	0.66
1:A:575:ARG:NH1	14:A:831:CLA:O1D	2.27	0.66
2:B:313:LYS:O	2:B:313:LYS:HG3	1.94	0.66
8:J:40:PRO:HD2	16:J:105:BCR:H382	1.77	0.66
2:B:181:LEU:CD2	14:B:3014:CLA:H43	2.25	0.66
5:E:62:LEU:HD23	5:E:62:LEU:H	1.60	0.66
14:B:3033:CLA:HBB1	14:B:3033:CLA:HMB1	1.77	0.66
1:A:65:LEU:HD12	1:A:65:LEU:O	1.96	0.66
1:A:405:VAL:HG13	16:A:850:BCR:H342	1.79	0.65
1:A:68:ILE:O	1:A:72:ILE:HG13	1.96	0.65
1:A:249:MET:HB2	1:A:258:TRP:CZ3	2.31	0.65
14:A:845:CLA:HMC1	14:A:845:CLA:HBC2	1.78	0.65
1:A:305:ALA:O	1:A:309:ILE:HD12	1.96	0.65
1:A:164:GLY:O	1:A:167:VAL:HG12	1.97	0.65
14:B:3024:CLA:HBC2	16:B:3051:BCR:H343	1.77	0.65
2:B:167:PHE:O	2:B:173:ARG:NH1	2.29	0.65
5:E:56:ASN:OD1	5:E:57:THR:HG23	1.95	0.65
1:A:188:GLU:OE1	1:A:188:GLU:N	2.29	0.65
8:J:17:ILE:HA	8:J:20:THR:HG22	1.78	0.65
4:D:38:VAL:O	4:D:75:ARG:NH1	2.30	0.64
1:A:524:VAL:HG12	1:A:525:ALA:N	2.13	0.64
14:A:810:CLA:HMB1	14:A:810:CLA:HBB1	1.79	0.64
11:M:27:THR:OG1	14:M:102:CLA:HED3	1.98	0.64
1:A:583:ARG:HA	3:C:76:MET:HA	1.80	0.64
14:A:811:CLA:O1A	14:A:813:CLA:H42	1.98	0.64
1:A:154:ASN:OD1	1:A:157:GLN:NE2	2.31	0.63
14:A:804:CLA:HED3	15:A:846:PQN:H262	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:ARG:NE	2:B:237:ASP:OD1	2.32	0.63
1:A:256:VAL:HB	1:A:258:TRP:HE1	1.64	0.63
4:D:9:LEU:HB2	4:D:48:VAL:HG12	1.79	0.63
16:A:851:BCR:H372	2:B:441:VAL:HG11	1.80	0.63
3:C:51:LYS:O	3:C:55:THR:HG23	1.98	0.63
16:J:103:BCR:H321	16:J:103:BCR:HC8	1.81	0.63
14:B:3033:CLA:H142	16:F:203:BCR:H333	1.80	0.63
14:A:822:CLA:HMB1	14:A:822:CLA:HBB1	1.79	0.62
14:B:3041:CLA:HBC3	14:B:3041:CLA:HHB	1.81	0.62
5:E:11:ARG:HG2	5:E:13:GLU:OE1	1.98	0.62
14:A:822:CLA:OBD	14:A:824:CLA:HMD3	1.99	0.62
6:F:1:ASP:OD2	6:F:42:LEU:HD21	2.00	0.62
1:A:177:TRP:HB2	14:A:812:CLA:HMC3	1.80	0.62
16:A:851:BCR:H23C	16:A:851:BCR:H403	1.82	0.62
2:B:300:ILE:HD12	2:B:300:ILE:H	1.64	0.62
16:A:849:BCR:H333	16:A:850:BCR:H333	1.81	0.62
2:B:472:LYS:NZ	2:B:517:THR:OG1	2.32	0.62
6:F:54:ASP:OD2	16:F:203:BCR:H393	1.99	0.62
9:K:21:LEU:HD12	14:K:101:CLA:CAD	2.30	0.62
14:B:3024:CLA:CBC	16:B:3051:BCR:H343	2.30	0.62
2:B:304:MET:CE	2:B:325:ILE:HD11	2.29	0.62
3:C:28:VAL:HG12	4:D:109:ARG:HB3	1.82	0.62
6:F:64:LEU:O	6:F:67:SER:OG	2.15	0.62
14:A:828:CLA:HBB1	14:A:828:CLA:HMB1	1.82	0.61
2:B:528:ALA:CB	14:B:3003:CLA:H192	2.30	0.61
14:B:3017:CLA:HMB1	14:B:3017:CLA:HBB1	1.81	0.61
8:J:23:ALA:O	8:J:27:ILE:HD12	1.99	0.61
9:K:22:CYS:HA	9:K:25:PHE:HB2	1.81	0.61
9:K:65:PHE:CD2	16:K:102:BCR:H402	2.35	0.61
1:A:143:LEU:HD22	1:A:146:LEU:CD2	2.31	0.61
5:E:1:VAL:N	5:E:5:SER:OG	2.34	0.61
2:B:291:ARG:HE	2:B:299:SER:HB3	1.65	0.61
2:B:318:PHE:HB2	14:B:3024:CLA:HMA1	1.83	0.61
14:B:3027:CLA:HMB1	14:B:3027:CLA:HBB1	1.82	0.60
1:A:143:LEU:HD22	1:A:146:LEU:HD22	1.83	0.60
9:K:29:LEU:HB3	9:K:62:THR:HG21	1.84	0.60
2:B:498:VAL:HG11	14:B:3017:CLA:HED1	1.83	0.60
1:A:339:ALA:HB3	1:A:428:ASN:HA	1.82	0.60
1:A:68:ILE:HD12	1:A:69:SER:H	1.65	0.60
14:A:820:CLA:HMB1	14:A:820:CLA:HBB1	1.83	0.60
2:B:401:TYR:O	4:D:126:SER:OG	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ALA:HB2	1:A:381:PRO:HD3	1.83	0.60
1:A:143:LEU:O	1:A:146:LEU:HB3	2.01	0.60
2:B:647:ASN:OD1	2:B:649:LEU:N	2.31	0.60
2:B:180:GLY:O	2:B:184:VAL:HG22	2.01	0.60
4:D:2:THR:HG22	4:D:3:LEU:H	1.67	0.60
10:L:106:SER:OG	10:L:107:SER:N	2.31	0.59
1:A:66:GLU:HA	1:A:187:LEU:HD13	1.84	0.59
2:B:483:ASN:OD1	2:B:486:SER:N	2.35	0.59
2:B:580:ASP:OD1	2:B:712:ARG:NH1	2.35	0.59
1:A:697:TRP:CZ2	15:A:846:PQN:H2M3	2.37	0.59
1:A:179:HIS:CE1	14:A:811:CLA:NA	2.70	0.59
4:D:3:LEU:CD2	4:D:91:THR:HG21	2.31	0.59
1:A:282:ASN:O	1:A:506:ALA:N	2.33	0.59
1:A:358:ILE:HG22	16:A:849:BCR:HC7	1.85	0.59
1:A:489:TRP:O	1:A:493:LEU:HD23	2.03	0.59
1:A:495:THR:HG21	1:A:514:GLY:CA	2.33	0.59
14:B:3022:CLA:C3B	14:B:3023:CLA:HMD2	2.33	0.59
1:A:48:ILE:HD13	14:A:842:CLA:HMB3	1.85	0.58
2:B:176:HIS:CE1	14:B:3013:CLA:NA	2.71	0.58
1:A:681:PHE:CD2	16:A:851:BCR:H363	2.38	0.58
2:B:337:LEU:HD23	2:B:392:HIS:ND1	2.18	0.58
6:F:54:ASP:OD1	6:F:55:GLY:N	2.37	0.58
1:A:319:TRP:HZ3	14:A:813:CLA:HMA1	1.68	0.58
14:A:825:CLA:HBB1	14:A:825:CLA:HMB1	1.84	0.58
1:A:70:ARG:NH1	1:A:184:ALA:O	2.37	0.58
1:A:436:HIS:CE1	14:A:832:CLA:ND	2.71	0.58
1:A:66:GLU:OE1	1:A:70:ARG:NH2	2.37	0.58
14:A:817:CLA:HBC3	14:A:817:CLA:HHD	1.85	0.57
14:A:839:CLA:HMB2	14:A:840:CLA:C3D	2.34	0.57
2:B:390:PHE:CE1	16:B:3047:BCR:H373	2.39	0.57
1:A:280:THR:HG21	1:A:282:ASN:OD1	2.03	0.57
7:I:30:LEU:HD21	17:I:102:LMG:H151	1.87	0.57
1:A:249:MET:HB2	1:A:258:TRP:CH2	2.40	0.57
5:E:24:ALA:O	5:E:25:SER:O	2.22	0.57
1:A:358:ILE:HD11	23:A:902:HOH:O	2.03	0.57
14:B:3038:CLA:HMB1	14:B:3038:CLA:HBB1	1.86	0.57
14:F:202:CLA:HBC2	8:J:19:MET:HE3	1.84	0.57
16:L:209:BCR:H343	16:L:209:BCR:H311	1.86	0.57
8:J:36:LEU:HD12	16:J:105:BCR:C21	2.34	0.57
1:A:146:LEU:HA	1:A:380:TYR:CE2	2.40	0.57
1:A:463:ASP:OD2	1:A:646:ILE:HG12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:VAL:HG11	16:B:3045:BCR:C33	2.34	0.57
2:B:435:HIS:CG	16:J:105:BCR:H333	2.40	0.57
14:A:829:CLA:HBB1	14:A:829:CLA:HMB1	1.86	0.57
3:C:61:PHE:HE2	3:C:65:ARG:NH1	2.02	0.57
6:F:8:CYS:HB3	6:F:14:PHE:CD2	2.40	0.57
6:F:133:ASP:HA	6:F:136:ILE:HD11	1.87	0.57
14:A:813:CLA:HMB3	14:A:821:CLA:C3D	2.35	0.56
14:A:827:CLA:HBB1	14:A:827:CLA:HMB1	1.85	0.56
6:F:80:VAL:HG21	6:F:110:MET:HA	1.86	0.56
14:A:841:CLA:H143	14:F:202:CLA:HAC1	1.87	0.56
2:B:337:LEU:HD23	2:B:392:HIS:CG	2.40	0.56
1:A:495:THR:HG21	1:A:514:GLY:HA3	1.86	0.56
14:B:3004:CLA:CGA	14:B:3004:CLA:H3A	2.35	0.56
14:B:3039:CLA:HMB2	14:B:3040:CLA:C2D	2.35	0.56
6:F:80:VAL:HG23	6:F:109:CYS:O	2.05	0.56
9:K:65:PHE:CE1	9:K:69:LEU:HD11	2.41	0.56
10:L:47:GLY:O	10:L:124:PHE:HA	2.04	0.56
14:A:809:CLA:CHC	14:A:810:CLA:HMD2	2.35	0.56
14:B:3007:CLA:CBB	16:B:3045:BCR:H402	2.36	0.56
1:A:367:SER:OG	1:A:400:ILE:HD11	2.06	0.56
1:A:459:TYR:HB3	1:A:646:ILE:HD11	1.87	0.56
12:X:12:ARG:HG2	12:X:12:ARG:HH11	1.71	0.56
1:A:609:VAL:HG11	14:A:838:CLA:HBB2	1.88	0.56
2:B:278:ALA:HA	14:B:3017:CLA:HMC3	1.86	0.56
2:B:116:TYR:HA	2:B:370:THR:HG22	1.88	0.56
2:B:300:ILE:O	2:B:304:MET:HG2	2.06	0.56
2:B:554:PRO:HD2	3:C:61:PHE:CZ	2.41	0.56
8:J:23:ALA:C	8:J:27:ILE:HD12	2.26	0.56
10:L:64:LYS:O	10:L:65:LEU:HD23	2.06	0.56
1:A:296:ASP:HB2	14:A:819:CLA:HMA1	1.88	0.56
1:A:575:ARG:HD2	1:A:725:ILE:HG21	1.88	0.56
2:B:325:ILE:HA	2:B:328:THR:HG22	1.87	0.56
2:B:662:VAL:HG12	2:B:718:HIS:O	2.06	0.56
14:A:841:CLA:HBC1	15:A:846:PQN:H212	1.88	0.55
1:A:219:VAL:HG13	1:A:239:PRO:HB3	1.88	0.55
15:A:846:PQN:C19	16:F:201:BCR:H382	2.35	0.55
14:B:3030:CLA:HBB1	14:B:3030:CLA:HMB1	1.88	0.55
9:K:29:LEU:HB3	9:K:62:THR:OG1	2.06	0.55
10:L:66:GLY:O	10:L:69:ARG:NH1	2.38	0.55
1:A:333:LYS:O	14:A:845:CLA:HBC3	2.07	0.55
14:B:3041:CLA:HED3	7:I:31:PHE:HZ	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:47:GLY:O	6:F:48:LEU:HD23	2.07	0.55
1:A:680:HIS:CE1	1:A:742:THR:HG21	2.42	0.55
14:B:3039:CLA:HMB2	14:B:3040:CLA:C3D	2.37	0.55
2:B:255:THR:OG1	2:B:271:ASP:OD1	2.24	0.55
16:L:208:BCR:H23C	16:L:208:BCR:H392	1.89	0.55
14:A:804:CLA:HMA1	14:A:809:CLA:H203	1.88	0.54
12:X:24:PHE:CD1	14:X:1701:CLA:HMA1	2.42	0.54
2:B:566:ASP:H	2:B:573:THR:HG23	1.72	0.54
1:A:367:SER:OG	1:A:397:HIS:O	2.22	0.54
14:A:856:CLA:HBB1	14:A:856:CLA:HMB1	1.89	0.54
1:A:280:THR:HG22	1:A:281:PHE:N	2.22	0.54
2:B:724:ILE:HG23	14:B:3028:CLA:HAB	1.88	0.54
16:I:101:BCR:H382	16:I:101:BCR:H23C	1.90	0.54
2:B:114:ILE:HD11	2:B:116:TYR:OH	2.07	0.54
14:J:101:CLA:HBB1	14:J:101:CLA:HMB1	1.89	0.54
2:B:69:TRP:HA	11:M:3:LEU:HD22	1.90	0.54
14:A:841:CLA:H93	15:A:846:PQN:H293	1.88	0.54
2:B:96:GLY:O	2:B:100:VAL:HG23	2.08	0.54
2:B:117:SER:OG	2:B:119:VAL:HG13	2.08	0.54
2:B:637:LEU:HD13	2:B:733:ALA:CB	2.37	0.54
6:F:88:VAL:HG11	6:F:97:LYS:HB2	1.90	0.54
14:B:3024:CLA:HAB	14:B:3031:CLA:HMD2	1.90	0.54
14:A:811:CLA:CHB	14:A:813:CLA:HMD1	2.38	0.53
2:B:47:ALA:HB2	2:B:156:LEU:HG	1.89	0.53
9:K:65:PHE:HE1	9:K:69:LEU:HD11	1.74	0.53
14:A:818:CLA:CBC	14:A:819:CLA:HMC2	2.38	0.53
2:B:416:GLN:O	6:F:141:ARG:NH2	2.41	0.53
1:A:690:LEU:HD13	2:B:671:ILE:HD13	1.91	0.53
14:A:804:CLA:H193	14:A:843:CLA:H18	1.89	0.53
2:B:724:ILE:HD13	14:B:3028:CLA:HMC2	1.90	0.53
10:L:44:ILE:HG23	10:L:45:LEU:N	2.23	0.53
9:K:56:LEU:HD12	9:K:59:LEU:HD23	1.89	0.53
1:A:25:PHE:CE2	8:J:4:PHE:CD2	2.97	0.53
1:A:317:THR:HG22	14:A:821:CLA:O1D	2.09	0.53
2:B:279:ILE:HD11	14:B:3018:CLA:C3C	2.38	0.53
1:A:602:MET:HB2	14:A:827:CLA:HBC1	1.91	0.53
2:B:398:VAL:HG23	2:B:547:ALA:HB1	1.89	0.53
2:B:17:THR:HG23	2:B:702:LYS:O	2.09	0.53
1:A:172:MET:HA	1:A:175:ALA:HB3	1.90	0.53
14:B:3009:CLA:HMC3	14:B:3010:CLA:C3D	2.38	0.53
4:D:119:ILE:HD12	4:D:119:ILE:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:PRO:HG2	1:A:242:PHE:CZ	2.44	0.52
2:B:282:LEU:O	2:B:285:VAL:HG12	2.09	0.52
2:B:567:GLY:O	2:B:573:THR:HG22	2.09	0.52
2:B:600:TRP:HB2	14:B:3038:CLA:HMC1	1.91	0.52
1:A:416:MET:HE1	1:A:434:LEU:HD11	1.91	0.52
1:A:338:GLY:H	1:A:432:ARG:CZ	2.22	0.52
1:A:451:LEU:HD13	1:A:544:PHE:HA	1.91	0.52
2:B:72:ASN:O	2:B:76:TRP:HB2	2.10	0.52
14:B:3030:CLA:H2A	14:B:3030:CLA:O2D	2.09	0.52
6:F:84:TYR:CE1	6:F:88:VAL:HG21	2.44	0.52
2:B:176:HIS:CG	14:B:3014:CLA:HMC2	2.45	0.52
2:B:437:LEU:O	2:B:441:VAL:HG12	2.09	0.52
14:A:825:CLA:HAB	14:A:832:CLA:HMD2	1.91	0.52
14:B:3035:CLA:HMD2	14:B:3036:CLA:CHC	2.40	0.52
6:F:101:ILE:HD11	6:F:106:ALA:HB2	1.91	0.52
16:I:101:BCR:H331	16:I:101:BCR:C8	2.40	0.52
1:A:149:ALA:O	1:A:220:SER:OG	2.26	0.52
14:A:810:CLA:H92	14:A:810:CLA:C3	2.40	0.52
2:B:291:ARG:N	2:B:298:HIS:O	2.43	0.52
12:X:24:PHE:CE1	14:X:1701:CLA:HMA1	2.44	0.52
1:A:711:LEU:HD11	14:B:3032:CLA:H3A	1.90	0.52
18:B:3050:LHG:O3	12:X:12:ARG:NH2	2.43	0.52
14:A:833:CLA:HMB1	14:A:833:CLA:HBB1	1.92	0.52
2:B:142:LEU:HD13	11:M:14:ILE:HG22	1.92	0.52
2:B:184:VAL:HG11	16:B:3045:BCR:H332	1.90	0.52
2:B:493:PRO:HG3	14:B:3037:CLA:C1D	2.40	0.52
1:A:89:GLY:CA	14:A:808:CLA:HMC3	2.39	0.52
2:B:727:TYR:HB2	14:B:3003:CLA:HED3	1.92	0.52
16:J:103:BCR:C8	16:J:103:BCR:H311	2.39	0.52
1:A:52:HIS:CE1	14:A:804:CLA:ND	2.76	0.52
1:A:286:ASN:HB3	1:A:289:THR:OG1	2.10	0.52
1:A:344:LEU:HA	1:A:347:VAL:HG22	1.90	0.52
14:A:820:CLA:C2D	14:A:830:CLA:H41	2.40	0.52
1:A:628:ASP:N	1:A:628:ASP:OD1	2.43	0.51
2:B:536:THR:HG21	14:B:3026:CLA:HBC3	1.92	0.51
3:C:17:VAL:HG22	3:C:25:LEU:HB2	1.91	0.51
6:F:55:GLY:HA2	12:X:31:PHE:CZ	2.45	0.51
1:A:73:PHE:CE2	1:A:189:TRP:HH2	2.29	0.51
3:C:25:LEU:HD23	3:C:41:SER:HA	1.92	0.51
6:F:57:LEU:HA	6:F:60:ALA:HB2	1.93	0.51
10:L:85:LEU:O	10:L:88:VAL:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:GLN:HA	1:A:220:SER:H	1.76	0.51
2:B:275:HIS:HB2	14:B:3018:CLA:CHB	2.40	0.51
2:B:651:VAL:HG13	14:B:3010:CLA:HAC1	1.92	0.51
14:B:3007:CLA:HBB2	16:B:3045:BCR:H402	1.93	0.51
5:E:53:SER:OG	5:E:54:GLY:N	2.43	0.51
12:X:9:TYR:HA	12:X:12:ARG:NH1	2.26	0.51
1:A:216:GLN:HE22	1:A:297:THR:HG22	1.75	0.51
14:A:802:CLA:H201	14:B:3010:CLA:H2	1.92	0.51
2:B:470:HIS:CE1	14:B:3035:CLA:NB	2.77	0.51
14:B:3041:CLA:H193	16:I:101:BCR:H362	1.92	0.51
1:A:256:VAL:HG12	1:A:258:TRP:CD1	2.45	0.51
1:A:337:THR:HG22	14:A:832:CLA:OBD	2.09	0.51
1:A:682:ILE:HD13	1:A:737:LEU:HD23	1.92	0.51
14:A:841:CLA:C9	14:A:841:CLA:HMC2	2.41	0.51
2:B:31:GLU:OE1	2:B:334:HIS:NE2	2.36	0.51
2:B:424:HIS:CD2	14:B:3031:CLA:HMB1	2.45	0.51
6:F:24:THR:OG1	6:F:34:ARG:NH1	2.44	0.51
9:K:59:LEU:O	9:K:62:THR:HG22	2.11	0.51
1:A:201:LEU:HD12	1:A:312:GLY:N	2.25	0.51
1:A:282:ASN:O	1:A:506:ALA:HB3	2.10	0.51
14:A:804:CLA:HED1	14:A:842:CLA:HAA1	1.92	0.51
14:A:826:CLA:HBB1	14:A:826:CLA:HMB1	1.91	0.51
1:A:432:ARG:O	14:A:832:CLA:HED1	2.11	0.51
14:B:3010:CLA:HMB3	14:B:3011:CLA:CHC	2.41	0.51
14:A:809:CLA:HBB1	14:A:809:CLA:HMB1	1.92	0.51
14:A:856:CLA:HBC2	2:B:591:ASN:HB2	1.93	0.51
2:B:275:HIS:HE1	14:B:3018:CLA:ND	2.09	0.51
2:B:321:PRO:HG3	2:B:413:ARG:HH21	1.75	0.51
4:D:41:MET:O	4:D:44:ALA:N	2.44	0.51
1:A:120:ILE:HG22	1:A:123:GLN:HG2	1.92	0.51
1:A:306:VAL:HG12	1:A:310:ILE:HD12	1.92	0.51
2:B:339:TRP:HH2	16:B:3051:BCR:H341	1.76	0.51
8:J:1:MET:O	8:J:4:PHE:N	2.44	0.51
10:L:41:LEU:HD13	10:L:45:LEU:HD23	1.93	0.51
10:L:79:LEU:O	10:L:83:ILE:HG12	2.11	0.51
1:A:67:ASP:OD1	1:A:71:LYS:HE3	2.11	0.50
1:A:120:ILE:HG23	1:A:121:VAL:HG22	1.93	0.50
2:B:117:SER:CB	2:B:119:VAL:HG13	2.41	0.50
6:F:73:ILE:O	6:F:77:ILE:HG12	2.11	0.50
6:F:80:VAL:CG2	6:F:110:MET:HA	2.41	0.50
14:A:802:CLA:HBB1	14:A:802:CLA:HMB1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:39:LYS:CE	9:K:56:LEU:HD13	2.41	0.50
10:L:58:LEU:O	10:L:61:PRO:HD2	2.11	0.50
12:X:20:LEU:HD13	12:X:20:LEU:O	2.12	0.50
1:A:490:VAL:HA	1:A:493:LEU:CD2	2.41	0.50
1:A:606:ILE:HA	1:A:609:VAL:HG22	1.94	0.50
14:A:822:CLA:CMB	14:A:826:CLA:HMA3	2.40	0.50
1:A:464:THR:HG23	14:B:3010:CLA:HMC3	1.93	0.50
2:B:242:VAL:HG23	2:B:242:VAL:O	2.10	0.50
11:M:31:LYS:HE3	18:M:101:LHG:HC12	1.93	0.50
1:A:654:LEU:HD22	13:A:801:CL0:H26	1.94	0.50
2:B:19:ARG:NH2	7:I:34:ILE:O	2.45	0.50
2:B:579:TRP:HZ2	2:B:713:LEU:HD13	1.77	0.50
14:F:202:CLA:HBC2	8:J:19:MET:CE	2.41	0.50
7:I:22:MET:N	7:I:23:PRO:HD2	2.27	0.50
2:B:459:GLU:OE1	2:B:464:GLN:NE2	2.38	0.50
2:B:474:LEU:H	2:B:474:LEU:HD22	1.77	0.50
4:D:105:VAL:HG12	4:D:106:ASN:N	2.27	0.50
1:A:373:HIS:CD2	14:A:828:CLA:NC	2.79	0.50
14:A:811:CLA:HMB2	14:A:813:CLA:HMD3	1.94	0.50
2:B:642:ASN:HB2	2:B:643:PRO:CD	2.42	0.50
14:K:101:CLA:HBB1	14:K:101:CLA:HMB1	1.94	0.50
1:A:168:MET:HA	1:A:171:LEU:CD2	2.41	0.49
14:B:3012:CLA:HBA1	14:B:3013:CLA:HMD1	1.94	0.49
4:D:101:PHE:HB3	4:D:103:GLU:OE1	2.12	0.49
5:E:36:VAL:HG12	5:E:60:PHE:O	2.11	0.49
9:K:60:LEU:O	9:K:62:THR:N	2.45	0.49
1:A:19:ASP:HB2	1:A:182:LYS:HD2	1.94	0.49
1:A:409:ALA:HA	16:A:850:BCR:H332	1.93	0.49
1:A:494:HIS:HB3	1:A:513:PHE:HD2	1.76	0.49
14:A:830:CLA:HMB1	14:A:830:CLA:HBB1	1.92	0.49
3:C:60:ASP:HB2	5:E:58:ASN:CG	2.33	0.49
6:F:2:VAL:O	6:F:5:LEU:HD13	2.12	0.49
10:L:33:ASN:CA	10:L:38:ARG:HD3	2.42	0.49
12:X:20:LEU:HD13	12:X:20:LEU:C	2.32	0.49
2:B:570:ARG:N	5:E:47:GLY:O	2.46	0.49
14:B:3018:CLA:HMB1	14:B:3018:CLA:HBB1	1.95	0.49
1:A:461:HIS:HE1	14:A:835:CLA:NA	2.10	0.49
14:A:825:CLA:HHB	14:A:845:CLA:CBB	2.42	0.49
2:B:57:PHE:CD2	2:B:144:LEU:HB3	2.48	0.49
2:B:569:GLY:CA	3:C:55:THR:HG22	2.41	0.49
1:A:249:MET:HB2	1:A:258:TRP:HZ3	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:18:VAL:O	7:I:23:PRO:HD2	2.13	0.49
16:J:104:BCR:H403	16:J:104:BCR:H23C	1.94	0.49
1:A:487:ALA:O	1:A:491:GLN:HG2	2.12	0.49
2:B:184:VAL:CG1	16:B:3045:BCR:H332	2.43	0.49
2:B:329:TYR:CZ	14:B:3025:CLA:NC	2.81	0.49
2:B:537:THR:HG21	14:B:3026:CLA:HAB	1.93	0.49
1:A:112:PRO:HB2	1:A:139:ILE:HG13	1.95	0.49
1:A:219:VAL:O	1:A:223:ILE:HG22	2.12	0.49
2:B:222:ALA:O	2:B:224:PHE:N	2.46	0.49
2:B:255:THR:HG23	2:B:270:THR:HB	1.94	0.49
2:B:338:GLY:HA2	2:B:389:ALA:HA	1.93	0.49
6:F:118:LEU:HD22	6:F:121:LEU:HD23	1.95	0.49
1:A:70:ARG:NH1	1:A:185:PRO:O	2.46	0.49
14:A:804:CLA:HMC3	14:A:812:CLA:C5	2.43	0.49
2:B:290:TYR:HA	2:B:298:HIS:O	2.13	0.49
6:F:34:ARG:HG3	8:J:35:ASP:HB3	1.95	0.49
11:M:14:ILE:O	11:M:18:PRO:HD2	2.13	0.49
1:A:460:VAL:HG23	14:A:835:CLA:HMC3	1.95	0.49
14:A:826:CLA:C14	14:A:826:CLA:HMD2	2.43	0.49
2:B:637:LEU:HD13	2:B:733:ALA:HB3	1.94	0.49
6:F:17:ARG:NE	6:F:48:LEU:HD21	2.27	0.49
6:F:59:ARG:NH2	6:F:62:ASP:OD1	2.45	0.49
7:I:18:VAL:O	7:I:23:PRO:CD	2.61	0.49
7:I:22:MET:HG3	7:I:23:PRO:HD3	1.95	0.49
1:A:302:LEU:O	1:A:306:VAL:HG23	2.13	0.49
1:A:524:VAL:HG12	1:A:525:ALA:H	1.77	0.49
1:A:682:ILE:CD1	1:A:737:LEU:HD23	2.43	0.49
2:B:307:LYS:C	2:B:314:VAL:HG23	2.33	0.49
4:D:100:VAL:HG23	4:D:109:ARG:NH2	2.28	0.49
6:F:25:THR:OG1	6:F:26:ALA:N	2.46	0.49
1:A:494:HIS:HB3	1:A:513:PHE:CD2	2.48	0.48
1:A:726:GLN:HG3	18:A:853:LHG:C8	2.43	0.48
2:B:173:ARG:CA	14:B:3014:CLA:HBC2	2.43	0.48
3:C:40:SER:OG	4:D:112:VAL:HG12	2.13	0.48
7:I:17:VAL:O	7:I:18:VAL:C	2.52	0.48
10:L:35:PRO:HG3	14:L:205:CLA:HED2	1.95	0.48
10:L:49:GLU:HB2	14:L:204:CLA:HED1	1.93	0.48
1:A:209:SER:OG	1:A:305:ALA:HB2	2.13	0.48
2:B:451:THR:O	2:B:451:THR:OG1	2.30	0.48
4:D:120:GLY:N	5:E:13:GLU:OE2	2.47	0.48
8:J:21:ILE:HG13	8:J:22:THR:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:ARG:NH2	2:B:302:GLU:OE2	2.46	0.48
2:B:412:ASP:OD1	2:B:416:GLN:NE2	2.44	0.48
6:F:111:LEU:HD12	6:F:111:LEU:H	1.79	0.48
1:A:72:ILE:HD12	1:A:352:TRP:CE2	2.48	0.48
1:A:185:PRO:HB2	1:A:189:TRP:CE3	2.49	0.48
1:A:66:GLU:O	1:A:70:ARG:HG3	2.14	0.48
1:A:451:LEU:HD21	14:A:839:CLA:HBB1	1.96	0.48
8:J:36:LEU:HD11	16:J:105:BCR:H392	1.94	0.48
1:A:120:ILE:CD1	8:J:31:ARG:HB2	2.43	0.48
14:A:841:CLA:H143	14:F:202:CLA:CAC	2.43	0.48
2:B:41:LEU:O	2:B:45:ILE:HG12	2.12	0.48
6:F:73:ILE:O	6:F:76:TRP:HB3	2.14	0.48
7:I:18:VAL:HA	7:I:22:MET:HG2	1.96	0.48
8:J:11:ALA:N	8:J:12:PRO:HD2	2.29	0.48
2:B:190:ALA:O	2:B:194:ILE:HG13	2.14	0.48
14:B:3033:CLA:O1A	14:B:3033:CLA:C2	2.60	0.48
10:L:33:ASN:HA	10:L:38:ARG:HD3	1.95	0.48
1:A:147:TRP:CE3	1:A:158:LEU:HD21	2.49	0.48
14:A:831:CLA:HMB1	14:A:831:CLA:HBB1	1.96	0.48
2:B:139:ILE:HG23	11:M:14:ILE:HD13	1.96	0.48
2:B:324:GLY:HA2	2:B:327:GLU:OE1	2.14	0.48
2:B:517:THR:O	2:B:603:LYS:NZ	2.45	0.48
10:L:47:GLY:HA2	10:L:120:PHE:CE1	2.49	0.48
13:A:801:CL0:H13	14:A:856:CLA:OBD	2.14	0.47
16:B:3047:BCR:H331	16:B:3047:BCR:C8	2.43	0.47
4:D:95:HIS:HB3	4:D:96:PRO:CD	2.44	0.47
11:M:12:LEU:HB3	16:M:103:BCR:H21C	1.96	0.47
1:A:127:ASN:OD1	1:A:136:GLY:HA2	2.14	0.47
1:A:722:LEU:HD21	14:A:843:CLA:HMD1	1.95	0.47
3:C:62:LEU:O	4:D:119:ILE:HD11	2.13	0.47
6:F:77:ILE:O	6:F:80:VAL:HG12	2.14	0.47
1:A:177:TRP:O	1:A:181:HIS:HB2	2.15	0.47
1:A:186:LYS:HG3	1:A:187:LEU:H	1.78	0.47
18:B:3050:LHG:O1	12:X:12:ARG:NH2	2.42	0.47
1:A:146:LEU:HA	1:A:380:TYR:CD2	2.49	0.47
2:B:146:SER:HB3	11:M:21:LEU:HD12	1.97	0.47
2:B:173:ARG:HD2	14:B:3014:CLA:HMD2	1.96	0.47
2:B:369:THR:HA	2:B:735:THR:HG21	1.97	0.47
14:B:3031:CLA:H3A	14:B:3032:CLA:OBD	2.15	0.47
6:F:103:VAL:HG22	6:F:107:ILE:HD12	1.97	0.47
1:A:593:ASP:OD1	1:A:728:ARG:NH1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:847:BCR:C38	16:K:102:BCR:H10C	2.45	0.47
14:B:3014:CLA:H41	14:B:3019:CLA:HBC3	1.96	0.47
6:F:53:VAL:O	6:F:64:LEU:HD11	2.13	0.47
9:K:65:PHE:HE2	16:K:102:BCR:H272	1.80	0.47
1:A:392:SER:HB3	14:A:829:CLA:HHB	1.97	0.47
14:A:811:CLA:CGA	14:A:813:CLA:H42	2.44	0.47
2:B:184:VAL:CG2	16:B:3045:BCR:H352	2.42	0.47
2:B:435:HIS:CB	16:J:105:BCR:H333	2.44	0.47
3:C:1:ALA:HA	3:C:70:ALA:O	2.14	0.47
8:J:28:GLU:OE2	14:J:101:CLA:NA	2.47	0.47
1:A:517:VAL:HG12	1:A:518:VAL:N	2.30	0.47
14:A:845:CLA:HMB3	18:A:854:LHG:C6	2.45	0.47
2:B:229:TRP:O	14:B:3017:CLA:H3A	2.14	0.47
2:B:411:LEU:O	2:B:415:LEU:HD23	2.15	0.47
14:B:3005:CLA:HHC	14:B:3007:CLA:OBD	2.14	0.47
16:B:3046:BCR:C8	16:B:3046:BCR:H331	2.44	0.47
12:X:34:LEU:C	12:X:35:LYS:HG3	2.35	0.47
14:A:839:CLA:HMB2	14:A:840:CLA:C2D	2.45	0.47
2:B:92:ASP:O	2:B:94:GLN:N	2.47	0.47
2:B:264:THR:OG1	2:B:266:SER:HB3	2.15	0.47
2:B:304:MET:HE3	2:B:322:HIS:HB3	1.97	0.47
11:M:13:VAL:O	11:M:16:LEU:HB2	2.15	0.47
1:A:28:TRP:NE1	14:A:812:CLA:HMB2	2.30	0.47
1:A:201:LEU:O	1:A:201:LEU:HD13	2.14	0.47
1:A:437:ARG:HH22	1:A:562:SER:HB2	1.80	0.47
14:A:841:CLA:O1A	2:B:427:TRP:HD1	1.98	0.47
2:B:103:PHE:O	2:B:111:PRO:HA	2.15	0.47
6:F:109:CYS:O	6:F:112:THR:HG22	2.15	0.47
1:A:300:HIS:HE2	14:A:820:CLA:C2B	2.28	0.47
1:A:524:VAL:CG1	1:A:525:ALA:N	2.78	0.47
1:A:625:VAL:HA	1:A:631:VAL:HA	1.97	0.47
2:B:335:PHE:O	2:B:339:TRP:HB2	2.15	0.47
2:B:376:THR:HG21	2:B:731:LEU:HD13	1.96	0.47
2:B:490:THR:HG22	2:B:492:TRP:HA	1.96	0.47
14:B:3029:CLA:HMB1	14:B:3029:CLA:HBB1	1.97	0.47
3:C:61:PHE:CE2	3:C:65:ARG:NH1	2.83	0.47
1:A:201:LEU:CD1	1:A:308:PHE:O	2.63	0.46
1:A:310:ILE:O	14:A:823:CLA:HBC1	2.15	0.46
6:F:101:ILE:HD11	6:F:106:ALA:CB	2.45	0.46
9:K:70:ALA:O	9:K:74:VAL:HG23	2.15	0.46
1:A:74:SER:HB3	1:A:180:TYR:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:851:BCR:HB3	2:B:437:LEU:CD1	2.45	0.46
2:B:242:VAL:HG22	2:B:247:GLN:HB3	1.95	0.46
14:B:3010:CLA:H203	7:I:26:VAL:CG2	2.45	0.46
9:K:63:THR:HG23	9:K:64:SER:N	2.31	0.46
14:B:3020:CLA:H2A	14:B:3020:CLA:HED3	1.98	0.46
9:K:29:LEU:HB3	9:K:62:THR:CG2	2.44	0.46
2:B:537:THR:CG2	14:B:3026:CLA:HMC2	2.45	0.46
2:B:668:MET:HB2	14:B:3004:CLA:C1C	2.46	0.46
3:C:7:TYR:HB3	4:D:117:ARG:O	2.15	0.46
1:A:152:ILE:HG23	1:A:157:GLN:HB2	1.98	0.46
1:A:433:VAL:HA	1:A:436:HIS:CE1	2.49	0.46
1:A:462:ASN:OD1	1:A:475:PHE:N	2.33	0.46
2:B:525:VAL:HG21	2:B:599:TYR:CD1	2.50	0.46
7:I:26:VAL:O	7:I:30:LEU:HG	2.15	0.46
9:K:41:PRO:HD2	9:K:56:LEU:HD22	1.98	0.46
10:L:43:PRO:HB3	10:L:111:LEU:CD1	2.46	0.46
14:A:813:CLA:HHC	14:A:813:CLA:HBB1	1.98	0.46
2:B:596:VAL:HG21	14:B:3038:CLA:HBB2	1.96	0.46
8:J:33:TYR:CD2	16:J:105:BCR:H401	2.51	0.46
1:A:115:GLN:CG	1:A:115:GLN:O	2.63	0.46
2:B:194:ILE:O	2:B:199:PRO:HD2	2.16	0.46
3:C:72:THR:N	3:C:75:SER:OG	2.46	0.46
6:F:110:MET:HG2	14:F:202:CLA:OBD	2.16	0.46
2:B:466:ILE:CD1	14:B:3035:CLA:HMC3	2.46	0.46
6:F:76:TRP:CE2	14:F:202:CLA:HBD	2.51	0.46
9:K:39:LYS:HD2	9:K:56:LEU:HD13	1.97	0.46
10:L:93:LEU:HD21	16:L:208:BCR:H383	1.98	0.46
1:A:201:LEU:HD13	1:A:201:LEU:C	2.36	0.46
14:A:814:CLA:HMB1	14:A:814:CLA:HBB1	1.98	0.46
14:A:833:CLA:HMB1	14:A:844:CLA:HAA2	1.97	0.46
2:B:121:HIS:HB2	2:B:364:ILE:HD13	1.97	0.46
2:B:332:SER:HB2	2:B:400:ASP:HB3	1.98	0.46
14:B:3014:CLA:HBB1	14:B:3014:CLA:HMB1	1.98	0.46
6:F:32:GLN:O	6:F:36:GLU:HG3	2.16	0.46
9:K:24:LEU:HD21	9:K:70:ALA:HB2	1.98	0.46
1:A:300:HIS:HE1	14:A:819:CLA:ND	2.08	0.45
1:A:584:GLY:HA3	3:C:76:MET:HE2	1.97	0.45
14:B:3025:CLA:HBB1	14:B:3025:CLA:HMB1	1.97	0.45
11:M:17:LEU:HB3	11:M:18:PRO:CD	2.45	0.45
1:A:202:ALA:HB2	1:A:312:GLY:HA3	1.97	0.45
1:A:207:LEU:CD1	16:A:847:BCR:H361	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:GLY:HA3	14:A:831:CLA:C2C	2.45	0.45
2:B:155:HIS:HE1	14:B:3012:CLA:ND	2.13	0.45
2:B:531:LEU:O	2:B:535:THR:HG22	2.16	0.45
2:B:571:GLY:HA2	5:E:49:SER:HA	1.99	0.45
2:B:711:ALA:CB	15:B:3043:PQN:C8	2.95	0.45
6:F:99:ILE:HG13	6:F:100:ILE:HD12	1.97	0.45
8:J:17:ILE:HG13	8:J:18:TRP:N	2.31	0.45
11:M:24:ARG:HH11	14:M:102:CLA:HMA1	1.81	0.45
1:A:470:ARG:NH1	2:B:94:GLN:O	2.45	0.45
1:A:508:THR:HG22	1:A:510:SER:H	1.81	0.45
1:A:548:VAL:HG11	1:A:601:TRP:CE2	2.52	0.45
14:A:826:CLA:HMD2	14:A:826:CLA:H142	1.99	0.45
2:B:277:LEU:C	2:B:277:LEU:HD23	2.37	0.45
2:B:360:PRO:HG3	14:B:3019:CLA:HBA2	1.99	0.45
9:K:21:LEU:HD12	14:K:101:CLA:C2D	2.46	0.45
22:L:207:DGD:O5D	22:L:207:DGD:O4D	2.21	0.45
1:A:256:VAL:HB	1:A:258:TRP:NE1	2.30	0.45
1:A:359:ASN:ND2	14:A:806:CLA:OBD	2.47	0.45
1:A:730:VAL:HG22	14:A:843:CLA:CAD	2.46	0.45
14:A:842:CLA:CBB	14:A:842:CLA:HHC	2.47	0.45
2:B:339:TRP:HE1	14:B:3025:CLA:C3B	2.29	0.45
4:D:41:MET:HE1	4:D:56:VAL:HG11	1.97	0.45
14:A:844:CLA:C19	16:L:201:BCR:H363	2.46	0.45
1:A:152:ILE:CD1	1:A:157:GLN:HB3	2.47	0.45
1:A:165:GLY:N	16:A:847:BCR:HC21	2.32	0.45
1:A:337:THR:HG1	18:A:854:LHG:H02	1.61	0.45
2:B:690:ARG:HD2	10:L:16:HIS:CG	2.51	0.45
14:B:3034:CLA:H62	14:B:3034:CLA:H41	1.86	0.45
10:L:42:SER:O	10:L:46:ARG:HG3	2.15	0.45
14:A:844:CLA:HHC	14:A:844:CLA:HBB1	1.99	0.45
2:B:117:SER:HB2	2:B:119:VAL:HG13	1.99	0.45
2:B:275:HIS:HB2	14:B:3018:CLA:C1B	2.46	0.45
14:B:3016:CLA:CMB	16:B:3046:BCR:H352	2.46	0.45
1:A:139:ILE:C	1:A:139:ILE:HD12	2.37	0.45
1:A:396:HIS:HE1	14:A:829:CLA:C1D	2.30	0.45
1:A:612:HIS:ND1	14:A:838:CLA:HMC2	2.32	0.45
2:B:42:TYR:CD2	2:B:167:PHE:HB3	2.52	0.45
2:B:651:VAL:CG1	14:B:3010:CLA:CHD	2.95	0.45
1:A:429:VAL:O	1:A:433:VAL:HG13	2.17	0.45
2:B:446:VAL:HG22	2:B:451:THR:HG1	1.81	0.45
8:J:37:LEU:HD23	8:J:37:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:TRP:HB3	9:K:58:GLU:OE2	2.17	0.45
1:A:432:ARG:HD3	14:A:832:CLA:OBD	2.17	0.45
1:A:482:LEU:O	1:A:533:THR:HA	2.17	0.45
1:A:602:MET:HG3	1:A:603:TYR:N	2.32	0.45
7:I:37:GLU:O	7:I:38:ALA:OXT	2.35	0.45
1:A:178:PHE:O	1:A:182:LYS:O	2.35	0.44
1:A:379:PRO:HB2	14:A:820:CLA:HAA2	1.99	0.44
2:B:321:PRO:HB2	2:B:409:ASN:HA	1.99	0.44
2:B:339:TRP:CH2	16:B:3051:BCR:H341	2.52	0.44
4:D:105:VAL:HG12	4:D:106:ASN:H	1.82	0.44
4:D:123:PRO:HD2	4:D:135:PRO:HA	1.98	0.44
8:J:33:TYR:O	8:J:36:LEU:HD23	2.16	0.44
1:A:217:ILE:CG2	1:A:298:ALA:HB1	2.47	0.44
1:A:443:HIS:CD2	14:A:833:CLA:NC	2.86	0.44
1:A:726:GLN:HG3	18:A:853:LHG:HC82	1.99	0.44
14:A:834:CLA:HMD2	14:A:835:CLA:C14	2.38	0.44
2:B:446:VAL:HG21	2:B:454:LYS:CB	2.47	0.44
2:B:696:LEU:HD11	10:L:37:TYR:OH	2.17	0.44
4:D:49:MET:HB3	4:D:54:ASN:HD21	1.82	0.44
7:I:5:TYR:CE1	7:I:8:SER:HA	2.52	0.44
10:L:21:ILE:O	10:L:27:VAL:HG21	2.17	0.44
1:A:347:VAL:HG12	1:A:424:MET:SD	2.58	0.44
2:B:377:HIS:O	2:B:381:ILE:HG12	2.18	0.44
2:B:471:GLY:HA3	2:B:504:LEU:HD21	1.98	0.44
14:B:3033:CLA:HBC2	14:B:3033:CLA:HHD	1.98	0.44
5:E:15:TYR:CD2	5:E:44:ASN:HA	2.53	0.44
16:J:104:BCR:H15C	16:J:104:BCR:H351	1.87	0.44
1:A:226:LEU:HB2	1:A:236:ILE:HD12	2.00	0.44
1:A:298:ALA:O	1:A:302:LEU:HD23	2.17	0.44
14:A:803:CLA:HED1	2:B:426:SER:OG	2.18	0.44
16:A:847:BCR:H383	16:K:102:BCR:HC8	2.00	0.44
3:C:30:TRP:HE3	3:C:33:CYS:HG	1.66	0.44
6:F:132:LYS:HG2	6:F:133:ASP:H	1.81	0.44
9:K:58:GLU:HA	9:K:60:LEU:HD22	2.00	0.44
1:A:217:ILE:HG22	1:A:298:ALA:HB1	1.99	0.44
2:B:453:GLU:OE2	6:F:34:ARG:NH2	2.51	0.44
2:B:525:VAL:HG11	2:B:625:TRP:CZ2	2.52	0.44
6:F:79:TRP:CH2	6:F:120:ALA:HA	2.52	0.44
9:K:35:GLN:O	9:K:36:SER:HB3	2.18	0.44
1:A:249:MET:CB	1:A:258:TRP:CH2	3.01	0.44
1:A:336:PHE:CE2	14:A:845:CLA:HMA3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:GLY:HA2	1:A:401:GLY:HA2	2.00	0.44
1:A:710:LYS:HE3	6:F:132:LYS:HA	1.99	0.44
14:A:807:CLA:H42	14:A:831:CLA:H2	1.99	0.44
14:A:812:CLA:HMB1	14:A:812:CLA:HBB1	2.00	0.44
2:B:59:TRP:NE1	14:B:3028:CLA:OBD	2.50	0.44
2:B:430:LEU:HD21	16:F:201:BCR:H402	1.98	0.44
9:K:25:PHE:O	9:K:29:LEU:HD23	2.18	0.44
1:A:67:ASP:OD1	1:A:71:LYS:CE	2.66	0.44
1:A:414:ILE:HD13	14:A:831:CLA:CED	2.47	0.44
1:A:722:LEU:HD12	15:A:846:PQN:C4	2.48	0.44
2:B:171:GLU:HG3	2:B:300:ILE:HD12	1.99	0.44
2:B:475:TYR:O	6:F:3:ALA:HA	2.17	0.44
16:B:3044:BCR:HC41	16:B:3046:BCR:H322	1.99	0.44
1:A:24:SER:H	14:A:812:CLA:HMA1	1.83	0.44
1:A:126:LEU:HB3	1:A:137:ILE:HD11	2.00	0.44
1:A:713:VAL:O	1:A:713:VAL:HG22	2.17	0.44
14:A:829:CLA:H41	14:A:829:CLA:H72	2.00	0.44
8:J:38:PHE:O	8:J:40:PRO:HD3	2.17	0.44
1:A:120:ILE:HD11	8:J:31:ARG:HB2	1.99	0.43
1:A:300:HIS:HB2	14:A:819:CLA:C1B	2.48	0.43
1:A:654:LEU:HD22	13:A:801:CL0:CMD	2.48	0.43
1:A:680:HIS:HB3	14:A:856:CLA:O1D	2.19	0.43
16:B:3045:BCR:H321	16:B:3045:BCR:C8	2.48	0.43
5:E:11:ARG:HD3	5:E:64:GLU:CD	2.39	0.43
6:F:103:VAL:N	6:F:104:PRO:HD3	2.33	0.43
17:I:102:LMG:C21	18:M:101:LHG:H382	2.47	0.43
16:J:105:BCR:H15C	16:J:105:BCR:H351	1.89	0.43
2:B:72:ASN:O	2:B:72:ASN:OD1	2.36	0.43
6:F:65:ILE:HB	6:F:66:PRO:HD3	1.99	0.43
9:K:31:ARG:HH11	9:K:34:ILE:HG13	1.83	0.43
1:A:396:HIS:HE1	14:A:829:CLA:ND	2.11	0.43
2:B:18:ARG:O	2:B:22:TYR:HB2	2.18	0.43
2:B:342:ALA:HB2	16:B:3047:BCR:H372	1.99	0.43
6:F:101:ILE:O	6:F:101:ILE:HG23	2.19	0.43
9:K:40:GLY:N	9:K:41:PRO:CD	2.82	0.43
1:A:289:THR:O	1:A:382:TYR:N	2.33	0.43
1:A:433:VAL:CG1	14:A:832:CLA:HMD3	2.48	0.43
2:B:6:LYS:NZ	11:M:30:TYR:CD2	2.86	0.43
2:B:179:ALA:O	2:B:183:GLY:HA3	2.18	0.43
2:B:377:HIS:HE1	14:B:3028:CLA:ND	2.06	0.43
2:B:541:VAL:O	2:B:545:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:GLY:O	1:A:98:SER:HB3	2.19	0.43
1:A:161:THR:N	14:A:815:CLA:O1A	2.52	0.43
1:A:172:MET:HA	1:A:175:ALA:CB	2.48	0.43
14:A:829:CLA:C1A	14:A:829:CLA:CGA	2.95	0.43
14:A:829:CLA:O1D	14:A:830:CLA:HHB	2.19	0.43
2:B:130:THR:HG23	2:B:133:ASP:H	1.83	0.43
1:A:267:PHE:HD2	1:A:268:PHE:CD2	2.35	0.43
1:A:367:SER:CB	1:A:400:ILE:HD11	2.48	0.43
1:A:439:ALA:HA	2:B:686:TRP:CZ3	2.53	0.43
14:A:842:CLA:HBB2	15:A:846:PQN:H141	1.99	0.43
2:B:266:SER:OG	2:B:267:LEU:N	2.50	0.43
2:B:589:MET:SD	2:B:589:MET:C	2.97	0.43
14:B:3004:CLA:H42	14:B:3004:CLA:O1A	2.19	0.43
14:B:3039:CLA:H43	14:X:1701:CLA:C3D	2.48	0.43
3:C:22:THR:HA	4:D:65:LEU:HD12	2.00	0.43
4:D:67:LEU:HD12	4:D:71:GLN:HB2	2.00	0.43
1:A:95:ALA:HA	1:A:158:LEU:HD13	2.01	0.43
1:A:352:TRP:CD1	14:A:826:CLA:H202	2.53	0.43
1:A:726:GLN:HG3	18:A:853:LHG:C7	2.48	0.43
6:F:16:LYS:O	6:F:19:ALA:HB3	2.19	0.43
6:F:84:TYR:CD1	6:F:84:TYR:C	2.92	0.43
9:K:60:LEU:O	9:K:61:ALA:C	2.57	0.43
12:X:15:TRP:O	12:X:19:LEU:HG	2.18	0.43
1:A:90:MET:HE1	14:A:809:CLA:H2A	2.01	0.43
1:A:175:ALA:HA	14:A:811:CLA:HBC2	2.00	0.43
1:A:201:LEU:HD11	1:A:311:ALA:HB3	1.99	0.43
1:A:246:PRO:O	1:A:250:ALA:HB2	2.19	0.43
1:A:396:HIS:HB2	14:A:829:CLA:C1B	2.48	0.43
1:A:411:HIS:CE1	14:A:831:CLA:NA	2.86	0.43
14:A:836:CLA:HHC	14:A:836:CLA:HBB1	1.99	0.43
2:B:45:ILE:HD12	14:B:3006:CLA:C2C	2.49	0.43
2:B:154:LEU:HD23	2:B:155:HIS:CE1	2.54	0.43
2:B:403:PRO:O	2:B:407:LYS:HB2	2.19	0.43
2:B:531:LEU:O	2:B:532:GLY:C	2.57	0.43
8:J:2:LYS:HD2	8:J:2:LYS:O	2.18	0.43
14:K:103:CLA:HBA2	14:K:103:CLA:H3A	1.80	0.43
10:L:54:HIS:HA	10:L:57:PHE:CE2	2.53	0.43
1:A:444:LEU:O	1:A:447:VAL:HG12	2.18	0.43
1:A:653:PHE:O	1:A:657:GLN:HG3	2.19	0.43
14:A:815:CLA:HBC2	14:A:817:CLA:HMC3	2.01	0.43
3:C:26:GLU:HA	4:D:102:PRO:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:131:SER:O	10:L:134:VAL:HG12	2.19	0.43
1:A:384:ALA:CB	1:A:525:ALA:HB1	2.49	0.43
1:A:410:ALA:HA	1:A:595:VAL:HG11	2.01	0.43
1:A:455:SER:OG	1:A:456:PHE:N	2.52	0.43
14:A:845:CLA:HMB3	18:A:854:LHG:HC62	2.01	0.43
2:B:360:PRO:HG3	14:B:3019:CLA:CBA	2.49	0.43
9:K:58:GLU:HB2	9:K:60:LEU:HD22	2.01	0.43
1:A:399:TRP:CE3	1:A:606:ILE:HG21	2.54	0.42
1:A:472:GLN:OE1	1:A:472:GLN:N	2.44	0.42
4:D:60:ARG:HB2	4:D:63:GLN:HG3	2.00	0.42
1:A:45:THR:CG2	1:A:719:PRO:HA	2.49	0.42
1:A:120:ILE:HG23	1:A:121:VAL:N	2.34	0.42
1:A:255:LYS:HE3	1:A:276:SER:OG	2.19	0.42
1:A:660:GLN:HB2	1:A:750:ARG:HA	2.02	0.42
1:A:747:PHE:O	1:A:751:ILE:HG22	2.19	0.42
14:A:832:CLA:HMA2	10:L:19:THR:HG21	2.01	0.42
2:B:430:LEU:HD21	16:F:201:BCR:C40	2.49	0.42
2:B:651:VAL:CG1	14:B:3010:CLA:HHD	2.49	0.42
14:B:3013:CLA:HMB3	14:B:3021:CLA:C4D	2.49	0.42
4:D:68:ALA:HA	4:D:72:LEU:HD12	2.02	0.42
12:X:13:THR:O	12:X:17:VAL:HG22	2.19	0.42
1:A:343:GLY:O	1:A:347:VAL:HG13	2.19	0.42
1:A:385:THR:HG21	1:A:520:VAL:HG12	2.00	0.42
14:A:804:CLA:H193	14:A:843:CLA:C18	2.48	0.42
2:B:339:TRP:HE1	14:B:3025:CLA:C2B	2.32	0.42
3:C:24:VAL:HB	19:C:101:SF4:S1	2.59	0.42
12:X:20:LEU:O	12:X:23:ASN:HB3	2.19	0.42
1:A:165:GLY:CA	16:A:847:BCR:HC21	2.49	0.42
1:A:242:PHE:HB3	1:A:249:MET:SD	2.60	0.42
14:A:832:CLA:HMB2	14:A:833:CLA:C1D	2.50	0.42
16:A:847:BCR:H381	16:K:102:BCR:H10C	2.02	0.42
2:B:99:ALA:O	2:B:103:PHE:HD2	2.03	0.42
2:B:566:ASP:H	2:B:573:THR:CG2	2.31	0.42
2:B:627:ARG:HH21	2:B:628:ASP:CG	2.23	0.42
2:B:711:ALA:HB2	15:B:3043:PQN:C7	2.49	0.42
1:A:69:SER:HB3	1:A:190:PHE:CD2	2.55	0.42
1:A:143:LEU:HD22	1:A:146:LEU:HD23	2.02	0.42
1:A:201:LEU:O	1:A:205:LEU:HB3	2.20	0.42
1:A:300:HIS:HE1	14:A:819:CLA:C1D	2.32	0.42
1:A:706:TRP:CD1	6:F:138:VAL:HG12	2.54	0.42
14:A:804:CLA:C2C	14:A:805:CLA:HMD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:813:CLA:C2B	14:A:821:CLA:HMD2	2.49	0.42
14:A:828:CLA:HMB3	14:A:836:CLA:HBA1	2.01	0.42
2:B:275:HIS:HE1	14:B:3018:CLA:C1D	2.32	0.42
14:B:3008:CLA:CGD	7:I:11:PRO:HG3	2.50	0.42
4:D:2:THR:HB	4:D:3:LEU:HD22	2.00	0.42
4:D:120:GLY:HA3	5:E:13:GLU:OE2	2.20	0.42
6:F:16:LYS:N	6:F:16:LYS:HE2	2.34	0.42
10:L:18:SER:CB	10:L:23:ASP:HB3	2.49	0.42
16:L:201:BCR:H24C	16:L:201:BCR:H371	1.80	0.42
2:B:192:HIS:O	2:B:193:LEU:C	2.58	0.42
2:B:342:ALA:O	2:B:346:VAL:HG22	2.19	0.42
2:B:442:HIS:HE1	14:B:3034:CLA:NA	2.14	0.42
2:B:509:SER:C	2:B:511:THR:H	2.23	0.42
14:B:3034:CLA:H2A	14:B:3034:CLA:HED2	2.00	0.42
3:C:60:ASP:OD1	3:C:60:ASP:O	2.38	0.42
6:F:1:ASP:OD2	6:F:42:LEU:CD2	2.68	0.42
6:F:77:ILE:HD12	14:F:202:CLA:C1D	2.50	0.42
12:X:25:LEU:C	12:X:25:LEU:HD23	2.39	0.42
1:A:91:TYR:CE1	1:A:147:TRP:NE1	2.87	0.42
1:A:93:HIS:HE1	14:A:808:CLA:C4B	2.33	0.42
1:A:249:MET:CB	1:A:258:TRP:HH2	2.33	0.42
1:A:681:PHE:CG	16:A:851:BCR:H363	2.53	0.42
14:A:818:CLA:HBC3	14:A:819:CLA:HMC2	2.01	0.42
17:A:855:LMG:HC5	22:L:207:DGD:HA42	2.01	0.42
2:B:49:HIS:CD2	14:B:3006:CLA:C4A	3.03	0.42
2:B:277:LEU:HD23	2:B:277:LEU:O	2.19	0.42
2:B:426:SER:HA	2:B:538:LEU:HD22	2.00	0.42
6:F:59:ARG:HA	6:F:59:ARG:HD2	1.93	0.42
10:L:143:LEU:N	10:L:143:LEU:HD22	2.35	0.42
1:A:93:HIS:HE1	14:A:808:CLA:NB	2.13	0.42
1:A:371:ALA:HB1	1:A:394:PHE:HA	2.02	0.42
1:A:696:TYR:OH	2:B:539:ILE:HA	2.20	0.42
14:A:820:CLA:O1A	14:A:830:CLA:HMD1	2.20	0.42
14:B:3034:CLA:HMB3	16:J:105:BCR:H12C	2.02	0.42
16:L:209:BCR:H20C	16:L:209:BCR:H361	1.83	0.42
1:A:410:ALA:O	1:A:414:ILE:HG13	2.20	0.42
1:A:706:TRP:HD1	6:F:138:VAL:HG12	1.85	0.42
14:A:828:CLA:HMB1	14:A:828:CLA:CBB	2.47	0.42
14:A:830:CLA:H2A	14:A:830:CLA:O2D	2.19	0.42
2:B:18:ARG:HG2	2:B:22:TYR:CD1	2.55	0.42
2:B:121:HIS:CB	2:B:364:ILE:HD13	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:12:PRO:HB2	16:J:104:BCR:H391	2.02	0.42
16:J:104:BCR:C8	16:J:104:BCR:H321	2.50	0.42
16:J:104:BCR:H321	16:J:104:BCR:HC8	2.02	0.42
9:K:29:LEU:HD13	9:K:62:THR:HG21	2.01	0.42
9:K:69:LEU:O	9:K:73:VAL:HG23	2.20	0.42
1:A:231:VAL:HB	1:A:236:ILE:HD11	2.02	0.42
1:A:673:GLY:O	1:A:676:PHE:HB3	2.20	0.42
1:A:693:GLY:HA3	2:B:574:CYS:HB2	2.02	0.42
2:B:428:VAL:HG21	14:B:3040:CLA:C2C	2.49	0.42
2:B:471:GLY:HA3	2:B:504:LEU:CD2	2.50	0.42
2:B:516:LEU:HD12	2:B:516:LEU:N	2.35	0.42
3:C:5:LYS:HG3	4:D:136:TYR:HB2	2.02	0.42
9:K:56:LEU:N	9:K:59:LEU:HD23	2.35	0.42
1:A:141:SER:OG	14:A:809:CLA:O1D	2.28	0.41
1:A:152:ILE:HD13	14:A:815:CLA:O1D	2.20	0.41
1:A:292:LEU:HD12	1:A:379:PRO:HA	2.02	0.41
1:A:360:LEU:HD23	14:A:806:CLA:HED1	2.02	0.41
1:A:672:TYR:CE2	1:A:748:LEU:HB3	2.55	0.41
2:B:54:ALA:CB	2:B:149:LEU:HG	2.50	0.41
2:B:692:PRO:O	2:B:693:LEU:HB2	2.20	0.41
14:B:3018:CLA:HBA1	14:B:3018:CLA:H3A	1.91	0.41
4:D:4:THR:HG23	4:D:53:GLU:OE2	2.19	0.41
6:F:38:TYR:O	6:F:41:ALA:HB3	2.20	0.41
6:F:48:LEU:HB3	6:F:49:PRO:CD	2.50	0.41
14:L:206:CLA:HBB1	14:L:206:CLA:HMB1	2.02	0.41
16:M:103:BCR:H15C	16:M:103:BCR:H351	1.96	0.41
12:X:34:LEU:O	12:X:35:LYS:HG3	2.20	0.41
2:B:159:LYS:HB2	2:B:160:PHE:CE1	2.55	0.41
2:B:298:HIS:CE1	14:B:3023:CLA:HMD1	2.55	0.41
2:B:636:GLN:OE1	2:B:737:ALA:HB1	2.20	0.41
6:F:84:TYR:CZ	6:F:88:VAL:HG21	2.55	0.41
6:F:103:VAL:N	6:F:104:PRO:CD	2.84	0.41
16:F:203:BCR:H20C	16:F:203:BCR:H361	1.95	0.41
14:J:102:CLA:HMD3	16:J:105:BCR:H292	2.02	0.41
1:A:356:LEU:O	1:A:360:LEU:HG	2.20	0.41
1:A:416:MET:HE1	1:A:434:LEU:HD21	2.02	0.41
1:A:544:PHE:CE1	1:A:548:VAL:HG21	2.55	0.41
2:B:655:MET:HA	2:B:658:PHE:HB3	2.03	0.41
14:B:3011:CLA:O2A	14:B:3011:CLA:H2A	2.20	0.41
14:B:3037:CLA:HHC	14:B:3037:CLA:HBB1	2.03	0.41
6:F:8:CYS:SG	6:F:42:LEU:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:57:LEU:HD12	6:F:57:LEU:H	1.84	0.41
1:A:17:ASP:O	1:A:20:PRO:HD3	2.20	0.41
1:A:297:THR:HG23	14:A:820:CLA:HMA3	2.01	0.41
1:A:341:HIS:HB3	1:A:344:LEU:HD12	2.03	0.41
2:B:523:PHE:CE2	2:B:527:HIS:CE1	3.08	0.41
14:B:3008:CLA:O1A	7:I:14:PHE:HB3	2.20	0.41
6:F:56:ARG:HG3	6:F:57:LEU:H	1.85	0.41
1:A:76:HIS:CD2	14:A:806:CLA:NA	2.88	0.41
1:A:306:VAL:HG21	14:A:818:CLA:CMC	2.50	0.41
1:A:457:GLY:HA2	1:A:460:VAL:HG22	2.03	0.41
1:A:697:TRP:NE1	15:A:846:PQN:C1	2.84	0.41
14:A:844:CLA:H192	16:L:201:BCR:H363	2.02	0.41
4:D:9:LEU:HD22	4:D:50:ARG:HD3	2.03	0.41
6:F:84:TYR:CE2	6:F:101:ILE:CD1	3.03	0.41
7:I:33:TYR:HB2	17:I:102:LMG:H111	2.03	0.41
10:L:54:HIS:HE1	14:L:205:CLA:C4D	2.33	0.41
11:M:17:LEU:HB3	11:M:18:PRO:HD3	2.02	0.41
2:B:192:HIS:HB2	14:B:3015:CLA:CHC	2.51	0.41
2:B:215:MET:HE2	2:B:218:PRO:O	2.21	0.41
3:C:65:ARG:HB3	3:C:67:TYR:CE1	2.56	0.41
1:A:232:ALA:O	1:A:236:ILE:HG12	2.19	0.41
1:A:490:VAL:HA	1:A:493:LEU:HD21	2.03	0.41
2:B:452:PRO:O	6:F:48:LEU:HD13	2.21	0.41
14:B:3026:CLA:HBD	14:B:3038:CLA:HMB3	2.02	0.41
14:B:3030:CLA:HMB1	14:B:3030:CLA:CBB	2.50	0.41
1:A:202:ALA:CB	1:A:309:ILE:HA	2.51	0.41
1:A:272:TRP:O	1:A:275:TYR:HB2	2.20	0.41
1:A:306:VAL:HG21	14:A:818:CLA:HMC2	2.03	0.41
1:A:354:ALA:O	1:A:358:ILE:HG23	2.21	0.41
1:A:638:ASN:OD1	1:A:638:ASN:N	2.52	0.41
2:B:498:VAL:HG12	2:B:498:VAL:O	2.21	0.41
6:F:73:ILE:HD13	14:F:202:CLA:H3A	2.02	0.41
6:F:105:LEU:HD12	6:F:106:ALA:N	2.35	0.41
7:I:22:MET:HG3	7:I:23:PRO:CD	2.49	0.41
8:J:28:GLU:HG2	8:J:31:ARG:NH2	2.36	0.41
9:K:23:ASN:OD1	9:K:23:ASN:N	2.53	0.41
9:K:59:LEU:O	9:K:59:LEU:HD12	2.20	0.41
9:K:60:LEU:HG	9:K:63:THR:CG2	2.51	0.41
1:A:51:LEU:C	1:A:51:LEU:HD23	2.41	0.41
1:A:490:VAL:HA	1:A:493:LEU:HD23	2.03	0.41
14:A:818:CLA:CBC	14:A:819:CLA:CMC	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:456:ILE:HG22	2:B:458:ILE:HD11	2.02	0.41
6:F:116:TRP:N	6:F:117:PRO:CD	2.83	0.41
16:I:101:BCR:H15C	16:I:101:BCR:H351	1.80	0.41
10:L:6:LYS:HB2	10:L:7:PRO:HD2	2.03	0.41
1:A:196:MET:HB2	14:A:814:CLA:HBC2	2.02	0.41
1:A:327:GLU:O	1:A:331:ALA:HB2	2.21	0.41
1:A:356:LEU:HD23	1:A:411:HIS:CG	2.56	0.41
1:A:688:MET:HB2	14:A:803:CLA:CHC	2.51	0.41
14:A:804:CLA:HMC2	14:A:805:CLA:C2D	2.51	0.41
14:A:856:CLA:H11	2:B:622:LEU:HD12	2.03	0.41
2:B:178:LEU:O	2:B:182:PHE:HB2	2.21	0.41
2:B:500:LEU:N	2:B:501:PRO:CD	2.84	0.41
14:B:3013:CLA:HBB1	14:B:3021:CLA:HBC2	2.02	0.41
14:B:3020:CLA:HED1	14:B:3024:CLA:O1D	2.21	0.41
1:A:94:GLY:HA3	1:A:147:TRP:CH2	2.56	0.40
1:A:180:TYR:HA	1:A:184:ALA:HB2	2.03	0.40
1:A:714:ALA:O	6:F:89:ARG:NH1	2.54	0.40
14:A:803:CLA:HMD2	2:B:539:ILE:HD13	2.03	0.40
14:A:823:CLA:CGA	14:A:823:CLA:H3A	2.51	0.40
2:B:129:ARG:HG3	2:B:200:GLU:OE1	2.21	0.40
9:K:24:LEU:HD13	9:K:69:LEU:HB3	2.02	0.40
10:L:33:ASN:HB3	10:L:38:ARG:HD3	2.02	0.40
1:A:31:PRO:HB3	14:A:804:CLA:HAC1	2.04	0.40
1:A:299:HIS:O	1:A:303:ALA:CB	2.69	0.40
1:A:380:TYR:O	1:A:383:LEU:CD2	2.68	0.40
1:A:462:ASN:O	1:A:463:ASP:C	2.59	0.40
1:A:730:VAL:HA	14:A:843:CLA:O1D	2.21	0.40
14:A:808:CLA:C6	14:J:101:CLA:HBC1	2.50	0.40
16:A:847:BCR:H24C	16:A:847:BCR:H371	1.92	0.40
2:B:299:SER:OG	2:B:302:GLU:HG3	2.21	0.40
2:B:329:TYR:CE1	2:B:336:GLN:HG2	2.56	0.40
16:F:203:BCR:H24C	16:F:203:BCR:H371	1.87	0.40
10:L:72:ASP:N	10:L:72:ASP:OD1	2.53	0.40
14:L:204:CLA:C1B	14:L:205:CLA:HED1	2.51	0.40
1:A:103:TRP:CE3	1:A:144:PHE:HB3	2.56	0.40
1:A:121:VAL:HA	6:F:24:THR:HG22	2.04	0.40
1:A:192:ASN:OD1	14:A:813:CLA:HED1	2.21	0.40
14:A:829:CLA:H193	16:J:103:BCR:C14	2.52	0.40
2:B:289:MET:HA	14:B:3022:CLA:HAC2	2.02	0.40
3:C:51:LYS:HD3	3:C:54:GLU:OE1	2.22	0.40
9:K:27:ILE:HD13	9:K:27:ILE:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LEU:O	1:A:104:LEU:HD12	2.22	0.40
1:A:337:THR:OG1	18:A:854:LHG:O2	2.32	0.40
1:A:379:PRO:HG2	1:A:380:TYR:CD1	2.56	0.40
1:A:385:THR:O	1:A:523:LYS:NZ	2.50	0.40
1:A:391:LEU:HD12	1:A:613:PHE:HE1	1.86	0.40
16:A:851:BCR:H20C	16:A:851:BCR:H361	1.82	0.40
2:B:525:VAL:HG11	2:B:625:TRP:HZ2	1.86	0.40
2:B:652:TRP:HE3	2:B:729:ALA:HA	1.86	0.40
14:B:3004:CLA:H161	14:B:3004:CLA:H141	1.86	0.40
4:D:21:ALA:HB1	4:D:26:LYS:HB3	2.04	0.40
1:A:215:HIS:HB2	14:A:815:CLA:CHC	2.51	0.40
1:A:286:ASN:OD1	1:A:288:VAL:HG12	2.21	0.40
1:A:483:GLN:O	1:A:485:VAL:N	2.55	0.40
1:A:494:HIS:HE1	14:A:836:CLA:C1B	2.35	0.40
1:A:665:TYR:OH	1:A:674:LEU:HD23	2.22	0.40
1:A:686:SER:OG	1:A:735:TYR:HB2	2.20	0.40
2:B:664:ALA:O	2:B:667:PHE:HB2	2.20	0.40
14:B:3042:CLA:C20	7:I:28:GLY:HA2	2.52	0.40
9:K:62:THR:HA	9:K:65:PHE:HB3	2.03	0.40
14:M:102:CLA:HED2	14:M:102:CLA:C2A	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	736/755 (98%)	671 (91%)	65 (9%)	0	100	100
2	B	737/740 (100%)	680 (92%)	56 (8%)	1 (0%)	51	85
3	C	78/80 (98%)	71 (91%)	7 (9%)	0	100	100
4	D	136/138 (99%)	122 (90%)	14 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	67/75 (89%)	56 (84%)	10 (15%)	1 (2%)	10	42
6	F	139/164 (85%)	121 (87%)	18 (13%)	0	100	100
7	I	36/38 (95%)	30 (83%)	6 (17%)	0	100	100
8	J	39/41 (95%)	35 (90%)	4 (10%)	0	100	100
9	K	43/83 (52%)	35 (81%)	8 (19%)	0	100	100
10	L	149/154 (97%)	136 (91%)	13 (9%)	0	100	100
11	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
12	X	27/35 (77%)	24 (89%)	3 (11%)	0	100	100
All	All	2216/2334 (95%)	2009 (91%)	205 (9%)	2 (0%)	51	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	25	SER
2	B	194	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	589/603 (98%)	577 (98%)	12 (2%)	55	83
2	B	597/597 (100%)	583 (98%)	14 (2%)	50	80
3	C	67/67 (100%)	64 (96%)	3 (4%)	27	64
4	D	115/115 (100%)	114 (99%)	1 (1%)	78	92
5	E	59/64 (92%)	57 (97%)	2 (3%)	37	72
6	F	109/128 (85%)	108 (99%)	1 (1%)	78	92
7	I	32/32 (100%)	32 (100%)	0	100	100
8	J	36/36 (100%)	36 (100%)	0	100	100
9	K	33/61 (54%)	30 (91%)	3 (9%)	9	34
10	L	117/119 (98%)	116 (99%)	1 (1%)	78	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	M	26/26 (100%)	26 (100%)	0	100	100
12	X	23/27 (85%)	20 (87%)	3 (13%)	4	19
All	All	1803/1875 (96%)	1763 (98%)	40 (2%)	52	81

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	43	GLN
1	A	59	ASP
1	A	84	PHE
1	A	207	LEU
1	A	257	ASP
1	A	260	PHE
1	A	302	LEU
1	A	333	LYS
1	A	345	TYR
1	A	720	ARG
1	A	723	SER
2	B	95	PHE
2	B	155	HIS
2	B	212	LEU
2	B	256	PHE
2	B	291	ARG
2	B	323	GLN
2	B	378	HIS
2	B	396	PHE
2	B	424	HIS
2	B	522	ASP
2	B	526	HIS
2	B	583	TYR
2	B	621	TYR
2	B	635	SER
3	C	13	CYS
3	C	16	CYS
3	C	18	ARG
4	D	33	SER
5	E	25	SER
5	E	53	SER
6	F	95	ASN
9	K	25	PHE

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Mol	Chain	Res	Type
9	K	43	LEU
9	K	60	LEU
10	L	72	ASP
12	X	12	ARG
12	X	23	ASN
12	X	30	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	138	GLN
1	A	191	GLN
1	A	245	ASN
1	A	542	HIS
1	A	657	GLN
1	A	718	GLN
2	B	105	GLN
2	B	121	HIS
2	B	228	ASN
2	B	319	ASN
2	B	336	GLN
2	B	377	HIS
2	B	467	GLN
2	B	591	ASN
3	C	37	GLN
4	D	78	ASN
5	E	59	ASN
6	F	90	ASN
6	F	134	ASN
8	J	3	HIS
8	J	30	ASN
10	L	75	ASN
11	M	7	GLN

5.3.3 RNA ⓘ

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](#)

Of 135 ligands modelled in this entry, 2 are monoatomic - leaving 133 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	825	-	50,67,73	1.67	4 (8%)	47,105,113	1.57	8 (17%)
14	CLA	A	816	-	33,53,73	2.00	5 (15%)	27,89,113	2.27	11 (40%)
14	CLA	B	3036	23	33,53,73	2.14	5 (15%)	27,89,113	1.98	9 (33%)
14	CLA	K	101	-	29,49,73	2.10	4 (13%)	20,83,113	2.25	6 (30%)
16	BCR	B	3047	-	41,41,41	1.15	3 (7%)	56,56,56	1.34	8 (14%)
14	CLA	K	103	-	33,53,73	2.06	5 (15%)	27,89,113	1.99	9 (33%)
14	CLA	A	839	-	56,73,73	1.56	5 (8%)	55,113,113	1.70	11 (20%)
14	CLA	B	3035	-	33,53,73	2.12	5 (15%)	27,89,113	1.91	7 (25%)
14	CLA	L	206	23	56,73,73	1.59	5 (8%)	55,113,113	1.68	9 (16%)
19	SF4	C	102	3	0,12,12	-	-	-	-	-
14	CLA	A	820	-	56,73,73	1.55	5 (8%)	55,113,113	1.73	12 (21%)
16	BCR	L	208	-	41,41,41	1.12	3 (7%)	56,56,56	1.44	12 (21%)
14	CLA	A	808	-	42,59,73	1.93	4 (9%)	38,96,113	1.63	7 (18%)
15	PQN	A	846	-	34,34,34	2.03	7 (20%)	42,45,45	1.29	6 (14%)
14	CLA	A	856	23	56,73,73	1.59	5 (8%)	55,113,113	1.60	9 (16%)
14	CLA	B	3033	-	56,73,73	1.59	5 (8%)	55,113,113	1.64	10 (18%)
14	CLA	B	3007	-	56,73,73	1.59	6 (10%)	55,113,113	1.53	9 (16%)
17	LMG	A	852	-	48,48,55	0.86	2 (4%)	56,56,63	1.27	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	818	-	45,62,73	1.85	6 (13%)	41,99,113	1.70	8 (19%)
16	BCR	F	203	-	41,41,41	1.12	3 (7%)	56,56,56	1.31	7 (12%)
14	CLA	B	3030	-	56,73,73	1.62	7 (12%)	55,113,113	1.71	13 (23%)
16	BCR	L	201	-	41,41,41	1.13	3 (7%)	56,56,56	1.21	5 (8%)
14	CLA	B	3013	-	33,53,73	2.07	6 (18%)	27,89,113	2.06	8 (29%)
16	BCR	L	209	-	41,41,41	1.17	3 (7%)	56,56,56	1.31	7 (12%)
14	CLA	A	813	-	45,62,73	1.78	6 (13%)	41,99,113	1.83	10 (24%)
16	BCR	B	3045	-	41,41,41	1.14	3 (7%)	56,56,56	1.26	6 (10%)
14	CLA	B	3017	-	46,63,73	1.78	4 (8%)	43,101,113	1.71	8 (18%)
14	CLA	B	3023	23	46,63,73	1.74	6 (13%)	43,101,113	1.67	7 (16%)
14	CLA	B	3028	-	56,73,73	1.57	7 (12%)	55,113,113	1.65	7 (12%)
14	CLA	B	3020	23	56,73,73	1.58	6 (10%)	55,113,113	1.68	11 (20%)
17	LMG	I	102	-	40,40,55	1.37	6 (15%)	48,48,63	1.23	4 (8%)
14	CLA	A	810	1	56,73,73	1.62	5 (8%)	55,113,113	1.48	8 (14%)
18	LHG	A	853	-	48,48,48	0.69	2 (4%)	51,54,54	1.23	6 (11%)
14	CLA	B	3041	23	56,73,73	1.78	7 (12%)	55,113,113	1.42	5 (9%)
14	CLA	B	3022	-	33,53,73	2.05	5 (15%)	27,89,113	2.08	9 (33%)
16	BCR	A	850	-	41,41,41	1.07	3 (7%)	56,56,56	1.20	4 (7%)
14	CLA	A	806	-	56,73,73	1.55	6 (10%)	55,113,113	1.69	9 (16%)
16	BCR	M	103	-	41,41,41	1.16	3 (7%)	56,56,56	1.14	2 (3%)
14	CLA	A	827	23	56,73,73	1.63	6 (10%)	55,113,113	1.55	9 (16%)
14	CLA	A	830	-	56,73,73	1.59	5 (8%)	55,113,113	1.59	9 (16%)
14	CLA	B	3027	-	56,73,73	1.63	6 (10%)	55,113,113	1.51	8 (14%)
16	BCR	B	3044	-	41,41,41	1.10	3 (7%)	56,56,56	1.21	6 (10%)
16	BCR	B	3051	-	41,41,41	1.16	3 (7%)	56,56,56	1.18	3 (5%)
14	CLA	A	812	14	56,73,73	1.62	8 (14%)	55,113,113	1.56	9 (16%)
14	CLA	A	824	-	42,59,73	1.81	5 (11%)	38,96,113	1.88	9 (23%)
14	CLA	B	3034	-	49,66,73	1.67	4 (8%)	46,104,113	1.69	12 (26%)
14	CLA	B	3038	-	51,68,73	1.65	6 (11%)	49,107,113	1.66	9 (18%)
14	CLA	B	3008	-	56,73,73	1.65	7 (12%)	55,113,113	1.62	9 (16%)
16	BCR	J	105	-	41,41,41	1.12	3 (7%)	56,56,56	1.35	9 (16%)
14	CLA	J	102	-	28,45,73	2.23	5 (17%)	19,78,113	2.03	6 (31%)
14	CLA	A	811	-	33,53,73	2.00	5 (15%)	27,89,113	2.04	9 (33%)
14	CLA	A	822	23	56,73,73	1.54	4 (7%)	55,113,113	1.55	11 (20%)
14	CLA	B	3004	-	56,73,73	1.58	7 (12%)	55,113,113	1.62	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	3015	-	56,73,73	1.64	5 (8%)	55,113,113	1.37	9 (16%)
14	CLA	A	817	23	40,57,73	1.92	5 (12%)	34,93,113	1.87	7 (20%)
14	CLA	B	3032	-	40,57,73	1.84	5 (12%)	34,93,113	1.97	10 (29%)
14	CLA	A	814	-	51,68,73	1.74	5 (9%)	49,107,113	1.50	9 (18%)
15	PQN	B	3043	-	34,34,34	2.15	7 (20%)	42,45,45	1.22	5 (11%)
14	CLA	A	844	23	56,73,73	1.63	5 (8%)	55,113,113	1.70	9 (16%)
14	CLA	A	835	-	56,73,73	1.60	5 (8%)	55,113,113	1.66	10 (18%)
14	CLA	B	3031	-	33,53,73	2.14	5 (15%)	27,89,113	2.06	6 (22%)
22	DGD	L	207	-	67,67,67	1.04	3 (4%)	81,81,81	1.18	8 (9%)
17	LMG	A	855	-	30,30,55	1.40	4 (13%)	37,37,63	1.32	4 (10%)
18	LHG	B	3050	-	22,22,48	1.57	5 (22%)	25,28,54	1.24	3 (12%)
14	CLA	B	3010	2	56,73,73	1.64	8 (14%)	55,113,113	1.79	12 (21%)
14	CLA	B	3042	-	56,73,73	1.62	6 (10%)	55,113,113	1.71	7 (12%)
18	LHG	A	854	14	26,26,48	0.97	1 (3%)	29,32,54	1.32	3 (10%)
16	BCR	J	104	-	41,41,41	1.18	3 (7%)	56,56,56	1.30	6 (10%)
14	CLA	B	3006	-	56,73,73	1.61	6 (10%)	55,113,113	1.56	9 (16%)
16	BCR	F	201	-	41,41,41	1.14	3 (7%)	56,56,56	1.26	6 (10%)
16	BCR	A	847	-	41,41,41	1.17	3 (7%)	56,56,56	1.25	6 (10%)
14	CLA	A	837	1	33,53,73	2.04	6 (18%)	27,89,113	2.11	8 (29%)
16	BCR	J	103	-	41,41,41	1.10	3 (7%)	56,56,56	1.20	2 (3%)
14	CLA	B	3019	-	51,68,73	1.66	4 (7%)	49,107,113	1.72	12 (24%)
14	CLA	A	843	-	56,73,73	1.66	5 (8%)	55,113,113	1.65	9 (16%)
14	CLA	B	3018	-	50,67,73	1.66	5 (10%)	47,105,113	1.81	9 (19%)
14	CLA	A	841	-	56,73,73	1.58	5 (8%)	55,113,113	1.63	12 (21%)
16	BCR	K	102	-	41,41,41	1.10	3 (7%)	56,56,56	1.36	8 (14%)
14	CLA	A	828	-	56,73,73	1.68	7 (12%)	55,113,113	1.50	7 (12%)
18	LHG	M	101	-	48,48,48	0.71	1 (2%)	51,54,54	1.20	3 (5%)
14	CLA	B	3037	23	33,53,73	2.13	6 (18%)	27,89,113	2.00	7 (25%)
14	CLA	A	815	-	33,53,73	2.09	5 (15%)	27,89,113	1.90	6 (22%)
14	CLA	B	3029	-	56,73,73	1.62	4 (7%)	55,113,113	1.57	10 (18%)
14	CLA	B	3014	-	56,73,73	1.64	5 (8%)	55,113,113	1.54	9 (16%)
14	CLA	A	807	-	56,73,73	1.64	4 (7%)	55,113,113	1.43	10 (18%)
16	BCR	A	848	-	41,41,41	1.14	3 (7%)	56,56,56	1.22	6 (10%)
14	CLA	B	3003	-	56,73,73	1.63	7 (12%)	55,113,113	1.61	7 (12%)
14	CLA	A	802	23	56,73,73	1.62	6 (10%)	55,113,113	1.61	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CL0	A	801	-	59,73,73	1.48	5 (8%)	67,113,113	1.40	10 (14%)
14	CLA	A	803	-	56,73,73	1.62	6 (10%)	55,113,113	1.69	10 (18%)
14	CLA	A	831	-	56,73,73	1.58	6 (10%)	55,113,113	1.59	11 (20%)
14	CLA	X	1701	12	33,53,73	2.08	6 (18%)	27,89,113	2.02	8 (29%)
14	CLA	B	3021	-	38,55,73	1.96	6 (15%)	33,91,113	1.88	8 (24%)
14	CLA	A	805	14	50,67,73	1.74	5 (10%)	47,105,113	1.54	5 (10%)
14	CLA	A	829	-	56,73,73	1.57	6 (10%)	55,113,113	1.55	9 (16%)
19	SF4	C	101	3	0,12,12	-	-	-	-	-
14	CLA	B	3012	-	33,53,73	2.04	5 (15%)	27,89,113	2.26	9 (33%)
14	CLA	B	3040	-	38,55,73	1.95	4 (10%)	33,91,113	2.02	10 (30%)
14	CLA	L	204	10	56,73,73	1.56	7 (12%)	55,113,113	1.82	13 (23%)
14	CLA	A	838	-	42,59,73	1.86	6 (14%)	38,96,113	1.89	10 (26%)
14	CLA	A	821	-	33,50,73	2.01	4 (12%)	26,84,113	2.28	10 (38%)
14	CLA	B	3016	-	33,53,73	2.03	5 (15%)	27,89,113	1.92	6 (22%)
21	LMT	L	202	-	36,36,36	1.15	5 (13%)	47,47,47	1.36	7 (14%)
14	CLA	A	836	-	45,62,73	1.80	6 (13%)	41,99,113	1.78	9 (21%)
14	CLA	A	845	18	43,60,73	1.77	5 (11%)	39,97,113	1.87	12 (30%)
16	BCR	B	3046	-	41,41,41	1.13	3 (7%)	56,56,56	1.26	7 (12%)
14	CLA	B	3005	-	45,62,73	1.77	6 (13%)	41,99,113	1.87	9 (21%)
14	CLA	J	101	8	33,53,73	2.07	4 (12%)	27,89,113	1.96	9 (33%)
16	BCR	A	849	-	41,41,41	1.14	3 (7%)	56,56,56	1.32	7 (12%)
14	CLA	B	3009	-	56,73,73	1.60	6 (10%)	55,113,113	1.59	10 (18%)
16	BCR	B	3048	-	41,41,41	1.10	3 (7%)	56,56,56	1.18	4 (7%)
14	CLA	B	3024	-	33,53,73	2.11	4 (12%)	27,89,113	1.88	7 (25%)
14	CLA	F	202	23	33,53,73	2.10	4 (12%)	27,89,113	2.06	9 (33%)
14	CLA	L	205	-	56,73,73	1.56	5 (8%)	55,113,113	1.60	10 (18%)
17	LMG	B	3049	-	55,55,55	0.81	1 (1%)	63,63,63	1.36	4 (6%)
16	BCR	A	851	-	41,41,41	1.16	3 (7%)	56,56,56	1.40	8 (14%)
14	CLA	A	833	-	56,73,73	1.55	7 (12%)	55,113,113	1.59	10 (18%)
14	CLA	B	3025	2	45,62,73	1.77	4 (8%)	41,99,113	1.91	13 (31%)
16	BCR	I	101	-	41,41,41	1.03	2 (4%)	56,56,56	1.26	7 (12%)
14	CLA	M	102	23	33,53,73	2.15	6 (18%)	27,89,113	1.98	12 (44%)
14	CLA	A	823	-	40,57,73	1.88	5 (12%)	34,93,113	1.97	10 (29%)
14	CLA	A	809	1	56,73,73	1.62	6 (10%)	55,113,113	1.55	7 (12%)
14	CLA	A	832	-	41,58,73	1.82	6 (14%)	37,95,113	1.87	10 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	804	-	56,73,73	1.62	6 (10%)	55,113,113	1.44	6 (10%)
14	CLA	A	826	-	56,73,73	1.59	5 (8%)	55,113,113	1.55	11 (20%)
14	CLA	B	3011	2	56,73,73	1.58	4 (7%)	55,113,113	1.53	11 (20%)
14	CLA	B	3026	23	37,54,73	1.97	7 (18%)	32,90,113	1.96	8 (25%)
14	CLA	A	842	23	42,59,73	1.76	7 (16%)	38,96,113	2.00	10 (26%)
14	CLA	B	3039	-	56,73,73	1.65	6 (10%)	55,113,113	1.56	9 (16%)
14	CLA	A	834	-	56,73,73	1.66	7 (12%)	55,113,113	1.56	8 (14%)
14	CLA	A	819	-	45,62,73	1.75	7 (15%)	41,99,113	1.90	10 (24%)
14	CLA	A	840	-	38,55,73	2.04	6 (15%)	33,91,113	1.99	10 (30%)
19	SF4	B	3001	1,2	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	825	-	1/1/18/20	13/30/108/115	-
14	CLA	A	816	-	1/1/15/20	4/11/91/115	-
14	CLA	B	3036	23	1/1/15/20	4/11/91/115	-
14	CLA	K	101	-	1/1/13/20	2/5/81/115	-
16	BCR	B	3047	-	-	15/29/63/63	0/2/2/2
14	CLA	K	103	-	1/1/15/20	5/11/91/115	-
14	CLA	A	839	-	1/1/20/20	9/37/115/115	-
14	CLA	B	3035	-	1/1/15/20	4/11/91/115	-
14	CLA	L	206	23	1/1/20/20	7/37/115/115	-
19	SF4	C	102	3	-	-	0/6/5/5
14	CLA	A	820	-	1/1/20/20	20/37/115/115	-
16	BCR	L	208	-	-	15/29/63/63	0/2/2/2
14	CLA	A	808	-	1/1/17/20	10/21/99/115	-
15	PQN	A	846	-	-	10/23/43/43	0/2/2/2
14	CLA	A	856	23	1/1/20/20	16/37/115/115	-
14	CLA	B	3033	-	1/1/20/20	18/37/115/115	-
14	CLA	B	3007	-	1/1/20/20	10/37/115/115	-
17	LMG	A	852	-	-	27/43/63/70	0/1/1/1
14	CLA	A	818	-	1/1/17/20	5/24/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	F	203	-	-	11/29/63/63	0/2/2/2
14	CLA	B	3030	-	1/1/20/20	15/37/115/115	-
16	BCR	L	201	-	-	8/29/63/63	0/2/2/2
14	CLA	B	3013	-	1/1/15/20	3/11/91/115	-
16	BCR	L	209	-	-	10/29/63/63	0/2/2/2
14	CLA	A	813	-	1/1/17/20	7/24/102/115	-
16	BCR	B	3045	-	-	11/29/63/63	0/2/2/2
14	CLA	B	3017	-	1/1/18/20	4/25/103/115	-
14	CLA	B	3023	23	1/1/18/20	9/25/103/115	-
14	CLA	B	3028	-	1/1/20/20	13/37/115/115	-
14	CLA	B	3020	23	1/1/20/20	14/37/115/115	-
17	LMG	I	102	-	-	11/35/55/70	0/1/1/1
14	CLA	A	810	1	1/1/20/20	10/37/115/115	-
18	LHG	A	853	-	-	27/53/53/53	-
14	CLA	B	3041	23	1/1/20/20	11/37/115/115	-
14	CLA	B	3022	-	1/1/15/20	8/11/91/115	-
16	BCR	A	850	-	-	11/29/63/63	0/2/2/2
14	CLA	A	806	-	1/1/20/20	21/37/115/115	-
16	BCR	M	103	-	-	7/29/63/63	0/2/2/2
14	CLA	A	827	23	1/1/20/20	10/37/115/115	-
14	CLA	A	830	-	1/1/20/20	15/37/115/115	-
14	CLA	B	3027	-	1/1/20/20	16/37/115/115	-
16	BCR	B	3044	-	-	8/29/63/63	0/2/2/2
16	BCR	B	3051	-	-	12/29/63/63	0/2/2/2
14	CLA	A	812	14	1/1/20/20	11/37/115/115	-
14	CLA	A	824	-	1/1/17/20	6/21/99/115	-
14	CLA	B	3034	-	1/1/18/20	11/29/107/115	-
14	CLA	B	3038	-	-	6/31/109/115	-
14	CLA	B	3008	-	1/1/20/20	5/37/115/115	-
16	BCR	J	105	-	-	12/29/63/63	0/2/2/2
14	CLA	J	102	-	1/1/12/20	0/2/76/115	-
14	CLA	A	811	-	1/1/15/20	9/11/91/115	-
14	CLA	A	822	23	1/1/20/20	15/37/115/115	-
14	CLA	B	3004	-	1/1/20/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	3015	-	1/1/20/20	13/37/115/115	-
14	CLA	A	817	23	1/1/16/20	8/18/96/115	-
14	CLA	B	3032	-	1/1/16/20	9/18/96/115	-
14	CLA	A	814	-	1/1/19/20	6/31/109/115	-
15	PQN	B	3043	-	-	8/23/43/43	0/2/2/2
14	CLA	A	844	23	1/1/20/20	13/37/115/115	-
14	CLA	A	835	-	1/1/20/20	14/37/115/115	-
14	CLA	B	3031	-	1/1/15/20	4/11/91/115	-
22	DGD	L	207	-	-	22/55/95/95	0/2/2/2
17	LMG	A	855	-	-	15/23/43/70	0/1/1/1
18	LHG	B	3050	-	-	11/26/26/53	-
14	CLA	B	3010	2	1/1/20/20	11/37/115/115	-
14	CLA	B	3042	-	1/1/20/20	7/37/115/115	-
18	LHG	A	854	14	-	14/31/31/53	-
16	BCR	J	104	-	-	15/29/63/63	0/2/2/2
14	CLA	B	3006	-	1/1/20/20	16/37/115/115	-
16	BCR	F	201	-	-	7/29/63/63	0/2/2/2
16	BCR	A	847	-	-	16/29/63/63	0/2/2/2
14	CLA	A	837	1	1/1/15/20	7/11/91/115	-
16	BCR	J	103	-	-	14/29/63/63	0/2/2/2
14	CLA	B	3019	-	1/1/19/20	11/31/109/115	-
14	CLA	A	843	-	1/1/20/20	7/37/115/115	-
14	CLA	B	3018	-	1/1/18/20	11/30/108/115	-
14	CLA	A	841	-	1/1/20/20	6/37/115/115	-
16	BCR	K	102	-	-	12/29/63/63	0/2/2/2
14	CLA	A	828	-	1/1/20/20	8/37/115/115	-
18	LHG	M	101	-	-	26/53/53/53	-
14	CLA	B	3037	23	1/1/15/20	2/11/91/115	-
14	CLA	A	815	-	1/1/15/20	0/11/91/115	-
14	CLA	B	3029	-	1/1/20/20	21/37/115/115	-
14	CLA	B	3014	-	1/1/20/20	12/37/115/115	-
14	CLA	A	807	-	1/1/20/20	15/37/115/115	-
16	BCR	A	848	-	-	7/29/63/63	0/2/2/2
14	CLA	B	3003	-	1/1/20/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	802	23	1/1/20/20	10/37/115/115	-
13	CL0	A	801	-	3/3/25/25	11/37/135/135	-
14	CLA	A	803	-	1/1/20/20	8/37/115/115	-
14	CLA	A	831	-	1/1/20/20	10/37/115/115	-
14	CLA	X	1701	12	1/1/15/20	1/11/91/115	-
14	CLA	B	3021	-	1/1/15/20	13/16/94/115	-
14	CLA	A	805	14	1/1/18/20	5/30/108/115	-
14	CLA	A	829	-	1/1/20/20	13/37/115/115	-
19	SF4	C	101	3	-	-	0/6/5/5
14	CLA	B	3012	-	1/1/15/20	5/11/91/115	-
14	CLA	B	3040	-	-	5/16/94/115	-
14	CLA	L	204	10	1/1/20/20	11/37/115/115	-
14	CLA	A	838	-	1/1/17/20	5/21/99/115	-
14	CLA	A	821	-	1/1/14/20	4/8/86/115	-
14	CLA	B	3016	-	1/1/15/20	7/11/91/115	-
21	LMT	L	202	-	-	12/21/61/61	0/2/2/2
14	CLA	A	836	-	1/1/17/20	11/24/102/115	-
14	CLA	A	845	18	1/1/17/20	9/22/100/115	-
16	BCR	B	3046	-	-	11/29/63/63	0/2/2/2
14	CLA	B	3005	-	1/1/17/20	8/24/102/115	-
14	CLA	J	101	8	1/1/15/20	4/11/91/115	-
16	BCR	A	849	-	-	12/29/63/63	0/2/2/2
14	CLA	B	3009	-	1/1/20/20	11/37/115/115	-
16	BCR	B	3048	-	-	4/29/63/63	0/2/2/2
14	CLA	B	3024	-	1/1/15/20	4/11/91/115	-
14	CLA	F	202	23	1/1/15/20	2/11/91/115	-
14	CLA	L	205	-	1/1/20/20	3/37/115/115	-
17	LMG	B	3049	-	-	23/50/70/70	0/1/1/1
16	BCR	A	851	-	-	17/29/63/63	0/2/2/2
14	CLA	A	833	-	1/1/20/20	9/37/115/115	-
14	CLA	B	3025	2	-	7/24/102/115	-
16	BCR	I	101	-	-	4/29/63/63	0/2/2/2
14	CLA	M	102	23	1/1/15/20	5/11/91/115	-
14	CLA	A	823	-	1/1/16/20	12/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	809	1	1/1/20/20	19/37/115/115	-
14	CLA	A	832	-	1/1/17/20	6/19/97/115	-
14	CLA	A	804	-	1/1/20/20	8/37/115/115	-
14	CLA	A	826	-	1/1/20/20	15/37/115/115	-
14	CLA	B	3011	2	1/1/20/20	17/37/115/115	-
14	CLA	B	3026	23	1/1/15/20	2/15/93/115	-
14	CLA	A	842	23	1/1/17/20	7/21/99/115	-
14	CLA	B	3039	-	1/1/20/20	9/37/115/115	-
14	CLA	A	834	-	1/1/20/20	8/37/115/115	-
14	CLA	A	819	-	1/1/17/20	6/24/102/115	-
14	CLA	A	840	-	1/1/15/20	5/16/94/115	-
19	SF4	B	3001	1,2	-	-	0/6/5/5

All (635) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3041	CLA	C4B-NB	8.54	1.42	1.35
14	B	3037	CLA	C4B-NB	8.31	1.42	1.35
14	A	828	CLA	C4B-NB	8.31	1.42	1.35
14	A	843	CLA	C4B-NB	8.28	1.42	1.35
14	A	817	CLA	C4B-NB	8.25	1.42	1.35
14	A	805	CLA	C4B-NB	8.24	1.42	1.35
14	A	840	CLA	C4B-NB	8.22	1.42	1.35
14	B	3013	CLA	C4B-NB	8.17	1.42	1.35
14	B	3030	CLA	C4B-NB	8.13	1.42	1.35
14	B	3036	CLA	C4B-NB	8.11	1.42	1.35
14	B	3031	CLA	C4B-NB	8.10	1.42	1.35
14	B	3026	CLA	C4B-NB	8.08	1.42	1.35
14	A	807	CLA	C4B-NB	8.05	1.42	1.35
14	B	3040	CLA	C4B-NB	8.04	1.42	1.35
14	B	3042	CLA	C4B-NB	8.02	1.42	1.35
14	A	834	CLA	C4B-NB	8.02	1.42	1.35
14	A	812	CLA	C4B-NB	8.02	1.42	1.35
14	A	808	CLA	C4B-NB	8.01	1.42	1.35
14	B	3035	CLA	C4B-NB	7.99	1.42	1.35
14	B	3039	CLA	C4B-NB	7.99	1.42	1.35
14	B	3027	CLA	C4B-NB	7.95	1.42	1.35
14	A	809	CLA	C4B-NB	7.95	1.42	1.35
14	J	101	CLA	C4B-NB	7.94	1.42	1.35
13	A	801	CL0	C4B-NB	7.93	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	804	CLA	C4B-NB	7.93	1.42	1.35
14	A	837	CLA	C4B-NB	7.92	1.42	1.35
14	B	3029	CLA	C4B-NB	7.92	1.42	1.35
14	X	1701	CLA	C4B-NB	7.89	1.42	1.35
14	B	3003	CLA	C4B-NB	7.89	1.42	1.35
14	B	3033	CLA	C4B-NB	7.89	1.42	1.35
14	A	823	CLA	C4B-NB	7.87	1.42	1.35
14	A	818	CLA	C4B-NB	7.85	1.42	1.35
14	A	814	CLA	C4B-NB	7.83	1.42	1.35
14	B	3021	CLA	C4B-NB	7.81	1.42	1.35
14	B	3014	CLA	C4B-NB	7.80	1.42	1.35
14	B	3008	CLA	C4B-NB	7.80	1.42	1.35
14	A	803	CLA	C4B-NB	7.78	1.42	1.35
14	F	202	CLA	C4B-NB	7.78	1.42	1.35
14	A	802	CLA	C4B-NB	7.77	1.42	1.35
14	A	844	CLA	C4B-NB	7.76	1.42	1.35
14	B	3024	CLA	C4B-NB	7.74	1.42	1.35
14	J	102	CLA	C4B-NB	7.73	1.42	1.35
14	A	813	CLA	C4B-NB	7.72	1.42	1.35
14	A	827	CLA	C4B-NB	7.72	1.42	1.35
14	B	3018	CLA	C4B-NB	7.72	1.42	1.35
14	B	3012	CLA	C4B-NB	7.72	1.42	1.35
14	B	3015	CLA	C4B-NB	7.72	1.42	1.35
14	A	815	CLA	C4B-NB	7.71	1.42	1.35
14	B	3017	CLA	C4B-NB	7.69	1.42	1.35
14	B	3022	CLA	C4B-NB	7.68	1.42	1.35
14	B	3009	CLA	C4B-NB	7.67	1.42	1.35
14	A	821	CLA	C4B-NB	7.67	1.42	1.35
14	B	3025	CLA	C4B-NB	7.67	1.42	1.35
14	B	3019	CLA	C4B-NB	7.66	1.42	1.35
14	A	836	CLA	C4B-NB	7.64	1.42	1.35
14	A	830	CLA	C4B-NB	7.62	1.42	1.35
14	B	3010	CLA	C4B-NB	7.62	1.42	1.35
14	A	829	CLA	C4B-NB	7.60	1.42	1.35
14	M	102	CLA	C4B-NB	7.60	1.42	1.35
14	A	810	CLA	C4B-NB	7.58	1.42	1.35
14	B	3028	CLA	C4B-NB	7.57	1.42	1.35
14	A	856	CLA	C4B-NB	7.57	1.42	1.35
14	B	3038	CLA	C4B-NB	7.55	1.41	1.35
14	A	825	CLA	C4B-NB	7.55	1.41	1.35
14	B	3006	CLA	C4B-NB	7.54	1.41	1.35
14	K	101	CLA	C4B-NB	7.54	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	838	CLA	C4B-NB	7.54	1.41	1.35
14	A	806	CLA	C4B-NB	7.53	1.41	1.35
14	B	3032	CLA	C4B-NB	7.51	1.41	1.35
14	K	103	CLA	C4B-NB	7.48	1.41	1.35
14	A	824	CLA	C4B-NB	7.47	1.41	1.35
14	A	831	CLA	C4B-NB	7.42	1.41	1.35
14	A	820	CLA	C4B-NB	7.39	1.41	1.35
14	B	3004	CLA	C4B-NB	7.38	1.41	1.35
14	B	3007	CLA	C4B-NB	7.38	1.41	1.35
14	B	3023	CLA	C4B-NB	7.35	1.41	1.35
14	A	832	CLA	C4B-NB	7.34	1.41	1.35
14	B	3020	CLA	C4B-NB	7.34	1.41	1.35
14	A	841	CLA	C4B-NB	7.33	1.41	1.35
14	B	3011	CLA	C4B-NB	7.33	1.41	1.35
14	A	816	CLA	C4B-NB	7.32	1.41	1.35
14	B	3005	CLA	C4B-NB	7.32	1.41	1.35
14	A	826	CLA	C4B-NB	7.27	1.41	1.35
14	A	839	CLA	C4B-NB	7.27	1.41	1.35
14	A	822	CLA	C4B-NB	7.26	1.41	1.35
14	L	206	CLA	C4B-NB	7.26	1.41	1.35
14	B	3016	CLA	C4B-NB	7.24	1.41	1.35
14	L	204	CLA	C4B-NB	7.24	1.41	1.35
14	A	833	CLA	C4B-NB	7.23	1.41	1.35
14	A	842	CLA	C4B-NB	7.20	1.41	1.35
14	A	811	CLA	C4B-NB	7.17	1.41	1.35
14	A	845	CLA	C4B-NB	7.16	1.41	1.35
14	A	835	CLA	C4B-NB	7.14	1.41	1.35
14	A	819	CLA	C4B-NB	7.12	1.41	1.35
14	L	205	CLA	C4B-NB	7.04	1.41	1.35
14	B	3034	CLA	C4B-NB	6.98	1.41	1.35
14	M	102	CLA	C4C-NC	6.44	1.41	1.35
14	B	3041	CLA	C4C-NC	6.36	1.40	1.35
14	A	814	CLA	C4C-NC	6.17	1.40	1.35
14	A	810	CLA	C4C-NC	6.13	1.40	1.35
14	B	3036	CLA	C4C-NC	6.13	1.40	1.35
14	B	3014	CLA	C4C-NC	6.09	1.40	1.35
14	A	808	CLA	C4C-NC	6.08	1.40	1.35
14	K	103	CLA	C4C-NC	6.06	1.40	1.35
14	A	827	CLA	C4C-NC	6.01	1.40	1.35
14	B	3015	CLA	C4C-NC	5.99	1.40	1.35
14	A	818	CLA	C4C-NC	5.97	1.40	1.35
15	B	3043	PQN	O1-C1	5.95	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3024	CLA	C4C-NC	5.94	1.40	1.35
14	A	835	CLA	C4C-NC	5.93	1.40	1.35
14	A	828	CLA	C4C-NC	5.92	1.40	1.35
14	L	206	CLA	C4C-NC	5.92	1.40	1.35
15	A	846	PQN	O1-C1	5.89	1.35	1.23
14	A	840	CLA	C4C-NC	5.88	1.40	1.35
14	B	3008	CLA	C4C-NC	5.87	1.40	1.35
14	J	102	CLA	C4C-NC	5.87	1.40	1.35
14	A	843	CLA	C4C-NC	5.87	1.40	1.35
15	A	846	PQN	O4-C4	5.86	1.35	1.23
14	A	826	CLA	C4C-NC	5.86	1.40	1.35
15	B	3043	PQN	O4-C4	5.85	1.35	1.23
14	B	3006	CLA	C4C-NC	5.83	1.40	1.35
14	B	3035	CLA	C4C-NC	5.82	1.40	1.35
14	A	844	CLA	C4C-NC	5.80	1.40	1.35
14	B	3034	CLA	C4C-NC	5.79	1.40	1.35
14	B	3031	CLA	C4C-NC	5.77	1.40	1.35
14	F	202	CLA	C4C-NC	5.74	1.40	1.35
14	A	809	CLA	C4C-NC	5.73	1.40	1.35
14	B	3017	CLA	C4C-NC	5.71	1.40	1.35
14	J	101	CLA	C4C-NC	5.70	1.40	1.35
14	B	3016	CLA	C4C-NC	5.69	1.40	1.35
14	B	3022	CLA	C4C-NC	5.69	1.40	1.35
14	A	825	CLA	C4C-NC	5.67	1.40	1.35
14	A	815	CLA	C4C-NC	5.65	1.40	1.35
15	B	3043	PQN	C10-C1	-5.65	1.37	1.48
14	A	830	CLA	C4C-NC	5.63	1.40	1.35
14	B	3011	CLA	C4C-NC	5.62	1.40	1.35
14	A	811	CLA	C4C-NC	5.62	1.40	1.35
14	B	3027	CLA	C4C-NC	5.62	1.40	1.35
14	A	804	CLA	C4C-NC	5.61	1.40	1.35
14	A	839	CLA	C4C-NC	5.61	1.40	1.35
14	B	3005	CLA	C4C-NC	5.60	1.40	1.35
14	B	3020	CLA	C4C-NC	5.58	1.40	1.35
14	B	3009	CLA	C4C-NC	5.57	1.40	1.35
14	B	3003	CLA	C4C-NC	5.57	1.40	1.35
14	A	834	CLA	C4C-NC	5.56	1.40	1.35
14	A	836	CLA	C4C-NC	5.55	1.40	1.35
14	A	831	CLA	C4C-NC	5.54	1.40	1.35
14	A	841	CLA	C4C-NC	5.54	1.40	1.35
14	A	820	CLA	C4C-NC	5.53	1.40	1.35
14	B	3023	CLA	C4C-NC	5.51	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	805	CLA	C4C-NC	5.51	1.40	1.35
14	A	845	CLA	C4C-NC	5.50	1.40	1.35
14	A	807	CLA	C4C-NC	5.50	1.40	1.35
14	B	3019	CLA	C4C-NC	5.49	1.40	1.35
14	A	832	CLA	C4C-NC	5.49	1.40	1.35
14	B	3007	CLA	C4C-NC	5.48	1.40	1.35
14	A	813	CLA	C4C-NC	5.47	1.40	1.35
14	A	838	CLA	C4C-NC	5.46	1.40	1.35
14	A	856	CLA	C4C-NC	5.43	1.40	1.35
14	A	802	CLA	C4C-NC	5.43	1.40	1.35
14	B	3029	CLA	C4C-NC	5.43	1.40	1.35
14	B	3021	CLA	C4C-NC	5.40	1.40	1.35
14	K	101	CLA	C4C-NC	5.38	1.40	1.35
14	B	3025	CLA	C4C-NC	5.38	1.40	1.35
14	A	819	CLA	C4C-NC	5.37	1.40	1.35
14	B	3004	CLA	C4C-NC	5.37	1.40	1.35
14	B	3032	CLA	C4C-NC	5.36	1.40	1.35
14	X	1701	CLA	C4C-NC	5.36	1.40	1.35
14	B	3039	CLA	C4C-NC	5.35	1.40	1.35
14	B	3040	CLA	C4C-NC	5.34	1.40	1.35
14	L	205	CLA	C4C-NC	5.33	1.40	1.35
14	A	803	CLA	C4C-NC	5.33	1.40	1.35
14	A	824	CLA	C4C-NC	5.31	1.39	1.35
14	B	3030	CLA	C4C-NC	5.29	1.39	1.35
14	B	3042	CLA	C4C-NC	5.29	1.39	1.35
14	A	822	CLA	C4C-NC	5.28	1.39	1.35
14	A	829	CLA	C4C-NC	5.26	1.39	1.35
14	B	3012	CLA	C4C-NC	5.26	1.39	1.35
14	B	3028	CLA	C4C-NC	5.26	1.39	1.35
14	B	3033	CLA	C4C-NC	5.25	1.39	1.35
14	A	816	CLA	C4C-NC	5.25	1.39	1.35
14	B	3018	CLA	C4C-NC	5.22	1.39	1.35
14	A	821	CLA	C4C-NC	5.22	1.39	1.35
14	A	837	CLA	C4C-NC	5.18	1.39	1.35
14	B	3038	CLA	C4C-NC	5.16	1.39	1.35
14	A	833	CLA	C4C-NC	5.16	1.39	1.35
14	B	3037	CLA	C4C-NC	5.15	1.39	1.35
14	A	823	CLA	C4C-NC	5.11	1.39	1.35
14	B	3013	CLA	C4C-NC	5.11	1.39	1.35
14	A	817	CLA	C4C-NC	5.10	1.39	1.35
14	B	3010	CLA	C4C-NC	5.10	1.39	1.35
14	A	842	CLA	C4C-NC	5.08	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	812	CLA	C4C-NC	5.02	1.39	1.35
14	B	3026	CLA	C4C-NC	4.98	1.39	1.35
14	L	204	CLA	C4C-NC	4.91	1.39	1.35
14	A	806	CLA	C4C-NC	4.58	1.39	1.35
17	A	855	LMG	O7-C8	-4.55	1.39	1.47
15	A	846	PQN	C10-C1	-4.20	1.40	1.48
15	B	3043	PQN	C5-C4	-4.10	1.40	1.48
17	I	102	LMG	C7-C8	4.05	1.63	1.50
16	L	209	BCR	C1-C6	-3.99	1.48	1.53
16	M	103	BCR	C1-C6	-3.92	1.48	1.53
17	I	102	LMG	O1-C1	3.89	1.46	1.40
16	B	3045	BCR	C1-C6	-3.88	1.48	1.53
18	B	3050	LHG	P-O6	3.88	1.75	1.59
16	J	104	BCR	C1-C6	-3.79	1.48	1.53
16	B	3051	BCR	C30-C25	-3.71	1.48	1.53
16	L	201	BCR	C1-C6	-3.70	1.48	1.53
15	A	846	PQN	C5-C4	-3.65	1.41	1.48
16	A	848	BCR	C1-C6	-3.58	1.48	1.53
16	A	849	BCR	C1-C6	-3.54	1.48	1.53
16	B	3046	BCR	C1-C6	-3.54	1.48	1.53
16	A	851	BCR	C1-C6	-3.53	1.48	1.53
16	A	847	BCR	C1-C6	-3.51	1.48	1.53
16	J	103	BCR	C1-C6	-3.40	1.49	1.53
16	J	105	BCR	C30-C25	-3.39	1.49	1.53
16	F	203	BCR	C1-C6	-3.35	1.49	1.53
13	A	801	CL0	CHC-C1C	3.35	1.43	1.35
16	B	3051	BCR	C1-C6	-3.35	1.49	1.53
16	K	102	BCR	C1-C6	-3.34	1.49	1.53
16	B	3044	BCR	C1-C6	-3.30	1.49	1.53
15	A	846	PQN	C3-C2	3.30	1.41	1.35
16	M	103	BCR	C30-C25	-3.29	1.49	1.53
16	F	201	BCR	C1-C6	-3.25	1.49	1.53
14	B	3010	CLA	CMB-C2B	-3.22	1.44	1.51
18	B	3050	LHG	C4-C5	3.20	1.60	1.50
16	B	3048	BCR	C1-C6	-3.20	1.49	1.53
16	B	3047	BCR	C30-C25	-3.17	1.49	1.53
16	J	104	BCR	C30-C25	-3.15	1.49	1.53
16	L	208	BCR	C1-C6	-3.14	1.49	1.53
16	J	105	BCR	C1-C6	-3.13	1.49	1.53
15	B	3043	PQN	C3-C2	3.13	1.40	1.35
16	L	208	BCR	C30-C25	-3.11	1.49	1.53
16	A	848	BCR	C30-C25	-3.07	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	835	CLA	C1D-C2D	3.06	1.49	1.42
16	A	847	BCR	C30-C25	-3.06	1.49	1.53
16	A	850	BCR	C1-C6	-3.03	1.49	1.53
16	F	203	BCR	C30-C25	-3.03	1.49	1.53
14	B	3041	CLA	C1D-C2D	3.03	1.49	1.42
16	F	201	BCR	C30-C25	-3.02	1.49	1.53
15	B	3043	PQN	C3-C4	-3.00	1.39	1.47
14	A	808	CLA	C1D-C2D	2.97	1.49	1.42
16	B	3047	BCR	C1-C6	-2.94	1.49	1.53
15	A	846	PQN	C3-C4	-2.92	1.39	1.47
16	I	101	BCR	C1-C6	-2.91	1.49	1.53
14	A	831	CLA	CMB-C2B	-2.91	1.45	1.51
14	B	3035	CLA	C1D-C2D	2.89	1.49	1.42
17	A	852	LMG	C7-C8	2.89	1.59	1.50
14	B	3024	CLA	C1D-C2D	2.88	1.49	1.42
14	B	3016	CLA	C1D-C2D	2.87	1.49	1.42
14	X	1701	CLA	C1D-C2D	2.86	1.49	1.42
18	B	3050	LHG	C6-C5	2.86	1.59	1.50
14	J	102	CLA	C1D-C2D	2.85	1.49	1.42
14	B	3010	CLA	C3B-C2B	-2.85	1.36	1.40
14	A	834	CLA	C1D-C2D	2.83	1.49	1.42
16	L	209	BCR	C30-C25	-2.81	1.49	1.53
14	L	205	CLA	C1D-C2D	2.81	1.48	1.42
14	A	802	CLA	C1D-C2D	2.81	1.48	1.42
14	L	206	CLA	C1D-C2D	2.80	1.48	1.42
17	A	855	LMG	C7-C8	2.80	1.57	1.50
14	A	807	CLA	C1D-C2D	2.80	1.48	1.42
14	B	3015	CLA	C1D-C2D	2.80	1.48	1.42
14	A	841	CLA	C1D-C2D	2.79	1.48	1.42
16	K	102	BCR	C30-C25	-2.79	1.49	1.53
16	L	201	BCR	C30-C25	-2.79	1.49	1.53
16	B	3048	BCR	C30-C25	-2.78	1.49	1.53
14	A	822	CLA	C1D-C2D	2.78	1.48	1.42
14	A	826	CLA	C1D-C2D	2.77	1.48	1.42
14	B	3039	CLA	C1D-C2D	2.77	1.48	1.42
15	B	3043	PQN	C2-C1	-2.77	1.42	1.48
14	A	818	CLA	C1D-C2D	2.77	1.48	1.42
14	A	814	CLA	C1D-C2D	2.76	1.48	1.42
16	I	101	BCR	C30-C25	-2.75	1.50	1.53
14	A	821	CLA	C1D-C2D	2.74	1.48	1.42
14	A	823	CLA	C1D-C2D	2.74	1.48	1.42
14	B	3026	CLA	CMB-C2B	-2.74	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3034	CLA	C1D-C2D	2.71	1.48	1.42
18	A	854	LHG	P-O6	2.71	1.70	1.59
14	B	3006	CLA	C1D-C2D	2.71	1.48	1.42
14	A	816	CLA	C1D-C2D	2.70	1.48	1.42
14	B	3011	CLA	C1D-C2D	2.70	1.48	1.42
14	F	202	CLA	CMB-C2B	-2.69	1.46	1.51
14	A	810	CLA	C1D-C2D	2.69	1.48	1.42
16	A	850	BCR	C30-C25	-2.69	1.50	1.53
14	L	204	CLA	CMB-C2B	-2.69	1.46	1.51
13	A	801	CL0	C1D-C2D	2.69	1.48	1.42
14	A	836	CLA	C1D-C2D	2.69	1.48	1.42
16	B	3046	BCR	C30-C25	-2.68	1.50	1.53
14	A	819	CLA	CMB-C2B	-2.68	1.46	1.51
14	A	825	CLA	C1D-C2D	2.68	1.48	1.42
21	L	202	LMT	O3B-C3B	-2.68	1.36	1.43
14	A	824	CLA	C1D-C2D	2.68	1.48	1.42
14	B	3032	CLA	C1D-C2D	2.67	1.48	1.42
15	A	846	PQN	C2-C1	-2.67	1.42	1.48
14	B	3037	CLA	CMB-C2B	-2.67	1.46	1.51
14	B	3003	CLA	CMB-C2B	-2.67	1.46	1.51
14	K	103	CLA	C1D-C2D	2.66	1.48	1.42
14	A	812	CLA	C1D-C2D	2.65	1.48	1.42
14	J	101	CLA	C1D-C2D	2.65	1.48	1.42
14	B	3021	CLA	C1D-C2D	2.64	1.48	1.42
14	A	811	CLA	C1D-C2D	2.64	1.48	1.42
14	B	3012	CLA	C1D-C2D	2.64	1.48	1.42
14	M	102	CLA	C1D-C2D	2.64	1.48	1.42
14	B	3007	CLA	CMB-C2B	-2.63	1.46	1.51
14	A	840	CLA	C1D-C2D	2.63	1.48	1.42
14	A	806	CLA	C1D-C2D	2.62	1.48	1.42
14	A	815	CLA	C1D-C2D	2.62	1.48	1.42
14	A	836	CLA	CMB-C2B	-2.62	1.46	1.51
14	F	202	CLA	C1D-C2D	2.62	1.48	1.42
16	A	851	BCR	C30-C25	-2.62	1.50	1.53
14	M	102	CLA	CMB-C2B	-2.62	1.46	1.51
14	A	832	CLA	C1D-C2D	2.61	1.48	1.42
14	A	844	CLA	CMB-C2B	-2.60	1.46	1.51
14	A	803	CLA	C1D-C2D	2.60	1.48	1.42
14	B	3031	CLA	CMB-C2B	-2.60	1.46	1.51
14	B	3017	CLA	C1D-C2D	2.59	1.48	1.42
14	A	839	CLA	C1D-C2D	2.57	1.48	1.42
14	A	845	CLA	C1D-C2D	2.56	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3008	CLA	C1D-C2D	2.55	1.48	1.42
14	B	3004	CLA	CMB-C2B	-2.55	1.46	1.51
14	B	3031	CLA	C1D-C2D	2.55	1.48	1.42
17	I	102	LMG	C4-C5	2.55	1.58	1.53
14	A	829	CLA	C1D-C2D	2.55	1.48	1.42
16	J	103	BCR	C30-C25	-2.55	1.50	1.53
14	B	3020	CLA	CMB-C2B	-2.54	1.46	1.51
14	A	817	CLA	CMB-C2B	-2.54	1.46	1.51
14	B	3038	CLA	CMB-C2B	-2.53	1.46	1.51
14	B	3039	CLA	CMB-C2B	-2.53	1.46	1.51
14	A	820	CLA	C1D-C2D	2.53	1.48	1.42
14	B	3023	CLA	C1D-C2D	2.53	1.48	1.42
14	B	3041	CLA	C1B-NB	2.53	1.37	1.35
14	B	3033	CLA	C1D-C2D	2.53	1.48	1.42
14	A	833	CLA	C1D-C2D	2.52	1.48	1.42
14	B	3013	CLA	C1D-C2D	2.52	1.48	1.42
14	B	3029	CLA	C1D-C2D	2.52	1.48	1.42
14	A	815	CLA	CMB-C2B	-2.52	1.46	1.51
14	B	3010	CLA	C1D-C2D	2.51	1.48	1.42
14	B	3038	CLA	C1D-C2D	2.51	1.48	1.42
22	L	207	DGD	O2G-C2G	-2.51	1.40	1.46
16	B	3044	BCR	C30-C25	-2.51	1.50	1.53
14	A	823	CLA	CMB-C2B	-2.51	1.46	1.51
14	B	3037	CLA	C1D-C2D	2.51	1.48	1.42
14	B	3014	CLA	C1D-C2D	2.51	1.48	1.42
14	B	3042	CLA	CMB-C2B	-2.50	1.46	1.51
14	B	3027	CLA	C1D-C2D	2.50	1.48	1.42
14	A	805	CLA	C1D-C2D	2.50	1.48	1.42
14	A	803	CLA	CMB-C2B	-2.50	1.46	1.51
13	A	801	CL0	CMB-C2B	-2.50	1.46	1.51
14	B	3042	CLA	C1D-C2D	2.49	1.48	1.42
14	A	812	CLA	CMB-C2B	-2.49	1.46	1.51
14	B	3036	CLA	C1D-C2D	2.49	1.48	1.42
14	B	3019	CLA	C1D-C2D	2.49	1.48	1.42
14	B	3031	CLA	C3B-C2B	-2.48	1.36	1.40
14	B	3004	CLA	C1D-C2D	2.48	1.48	1.42
14	A	806	CLA	CMB-C2B	-2.48	1.46	1.51
14	A	809	CLA	C1D-C2D	2.48	1.48	1.42
14	B	3020	CLA	C1D-C2D	2.48	1.48	1.42
14	B	3023	CLA	CMB-C2B	-2.47	1.46	1.51
14	B	3009	CLA	CMB-C2B	-2.47	1.46	1.51
14	L	205	CLA	CMB-C2B	-2.47	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3030	CLA	CMB-C2B	-2.47	1.46	1.51
14	A	821	CLA	CMB-C2B	-2.47	1.46	1.51
14	B	3005	CLA	CMB-C2B	-2.47	1.46	1.51
14	A	843	CLA	CMB-C2B	-2.47	1.46	1.51
14	A	816	CLA	CMB-C2B	-2.46	1.46	1.51
18	M	101	LHG	P-O6	2.46	1.69	1.59
14	A	804	CLA	CMC-C2C	-2.46	1.45	1.51
14	A	844	CLA	C1D-C2D	2.46	1.48	1.42
14	A	819	CLA	CMC-C2C	-2.46	1.45	1.51
14	B	3021	CLA	CMB-C2B	-2.46	1.46	1.51
14	B	3005	CLA	C1D-C2D	2.46	1.48	1.42
14	L	204	CLA	C1D-C2D	2.46	1.48	1.42
14	A	844	CLA	CMD-C2D	-2.45	1.45	1.51
14	B	3003	CLA	C1D-C2D	2.45	1.48	1.42
14	A	827	CLA	C1D-C2D	2.45	1.48	1.42
14	A	819	CLA	C1D-C2D	2.45	1.48	1.42
14	X	1701	CLA	CMB-C2B	-2.45	1.46	1.51
14	A	817	CLA	C1D-C2D	2.45	1.48	1.42
14	A	838	CLA	CMB-C2B	-2.45	1.46	1.51
14	A	826	CLA	CMB-C2B	-2.45	1.46	1.51
14	B	3019	CLA	CMB-C2B	-2.45	1.46	1.51
14	B	3030	CLA	C1D-C2D	2.44	1.48	1.42
14	A	840	CLA	CMB-C2B	-2.44	1.46	1.51
14	B	3013	CLA	CMB-C2B	-2.44	1.46	1.51
14	B	3022	CLA	CMB-C2B	-2.44	1.46	1.51
14	B	3040	CLA	CMB-C2B	-2.44	1.46	1.51
14	A	805	CLA	CMB-C2B	-2.43	1.46	1.51
14	B	3040	CLA	C1D-C2D	2.43	1.48	1.42
14	B	3012	CLA	CMB-C2B	-2.43	1.46	1.51
14	A	808	CLA	CMB-C2B	-2.43	1.46	1.51
14	A	830	CLA	CMB-C2B	-2.43	1.46	1.51
14	B	3041	CLA	CMB-C2B	-2.43	1.46	1.51
14	K	101	CLA	C1D-C2D	2.42	1.48	1.42
14	K	101	CLA	CMB-C2B	-2.42	1.46	1.51
14	A	856	CLA	CMB-C2B	-2.42	1.46	1.51
14	A	833	CLA	CMB-C2B	-2.42	1.46	1.51
17	A	855	LMG	O1-C1	2.42	1.44	1.40
14	A	842	CLA	CMB-C2B	-2.41	1.46	1.51
14	B	3027	CLA	CMB-C2B	-2.41	1.46	1.51
16	A	849	BCR	C30-C25	-2.41	1.50	1.53
14	A	828	CLA	C1D-C2D	2.41	1.48	1.42
14	A	830	CLA	C1D-C2D	2.41	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3035	CLA	CMB-C2B	-2.41	1.46	1.51
14	B	3023	CLA	CMD-C2D	-2.40	1.45	1.51
14	B	3034	CLA	CMB-C2B	-2.40	1.46	1.51
14	A	813	CLA	CMB-C2B	-2.40	1.46	1.51
14	B	3025	CLA	CMB-C2B	-2.40	1.46	1.51
16	F	203	BCR	C33-C5	-2.40	1.47	1.50
14	A	813	CLA	CMD-C2D	-2.39	1.45	1.51
14	A	811	CLA	CMB-C2B	-2.39	1.46	1.51
14	A	837	CLA	CMB-C2B	-2.39	1.46	1.51
17	B	3049	LMG	O8-C9	-2.39	1.39	1.45
14	B	3022	CLA	C1D-C2D	2.39	1.48	1.42
14	A	825	CLA	CMB-C2B	-2.39	1.46	1.51
16	B	3047	BCR	C33-C5	-2.39	1.47	1.50
14	A	843	CLA	C1D-C2D	2.39	1.48	1.42
14	J	102	CLA	CMB-C2B	-2.38	1.46	1.51
14	A	810	CLA	CMB-C2B	-2.38	1.46	1.51
14	A	839	CLA	CMB-C2B	-2.38	1.46	1.51
14	B	3018	CLA	CMB-C2B	-2.38	1.46	1.51
16	B	3045	BCR	C33-C5	-2.38	1.47	1.50
14	A	845	CLA	CMB-C2B	-2.38	1.46	1.51
16	L	208	BCR	C33-C5	-2.38	1.47	1.50
14	A	822	CLA	CMB-C2B	-2.38	1.46	1.51
14	B	3016	CLA	CMB-C2B	-2.37	1.46	1.51
14	B	3032	CLA	CMB-C2B	-2.37	1.46	1.51
14	B	3008	CLA	CMB-C2B	-2.37	1.46	1.51
14	A	838	CLA	C1D-C2D	2.37	1.47	1.42
14	B	3007	CLA	C1D-C2D	2.37	1.47	1.42
21	L	202	LMT	O4'-C4B	-2.37	1.37	1.43
14	A	841	CLA	CMB-C2B	-2.37	1.46	1.51
14	B	3028	CLA	CMB-C2B	-2.37	1.46	1.51
14	B	3014	CLA	CMB-C2B	-2.36	1.46	1.51
14	B	3026	CLA	C1D-C2D	2.36	1.47	1.42
18	B	3050	LHG	O8-C6	2.36	1.50	1.45
14	B	3015	CLA	CMB-C2B	-2.36	1.46	1.51
14	M	102	CLA	CMD-C2D	-2.36	1.46	1.51
14	B	3024	CLA	CMB-C2B	-2.35	1.46	1.51
17	I	102	LMG	O1-C7	2.35	1.48	1.43
14	B	3028	CLA	C1D-C2D	2.35	1.47	1.42
14	A	804	CLA	CMB-C2B	-2.35	1.46	1.51
16	J	105	BCR	C33-C5	-2.34	1.47	1.50
14	A	807	CLA	CMB-C2B	-2.33	1.46	1.51
14	A	814	CLA	CMB-C2B	-2.33	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	819	CLA	C3B-CAB	-2.33	1.43	1.47
16	J	104	BCR	C33-C5	-2.32	1.47	1.50
14	A	804	CLA	C1D-C2D	2.32	1.47	1.42
17	I	102	LMG	O8-C28	2.32	1.40	1.33
14	A	837	CLA	C1D-C2D	2.32	1.47	1.42
14	B	3033	CLA	CMB-C2B	-2.30	1.46	1.51
14	B	3007	CLA	CMD-C2D	-2.30	1.46	1.51
14	A	802	CLA	CMB-C2B	-2.30	1.46	1.51
14	A	842	CLA	C1D-C2D	2.29	1.47	1.42
14	A	828	CLA	CMB-C2B	-2.29	1.46	1.51
14	B	3017	CLA	CMB-C2B	-2.29	1.46	1.51
14	B	3005	CLA	CMD-C2D	-2.28	1.46	1.51
16	A	847	BCR	C33-C5	-2.28	1.47	1.50
14	A	809	CLA	CMB-C2B	-2.28	1.46	1.51
16	B	3045	BCR	C30-C25	-2.28	1.50	1.53
14	B	3018	CLA	C1D-C2D	2.28	1.47	1.42
14	L	206	CLA	CMB-C2B	-2.28	1.46	1.51
21	L	202	LMT	O2B-C2B	-2.28	1.37	1.43
16	A	849	BCR	C33-C5	-2.28	1.47	1.50
14	A	827	CLA	CMD-C2D	-2.27	1.46	1.51
21	L	202	LMT	O2'-C2'	-2.27	1.37	1.43
14	B	3004	CLA	CMD-C2D	-2.27	1.46	1.51
14	B	3006	CLA	CMB-C2B	-2.27	1.46	1.51
14	B	3032	CLA	O2D-CGD	2.27	1.38	1.33
14	B	3009	CLA	C1D-C2D	2.26	1.47	1.42
14	A	831	CLA	C1D-C2D	2.26	1.47	1.42
14	A	832	CLA	CMB-C2B	-2.26	1.46	1.51
14	B	3025	CLA	C1D-C2D	2.26	1.47	1.42
14	K	103	CLA	CMB-C2B	-2.25	1.47	1.51
14	A	803	CLA	CMD-C2D	-2.25	1.46	1.51
14	A	820	CLA	CMB-C2B	-2.25	1.47	1.51
14	A	834	CLA	CMB-C2B	-2.25	1.47	1.51
14	A	818	CLA	CMB-C2B	-2.25	1.47	1.51
22	L	207	DGD	O3G-C1D	2.24	1.44	1.40
16	B	3046	BCR	C33-C5	-2.24	1.47	1.50
14	A	843	CLA	CMD-C2D	-2.24	1.46	1.51
14	B	3036	CLA	CMB-C2B	-2.24	1.47	1.51
14	A	809	CLA	C1C-C2C	2.24	1.47	1.42
16	B	3044	BCR	C33-C5	-2.24	1.47	1.50
14	A	827	CLA	CMB-C2B	-2.23	1.47	1.51
14	B	3020	CLA	CMD-C2D	-2.23	1.46	1.51
14	B	3029	CLA	CMB-C2B	-2.23	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	J	101	CLA	CMB-C2B	-2.23	1.47	1.51
14	A	856	CLA	CMD-C2D	-2.23	1.46	1.51
14	B	3003	CLA	CMD-C2D	-2.23	1.46	1.51
14	A	824	CLA	CMB-C2B	-2.22	1.47	1.51
21	L	202	LMT	O3'-C3'	-2.22	1.37	1.43
14	B	3010	CLA	C3B-CAB	-2.21	1.43	1.47
14	B	3039	CLA	C3B-C2B	-2.21	1.37	1.40
16	F	201	BCR	C33-C5	-2.21	1.47	1.50
14	A	834	CLA	CAC-C3C	-2.21	1.46	1.52
16	A	848	BCR	C33-C5	-2.21	1.47	1.50
17	I	102	LMG	C9-C8	2.21	1.57	1.50
22	L	207	DGD	C3G-C2G	2.21	1.57	1.50
14	A	856	CLA	C1D-C2D	2.21	1.47	1.42
14	B	3021	CLA	CMD-C2D	-2.20	1.46	1.51
16	L	209	BCR	C33-C5	-2.20	1.47	1.50
14	B	3042	CLA	C3B-C2B	-2.19	1.37	1.40
14	B	3010	CLA	CMD-C2D	-2.19	1.46	1.51
16	B	3051	BCR	C33-C5	-2.18	1.47	1.50
14	A	832	CLA	CMC-C2C	-2.18	1.46	1.51
14	B	3008	CLA	CMD-C2D	-2.18	1.46	1.51
13	A	801	CL0	CMD-C2D	-2.17	1.46	1.51
14	B	3028	CLA	CMC-C2C	-2.17	1.46	1.51
14	A	811	CLA	CMD-C2D	-2.16	1.46	1.51
14	B	3028	CLA	CAC-C3C	-2.16	1.46	1.52
14	A	828	CLA	C1C-C2C	2.16	1.47	1.42
14	A	833	CLA	CMC-C2C	-2.16	1.46	1.51
14	A	815	CLA	CMD-C2D	-2.16	1.46	1.51
14	B	3020	CLA	CMC-C2C	-2.16	1.46	1.51
16	B	3048	BCR	C33-C5	-2.15	1.47	1.50
16	M	103	BCR	C33-C5	-2.15	1.47	1.50
14	A	829	CLA	CMD-C2D	-2.15	1.46	1.51
14	A	838	CLA	C3B-CAB	-2.15	1.43	1.47
14	A	806	CLA	C3B-C2B	-2.15	1.37	1.40
16	K	102	BCR	C33-C5	-2.14	1.47	1.50
14	A	818	CLA	CMC-C2C	-2.14	1.46	1.51
14	B	3027	CLA	CMC-C2C	-2.14	1.46	1.51
14	A	834	CLA	CMC-C2C	-2.14	1.46	1.51
14	A	812	CLA	CAC-C3C	-2.14	1.46	1.52
16	J	103	BCR	C33-C5	-2.13	1.47	1.50
14	B	3026	CLA	CAC-C3C	-2.13	1.47	1.52
14	A	835	CLA	CMB-C2B	-2.13	1.47	1.51
14	A	819	CLA	CMD-C2D	-2.13	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	830	CLA	CMC-C2C	-2.13	1.46	1.51
14	B	3037	CLA	C3B-C2B	-2.13	1.37	1.40
14	B	3028	CLA	CMD-C2D	-2.13	1.46	1.51
14	A	834	CLA	CMD-C2D	-2.13	1.46	1.51
14	L	204	CLA	C3B-C2B	-2.13	1.37	1.40
14	B	3003	CLA	C3B-C2B	-2.12	1.37	1.40
14	B	3039	CLA	C3B-CAB	-2.12	1.43	1.47
14	B	3008	CLA	C3B-C2B	-2.12	1.37	1.40
14	B	3016	CLA	CMD-C2D	-2.12	1.46	1.51
16	A	850	BCR	C33-C5	-2.12	1.47	1.50
14	L	206	CLA	CMD-C2D	-2.12	1.46	1.51
16	A	851	BCR	C33-C5	-2.11	1.47	1.50
14	B	3022	CLA	CMD-C2D	-2.11	1.46	1.51
14	A	839	CLA	CMD-C2D	-2.11	1.46	1.51
14	A	820	CLA	CMC-C2C	-2.11	1.46	1.51
14	B	3005	CLA	CAC-C3C	-2.11	1.47	1.52
14	A	840	CLA	C3B-C2B	-2.11	1.37	1.40
14	A	829	CLA	CMB-C2B	-2.10	1.47	1.51
14	A	835	CLA	C3B-CAB	-2.10	1.43	1.47
17	A	855	LMG	C3-C2	2.10	1.57	1.52
14	A	817	CLA	CMD-C2D	-2.10	1.46	1.51
14	A	836	CLA	CMD-C2D	-2.10	1.46	1.51
14	A	816	CLA	O2D-CGD	2.10	1.38	1.33
14	B	3026	CLA	C3B-C2B	-2.09	1.37	1.40
14	B	3021	CLA	C1B-NB	2.09	1.37	1.35
14	B	3010	CLA	CMC-C2C	-2.09	1.46	1.51
16	L	201	BCR	C33-C5	-2.09	1.47	1.50
14	B	3030	CLA	C3B-C2B	-2.09	1.37	1.40
14	B	3008	CLA	CMC-C2C	-2.09	1.46	1.51
14	A	838	CLA	CMD-C2D	-2.09	1.46	1.51
14	A	813	CLA	CMC-C2C	-2.09	1.46	1.51
14	B	3030	CLA	CMD-C2D	-2.09	1.46	1.51
14	X	1701	CLA	CAC-C3C	-2.09	1.47	1.52
14	B	3038	CLA	CAC-C3C	-2.09	1.47	1.52
14	A	803	CLA	CAC-C3C	-2.08	1.47	1.52
14	A	823	CLA	CAC-C3C	-2.08	1.47	1.52
14	B	3033	CLA	CMD-C2D	-2.08	1.46	1.51
14	A	836	CLA	CMC-C2C	-2.08	1.46	1.51
14	B	3009	CLA	CMD-C2D	-2.08	1.46	1.51
14	A	805	CLA	CMD-C2D	-2.08	1.46	1.51
14	A	837	CLA	CMD-C2D	-2.08	1.46	1.51
14	A	845	CLA	C3B-C2B	-2.07	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3004	CLA	C3B-CAB	-2.07	1.43	1.47
14	L	204	CLA	CAC-C3C	-2.07	1.47	1.52
14	B	3014	CLA	CMC-C2C	-2.07	1.46	1.51
14	L	205	CLA	CMD-C2D	-2.07	1.46	1.51
14	M	102	CLA	C1A-CHA	-2.07	1.34	1.43
14	A	828	CLA	CMD-C2D	-2.07	1.46	1.51
18	A	853	LHG	O7-C5	-2.07	1.41	1.46
14	J	102	CLA	CMD-C2D	-2.06	1.46	1.51
14	A	833	CLA	CAC-C3C	-2.06	1.47	1.52
14	A	809	CLA	CMD-C2D	-2.06	1.46	1.51
14	A	833	CLA	CMD-C2D	-2.06	1.46	1.51
14	A	840	CLA	CMD-C2D	-2.06	1.46	1.51
14	A	818	CLA	C1C-C2C	2.06	1.47	1.42
14	A	842	CLA	CMC-C2C	-2.06	1.46	1.51
14	A	812	CLA	CMC-C2C	-2.06	1.46	1.51
14	A	813	CLA	C1D-C2D	2.06	1.47	1.42
14	A	829	CLA	CAC-C3C	-2.06	1.47	1.52
14	B	3026	CLA	CMD-C2D	-2.05	1.46	1.51
14	B	3041	CLA	CMD-C2D	-2.05	1.46	1.51
14	A	806	CLA	CMD-C2D	-2.05	1.46	1.51
14	A	824	CLA	CMC-C2C	-2.05	1.46	1.51
18	A	853	LHG	P-O6	2.05	1.67	1.59
14	A	802	CLA	CAC-C3C	-2.05	1.47	1.52
14	A	842	CLA	CMD-C2D	-2.05	1.46	1.51
14	B	3038	CLA	CMC-C2C	-2.04	1.46	1.51
14	X	1701	CLA	CMD-C2D	-2.04	1.46	1.51
14	B	3006	CLA	CMD-C2D	-2.04	1.46	1.51
14	B	3013	CLA	C1C-C2C	2.04	1.47	1.42
14	B	3012	CLA	CMD-C2D	-2.04	1.46	1.51
14	K	103	CLA	CMD-C2D	-2.04	1.46	1.51
14	A	841	CLA	CAC-C3C	-2.04	1.47	1.52
14	A	812	CLA	O2D-CGD	2.04	1.38	1.33
14	B	3036	CLA	CMD-C2D	-2.04	1.46	1.51
14	A	831	CLA	CMD-C2D	-2.04	1.46	1.51
14	A	831	CLA	C3B-C2B	-2.04	1.37	1.40
14	A	802	CLA	CMD-C2D	-2.03	1.46	1.51
14	A	810	CLA	CMD-C2D	-2.03	1.46	1.51
14	A	812	CLA	CMD-C2D	-2.03	1.46	1.51
14	B	3023	CLA	CMC-C2C	-2.03	1.46	1.51
14	B	3042	CLA	CAC-C3C	-2.03	1.47	1.52
14	B	3011	CLA	CMC-C2C	-2.03	1.46	1.51
14	B	3009	CLA	C3B-C2B	-2.03	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	842	CLA	CAC-C3C	-2.03	1.47	1.52
14	A	826	CLA	CMD-C2D	-2.03	1.46	1.51
14	A	804	CLA	CMD-C2D	-2.03	1.46	1.51
14	B	3018	CLA	CMD-C2D	-2.03	1.46	1.51
17	A	852	LMG	O1-C1	2.02	1.43	1.40
14	B	3041	CLA	C3B-C2B	-2.02	1.37	1.40
14	A	832	CLA	CMD-C2D	-2.02	1.46	1.51
14	B	3037	CLA	C1C-C2C	2.02	1.47	1.42
14	B	3015	CLA	CMD-C2D	-2.02	1.46	1.51
14	B	3035	CLA	CMD-C2D	-2.02	1.46	1.51
14	B	3007	CLA	CAC-C3C	-2.01	1.47	1.52
14	A	814	CLA	CMD-C2D	-2.01	1.46	1.51
14	A	837	CLA	C1C-C2C	2.01	1.47	1.42
14	B	3003	CLA	CMC-C2C	-2.01	1.46	1.51
14	B	3030	CLA	CMC-C2C	-2.01	1.46	1.51
18	B	3050	LHG	P-O3	2.01	1.67	1.59
14	B	3006	CLA	CMC-C2C	-2.01	1.46	1.51
14	B	3004	CLA	C3B-C2B	-2.00	1.37	1.40
14	A	828	CLA	CMC-C2C	-2.00	1.46	1.51
14	B	3013	CLA	CMD-C2D	-2.00	1.46	1.51
14	L	204	CLA	CMC-C2C	-2.00	1.46	1.51
14	A	827	CLA	CMC-C2C	-2.00	1.46	1.51
14	B	3027	CLA	CMD-C2D	-2.00	1.46	1.51

All (1062) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	842	CLA	C4A-NA-C1A	8.06	110.33	106.71
14	A	806	CLA	C4A-NA-C1A	7.97	110.29	106.71
14	B	3042	CLA	C4A-NA-C1A	7.78	110.20	106.71
14	B	3033	CLA	C4A-NA-C1A	7.66	110.15	106.71
14	A	803	CLA	C4A-NA-C1A	7.63	110.14	106.71
14	B	3005	CLA	C4A-NA-C1A	7.50	110.08	106.71
14	B	3028	CLA	C4A-NA-C1A	7.42	110.04	106.71
14	B	3003	CLA	C4A-NA-C1A	7.34	110.01	106.71
14	A	812	CLA	C4A-NA-C1A	7.15	109.92	106.71
14	B	3031	CLA	C4A-NA-C1A	7.14	109.92	106.71
14	B	3012	CLA	C4A-NA-C1A	7.14	109.92	106.71
14	B	3004	CLA	C4A-NA-C1A	7.10	109.90	106.71
14	B	3008	CLA	C4A-NA-C1A	7.05	109.87	106.71
14	B	3026	CLA	C4A-NA-C1A	7.04	109.87	106.71
14	A	832	CLA	C4A-NA-C1A	7.04	109.87	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L	204	CLA	C4A-NA-C1A	6.99	109.85	106.71
14	A	820	CLA	C4A-NA-C1A	6.95	109.83	106.71
14	A	843	CLA	C4A-NA-C1A	6.94	109.82	106.71
14	B	3040	CLA	C4A-NA-C1A	6.92	109.82	106.71
14	A	828	CLA	C4A-NA-C1A	6.92	109.81	106.71
14	B	3041	CLA	C4A-NA-C1A	6.86	109.79	106.71
14	B	3006	CLA	C4A-NA-C1A	6.84	109.78	106.71
14	A	840	CLA	C4A-NA-C1A	6.79	109.76	106.71
14	B	3007	CLA	C4A-NA-C1A	6.78	109.75	106.71
14	L	205	CLA	C4A-NA-C1A	6.75	109.74	106.71
14	A	817	CLA	C4A-NA-C1A	6.74	109.74	106.71
14	A	844	CLA	C4A-NA-C1A	6.74	109.74	106.71
14	B	3039	CLA	C4A-NA-C1A	6.70	109.72	106.71
14	B	3020	CLA	C4A-NA-C1A	6.70	109.72	106.71
14	B	3010	CLA	C4A-NA-C1A	6.69	109.71	106.71
14	A	837	CLA	C4A-NA-C1A	6.65	109.70	106.71
14	B	3030	CLA	C4A-NA-C1A	6.52	109.64	106.71
14	B	3017	CLA	C4A-NA-C1A	6.51	109.63	106.71
14	A	824	CLA	C4A-NA-C1A	6.50	109.63	106.71
14	A	833	CLA	C4A-NA-C1A	6.48	109.62	106.71
14	A	845	CLA	C4A-NA-C1A	6.45	109.61	106.71
14	A	829	CLA	C4A-NA-C1A	6.45	109.61	106.71
14	B	3018	CLA	C4A-NA-C1A	6.44	109.60	106.71
14	A	838	CLA	C4A-NA-C1A	6.43	109.60	106.71
14	A	823	CLA	C4A-NA-C1A	6.40	109.58	106.71
14	A	816	CLA	C4A-NA-C1A	6.39	109.58	106.71
14	B	3013	CLA	C4A-NA-C1A	6.34	109.56	106.71
14	A	839	CLA	C4A-NA-C1A	6.33	109.55	106.71
14	B	3009	CLA	C4A-NA-C1A	6.27	109.53	106.71
14	A	841	CLA	C4A-NA-C1A	6.23	109.51	106.71
14	B	3037	CLA	C4A-NA-C1A	6.22	109.50	106.71
14	B	3038	CLA	C4A-NA-C1A	6.21	109.50	106.71
14	A	826	CLA	C4A-NA-C1A	6.20	109.50	106.71
14	B	3021	CLA	C4A-NA-C1A	6.17	109.48	106.71
14	A	830	CLA	C4A-NA-C1A	6.17	109.48	106.71
14	A	831	CLA	C4A-NA-C1A	6.15	109.47	106.71
14	A	818	CLA	C4A-NA-C1A	6.14	109.47	106.71
13	A	801	CL0	C4A-NA-C1A	6.13	109.46	106.71
14	A	834	CLA	C4A-NA-C1A	6.07	109.44	106.71
14	B	3032	CLA	C4A-NA-C1A	6.07	109.43	106.71
14	A	813	CLA	C4A-NA-C1A	6.05	109.42	106.71
14	B	3029	CLA	C4A-NA-C1A	6.04	109.42	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3016	CLA	C4A-NA-C1A	6.04	109.42	106.71
14	B	3022	CLA	C4A-NA-C1A	6.00	109.40	106.71
14	A	805	CLA	C4A-NA-C1A	5.99	109.40	106.71
14	A	809	CLA	C4A-NA-C1A	5.95	109.38	106.71
14	B	3011	CLA	C4A-NA-C1A	5.89	109.35	106.71
14	A	815	CLA	C4A-NA-C1A	5.87	109.35	106.71
14	A	804	CLA	C4A-NA-C1A	5.87	109.34	106.71
14	B	3027	CLA	C4A-NA-C1A	5.87	109.34	106.71
14	A	836	CLA	C4A-NA-C1A	5.84	109.33	106.71
14	X	1701	CLA	C4A-NA-C1A	5.84	109.33	106.71
14	A	821	CLA	C4A-NA-C1A	5.82	109.32	106.71
14	A	819	CLA	C4A-NA-C1A	5.74	109.29	106.71
14	A	835	CLA	C4A-NA-C1A	5.71	109.27	106.71
14	J	101	CLA	C4A-NA-C1A	5.68	109.26	106.71
14	A	802	CLA	C4A-NA-C1A	5.68	109.26	106.71
14	B	3019	CLA	C4A-NA-C1A	5.67	109.26	106.71
14	A	825	CLA	C4A-NA-C1A	5.62	109.23	106.71
14	K	101	CLA	C4A-NA-C1A	5.62	109.23	106.71
14	A	856	CLA	C4A-NA-C1A	5.59	109.22	106.71
14	A	808	CLA	C4A-NA-C1A	5.55	109.20	106.71
14	B	3035	CLA	C4A-NA-C1A	5.52	109.19	106.71
14	A	822	CLA	C4A-NA-C1A	5.52	109.19	106.71
14	J	102	CLA	C4A-NA-C1A	5.51	109.18	106.71
14	B	3023	CLA	C4A-NA-C1A	5.47	109.16	106.71
14	B	3015	CLA	C4A-NA-C1A	5.43	109.14	106.71
14	B	3014	CLA	C4A-NA-C1A	5.27	109.07	106.71
14	A	810	CLA	C4A-NA-C1A	5.24	109.06	106.71
14	B	3025	CLA	C4A-NA-C1A	5.23	109.06	106.71
14	A	827	CLA	C4A-NA-C1A	5.16	109.02	106.71
14	A	807	CLA	C4A-NA-C1A	5.13	109.01	106.71
14	A	814	CLA	C4A-NA-C1A	5.10	109.00	106.71
14	A	811	CLA	C4A-NA-C1A	5.06	108.98	106.71
14	B	3034	CLA	C4A-NA-C1A	5.05	108.98	106.71
14	K	103	CLA	C4A-NA-C1A	5.03	108.97	106.71
14	L	206	CLA	CMB-C2B-C1B	-5.02	120.75	128.46
14	L	206	CLA	C4A-NA-C1A	5.01	108.96	106.71
14	B	3036	CLA	C4A-NA-C1A	4.97	108.94	106.71
14	A	821	CLA	CMB-C2B-C1B	-4.91	120.91	128.46
14	A	819	CLA	CMB-C2B-C1B	-4.82	121.06	128.46
14	A	844	CLA	CMB-C2B-C1B	-4.74	121.17	128.46
14	L	206	CLA	CMB-C2B-C3B	4.67	133.41	124.68
14	B	3024	CLA	C4A-NA-C1A	4.63	108.79	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	802	CLA	CMB-C2B-C1B	-4.59	121.40	128.46
14	A	816	CLA	O2D-CGD-CBD	4.45	119.18	111.27
16	F	203	BCR	C35-C13-C14	-4.39	116.77	122.92
14	B	3010	CLA	CMB-C2B-C1B	-4.39	121.72	128.46
14	B	3023	CLA	CMB-C2B-C1B	-4.29	121.88	128.46
18	A	854	LHG	O4-P-O5	4.23	133.18	112.24
14	A	836	CLA	CMB-C2B-C1B	-4.23	121.97	128.46
14	A	802	CLA	CMB-C2B-C3B	4.19	132.52	124.68
14	A	835	CLA	C1-C2-C3	-4.15	118.86	126.04
18	M	101	LHG	O4-P-O5	4.14	132.73	112.24
14	K	101	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
18	A	853	LHG	O4-P-O5	4.12	132.62	112.24
14	B	3019	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
14	A	819	CLA	CMB-C2B-C3B	4.06	132.27	124.68
14	A	821	CLA	CMB-C2B-C3B	4.01	132.18	124.68
14	F	202	CLA	C4A-NA-C1A	4.01	108.51	106.71
14	A	827	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
16	K	102	BCR	C2-C1-C6	3.96	116.58	110.48
14	B	3032	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
14	B	3020	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
18	B	3050	LHG	O4-P-O5	3.91	131.59	112.24
14	L	204	CLA	C1-C2-C3	-3.91	119.29	126.04
14	A	803	CLA	CAA-C2A-C1A	-3.88	99.25	111.97
14	B	3019	CLA	CMD-C2D-C3D	3.84	131.87	124.68
14	A	824	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
18	A	854	LHG	O8-C23-C24	3.80	121.35	111.38
14	B	3012	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
14	A	822	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
14	A	831	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
14	K	103	CLA	O2D-CGD-O1D	-3.74	116.52	123.84
14	B	3030	CLA	CAA-C2A-C3A	-3.73	102.56	112.78
16	A	851	BCR	C2-C1-C6	3.70	116.17	110.48
14	B	3013	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
14	B	3018	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
14	A	843	CLA	O2D-CGD-O1D	-3.67	116.66	123.84
14	A	839	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
16	F	201	BCR	C2-C1-C6	3.65	116.11	110.48
14	B	3022	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
14	A	856	CLA	O2D-CGD-O1D	-3.63	116.74	123.84
14	A	804	CLA	CMB-C2B-C1B	-3.62	122.89	128.46
14	A	811	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
14	F	202	CLA	C4D-C3D-CAD	-3.61	106.46	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	837	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
14	A	817	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
14	A	829	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
14	B	3032	CLA	O2D-CGD-O1D	-3.55	116.89	123.84
14	A	809	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
14	B	3040	CLA	CMD-C2D-C3D	3.54	131.30	124.68
14	A	813	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
14	A	830	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
14	B	3025	CLA	CMD-C2D-C3D	3.52	131.26	124.68
14	A	839	CLA	O2D-CGD-CBD	3.52	117.52	111.27
14	M	102	CLA	CMB-C2B-C1B	-3.51	123.08	128.46
14	F	202	CLA	CMD-C2D-C3D	3.51	131.24	124.68
14	K	101	CLA	CMB-C2B-C3B	3.49	131.22	124.68
14	B	3023	CLA	CMB-C2B-C3B	3.49	131.21	124.68
14	A	824	CLA	CMB-C2B-C3B	3.49	131.20	124.68
14	X	1701	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
14	K	101	CLA	CMD-C2D-C3D	3.46	131.15	124.68
14	A	829	CLA	CMB-C2B-C3B	3.45	131.13	124.68
14	B	3025	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
14	A	827	CLA	CMB-C2B-C3B	3.44	131.11	124.68
14	B	3014	CLA	C4D-C3D-CAD	-3.44	106.55	108.47
14	B	3006	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
14	F	202	CLA	O2D-CGD-O1D	-3.43	117.12	123.84
14	M	102	CLA	CMD-C2D-C3D	3.43	131.10	124.68
14	A	810	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
14	F	202	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
14	B	3020	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
14	B	3038	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
14	A	816	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
14	B	3009	CLA	O2A-CGA-O1A	-3.42	114.96	123.59
14	A	804	CLA	CMD-C2D-C3D	3.41	131.06	124.68
14	A	825	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
21	L	202	LMT	C2'-C3'-C4'	3.40	117.45	109.68
14	A	826	CLA	O2D-CGD-O1D	-3.40	117.18	123.84
14	B	3027	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
14	K	103	CLA	O2D-CGD-CBD	3.39	117.30	111.27
14	B	3018	CLA	CMD-C2D-C3D	3.39	131.02	124.68
14	B	3034	CLA	C4D-C3D-CAD	-3.39	106.58	108.47
14	B	3019	CLA	CMB-C2B-C3B	3.37	130.99	124.68
14	B	3035	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
14	A	802	CLA	C1B-CHB-C4A	-3.35	123.48	130.12
14	A	813	CLA	O2D-CGD-O1D	-3.35	117.30	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3032	CLA	CED-O2D-CGD	3.34	123.50	115.94
14	B	3004	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
14	B	3010	CLA	C1-C2-C3	-3.32	120.30	126.04
14	A	816	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
14	B	3009	CLA	O2D-CGD-O1D	-3.31	117.38	123.84
14	A	842	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
16	L	209	BCR	C15-C16-C17	-3.29	116.73	123.47
14	A	836	CLA	CMB-C2B-C3B	3.29	130.83	124.68
14	M	102	CLA	C4A-NA-C1A	3.29	108.18	106.71
14	A	831	CLA	CMD-C2D-C3D	3.27	130.80	124.68
14	B	3039	CLA	C4D-C3D-CAD	-3.26	106.65	108.47
16	B	3047	BCR	C2-C1-C6	3.26	115.50	110.48
14	A	839	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
14	B	3029	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
14	B	3036	CLA	CMD-C2D-C3D	3.24	130.75	124.68
14	A	830	CLA	CMD-C2D-C3D	3.24	130.73	124.68
16	M	103	BCR	C33-C5-C6	-3.23	120.90	124.53
15	B	3043	PQN	O1-C1-C10	-3.23	116.33	121.56
14	A	820	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
14	A	835	CLA	C5-C3-C2	3.23	127.65	121.12
14	A	823	CLA	CHB-C4A-NA	3.23	128.97	124.51
14	A	818	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
14	B	3032	CLA	CMB-C2B-C3B	3.21	130.68	124.68
14	A	833	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
14	A	856	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
14	M	102	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
14	B	3040	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
14	A	835	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
16	F	201	BCR	C27-C26-C25	3.19	127.37	122.73
14	B	3030	CLA	CHB-C4A-NA	3.19	128.92	124.51
14	A	806	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
14	A	809	CLA	CMB-C2B-C3B	3.19	130.64	124.68
14	A	840	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
14	J	101	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
14	B	3012	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
18	M	101	LHG	O8-C23-C24	3.18	121.88	111.91
14	A	821	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
14	B	3021	CLA	C1B-CHB-C4A	-3.18	123.82	130.12
14	B	3025	CLA	CMB-C2B-C3B	3.18	130.62	124.68
14	A	811	CLA	CMB-C2B-C3B	3.17	130.60	124.68
14	A	844	CLA	CMB-C2B-C3B	3.16	130.59	124.68
14	B	3014	CLA	CMD-C2D-C3D	3.16	130.59	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	813	CLA	CMD-C2D-C3D	3.15	130.57	124.68
14	B	3042	CLA	CMD-C2D-C3D	3.15	130.57	124.68
16	I	101	BCR	C35-C13-C14	-3.15	118.51	122.92
14	A	811	CLA	CMD-C2D-C3D	3.15	130.57	124.68
14	A	822	CLA	CMB-C2B-C3B	3.15	130.56	124.68
14	A	843	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
14	L	205	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
14	A	830	CLA	CMB-C2B-C3B	3.14	130.55	124.68
14	B	3014	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
14	A	805	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
16	J	105	BCR	C7-C8-C9	-3.12	121.51	126.23
15	A	846	PQN	O1-C1-C10	-3.12	116.50	121.56
14	A	843	CLA	CHB-C4A-NA	3.12	128.83	124.51
14	B	3037	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
14	B	3007	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
14	B	3028	CLA	CMD-C2D-C3D	3.11	130.50	124.68
14	A	825	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
16	B	3044	BCR	C29-C30-C25	3.11	115.27	110.48
14	A	820	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
14	B	3036	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
14	A	820	CLA	CAA-C2A-C1A	-3.11	101.79	111.97
14	B	3018	CLA	CHB-C4A-NA	3.11	128.81	124.51
14	B	3042	CLA	CHB-C4A-NA	3.11	128.81	124.51
21	L	202	LMT	C1'-C2'-C3'	3.10	116.46	110.00
14	B	3018	CLA	CMB-C2B-C3B	3.10	130.48	124.68
14	A	822	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
14	B	3005	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
14	A	820	CLA	CMB-C2B-C3B	3.08	130.44	124.68
14	A	827	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
17	B	3049	LMG	O6-C1-O1	-3.08	102.69	109.97
14	B	3024	CLA	C4D-C3D-CAD	-3.08	106.75	108.47
14	B	3040	CLA	C4D-C3D-CAD	-3.08	106.75	108.47
14	A	823	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
14	B	3012	CLA	CMB-C2B-C3B	3.07	130.43	124.68
14	B	3037	CLA	CMD-C2D-C3D	3.07	130.42	124.68
16	L	208	BCR	C27-C26-C25	3.07	127.18	122.73
14	A	823	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
14	B	3010	CLA	CMB-C2B-C3B	3.06	130.41	124.68
14	A	808	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
16	L	201	BCR	C24-C23-C22	-3.05	121.62	126.23
14	B	3017	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
14	X	1701	CLA	CMB-C2B-C1B	-3.05	123.78	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3042	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
14	B	3020	CLA	CMB-C2B-C3B	3.04	130.37	124.68
14	A	811	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
14	A	839	CLA	CHB-C4A-NA	3.04	128.71	124.51
14	B	3011	CLA	CHB-C4A-NA	3.03	128.71	124.51
16	K	102	BCR	C27-C26-C25	3.03	127.13	122.73
14	B	3020	CLA	CMD-C2D-C3D	3.03	130.34	124.68
14	A	830	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
14	A	856	CLA	CMD-C2D-C3D	3.02	130.34	124.68
13	A	801	CL0	CMB-C2B-C1B	-3.02	123.83	128.46
16	A	849	BCR	C15-C14-C13	-3.02	123.01	127.31
14	B	3029	CLA	CMB-C2B-C3B	3.01	130.32	124.68
14	A	843	CLA	CMD-C2D-C3D	3.01	130.31	124.68
14	A	837	CLA	CMD-C2D-C3D	3.01	130.31	124.68
14	B	3038	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
14	A	826	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
14	A	805	CLA	CMD-C2D-C3D	3.00	130.30	124.68
14	A	844	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
14	B	3034	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
14	A	829	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
14	B	3030	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
14	A	837	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
16	A	850	BCR	C37-C22-C21	-2.99	118.73	122.92
14	A	837	CLA	CMB-C2B-C3B	2.99	130.28	124.68
14	A	839	CLA	CMB-C2B-C3B	2.99	130.28	124.68
14	B	3004	CLA	CHB-C4A-NA	2.99	128.65	124.51
14	A	841	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
14	B	3025	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
14	A	822	CLA	CMC-C2C-C3C	2.98	130.55	124.94
14	K	103	CLA	CMB-C2B-C1B	-2.97	123.89	128.46
14	A	843	CLA	O2D-CGD-CBD	2.97	116.55	111.27
14	B	3019	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
16	A	847	BCR	C33-C5-C6	-2.97	121.19	124.53
14	A	814	CLA	CMB-C2B-C1B	-2.97	123.91	128.46
14	A	803	CLA	CMC-C2C-C3C	2.96	130.53	124.94
14	B	3010	CLA	CBA-CAA-C2A	-2.96	105.12	113.86
14	A	809	CLA	CMD-C2D-C3D	2.96	130.22	124.68
14	A	844	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
14	A	845	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
14	B	3016	CLA	CMB-C2B-C1B	-2.95	123.92	128.46
14	A	825	CLA	CMB-C2B-C3B	2.95	130.21	124.68
14	A	836	CLA	C4D-C3D-CAD	-2.95	106.82	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	805	CLA	CMB-C2B-C1B	-2.95	123.94	128.46
17	A	852	LMG	C7-O1-C1	2.94	119.48	113.74
14	L	204	CLA	C5-C3-C2	2.94	127.06	121.12
14	B	3018	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
14	L	206	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
14	A	834	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
14	A	839	CLA	CMD-C2D-C3D	2.93	130.16	124.68
16	L	208	BCR	C33-C5-C6	-2.93	121.24	124.53
14	B	3023	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
14	B	3033	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
16	A	851	BCR	C28-C27-C26	-2.92	108.86	114.08
14	A	841	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
14	A	808	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
14	A	836	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
14	B	3029	CLA	C4D-C3D-CAD	-2.90	106.85	108.47
14	B	3027	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
16	B	3045	BCR	C33-C5-C6	-2.90	121.27	124.53
14	A	807	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
14	A	820	CLA	CHB-C4A-NA	2.90	128.52	124.51
16	J	104	BCR	C24-C23-C22	-2.90	121.86	126.23
14	B	3013	CLA	CMB-C2B-C3B	2.90	130.10	124.68
14	A	814	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
14	B	3024	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
14	B	3012	CLA	CHB-C4A-NA	2.89	128.51	124.51
14	A	840	CLA	O2D-CGD-CBD	2.89	116.40	111.27
14	B	3036	CLA	C4D-C3D-CAD	-2.88	106.86	108.47
14	A	819	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
14	X	1701	CLA	CHB-C4A-NA	2.88	128.49	124.51
14	L	204	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
14	K	103	CLA	CMB-C2B-C3B	2.88	130.06	124.68
14	A	816	CLA	CMD-C2D-C3D	2.88	130.06	124.68
16	B	3051	BCR	C27-C26-C25	2.88	126.91	122.73
14	B	3029	CLA	CHB-C4A-NA	2.88	128.49	124.51
14	B	3035	CLA	CMB-C2B-C1B	-2.88	124.05	128.46
14	B	3025	CLA	C4-C3-C5	2.87	120.10	115.27
14	A	839	CLA	C4D-C3D-CAD	-2.87	106.87	108.47
14	B	3022	CLA	CMB-C2B-C3B	2.87	130.04	124.68
14	B	3031	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
14	B	3036	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
14	A	856	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
14	A	803	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
16	F	201	BCR	C16-C15-C14	-2.85	117.64	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3033	CLA	CMC-C2C-C3C	2.85	130.31	124.94
14	A	831	CLA	CMB-C2B-C3B	2.85	130.01	124.68
14	B	3024	CLA	CMB-C2B-C1B	-2.85	124.09	128.46
14	B	3034	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
14	B	3037	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
14	J	102	CLA	CMB-C2B-C1B	-2.85	124.09	128.46
14	A	842	CLA	CMD-C2D-C3D	2.84	129.99	124.68
14	B	3008	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
14	A	827	CLA	CMD-C2D-C3D	2.84	129.99	124.68
14	A	844	CLA	CMD-C2D-C3D	2.84	129.99	124.68
14	A	810	CLA	CMB-C2B-C3B	2.84	129.99	124.68
14	B	3038	CLA	CMD-C2D-C3D	2.84	129.99	124.68
14	A	817	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
21	L	202	LMT	C1'-O5'-C5'	-2.83	108.12	113.69
14	A	817	CLA	CMB-C2B-C3B	2.83	129.98	124.68
14	B	3004	CLA	CMB-C2B-C3B	2.83	129.98	124.68
16	A	851	BCR	C7-C8-C9	-2.83	121.95	126.23
14	B	3022	CLA	CMD-C2D-C3D	2.83	129.97	124.68
16	B	3047	BCR	C15-C16-C17	-2.82	117.69	123.47
14	B	3013	CLA	CMD-C2D-C3D	2.82	129.96	124.68
14	B	3010	CLA	C6-C5-C3	-2.82	106.05	113.45
14	F	202	CLA	OBD-CAD-CBD	-2.82	121.86	125.89
16	A	849	BCR	C15-C16-C17	-2.82	117.70	123.47
14	B	3015	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
14	A	803	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
14	A	816	CLA	C4D-C3D-CAD	-2.81	106.90	108.47
16	L	208	BCR	C15-C16-C17	-2.81	117.71	123.47
14	J	101	CLA	CMB-C2B-C3B	2.81	129.94	124.68
14	A	828	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
14	A	839	CLA	CMC-C2C-C3C	2.81	130.24	124.94
14	A	809	CLA	CHB-C4A-NA	2.81	128.40	124.51
14	B	3040	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
14	A	807	CLA	CMB-C2B-C1B	-2.80	124.15	128.46
14	A	839	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
14	A	809	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
14	B	3025	CLA	CHB-C4A-NA	2.80	128.38	124.51
14	M	102	CLA	O2D-CGD-CBD	2.80	116.24	111.27
14	A	833	CLA	CMB-C2B-C3B	2.80	129.91	124.68
16	L	201	BCR	C2-C1-C6	2.80	114.78	110.48
14	B	3025	CLA	C2A-C1A-CHA	2.79	128.74	123.86
14	B	3013	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
16	B	3047	BCR	C27-C26-C25	2.79	126.78	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	J	105	BCR	C2-C1-C6	2.79	114.77	110.48
14	L	204	CLA	CMD-C2D-C3D	2.79	129.89	124.68
14	A	815	CLA	CMB-C2B-C1B	-2.79	124.18	128.46
16	F	203	BCR	C2-C1-C6	2.78	114.77	110.48
16	B	3047	BCR	C11-C10-C9	-2.78	123.34	127.31
13	A	801	CL0	O2D-CGD-O1D	-2.78	118.40	123.84
14	A	816	CLA	CMB-C2B-C3B	2.78	129.88	124.68
14	A	804	CLA	CMB-C2B-C3B	2.78	129.87	124.68
14	A	817	CLA	CMD-C2D-C3D	2.78	129.87	124.68
16	J	105	BCR	C27-C26-C25	2.78	126.76	122.73
14	B	3008	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
14	B	3010	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
14	A	812	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
14	L	204	CLA	CMC-C2C-C3C	2.77	130.16	124.94
14	A	813	CLA	CMB-C2B-C3B	2.77	129.86	124.68
14	B	3014	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
14	B	3016	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
16	A	851	BCR	C24-C23-C22	-2.76	122.06	126.23
14	B	3029	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
16	L	208	BCR	C24-C23-C22	-2.76	122.07	126.23
14	B	3007	CLA	CMD-C2D-C3D	2.76	129.84	124.68
14	B	3034	CLA	CMB-C2B-C3B	2.76	129.84	124.68
14	B	3034	CLA	CMD-C2D-C3D	2.76	129.84	124.68
16	A	848	BCR	C2-C1-C6	2.76	114.72	110.48
14	A	818	CLA	O2D-CGD-CBD	2.76	116.16	111.27
14	A	812	CLA	CHB-C4A-NA	2.75	128.32	124.51
14	A	838	CLA	CMD-C2D-C3D	2.75	129.82	124.68
14	A	824	CLA	CHB-C4A-NA	2.75	128.31	124.51
14	B	3039	CLA	CMB-C2B-C1B	-2.75	124.24	128.46
14	B	3021	CLA	CMB-C2B-C1B	-2.75	124.24	128.46
14	B	3028	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
14	B	3031	CLA	CMD-C2D-C3D	2.74	129.81	124.68
14	A	838	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
14	A	834	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
14	A	813	CLA	O2D-CGD-CBD	2.73	116.12	111.27
17	I	102	LMG	O6-C5-C4	2.73	114.65	109.69
14	A	842	CLA	CMB-C2B-C3B	2.73	129.78	124.68
17	A	855	LMG	C1-O6-C5	-2.73	108.34	113.69
14	B	3029	CLA	CMD-C2D-C3D	2.72	129.78	124.68
14	A	824	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
14	L	205	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
16	A	848	BCR	C27-C26-C25	2.72	126.67	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	208	BCR	C37-C22-C21	-2.72	119.12	122.92
14	A	806	CLA	CHB-C4A-NA	2.72	128.27	124.51
14	L	205	CLA	CMB-C2B-C3B	2.72	129.76	124.68
16	B	3046	BCR	C33-C5-C6	-2.71	121.48	124.53
14	B	3041	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
14	A	838	CLA	CMB-C2B-C1B	-2.71	124.30	128.46
15	A	846	PQN	C2M-C2-C1	2.71	120.76	116.27
14	A	832	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
14	B	3032	CLA	CHB-C4A-NA	2.71	128.26	124.51
14	A	856	CLA	CMB-C2B-C3B	2.70	129.73	124.68
14	A	840	CLA	C4D-C3D-CAD	-2.70	106.96	108.47
16	B	3046	BCR	C24-C23-C22	-2.70	122.16	126.23
14	B	3033	CLA	CMB-C2B-C1B	-2.70	124.32	128.46
14	B	3009	CLA	O2D-CGD-CBD	2.70	116.06	111.27
16	B	3044	BCR	C2-C1-C6	2.69	114.63	110.48
14	B	3033	CLA	O2D-CGD-CBD	2.69	116.05	111.27
14	B	3007	CLA	CMC-C2C-C3C	2.69	130.01	124.94
16	J	104	BCR	C15-C16-C17	-2.69	117.97	123.47
14	A	817	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
14	B	3026	CLA	CHB-C4A-NA	2.69	128.23	124.51
14	A	815	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
14	B	3017	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
14	B	3005	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
14	A	845	CLA	CHB-C4A-NA	2.67	128.20	124.51
14	A	833	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
14	B	3033	CLA	CHB-C4A-NA	2.67	128.20	124.51
14	B	3004	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
14	A	834	CLA	CMB-C2B-C3B	2.66	129.65	124.68
14	B	3041	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
14	A	840	CLA	CMD-C2D-C3D	2.66	129.65	124.68
14	B	3005	CLA	CHB-C4A-NA	2.66	128.18	124.51
14	A	819	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
14	B	3026	CLA	C2A-C1A-CHA	2.65	128.50	123.86
16	L	209	BCR	C8-C7-C6	-2.65	119.76	127.20
14	B	3038	CLA	CMB-C2B-C3B	2.65	129.64	124.68
14	B	3017	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
16	J	103	BCR	C27-C26-C25	2.64	126.56	122.73
14	A	814	CLA	O2D-CGD-CBD	2.63	115.95	111.27
14	A	838	CLA	O2A-CGA-O1A	-2.63	116.95	123.59
14	B	3035	CLA	O2D-CGD-CBD	2.63	115.94	111.27
14	A	827	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
14	A	826	CLA	CMB-C2B-C3B	2.63	129.59	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	819	CLA	CHB-C4A-NA	2.62	128.14	124.51
14	A	832	CLA	CMB-C2B-C1B	-2.62	124.44	128.46
14	K	101	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
14	A	810	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
14	B	3027	CLA	CMB-C2B-C3B	2.61	129.55	124.68
14	A	841	CLA	O2A-CGA-O1A	-2.60	117.02	123.59
14	B	3015	CLA	CMB-C2B-C1B	-2.60	124.47	128.46
14	J	101	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
14	B	3021	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
14	B	3014	CLA	CMB-C2B-C3B	2.60	129.54	124.68
16	B	3047	BCR	C35-C13-C14	-2.60	119.28	122.92
14	A	842	CLA	CHB-C4A-NA	2.60	128.10	124.51
14	B	3040	CLA	CMB-C2B-C3B	2.60	129.53	124.68
14	B	3020	CLA	C1B-CHB-C4A	-2.60	124.98	130.12
14	A	818	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
14	B	3022	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
14	B	3011	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
14	B	3003	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
16	A	851	BCR	C3-C4-C5	-2.59	109.45	114.08
14	A	807	CLA	CMC-C2C-C3C	2.59	129.82	124.94
14	A	815	CLA	C1B-CHB-C4A	-2.59	125.00	130.12
21	L	202	LMT	O1B-C4'-C3'	2.59	114.16	107.28
14	B	3039	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
14	B	3033	CLA	CMD-C2D-C3D	2.58	129.51	124.68
14	B	3025	CLA	C4D-C3D-CAD	-2.58	107.03	108.47
14	A	803	CLA	CHB-C4A-NA	2.58	128.08	124.51
14	B	3030	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
15	A	846	PQN	C2M-C2-C3	-2.58	120.19	124.40
16	A	849	BCR	C33-C5-C6	-2.58	121.64	124.53
14	B	3022	CLA	C4D-C3D-CAD	-2.58	107.03	108.47
14	B	3028	CLA	CMB-C2B-C1B	-2.57	124.51	128.46
14	B	3005	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
14	B	3008	CLA	CHB-C4A-NA	2.57	128.06	124.51
14	B	3017	CLA	CHB-C4A-NA	2.57	128.06	124.51
16	J	103	BCR	C33-C5-C6	-2.57	121.64	124.53
14	B	3010	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
14	A	806	CLA	C4D-C3D-CAD	-2.57	107.04	108.47
14	B	3010	CLA	C4D-C3D-CAD	-2.57	107.04	108.47
14	A	814	CLA	CMB-C2B-C3B	2.57	129.48	124.68
14	B	3009	CLA	CHB-C4A-NA	2.57	128.06	124.51
14	A	815	CLA	CMD-C2D-C3D	2.57	129.48	124.68
14	B	3017	CLA	CMD-C2D-C3D	2.57	129.48	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3023	CLA	C1B-CHB-C4A	-2.57	125.04	130.12
14	L	204	CLA	CMB-C2B-C1B	-2.56	124.53	128.46
14	B	3004	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
14	B	3012	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
14	B	3027	CLA	CHB-C4A-NA	2.56	128.05	124.51
16	L	201	BCR	C33-C5-C6	-2.56	121.66	124.53
14	B	3019	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
16	B	3046	BCR	C15-C16-C17	-2.56	118.24	123.47
14	L	206	CLA	CHB-C4A-NA	2.55	128.04	124.51
14	B	3031	CLA	CHB-C4A-NA	2.55	128.04	124.51
14	A	819	CLA	CMD-C2D-C3D	2.55	129.45	124.68
14	B	3008	CLA	CMD-C2D-C3D	2.55	129.45	124.68
14	A	835	CLA	CHB-C4A-NA	2.55	128.03	124.51
14	B	3035	CLA	CHB-C4A-NA	2.55	128.03	124.51
14	A	838	CLA	CHB-C4A-NA	2.54	128.03	124.51
14	L	205	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
16	J	105	BCR	C11-C10-C9	-2.54	123.68	127.31
14	B	3016	CLA	CHB-C4A-NA	2.54	128.03	124.51
14	A	820	CLA	CMD-C2D-C3D	2.54	129.43	124.68
14	B	3011	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
14	A	831	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
14	A	840	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
16	L	208	BCR	C11-C10-C9	-2.54	123.69	127.31
14	B	3009	CLA	CMD-C2D-C3D	2.54	129.42	124.68
16	F	203	BCR	C27-C26-C25	2.53	126.41	122.73
14	A	829	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
14	A	833	CLA	CMD-C2D-C3D	2.53	129.41	124.68
14	L	204	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
14	B	3017	CLA	CMB-C2B-C3B	2.53	129.41	124.68
14	B	3021	CLA	CMB-C2B-C3B	2.53	129.41	124.68
14	A	813	CLA	C4D-C3D-CAD	-2.53	107.06	108.47
17	I	102	LMG	O3-C3-C2	-2.53	104.51	110.35
14	B	3008	CLA	CMB-C2B-C1B	-2.53	124.58	128.46
16	A	847	BCR	C24-C23-C22	-2.53	122.42	126.23
22	L	207	DGD	O3G-C3G-C2G	-2.52	104.81	110.90
14	A	845	CLA	CMB-C2B-C1B	-2.52	124.59	128.46
14	A	841	CLA	CMD-C2D-C3D	2.52	129.40	124.68
16	L	208	BCR	C30-C25-C26	-2.52	119.06	122.61
16	A	848	BCR	C33-C5-C6	-2.52	121.70	124.53
14	B	3037	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
14	A	820	CLA	C2A-C1A-CHA	2.52	128.27	123.86
14	B	3030	CLA	C2A-C1A-CHA	2.52	128.27	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	X	1701	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
16	B	3048	BCR	C27-C26-C25	2.52	126.39	122.73
14	B	3019	CLA	CHB-C4A-NA	2.52	127.99	124.51
14	B	3016	CLA	CMB-C2B-C3B	2.52	129.39	124.68
14	X	1701	CLA	CMB-C2B-C3B	2.52	129.39	124.68
14	A	822	CLA	CHB-C4A-NA	2.52	127.99	124.51
14	B	3006	CLA	CMC-C2C-C3C	2.52	129.69	124.94
14	B	3018	CLA	C1-C2-C3	-2.51	121.69	126.04
14	B	3022	CLA	CHB-C4A-NA	2.51	127.99	124.51
14	B	3021	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
16	B	3051	BCR	C30-C25-C26	-2.51	119.08	122.61
14	B	3036	CLA	CMB-C2B-C3B	2.51	129.37	124.68
14	A	811	CLA	C4D-C3D-CAD	-2.51	107.07	108.47
14	A	832	CLA	CHB-C4A-NA	2.51	127.98	124.51
14	A	840	CLA	CMB-C2B-C1B	-2.51	124.61	128.46
16	L	201	BCR	C8-C7-C6	-2.51	120.16	127.20
14	B	3039	CLA	CMD-C2D-C3D	2.50	129.36	124.68
14	B	3026	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
14	B	3019	CLA	CMC-C2C-C3C	2.50	129.65	124.94
16	J	104	BCR	C33-C5-C6	-2.50	121.72	124.53
14	A	845	CLA	CMD-C2D-C3D	2.50	129.35	124.68
14	K	103	CLA	CMD-C2D-C3D	2.49	129.35	124.68
16	A	850	BCR	C33-C5-C6	-2.49	121.73	124.53
14	B	3007	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
14	A	816	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
16	A	850	BCR	C27-C26-C25	2.49	126.34	122.73
14	A	814	CLA	CHB-C4A-NA	2.49	127.95	124.51
14	A	806	CLA	CMC-C2C-C3C	2.49	129.63	124.94
14	B	3011	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
14	A	823	CLA	CMC-C2C-C3C	2.48	129.63	124.94
14	B	3027	CLA	CMD-C2D-C3D	2.48	129.32	124.68
14	F	202	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
14	A	828	CLA	CHB-C4A-NA	2.48	127.94	124.51
14	L	206	CLA	C4D-C3D-CAD	-2.48	107.09	108.47
14	A	827	CLA	O2D-CGD-CBD	2.48	115.67	111.27
14	A	823	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
14	A	843	CLA	CMB-C2B-C3B	2.48	129.31	124.68
14	A	826	CLA	CMC-C2C-C3C	2.47	129.60	124.94
14	B	3025	CLA	CHA-C1A-NA	-2.47	120.74	126.40
14	A	807	CLA	CHB-C4A-NA	2.47	127.93	124.51
14	L	204	CLA	C4D-C3D-CAD	-2.47	107.09	108.47
14	B	3011	CLA	CBC-CAC-C3C	2.47	118.55	112.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3024	CLA	CMB-C2B-C3B	2.47	129.29	124.68
14	A	821	CLA	C4D-C3D-CAD	-2.46	107.10	108.47
14	B	3038	CLA	CMC-C2C-C3C	2.46	129.58	124.94
14	B	3030	CLA	C3A-C2A-C1A	2.46	105.02	101.34
14	B	3026	CLA	CMB-C2B-C1B	-2.46	124.69	128.46
16	A	849	BCR	C27-C26-C25	2.46	126.30	122.73
14	B	3009	CLA	CGD-CBD-CAD	-2.46	102.78	110.73
14	B	3016	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
14	B	3028	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
13	A	801	CL0	CHB-C4A-NA	2.45	127.90	124.51
14	A	828	CLA	CMB-C2B-C1B	-2.45	124.69	128.46
14	A	841	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
14	A	803	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
14	B	3030	CLA	CMD-C2D-C3D	2.45	129.26	124.68
21	L	202	LMT	C1B-O1B-C4'	2.45	124.03	117.96
14	B	3026	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
16	L	209	BCR	C33-C5-C6	-2.45	121.78	124.53
14	B	3007	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
14	B	3020	CLA	CMC-C2C-C3C	2.45	129.55	124.94
14	A	833	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
16	I	101	BCR	C15-C16-C17	-2.45	118.47	123.47
14	J	101	CLA	CHB-C4A-NA	2.44	127.89	124.51
22	L	207	DGD	O3G-C1D-C2D	-2.44	104.49	108.30
14	A	840	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
14	A	834	CLA	O2D-CGD-CBD	2.44	115.60	111.27
14	B	3030	CLA	CMB-C2B-C3B	2.44	129.24	124.68
14	A	832	CLA	C4D-C3D-CAD	-2.44	107.11	108.47
14	A	802	CLA	C7-C6-C5	-2.44	106.74	113.36
14	A	806	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
14	B	3003	CLA	CHB-C4A-NA	2.43	127.87	124.51
14	B	3028	CLA	CMB-C2B-C3B	2.43	129.22	124.68
14	B	3018	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
16	B	3051	BCR	C33-C5-C6	-2.43	121.80	124.53
14	M	102	CLA	CMB-C2B-C3B	2.43	129.22	124.68
14	A	819	CLA	C1-C2-C3	-2.43	121.84	126.04
14	A	824	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
14	B	3003	CLA	CMB-C2B-C1B	-2.42	124.74	128.46
14	A	835	CLA	CMB-C2B-C3B	2.42	129.21	124.68
16	B	3045	BCR	C16-C15-C14	-2.42	118.52	123.47
14	M	102	CLA	CMA-C3A-C4A	2.42	118.28	111.77
14	A	829	CLA	CMD-C2D-C3D	2.42	129.21	124.68
14	A	856	CLA	CMC-C2C-C3C	2.42	129.50	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	842	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
14	A	804	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
14	B	3008	CLA	CMC-C2C-C3C	2.42	129.50	124.94
14	L	204	CLA	O2A-CGA-O1A	-2.42	117.50	123.59
14	A	834	CLA	C1B-CHB-C4A	-2.41	125.33	130.12
16	L	209	BCR	C27-C26-C25	2.41	126.23	122.73
14	L	204	CLA	CHB-C4A-NA	2.41	127.85	124.51
14	B	3039	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
14	B	3009	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
14	A	811	CLA	CAA-C2A-C3A	2.41	119.38	112.78
16	L	208	BCR	C15-C14-C13	-2.41	123.87	127.31
14	B	3020	CLA	O2D-CGD-CBD	2.41	115.55	111.27
14	B	3011	CLA	CMB-C2B-C3B	2.41	129.18	124.68
14	A	842	CLA	O2A-CGA-O1A	-2.40	117.52	123.59
14	B	3027	CLA	O2D-CGD-CBD	2.40	115.54	111.27
14	B	3034	CLA	O2A-CGA-O1A	-2.40	117.52	123.59
14	B	3030	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
17	B	3049	LMG	C9-C8-C7	-2.40	106.10	111.79
14	A	821	CLA	CHB-C4A-NA	2.40	127.83	124.51
14	B	3008	CLA	C4D-C3D-CAD	-2.40	107.13	108.47
17	A	852	LMG	O3-C3-C2	-2.40	104.80	110.35
14	A	823	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
14	K	101	CLA	CHB-C4A-NA	2.40	127.83	124.51
14	M	102	CLA	CBC-CAC-C3C	2.40	118.37	112.27
13	A	801	CL0	C1B-CHB-C4A	-2.40	125.37	130.12
14	A	828	CLA	CMD-C2D-C3D	2.40	129.16	124.68
14	B	3034	CLA	C1B-CHB-C4A	-2.39	125.37	130.12
16	A	850	BCR	C2-C1-C6	2.39	114.16	110.48
14	A	842	CLA	CMC-C2C-C3C	2.39	129.45	124.94
14	B	3031	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
14	B	3029	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
14	A	832	CLA	CMB-C2B-C3B	2.38	129.14	124.68
14	A	835	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
14	A	826	CLA	CHB-C4A-NA	2.38	127.81	124.51
14	A	810	CLA	CHB-C4A-NA	2.38	127.81	124.51
14	A	818	CLA	CMB-C2B-C3B	2.38	129.14	124.68
14	A	808	CLA	O2D-CGD-CBD	2.38	115.50	111.27
14	A	816	CLA	CMC-C2C-C3C	2.38	129.43	124.94
14	B	3007	CLA	CHB-C4A-NA	2.38	127.80	124.51
14	A	816	CLA	CHB-C4A-NA	2.38	127.80	124.51
14	B	3008	CLA	CMB-C2B-C3B	2.38	129.13	124.68
14	J	101	CLA	CMD-C2D-C3D	2.38	129.13	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	801	CL0	CMB-C2B-C3B	2.38	129.12	124.68
14	B	3010	CLA	CMD-C2D-C3D	2.38	129.12	124.68
14	B	3028	CLA	CHB-C4A-NA	2.38	127.80	124.51
14	A	821	CLA	O2D-CGD-CBD	2.38	115.49	111.27
14	A	844	CLA	C1-C2-C3	-2.38	121.94	126.04
17	A	855	LMG	O6-C1-C2	-2.37	105.33	110.35
14	A	821	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
14	A	812	CLA	C7-C6-C5	-2.37	106.92	113.36
14	A	807	CLA	CMD-C2D-C3D	2.37	129.11	124.68
14	A	833	CLA	C4D-C3D-CAD	-2.37	107.15	108.47
16	A	851	BCR	C15-C16-C17	-2.37	118.62	123.47
14	B	3030	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
14	B	3006	CLA	CHB-C4A-NA	2.37	127.79	124.51
14	A	829	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
14	B	3026	CLA	CMD-C2D-C3D	2.37	129.11	124.68
14	B	3034	CLA	CHB-C4A-NA	2.37	127.78	124.51
17	I	102	LMG	C8-O7-C10	2.37	123.62	117.79
16	A	847	BCR	C27-C26-C25	2.37	126.17	122.73
14	B	3038	CLA	CHB-C4A-NA	2.37	127.78	124.51
16	I	101	BCR	C8-C7-C6	-2.37	120.56	127.20
16	B	3048	BCR	C15-C16-C17	-2.37	118.63	123.47
14	B	3003	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
14	A	842	CLA	C4D-C3D-CAD	-2.36	107.15	108.47
14	A	830	CLA	C3A-C2A-C1A	2.36	104.88	101.34
14	A	809	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
14	A	830	CLA	CHB-C4A-NA	2.36	127.78	124.51
14	B	3027	CLA	CMC-C2C-C3C	2.36	129.39	124.94
14	A	808	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
14	B	3033	CLA	C1-C2-C3	-2.36	121.97	126.04
14	B	3003	CLA	CMC-C2C-C3C	2.35	129.38	124.94
14	J	102	CLA	CMB-C2B-C3B	2.35	129.08	124.68
16	B	3045	BCR	C8-C7-C6	-2.35	120.60	127.20
14	B	3042	CLA	CMB-C2B-C1B	-2.35	124.86	128.46
14	A	810	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
13	A	801	CL0	O1D-CGD-CBD	2.35	129.29	124.48
16	A	848	BCR	C35-C13-C14	-2.35	119.64	122.92
14	L	205	CLA	CHB-C4A-NA	2.35	127.75	124.51
14	A	812	CLA	CMB-C2B-C1B	-2.34	124.86	128.46
14	B	3036	CLA	CBC-CAC-C3C	2.34	118.24	112.27
14	B	3010	CLA	CMC-C2C-C3C	2.34	129.36	124.94
14	B	3006	CLA	O2D-CGD-CBD	2.34	115.43	111.27
14	B	3020	CLA	CHB-C4A-NA	2.34	127.75	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	202	CLA	CMB-C2B-C3B	2.34	129.06	124.68
16	F	203	BCR	C38-C26-C25	-2.34	121.90	124.53
14	A	832	CLA	C1-C2-C3	-2.34	122.97	126.75
14	A	837	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
14	A	802	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
16	B	3048	BCR	C2-C1-C6	2.34	114.08	110.48
16	J	105	BCR	C3-C4-C5	-2.34	109.90	114.08
14	A	807	CLA	C4D-C3D-CAD	-2.34	107.17	108.47
14	A	836	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
14	B	3011	CLA	C2A-C1A-CHA	2.34	127.94	123.86
14	A	826	CLA	C4D-C3D-CAD	-2.33	107.17	108.47
14	B	3011	CLA	O1D-CGD-CBD	2.33	129.26	124.48
14	A	840	CLA	CHB-C4A-NA	2.33	127.74	124.51
14	A	814	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
14	A	839	CLA	OBD-CAD-CBD	-2.33	122.57	125.89
14	A	818	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
14	B	3041	CLA	CHB-C4A-NA	2.33	127.73	124.51
14	A	812	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
14	B	3020	CLA	C1-C2-C3	-2.32	122.02	126.04
14	L	206	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
22	L	207	DGD	O6E-C1E-O5D	-2.32	104.47	109.97
14	B	3039	CLA	CHB-C4A-NA	2.32	127.72	124.51
16	A	851	BCR	C33-C5-C6	-2.32	121.92	124.53
14	A	824	CLA	CMD-C2D-C3D	2.32	129.02	124.68
14	A	825	CLA	CHB-C4A-NA	2.32	127.72	124.51
14	X	1701	CLA	O2D-CGD-CBD	2.32	115.39	111.27
14	A	837	CLA	CHB-C4A-NA	2.32	127.72	124.51
16	M	103	BCR	C8-C7-C6	-2.32	120.70	127.20
14	A	838	CLA	CHA-C1A-NA	-2.32	121.10	126.40
14	A	829	CLA	C1-C2-C3	-2.31	122.04	126.04
16	K	102	BCR	C40-C30-C25	2.31	114.05	110.30
14	B	3035	CLA	CMB-C2B-C3B	2.31	129.00	124.68
16	K	102	BCR	C24-C23-C22	-2.31	122.74	126.23
14	A	831	CLA	C1-C2-C3	-2.31	122.05	126.04
16	B	3046	BCR	C2-C1-C6	2.31	114.04	110.48
16	A	849	BCR	C8-C7-C6	-2.31	120.71	127.20
14	B	3022	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
14	X	1701	CLA	CMC-C2C-C3C	2.31	129.29	124.94
16	B	3044	BCR	C30-C25-C26	-2.31	119.37	122.61
14	K	103	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
14	B	3022	CLA	CMC-C2C-C3C	2.30	129.29	124.94
17	I	102	LMG	O2-C2-C1	-2.30	104.45	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3012	CLA	CED-O2D-CGD	2.30	121.14	115.94
14	A	841	CLA	CMB-C2B-C3B	2.30	128.99	124.68
16	L	208	BCR	C7-C8-C9	-2.30	122.76	126.23
14	B	3042	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
14	A	825	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
14	L	205	CLA	CAA-C2A-C1A	-2.30	104.44	111.97
14	A	832	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
14	A	842	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
14	A	822	CLA	CMD-C2D-C3D	2.30	128.98	124.68
16	F	203	BCR	C33-C5-C6	-2.30	121.95	124.53
21	L	202	LMT	O5B-C5B-C4B	2.30	113.87	109.69
14	A	818	CLA	CHB-C4A-NA	2.29	127.69	124.51
16	L	208	BCR	C20-C21-C22	-2.29	124.04	127.31
14	A	820	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
14	A	820	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
14	A	836	CLA	CHB-C4A-NA	2.29	127.68	124.51
14	A	843	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
14	A	845	CLA	C6-C5-C3	2.29	118.36	114.62
14	B	3007	CLA	CMB-C2B-C3B	2.29	128.96	124.68
14	A	806	CLA	CMD-C2D-C3D	2.29	128.96	124.68
14	B	3004	CLA	CMC-C2C-C3C	2.29	129.25	124.94
14	J	101	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
14	A	811	CLA	O2D-CGD-CBD	2.29	115.33	111.27
15	A	846	PQN	C5-C4-C3	2.29	122.61	118.42
14	A	822	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
14	B	3006	CLA	C4D-C3D-CAD	-2.28	107.20	108.47
14	A	843	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
17	A	855	LMG	O2-C2-C1	-2.28	104.51	110.05
14	B	3031	CLA	C4D-C3D-CAD	-2.28	107.20	108.47
14	M	102	CLA	CMA-C3A-C2A	-2.28	104.64	113.83
14	B	3015	CLA	O1D-CGD-CBD	2.28	129.14	124.48
14	A	813	CLA	C3A-C2A-C1A	2.28	104.75	101.34
16	B	3045	BCR	C28-C27-C26	-2.28	110.01	114.08
14	B	3025	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
14	L	205	CLA	C4D-C3D-CAD	-2.27	107.20	108.47
16	L	209	BCR	C15-C14-C13	-2.27	124.07	127.31
14	B	3025	CLA	O2D-CGD-CBD	2.27	115.31	111.27
14	B	3013	CLA	CHB-C4A-NA	2.27	127.65	124.51
14	A	831	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
14	A	803	CLA	CMB-C2B-C3B	2.27	128.92	124.68
16	F	203	BCR	C16-C15-C14	-2.27	118.83	123.47
14	A	832	CLA	C1B-CHB-C4A	-2.27	125.63	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	849	BCR	C35-C13-C14	-2.26	119.75	122.92
16	I	101	BCR	C27-C26-C25	2.26	126.01	122.73
14	A	819	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
14	A	845	CLA	CMC-C2C-C3C	2.26	129.20	124.94
14	B	3030	CLA	CAA-CBA-CGA	-2.26	106.66	113.25
14	B	3015	CLA	CHB-C4A-NA	2.26	127.63	124.51
16	F	201	BCR	C33-C5-C6	-2.26	121.99	124.53
14	A	830	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
14	A	845	CLA	CMB-C2B-C3B	2.25	128.90	124.68
14	A	838	CLA	CMB-C2B-C3B	2.25	128.89	124.68
14	A	841	CLA	CHB-C4A-NA	2.25	127.62	124.51
14	B	3042	CLA	O2D-CGD-CBD	2.25	115.27	111.27
14	A	834	CLA	CBC-CAC-C3C	-2.25	106.54	112.27
14	A	823	CLA	C2A-C1A-CHA	2.25	127.79	123.86
14	B	3010	CLA	C6-C7-C8	-2.25	108.66	115.92
14	B	3014	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
14	B	3015	CLA	CMC-C2C-C3C	2.25	129.18	124.94
16	J	105	BCR	C15-C16-C17	-2.25	118.87	123.47
16	J	104	BCR	C8-C7-C6	-2.24	120.90	127.20
14	A	807	CLA	CMB-C2B-C3B	2.24	128.87	124.68
14	A	835	CLA	C4-C3-C2	-2.24	117.93	123.68
16	F	201	BCR	C37-C22-C21	-2.24	119.78	122.92
18	A	853	LHG	C18-C17-C16	-2.24	103.05	114.42
15	B	3043	PQN	C10-C1-C2	2.24	122.15	118.95
14	A	826	CLA	CMD-C2D-C3D	2.24	128.86	124.68
14	B	3005	CLA	C3A-C2A-C1A	2.24	104.69	101.34
14	A	806	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
14	A	827	CLA	CHB-C4A-NA	2.23	127.60	124.51
14	B	3037	CLA	CMB-C2B-C3B	2.23	128.85	124.68
16	K	102	BCR	C8-C7-C6	-2.23	120.94	127.20
16	I	101	BCR	C33-C5-C6	-2.23	122.02	124.53
14	B	3012	CLA	O2D-CGD-CBD	2.23	115.23	111.27
16	L	201	BCR	C28-C27-C26	-2.23	110.10	114.08
21	L	202	LMT	O1'-C1'-C2'	2.23	111.78	108.30
14	A	808	CLA	CMB-C2B-C3B	2.23	128.85	124.68
16	B	3047	BCR	C37-C22-C21	-2.23	119.80	122.92
14	A	844	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
14	A	807	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
14	A	844	CLA	CMC-C2C-C3C	2.22	129.13	124.94
16	A	847	BCR	C35-C13-C14	-2.22	119.81	122.92
15	A	846	PQN	O4-C4-C3	-2.22	116.98	120.56
16	L	208	BCR	C38-C26-C27	-2.22	109.35	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	833	CLA	C3A-C2A-C1A	2.22	104.67	101.34
14	A	831	CLA	CHB-C4A-NA	2.22	127.58	124.51
16	J	105	BCR	C15-C14-C13	-2.22	124.14	127.31
14	A	823	CLA	CMB-C2B-C3B	2.22	128.83	124.68
14	A	822	CLA	OBD-CAD-CBD	-2.22	122.73	125.89
15	B	3043	PQN	O4-C4-C3	-2.22	117.00	120.56
14	A	819	CLA	C4D-C3D-CAD	-2.22	107.23	108.47
14	A	828	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
17	A	855	LMG	O3-C3-C2	-2.21	105.23	110.35
16	I	101	BCR	C11-C10-C9	-2.21	124.15	127.31
14	J	102	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
14	B	3006	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
14	B	3024	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
14	B	3012	CLA	CMC-C2C-C3C	2.21	129.11	124.94
14	A	841	CLA	O2A-C1-C2	-2.21	102.83	108.64
17	A	852	LMG	O2-C2-C1	-2.21	104.68	110.05
14	B	3039	CLA	CMC-C2C-C3C	2.21	129.10	124.94
22	L	207	DGD	CBB-CAB-C9B	-2.21	103.22	114.42
16	B	3047	BCR	C15-C14-C13	-2.21	124.16	127.31
14	K	103	CLA	CHB-C4A-NA	2.20	127.56	124.51
14	B	3018	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
14	B	3024	CLA	CHB-C4A-NA	2.20	127.56	124.51
14	B	3034	CLA	CAA-C2A-C1A	-2.20	104.77	111.97
17	B	3049	LMG	O2-C2-C1	-2.20	104.70	110.05
14	B	3040	CLA	CHB-C4A-NA	2.20	127.55	124.51
14	B	3009	CLA	CMC-C2C-C3C	2.20	129.09	124.94
14	A	806	CLA	CMB-C2B-C1B	-2.20	125.08	128.46
14	B	3015	CLA	CMB-C2B-C3B	2.20	128.79	124.68
14	B	3038	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
14	B	3023	CLA	CMD-C2D-C3D	2.20	128.79	124.68
14	B	3039	CLA	CMB-C2B-C3B	2.19	128.78	124.68
14	B	3004	CLA	C2A-C1A-CHA	2.19	127.70	123.86
14	A	845	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
16	B	3045	BCR	C2-C1-C6	2.19	113.85	110.48
14	B	3034	CLA	O2D-CGD-CBD	2.19	115.16	111.27
14	B	3019	CLA	O2D-CGD-CBD	2.19	115.16	111.27
16	K	102	BCR	C33-C5-C6	-2.19	122.07	124.53
16	A	847	BCR	C36-C18-C17	-2.18	119.86	122.92
14	A	815	CLA	CMB-C2B-C3B	2.18	128.76	124.68
14	A	820	CLA	C4D-C3D-CAD	-2.18	107.25	108.47
14	A	822	CLA	C4D-C3D-CAD	-2.18	107.25	108.47
14	A	833	CLA	CHB-C4A-NA	2.18	127.53	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	209	BCR	C37-C22-C21	-2.18	119.87	122.92
14	A	828	CLA	O2D-CGD-CBD	2.18	115.14	111.27
14	J	101	CLA	C4D-C3D-CAD	-2.18	107.26	108.47
14	A	824	CLA	O2A-CGA-O1A	-2.17	118.10	123.59
14	B	3005	CLA	CMC-C2C-C3C	2.17	129.04	124.94
14	A	812	CLA	CMD-C2D-C3D	2.17	128.75	124.68
14	B	3033	CLA	CMB-C2B-C3B	2.17	128.74	124.68
14	L	205	CLA	CMC-C2C-C3C	2.17	129.04	124.94
16	J	104	BCR	C15-C14-C13	-2.17	124.21	127.31
14	A	821	CLA	CMD-C2D-C3D	2.17	128.74	124.68
14	A	823	CLA	CMD-C2D-C3D	2.17	128.74	124.68
14	B	3040	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
14	A	813	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
14	A	821	CLA	CMA-C3A-C2A	-2.17	111.04	116.10
16	J	104	BCR	C27-C26-C25	2.16	125.87	122.73
14	B	3032	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
14	M	102	CLA	C4D-C3D-CAD	-2.16	107.26	108.47
14	A	835	CLA	CMB-C2B-C1B	-2.16	125.14	128.46
14	A	837	CLA	O2D-CGD-CBD	2.16	115.11	111.27
14	M	102	CLA	CGD-CBD-CAD	2.16	117.73	110.73
14	B	3014	CLA	CHB-C4A-NA	2.16	127.50	124.51
14	B	3009	CLA	CMB-C2B-C1B	-2.16	125.15	128.46
14	A	824	CLA	C4D-C3D-CAD	-2.16	107.27	108.47
14	A	831	CLA	C4D-C3D-CAD	-2.16	107.27	108.47
14	A	838	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
18	B	3050	LHG	O8-C23-C24	2.15	121.77	112.38
14	A	818	CLA	C4D-C3D-CAD	-2.15	107.27	108.47
13	A	801	CL0	C1D-CHD-C4C	2.15	125.40	122.56
14	B	3021	CLA	CHB-C4A-NA	2.15	127.49	124.51
18	A	854	LHG	C11-C10-C9	-2.15	103.52	114.42
14	B	3023	CLA	OBD-CAD-CBD	-2.15	122.83	125.89
14	B	3032	CLA	O1D-CGD-CBD	2.15	128.87	124.48
16	A	847	BCR	C15-C16-C17	-2.15	119.08	123.47
16	J	105	BCR	C33-C5-C6	-2.14	122.12	124.53
14	A	807	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
14	B	3040	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
14	A	820	CLA	C3A-C2A-C1A	2.14	104.55	101.34
14	L	206	CLA	CMD-C2D-C3D	2.14	128.69	124.68
16	L	209	BCR	C40-C30-C25	2.14	113.77	110.30
15	A	846	PQN	C10-C1-C2	2.14	122.00	118.95
18	A	853	LHG	O8-C23-C24	2.14	118.62	111.91
14	A	856	CLA	C4-C3-C5	2.14	118.87	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	848	BCR	C8-C7-C6	-2.14	121.19	127.20
14	L	206	CLA	CAA-C2A-C1A	-2.14	104.97	111.97
14	A	812	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
14	L	204	CLA	C11-C10-C8	-2.14	109.02	115.92
16	F	203	BCR	C1-C6-C5	-2.13	119.61	122.61
14	A	832	CLA	CMD-C2D-C3D	2.13	128.66	124.68
14	B	3005	CLA	CMB-C2B-C3B	2.13	128.66	124.68
16	A	848	BCR	C37-C22-C21	-2.13	119.94	122.92
14	B	3029	CLA	C2A-C1A-CHA	2.13	127.58	123.86
14	B	3026	CLA	CMC-C2C-C3C	2.13	128.95	124.94
14	A	845	CLA	CAA-CBA-CGA	-2.13	107.04	113.25
16	I	101	BCR	C15-C14-C13	-2.13	124.28	127.31
14	B	3005	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
14	B	3020	CLA	C4-C3-C5	2.13	118.85	115.27
14	A	805	CLA	CMB-C2B-C3B	2.12	128.65	124.68
14	B	3033	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
16	J	105	BCR	C35-C13-C14	-2.12	119.95	122.92
16	L	208	BCR	C35-C13-C14	-2.12	119.95	122.92
14	A	811	CLA	CMC-C2C-C3C	2.12	128.94	124.94
14	B	3019	CLA	C4D-C3D-CAD	-2.12	107.29	108.47
16	B	3047	BCR	C33-C5-C6	-2.12	122.15	124.53
15	B	3043	PQN	C2M-C2-C1	2.12	119.78	116.27
16	B	3046	BCR	C28-C27-C26	-2.12	110.29	114.08
14	J	102	CLA	CMA-C3A-C2A	-2.12	111.16	116.10
14	B	3041	CLA	O2A-CGA-O1A	-2.11	118.25	123.59
14	A	841	CLA	C4-C3-C5	2.11	118.83	115.27
16	B	3044	BCR	C11-C10-C9	-2.11	124.30	127.31
14	B	3038	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
14	B	3013	CLA	C4D-C3D-CAD	-2.11	107.29	108.47
17	A	852	LMG	C1-O6-C5	-2.11	109.55	113.69
14	B	3006	CLA	CMB-C2B-C1B	-2.11	125.22	128.46
14	A	803	CLA	CMD-C2D-C3D	2.10	128.62	124.68
14	A	813	CLA	CMC-C2C-C3C	2.10	128.91	124.94
14	B	3013	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
14	A	812	CLA	CMC-C2C-C3C	2.10	128.91	124.94
14	A	831	CLA	O1D-CGD-CBD	2.10	128.78	124.48
14	B	3014	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
14	A	814	CLA	CMD-C2D-C3D	2.10	128.61	124.68
14	A	825	CLA	C4D-C3D-CAD	-2.10	107.30	108.47
14	B	3011	CLA	CHA-C1A-NA	-2.10	121.59	126.40
14	L	205	CLA	CMD-C2D-C3D	2.10	128.60	124.68
14	B	3037	CLA	C4D-C3D-CAD	-2.10	107.30	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	841	CLA	C4D-C3D-CAD	-2.10	107.30	108.47
14	A	826	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
14	A	816	CLA	OBD-CAD-CBD	-2.09	122.90	125.89
14	B	3015	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
14	A	822	CLA	O2D-CGD-CBD	2.09	114.98	111.27
13	A	801	CL0	CED-O2D-CGD	2.09	120.66	115.94
18	B	3050	LHG	O10-C23-C24	-2.09	117.20	124.81
16	B	3044	BCR	C33-C5-C6	-2.09	122.18	124.53
14	A	803	CLA	CAA-CBA-CGA	-2.09	107.16	113.25
16	B	3044	BCR	C8-C7-C6	-2.08	121.35	127.20
14	A	845	CLA	C5-C3-C2	2.08	125.33	121.12
16	F	201	BCR	C38-C26-C27	-2.08	109.62	113.62
14	A	826	CLA	O2D-CGD-CBD	2.08	114.96	111.27
15	B	3043	PQN	C5-C4-C3	2.08	122.23	118.42
14	B	3035	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
14	A	845	CLA	O2A-CGA-O1A	-2.08	118.36	123.59
14	M	102	CLA	OBD-CAD-CBD	-2.07	122.93	125.89
14	A	841	CLA	C5-C3-C2	-2.07	116.92	121.12
14	A	808	CLA	CHB-C4A-NA	2.07	127.37	124.51
22	L	207	DGD	C5B-C4B-C3B	-2.07	103.92	114.42
14	B	3036	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
14	A	838	CLA	CMC-C2C-C3C	2.07	128.84	124.94
17	A	852	LMG	C6-C5-C4	-2.07	108.16	113.00
14	J	101	CLA	O1D-CGD-CBD	2.07	128.71	124.48
14	A	804	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
14	A	833	CLA	CMC-C2C-C3C	2.06	128.83	124.94
14	B	3021	CLA	CMC-C2C-C3C	2.06	128.82	124.94
16	B	3046	BCR	C8-C7-C6	-2.06	121.42	127.20
14	B	3025	CLA	CMC-C2C-C3C	2.06	128.82	124.94
16	K	102	BCR	C30-C25-C26	-2.06	119.72	122.61
14	A	856	CLA	C1-C2-C3	-2.05	122.49	126.04
14	B	3015	CLA	CMD-C2D-C3D	2.05	128.52	124.68
14	A	810	CLA	O1D-CGD-CBD	2.05	128.68	124.48
14	B	3017	CLA	CMC-C2C-C3C	2.05	128.81	124.94
16	A	849	BCR	C30-C25-C26	-2.05	119.73	122.61
18	A	853	LHG	C20-C19-C18	-2.05	104.03	114.42
14	J	102	CLA	OBD-CAD-C3D	2.05	129.28	127.19
14	B	3036	CLA	CHB-C4A-NA	2.05	127.34	124.51
14	B	3019	CLA	C1-O2A-CGA	2.05	121.81	116.44
14	B	3011	CLA	C11-C12-C13	-2.04	109.32	115.92
14	A	840	CLA	CBA-CAA-C2A	2.04	119.89	113.86
14	A	829	CLA	CHB-C4A-NA	2.04	127.33	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	801	CL0	O2A-CGA-O1A	-2.04	118.44	123.59
14	K	103	CLA	CAA-C2A-C1A	-2.04	105.29	111.97
18	A	853	LHG	C11-C10-C9	-2.04	104.08	114.42
14	A	825	CLA	O2D-CGD-CBD	2.04	114.89	111.27
22	L	207	DGD	O3E-C3E-C2E	-2.04	105.64	110.35
14	B	3029	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
14	B	3032	CLA	CMC-C2C-C3C	2.03	128.78	124.94
14	F	202	CLA	CMC-C2C-C3C	2.03	128.78	124.94
14	A	830	CLA	C4D-C3D-CAD	-2.03	107.34	108.47
22	L	207	DGD	O6D-C1D-O3G	-2.03	105.18	109.97
14	B	3030	CLA	OBD-CAD-CBD	-2.03	123.00	125.89
14	A	831	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
14	A	836	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
17	B	3049	LMG	C40-C39-C38	-2.02	104.15	114.42
16	K	102	BCR	C38-C26-C27	-2.02	109.73	113.62
14	L	204	CLA	C6-C7-C8	-2.02	109.39	115.92
14	A	810	CLA	CHA-C1A-NA	-2.02	121.77	126.40
14	A	836	CLA	CMC-C2C-C3C	2.02	128.75	124.94
14	A	834	CLA	C6-C7-C8	-2.02	109.39	115.92
14	A	835	CLA	C6-C5-C3	2.02	118.74	113.45
14	B	3040	CLA	CMC-C2C-C3C	2.02	128.74	124.94
14	B	3019	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
14	A	814	CLA	C4D-C3D-CAD	-2.01	107.35	108.47
14	B	3034	CLA	CAA-CBA-CGA	-2.01	107.37	113.25
14	A	827	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
18	M	101	LHG	C20-C19-C18	-2.01	104.22	114.42
18	A	853	LHG	C10-C9-C8	-2.01	105.96	113.19
16	B	3048	BCR	C8-C7-C6	-2.01	121.56	127.20
14	A	826	CLA	C11-C10-C8	-2.01	109.43	115.92
16	B	3046	BCR	C27-C26-C25	2.01	125.65	122.73
22	L	207	DGD	C1E-O6E-C5E	2.01	117.62	113.69
17	A	852	LMG	O7-C10-O9	-2.01	118.86	123.70
14	B	3007	CLA	C4D-C3D-CAD	-2.00	107.35	108.47
14	B	3032	CLA	C1B-CHB-C4A	-2.00	126.15	130.12
16	A	851	BCR	C35-C13-C14	-2.00	120.12	122.92
16	B	3045	BCR	C35-C13-C14	-2.00	120.12	122.92
14	B	3003	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
14	A	817	CLA	CHB-C4A-NA	2.00	127.28	124.51
14	B	3006	CLA	CMB-C2B-C3B	2.00	128.42	124.68

All (95) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	801	CL0	NA
13	A	801	CL0	NC
13	A	801	CL0	ND
14	A	802	CLA	ND
14	A	803	CLA	ND
14	A	804	CLA	ND
14	A	805	CLA	ND
14	A	806	CLA	ND
14	A	807	CLA	ND
14	A	808	CLA	ND
14	A	809	CLA	ND
14	A	810	CLA	ND
14	A	811	CLA	ND
14	A	812	CLA	ND
14	A	813	CLA	ND
14	A	814	CLA	ND
14	A	815	CLA	ND
14	A	816	CLA	ND
14	A	817	CLA	ND
14	A	818	CLA	ND
14	A	819	CLA	ND
14	A	820	CLA	ND
14	A	821	CLA	ND
14	A	822	CLA	ND
14	A	823	CLA	ND
14	A	824	CLA	ND
14	A	825	CLA	ND
14	A	826	CLA	ND
14	A	827	CLA	ND
14	A	828	CLA	ND
14	A	829	CLA	ND
14	A	830	CLA	ND
14	A	831	CLA	ND
14	A	832	CLA	ND
14	A	833	CLA	ND
14	A	834	CLA	ND
14	A	835	CLA	ND
14	A	836	CLA	ND
14	A	837	CLA	ND
14	A	838	CLA	ND
14	A	839	CLA	ND
14	A	840	CLA	ND
14	A	841	CLA	ND

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Mol	Chain	Res	Type	Atom
14	A	842	CLA	ND
14	A	843	CLA	ND
14	A	844	CLA	ND
14	A	845	CLA	ND
14	A	856	CLA	ND
14	B	3003	CLA	ND
14	B	3004	CLA	ND
14	B	3005	CLA	ND
14	B	3006	CLA	ND
14	B	3007	CLA	ND
14	B	3008	CLA	ND
14	B	3009	CLA	ND
14	B	3010	CLA	ND
14	B	3011	CLA	ND
14	B	3012	CLA	ND
14	B	3013	CLA	ND
14	B	3014	CLA	ND
14	B	3015	CLA	ND
14	B	3016	CLA	ND
14	B	3017	CLA	ND
14	B	3018	CLA	ND
14	B	3019	CLA	ND
14	B	3020	CLA	ND
14	B	3021	CLA	ND
14	B	3022	CLA	ND
14	B	3023	CLA	ND
14	B	3024	CLA	ND
14	B	3026	CLA	ND
14	B	3027	CLA	ND
14	B	3028	CLA	ND
14	B	3029	CLA	ND
14	B	3030	CLA	ND
14	B	3031	CLA	ND
14	B	3032	CLA	ND
14	B	3033	CLA	ND
14	B	3034	CLA	ND
14	B	3035	CLA	ND
14	B	3036	CLA	ND
14	B	3037	CLA	ND
14	B	3039	CLA	ND
14	B	3041	CLA	ND
14	B	3042	CLA	ND

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Mol	Chain	Res	Type	Atom
14	F	202	CLA	ND
14	J	101	CLA	ND
14	J	102	CLA	ND
14	K	101	CLA	ND
14	K	103	CLA	ND
14	L	204	CLA	ND
14	L	205	CLA	ND
14	L	206	CLA	ND
14	M	102	CLA	ND
14	X	1701	CLA	ND

All (1307) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	801	CL0	C1A-C2A-CAA-CBA
13	A	801	CL0	C3A-C2A-CAA-CBA
14	A	806	CLA	C1A-C2A-CAA-CBA
14	A	806	CLA	CAD-CBD-CGD-O1D
14	A	806	CLA	CAD-CBD-CGD-O2D
14	A	806	CLA	C2-C3-C5-C6
14	A	806	CLA	C4-C3-C5-C6
14	A	807	CLA	CHA-CBD-CGD-O1D
14	A	807	CLA	CHA-CBD-CGD-O2D
14	A	807	CLA	CBD-CGD-O2D-CED
14	A	808	CLA	C1A-C2A-CAA-CBA
14	A	808	CLA	C2-C3-C5-C6
14	A	808	CLA	C4-C3-C5-C6
14	A	809	CLA	C1A-C2A-CAA-CBA
14	A	809	CLA	C3A-C2A-CAA-CBA
14	A	811	CLA	C3A-C2A-CAA-CBA
14	A	812	CLA	C1A-C2A-CAA-CBA
14	A	812	CLA	C3A-C2A-CAA-CBA
14	A	817	CLA	CBD-CGD-O2D-CED
14	A	819	CLA	C3A-C2A-CAA-CBA
14	A	819	CLA	CBD-CGD-O2D-CED
14	A	820	CLA	C1A-C2A-CAA-CBA
14	A	820	CLA	C3A-C2A-CAA-CBA
14	A	820	CLA	CBD-CGD-O2D-CED
14	A	821	CLA	CHA-CBD-CGD-O1D
14	A	821	CLA	CHA-CBD-CGD-O2D
14	A	822	CLA	CBD-CGD-O2D-CED
14	A	823	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	A	823	CLA	CAD-CBD-CGD-O1D
14	A	823	CLA	CAD-CBD-CGD-O2D
14	A	824	CLA	C3A-C2A-CAA-CBA
14	A	824	CLA	CHA-CBD-CGD-O1D
14	A	824	CLA	CHA-CBD-CGD-O2D
14	A	829	CLA	CHA-CBD-CGD-O1D
14	A	829	CLA	CHA-CBD-CGD-O2D
14	A	829	CLA	CBD-CGD-O2D-CED
14	A	832	CLA	C1A-C2A-CAA-CBA
14	A	832	CLA	C3A-C2A-CAA-CBA
14	A	835	CLA	C1A-C2A-CAA-CBA
14	A	835	CLA	C3A-C2A-CAA-CBA
14	A	837	CLA	C1A-C2A-CAA-CBA
14	A	837	CLA	C3A-C2A-CAA-CBA
14	A	837	CLA	CHA-CBD-CGD-O1D
14	A	837	CLA	CHA-CBD-CGD-O2D
14	A	838	CLA	CBD-CGD-O2D-CED
14	A	840	CLA	CHA-CBD-CGD-O1D
14	A	840	CLA	CHA-CBD-CGD-O2D
14	A	842	CLA	CBD-CGD-O2D-CED
14	A	843	CLA	C1A-C2A-CAA-CBA
14	A	843	CLA	C3A-C2A-CAA-CBA
14	A	844	CLA	CBD-CGD-O2D-CED
14	A	845	CLA	C2C-C3C-CAC-CBC
14	A	845	CLA	CBD-CGD-O2D-CED
14	A	845	CLA	O1D-CGD-O2D-CED
14	A	856	CLA	C2-C3-C5-C6
14	A	856	CLA	C4-C3-C5-C6
14	B	3003	CLA	CHA-CBD-CGD-O1D
14	B	3003	CLA	CHA-CBD-CGD-O2D
14	B	3003	CLA	CBD-CGD-O2D-CED
14	B	3004	CLA	CBD-CGD-O2D-CED
14	B	3005	CLA	CBD-CGD-O2D-CED
14	B	3006	CLA	C1A-C2A-CAA-CBA
14	B	3006	CLA	C3A-C2A-CAA-CBA
14	B	3006	CLA	CBD-CGD-O2D-CED
14	B	3009	CLA	CHA-CBD-CGD-O1D
14	B	3009	CLA	CHA-CBD-CGD-O2D
14	B	3012	CLA	CBD-CGD-O2D-CED
14	B	3012	CLA	O1D-CGD-O2D-CED
14	B	3013	CLA	C2A-CAA-CBA-CGA
14	B	3018	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	B	3018	CLA	C3A-C2A-CAA-CBA
14	B	3019	CLA	C3A-C2A-CAA-CBA
14	B	3021	CLA	C1A-C2A-CAA-CBA
14	B	3021	CLA	C3A-C2A-CAA-CBA
14	B	3021	CLA	CHA-CBD-CGD-O1D
14	B	3021	CLA	CHA-CBD-CGD-O2D
14	B	3021	CLA	CAD-CBD-CGD-O1D
14	B	3022	CLA	C1A-C2A-CAA-CBA
14	B	3022	CLA	C3A-C2A-CAA-CBA
14	B	3025	CLA	C2-C3-C5-C6
14	B	3025	CLA	C4-C3-C5-C6
14	B	3029	CLA	C1A-C2A-CAA-CBA
14	B	3029	CLA	C3A-C2A-CAA-CBA
14	B	3029	CLA	CHA-CBD-CGD-O1D
14	B	3030	CLA	CHA-CBD-CGD-O2D
14	B	3031	CLA	CHA-CBD-CGD-O1D
14	B	3031	CLA	CHA-CBD-CGD-O2D
14	B	3031	CLA	CAD-CBD-CGD-O1D
14	B	3031	CLA	CAD-CBD-CGD-O2D
14	B	3032	CLA	CBD-CGD-O2D-CED
14	B	3033	CLA	C1A-C2A-CAA-CBA
14	B	3033	CLA	C3A-C2A-CAA-CBA
14	B	3035	CLA	CBD-CGD-O2D-CED
14	B	3036	CLA	C1A-C2A-CAA-CBA
14	B	3036	CLA	C3A-C2A-CAA-CBA
14	B	3037	CLA	CBD-CGD-O2D-CED
14	B	3041	CLA	C2A-CAA-CBA-CGA
14	B	3041	CLA	C2C-C3C-CAC-CBC
14	B	3041	CLA	C4C-C3C-CAC-CBC
14	B	3042	CLA	C1A-C2A-CAA-CBA
14	F	202	CLA	CBD-CGD-O2D-CED
14	J	101	CLA	C1A-C2A-CAA-CBA
14	J	101	CLA	C3A-C2A-CAA-CBA
14	K	103	CLA	C1A-C2A-CAA-CBA
14	K	103	CLA	C3A-C2A-CAA-CBA
14	L	204	CLA	C1A-C2A-CAA-CBA
14	L	204	CLA	C3A-C2A-CAA-CBA
14	M	102	CLA	C2C-C3C-CAC-CBC
14	M	102	CLA	CBD-CGD-O2D-CED
16	A	847	BCR	C11-C12-C13-C14
16	A	847	BCR	C15-C16-C17-C18
16	A	847	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
16	A	847	BCR	C18-C19-C20-C21
16	A	847	BCR	C22-C23-C24-C25
16	A	848	BCR	C7-C8-C9-C34
16	A	848	BCR	C11-C10-C9-C8
16	A	848	BCR	C11-C12-C13-C35
16	A	848	BCR	C20-C21-C22-C37
16	A	849	BCR	C5-C6-C7-C8
16	A	849	BCR	C23-C24-C25-C26
16	A	850	BCR	C7-C8-C9-C10
16	A	850	BCR	C7-C8-C9-C34
16	A	850	BCR	C20-C21-C22-C37
16	A	850	BCR	C22-C23-C24-C25
16	A	851	BCR	C7-C8-C9-C34
16	A	851	BCR	C11-C10-C9-C8
16	A	851	BCR	C11-C10-C9-C34
16	A	851	BCR	C11-C12-C13-C35
16	A	851	BCR	C20-C21-C22-C37
16	A	851	BCR	C21-C22-C23-C24
16	A	851	BCR	C22-C23-C24-C25
16	A	851	BCR	C23-C24-C25-C26
16	A	851	BCR	C23-C24-C25-C30
16	B	3044	BCR	C7-C8-C9-C10
16	B	3044	BCR	C21-C22-C23-C24
16	B	3044	BCR	C37-C22-C23-C24
16	B	3045	BCR	C6-C7-C8-C9
16	B	3045	BCR	C7-C8-C9-C10
16	B	3045	BCR	C11-C12-C13-C35
16	B	3045	BCR	C21-C22-C23-C24
16	B	3046	BCR	C7-C8-C9-C34
16	B	3046	BCR	C11-C10-C9-C8
16	B	3046	BCR	C11-C10-C9-C34
16	B	3046	BCR	C10-C11-C12-C13
16	B	3046	BCR	C22-C23-C24-C25
16	B	3047	BCR	C7-C8-C9-C10
16	B	3047	BCR	C7-C8-C9-C34
16	B	3047	BCR	C10-C11-C12-C13
16	B	3047	BCR	C11-C12-C13-C14
16	B	3047	BCR	C16-C17-C18-C36
16	B	3048	BCR	C18-C19-C20-C21
16	B	3051	BCR	C11-C10-C9-C34
16	B	3051	BCR	C11-C12-C13-C35
16	F	201	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
16	F	203	BCR	C7-C8-C9-C34
16	F	203	BCR	C12-C13-C14-C15
16	F	203	BCR	C20-C21-C22-C37
16	I	101	BCR	C7-C8-C9-C34
16	I	101	BCR	C22-C23-C24-C25
16	J	103	BCR	C6-C7-C8-C9
16	J	103	BCR	C11-C12-C13-C35
16	J	103	BCR	C35-C13-C14-C15
16	J	103	BCR	C37-C22-C23-C24
16	J	104	BCR	C1-C6-C7-C8
16	J	104	BCR	C5-C6-C7-C8
16	J	104	BCR	C7-C8-C9-C34
16	J	104	BCR	C11-C12-C13-C35
16	J	104	BCR	C23-C24-C25-C26
16	J	105	BCR	C7-C8-C9-C10
16	J	105	BCR	C7-C8-C9-C34
16	J	105	BCR	C11-C12-C13-C14
16	J	105	BCR	C11-C12-C13-C35
16	J	105	BCR	C16-C17-C18-C36
16	J	105	BCR	C22-C23-C24-C25
16	K	102	BCR	C11-C10-C9-C34
16	K	102	BCR	C16-C17-C18-C36
16	K	102	BCR	C18-C19-C20-C21
16	K	102	BCR	C21-C22-C23-C24
16	K	102	BCR	C23-C24-C25-C26
16	L	201	BCR	C7-C8-C9-C34
16	L	201	BCR	C11-C10-C9-C8
16	L	201	BCR	C20-C21-C22-C37
16	L	208	BCR	C7-C8-C9-C34
16	L	208	BCR	C11-C10-C9-C34
16	L	208	BCR	C11-C12-C13-C14
16	L	208	BCR	C11-C12-C13-C35
16	L	208	BCR	C36-C18-C19-C20
16	L	209	BCR	C6-C7-C8-C9
16	L	209	BCR	C7-C8-C9-C10
16	L	209	BCR	C7-C8-C9-C34
16	L	209	BCR	C11-C10-C9-C8
16	L	209	BCR	C11-C10-C9-C34
16	L	209	BCR	C11-C12-C13-C35
16	M	103	BCR	C1-C6-C7-C8
16	M	103	BCR	C5-C6-C7-C8
17	A	855	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
17	A	855	LMG	O9-C10-O7-C8
17	A	855	LMG	C11-C10-O7-C8
17	B	3049	LMG	C2-C1-O1-C7
17	B	3049	LMG	O6-C1-O1-C7
17	I	102	LMG	C2-C1-O1-C7
17	I	102	LMG	O6-C1-O1-C7
18	A	853	LHG	C3-O3-P-O5
18	A	854	LHG	C1-C2-C3-O3
18	M	101	LHG	O1-C1-C2-C3
18	M	101	LHG	C3-O3-P-O4
18	M	101	LHG	C3-O3-P-O5
18	M	101	LHG	C3-O3-P-O6
21	L	202	LMT	C2'-C1'-O1'-C1
21	L	202	LMT	O5'-C1'-O1'-C1
22	L	207	DGD	O6D-C1D-O3G-C3G
22	L	207	DGD	C2E-C1E-O5D-C6D
22	L	207	DGD	O6E-C1E-O5D-C6D
14	A	817	CLA	O1D-CGD-O2D-CED
14	B	3003	CLA	O1D-CGD-O2D-CED
14	B	3013	CLA	O1D-CGD-O2D-CED
14	B	3035	CLA	O1D-CGD-O2D-CED
14	A	807	CLA	O1D-CGD-O2D-CED
14	A	820	CLA	O1D-CGD-O2D-CED
14	A	823	CLA	O1D-CGD-O2D-CED
14	A	829	CLA	O1D-CGD-O2D-CED
14	B	3004	CLA	O1D-CGD-O2D-CED
14	B	3032	CLA	O1D-CGD-O2D-CED
14	A	806	CLA	CBD-CGD-O2D-CED
14	A	823	CLA	CBD-CGD-O2D-CED
14	A	830	CLA	CBD-CGD-O2D-CED
14	A	841	CLA	CBD-CGD-O2D-CED
14	B	3013	CLA	CBD-CGD-O2D-CED
14	B	3016	CLA	CBD-CGD-O2D-CED
14	B	3020	CLA	CBD-CGD-O2D-CED
14	B	3022	CLA	CBD-CGD-O2D-CED
14	B	3034	CLA	CBD-CGD-O2D-CED
14	B	3036	CLA	CBD-CGD-O2D-CED
14	A	845	CLA	O1A-CGA-O2A-C1
14	A	819	CLA	O1D-CGD-O2D-CED
14	A	844	CLA	O1D-CGD-O2D-CED
14	B	3022	CLA	O1D-CGD-O2D-CED
14	A	838	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	B	3005	CLA	O1D-CGD-O2D-CED
14	B	3006	CLA	O1D-CGD-O2D-CED
14	M	102	CLA	O1D-CGD-O2D-CED
13	A	801	CL0	CBA-CGA-O2A-C1
14	A	820	CLA	CBA-CGA-O2A-C1
14	A	813	CLA	CBD-CGD-O2D-CED
14	A	856	CLA	CBD-CGD-O2D-CED
14	B	3015	CLA	CBD-CGD-O2D-CED
13	A	801	CL0	O1A-CGA-O2A-C1
14	A	806	CLA	O1A-CGA-O2A-C1
14	A	820	CLA	O1A-CGA-O2A-C1
18	M	101	LHG	O10-C23-O8-C6
14	A	822	CLA	O1D-CGD-O2D-CED
14	B	3037	CLA	O1D-CGD-O2D-CED
14	F	202	CLA	O1D-CGD-O2D-CED
14	A	842	CLA	O1D-CGD-O2D-CED
21	L	202	LMT	C3'-C4'-O1B-C1B
14	A	806	CLA	O1D-CGD-O2D-CED
14	A	830	CLA	C3-C5-C6-C7
14	B	3003	CLA	C3-C5-C6-C7
14	B	3005	CLA	C3-C5-C6-C7
14	B	3018	CLA	C3-C5-C6-C7
14	B	3027	CLA	C3-C5-C6-C7
14	B	3033	CLA	C3-C5-C6-C7
14	B	3041	CLA	C3-C5-C6-C7
14	A	806	CLA	CBA-CGA-O2A-C1
14	A	838	CLA	CBA-CGA-O2A-C1
14	A	845	CLA	CBA-CGA-O2A-C1
14	B	3016	CLA	O1D-CGD-O2D-CED
14	B	3020	CLA	O1D-CGD-O2D-CED
14	B	3034	CLA	O1D-CGD-O2D-CED
14	B	3036	CLA	O1D-CGD-O2D-CED
14	B	3034	CLA	C4-C3-C5-C6
14	B	3034	CLA	C2-C3-C5-C6
14	B	3029	CLA	CBD-CGD-O2D-CED
14	B	3030	CLA	CBD-CGD-O2D-CED
14	A	808	CLA	C2A-CAA-CBA-CGA
14	A	820	CLA	C2A-CAA-CBA-CGA
14	A	830	CLA	C2A-CAA-CBA-CGA
14	B	3029	CLA	C2A-CAA-CBA-CGA
14	A	820	CLA	C3-C5-C6-C7
14	A	817	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	A	825	CLA	CBA-CGA-O2A-C1
14	A	829	CLA	CBA-CGA-O2A-C1
14	B	3032	CLA	CBA-CGA-O2A-C1
14	L	204	CLA	CBA-CGA-O2A-C1
18	M	101	LHG	C24-C23-O8-C6
14	A	830	CLA	O1D-CGD-O2D-CED
14	B	3025	CLA	CBD-CGD-O2D-CED
14	A	841	CLA	O1D-CGD-O2D-CED
18	B	3050	LHG	O9-C7-O7-C5
14	A	817	CLA	O1A-CGA-O2A-C1
14	A	829	CLA	O1A-CGA-O2A-C1
14	A	838	CLA	O1A-CGA-O2A-C1
14	B	3016	CLA	C2A-CAA-CBA-CGA
14	K	103	CLA	C2A-CAA-CBA-CGA
16	B	3047	BCR	C19-C20-C21-C22
13	A	801	CL0	CBD-CGD-O2D-CED
14	A	803	CLA	CBD-CGD-O2D-CED
14	A	825	CLA	CBD-CGD-O2D-CED
14	A	827	CLA	CBD-CGD-O2D-CED
14	A	831	CLA	CBD-CGD-O2D-CED
14	B	3021	CLA	CBD-CGD-O2D-CED
14	B	3023	CLA	CBD-CGD-O2D-CED
14	B	3040	CLA	CBD-CGD-O2D-CED
18	A	854	LHG	O2-C2-C3-O3
14	A	823	CLA	CBA-CGA-O2A-C1
22	L	207	DGD	C2A-C1A-O1G-C1G
18	B	3050	LHG	C8-C7-O7-C5
14	A	836	CLA	CBD-CGD-O2D-CED
14	B	3028	CLA	CBD-CGD-O2D-CED
17	A	855	LMG	O6-C5-C6-O5
17	B	3049	LMG	O6-C5-C6-O5
14	A	825	CLA	O1A-CGA-O2A-C1
14	B	3032	CLA	O1A-CGA-O2A-C1
14	L	204	CLA	O1A-CGA-O2A-C1
15	A	846	PQN	C14-C13-C15-C16
15	A	846	PQN	C12-C13-C15-C16
14	A	856	CLA	C2A-CAA-CBA-CGA
21	L	202	LMT	O5B-C5B-C6B-O6B
14	A	823	CLA	O1A-CGA-O2A-C1
22	L	207	DGD	O1A-C1A-O1G-C1G
14	A	805	CLA	CBA-CGA-O2A-C1
14	A	812	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	B	3015	CLA	O1D-CGD-O2D-CED
14	A	812	CLA	CBD-CGD-O2D-CED
14	B	3011	CLA	CBD-CGD-O2D-CED
18	B	3050	LHG	C1-C2-C3-O3
14	A	808	CLA	CBA-CGA-O2A-C1
14	A	809	CLA	CBA-CGA-O2A-C1
14	A	826	CLA	CBA-CGA-O2A-C1
14	A	843	CLA	CBA-CGA-O2A-C1
14	A	856	CLA	CBA-CGA-O2A-C1
14	B	3017	CLA	CBA-CGA-O2A-C1
14	B	3018	CLA	CBA-CGA-O2A-C1
14	B	3021	CLA	CBA-CGA-O2A-C1
21	L	202	LMT	C4B-C5B-C6B-O6B
14	A	816	CLA	C2A-CAA-CBA-CGA
17	B	3049	LMG	C4-C5-C6-O5
14	A	829	CLA	C13-C15-C16-C17
14	A	830	CLA	C8-C10-C11-C12
14	B	3004	CLA	C10-C11-C12-C13
14	B	3030	CLA	C15-C16-C17-C18
14	A	845	CLA	C3-C5-C6-C7
17	A	855	LMG	C2-C1-O1-C7
14	A	812	CLA	O1A-CGA-O2A-C1
14	A	802	CLA	C14-C13-C15-C16
14	A	803	CLA	C14-C13-C15-C16
14	A	812	CLA	C14-C13-C15-C16
14	B	3020	CLA	C11-C12-C13-C14
14	B	3027	CLA	C11-C10-C8-C9
14	B	3041	CLA	C14-C13-C15-C16
15	A	846	PQN	C16-C17-C18-C19
16	A	847	BCR	C11-C12-C13-C35
16	B	3045	BCR	C7-C8-C9-C34
16	B	3047	BCR	C11-C12-C13-C35
16	B	3051	BCR	C37-C22-C23-C24
16	J	104	BCR	C37-C22-C23-C24
16	K	102	BCR	C37-C22-C23-C24
14	A	809	CLA	O1A-CGA-O2A-C1
14	A	826	CLA	O1A-CGA-O2A-C1
14	A	843	CLA	O1A-CGA-O2A-C1
14	B	3017	CLA	O1A-CGA-O2A-C1
14	B	3018	CLA	O1A-CGA-O2A-C1
18	A	853	LHG	O10-C23-O8-C6
14	B	3004	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
15	B	3043	PQN	C20-C21-C22-C23
15	B	3043	PQN	C23-C25-C26-C27
17	A	852	LMG	C4-C5-C6-O5
14	A	809	CLA	C3-C5-C6-C7
14	A	836	CLA	CBA-CGA-O2A-C1
14	B	3023	CLA	C5-C6-C7-C8
14	A	813	CLA	O1D-CGD-O2D-CED
14	A	808	CLA	O1A-CGA-O2A-C1
14	A	825	CLA	C8-C10-C11-C12
14	A	802	CLA	C15-C16-C17-C18
14	A	806	CLA	C2-C1-O2A-CGA
14	A	826	CLA	C2-C1-O2A-CGA
14	B	3028	CLA	C8-C10-C11-C12
14	B	3034	CLA	C5-C6-C7-C8
14	A	837	CLA	C2A-CAA-CBA-CGA
14	K	101	CLA	C2A-CAA-CBA-CGA
14	M	102	CLA	C2A-CAA-CBA-CGA
14	B	3027	CLA	C6-C7-C8-C10
14	A	856	CLA	C3-C5-C6-C7
14	A	831	CLA	C10-C11-C12-C13
14	B	3010	CLA	C8-C10-C11-C12
14	A	856	CLA	O1A-CGA-O2A-C1
13	A	801	CL0	C13-C15-C16-C17
14	A	803	CLA	C13-C15-C16-C17
15	A	846	PQN	C25-C26-C27-C28
16	B	3044	BCR	C18-C19-C20-C21
16	B	3051	BCR	C10-C11-C12-C13
16	F	201	BCR	C10-C11-C12-C13
16	J	105	BCR	C18-C19-C20-C21
16	L	201	BCR	C10-C11-C12-C13
18	B	3050	LHG	O2-C2-C3-O3
14	B	3003	CLA	C8-C10-C11-C12
14	B	3014	CLA	C13-C15-C16-C17
14	B	3029	CLA	C15-C16-C17-C18
14	A	856	CLA	O1D-CGD-O2D-CED
14	A	805	CLA	O1A-CGA-O2A-C1
14	B	3021	CLA	O1A-CGA-O2A-C1
17	A	852	LMG	C28-C29-C30-C31
14	A	804	CLA	C10-C11-C12-C13
14	A	820	CLA	C13-C15-C16-C17
14	A	822	CLA	C15-C16-C17-C18
14	A	826	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
14	B	3029	CLA	O1D-CGD-O2D-CED
14	A	810	CLA	C15-C16-C17-C18
14	A	833	CLA	C10-C11-C12-C13
14	A	834	CLA	C5-C6-C7-C8
14	B	3004	CLA	C15-C16-C17-C18
14	B	3006	CLA	C13-C15-C16-C17
14	B	3041	CLA	C8-C10-C11-C12
18	B	3050	LHG	C4-O6-P-O3
18	M	101	LHG	C4-O6-P-O3
14	A	818	CLA	CBA-CGA-O2A-C1
14	B	3034	CLA	CBA-CGA-O2A-C1
14	A	809	CLA	CBD-CGD-O2D-CED
14	A	807	CLA	C5-C6-C7-C8
14	A	814	CLA	C8-C10-C11-C12
17	A	852	LMG	O9-C10-O7-C8
14	B	3030	CLA	C8-C10-C11-C12
14	A	818	CLA	CBD-CGD-O2D-CED
14	B	3005	CLA	C2A-CAA-CBA-CGA
14	B	3021	CLA	C2A-CAA-CBA-CGA
14	A	804	CLA	CBA-CGA-O2A-C1
14	A	840	CLA	CBA-CGA-O2A-C1
14	B	3011	CLA	C13-C15-C16-C17
14	A	821	CLA	CBD-CGD-O2D-CED
14	A	839	CLA	C8-C10-C11-C12
17	A	852	LMG	C11-C10-O7-C8
16	A	849	BCR	C16-C17-C18-C36
16	A	849	BCR	C20-C21-C22-C37
16	A	850	BCR	C35-C13-C14-C15
16	A	850	BCR	C16-C17-C18-C36
16	B	3044	BCR	C20-C21-C22-C37
16	B	3045	BCR	C35-C13-C14-C15
16	B	3045	BCR	C20-C21-C22-C37
16	B	3046	BCR	C35-C13-C14-C15
16	B	3047	BCR	C20-C21-C22-C37
16	F	203	BCR	C16-C17-C18-C36
16	J	103	BCR	C16-C17-C18-C36
16	J	104	BCR	C11-C10-C9-C34
16	L	201	BCR	C11-C10-C9-C34
16	M	103	BCR	C11-C10-C9-C34
14	A	804	CLA	C3-C5-C6-C7
14	A	806	CLA	C16-C17-C18-C20
15	A	846	PQN	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
15	A	846	PQN	C26-C27-C28-C30
17	A	852	LMG	C23-C24-C25-C26
14	B	3038	CLA	C5-C6-C7-C8
17	A	852	LMG	C17-C18-C19-C20
17	I	102	LMG	C18-C19-C20-C21
14	A	825	CLA	O1D-CGD-O2D-CED
14	B	3040	CLA	O1D-CGD-O2D-CED
17	A	855	LMG	C18-C19-C20-C21
14	B	3030	CLA	O1D-CGD-O2D-CED
14	A	833	CLA	C3-C5-C6-C7
18	M	101	LHG	C23-C24-C25-C26
16	A	849	BCR	C12-C13-C14-C15
16	A	850	BCR	C20-C21-C22-C23
16	A	851	BCR	C20-C21-C22-C23
16	B	3044	BCR	C11-C10-C9-C8
16	B	3046	BCR	C12-C13-C14-C15
16	B	3047	BCR	C12-C13-C14-C15
16	B	3047	BCR	C16-C17-C18-C19
16	B	3048	BCR	C11-C10-C9-C8
16	F	203	BCR	C11-C10-C9-C8
16	I	101	BCR	C11-C10-C9-C8
16	J	103	BCR	C12-C13-C14-C15
16	J	103	BCR	C16-C17-C18-C19
16	J	105	BCR	C11-C10-C9-C8
16	J	105	BCR	C16-C17-C18-C19
16	K	102	BCR	C11-C10-C9-C8
16	K	102	BCR	C12-C13-C14-C15
16	L	201	BCR	C20-C21-C22-C23
16	L	208	BCR	C11-C10-C9-C8
16	L	208	BCR	C20-C21-C22-C23
16	M	103	BCR	C11-C10-C9-C8
14	A	807	CLA	CBA-CGA-O2A-C1
14	B	3019	CLA	CBA-CGA-O2A-C1
14	B	3009	CLA	C13-C15-C16-C17
15	A	846	PQN	C20-C21-C22-C23
14	A	836	CLA	O1A-CGA-O2A-C1
14	B	3034	CLA	O1A-CGA-O2A-C1
13	A	801	CL0	C16-C17-C18-C20
14	A	839	CLA	C16-C17-C18-C20
14	B	3025	CLA	O1D-CGD-O2D-CED
17	A	852	LMG	O6-C5-C6-O5
14	A	835	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
17	A	855	LMG	C16-C17-C18-C19
18	A	853	LHG	C12-C13-C14-C15
15	B	3043	PQN	C21-C22-C23-C24
22	L	207	DGD	C4B-C5B-C6B-C7B
22	L	207	DGD	C5B-C6B-C7B-C8B
14	B	3033	CLA	C5-C6-C7-C8
13	A	801	CL0	C2A-CAA-CBA-CGA
14	A	802	CLA	C2A-CAA-CBA-CGA
17	B	3049	LMG	C35-C36-C37-C38
18	M	101	LHG	C25-C26-C27-C28
16	B	3051	BCR	C21-C22-C23-C24
14	A	809	CLA	C5-C6-C7-C8
17	A	852	LMG	C11-C12-C13-C14
17	A	852	LMG	C30-C31-C32-C33
18	M	101	LHG	C14-C15-C16-C17
18	M	101	LHG	C32-C33-C34-C35
18	M	101	LHG	C33-C34-C35-C36
14	A	806	CLA	C16-C17-C18-C19
14	A	820	CLA	C16-C17-C18-C19
14	A	820	CLA	C16-C17-C18-C20
14	B	3010	CLA	C16-C17-C18-C20
14	L	206	CLA	C16-C17-C18-C19
14	B	3011	CLA	C5-C6-C7-C8
22	L	207	DGD	C2B-C3B-C4B-C5B
14	A	831	CLA	O1D-CGD-O2D-CED
14	A	830	CLA	C5-C6-C7-C8
15	A	846	PQN	C15-C16-C17-C18
14	A	811	CLA	C2A-CAA-CBA-CGA
14	J	101	CLA	C2A-CAA-CBA-CGA
17	I	102	LMG	C15-C16-C17-C18
14	A	803	CLA	O1D-CGD-O2D-CED
14	B	3021	CLA	O1D-CGD-O2D-CED
14	B	3023	CLA	O1D-CGD-O2D-CED
14	A	802	CLA	C3A-C2A-CAA-CBA
14	A	804	CLA	C3A-C2A-CAA-CBA
14	A	806	CLA	C3A-C2A-CAA-CBA
14	A	826	CLA	C3A-C2A-CAA-CBA
14	A	842	CLA	C3A-C2A-CAA-CBA
14	L	206	CLA	C10-C11-C12-C13
21	L	202	LMT	C2-C1-O1'-C1'
14	A	818	CLA	O1A-CGA-O2A-C1
14	A	839	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
17	A	852	LMG	C20-C21-C22-C23
17	A	852	LMG	C33-C34-C35-C36
17	A	855	LMG	C13-C14-C15-C16
17	B	3049	LMG	C17-C18-C19-C20
14	A	856	CLA	O2A-C1-C2-C3
16	F	201	BCR	C14-C15-C16-C17
14	A	820	CLA	C15-C16-C17-C18
14	B	3019	CLA	C8-C10-C11-C12
14	B	3033	CLA	C2-C3-C5-C6
18	A	853	LHG	C8-C7-O7-C5
17	A	855	LMG	C4-C5-C6-O5
18	M	101	LHG	O1-C1-C2-O2
18	M	101	LHG	C26-C27-C28-C29
14	A	840	CLA	O1A-CGA-O2A-C1
14	L	206	CLA	C16-C17-C18-C20
14	B	3041	CLA	C15-C16-C17-C18
14	B	3028	CLA	C3-C5-C6-C7
18	M	101	LHG	C30-C31-C32-C33
14	A	804	CLA	O1A-CGA-O2A-C1
14	B	3019	CLA	O1A-CGA-O2A-C1
17	A	855	LMG	C10-C11-C12-C13
14	A	808	CLA	C2-C1-O2A-CGA
14	A	830	CLA	C10-C11-C12-C13
14	A	807	CLA	O1A-CGA-O2A-C1
18	A	853	LHG	C24-C25-C26-C27
14	A	819	CLA	C3-C5-C6-C7
14	B	3020	CLA	C3-C5-C6-C7
16	A	847	BCR	C23-C24-C25-C26
16	A	847	BCR	C23-C24-C25-C30
16	A	849	BCR	C1-C6-C7-C8
16	A	849	BCR	C23-C24-C25-C30
16	A	851	BCR	C1-C6-C7-C8
16	A	851	BCR	C5-C6-C7-C8
16	B	3045	BCR	C1-C6-C7-C8
16	B	3045	BCR	C5-C6-C7-C8
16	B	3051	BCR	C1-C6-C7-C8
16	B	3051	BCR	C5-C6-C7-C8
16	B	3051	BCR	C23-C24-C25-C26
16	B	3051	BCR	C23-C24-C25-C30
16	F	203	BCR	C1-C6-C7-C8
16	F	203	BCR	C5-C6-C7-C8
16	F	203	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
16	F	203	BCR	C23-C24-C25-C30
16	J	103	BCR	C1-C6-C7-C8
16	J	103	BCR	C5-C6-C7-C8
16	J	104	BCR	C23-C24-C25-C30
16	J	105	BCR	C1-C6-C7-C8
16	J	105	BCR	C5-C6-C7-C8
16	K	102	BCR	C23-C24-C25-C30
16	L	208	BCR	C23-C24-C25-C26
16	L	208	BCR	C23-C24-C25-C30
16	L	209	BCR	C1-C6-C7-C8
16	L	209	BCR	C5-C6-C7-C8
16	M	103	BCR	C23-C24-C25-C26
16	M	103	BCR	C23-C24-C25-C30
14	A	833	CLA	C5-C6-C7-C8
14	A	844	CLA	C15-C16-C17-C18
17	A	852	LMG	C16-C17-C18-C19
14	B	3033	CLA	C4-C3-C5-C6
14	A	802	CLA	C12-C13-C15-C16
14	A	812	CLA	C12-C13-C15-C16
14	A	822	CLA	C12-C13-C15-C16
14	A	826	CLA	C2-C3-C5-C6
14	A	827	CLA	C12-C13-C15-C16
14	A	833	CLA	C11-C10-C8-C7
14	A	835	CLA	C2-C3-C5-C6
14	B	3018	CLA	C11-C10-C8-C7
14	B	3027	CLA	C11-C10-C8-C7
14	B	3041	CLA	C12-C13-C15-C16
15	B	3043	PQN	C21-C22-C23-C25
14	B	3009	CLA	C15-C16-C17-C18
13	A	801	CL0	O1D-CGD-O2D-CED
18	M	101	LHG	C7-C8-C9-C10
18	A	853	LHG	C24-C23-O8-C6
14	A	844	CLA	C2A-CAA-CBA-CGA
14	A	844	CLA	C5-C6-C7-C8
14	B	3019	CLA	C5-C6-C7-C8
14	B	3028	CLA	C15-C16-C17-C18
14	A	827	CLA	O1D-CGD-O2D-CED
21	L	202	LMT	C1-C2-C3-C4
17	A	852	LMG	C18-C19-C20-C21
17	B	3049	LMG	C34-C35-C36-C37
14	A	836	CLA	O1D-CGD-O2D-CED
14	B	3011	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	B	3028	CLA	O1D-CGD-O2D-CED
17	A	852	LMG	C22-C23-C24-C25
17	B	3049	LMG	C31-C32-C33-C34
14	B	3019	CLA	C3-C5-C6-C7
14	A	836	CLA	C5-C6-C7-C8
16	J	103	BCR	C22-C23-C24-C25
16	J	104	BCR	C6-C7-C8-C9
16	J	104	BCR	C22-C23-C24-C25
14	B	3003	CLA	CBA-CGA-O2A-C1
14	B	3040	CLA	CBA-CGA-O2A-C1
14	B	3033	CLA	C16-C17-C18-C20
18	A	853	LHG	C23-C24-C25-C26
16	J	103	BCR	C18-C19-C20-C21
14	A	820	CLA	C8-C10-C11-C12
14	B	3009	CLA	C8-C10-C11-C12
14	B	3039	CLA	C5-C6-C7-C8
18	A	854	LHG	O9-C7-O7-C5
18	A	853	LHG	O7-C5-C6-O8
14	B	3007	CLA	C16-C17-C18-C20
18	M	101	LHG	C11-C10-C9-C8
14	A	825	CLA	C5-C6-C7-C8
14	A	826	CLA	C4-C3-C5-C6
17	B	3049	LMG	C28-C29-C30-C31
14	A	827	CLA	C14-C13-C15-C16
14	A	833	CLA	C11-C10-C8-C9
14	B	3009	CLA	C14-C13-C15-C16
14	B	3010	CLA	C6-C7-C8-C9
14	B	3018	CLA	C11-C10-C8-C9
14	L	204	CLA	C11-C12-C13-C14
14	B	3018	CLA	C10-C11-C12-C13
14	A	813	CLA	C2A-CAA-CBA-CGA
14	B	3033	CLA	C2A-CAA-CBA-CGA
16	A	849	BCR	C36-C18-C19-C20
14	A	804	CLA	C1A-C2A-CAA-CBA
14	A	811	CLA	C1A-C2A-CAA-CBA
14	A	819	CLA	C1A-C2A-CAA-CBA
14	A	824	CLA	C1A-C2A-CAA-CBA
14	A	826	CLA	C1A-C2A-CAA-CBA
14	A	842	CLA	C1A-C2A-CAA-CBA
14	B	3019	CLA	C1A-C2A-CAA-CBA
14	B	3028	CLA	C1A-C2A-CAA-CBA
14	B	3030	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	A	801	CL0	C16-C17-C18-C19
14	B	3033	CLA	C16-C17-C18-C19
14	B	3041	CLA	C10-C11-C12-C13
14	A	834	CLA	C3-C5-C6-C7
14	B	3015	CLA	C5-C6-C7-C8
14	B	3028	CLA	CBA-CGA-O2A-C1
14	A	812	CLA	O1D-CGD-O2D-CED
14	B	3010	CLA	C16-C17-C18-C19
14	A	811	CLA	CBD-CGD-O2D-CED
14	A	826	CLA	C10-C11-C12-C13
17	B	3049	LMG	C14-C15-C16-C17
18	A	853	LHG	C9-C10-C11-C12
14	B	3029	CLA	C5-C6-C7-C8
18	A	853	LHG	C4-C5-C6-O8
18	M	101	LHG	C4-C5-C6-O8
18	A	853	LHG	C19-C20-C21-C22
18	A	854	LHG	C11-C10-C9-C8
14	B	3040	CLA	O1A-CGA-O2A-C1
17	B	3049	LMG	C23-C24-C25-C26
17	B	3049	LMG	C30-C31-C32-C33
14	A	825	CLA	C11-C12-C13-C14
17	A	852	LMG	C21-C22-C23-C24
14	A	810	CLA	C10-C11-C12-C13
22	L	207	DGD	CAA-CBA-CCA-CDA
14	A	822	CLA	C13-C15-C16-C17
14	B	3015	CLA	C8-C10-C11-C12
16	A	847	BCR	C20-C21-C22-C37
16	B	3046	BCR	C20-C21-C22-C37
16	F	201	BCR	C20-C21-C22-C37
16	K	102	BCR	C35-C13-C14-C15
16	M	103	BCR	C16-C17-C18-C36
14	A	822	CLA	C4-C3-C5-C6
22	L	207	DGD	C9B-CAB-CBB-CCB
17	A	852	LMG	C14-C15-C16-C17
14	B	3033	CLA	C2-C1-O2A-CGA
14	B	3025	CLA	C5-C6-C7-C8
14	A	822	CLA	C3-C5-C6-C7
18	A	854	LHG	C9-C10-C11-C12
17	A	855	LMG	C12-C13-C14-C15
14	B	3027	CLA	CBA-CGA-O2A-C1
14	B	3028	CLA	O1A-CGA-O2A-C1
14	A	839	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	B	3003	CLA	O1A-CGA-O2A-C1
14	B	3039	CLA	C13-C15-C16-C17
17	A	852	LMG	C2-C1-O1-C7
14	B	3033	CLA	C10-C11-C12-C13
14	A	807	CLA	C11-C12-C13-C15
14	A	822	CLA	C6-C7-C8-C10
14	A	828	CLA	C11-C10-C8-C7
14	A	834	CLA	C11-C10-C8-C7
14	A	834	CLA	C12-C13-C15-C16
14	A	856	CLA	C11-C10-C8-C7
14	B	3009	CLA	C11-C10-C8-C7
14	B	3010	CLA	C6-C7-C8-C10
14	B	3010	CLA	C11-C10-C8-C7
14	B	3011	CLA	C11-C12-C13-C15
14	B	3020	CLA	C11-C10-C8-C7
14	B	3027	CLA	C11-C12-C13-C15
14	B	3029	CLA	C12-C13-C15-C16
14	B	3039	CLA	C11-C10-C8-C7
14	B	3039	CLA	C11-C12-C13-C15
14	B	3042	CLA	C11-C10-C8-C7
14	L	204	CLA	C11-C12-C13-C15
14	L	206	CLA	C6-C7-C8-C10
15	A	846	PQN	C16-C17-C18-C20
17	A	852	LMG	C35-C36-C37-C38
14	A	805	CLA	C6-C7-C8-C9
14	A	807	CLA	C11-C12-C13-C14
14	A	809	CLA	C6-C7-C8-C9
14	A	827	CLA	C11-C12-C13-C14
14	A	828	CLA	C11-C10-C8-C9
14	A	830	CLA	C11-C12-C13-C14
14	A	834	CLA	C11-C10-C8-C9
14	A	834	CLA	C14-C13-C15-C16
14	A	841	CLA	C6-C7-C8-C9
14	A	856	CLA	C11-C10-C8-C9
14	B	3007	CLA	C11-C12-C13-C14
14	B	3009	CLA	C11-C10-C8-C9
14	B	3020	CLA	C11-C10-C8-C9
14	B	3029	CLA	C14-C13-C15-C16
14	B	3030	CLA	C11-C10-C8-C9
14	B	3039	CLA	C11-C10-C8-C9
14	B	3039	CLA	C11-C12-C13-C14
16	K	102	BCR	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
14	A	827	CLA	C5-C6-C7-C8
14	B	3011	CLA	C8-C10-C11-C12
14	A	818	CLA	O1D-CGD-O2D-CED
14	B	3039	CLA	C16-C17-C18-C20
16	B	3051	BCR	C11-C12-C13-C14
16	J	104	BCR	C7-C8-C9-C10
14	A	804	CLA	C5-C6-C7-C8
14	A	841	CLA	C5-C6-C7-C8
14	A	835	CLA	C5-C6-C7-C8
22	L	207	DGD	C7A-C8A-C9A-CAA
14	B	3019	CLA	C10-C11-C12-C13
14	B	3028	CLA	C10-C11-C12-C13
14	A	822	CLA	C2-C3-C5-C6
14	A	831	CLA	C16-C17-C18-C20
14	A	835	CLA	C16-C17-C18-C20
14	A	809	CLA	O1D-CGD-O2D-CED
14	A	821	CLA	O1D-CGD-O2D-CED
14	A	808	CLA	C3A-C2A-CAA-CBA
14	A	823	CLA	C3A-C2A-CAA-CBA
14	A	836	CLA	C3A-C2A-CAA-CBA
14	B	3020	CLA	C3A-C2A-CAA-CBA
14	B	3030	CLA	C3A-C2A-CAA-CBA
14	B	3042	CLA	C3A-C2A-CAA-CBA
14	A	813	CLA	C6-C7-C8-C9
17	B	3049	LMG	C41-C42-C43-C44
16	B	3047	BCR	C9-C10-C11-C12
17	I	102	LMG	C32-C33-C34-C35
14	A	835	CLA	C16-C17-C18-C19
14	A	822	CLA	CBA-CGA-O2A-C1
17	A	855	LMG	C17-C18-C19-C20
17	B	3049	LMG	O1-C7-C8-C9
18	M	101	LHG	C17-C18-C19-C20
14	B	3039	CLA	C16-C17-C18-C19
17	I	102	LMG	C11-C10-O7-C8
14	A	822	CLA	C2A-CAA-CBA-CGA
18	A	853	LHG	O1-C1-C2-O2
18	M	101	LHG	O7-C5-C6-O8
14	A	831	CLA	C13-C15-C16-C17
14	B	3007	CLA	C16-C17-C18-C19
14	B	3038	CLA	C11-C12-C13-C15
14	B	3010	CLA	C10-C11-C12-C13
17	B	3049	LMG	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
22	L	207	DGD	O1B-C1B-O2G-C2G
14	B	3028	CLA	C2-C1-O2A-CGA
14	A	822	CLA	C14-C13-C15-C16
14	A	828	CLA	C14-C13-C15-C16
14	A	833	CLA	C14-C13-C15-C16
14	B	3003	CLA	C6-C7-C8-C9
14	B	3004	CLA	C11-C10-C8-C9
14	B	3011	CLA	C11-C12-C13-C14
14	B	3033	CLA	C11-C12-C13-C14
14	B	3042	CLA	C11-C10-C8-C9
14	L	204	CLA	C14-C13-C15-C16
14	L	205	CLA	C14-C13-C15-C16
18	A	854	LHG	C2-C3-O3-P
14	B	3027	CLA	O1A-CGA-O2A-C1
14	A	831	CLA	C16-C17-C18-C19
14	B	3042	CLA	C16-C17-C18-C20
16	A	847	BCR	C1-C6-C7-C8
16	A	847	BCR	C5-C6-C7-C8
16	A	848	BCR	C5-C6-C7-C8
16	A	850	BCR	C1-C6-C7-C8
16	A	850	BCR	C5-C6-C7-C8
16	B	3047	BCR	C23-C24-C25-C26
16	B	3047	BCR	C23-C24-C25-C30
16	B	3047	BCR	C36-C18-C19-C20
14	B	3014	CLA	CBA-CGA-O2A-C1
16	A	849	BCR	C21-C22-C23-C24
16	A	851	BCR	C11-C12-C13-C14
16	F	203	BCR	C7-C8-C9-C10
16	J	104	BCR	C11-C12-C13-C14
16	L	209	BCR	C11-C12-C13-C14
14	B	3042	CLA	C16-C17-C18-C19
14	B	3011	CLA	C15-C16-C17-C18
14	A	839	CLA	C6-C7-C8-C10
14	A	841	CLA	C6-C7-C8-C10
14	B	3003	CLA	C6-C7-C8-C10
14	B	3004	CLA	C11-C10-C8-C7
14	B	3011	CLA	C6-C7-C8-C10
14	B	3030	CLA	C11-C10-C8-C7
14	B	3030	CLA	C12-C13-C15-C16
14	B	3033	CLA	C11-C12-C13-C15
14	L	204	CLA	C6-C7-C8-C10
14	L	204	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	L	205	CLA	C12-C13-C15-C16
14	A	839	CLA	C10-C11-C12-C13
14	B	3024	CLA	CBD-CGD-O2D-CED
14	B	3023	CLA	C2A-CAA-CBA-CGA
14	A	845	CLA	C4C-C3C-CAC-CBC
16	B	3044	BCR	C35-C13-C14-C15
16	B	3047	BCR	C11-C10-C9-C34
16	B	3051	BCR	C16-C17-C18-C36
16	J	104	BCR	C20-C21-C22-C37
16	K	102	BCR	C20-C21-C22-C37
16	L	208	BCR	C20-C21-C22-C37
18	A	853	LHG	C33-C34-C35-C36
14	B	3020	CLA	CBA-CGA-O2A-C1
14	B	3029	CLA	CBA-CGA-O2A-C1
14	A	816	CLA	CAD-CBD-CGD-O2D
14	A	830	CLA	CAD-CBD-CGD-O2D
14	A	834	CLA	CAD-CBD-CGD-O2D
14	A	842	CLA	CAD-CBD-CGD-O2D
14	B	3006	CLA	CAD-CBD-CGD-O2D
14	B	3023	CLA	CAD-CBD-CGD-O2D
14	B	3028	CLA	CAD-CBD-CGD-O2D
14	B	3041	CLA	CAD-CBD-CGD-O2D
14	J	101	CLA	CAD-CBD-CGD-O2D
14	K	103	CLA	CAD-CBD-CGD-O2D
14	A	807	CLA	C13-C15-C16-C17
14	B	3028	CLA	C5-C6-C7-C8
14	B	3039	CLA	C15-C16-C17-C18
17	I	102	LMG	C28-C29-C30-C31
16	B	3046	BCR	C6-C7-C8-C9
14	B	3008	CLA	CBA-CGA-O2A-C1
14	B	3023	CLA	CBA-CGA-O2A-C1
14	B	3010	CLA	C2C-C3C-CAC-CBC
14	A	828	CLA	C8-C10-C11-C12
14	A	817	CLA	O2A-C1-C2-C3
14	B	3032	CLA	O2A-C1-C2-C3
14	A	835	CLA	CBD-CGD-O2D-CED
14	A	805	CLA	CHA-CBD-CGD-O1D
14	A	805	CLA	CHA-CBD-CGD-O2D
14	A	809	CLA	CHA-CBD-CGD-O1D
14	A	809	CLA	CHA-CBD-CGD-O2D
14	A	825	CLA	CHA-CBD-CGD-O1D
14	A	828	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	A	828	CLA	CHA-CBD-CGD-O2D
14	A	831	CLA	CHA-CBD-CGD-O1D
14	A	831	CLA	CHA-CBD-CGD-O2D
14	B	3006	CLA	CHA-CBD-CGD-O1D
14	B	3024	CLA	CHA-CBD-CGD-O1D
14	B	3024	CLA	CHA-CBD-CGD-O2D
14	B	3025	CLA	CHA-CBD-CGD-O1D
14	B	3025	CLA	CHA-CBD-CGD-O2D
14	B	3026	CLA	CHA-CBD-CGD-O1D
14	B	3026	CLA	CHA-CBD-CGD-O2D
14	B	3027	CLA	CHA-CBD-CGD-O1D
14	B	3027	CLA	CHA-CBD-CGD-O2D
14	B	3030	CLA	CHA-CBD-CGD-O1D
14	B	3034	CLA	CHA-CBD-CGD-O1D
14	B	3035	CLA	CHA-CBD-CGD-O1D
14	B	3035	CLA	CHA-CBD-CGD-O2D
14	A	822	CLA	O1A-CGA-O2A-C1
14	B	3023	CLA	O1A-CGA-O2A-C1
16	A	847	BCR	C11-C10-C9-C8
16	B	3048	BCR	C20-C21-C22-C23
17	B	3049	LMG	O1-C7-C8-O7
14	A	837	CLA	CBD-CGD-O2D-CED
14	B	3014	CLA	O1A-CGA-O2A-C1
14	A	824	CLA	CBA-CGA-O2A-C1
14	B	3007	CLA	C6-C7-C8-C9
14	B	3019	CLA	C6-C7-C8-C9
14	B	3024	CLA	O1D-CGD-O2D-CED
14	A	824	CLA	O1A-CGA-O2A-C1
14	A	817	CLA	C2A-CAA-CBA-CGA
22	L	207	DGD	CEB-CFB-CGB-CHB
16	B	3046	BCR	C7-C8-C9-C10
14	A	829	CLA	C3-C5-C6-C7
14	A	802	CLA	C1A-C2A-CAA-CBA
14	B	3014	CLA	C15-C16-C17-C18
14	A	832	CLA	CBA-CGA-O2A-C1
14	A	835	CLA	CBA-CGA-O2A-C1
14	B	3029	CLA	O1A-CGA-O2A-C1
14	A	806	CLA	C15-C16-C17-C18
14	A	837	CLA	O1D-CGD-O2D-CED
22	L	207	DGD	C3A-C4A-C5A-C6A
14	A	810	CLA	C3-C5-C6-C7
14	A	813	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
14	B	3008	CLA	O1A-CGA-O2A-C1
18	B	3050	LHG	C4-O6-P-O5
18	M	101	LHG	C4-O6-P-O5
14	A	823	CLA	O2A-C1-C2-C3
14	A	827	CLA	C13-C15-C16-C17
14	B	3029	CLA	C13-C15-C16-C17
14	B	3006	CLA	CBA-CGA-O2A-C1
14	B	3030	CLA	CBA-CGA-O2A-C1
14	A	825	CLA	C3-C5-C6-C7
21	L	202	LMT	C9-C10-C11-C12
17	A	852	LMG	C29-C30-C31-C32
14	A	828	CLA	CAD-CBD-CGD-O1D
14	A	842	CLA	C2-C3-C5-C6
14	B	3017	CLA	CAD-CBD-CGD-O1D
14	A	802	CLA	C6-C7-C8-C10
14	A	807	CLA	C12-C13-C15-C16
14	A	826	CLA	C11-C10-C8-C7
14	A	827	CLA	C11-C10-C8-C7
14	A	829	CLA	C6-C7-C8-C10
14	A	830	CLA	C6-C7-C8-C10
14	A	844	CLA	C11-C12-C13-C15
14	B	3005	CLA	C3A-C2A-CAA-CBA
14	B	3006	CLA	C12-C13-C15-C16
14	B	3007	CLA	C11-C10-C8-C7
14	B	3007	CLA	C11-C12-C13-C15
14	B	3015	CLA	C12-C13-C15-C16
14	B	3019	CLA	C6-C7-C8-C10
14	B	3020	CLA	C12-C13-C15-C16
14	B	3029	CLA	C6-C7-C8-C10
14	B	3033	CLA	C6-C7-C8-C10
15	B	3043	PQN	C22-C23-C25-C26
22	L	207	DGD	C1B-C2B-C3B-C4B
14	B	3006	CLA	O1A-CGA-O2A-C1
14	B	3028	CLA	C13-C15-C16-C17
14	B	3020	CLA	O1A-CGA-O2A-C1
14	B	3009	CLA	O1D-CGD-O2D-CED
17	I	102	LMG	O1-C7-C8-C9
17	I	102	LMG	O1-C7-C8-O7
18	A	853	LHG	C30-C31-C32-C33
14	A	835	CLA	O1A-CGA-O2A-C1
14	A	806	CLA	C13-C15-C16-C17
18	A	853	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	A	826	CLA	C13-C15-C16-C17
14	B	3038	CLA	C8-C10-C11-C12
14	A	822	CLA	C6-C7-C8-C9
14	A	827	CLA	C11-C10-C8-C9
14	A	839	CLA	C6-C7-C8-C9
14	B	3006	CLA	C11-C10-C8-C9
14	B	3010	CLA	C11-C10-C8-C9
14	B	3027	CLA	C6-C7-C8-C9
14	B	3029	CLA	C11-C10-C8-C9
14	B	3030	CLA	C14-C13-C15-C16
14	L	206	CLA	C6-C7-C8-C9
15	B	3043	PQN	C24-C23-C25-C26
16	A	851	BCR	C6-C7-C8-C9
14	B	3030	CLA	O1A-CGA-O2A-C1
21	L	202	LMT	C5'-C4'-O1B-C1B
16	A	849	BCR	C7-C8-C9-C34
16	A	850	BCR	C11-C12-C13-C35
22	L	207	DGD	C9A-CAA-CBA-CCA
14	A	830	CLA	C4-C3-C5-C6
18	M	101	LHG	C16-C17-C18-C19
14	B	3010	CLA	C15-C16-C17-C18
18	A	853	LHG	C13-C14-C15-C16
14	A	823	CLA	C1-C2-C3-C4
14	B	3032	CLA	C1-C2-C3-C4
14	A	803	CLA	C3-C5-C6-C7
14	B	3032	CLA	C2A-CAA-CBA-CGA
14	B	3015	CLA	C2-C1-O2A-CGA
14	L	205	CLA	C2-C1-O2A-CGA
16	L	209	BCR	C14-C15-C16-C17
16	A	848	BCR	C1-C6-C7-C8
16	L	208	BCR	C5-C6-C7-C8
14	B	3005	CLA	O1A-CGA-O2A-C1
17	A	852	LMG	C32-C33-C34-C35
17	B	3049	LMG	C36-C37-C38-C39
14	B	3038	CLA	C11-C12-C13-C14
16	A	849	BCR	C20-C21-C22-C23
16	B	3045	BCR	C11-C10-C9-C8
16	B	3051	BCR	C11-C10-C9-C8
18	A	853	LHG	C11-C12-C13-C14
18	A	853	LHG	C3-O3-P-O6
18	A	854	LHG	C3-O3-P-O6
18	B	3050	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
17	B	3049	LMG	C42-C43-C44-C45
14	A	809	CLA	C4-C3-C5-C6
14	A	809	CLA	C6-C7-C8-C10
14	A	830	CLA	C11-C12-C13-C15
14	B	3020	CLA	C11-C12-C13-C15
14	A	807	CLA	C14-C13-C15-C16
14	A	830	CLA	C6-C7-C8-C9
14	B	3011	CLA	C14-C13-C15-C16
14	B	3033	CLA	C6-C7-C8-C9
14	L	204	CLA	C6-C7-C8-C9
14	A	856	CLA	C13-C15-C16-C17
14	A	811	CLA	O1D-CGD-O2D-CED
17	B	3049	LMG	C22-C23-C24-C25
14	A	832	CLA	O1A-CGA-O2A-C1
18	A	854	LHG	O10-C23-O8-C6
16	F	201	BCR	C7-C8-C9-C34
14	B	3005	CLA	CBA-CGA-O2A-C1
21	L	202	LMT	C3-C4-C5-C6
16	A	847	BCR	C13-C14-C15-C16
16	A	850	BCR	C19-C20-C21-C22
16	J	103	BCR	C9-C10-C11-C12
18	B	3050	LHG	O6-C4-C5-C6
16	J	104	BCR	C18-C19-C20-C21
17	A	852	LMG	C13-C14-C15-C16
14	A	829	CLA	C16-C17-C18-C19
22	L	207	DGD	C2D-C1D-O3G-C3G
14	A	809	CLA	C2A-CAA-CBA-CGA
18	A	853	LHG	C31-C32-C33-C34
14	A	816	CLA	C3A-C2A-CAA-CBA
14	A	820	CLA	C5-C6-C7-C8
18	A	853	LHG	C34-C35-C36-C37
14	A	820	CLA	C6-C7-C8-C9
14	A	829	CLA	C6-C7-C8-C9
14	A	841	CLA	C11-C10-C8-C9
14	A	844	CLA	C11-C12-C13-C14
14	B	3006	CLA	C14-C13-C15-C16
14	B	3018	CLA	C6-C7-C8-C9
14	B	3029	CLA	C11-C12-C13-C14
14	L	206	CLA	C11-C10-C8-C9
16	A	851	BCR	C16-C17-C18-C36
16	B	3045	BCR	C11-C10-C9-C34
16	F	203	BCR	C35-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
14	A	844	CLA	O2A-C1-C2-C3
16	A	848	BCR	C14-C15-C16-C17
16	J	104	BCR	C21-C22-C23-C24
14	A	830	CLA	C13-C15-C16-C17
14	A	810	CLA	C1A-C2A-CAA-CBA
14	A	836	CLA	C1A-C2A-CAA-CBA
14	B	3005	CLA	C1A-C2A-CAA-CBA
14	B	3010	CLA	C1A-C2A-CAA-CBA
14	B	3020	CLA	C1A-C2A-CAA-CBA
14	A	806	CLA	C11-C12-C13-C15
14	A	810	CLA	C6-C7-C8-C10
14	A	814	CLA	C11-C10-C8-C7
14	A	828	CLA	C12-C13-C15-C16
14	A	829	CLA	C11-C12-C13-C15
14	A	835	CLA	C11-C12-C13-C15
14	A	843	CLA	C11-C10-C8-C7
14	B	3006	CLA	C11-C10-C8-C7
14	B	3007	CLA	C6-C7-C8-C10
14	B	3015	CLA	C11-C10-C8-C7
14	B	3029	CLA	C11-C10-C8-C7
14	B	3009	CLA	C5-C6-C7-C8
14	B	3014	CLA	C5-C6-C7-C8
18	B	3050	LHG	O6-C4-C5-O7
14	A	820	CLA	C4-C3-C5-C6
17	A	855	LMG	C15-C16-C17-C18
16	A	847	BCR	C16-C17-C18-C19
16	A	851	BCR	C16-C17-C18-C19
16	B	3046	BCR	C20-C21-C22-C23
16	F	201	BCR	C11-C10-C9-C8
16	J	105	BCR	C6-C7-C8-C9
16	L	201	BCR	C22-C23-C24-C25
14	A	826	CLA	O1D-CGD-O2D-CED
14	A	835	CLA	O1D-CGD-O2D-CED
14	B	3042	CLA	C15-C16-C17-C18
15	B	3043	PQN	C25-C26-C27-C28
14	B	3038	CLA	C4-C3-C5-C6
14	A	844	CLA	O1A-CGA-O2A-C1
18	M	101	LHG	C28-C29-C30-C31
14	A	842	CLA	C4-C3-C5-C6
14	A	819	CLA	CAA-CBA-CGA-O2A
14	B	3008	CLA	C2A-CAA-CBA-CGA
14	A	856	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
14	A	844	CLA	CBA-CGA-O2A-C1
16	F	201	BCR	C23-C24-C25-C30
16	L	208	BCR	C1-C6-C7-C8
18	A	853	LHG	O1-C1-C2-C3
14	B	3011	CLA	C4-C3-C5-C6
16	J	103	BCR	C21-C22-C23-C24
14	A	809	CLA	C8-C10-C11-C12
15	A	846	PQN	C23-C25-C26-C27
14	A	809	CLA	C2-C3-C5-C6
14	A	830	CLA	C2-C3-C5-C6
14	A	802	CLA	C10-C11-C12-C13
17	A	855	LMG	C8-C7-O1-C1
14	B	3018	CLA	C11-C12-C13-C14
14	B	3027	CLA	C16-C17-C18-C20
13	A	801	CL0	C8-C10-C11-C12
14	A	810	CLA	C5-C6-C7-C8
14	B	3027	CLA	C2A-CAA-CBA-CGA
18	A	854	LHG	O6-C4-C5-C6
14	A	807	CLA	C4-C3-C5-C6
14	A	812	CLA	C4-C3-C5-C6
14	A	833	CLA	C12-C13-C15-C16
14	B	3011	CLA	C2-C3-C5-C6
14	B	3011	CLA	C12-C13-C15-C16
14	A	826	CLA	CBD-CGD-O2D-CED
14	B	3014	CLA	C8-C10-C11-C12
17	A	852	LMG	O1-C7-C8-O7
17	A	852	LMG	O10-C28-O8-C9
22	L	207	DGD	CFB-CGB-CHB-CIB
17	B	3049	LMG	O7-C10-C11-C12
14	A	811	CLA	C4C-C3C-CAC-CBC
14	A	817	CLA	C4C-C3C-CAC-CBC
14	B	3022	CLA	C4C-C3C-CAC-CBC
16	A	847	BCR	C11-C10-C9-C34
16	A	847	BCR	C35-C13-C14-C15
16	L	208	BCR	C16-C17-C18-C36
14	A	808	CLA	CAA-CBA-CGA-O2A
14	A	825	CLA	C4-C3-C5-C6
14	A	834	CLA	C4-C3-C5-C6
14	A	839	CLA	C4-C3-C5-C6
14	B	3003	CLA	C4-C3-C5-C6
14	A	844	CLA	C8-C10-C11-C12
14	B	3038	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	L	202	LMT	C6-C7-C8-C9
14	A	802	CLA	C6-C7-C8-C9
14	A	810	CLA	C6-C7-C8-C9
14	A	826	CLA	C11-C10-C8-C9
14	A	835	CLA	C11-C12-C13-C14
14	B	3007	CLA	C11-C10-C8-C9
14	B	3011	CLA	C6-C7-C8-C9
14	B	3015	CLA	C11-C10-C8-C9
14	B	3029	CLA	C6-C7-C8-C9
14	A	810	CLA	C3A-C2A-CAA-CBA
14	A	825	CLA	C3A-C2A-CAA-CBA
14	A	831	CLA	C3A-C2A-CAA-CBA
14	B	3016	CLA	C3A-C2A-CAA-CBA
14	B	3034	CLA	C3A-C2A-CAA-CBA
14	A	840	CLA	C2-C1-O2A-CGA
14	A	827	CLA	C8-C10-C11-C12
14	A	802	CLA	CAD-CBD-CGD-O2D
14	A	804	CLA	CAD-CBD-CGD-O2D
14	A	812	CLA	CAD-CBD-CGD-O2D
14	A	813	CLA	CAD-CBD-CGD-O2D
14	A	818	CLA	CAD-CBD-CGD-O2D
14	A	822	CLA	CAD-CBD-CGD-O2D
14	A	833	CLA	CAD-CBD-CGD-O2D
14	A	856	CLA	CAD-CBD-CGD-O2D
14	B	3014	CLA	CAD-CBD-CGD-O2D
14	B	3015	CLA	CAD-CBD-CGD-O2D
14	B	3018	CLA	CAD-CBD-CGD-O2D
14	B	3021	CLA	CAD-CBD-CGD-O2D
14	B	3033	CLA	CAD-CBD-CGD-O2D
14	B	3034	CLA	CAD-CBD-CGD-O2D
14	L	204	CLA	CAD-CBD-CGD-O2D
14	L	206	CLA	CAD-CBD-CGD-O2D
21	L	202	LMT	C4-C5-C6-C7
18	B	3050	LHG	O7-C7-C8-C9
16	B	3044	BCR	C6-C7-C8-C9
17	A	852	LMG	C15-C16-C17-C18
14	A	856	CLA	C16-C17-C18-C19
14	A	820	CLA	C2-C3-C5-C6
14	B	3003	CLA	C2-C3-C5-C6
16	I	101	BCR	C17-C18-C19-C20
16	J	103	BCR	C11-C12-C13-C14
16	L	201	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
16	L	208	BCR	C21-C22-C23-C24
14	A	810	CLA	C2C-C3C-CAC-CBC
14	A	811	CLA	C2C-C3C-CAC-CBC
14	A	813	CLA	C2C-C3C-CAC-CBC
14	A	817	CLA	C2C-C3C-CAC-CBC
14	A	838	CLA	C2C-C3C-CAC-CBC
14	A	843	CLA	C2C-C3C-CAC-CBC
14	A	844	CLA	C2C-C3C-CAC-CBC
14	B	3014	CLA	C2C-C3C-CAC-CBC
14	B	3015	CLA	C2C-C3C-CAC-CBC
14	B	3017	CLA	C2C-C3C-CAC-CBC
14	B	3020	CLA	C2C-C3C-CAC-CBC
14	B	3022	CLA	C2C-C3C-CAC-CBC
14	B	3023	CLA	C2C-C3C-CAC-CBC
14	B	3032	CLA	C2C-C3C-CAC-CBC
14	B	3033	CLA	C2C-C3C-CAC-CBC
14	K	101	CLA	C2C-C3C-CAC-CBC
14	K	103	CLA	C2C-C3C-CAC-CBC
18	M	101	LHG	C5-C4-O6-P
18	A	854	LHG	O6-C4-C5-O7
17	A	852	LMG	O8-C28-C29-C30
17	A	852	LMG	C19-C20-C21-C22
18	M	101	LHG	C10-C11-C12-C13
22	L	207	DGD	CBB-CCB-CDB-CEB
14	A	806	CLA	O2A-C1-C2-C3
14	A	833	CLA	O2A-C1-C2-C3
14	B	3033	CLA	O2A-C1-C2-C3
14	B	3027	CLA	C13-C15-C16-C17
15	B	3043	PQN	C26-C27-C28-C29
14	A	806	CLA	CHA-CBD-CGD-O1D
14	A	806	CLA	CHA-CBD-CGD-O2D
14	A	811	CLA	CHA-CBD-CGD-O1D
14	A	811	CLA	CHA-CBD-CGD-O2D
14	A	814	CLA	CHA-CBD-CGD-O1D
14	A	823	CLA	CHA-CBD-CGD-O1D
14	A	823	CLA	CHA-CBD-CGD-O2D
14	A	825	CLA	CHA-CBD-CGD-O2D
14	A	826	CLA	CHA-CBD-CGD-O1D
14	A	835	CLA	CHA-CBD-CGD-O1D
14	A	836	CLA	CHA-CBD-CGD-O1D
14	A	836	CLA	CHA-CBD-CGD-O2D
14	B	3008	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	B	3008	CLA	CHA-CBD-CGD-O2D
14	B	3012	CLA	CHA-CBD-CGD-O1D
14	B	3012	CLA	CHA-CBD-CGD-O2D
14	B	3016	CLA	CHA-CBD-CGD-O1D
14	B	3019	CLA	CHA-CBD-CGD-O2D
14	B	3022	CLA	CHA-CBD-CGD-O1D
14	B	3022	CLA	CHA-CBD-CGD-O2D
14	B	3029	CLA	CHA-CBD-CGD-O2D
14	M	102	CLA	CHA-CBD-CGD-O1D
14	A	803	CLA	CAA-CBA-CGA-O2A
14	A	807	CLA	CAA-CBA-CGA-O2A
14	B	3014	CLA	CAA-CBA-CGA-O2A
14	B	3006	CLA	CAA-CBA-CGA-O2A
14	A	845	CLA	CAA-CBA-CGA-O2A
14	B	3030	CLA	C4-C3-C5-C6
14	A	803	CLA	C12-C13-C15-C16
14	B	3041	CLA	C11-C12-C13-C15
14	B	3011	CLA	CAA-CBA-CGA-O2A
14	A	806	CLA	C11-C12-C13-C14
14	A	814	CLA	C11-C10-C8-C9
14	B	3015	CLA	C14-C13-C15-C16
14	B	3020	CLA	C14-C13-C15-C16
18	A	854	LHG	O8-C23-C24-C25
17	A	855	LMG	C19-C20-C21-C22
17	B	3049	LMG	C16-C17-C18-C19
14	A	808	CLA	CAA-CBA-CGA-O1A
14	A	809	CLA	C15-C16-C17-C18
14	A	829	CLA	C16-C17-C18-C20
14	A	836	CLA	C6-C7-C8-C9
18	B	3050	LHG	O1-C1-C2-C3
18	A	853	LHG	O10-C23-C24-C25
16	A	849	BCR	C7-C8-C9-C10
14	A	816	CLA	C1A-C2A-CAA-CBA
14	A	825	CLA	C1A-C2A-CAA-CBA
14	A	831	CLA	C1A-C2A-CAA-CBA
14	B	3003	CLA	C1A-C2A-CAA-CBA
14	B	3014	CLA	C1A-C2A-CAA-CBA
14	B	3016	CLA	C1A-C2A-CAA-CBA
14	B	3032	CLA	C1A-C2A-CAA-CBA
14	B	3034	CLA	C1A-C2A-CAA-CBA
17	A	852	LMG	O10-C28-C29-C30
17	B	3049	LMG	O9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
14	B	3040	CLA	C2-C1-O2A-CGA
14	B	3009	CLA	CBD-CGD-O2D-CED
14	B	3029	CLA	CAA-CBA-CGA-O2A
18	M	101	LHG	O9-C7-C8-C9
14	B	3006	CLA	C15-C16-C17-C18
22	L	207	DGD	C2A-C3A-C4A-C5A
18	A	854	LHG	C4-O6-P-O5
14	A	845	CLA	CAA-CBA-CGA-O1A
14	B	3006	CLA	CAA-CBA-CGA-O1A
16	B	3048	BCR	C11-C10-C9-C34
17	B	3049	LMG	C19-C20-C21-C22
14	B	3027	CLA	C16-C17-C18-C19
16	A	851	BCR	C18-C19-C20-C21
17	I	102	LMG	O9-C10-C11-C12
14	A	809	CLA	CAA-CBA-CGA-O2A
14	B	3015	CLA	CAA-CBA-CGA-O2A
18	A	853	LHG	C17-C18-C19-C20
14	B	3011	CLA	CAA-CBA-CGA-O1A
18	A	854	LHG	C8-C7-O7-C5
14	A	809	CLA	C16-C17-C18-C20
14	A	810	CLA	CAD-CBD-CGD-O1D
14	A	814	CLA	CAD-CBD-CGD-O1D
14	A	836	CLA	CAD-CBD-CGD-O1D
14	B	3011	CLA	CAD-CBD-CGD-O1D
14	B	3012	CLA	CAD-CBD-CGD-O1D
14	B	3016	CLA	CAD-CBD-CGD-O1D
14	B	3027	CLA	CAD-CBD-CGD-O1D
14	X	1701	CLA	CAD-CBD-CGD-O1D
14	A	820	CLA	CAA-CBA-CGA-O2A
14	B	3007	CLA	CAA-CBA-CGA-O2A
14	A	843	CLA	C11-C10-C8-C9
14	A	814	CLA	C3-C5-C6-C7
14	B	3021	CLA	CAA-CBA-CGA-O2A
22	L	207	DGD	CDB-CEB-CFB-CGB
14	A	803	CLA	CAA-CBA-CGA-O1A
22	L	207	DGD	CEA-CFA-CGA-CHA
14	A	832	CLA	CAA-CBA-CGA-O2A
14	A	806	CLA	C10-C11-C12-C13
14	B	3021	CLA	CAA-CBA-CGA-O1A
14	B	3023	CLA	C4-C3-C5-C6
14	A	820	CLA	C6-C7-C8-C10
14	A	820	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
14	A	839	CLA	C11-C12-C13-C15
14	B	3014	CLA	C11-C10-C8-C7
14	B	3029	CLA	CAA-CBA-CGA-O1A
17	I	102	LMG	O7-C10-C11-C12
18	A	853	LHG	C28-C29-C30-C31
16	L	208	BCR	C7-C8-C9-C10
14	A	832	CLA	CAA-CBA-CGA-O1A
14	B	3007	CLA	CAA-CBA-CGA-O1A
14	B	3014	CLA	CAA-CBA-CGA-O1A
14	B	3015	CLA	CAA-CBA-CGA-O1A
18	A	854	LHG	O9-C7-C8-C9
14	B	3027	CLA	CAA-CBA-CGA-O2A
18	A	853	LHG	O7-C7-C8-C9
18	A	853	LHG	C35-C36-C37-C38
14	A	807	CLA	CAA-CBA-CGA-O1A
18	A	853	LHG	C15-C16-C17-C18
14	A	812	CLA	CAA-CBA-CGA-O2A
14	A	844	CLA	C13-C15-C16-C17
14	A	856	CLA	C8-C10-C11-C12

There are no ring outliers.

124 monomers are involved in 376 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	825	CLA	3	0
14	B	3036	CLA	1	0
14	K	101	CLA	4	0
16	B	3047	BCR	3	0
14	K	103	CLA	1	0
14	A	839	CLA	3	0
14	B	3035	CLA	3	0
14	L	206	CLA	1	0
14	A	820	CLA	6	0
16	L	208	BCR	2	0
14	A	808	CLA	4	0
15	A	846	PQN	9	0
14	A	856	CLA	7	0
14	B	3033	CLA	4	0
14	B	3007	CLA	3	0
14	A	818	CLA	5	0
16	F	203	BCR	4	0
14	B	3030	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	L	201	BCR	3	0
14	B	3013	CLA	4	0
16	L	209	BCR	2	0
14	A	813	CLA	9	0
16	B	3045	BCR	8	0
14	B	3017	CLA	4	0
14	B	3023	CLA	2	0
14	B	3028	CLA	4	0
14	B	3020	CLA	2	0
17	I	102	LMG	3	0
14	A	810	CLA	3	0
18	A	853	LHG	3	0
14	B	3041	CLA	3	0
14	B	3022	CLA	2	0
16	A	850	BCR	4	0
14	A	806	CLA	3	0
16	M	103	BCR	2	0
14	A	827	CLA	2	0
14	A	830	CLA	5	0
14	B	3027	CLA	1	0
16	B	3044	BCR	1	0
16	B	3051	BCR	4	0
14	A	812	CLA	5	0
14	A	824	CLA	1	0
14	B	3034	CLA	5	0
14	B	3038	CLA	4	0
14	B	3008	CLA	3	0
16	J	105	BCR	11	0
14	J	102	CLA	1	0
14	A	811	CLA	7	0
14	A	822	CLA	4	0
14	B	3004	CLA	4	0
14	B	3015	CLA	1	0
14	A	817	CLA	3	0
14	B	3032	CLA	2	0
14	A	814	CLA	2	0
15	B	3043	PQN	2	0
14	A	844	CLA	4	0
14	A	835	CLA	4	0
14	B	3031	CLA	3	0
22	L	207	DGD	2	0
17	A	855	LMG	1	0

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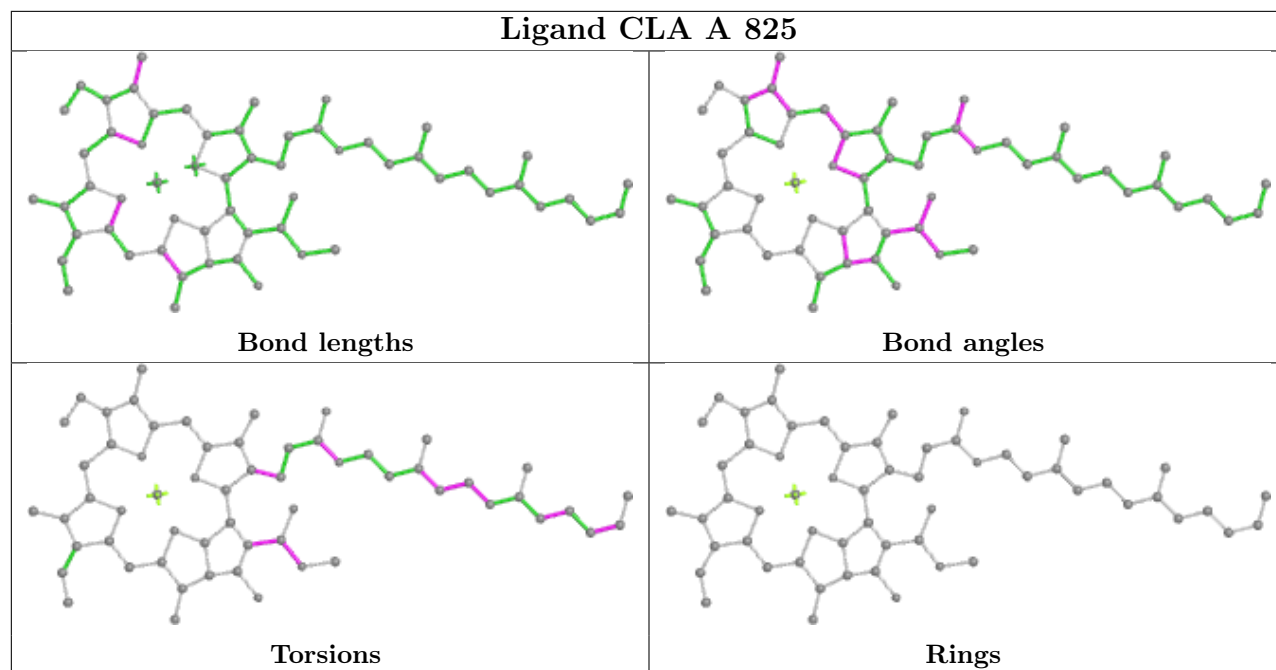
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	3050	LHG	2	0
14	B	3010	CLA	8	0
14	B	3042	CLA	1	0
18	A	854	LHG	4	0
16	J	104	BCR	6	0
14	B	3006	CLA	2	0
16	F	201	BCR	4	0
16	A	847	BCR	7	0
16	J	103	BCR	3	0
14	B	3019	CLA	3	0
14	A	843	CLA	5	0
14	B	3018	CLA	7	0
14	A	841	CLA	6	0
16	K	102	BCR	5	0
14	A	828	CLA	5	0
18	M	101	LHG	3	0
14	B	3037	CLA	2	0
14	A	815	CLA	4	0
14	B	3029	CLA	1	0
14	B	3014	CLA	7	0
14	A	807	CLA	1	0
14	B	3003	CLA	4	0
14	A	802	CLA	3	0
13	A	801	CL0	3	0
14	A	803	CLA	3	0
14	A	831	CLA	6	0
14	X	1701	CLA	3	0
14	B	3021	CLA	2	0
14	A	805	CLA	2	0
14	A	829	CLA	9	0
19	C	101	SF4	1	0
14	B	3012	CLA	2	0
14	B	3040	CLA	3	0
14	L	204	CLA	2	0
14	A	838	CLA	2	0
14	A	821	CLA	3	0
14	B	3016	CLA	1	0
14	A	836	CLA	3	0
14	A	845	CLA	6	0
16	B	3046	BCR	3	0
14	B	3005	CLA	2	0
14	J	101	CLA	3	0

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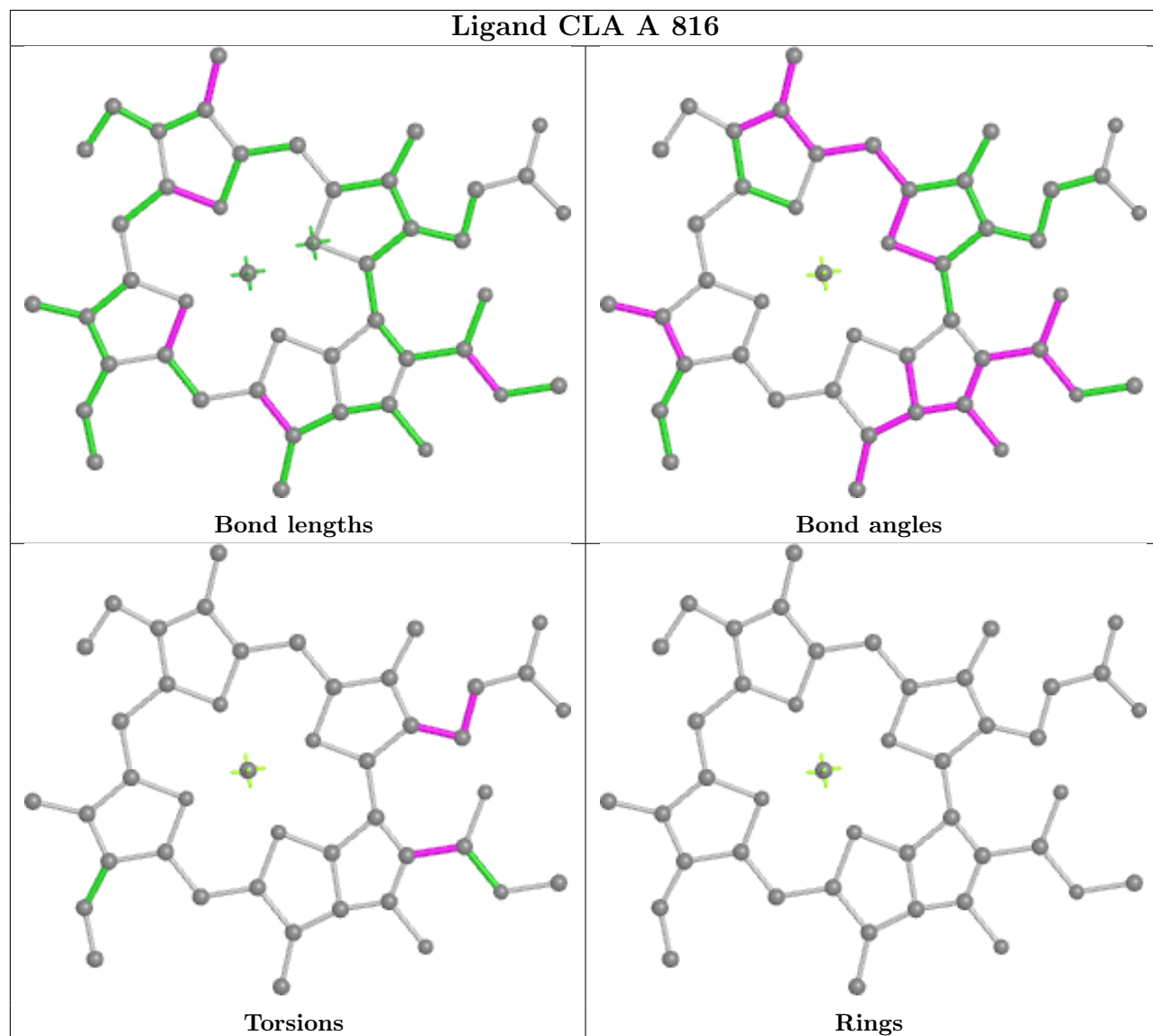
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	849	BCR	2	0
14	B	3009	CLA	1	0
14	B	3024	CLA	5	0
14	F	202	CLA	8	0
14	L	205	CLA	3	0
16	A	851	BCR	8	0
14	A	833	CLA	4	0
14	B	3025	CLA	4	0
16	I	101	BCR	4	0
14	M	102	CLA	4	0
14	A	823	CLA	2	0
14	A	809	CLA	6	0
14	A	832	CLA	8	0
14	A	804	CLA	10	0
14	A	826	CLA	8	0
14	B	3011	CLA	2	0
14	B	3026	CLA	5	0
14	A	842	CLA	4	0
14	B	3039	CLA	3	0
14	A	834	CLA	2	0
14	A	819	CLA	7	0
14	A	840	CLA	2	0

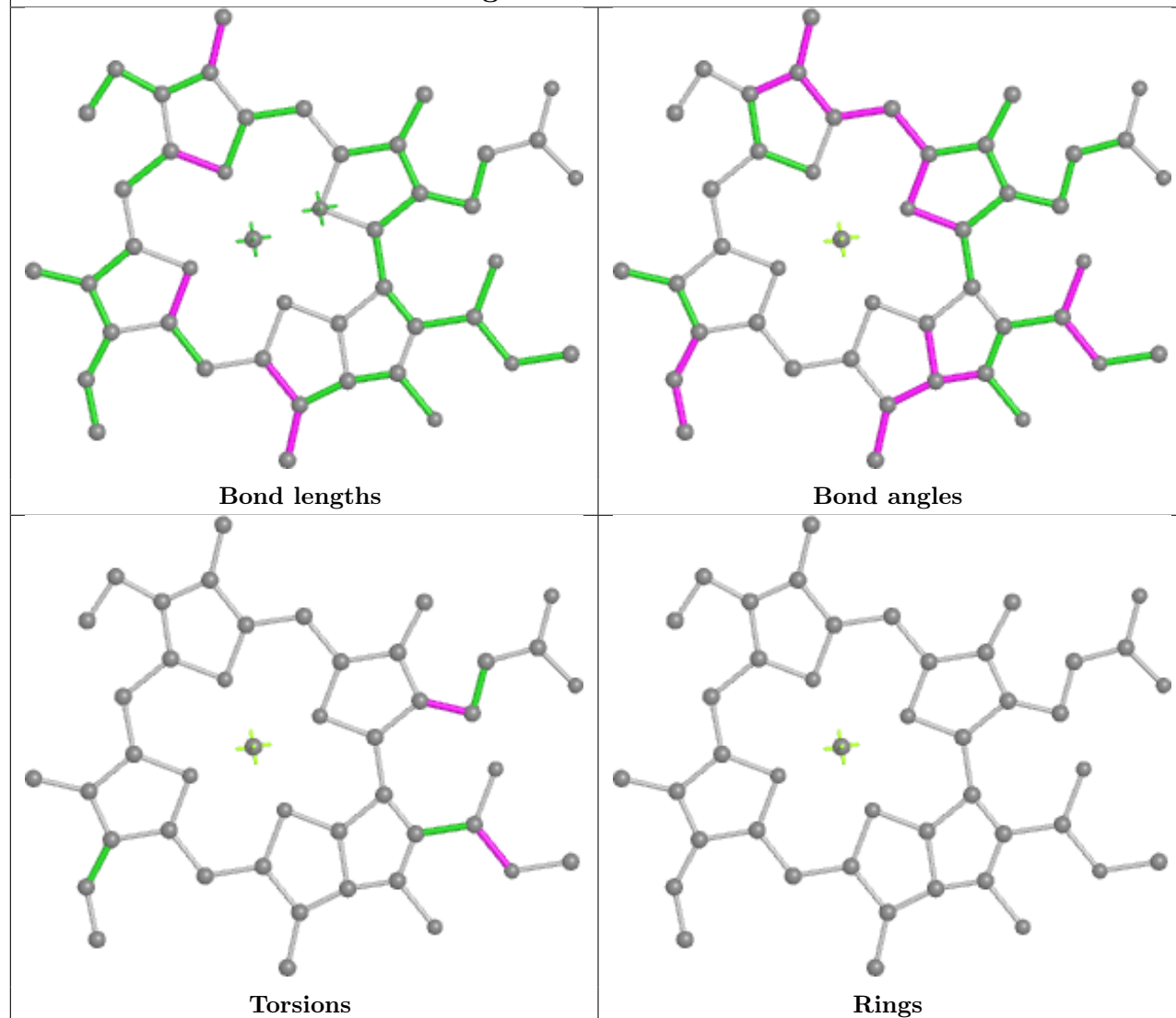
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



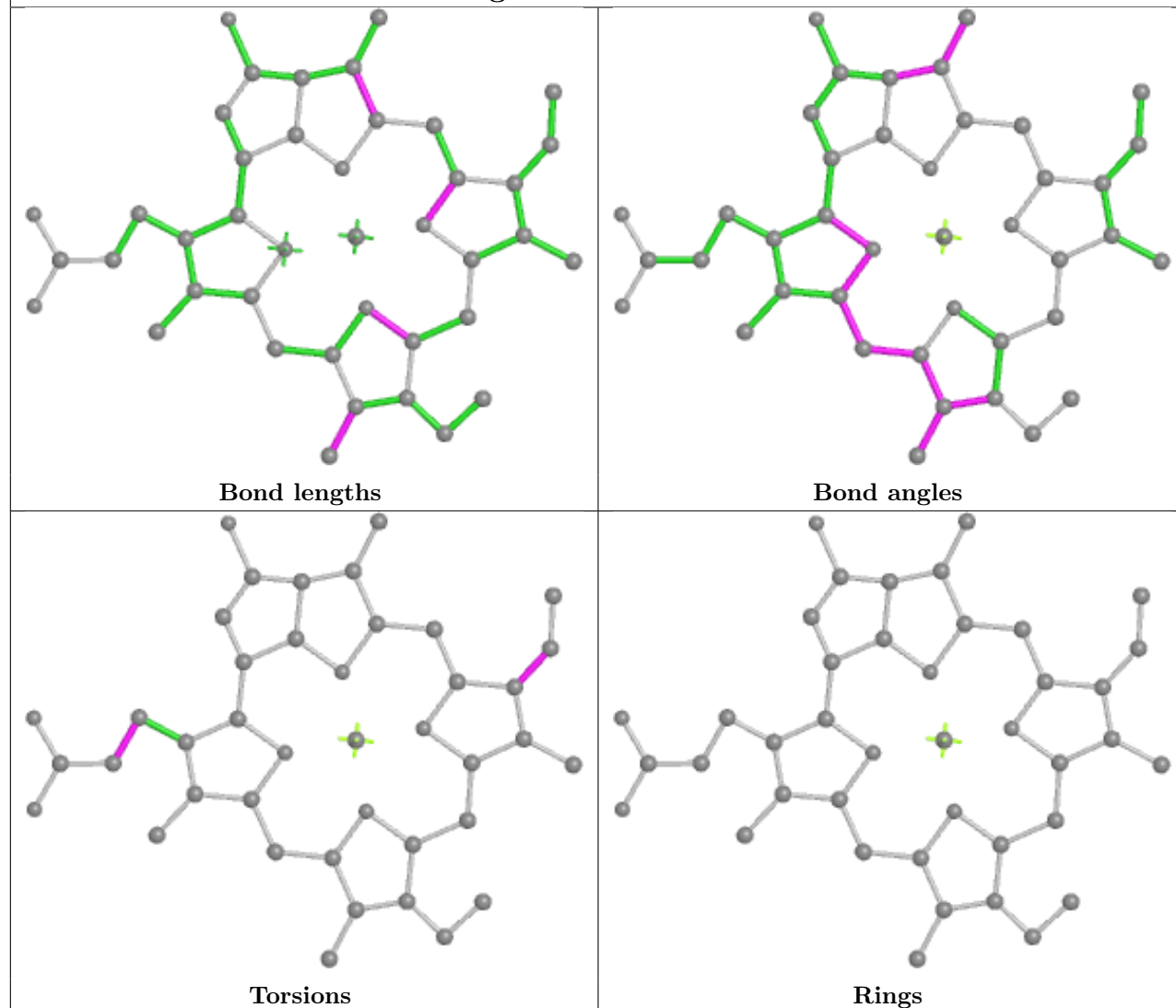
Ligand CLA A 816



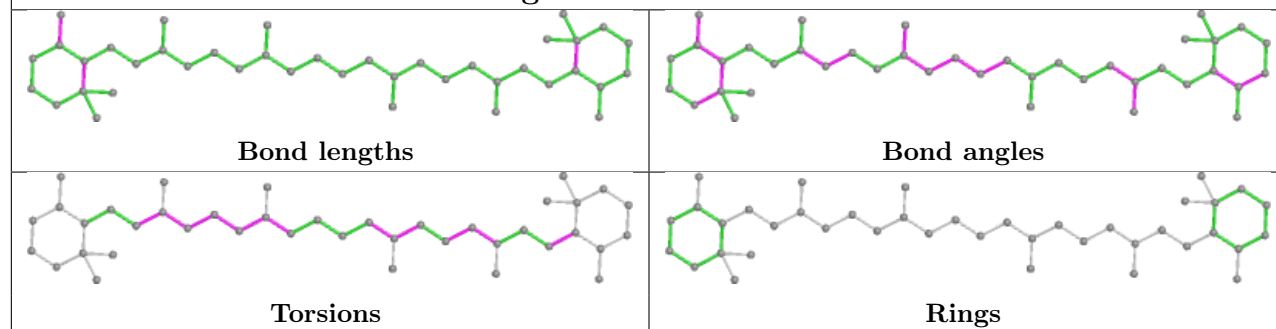
Ligand CLA B 3036



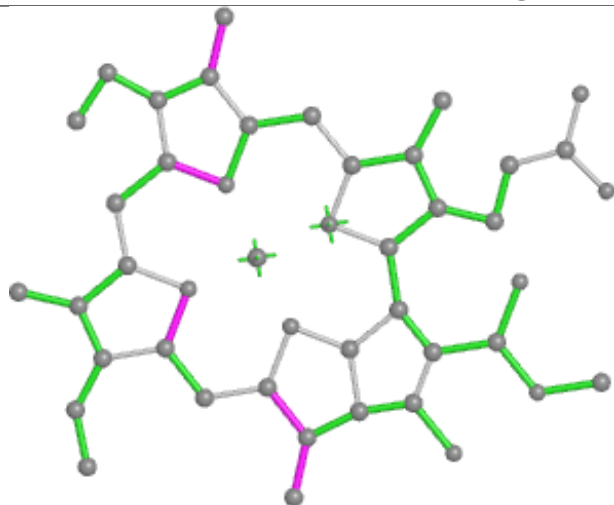
Ligand CLA K 101



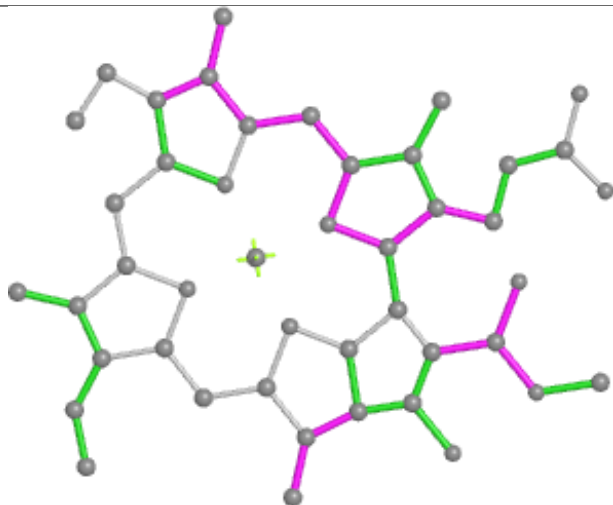
Ligand BCR B 3047



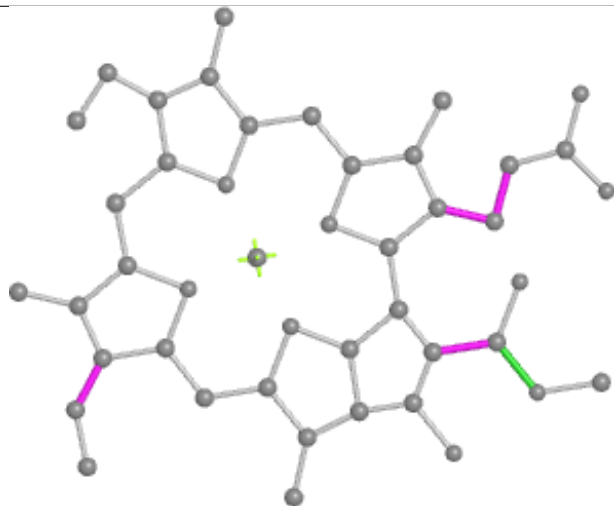
Ligand CLA K 103



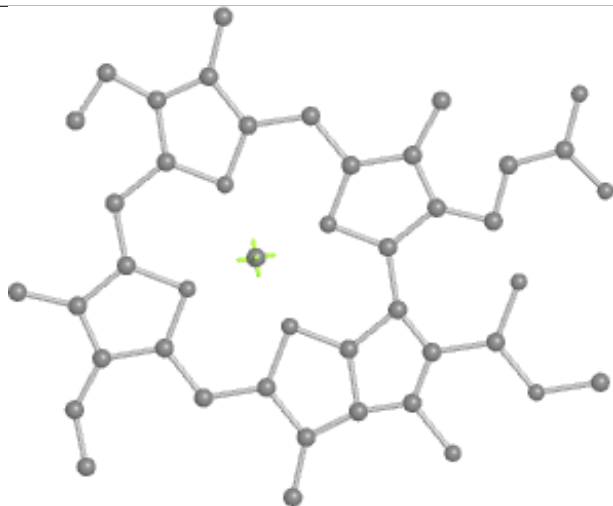
Bond lengths



Bond angles

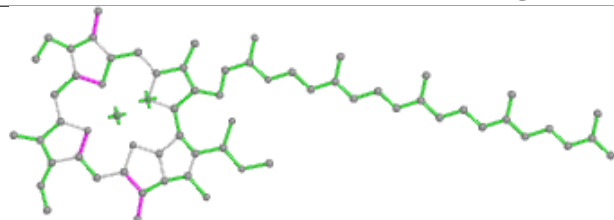


Torsions

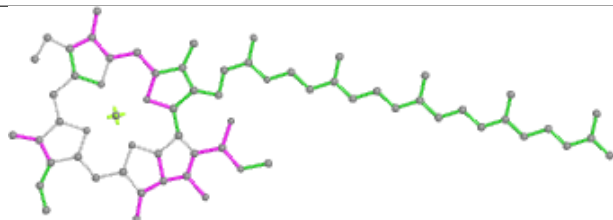


Rings

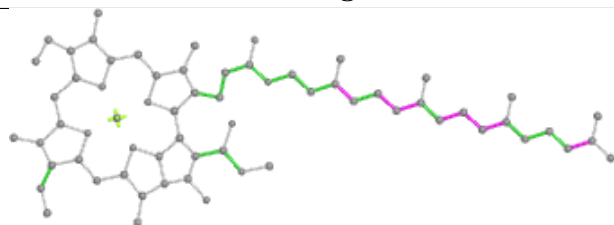
Ligand CLA A 839



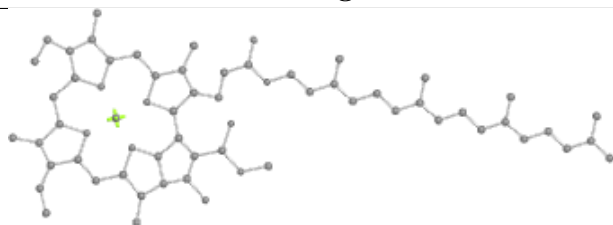
Bond lengths



Bond angles

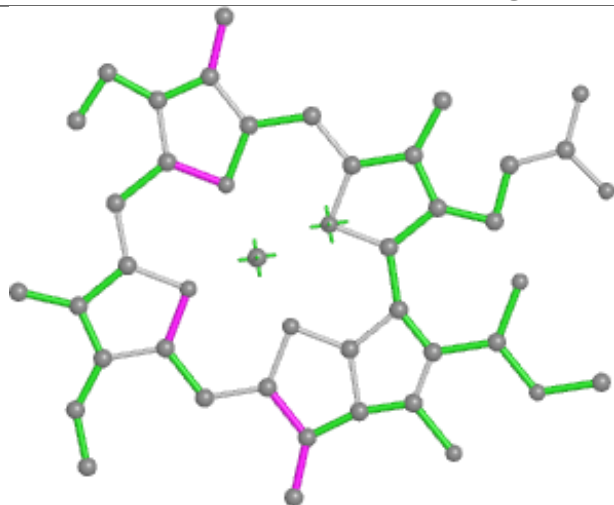


Torsions

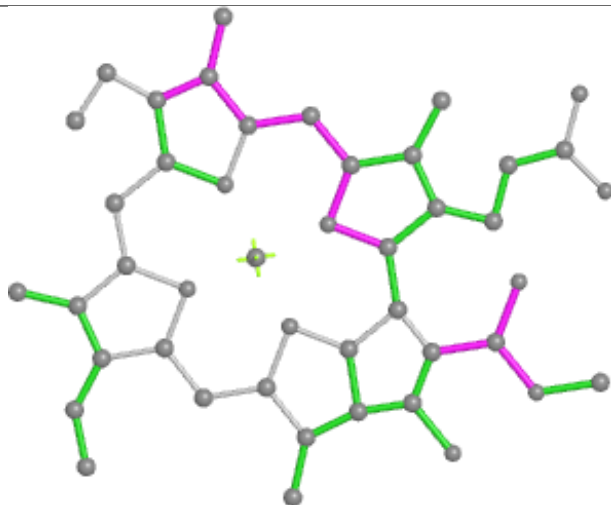


Rings

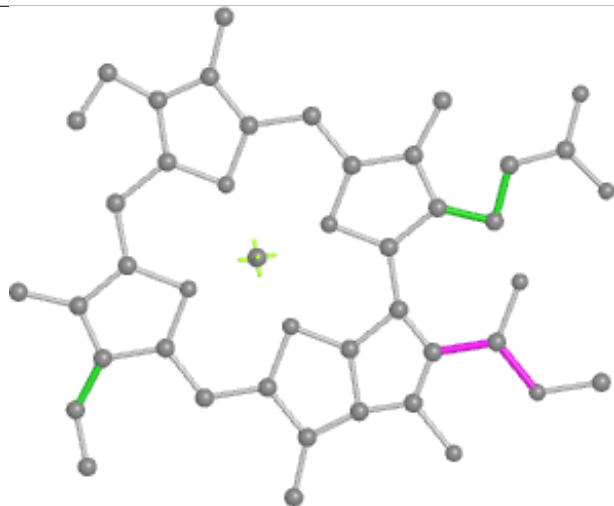
Ligand CLA B 3035



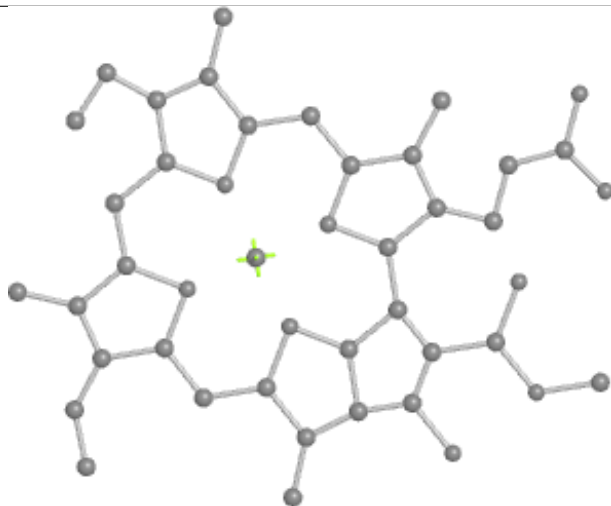
Bond lengths



Bond angles

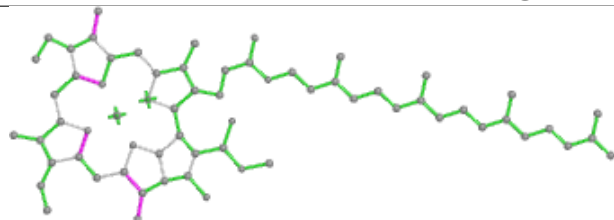


Torsions

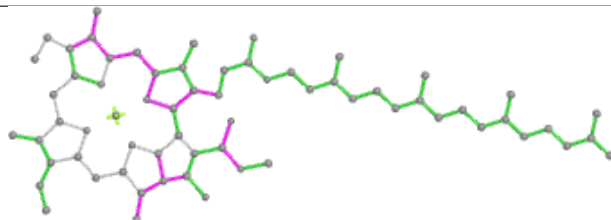


Rings

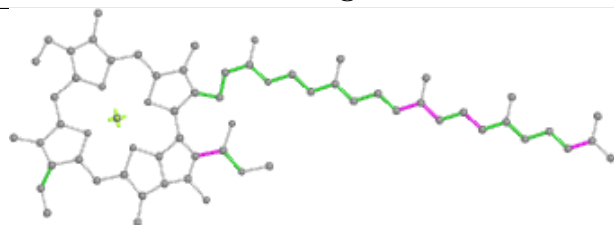
Ligand CLA L 206



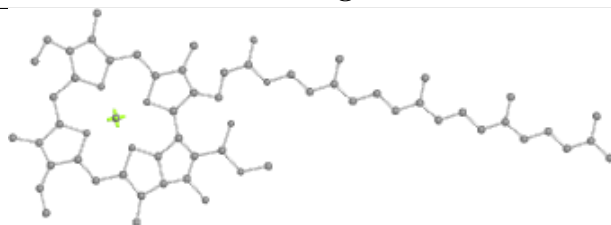
Bond lengths



Bond angles

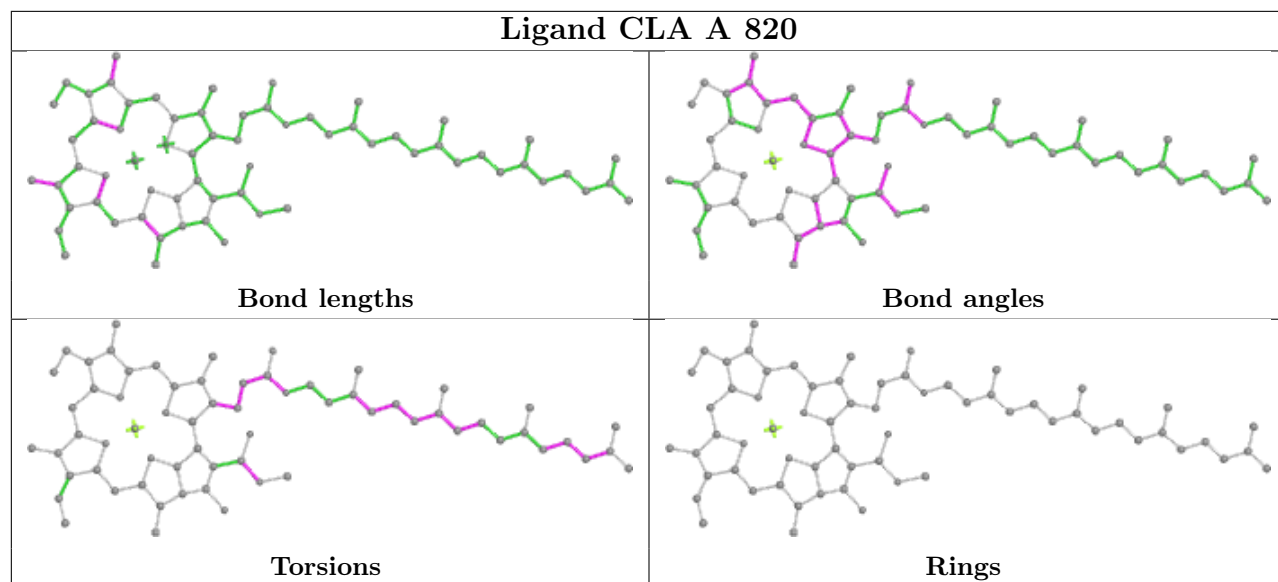


Torsions

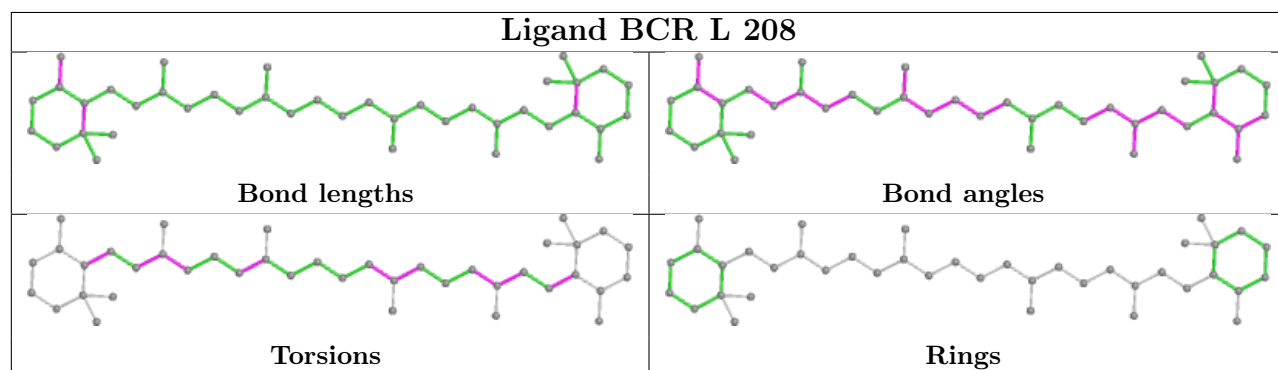


Rings

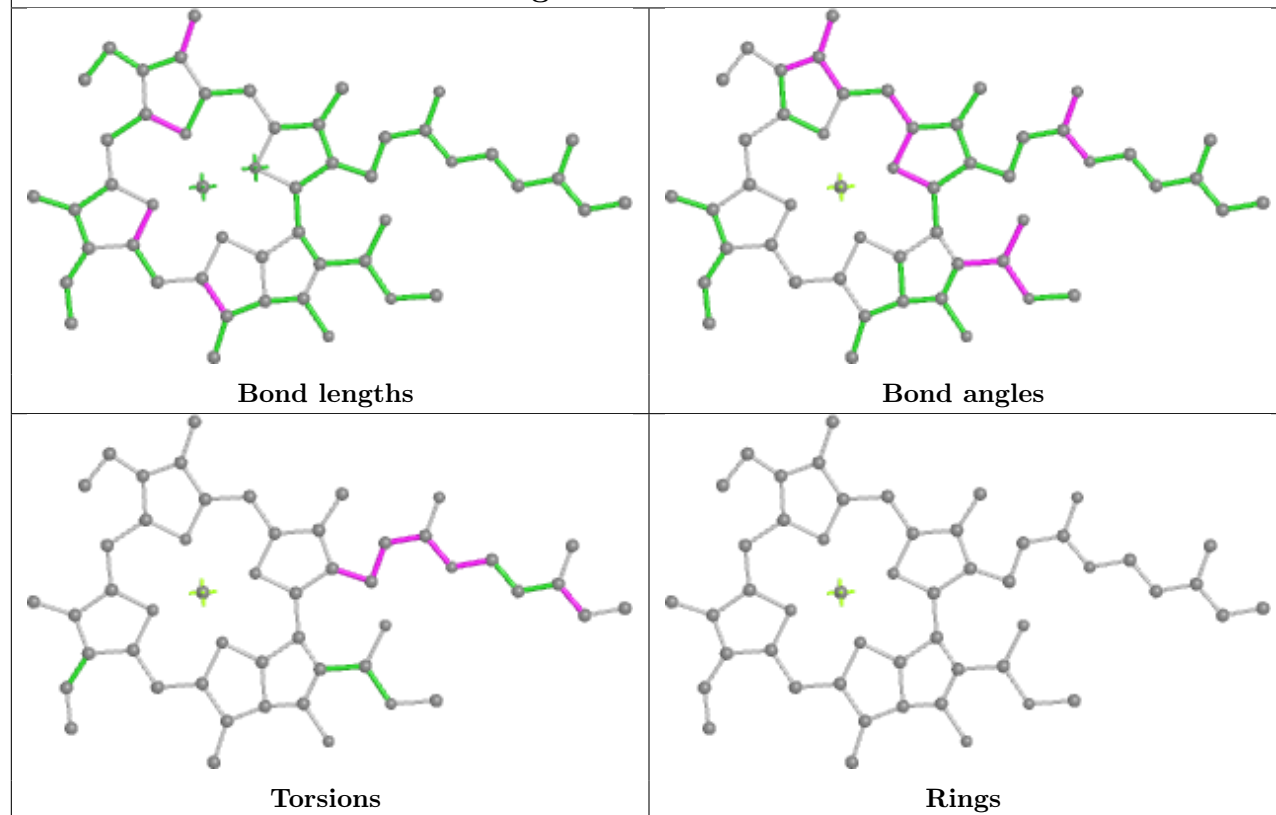
Ligand CLA A 820



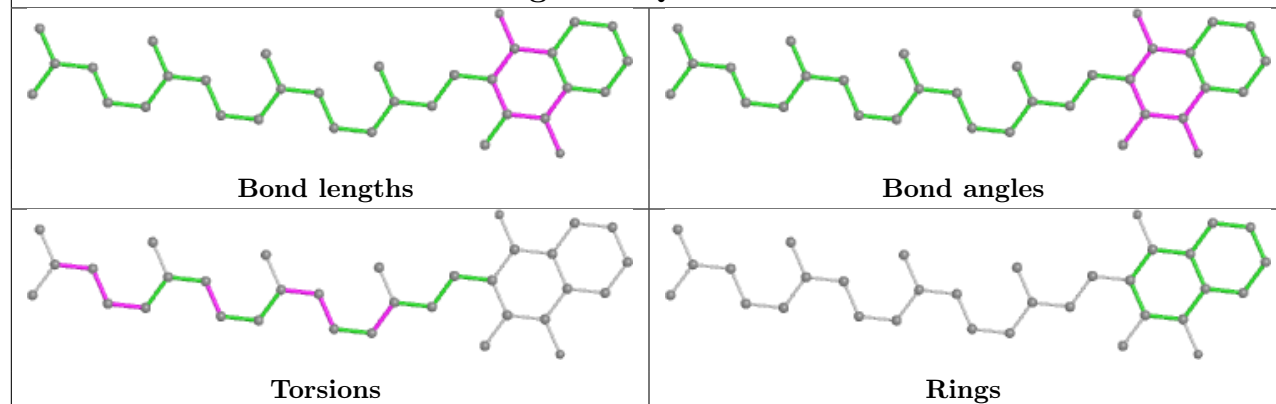
Ligand BCR L 208



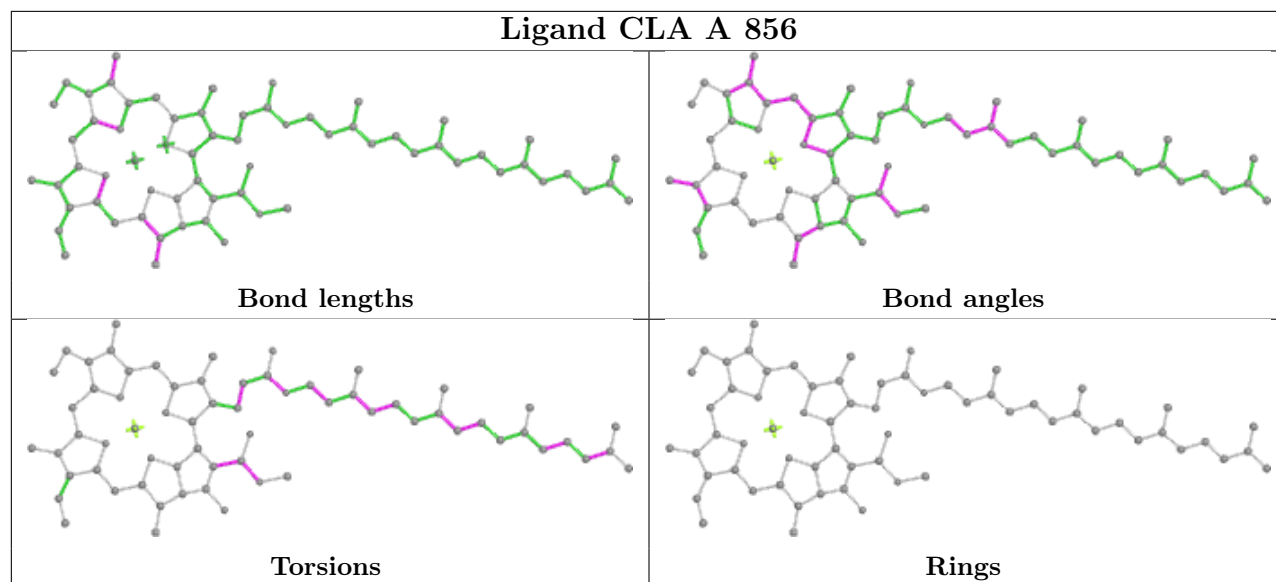
Ligand CLA A 808



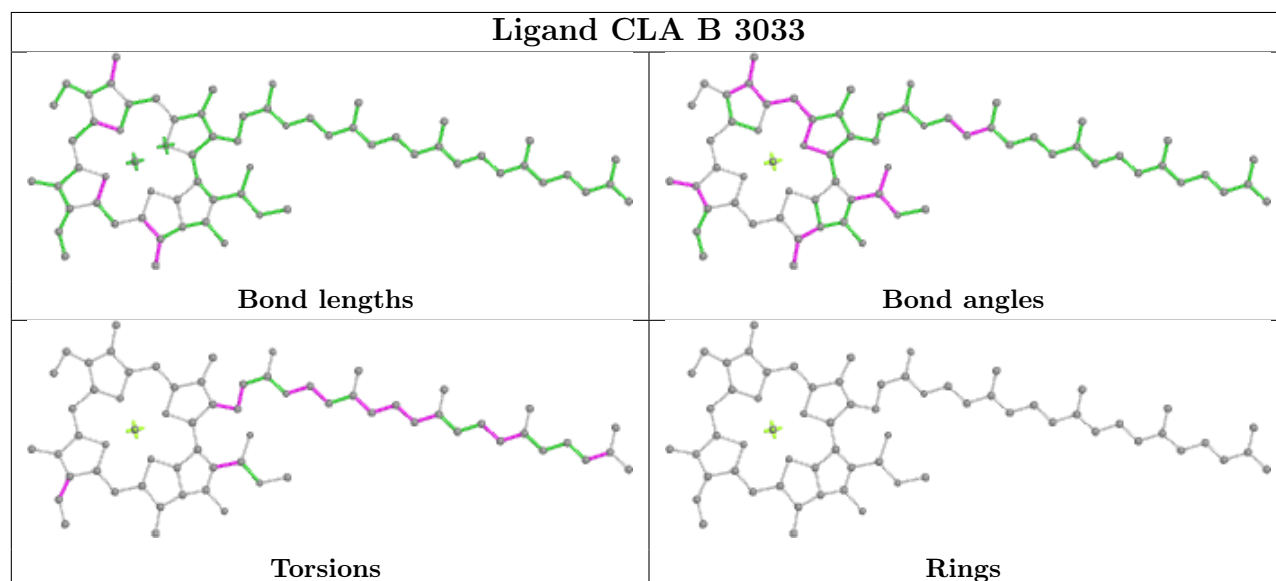
Ligand PQN A 846



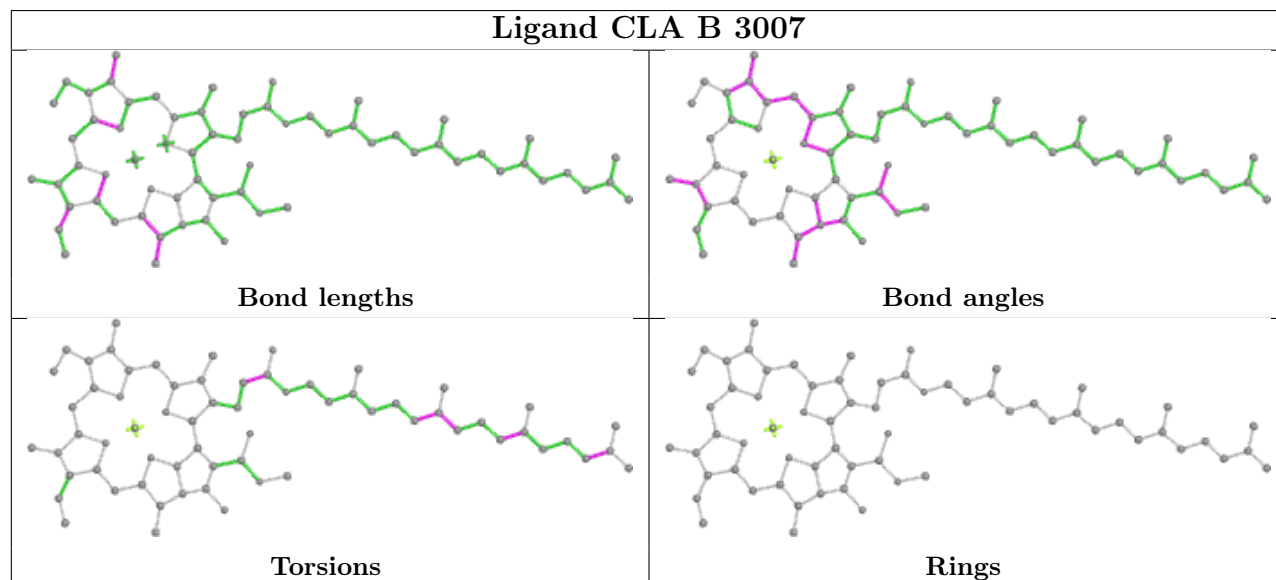
Ligand CLA A 856

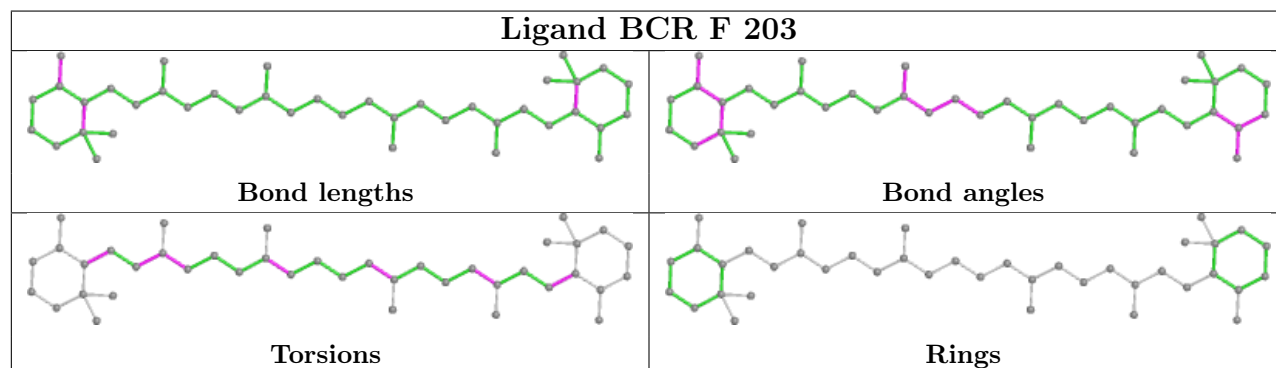
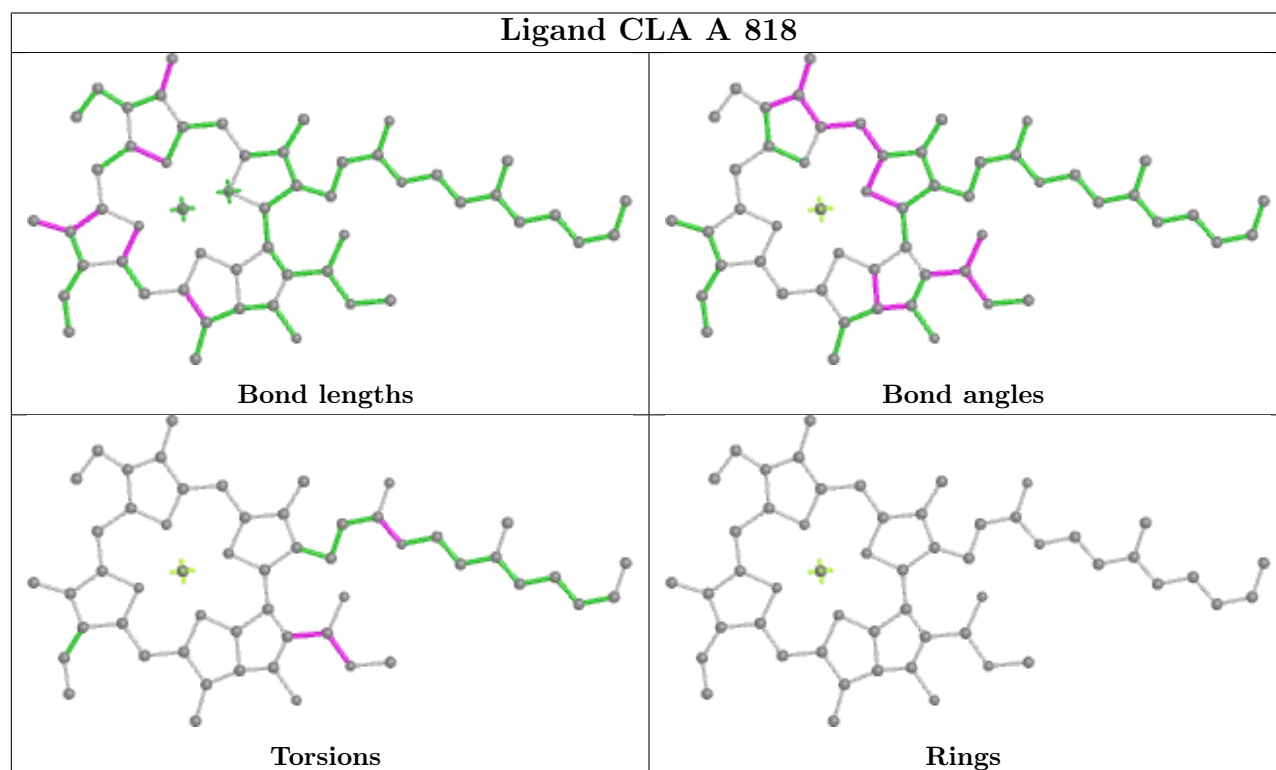
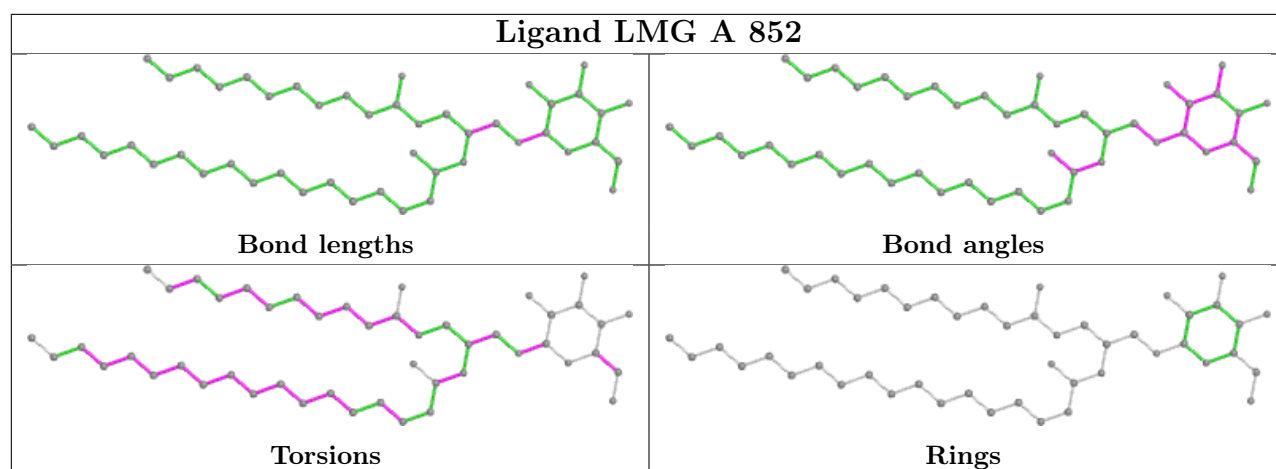


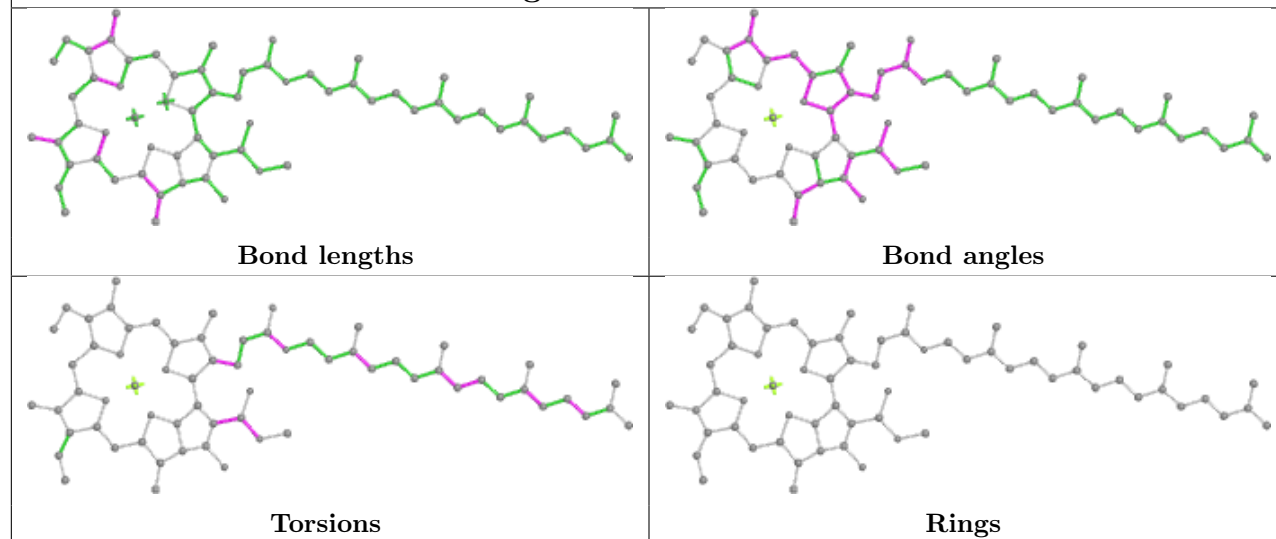
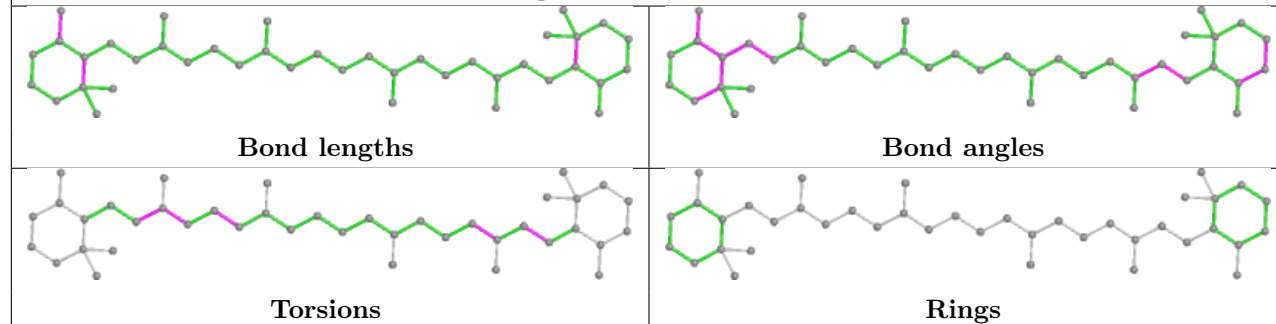
Ligand CLA B 3033



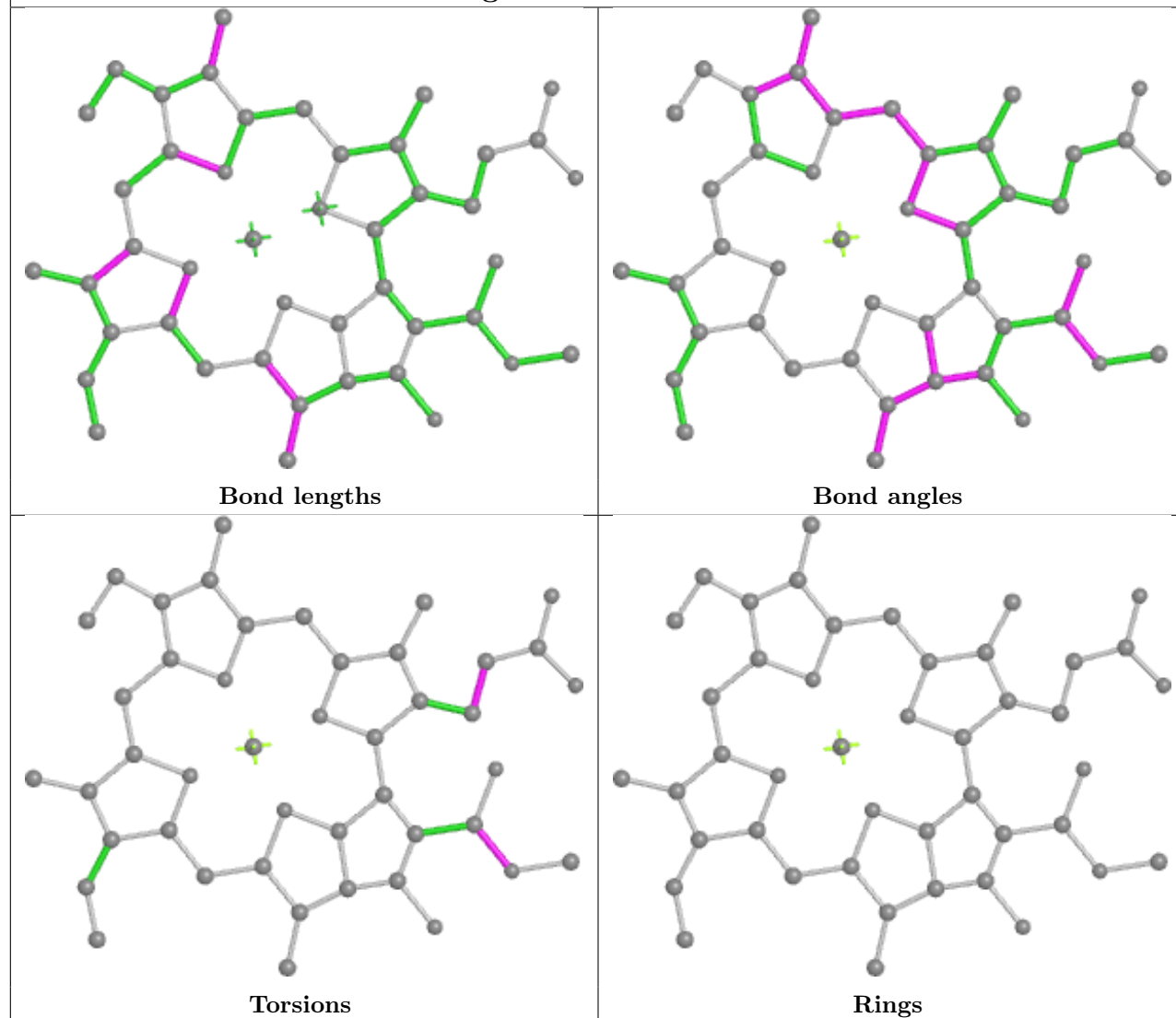
Ligand CLA B 3007



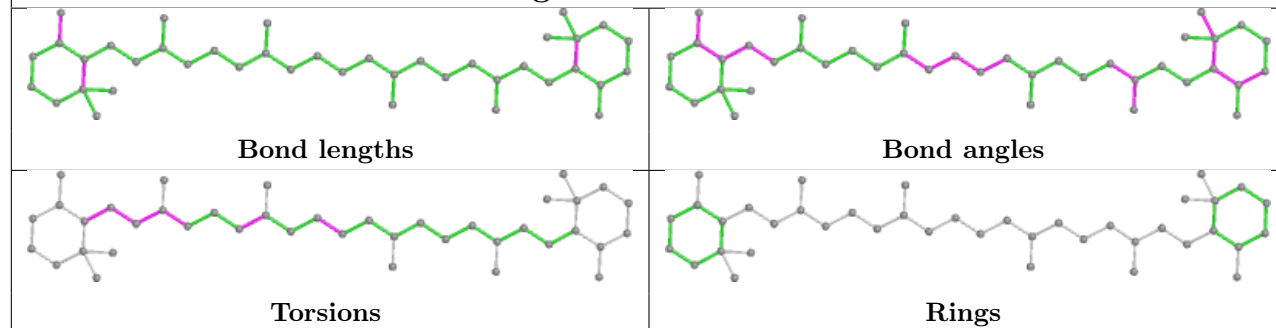


Ligand CLA B 3030**Ligand BCR L 201**

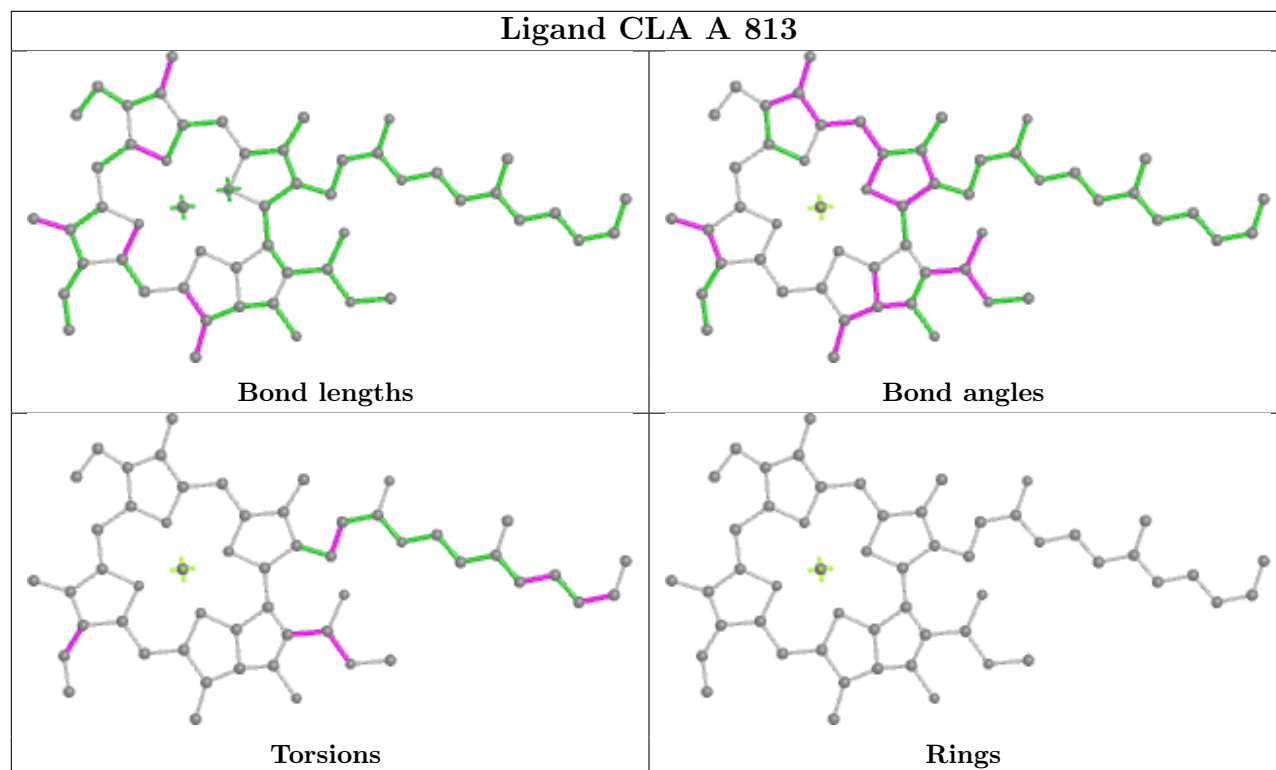
Ligand CLA B 3013



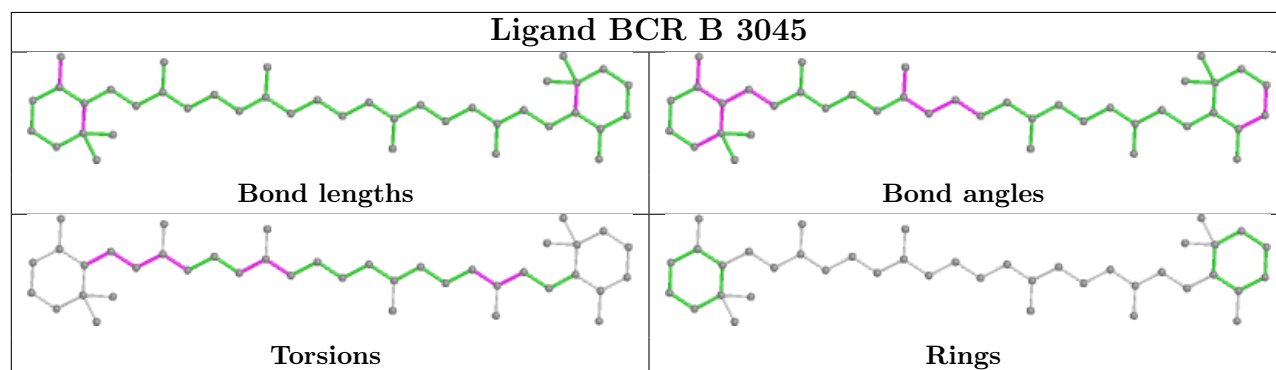
Ligand BCR L 209



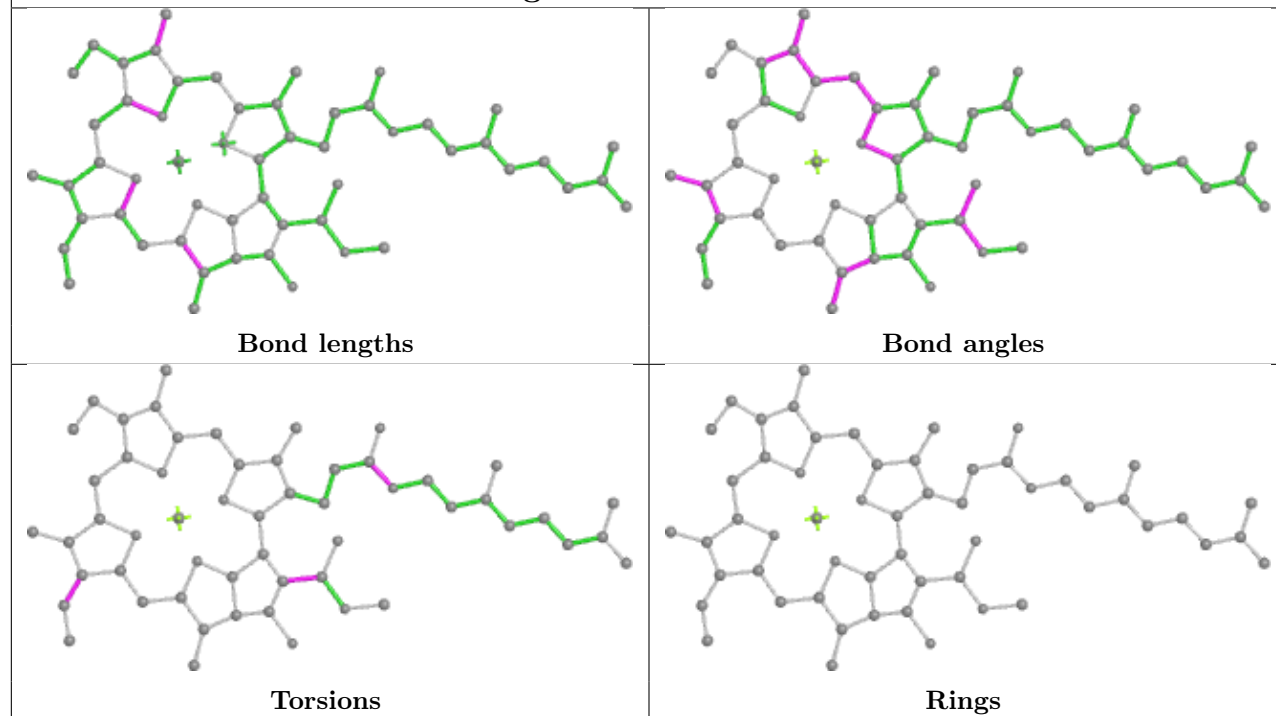
Ligand CLA A 813



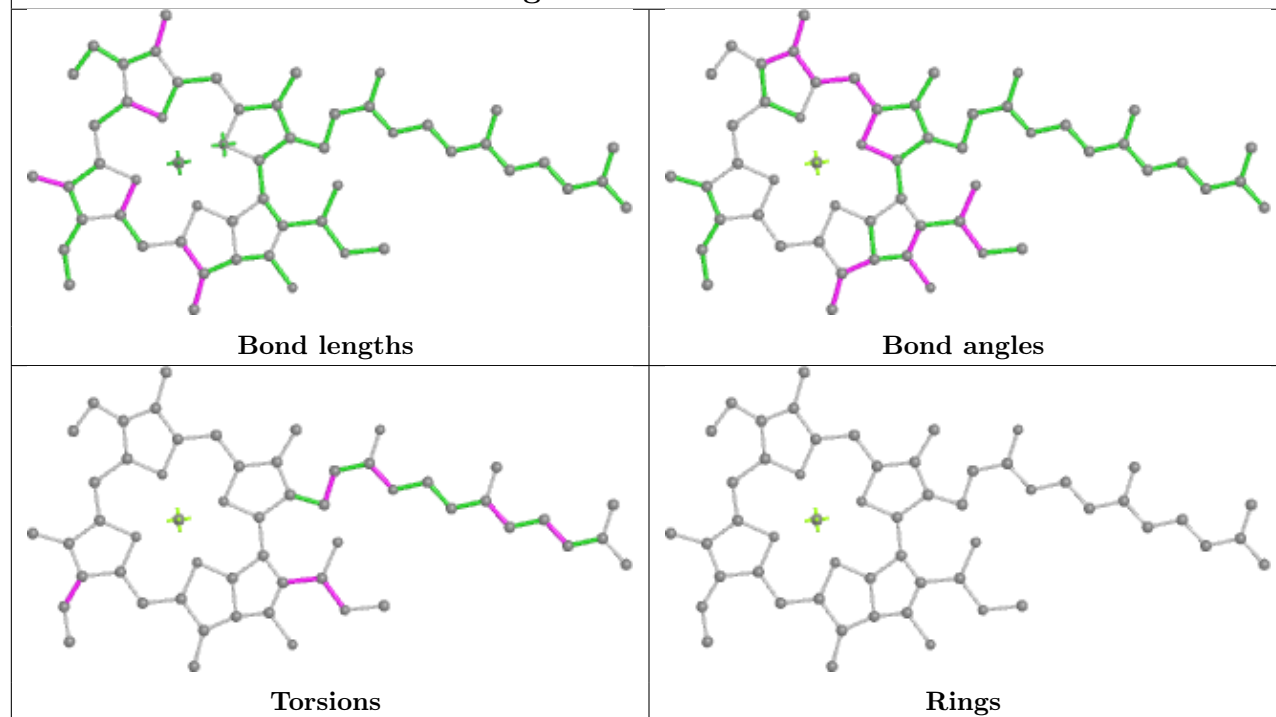
Ligand BCR B 3045

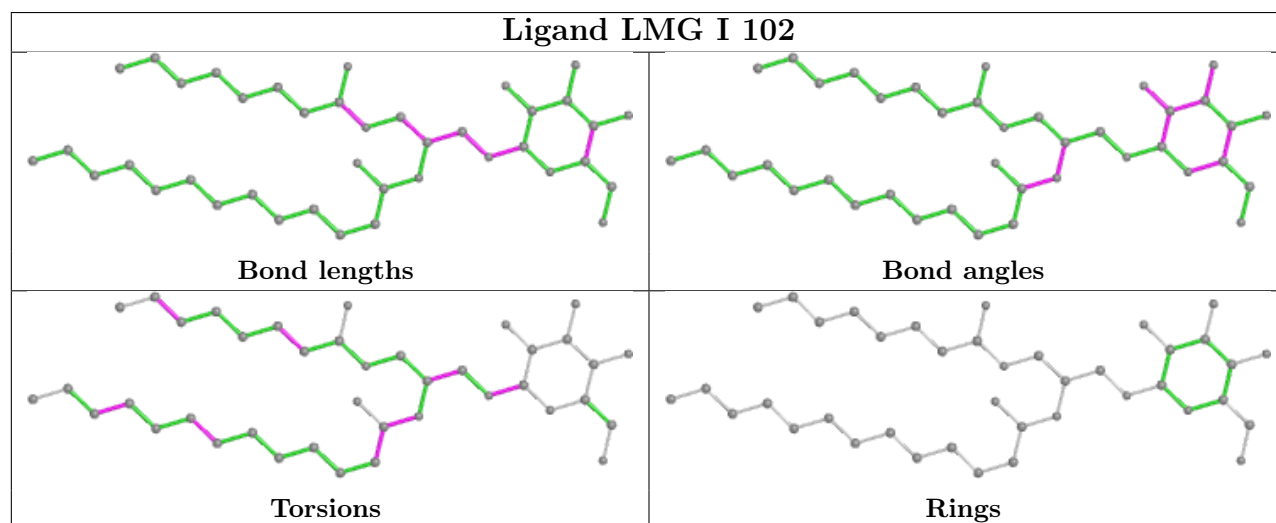
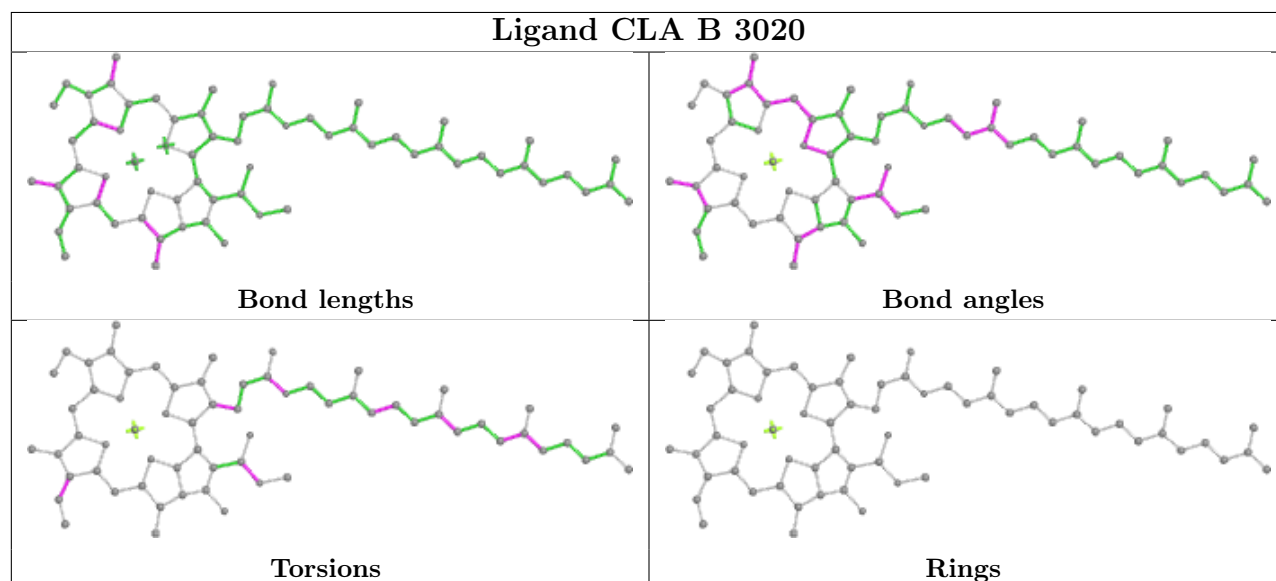
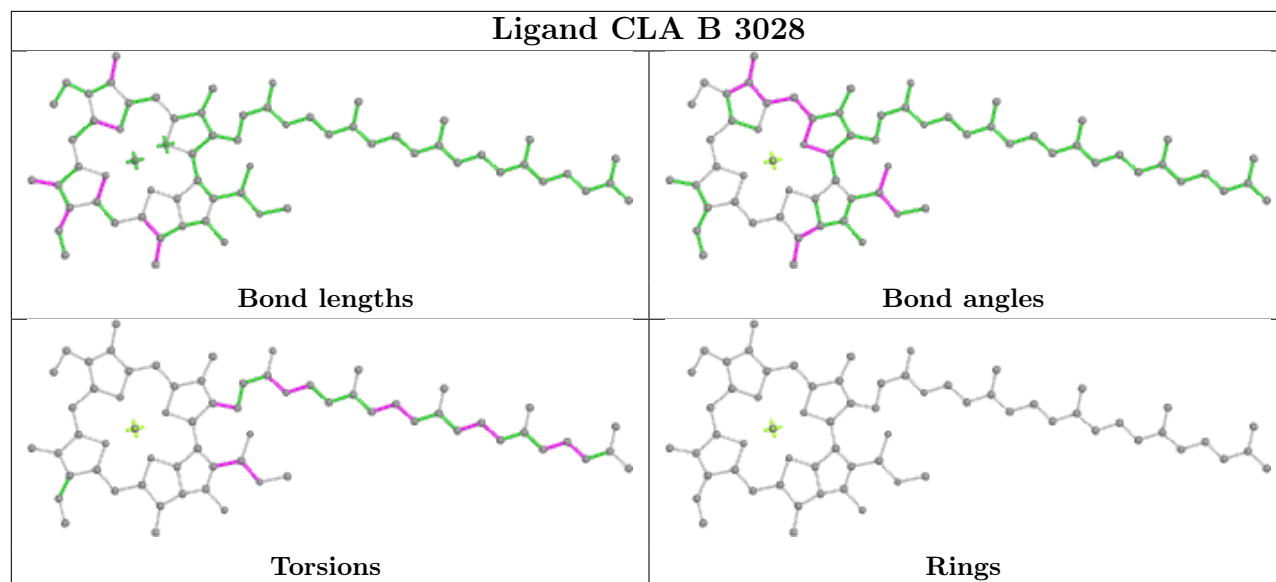


Ligand CLA B 3017

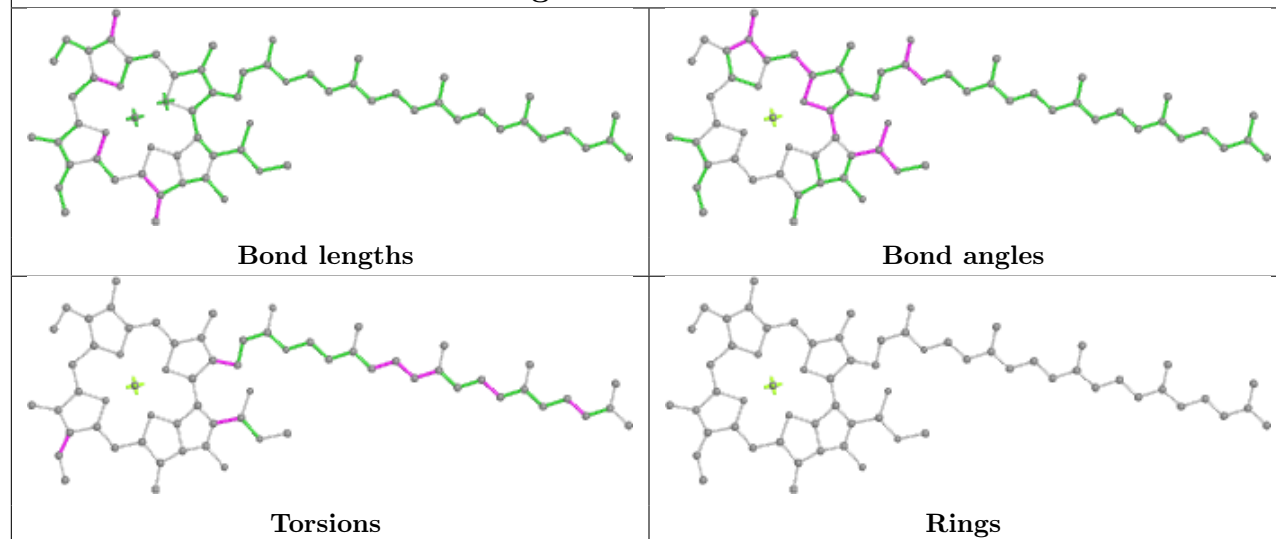


Ligand CLA B 3023

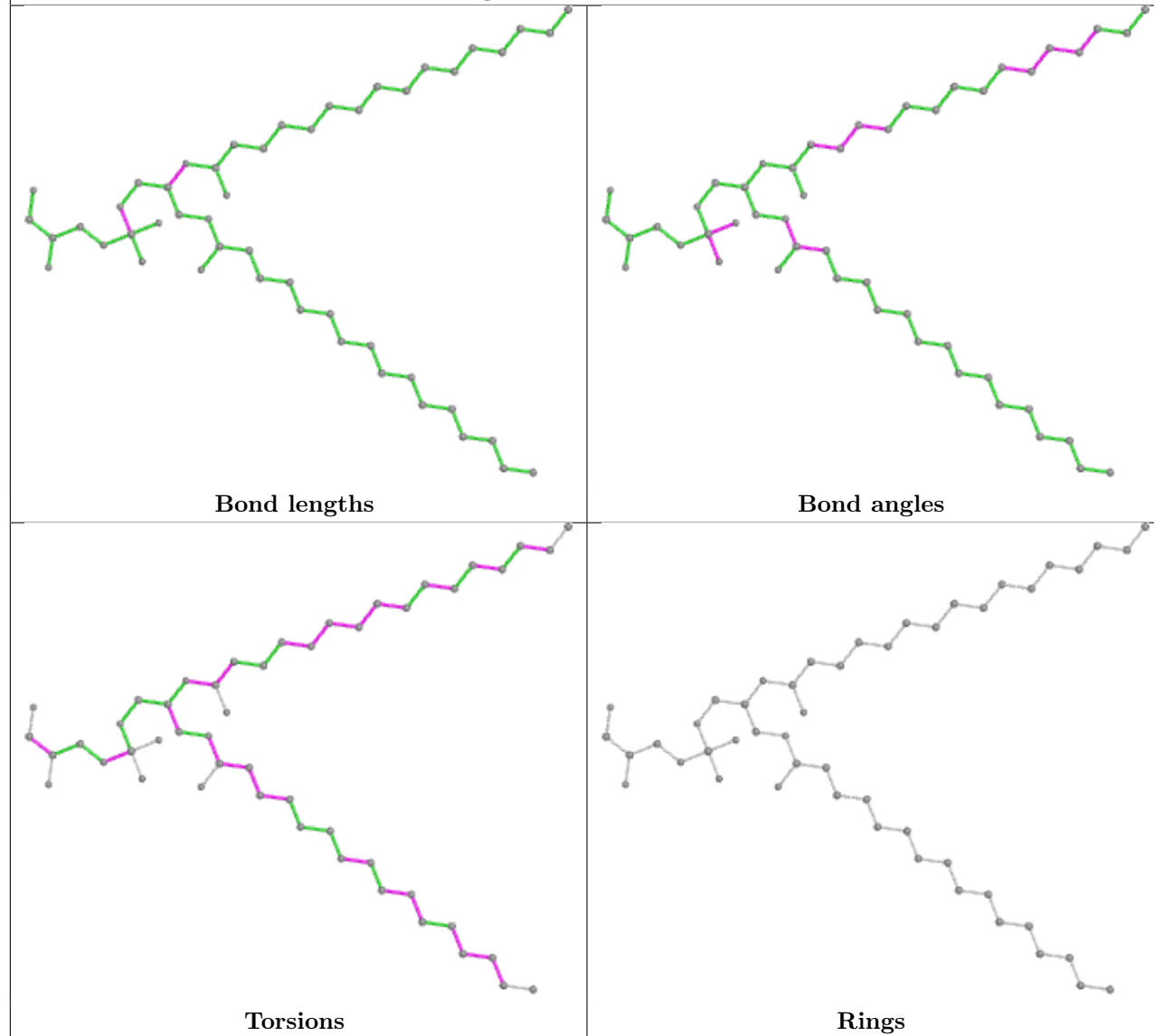




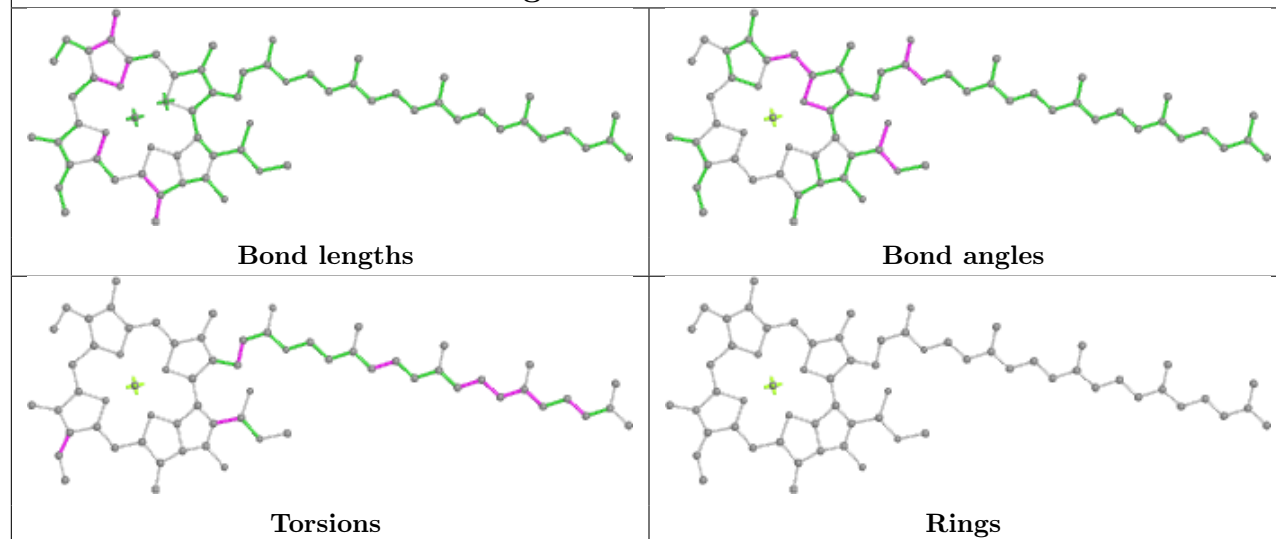
Ligand CLA A 810



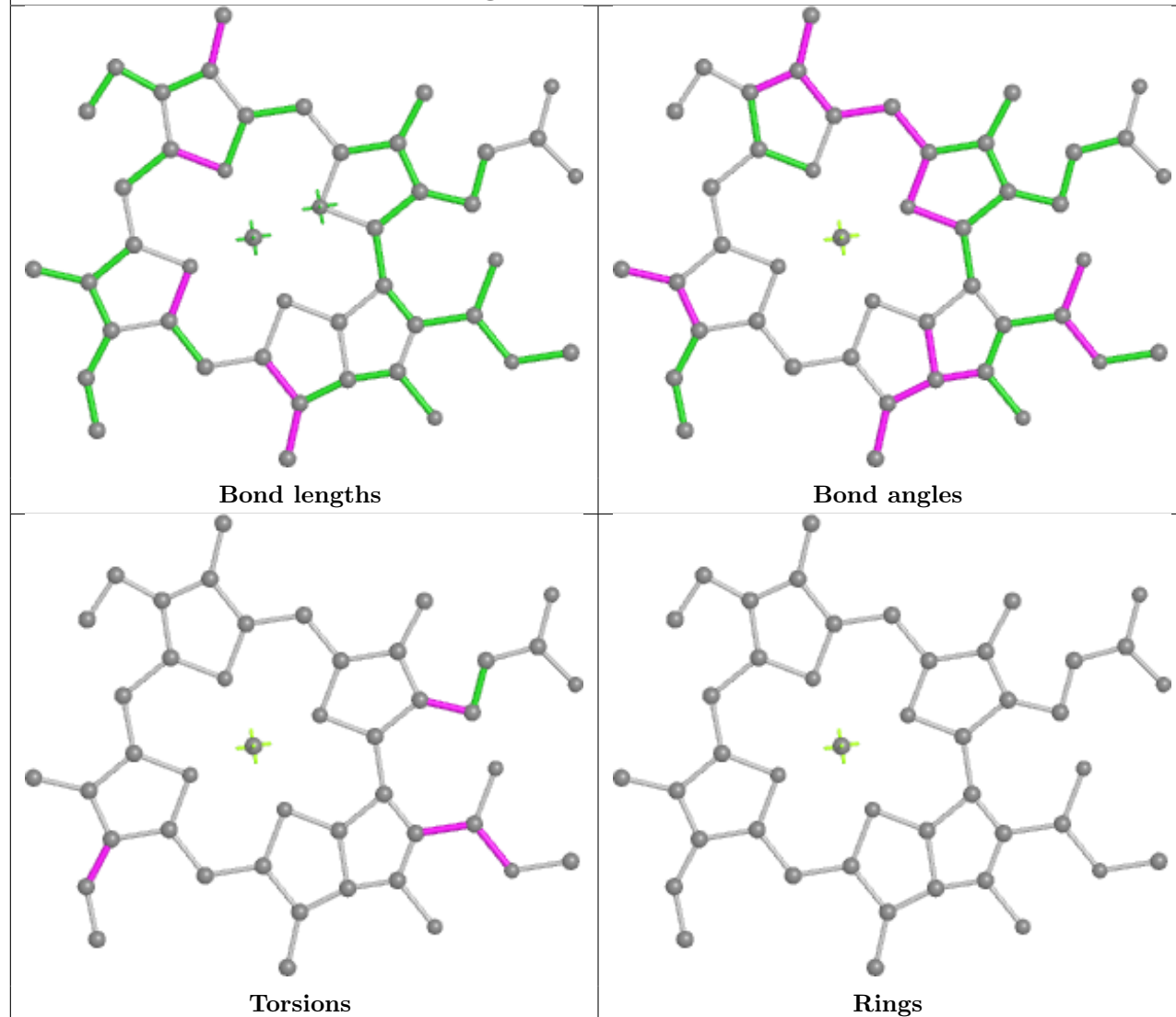
Ligand LHG A 853

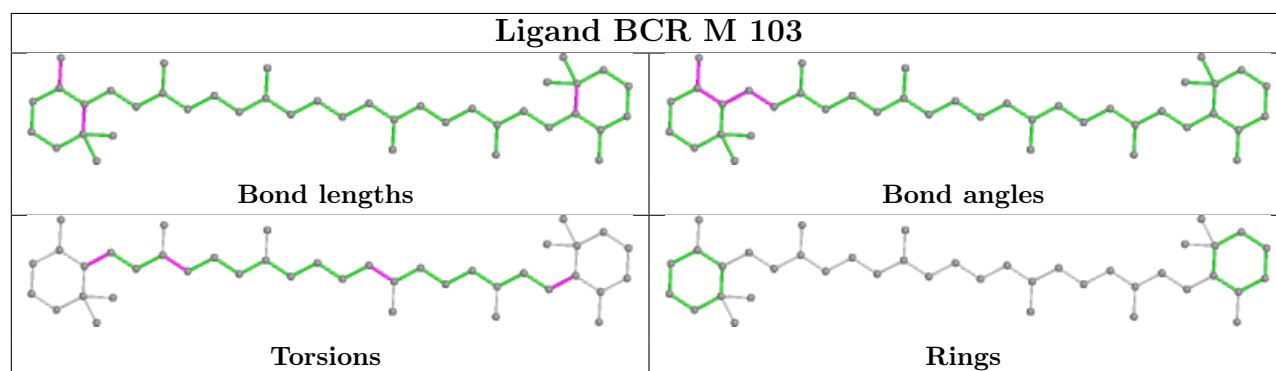
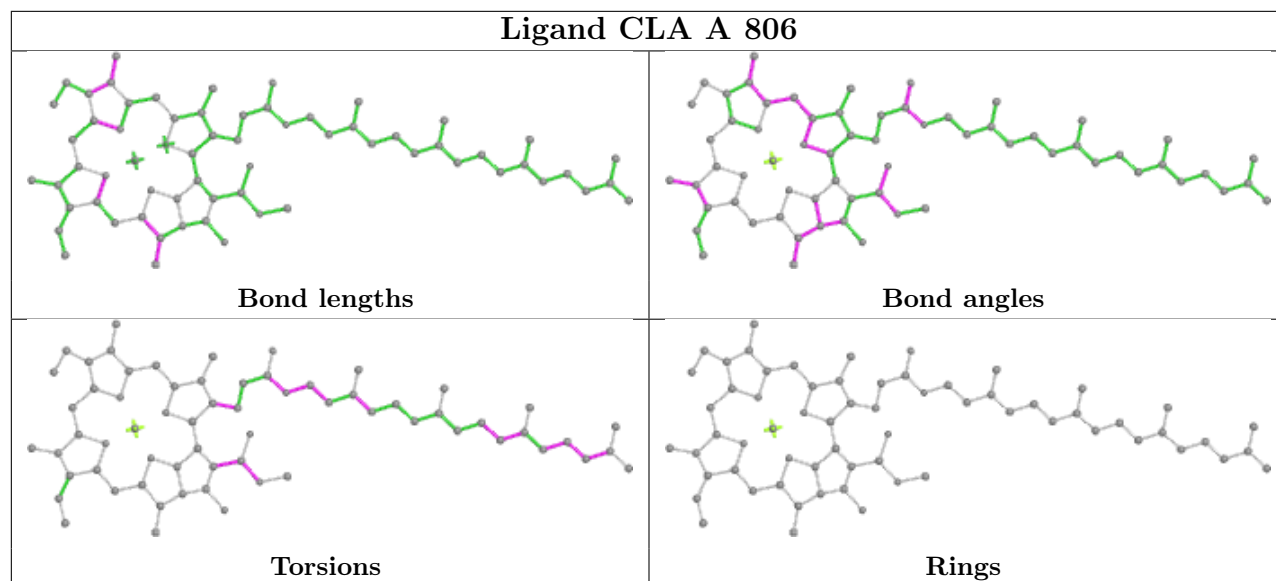
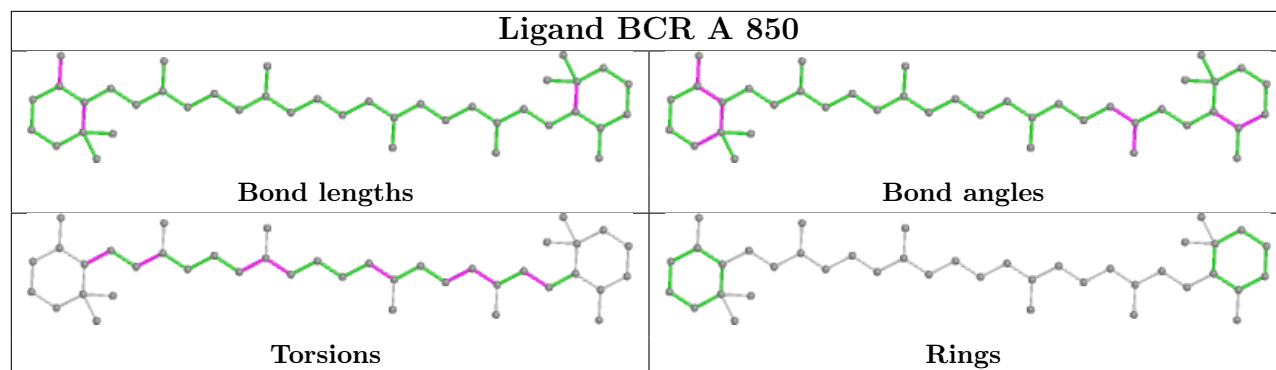


Ligand CLA B 3041

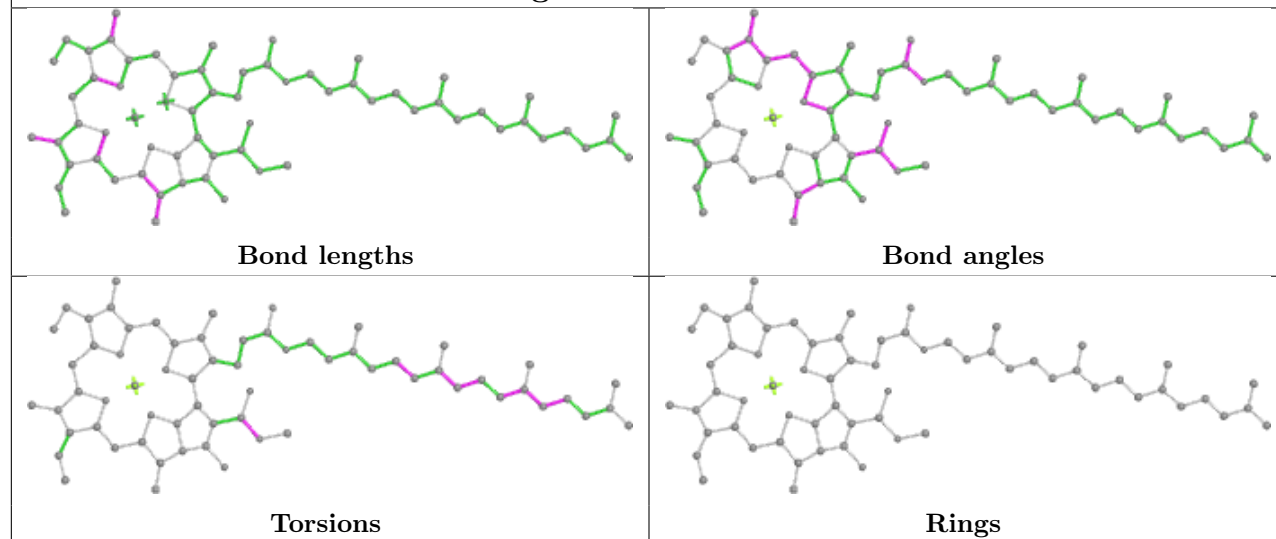


Ligand CLA B 3022

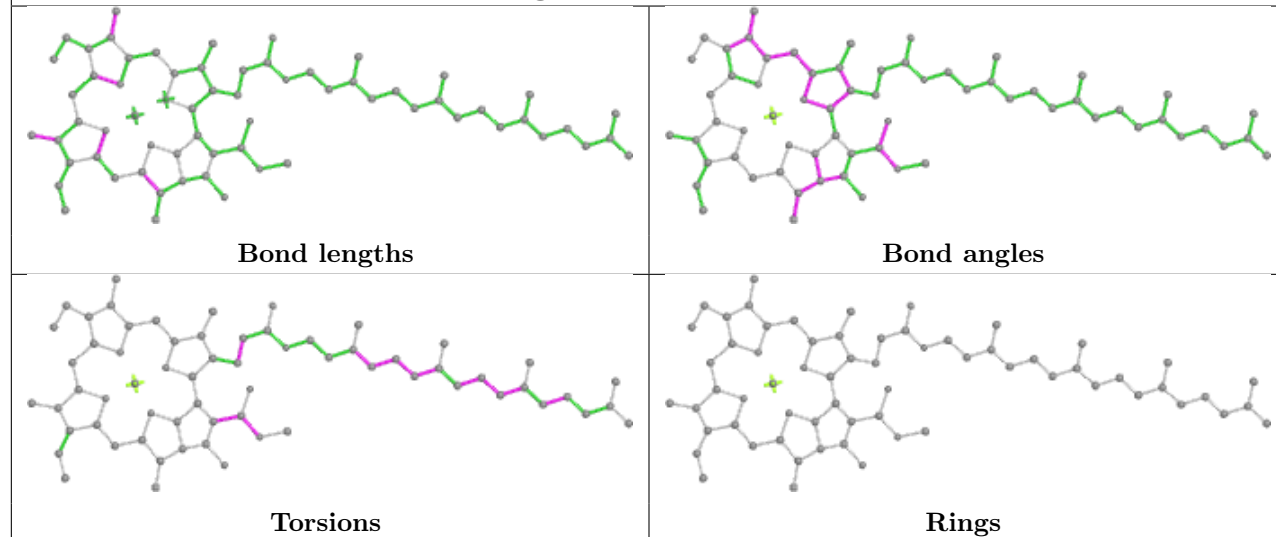




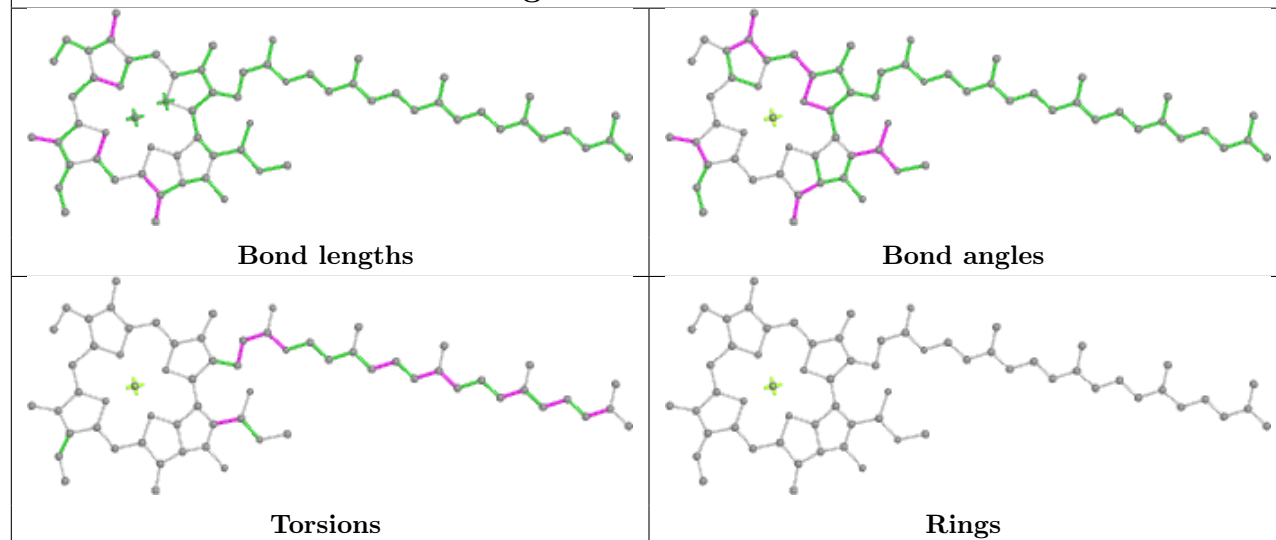
Ligand CLA A 827

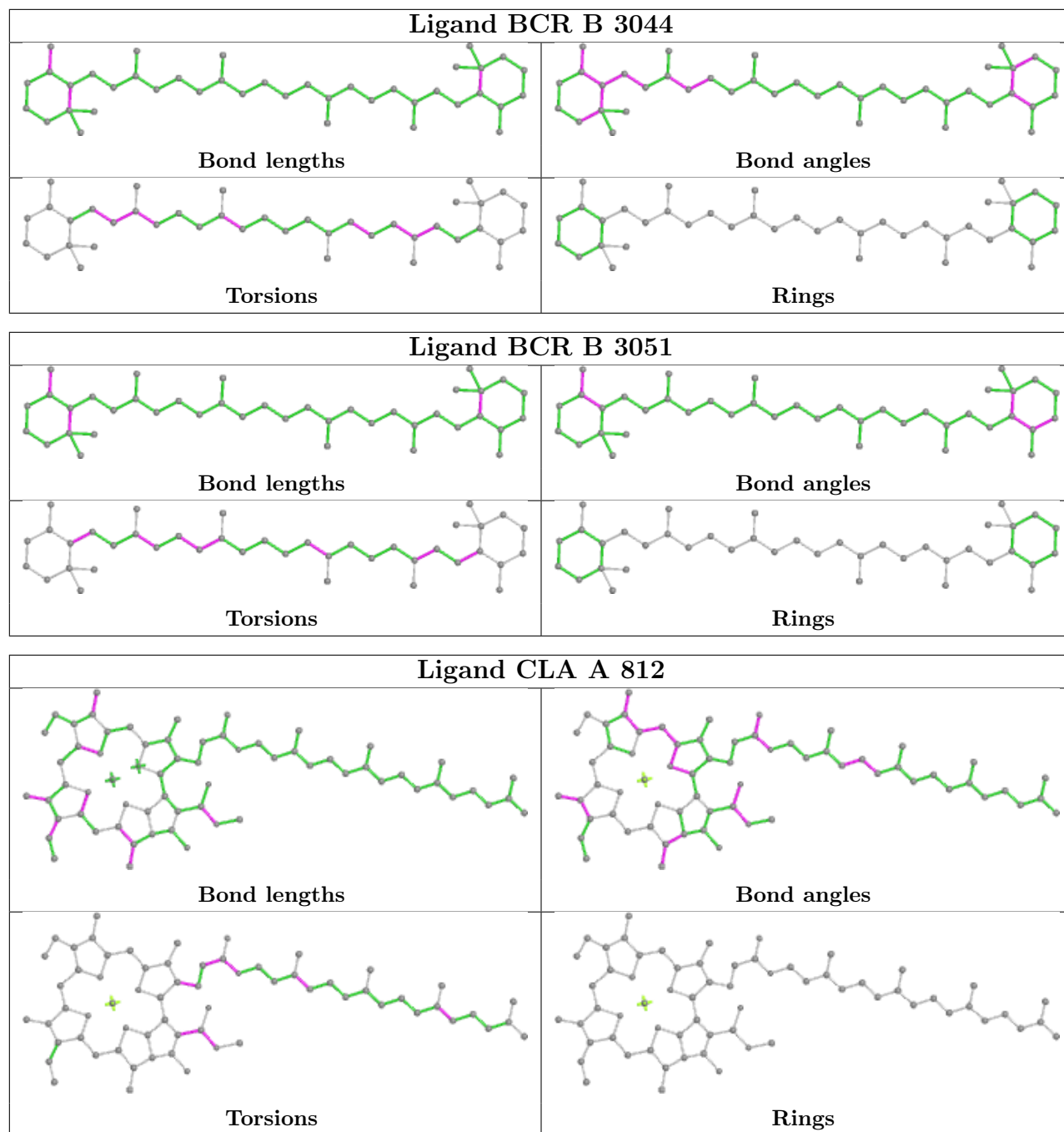


Ligand CLA A 830

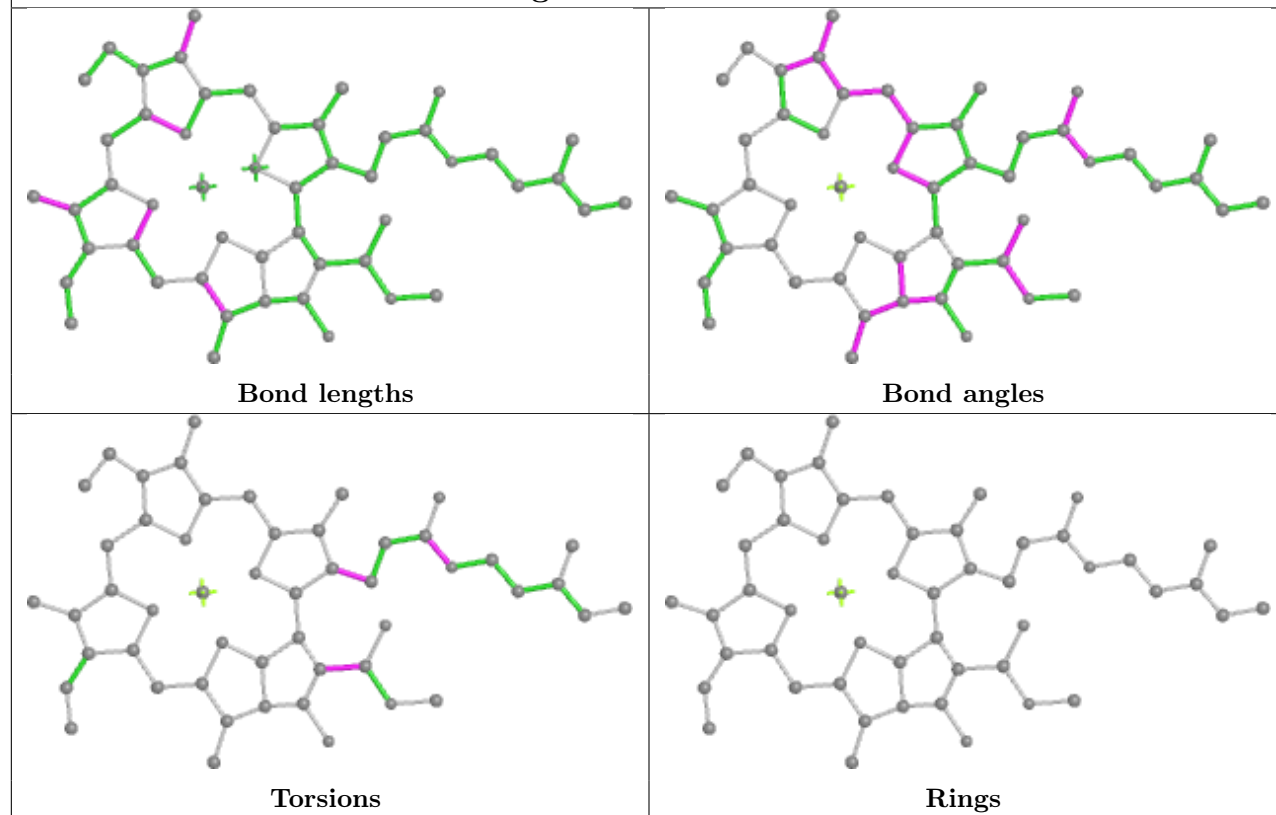


Ligand CLA B 3027

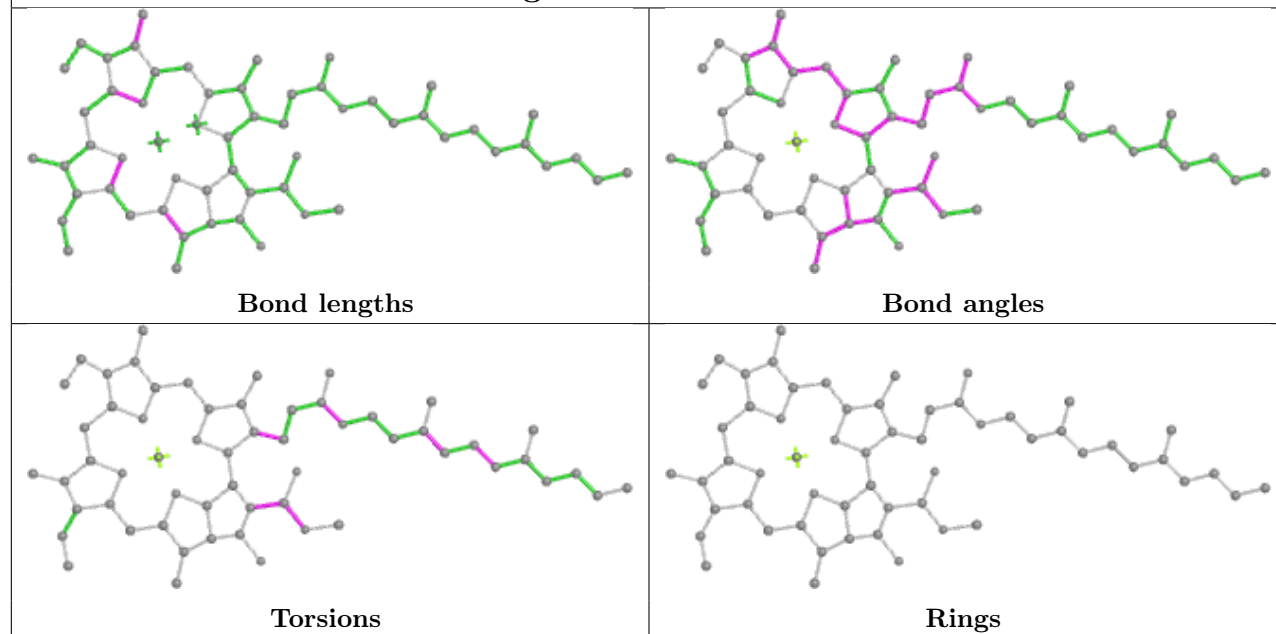


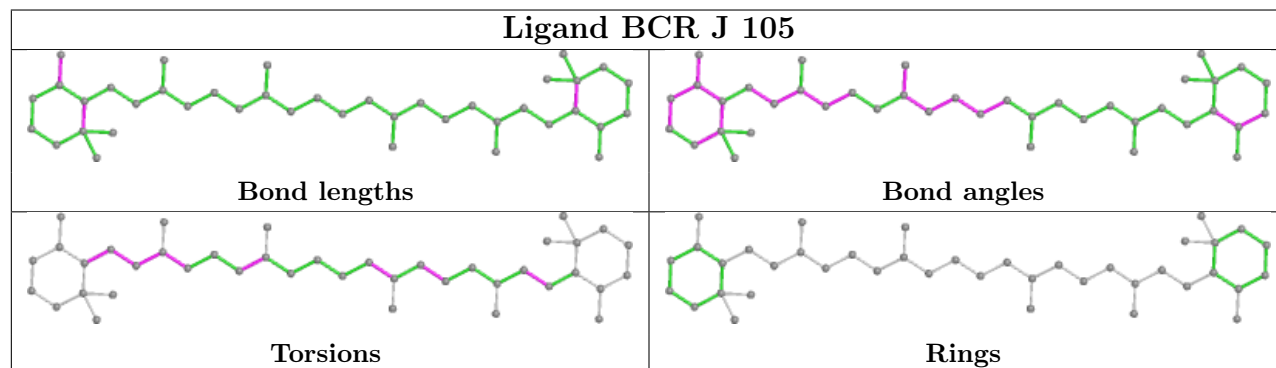
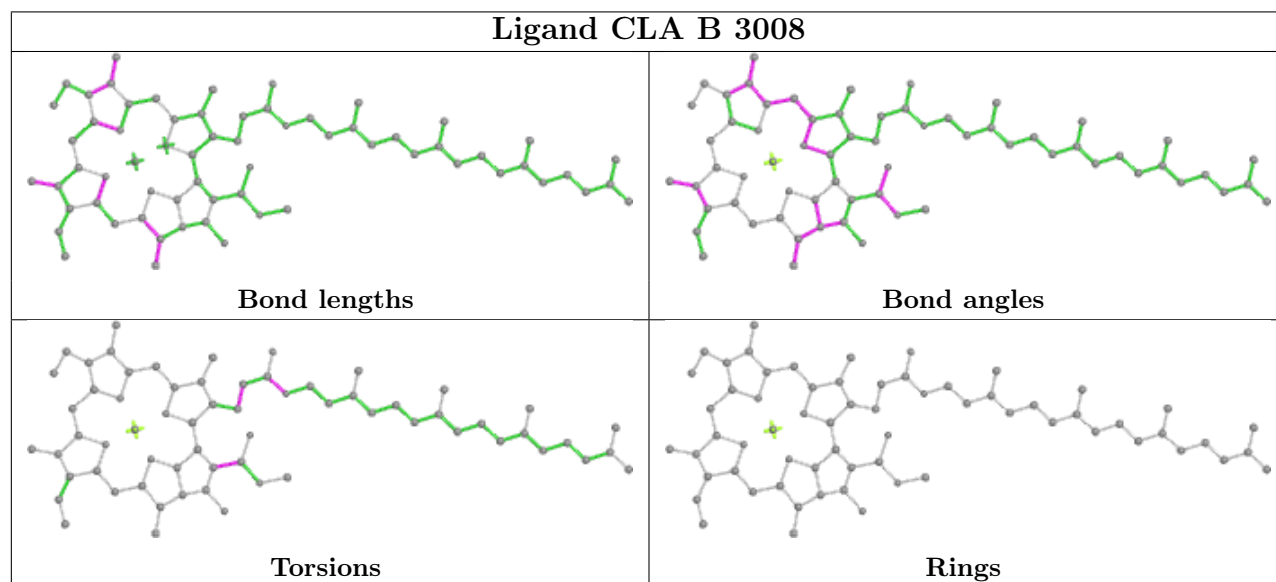
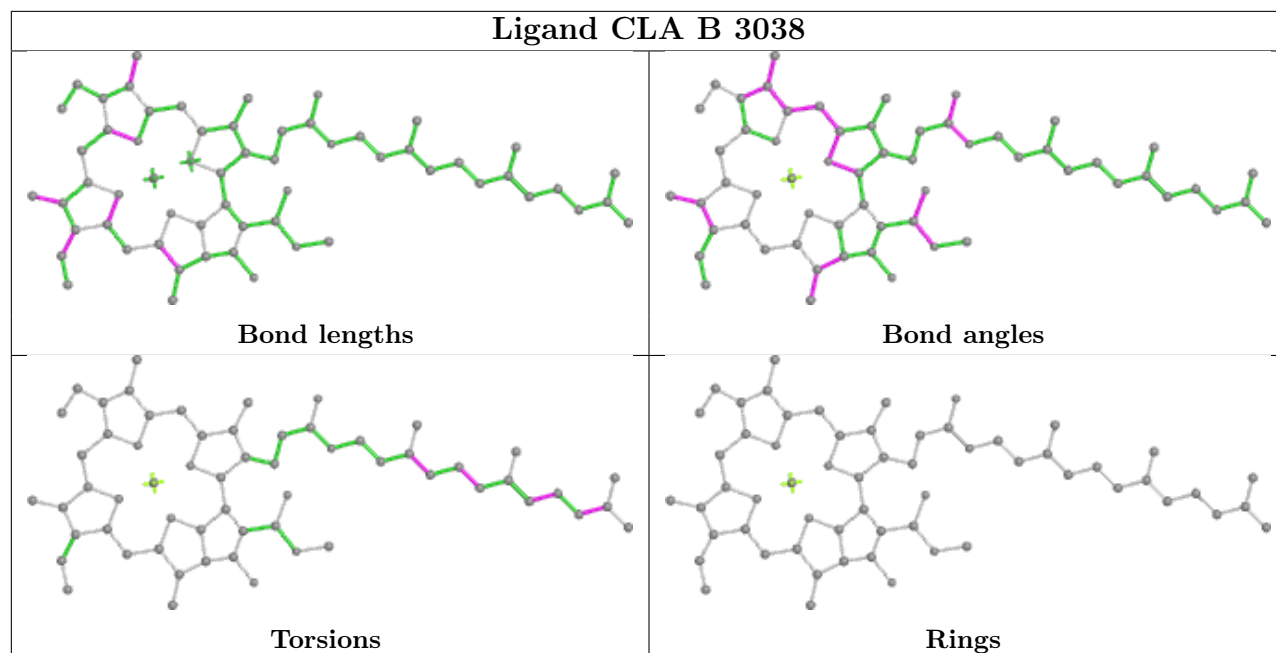


Ligand CLA A 824

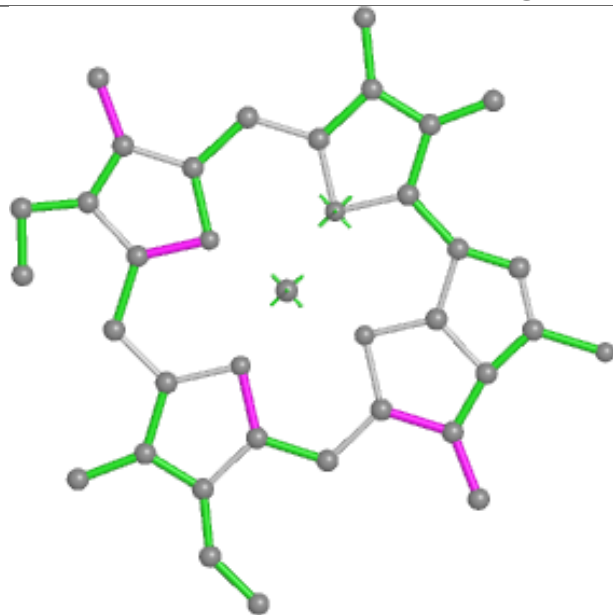


Ligand CLA B 3034

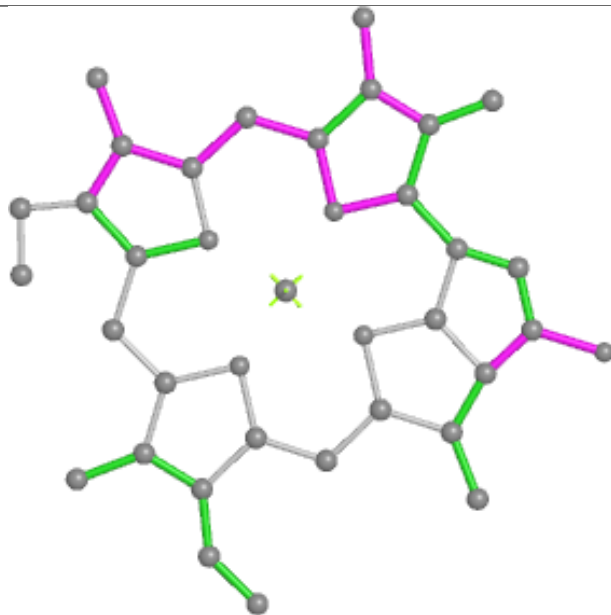




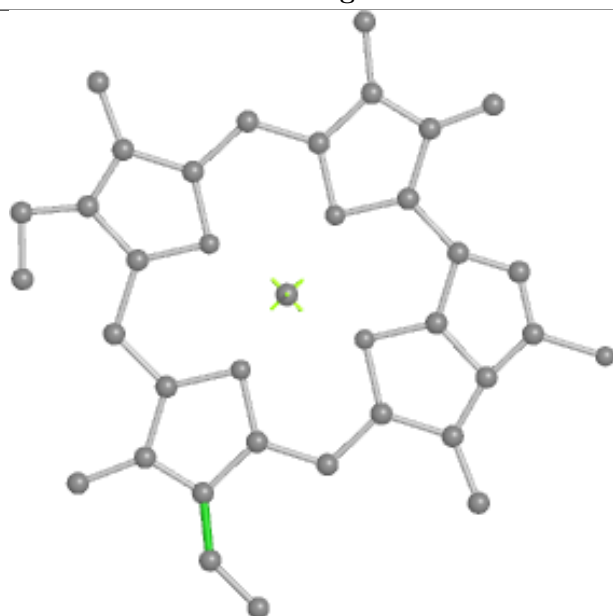
Ligand CLA J 102



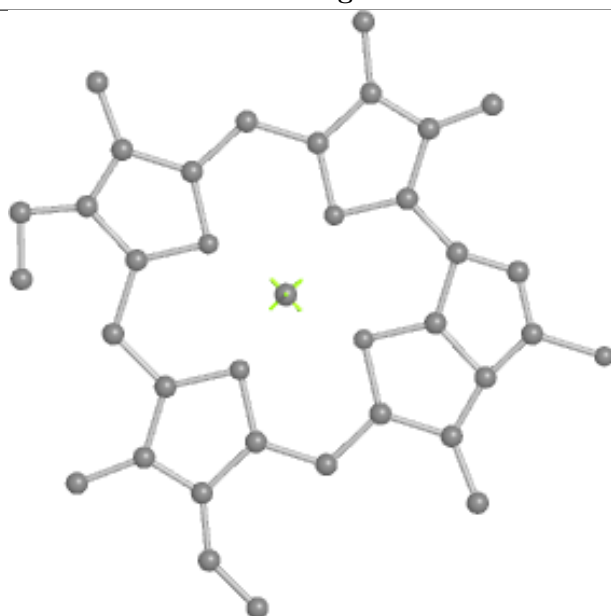
Bond lengths



Bond angles

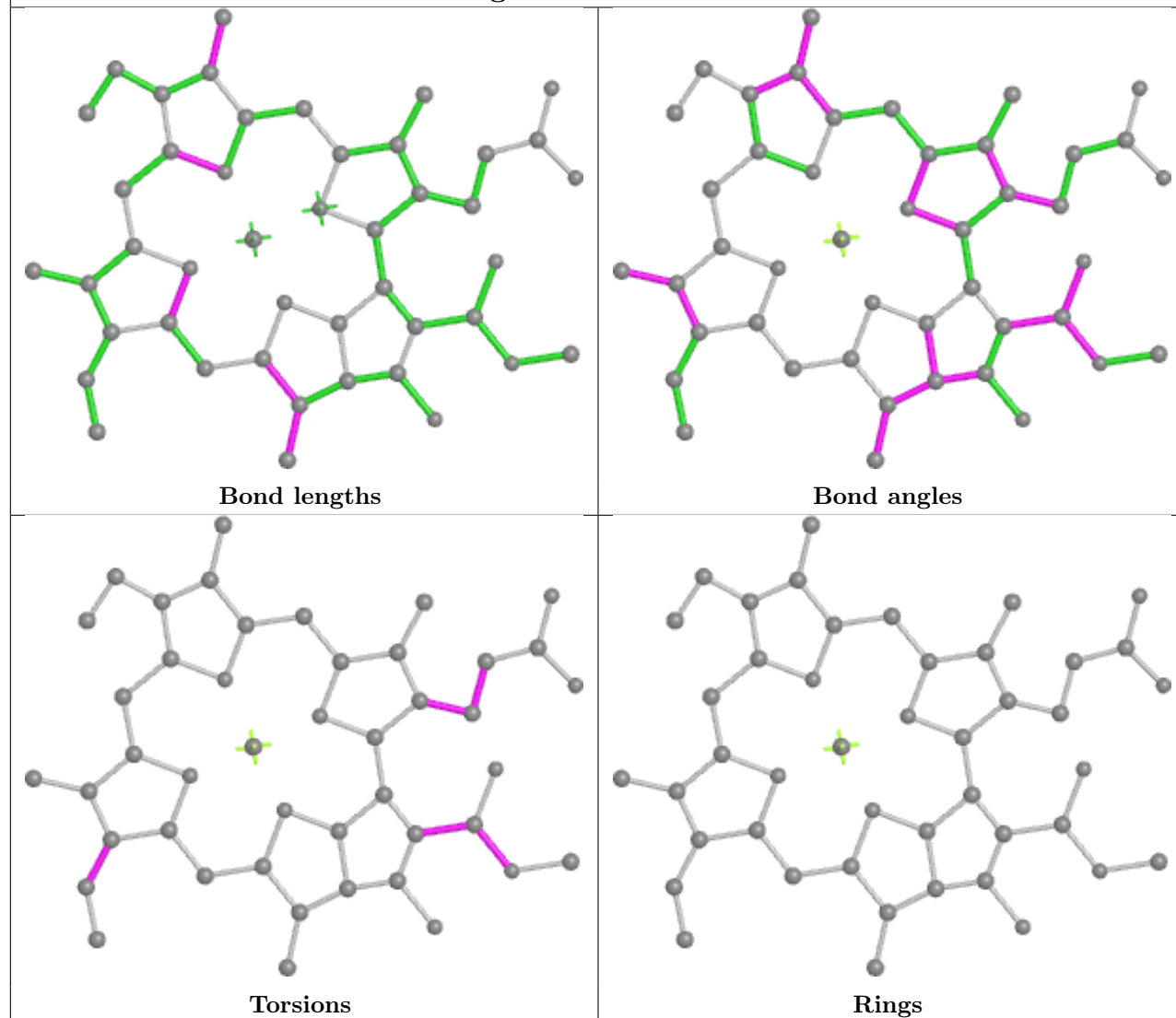


Torsions

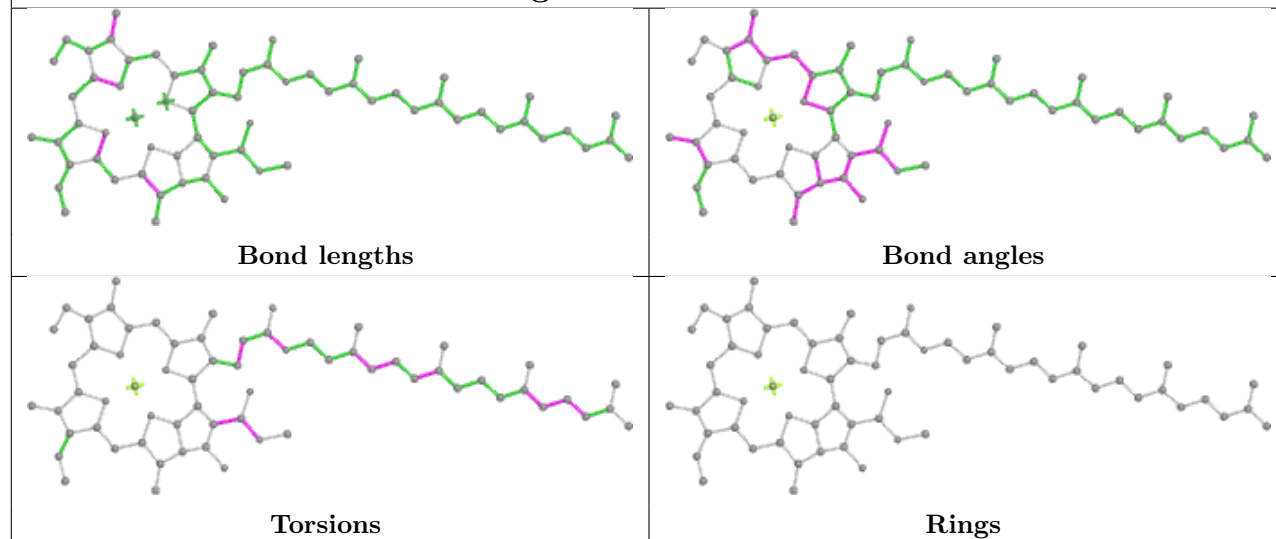


Rings

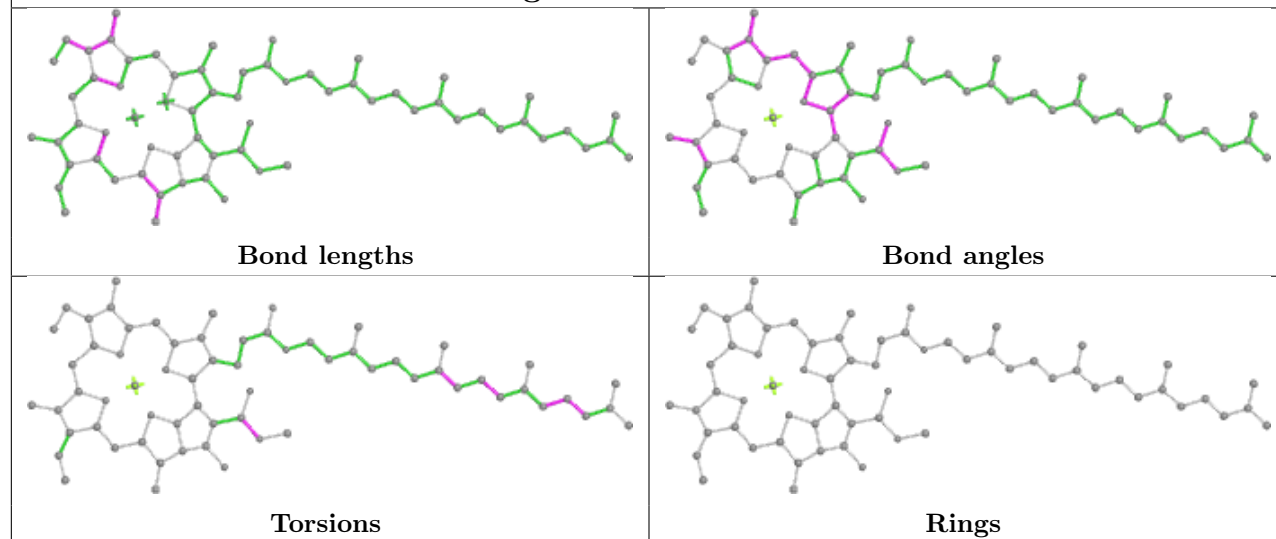
Ligand CLA A 811



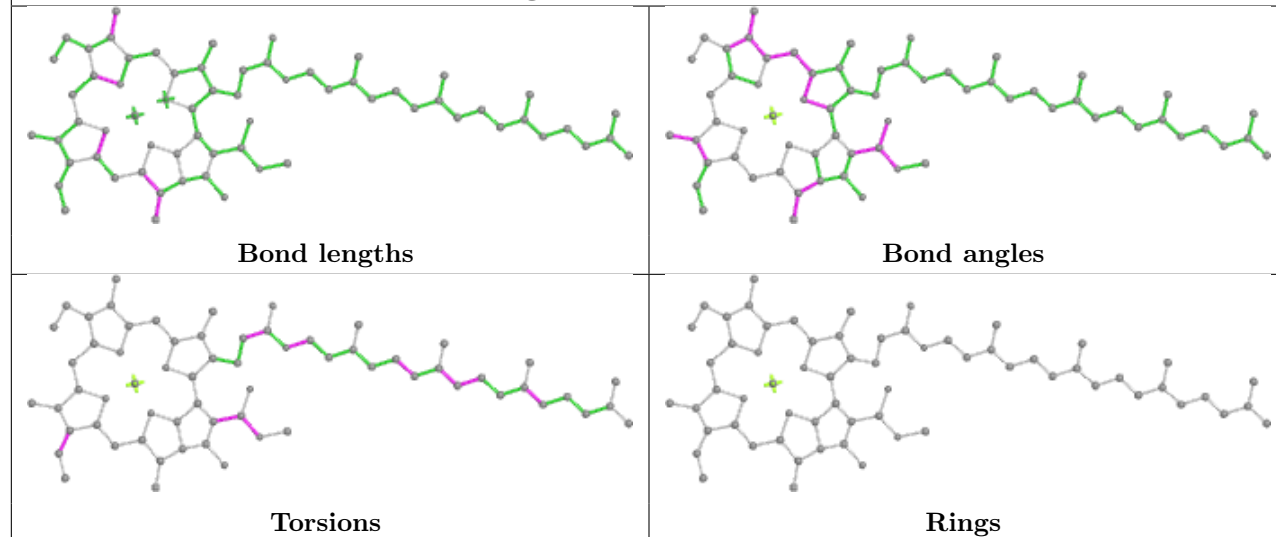
Ligand CLA A 822



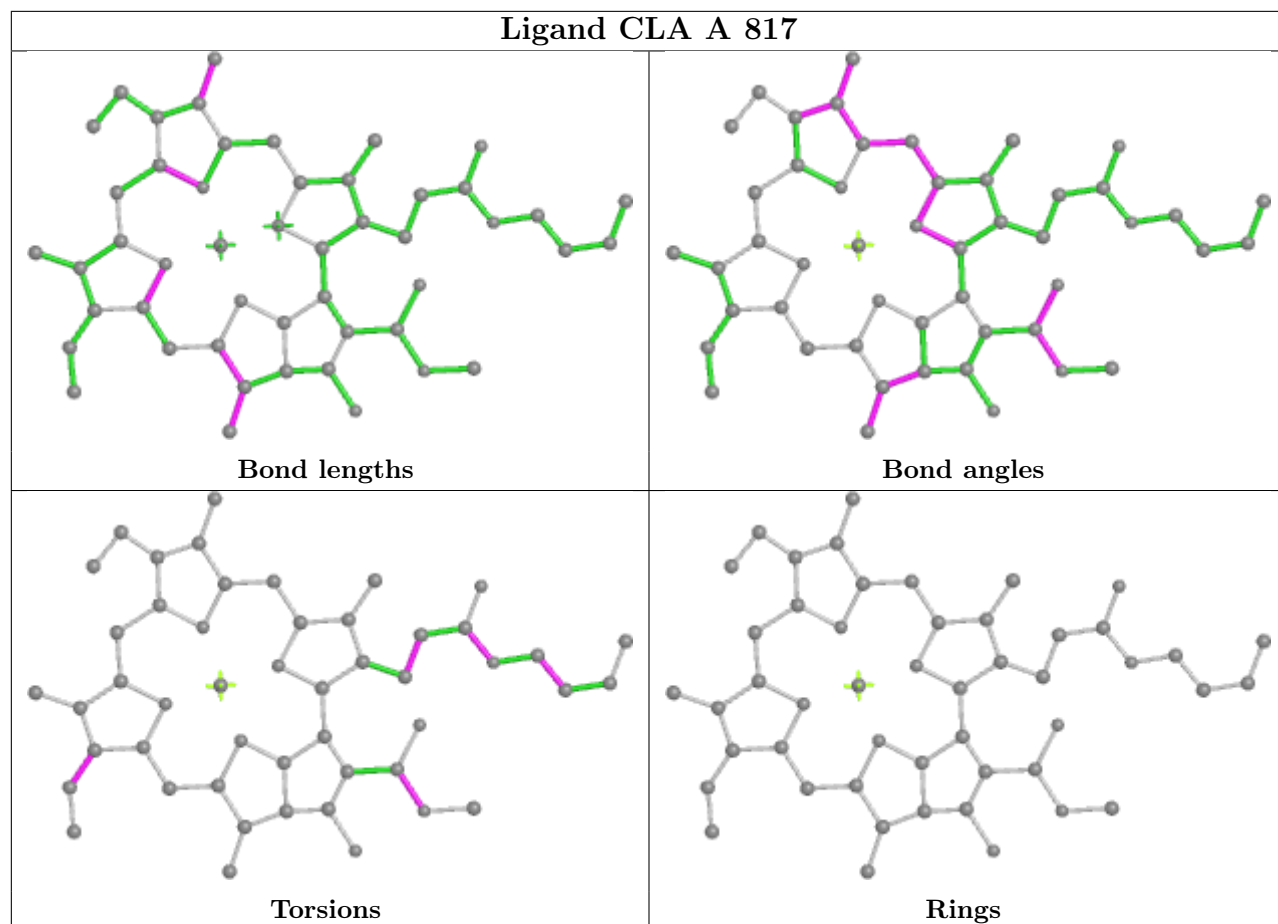
Ligand CLA B 3004



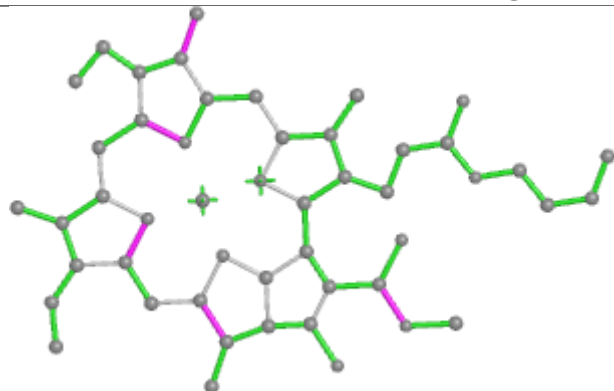
Ligand CLA B 3015



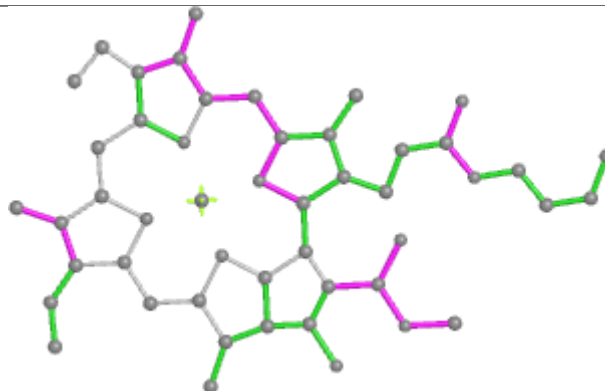
Ligand CLA A 817



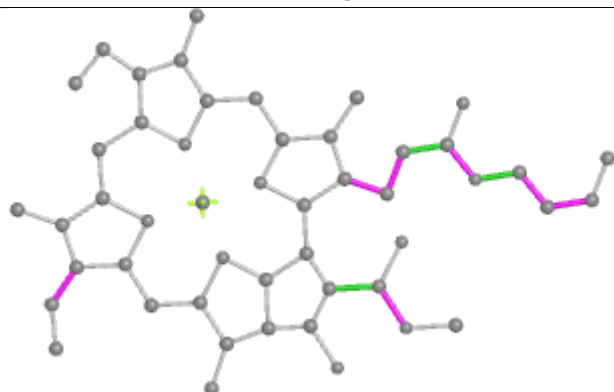
Ligand CLA B 3032



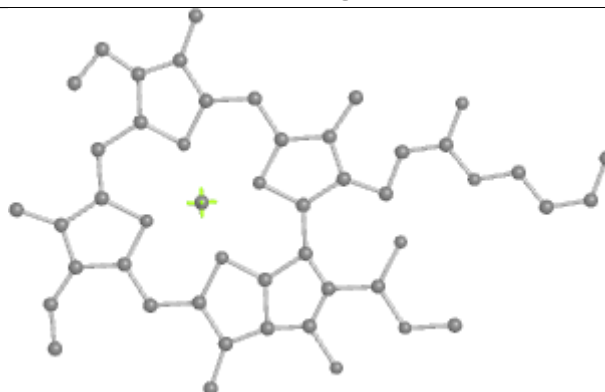
Bond lengths



Bond angles

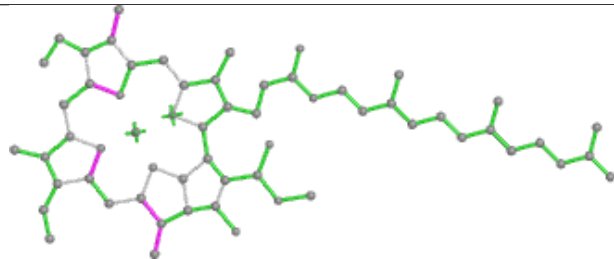


Torsions

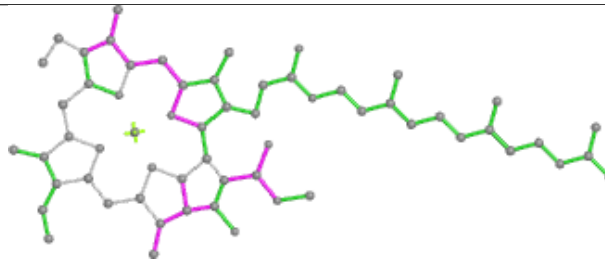


Rings

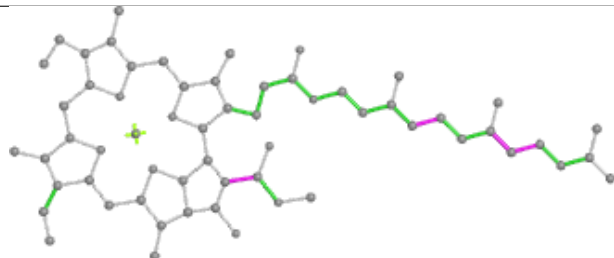
Ligand CLA A 814



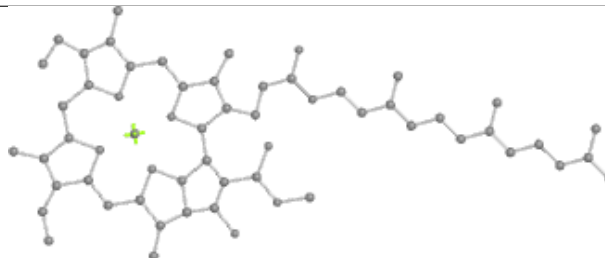
Bond lengths



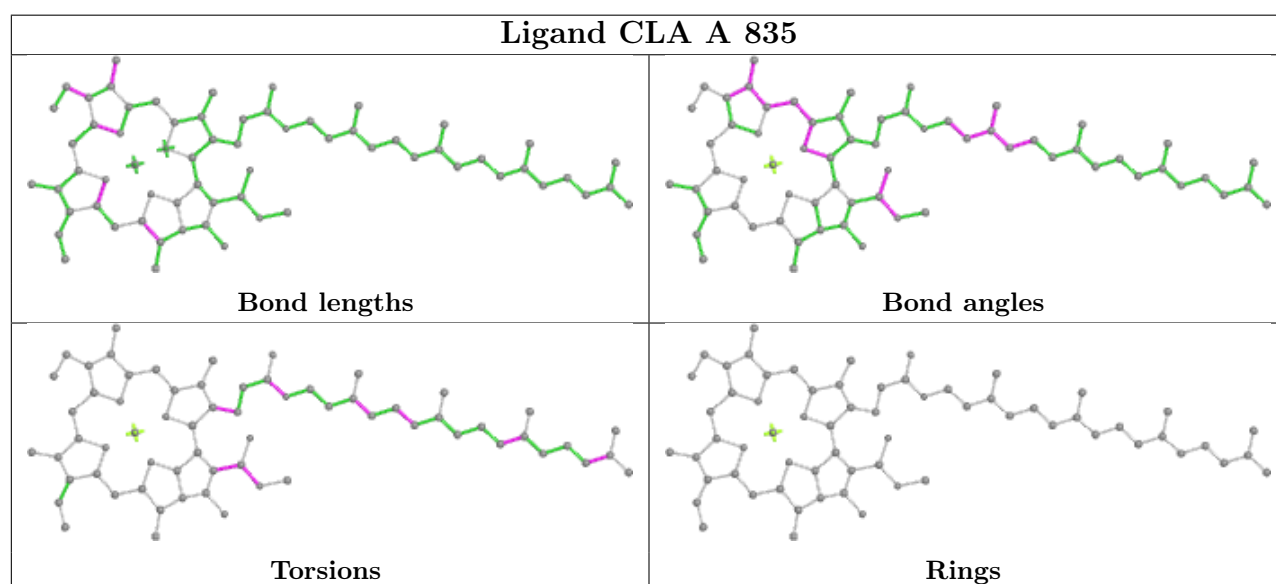
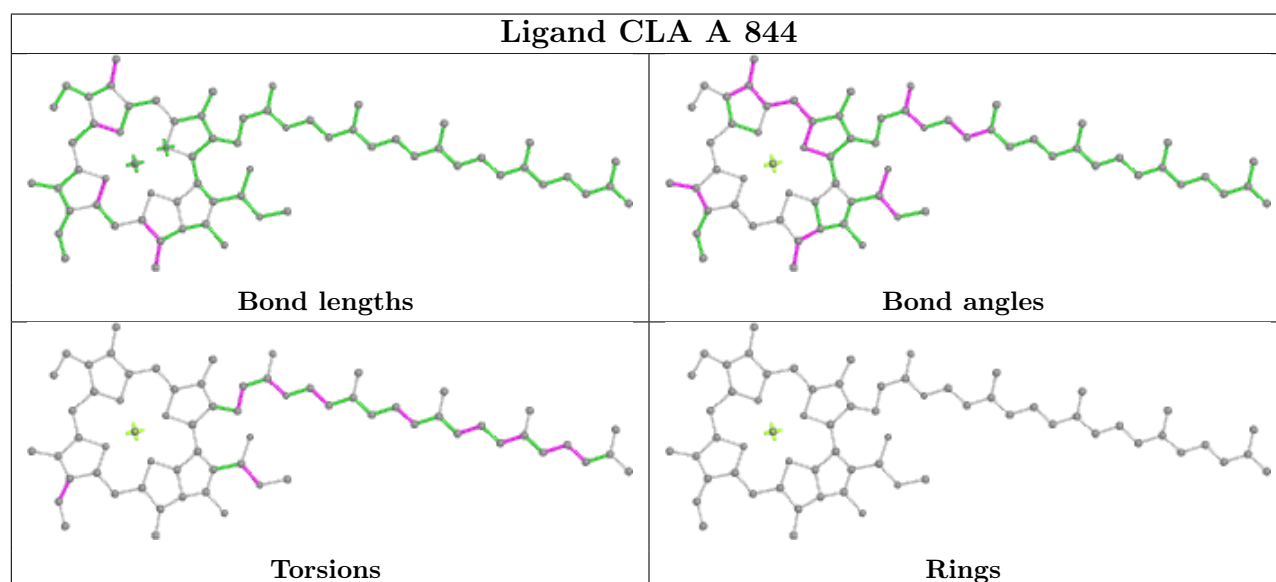
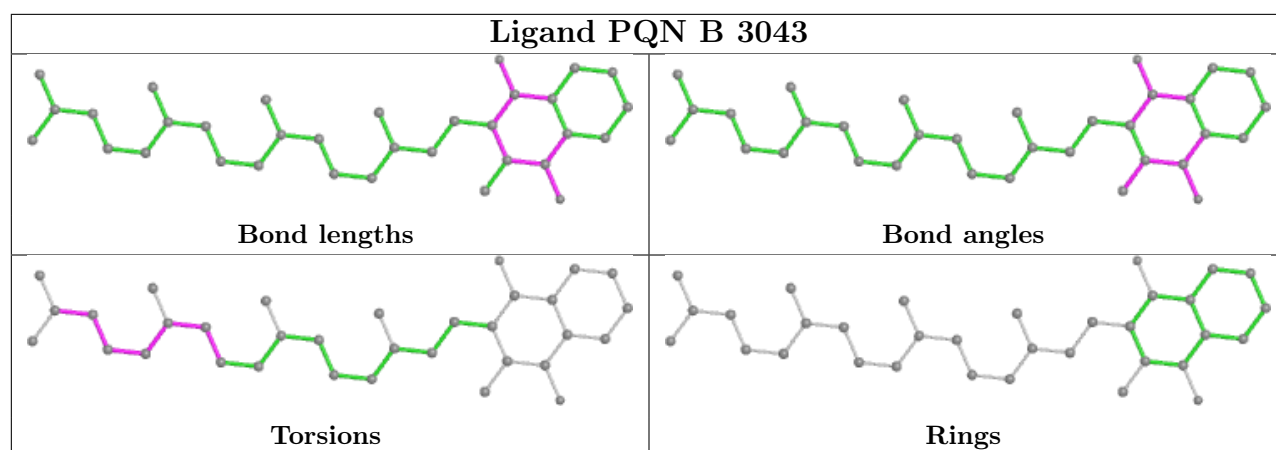
Bond angles



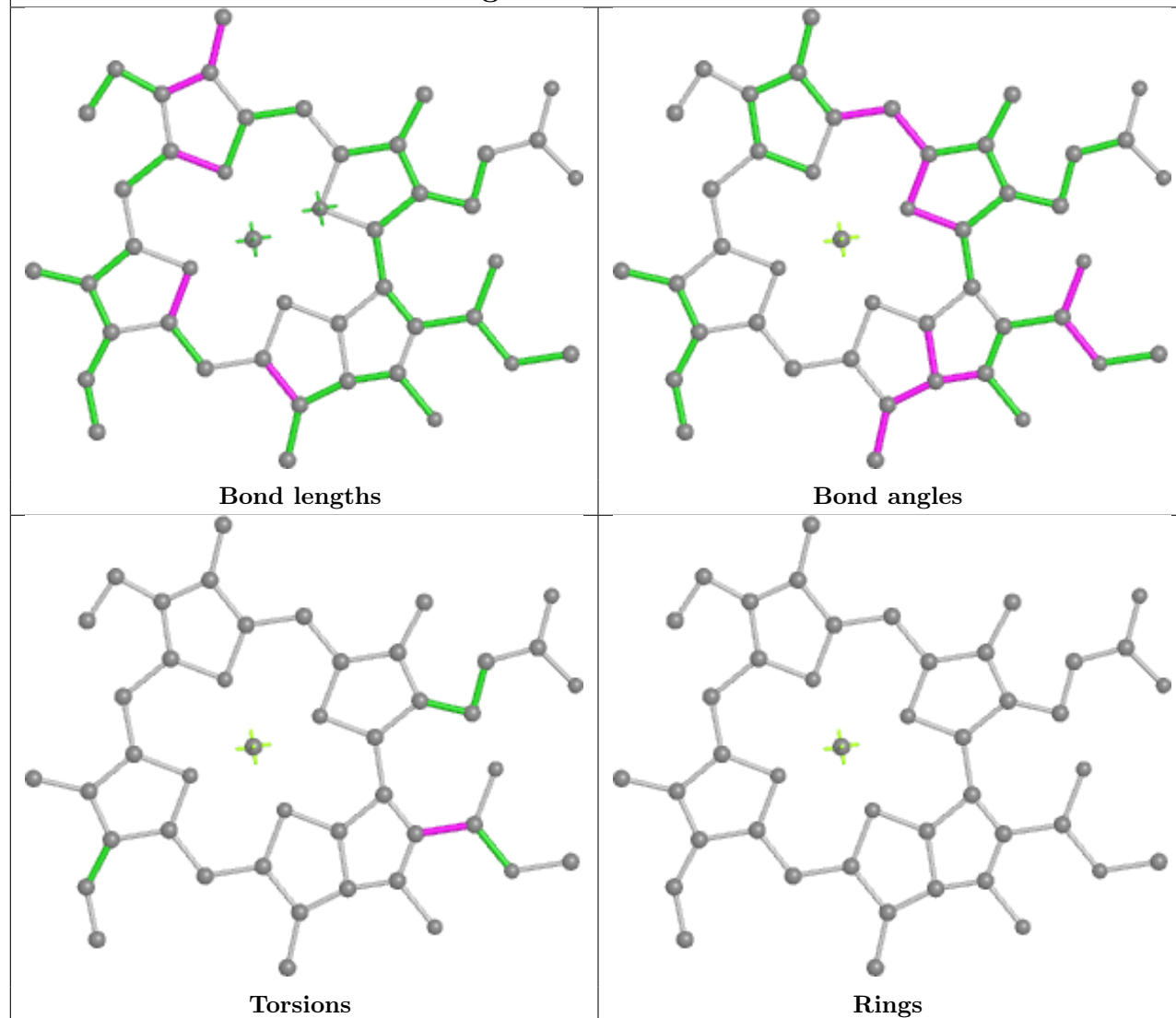
Torsions



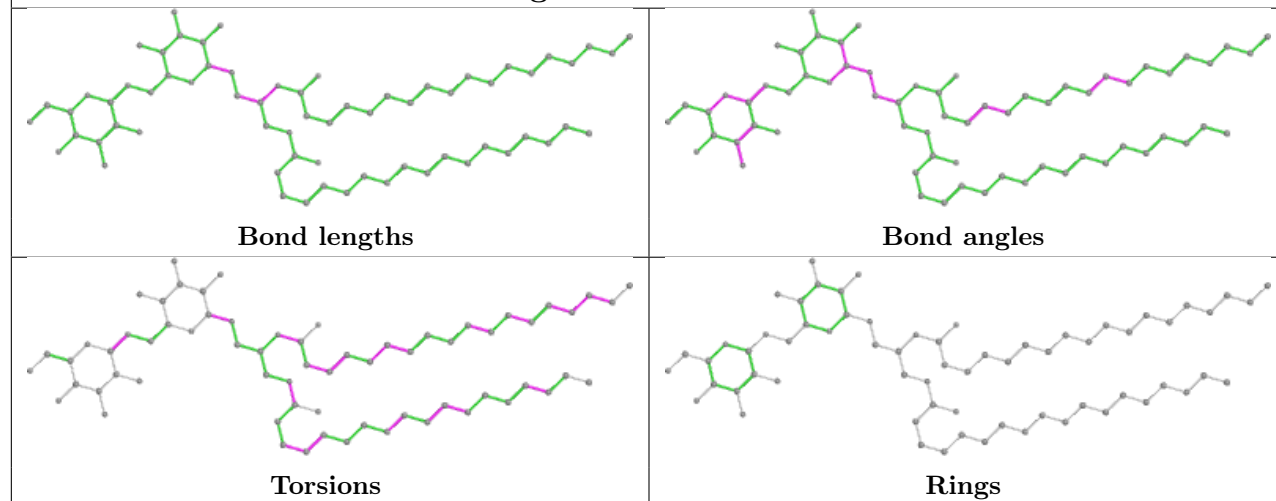
Rings

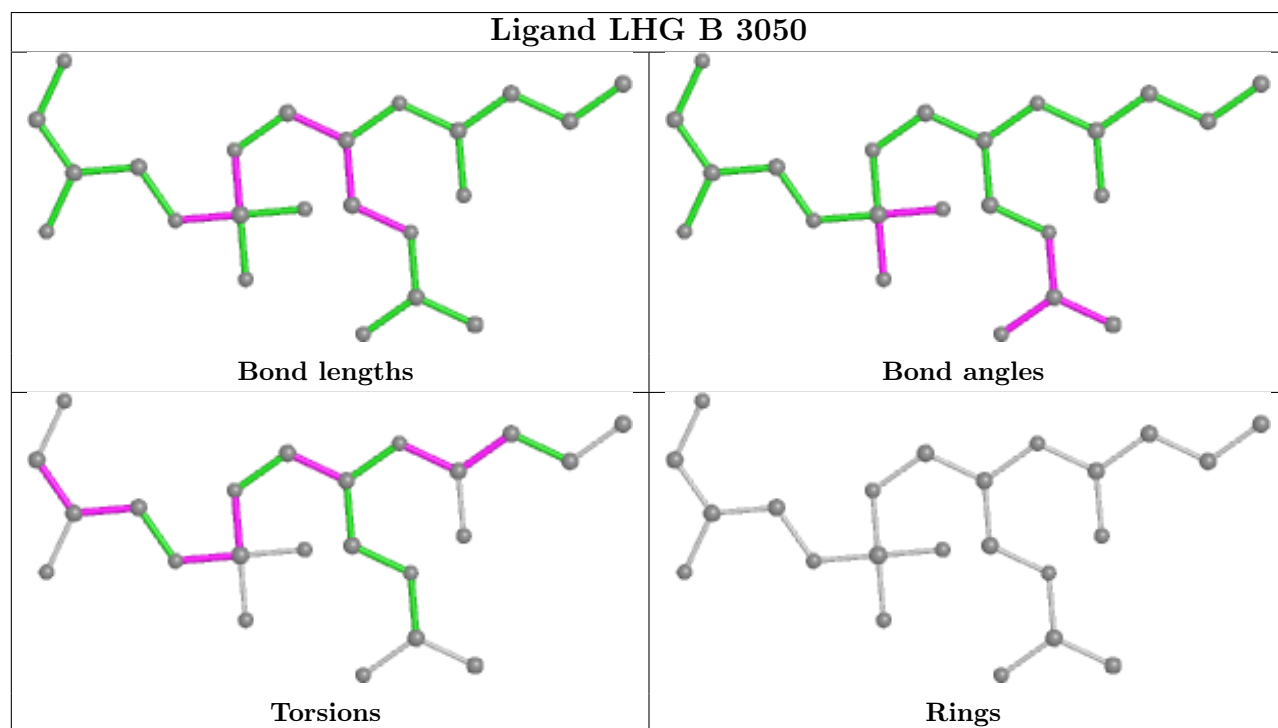
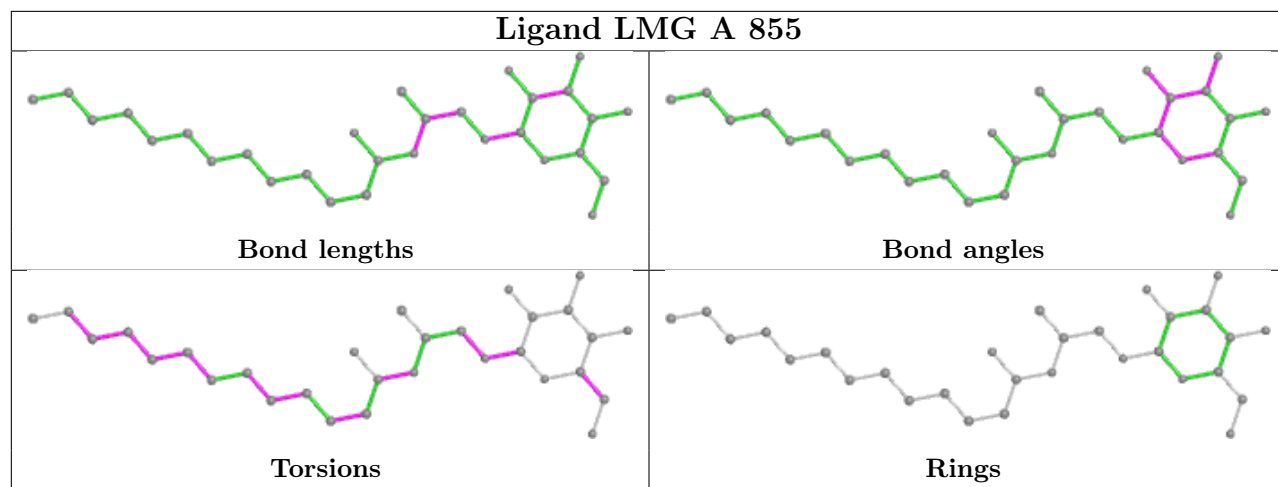


Ligand CLA B 3031

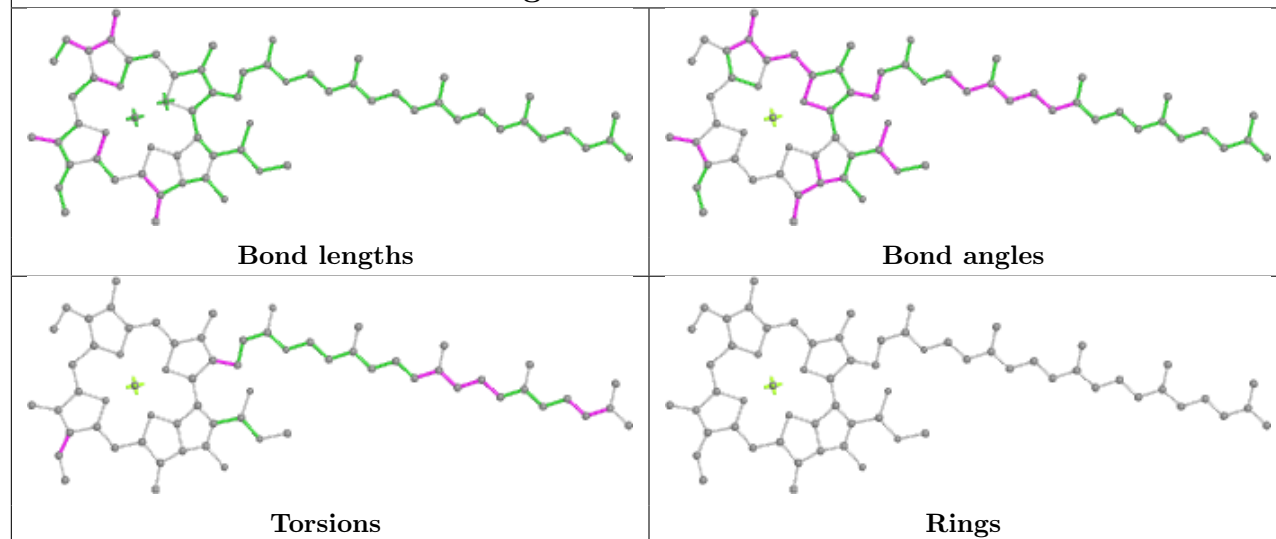


Ligand DGD L 207

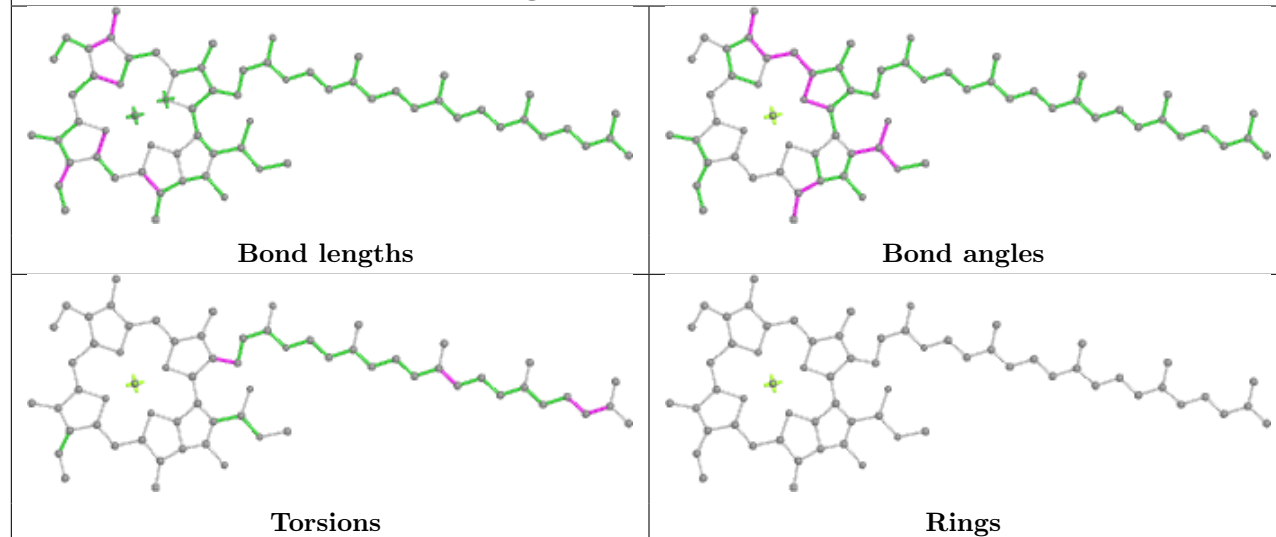


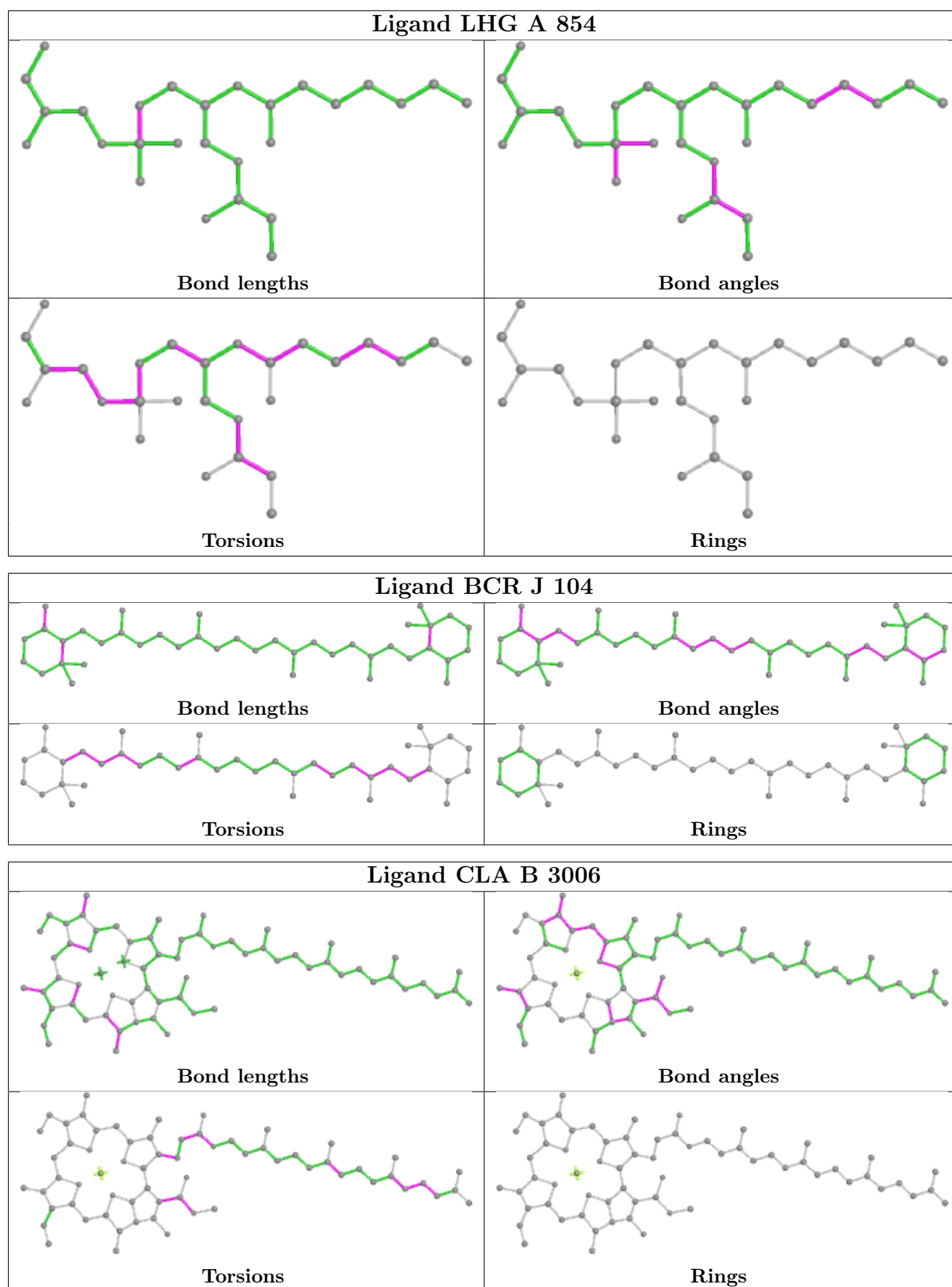


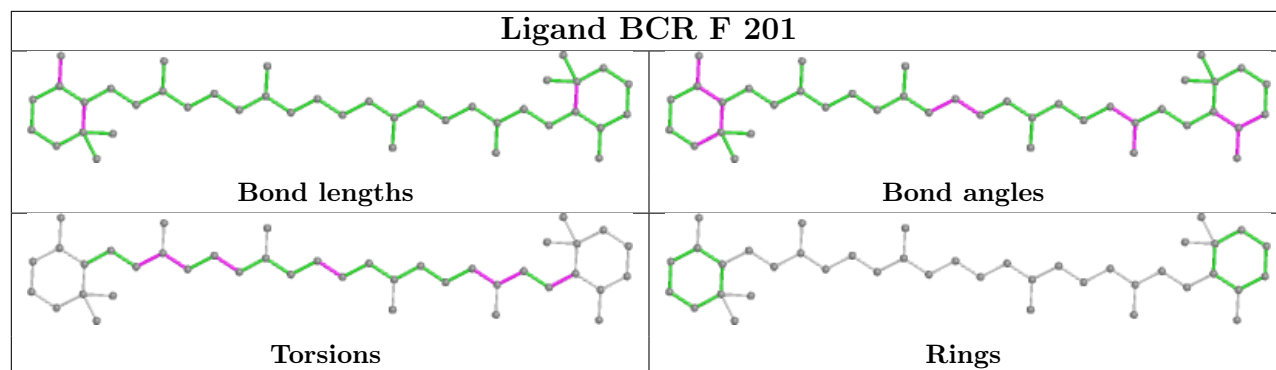
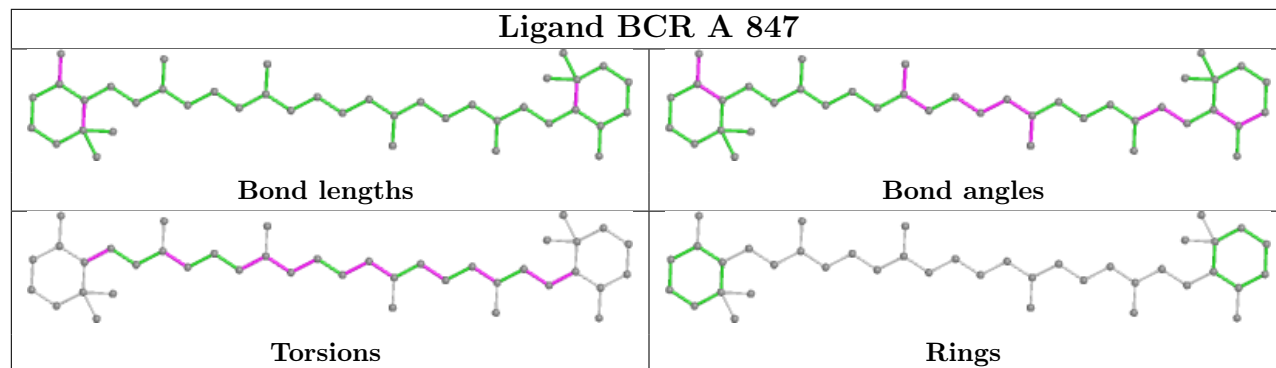
Ligand CLA B 3010



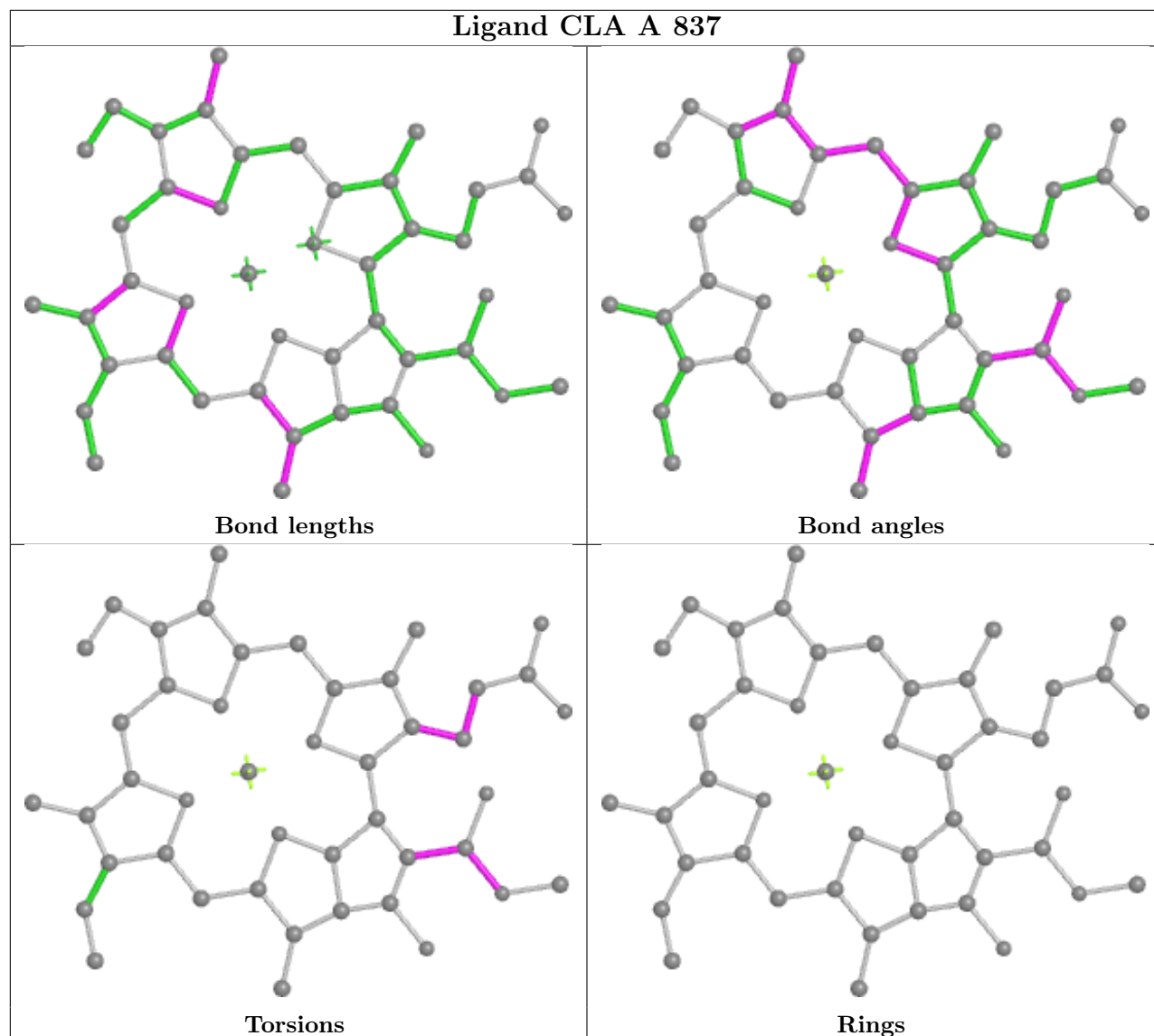
Ligand CLA B 3042



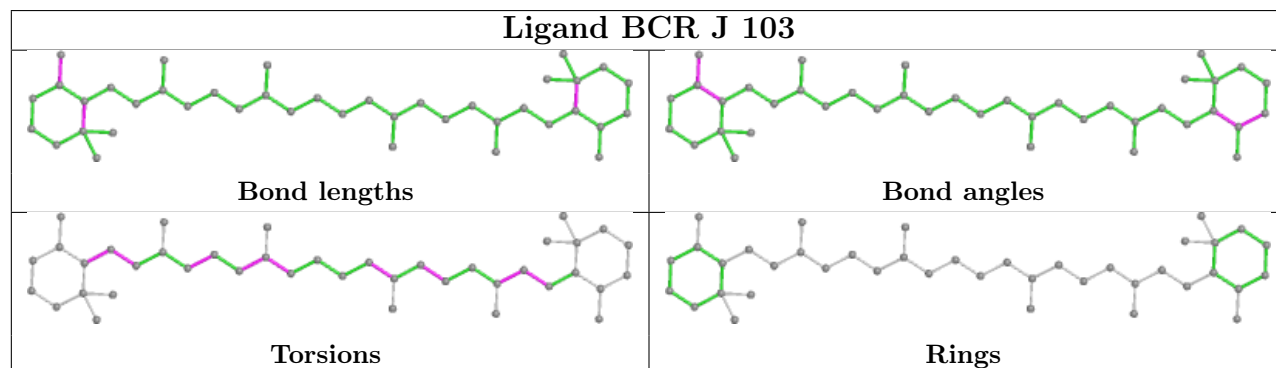


Ligand BCR F 201**Ligand BCR A 847**

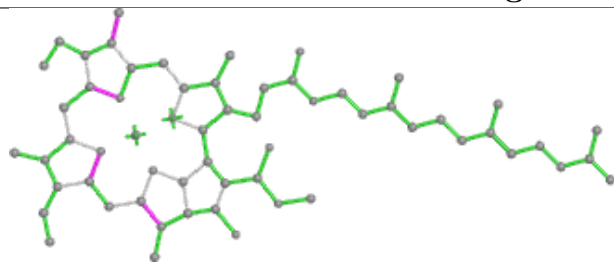
Ligand CLA A 837



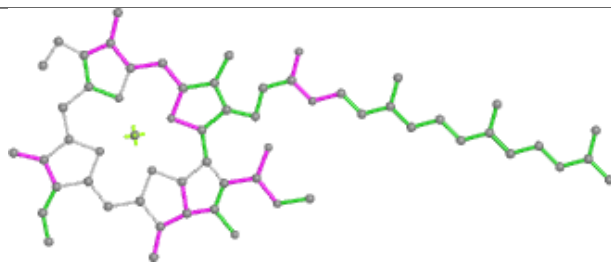
Ligand BCR J 103



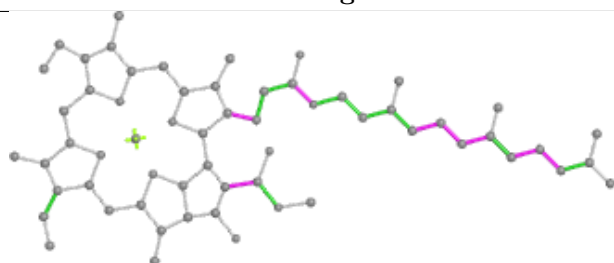
Ligand CLA B 3019



Bond lengths



Bond angles

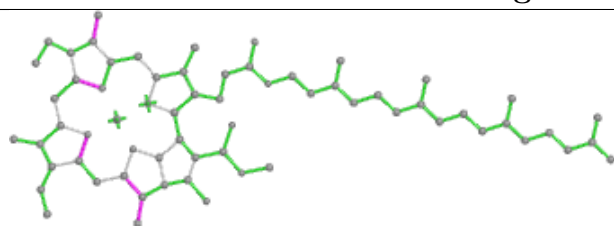


Torsions

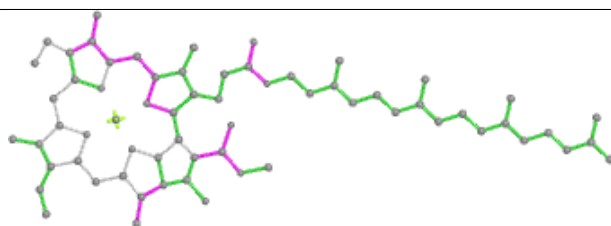


Rings

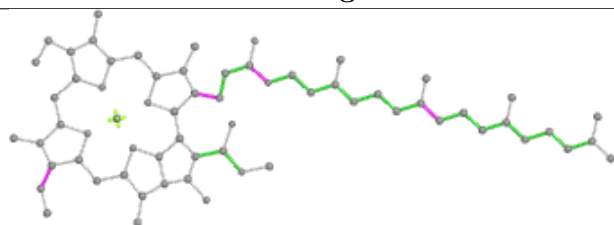
Ligand CLA A 843



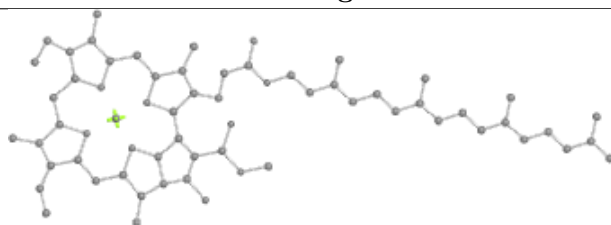
Bond lengths



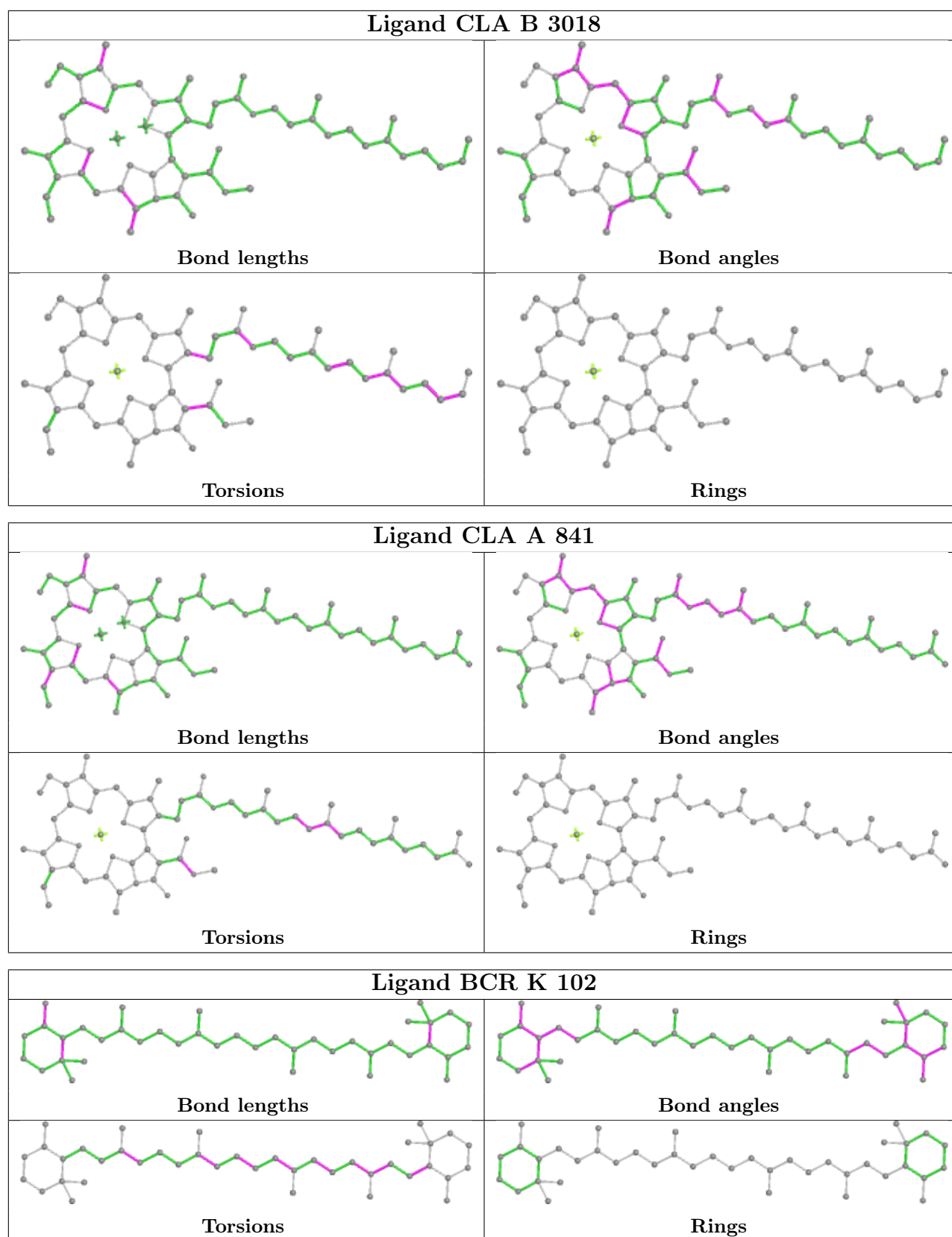
Bond angles



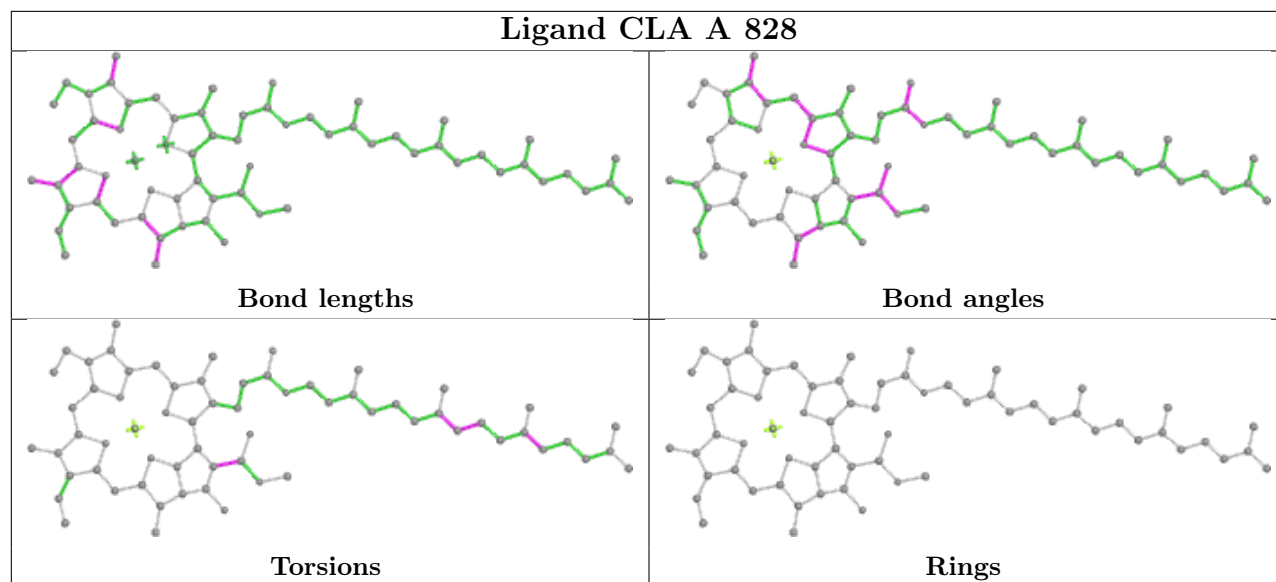
Torsions



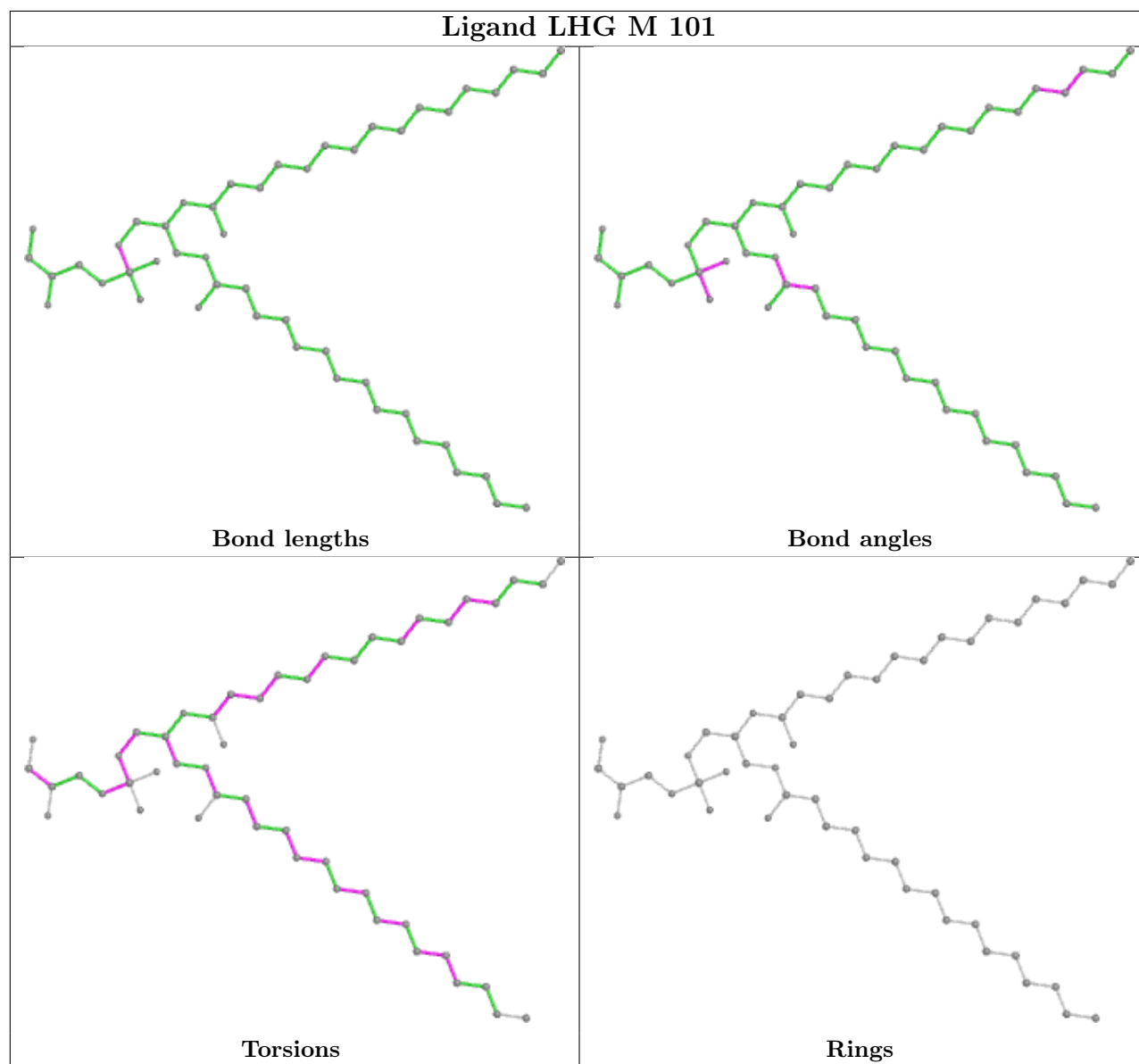
Rings



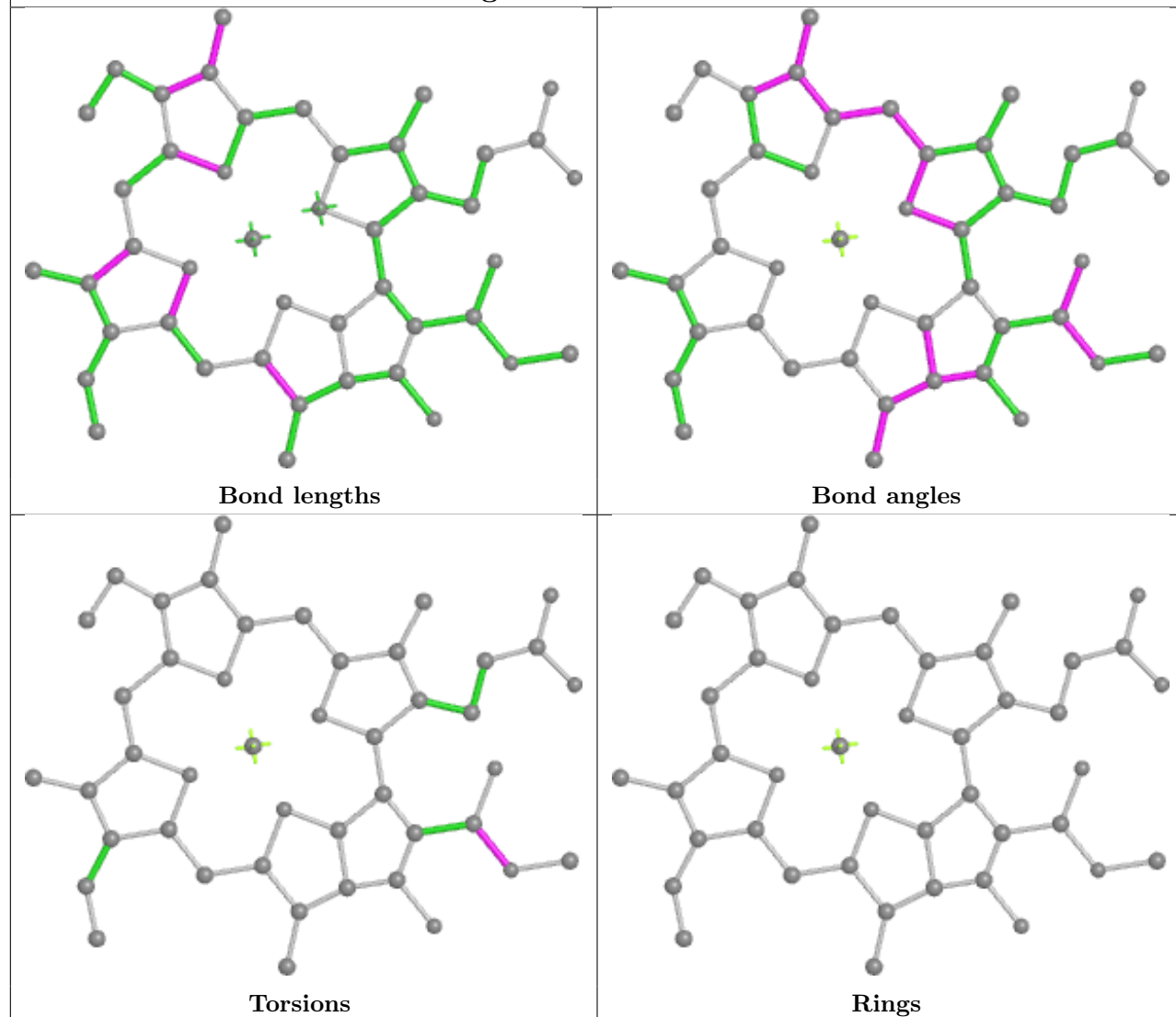
Ligand CLA A 828



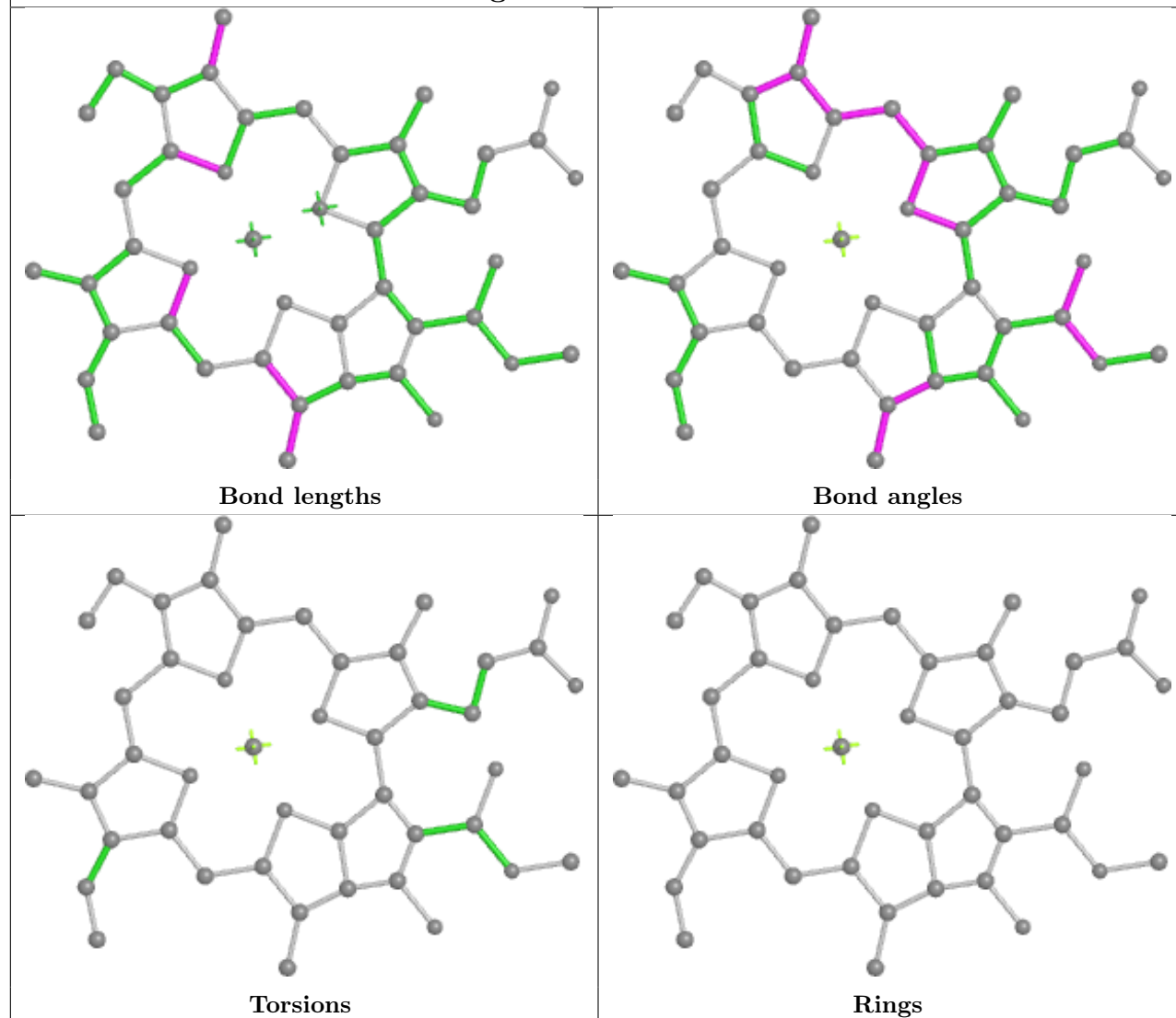
Ligand LHG M 101



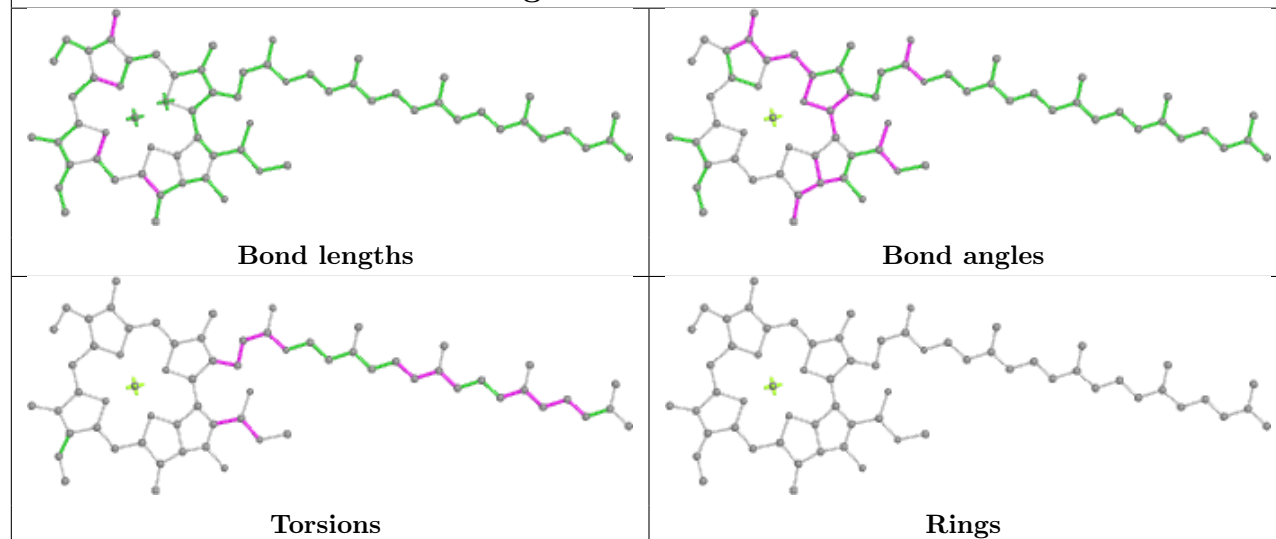
Ligand CLA B 3037



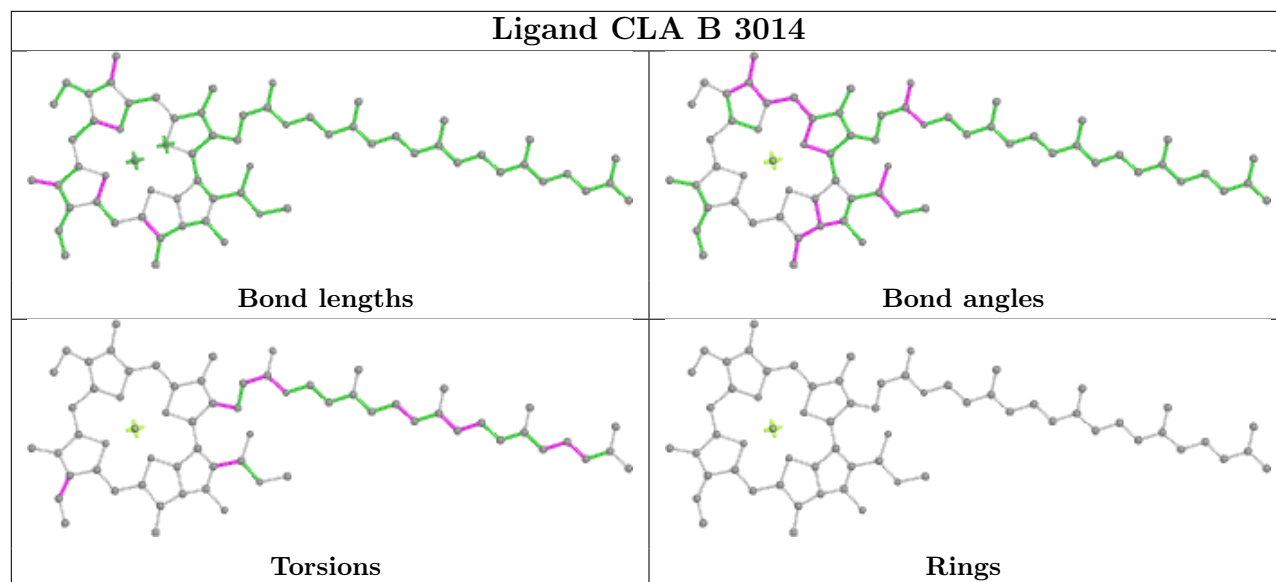
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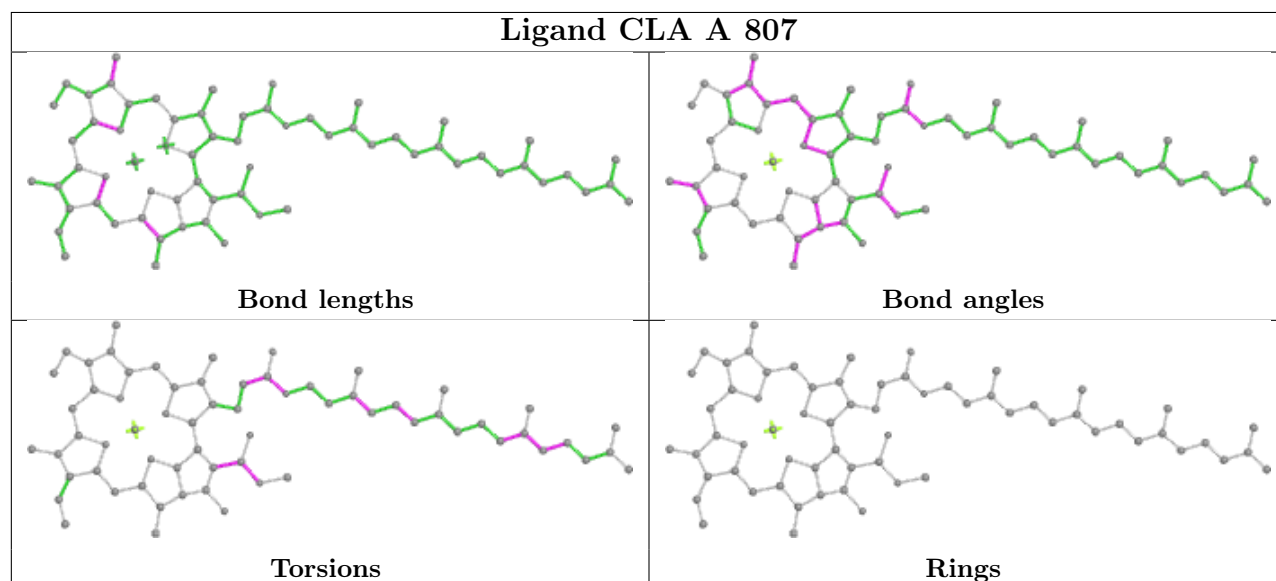
Ligand CLA B 3029



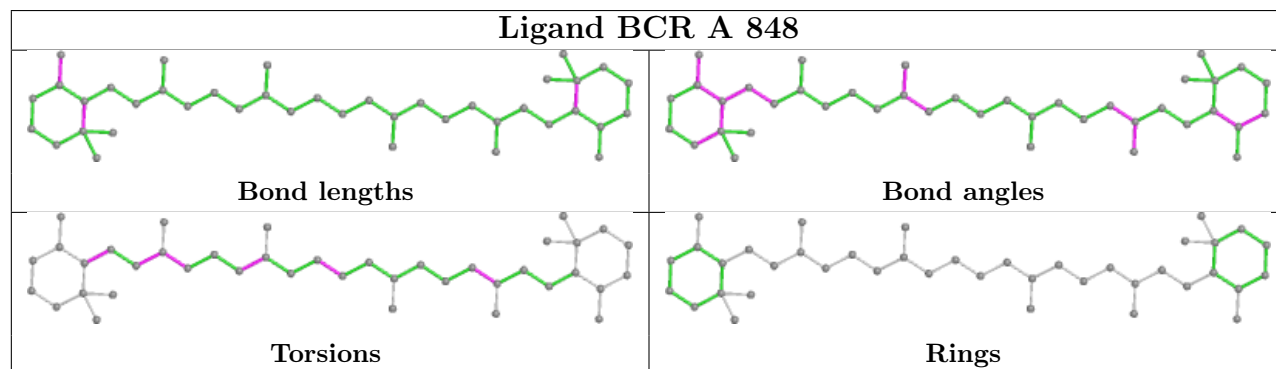
Ligand CLA B 3014



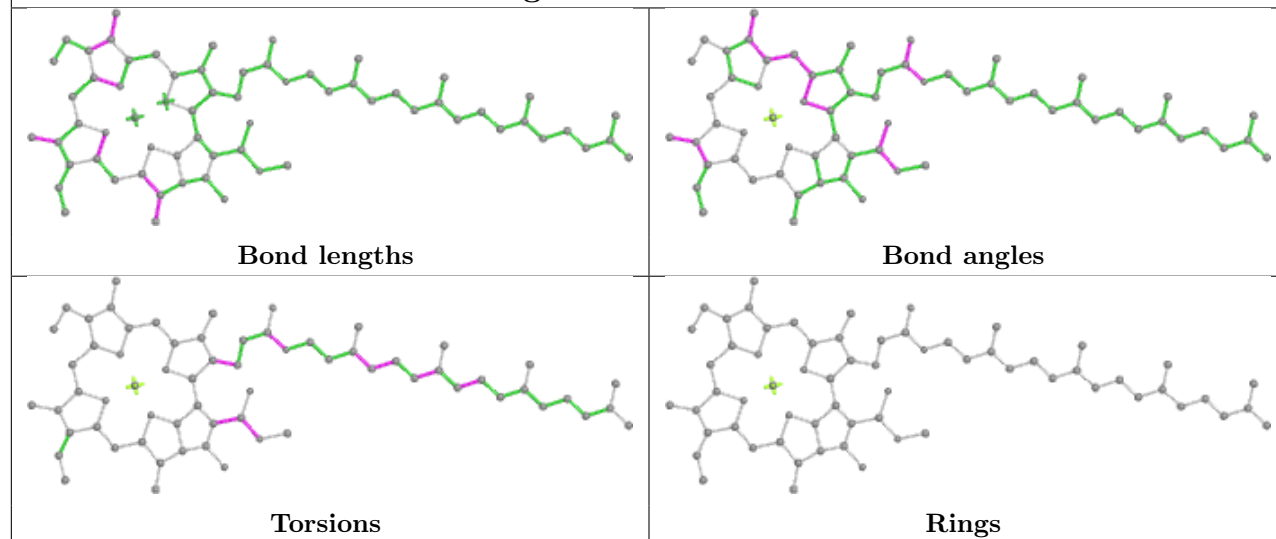
Ligand CLA A 807



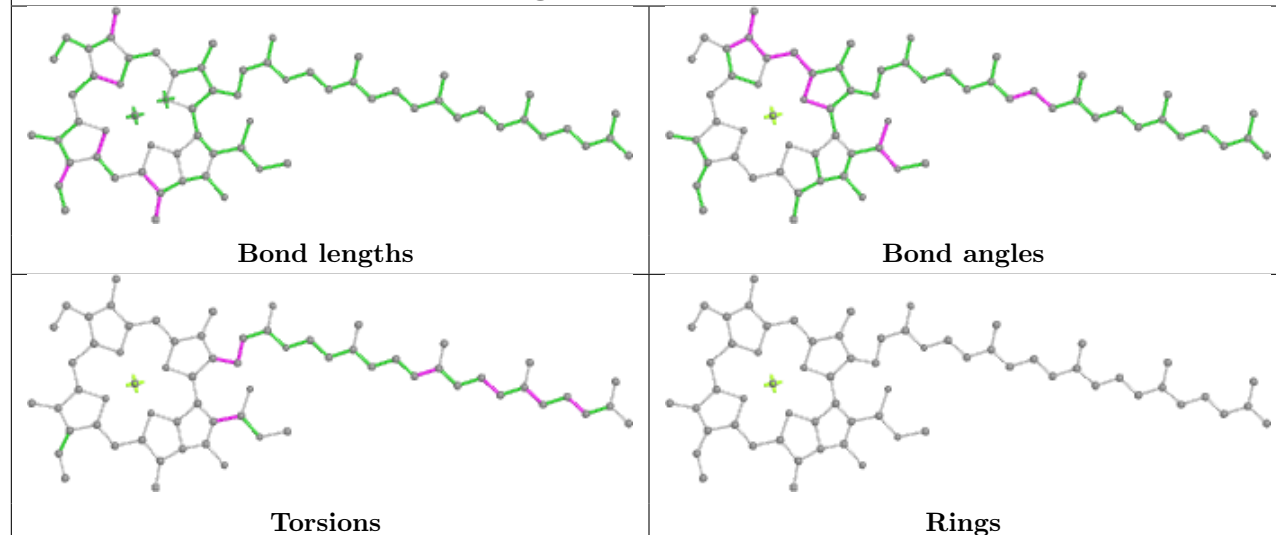
Ligand BCR A 848



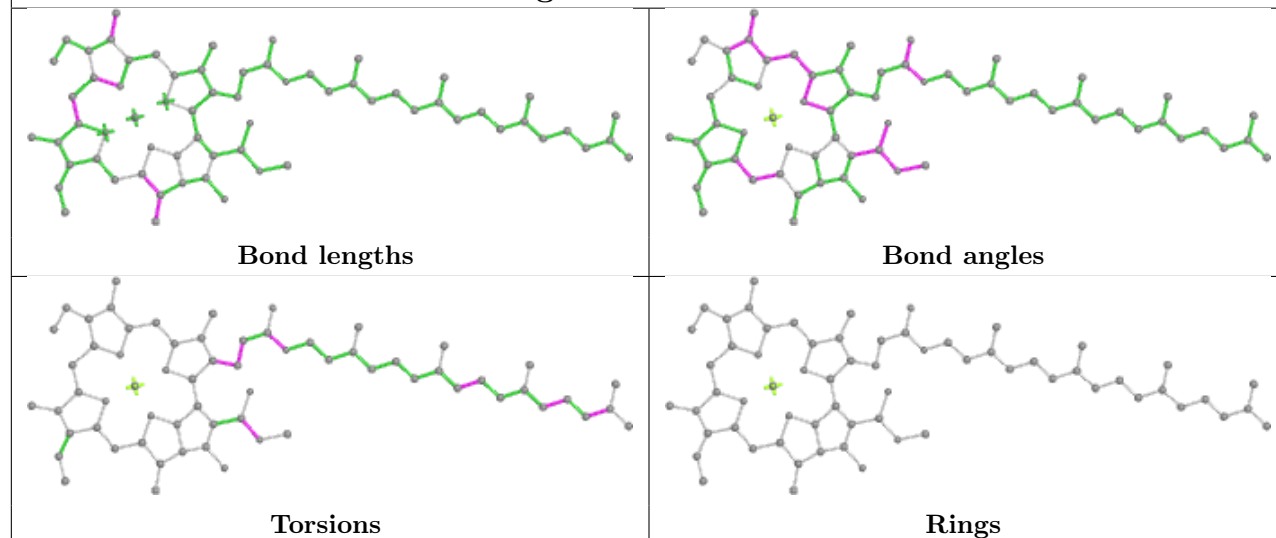
Ligand CLA B 3003



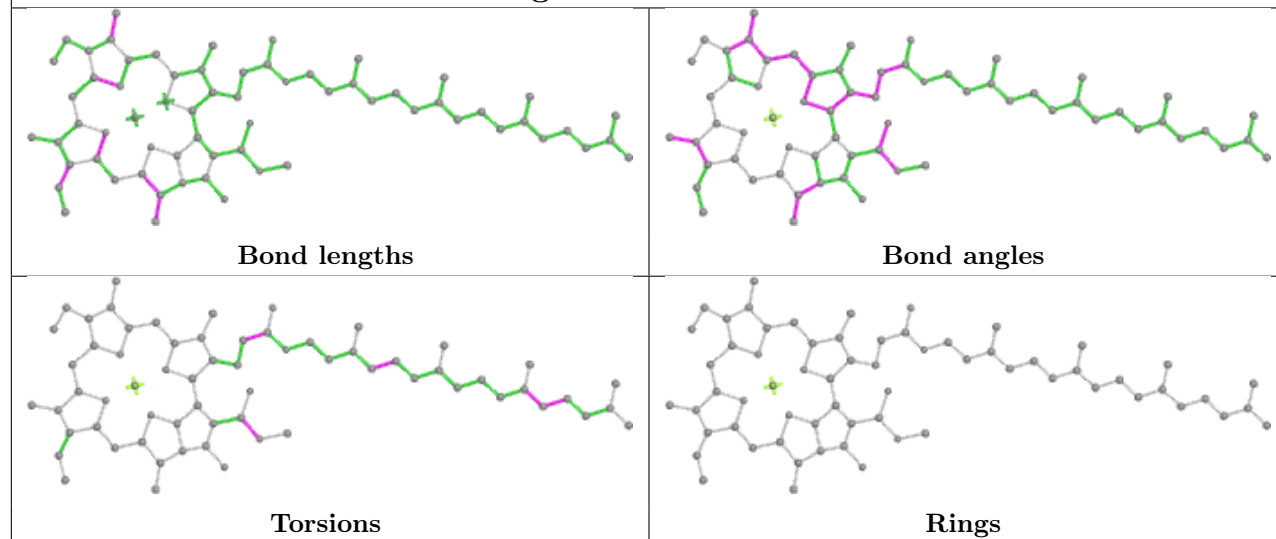
Ligand CLA A 802



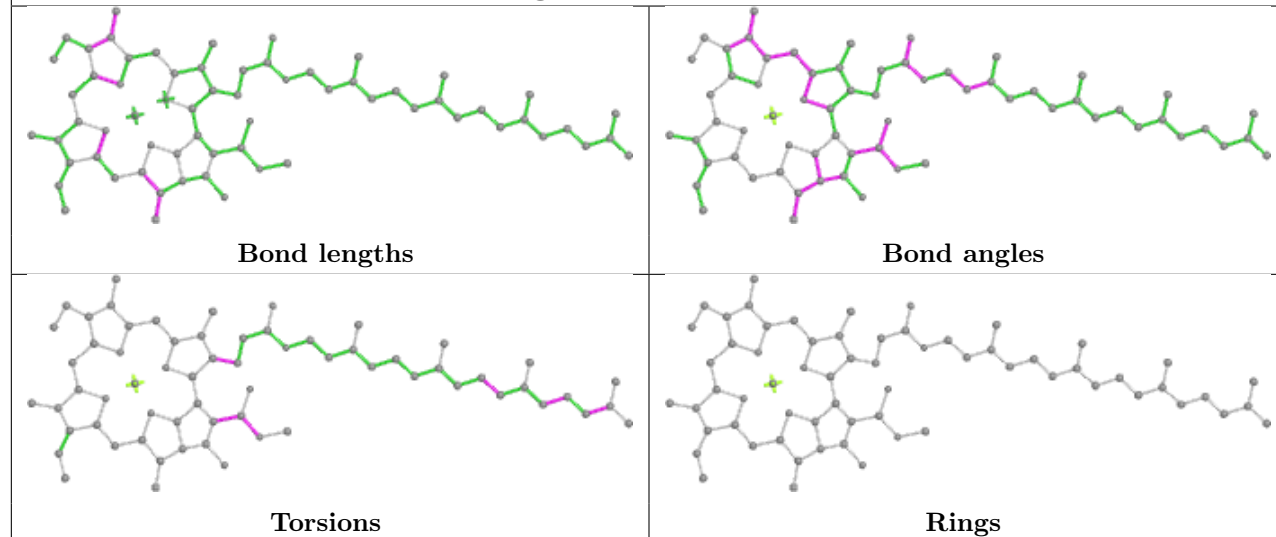
Ligand CL0 A 801



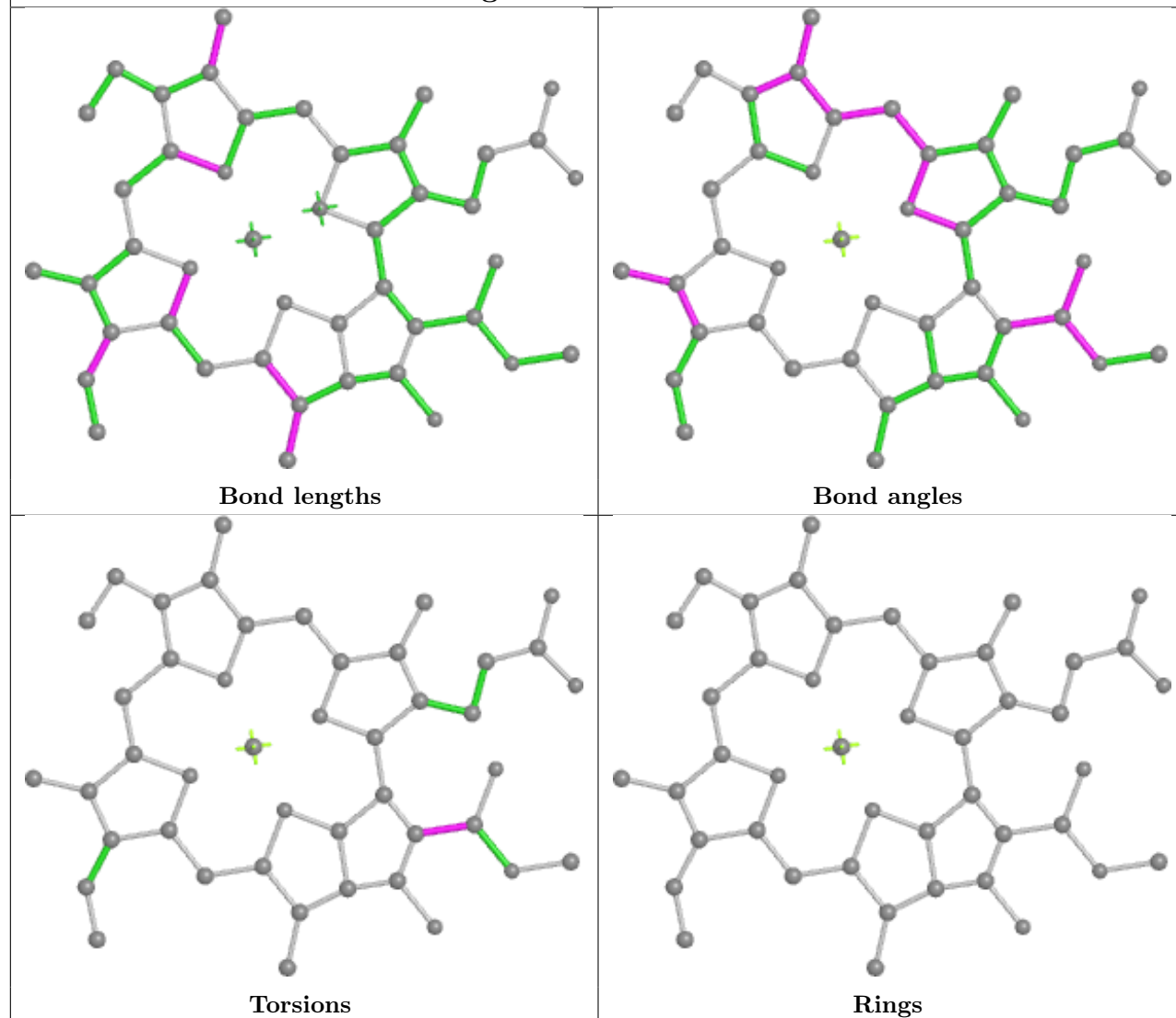
Ligand CLA A 803



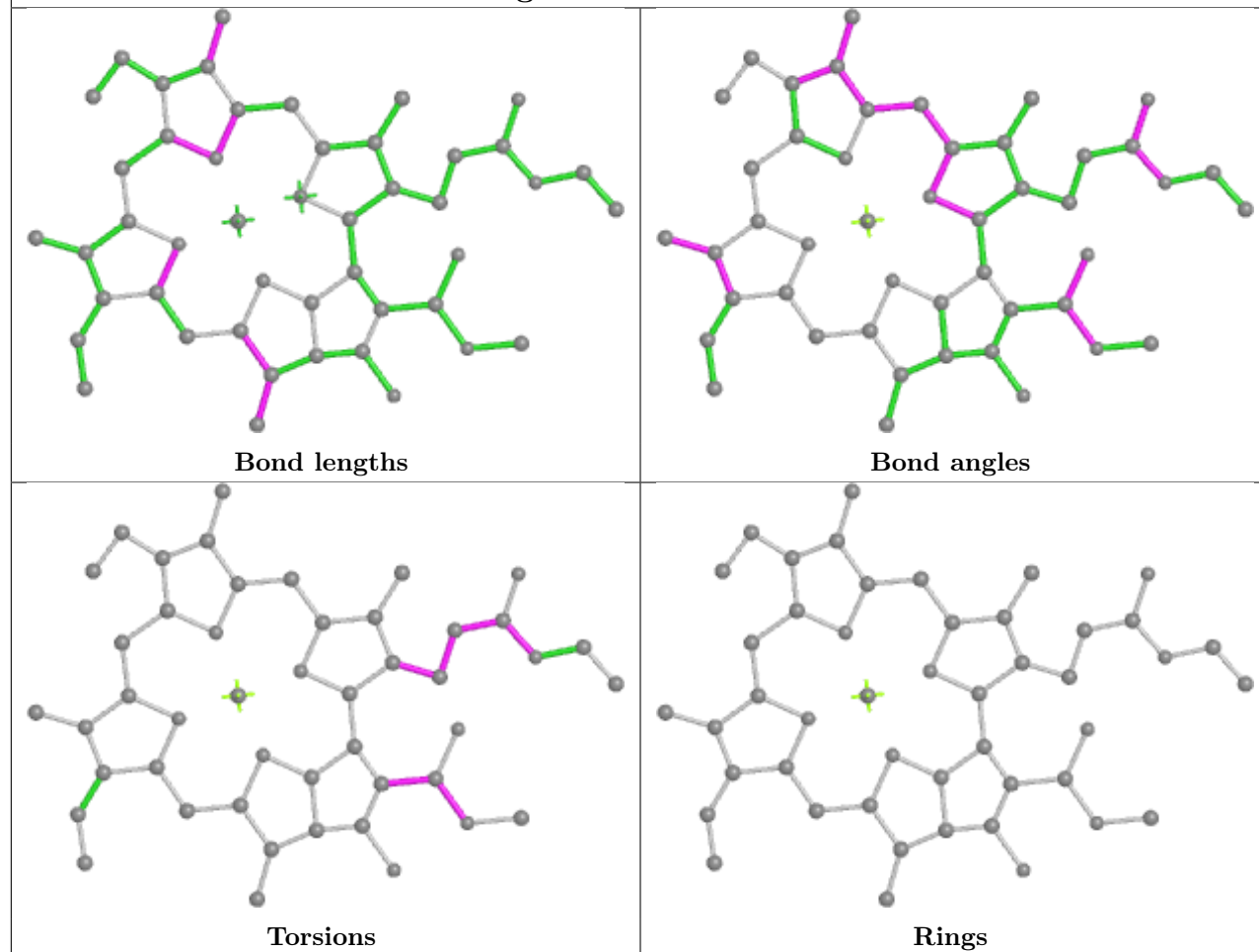
Ligand CLA A 831



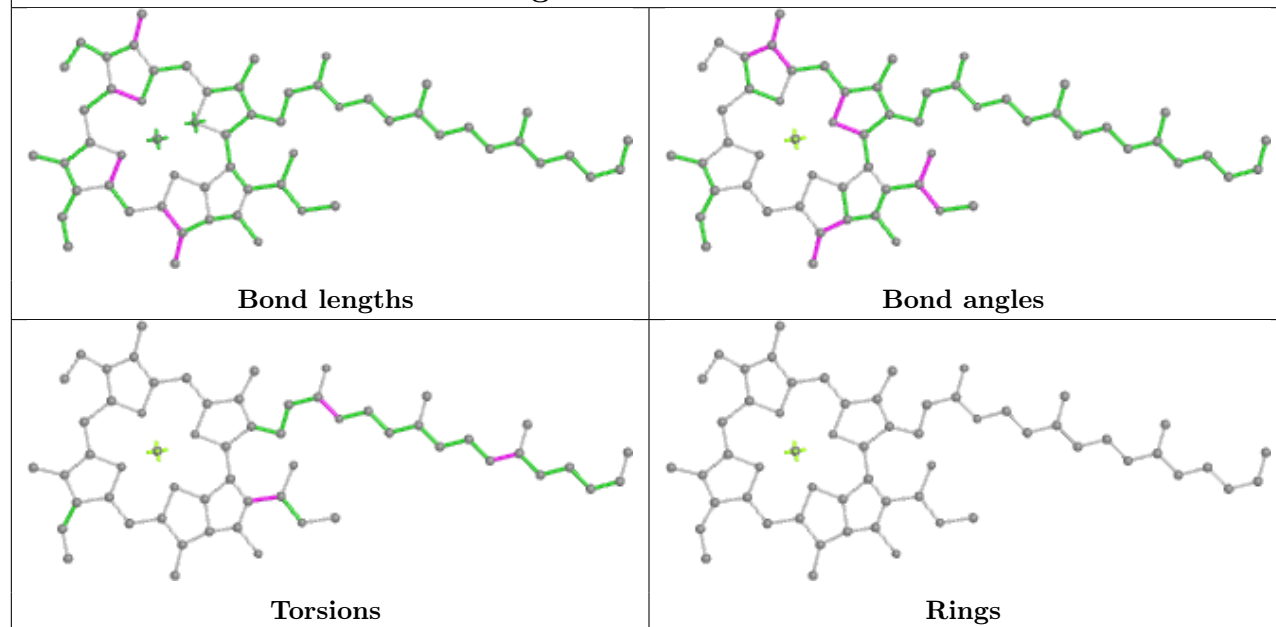
Ligand CLA X 1701



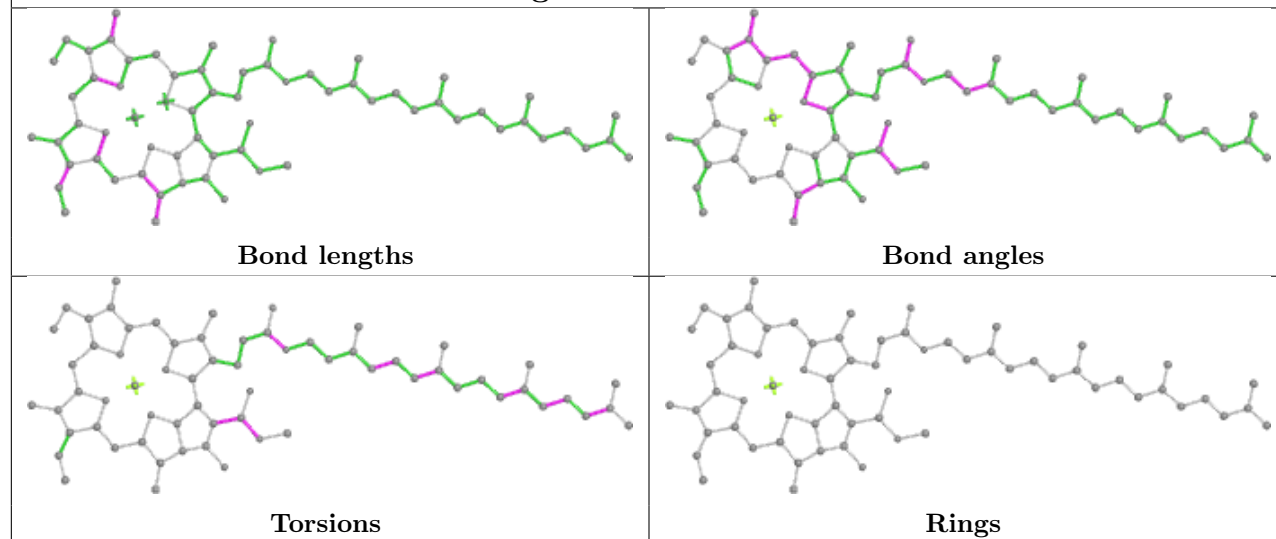
Ligand CLA B 3021



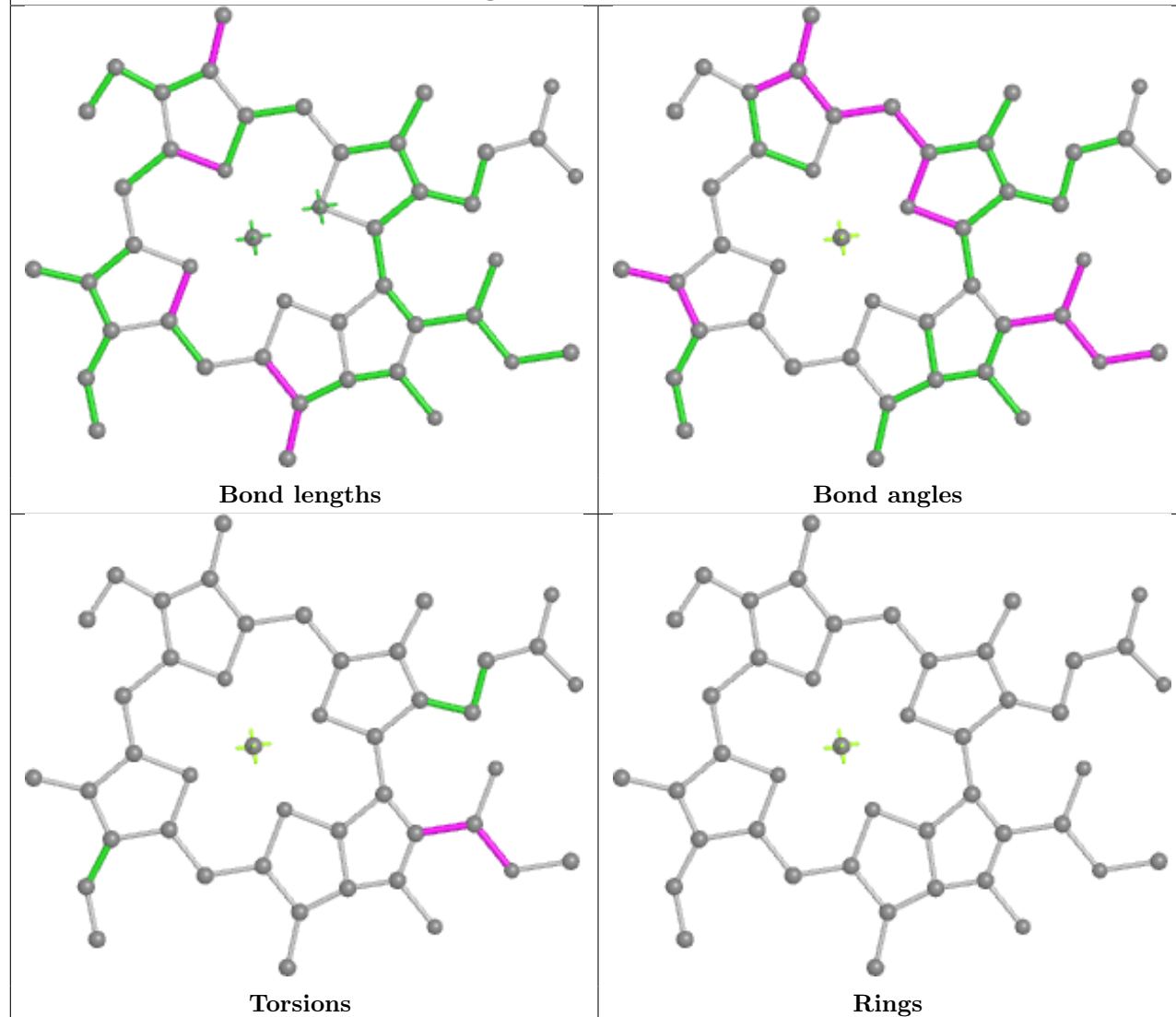
Ligand CLA A 805

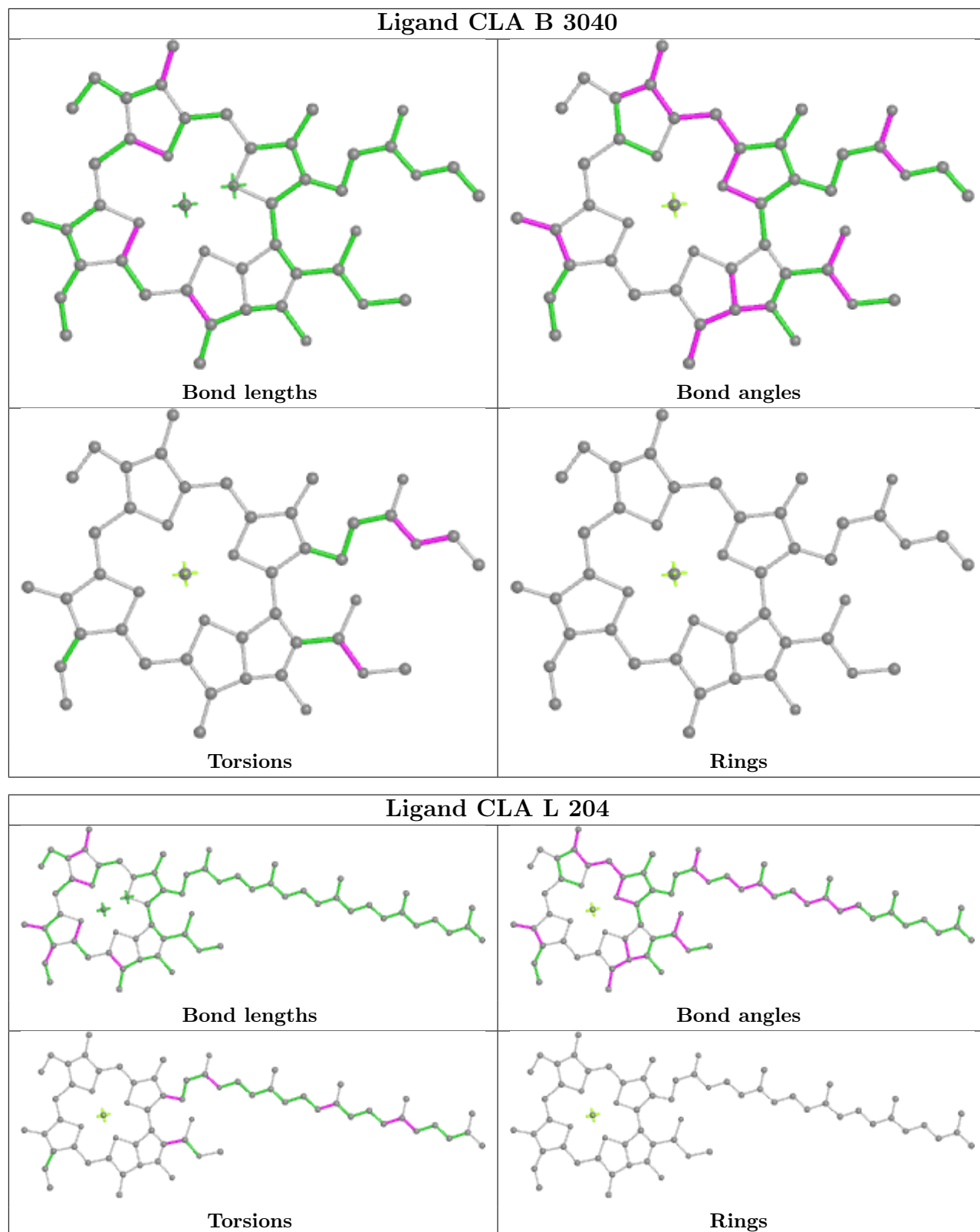


Ligand CLA A 829

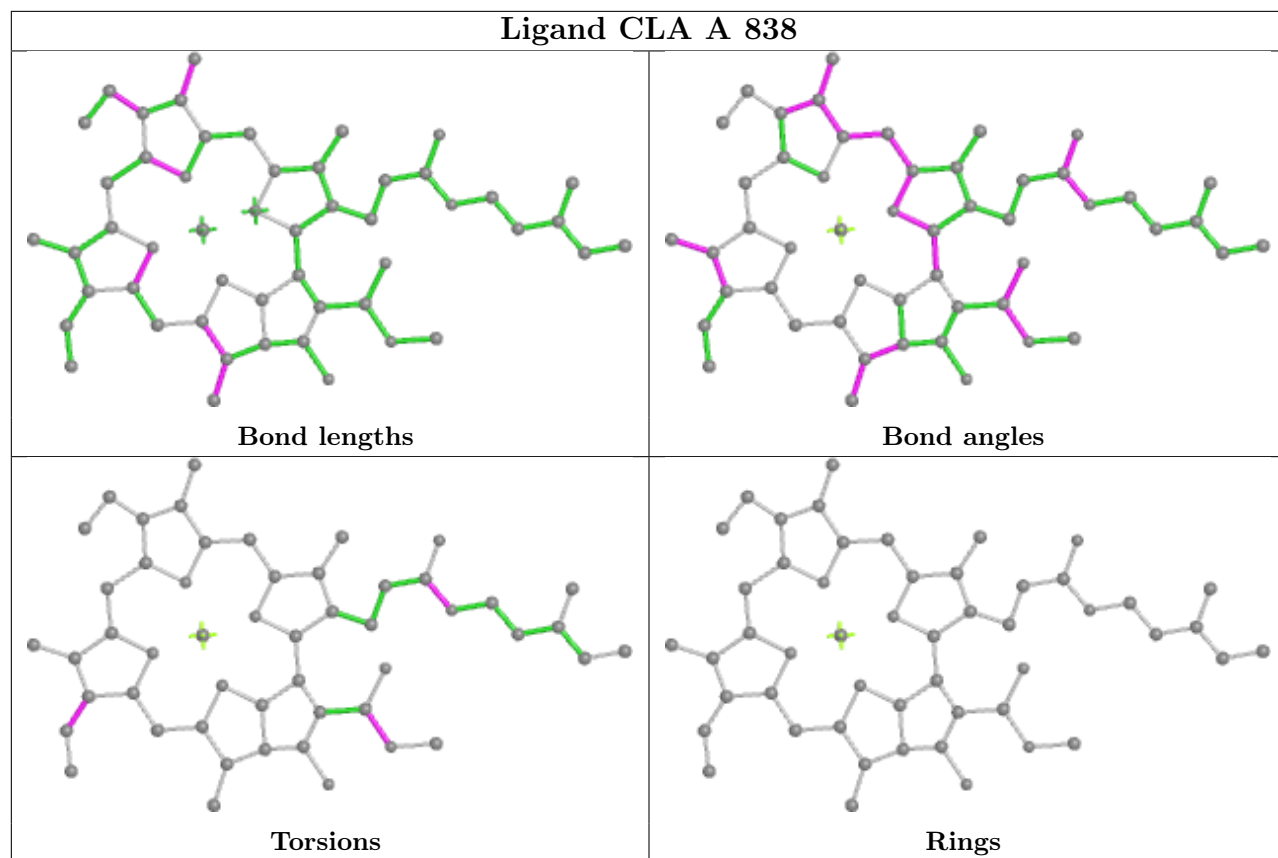


Ligand CLA B 3012

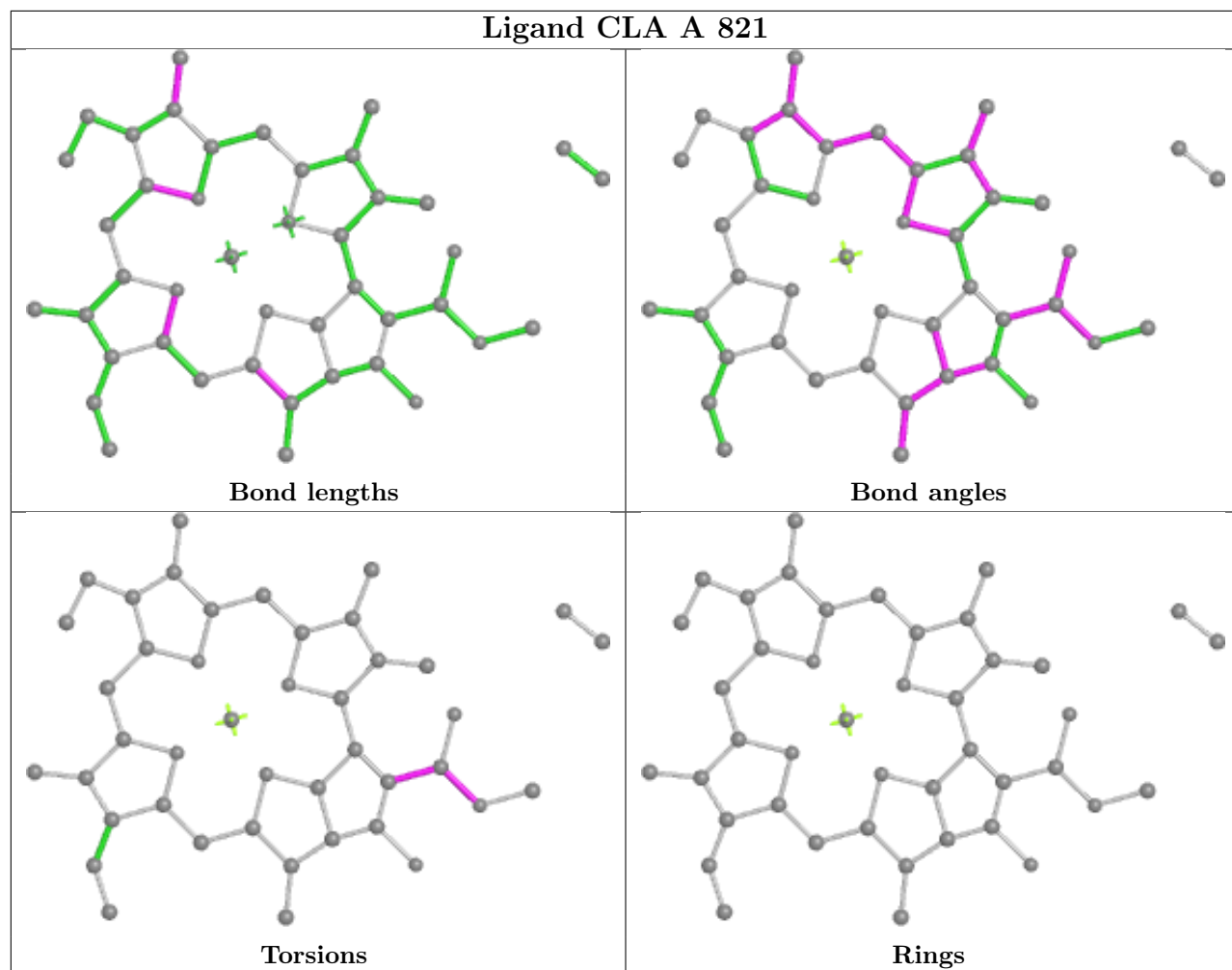


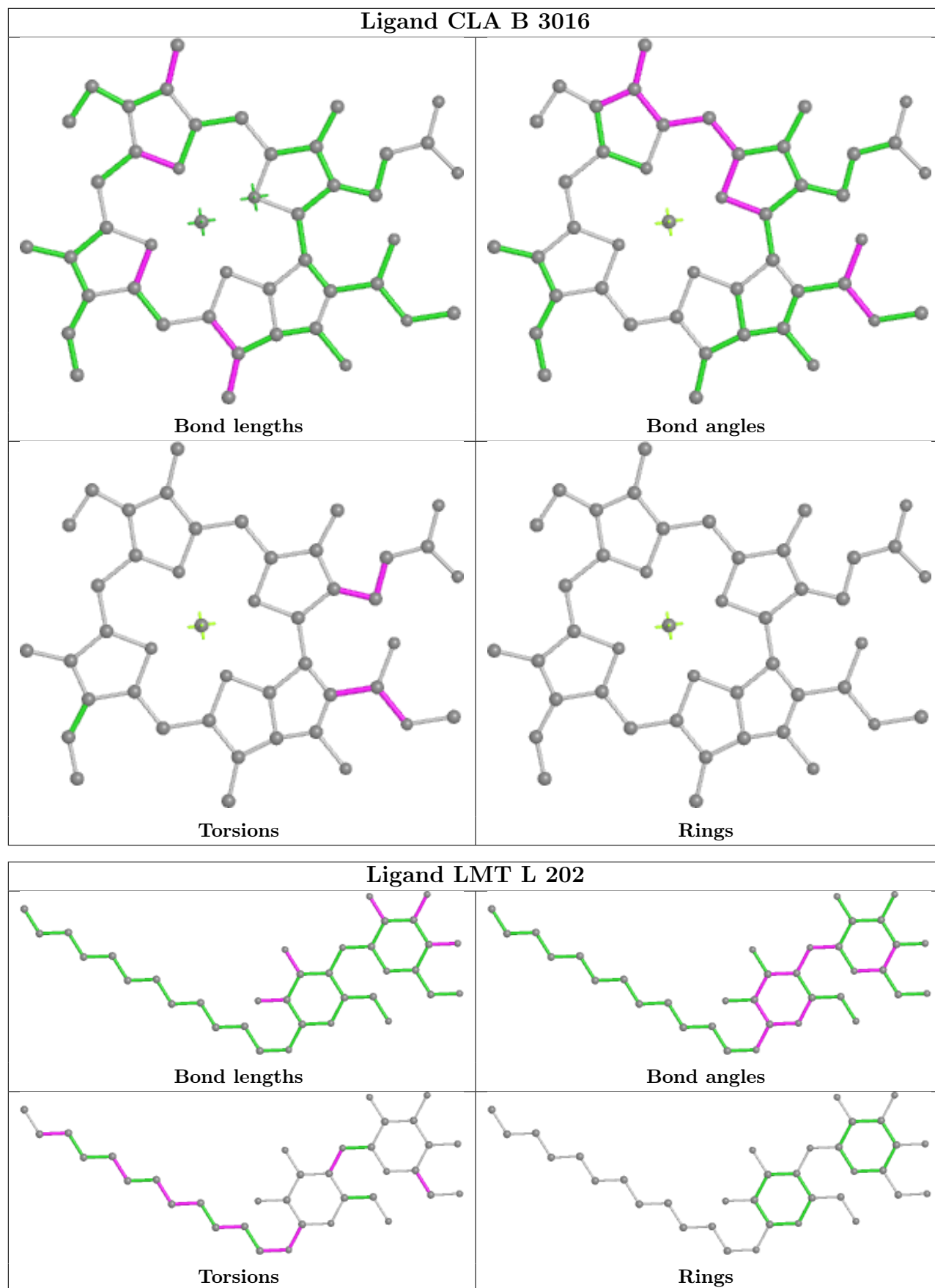


Ligand CLA A 838

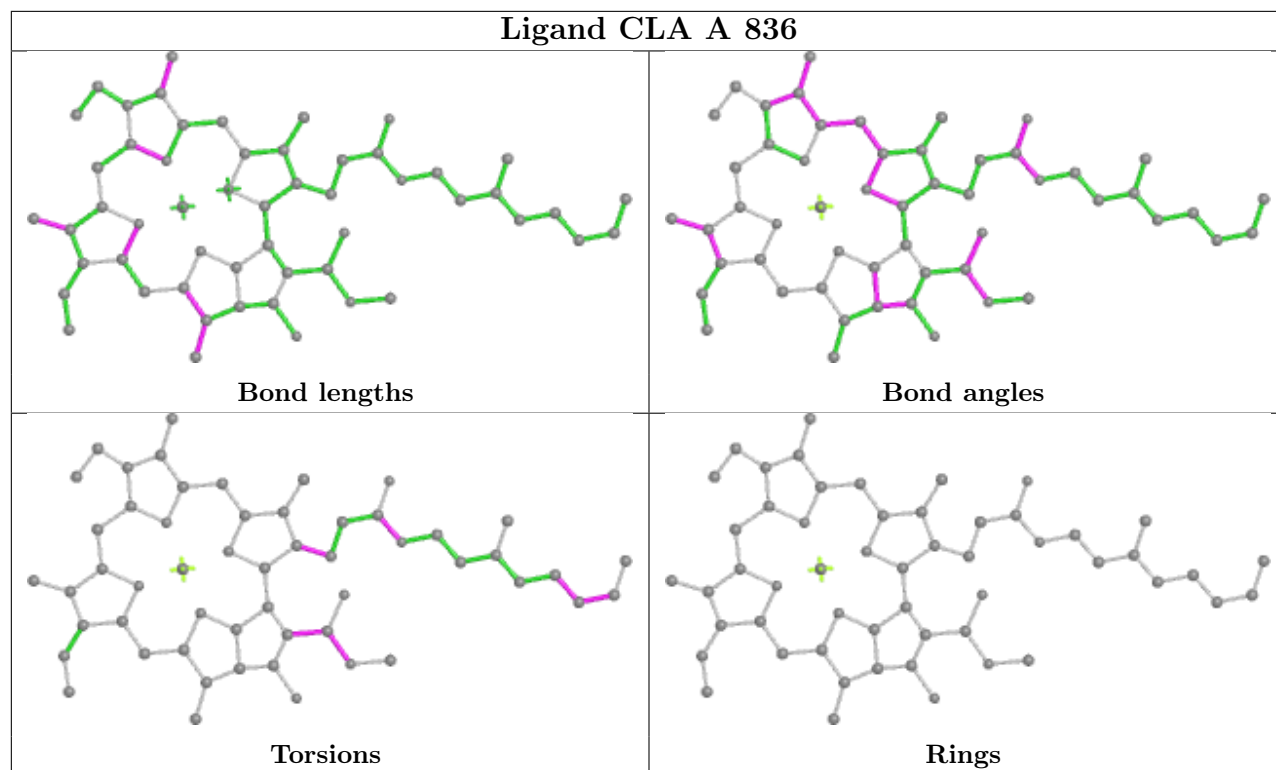


Ligand CLA A 821

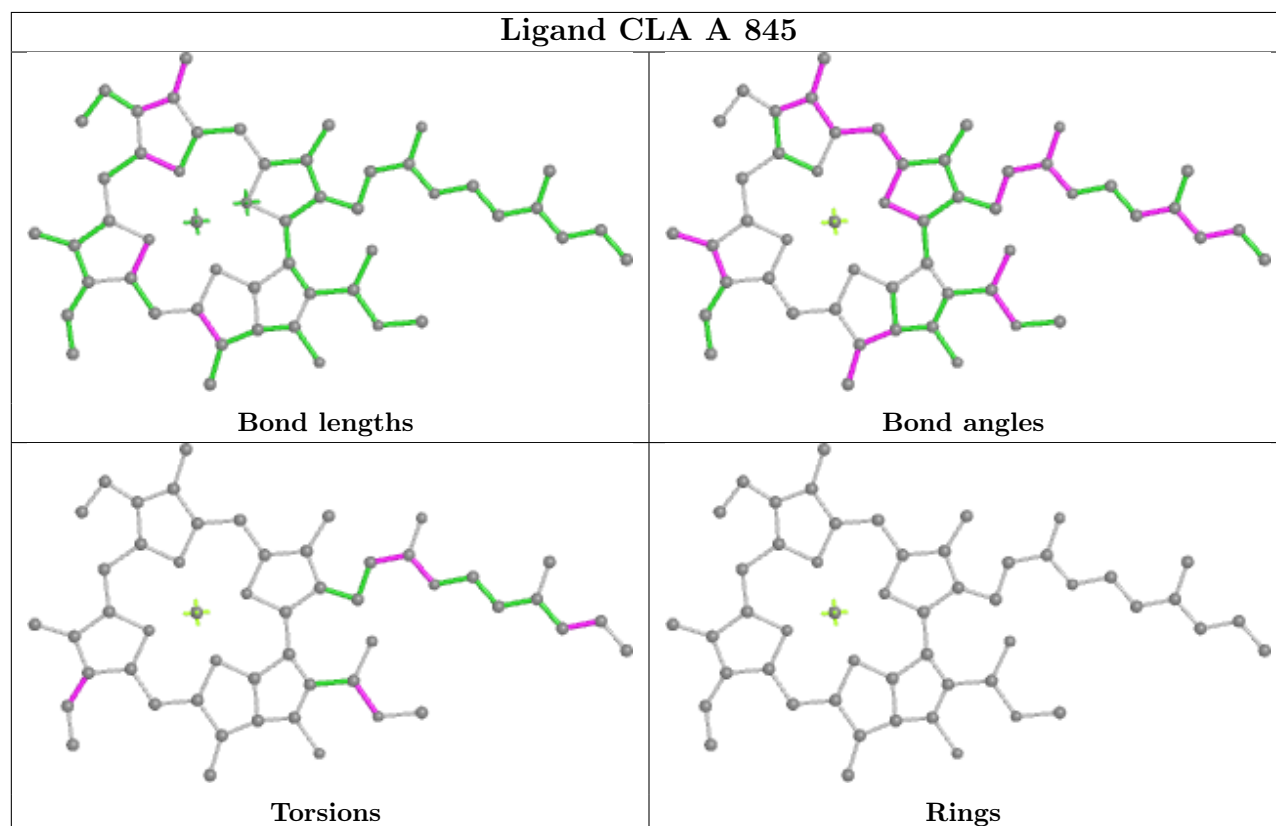


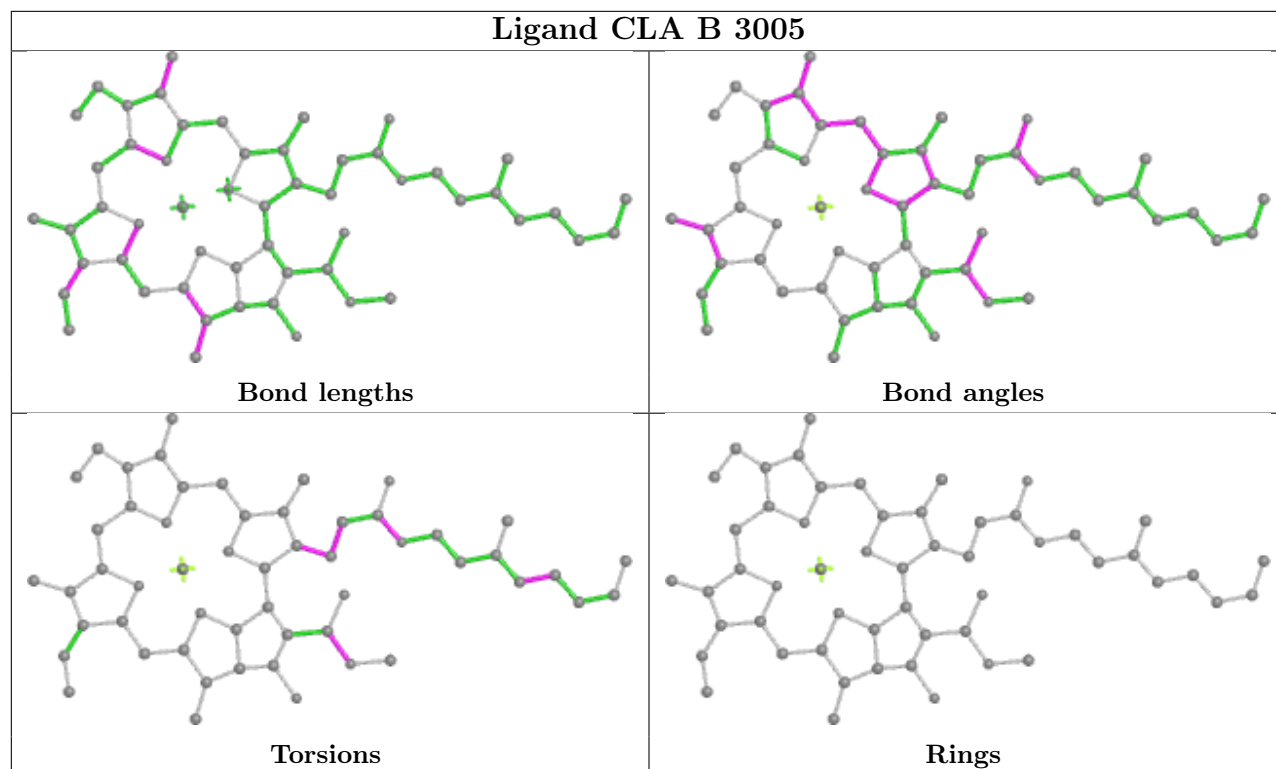
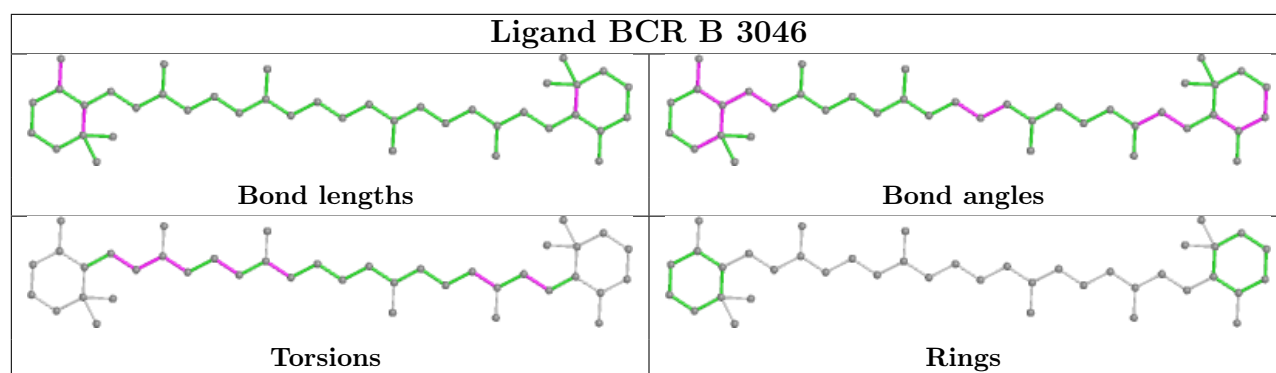


Ligand CLA A 836

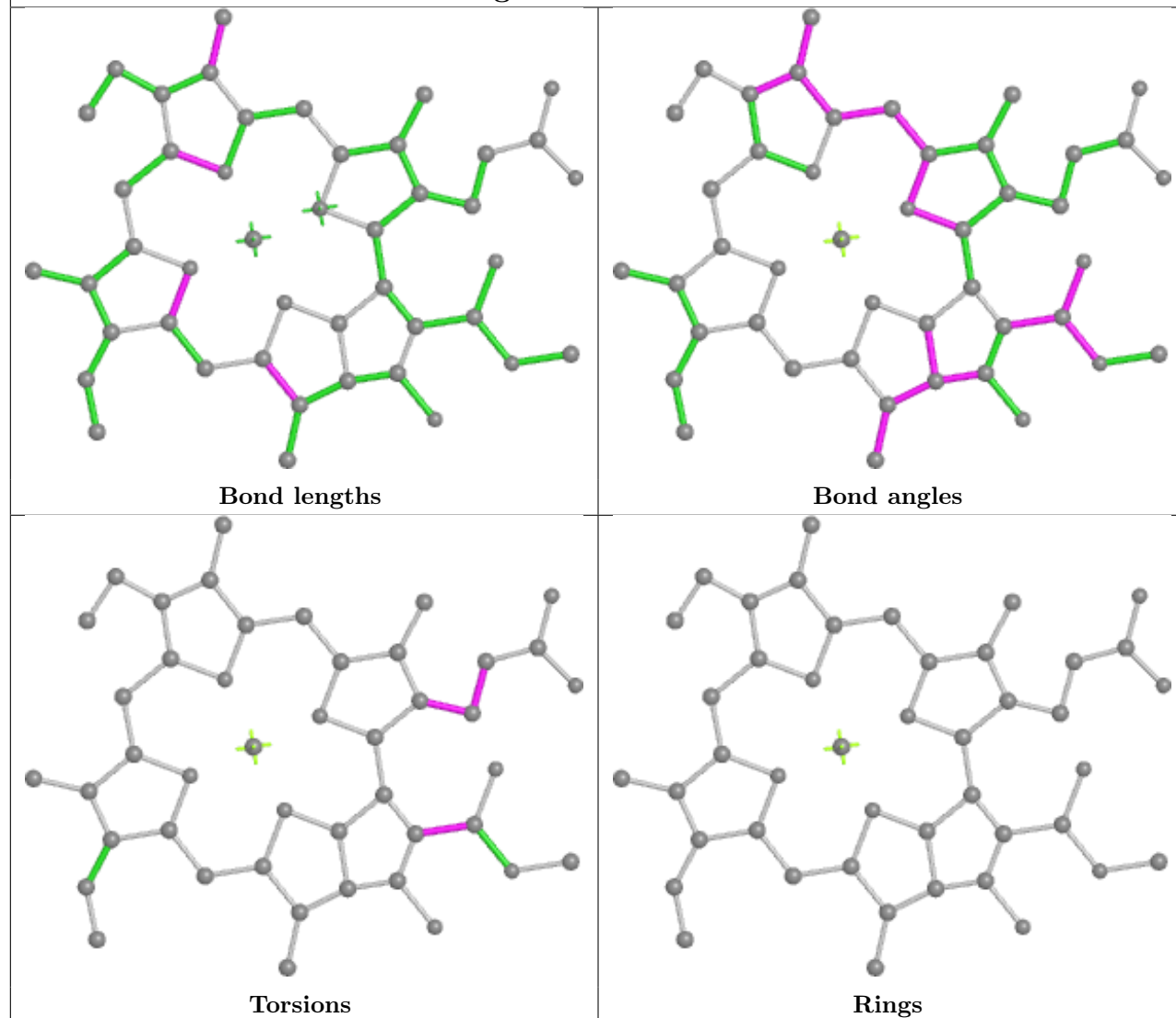


Ligand CLA A 845

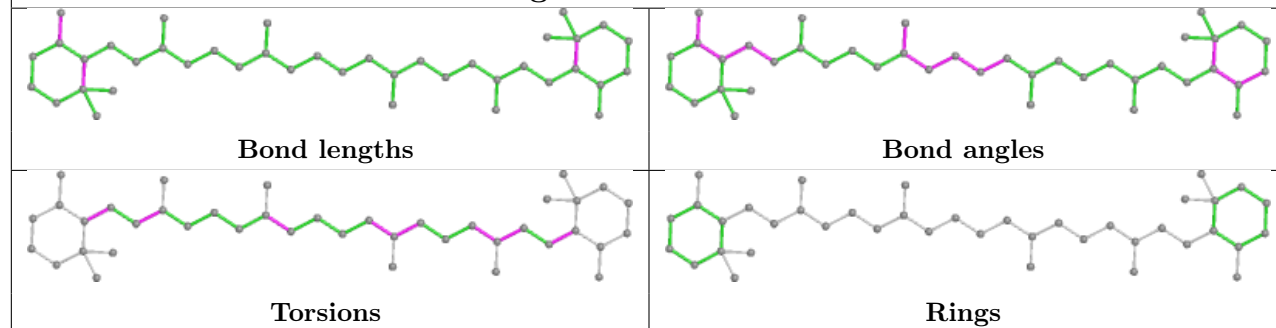


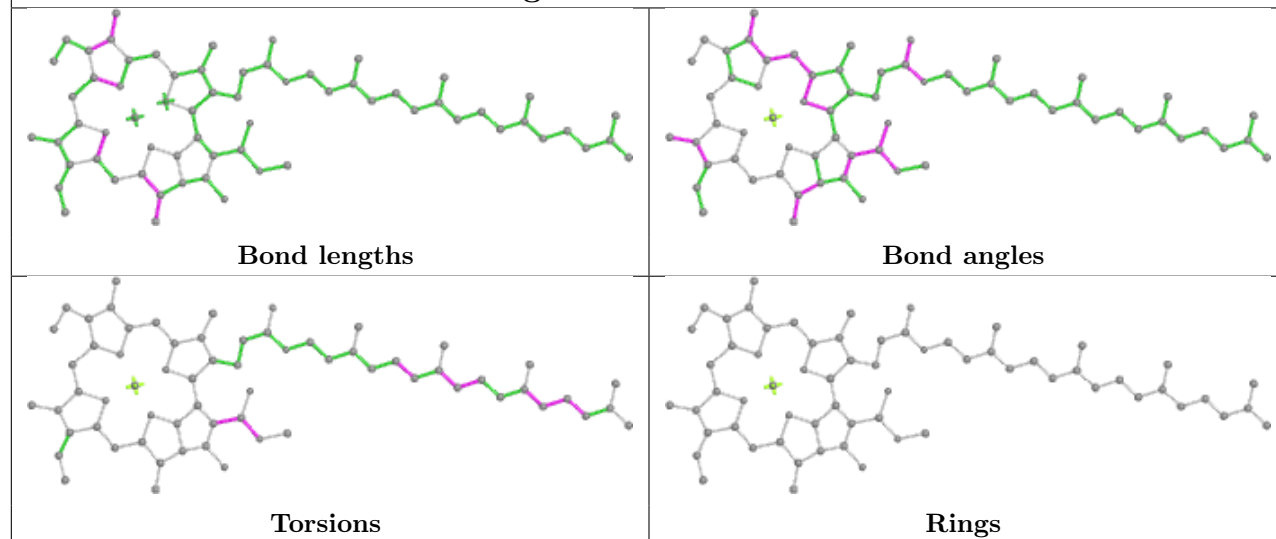
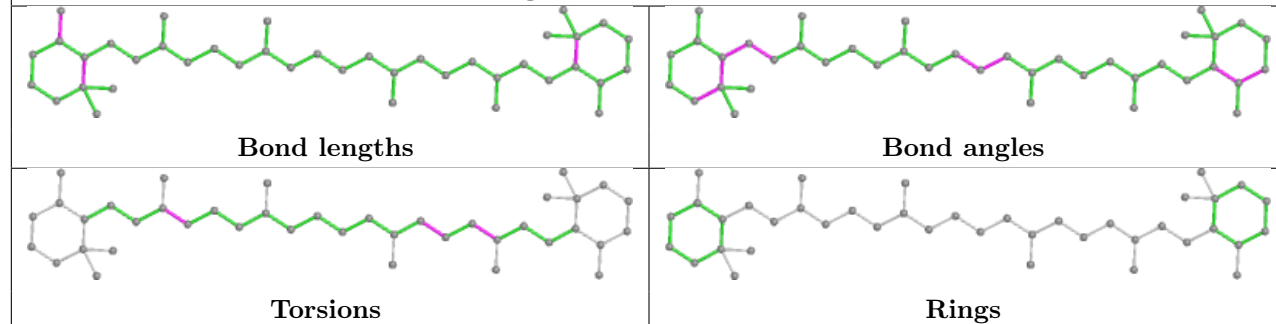


Ligand CLA J 101

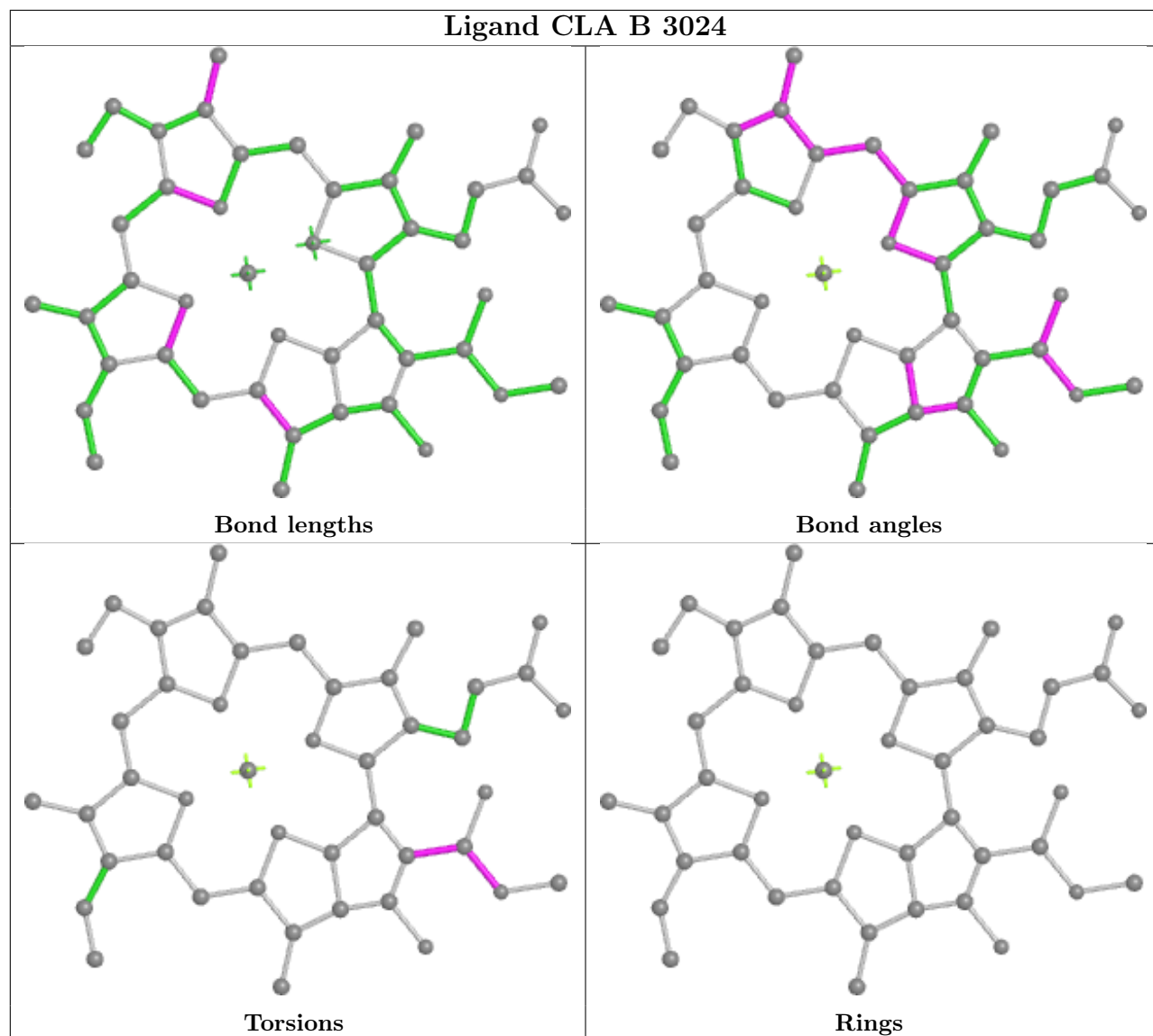


Ligand BCR A 849

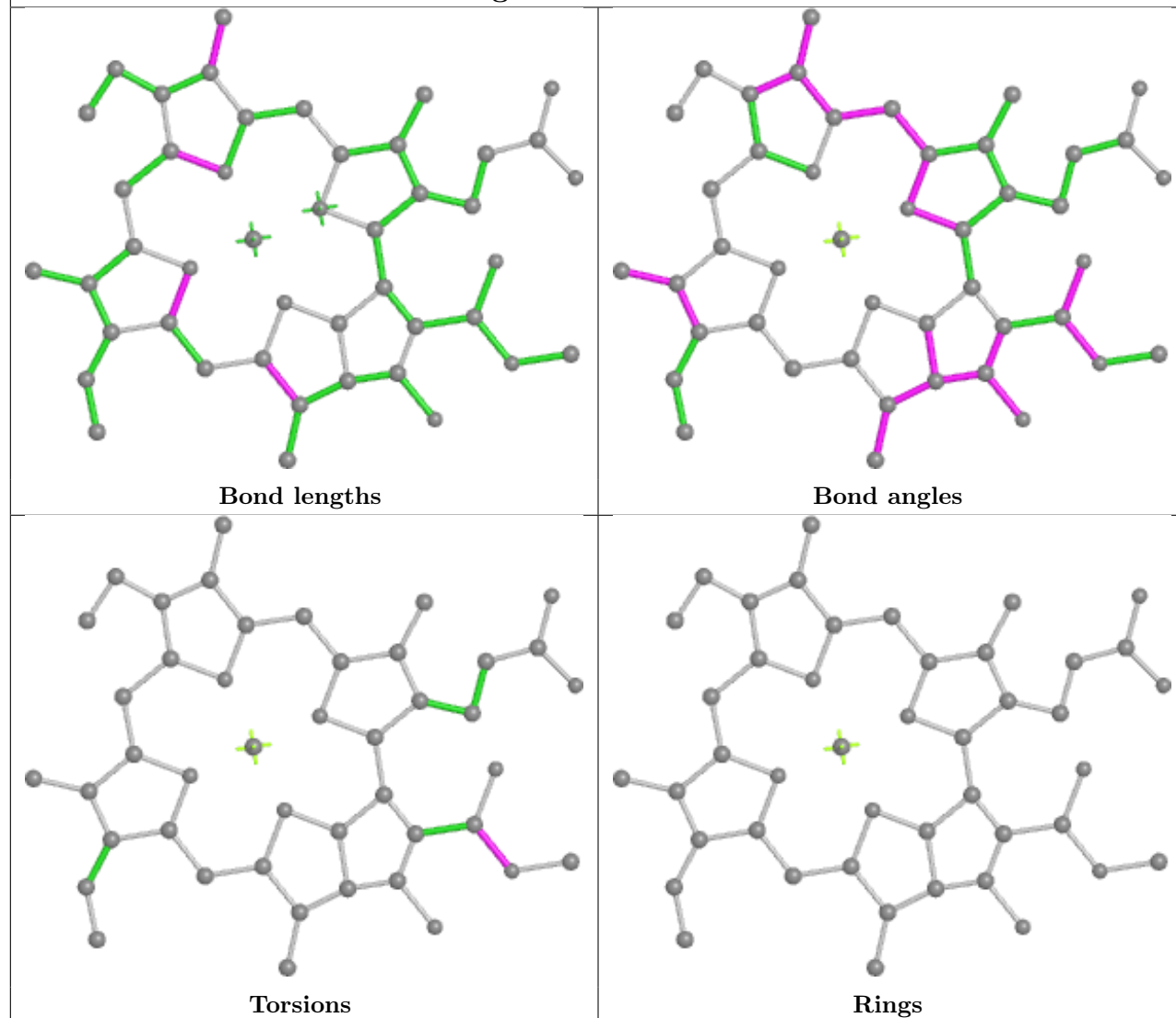


Ligand CLA B 3009**Ligand BCR B 3048**

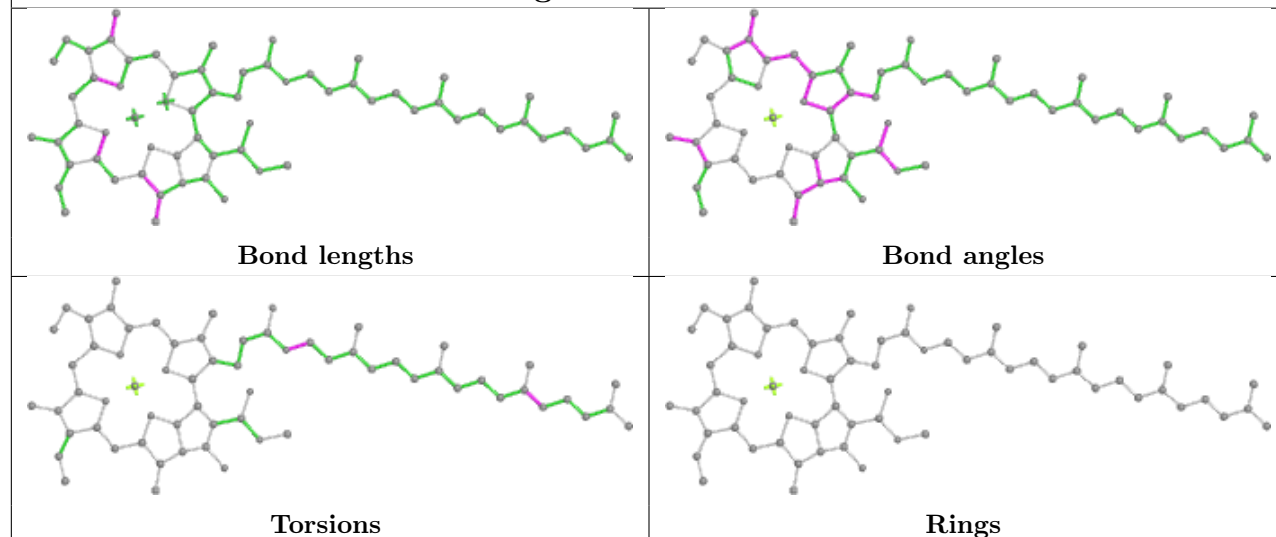
Ligand CLA B 3024

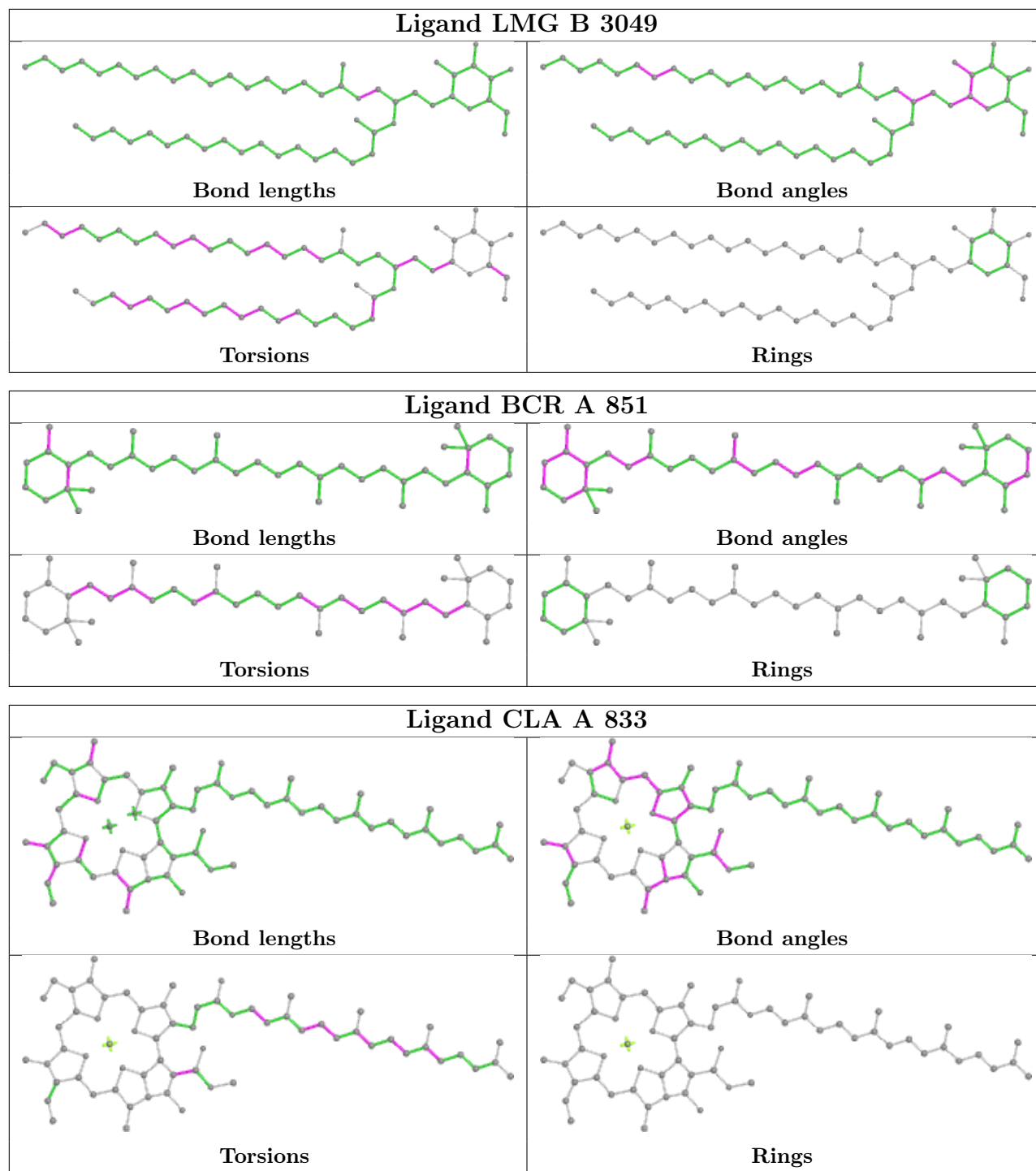


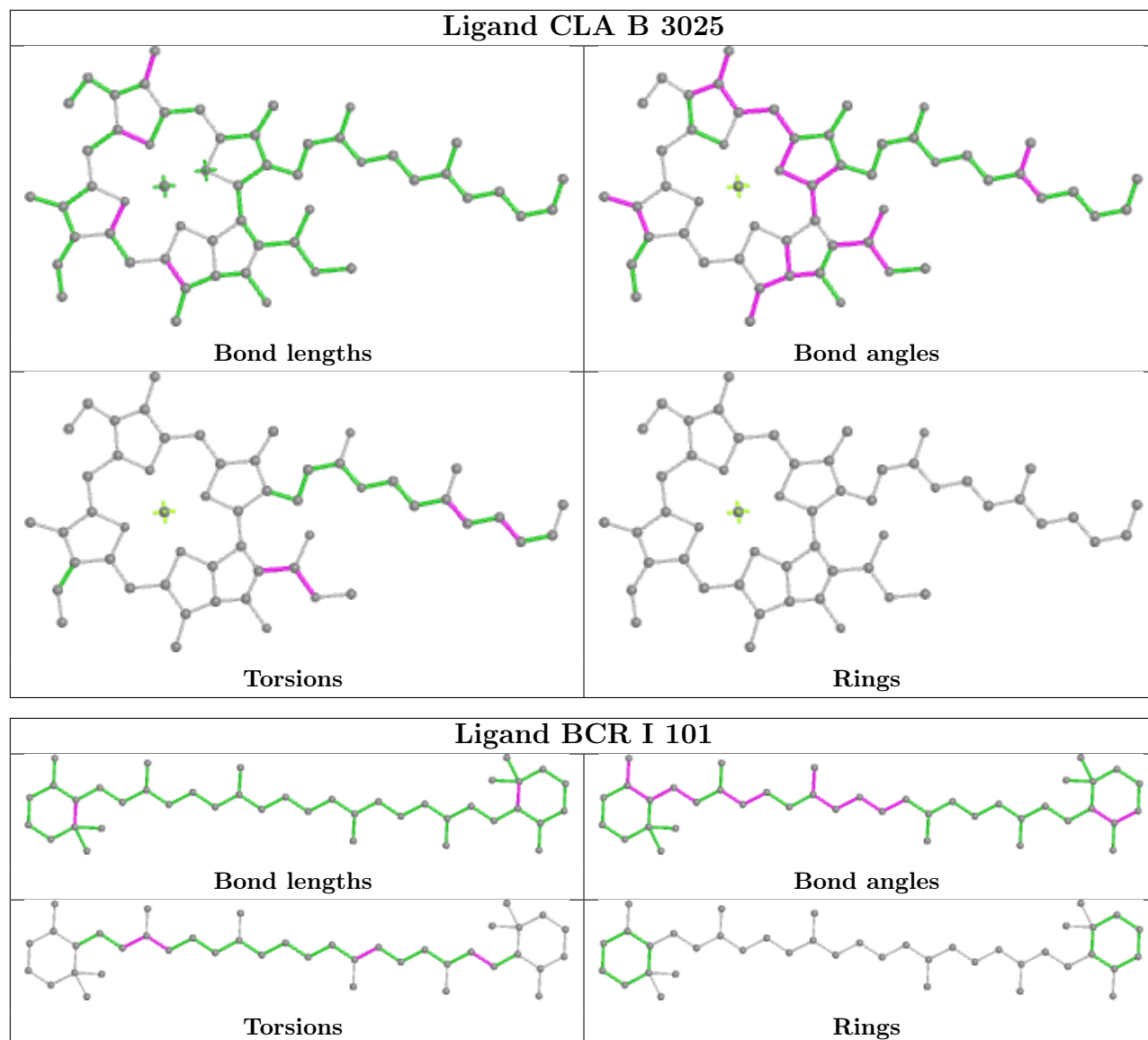
Ligand CLA F 202

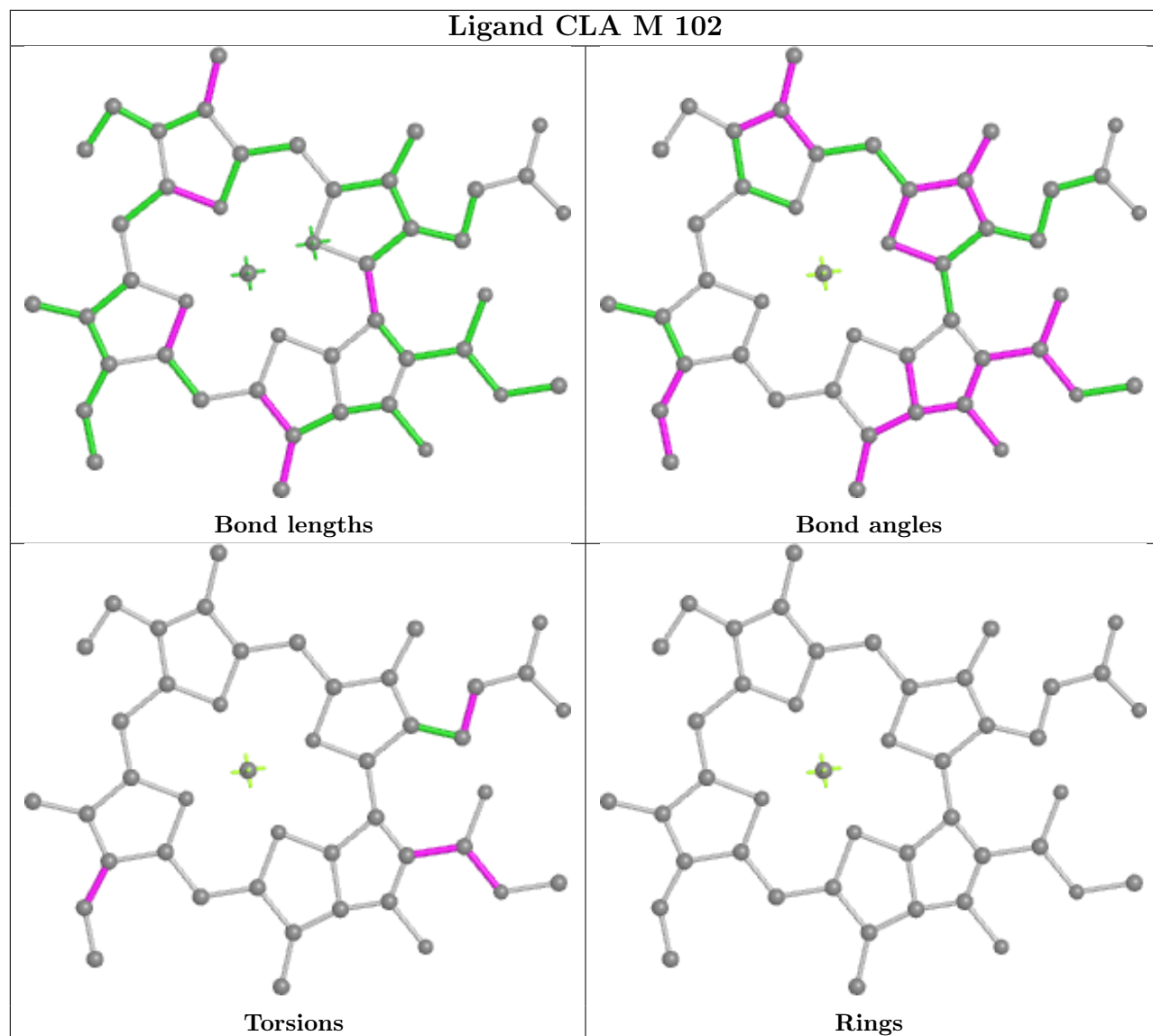


Ligand CLA L 205

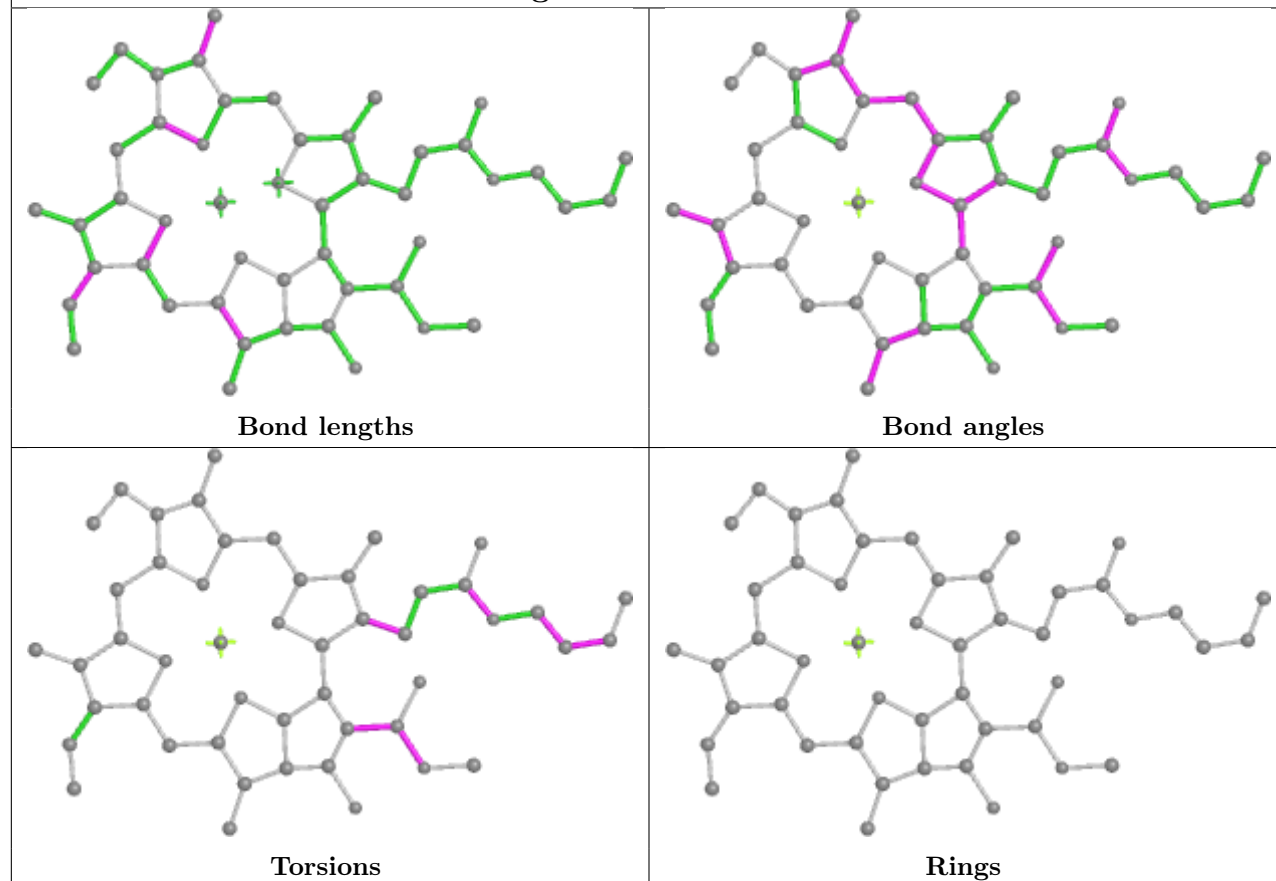




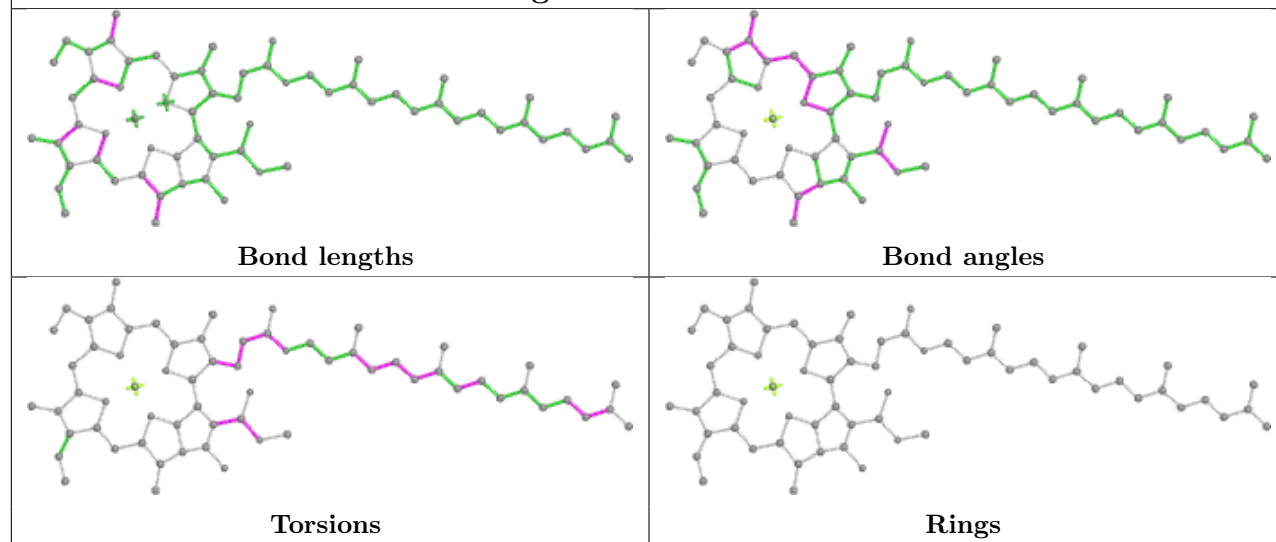




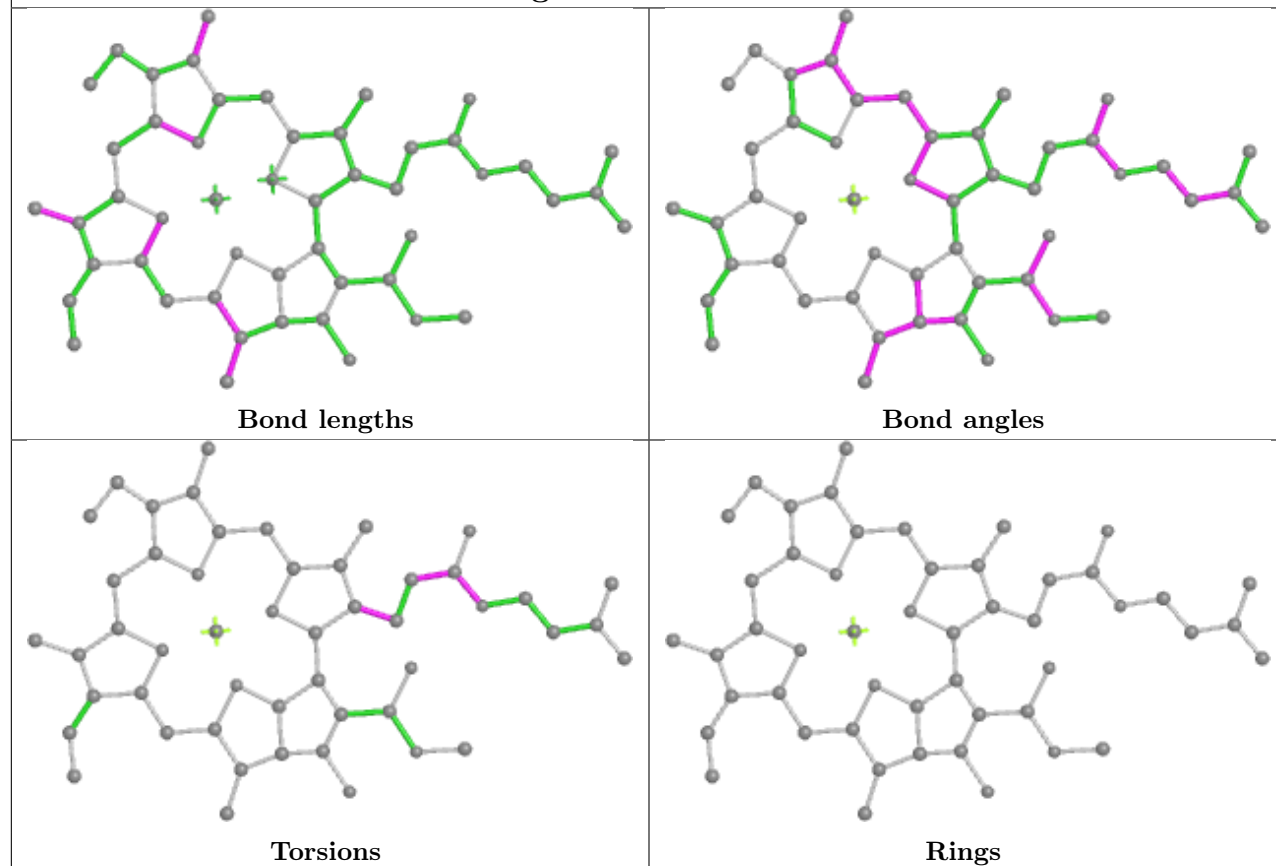
Ligand CLA A 823



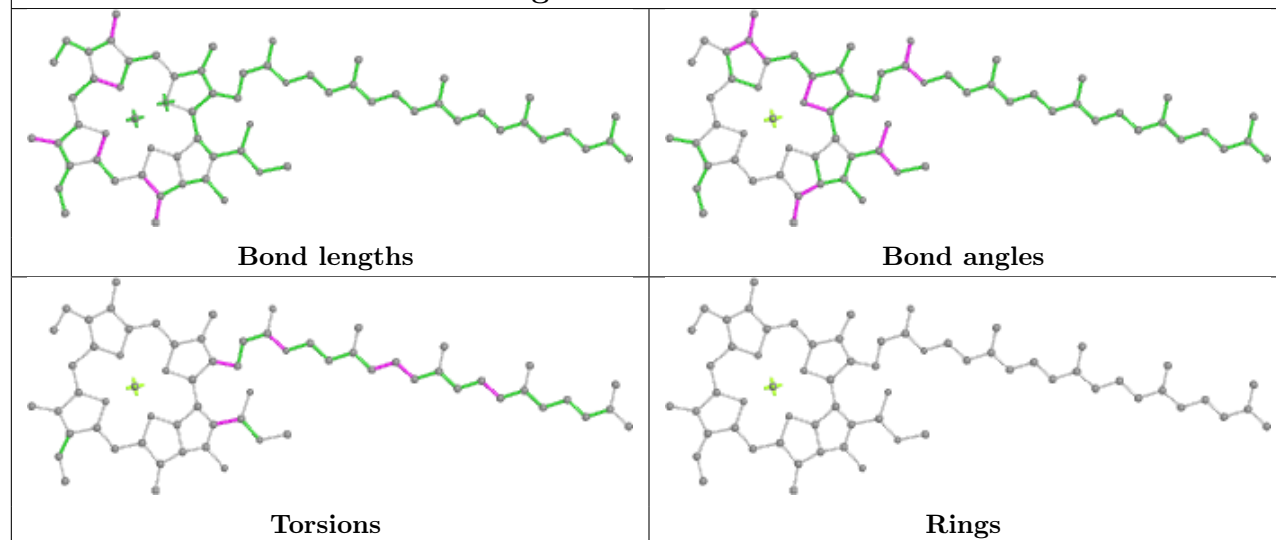
Ligand CLA A 809



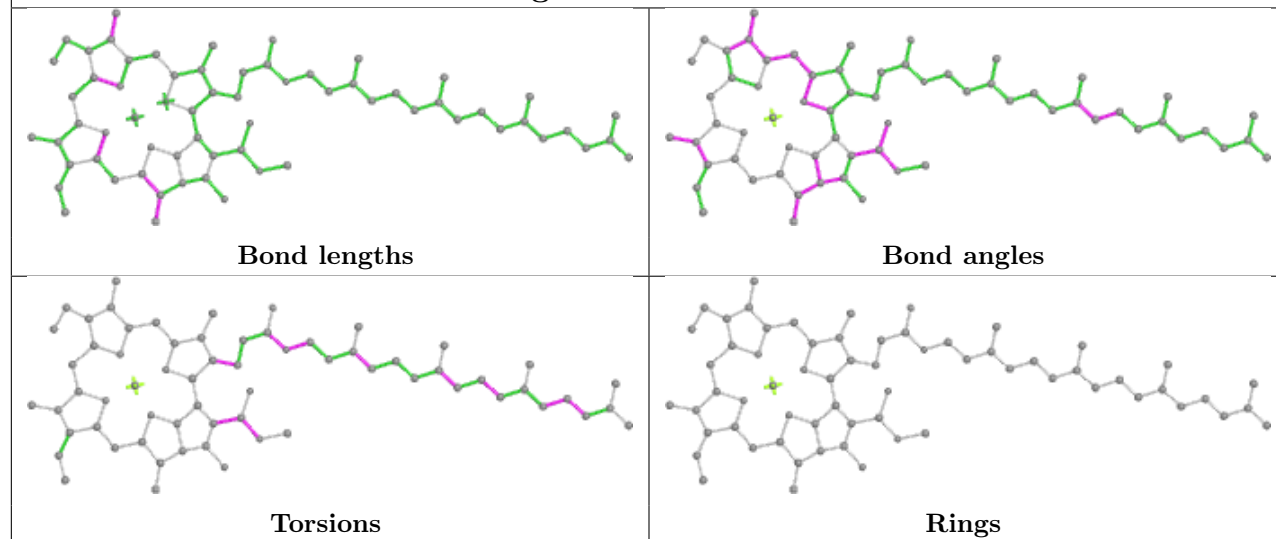
Ligand CLA A 832



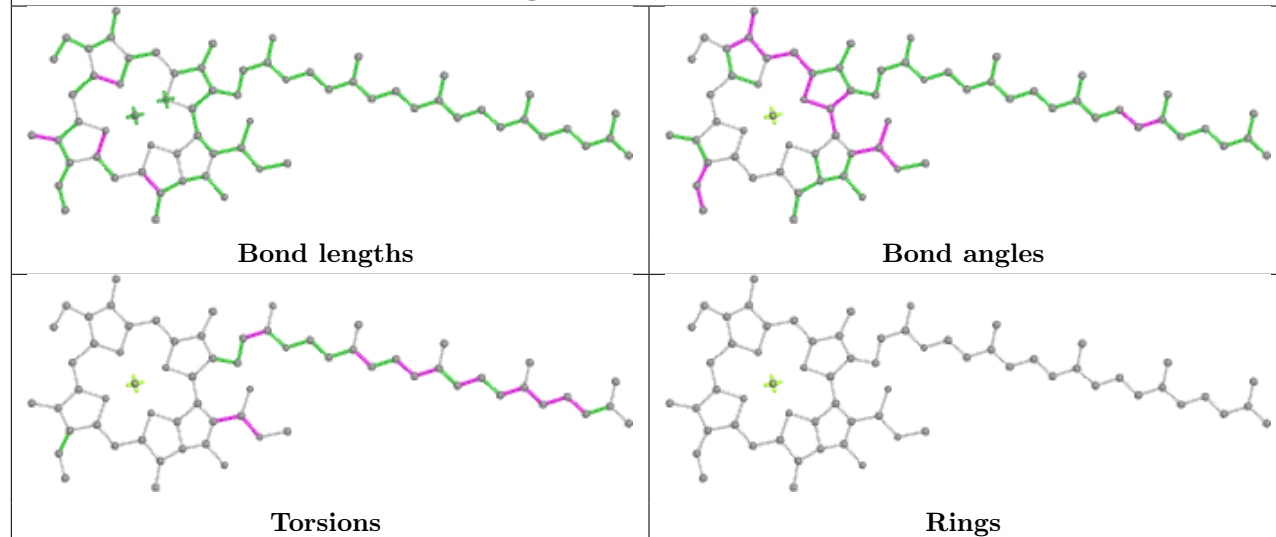
Ligand CLA A 804



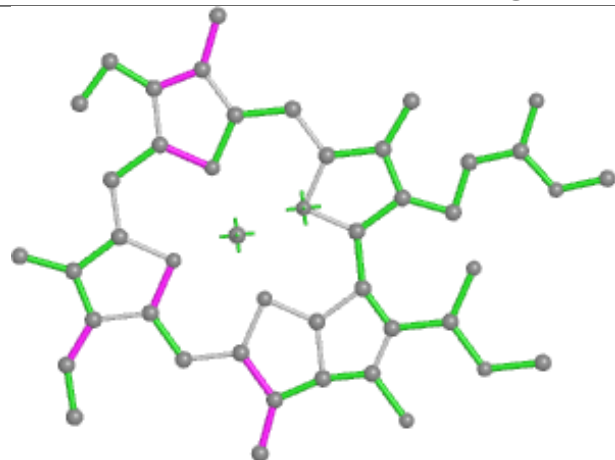
Ligand CLA A 826



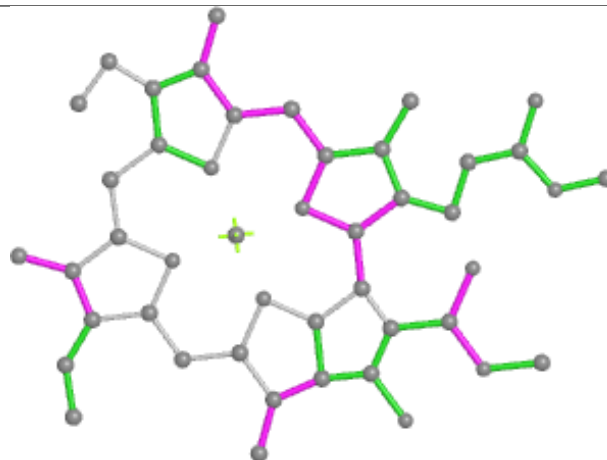
Ligand CLA B 3011



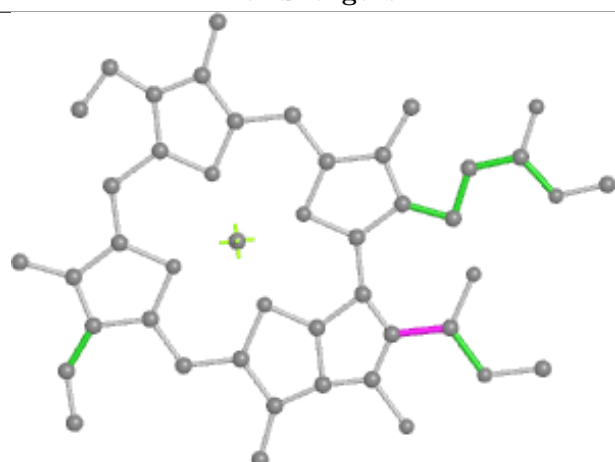
Ligand CLA B 3026



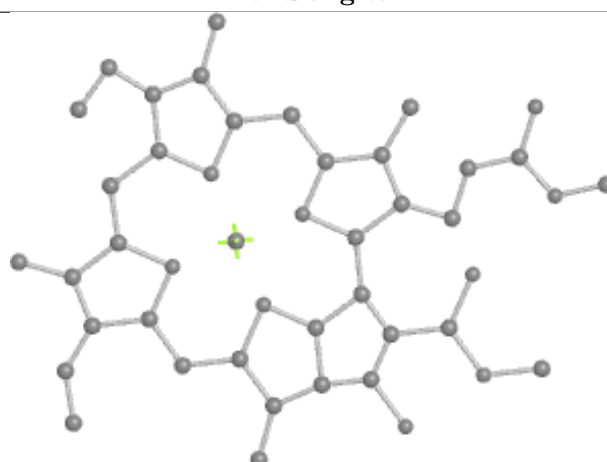
Bond lengths



Bond angles

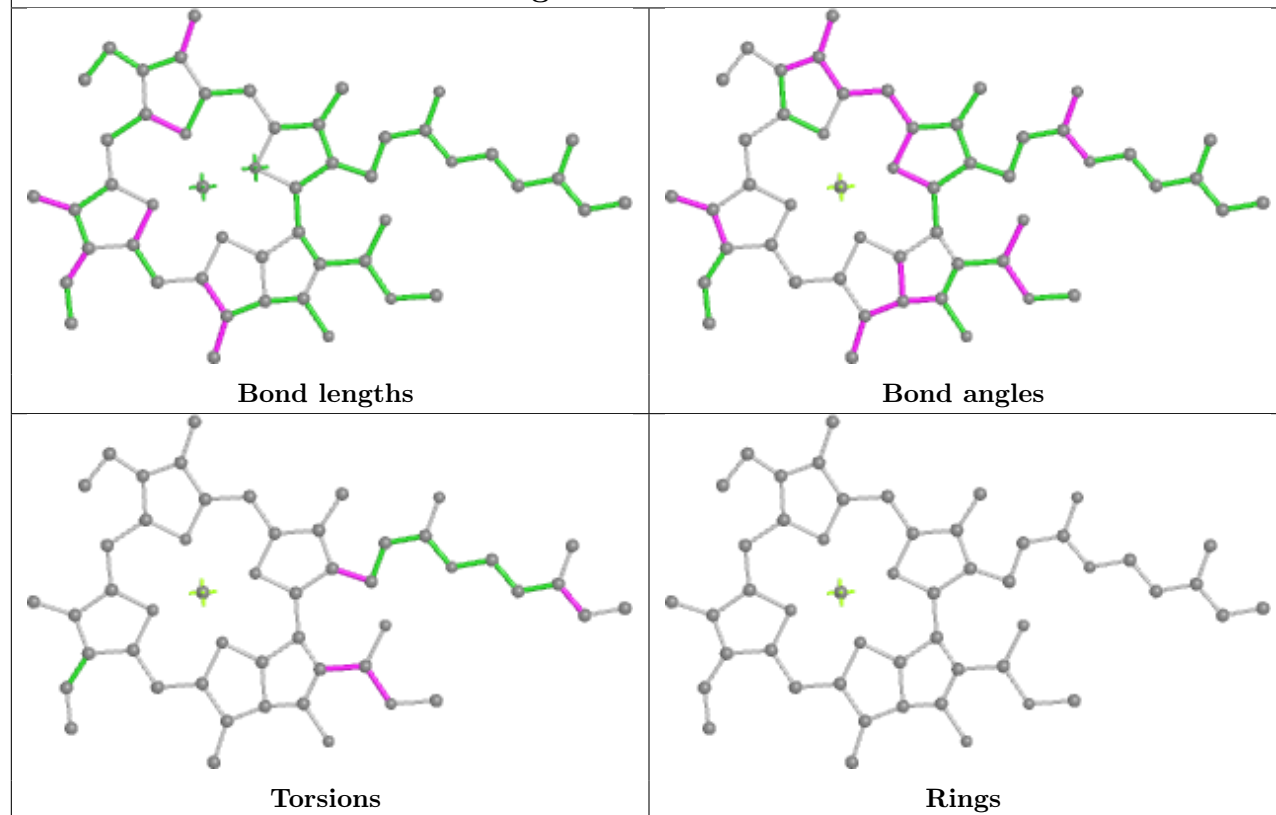


Torsions

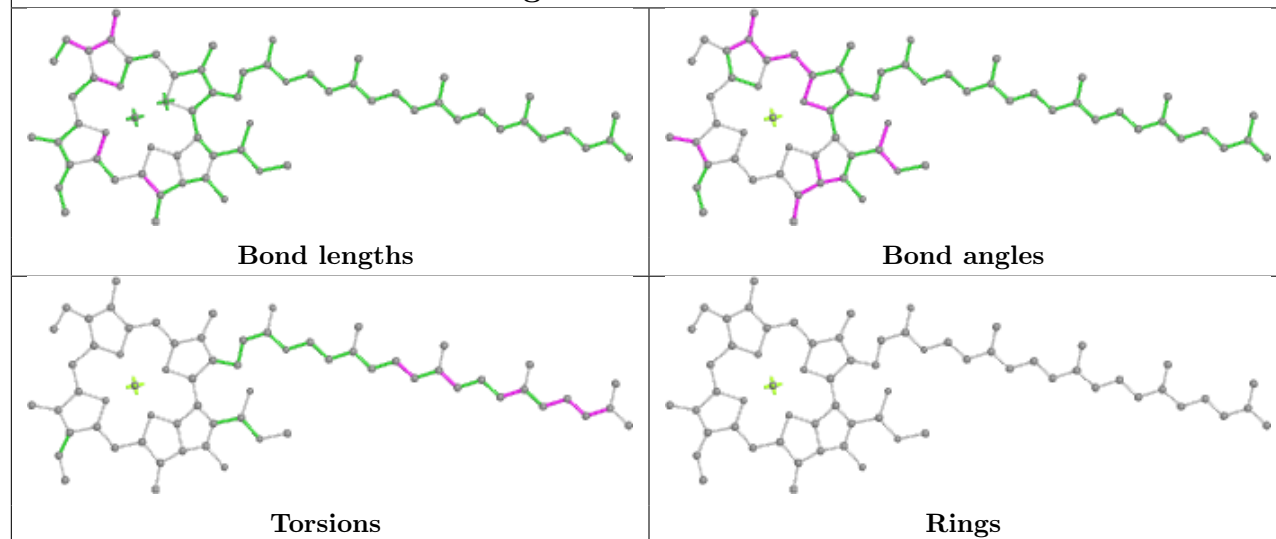


Rings

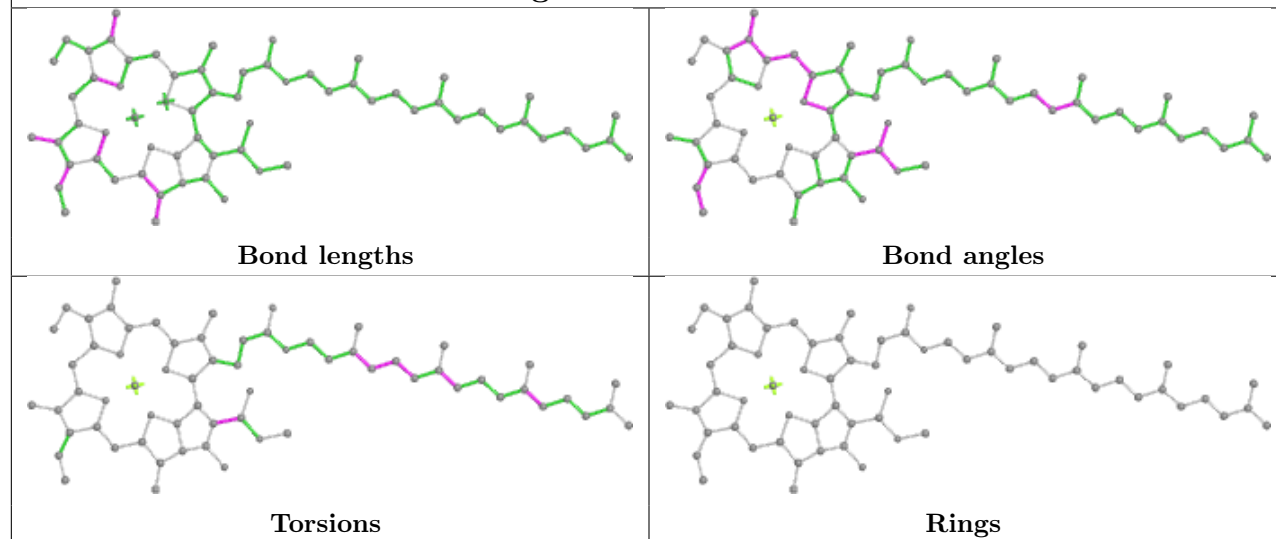
Ligand CLA A 842



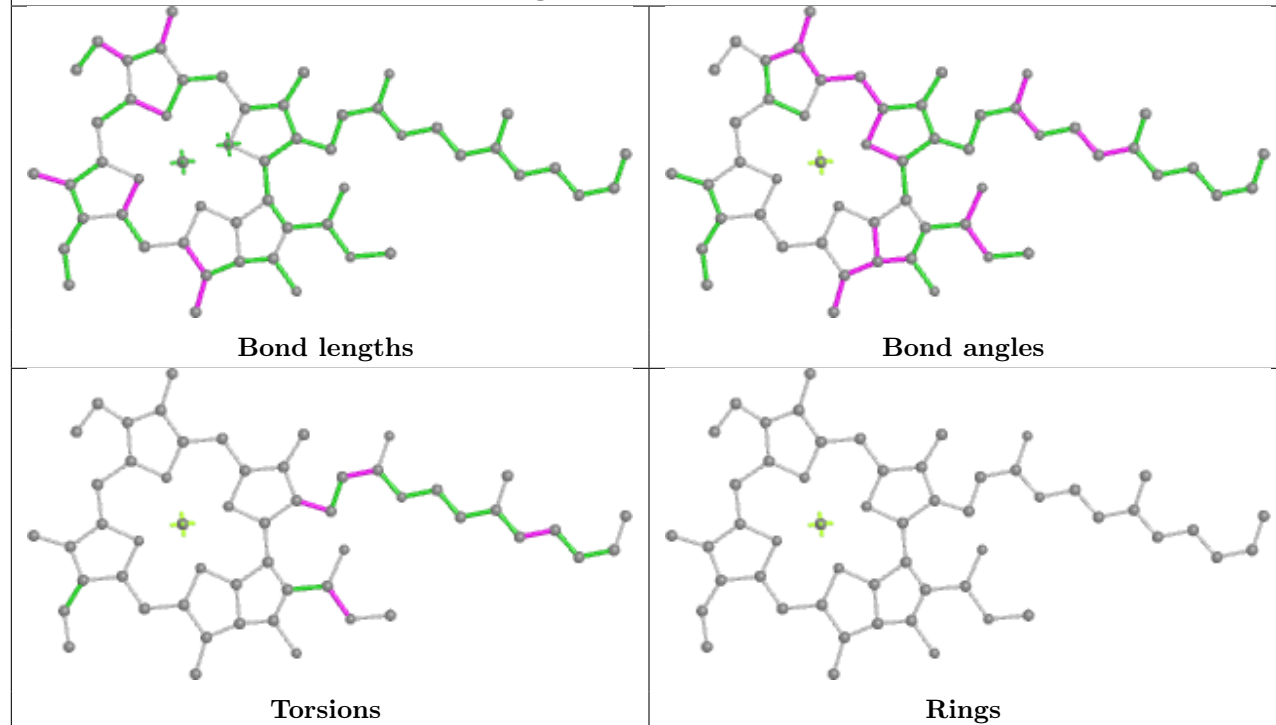
Ligand CLA B 3039

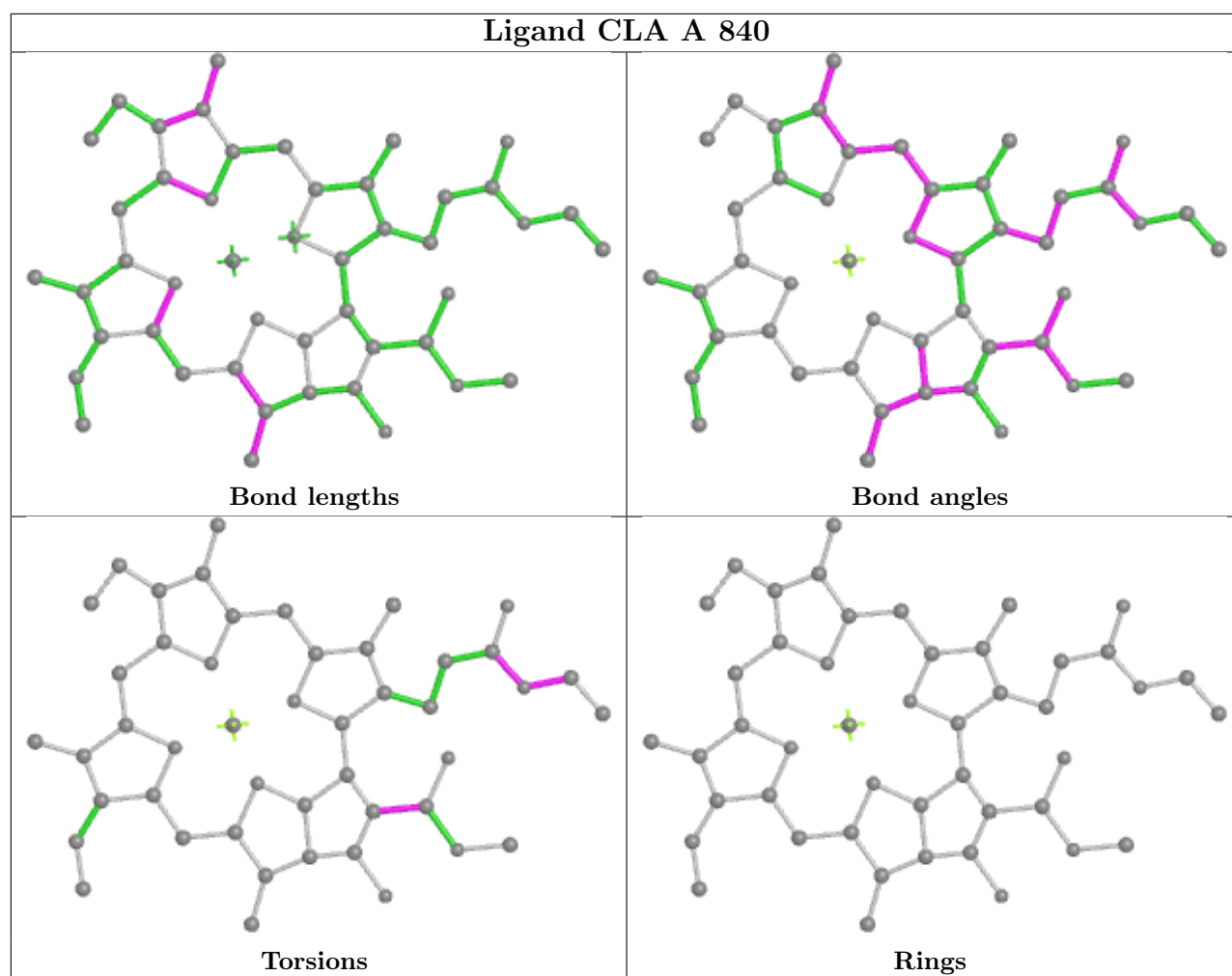


Ligand CLA A 834



Ligand CLA A 819





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	740/755 (98%)	-0.68	1 (0%) 95 89	17, 77, 124, 161	0
2	B	739/740 (99%)	-0.62	0 100 100	11, 52, 94, 129	0
3	C	80/80 (100%)	-0.69	0 100 100	13, 46, 70, 76	0
4	D	138/138 (100%)	-0.74	0 100 100	24, 57, 81, 127	0
5	E	69/75 (92%)	-0.91	0 100 100	48, 71, 92, 105	0
6	F	141/164 (85%)	-0.75	0 100 100	46, 94, 111, 118	0
7	I	38/38 (100%)	-0.46	0 100 100	14, 27, 55, 79	0
8	J	41/41 (100%)	-0.76	0 100 100	88, 105, 117, 132	0
9	K	47/83 (56%)	-0.54	0 100 100	113, 149, 164, 180	0
10	L	151/154 (98%)	-0.44	0 100 100	8, 26, 60, 110	0
11	M	31/31 (100%)	-0.54	0 100 100	26, 42, 64, 92	0
12	X	29/35 (82%)	-0.64	0 100 100	57, 78, 104, 118	0
All	All	2244/2334 (96%)	-0.65	1 (0%) 100 100	8, 61, 118, 180	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	ALA	2.1

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 ⓘ

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
17	LMG	I	102	40/55	0.83	0.33	49,85,120,144	0
14	CLA	M	102	45/65	0.84	0.30	83,131,166,180	0
18	LHG	M	101	49/49	0.85	0.36	47,89,164,181	0
16	BCR	K	102	40/40	0.87	0.44	107,147,166,175	0
17	LMG	A	855	30/55	0.87	0.27	32,83,145,162	0
16	BCR	A	848	40/40	0.88	0.57	77,119,171,177	0
16	BCR	J	105	40/40	0.88	0.40	67,114,154,161	0
16	BCR	A	847	40/40	0.89	0.44	96,131,161,175	0
16	BCR	J	104	40/40	0.89	0.31	78,116,145,150	0
17	LMG	A	852	48/55	0.89	0.36	56,113,152,160	0
21	LMT	L	202	35/35	0.89	0.28	74,142,179,192	0
22	DGD	L	207	66/66	0.90	0.25	45,99,155,168	0
16	BCR	B	3044	40/40	0.91	0.47	75,110,143,161	0
14	CLA	J	101	45/65	0.91	0.25	118,137,171,176	0
14	CLA	A	816	45/65	0.92	0.21	105,143,169,179	0
18	LHG	B	3050	23/49	0.92	0.18	73,111,139,145	0
14	CLA	K	101	41/65	0.92	0.17	112,149,185,194	0
14	CLA	K	103	45/65	0.92	0.23	101,132,164,166	0
17	LMG	B	3049	55/55	0.92	0.24	20,58,84,87	0
14	CLA	F	202	45/65	0.93	0.19	86,115,145,151	0
16	BCR	A	849	40/40	0.93	0.41	61,91,155,157	0
14	CLA	A	811	45/65	0.94	0.18	92,125,152,159	0
14	CLA	A	817	49/65	0.94	0.20	63,127,159,160	0
14	CLA	J	102	37/65	0.94	0.26	102,125,149,163	0
14	CLA	A	821	43/65	0.94	0.27	72,130,170,176	0
16	BCR	B	3046	40/40	0.94	0.36	43,76,131,143	0
16	BCR	B	3051	40/40	0.94	0.38	46,84,127,134	0
16	BCR	F	203	40/40	0.94	0.30	43,94,126,147	0
14	CLA	A	823	49/65	0.94	0.20	78,116,146,158	0
14	CLA	A	845	52/65	0.94	0.19	44,84,111,120	0
14	CLA	B	3022	45/65	0.95	0.21	67,93,119,120	0
16	BCR	B	3045	40/40	0.95	0.28	48,74,114,123	0
14	CLA	A	818	54/65	0.95	0.26	95,124,151,161	0
14	CLA	A	837	45/65	0.95	0.17	80,104,127,137	0
16	BCR	F	201	40/40	0.95	0.39	45,91,124,132	0
18	LHG	A	853	49/49	0.95	0.30	38,84,108,118	0
14	CLA	A	812	65/65	0.95	0.24	81,114,144,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
16	BCR	J	103	40/40	0.95	0.41	60,102,125,129	0
20	CA	B	3002	1/1	0.95	0.15	69,69,69,69	0
14	CLA	B	3020	65/65	0.95	0.31	48,91,121,132	0
16	BCR	A	850	40/40	0.95	0.36	41,74,108,125	0
14	CLA	A	808	51/65	0.96	0.20	81,103,130,133	0
14	CLA	B	3031	45/65	0.96	0.20	46,73,95,113	0
14	CLA	B	3032	49/65	0.96	0.22	34,69,97,122	0
16	BCR	B	3047	40/40	0.96	0.44	54,79,99,106	0
14	CLA	B	3034	58/65	0.96	0.28	63,98,137,141	0
14	CLA	B	3036	45/65	0.96	0.19	44,79,107,111	0
14	CLA	B	3037	45/65	0.96	0.19	64,88,120,121	0
14	CLA	B	3038	60/65	0.96	0.21	41,81,112,122	0
14	CLA	B	3039	65/65	0.96	0.28	42,88,128,143	0
14	CLA	A	826	65/65	0.96	0.25	71,100,131,134	0
14	CLA	A	828	65/65	0.96	0.24	59,93,128,135	0
16	BCR	M	103	40/40	0.96	0.23	21,48,76,82	0
14	CLA	A	819	54/65	0.96	0.20	61,94,116,132	0
14	CLA	A	813	54/65	0.96	0.20	74,100,128,136	0
14	CLA	B	3012	45/65	0.96	0.19	45,67,88,111	0
14	CLA	B	3013	45/65	0.96	0.17	57,89,115,119	0
14	CLA	X	1701	45/65	0.96	0.17	75,104,134,140	0
15	PQN	A	846	33/33	0.96	0.27	61,89,118,121	0
14	CLA	B	3015	65/65	0.96	0.28	45,77,112,117	0
14	CLA	B	3017	55/65	0.96	0.28	61,96,133,166	0
14	CLA	A	822	65/65	0.96	0.28	51,87,121,127	0
14	CLA	B	3021	47/65	0.96	0.21	69,98,129,135	0
14	CLA	L	206	65/65	0.97	0.23	21,46,75,85	0
14	CLA	A	807	65/65	0.97	0.25	56,84,110,116	0
14	CLA	A	856	65/65	0.97	0.24	38,65,91,102	0
13	CL0	A	801	65/65	0.97	0.22	2,46,71,74	0
14	CLA	A	810	65/65	0.97	0.24	44,99,148,161	0
14	CLA	A	820	65/65	0.97	0.25	65,100,125,134	0
14	CLA	B	3016	45/65	0.97	0.21	61,82,115,118	0
14	CLA	A	803	65/65	0.97	0.24	42,67,87,108	0
16	BCR	A	851	40/40	0.97	0.28	20,63,90,93	0
14	CLA	B	3018	59/65	0.97	0.24	47,81,109,117	0
14	CLA	A	804	65/65	0.97	0.27	59,98,125,132	0
14	CLA	A	805	59/65	0.97	0.21	75,98,125,141	0
14	CLA	A	824	51/65	0.97	0.22	67,101,132,138	0
14	CLA	B	3023	55/65	0.97	0.21	69,94,122,122	0
14	CLA	B	3027	65/65	0.97	0.25	38,65,91,97	0
14	CLA	B	3028	65/65	0.97	0.25	15,48,100,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	CLA	B	3029	65/65	0.97	0.23	27,61,79,97	0
14	CLA	A	825	59/65	0.97	0.30	49,83,123,135	0
14	CLA	A	814	60/65	0.97	0.28	73,115,140,141	0
14	CLA	A	827	65/65	0.97	0.30	29,68,145,167	0
14	CLA	B	3035	45/65	0.97	0.20	55,73,95,97	0
14	CLA	A	815	45/65	0.97	0.17	85,114,150,156	0
14	CLA	A	829	65/65	0.97	0.27	59,85,110,117	0
14	CLA	A	830	65/65	0.97	0.22	55,88,118,121	0
14	CLA	A	833	65/65	0.97	0.27	24,63,135,140	0
14	CLA	B	3040	47/65	0.97	0.21	49,74,93,105	0
18	LHG	A	854	27/49	0.97	0.21	46,79,116,117	0
14	CLA	A	836	54/65	0.97	0.26	47,87,128,136	0
14	CLA	A	806	65/65	0.97	0.24	67,101,136,142	0
14	CLA	A	839	65/65	0.97	0.26	21,59,97,120	0
14	CLA	A	840	47/65	0.97	0.22	22,55,75,93	0
14	CLA	A	844	65/65	0.97	0.24	2,17,50,59	0
14	CLA	B	3024	45/65	0.98	0.20	30,61,94,106	0
15	PQN	B	3043	33/33	0.98	0.24	27,47,66,70	0
14	CLA	B	3025	54/65	0.98	0.19	48,64,87,87	0
14	CLA	B	3026	46/65	0.98	0.21	36,64,89,90	0
14	CLA	B	3004	65/65	0.98	0.21	9,33,53,64	0
14	CLA	B	3005	54/65	0.98	0.20	23,48,67,74	0
14	CLA	B	3006	65/65	0.98	0.25	26,56,90,101	0
14	CLA	B	3030	65/65	0.98	0.23	20,47,80,98	0
14	CLA	B	3007	65/65	0.98	0.25	22,50,77,90	0
14	CLA	B	3008	65/65	0.98	0.24	10,35,66,89	0
14	CLA	B	3033	65/65	0.98	0.26	56,86,112,121	0
16	BCR	B	3048	40/40	0.98	0.24	14,34,61,61	0
14	CLA	B	3009	65/65	0.98	0.24	10,39,72,76	0
14	CLA	B	3010	65/65	0.98	0.22	5,38,66,90	0
14	CLA	B	3011	65/65	0.98	0.24	2,24,59,69	0
16	BCR	I	101	40/40	0.98	0.24	2,28,50,68	0
14	CLA	A	838	51/65	0.98	0.20	36,59,79,102	0
14	CLA	A	832	50/65	0.98	0.21	33,61,91,117	0
14	CLA	B	3014	65/65	0.98	0.21	42,72,99,102	0
14	CLA	A	809	65/65	0.98	0.28	38,84,123,129	0
16	BCR	L	201	40/40	0.98	0.24	2,34,59,61	0
16	BCR	L	208	40/40	0.98	0.27	3,28,48,65	0
16	BCR	L	209	40/40	0.98	0.24	2,38,86,98	0
14	CLA	B	3041	65/65	0.98	0.22	2,18,52,58	0
14	CLA	B	3042	65/65	0.98	0.25	4,29,52,55	0
14	CLA	A	841	65/65	0.98	0.24	32,69,123,132	0

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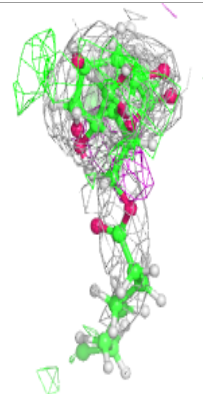
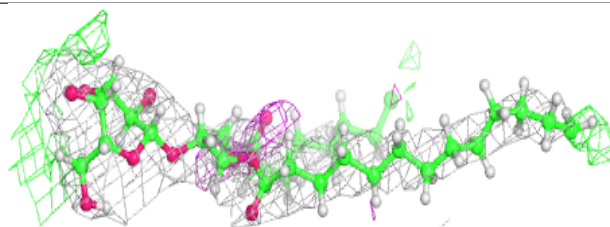
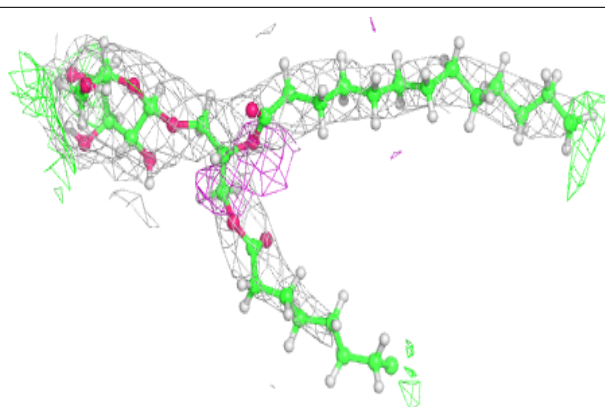
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	CLA	A	842	51/65	0.98	0.26	36,75,124,143	0
14	CLA	A	843	65/65	0.98	0.27	37,73,117,135	0
14	CLA	B	3019	60/65	0.98	0.25	49,70,100,107	0
14	CLA	A	834	65/65	0.98	0.24	10,37,65,71	0
14	CLA	L	204	65/65	0.98	0.23	11,41,72,93	0
14	CLA	L	205	65/65	0.98	0.25	8,45,117,130	0
14	CLA	A	802	65/65	0.98	0.21	20,38,54,75	0
14	CLA	A	831	65/65	0.98	0.25	55,87,110,118	0
14	CLA	B	3003	65/65	0.98	0.23	16,49,70,76	0
20	CA	L	203	1/1	0.99	0.19	27,27,27,27	0
19	SF4	B	3001	8/8	0.99	0.30	29,46,88,118	0
14	CLA	A	835	65/65	0.99	0.23	2,32,62,90	0
19	SF4	C	101	8/8	1.00	0.29	23,51,58,71	0
19	SF4	C	102	8/8	1.00	0.28	38,45,62,64	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.

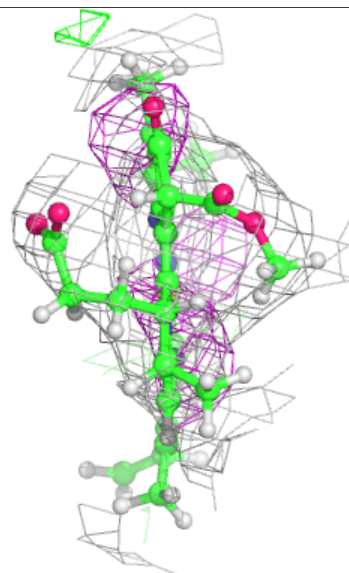
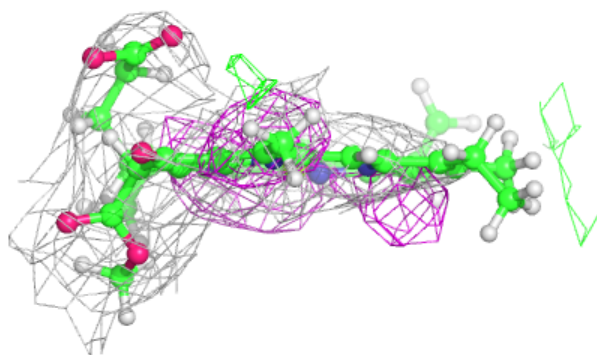
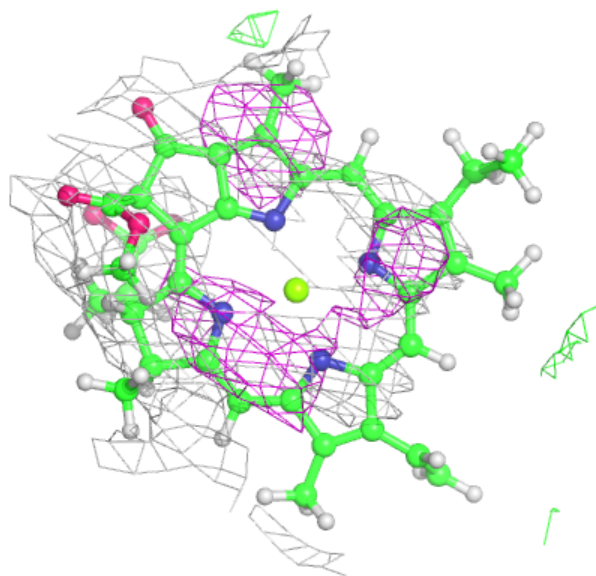
Electron density around LMG I 102:

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



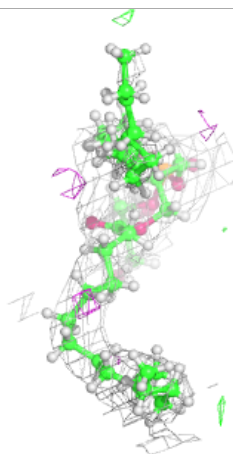
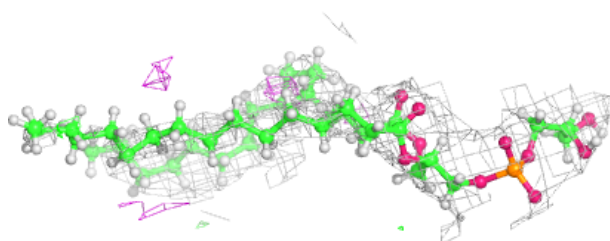
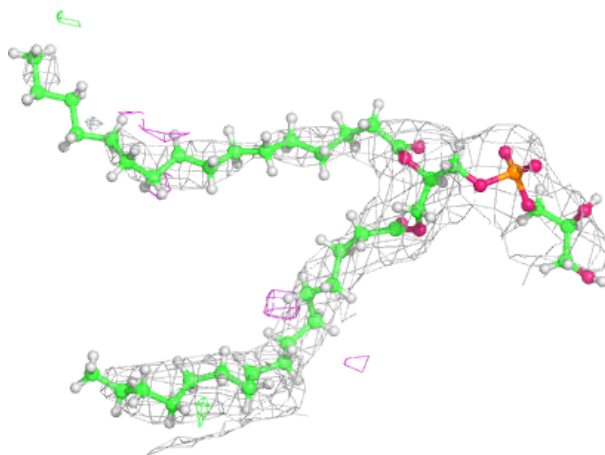
Electron density around CLA M 102:

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



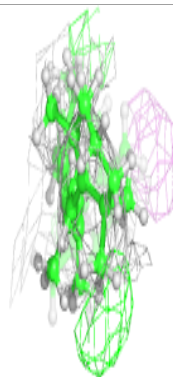
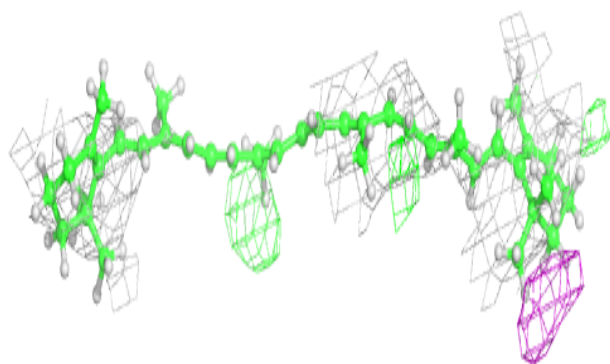
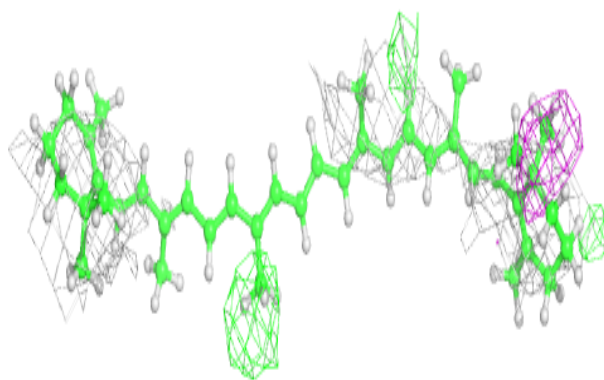
Electron density around LHG M 101:

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

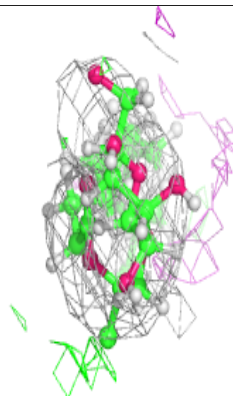
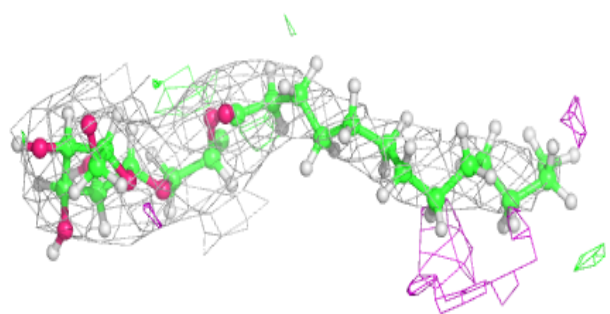
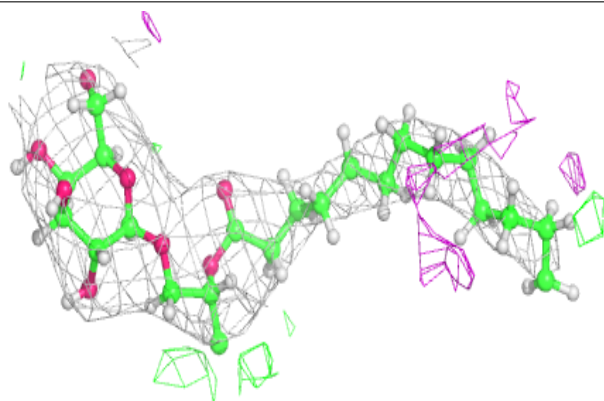


Electron density around BCR K 102:

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

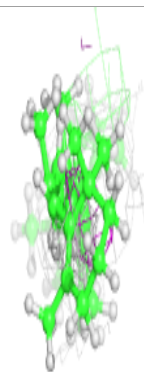
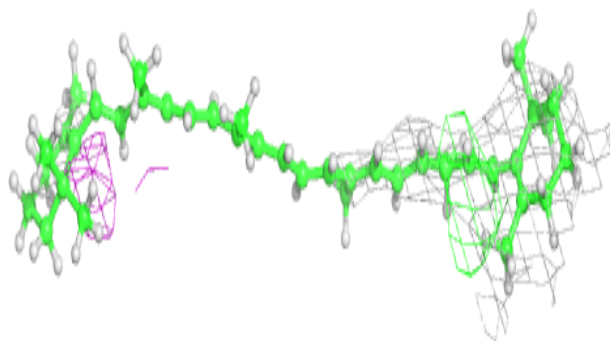
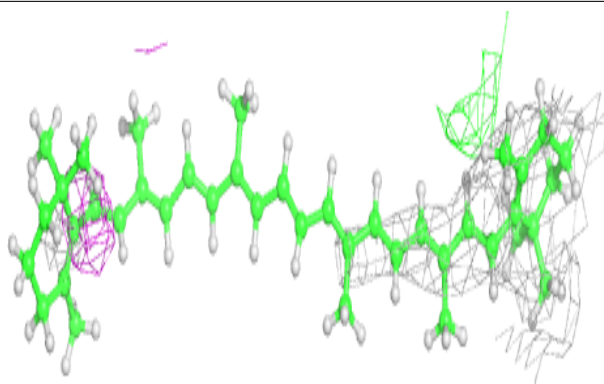
**Electron density around LMG A 855:**

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

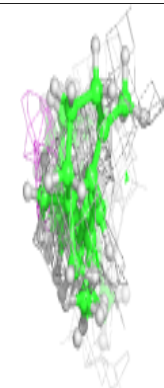
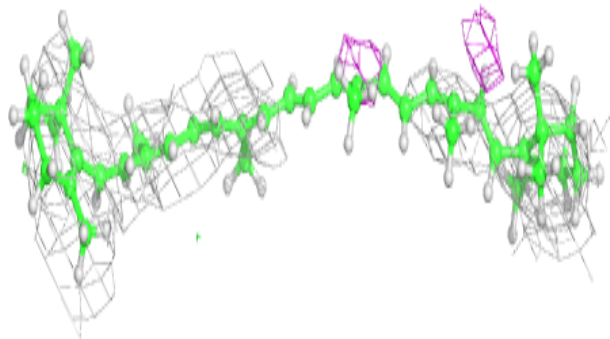
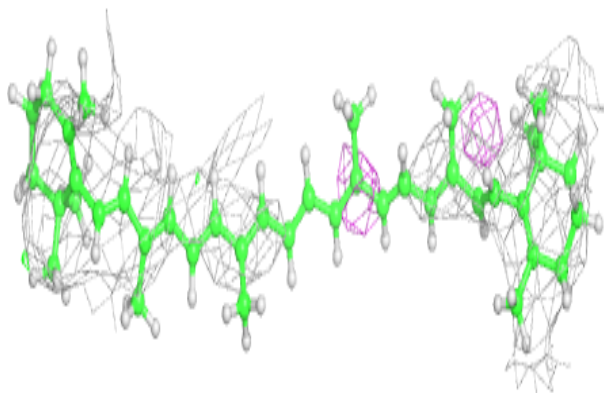


Electron density around BCR A 848:

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

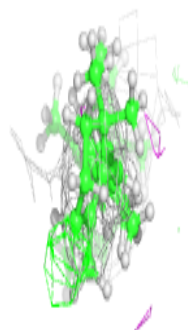
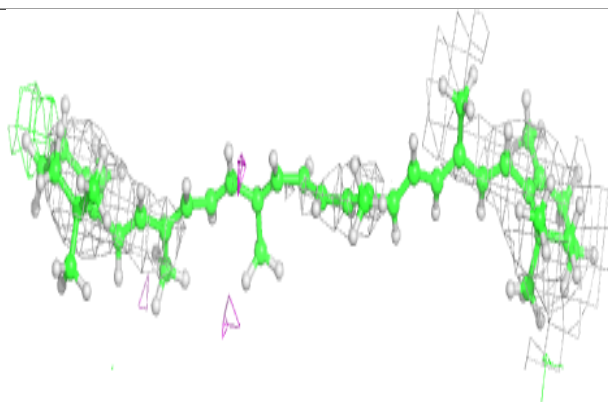
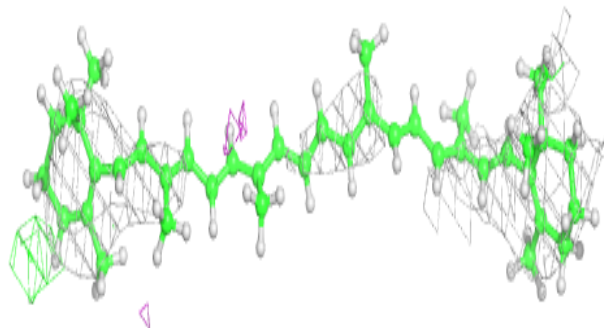
**Electron density around BCR J 105:**

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

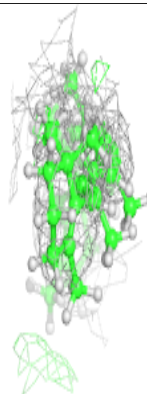
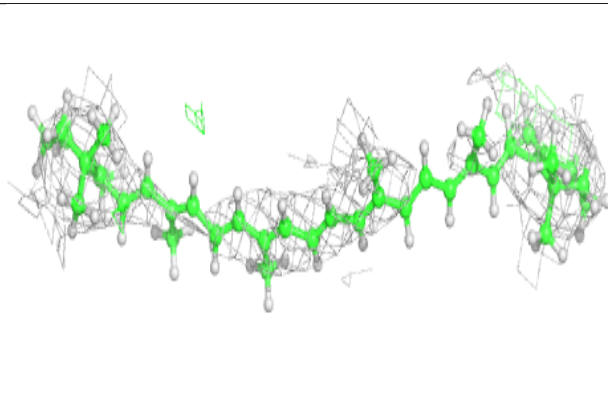
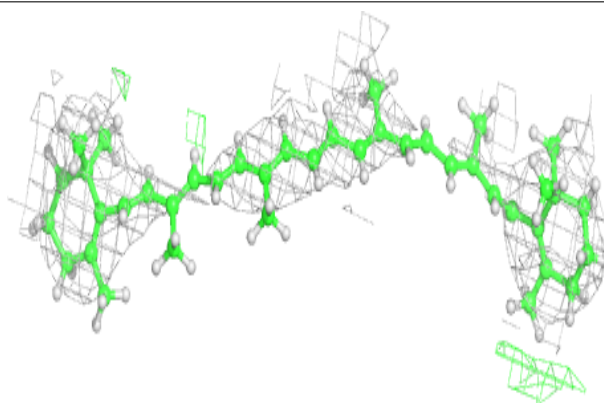


Electron density around BCR A 847:

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

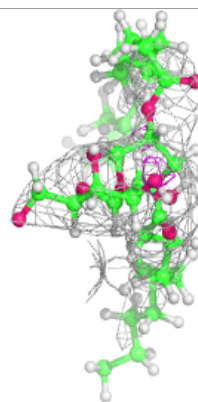
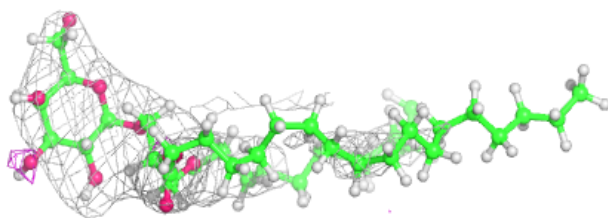
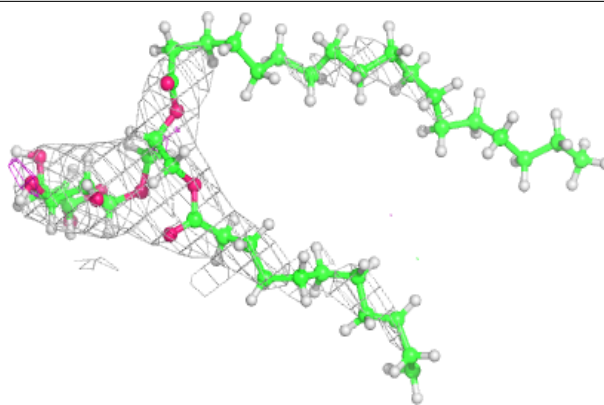
**Electron density around BCR J 104:**

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

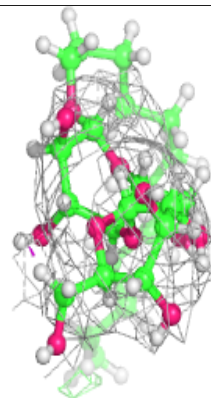
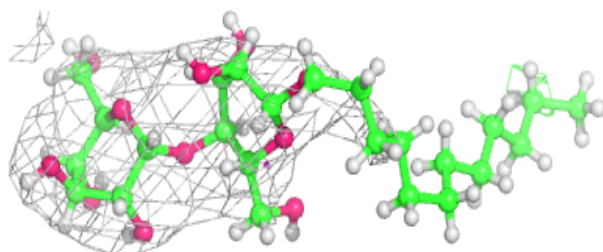
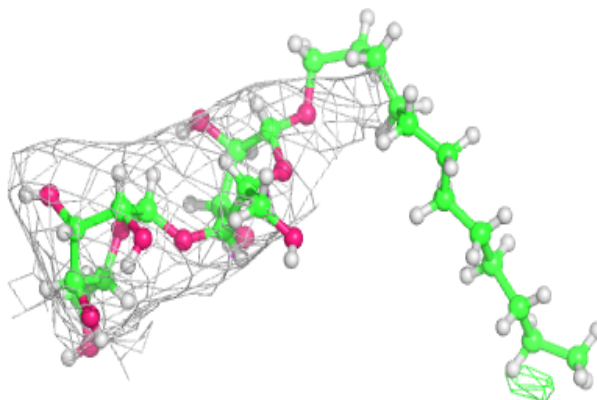


Electron density around LMG A 852:

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and green (positive)

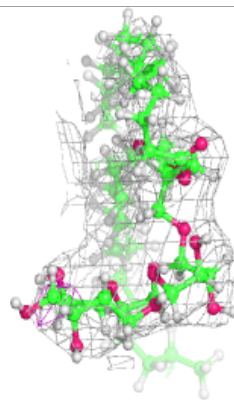
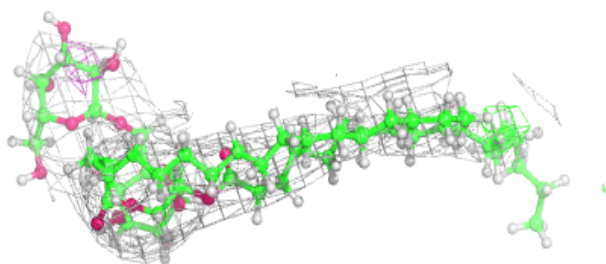
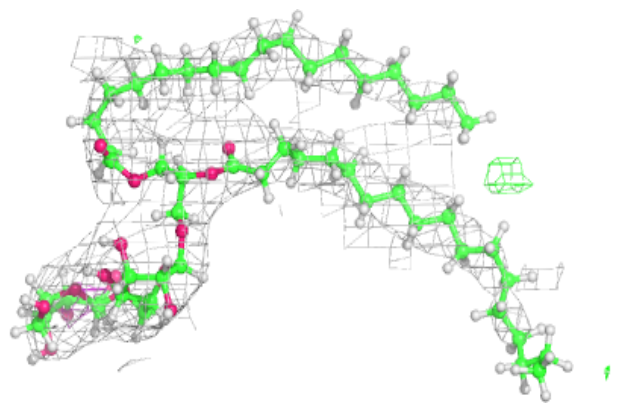
**Electron density around LMT L 202:**

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

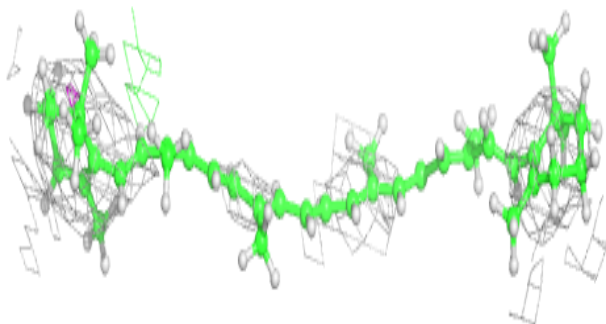
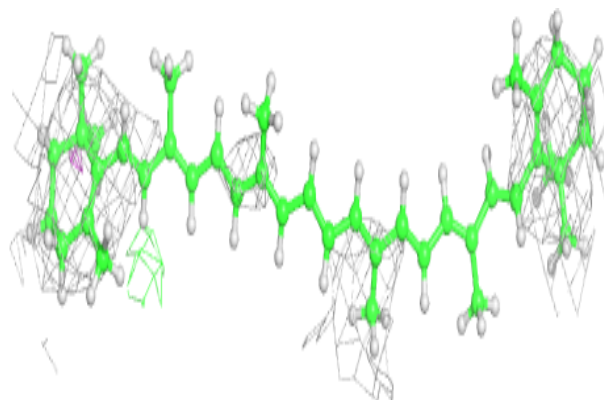


Electron density around DGD L 207:

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

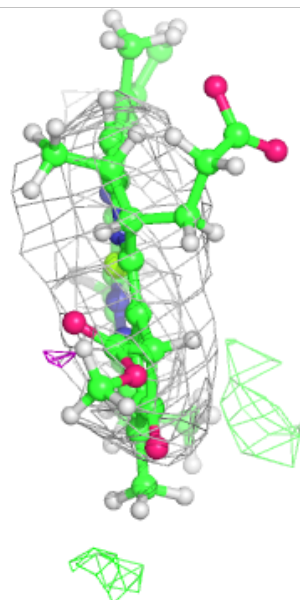
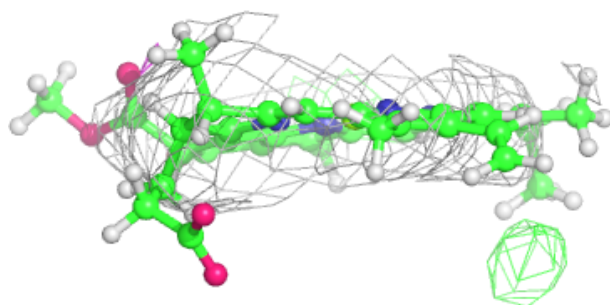
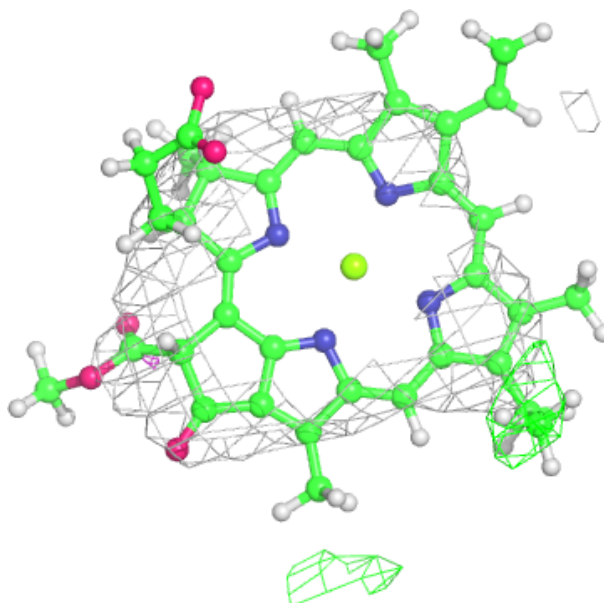
**Electron density around BCR B 3044:**

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



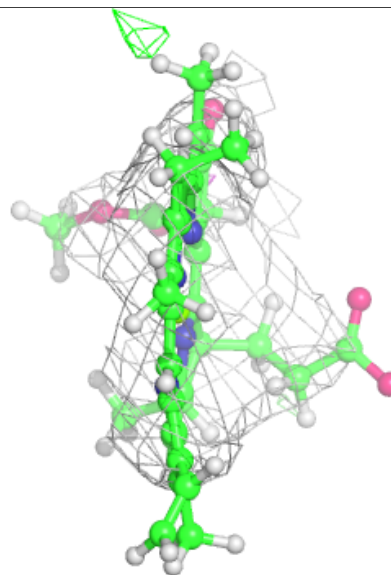
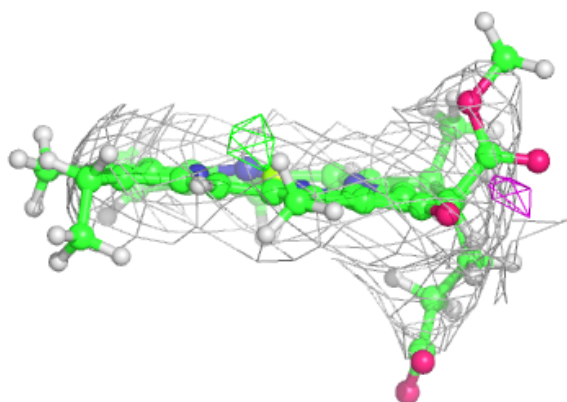
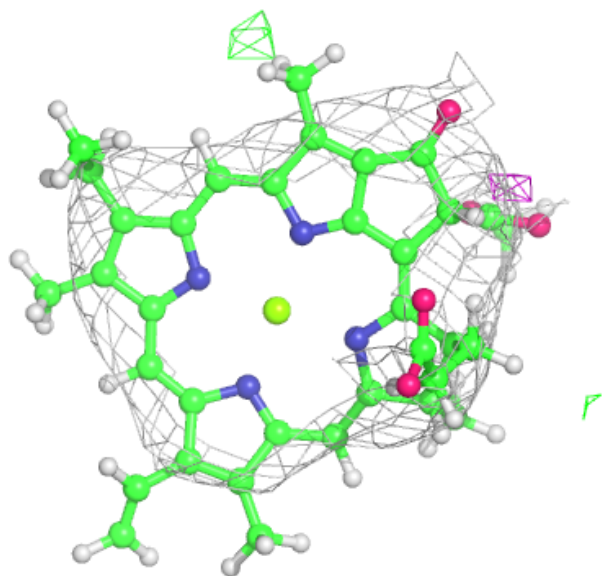
Electron density around CLA J 101:

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



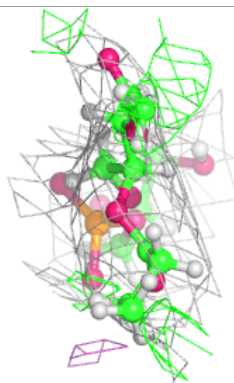
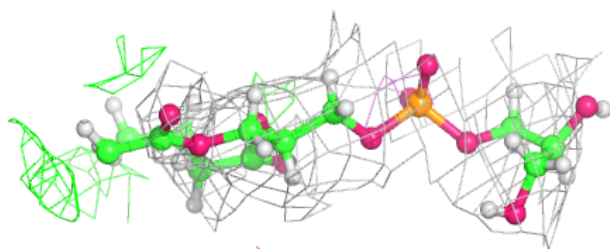
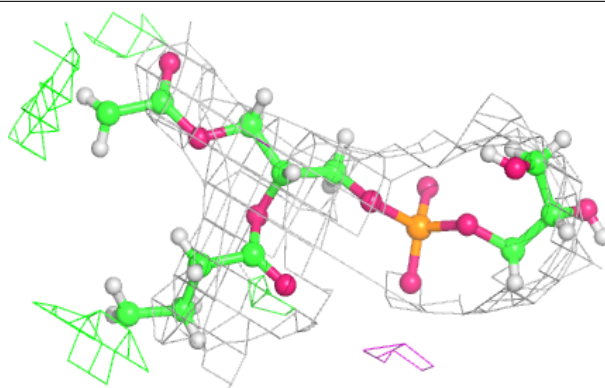
Electron density around CLA A 816:

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



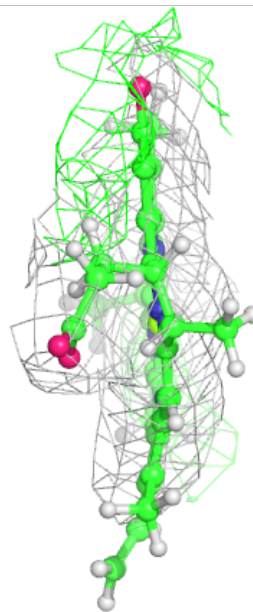
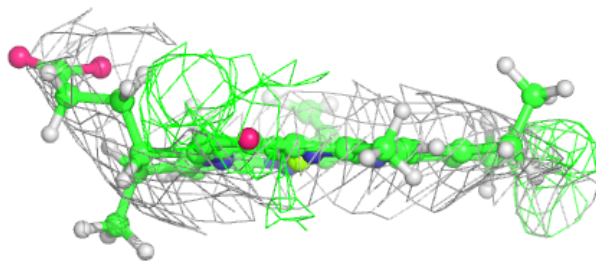
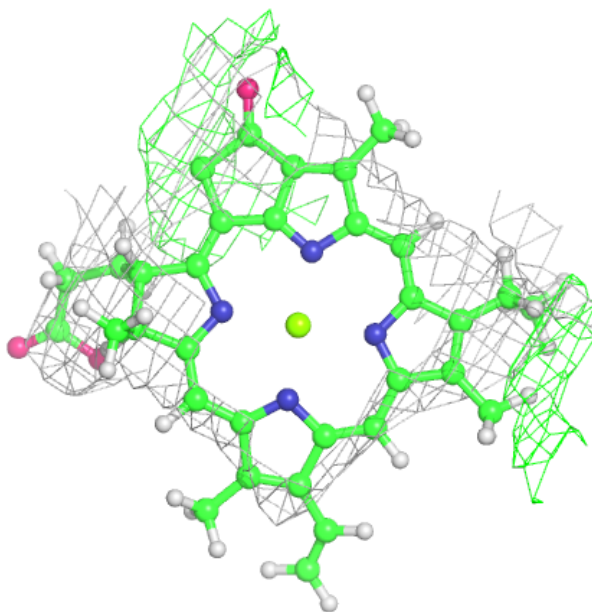
Electron density around LHG B 3050:

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



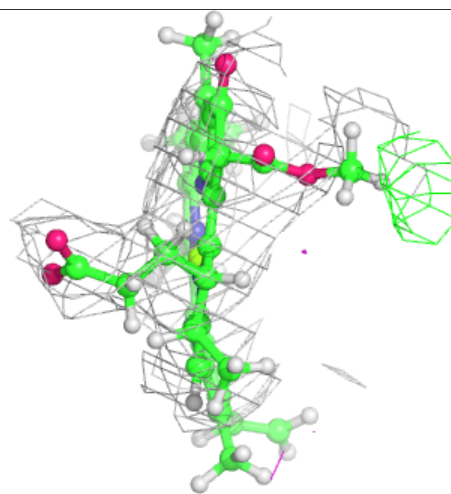
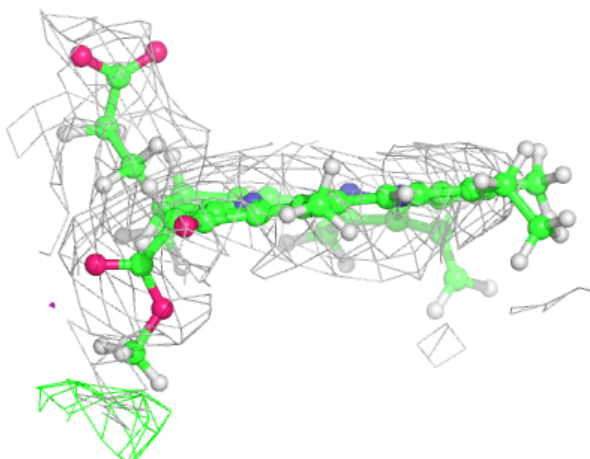
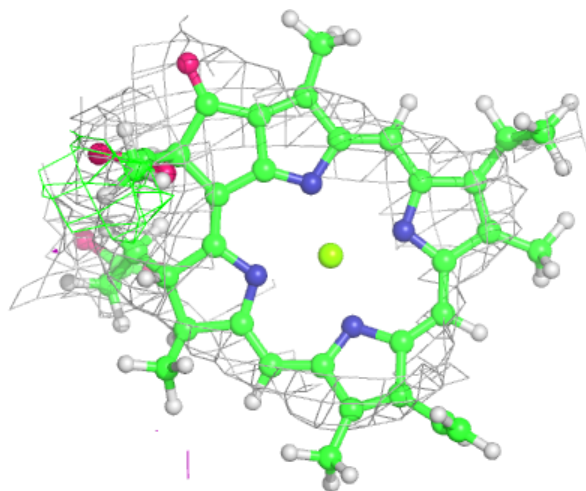
Electron density around CLA K 101:

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and green (positive)



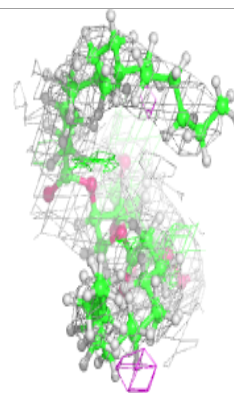
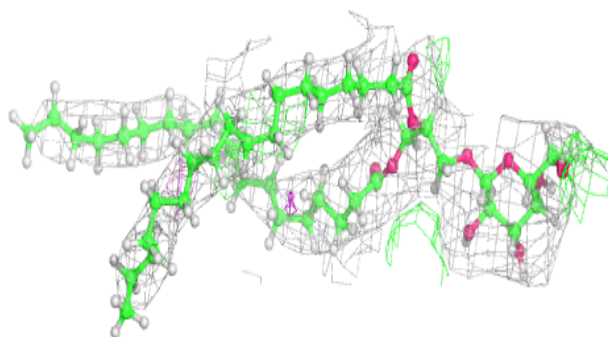
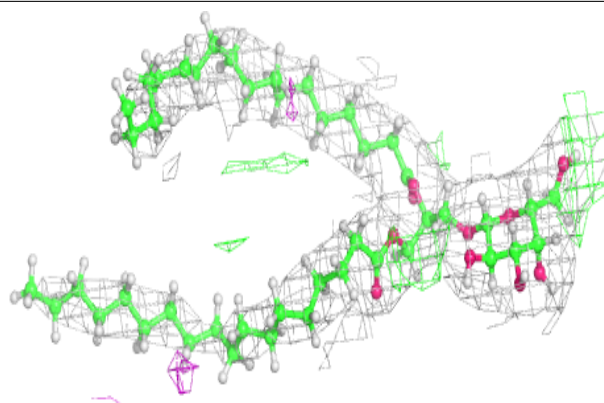
Electron density around CLA K 103:

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and green (positive)



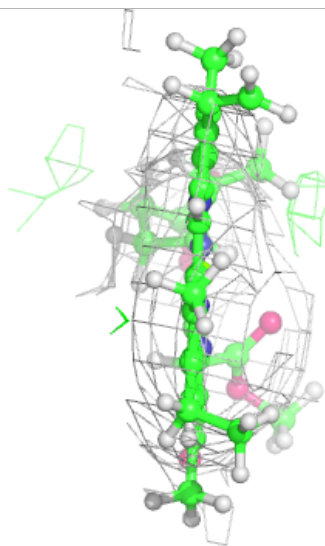
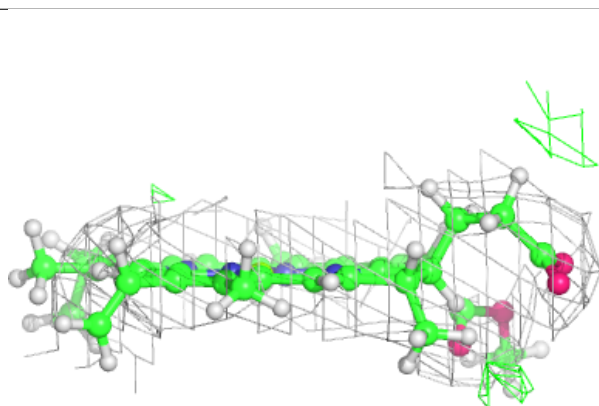
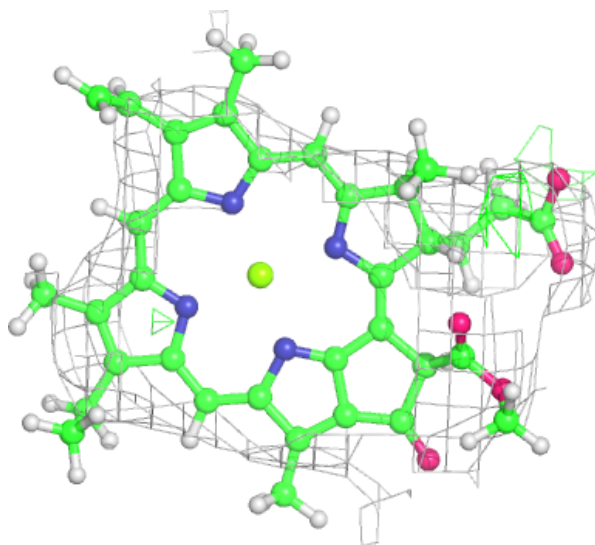
Electron density around LMG B 3049:

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and green (positive)



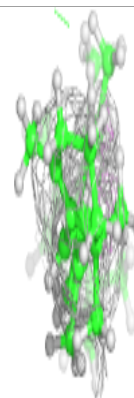
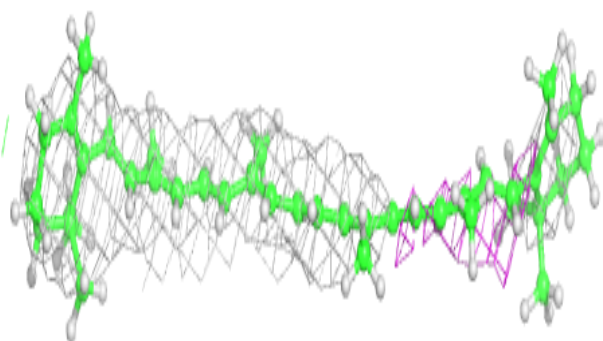
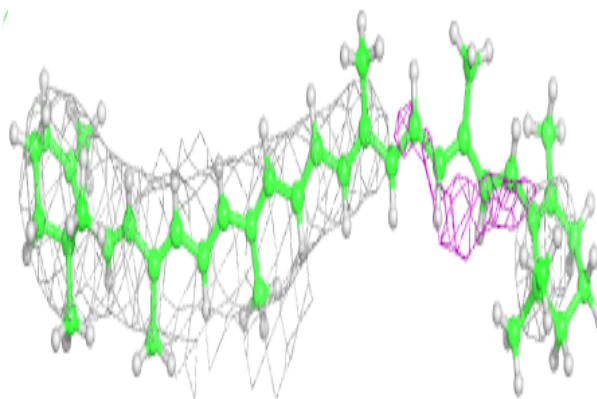
Electron density around CLA F 202:

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



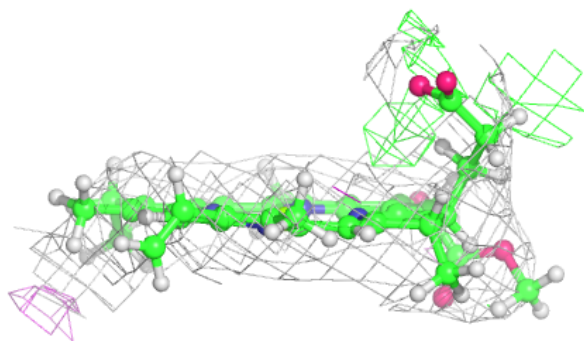
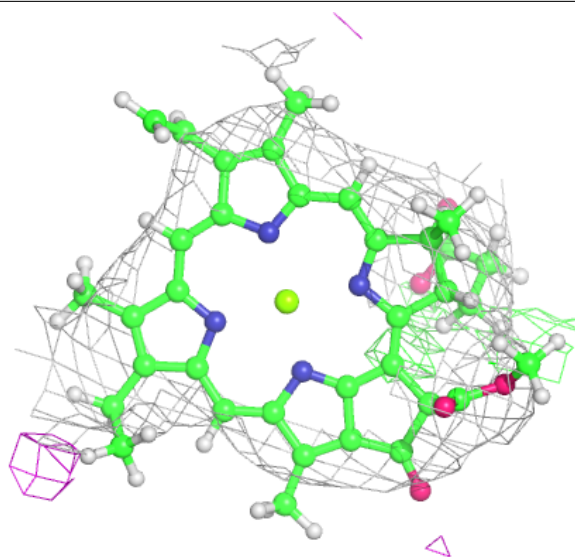
Electron density around BCR A 849:

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



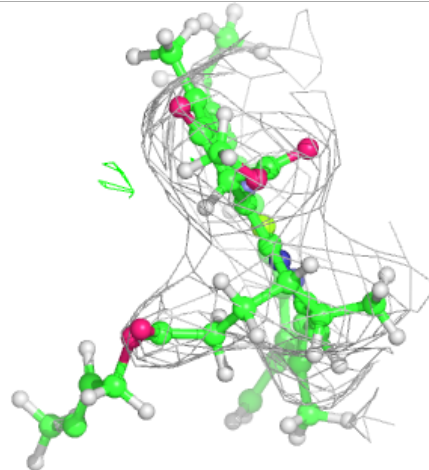
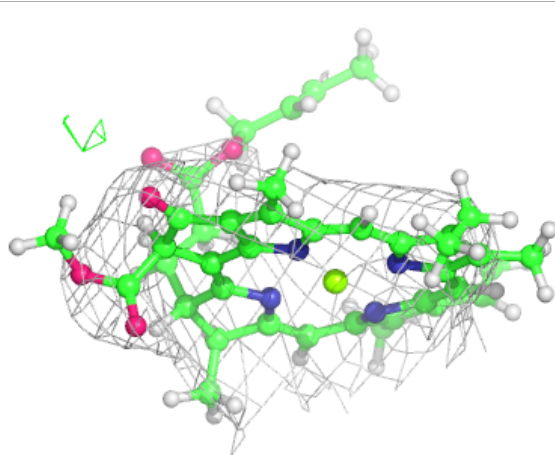
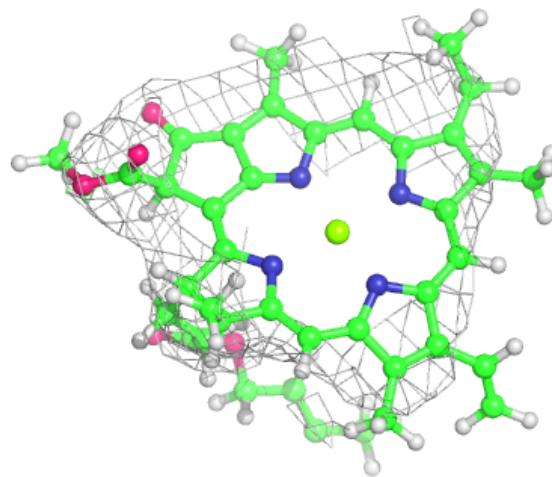
Electron density around CLA A 811:

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and green (positive)



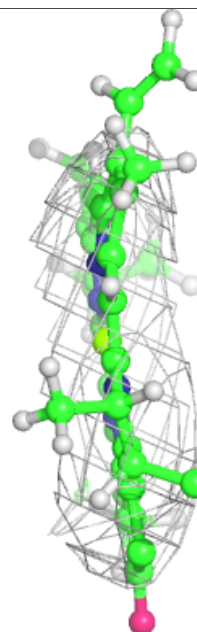
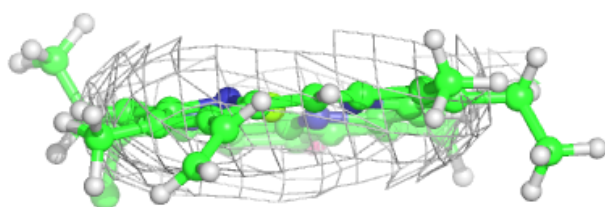
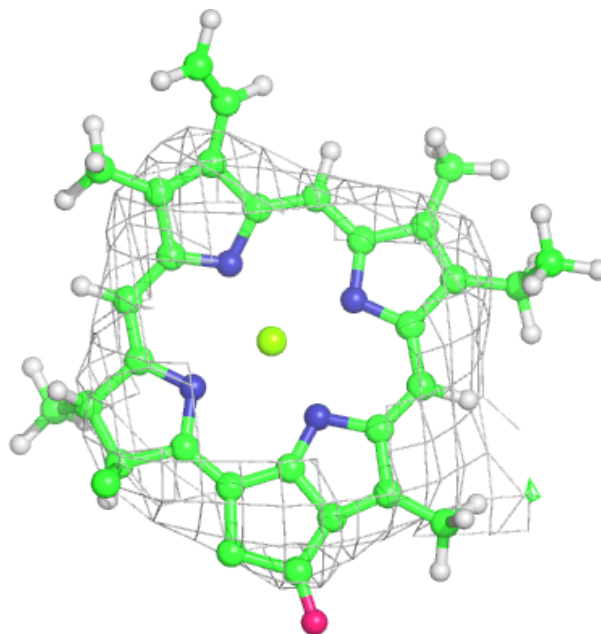
Electron density around CLA A 817:

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



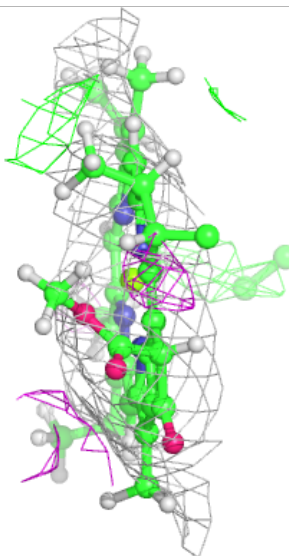
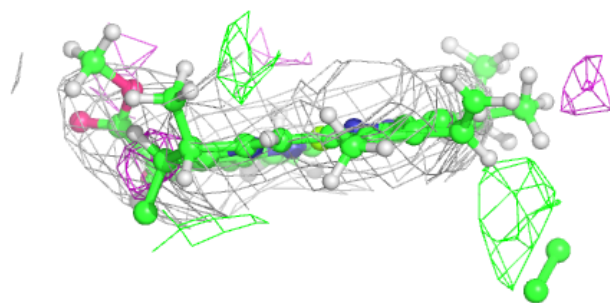
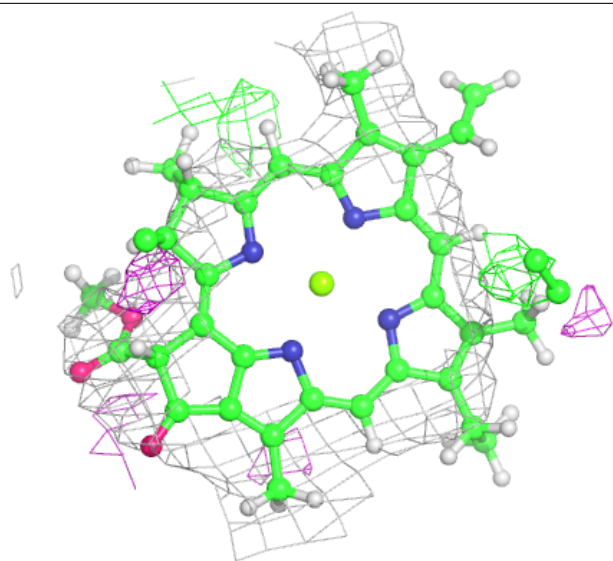
Electron density around CLA J 102:

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



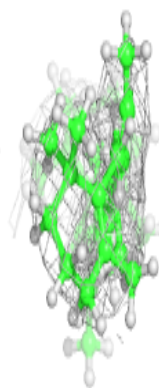
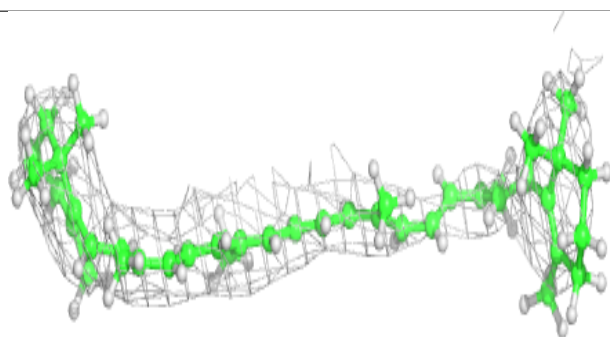
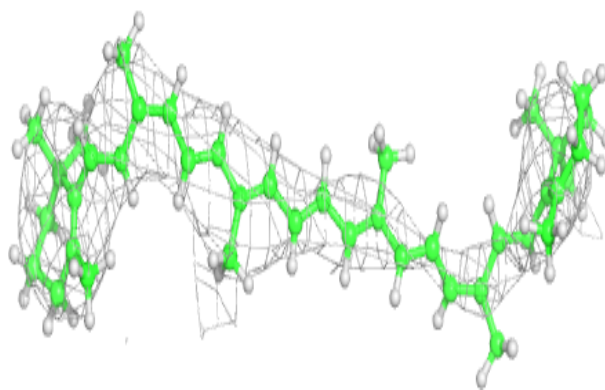
Electron density around CLA A 821:

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

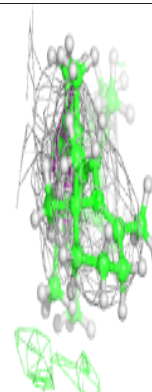
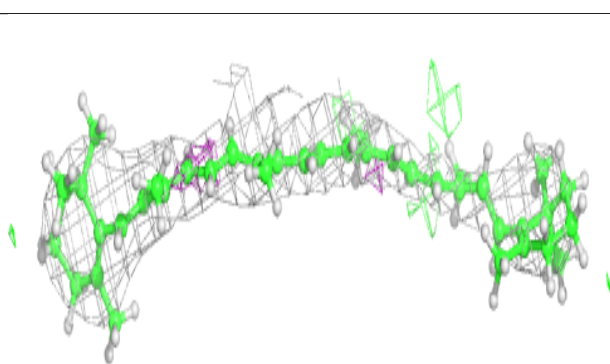
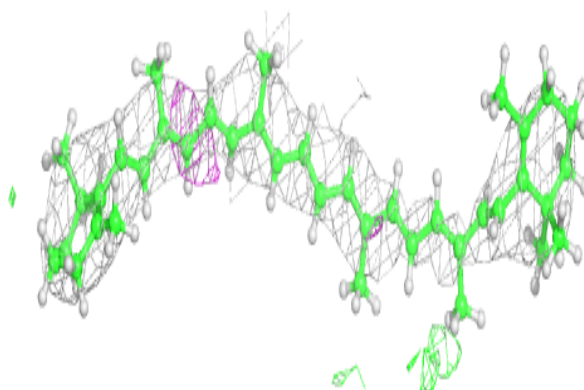


Electron density around BCR B 3046:

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

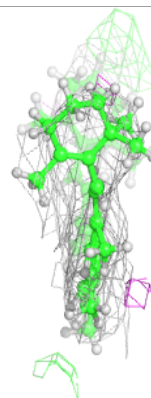
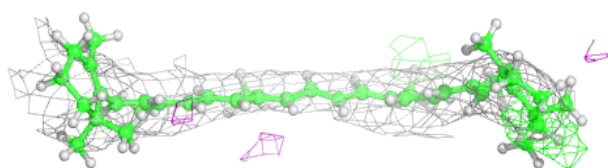
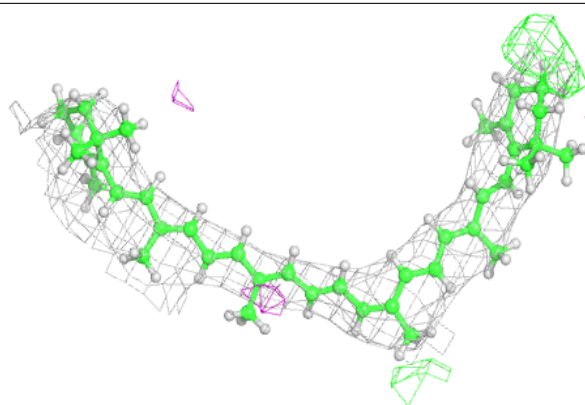
**Electron density around BCR B 3051:**

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



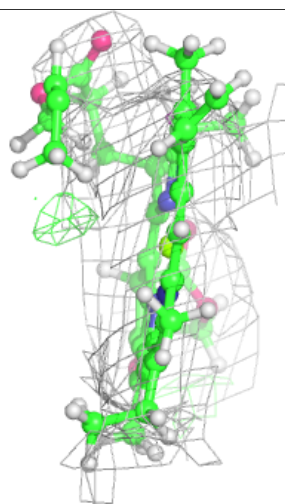
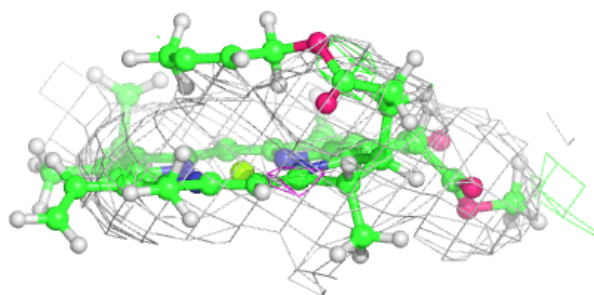
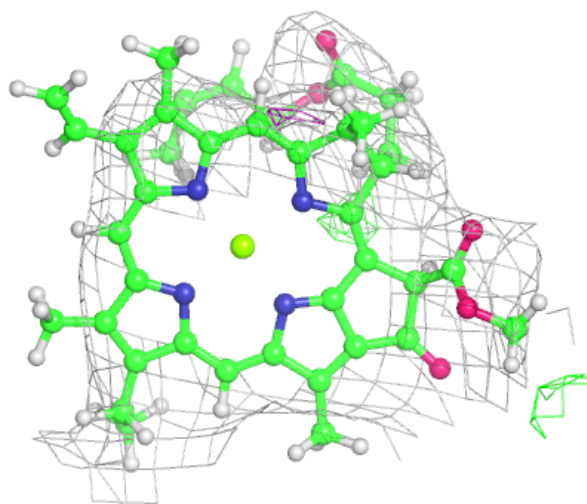
Electron density around BCR F 203:

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



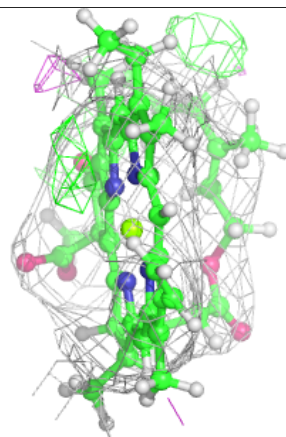
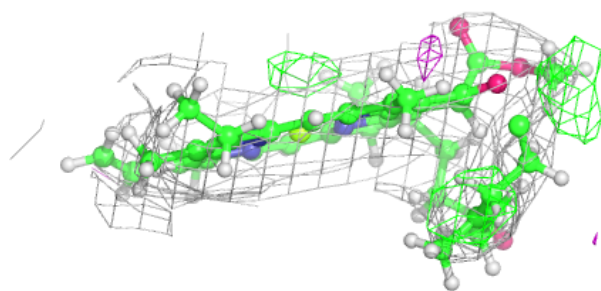
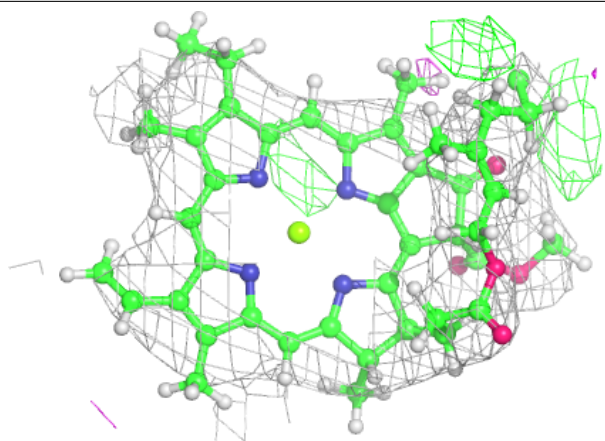
Electron density around CLA A 823:

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



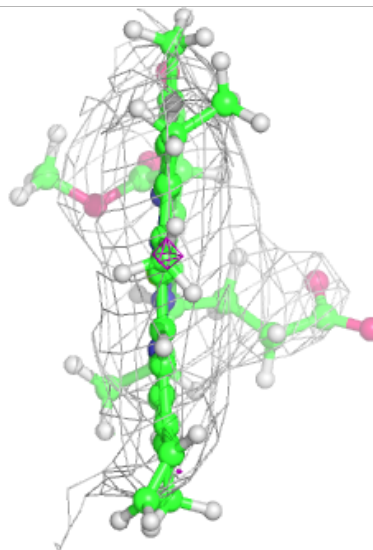
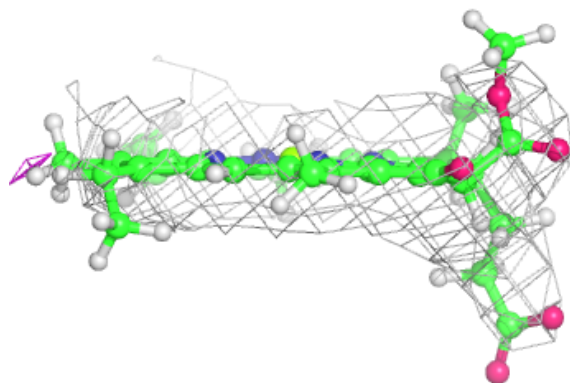
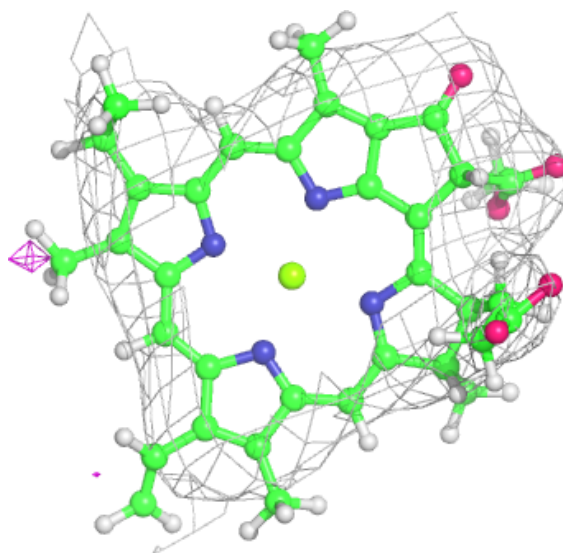
Electron density around CLA A 845:

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



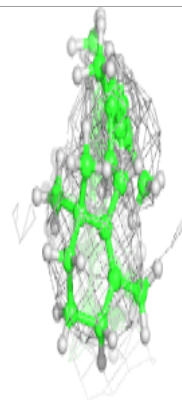
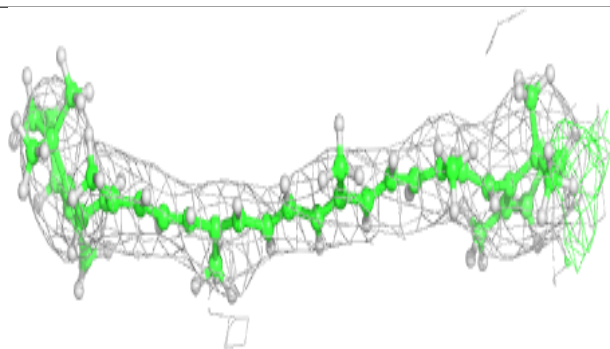
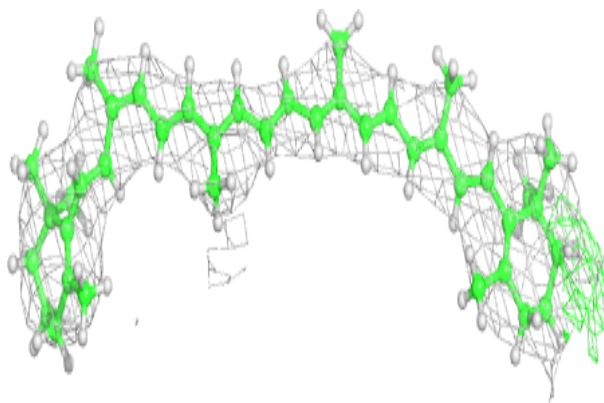
Electron density around CLA B 3022:

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



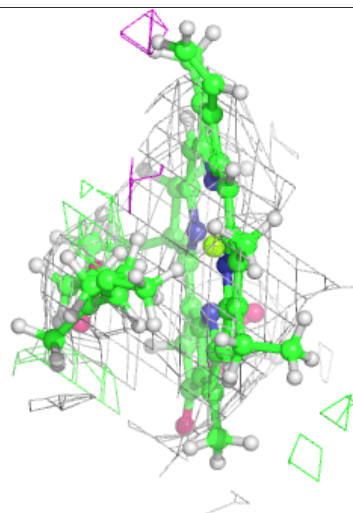
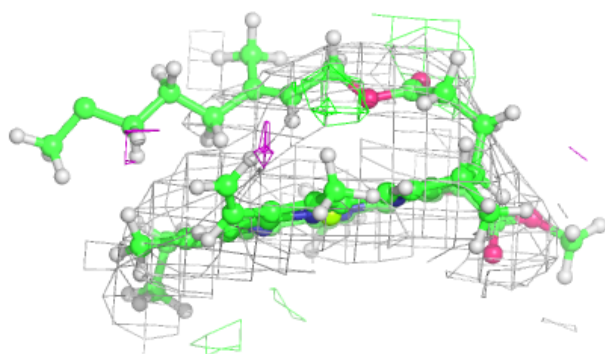
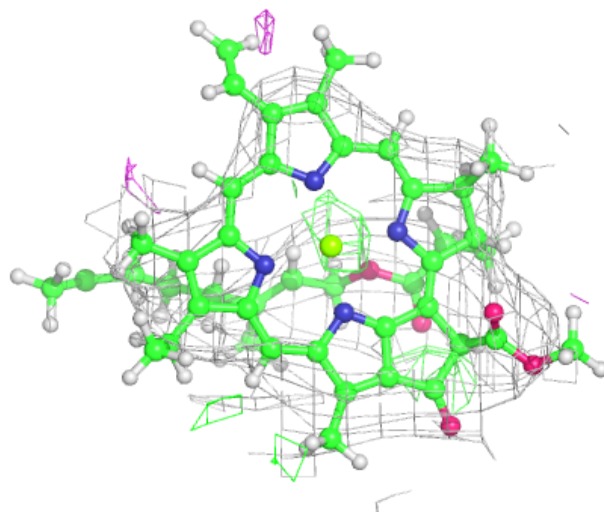
Electron density around BCR B 3045:

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



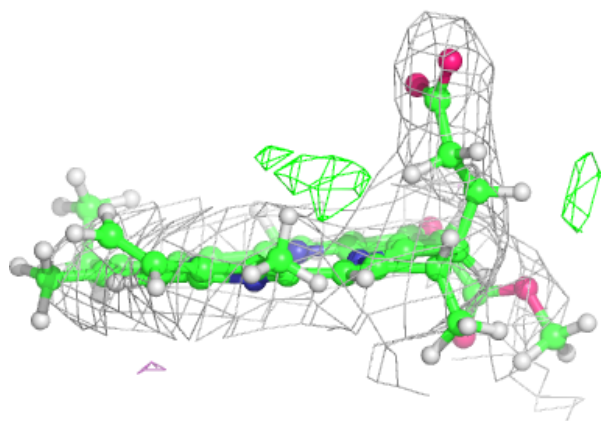
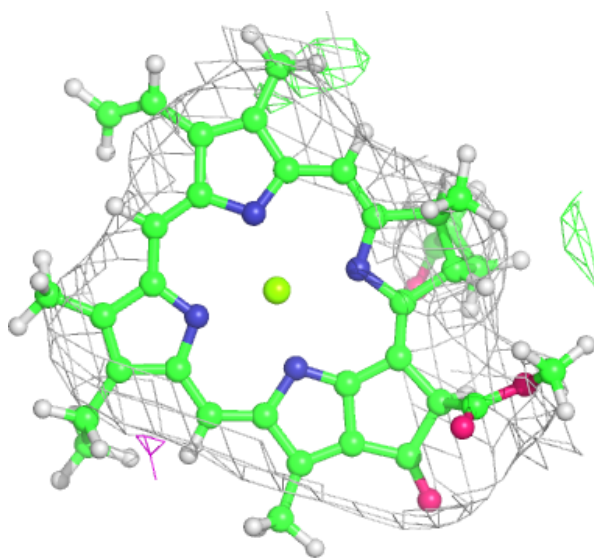
Electron density around CLA A 818:

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



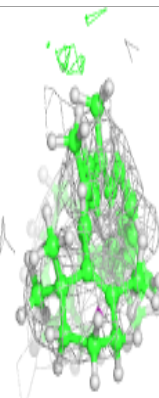
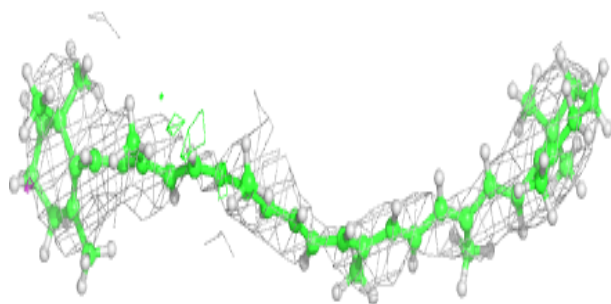
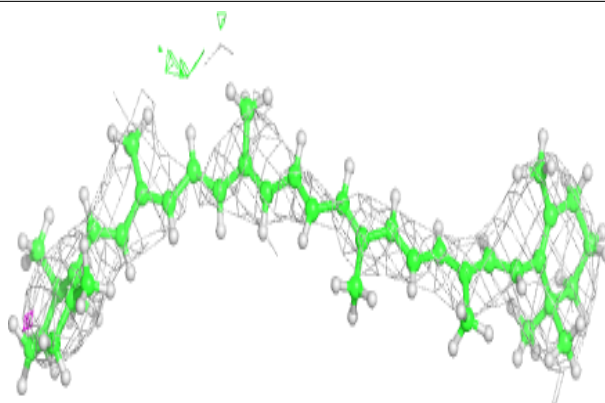
Electron density around CLA A 837:

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

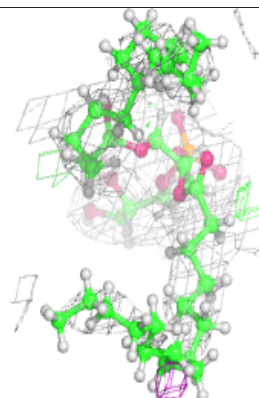
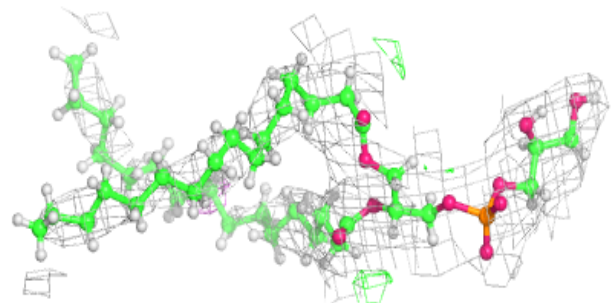
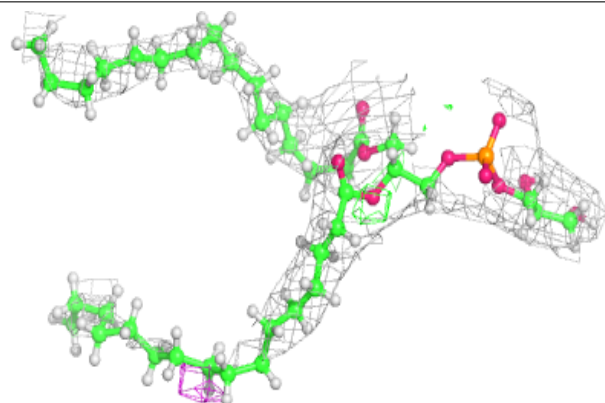


Electron density around BCR F 201:

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

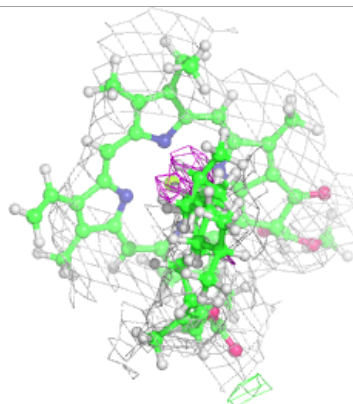
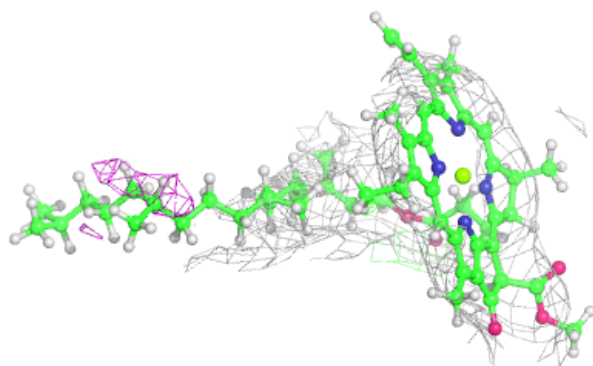
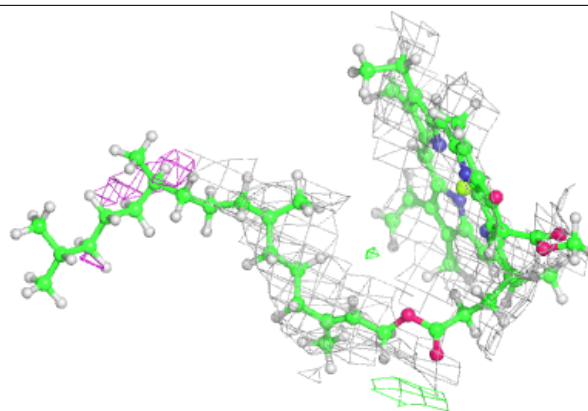
**Electron density around LHG A 853:**

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

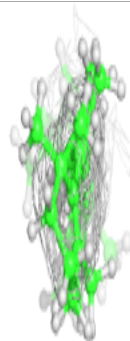
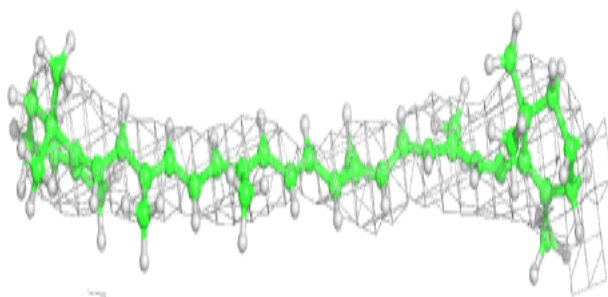
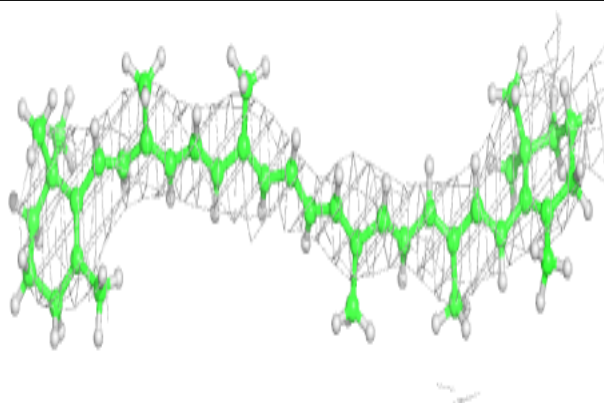


Electron density around CLA A 812:

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

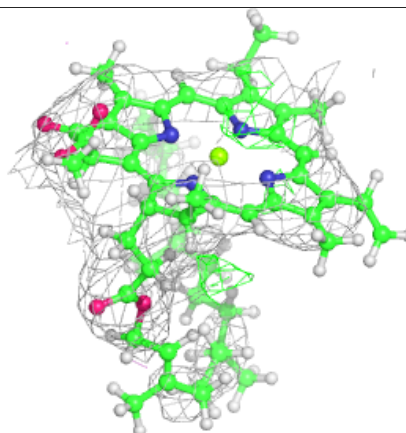
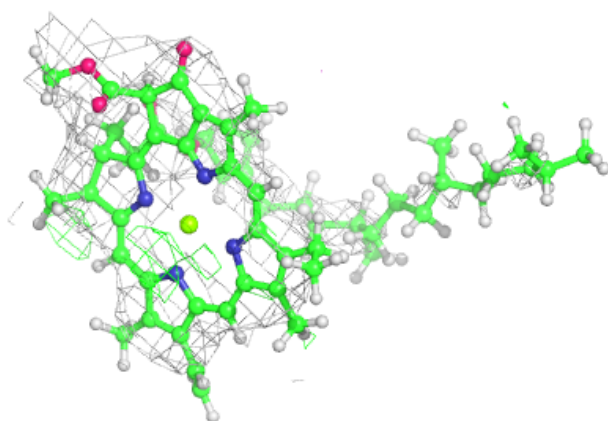
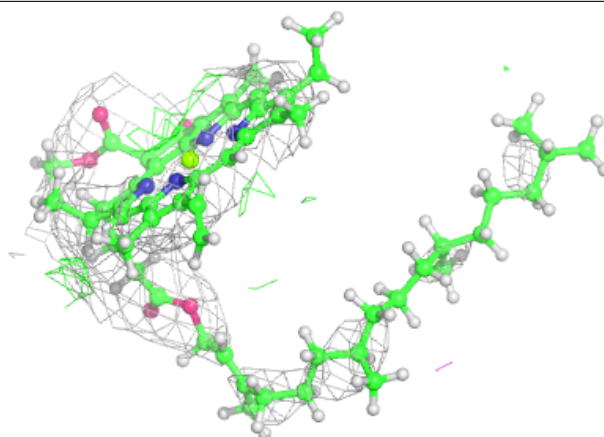
**Electron density around BCR J 103:**

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

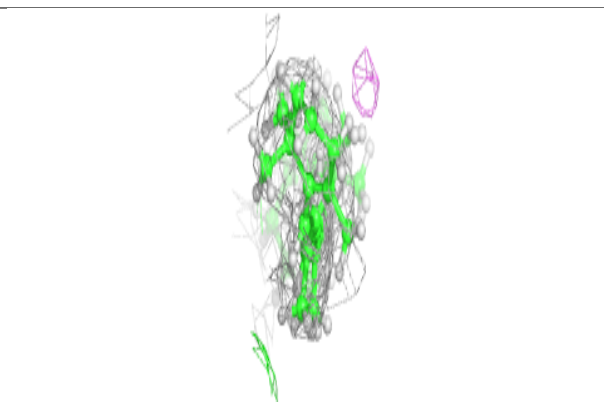
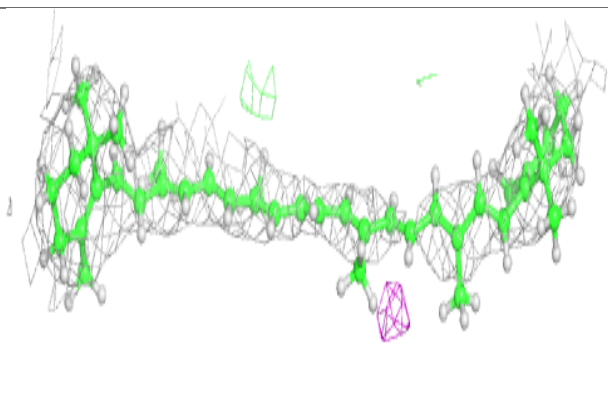
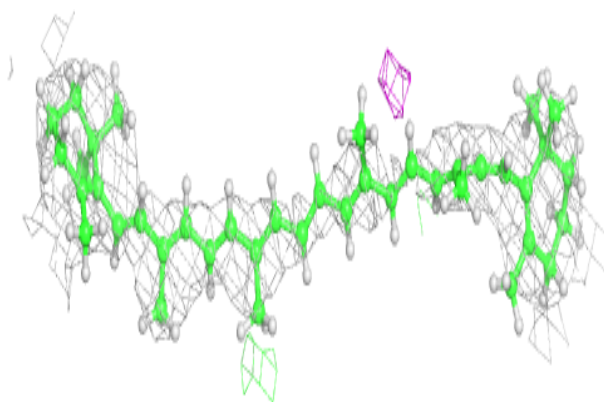


Electron density around CLA B 3020:

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

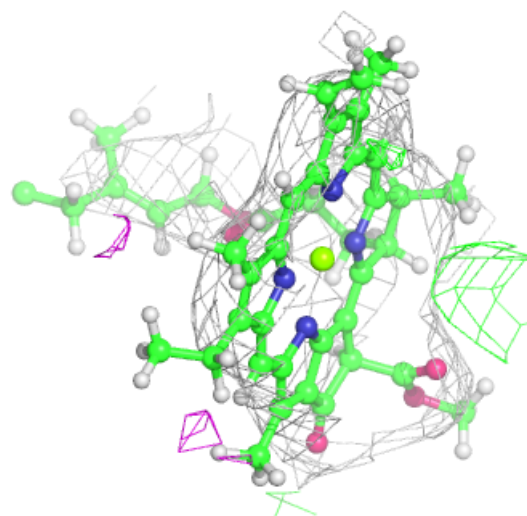
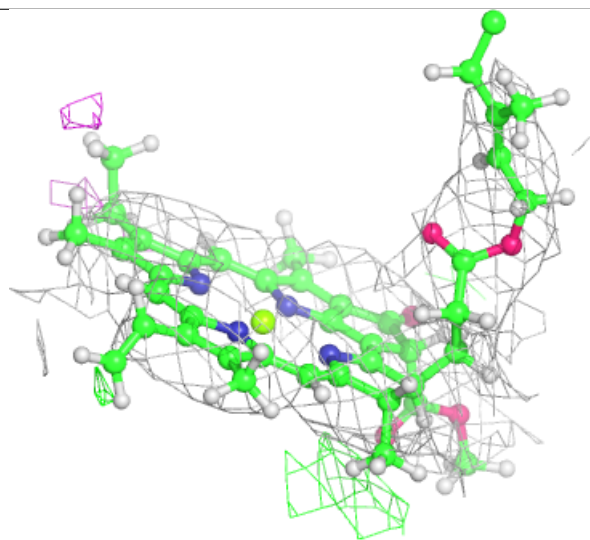
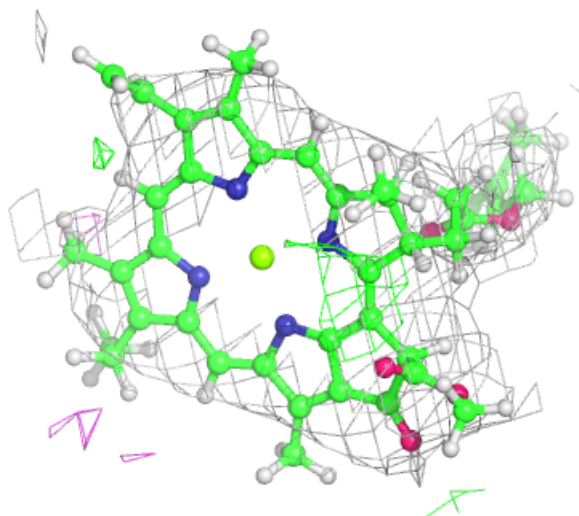
**Electron density around BCR A 850:**

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



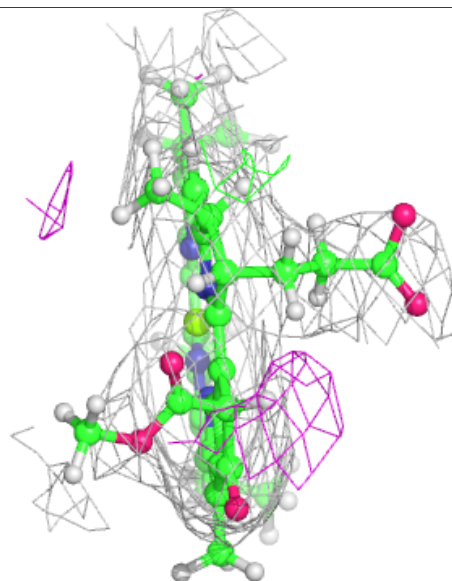
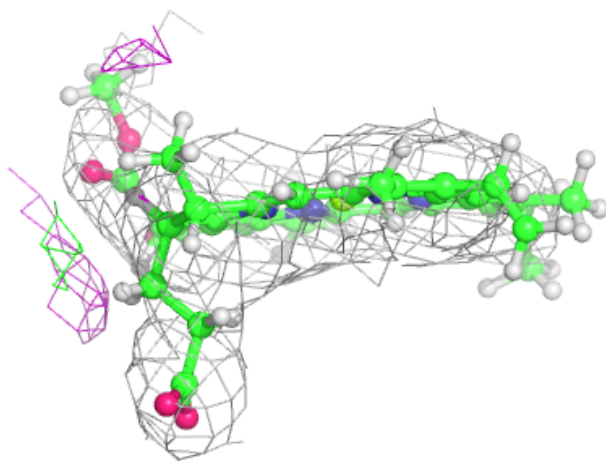
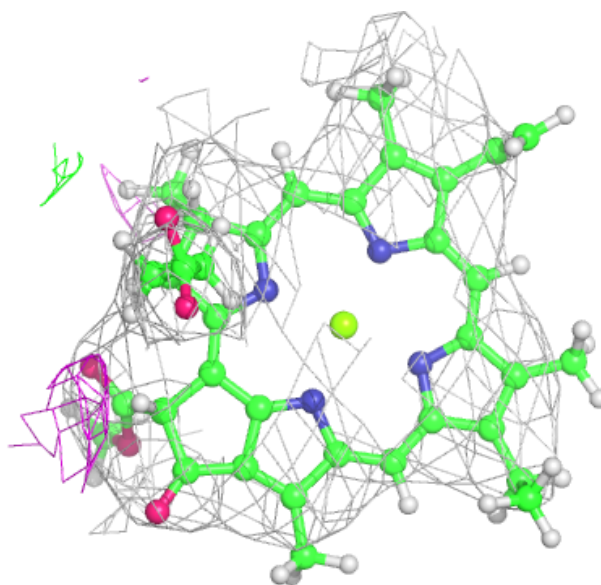
Electron density around CLA A 808:

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



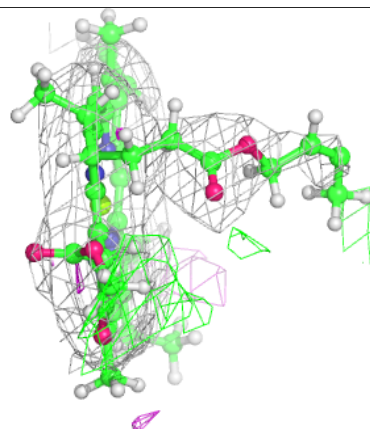
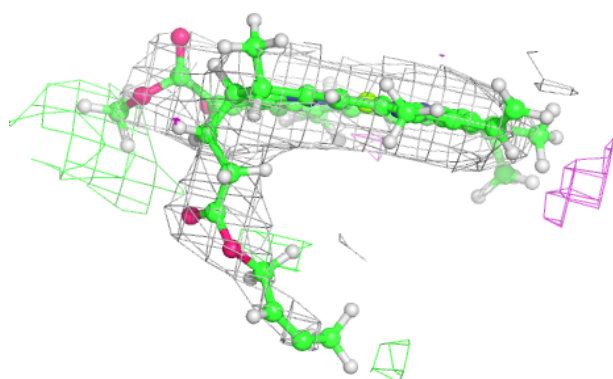
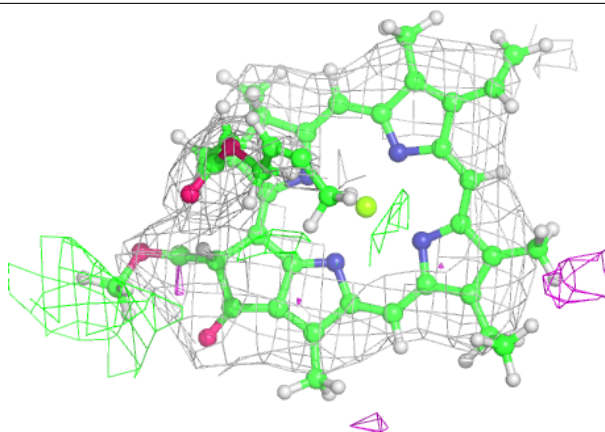
Electron density around CLA B 3031:

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

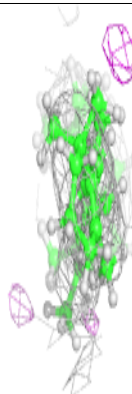
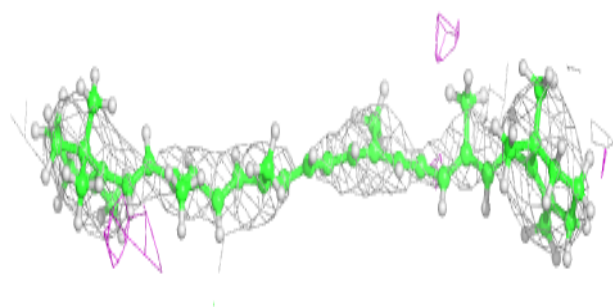
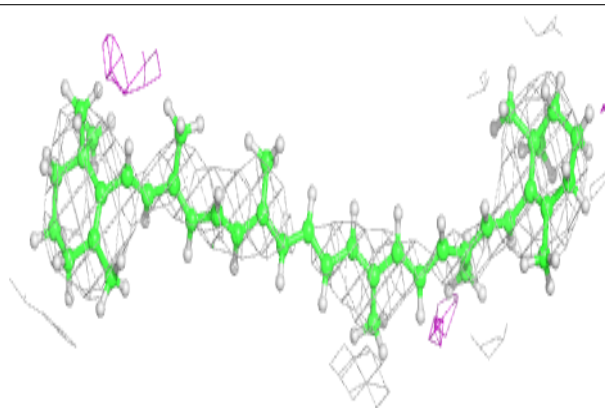


Electron density around CLA B 3032:

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

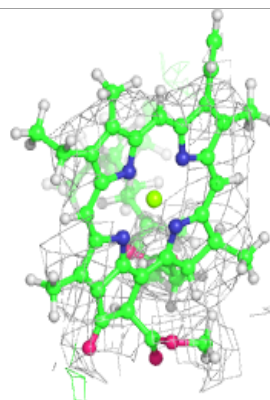
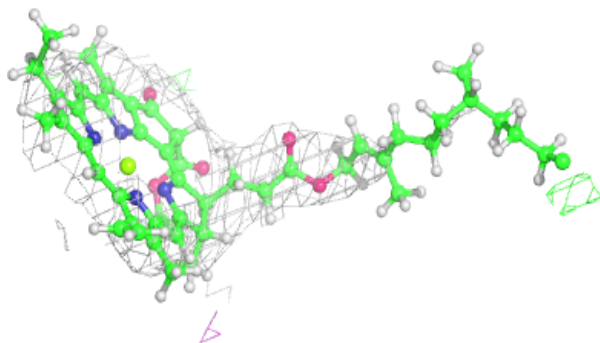
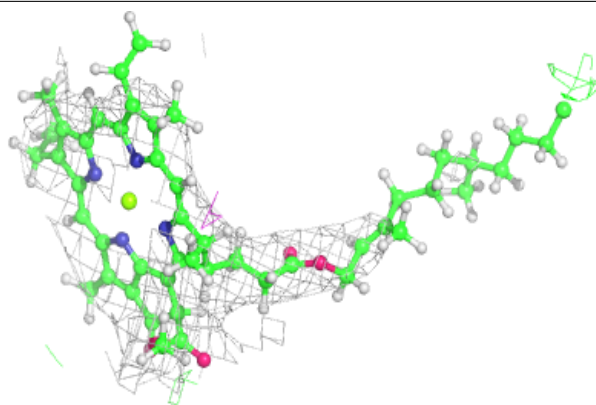
**Electron density around BCR B 3047:**

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



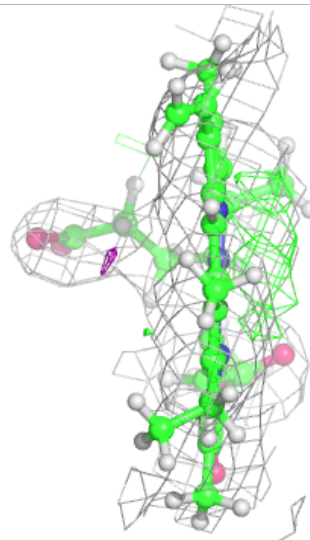
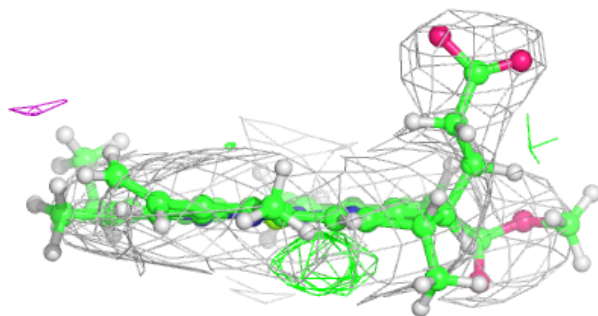
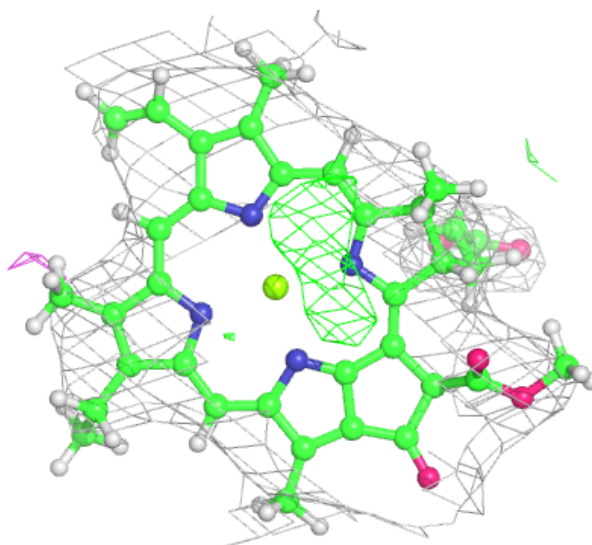
Electron density around CLA B 3034:

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



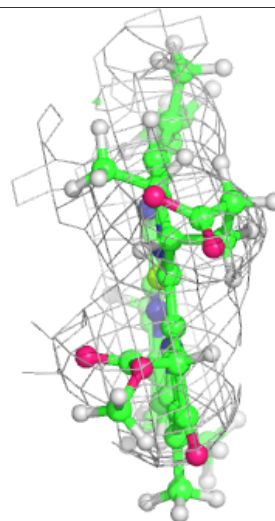
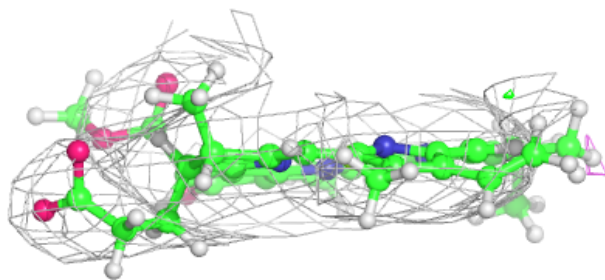
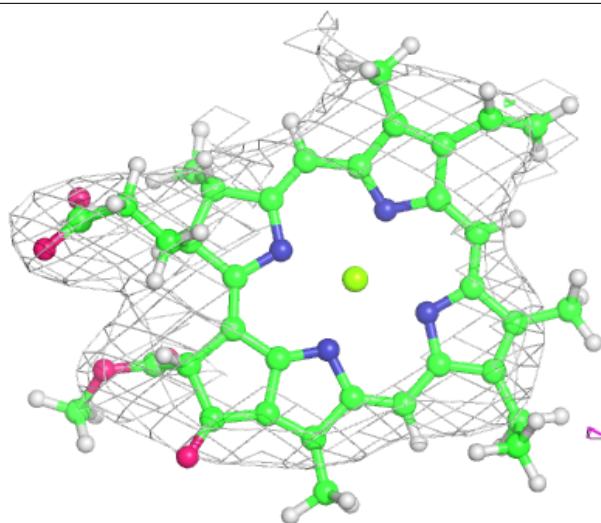
Electron density around CLA B 3036:

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



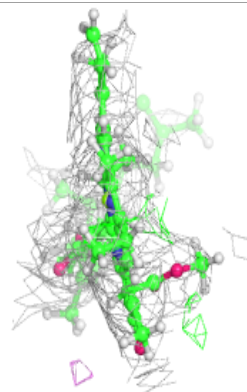
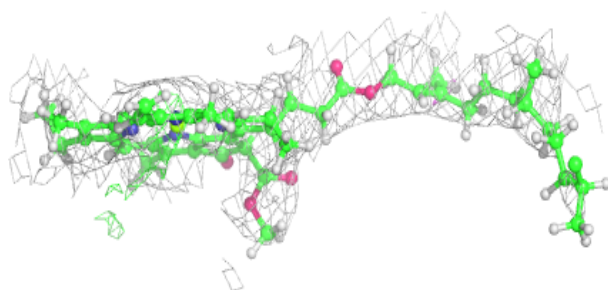
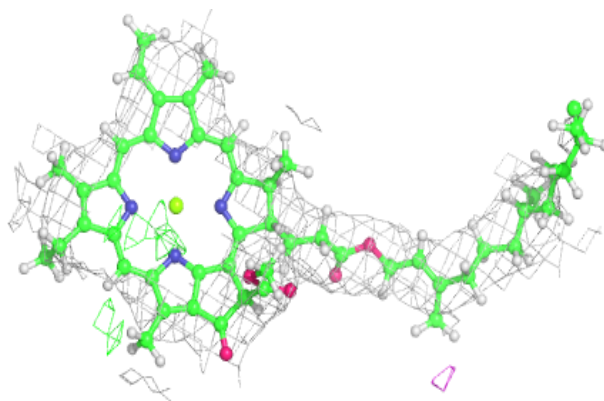
Electron density around CLA B 3037:

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

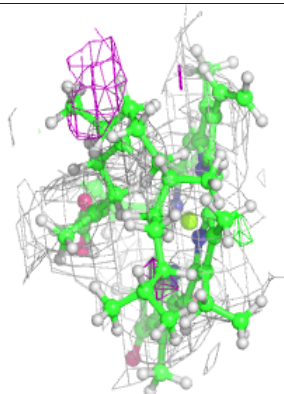
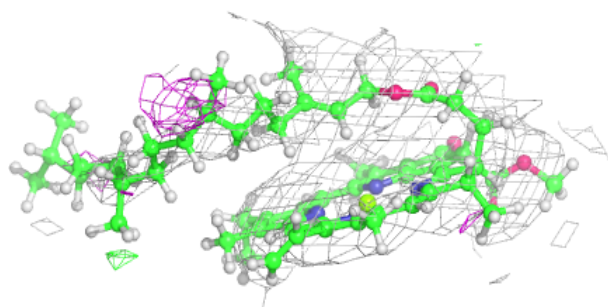
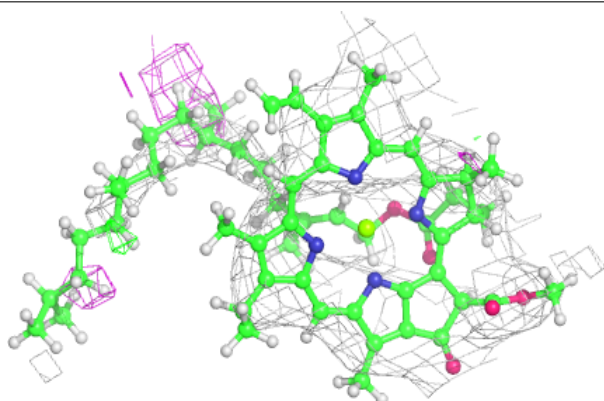


Electron density around CLA B 3038:

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

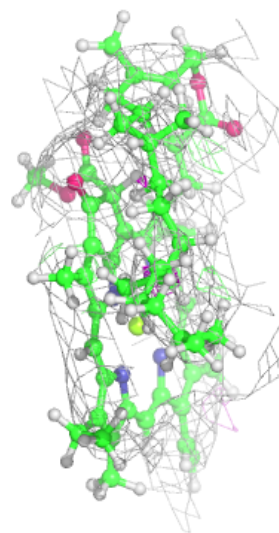
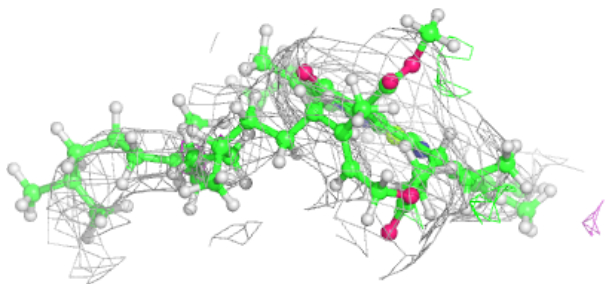
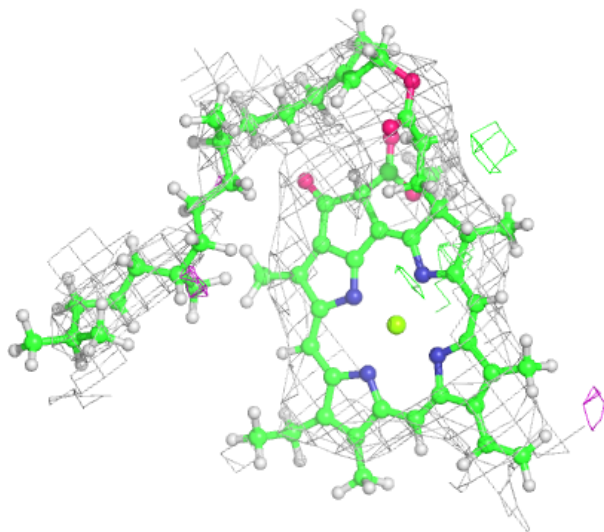
**Electron density around CLA B 3039:**

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



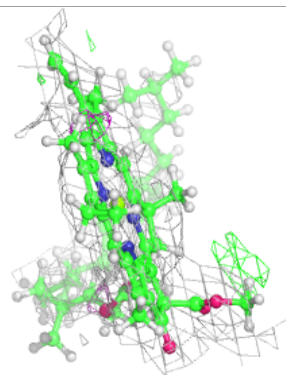
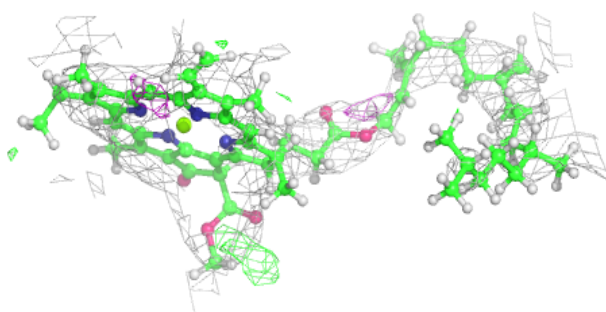
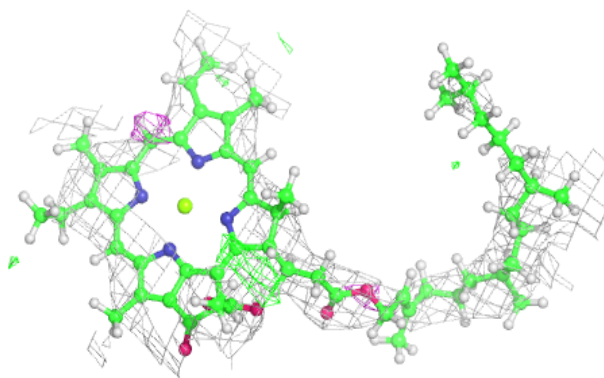
Electron density around CLA A 826:

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

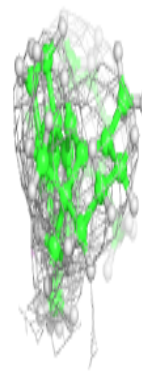
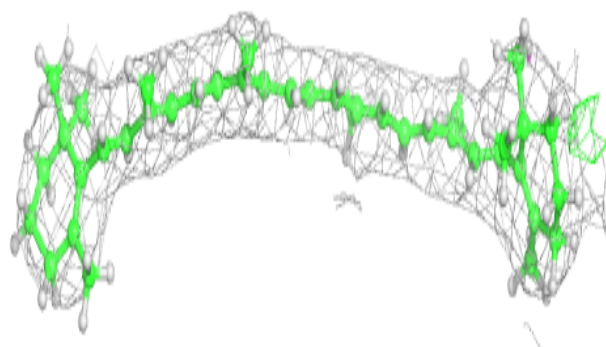
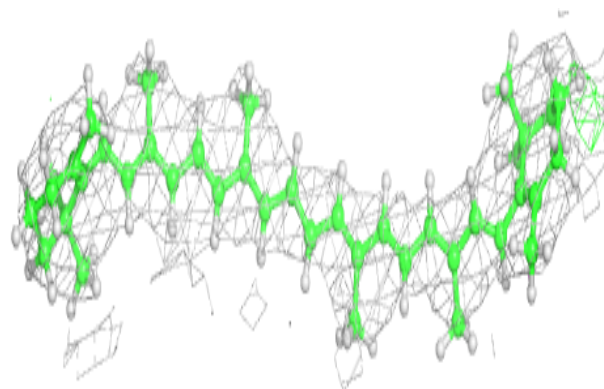


Electron density around CLA A 828:

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

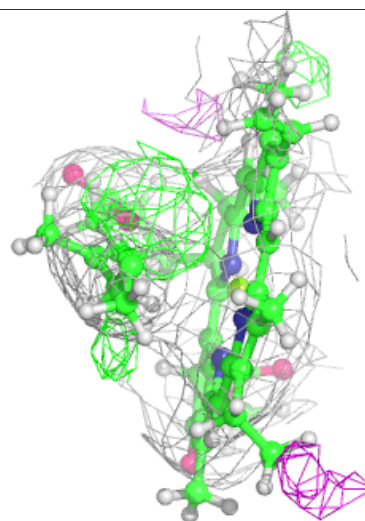
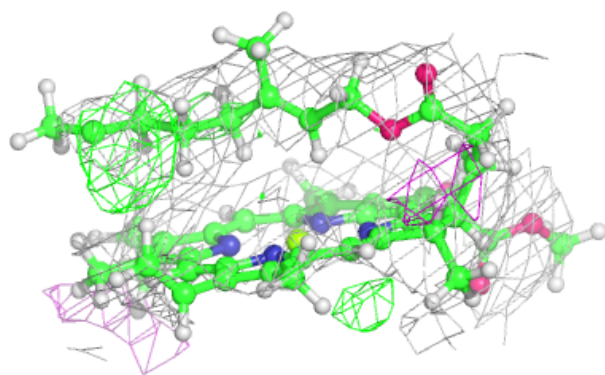
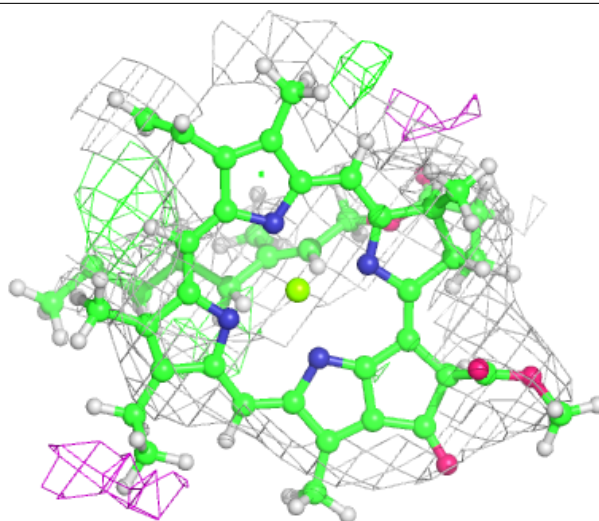
**Electron density around BCR M 103:**

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



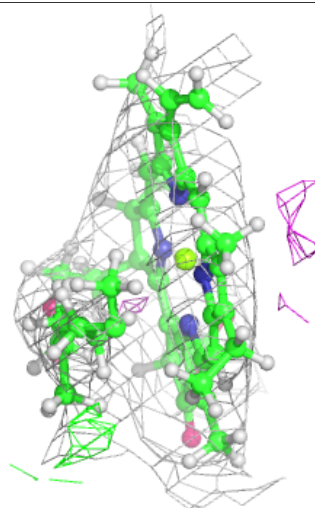
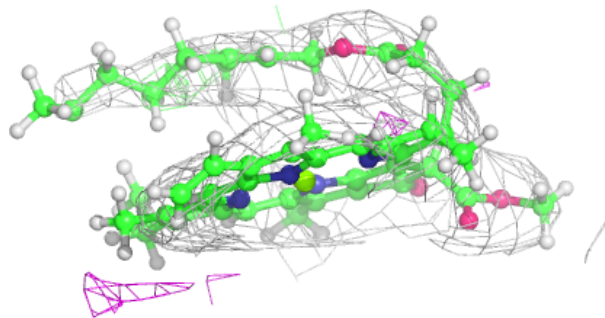
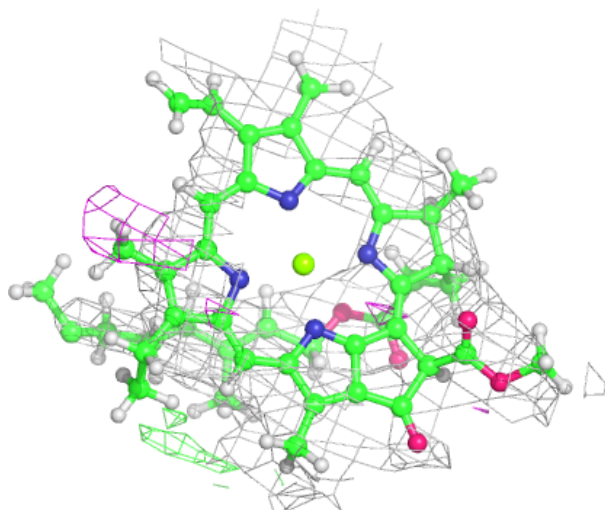
Electron density around CLA A 819:

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



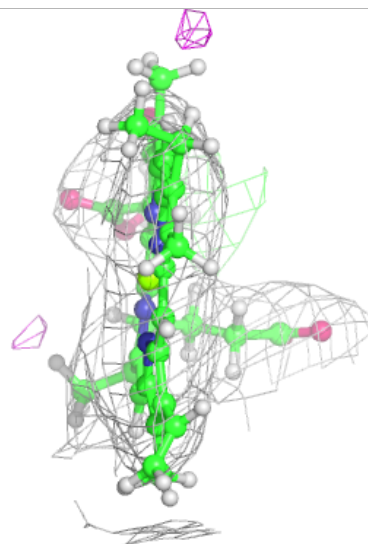
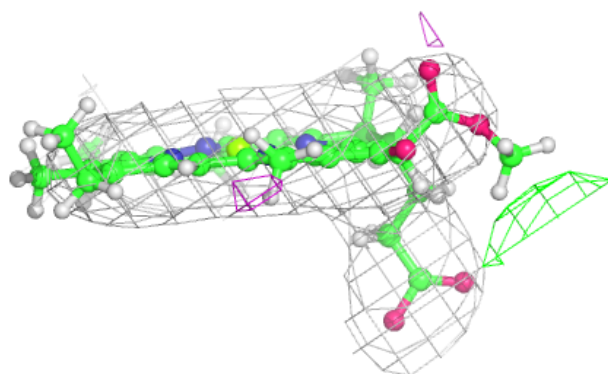
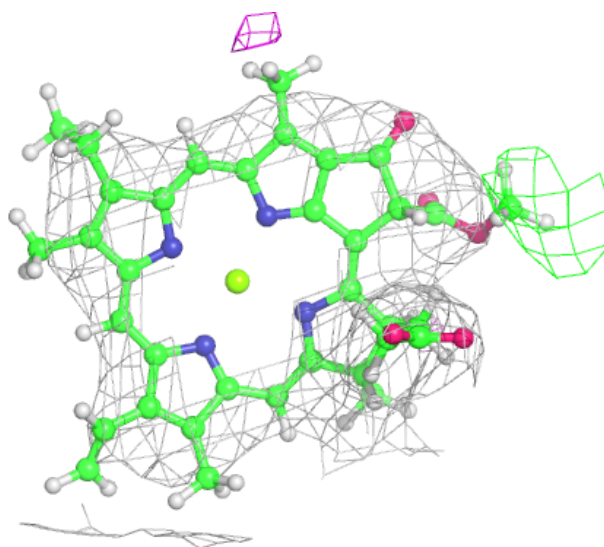
Electron density around CLA A 813:

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



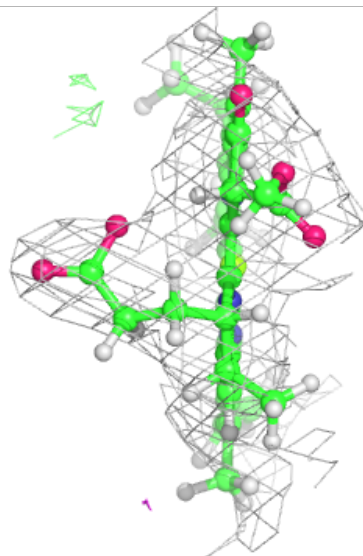
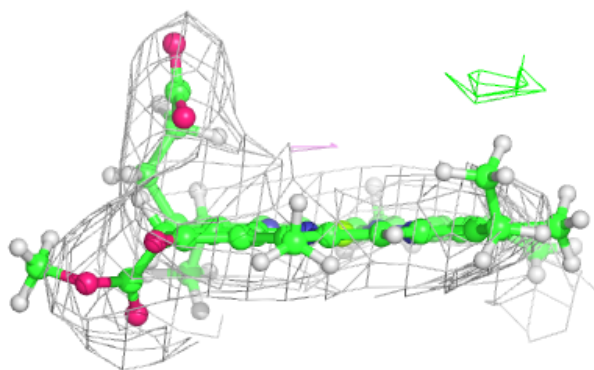
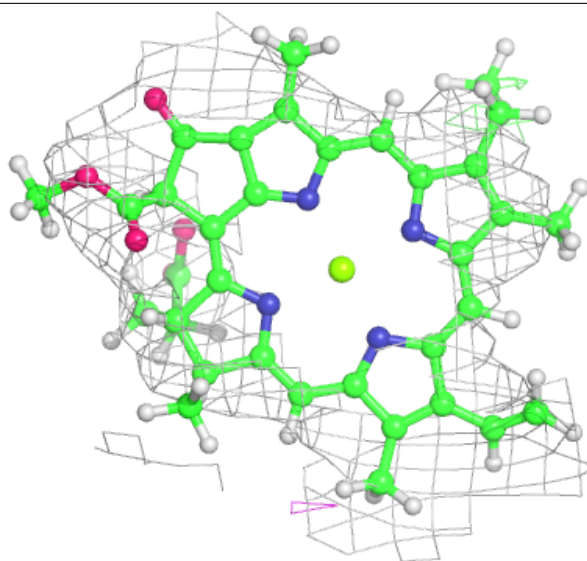
Electron density around CLA B 3012:

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



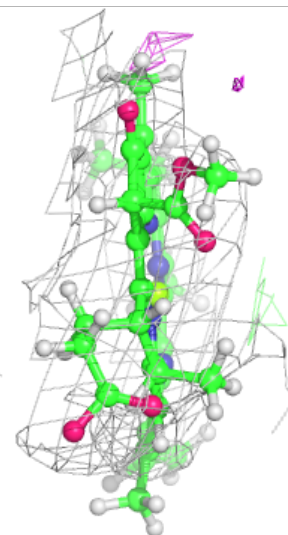
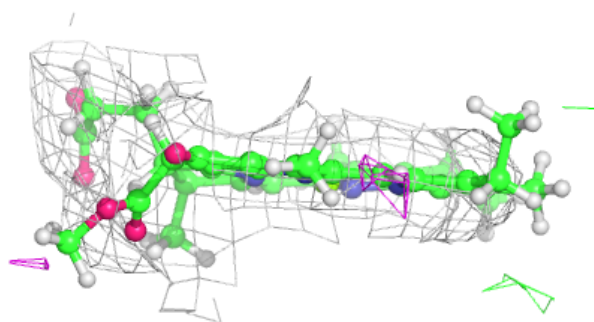
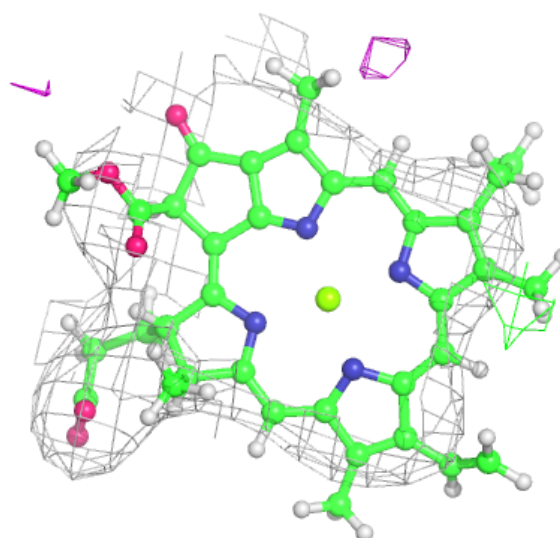
Electron density around CLA B 3013:

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



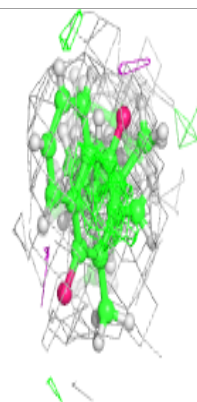
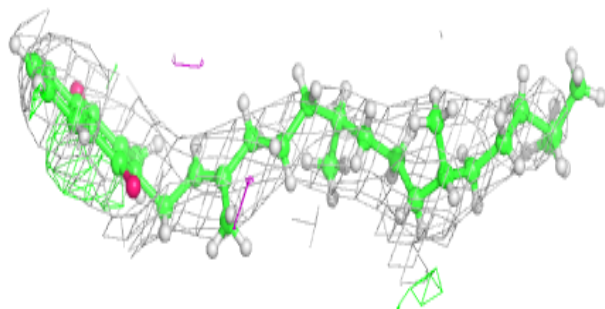
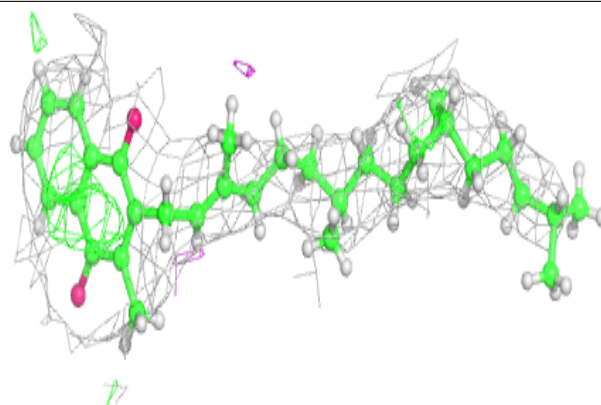
Electron density around CLA X 1701:

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

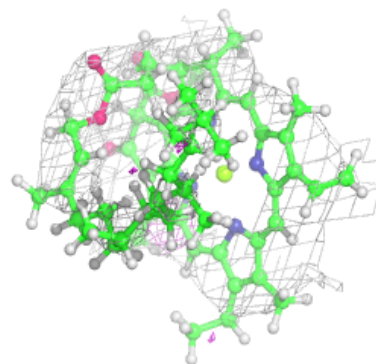
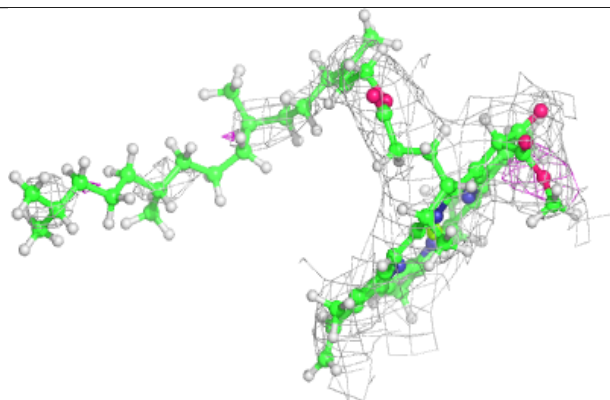
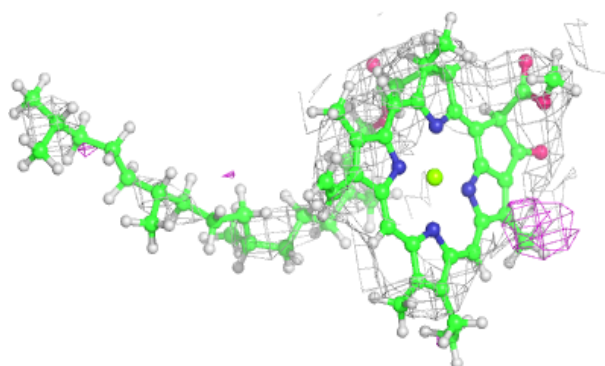


Electron density around PQN A 846:

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

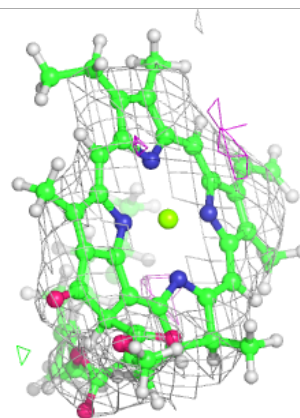
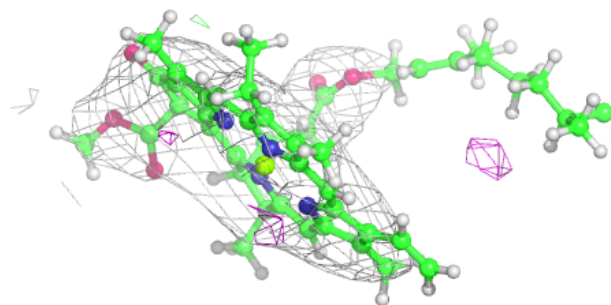
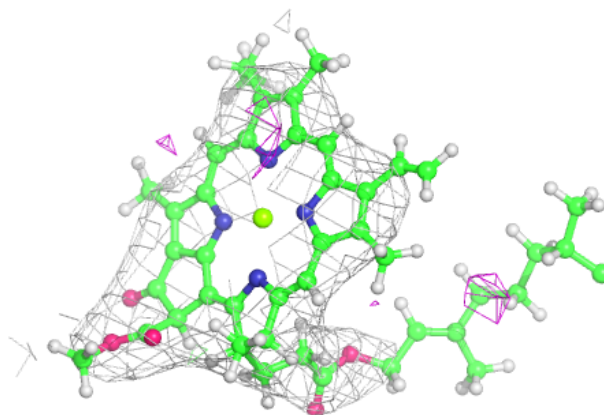
**Electron density around CLA B 3015:**

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



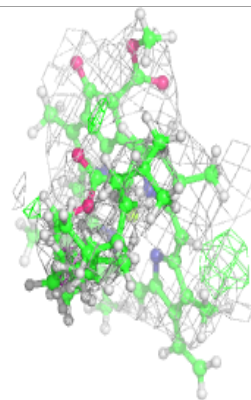
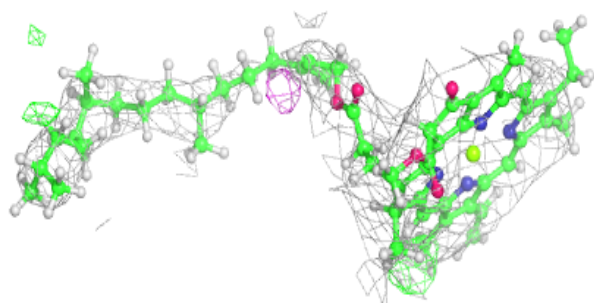
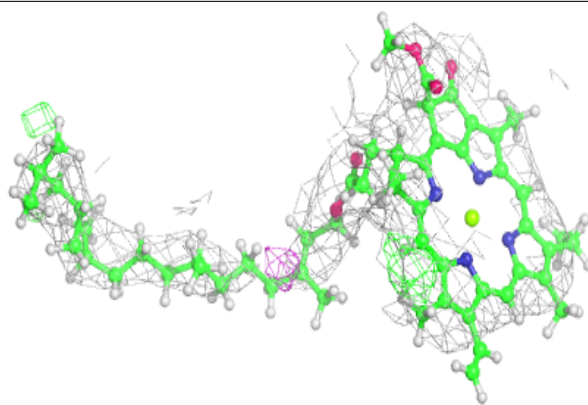
Electron density around CLA B 3017:

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



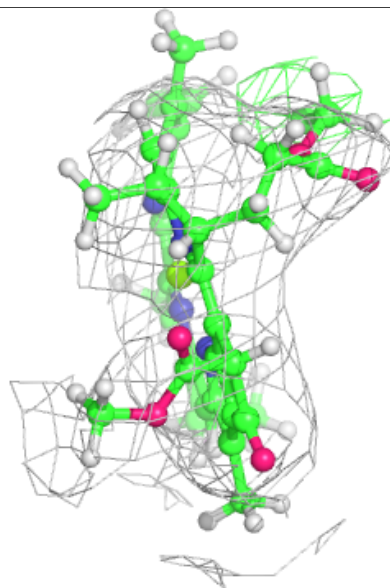
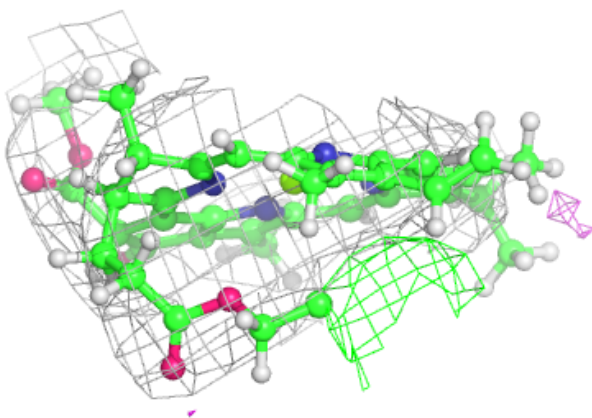
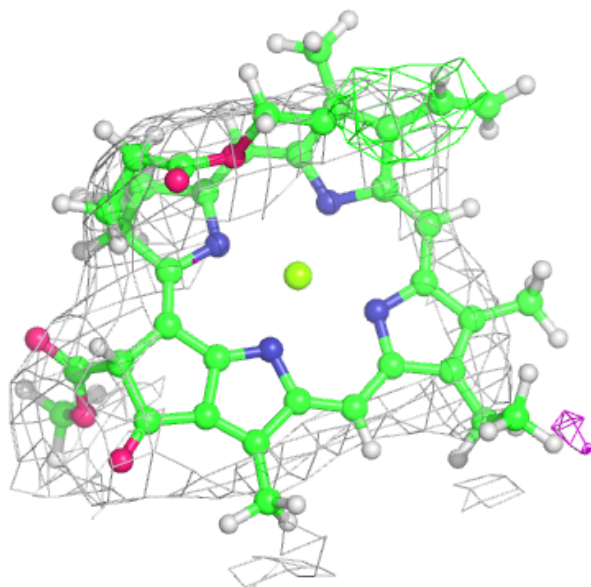
Electron density around CLA A 822:

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



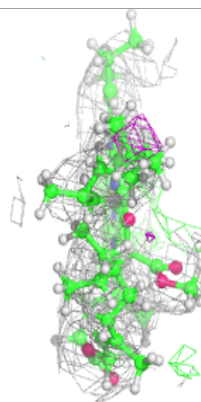
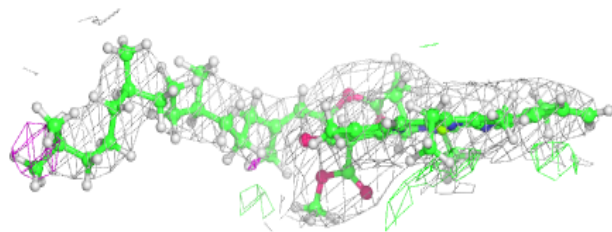
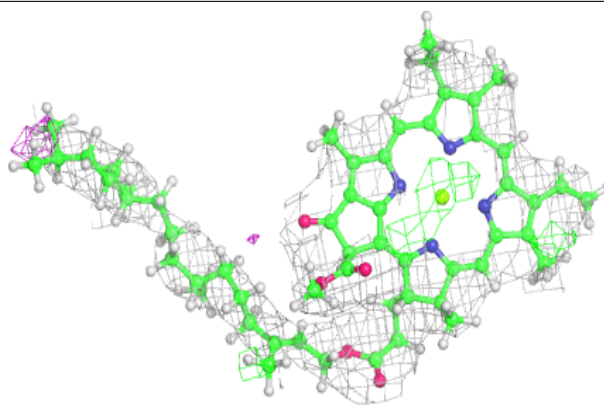
Electron density around CLA B 3021:

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

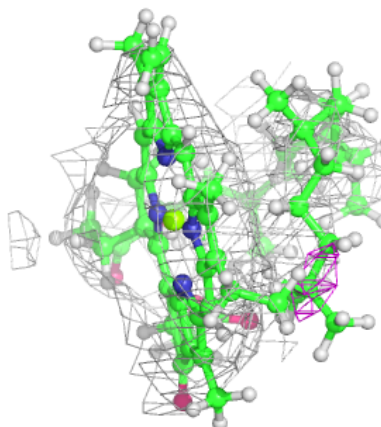
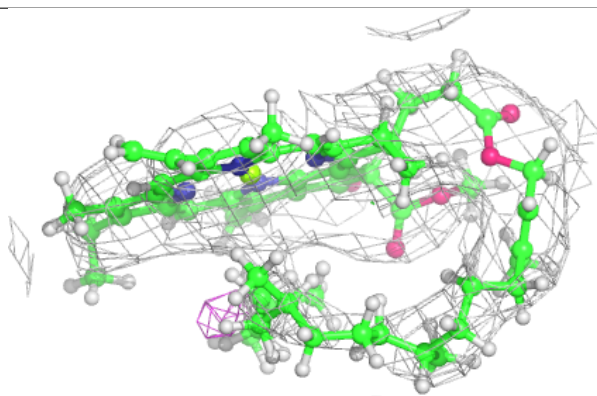
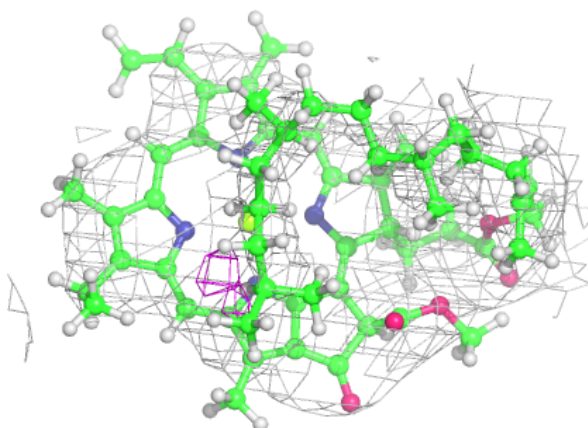


Electron density around CLA L 206:

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

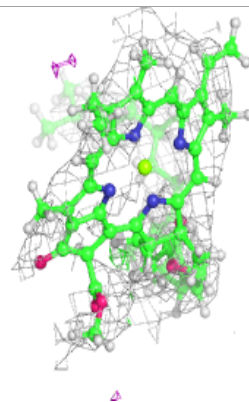
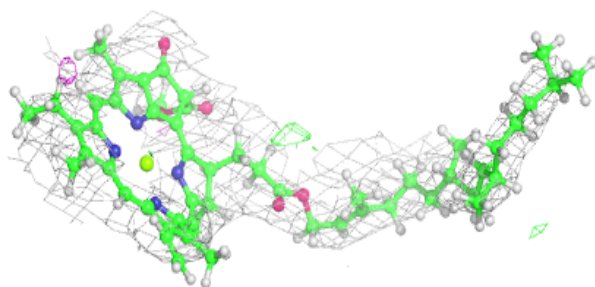
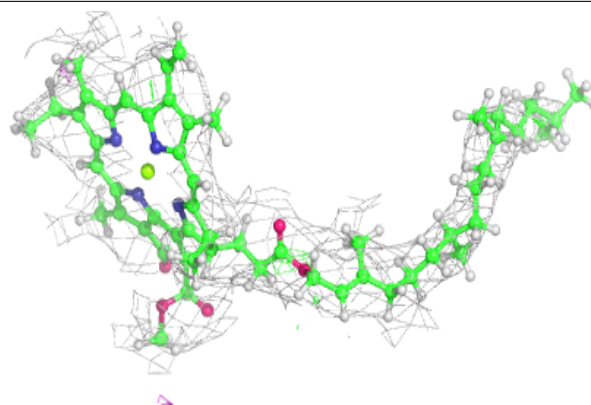
**Electron density around CLA A 807:**

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

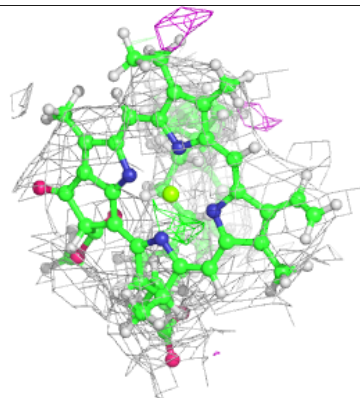
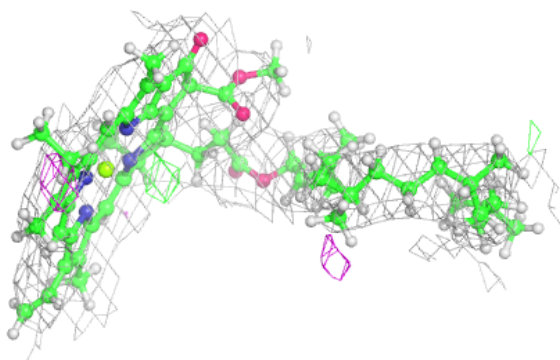
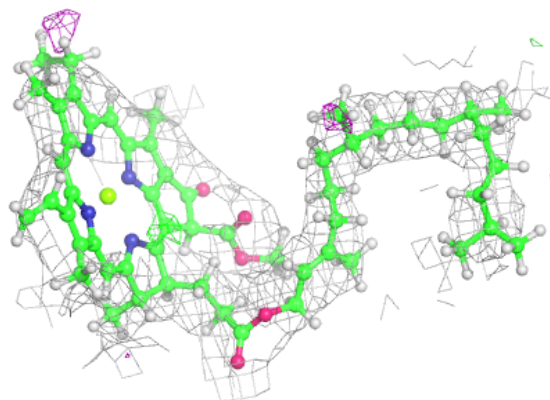


Electron density around CLA A 856:

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

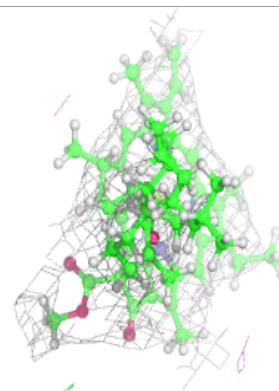
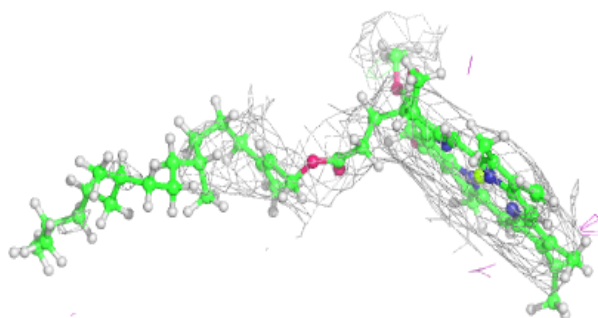
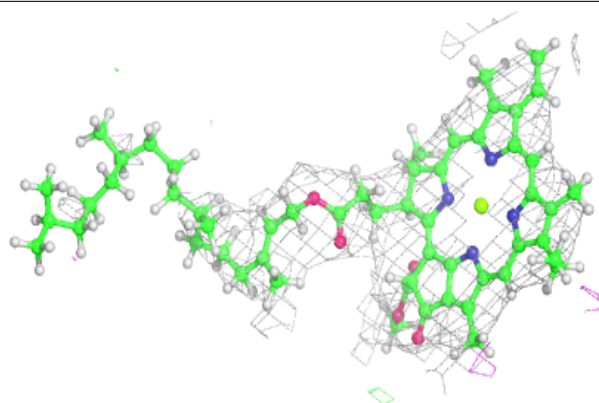
**Electron density around CL0 A 801:**

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

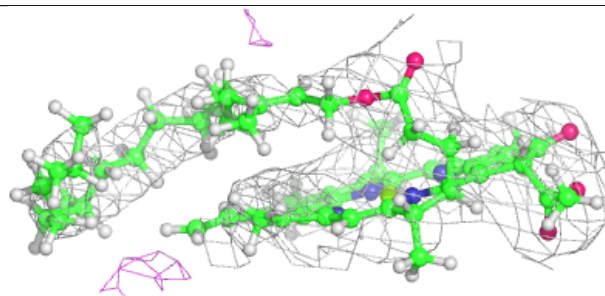
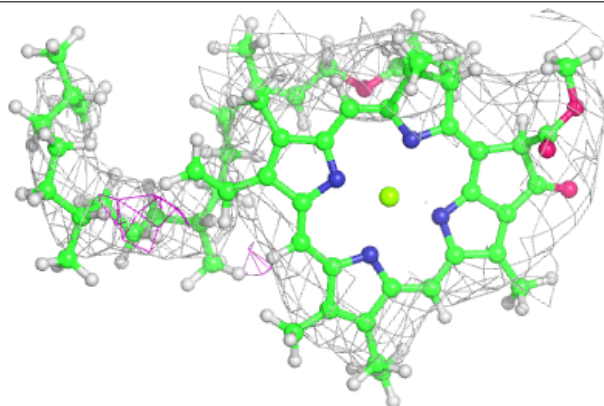


Electron density around CLA A 810:

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

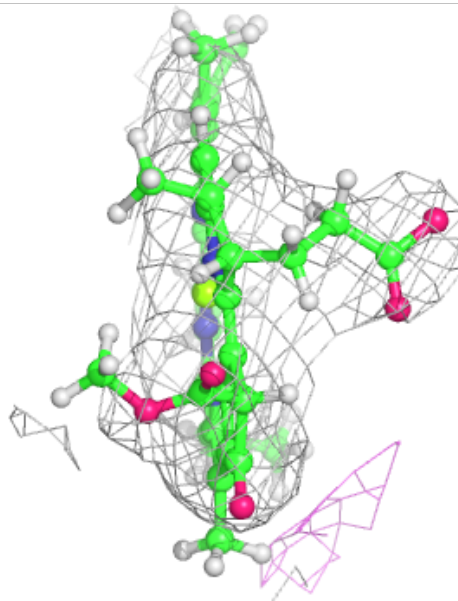
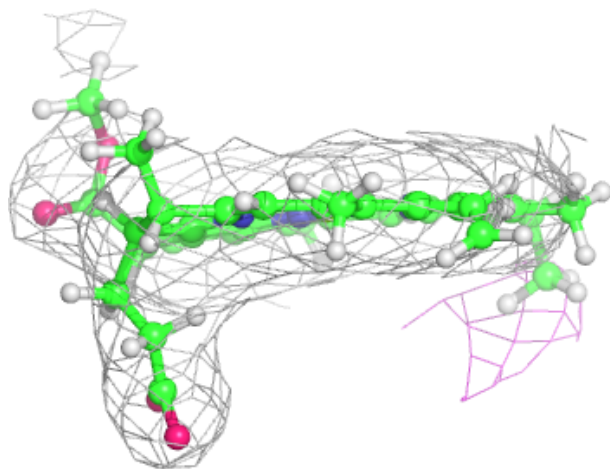
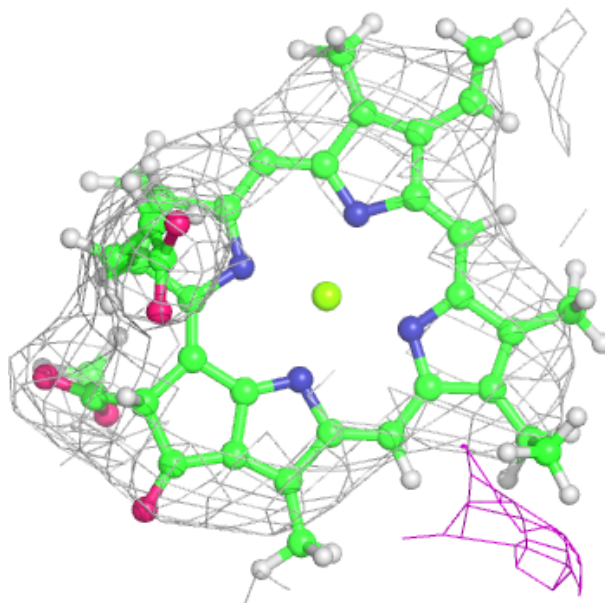
**Electron density around CLA A 820:**

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



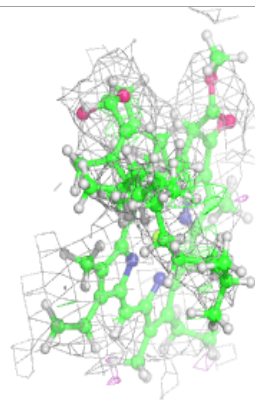
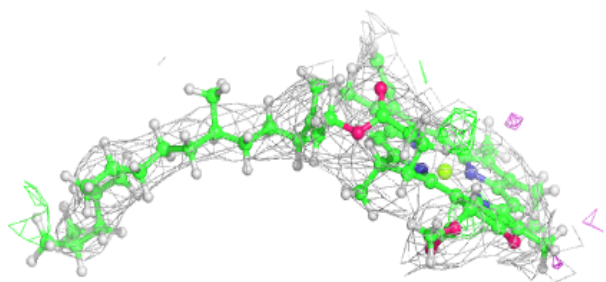
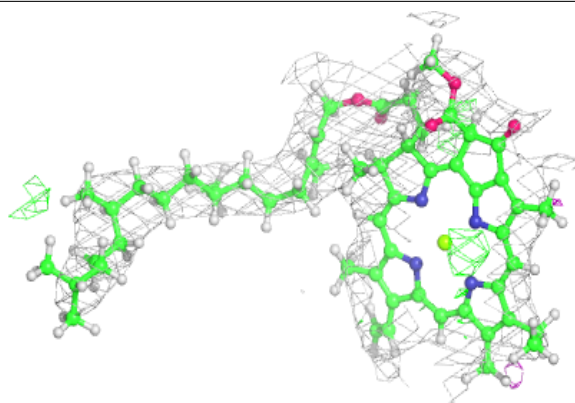
Electron density around CLA B 3016:

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

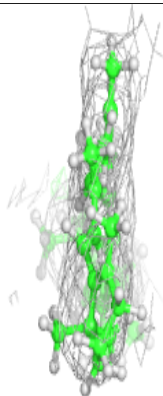
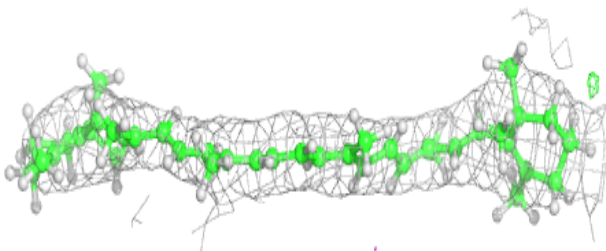
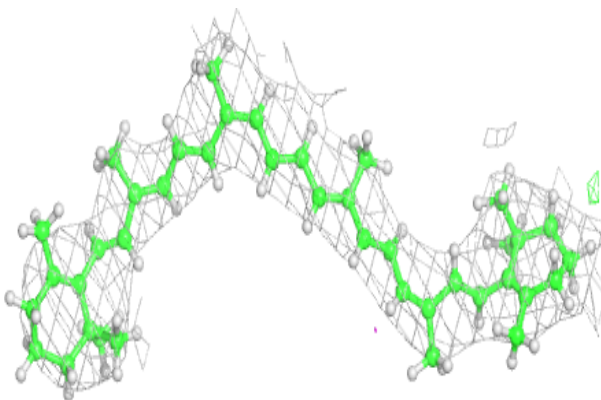


Electron density around CLA A 803:

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

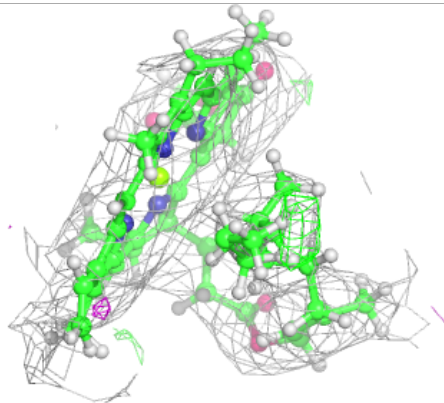
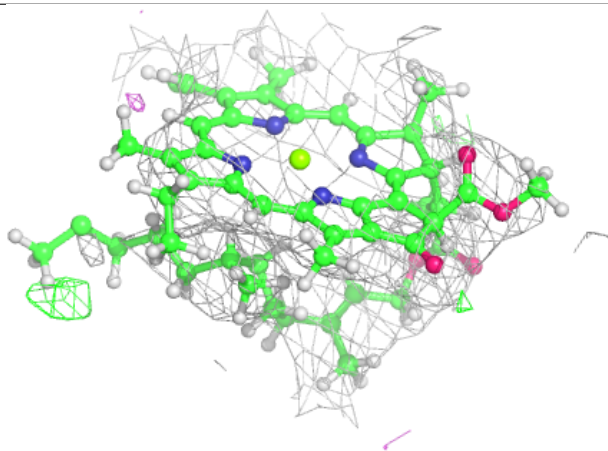
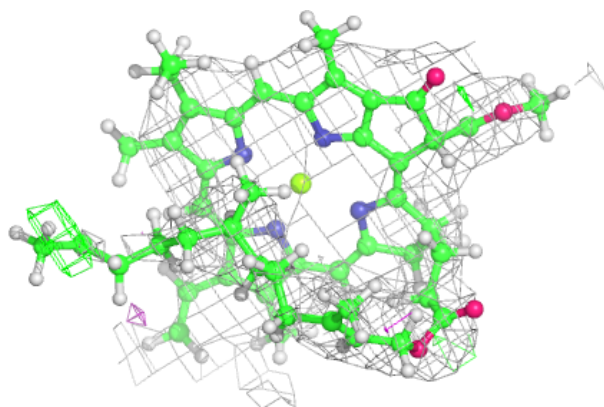
**Electron density around BCR A 851:**

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



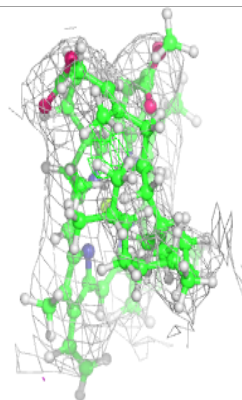
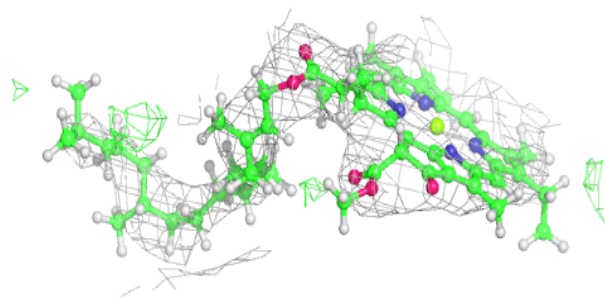
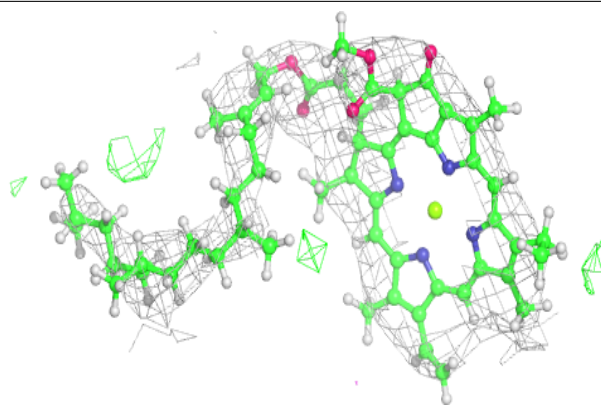
Electron density around CLA B 3018:

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



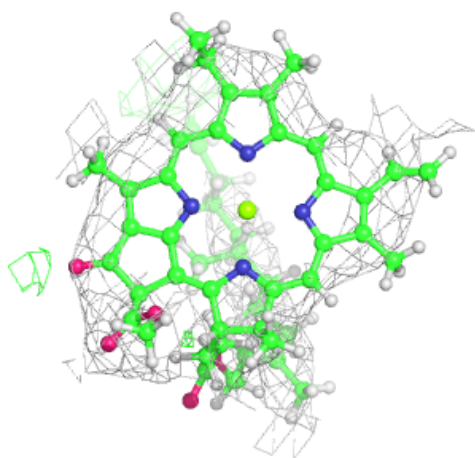
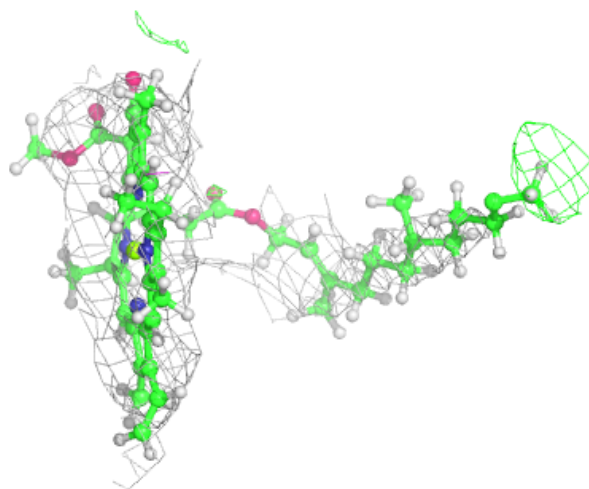
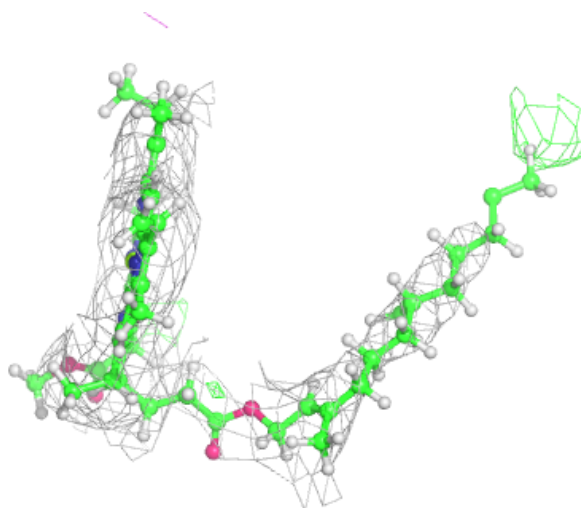
Electron density around CLA A 804:

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



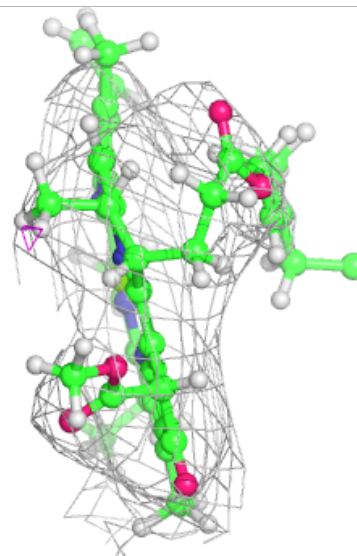
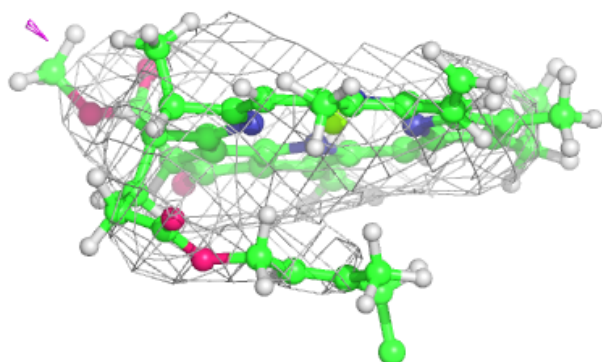
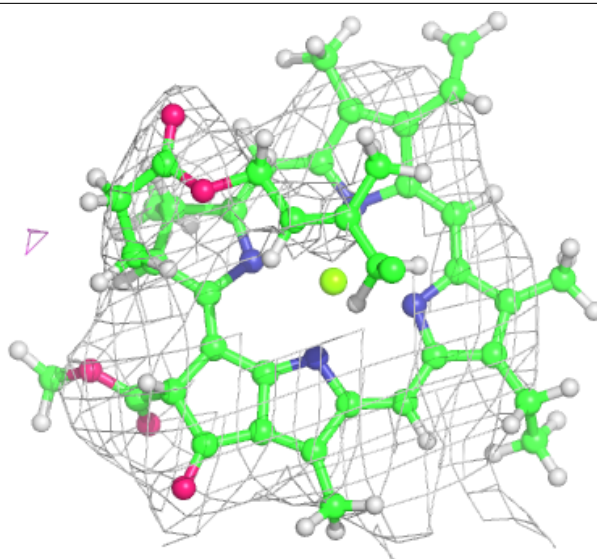
Electron density around CLA A 805:

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



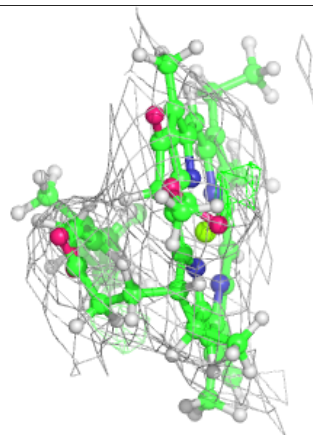
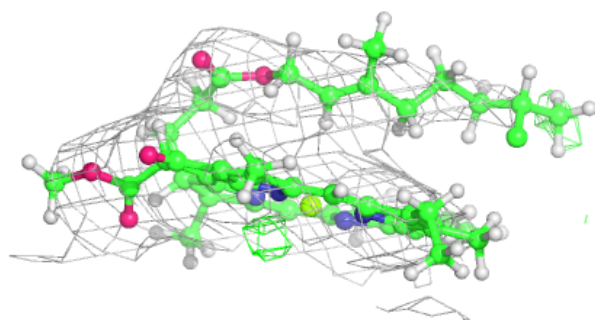
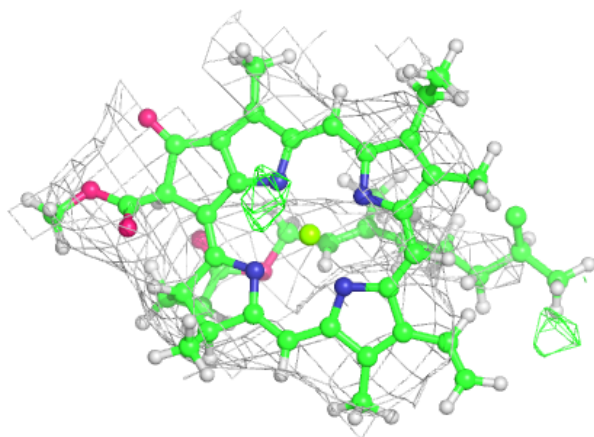
Electron density around CLA A 824:

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

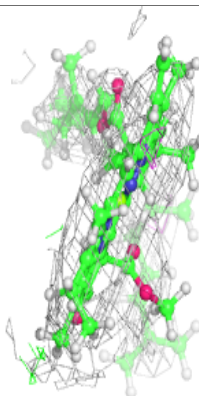
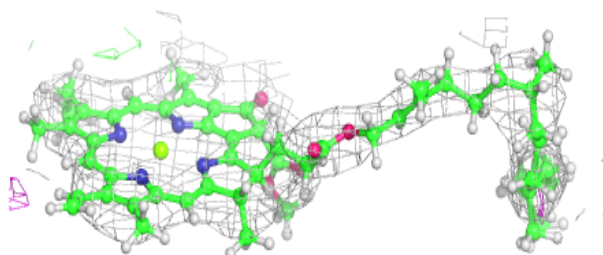
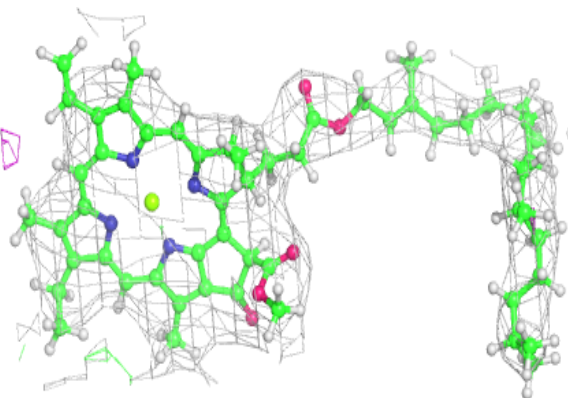


Electron density around CLA B 3023:

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

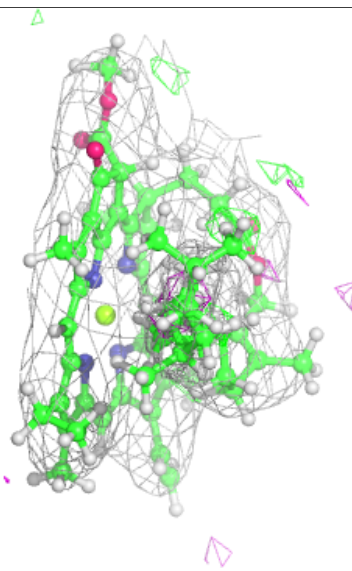
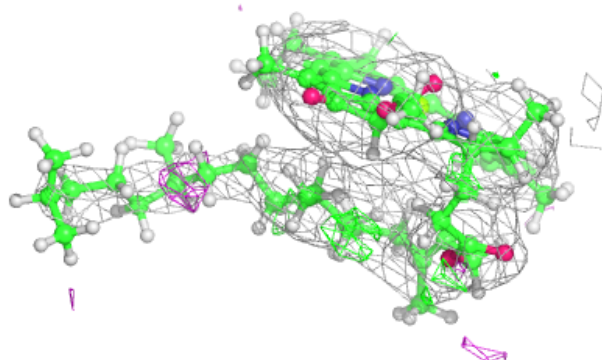
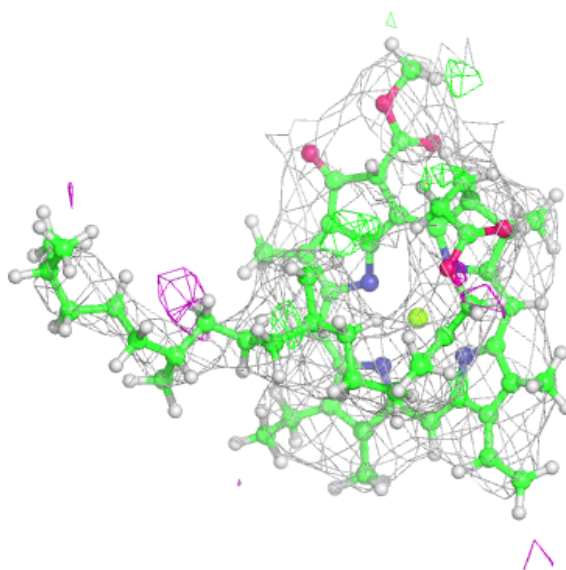
**Electron density around CLA B 3027:**

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



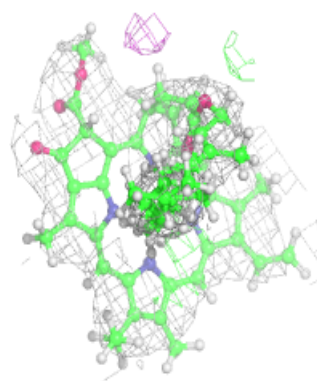
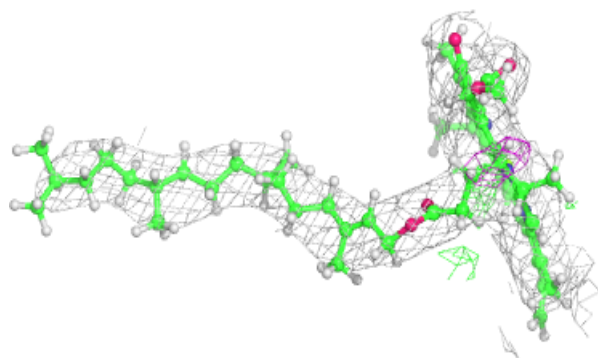
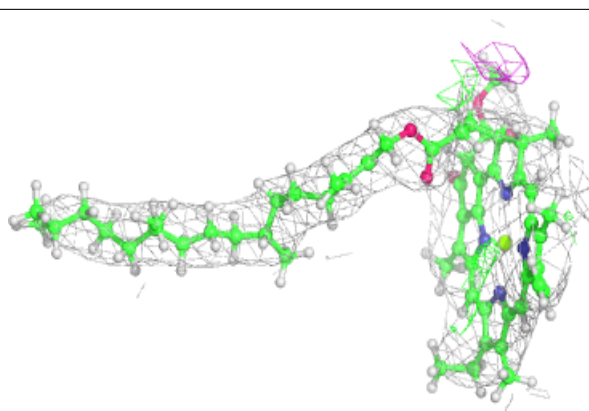
Electron density around CLA B 3028:

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



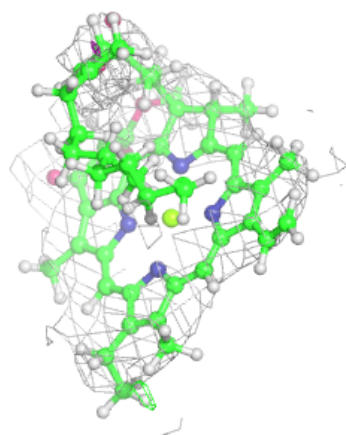
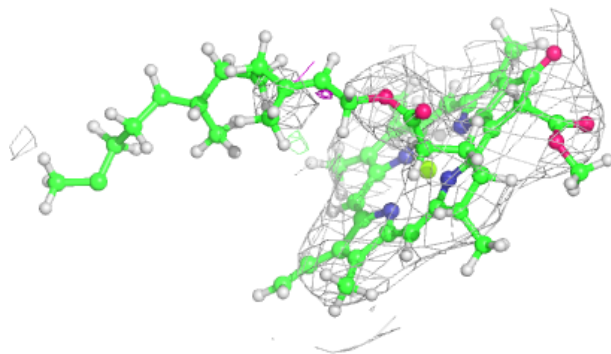
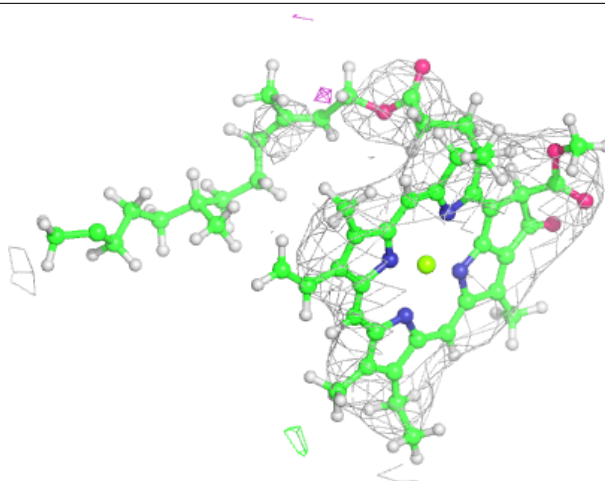
Electron density around CLA B 3029:

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



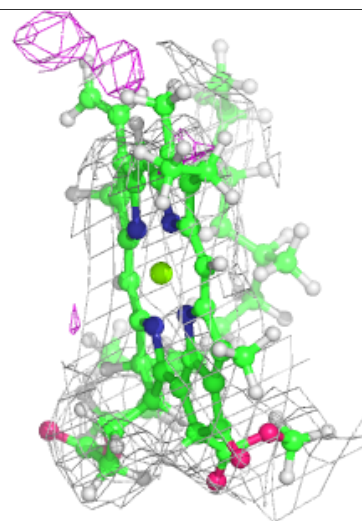
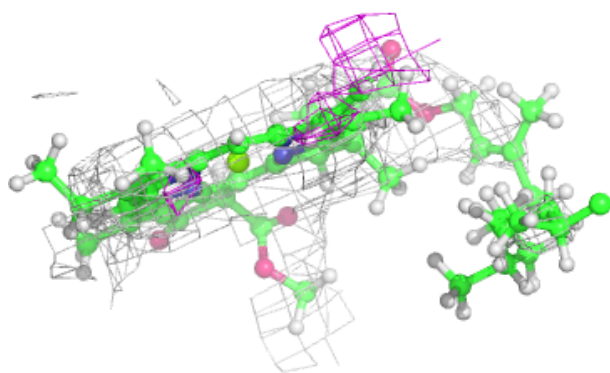
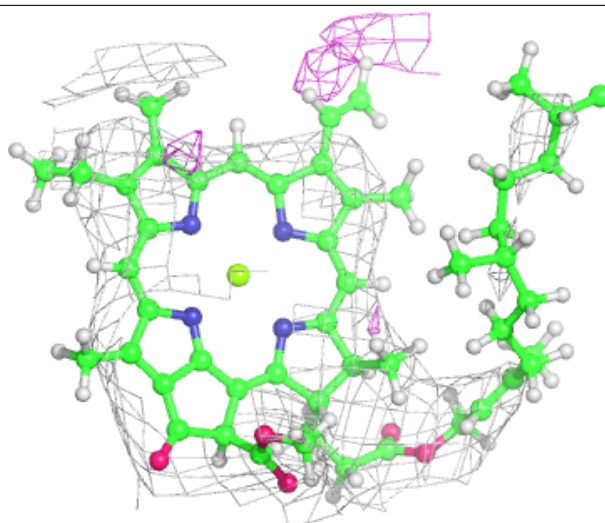
Electron density around CLA A 825:

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



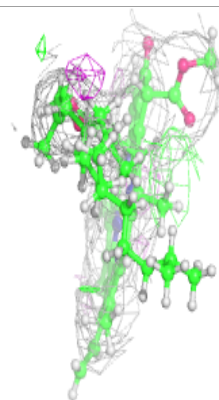
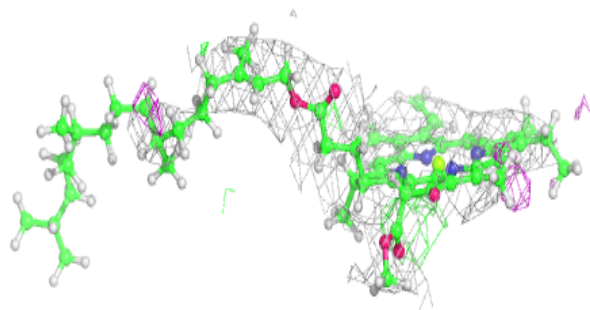
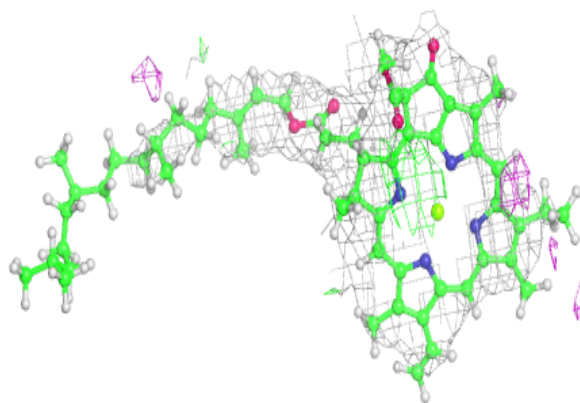
Electron density around CLA A 814:

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



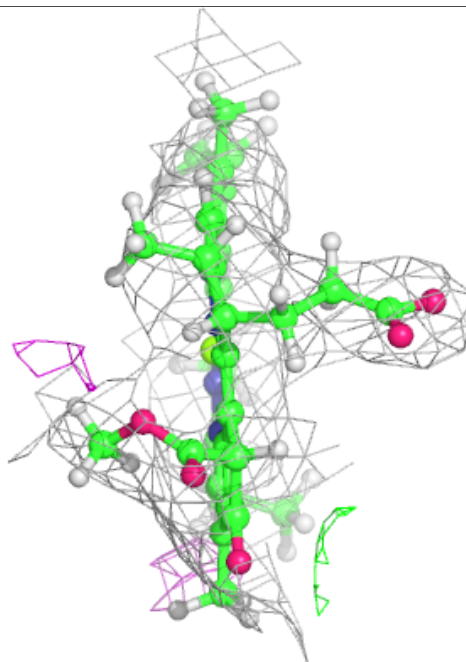
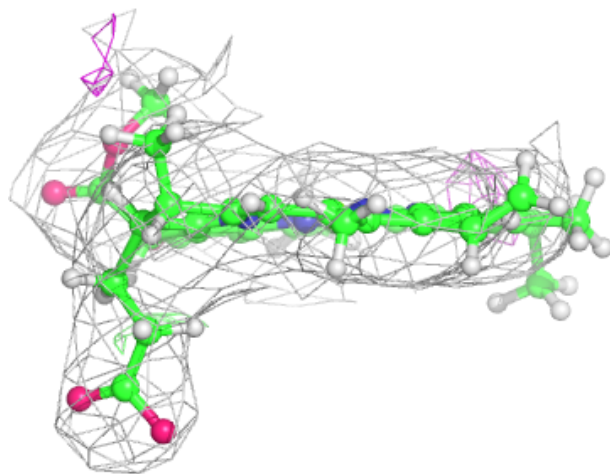
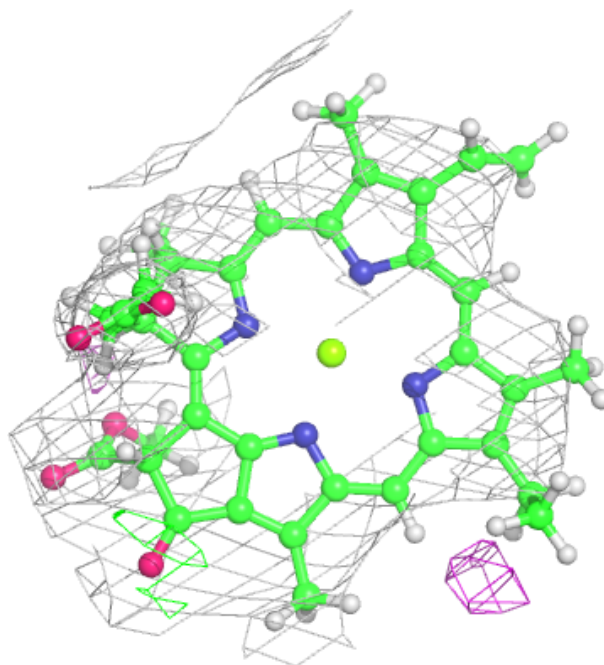
Electron density around CLA A 827:

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



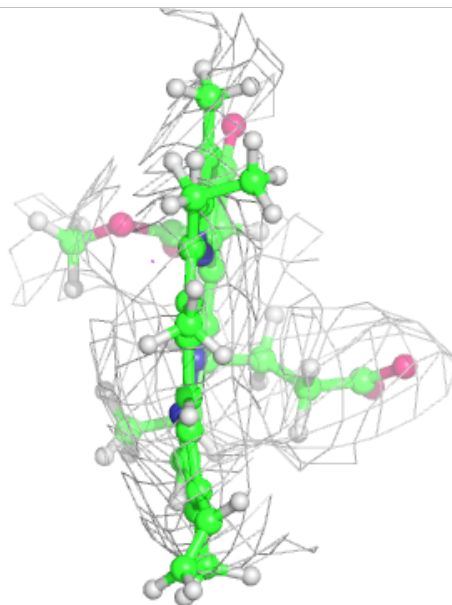
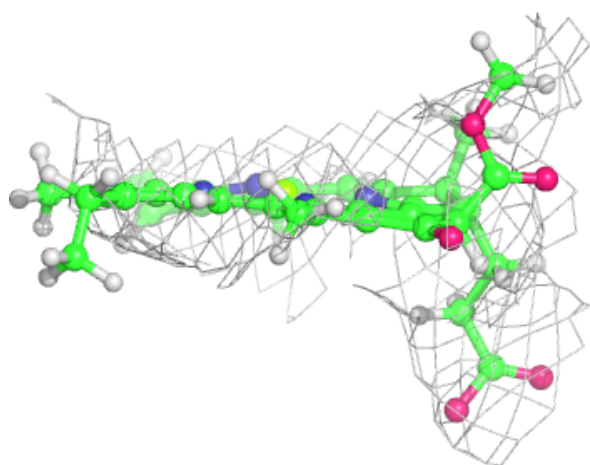
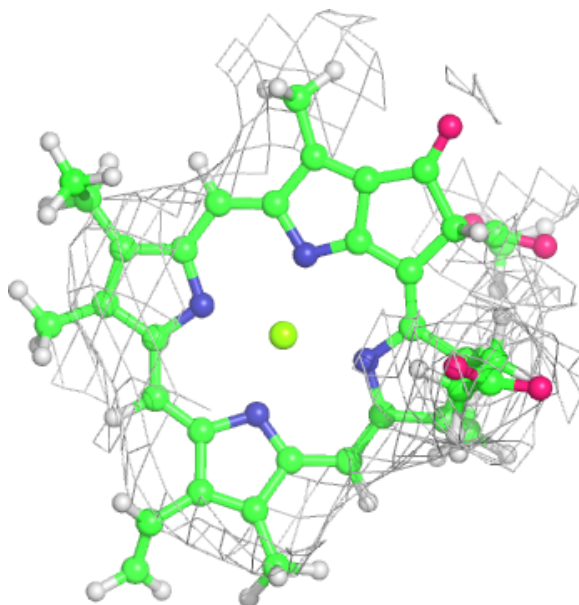
Electron density around CLA B 3035:

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



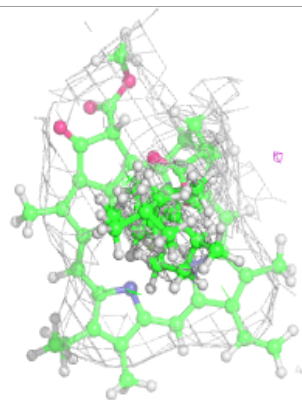
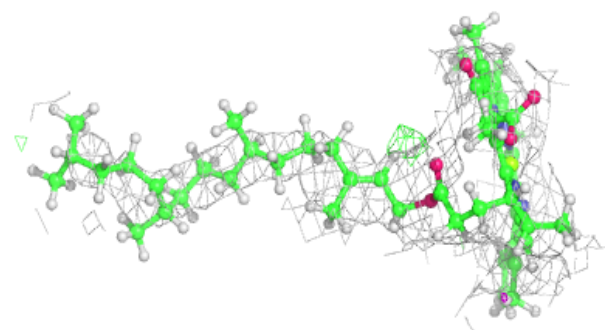
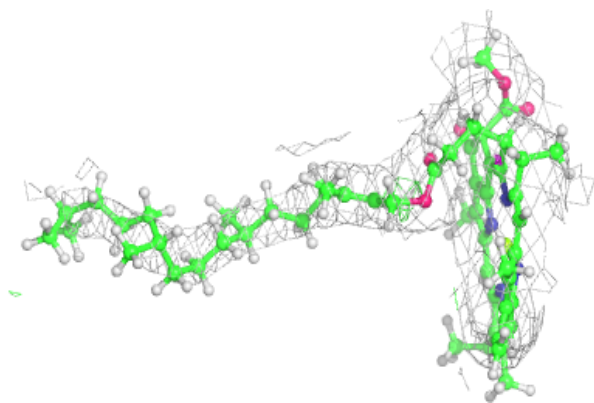
Electron density around CLA A 815:

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



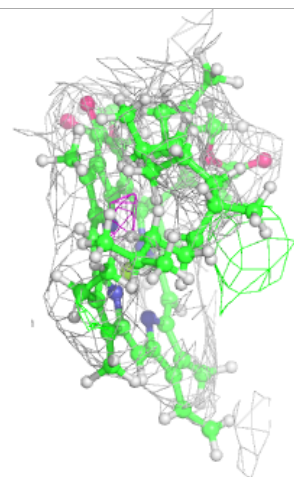
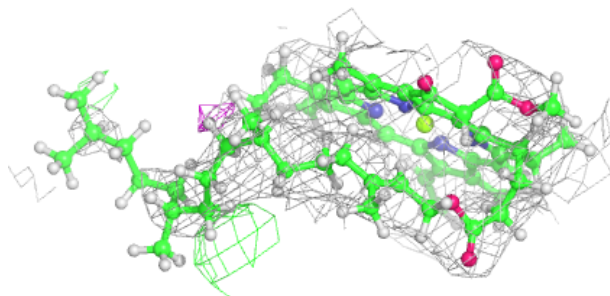
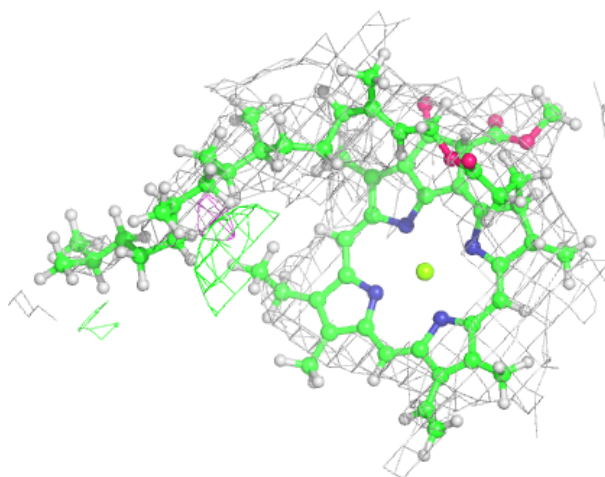
Electron density around CLA A 829:

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



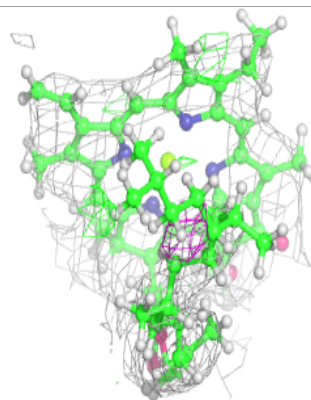
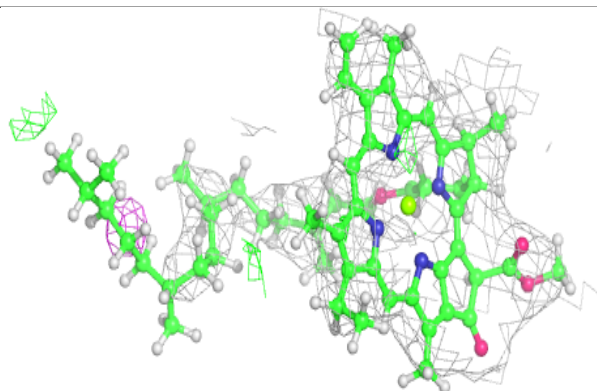
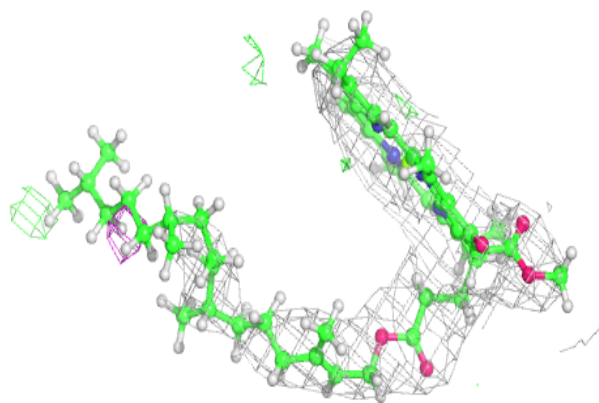
Electron density around CLA A 830:

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



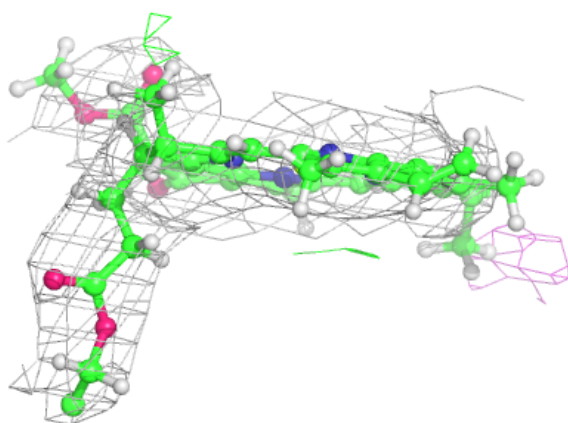
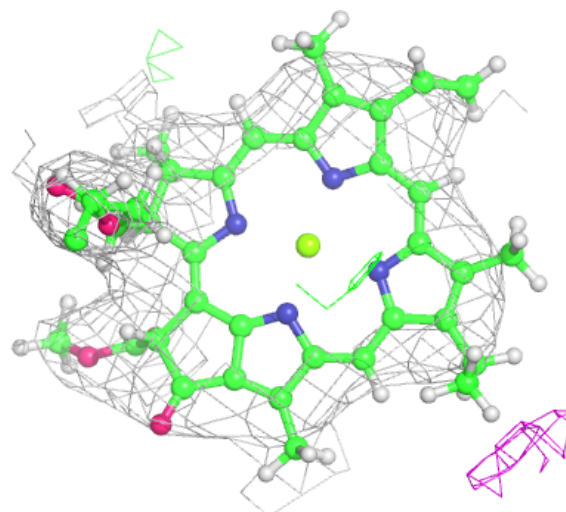
Electron density around CLA A 833:

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



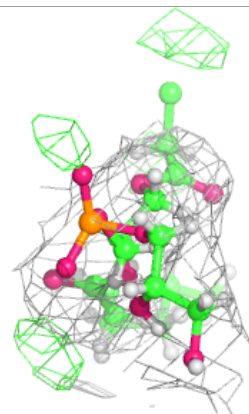
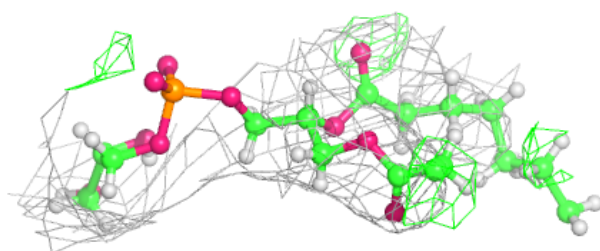
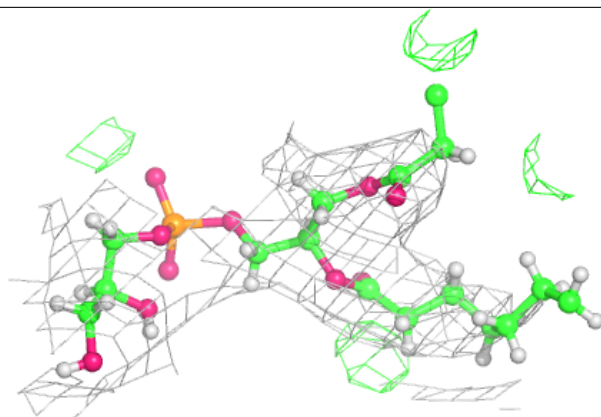
Electron density around CLA B 3040:

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



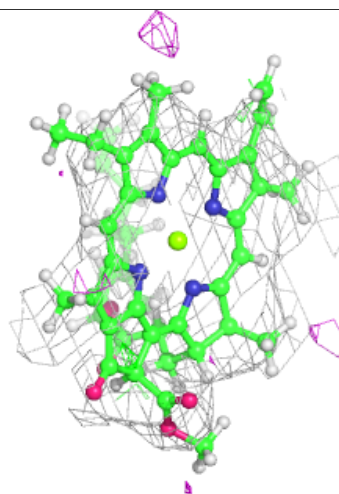
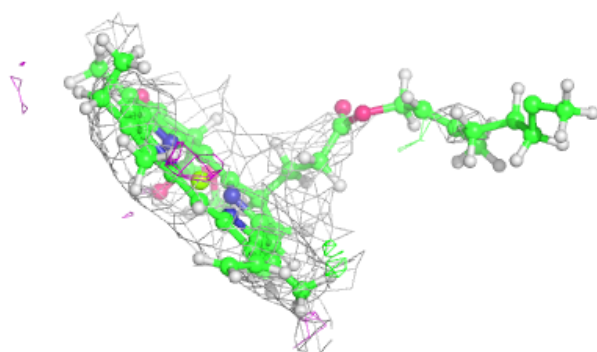
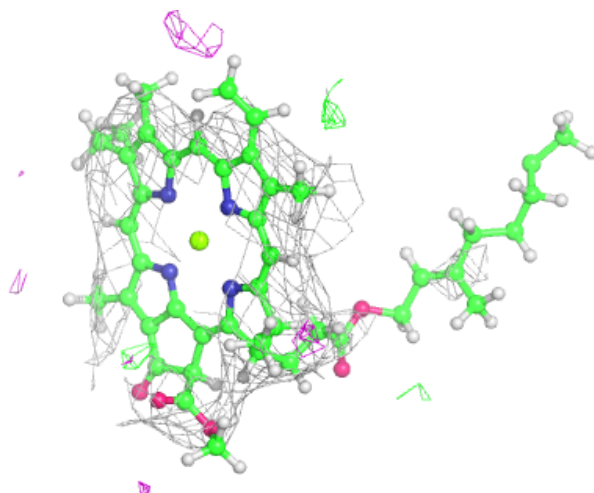
Electron density around LHG A 854:

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



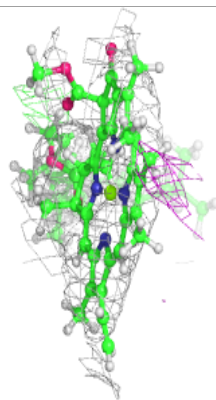
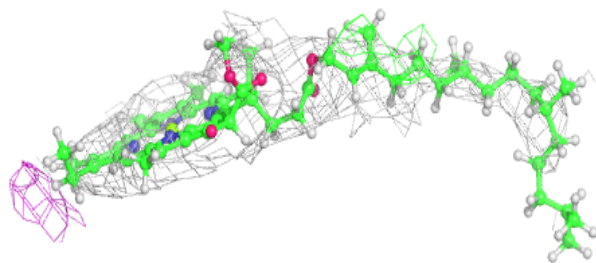
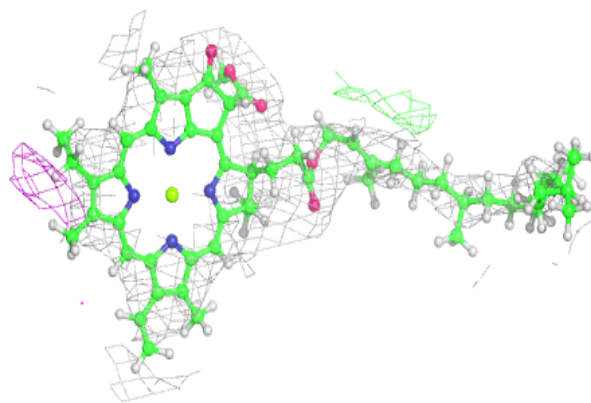
Electron density around CLA A 836:

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

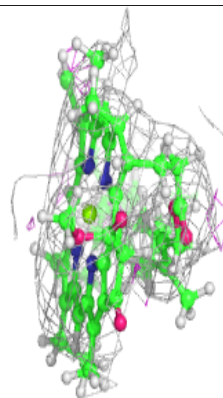
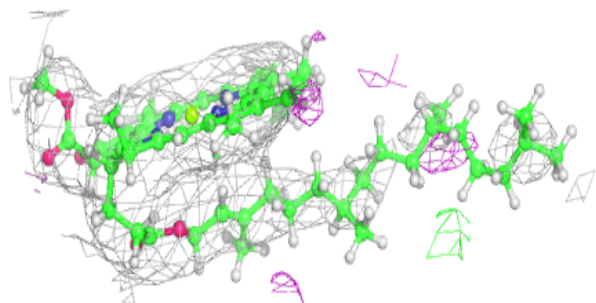
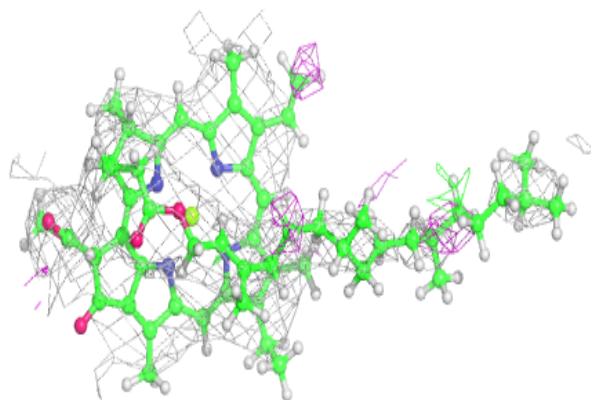


Electron density around CLA A 806:

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

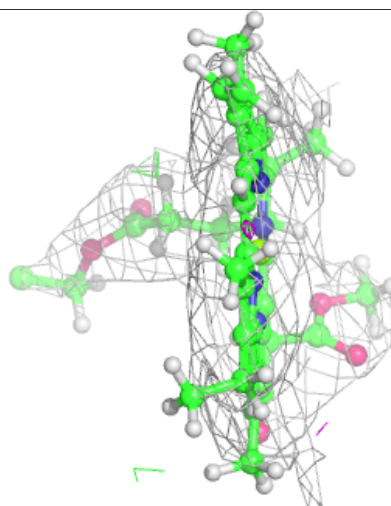
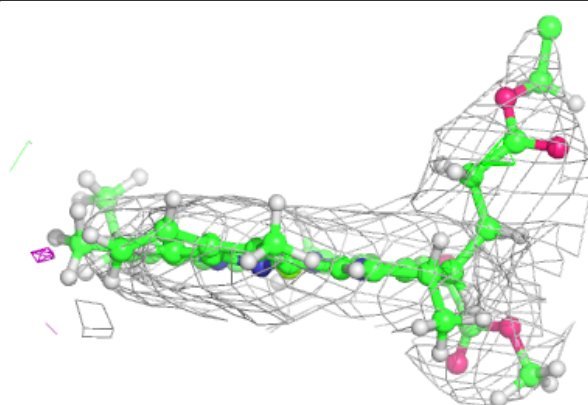
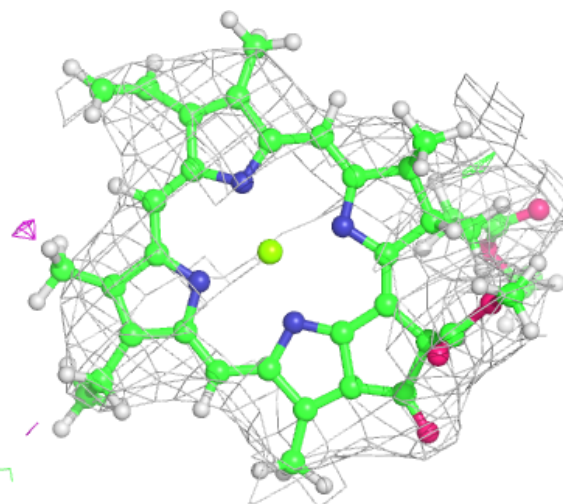
**Electron density around CLA A 839:**

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



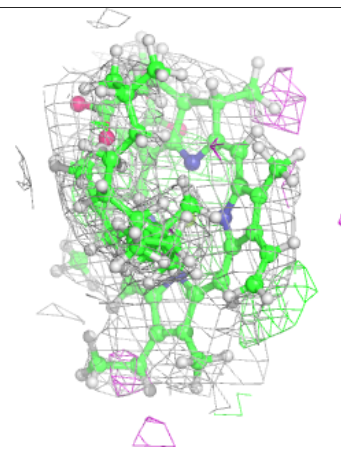
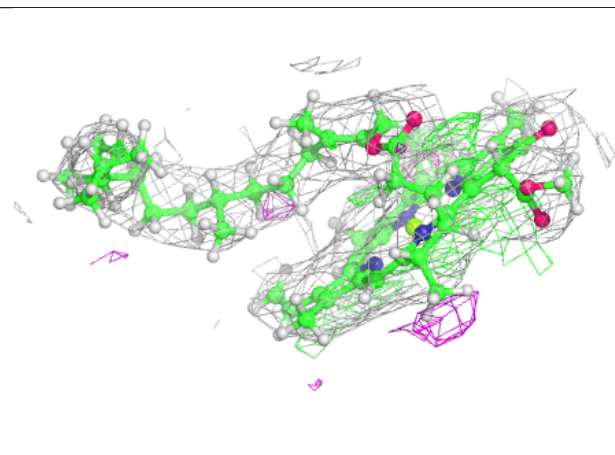
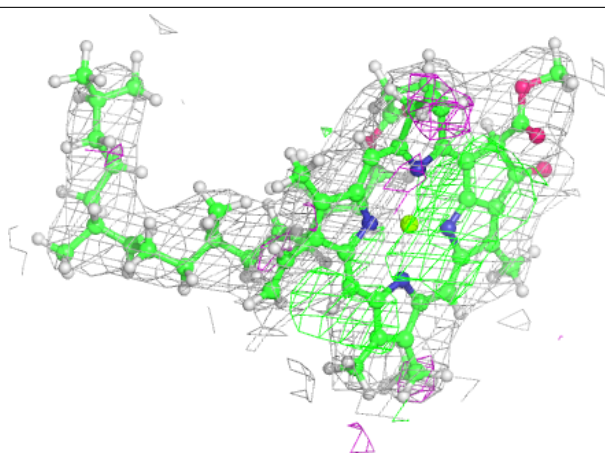
Electron density around CLA A 840:

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



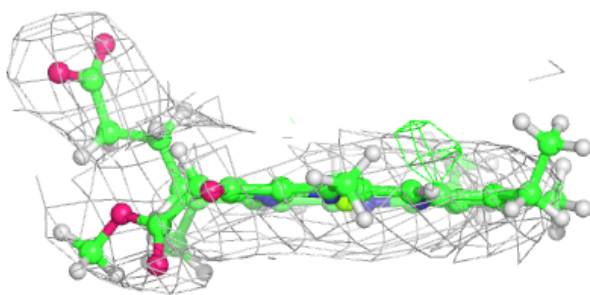
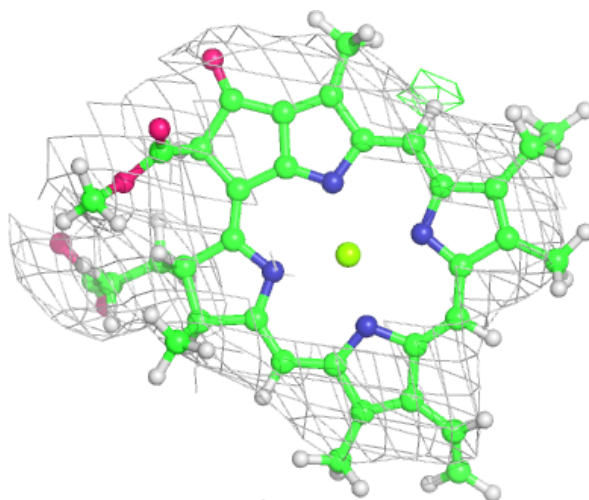
Electron density around CLA A 844:

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



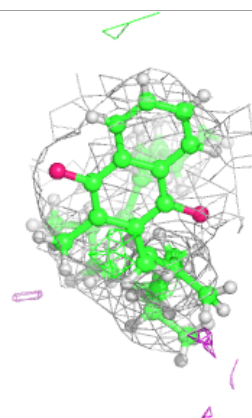
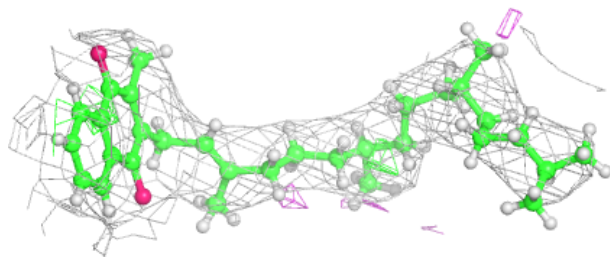
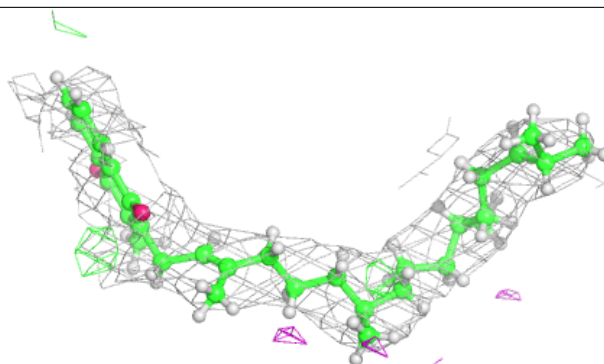
Electron density around CLA B 3024:

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



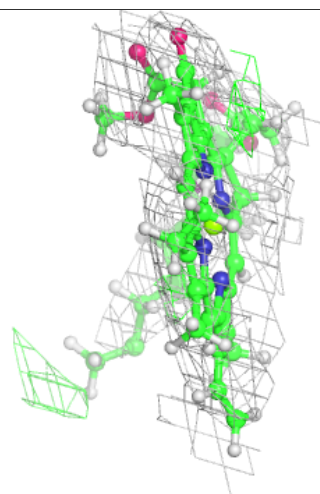
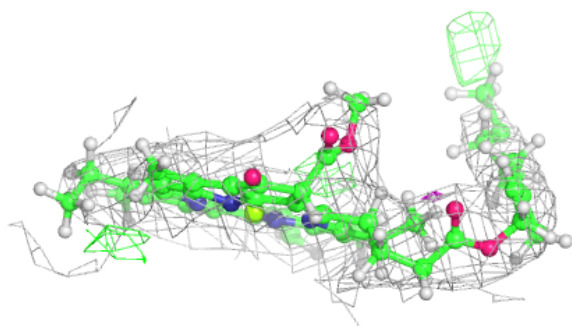
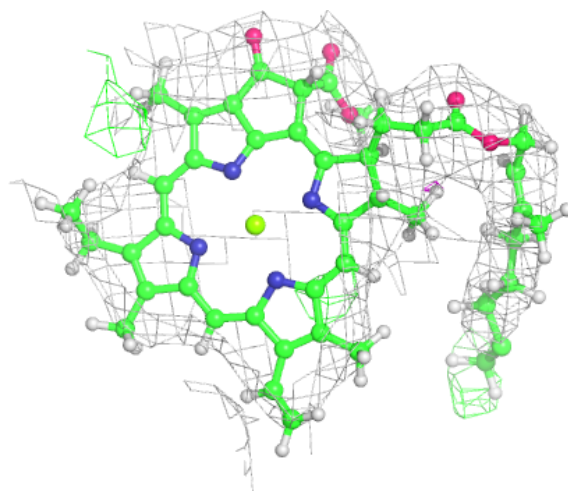
Electron density around PQN B 3043:

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



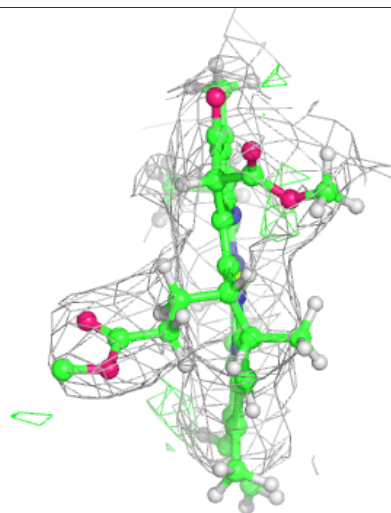
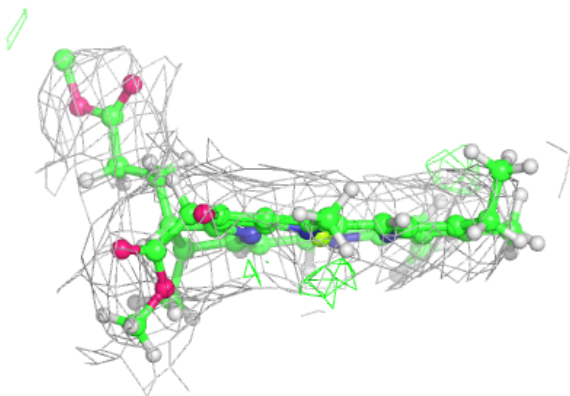
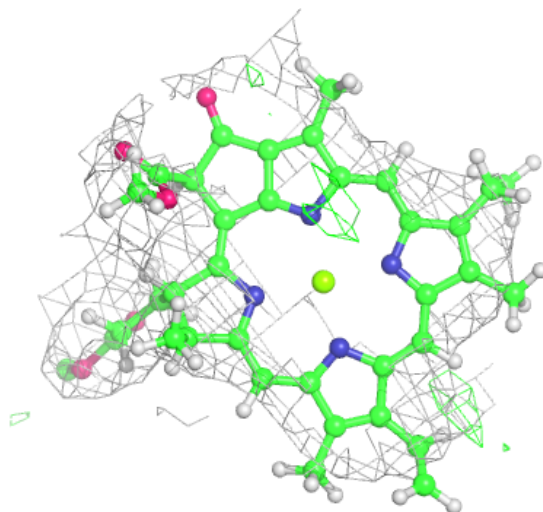
Electron density around CLA B 3025:

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



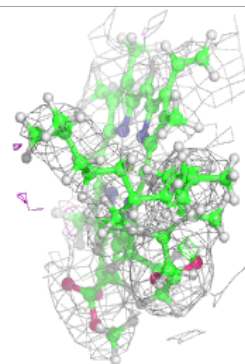
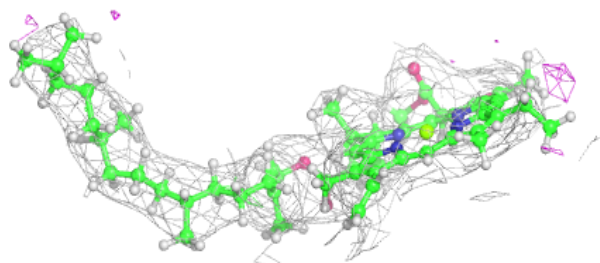
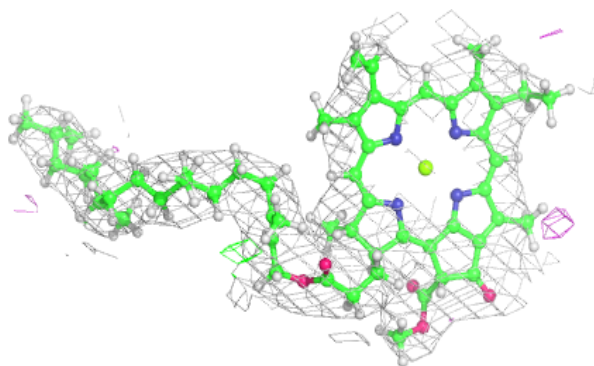
Electron density around CLA B 3026:

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



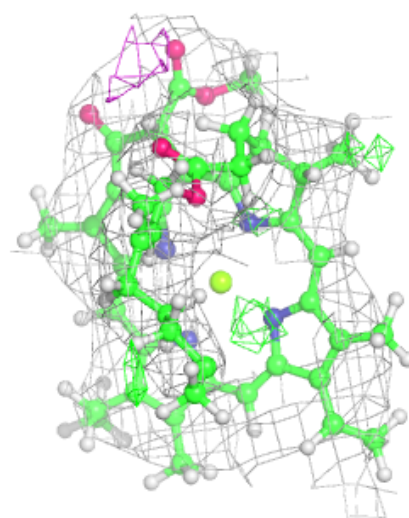
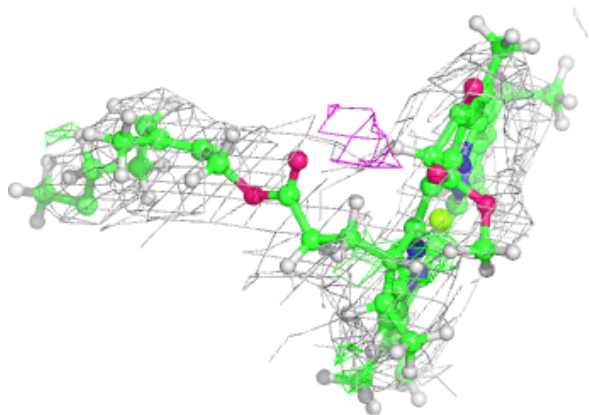
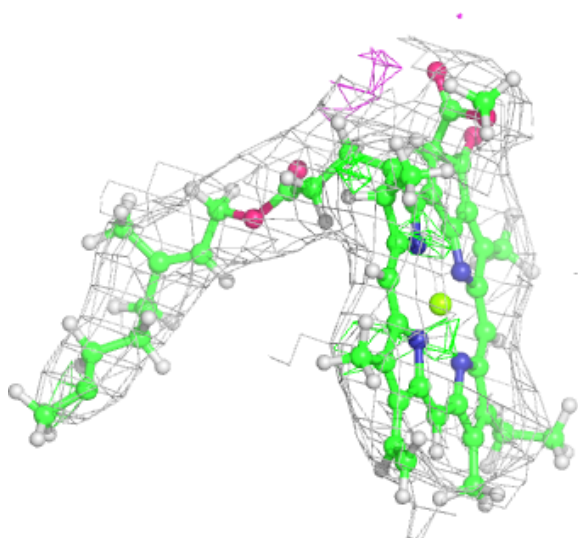
Electron density around CLA B 3004:

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



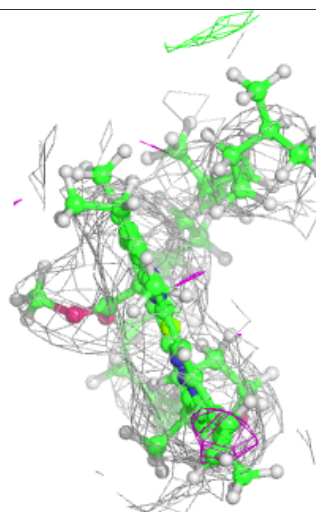
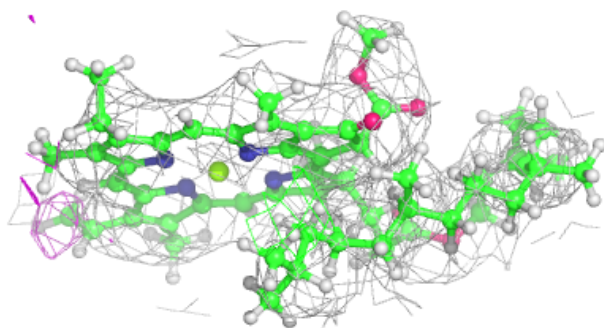
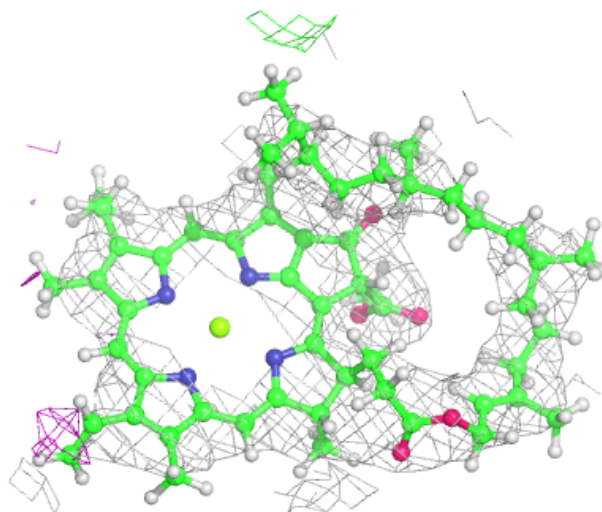
Electron density around CLA B 3005:

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



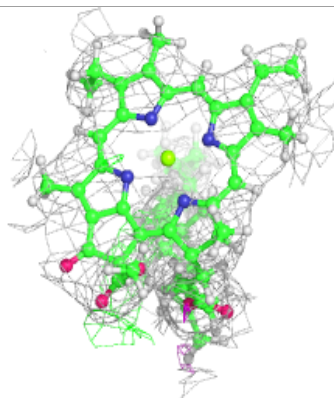
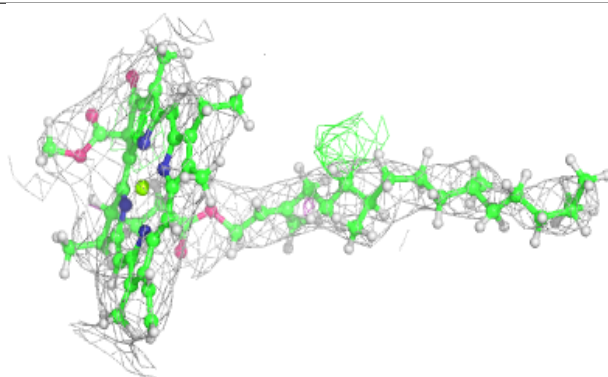
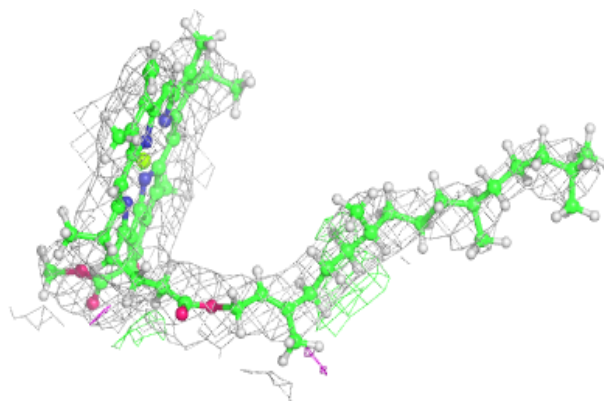
Electron density around CLA B 3006:

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



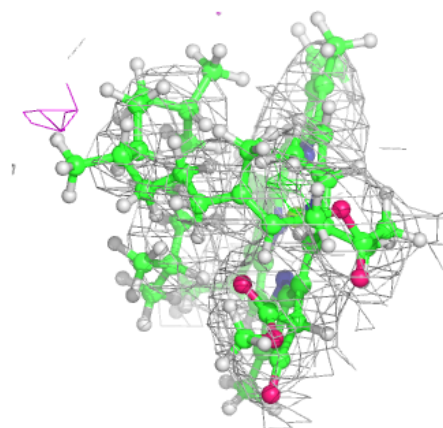
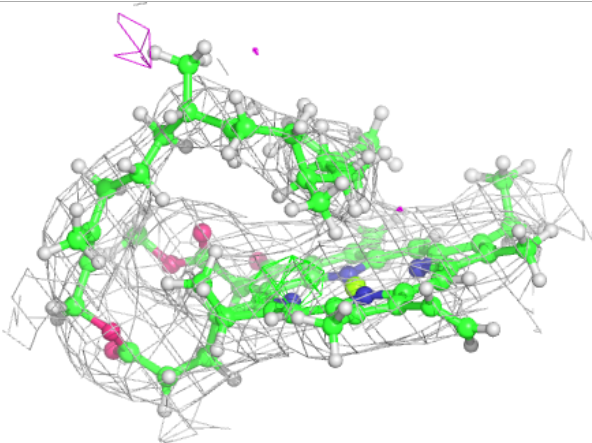
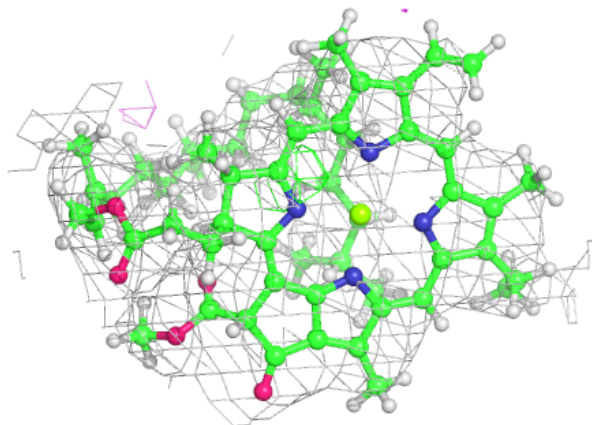
Electron density around CLA B 3030:

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



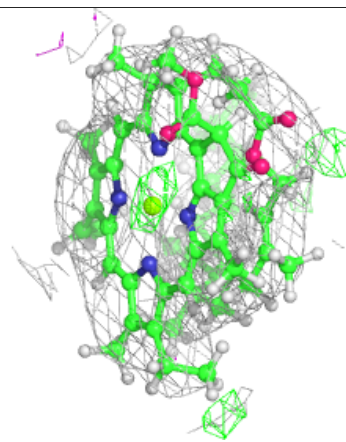
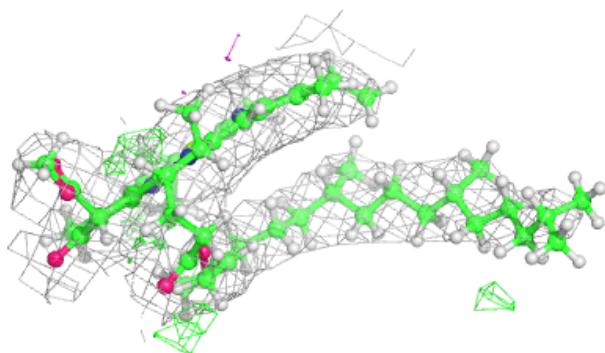
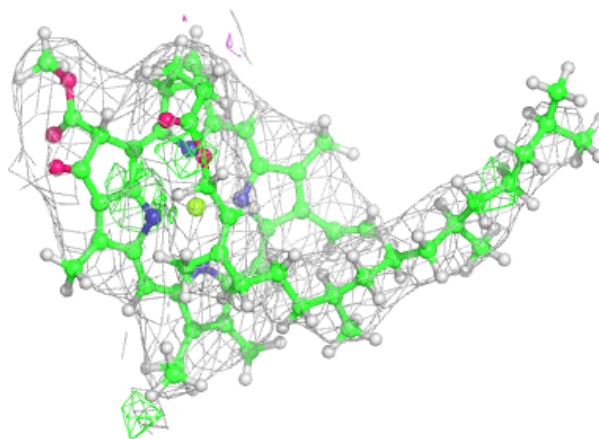
Electron density around CLA B 3007:

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



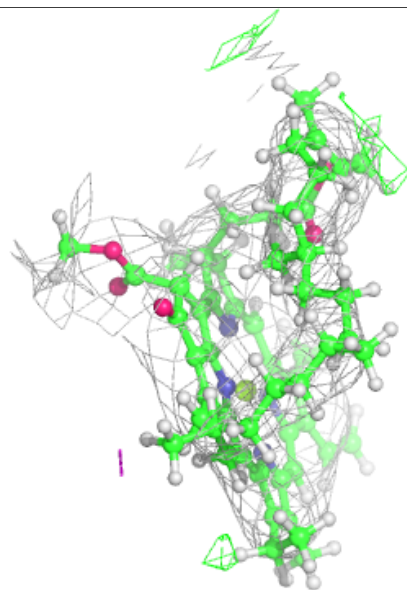
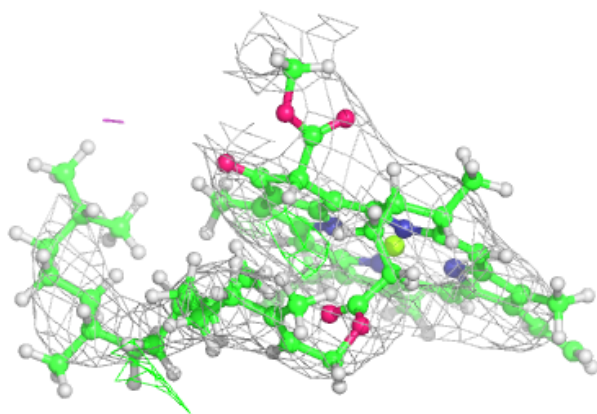
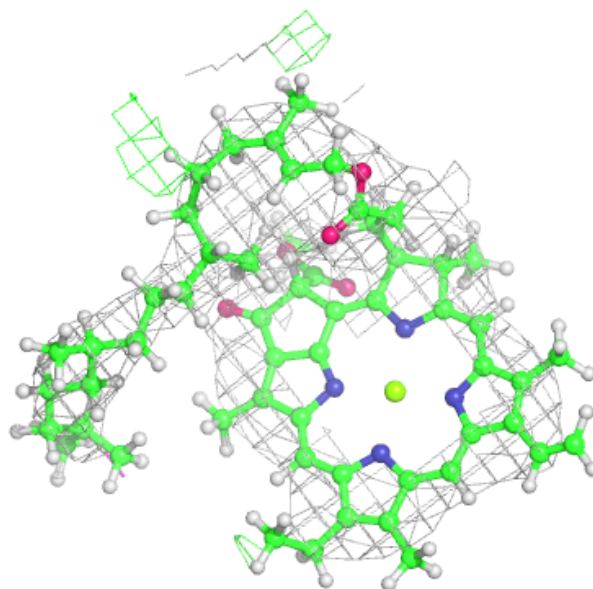
Electron density around CLA B 3008:

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



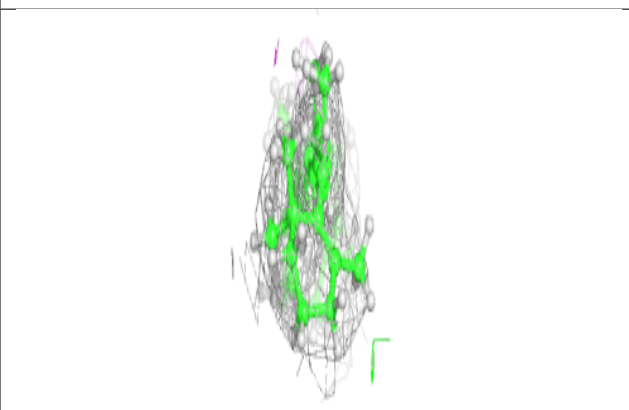
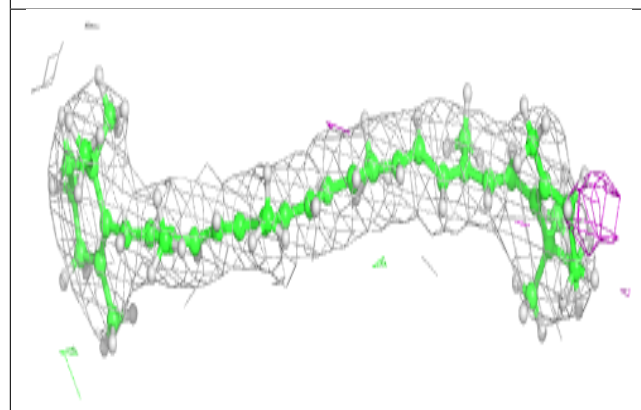
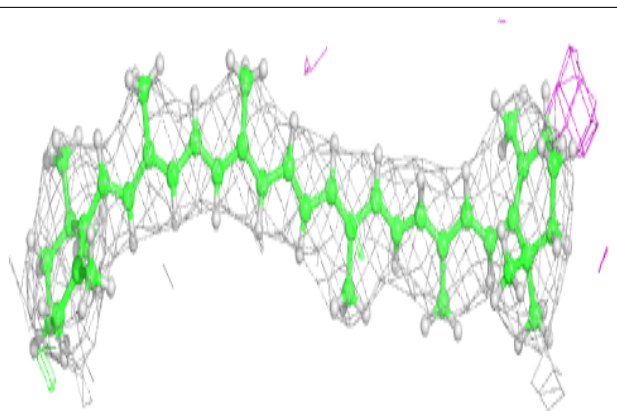
Electron density around CLA B 3033:

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



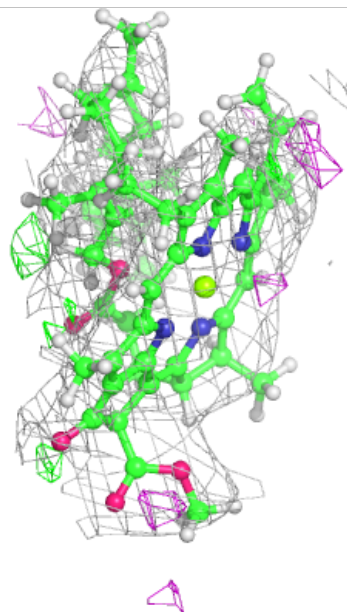
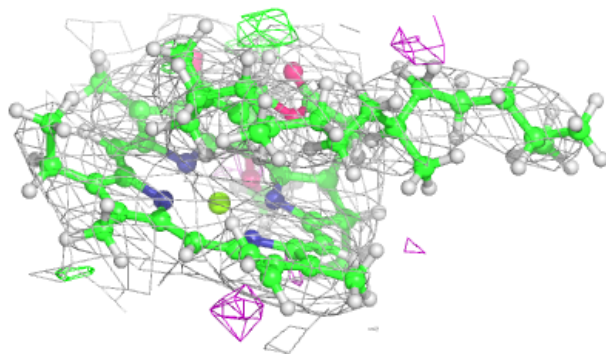
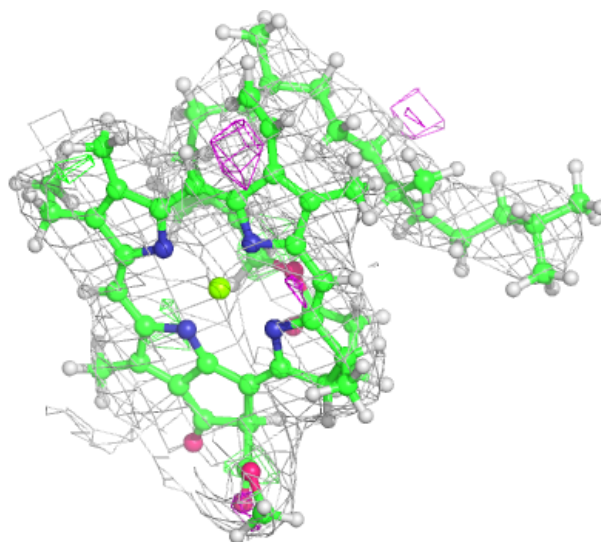
Electron density around BCR B 3048:

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



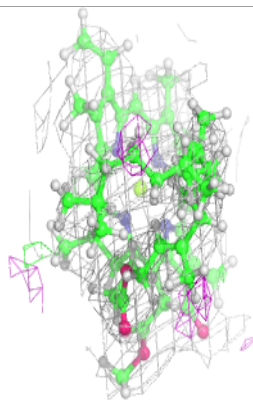
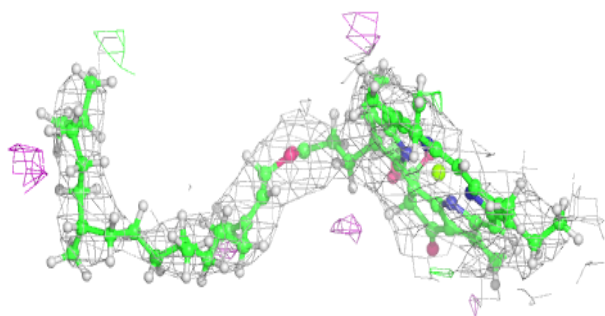
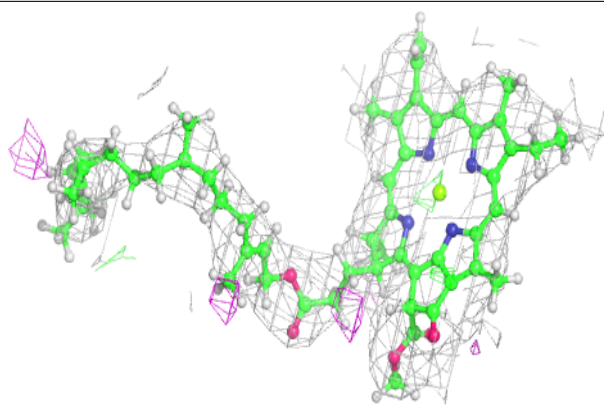
Electron density around CLA B 3009:

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

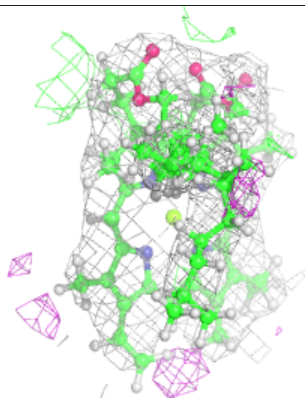
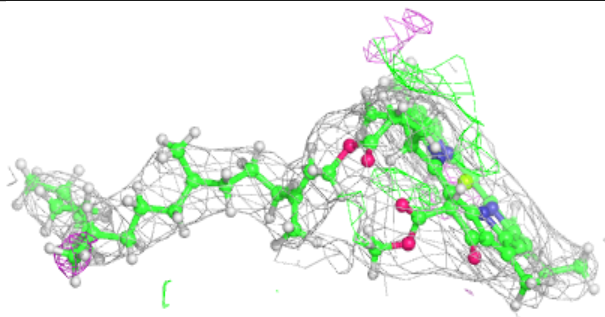
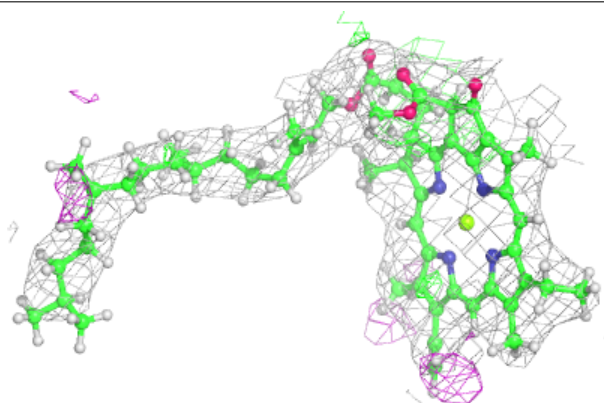


Electron density around CLA B 3010:

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

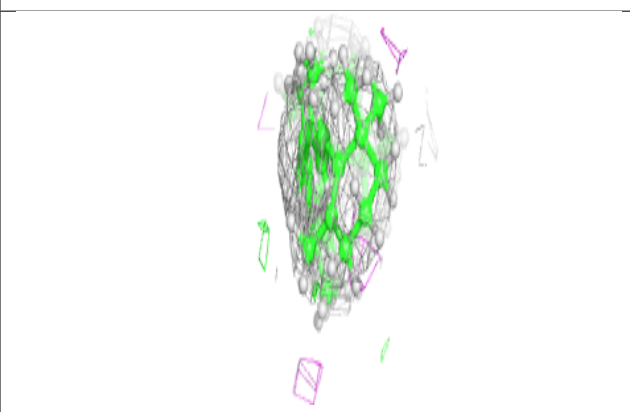
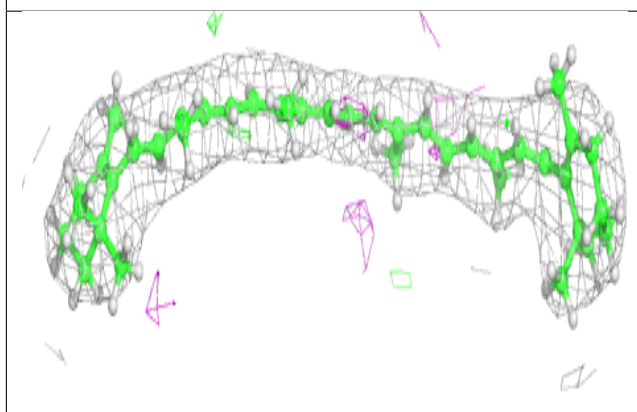
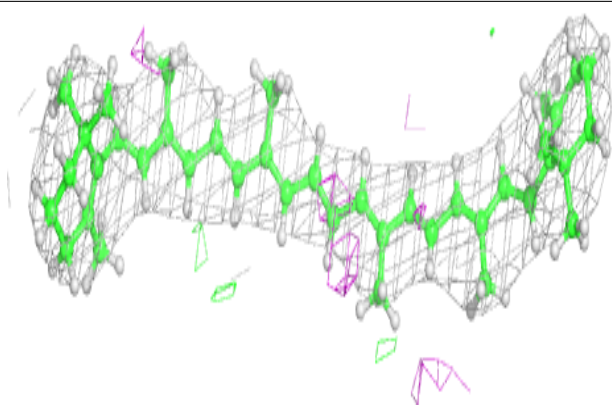
**Electron density around CLA B 3011:**

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

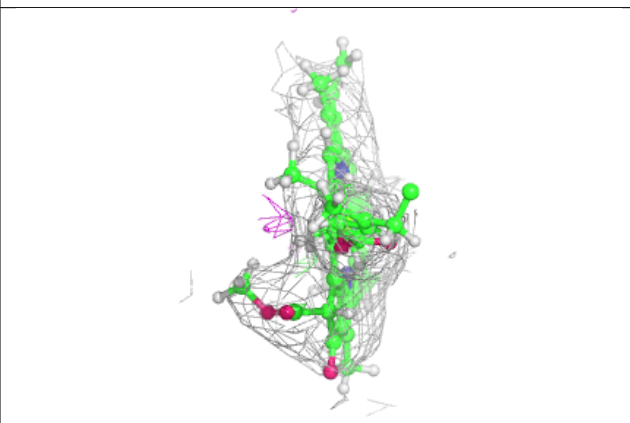
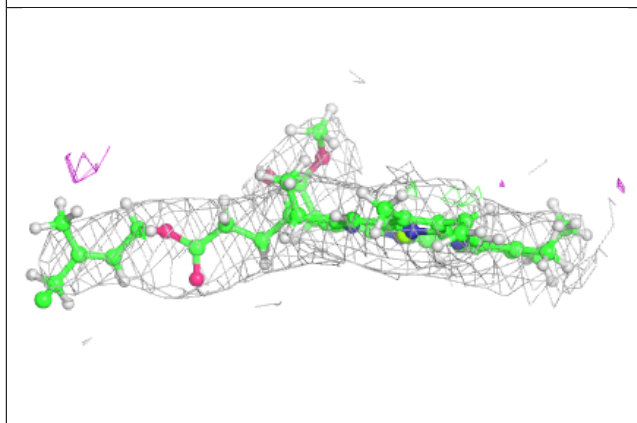
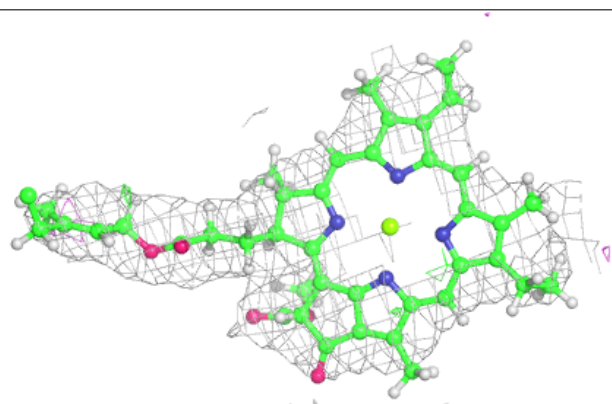


Electron density around BCR I 101:

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

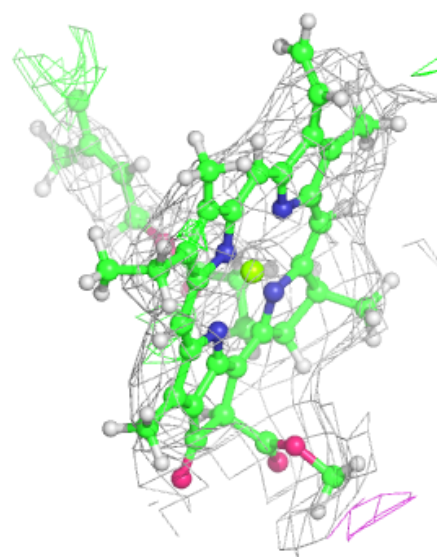
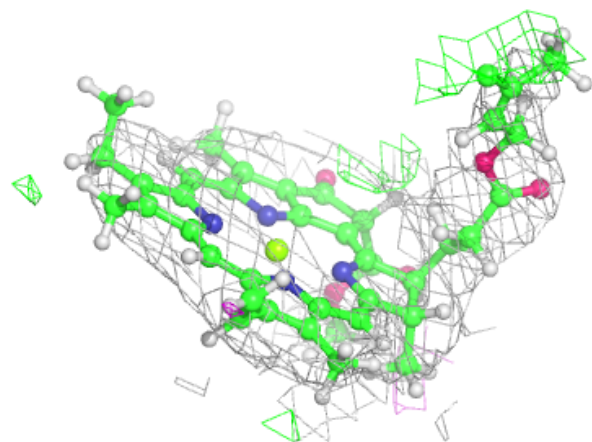
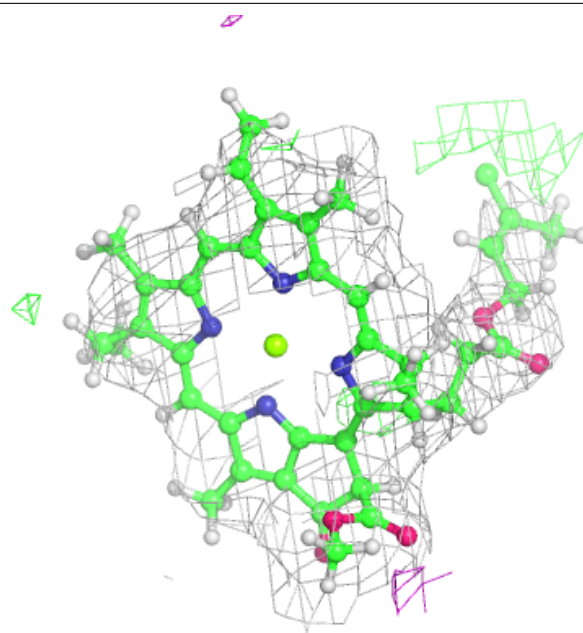
**Electron density around CLA A 838:**

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



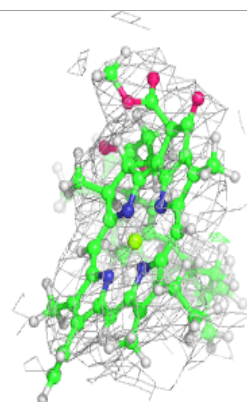
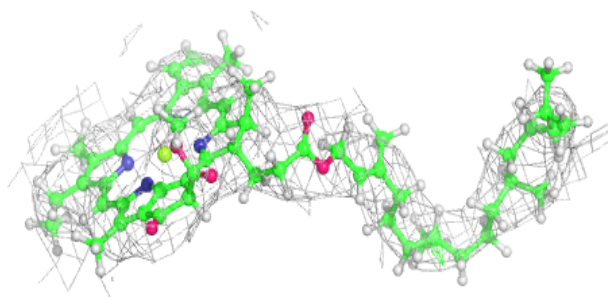
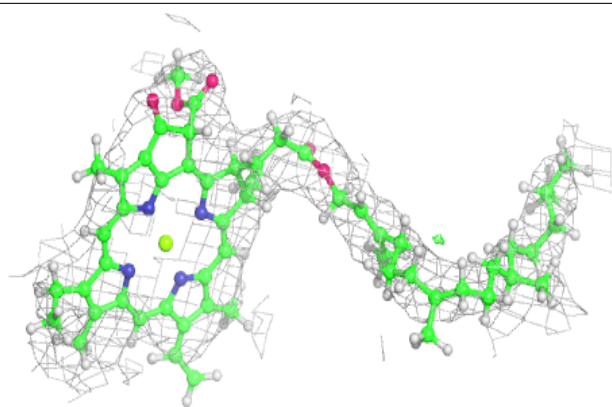
Electron density around CLA A 832:

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

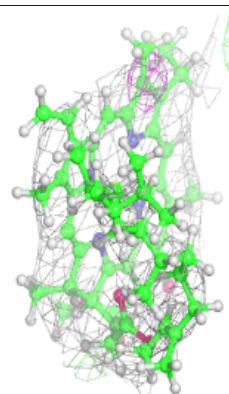
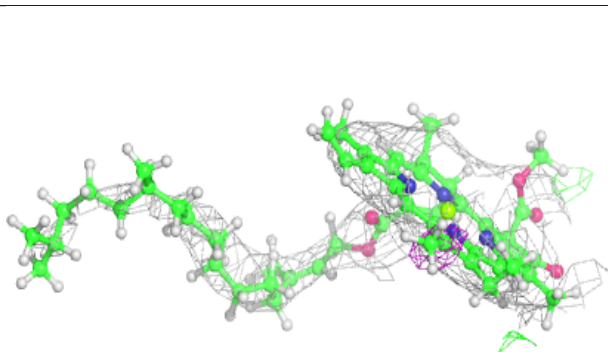
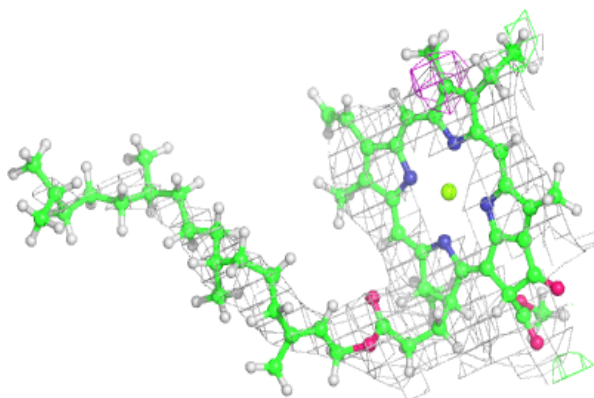


Electron density around CLA B 3014:

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

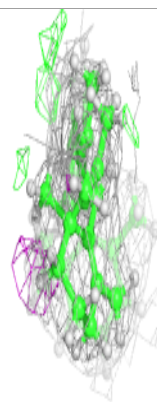
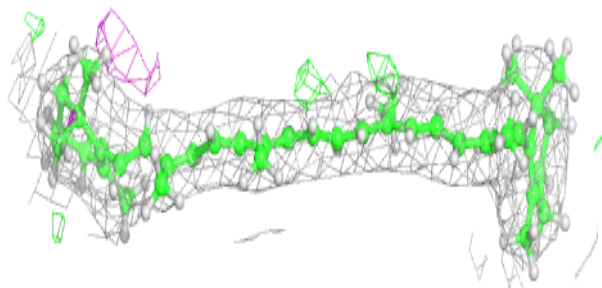
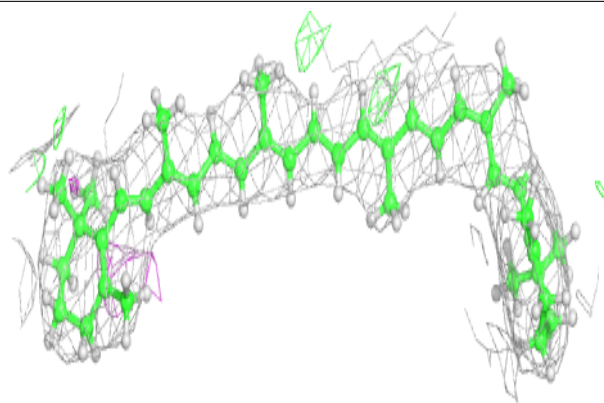
**Electron density around CLA A 809:**

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

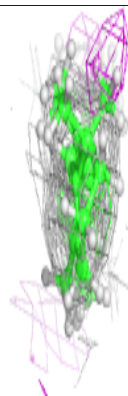
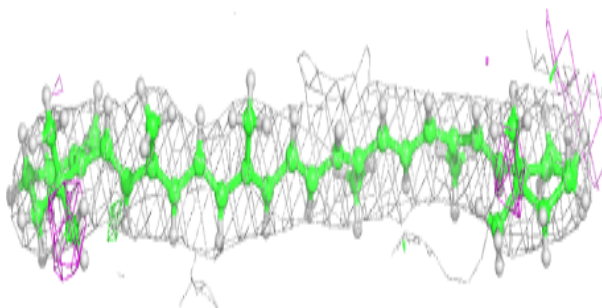
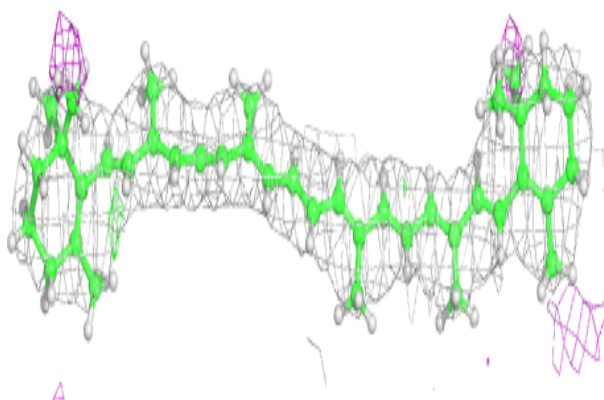


Electron density around BCR L 201:

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

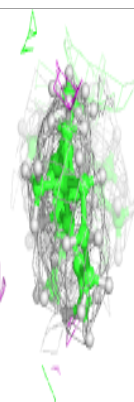
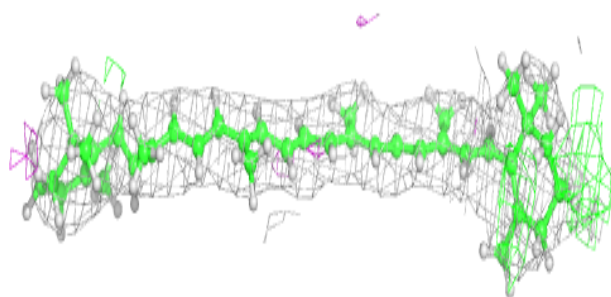
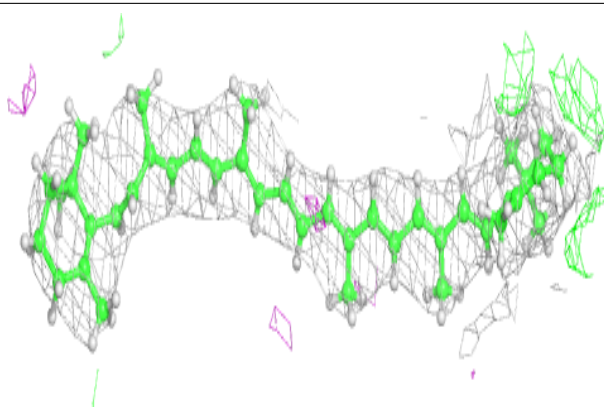
**Electron density around BCR L 208:**

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

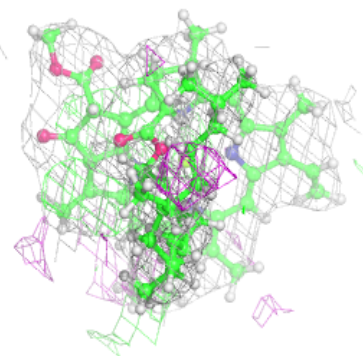
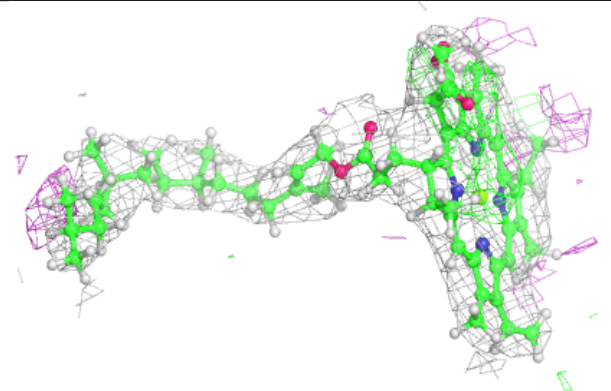
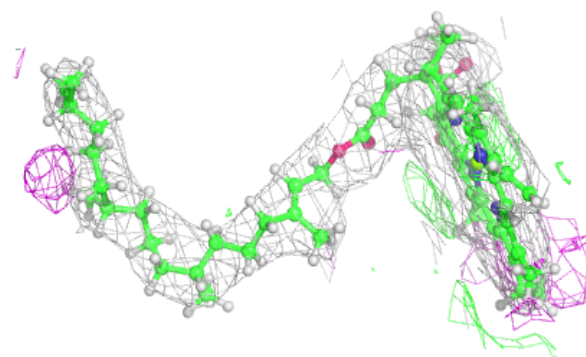


Electron density around BCR L 209:

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

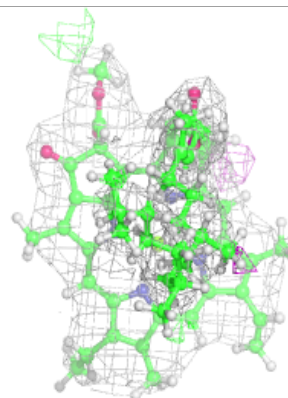
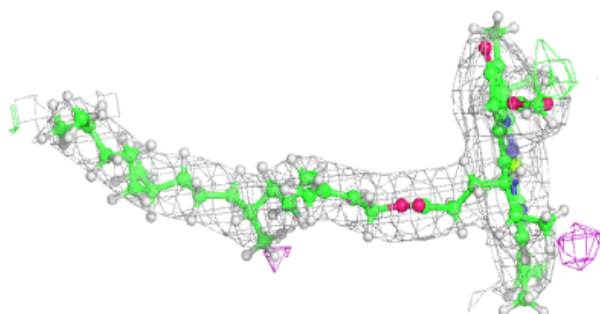
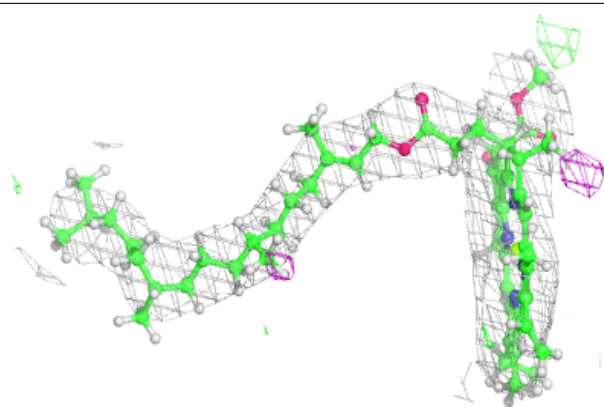
**Electron density around CLA B 3041:**

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

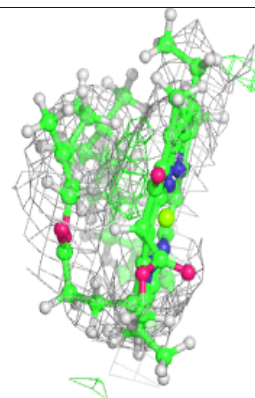
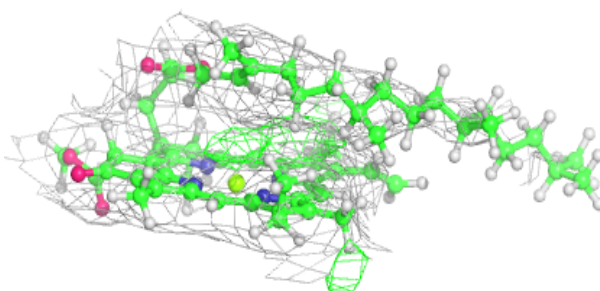
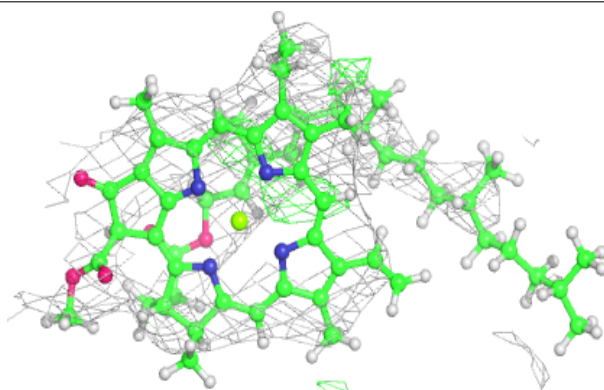


Electron density around CLA B 3042:

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

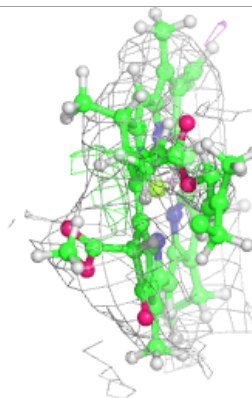
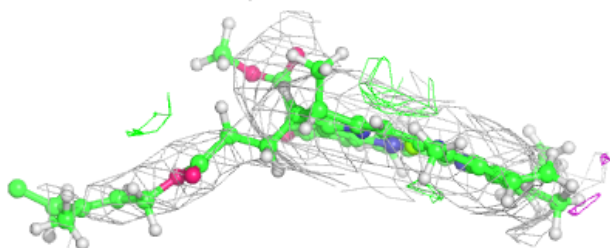
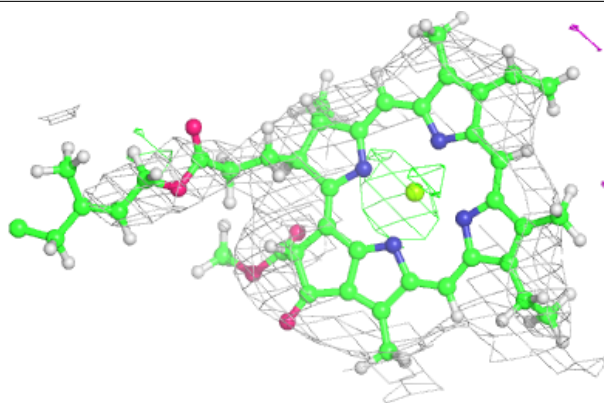
**Electron density around CLA A 841:**

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

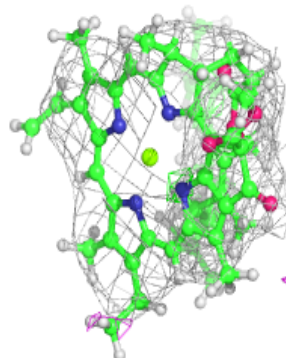
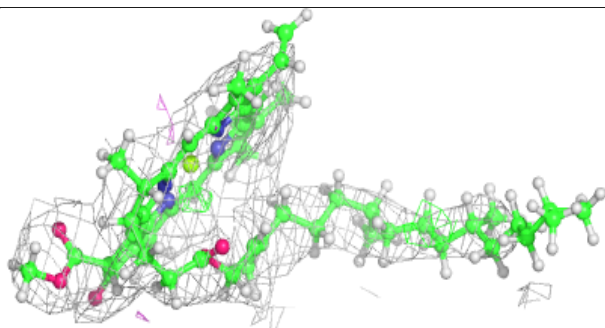
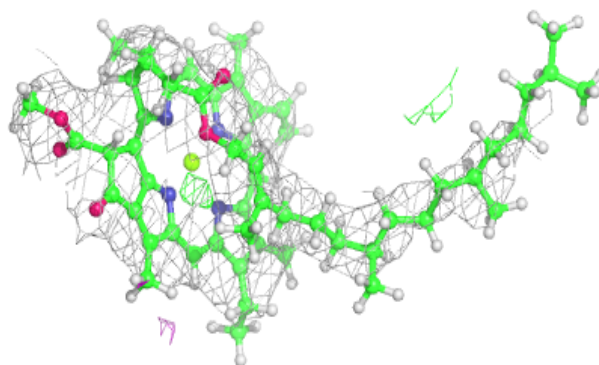


Electron density around CLA A 842:

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

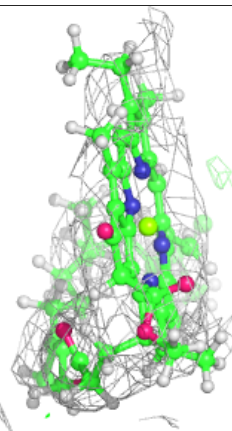
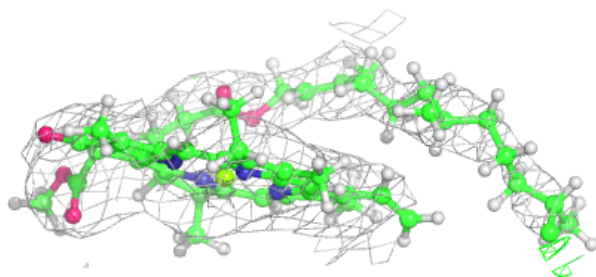
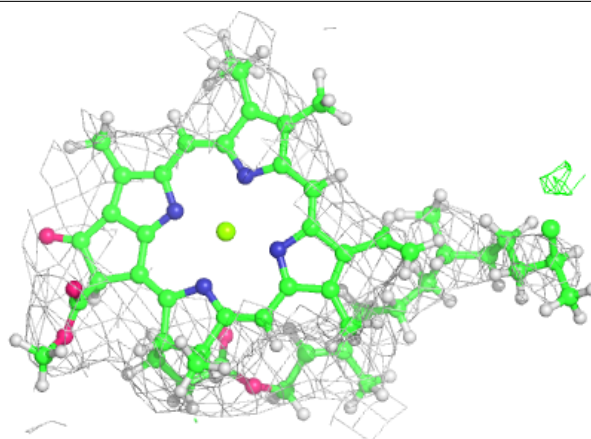
**Electron density around CLA A 843:**

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

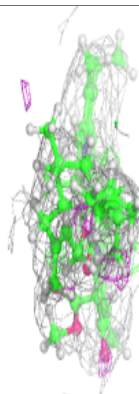
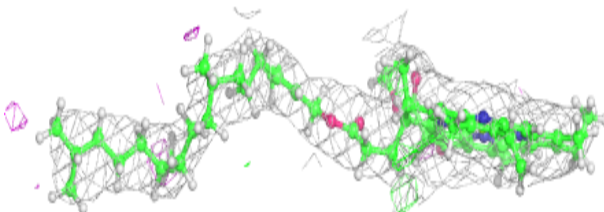
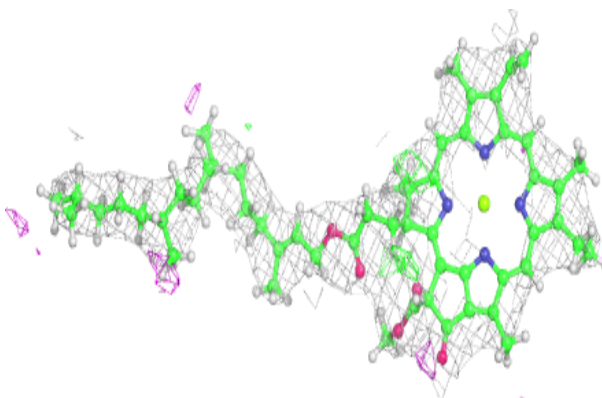


Electron density around CLA B 3019:

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

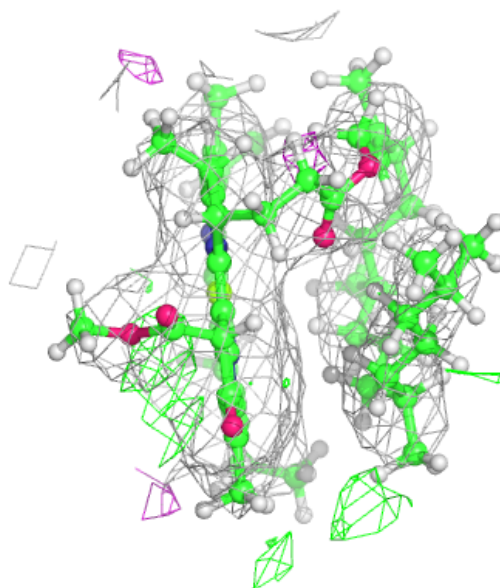
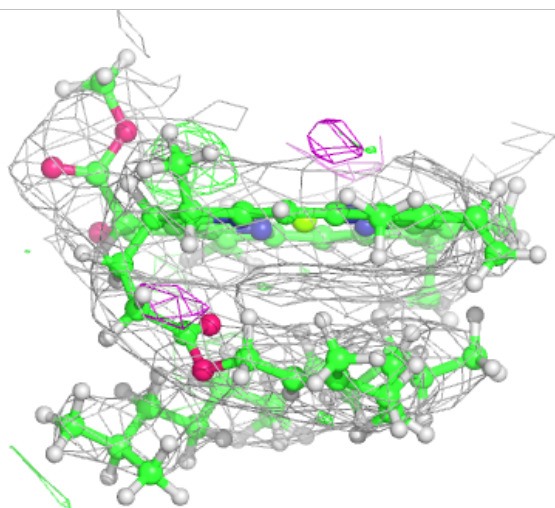
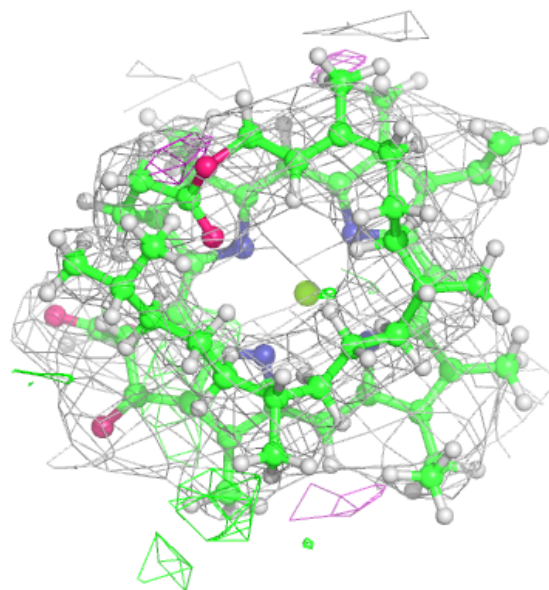
**Electron density around CLA A 834:**

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



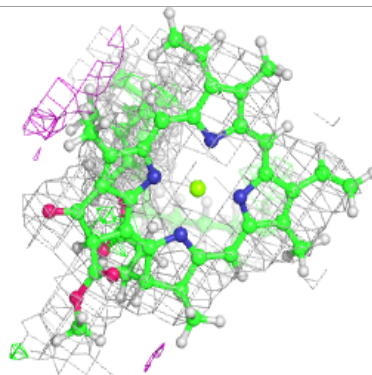
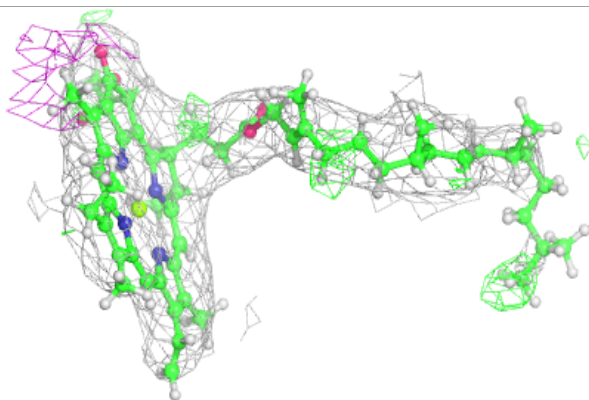
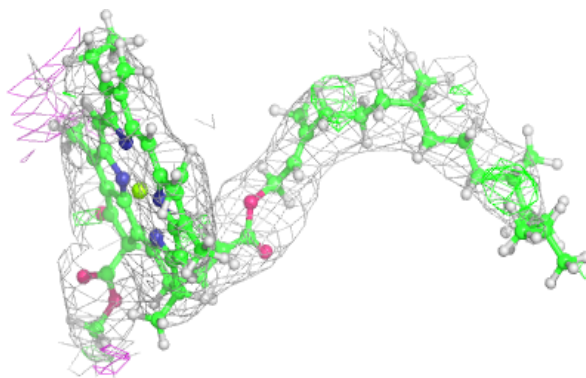
Electron density around CLA L 204:

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

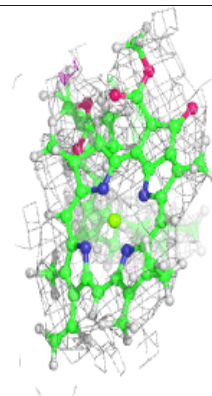
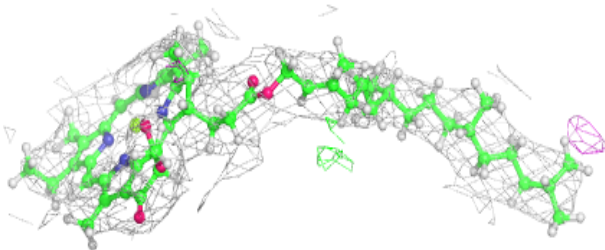
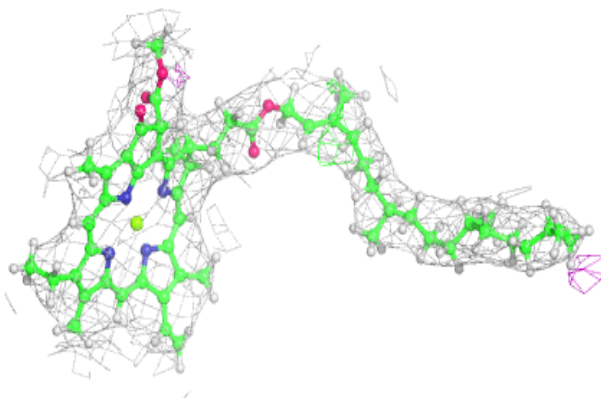


Electron density around CLA L 205:

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

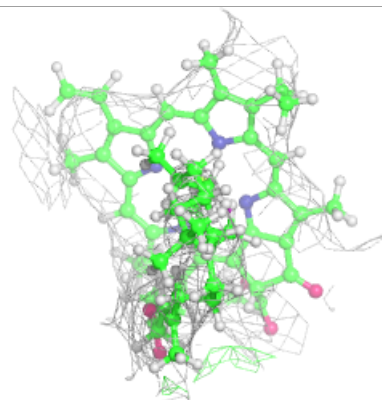
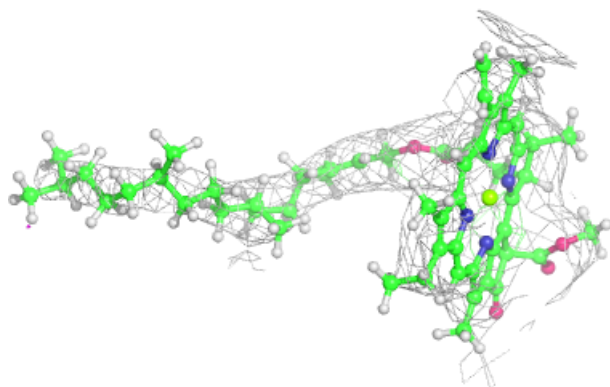
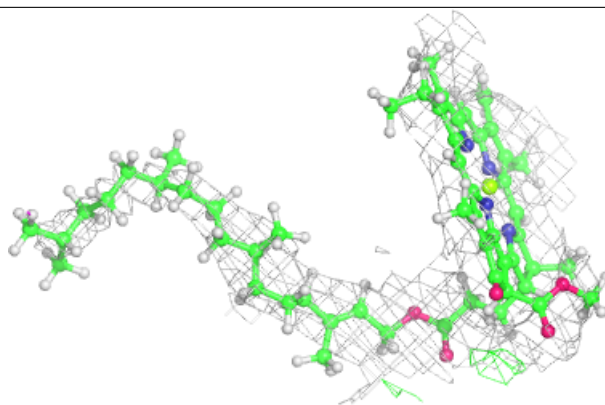
**Electron density around CLA A 802:**

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

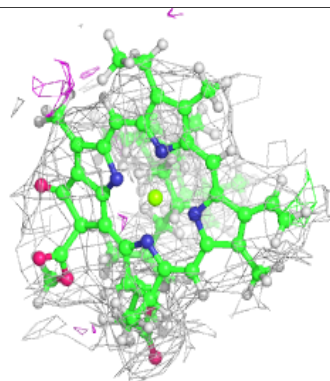
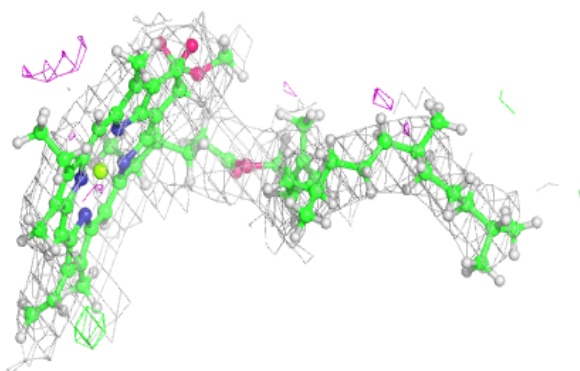
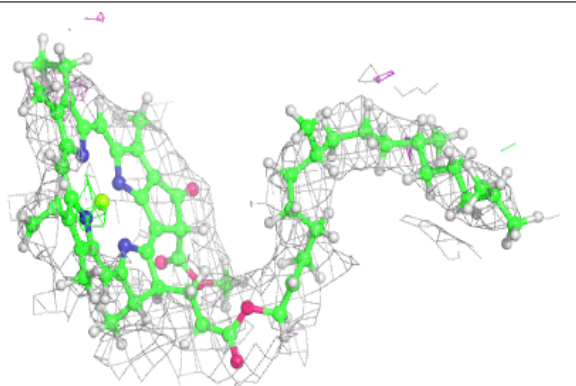


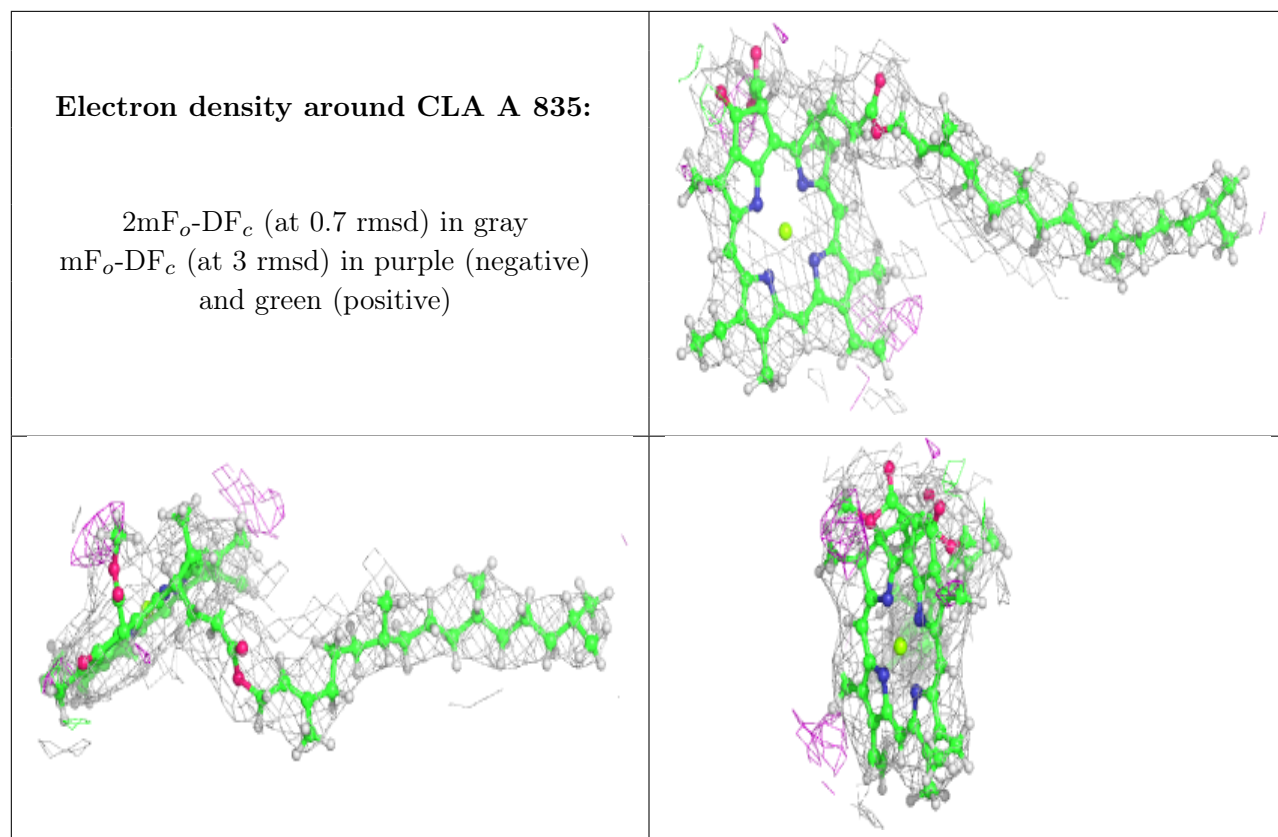
Electron density around CLA A 831:

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

**Electron density around CLA B 3003:**

$2mF_o-DF_c$ (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.