



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:51 PM UTC

PDB ID : 7M76 / pdb_00007m76
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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

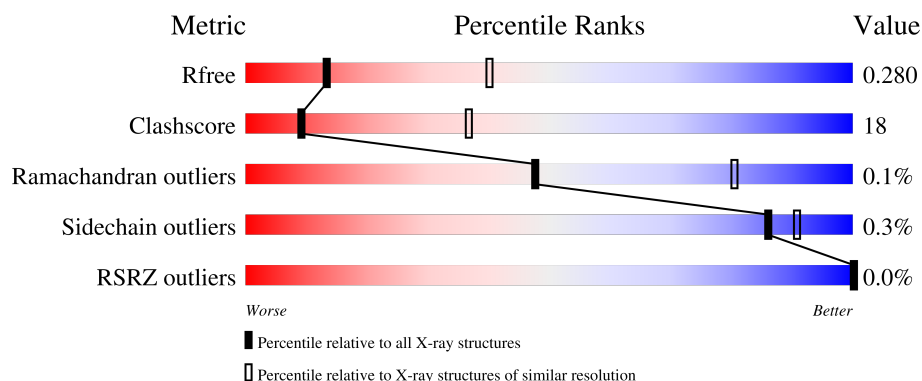
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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	59% 39% .
2	B	740	66% 34%
3	C	80	68% 31% .
4	D	138	68% 32%

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Mol	Chain	Length	Quality of chain
5	E	75	
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	824	X	-	-	-
14	CLA	A	825	X	-	-	-
14	CLA	A	826	X	-	-	-
14	CLA	A	827	X	-	-	-
14	CLA	A	828	X	-	-	-
14	CLA	A	829	X	-	-	-
14	CLA	A	830	X	-	-	-
14	CLA	A	831	X	-	-	-
14	CLA	A	832	X	-	-	-
14	CLA	A	833	X	-	-	-
14	CLA	A	834	X	-	-	-
14	CLA	A	835	X	-	-	-
14	CLA	A	836	X	-	-	-
14	CLA	A	837	X	-	-	-
14	CLA	A	838	X	-	-	-
14	CLA	A	839	X	-	-	-
14	CLA	A	840	X	-	-	-
14	CLA	A	841	X	-	-	-
14	CLA	A	842	X	-	-	-
14	CLA	A	843	X	-	-	-
14	CLA	A	844	X	-	-	-
14	CLA	A	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	3022	X	-	-	-
14	CLA	B	3023	X	-	-	-
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

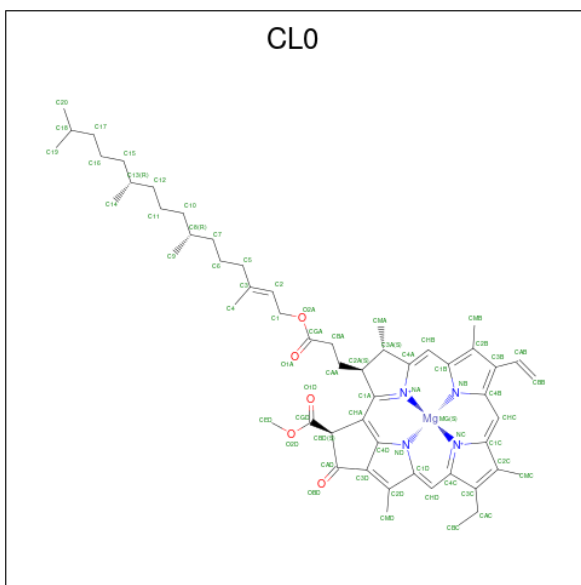
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

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.

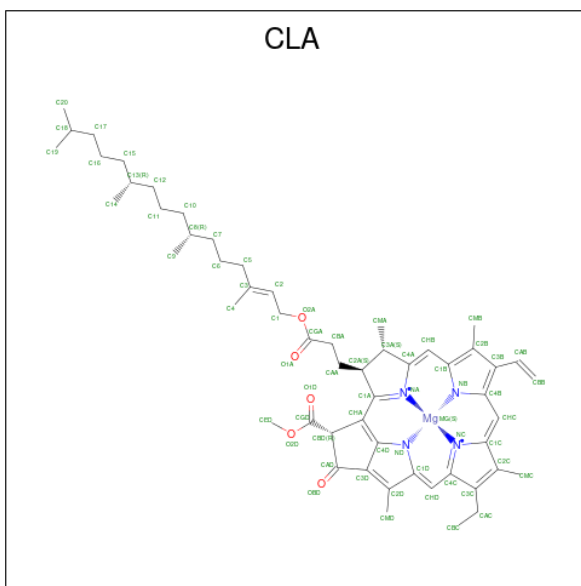
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	X	29	Total	C	H	N	O	0	0	0
			459	172	217	35	35			

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: 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 (CCD ID: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$) (labeled as "Ligand of Interest" by depositor).



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

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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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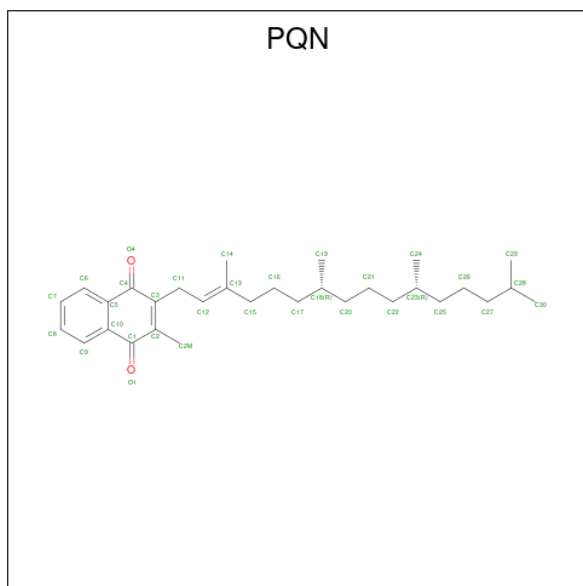
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
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			104	45	49	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			79	36	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	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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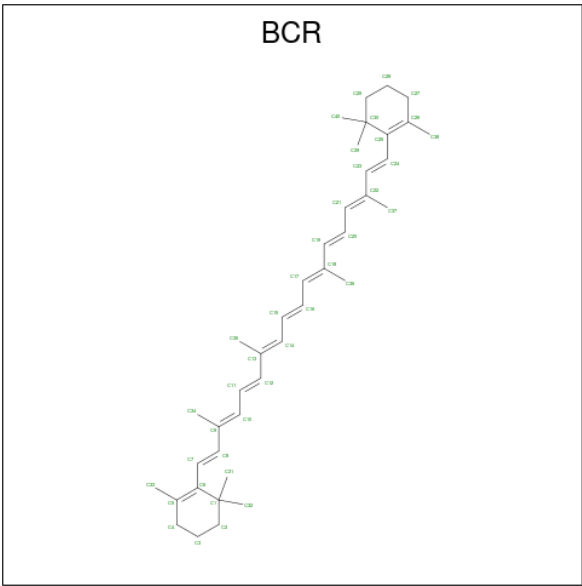
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
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			78	35	33	1	4	5		
14	J	1	Total	C	H	Mg	N	O	0	0
			62	31	25	1	4	1		
14	K	1	Total	C	H	Mg	N	O	0	0
			70	33	29	1	4	3		
14	K	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	L	1	Total	C	H	Mg	N	O	0	0
			137	55	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 (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



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 (CCD ID: BCR) (formula: C₄₀H₅₆).



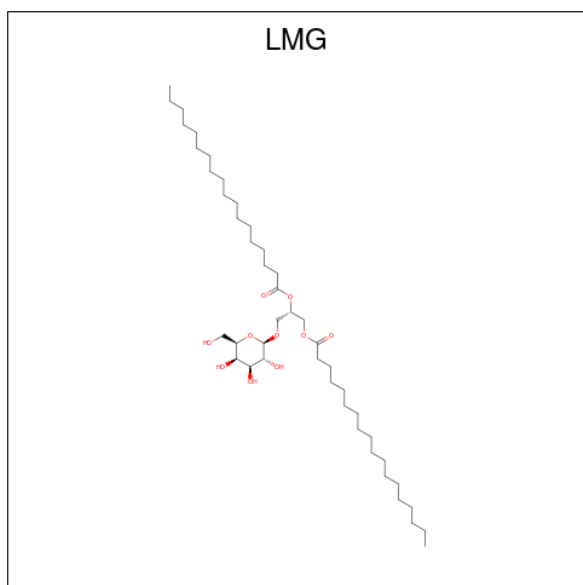
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	A	1	Total	C	H	0	0
			96	40	56		
16	A	1	Total	C	H	0	0
			96	40	56		
16	A	1	Total	C	H	0	0
			96	40	56		
16	A	1	Total	C	H	0	0
			96	40	56		
16	A	1	Total	C	H	0	0
			96	40	56		
16	B	1	Total	C	H	0	0
			96	40	56		
16	B	1	Total	C	H	0	0
			96	40	56		
16	B	1	Total	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 (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



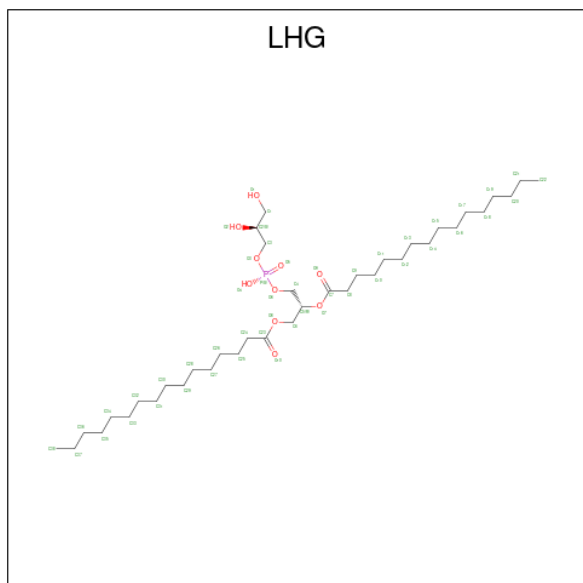
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	H	O	0	0
			118	38	70	10		
17	A	1	Total	C	H	O	0	0
			67	22	37	8		

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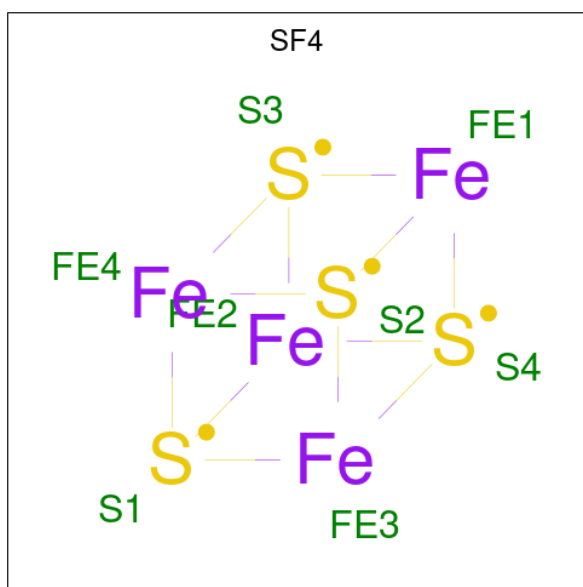
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	B	1	Total	C	H	O	0	0
			141	45	86	10		
17	I	1	Total	C	H	O	0	0
			91	30	51	10		

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: 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 (CCD ID: SF4) (formula: Fe_4S_4).

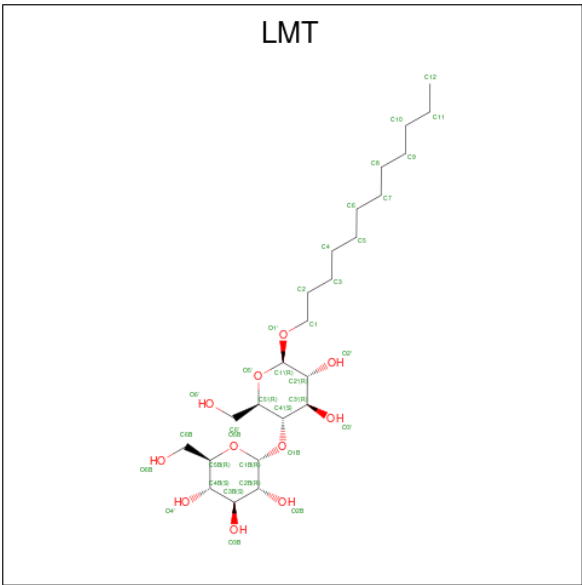


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	B	1	Total	Fe	S	0	0
			8	4	4		
19	C	1	Total	Fe	S	0	0
			8	4	4		
19	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 20 is CALCIUM ION (CCD ID: CA) (formula: Ca).

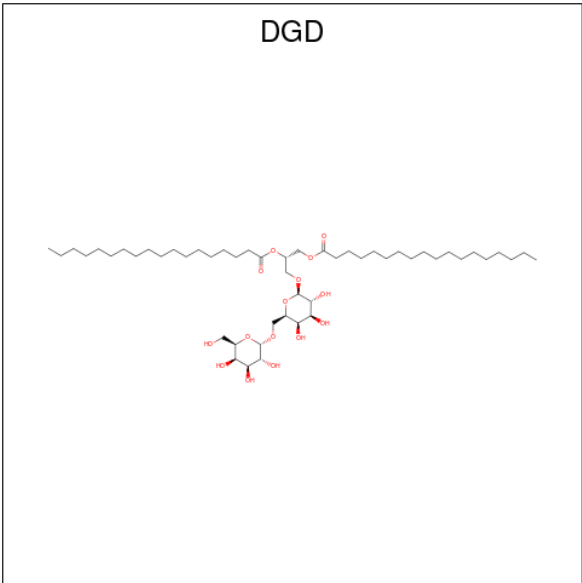
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	B	1	Total	Ca	0	0
			1	1		
20	L	1	Total	Ca	0	0
			1	1		

- Molecule 21 is DODECYL-BETA-D-MALTOSIDE (CCD ID: 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) (CCD ID: 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		

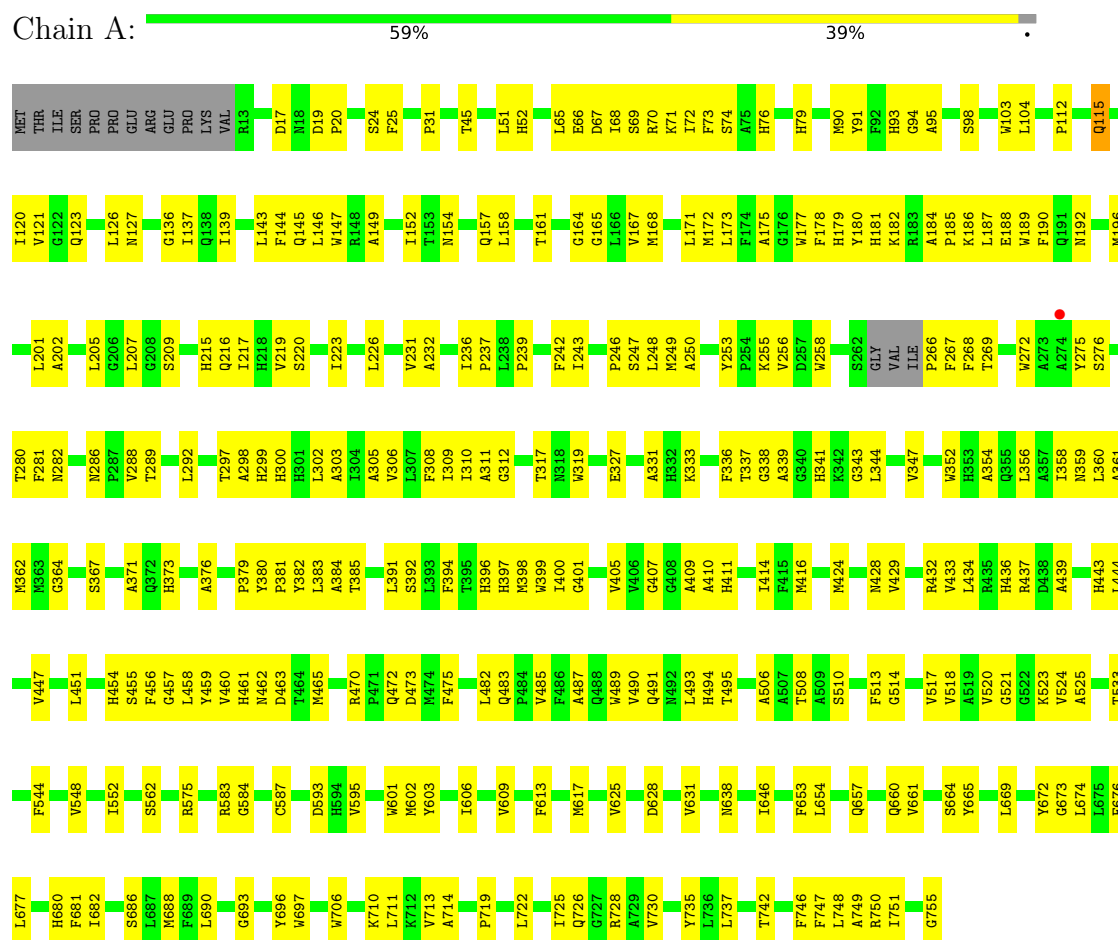
- Molecule 23 is water.

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

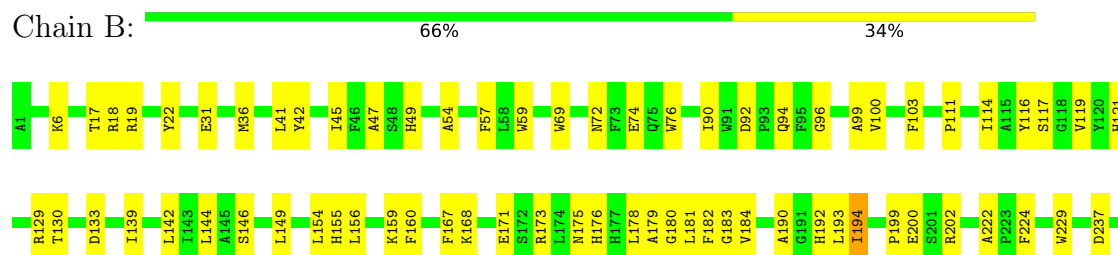
3 Residue-property plots

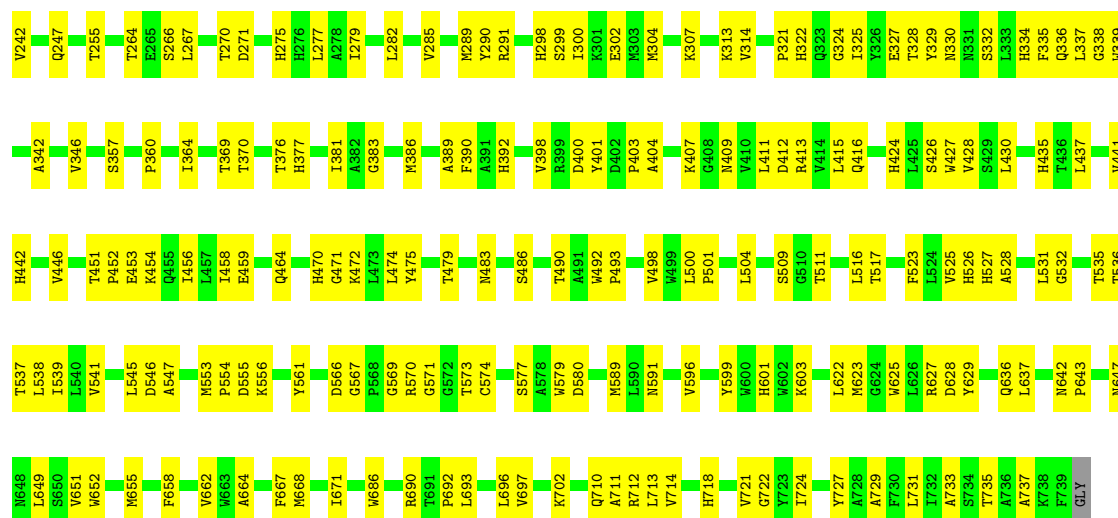
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





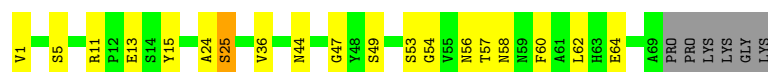
• Molecule 3: Photosystem I iron-sulfur center



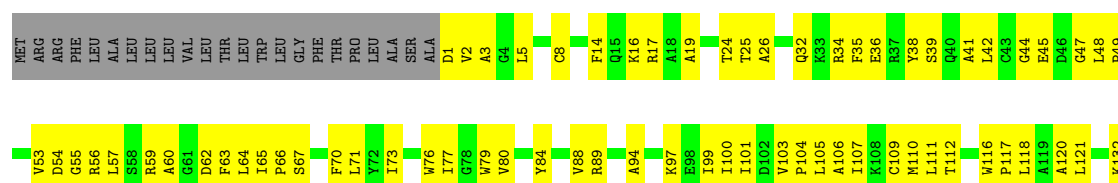
• Molecule 4: Photosystem I reaction center subunit II



• 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%



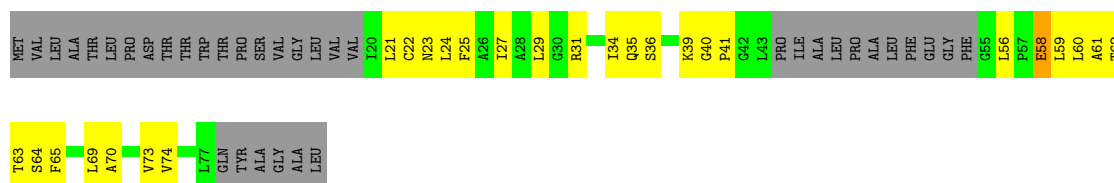
• Molecule 8: Photosystem I reaction center subunit IX

Chain J: 44% 56%



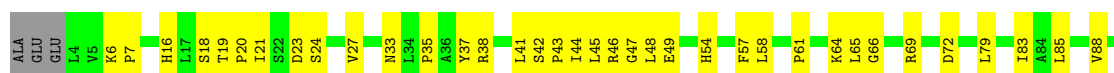
• Molecule 9: Photosystem I reaction center subunit PsaK

Chain K: 24% 31% 43%



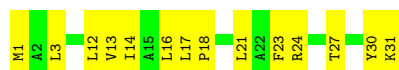
• Molecule 10: Photosystem I reaction center subunit XI

Chain L: 68% 31%



• Molecule 11: Photosystem I reaction center subunit XII

Chain M: 55% 45%



• Molecule 12: Photosystem I 4.8K protein

Chain X: 43% 40% 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 0.270 , 0.280	Depositor DCC
R_{free} test set	1997 reflections (1.31%)	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)	0.24 , 60.3	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	0.91	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: LHG, CL0, LMG, DGD, SF4, PQN, LMT, BCR, CLA, CA

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	0.27	0/5983	0.54	1/8158 (0.0%)
2	B	0.26	0/6107	0.51	0/8345
3	C	0.29	0/608	0.54	0/824
4	D	0.21	0/1101	0.50	0/1492
5	E	0.26	0/551	0.54	0/750
6	F	0.28	0/1087	0.54	0/1476
7	I	0.27	0/312	0.65	0/425
8	J	0.30	0/350	0.60	0/477
9	K	0.28	0/337	0.67	0/454
10	L	0.26	0/1148	0.55	0/1558
11	M	0.33	0/244	0.60	0/332
12	X	0.30	0/251	0.49	0/342
All	All	0.27	0/18079	0.54	1/24633 (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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	TYR	O-C-N	5.61	124.11	121.53

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	295	0
2	B	5889	5618	5649	227	0
3	C	598	576	580	28	0
4	D	1075	1077	1077	34	0
5	E	539	528	528	14	0
6	F	1065	1076	1077	75	0
7	I	301	306	306	18	0
8	J	338	347	347	28	0
9	K	333	354	354	44	0
10	L	1119	1125	1125	36	0
11	M	241	264	264	16	0
12	X	242	217	249	16	0
13	A	65	72	72	1	0
14	A	2628	2615	2615	112	0
14	B	2284	2232	2232	82	0
14	F	45	33	33	9	0
14	J	82	58	58	3	0
14	K	86	62	62	6	0
14	L	195	216	216	5	0
14	M	45	33	33	4	0
14	X	45	33	33	3	0
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	20	0
16	F	80	112	112	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	I	40	56	56	4	0
16	J	120	168	168	19	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	4	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	891	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 18.

All (891) 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
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
2:B:304:MET:HE2	2:B:325:ILE:HD11	1.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:479:THR:HG21	12:X:29:TYR:O	1.80	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
2:B:546:ASP:O	2:B:556:LYS:NZ	2.16	0.76
6:F:53:VAL:HG13	6:F:63:PHE:CD2	2.19	0.76
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
14:B:3008:CLA:H192	18:M:101:LHG:H383	1.68	0.74
1:A:376:ALA:O	1:A:510:SER:OG	2.06	0.74
1:A:465:MET:HE1	1:A:470:ARG:NH2	2.02	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: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
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
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
14:A:821:CLA:HMB2	9:K:64:SER:OG	1.95	0.67
1:A:66:GLU:OE1	1:A:186:LYS:HE2	1.95	0.67
1:A:722:LEU:HD23	1:A:726:GLN:OE1	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:306:VAL:HG21	14:A:818:CLA:HMC3	1.77	0.66
2:B:175:ASN:HB3	14:B:3021:CLA:HMD1	1.78	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
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
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
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
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:B:3041:CLA:HBC3	14:B:3041:CLA:HHD	1.81	0.62
5:E:11:ARG:HG2	5:E:13:GLU:OE1	1.98	0.62
6:F:1:ASP:OD2	6:F:42:LEU:HD21	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:528:ALA:CB	14:B:3003:CLA:H192	2.30	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
1:A:362:MET:HE3	14:A:828:CLA:H43	1.82	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
2:B:304:MET:CE	2:B:325:ILE:HD11	2.29	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
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
8:J:23:ALA:C	8:J:27:ILE:HD12	2.26	0.60
1:A:339:ALA:HB3	1:A:428:ASN:HA	1.82	0.60
2:B:553:MET:HE1	2:B:566:ASP:HB2	1.83	0.60
1:A:68:ILE:HD12	1:A:69:SER:H	1.65	0.60
2:B:401:TYR:O	4:D:126:SER:OG	2.15	0.60
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
14:F:202:CLA:HBC2	8:J:19:MET:HE3	1.82	0.59
1:A:179:HIS:CE1	14:A:811:CLA:NA	2.70	0.59
2:B:304:MET:HE2	2:B:325:ILE:CD1	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:802:CLA:OBD	14:B:3003:CLA:HMB2	2.02	0.58
14:A:844:CLA:HMB1	2:B:697:VAL:HG21	1.84	0.58
2:B:176:HIS:CE1	14:B:3013:CLA:NA	2.71	0.58
14:B:3016:CLA:HMB1	16:B:3046:BCR:H352	1.85	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
2:B:601:HIS:HD1	2:B:629:TYR:HE1	1.52	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
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
14:A:825:CLA:HBB1	14:A:825:CLA:HMB3	1.85	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
22:L:207:DGD:O5D	22:L:207:DGD:O4D	2.21	0.57
1:A:358:ILE:HD11	23:A:902:HOH:O	2.03	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
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
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:834:CLA:HMD1	14:A:835:CLA:H143	1.86	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
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:B:3007:CLA:CBB	16:B:3045:BCR:H402	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
10:L:64:LYS:O	10:L:65:LEU:HD23	2.06	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
2:B:304:MET:HE3	2:B:304:MET:HA	1.87	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
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
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
11:M:24:ARG:HD2	14:M:102:CLA:HMA2	1.88	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
12:X:20:LEU:C	12:X:20:LEU:HD13	2.32	0.55
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
1:A:280:THR:HG22	1:A:281:PHE:N	2.22	0.54
3:C:60:ASP:HB2	5:E:58:ASN:CG	2.33	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
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
2:B:307:LYS:C	2:B:314:VAL:HG23	2.33	0.54
2:B:47:ALA:HB2	2:B:156:LEU:HG	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:65:PHE:HE1	9:K:69:LEU:HD11	1.74	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
7:I:17:VAL:O	7:I:18:VAL:C	2.52	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
14:K:101:CLA:HMB3	14:K:101:CLA:HBB1	1.90	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
1:A:205:LEU:HD12	14:A:820:CLA:HMC3	1.90	0.53
4:D:119:ILE:HD12	4:D:119:ILE:H	1.74	0.53
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
14:A:812:CLA:HBB1	14:A:812:CLA:HMB3	1.90	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:437:LEU:O	2:B:441:VAL:HG12	2.09	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:X:34:LEU:C	12:X:35:LYS:HG3	2.35	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
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
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
2:B:31:GLU:OE1	2:B:334:HIS:NE2	2.36	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
1:A:432:ARG:O	14:A:832:CLA:HED1	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:584:GLY:HA3	3:C:76:MET:HE2	1.94	0.50
6:F:80:VAL:CG2	6:F:110:MET:HA	2.41	0.50
1:A:201:LEU:C	1:A:201:LEU:HD13	2.36	0.50
1:A:299:HIS:HB3	14:A:819:CLA:HMB2	1.93	0.50
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:306:VAL:CG2	14:A:818:CLA:HMC3	2.41	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
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
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
2:B:357:SER:CB	14:B:3027:CLA:HMC2	2.42	0.50
2:B:642:ASN:HB2	2:B:643:PRO:CD	2.42	0.50
1:A:139:ILE:C	1:A:139:ILE:HD12	2.37	0.49
1:A:168:MET:HA	1:A:171:LEU:CD2	2.41	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
2:B:277:LEU:C	2:B:277:LEU:HD23	2.37	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
2:B:570:ARG:N	5:E:47:GLY:O	2.46	0.49
5:E:53:SER:OG	5:E:54:GLY:N	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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
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
1:A:416:MET:HE1	1:A:434:LEU:HD21	1.95	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
2:B:291:ARG:NH2	2:B:302:GLU:OE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:ASP:OD1	2:B:416:GLN:NE2	2.44	0.48
5:E:11:ARG:HD3	5:E:64:GLU:CD	2.39	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
2:B:90:ILE:HD11	14:B:3010:CLA:HMD1	1.95	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:821:CLA:HMA3	9:K:61:ALA:CB	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
6:F:84:TYR:CD1	6:F:84:TYR:C	2.92	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
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
9:K:60:LEU:O	9:K:61:ALA:C	2.57	0.48
10:L:47:GLY:HA2	10:L:120:PHE:CE1	2.49	0.48
12:X:25:LEU:C	12:X:25:LEU:HD23	2.39	0.48
2:B:589:MET:SD	2:B:589:MET:C	2.97	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
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
1:A:337:THR:OG1	18:A:854:LHG:O2	2.32	0.47
18:B:3050:LHG:O1	12:X:12:ARG:NH2	2.42	0.47
1:A:79:HIS:CE1	14:A:806:CLA:HMA2	2.50	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:369:THR:HA	2:B:735:THR:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:B:627:ARG:HH21	2:B:628:ASP:CG	2.23	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
1:A:465:MET:HE3	1:A:473:ASP:CB	2.45	0.47
2:B:92:ASP:O	2:B:94:GLN:N	2.47	0.47
2:B:192:HIS:O	2:B:193:LEU:C	2.58	0.47
2:B:264:THR:OG1	2:B:266:SER:HB3	2.15	0.47
2:B:509:SER:C	2:B:511:THR:H	2.23	0.47
11:M:13:VAL:O	11:M:16:LEU:HB2	2.15	0.47
1:A:201:LEU:HD13	1:A:201:LEU:O	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:465:MET:HE1	1:A:470:ARG:CZ	2.45	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
16:A:851:BCR:H373	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: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
6:F:8:CYS:SG	6:F:42:LEU:C	2.98	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:90:ILE:CD1	14:B:3010:CLA:HMD1	2.45	0.46
2:B:531:LEU:O	2:B:532:GLY:C	2.57	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
9:K:21:LEU:CD1	14:K:101:CLA:HMD2	2.46	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
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:115:GLN:O	1:A:115:GLN:CG	2.63	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
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
11:M:17:LEU:HB3	11:M:18:PRO:CD	2.45	0.45
1:A:51:LEU:C	1:A:51:LEU:HD23	2.41	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
1:A:407:GLY:HA3	14:A:831:CLA:C2C	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:168:MET:HE3	1:A:171:LEU:HD21	1.99	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:811:CLA:CHB	14:A:813:CLA:HMD1	2.46	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
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
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
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
1:A:396:HIS:HE1	14:A:829:CLA:C1D	2.30	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:304:MET:HE3	2:B:322:HIS:HB3	1.99	0.45
2:B:357:SER:HB3	14:B:3027:CLA:HMC2	1.99	0.45
8:J:37:LEU:HD23	8:J:37:LEU:O	2.17	0.45
14:J:102:CLA:HMD2	16:J:105:BCR:H292	1.99	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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
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:286:ASN:OD1	1:A:286:ASN:C	2.61	0.44
1:A:414:ILE:HD13	14:A:831:CLA:CED	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:ASN:O	1:A:463:ASP:C	2.59	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
14:B:3016:CLA:CMB	16:B:3046:BCR:H352	2.46	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:266:PRO:C	1:A:269:THR:HG23	2.43	0.43
1:A:300:HIS:HB2	14:A:819:CLA:C1B	2.48	0.43
1:A:398:MET:CE	14:A:827:CLA:HMD2	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
6:F:35:PHE:O	6:F:39:SER:OG	2.31	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
2:B:173:ARG:CZ	14:B:3025:CLA:HMD3	2.48	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:70:PHE:O	6:F:71:LEU:C	2.60	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:677:LEU:HD13	2:B:623:MET:HE2	2.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:383:GLY:C	2:B:589:MET:HE2	2.43	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
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:552:ILE:CD1	14:B:3004:CLA:HMD3	2.49	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
12:X:15:TRP:O	12:X:19:LEU:HG	2.18	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
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:90:MET:HE1	14:A:809:CLA:H2A	2.01	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:835:CLA:H152	14:L:205:CLA:HMB3	2.01	0.43
3:C:26:GLU:HA	4:D:102:PRO:HB2	1.99	0.43
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:721:VAL:O	2:B:722:GLY:C	2.62	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:36:MET:HE2	2:B:41:LEU:HA	2.01	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
9:K:24:LEU:C	9:K:24:LEU:HD12	2.44	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
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: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
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
1:A:722:LEU:HD23	1:A:726:GLN:CD	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
11:M:30:TYR:O	11:M:31:LYS:C	2.62	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
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:103:TRP:O	1:A:104:LEU:C	2.63	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
4:D:41:MET:HE2	4:D:42:PRO:HD2	2.02	0.42
16:L:209:BCR:H20C	16:L:209:BCR:H361	1.83	0.42
1:A:67:ASP:OD1	1:A:67:ASP:C	2.62	0.42
1:A:247:SER:O	1:A:248:LEU:C	2.63	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: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
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:403:PRO:O	2:B:404:ALA:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
10:L:124:PHE:CD1	10:L:124:PHE:C	2.97	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
1:A:145:GLN:H	1:A:145:GLN:CD	2.27	0.41
2:B:159:LYS:HB2	2:B:160:PHE:CE1	2.55	0.41
2:B:555:ASP:CG	3:C:65:ARG:NH1	2.78	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
10:L:64:LYS:C	10:L:65:LEU:HD23	2.44	0.41
1:A:356:LEU:O	1:A:360:LEU:HG	2.20	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:57:LEU:HD12	6:F:57:LEU:H	1.84	0.41
6:F:107:ILE:HA	6:F:110:MET:HE3	2.01	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:386:MET:HE1	16:B:3047:BCR:C36	2.50	0.41
2:B:517:THR:O	2:B:603:LYS:NZ	2.45	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:457:GLY:HA2	1:A:460:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:44:GLY:O	6:F:45:GLU:C	2.63	0.41
6:F:80:VAL:HG11	14:F:202:CLA:HMD3	2.02	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
3:C:65:ARG:HB3	3:C:67:TYR:CE1	2.56	0.41
9:K:39:LYS:HZ1	9:K:59:LEU:CB	2.33	0.41
10:L:57:PHE:CD1	10:L:57:PHE:C	2.99	0.41
1:A:177:TRP:HB2	14:A:812:CLA:CMC	2.50	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
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: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
1:A:664:SER:HB2	1:A:669:LEU:C	2.45	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:173:LEU:C	1:A:173:LEU:HD23	2.46	0.41
1:A:465:MET:HE3	1:A:473:ASP:HB3	2.03	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
2:B:456:ILE:HG22	2:B:458:ILE:HD11	2.02	0.41
2:B:498:VAL:O	2:B:498:VAL:HG12	2.21	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
8:J:29:PHE:CD1	8:J:29:PHE:C	2.99	0.41
9:K:61:ALA:C	9:K:63:THR:H	2.29	0.41
10:L:6:LYS:HB2	10:L:7:PRO:HD2	2.03	0.41
10:L:48:LEU:O	10:L:49:GLU:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:C:22:THR:O	4:D:61:LYS:NZ	2.45	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:804:CLA:HMC2	14:A:812:CLA:C3	2.50	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:455:SER:OG	1:A:456:PHE:N	2.52	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
1:A:104:LEU:O	1:A:104:LEU:HD12	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:LEU:HD12	1:A:613:PHE:HE1	1.86	0.40
14:A:834:CLA:HMD1	14:A:835:CLA:C14	2.51	0.40
16:A:851:BCR:H20C	16:A:851:BCR:H361	1.82	0.40
2:B:304:MET:HE2	2:B:325:ILE:CG1	2.51	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
1:A:697:TRP:CZ2	15:A:846:PQN:H2M3	2.56	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%)	48	80
3	C	78/80 (98%)	71 (91%)	7 (9%)	0	100	100
4	D	136/138 (99%)	122 (90%)	14 (10%)	0	100	100
5	E	67/75 (89%)	56 (84%)	10 (15%)	1 (2%)	8	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	48	80

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%)	587 (100%)	2 (0%)	86	91
2	B	597/597 (100%)	595 (100%)	2 (0%)	86	91
3	C	67/67 (100%)	66 (98%)	1 (2%)	57	80
4	D	115/115 (100%)	115 (100%)	0	100	100
5	E	59/64 (92%)	59 (100%)	0	100	100
6	F	109/128 (85%)	109 (100%)	0	100	100
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%)	33 (100%)	0	100	100
10	L	117/119 (98%)	117 (100%)	0	100	100
11	M	26/26 (100%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	X	23/27 (85%)	23 (100%)	0	100	100
All	All	1803/1875 (96%)	1798 (100%)	5 (0%)	86	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	587	CYS
2	B	424	HIS
2	B	526	HIS
3	C	16	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	191	GLN
1	A	216	GLN
1	A	245	ASN
1	A	427	ASN
1	A	542	HIS
1	A	618	GLN
1	A	657	GLN
2	B	9	GLN
2	B	105	GLN
2	B	121	HIS
2	B	217	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
2	B	688	HIS
2	B	710	GLN
3	C	37	GLN
4	D	63	GLN
5	E	59	ASN
6	F	90	ASN
6	F	134	ASN
8	J	3	HIS

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Mol	Chain	Res	Type
10	L	75	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	833	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	5 (6%)
16	BCR	J	105	-	41,41,41	1.17	3 (7%)	56,56,56	1.36	8 (14%)
14	CLA	A	806	-	69,73,73	1.18	6 (8%)	82,113,113	1.38	5 (6%)
14	CLA	K	101	-	45,49,73	1.40	7 (15%)	54,83,113	1.34	5 (9%)
14	CLA	B	3027	-	69,73,73	1.23	7 (10%)	82,113,113	1.21	5 (6%)
14	CLA	B	3029	-	69,73,73	1.19	5 (7%)	82,113,113	1.26	6 (7%)
14	CLA	B	3019	-	64,68,73	1.22	6 (9%)	76,107,113	1.30	8 (10%)
16	BCR	A	849	-	41,41,41	1.16	3 (7%)	56,56,56	1.34	7 (12%)
14	CLA	B	3033	-	69,73,73	1.19	6 (8%)	82,113,113	1.29	6 (7%)
14	CLA	A	824	-	55,59,73	1.32	5 (9%)	64,96,113	1.38	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CL0	A	801	-	58,73,73	2.30	11 (18%)	60,113,113	1.61	14 (23%)
14	CLA	B	3003	-	69,73,73	1.20	7 (10%)	82,113,113	1.31	5 (6%)
14	CLA	B	3004	-	69,73,73	1.19	8 (11%)	82,113,113	1.36	5 (6%)
14	CLA	A	815	-	49,53,73	1.42	8 (16%)	58,89,113	1.33	3 (5%)
14	CLA	K	103	-	49,53,73	1.41	6 (12%)	58,89,113	1.44	6 (10%)
16	BCR	K	102	-	41,41,41	1.14	3 (7%)	56,56,56	1.39	7 (12%)
14	CLA	B	3017	-	59,63,73	1.32	6 (10%)	70,101,113	1.28	5 (7%)
14	CLA	B	3024	-	49,53,73	1.45	5 (10%)	58,89,113	1.36	6 (10%)
16	BCR	J	104	-	41,41,41	1.21	3 (7%)	56,56,56	1.31	7 (12%)
14	CLA	B	3039	-	69,73,73	1.21	7 (10%)	82,113,113	1.24	4 (4%)
14	CLA	A	835	-	69,73,73	1.20	7 (10%)	82,113,113	1.44	10 (12%)
14	CLA	B	3025	2	58,62,73	1.33	7 (12%)	68,99,113	1.41	8 (11%)
14	CLA	A	841	-	69,73,73	1.18	5 (7%)	82,113,113	1.36	7 (8%)
16	BCR	L	201	-	41,41,41	1.16	3 (7%)	56,56,56	1.23	5 (8%)
14	CLA	A	808	-	55,59,73	1.40	6 (10%)	64,96,113	1.41	7 (10%)
14	CLA	A	814	-	64,68,73	1.26	5 (7%)	76,107,113	1.24	5 (6%)
14	CLA	B	3032	-	53,57,73	1.38	6 (11%)	61,93,113	1.50	8 (13%)
14	CLA	L	205	-	69,73,73	1.17	7 (10%)	82,113,113	1.30	7 (8%)
14	CLA	A	817	23	53,57,73	1.35	7 (13%)	61,93,113	1.32	2 (3%)
14	CLA	A	816	-	49,53,73	1.40	7 (14%)	58,89,113	1.50	5 (8%)
14	CLA	A	838	-	55,59,73	1.37	8 (14%)	64,96,113	1.47	7 (10%)
16	BCR	B	3048	-	41,41,41	1.13	3 (7%)	56,56,56	1.20	7 (12%)
17	LMG	B	3049	-	55,55,55	0.81	1 (1%)	63,63,63	1.36	4 (6%)
14	CLA	B	3013	-	49,53,73	1.41	6 (12%)	58,89,113	1.38	4 (6%)
14	CLA	M	102	23	49,53,73	1.52	12 (24%)	58,89,113	1.57	12 (20%)
16	BCR	F	203	-	41,41,41	1.16	3 (7%)	56,56,56	1.30	8 (14%)
14	CLA	A	834	-	69,73,73	1.21	7 (10%)	82,113,113	1.29	6 (7%)
17	LMG	I	102	-	40,40,55	1.36	6 (15%)	48,48,63	1.24	5 (10%)
14	CLA	B	3031	-	49,53,73	1.43	7 (14%)	58,89,113	1.47	5 (8%)
14	CLA	A	819	-	58,62,73	1.29	8 (13%)	68,99,113	1.46	10 (14%)
14	CLA	A	823	-	53,57,73	1.36	6 (11%)	61,93,113	1.46	5 (8%)
14	CLA	B	3020	23	69,73,73	1.18	9 (13%)	82,113,113	1.33	7 (8%)
14	CLA	A	827	23	69,73,73	1.17	7 (10%)	82,113,113	1.27	7 (8%)
21	LMT	L	202	-	36,36,36	1.12	5 (13%)	47,47,47	1.38	7 (14%)
14	CLA	B	3041	23	69,73,73	1.25	7 (10%)	82,113,113	1.37	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	3026	23	50,54,73	1.40	5 (10%)	59,90,113	1.48	4 (6%)
16	BCR	B	3051	-	41,41,41	1.20	3 (7%)	56,56,56	1.20	3 (5%)
14	CLA	A	844	23	69,73,73	1.20	7 (10%)	82,113,113	1.39	6 (7%)
14	CLA	B	3035	-	49,53,73	1.44	6 (12%)	58,89,113	1.47	6 (10%)
18	LHG	B	3050	-	22,22,48	1.58	5 (22%)	25,28,54	1.27	3 (12%)
14	CLA	A	804	-	69,73,73	1.20	6 (8%)	82,113,113	1.17	4 (4%)
19	SF4	B	3001	1,2	0,12,12	-	-	-		
14	CLA	A	836	-	58,62,73	1.30	8 (13%)	68,99,113	1.34	6 (8%)
14	CLA	X	1701	12	49,53,73	1.42	6 (12%)	58,89,113	1.45	5 (8%)
14	CLA	A	803	-	69,73,73	1.18	7 (10%)	82,113,113	1.39	6 (7%)
14	CLA	L	206	23	69,73,73	1.19	7 (10%)	82,113,113	1.35	9 (10%)
14	CLA	A	822	23	69,73,73	1.18	6 (8%)	82,113,113	1.21	6 (7%)
14	CLA	A	828	-	69,73,73	1.24	6 (8%)	82,113,113	1.23	6 (7%)
18	LHG	M	101	-	48,48,48	0.72	1 (2%)	51,54,54	1.22	3 (5%)
14	CLA	B	3030	-	69,73,73	1.18	7 (10%)	82,113,113	1.37	9 (10%)
14	CLA	A	805	14	63,67,73	1.28	8 (12%)	74,105,113	1.21	4 (5%)
14	CLA	B	3042	-	69,73,73	1.20	7 (10%)	82,113,113	1.38	6 (7%)
14	CLA	A	842	23	55,59,73	1.33	7 (12%)	64,96,113	1.48	5 (7%)
16	BCR	I	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.25	7 (12%)
18	LHG	A	854	14	26,26,48	0.98	1 (3%)	29,32,54	1.31	3 (10%)
14	CLA	B	3011	2	69,73,73	1.20	6 (8%)	82,113,113	1.32	11 (13%)
14	CLA	L	204	10	69,73,73	1.19	5 (7%)	82,113,113	1.48	8 (9%)
14	CLA	J	101	8	49,53,73	1.44	5 (10%)	58,89,113	1.32	5 (8%)
14	CLA	A	845	18	56,60,73	1.32	6 (10%)	65,97,113	1.43	7 (10%)
16	BCR	J	103	-	41,41,41	1.12	3 (7%)	56,56,56	1.22	2 (3%)
17	LMG	A	855	-	30,30,55	1.40	4 (13%)	37,37,63	1.33	4 (10%)
16	BCR	L	208	-	41,41,41	1.15	3 (7%)	56,56,56	1.43	10 (17%)
14	CLA	A	802	23	69,73,73	1.20	6 (8%)	82,113,113	1.25	6 (7%)
16	BCR	M	103	-	41,41,41	1.20	3 (7%)	56,56,56	1.17	3 (5%)
14	CLA	B	3036	23	49,53,73	1.44	5 (10%)	58,89,113	1.40	6 (10%)
16	BCR	F	201	-	41,41,41	1.18	4 (9%)	56,56,56	1.29	4 (7%)
14	CLA	A	825	-	63,67,73	1.26	7 (11%)	74,105,113	1.28	6 (8%)
15	PQN	A	846	-	34,34,34	2.03	7 (20%)	43,45,45	1.28	6 (13%)
14	CLA	A	820	-	69,73,73	1.16	6 (8%)	82,113,113	1.38	8 (9%)
14	CLA	B	3021	-	51,55,73	1.36	7 (13%)	60,91,113	1.36	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	A	850	-	41,41,41	1.11	3 (7%)	56,56,56	1.20	4 (7%)
14	CLA	B	3040	-	51,55,73	1.39	7 (13%)	60,91,113	1.39	5 (8%)
14	CLA	B	3007	-	69,73,73	1.18	7 (10%)	82,113,113	1.25	4 (4%)
14	CLA	A	811	-	49,53,73	1.40	8 (16%)	58,89,113	1.39	6 (10%)
14	CLA	A	829	-	69,73,73	1.17	6 (8%)	82,113,113	1.23	6 (7%)
14	CLA	B	3010	2	69,73,73	1.21	9 (13%)	82,113,113	1.47	10 (12%)
16	BCR	B	3045	-	41,41,41	1.17	3 (7%)	56,56,56	1.27	6 (10%)
14	CLA	A	821	-	46,50,73	1.41	6 (13%)	54,84,113	1.50	9 (16%)
16	BCR	L	209	-	41,41,41	1.21	3 (7%)	56,56,56	1.33	6 (10%)
14	CLA	B	3037	23	49,53,73	1.43	7 (14%)	58,89,113	1.32	3 (5%)
16	BCR	B	3046	-	41,41,41	1.16	3 (7%)	56,56,56	1.28	7 (12%)
14	CLA	A	840	-	51,55,73	1.40	7 (13%)	60,91,113	1.48	7 (11%)
14	CLA	A	830	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
14	CLA	A	832	-	54,58,73	1.33	7 (12%)	64,95,113	1.41	6 (9%)
14	CLA	B	3006	-	69,73,73	1.20	5 (7%)	82,113,113	1.25	5 (6%)
15	PQN	B	3043	-	34,34,34	2.15	7 (20%)	43,45,45	1.21	4 (9%)
14	CLA	A	826	-	69,73,73	1.20	6 (8%)	82,113,113	1.28	5 (6%)
14	CLA	A	843	-	69,73,73	1.20	7 (10%)	82,113,113	1.37	6 (7%)
16	BCR	B	3047	-	41,41,41	1.18	3 (7%)	56,56,56	1.35	8 (14%)
14	CLA	A	837	1	49,53,73	1.40	7 (14%)	58,89,113	1.39	5 (8%)
14	CLA	A	839	-	69,73,73	1.16	6 (8%)	82,113,113	1.33	5 (6%)
14	CLA	B	3005	-	58,62,73	1.30	6 (10%)	68,99,113	1.45	5 (7%)
16	BCR	A	848	-	41,41,41	1.19	3 (7%)	56,56,56	1.23	4 (7%)
14	CLA	A	813	-	58,62,73	1.30	9 (15%)	68,99,113	1.36	5 (7%)
16	BCR	A	851	-	41,41,41	1.18	3 (7%)	56,56,56	1.41	8 (14%)
14	CLA	B	3012	-	49,53,73	1.42	6 (12%)	58,89,113	1.57	6 (10%)
14	CLA	A	831	-	69,73,73	1.18	6 (8%)	82,113,113	1.25	7 (8%)
22	DGD	L	207	-	67,67,67	1.05	3 (4%)	81,81,81	1.18	7 (8%)
14	CLA	B	3008	-	69,73,73	1.20	7 (10%)	82,113,113	1.29	4 (4%)
14	CLA	B	3009	-	69,73,73	1.19	7 (10%)	82,113,113	1.32	8 (9%)
14	CLA	A	809	1	69,73,73	1.19	6 (8%)	82,113,113	1.24	5 (6%)
14	CLA	A	818	-	58,62,73	1.31	6 (10%)	68,99,113	1.39	6 (8%)
16	BCR	B	3044	-	41,41,41	1.14	3 (7%)	56,56,56	1.24	6 (10%)
14	CLA	A	856	23	69,73,73	1.19	9 (13%)	82,113,113	1.24	6 (7%)
14	CLA	A	812	14	69,73,73	1.21	7 (10%)	82,113,113	1.32	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	810	1	69,73,73	1.23	5 (7%)	82,113,113	1.23	9 (10%)
14	CLA	B	3034	-	62,66,73	1.25	6 (9%)	73,104,113	1.34	9 (12%)
14	CLA	B	3018	-	63,67,73	1.23	6 (9%)	74,105,113	1.37	6 (8%)
14	CLA	J	102	-	41,45,73	1.51	7 (17%)	50,78,113	1.31	5 (10%)
14	CLA	A	807	-	69,73,73	1.22	5 (7%)	82,113,113	1.18	5 (6%)
19	SF4	C	101	3	0,12,12	-	-	-	-	-
14	CLA	B	3015	-	69,73,73	1.22	5 (7%)	82,113,113	1.14	5 (6%)
14	CLA	B	3028	-	69,73,73	1.18	7 (10%)	82,113,113	1.29	3 (3%)
17	LMG	A	852	-	48,48,55	0.85	2 (4%)	56,56,63	1.26	5 (8%)
16	BCR	A	847	-	41,41,41	1.20	4 (9%)	56,56,56	1.26	5 (8%)
19	SF4	C	102	3	0,12,12	-	-	-	-	-
18	LHG	A	853	-	48,48,48	0.70	3 (6%)	51,54,54	1.25	5 (9%)
14	CLA	B	3022	-	49,53,73	1.42	7 (14%)	58,89,113	1.37	5 (8%)
14	CLA	B	3038	-	64,68,73	1.24	7 (10%)	76,107,113	1.28	6 (7%)
14	CLA	F	202	23	49,53,73	1.43	7 (14%)	58,89,113	1.36	5 (8%)
14	CLA	B	3023	23	59,63,73	1.28	8 (13%)	70,101,113	1.27	4 (5%)
14	CLA	B	3016	-	49,53,73	1.41	5 (10%)	58,89,113	1.44	6 (10%)
14	CLA	B	3014	-	69,73,73	1.21	7 (10%)	82,113,113	1.23	6 (7%)

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	833	-	1/1/20/20	5/39/115/115	-
16	BCR	J	105	-	-	12/29/63/63	0/2/2/2
14	CLA	A	806	-	1/1/20/20	18/39/115/115	-
14	CLA	K	101	-	1/1/13/20	1/9/81/115	-
14	CLA	B	3027	-	1/1/20/20	13/39/115/115	-
14	CLA	B	3029	-	1/1/20/20	17/39/115/115	-
14	CLA	B	3019	-	1/1/19/20	10/33/109/115	-
16	BCR	A	849	-	-	12/29/63/63	0/2/2/2
14	CLA	B	3033	-	1/1/20/20	16/39/115/115	-
14	CLA	A	824	-	1/1/17/20	4/23/99/115	-
13	CL0	A	801	-	3/3/25/25	13/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	3003	-	1/1/20/20	13/39/115/115	-
14	CLA	B	3004	-	1/1/20/20	7/39/115/115	-
14	CLA	A	815	-	1/1/15/20	2/15/91/115	-
14	CLA	K	103	-	1/1/15/20	10/15/91/115	-
16	BCR	K	102	-	-	12/29/63/63	0/2/2/2
14	CLA	B	3017	-	1/1/18/20	5/27/103/115	-
14	CLA	B	3024	-	1/1/15/20	4/15/91/115	-
16	BCR	J	104	-	-	15/29/63/63	0/2/2/2
14	CLA	B	3039	-	1/1/20/20	9/39/115/115	-
14	CLA	A	835	-	1/1/20/20	16/39/115/115	-
14	CLA	B	3025	2	-	8/26/102/115	-
14	CLA	A	841	-	1/1/20/20	6/39/115/115	-
16	BCR	L	201	-	-	8/29/63/63	0/2/2/2
14	CLA	A	808	-	1/1/17/20	12/23/99/115	-
14	CLA	A	814	-	1/1/19/20	4/33/109/115	-
14	CLA	B	3032	-	1/1/16/20	7/20/96/115	-
14	CLA	L	205	-	1/1/20/20	4/39/115/115	-
14	CLA	A	817	23	1/1/16/20	8/20/96/115	-
14	CLA	A	816	-	1/1/15/20	2/15/91/115	-
14	CLA	A	838	-	1/1/17/20	6/23/99/115	-
16	BCR	B	3048	-	-	4/29/63/63	0/2/2/2
17	LMG	B	3049	-	-	23/50/70/70	0/1/1/1
14	CLA	B	3013	-	1/1/15/20	6/15/91/115	-
14	CLA	M	102	23	1/1/15/20	11/15/91/115	-
16	BCR	F	203	-	-	11/29/63/63	0/2/2/2
14	CLA	A	834	-	1/1/20/20	9/39/115/115	-
17	LMG	I	102	-	-	11/35/55/70	0/1/1/1
14	CLA	B	3031	-	1/1/15/20	6/15/91/115	-
14	CLA	A	819	-	1/1/17/20	8/26/102/115	-
14	CLA	A	823	-	1/1/16/20	10/20/96/115	-
14	CLA	B	3020	23	1/1/20/20	13/39/115/115	-
14	CLA	A	827	23	1/1/20/20	10/39/115/115	-
21	LMT	L	202	-	-	12/21/61/61	0/2/2/2
14	CLA	B	3041	23	1/1/20/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	3026	23	1/1/15/20	2/17/93/115	-
16	BCR	B	3051	-	-	12/29/63/63	0/2/2/2
14	CLA	A	844	23	1/1/20/20	12/39/115/115	-
14	CLA	B	3035	-	1/1/15/20	5/15/91/115	-
18	LHG	B	3050	-	-	10/26/26/53	-
14	CLA	A	804	-	1/1/20/20	7/39/115/115	-
19	SF4	B	3001	1,2	-	-	0/6/5/5
14	CLA	A	836	-	1/1/17/20	8/26/102/115	-
14	CLA	X	1701	12	1/1/15/20	3/15/91/115	-
14	CLA	A	803	-	1/1/20/20	8/39/115/115	-
14	CLA	L	206	23	1/1/20/20	6/39/115/115	-
14	CLA	A	822	23	1/1/20/20	15/39/115/115	-
14	CLA	A	828	-	1/1/20/20	5/39/115/115	-
18	LHG	M	101	-	-	26/53/53/53	-
14	CLA	B	3030	-	1/1/20/20	15/39/115/115	-
14	CLA	A	805	14	1/1/18/20	5/32/108/115	-
14	CLA	B	3042	-	1/1/20/20	8/39/115/115	-
14	CLA	A	842	23	1/1/17/20	6/23/99/115	-
16	BCR	I	101	-	-	4/29/63/63	0/2/2/2
18	LHG	A	854	14	-	10/31/31/53	-
14	CLA	B	3011	2	1/1/20/20	14/39/115/115	-
14	CLA	L	204	10	1/1/20/20	12/39/115/115	-
14	CLA	J	101	8	1/1/15/20	5/15/91/115	-
14	CLA	A	845	18	1/1/17/20	9/24/100/115	-
16	BCR	J	103	-	-	14/29/63/63	0/2/2/2
17	LMG	A	855	-	-	15/23/43/70	0/1/1/1
16	BCR	L	208	-	-	12/29/63/63	0/2/2/2
14	CLA	A	802	23	1/1/20/20	9/39/115/115	-
16	BCR	M	103	-	-	7/29/63/63	0/2/2/2
14	CLA	B	3036	23	1/1/15/20	6/15/91/115	-
16	BCR	F	201	-	-	6/29/63/63	0/2/2/2
14	CLA	A	825	-	1/1/18/20	10/32/108/115	-
15	PQN	A	846	-	-	9/23/43/43	0/2/2/2
14	CLA	A	820	-	1/1/20/20	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	3021	-	1/1/15/20	12/18/94/115	-
16	BCR	A	850	-	-	11/29/63/63	0/2/2/2
14	CLA	B	3040	-	-	5/18/94/115	-
14	CLA	B	3007	-	1/1/20/20	9/39/115/115	-
14	CLA	A	811	-	1/1/15/20	9/15/91/115	-
14	CLA	A	829	-	1/1/20/20	11/39/115/115	-
14	CLA	B	3010	2	1/1/20/20	14/39/115/115	-
16	BCR	B	3045	-	-	11/29/63/63	0/2/2/2
14	CLA	A	821	-	1/1/14/20	6/10/86/115	-
16	BCR	L	209	-	-	10/29/63/63	0/2/2/2
14	CLA	B	3037	23	1/1/15/20	4/15/91/115	-
16	BCR	B	3046	-	-	11/29/63/63	0/2/2/2
14	CLA	A	840	-	1/1/15/20	4/18/94/115	-
14	CLA	A	830	-	1/1/20/20	13/39/115/115	-
14	CLA	A	832	-	1/1/17/20	6/21/97/115	-
14	CLA	B	3006	-	1/1/20/20	14/39/115/115	-
15	PQN	B	3043	-	-	8/23/43/43	0/2/2/2
14	CLA	A	826	-	1/1/20/20	16/39/115/115	-
14	CLA	A	843	-	1/1/20/20	8/39/115/115	-
16	BCR	B	3047	-	-	15/29/63/63	0/2/2/2
14	CLA	A	837	1	1/1/15/20	6/15/91/115	-
14	CLA	A	839	-	1/1/20/20	9/39/115/115	-
14	CLA	B	3005	-	1/1/17/20	8/26/102/115	-
16	BCR	A	848	-	-	7/29/63/63	0/2/2/2
14	CLA	A	813	-	1/1/17/20	6/26/102/115	-
16	BCR	A	851	-	-	16/29/63/63	0/2/2/2
14	CLA	B	3012	-	1/1/15/20	2/15/91/115	-
14	CLA	A	831	-	1/1/20/20	9/39/115/115	-
22	DGD	L	207	-	-	23/55/95/95	0/2/2/2
14	CLA	B	3008	-	1/1/20/20	6/39/115/115	-
14	CLA	B	3009	-	1/1/20/20	10/39/115/115	-
14	CLA	A	809	1	1/1/20/20	18/39/115/115	-
14	CLA	A	818	-	1/1/17/20	4/26/102/115	-
16	BCR	B	3044	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	856	23	1/1/20/20	15/39/115/115	-
14	CLA	A	812	14	1/1/20/20	9/39/115/115	-
14	CLA	A	810	1	1/1/20/20	10/39/115/115	-
14	CLA	B	3034	-	1/1/18/20	9/31/107/115	-
14	CLA	B	3018	-	1/1/18/20	11/32/108/115	-
14	CLA	J	102	-	1/1/12/20	0/4/76/115	-
14	CLA	A	807	-	1/1/20/20	12/39/115/115	-
19	SF4	C	101	3	-	-	0/6/5/5
14	CLA	B	3015	-	1/1/20/20	11/39/115/115	-
14	CLA	B	3028	-	1/1/20/20	12/39/115/115	-
17	LMG	A	852	-	-	27/43/63/70	0/1/1/1
16	BCR	A	847	-	-	16/29/63/63	0/2/2/2
19	SF4	C	102	3	-	-	0/6/5/5
18	LHG	A	853	-	-	23/53/53/53	-
14	CLA	B	3022	-	1/1/15/20	8/15/91/115	-
14	CLA	B	3038	-	-	6/33/109/115	-
14	CLA	F	202	23	1/1/15/20	6/15/91/115	-
14	CLA	B	3023	23	1/1/18/20	8/27/103/115	-
14	CLA	B	3016	-	1/1/15/20	4/15/91/115	-
14	CLA	B	3014	-	1/1/20/20	13/39/115/115	-

All (755) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	801	CL0	C1B-C2B	9.16	1.50	1.39
13	A	801	CL0	C3B-C4B	8.43	1.49	1.41
13	A	801	CL0	C1D-C2D	8.00	1.48	1.39
15	B	3043	PQN	O1-C1	6.03	1.35	1.23
15	A	846	PQN	O1-C1	5.97	1.35	1.23
15	A	846	PQN	O4-C4	5.94	1.35	1.23
15	B	3043	PQN	O4-C4	5.93	1.35	1.23
15	B	3043	PQN	C10-C1	-5.52	1.37	1.48
17	A	855	LMG	O7-C8	-4.55	1.39	1.47
16	L	209	BCR	C1-C6	-4.30	1.48	1.53
16	M	103	BCR	C1-C6	-4.22	1.48	1.53
13	A	801	CL0	C3D-C4D	4.19	1.47	1.41
16	B	3045	BCR	C1-C6	-4.18	1.48	1.53
15	A	846	PQN	C10-C1	-4.10	1.40	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	J	104	BCR	C1-C6	-4.08	1.48	1.53
14	A	808	CLA	C1D-ND	4.03	1.43	1.37
15	B	3043	PQN	C5-C4	-4.00	1.40	1.48
16	B	3051	BCR	C30-C25	-4.00	1.48	1.53
18	B	3050	LHG	P-O6	3.99	1.75	1.59
17	I	102	LMG	O1-C1	3.99	1.46	1.40
14	B	3006	CLA	C1D-ND	3.98	1.43	1.37
16	L	201	BCR	C1-C6	-3.98	1.48	1.53
17	I	102	LMG	C7-C8	3.93	1.63	1.50
14	B	3005	CLA	C1D-ND	3.92	1.43	1.37
14	B	3017	CLA	C1D-ND	3.90	1.43	1.37
14	A	835	CLA	C1D-ND	3.89	1.43	1.37
16	A	848	BCR	C1-C6	-3.85	1.48	1.53
14	A	810	CLA	C1D-ND	3.85	1.42	1.37
14	B	3041	CLA	C1D-ND	3.81	1.42	1.37
16	A	849	BCR	C1-C6	-3.81	1.48	1.53
16	B	3046	BCR	C1-C6	-3.81	1.48	1.53
16	A	851	BCR	C1-C6	-3.80	1.48	1.53
14	A	826	CLA	C1D-ND	3.79	1.42	1.37
14	B	3041	CLA	C4B-NB	3.79	1.42	1.37
16	A	847	BCR	C1-C6	-3.78	1.48	1.53
14	A	823	CLA	C1D-ND	3.78	1.42	1.37
14	B	3011	CLA	C1D-ND	3.76	1.42	1.37
14	J	101	CLA	C1D-ND	3.76	1.42	1.37
14	A	828	CLA	C1D-ND	3.75	1.42	1.37
14	B	3012	CLA	C1D-ND	3.75	1.42	1.37
14	A	834	CLA	C1D-ND	3.75	1.42	1.37
14	A	818	CLA	C1D-ND	3.73	1.42	1.37
14	A	824	CLA	C1D-ND	3.72	1.42	1.37
14	A	832	CLA	C1D-ND	3.72	1.42	1.37
14	A	829	CLA	C1D-ND	3.72	1.42	1.37
14	A	825	CLA	C1D-ND	3.71	1.42	1.37
14	B	3008	CLA	C1D-ND	3.71	1.42	1.37
14	A	814	CLA	C1D-ND	3.70	1.42	1.37
14	A	819	CLA	C1D-ND	3.69	1.42	1.37
14	B	3014	CLA	C1D-ND	3.69	1.42	1.37
14	B	3028	CLA	C1D-ND	3.68	1.42	1.37
14	B	3032	CLA	C1D-ND	3.68	1.42	1.37
14	A	820	CLA	C1D-ND	3.67	1.42	1.37
16	J	103	BCR	C1-C6	-3.67	1.49	1.53
14	A	845	CLA	C1D-ND	3.66	1.42	1.37
14	B	3016	CLA	C1D-ND	3.65	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	J	105	BCR	C30-C25	-3.65	1.49	1.53
14	B	3015	CLA	C1D-ND	3.64	1.42	1.37
14	K	103	CLA	C1D-ND	3.64	1.42	1.37
14	B	3038	CLA	C1D-ND	3.63	1.42	1.37
14	A	828	CLA	C4B-NB	3.63	1.42	1.37
14	B	3037	CLA	C4B-NB	3.63	1.42	1.37
14	B	3040	CLA	C1D-ND	3.62	1.42	1.37
14	B	3034	CLA	C1D-ND	3.62	1.42	1.37
14	A	842	CLA	C1D-ND	3.61	1.42	1.37
16	B	3051	BCR	C1-C6	-3.61	1.49	1.53
16	F	203	BCR	C1-C6	-3.61	1.49	1.53
14	A	843	CLA	C4B-NB	3.60	1.42	1.37
14	B	3031	CLA	C1D-ND	3.60	1.42	1.37
16	K	102	BCR	C1-C6	-3.60	1.49	1.53
14	A	838	CLA	C1D-ND	3.60	1.42	1.37
14	J	102	CLA	C1D-ND	3.60	1.42	1.37
14	A	840	CLA	C1D-ND	3.59	1.42	1.37
14	B	3027	CLA	C1D-ND	3.58	1.42	1.37
14	A	817	CLA	C4B-NB	3.58	1.42	1.37
14	B	3039	CLA	C1D-ND	3.57	1.42	1.37
14	B	3009	CLA	C1D-ND	3.57	1.42	1.37
14	A	805	CLA	C4B-NB	3.57	1.42	1.37
14	B	3003	CLA	C1D-ND	3.56	1.42	1.37
14	X	1701	CLA	C1D-ND	3.56	1.42	1.37
14	A	802	CLA	C1D-ND	3.56	1.42	1.37
14	A	840	CLA	C4B-NB	3.56	1.42	1.37
14	B	3035	CLA	C1D-ND	3.56	1.42	1.37
15	A	846	PQN	C5-C4	-3.56	1.41	1.48
16	B	3044	BCR	C1-C6	-3.56	1.49	1.53
14	B	3033	CLA	C1D-ND	3.55	1.42	1.37
14	A	807	CLA	C1D-ND	3.55	1.42	1.37
14	L	206	CLA	C1D-ND	3.55	1.42	1.37
14	A	836	CLA	C1D-ND	3.55	1.42	1.37
14	B	3021	CLA	C1D-ND	3.55	1.42	1.37
14	B	3024	CLA	C1D-ND	3.54	1.42	1.37
14	A	805	CLA	C1D-ND	3.54	1.42	1.37
16	M	103	BCR	C30-C25	-3.54	1.49	1.53
14	F	202	CLA	C1D-ND	3.54	1.42	1.37
14	B	3013	CLA	C4B-NB	3.53	1.42	1.37
14	B	3030	CLA	C1D-ND	3.52	1.42	1.37
14	A	841	CLA	C1D-ND	3.51	1.42	1.37
14	B	3018	CLA	C1D-ND	3.51	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	822	CLA	C1D-ND	3.51	1.42	1.37
14	B	3030	CLA	C4B-NB	3.50	1.42	1.37
16	F	201	BCR	C1-C6	-3.50	1.49	1.53
14	A	812	CLA	C1D-ND	3.50	1.42	1.37
14	B	3036	CLA	C1D-ND	3.50	1.42	1.37
14	A	816	CLA	C1D-ND	3.49	1.42	1.37
14	B	3036	CLA	C4B-NB	3.49	1.42	1.37
14	B	3007	CLA	C1D-ND	3.49	1.42	1.37
14	B	3029	CLA	C1D-ND	3.49	1.42	1.37
14	B	3031	CLA	C4B-NB	3.48	1.42	1.37
14	A	806	CLA	C1D-ND	3.47	1.42	1.37
14	A	833	CLA	C1D-ND	3.47	1.42	1.37
14	B	3026	CLA	C4B-NB	3.47	1.42	1.37
14	B	3026	CLA	C1D-ND	3.45	1.42	1.37
16	B	3048	BCR	C1-C6	-3.45	1.49	1.53
14	A	807	CLA	C4B-NB	3.44	1.42	1.37
14	B	3040	CLA	C4B-NB	3.44	1.42	1.37
14	B	3042	CLA	C4B-NB	3.43	1.42	1.37
14	A	834	CLA	C4B-NB	3.43	1.42	1.37
14	A	844	CLA	C1D-ND	3.42	1.42	1.37
14	B	3037	CLA	C1D-ND	3.42	1.42	1.37
14	A	812	CLA	C4B-NB	3.42	1.42	1.37
14	L	205	CLA	C1D-ND	3.42	1.42	1.37
14	A	808	CLA	C4B-NB	3.42	1.42	1.37
16	B	3047	BCR	C30-C25	-3.41	1.49	1.53
14	A	839	CLA	C1D-ND	3.41	1.42	1.37
14	B	3035	CLA	C4B-NB	3.41	1.42	1.37
14	B	3039	CLA	C4B-NB	3.40	1.42	1.37
16	J	104	BCR	C30-C25	-3.40	1.49	1.53
14	B	3020	CLA	C1D-ND	3.39	1.42	1.37
14	A	837	CLA	C1D-ND	3.38	1.42	1.37
16	L	208	BCR	C1-C6	-3.38	1.49	1.53
14	B	3027	CLA	C4B-NB	3.38	1.42	1.37
14	A	809	CLA	C4B-NB	3.38	1.42	1.37
16	J	105	BCR	C1-C6	-3.38	1.49	1.53
14	A	809	CLA	C1D-ND	3.37	1.42	1.37
14	J	101	CLA	C4B-NB	3.37	1.42	1.37
14	B	3042	CLA	C1D-ND	3.37	1.42	1.37
14	A	804	CLA	C4B-NB	3.36	1.42	1.37
14	A	837	CLA	C4B-NB	3.36	1.42	1.37
14	A	831	CLA	C1D-ND	3.36	1.42	1.37
14	B	3029	CLA	C4B-NB	3.36	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	846	PQN	C3-C2	3.36	1.41	1.35
14	A	815	CLA	C1D-ND	3.35	1.42	1.37
16	L	208	BCR	C30-C25	-3.35	1.49	1.53
14	L	204	CLA	C1D-ND	3.35	1.42	1.37
14	X	1701	CLA	C4B-NB	3.34	1.42	1.37
14	B	3003	CLA	C4B-NB	3.34	1.42	1.37
14	B	3033	CLA	C4B-NB	3.34	1.42	1.37
14	A	827	CLA	C1D-ND	3.33	1.42	1.37
14	B	3004	CLA	C1D-ND	3.33	1.42	1.37
14	A	823	CLA	C4B-NB	3.33	1.42	1.37
14	A	818	CLA	C4B-NB	3.32	1.42	1.37
14	A	830	CLA	C1D-ND	3.32	1.42	1.37
14	B	3025	CLA	C1D-ND	3.32	1.42	1.37
14	B	3022	CLA	C1D-ND	3.31	1.42	1.37
16	A	848	BCR	C30-C25	-3.31	1.49	1.53
14	A	814	CLA	C4B-NB	3.30	1.42	1.37
16	A	847	BCR	C30-C25	-3.30	1.49	1.53
14	A	821	CLA	C1D-ND	3.30	1.42	1.37
14	B	3021	CLA	C4B-NB	3.28	1.42	1.37
14	B	3014	CLA	C4B-NB	3.28	1.42	1.37
14	B	3008	CLA	C4B-NB	3.28	1.42	1.37
14	B	3041	CLA	C1B-C2B	3.27	1.50	1.43
16	A	850	BCR	C1-C6	-3.27	1.49	1.53
16	F	203	BCR	C30-C25	-3.26	1.49	1.53
14	A	803	CLA	C4B-NB	3.26	1.42	1.37
14	F	202	CLA	C4B-NB	3.26	1.42	1.37
14	A	804	CLA	C1D-ND	3.26	1.42	1.37
14	A	802	CLA	C4B-NB	3.26	1.42	1.37
16	F	201	BCR	C30-C25	-3.25	1.49	1.53
14	A	844	CLA	C4B-NB	3.25	1.42	1.37
14	A	803	CLA	C1D-ND	3.25	1.42	1.37
14	B	3024	CLA	C4B-NB	3.24	1.42	1.37
14	A	843	CLA	C1D-ND	3.23	1.42	1.37
14	J	102	CLA	C4B-NB	3.23	1.42	1.37
14	A	813	CLA	C4B-NB	3.23	1.42	1.37
14	A	827	CLA	C4B-NB	3.23	1.42	1.37
14	B	3018	CLA	C4B-NB	3.22	1.42	1.37
14	B	3012	CLA	C4B-NB	3.22	1.42	1.37
14	A	815	CLA	C4B-NB	3.22	1.42	1.37
14	B	3015	CLA	C4B-NB	3.22	1.42	1.37
14	B	3017	CLA	C4B-NB	3.21	1.42	1.37
14	B	3023	CLA	C1D-ND	3.20	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3022	CLA	C4B-NB	3.20	1.42	1.37
14	B	3009	CLA	C4B-NB	3.19	1.42	1.37
15	B	3043	PQN	C3-C2	3.19	1.40	1.35
14	A	821	CLA	C4B-NB	3.19	1.42	1.37
14	B	3025	CLA	C4B-NB	3.19	1.42	1.37
14	B	3019	CLA	C4B-NB	3.18	1.42	1.37
14	A	805	CLA	C1B-C2B	3.18	1.50	1.43
14	B	3019	CLA	C1D-ND	3.18	1.42	1.37
14	A	836	CLA	C4B-NB	3.17	1.42	1.37
16	B	3047	BCR	C1-C6	-3.17	1.49	1.53
14	A	811	CLA	C1D-ND	3.16	1.42	1.37
14	B	3010	CLA	C4B-NB	3.15	1.42	1.37
14	B	3006	CLA	C1B-C2B	3.15	1.50	1.43
14	A	830	CLA	C4B-NB	3.15	1.42	1.37
14	B	3028	CLA	C1B-C2B	3.14	1.50	1.43
14	A	829	CLA	C4B-NB	3.14	1.42	1.37
14	A	812	CLA	C1B-C2B	3.14	1.50	1.43
16	I	101	BCR	C1-C6	-3.14	1.49	1.53
14	M	102	CLA	C4B-NB	3.13	1.42	1.37
14	A	828	CLA	C1B-C2B	3.13	1.50	1.43
14	A	810	CLA	C4B-NB	3.13	1.42	1.37
14	B	3028	CLA	C4B-NB	3.12	1.42	1.37
14	B	3013	CLA	C1D-ND	3.12	1.42	1.37
14	A	856	CLA	C4B-NB	3.12	1.42	1.37
14	B	3033	CLA	C1B-C2B	3.12	1.50	1.43
14	B	3038	CLA	C4B-NB	3.11	1.41	1.37
18	B	3050	LHG	C4-C5	3.11	1.60	1.50
14	A	825	CLA	C4B-NB	3.11	1.41	1.37
14	B	3006	CLA	C4B-NB	3.10	1.41	1.37
14	K	101	CLA	C4B-NB	3.10	1.41	1.37
14	A	841	CLA	C1B-C2B	3.10	1.50	1.43
14	A	838	CLA	C4B-NB	3.10	1.41	1.37
14	A	806	CLA	C4B-NB	3.10	1.41	1.37
14	A	856	CLA	C1D-ND	3.10	1.41	1.37
14	B	3032	CLA	C4B-NB	3.08	1.41	1.37
14	B	3010	CLA	C1D-ND	3.06	1.41	1.37
14	K	103	CLA	C4B-NB	3.06	1.41	1.37
14	A	824	CLA	C4B-NB	3.05	1.41	1.37
14	M	102	CLA	C1B-C2B	3.03	1.50	1.43
14	K	101	CLA	C1D-ND	3.03	1.41	1.37
16	L	209	BCR	C30-C25	-3.03	1.49	1.53
14	A	809	CLA	CHC-C1C	3.03	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	J	102	CLA	C1B-C2B	3.02	1.50	1.43
14	A	831	CLA	C4B-NB	3.02	1.41	1.37
14	A	808	CLA	C1B-C2B	3.02	1.50	1.43
14	B	3026	CLA	C1B-C2B	3.01	1.50	1.43
14	A	832	CLA	C1B-C2B	3.01	1.50	1.43
14	A	834	CLA	C1B-C2B	3.01	1.50	1.43
16	K	102	BCR	C30-C25	-3.01	1.49	1.53
16	L	201	BCR	C30-C25	-3.00	1.49	1.53
14	A	806	CLA	C1B-C2B	3.00	1.50	1.43
16	B	3048	BCR	C30-C25	-3.00	1.49	1.53
15	B	3043	PQN	C3-C4	-3.00	1.39	1.47
14	A	820	CLA	C4B-NB	3.00	1.41	1.37
14	B	3015	CLA	C1B-C2B	3.00	1.50	1.43
14	B	3005	CLA	C1B-C2B	2.99	1.50	1.43
14	B	3004	CLA	C4B-NB	2.99	1.41	1.37
14	B	3007	CLA	C4B-NB	2.99	1.41	1.37
14	A	817	CLA	C1D-ND	2.98	1.41	1.37
14	A	813	CLA	C1D-ND	2.97	1.41	1.37
14	B	3009	CLA	C1B-C2B	2.97	1.50	1.43
14	A	832	CLA	C4B-NB	2.97	1.41	1.37
14	B	3023	CLA	C4B-NB	2.97	1.41	1.37
14	B	3020	CLA	C4B-NB	2.97	1.41	1.37
16	I	101	BCR	C30-C25	-2.96	1.50	1.53
14	A	841	CLA	C4B-NB	2.96	1.41	1.37
14	B	3011	CLA	C4B-NB	2.96	1.41	1.37
14	A	816	CLA	C4B-NB	2.95	1.41	1.37
14	L	204	CLA	C1B-C2B	2.95	1.50	1.43
14	B	3005	CLA	C4B-NB	2.95	1.41	1.37
14	A	815	CLA	C1B-C2B	2.94	1.50	1.43
14	A	839	CLA	C1B-C2B	2.94	1.50	1.43
14	B	3042	CLA	C1B-C2B	2.93	1.50	1.43
14	A	826	CLA	C4B-NB	2.92	1.41	1.37
14	B	3027	CLA	C1B-C2B	2.92	1.50	1.43
14	A	839	CLA	C4B-NB	2.92	1.41	1.37
14	M	102	CLA	C1D-ND	2.92	1.41	1.37
15	A	846	PQN	C3-C4	-2.91	1.39	1.47
14	A	822	CLA	C4B-NB	2.91	1.41	1.37
14	L	206	CLA	C4B-NB	2.91	1.41	1.37
14	A	842	CLA	C1B-C2B	2.91	1.49	1.43
14	B	3024	CLA	C1B-C2B	2.91	1.49	1.43
14	B	3032	CLA	C1B-C2B	2.90	1.49	1.43
14	B	3017	CLA	C1B-C2B	2.90	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	850	BCR	C30-C25	-2.90	1.50	1.53
14	B	3016	CLA	C4B-NB	2.90	1.41	1.37
14	L	204	CLA	C4B-NB	2.89	1.41	1.37
16	B	3046	BCR	C30-C25	-2.89	1.50	1.53
14	A	823	CLA	C1B-C2B	2.89	1.49	1.43
14	A	816	CLA	C1B-C2B	2.89	1.49	1.43
14	A	833	CLA	C4B-NB	2.88	1.41	1.37
17	A	855	LMG	C7-C8	2.88	1.57	1.50
14	X	1701	CLA	C1B-C2B	2.88	1.49	1.43
14	B	3038	CLA	C1B-C2B	2.88	1.49	1.43
14	A	842	CLA	C4B-NB	2.87	1.41	1.37
14	A	840	CLA	C1B-C2B	2.86	1.49	1.43
14	A	856	CLA	C1B-C2B	2.86	1.49	1.43
14	B	3022	CLA	C1B-C2B	2.85	1.49	1.43
14	A	811	CLA	C4B-NB	2.85	1.41	1.37
14	A	835	CLA	C1B-C2B	2.85	1.49	1.43
14	B	3021	CLA	C1B-C2B	2.84	1.49	1.43
14	B	3016	CLA	C1B-C2B	2.84	1.49	1.43
14	A	810	CLA	C1B-C2B	2.84	1.49	1.43
14	B	3010	CLA	CMB-C2B	-2.84	1.44	1.50
14	A	845	CLA	C4B-NB	2.84	1.41	1.37
14	B	3034	CLA	C1B-C2B	2.83	1.49	1.43
14	B	3011	CLA	C1B-C2B	2.83	1.49	1.43
14	A	835	CLA	C4B-NB	2.83	1.41	1.37
14	A	833	CLA	C1B-C2B	2.83	1.49	1.43
14	A	826	CLA	C1B-C2B	2.82	1.49	1.43
16	A	851	BCR	C30-C25	-2.82	1.50	1.53
14	A	811	CLA	C1B-C2B	2.81	1.49	1.43
14	A	819	CLA	C4B-NB	2.81	1.41	1.37
14	B	3003	CLA	C1B-C2B	2.80	1.49	1.43
14	A	818	CLA	C1B-C2B	2.80	1.49	1.43
17	A	852	LMG	C7-C8	2.80	1.59	1.50
14	B	3007	CLA	C1B-C2B	2.79	1.49	1.43
14	B	3008	CLA	C1B-C2B	2.79	1.49	1.43
14	A	809	CLA	C3B-C4B	2.78	1.50	1.42
18	A	854	LHG	P-O6	2.78	1.70	1.59
14	B	3031	CLA	C1B-C2B	2.77	1.49	1.43
18	B	3050	LHG	C6-C5	2.77	1.59	1.50
14	J	101	CLA	C1B-C2B	2.77	1.49	1.43
14	A	803	CLA	C1B-C2B	2.77	1.49	1.43
14	A	829	CLA	C1B-C2B	2.76	1.49	1.43
14	B	3030	CLA	C1B-C2B	2.76	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3040	CLA	C1B-C2B	2.76	1.49	1.43
14	L	205	CLA	C4B-NB	2.76	1.41	1.37
14	L	205	CLA	C1B-C2B	2.76	1.49	1.43
14	B	3025	CLA	C3B-C4B	2.76	1.50	1.42
14	B	3023	CLA	C1B-C2B	2.76	1.49	1.43
14	B	3020	CLA	C1B-C2B	2.76	1.49	1.43
16	J	103	BCR	C30-C25	-2.74	1.50	1.53
14	A	818	CLA	CHC-C1C	2.74	1.44	1.38
14	J	101	CLA	C3B-C4B	2.73	1.50	1.42
14	A	804	CLA	C3B-C4B	2.73	1.50	1.42
14	B	3035	CLA	C1B-C2B	2.73	1.49	1.43
14	B	3025	CLA	CHC-C1C	2.72	1.43	1.38
14	K	103	CLA	C1B-C2B	2.72	1.49	1.43
14	A	817	CLA	C1B-C2B	2.72	1.49	1.43
14	A	838	CLA	C1B-C2B	2.72	1.49	1.43
14	B	3034	CLA	C4B-NB	2.72	1.41	1.37
14	A	807	CLA	C1B-C2B	2.72	1.49	1.43
16	B	3044	BCR	C30-C25	-2.71	1.50	1.53
14	A	814	CLA	CHC-C1C	2.71	1.43	1.38
14	A	845	CLA	C1B-C2B	2.70	1.49	1.43
14	B	3037	CLA	C1B-C2B	2.70	1.49	1.43
14	A	820	CLA	C1B-C2B	2.70	1.49	1.43
14	B	3014	CLA	C1B-C2B	2.69	1.49	1.43
14	A	824	CLA	C1B-C2B	2.69	1.49	1.43
14	A	837	CLA	C1B-C2B	2.68	1.49	1.43
22	L	207	DGD	O2G-C2G	-2.67	1.40	1.46
14	A	821	CLA	CHC-C1C	2.67	1.43	1.38
14	A	814	CLA	C1B-C2B	2.67	1.49	1.43
14	L	206	CLA	C3B-C4B	2.67	1.50	1.42
14	A	821	CLA	C3B-C4B	2.66	1.50	1.42
14	B	3012	CLA	C1B-C2B	2.66	1.49	1.43
14	B	3039	CLA	C1B-C2B	2.66	1.49	1.43
14	A	822	CLA	C1B-C2B	2.65	1.49	1.43
13	A	801	CL0	C1A-CHA	-2.65	1.37	1.40
14	B	3036	CLA	CHC-C1C	2.64	1.43	1.38
14	A	828	CLA	CHC-C1C	2.64	1.43	1.38
14	B	3011	CLA	C3B-C4B	2.63	1.50	1.42
14	A	807	CLA	C3B-C4B	2.63	1.50	1.42
14	A	804	CLA	C1B-C2B	2.63	1.49	1.43
14	A	825	CLA	C1B-C2B	2.63	1.49	1.43
14	B	3013	CLA	C3B-C4B	2.63	1.50	1.42
14	A	843	CLA	C1B-C2B	2.63	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3029	CLA	C1B-C2B	2.63	1.49	1.43
14	A	828	CLA	C3B-C4B	2.63	1.50	1.42
14	A	813	CLA	C1B-C2B	2.63	1.49	1.43
13	A	801	CL0	CMD-C2D	-2.62	1.46	1.51
14	B	3036	CLA	C1B-C2B	2.62	1.49	1.43
14	B	3019	CLA	C1B-C2B	2.61	1.49	1.43
14	F	202	CLA	C1B-C2B	2.61	1.49	1.43
14	J	101	CLA	CHC-C1C	2.61	1.43	1.38
14	B	3013	CLA	C1B-C2B	2.61	1.49	1.43
14	A	844	CLA	C1B-C2B	2.60	1.49	1.43
14	A	843	CLA	CHC-C1C	2.60	1.43	1.38
16	A	849	BCR	C30-C25	-2.60	1.50	1.53
14	K	101	CLA	C1B-C2B	2.60	1.49	1.43
14	B	3024	CLA	CHC-C1C	2.60	1.43	1.38
14	B	3036	CLA	C3B-C4B	2.60	1.50	1.42
14	B	3014	CLA	C3B-C4B	2.60	1.50	1.42
14	A	814	CLA	C3B-C4B	2.60	1.50	1.42
14	B	3014	CLA	CHC-C1C	2.59	1.43	1.38
13	A	801	CL0	CMB-C2B	-2.59	1.46	1.51
14	A	809	CLA	C1B-C2B	2.59	1.49	1.43
14	A	831	CLA	C1B-C2B	2.58	1.49	1.43
14	A	817	CLA	CHC-C1C	2.57	1.43	1.38
14	A	830	CLA	C1B-C2B	2.57	1.49	1.43
14	B	3029	CLA	C3B-C4B	2.57	1.50	1.42
14	A	825	CLA	C3B-C4B	2.57	1.50	1.42
14	B	3018	CLA	C1B-C2B	2.55	1.49	1.43
14	A	813	CLA	C3B-C4B	2.55	1.50	1.42
14	A	843	CLA	C3B-C4B	2.55	1.50	1.42
14	A	818	CLA	C3B-C4B	2.55	1.50	1.42
14	A	810	CLA	C3B-C4B	2.55	1.50	1.42
14	B	3030	CLA	C3B-C4B	2.55	1.50	1.42
14	A	822	CLA	C3B-C4B	2.54	1.50	1.42
21	L	202	LMT	O3B-C3B	-2.54	1.36	1.43
14	K	101	CLA	CHC-C1C	2.54	1.43	1.38
14	A	829	CLA	C3B-C4B	2.54	1.50	1.42
14	K	101	CLA	C3B-C4B	2.53	1.50	1.42
14	B	3017	CLA	C3B-C4B	2.53	1.50	1.42
14	B	3004	CLA	C1B-C2B	2.53	1.49	1.43
14	A	836	CLA	C3B-C4B	2.53	1.50	1.42
14	B	3027	CLA	C3B-C4B	2.53	1.50	1.42
14	A	831	CLA	CMB-C2B	-2.53	1.45	1.50
14	B	3033	CLA	C3B-C4B	2.53	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3011	CLA	CHC-C1C	2.53	1.43	1.38
14	A	827	CLA	CHC-C1C	2.52	1.43	1.38
17	I	102	LMG	C4-C5	2.52	1.58	1.53
18	M	101	LHG	P-O6	2.52	1.69	1.59
14	B	3008	CLA	C3B-C4B	2.52	1.50	1.42
14	L	206	CLA	CHC-C1C	2.51	1.43	1.38
14	A	827	CLA	C1B-C2B	2.51	1.49	1.43
14	B	3013	CLA	CHC-C1C	2.51	1.43	1.38
14	M	102	CLA	C4C-C3C	2.50	1.49	1.45
14	A	844	CLA	C3B-C4B	2.50	1.50	1.42
14	B	3029	CLA	CHC-C1C	2.50	1.43	1.38
14	A	827	CLA	C3B-C4B	2.49	1.50	1.42
13	A	801	CL0	CAC-C3C	-2.49	1.47	1.51
14	B	3024	CLA	C3B-C4B	2.49	1.50	1.42
14	A	820	CLA	C3B-C4B	2.48	1.50	1.42
14	B	3025	CLA	C1B-C2B	2.48	1.48	1.43
14	A	817	CLA	C3B-C4B	2.48	1.49	1.42
14	B	3027	CLA	CHC-C1C	2.48	1.43	1.38
14	A	819	CLA	CHC-C1C	2.48	1.43	1.38
16	F	203	BCR	C33-C5	-2.47	1.47	1.50
14	A	830	CLA	CHC-C1C	2.47	1.43	1.38
17	A	855	LMG	O1-C1	2.47	1.44	1.40
14	A	804	CLA	CMC-C2C	-2.47	1.45	1.50
14	B	3035	CLA	C3B-C4B	2.47	1.49	1.42
14	A	837	CLA	C3B-C4B	2.47	1.49	1.42
16	B	3047	BCR	C33-C5	-2.47	1.47	1.50
14	A	819	CLA	CMC-C2C	-2.47	1.45	1.50
14	A	823	CLA	C3B-C4B	2.46	1.49	1.42
14	A	844	CLA	CMD-C2D	-2.46	1.45	1.50
16	B	3045	BCR	C30-C25	-2.46	1.50	1.53
16	B	3045	BCR	C33-C5	-2.46	1.47	1.50
17	I	102	LMG	O1-C7	2.45	1.48	1.43
14	B	3015	CLA	CHC-C1C	2.45	1.43	1.38
14	B	3010	CLA	MG-NB	-2.45	2.00	2.05
14	B	3003	CLA	C3B-C4B	2.45	1.49	1.42
16	L	208	BCR	C33-C5	-2.45	1.47	1.50
17	B	3049	LMG	O8-C9	-2.45	1.39	1.45
14	A	803	CLA	CHC-C1C	2.44	1.43	1.38
14	B	3012	CLA	C3B-C4B	2.44	1.49	1.42
14	A	821	CLA	C1B-C2B	2.44	1.48	1.43
14	B	3041	CLA	C3B-C4B	2.43	1.49	1.42
14	A	824	CLA	C3B-C4B	2.43	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	802	CLA	CHC-C1C	2.43	1.43	1.38
14	M	102	CLA	MG-NB	-2.43	2.01	2.05
14	B	3031	CLA	C3B-C4B	2.42	1.49	1.42
14	B	3018	CLA	C3B-C4B	2.42	1.49	1.42
16	J	105	BCR	C33-C5	-2.42	1.47	1.50
14	B	3022	CLA	C3B-C4B	2.42	1.49	1.42
15	B	3043	PQN	C2-C1	-2.42	1.42	1.47
14	B	3037	CLA	C3B-C4B	2.41	1.49	1.42
14	A	830	CLA	C3B-C4B	2.41	1.49	1.42
14	X	1701	CLA	C3B-C4B	2.41	1.49	1.42
14	B	3018	CLA	CHC-C1C	2.41	1.43	1.38
14	B	3008	CLA	CHC-C1C	2.41	1.43	1.38
14	A	845	CLA	C3B-C4B	2.41	1.49	1.42
14	A	802	CLA	C3B-C4B	2.41	1.49	1.42
14	B	3023	CLA	CMD-C2D	-2.40	1.45	1.50
18	B	3050	LHG	O8-C6	2.40	1.50	1.45
14	A	807	CLA	CHC-C1C	2.40	1.43	1.38
14	A	835	CLA	CHC-C1C	2.40	1.43	1.38
14	J	102	CLA	C3B-C4B	2.40	1.49	1.42
14	A	836	CLA	C1B-C2B	2.40	1.48	1.43
14	A	805	CLA	CHC-C1C	2.40	1.43	1.38
14	A	804	CLA	CHC-C1C	2.40	1.43	1.38
14	A	835	CLA	C3B-C4B	2.40	1.49	1.42
16	J	104	BCR	C33-C5	-2.40	1.47	1.50
14	A	813	CLA	CMD-C2D	-2.40	1.45	1.50
14	L	205	CLA	MG-NB	-2.39	2.01	2.05
14	B	3040	CLA	C3B-C4B	2.39	1.49	1.42
14	B	3030	CLA	CHC-C1C	2.39	1.43	1.38
14	B	3003	CLA	CHC-C1C	2.39	1.43	1.38
14	A	812	CLA	C3B-C4B	2.38	1.49	1.42
14	A	802	CLA	C1B-C2B	2.38	1.48	1.43
14	A	803	CLA	C3B-C4B	2.38	1.49	1.42
14	B	3042	CLA	C3B-C4B	2.38	1.49	1.42
14	B	3019	CLA	CHC-C1C	2.37	1.43	1.38
14	A	856	CLA	CHC-C1C	2.37	1.43	1.38
14	A	837	CLA	CHC-C1C	2.37	1.43	1.38
14	A	810	CLA	CHC-C1C	2.37	1.43	1.38
14	B	3039	CLA	CHC-C1C	2.36	1.43	1.38
14	A	833	CLA	CHC-C1C	2.36	1.43	1.38
14	A	826	CLA	C3B-C4B	2.36	1.49	1.42
14	A	840	CLA	C3B-C4B	2.36	1.49	1.42
14	A	808	CLA	CHC-C1C	2.36	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3019	CLA	C3B-C4B	2.36	1.49	1.42
14	A	838	CLA	MG-NB	-2.36	2.01	2.05
14	B	3009	CLA	CHC-C1C	2.36	1.43	1.38
16	A	847	BCR	C33-C5	-2.36	1.47	1.50
14	B	3009	CLA	C3B-C4B	2.36	1.49	1.42
14	B	3026	CLA	CMB-C2B	-2.35	1.45	1.50
14	M	102	CLA	CMD-C2D	-2.35	1.46	1.50
16	A	849	BCR	C33-C5	-2.35	1.47	1.50
14	B	3004	CLA	CHC-C1C	2.35	1.43	1.38
14	A	811	CLA	MG-NB	-2.35	2.01	2.05
14	B	3035	CLA	CHC-C1C	2.34	1.43	1.38
14	A	813	CLA	CHC-C1C	2.34	1.43	1.38
13	A	801	CL0	CMC-C2C	-2.33	1.47	1.50
14	A	819	CLA	C3B-C4B	2.33	1.49	1.42
14	A	836	CLA	CHC-C1C	2.33	1.43	1.38
15	A	846	PQN	C2-C1	-2.33	1.42	1.47
14	A	822	CLA	CHC-C1C	2.33	1.43	1.38
14	B	3039	CLA	C3B-C4B	2.33	1.49	1.42
14	B	3037	CLA	CHC-C1C	2.32	1.43	1.38
14	F	202	CLA	C3B-C4B	2.32	1.49	1.42
14	A	825	CLA	CHC-C1C	2.32	1.43	1.38
14	B	3004	CLA	C3B-C4B	2.32	1.49	1.42
14	B	3015	CLA	C3B-C4B	2.32	1.49	1.42
17	I	102	LMG	O8-C28	2.32	1.40	1.33
14	A	824	CLA	CHC-C1C	2.32	1.43	1.38
14	B	3032	CLA	C3B-C4B	2.31	1.49	1.42
16	B	3046	BCR	C33-C5	-2.31	1.47	1.50
14	A	834	CLA	CHC-C1C	2.31	1.43	1.38
14	F	202	CLA	CMB-C2B	-2.31	1.46	1.50
14	M	102	CLA	MG-ND	-2.31	2.01	2.05
14	J	102	CLA	CHC-C1C	2.31	1.43	1.38
16	B	3044	BCR	C33-C5	-2.31	1.47	1.50
14	B	3017	CLA	CHC-C1C	2.31	1.43	1.38
14	L	204	CLA	CMB-C2B	-2.30	1.46	1.50
14	A	834	CLA	C3B-C4B	2.30	1.49	1.42
14	A	842	CLA	C3B-C4B	2.30	1.49	1.42
14	K	103	CLA	C3B-C4B	2.30	1.49	1.42
14	A	819	CLA	CMB-C2B	-2.29	1.46	1.50
14	A	815	CLA	CHC-C1C	2.29	1.43	1.38
14	B	3021	CLA	C3B-C4B	2.29	1.49	1.42
14	A	819	CLA	MG-NB	-2.29	2.01	2.05
22	L	207	DGD	O3G-C1D	2.29	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3037	CLA	CMB-C2B	-2.29	1.46	1.50
14	B	3003	CLA	CMB-C2B	-2.29	1.46	1.50
14	F	202	CLA	CHC-C1C	2.28	1.43	1.38
14	B	3007	CLA	CMD-C2D	-2.28	1.46	1.50
16	F	201	BCR	C33-C5	-2.28	1.47	1.50
14	B	3033	CLA	CHC-C1C	2.28	1.43	1.38
16	A	848	BCR	C33-C5	-2.28	1.47	1.50
14	A	842	CLA	MG-NB	-2.28	2.01	2.05
14	A	829	CLA	CHC-C1C	2.27	1.43	1.38
14	B	3038	CLA	C3B-C4B	2.27	1.49	1.42
16	L	209	BCR	C33-C5	-2.27	1.47	1.50
14	B	3005	CLA	CMD-C2D	-2.27	1.46	1.50
14	B	3041	CLA	CHC-C1C	2.26	1.43	1.38
14	A	815	CLA	MG-NB	-2.26	2.01	2.05
14	K	103	CLA	CHC-C1C	2.26	1.43	1.38
14	A	831	CLA	MG-NB	-2.26	2.01	2.05
16	B	3051	BCR	C33-C5	-2.25	1.47	1.50
14	B	3022	CLA	CHC-C1C	2.25	1.43	1.38
14	F	202	CLA	MG-NB	-2.25	2.01	2.05
14	A	827	CLA	CMD-C2D	-2.25	1.46	1.50
14	B	3016	CLA	C3B-C4B	2.25	1.49	1.42
14	A	856	CLA	C3B-C4B	2.25	1.49	1.42
14	A	826	CLA	CHC-C1C	2.25	1.43	1.38
14	B	3004	CLA	CMD-C2D	-2.25	1.46	1.50
14	B	3007	CLA	CMB-C2B	-2.25	1.46	1.50
14	A	833	CLA	C3B-C4B	2.25	1.49	1.42
21	L	202	LMT	O4'-C4B	-2.25	1.37	1.43
14	B	3031	CLA	CHC-C1C	2.24	1.43	1.38
14	A	856	CLA	MG-NB	-2.24	2.01	2.05
14	B	3032	CLA	O2D-CGD	2.24	1.38	1.33
14	B	3010	CLA	C3B-C4B	2.24	1.49	1.42
14	A	813	CLA	MG-NB	-2.23	2.01	2.05
14	A	836	CLA	CMB-C2B	-2.23	1.46	1.50
14	M	102	CLA	CMB-C2B	-2.23	1.46	1.50
14	A	811	CLA	CHC-C1C	2.23	1.43	1.38
14	L	204	CLA	MG-NB	-2.23	2.01	2.05
14	A	803	CLA	CMD-C2D	-2.23	1.46	1.50
14	B	3028	CLA	C3B-C4B	2.23	1.49	1.42
14	A	840	CLA	CHC-C1C	2.23	1.42	1.38
14	X	1701	CLA	CHC-C1C	2.22	1.42	1.38
16	B	3048	BCR	C33-C5	-2.22	1.47	1.50
14	B	3034	CLA	C3B-C4B	2.22	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3023	CLA	MG-NB	-2.22	2.01	2.05
14	A	844	CLA	CMB-C2B	-2.22	1.46	1.50
16	M	103	BCR	C33-C5	-2.22	1.47	1.50
14	A	843	CLA	CMD-C2D	-2.22	1.46	1.50
16	K	102	BCR	C33-C5	-2.21	1.47	1.50
14	B	3026	CLA	C3B-C4B	2.21	1.49	1.42
14	B	3020	CLA	CMD-C2D	-2.21	1.46	1.50
14	B	3031	CLA	CMB-C2B	-2.21	1.46	1.50
14	A	811	CLA	C3B-C4B	2.21	1.49	1.42
14	B	3023	CLA	C3B-C4B	2.21	1.49	1.42
13	A	801	CL0	CHC-C1C	2.20	1.43	1.39
14	A	805	CLA	C3B-C4B	2.20	1.49	1.42
16	J	103	BCR	C33-C5	-2.20	1.47	1.50
14	A	856	CLA	CMD-C2D	-2.20	1.46	1.50
14	B	3003	CLA	CMD-C2D	-2.20	1.46	1.50
18	A	853	LHG	O7-C5	-2.20	1.41	1.46
14	A	845	CLA	MG-NB	-2.19	2.01	2.05
14	M	102	CLA	CHC-C1C	2.19	1.42	1.38
16	A	850	BCR	C33-C5	-2.19	1.47	1.50
14	A	808	CLA	C3B-C4B	2.19	1.49	1.42
16	A	851	BCR	C33-C5	-2.18	1.47	1.50
14	A	806	CLA	C3B-C4B	2.18	1.49	1.42
14	B	3006	CLA	C3B-C4B	2.18	1.49	1.42
14	B	3040	CLA	CHC-C1C	2.18	1.42	1.38
14	B	3007	CLA	C3B-C4B	2.18	1.49	1.42
14	A	839	CLA	C3B-C4B	2.17	1.49	1.42
14	J	102	CLA	CBD-CAD	2.17	1.56	1.51
14	A	827	CLA	MG-NB	-2.17	2.01	2.05
14	B	3021	CLA	CMD-C2D	-2.17	1.46	1.50
14	B	3034	CLA	CHC-C1C	2.17	1.42	1.38
14	L	206	CLA	C1B-C2B	2.17	1.48	1.43
14	B	3006	CLA	CHC-C1C	2.17	1.42	1.38
14	K	101	CLA	CBD-CAD	2.17	1.56	1.51
14	B	3004	CLA	CMB-C2B	-2.17	1.46	1.50
14	M	102	CLA	C3B-C4B	2.16	1.49	1.42
14	M	102	CLA	MG-NC	2.16	2.11	2.06
14	B	3012	CLA	CHC-C1C	2.16	1.42	1.38
14	A	816	CLA	C3B-C4B	2.16	1.49	1.42
14	B	3020	CLA	C3B-C4B	2.16	1.49	1.42
16	L	201	BCR	C33-C5	-2.16	1.47	1.50
21	L	202	LMT	O2B-C2B	-2.16	1.37	1.43
14	B	3004	CLA	MG-NB	-2.16	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3010	CLA	CMD-C2D	-2.15	1.46	1.50
14	B	3020	CLA	CMB-C2B	-2.15	1.46	1.50
14	B	3039	CLA	CMB-C2B	-2.15	1.46	1.50
14	A	817	CLA	CMB-C2B	-2.15	1.46	1.50
21	L	202	LMT	O2'-C2'	-2.15	1.37	1.43
14	A	832	CLA	C3B-C4B	2.15	1.49	1.42
14	A	832	CLA	CMC-C2C	-2.15	1.46	1.50
14	B	3038	CLA	CMB-C2B	-2.15	1.46	1.50
14	B	3008	CLA	CMD-C2D	-2.15	1.46	1.50
14	L	206	CLA	MG-NB	-2.14	2.01	2.05
14	B	3038	CLA	CHC-C1C	2.14	1.42	1.38
14	B	3028	CLA	CMC-C2C	-2.13	1.46	1.50
22	L	207	DGD	C3G-C2G	2.13	1.57	1.50
17	I	102	LMG	C9-C8	2.13	1.57	1.50
14	A	815	CLA	CMB-C2B	-2.13	1.46	1.50
14	A	832	CLA	CHC-C1C	2.13	1.42	1.38
14	A	811	CLA	CMD-C2D	-2.13	1.46	1.50
14	B	3005	CLA	C3B-C4B	2.12	1.48	1.42
14	A	841	CLA	MG-NB	-2.12	2.01	2.05
14	A	833	CLA	CMC-C2C	-2.12	1.46	1.50
14	A	815	CLA	CMD-C2D	-2.12	1.46	1.50
14	A	823	CLA	CMB-C2B	-2.12	1.46	1.50
14	B	3020	CLA	CMC-C2C	-2.12	1.46	1.50
14	B	3042	CLA	CHC-C1C	2.12	1.42	1.38
14	B	3028	CLA	CHC-C1C	2.12	1.42	1.38
14	B	3042	CLA	CMB-C2B	-2.12	1.46	1.50
14	B	3040	CLA	MG-NB	-2.12	2.01	2.05
14	A	816	CLA	MG-NB	-2.11	2.01	2.05
14	A	815	CLA	C3B-C4B	2.11	1.48	1.42
14	A	844	CLA	MG-NB	-2.11	2.01	2.05
14	A	829	CLA	CMD-C2D	-2.11	1.46	1.50
14	A	835	CLA	C1D-C2D	2.11	1.49	1.45
14	B	3007	CLA	MG-NB	-2.11	2.01	2.05
14	A	803	CLA	CMB-C2B	-2.11	1.46	1.50
21	L	202	LMT	O3'-C3'	-2.11	1.37	1.43
14	A	812	CLA	CMB-C2B	-2.11	1.46	1.50
14	B	3020	CLA	MG-NB	-2.10	2.01	2.05
14	B	3027	CLA	CMC-C2C	-2.10	1.46	1.50
14	A	818	CLA	CMC-C2C	-2.10	1.46	1.50
14	A	834	CLA	CMC-C2C	-2.10	1.46	1.50
14	B	3011	CLA	MG-ND	-2.09	2.01	2.05
18	A	853	LHG	P-O6	2.09	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	806	CLA	CMB-C2B	-2.09	1.46	1.50
14	A	820	CLA	CHC-C1C	2.09	1.42	1.38
14	B	3023	CLA	CMB-C2B	-2.09	1.46	1.50
14	A	819	CLA	CMD-C2D	-2.09	1.46	1.50
14	A	830	CLA	CMC-C2C	-2.09	1.46	1.50
14	A	841	CLA	C3B-C4B	2.09	1.48	1.42
14	A	839	CLA	CHC-C1C	2.09	1.42	1.38
14	B	3028	CLA	CMD-C2D	-2.09	1.46	1.50
14	A	834	CLA	CMD-C2D	-2.09	1.46	1.50
14	B	3009	CLA	CMB-C2B	-2.08	1.46	1.50
14	L	205	CLA	CMB-C2B	-2.08	1.46	1.50
14	A	802	CLA	MG-NB	-2.08	2.01	2.05
14	M	102	CLA	C1A-CHA	-2.08	1.34	1.43
14	B	3039	CLA	MG-NB	-2.08	2.01	2.05
14	B	3030	CLA	CMB-C2B	-2.08	1.46	1.50
14	K	103	CLA	MG-NB	-2.08	2.01	2.05
14	A	821	CLA	CMB-C2B	-2.08	1.46	1.50
14	B	3005	CLA	CMB-C2B	-2.08	1.46	1.50
14	B	3010	CLA	C1B-C2B	2.08	1.48	1.43
14	A	843	CLA	CMB-C2B	-2.08	1.46	1.50
14	B	3018	CLA	MG-NB	-2.08	2.01	2.05
14	B	3017	CLA	MG-NB	-2.07	2.01	2.05
14	B	3016	CLA	CMD-C2D	-2.07	1.46	1.50
14	A	816	CLA	CMB-C2B	-2.07	1.46	1.50
14	A	816	CLA	O2D-CGD	2.07	1.38	1.33
14	B	3037	CLA	MG-NB	-2.07	2.01	2.05
14	L	206	CLA	CMD-C2D	-2.07	1.46	1.50
14	B	3022	CLA	CMD-C2D	-2.07	1.46	1.50
14	A	806	CLA	CHC-C1C	2.07	1.42	1.38
14	B	3042	CLA	MG-NB	-2.07	2.01	2.05
14	A	839	CLA	CMD-C2D	-2.07	1.46	1.50
14	B	3010	CLA	CHC-C1C	2.07	1.42	1.38
14	B	3021	CLA	CHC-C1C	2.07	1.42	1.38
14	B	3041	CLA	C1D-C2D	2.07	1.49	1.45
17	A	852	LMG	O1-C1	2.07	1.43	1.40
14	A	831	CLA	C3B-C4B	2.07	1.48	1.42
14	A	845	CLA	CHC-C1C	2.06	1.42	1.38
14	A	820	CLA	CMC-C2C	-2.06	1.46	1.50
14	B	3021	CLA	CMB-C2B	-2.06	1.46	1.50
14	X	1701	CLA	CMB-C2B	-2.06	1.46	1.50
16	A	847	BCR	C38-C26	-2.06	1.47	1.50
14	B	3020	CLA	CHC-C1C	2.06	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	838	CLA	CMB-C2B	-2.06	1.46	1.50
14	B	3019	CLA	CMB-C2B	-2.06	1.46	1.50
14	B	3014	CLA	MG-NB	-2.06	2.01	2.05
17	A	855	LMG	C3-C2	2.05	1.57	1.52
14	B	3038	CLA	MG-NB	-2.05	2.01	2.05
14	A	826	CLA	CMB-C2B	-2.05	1.46	1.50
14	A	817	CLA	CMD-C2D	-2.05	1.46	1.50
14	A	840	CLA	CMB-C2B	-2.05	1.46	1.50
18	B	3050	LHG	P-O3	2.05	1.67	1.59
14	B	3013	CLA	CMB-C2B	-2.05	1.46	1.50
14	A	833	CLA	MG-NB	-2.05	2.01	2.05
14	A	836	CLA	CMD-C2D	-2.05	1.46	1.50
14	B	3022	CLA	CMB-C2B	-2.05	1.46	1.50
14	B	3040	CLA	CMB-C2B	-2.05	1.46	1.50
14	B	3023	CLA	CHC-C1C	2.05	1.42	1.38
14	A	805	CLA	MG-NB	-2.05	2.01	2.05
14	A	805	CLA	CMB-C2B	-2.05	1.46	1.50
14	B	3031	CLA	O2A-CGA	2.05	1.37	1.30
14	B	3010	CLA	CMC-C2C	-2.04	1.46	1.50
14	B	3012	CLA	CMB-C2B	-2.04	1.46	1.50
14	A	808	CLA	CMB-C2B	-2.04	1.46	1.50
14	A	830	CLA	CMB-C2B	-2.04	1.46	1.50
14	A	838	CLA	C3B-C4B	2.04	1.48	1.42
14	B	3008	CLA	CMC-C2C	-2.04	1.46	1.50
14	B	3041	CLA	CMB-C2B	-2.04	1.46	1.50
14	A	838	CLA	CMD-C2D	-2.04	1.46	1.50
14	A	813	CLA	CMC-C2C	-2.04	1.46	1.50
14	B	3030	CLA	CMD-C2D	-2.04	1.46	1.50
14	A	823	CLA	CHC-C1C	2.04	1.42	1.38
14	L	205	CLA	C3B-C4B	2.04	1.48	1.42
14	A	822	CLA	MG-NB	-2.03	2.01	2.05
14	K	101	CLA	CMB-C2B	-2.03	1.46	1.50
14	A	833	CLA	CMB-C2B	-2.03	1.46	1.50
14	A	856	CLA	CMB-C2B	-2.03	1.46	1.50
14	A	835	CLA	MG-NB	-2.03	2.01	2.05
14	A	836	CLA	CMC-C2C	-2.03	1.46	1.50
14	B	3009	CLA	CMD-C2D	-2.03	1.46	1.50
14	B	3033	CLA	CMD-C2D	-2.03	1.46	1.50
14	A	805	CLA	CMD-C2D	-2.03	1.46	1.50
13	A	801	CL0	MG-NB	-2.03	2.01	2.05
14	A	842	CLA	CMB-C2B	-2.03	1.46	1.50
14	B	3027	CLA	CMB-C2B	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	837	CLA	CMD-C2D	-2.02	1.46	1.50
14	A	837	CLA	O2A-CGA	2.02	1.37	1.30
14	A	830	CLA	MG-NB	-2.02	2.01	2.05
14	A	825	CLA	MG-NB	-2.02	2.01	2.05
14	A	832	CLA	MG-NB	-2.02	2.01	2.05
14	B	3014	CLA	CMC-C2C	-2.02	1.46	1.50
14	L	205	CLA	CMD-C2D	-2.02	1.46	1.50
14	B	3032	CLA	CHC-C1C	2.02	1.42	1.38
16	F	201	BCR	C38-C26	-2.02	1.47	1.50
18	A	853	LHG	O8-C6	-2.02	1.40	1.45
14	A	838	CLA	CHC-C1C	2.02	1.42	1.38
14	A	828	CLA	CMD-C2D	-2.02	1.46	1.50
14	B	3035	CLA	CMB-C2B	-2.02	1.46	1.50
14	A	856	CLA	MG-ND	-2.01	2.01	2.05
14	B	3034	CLA	CMB-C2B	-2.01	1.46	1.50
14	J	102	CLA	CMD-C2D	-2.01	1.46	1.50
14	A	812	CLA	O2D-CGD	2.01	1.38	1.33
14	A	809	CLA	CMD-C2D	-2.01	1.46	1.50
14	B	3025	CLA	C3D-C4D	2.01	1.48	1.44
14	B	3025	CLA	CMB-C2B	-2.01	1.46	1.50
14	A	833	CLA	CMD-C2D	-2.01	1.46	1.50
14	A	813	CLA	CMB-C2B	-2.01	1.46	1.50
14	A	811	CLA	CMB-C2B	-2.01	1.46	1.50
14	A	840	CLA	CMD-C2D	-2.00	1.46	1.50
14	A	842	CLA	CMC-C2C	-2.00	1.46	1.50
14	A	825	CLA	CMB-C2B	-2.00	1.46	1.50
14	A	812	CLA	CMC-C2C	-2.00	1.46	1.50

All (773) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	842	CLA	C4A-NA-C1A	8.00	110.33	106.68
14	A	806	CLA	C4A-NA-C1A	7.90	110.28	106.68
14	B	3042	CLA	C4A-NA-C1A	7.73	110.20	106.68
14	B	3033	CLA	C4A-NA-C1A	7.62	110.16	106.68
14	A	803	CLA	C4A-NA-C1A	7.58	110.14	106.68
14	B	3005	CLA	C4A-NA-C1A	7.45	110.08	106.68
14	B	3028	CLA	C4A-NA-C1A	7.37	110.04	106.68
14	B	3003	CLA	C4A-NA-C1A	7.29	110.01	106.68
14	A	812	CLA	C4A-NA-C1A	7.12	109.93	106.68
14	B	3031	CLA	C4A-NA-C1A	7.10	109.92	106.68
14	B	3012	CLA	C4A-NA-C1A	7.10	109.92	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3004	CLA	C4A-NA-C1A	7.07	109.90	106.68
14	A	832	CLA	C4A-NA-C1A	7.01	109.88	106.68
14	B	3008	CLA	C4A-NA-C1A	7.00	109.87	106.68
14	B	3026	CLA	C4A-NA-C1A	7.00	109.87	106.68
14	L	204	CLA	C4A-NA-C1A	6.95	109.85	106.68
14	A	820	CLA	C4A-NA-C1A	6.91	109.83	106.68
14	B	3040	CLA	C4A-NA-C1A	6.89	109.82	106.68
14	A	843	CLA	C4A-NA-C1A	6.89	109.82	106.68
14	A	828	CLA	C4A-NA-C1A	6.87	109.81	106.68
14	B	3041	CLA	C4A-NA-C1A	6.81	109.79	106.68
14	B	3006	CLA	C4A-NA-C1A	6.80	109.78	106.68
14	A	840	CLA	C4A-NA-C1A	6.75	109.76	106.68
14	B	3007	CLA	C4A-NA-C1A	6.74	109.76	106.68
14	L	205	CLA	C4A-NA-C1A	6.71	109.74	106.68
14	A	817	CLA	C4A-NA-C1A	6.71	109.74	106.68
14	A	844	CLA	C4A-NA-C1A	6.70	109.74	106.68
14	B	3020	CLA	C4A-NA-C1A	6.66	109.72	106.68
14	B	3010	CLA	C4A-NA-C1A	6.66	109.72	106.68
14	B	3039	CLA	C4A-NA-C1A	6.65	109.71	106.68
14	A	837	CLA	C4A-NA-C1A	6.62	109.70	106.68
14	B	3017	CLA	C4A-NA-C1A	6.47	109.63	106.68
14	B	3030	CLA	C4A-NA-C1A	6.47	109.63	106.68
14	A	824	CLA	C4A-NA-C1A	6.46	109.63	106.68
14	A	833	CLA	C4A-NA-C1A	6.45	109.62	106.68
14	A	829	CLA	C4A-NA-C1A	6.42	109.61	106.68
14	A	845	CLA	C4A-NA-C1A	6.42	109.61	106.68
14	B	3018	CLA	C4A-NA-C1A	6.40	109.60	106.68
14	A	838	CLA	C4A-NA-C1A	6.39	109.60	106.68
14	A	823	CLA	C4A-NA-C1A	6.37	109.59	106.68
14	A	816	CLA	C4A-NA-C1A	6.35	109.58	106.68
14	B	3013	CLA	C4A-NA-C1A	6.31	109.56	106.68
14	A	839	CLA	C4A-NA-C1A	6.30	109.55	106.68
13	A	801	CL0	C1B-CHB-C4A	6.29	125.37	121.32
14	B	3009	CLA	C4A-NA-C1A	6.24	109.53	106.68
14	A	841	CLA	C4A-NA-C1A	6.20	109.51	106.68
14	B	3037	CLA	C4A-NA-C1A	6.19	109.50	106.68
14	B	3038	CLA	C4A-NA-C1A	6.17	109.50	106.68
14	A	826	CLA	C4A-NA-C1A	6.17	109.49	106.68
14	A	830	CLA	C4A-NA-C1A	6.14	109.48	106.68
14	B	3021	CLA	C4A-NA-C1A	6.13	109.48	106.68
14	A	831	CLA	C4A-NA-C1A	6.12	109.47	106.68
14	A	818	CLA	C4A-NA-C1A	6.11	109.47	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	834	CLA	C4A-NA-C1A	6.04	109.44	106.68
14	B	3032	CLA	C4A-NA-C1A	6.04	109.43	106.68
14	B	3029	CLA	C4A-NA-C1A	6.03	109.43	106.68
14	A	813	CLA	C4A-NA-C1A	6.02	109.42	106.68
14	B	3016	CLA	C4A-NA-C1A	6.01	109.42	106.68
14	B	3022	CLA	C4A-NA-C1A	5.97	109.40	106.68
14	A	805	CLA	C4A-NA-C1A	5.96	109.40	106.68
14	A	809	CLA	C4A-NA-C1A	5.92	109.38	106.68
14	B	3011	CLA	C4A-NA-C1A	5.86	109.35	106.68
14	A	815	CLA	C4A-NA-C1A	5.85	109.35	106.68
14	A	804	CLA	C4A-NA-C1A	5.84	109.34	106.68
14	B	3027	CLA	C4A-NA-C1A	5.84	109.34	106.68
14	A	836	CLA	C4A-NA-C1A	5.82	109.33	106.68
14	X	1701	CLA	C4A-NA-C1A	5.82	109.33	106.68
14	A	821	CLA	C4A-NA-C1A	5.79	109.32	106.68
14	A	819	CLA	C4A-NA-C1A	5.72	109.29	106.68
14	A	835	CLA	C4A-NA-C1A	5.68	109.27	106.68
14	A	802	CLA	C4A-NA-C1A	5.66	109.26	106.68
14	B	3019	CLA	C4A-NA-C1A	5.65	109.26	106.68
14	J	101	CLA	C4A-NA-C1A	5.65	109.26	106.68
14	A	825	CLA	C4A-NA-C1A	5.60	109.23	106.68
14	K	101	CLA	C4A-NA-C1A	5.60	109.23	106.68
14	A	856	CLA	C4A-NA-C1A	5.57	109.22	106.68
14	A	808	CLA	C4A-NA-C1A	5.53	109.20	106.68
14	A	822	CLA	C4A-NA-C1A	5.50	109.19	106.68
14	B	3035	CLA	C4A-NA-C1A	5.50	109.19	106.68
14	J	102	CLA	C4A-NA-C1A	5.48	109.18	106.68
14	B	3023	CLA	C4A-NA-C1A	5.45	109.16	106.68
14	B	3015	CLA	C4A-NA-C1A	5.41	109.14	106.68
14	B	3014	CLA	C4A-NA-C1A	5.25	109.07	106.68
14	A	810	CLA	C4A-NA-C1A	5.23	109.06	106.68
14	B	3025	CLA	C4A-NA-C1A	5.21	109.06	106.68
14	A	827	CLA	C4A-NA-C1A	5.13	109.02	106.68
14	A	807	CLA	C4A-NA-C1A	5.12	109.01	106.68
14	A	814	CLA	C4A-NA-C1A	5.08	109.00	106.68
14	A	811	CLA	C4A-NA-C1A	5.06	108.99	106.68
14	B	3034	CLA	C4A-NA-C1A	5.05	108.98	106.68
14	K	103	CLA	C4A-NA-C1A	5.02	108.97	106.68
14	L	206	CLA	C4A-NA-C1A	4.99	108.96	106.68
14	B	3036	CLA	C4A-NA-C1A	4.96	108.94	106.68
14	B	3024	CLA	C4A-NA-C1A	4.62	108.78	106.68
14	A	816	CLA	O2D-CGD-CBD	4.55	119.19	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	835	CLA	C1-C2-C3	-4.48	118.86	126.20
18	A	854	LHG	O4-P-O5	4.46	133.18	112.44
18	M	101	LHG	O4-P-O5	4.36	132.73	112.44
18	A	853	LHG	O4-P-O5	4.34	132.62	112.44
16	K	102	BCR	C2-C1-C6	4.23	116.58	110.44
14	L	204	CLA	C1-C2-C3	-4.22	119.29	126.20
18	B	3050	LHG	O4-P-O5	4.11	131.59	112.44
14	F	202	CLA	C4A-NA-C1A	4.01	108.51	106.68
16	A	851	BCR	C2-C1-C6	3.94	116.17	110.44
14	A	819	CLA	C3B-C4B-NB	-3.91	107.04	110.53
16	F	201	BCR	C2-C1-C6	3.90	116.11	110.44
14	A	803	CLA	CAA-C2A-C1A	-3.88	99.26	111.97
14	B	3030	CLA	CAA-C2A-C3A	-3.86	102.56	113.00
14	A	827	CLA	C3B-C4B-NB	-3.81	107.13	110.53
14	B	3025	CLA	C3B-C4B-NB	-3.80	107.14	110.53
14	K	103	CLA	O2D-CGD-O1D	-3.77	116.52	123.85
14	A	843	CLA	C3B-C4B-NB	-3.75	107.18	110.53
16	F	203	BCR	C35-C13-C14	-3.73	116.77	122.82
14	A	843	CLA	O2D-CGD-O1D	-3.69	116.66	123.85
14	A	809	CLA	C3B-C4B-NB	-3.65	107.27	110.53
14	A	856	CLA	O2D-CGD-O1D	-3.65	116.74	123.85
14	B	3036	CLA	C3B-C4B-NB	-3.63	107.29	110.53
14	B	3010	CLA	C1-C2-C3	-3.60	120.30	126.20
14	A	839	CLA	O2D-CGD-CBD	3.60	117.52	111.23
14	B	3032	CLA	O2D-CGD-O1D	-3.57	116.89	123.85
14	A	818	CLA	C3B-C4B-NB	-3.55	107.36	110.53
14	B	3014	CLA	C3B-C4B-NB	-3.52	107.39	110.53
16	B	3047	BCR	C2-C1-C6	3.49	115.50	110.44
14	X	1701	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
14	B	3003	CLA	C3B-C4B-NB	-3.49	107.42	110.53
14	K	103	CLA	O2D-CGD-CBD	3.47	117.29	111.23
14	B	3009	CLA	O2A-CGA-O1A	-3.46	114.96	123.63
14	A	814	CLA	C3B-C4B-NB	-3.46	107.44	110.53
14	B	3039	CLA	C3B-C4B-NB	-3.46	107.44	110.53
14	B	3013	CLA	C3B-C4B-NB	-3.46	107.44	110.53
14	B	3006	CLA	O2D-CGD-O1D	-3.46	117.12	123.85
16	F	201	BCR	C27-C26-C25	3.45	127.37	122.70
14	F	202	CLA	O2D-CGD-O1D	-3.45	117.12	123.85
14	B	3020	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
14	A	816	CLA	O2D-CGD-O1D	-3.44	117.14	123.85
14	A	826	CLA	O2D-CGD-O1D	-3.42	117.18	123.85
21	L	202	LMT	C2'-C3'-C4'	3.42	117.45	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3035	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
14	A	813	CLA	C3B-C4B-NB	-3.38	107.52	110.53
14	A	813	CLA	O2D-CGD-O1D	-3.37	117.30	123.85
18	A	854	LHG	O8-C23-C24	3.36	121.35	111.15
14	L	206	CLA	C3B-C4B-NB	-3.36	107.53	110.53
14	B	3032	CLA	CED-O2D-CGD	3.34	123.50	115.92
14	B	3009	CLA	O2D-CGD-O1D	-3.33	117.38	123.85
16	B	3044	BCR	C29-C30-C25	3.32	115.27	110.44
16	L	209	BCR	C15-C16-C17	-3.32	116.74	123.52
16	L	208	BCR	C27-C26-C25	3.31	127.18	122.70
14	A	838	CLA	C3B-C4B-NB	-3.30	107.58	110.53
18	M	101	LHG	O8-C23-C24	3.29	121.88	111.83
16	M	103	BCR	C33-C5-C6	-3.29	120.89	124.48
14	M	102	CLA	C4A-NA-C1A	3.29	108.18	106.68
15	B	3043	PQN	O1-C1-C10	-3.28	116.33	121.57
16	K	102	BCR	C27-C26-C25	3.28	127.13	122.70
14	A	839	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
14	A	830	CLA	C3B-C4B-NB	-3.25	107.63	110.53
14	A	818	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
14	M	102	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
14	A	835	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
14	A	806	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
14	L	205	CLA	C3B-C4B-NB	-3.21	107.67	110.53
14	A	840	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
14	B	3012	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
14	A	821	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
16	J	105	BCR	C7-C8-C9	-3.19	121.51	126.23
14	M	102	CLA	CAC-C3C-C4C	3.19	128.94	124.79
14	F	202	CLA	C3B-C4B-NB	-3.19	107.68	110.53
13	A	801	CL0	CHA-C1A-C2A	-3.19	125.82	133.31
14	A	823	CLA	CHB-C4A-NA	3.17	128.98	124.40
15	A	846	PQN	O1-C1-C10	-3.17	116.50	121.57
14	B	3018	CLA	C3B-C4B-NB	-3.16	107.70	110.53
14	B	3041	CLA	CAC-C3C-C4C	3.16	128.91	124.79
14	B	3004	CLA	C3B-C4B-NB	-3.15	107.72	110.53
14	A	805	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
14	B	3030	CLA	CHB-C4A-NA	3.13	128.92	124.40
14	A	825	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
14	A	820	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
14	M	102	CLA	C2D-C1D-ND	-3.13	107.03	110.13
14	A	828	CLA	C3B-C4B-NB	-3.12	107.74	110.53
14	B	3036	CLA	O2D-CGD-O1D	-3.12	117.77	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	201	BCR	C24-C23-C22	-3.12	121.62	126.23
17	B	3049	LMG	O6-C1-O1	-3.11	102.69	110.04
14	A	822	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
14	B	3005	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
16	B	3051	BCR	C27-C26-C25	3.11	126.91	122.70
14	B	3031	CLA	C3B-C4B-NB	-3.11	107.75	110.53
14	A	820	CLA	CAA-C2A-C1A	-3.11	101.79	111.97
14	A	836	CLA	C3B-C4B-NB	-3.11	107.76	110.53
14	B	3029	CLA	C3B-C4B-NB	-3.10	107.76	110.53
14	A	827	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
14	A	823	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
14	B	3027	CLA	C3B-C4B-NB	-3.08	107.78	110.53
14	A	833	CLA	C3B-C4B-NB	-3.08	107.78	110.53
14	A	808	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
14	B	3042	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
14	L	206	CLA	CMB-C2B-C1B	-3.07	120.75	125.42
14	A	843	CLA	CHB-C4A-NA	3.07	128.83	124.40
21	L	202	LMT	C1'-C2'-C3'	3.07	116.46	110.01
14	A	811	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
14	B	3018	CLA	CHB-C4A-NA	3.06	128.81	124.40
14	B	3042	CLA	CHB-C4A-NA	3.05	128.81	124.40
14	A	830	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
14	B	3010	CLA	C6-C5-C3	-3.04	106.05	113.47
14	A	843	CLA	O2D-CGD-CBD	3.04	116.55	111.23
16	A	849	BCR	C15-C14-C13	-3.04	123.01	127.28
14	A	835	CLA	C3B-C4B-NB	-3.03	107.83	110.53
14	B	3038	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
16	B	3047	BCR	C27-C26-C25	3.02	126.78	122.70
16	A	847	BCR	C33-C5-C6	-3.02	121.19	124.48
14	A	829	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
14	A	837	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
13	A	801	CL0	O1D-CGD-CBD	3.01	129.29	124.72
14	A	841	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
16	J	105	BCR	C27-C26-C25	3.00	126.76	122.70
14	B	3025	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
16	L	201	BCR	C2-C1-C6	2.99	114.78	110.44
14	B	3019	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
14	A	803	CLA	C3B-C4B-NB	-2.99	107.86	110.53
14	B	3011	CLA	CHB-C4A-NA	2.98	128.71	124.40
16	J	105	BCR	C2-C1-C6	2.98	114.77	110.44
14	A	839	CLA	CHB-C4A-NA	2.98	128.71	124.40
16	F	203	BCR	C2-C1-C6	2.98	114.77	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	844	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
14	A	845	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
16	L	208	BCR	C33-C5-C6	-2.97	121.24	124.48
14	A	804	CLA	C3B-C4B-NB	-2.97	107.88	110.53
14	A	821	CLA	CMB-C2B-C1B	-2.96	120.91	125.42
14	A	840	CLA	O2D-CGD-CBD	2.96	116.40	111.23
14	B	3018	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
16	J	104	BCR	C24-C23-C22	-2.96	121.86	126.23
14	B	3024	CLA	C3B-C4B-NB	-2.95	107.89	110.53
14	L	206	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
16	A	848	BCR	C2-C1-C6	2.95	114.72	110.44
16	B	3045	BCR	C33-C5-C6	-2.95	121.27	124.48
14	B	3023	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
14	B	3004	CLA	CHB-C4A-NA	2.95	128.65	124.40
14	B	3033	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
16	A	848	BCR	C27-C26-C25	2.94	126.67	122.70
14	A	836	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
14	A	811	CLA	C3B-C4B-NB	-2.92	107.92	110.53
14	B	3027	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
14	L	206	CLA	CMB-C2B-C3B	2.92	133.41	126.55
14	A	807	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
14	B	3010	CLA	CBA-CAA-C2A	-2.91	105.12	113.79
16	A	851	BCR	C28-C27-C26	-2.91	108.86	114.06
14	A	814	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
14	B	3024	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
14	B	3034	CLA	CAC-C3C-C4C	2.90	128.57	124.79
16	A	851	BCR	C7-C8-C9	-2.90	121.95	126.23
14	L	204	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
14	A	835	CLA	C5-C3-C2	2.89	127.65	121.17
14	A	807	CLA	C3B-C4B-NB	-2.89	107.95	110.53
14	K	101	CLA	C3B-C4B-NB	-2.89	107.95	110.53
16	B	3044	BCR	C2-C1-C6	2.88	114.63	110.44
16	F	201	BCR	C16-C15-C14	-2.87	117.64	123.52
14	B	3031	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
14	B	3034	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
21	L	202	LMT	C1'-O5'-C5'	-2.87	108.12	113.72
14	B	3019	CLA	C3B-C4B-NB	-2.87	107.97	110.53
14	M	102	CLA	O2D-CGD-CBD	2.86	116.24	111.23
14	A	805	CLA	C3B-C4B-NB	-2.86	107.97	110.53
14	B	3037	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
14	B	3008	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
14	B	3035	CLA	C3B-C4B-NB	-2.86	107.98	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	819	CLA	CMB-C2B-C1B	-2.86	121.06	125.42
14	B	3007	CLA	C3B-C4B-NB	-2.86	107.98	110.53
14	B	3015	CLA	C3B-C4B-NB	-2.86	107.98	110.53
14	A	820	CLA	CHB-C4A-NA	2.85	128.52	124.40
14	A	817	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
16	J	103	BCR	C27-C26-C25	2.85	126.56	122.70
16	B	3047	BCR	C15-C16-C17	-2.85	117.69	123.52
14	A	832	CLA	C3B-C4B-NB	-2.85	107.99	110.53
14	B	3012	CLA	CHB-C4A-NA	2.85	128.51	124.40
16	A	849	BCR	C15-C16-C17	-2.85	117.70	123.52
14	B	3015	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
16	L	208	BCR	C15-C16-C17	-2.84	117.71	123.52
14	B	3029	CLA	CHB-C4A-NA	2.84	128.49	124.40
14	A	845	CLA	C3B-C4B-NB	-2.83	108.00	110.53
14	X	1701	CLA	CHB-C4A-NA	2.83	128.49	124.40
14	A	837	CLA	C3B-C4B-NB	-2.83	108.00	110.53
14	A	828	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
14	A	818	CLA	O2D-CGD-CBD	2.83	116.17	111.23
14	B	3040	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
14	B	3024	CLA	CAC-C3C-C4C	2.82	128.46	124.79
16	A	851	BCR	C24-C23-C22	-2.82	122.06	126.23
14	A	809	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
14	B	3013	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
16	L	208	BCR	C24-C23-C22	-2.81	122.07	126.23
14	B	3025	CLA	C2A-C1A-CHA	2.81	128.74	123.87
16	B	3047	BCR	C11-C10-C9	-2.81	123.34	127.28
14	B	3025	CLA	C4-C3-C5	2.81	120.10	115.23
13	A	801	CL0	O2D-CGD-O1D	-2.80	118.40	123.85
14	A	813	CLA	O2D-CGD-CBD	2.80	116.12	111.23
14	A	812	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
14	A	844	CLA	CMB-C2B-C1B	-2.79	121.17	125.42
14	B	3014	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
14	B	3016	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
14	B	3029	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
14	A	809	CLA	CHB-C4A-NA	2.77	128.40	124.40
14	B	3010	CLA	C3B-C4B-NB	-2.77	108.06	110.53
14	B	3028	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
14	B	3009	CLA	O2D-CGD-CBD	2.76	116.06	111.23
14	A	838	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
14	B	3033	CLA	O2D-CGD-CBD	2.76	116.05	111.23
14	A	834	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
16	B	3046	BCR	C24-C23-C22	-2.76	122.16	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	855	LMG	C1-O6-C5	-2.76	108.34	113.72
14	B	3025	CLA	CHB-C4A-NA	2.76	128.38	124.40
16	B	3046	BCR	C33-C5-C6	-2.75	121.48	124.48
14	B	3018	CLA	C1-C2-C3	-2.75	121.69	126.20
17	I	102	LMG	O6-C5-C4	2.75	114.65	109.70
14	A	831	CLA	C3B-C4B-NB	-2.74	108.08	110.53
16	F	203	BCR	C27-C26-C25	2.74	126.41	122.70
14	L	205	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
14	B	3011	CLA	C3B-C4B-NB	-2.73	108.09	110.53
14	K	103	CLA	C3B-C4B-NB	-2.73	108.09	110.53
21	L	202	LMT	O1B-C4'-C3'	2.73	114.16	107.23
14	A	832	CLA	O2D-CGD-O1D	-2.72	118.54	123.85
16	B	3048	BCR	C27-C26-C25	2.72	126.39	122.70
14	A	825	CLA	C3B-C4B-NB	-2.72	108.10	110.53
14	A	812	CLA	CHB-C4A-NA	2.72	128.32	124.40
16	J	104	BCR	C15-C16-C17	-2.71	117.97	123.52
14	A	824	CLA	CHB-C4A-NA	2.71	128.31	124.40
16	L	209	BCR	C8-C7-C6	-2.71	119.76	127.00
14	A	810	CLA	C3B-C4B-NB	-2.70	108.12	110.53
14	A	815	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
14	A	814	CLA	O2D-CGD-CBD	2.70	115.95	111.23
14	A	821	CLA	C3B-C4B-NB	-2.70	108.12	110.53
14	B	3035	CLA	O2D-CGD-CBD	2.70	115.94	111.23
16	A	850	BCR	C27-C26-C25	2.69	126.34	122.70
14	A	833	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
14	A	806	CLA	CHB-C4A-NA	2.68	128.27	124.40
14	B	3037	CLA	C3B-C4B-NB	-2.68	108.14	110.53
14	B	3041	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
14	B	3032	CLA	CHB-C4A-NA	2.67	128.26	124.40
14	A	819	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
14	B	3026	CLA	C2A-C1A-CHA	2.67	128.50	123.87
14	A	838	CLA	O2A-CGA-O1A	-2.67	116.95	123.63
14	B	3017	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
14	A	808	CLA	CAC-C3C-C4C	2.66	128.26	124.79
16	A	849	BCR	C27-C26-C25	2.66	126.30	122.70
16	I	101	BCR	C35-C13-C14	-2.66	118.51	122.82
14	A	819	CLA	C1-C2-C3	-2.66	121.84	126.20
13	A	801	CL0	C1C-CHC-C4B	2.65	125.56	116.07
14	B	3026	CLA	CHB-C4A-NA	2.65	128.23	124.40
17	A	852	LMG	C7-O1-C1	2.65	119.48	113.80
14	A	841	CLA	O2A-CGA-O1A	-2.64	117.02	123.63
14	A	840	CLA	C3B-C4B-NB	-2.64	108.17	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3021	CLA	O2A-CGA-O1A	-2.64	117.03	123.63
14	B	3033	CLA	CHB-C4A-NA	2.64	128.21	124.40
14	A	802	CLA	CMB-C2B-C1B	-2.64	121.41	125.42
14	A	845	CLA	CHB-C4A-NA	2.63	128.20	124.40
14	J	101	CLA	C3B-C4B-NB	-2.63	108.18	110.53
14	L	204	CLA	C5-C3-C2	2.63	127.06	121.17
14	A	810	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
14	B	3005	CLA	CHB-C4A-NA	2.62	128.18	124.40
14	J	101	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
16	L	208	BCR	C30-C25-C26	-2.61	119.06	122.64
16	L	209	BCR	C27-C26-C25	2.61	126.23	122.70
14	B	3022	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
16	A	849	BCR	C33-C5-C6	-2.61	121.64	124.48
13	A	801	CL0	C4C-CHD-C1D	2.61	125.40	116.07
14	B	3003	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
16	B	3051	BCR	C30-C25-C26	-2.60	119.08	122.64
16	J	103	BCR	C33-C5-C6	-2.60	121.64	124.48
14	A	844	CLA	C1-C2-C3	-2.60	121.94	126.20
14	B	3030	CLA	O2D-CGD-O1D	-2.60	118.80	123.85
15	A	846	PQN	C2M-C2-C3	-2.59	120.19	124.45
14	A	815	CLA	C3B-C4B-NB	-2.59	108.22	110.53
16	L	201	BCR	C33-C5-C6	-2.59	121.66	124.48
14	A	819	CLA	CHB-C4A-NA	2.59	128.14	124.40
14	B	3010	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
14	B	3033	CLA	C1-C2-C3	-2.58	121.97	126.20
16	A	851	BCR	C3-C4-C5	-2.58	109.45	114.06
14	A	808	CLA	C3B-C4B-NB	-2.58	108.23	110.53
16	B	3046	BCR	C15-C16-C17	-2.58	118.24	123.52
16	A	847	BCR	C24-C23-C22	-2.58	122.42	126.23
14	B	3004	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
14	A	840	CLA	O2A-CGA-O1A	-2.57	117.19	123.63
14	A	842	CLA	CHB-C4A-NA	2.57	128.10	124.40
16	A	850	BCR	C2-C1-C6	2.56	114.16	110.44
16	J	105	BCR	C11-C10-C9	-2.56	123.68	127.28
16	A	847	BCR	C27-C26-C25	2.56	126.17	122.70
16	L	201	BCR	C8-C7-C6	-2.56	120.16	127.00
14	A	822	CLA	C3B-C4B-NB	-2.56	108.25	110.53
14	A	826	CLA	C3B-C4B-NB	-2.56	108.25	110.53
16	L	208	BCR	C11-C10-C9	-2.56	123.69	127.28
16	A	848	BCR	C33-C5-C6	-2.56	121.70	124.48
14	A	831	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
21	L	202	LMT	C1B-O1B-C4'	2.55	124.03	117.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	803	CLA	CHB-C4A-NA	2.55	128.08	124.40
14	B	3020	CLA	C1-C2-C3	-2.55	122.02	126.20
14	A	827	CLA	O2D-CGD-CBD	2.54	115.67	111.23
14	B	3008	CLA	CHB-C4A-NA	2.54	128.06	124.40
14	B	3017	CLA	CHB-C4A-NA	2.54	128.06	124.40
14	A	829	CLA	C1-C2-C3	-2.54	122.04	126.20
14	A	802	CLA	CMB-C2B-C3B	2.54	132.52	126.55
14	B	3009	CLA	CHB-C4A-NA	2.54	128.06	124.40
14	A	820	CLA	C2A-C1A-CHA	2.54	128.27	123.87
14	B	3030	CLA	C2A-C1A-CHA	2.54	128.27	123.87
14	A	831	CLA	C1-C2-C3	-2.53	122.05	126.20
14	B	3036	CLA	CAC-C3C-C4C	2.53	128.09	124.79
14	B	3027	CLA	CHB-C4A-NA	2.53	128.05	124.40
16	J	104	BCR	C33-C5-C6	-2.53	121.72	124.48
14	B	3021	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
16	A	850	BCR	C33-C5-C6	-2.52	121.73	124.48
14	B	3031	CLA	CHB-C4A-NA	2.52	128.04	124.40
14	L	206	CLA	CHB-C4A-NA	2.52	128.04	124.40
16	A	850	BCR	C37-C22-C21	-2.52	118.73	122.82
13	A	801	CL0	CMA-C3A-C4A	-2.52	109.18	114.61
14	A	835	CLA	CHB-C4A-NA	2.52	128.03	124.40
14	B	3035	CLA	CHB-C4A-NA	2.52	128.03	124.40
14	A	842	CLA	C3B-C4B-NB	-2.52	108.28	110.53
14	A	823	CLA	O2A-CGA-O1A	-2.52	117.34	123.63
14	A	838	CLA	CHB-C4A-NA	2.51	128.03	124.40
14	A	806	CLA	C3B-C4B-NB	-2.51	108.29	110.53
14	B	3016	CLA	CHB-C4A-NA	2.51	128.03	124.40
14	B	3014	CLA	CAC-C3C-C4C	2.51	128.06	124.79
16	B	3048	BCR	C2-C1-C6	2.51	114.08	110.44
14	A	834	CLA	O2D-CGD-CBD	2.50	115.61	111.23
14	B	3016	CLA	CAC-C3C-C4C	2.50	128.05	124.79
14	B	3011	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
14	B	3023	CLA	C3B-C4B-NB	-2.50	108.30	110.53
14	B	3025	CLA	CHA-C1A-NA	-2.49	120.74	126.39
14	J	102	CLA	CAC-C3C-C4C	2.49	128.03	124.79
14	B	3009	CLA	CGD-CBD-CAD	-2.49	102.78	110.85
14	B	3019	CLA	CHB-C4A-NA	2.49	127.99	124.40
22	L	207	DGD	O3G-C1D-C2D	-2.49	104.49	108.27
17	I	102	LMG	O3-C3-C2	-2.49	104.51	110.38
14	A	822	CLA	CHB-C4A-NA	2.49	127.99	124.40
14	B	3022	CLA	CHB-C4A-NA	2.48	127.99	124.40
14	A	832	CLA	CHB-C4A-NA	2.48	127.98	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	209	BCR	C33-C5-C6	-2.48	121.78	124.48
14	A	834	CLA	C3B-C4B-NB	-2.48	108.32	110.53
16	B	3046	BCR	C2-C1-C6	2.48	114.04	110.44
22	L	207	DGD	O3G-C3G-C2G	-2.47	104.81	110.82
16	I	101	BCR	C15-C16-C17	-2.47	118.47	123.52
14	B	3020	CLA	O2D-CGD-CBD	2.47	115.55	111.23
14	A	803	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
14	A	806	CLA	O2A-CGA-O1A	-2.47	117.45	123.63
14	B	3027	CLA	O2D-CGD-CBD	2.47	115.54	111.23
14	A	824	CLA	C3B-C4B-NB	-2.47	108.33	110.53
14	B	3026	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
14	B	3007	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
14	A	814	CLA	CHB-C4A-NA	2.46	127.95	124.40
16	B	3051	BCR	C33-C5-C6	-2.46	121.80	124.48
14	B	3030	CLA	C3A-C2A-C1A	2.46	105.02	101.34
14	A	828	CLA	CHB-C4A-NA	2.46	127.94	124.40
14	A	841	CLA	CAC-C3C-C4C	2.46	127.98	124.79
17	A	855	LMG	O6-C1-C2	-2.46	105.33	110.37
16	I	101	BCR	C27-C26-C25	2.45	126.02	122.70
14	L	204	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
14	A	802	CLA	C7-C6-C5	-2.45	106.74	113.26
16	B	3045	BCR	C16-C15-C14	-2.45	118.52	123.52
14	A	807	CLA	CHB-C4A-NA	2.44	127.93	124.40
14	A	808	CLA	O2D-CGD-CBD	2.44	115.50	111.23
14	A	824	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
14	B	3034	CLA	O2A-CGA-O1A	-2.44	117.52	123.63
14	A	842	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
17	B	3049	LMG	C9-C8-C7	-2.44	106.10	111.78
14	A	821	CLA	O2D-CGD-CBD	2.44	115.49	111.23
14	B	3010	CLA	CMB-C2B-C1B	-2.44	121.71	125.42
14	B	3008	CLA	C3B-C4B-NB	-2.44	108.36	110.53
17	I	102	LMG	C8-O7-C10	2.43	123.62	117.80
14	A	819	CLA	CMB-C2B-C3B	2.43	132.27	126.55
14	A	804	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
16	L	208	BCR	C15-C14-C13	-2.43	123.87	127.28
14	B	3039	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
16	K	102	BCR	C40-C30-C25	2.43	114.05	110.24
14	B	3038	CLA	C3B-C4B-NB	-2.43	108.36	110.53
14	B	3034	CLA	C3B-C4B-NB	-2.42	108.37	110.53
14	M	102	CLA	CMA-C3A-C4A	2.42	118.28	111.77
14	J	101	CLA	CHB-C4A-NA	2.42	127.89	124.40
14	M	102	CLA	CMA-C3A-C2A	-2.42	104.64	113.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	101	BCR	C8-C7-C6	-2.41	120.56	127.00
14	B	3040	CLA	C3B-C4B-NB	-2.41	108.38	110.53
14	B	3030	CLA	O2A-CGA-O1A	-2.40	117.61	123.63
14	B	3011	CLA	O1D-CGD-CBD	2.40	129.26	124.52
14	A	829	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
14	B	3003	CLA	CHB-C4A-NA	2.40	127.87	124.40
14	B	3006	CLA	O2D-CGD-CBD	2.40	115.43	111.23
16	B	3045	BCR	C8-C7-C6	-2.40	120.60	127.00
16	A	851	BCR	C15-C16-C17	-2.40	118.62	123.52
14	A	821	CLA	CMB-C2B-C3B	2.39	132.18	126.55
14	A	808	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
14	B	3032	CLA	C4D-CHA-C1A	-2.39	118.39	121.24
16	B	3044	BCR	C30-C25-C26	-2.39	119.37	122.64
14	L	204	CLA	CHB-C4A-NA	2.39	127.85	124.40
16	B	3048	BCR	C15-C16-C17	-2.39	118.63	123.52
14	B	3006	CLA	C3B-C4B-NB	-2.39	108.40	110.53
14	B	3042	CLA	C3B-C4B-NB	-2.39	108.40	110.53
14	A	810	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
13	A	801	CL0	C4D-CHA-CBD	-2.38	106.57	108.97
14	A	812	CLA	C7-C6-C5	-2.38	106.92	113.26
14	A	821	CLA	CHB-C4A-NA	2.38	127.83	124.40
14	K	101	CLA	CHB-C4A-NA	2.38	127.83	124.40
14	X	1701	CLA	O2D-CGD-CBD	2.38	115.39	111.23
14	A	819	CLA	CHB-C1B-NB	2.37	127.61	124.05
15	A	846	PQN	C5-C4-C3	2.37	122.61	118.27
16	F	203	BCR	C38-C26-C25	-2.37	121.90	124.48
14	B	3020	CLA	C3B-C4B-NB	-2.37	108.42	110.53
17	A	852	LMG	O3-C3-C2	-2.37	104.80	110.38
14	A	830	CLA	C3A-C2A-C1A	2.36	104.88	101.34
14	A	811	CLA	CAA-C2A-C3A	2.36	119.39	113.00
17	I	102	LMG	O2-C2-C1	-2.36	104.45	110.08
14	A	810	CLA	CHB-C4A-NA	2.36	127.81	124.40
14	B	3007	CLA	CHB-C4A-NA	2.36	127.81	124.40
16	K	102	BCR	C24-C23-C22	-2.36	122.74	126.23
14	A	816	CLA	CHB-C4A-NA	2.36	127.80	124.40
16	M	103	BCR	C8-C7-C6	-2.36	120.70	127.00
14	A	826	CLA	CHB-C4A-NA	2.36	127.80	124.40
14	A	802	CLA	O2D-CGD-O1D	-2.36	119.26	123.85
22	L	207	DGD	O6E-C1E-O5D	-2.36	104.47	110.04
14	B	3028	CLA	CHB-C4A-NA	2.35	127.80	124.40
16	A	849	BCR	C8-C7-C6	-2.35	120.71	127.00
14	M	102	CLA	CHD-C4C-C3C	2.35	128.20	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	208	BCR	C7-C8-C9	-2.35	122.76	126.23
16	B	3045	BCR	C2-C1-C6	2.35	113.85	110.44
14	B	3011	CLA	C2A-C1A-CHA	2.35	127.94	123.87
16	A	851	BCR	C33-C5-C6	-2.35	121.92	124.48
14	B	3015	CLA	O1D-CGD-CBD	2.35	129.15	124.52
14	B	3034	CLA	CHB-C4A-NA	2.35	127.79	124.40
14	B	3006	CLA	CHB-C4A-NA	2.35	127.79	124.40
14	B	3038	CLA	CHB-C4A-NA	2.35	127.79	124.40
16	J	104	BCR	C27-C26-C25	2.35	125.87	122.70
14	A	856	CLA	C3B-C4B-NB	-2.35	108.44	110.53
14	A	832	CLA	C1-C2-C3	-2.35	122.97	126.76
14	A	811	CLA	O2D-CGD-CBD	2.35	115.33	111.23
14	A	830	CLA	CHB-C4A-NA	2.34	127.78	124.40
14	A	838	CLA	CHA-C1A-NA	-2.34	121.10	126.39
14	A	825	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
17	A	855	LMG	O2-C2-C1	-2.34	104.51	110.08
14	A	832	CLA	O2A-CGA-O1A	-2.33	117.79	123.63
14	B	3025	CLA	O2D-CGD-CBD	2.33	115.31	111.23
16	J	105	BCR	C3-C4-C5	-2.33	109.90	114.06
16	F	203	BCR	C33-C5-C6	-2.33	121.94	124.48
14	A	820	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
14	L	205	CLA	CHB-C4A-NA	2.32	127.75	124.40
14	B	3023	CLA	CMB-C2B-C1B	-2.32	121.88	125.42
14	B	3020	CLA	CHB-C4A-NA	2.32	127.75	124.40
14	J	102	CLA	C3B-C4B-NB	-2.32	108.46	110.53
14	A	843	CLA	O2A-CGA-O1A	-2.32	117.84	123.63
14	A	842	CLA	O2D-CGD-O1D	-2.32	119.34	123.85
14	A	812	CLA	CAC-C3C-C4C	2.31	127.80	124.79
14	A	840	CLA	CHB-C4A-NA	2.31	127.74	124.40
13	A	801	CL0	C3C-C4C-NC	-2.31	109.00	114.65
21	L	202	LMT	O5B-C5B-C4B	2.31	113.87	109.70
21	L	202	LMT	O1'-C1'-C2'	2.31	111.78	108.27
16	L	208	BCR	C20-C21-C22	-2.31	124.04	127.28
14	B	3041	CLA	CHB-C4A-NA	2.31	127.73	124.40
14	B	3042	CLA	O2D-CGD-CBD	2.31	115.27	111.23
14	B	3012	CLA	CED-O2D-CGD	2.31	121.15	115.92
14	B	3030	CLA	CAA-CBA-CGA	-2.31	106.66	113.21
14	B	3022	CLA	C3B-C4B-NB	-2.30	108.47	110.53
14	L	205	CLA	CAA-C2A-C1A	-2.30	104.44	111.97
14	A	825	CLA	CHB-C4A-NA	2.30	127.72	124.40
15	A	846	PQN	O4-C4-C3	-2.30	116.98	120.67
14	A	837	CLA	CHB-C4A-NA	2.30	127.72	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3039	CLA	CHB-C4A-NA	2.30	127.72	124.40
14	A	819	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
16	F	203	BCR	C16-C15-C14	-2.29	118.83	123.52
16	L	209	BCR	C15-C14-C13	-2.29	124.07	127.28
15	B	3043	PQN	O4-C4-C3	-2.29	117.00	120.67
14	B	3032	CLA	CHA-C4D-ND	2.29	137.27	132.55
14	B	3012	CLA	O2D-CGD-CBD	2.29	115.23	111.23
15	B	3043	PQN	C10-C1-C2	2.29	122.15	118.97
16	F	201	BCR	C33-C5-C6	-2.28	121.99	124.48
16	L	208	BCR	C37-C22-C21	-2.28	119.12	122.82
16	J	104	BCR	C8-C7-C6	-2.28	120.90	127.00
14	B	3014	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
14	A	818	CLA	CHB-C4A-NA	2.28	127.69	124.40
14	A	813	CLA	C3A-C2A-C1A	2.28	104.75	101.34
14	M	102	CLA	C3B-C4B-NB	-2.27	108.50	110.53
14	B	3035	CLA	CAC-C3C-C4C	2.27	127.75	124.79
14	A	836	CLA	CHB-C4A-NA	2.27	127.68	124.40
14	B	3033	CLA	C3B-C4B-NB	-2.27	108.50	110.53
16	J	105	BCR	C15-C16-C17	-2.27	118.87	123.52
16	K	102	BCR	C8-C7-C6	-2.27	120.94	127.00
16	B	3045	BCR	C28-C27-C26	-2.27	110.01	114.06
14	A	836	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
17	A	852	LMG	O2-C2-C1	-2.26	104.68	110.08
14	B	3011	CLA	CBC-CAC-C3C	2.26	118.55	112.42
14	A	844	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
14	A	821	CLA	CMA-C3A-C2A	-2.26	111.04	116.23
14	A	823	CLA	C2A-C1A-CHA	2.26	127.79	123.87
14	A	856	CLA	C1-C2-C3	-2.26	122.50	126.20
17	B	3049	LMG	O2-C2-C1	-2.26	104.70	110.08
14	B	3013	CLA	CHB-C4A-NA	2.25	127.65	124.40
14	B	3009	CLA	C3B-C4B-NB	-2.25	108.52	110.53
16	L	209	BCR	C40-C30-C25	2.25	113.77	110.24
14	A	828	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
16	I	101	BCR	C33-C5-C6	-2.25	122.03	124.48
14	B	3034	CLA	O2D-CGD-CBD	2.25	115.16	111.23
14	B	3019	CLA	O2D-CGD-CBD	2.25	115.16	111.23
14	B	3015	CLA	CHB-C4A-NA	2.24	127.63	124.40
18	A	853	LHG	C18-C17-C16	-2.24	103.05	114.37
16	J	105	BCR	C15-C14-C13	-2.24	124.14	127.28
14	F	202	CLA	CHB-C1B-NB	2.24	127.41	124.05
14	A	828	CLA	O2D-CGD-CBD	2.24	115.14	111.23
14	B	3005	CLA	C3A-C2A-C1A	2.24	104.69	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3018	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
14	A	841	CLA	CHB-C4A-NA	2.23	127.62	124.40
16	I	101	BCR	C11-C10-C9	-2.23	124.16	127.28
18	A	853	LHG	O8-C23-C24	2.23	118.62	111.83
14	F	202	CLA	C4D-CHA-C1A	2.22	123.90	121.24
14	A	818	CLA	CHD-C1D-ND	-2.22	121.67	124.80
16	B	3047	BCR	C15-C14-C13	-2.22	124.16	127.28
13	A	801	CL0	CMB-C2B-C3B	2.22	129.12	124.68
15	A	846	PQN	C2M-C2-C1	2.22	120.77	116.68
14	A	833	CLA	C3A-C2A-C1A	2.22	104.67	101.34
16	L	201	BCR	C28-C27-C26	-2.22	110.09	114.06
13	A	801	CL0	C3D-C4D-CHA	2.22	111.92	108.54
16	F	203	BCR	C1-C6-C5	-2.22	119.60	122.64
14	A	835	CLA	C4-C3-C2	-2.22	117.93	123.63
14	A	837	CLA	O2D-CGD-CBD	2.22	115.11	111.23
18	B	3050	LHG	O8-C23-C24	2.21	121.78	112.38
14	A	827	CLA	CHB-C4A-NA	2.21	127.59	124.40
14	B	3017	CLA	C3B-C4B-NB	-2.21	108.56	110.53
14	J	102	CLA	CMA-C3A-C2A	-2.21	111.16	116.23
16	K	102	BCR	C33-C5-C6	-2.21	122.07	124.48
14	B	3032	CLA	O1D-CGD-CBD	2.21	128.87	124.52
14	A	844	CLA	CHB-C1B-NB	2.21	127.36	124.05
14	M	102	CLA	CMD-C2D-C1D	-2.21	120.84	124.73
14	A	824	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
14	B	3004	CLA	C2A-C1A-CHA	2.21	127.70	123.87
14	A	831	CLA	CHB-C4A-NA	2.21	127.58	124.40
22	L	207	DGD	CBB-CAB-C9B	-2.21	103.22	114.37
13	A	801	CL0	CBC-CAC-C3C	-2.20	109.72	112.87
14	B	3034	CLA	CAA-C2A-C1A	-2.20	104.77	111.97
14	B	3010	CLA	C6-C7-C8	-2.20	108.66	115.97
14	B	3032	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
14	M	102	CLA	CBC-CAC-C3C	2.20	118.37	112.42
14	B	3010	CLA	CHB-C1B-NB	2.19	127.33	124.05
14	K	103	CLA	CHB-C4A-NA	2.19	127.56	124.40
16	J	104	BCR	C15-C14-C13	-2.19	124.21	127.28
14	B	3040	CLA	CHB-C4A-NA	2.19	127.55	124.40
14	K	101	CLA	O2A-CGA-O1A	-2.19	117.71	123.33
17	A	855	LMG	O3-C3-C2	-2.18	105.23	110.38
16	B	3047	BCR	C35-C13-C14	-2.18	119.28	122.82
15	A	846	PQN	C10-C1-C2	2.18	122.00	118.97
14	L	204	CLA	C3B-C4B-NB	-2.18	108.58	110.53
14	B	3024	CLA	CHB-C4A-NA	2.18	127.55	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	3046	BCR	C27-C26-C25	2.18	125.65	122.70
14	A	807	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
14	B	3040	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
14	A	845	CLA	CAA-CBA-CGA	-2.17	107.04	113.21
16	A	848	BCR	C8-C7-C6	-2.17	121.19	127.00
14	A	834	CLA	CBC-CAC-C3C	-2.17	106.54	112.42
14	A	812	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
16	A	847	BCR	C15-C16-C17	-2.17	119.08	123.52
14	A	833	CLA	CHB-C4A-NA	2.17	127.53	124.40
14	A	809	CLA	C1-C2-C3	-2.17	122.65	126.20
16	J	105	BCR	C33-C5-C6	-2.17	122.12	124.48
14	K	101	CLA	CMB-C2B-C1B	-2.17	122.12	125.42
14	A	835	CLA	C6-C5-C3	2.17	118.74	113.47
14	A	831	CLA	O1D-CGD-CBD	2.16	128.79	124.52
15	B	3043	PQN	C5-C4-C3	2.16	122.23	118.27
14	B	3041	CLA	CHC-C1C-NC	2.16	127.57	124.31
14	B	3005	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
16	M	103	BCR	C27-C26-C25	2.15	125.61	122.70
14	B	3019	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
14	B	3041	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
14	B	3016	CLA	C3B-C4B-NB	-2.15	108.61	110.53
14	A	822	CLA	O2D-CGD-CBD	2.15	114.98	111.23
14	B	3036	CLA	CBC-CAC-C3C	2.15	118.24	112.42
14	B	3014	CLA	CHB-C4A-NA	2.15	127.50	124.40
18	A	854	LHG	C11-C10-C9	-2.15	103.52	114.37
14	B	3038	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
14	A	820	CLA	C3A-C2A-C1A	2.14	104.55	101.34
16	B	3047	BCR	C33-C5-C6	-2.14	122.15	124.48
14	B	3029	CLA	C2A-C1A-CHA	2.14	127.58	123.87
16	I	101	BCR	C15-C14-C13	-2.14	124.28	127.28
14	B	3021	CLA	CHB-C4A-NA	2.14	127.49	124.40
14	L	206	CLA	CAA-C2A-C1A	-2.14	104.97	111.97
17	A	852	LMG	C1-O6-C5	-2.14	109.55	113.72
18	B	3050	LHG	O10-C23-C24	-2.14	117.20	124.77
14	A	826	CLA	O2D-CGD-CBD	2.14	114.96	111.23
16	K	102	BCR	C30-C25-C26	-2.14	119.72	122.64
14	A	821	CLA	CHD-C1D-ND	-2.13	121.80	124.80
14	B	3019	CLA	C1-O2A-CGA	2.13	121.81	116.65
14	A	803	CLA	CAA-CBA-CGA	-2.13	107.16	113.21
16	A	849	BCR	C30-C25-C26	-2.13	119.73	122.64
14	J	101	CLA	O1D-CGD-CBD	2.13	128.71	124.52
16	B	3044	BCR	C11-C10-C9	-2.13	124.30	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	102	CLA	CGD-CBD-CAD	2.13	117.73	110.85
14	B	3011	CLA	CHA-C1A-NA	-2.12	121.59	126.39
14	A	841	CLA	C3B-C4B-NB	-2.12	108.64	110.53
16	B	3044	BCR	C8-C7-C6	-2.12	121.35	127.00
14	A	810	CLA	O1D-CGD-CBD	2.11	128.68	124.52
16	B	3046	BCR	C28-C27-C26	-2.11	110.29	114.06
14	B	3011	CLA	CHA-C4D-ND	2.11	136.90	132.55
14	A	845	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
16	B	3044	BCR	C33-C5-C6	-2.11	122.18	124.48
14	A	804	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
14	A	856	CLA	C4-C3-C5	2.10	118.87	115.23
13	A	801	CL0	CED-O2D-CGD	2.09	120.66	115.92
14	A	835	CLA	C2D-C1D-ND	-2.09	108.06	110.13
14	L	204	CLA	C11-C10-C8	-2.09	109.02	115.97
14	A	825	CLA	O2D-CGD-CBD	2.09	114.88	111.23
16	B	3046	BCR	C8-C7-C6	-2.09	121.42	127.00
14	B	3020	CLA	C4-C3-C5	2.08	118.85	115.23
14	B	3041	CLA	CAC-C3C-C2C	-2.08	123.73	127.56
14	B	3024	CLA	CHD-C1D-ND	-2.08	121.88	124.80
16	A	847	BCR	C4-C5-C6	2.08	125.51	122.70
14	B	3038	CLA	C1-C2-C3	-2.08	122.79	126.20
14	A	841	CLA	C4-C3-C5	2.08	118.83	115.23
14	B	3012	CLA	C3B-C4B-NB	-2.08	108.68	110.53
17	A	852	LMG	O7-C10-O9	-2.07	118.86	123.70
13	A	801	CL0	O2A-CGA-O1A	-2.07	118.44	123.63
14	A	802	CLA	C3B-C4B-NB	-2.07	108.68	110.53
14	X	1701	CLA	C3B-C4B-NB	-2.07	108.68	110.53
16	F	203	BCR	C4-C5-C6	2.07	125.50	122.70
22	L	207	DGD	C5B-C4B-C3B	-2.07	103.92	114.37
14	B	3029	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
14	L	206	CLA	CHB-C1B-C2B	-2.07	121.43	127.43
14	B	3041	CLA	C3B-C4B-NB	-2.07	108.69	110.53
14	B	3016	CLA	C2D-C1D-ND	-2.06	108.08	110.13
22	L	207	DGD	O6D-C1D-O3G	-2.06	105.17	110.04
14	A	808	CLA	CHB-C4A-NA	2.06	127.37	124.40
14	A	811	CLA	O2A-CGA-O1A	-2.06	118.03	123.33
14	A	836	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
14	A	831	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
14	B	3034	CLA	CAA-CBA-CGA	-2.06	107.37	113.21
14	A	834	CLA	CHD-C1D-ND	-2.05	121.92	124.80
14	A	820	CLA	C1-C2-C3	-2.05	122.84	126.20
14	B	3022	CLA	O2A-CGA-O1A	-2.05	118.06	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	840	CLA	CBA-CAA-C2A	2.05	119.89	113.79
14	A	816	CLA	O1A-CGA-CBA	2.05	129.59	123.09
14	A	835	CLA	CHD-C1D-C2D	2.05	129.75	125.49
14	B	3019	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
14	A	856	CLA	O2D-CGD-CBD	2.05	114.81	111.23
18	A	853	LHG	C20-C19-C18	-2.04	104.03	114.37
14	A	827	CLA	O2A-CGA-O1A	-2.04	118.51	123.63
14	A	829	CLA	CHD-C1D-ND	-2.04	121.92	124.80
14	B	3042	CLA	C1-C2-C3	-2.04	122.85	126.20
14	B	3009	CLA	CHA-C4D-ND	2.04	136.76	132.55
14	A	839	CLA	C1-C2-C3	-2.04	122.85	126.20
14	L	205	CLA	O2D-CGD-CBD	2.04	114.80	111.23
14	K	103	CLA	CAA-C2A-C1A	-2.04	105.29	111.97
14	A	810	CLA	CHA-C1A-NA	-2.04	121.77	126.39
14	B	3036	CLA	CHB-C4A-NA	2.04	127.34	124.40
14	A	822	CLA	CHD-C1D-ND	-2.04	121.94	124.80
16	B	3048	BCR	C8-C7-C6	-2.04	121.56	127.00
18	A	853	LHG	C11-C10-C9	-2.04	104.08	114.37
14	B	3003	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
14	A	829	CLA	CHB-C4A-NA	2.03	127.34	124.40
14	B	3011	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
14	L	206	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
17	I	102	LMG	O6-C1-O1	-2.03	105.25	110.04
14	A	845	CLA	O2D-CGD-CBD	2.03	114.77	111.23
16	A	849	BCR	C7-C8-C9	-2.03	123.24	126.23
14	A	819	CLA	CHD-C1D-ND	-2.02	121.95	124.80
16	B	3048	BCR	C16-C15-C14	-2.02	119.38	123.52
14	J	102	CLA	CAA-C2A-C3A	-2.02	111.59	116.23
16	J	104	BCR	C29-C30-C25	2.02	113.38	110.44
17	B	3049	LMG	C40-C39-C38	-2.02	104.15	114.37
14	A	810	CLA	CHA-C4D-ND	2.02	136.72	132.55
16	A	851	BCR	C29-C30-C25	2.02	113.37	110.44
16	B	3047	BCR	C38-C26-C25	-2.02	122.28	124.48
16	B	3048	BCR	C29-C30-C25	2.02	113.37	110.44
14	A	810	CLA	C6-C5-C3	2.01	118.38	113.47
14	A	805	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
14	L	205	CLA	CHC-C4B-NB	2.01	127.06	124.05
16	B	3048	BCR	C33-C5-C6	-2.01	122.29	124.48
14	B	3031	CLA	O2A-CGA-O1A	-2.01	118.17	123.33
18	M	101	LHG	C20-C19-C18	-2.01	104.22	114.37
14	B	3017	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
22	L	207	DGD	O3E-C3E-C2E	-2.01	105.64	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3010	CLA	CAC-C3C-C4C	2.00	127.40	124.79
14	B	3030	CLA	CHA-C4D-ND	2.00	136.68	132.55
14	A	827	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
16	B	3045	BCR	C27-C26-C25	2.00	125.41	122.70
14	B	3011	CLA	C11-C12-C13	-2.00	109.32	115.97
14	A	838	CLA	C2A-C1A-CHA	2.00	127.34	123.87

All (95) chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
14	A	831	CLA	ND
14	A	832	CLA	ND
14	A	833	CLA	ND
14	A	834	CLA	ND
14	A	835	CLA	ND
14	A	836	CLA	ND
14	A	837	CLA	ND
14	A	838	CLA	ND
14	A	839	CLA	ND
14	A	840	CLA	ND
14	A	841	CLA	ND
14	A	842	CLA	ND
14	A	843	CLA	ND
14	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

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Mol	Chain	Res	Type	Atom
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
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 (1265) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	801	CL0	C3A-C2A-CAA-CBA
14	A	805	CLA	CHA-CBD-CGD-O1D
14	A	805	CLA	CHA-CBD-CGD-O2D
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	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	809	CLA	CHA-CBD-CGD-O1D
14	A	809	CLA	CHA-CBD-CGD-O2D
14	A	811	CLA	C3A-C2A-CAA-CBA
14	A	811	CLA	C2B-C3B-CAB-CBB
14	A	811	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
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	C2B-C3B-CAB-CBB
14	A	819	CLA	C4B-C3B-CAB-CBB
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
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	829	CLA	CBD-CGD-O2D-CED
14	A	831	CLA	CHA-CBD-CGD-O1D
14	A	831	CLA	CHA-CBD-CGD-O2D
14	A	832	CLA	C1A-C2A-CAA-CBA
14	A	832	CLA	C3A-C2A-CAA-CBA
14	A	832	CLA	C4B-C3B-CAB-CBB
14	A	834	CLA	C4B-C3B-CAB-CBB
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	838	CLA	CBD-CGD-O2D-CED
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	CBD-CGD-O2D-CED
14	A	845	CLA	O1D-CGD-O2D-CED
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

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Mol	Chain	Res	Type	Atoms
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	3018	CLA	C1A-C2A-CAA-CBA
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	CAD-CBD-CGD-O1D
14	B	3021	CLA	CAD-CBD-CGD-O2D
14	B	3022	CLA	C1A-C2A-CAA-CBA
14	B	3022	CLA	C3A-C2A-CAA-CBA
14	B	3022	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	3029	CLA	C1A-C2A-CAA-CBA
14	B	3029	CLA	C3A-C2A-CAA-CBA
14	B	3030	CLA	CHA-CBD-CGD-O1D
14	B	3030	CLA	CHA-CBD-CGD-O2D
14	B	3031	CLA	C2B-C3B-CAB-CBB
14	B	3031	CLA	C4B-C3B-CAB-CBB
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	CHA-CBD-CGD-O1D
14	B	3035	CLA	CHA-CBD-CGD-O2D
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	3042	CLA	C1A-C2A-CAA-CBA
14	F	202	CLA	C2B-C3B-CAB-CBB
14	F	202	CLA	C4B-C3B-CAB-CBB
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

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Mol	Chain	Res	Type	Atoms
14	K	103	CLA	C2B-C3B-CAB-CBB
14	K	103	CLA	C4B-C3B-CAB-CBB
14	L	204	CLA	C1A-C2A-CAA-CBA
14	L	204	CLA	C3A-C2A-CAA-CBA
14	M	102	CLA	C2B-C3B-CAB-CBB
14	M	102	CLA	C4B-C3B-CAB-CBB
14	M	102	CLA	CHA-CBD-CGD-O2D
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
16	A	847	BCR	C18-C19-C20-C21
16	A	847	BCR	C22-C23-C24-C25
16	A	848	BCR	C11-C10-C9-C8
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	C11-C10-C9-C8
16	A	851	BCR	C11-C10-C9-C34
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	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

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Mol	Chain	Res	Type	Atoms
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	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	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	C11-C12-C13-C14
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	C11-C10-C9-C34
16	L	208	BCR	C11-C12-C13-C14
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	M	103	BCR	C1-C6-C7-C8
16	M	103	BCR	C5-C6-C7-C8
17	A	855	LMG	O6-C1-O1-C7
17	A	855	LMG	O9-C10-O7-C8
17	A	855	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
18	A	853	LHG	C3-O3-P-O5
18	A	854	LHG	C1-C2-C3-O3
18	B	3050	LHG	C4-O6-P-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
18	M	101	LHG	C4-O6-P-O3
22	L	207	DGD	O6D-C1D-O3G-C3G
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	B	3041	CLA	C2C-C3C-CAC-CBC
14	B	3022	CLA	O1D-CGD-O2D-CED
13	A	801	CL0	CBA-CGA-O2A-C1
14	A	820	CLA	CBA-CGA-O2A-C1
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	819	CLA	O1D-CGD-O2D-CED
14	A	844	CLA	O1D-CGD-O2D-CED
14	B	3006	CLA	O1D-CGD-O2D-CED
21	L	202	LMT	C3'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
14	A	822	CLA	O1D-CGD-O2D-CED
14	A	838	CLA	O1D-CGD-O2D-CED
14	B	3005	CLA	O1D-CGD-O2D-CED
14	B	3037	CLA	O1D-CGD-O2D-CED
14	F	202	CLA	O1D-CGD-O2D-CED
14	M	102	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	A	813	CLA	CBD-CGD-O2D-CED
14	A	856	CLA	CBD-CGD-O2D-CED
14	B	3015	CLA	CBD-CGD-O2D-CED
14	A	806	CLA	O1D-CGD-O2D-CED
14	A	842	CLA	O1D-CGD-O2D-CED
14	A	806	CLA	C4-C3-C5-C6
14	A	856	CLA	C4-C3-C5-C6
14	B	3025	CLA	C4-C3-C5-C6
14	B	3034	CLA	C4-C3-C5-C6
14	A	806	CLA	C2-C3-C5-C6
14	A	856	CLA	C2-C3-C5-C6
14	B	3025	CLA	C2-C3-C5-C6
14	B	3034	CLA	C2-C3-C5-C6
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	K	103	CLA	C2A-CAA-CBA-CGA
14	A	820	CLA	C3-C5-C6-C7
14	A	817	CLA	CBA-CGA-O2A-C1
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
16	B	3047	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
14	A	817	CLA	O1A-CGA-O2A-C1
14	A	829	CLA	O1A-CGA-O2A-C1
14	A	838	CLA	O1A-CGA-O2A-C1
18	B	3050	LHG	O9-C7-O7-C5
14	B	3041	CLA	C4C-C3C-CAC-CBC
14	A	845	CLA	C2C-C3C-CAC-CBC
14	A	830	CLA	O1D-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
14	A	841	CLA	O1D-CGD-O2D-CED
18	B	3050	LHG	C8-C7-O7-C5
14	B	3029	CLA	CBD-CGD-O2D-CED
14	B	3030	CLA	CBD-CGD-O2D-CED
15	A	846	PQN	C14-C13-C15-C16
15	A	846	PQN	C12-C13-C15-C16
14	A	825	CLA	O1A-CGA-O2A-C1
14	B	3032	CLA	O1A-CGA-O2A-C1
14	L	204	CLA	O1A-CGA-O2A-C1
14	B	3025	CLA	CBD-CGD-O2D-CED
17	A	855	LMG	O6-C5-C6-O5
14	A	820	CLA	C2A-CAA-CBA-CGA
14	A	830	CLA	C2A-CAA-CBA-CGA
14	A	823	CLA	O1A-CGA-O2A-C1
22	L	207	DGD	O1A-C1A-O1G-C1G
17	B	3049	LMG	O6-C1-O1-C7
17	I	102	LMG	O6-C1-O1-C7
21	L	202	LMT	O5'-C1'-O1'-C1
22	L	207	DGD	O6E-C1E-O5D-C6D
17	B	3049	LMG	O6-C5-C6-O5
14	A	805	CLA	CBA-CGA-O2A-C1
14	A	812	CLA	CBA-CGA-O2A-C1
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
21	L	202	LMT	O5B-C5B-C6B-O6B
14	A	836	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	B	3028	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	811	CLA	C2C-C3C-CAC-CBC
14	B	3015	CLA	O1D-CGD-O2D-CED
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
17	B	3049	LMG	C4-C5-C6-O5
17	B	3049	LMG	C2-C1-O1-C7
17	I	102	LMG	C2-C1-O1-C7
21	L	202	LMT	C2'-C1'-O1'-C1
22	L	207	DGD	C2E-C1E-O5D-C6D
14	A	812	CLA	O1A-CGA-O2A-C1
16	A	847	BCR	C11-C12-C13-C35
16	A	848	BCR	C7-C8-C9-C34
16	A	848	BCR	C11-C12-C13-C35
16	A	851	BCR	C7-C8-C9-C34
16	A	851	BCR	C11-C12-C13-C35
16	B	3045	BCR	C7-C8-C9-C34
16	B	3046	BCR	C7-C8-C9-C34
16	B	3047	BCR	C11-C12-C13-C35
16	B	3051	BCR	C37-C22-C23-C24
16	F	201	BCR	C37-C22-C23-C24
16	I	101	BCR	C7-C8-C9-C34
16	J	105	BCR	C7-C8-C9-C34
16	J	105	BCR	C11-C12-C13-C35
16	K	102	BCR	C37-C22-C23-C24
16	L	208	BCR	C7-C8-C9-C34
16	L	208	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
16	L	208	BCR	C36-C18-C19-C20
16	L	209	BCR	C11-C12-C13-C35
14	A	845	CLA	C3-C5-C6-C7
14	B	3016	CLA	C2A-CAA-CBA-CGA
14	B	3041	CLA	C2A-CAA-CBA-CGA
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	A	845	CLA	C4C-C3C-CAC-CBC
14	A	836	CLA	CBA-CGA-O2A-C1
14	A	806	CLA	C2-C1-O2A-CGA
14	A	826	CLA	C2-C1-O2A-CGA
14	A	808	CLA	O1A-CGA-O2A-C1
14	A	812	CLA	CBD-CGD-O2D-CED
14	B	3011	CLA	CBD-CGD-O2D-CED
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	809	CLA	C3-C5-C6-C7
14	B	3027	CLA	C6-C7-C8-C10
14	A	813	CLA	O1D-CGD-O2D-CED
17	A	852	LMG	C4-C5-C6-O5
14	A	856	CLA	C3-C5-C6-C7
15	B	3043	PQN	C20-C21-C22-C23
14	B	3004	CLA	C13-C15-C16-C17
14	B	3023	CLA	C5-C6-C7-C8
15	B	3043	PQN	C23-C25-C26-C27
14	A	808	CLA	C2A-CAA-CBA-CGA
14	A	816	CLA	C2A-CAA-CBA-CGA
14	B	3013	CLA	C2A-CAA-CBA-CGA
14	B	3029	CLA	C2A-CAA-CBA-CGA
16	F	201	BCR	C10-C11-C12-C13
14	A	856	CLA	O1A-CGA-O2A-C1
14	A	802	CLA	C15-C16-C17-C18
14	A	825	CLA	C8-C10-C11-C12
14	B	3034	CLA	C5-C6-C7-C8
18	B	3050	LHG	O2-C2-C3-O3
14	A	805	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	B	3021	CLA	O1A-CGA-O2A-C1
14	B	3028	CLA	C8-C10-C11-C12
14	A	831	CLA	C10-C11-C12-C13
14	A	818	CLA	CBA-CGA-O2A-C1
14	B	3034	CLA	CBA-CGA-O2A-C1
13	A	801	CL0	C13-C15-C16-C17
14	B	3010	CLA	C8-C10-C11-C12
14	A	803	CLA	C13-C15-C16-C17
15	A	846	PQN	C25-C26-C27-C28
17	A	852	LMG	O9-C10-O7-C8
14	A	856	CLA	C2A-CAA-CBA-CGA
14	B	3005	CLA	C2A-CAA-CBA-CGA
14	A	856	CLA	O1D-CGD-O2D-CED
14	A	804	CLA	CBA-CGA-O2A-C1
14	A	840	CLA	CBA-CGA-O2A-C1
14	A	804	CLA	C10-C11-C12-C13
14	B	3014	CLA	C13-C15-C16-C17
14	B	3029	CLA	C15-C16-C17-C18
14	B	3029	CLA	O1D-CGD-O2D-CED
14	A	810	CLA	C15-C16-C17-C18
14	A	820	CLA	C13-C15-C16-C17
14	A	822	CLA	C15-C16-C17-C18
14	A	826	CLA	C15-C16-C17-C18
14	A	833	CLA	C10-C11-C12-C13
14	B	3003	CLA	C8-C10-C11-C12
14	A	807	CLA	C5-C6-C7-C8
14	A	834	CLA	C5-C6-C7-C8
14	B	3006	CLA	C13-C15-C16-C17
14	B	3041	CLA	C8-C10-C11-C12
17	A	852	LMG	C28-C29-C30-C31
14	A	814	CLA	C8-C10-C11-C12
14	B	3004	CLA	C15-C16-C17-C18
14	A	804	CLA	C3-C5-C6-C7
17	A	852	LMG	C11-C10-O7-C8
14	B	3030	CLA	C8-C10-C11-C12
14	A	807	CLA	CBA-CGA-O2A-C1
14	B	3019	CLA	CBA-CGA-O2A-C1
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

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Mol	Chain	Res	Type	Atoms
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	809	CLA	CBD-CGD-O2D-CED
14	A	839	CLA	C8-C10-C11-C12
16	J	104	BCR	C37-C22-C23-C24
17	A	852	LMG	O6-C5-C6-O5
16	B	3051	BCR	C21-C22-C23-C24
14	A	836	CLA	O1A-CGA-O2A-C1
14	B	3034	CLA	O1A-CGA-O2A-C1
13	A	801	CL0	C2A-CAA-CBA-CGA
14	A	837	CLA	C2A-CAA-CBA-CGA
14	A	818	CLA	CBD-CGD-O2D-CED
14	A	806	CLA	C16-C17-C18-C20
15	A	846	PQN	C26-C27-C28-C29
15	A	846	PQN	C26-C27-C28-C30
14	A	833	CLA	C3-C5-C6-C7
14	B	3011	CLA	C13-C15-C16-C17
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

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Mol	Chain	Res	Type	Atoms
16	L	208	BCR	C20-C21-C22-C23
16	M	103	BCR	C11-C10-C9-C8
14	A	821	CLA	CBD-CGD-O2D-CED
14	A	825	CLA	O1D-CGD-O2D-CED
14	B	3040	CLA	O1D-CGD-O2D-CED
14	B	3009	CLA	C13-C15-C16-C17
15	A	846	PQN	C20-C21-C22-C23
14	B	3030	CLA	O1D-CGD-O2D-CED
13	A	801	CL0	C16-C17-C18-C20
14	A	806	CLA	C16-C17-C18-C19
14	A	839	CLA	C16-C17-C18-C20
14	L	206	CLA	C16-C17-C18-C19
14	B	3033	CLA	C5-C6-C7-C8
14	B	3038	CLA	C5-C6-C7-C8
16	F	201	BCR	C14-C15-C16-C17
14	A	809	CLA	C5-C6-C7-C8
14	A	818	CLA	O1A-CGA-O2A-C1
18	M	101	LHG	O1-C1-C2-O2
17	A	852	LMG	C23-C24-C25-C26
17	I	102	LMG	C18-C19-C20-C21
14	B	3025	CLA	O1D-CGD-O2D-CED
14	A	808	CLA	C4B-C3B-CAB-CBB
14	B	3006	CLA	C4B-C3B-CAB-CBB
14	B	3008	CLA	C4B-C3B-CAB-CBB
14	B	3010	CLA	C4B-C3B-CAB-CBB
18	M	101	LHG	C23-C24-C25-C26
17	A	852	LMG	C17-C18-C19-C20
14	A	820	CLA	C16-C17-C18-C19
14	A	820	CLA	C16-C17-C18-C20
14	A	839	CLA	C16-C17-C18-C19
14	L	206	CLA	C16-C17-C18-C20
14	B	3021	CLA	C2A-CAA-CBA-CGA
18	A	853	LHG	C8-C7-O7-C5
14	A	802	CLA	C12-C13-C15-C16
14	A	830	CLA	C5-C6-C7-C8
15	A	846	PQN	C15-C16-C17-C18
14	A	840	CLA	O1A-CGA-O2A-C1
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

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Mol	Chain	Res	Type	Atoms
17	A	855	LMG	C18-C19-C20-C21
18	A	853	LHG	C12-C13-C14-C15
14	B	3011	CLA	C5-C6-C7-C8
14	L	206	CLA	C10-C11-C12-C13
14	A	831	CLA	O1D-CGD-O2D-CED
14	B	3010	CLA	C16-C17-C18-C20
14	A	804	CLA	O1A-CGA-O2A-C1
14	B	3019	CLA	O1A-CGA-O2A-C1
17	B	3049	LMG	C35-C36-C37-C38
17	A	855	LMG	C4-C5-C6-O5
14	B	3021	CLA	O1D-CGD-O2D-CED
17	A	852	LMG	C30-C31-C32-C33
17	A	855	LMG	C16-C17-C18-C19
14	B	3028	CLA	C3-C5-C6-C7
14	A	820	CLA	C15-C16-C17-C18
14	B	3019	CLA	C8-C10-C11-C12
14	A	803	CLA	O1D-CGD-O2D-CED
18	M	101	LHG	C32-C33-C34-C35
14	A	807	CLA	O1A-CGA-O2A-C1
22	L	207	DGD	C5B-C6B-C7B-C8B
14	B	3023	CLA	O1D-CGD-O2D-CED
14	A	832	CLA	C2B-C3B-CAB-CBB
14	A	834	CLA	C2B-C3B-CAB-CBB
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	B	3045	BCR	C1-C6-C7-C8
16	B	3045	BCR	C5-C6-C7-C8
16	B	3051	BCR	C1-C6-C7-C8
16	F	203	BCR	C1-C6-C7-C8
16	F	203	BCR	C5-C6-C7-C8
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	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	M	103	BCR	C23-C24-C25-C26
16	M	103	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
18	A	853	LHG	C24-C23-O8-C6
14	B	3041	CLA	C15-C16-C17-C18
14	B	3020	CLA	C3-C5-C6-C7
14	M	102	CLA	C2C-C3C-CAC-CBC
14	A	802	CLA	C2A-CAA-CBA-CGA
14	K	101	CLA	C2A-CAA-CBA-CGA
17	A	852	LMG	C20-C21-C22-C23
18	M	101	LHG	C25-C26-C27-C28
22	L	207	DGD	C4B-C5B-C6B-C7B
16	B	3044	BCR	C18-C19-C20-C21
16	B	3051	BCR	C10-C11-C12-C13
16	J	105	BCR	C18-C19-C20-C21
16	L	201	BCR	C10-C11-C12-C13
14	A	830	CLA	C10-C11-C12-C13
17	A	852	LMG	C11-C12-C13-C14
18	M	101	LHG	C33-C34-C35-C36
18	M	101	LHG	C14-C15-C16-C17
16	J	103	BCR	C22-C23-C24-C25
16	J	104	BCR	C6-C7-C8-C9
16	J	104	BCR	C22-C23-C24-C25
21	L	202	LMT	C1-C2-C3-C4
17	A	855	LMG	C2-C1-O1-C7
14	A	833	CLA	C5-C6-C7-C8
22	L	207	DGD	C2B-C3B-C4B-C5B
14	A	819	CLA	C3-C5-C6-C7
14	B	3003	CLA	CBA-CGA-O2A-C1
14	B	3040	CLA	CBA-CGA-O2A-C1
17	A	855	LMG	C10-C11-C12-C13
14	A	811	CLA	C4C-C3C-CAC-CBC
18	A	853	LHG	C24-C25-C26-C27
14	B	3033	CLA	C2A-CAA-CBA-CGA
14	M	102	CLA	C2A-CAA-CBA-CGA
13	A	801	CL0	C16-C17-C18-C19
14	B	3033	CLA	C16-C17-C18-C19
14	B	3033	CLA	C16-C17-C18-C20
14	A	844	CLA	C15-C16-C17-C18
14	B	3019	CLA	C3-C5-C6-C7
14	B	3009	CLA	C15-C16-C17-C18
17	I	102	LMG	C15-C16-C17-C18
14	B	3028	CLA	C15-C16-C17-C18
14	B	3007	CLA	C16-C17-C18-C20
14	B	3010	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
13	A	801	CL0	O1D-CGD-O2D-CED
14	A	825	CLA	C5-C6-C7-C8
14	A	844	CLA	C5-C6-C7-C8
14	B	3019	CLA	C5-C6-C7-C8
17	A	852	LMG	C18-C19-C20-C21
18	A	853	LHG	O7-C5-C6-O8
17	A	855	LMG	C13-C14-C15-C16
17	B	3049	LMG	C17-C18-C19-C20
17	B	3049	LMG	C31-C32-C33-C34
14	B	3028	CLA	CBA-CGA-O2A-C1
17	A	852	LMG	C33-C34-C35-C36
18	M	101	LHG	C26-C27-C28-C29
14	A	808	CLA	C2-C1-O2A-CGA
14	B	3033	CLA	C2-C1-O2A-CGA
14	B	3039	CLA	C5-C6-C7-C8
14	A	836	CLA	C5-C6-C7-C8
18	M	101	LHG	C30-C31-C32-C33
18	A	854	LHG	O9-C7-O7-C5
14	B	3041	CLA	C10-C11-C12-C13
14	A	844	CLA	C2A-CAA-CBA-CGA
14	A	827	CLA	O1D-CGD-O2D-CED
14	A	836	CLA	O1D-CGD-O2D-CED
14	B	3011	CLA	O1D-CGD-O2D-CED
14	B	3028	CLA	O1D-CGD-O2D-CED
14	A	820	CLA	C8-C10-C11-C12
14	B	3009	CLA	C8-C10-C11-C12
18	M	101	LHG	C7-C8-C9-C10
14	A	834	CLA	C3-C5-C6-C7
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
17	A	852	LMG	C16-C17-C18-C19
14	A	807	CLA	C11-C12-C13-C15
14	A	828	CLA	C11-C10-C8-C7
14	A	834	CLA	C11-C10-C8-C7
14	A	834	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	A	856	CLA	C11-C10-C8-C7
14	B	3010	CLA	C6-C7-C8-C10
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	B	3040	CLA	O1A-CGA-O2A-C1
18	A	853	LHG	C23-C24-C25-C26
17	B	3049	LMG	C34-C35-C36-C37
14	B	3015	CLA	C5-C6-C7-C8
14	A	817	CLA	C2C-C3C-CAC-CBC
14	A	813	CLA	C2A-CAA-CBA-CGA
14	A	841	CLA	C6-C7-C8-C9
14	B	3007	CLA	C11-C12-C13-C14
14	B	3009	CLA	C14-C13-C15-C16
14	B	3010	CLA	C6-C7-C8-C9
14	B	3020	CLA	C11-C10-C8-C9
14	B	3029	CLA	C14-C13-C15-C16
14	L	204	CLA	C11-C12-C13-C14
14	B	3029	CLA	C5-C6-C7-C8
14	B	3015	CLA	C2C-C3C-CAC-CBC
18	A	853	LHG	C4-C5-C6-O8
18	M	101	LHG	C4-C5-C6-O8
17	A	852	LMG	C22-C23-C24-C25
14	A	826	CLA	C10-C11-C12-C13
17	B	3049	LMG	C14-C15-C16-C17
14	B	3027	CLA	CBA-CGA-O2A-C1
14	B	3028	CLA	O1A-CGA-O2A-C1
14	A	812	CLA	O1D-CGD-O2D-CED
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
18	A	854	LHG	C11-C10-C9-C8
17	B	3049	LMG	C28-C29-C30-C31
14	B	3003	CLA	O1A-CGA-O2A-C1
14	A	811	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	A	810	CLA	C10-C11-C12-C13
14	A	822	CLA	C13-C15-C16-C17
16	B	3051	BCR	C11-C12-C13-C14
16	J	104	BCR	C7-C8-C9-C10
14	B	3015	CLA	C8-C10-C11-C12
18	M	101	LHG	C11-C10-C9-C8
14	B	3018	CLA	C10-C11-C12-C13
14	A	856	CLA	O2A-C1-C2-C3
14	A	839	CLA	C5-C6-C7-C8
16	B	3047	BCR	C9-C10-C11-C12
14	B	3033	CLA	C2C-C3C-CAC-CBC
14	A	822	CLA	C3-C5-C6-C7
17	A	852	LMG	C21-C22-C23-C24
14	B	3033	CLA	C10-C11-C12-C13
14	B	3039	CLA	C16-C17-C18-C20
17	A	852	LMG	C14-C15-C16-C17
18	A	853	LHG	C9-C10-C11-C12
18	A	854	LHG	C9-C10-C11-C12
18	A	853	LHG	C19-C20-C21-C22
17	B	3049	LMG	C23-C24-C25-C26
17	B	3049	LMG	C30-C31-C32-C33
14	A	841	CLA	C5-C6-C7-C8
16	K	102	BCR	C14-C15-C16-C17
22	L	207	DGD	CAA-CBA-CCA-CDA
14	A	825	CLA	C11-C12-C13-C14
14	A	835	CLA	C5-C6-C7-C8
14	A	831	CLA	C16-C17-C18-C20
14	A	835	CLA	C16-C17-C18-C19
14	A	835	CLA	C16-C17-C18-C20
14	A	826	CLA	C2-C3-C5-C6
14	A	822	CLA	CBA-CGA-O2A-C1
14	B	3022	CLA	C2C-C3C-CAC-CBC
18	A	853	LHG	O1-C1-C2-O2
21	L	202	LMT	C2-C1-O1'-C1'
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	834	CLA	C11-C10-C8-C9
14	A	834	CLA	C14-C13-C15-C16
14	A	856	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
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	3030	CLA	C11-C10-C8-C9
14	B	3033	CLA	C11-C12-C13-C14
14	B	3039	CLA	C11-C10-C8-C9
14	B	3039	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
14	B	3025	CLA	C5-C6-C7-C8
22	L	207	DGD	C9B-CAB-CBB-CCB
14	B	3028	CLA	C10-C11-C12-C13
14	B	3039	CLA	C13-C15-C16-C17
14	A	821	CLA	C4B-C3B-CAB-CBB
14	B	3003	CLA	C4B-C3B-CAB-CBB
14	B	3039	CLA	C16-C17-C18-C19
17	A	855	LMG	C12-C13-C14-C15
14	A	822	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	3010	CLA	C11-C10-C8-C7
14	B	3030	CLA	C11-C10-C8-C7
14	B	3033	CLA	C11-C12-C13-C15
14	L	204	CLA	C12-C13-C15-C16
14	L	205	CLA	C12-C13-C15-C16
14	L	206	CLA	C6-C7-C8-C10
14	A	827	CLA	C5-C6-C7-C8
14	B	3011	CLA	C8-C10-C11-C12
17	A	852	LMG	C35-C36-C37-C38
14	A	808	CLA	C3A-C2A-CAA-CBA
14	A	822	CLA	C4-C3-C5-C6
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	B	3033	CLA	C2-C3-C5-C6
14	A	818	CLA	O1D-CGD-O2D-CED
14	A	804	CLA	C5-C6-C7-C8
16	A	849	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
14	M	102	CLA	C4C-C3C-CAC-CBC
17	I	102	LMG	C11-C10-O7-C8
14	A	822	CLA	C2A-CAA-CBA-CGA
17	B	3049	LMG	O1-C7-C8-C9
14	A	831	CLA	C16-C17-C18-C19
14	B	3019	CLA	C10-C11-C12-C13
13	A	801	CL0	C1A-C2A-CAA-CBA
22	L	207	DGD	C7A-C8A-C9A-CAA
14	A	826	CLA	C4-C3-C5-C6
14	B	3033	CLA	C4-C3-C5-C6
17	A	855	LMG	C17-C18-C19-C20
14	B	3042	CLA	C16-C17-C18-C19
14	B	3042	CLA	C16-C17-C18-C20
14	B	3027	CLA	O1A-CGA-O2A-C1
16	A	851	BCR	C5-C6-C7-C8
16	B	3051	BCR	C5-C6-C7-C8
16	B	3051	BCR	C23-C24-C25-C30
16	F	203	BCR	C23-C24-C25-C30
16	J	105	BCR	C1-C6-C7-C8
14	B	3014	CLA	CBA-CGA-O2A-C1
18	A	854	LHG	C2-C3-O3-P
17	B	3049	LMG	C41-C42-C43-C44
14	A	813	CLA	C6-C7-C8-C9
14	A	809	CLA	O1D-CGD-O2D-CED
14	A	831	CLA	C13-C15-C16-C17
17	I	102	LMG	C32-C33-C34-C35
14	A	821	CLA	O1D-CGD-O2D-CED
18	M	101	LHG	O7-C5-C6-O8
14	A	835	CLA	C4-C3-C5-C6
18	M	101	LHG	C17-C18-C19-C20
16	J	103	BCR	C18-C19-C20-C21
14	B	3007	CLA	C16-C17-C18-C19
14	A	822	CLA	C14-C13-C15-C16
14	B	3019	CLA	C6-C7-C8-C9
14	A	817	CLA	C4C-C3C-CAC-CBC
16	B	3046	BCR	C6-C7-C8-C9
14	A	817	CLA	O2A-C1-C2-C3
14	B	3032	CLA	O2A-C1-C2-C3
17	A	852	LMG	C2-C1-O1-C7
14	B	3010	CLA	C10-C11-C12-C13
14	B	3029	CLA	CBA-CGA-O2A-C1
14	A	822	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	A	835	CLA	C2-C3-C5-C6
17	B	3049	LMG	C20-C21-C22-C23
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
14	B	3020	CLA	CBA-CGA-O2A-C1
14	B	3023	CLA	CBA-CGA-O2A-C1
14	B	3038	CLA	C11-C12-C13-C15
14	A	813	CLA	C2C-C3C-CAC-CBC
14	A	827	CLA	C11-C10-C8-C7
14	A	839	CLA	C6-C7-C8-C10
14	B	3007	CLA	C11-C12-C13-C15
14	B	3011	CLA	C6-C7-C8-C10
14	B	3019	CLA	C6-C7-C8-C10
14	B	3030	CLA	C12-C13-C15-C16
14	L	204	CLA	C6-C7-C8-C10
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	3008	CLA	CBA-CGA-O2A-C1
14	A	822	CLA	O1A-CGA-O2A-C1
22	L	207	DGD	O1B-C1B-O2G-C2G
14	B	3023	CLA	O1A-CGA-O2A-C1
14	B	3011	CLA	C15-C16-C17-C18
14	B	3018	CLA	C2C-C3C-CAC-CBC
14	B	3014	CLA	O1A-CGA-O2A-C1
14	A	839	CLA	C10-C11-C12-C13
16	A	847	BCR	C11-C10-C9-C8
16	B	3048	BCR	C20-C21-C22-C23
14	A	823	CLA	O2A-C1-C2-C3
14	A	824	CLA	CBA-CGA-O2A-C1
14	B	3023	CLA	C2A-CAA-CBA-CGA
14	A	829	CLA	C3-C5-C6-C7
18	A	853	LHG	C33-C34-C35-C36
17	B	3049	LMG	O1-C7-C8-O7
14	A	827	CLA	C11-C10-C8-C9
14	A	824	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	B	3028	CLA	C5-C6-C7-C8
14	B	3039	CLA	C15-C16-C17-C18
14	A	810	CLA	C3-C5-C6-C7
14	B	3024	CLA	CBD-CGD-O2D-CED
14	A	807	CLA	C13-C15-C16-C17
14	B	3014	CLA	C15-C16-C17-C18
14	B	3025	CLA	C2C-C3C-CAC-CBC
14	A	828	CLA	C8-C10-C11-C12
14	B	3029	CLA	O1A-CGA-O2A-C1
14	A	832	CLA	CBA-CGA-O2A-C1
14	A	835	CLA	CBA-CGA-O2A-C1
14	A	806	CLA	C15-C16-C17-C18
14	B	3029	CLA	C13-C15-C16-C17
14	B	3008	CLA	O1A-CGA-O2A-C1
14	A	813	CLA	C3-C5-C6-C7
14	B	3008	CLA	C2C-C3C-CAC-CBC
14	B	3006	CLA	CBA-CGA-O2A-C1
17	I	102	LMG	C28-C29-C30-C31
16	B	3047	BCR	C36-C18-C19-C20
14	A	802	CLA	C1A-C2A-CAA-CBA
14	B	3007	CLA	C4B-C3B-CAB-CBB
14	B	3035	CLA	C4B-C3B-CAB-CBB
14	B	3030	CLA	CBA-CGA-O2A-C1
16	A	851	BCR	C6-C7-C8-C9
16	B	3046	BCR	C7-C8-C9-C10
14	A	825	CLA	C3-C5-C6-C7
14	A	817	CLA	C2A-CAA-CBA-CGA
22	L	207	DGD	CEB-CFB-CGB-CHB
21	L	202	LMT	C5'-C4'-O1B-C1B
14	A	842	CLA	C2-C3-C5-C6
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	829	CLA	C6-C7-C8-C10
14	A	830	CLA	C6-C7-C8-C10
14	A	844	CLA	C11-C12-C13-C15
14	B	3006	CLA	C12-C13-C15-C16
14	B	3007	CLA	C11-C10-C8-C7
14	B	3015	CLA	C12-C13-C15-C16
14	B	3020	CLA	C12-C13-C15-C16
14	B	3029	CLA	C6-C7-C8-C10
14	B	3033	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
15	B	3043	PQN	C22-C23-C25-C26
14	B	3024	CLA	O1D-CGD-O2D-CED
14	A	835	CLA	CBD-CGD-O2D-CED
14	B	3006	CLA	O1A-CGA-O2A-C1
22	L	207	DGD	C3A-C4A-C5A-C6A
14	B	3020	CLA	O1A-CGA-O2A-C1
14	A	830	CLA	C4-C3-C5-C6
14	B	3005	CLA	C3A-C2A-CAA-CBA
14	A	837	CLA	CBD-CGD-O2D-CED
14	A	822	CLA	C6-C7-C8-C9
14	A	839	CLA	C6-C7-C8-C9
14	B	3010	CLA	C11-C10-C8-C9
14	B	3027	CLA	C6-C7-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
14	A	835	CLA	O1A-CGA-O2A-C1
14	A	827	CLA	C13-C15-C16-C17
14	B	3010	CLA	C2C-C3C-CAC-CBC
14	A	823	CLA	C1-C2-C3-C4
14	B	3032	CLA	C1-C2-C3-C4
17	A	852	LMG	C29-C30-C31-C32
14	A	837	CLA	O1D-CGD-O2D-CED
17	I	102	LMG	O1-C7-C8-O7
17	I	102	LMG	O1-C7-C8-C9
21	L	202	LMT	C9-C10-C11-C12
14	A	828	CLA	CAD-CBD-CGD-O2D
14	B	3017	CLA	CAD-CBD-CGD-O2D
14	B	3030	CLA	O1A-CGA-O2A-C1
14	A	822	CLA	C2C-C3C-CAC-CBC
14	A	803	CLA	C3-C5-C6-C7
13	A	801	CL0	CHA-CBD-CGD-O1D
13	A	801	CL0	CHA-CBD-CGD-O2D
14	A	826	CLA	CHA-CBD-CGD-O1D
14	A	826	CLA	CHA-CBD-CGD-O2D
14	A	828	CLA	CAD-CBD-CGD-O1D
14	A	835	CLA	CHA-CBD-CGD-O1D
14	A	835	CLA	CHA-CBD-CGD-O2D
14	B	3013	CLA	CHA-CBD-CGD-O1D
14	B	3017	CLA	CAD-CBD-CGD-O1D
14	B	3022	CLA	CHA-CBD-CGD-O1D
14	M	102	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
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	C4-O6-P-O5
18	M	101	LHG	C4-O6-P-O5
18	A	853	LHG	C30-C31-C32-C33
14	A	809	CLA	C4-C3-C5-C6
14	A	808	CLA	C2B-C3B-CAB-CBB
14	B	3006	CLA	C2B-C3B-CAB-CBB
14	B	3010	CLA	C2B-C3B-CAB-CBB
16	J	105	BCR	C5-C6-C7-C8
14	B	3028	CLA	C13-C15-C16-C17
18	A	853	LHG	C10-C11-C12-C13
22	L	207	DGD	C1B-C2B-C3B-C4B
14	B	3010	CLA	C15-C16-C17-C18
14	A	806	CLA	C13-C15-C16-C17
14	B	3009	CLA	O1D-CGD-O2D-CED
14	B	3038	CLA	C11-C12-C13-C14
14	A	826	CLA	C13-C15-C16-C17
22	L	207	DGD	C9A-CAA-CBA-CCA
14	B	3038	CLA	C8-C10-C11-C12
14	B	3014	CLA	C2C-C3C-CAC-CBC
14	A	833	CLA	C11-C10-C8-C9
14	B	3033	CLA	C6-C7-C8-C9
14	L	204	CLA	C6-C7-C8-C9
14	A	833	CLA	C11-C10-C8-C7
14	B	3020	CLA	C11-C12-C13-C15
16	A	849	BCR	C20-C21-C22-C23
16	B	3045	BCR	C11-C10-C9-C8
16	B	3051	BCR	C11-C10-C9-C8
16	L	209	BCR	C14-C15-C16-C17
18	A	853	LHG	C13-C14-C15-C16
18	M	101	LHG	C16-C17-C18-C19
14	A	838	CLA	C4C-C3C-CAC-CBC
14	B	3005	CLA	O1A-CGA-O2A-C1
14	A	838	CLA	C2C-C3C-CAC-CBC
14	A	810	CLA	C2C-C3C-CAC-CBC
14	B	3032	CLA	C2A-CAA-CBA-CGA
14	B	3014	CLA	C4C-C3C-CAC-CBC
17	A	852	LMG	C32-C33-C34-C35
14	B	3017	CLA	C2C-C3C-CAC-CBC
16	A	849	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
16	A	850	BCR	C11-C12-C13-C35
17	A	855	LMG	C8-C7-O1-C1
17	B	3049	LMG	C36-C37-C38-C39
14	B	3005	CLA	CBA-CGA-O2A-C1
14	A	832	CLA	O1A-CGA-O2A-C1
18	A	854	LHG	O10-C23-O8-C6
14	A	807	CLA	C14-C13-C15-C16
14	A	830	CLA	C6-C7-C8-C9
17	B	3049	LMG	C42-C43-C44-C45
18	A	853	LHG	C11-C12-C13-C14
14	A	835	CLA	C4B-C3B-CAB-CBB
14	A	843	CLA	C4B-C3B-CAB-CBB
14	L	204	CLA	C4B-C3B-CAB-CBB
17	B	3049	LMG	C22-C23-C24-C25
14	A	856	CLA	C13-C15-C16-C17
14	A	820	CLA	C4-C3-C5-C6
14	X	1701	CLA	CAA-CBA-CGA-O2A
14	A	829	CLA	C11-C12-C13-C15
15	B	3043	PQN	C21-C22-C23-C25
14	A	816	CLA	C3A-C2A-CAA-CBA
14	B	3038	CLA	C4-C3-C5-C6
14	A	811	CLA	O1D-CGD-O2D-CED
16	A	851	BCR	C16-C17-C18-C36
16	B	3045	BCR	C11-C10-C9-C34
16	F	203	BCR	C35-C13-C14-C15
16	J	105	BCR	C6-C7-C8-C9
16	L	201	BCR	C22-C23-C24-C25
14	A	830	CLA	C13-C15-C16-C17
14	B	3009	CLA	C5-C6-C7-C8
16	F	201	BCR	C7-C8-C9-C34
14	X	1701	CLA	CAA-CBA-CGA-O1A
21	L	202	LMT	C3-C4-C5-C6
14	A	842	CLA	C4-C3-C5-C6
14	B	3014	CLA	C5-C6-C7-C8
16	J	104	BCR	C21-C22-C23-C24
14	B	3011	CLA	C4-C3-C5-C6
14	K	103	CLA	C4C-C3C-CAC-CBC
14	A	809	CLA	C2-C3-C5-C6
14	A	830	CLA	C2-C3-C5-C6
14	A	829	CLA	C16-C17-C18-C19
16	A	848	BCR	C14-C15-C16-C17
14	A	829	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
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	3018	CLA	C11-C10-C8-C9
14	B	3029	CLA	C11-C12-C13-C14
14	L	206	CLA	C11-C10-C8-C9
15	B	3043	PQN	C21-C22-C23-C24
17	A	852	LMG	C13-C14-C15-C16
18	A	853	LHG	C31-C32-C33-C34
14	A	820	CLA	C5-C6-C7-C8
14	B	3011	CLA	C2-C3-C5-C6
14	A	809	CLA	C2A-CAA-CBA-CGA
14	J	101	CLA	C2A-CAA-CBA-CGA
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
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
18	A	853	LHG	C34-C35-C36-C37
18	B	3050	LHG	O6-C4-C5-O7
14	A	821	CLA	C2B-C3B-CAB-CBB
14	B	3003	CLA	C2B-C3B-CAB-CBB
14	B	3007	CLA	C2B-C3B-CAB-CBB
14	L	204	CLA	C2B-C3B-CAB-CBB
16	A	847	BCR	C1-C6-C7-C8
16	A	850	BCR	C1-C6-C7-C8
16	B	3047	BCR	C23-C24-C25-C30
16	B	3051	BCR	C23-C24-C25-C26
16	F	203	BCR	C23-C24-C25-C26
16	L	209	BCR	C5-C6-C7-C8
14	A	810	CLA	C4C-C3C-CAC-CBC
14	B	3003	CLA	C4-C3-C5-C6
18	B	3050	LHG	O6-C4-C5-C6
14	B	3038	CLA	C2-C3-C5-C6
14	B	3024	CLA	CAA-CBA-CGA-O1A
14	K	103	CLA	CAA-CBA-CGA-O1A
15	B	3043	PQN	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
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	835	CLA	C11-C12-C13-C15
14	A	843	CLA	C11-C10-C8-C7
14	B	3015	CLA	C11-C10-C8-C7
14	B	3018	CLA	C11-C10-C8-C7
14	A	811	CLA	C2A-CAA-CBA-CGA
14	K	103	CLA	CAA-CBA-CGA-O2A
14	B	3024	CLA	CAA-CBA-CGA-O2A
14	A	807	CLA	C4-C3-C5-C6
14	A	812	CLA	C4-C3-C5-C6
14	A	820	CLA	C2-C3-C5-C6
14	B	3003	CLA	C2-C3-C5-C6
14	A	856	CLA	C16-C17-C18-C20
17	A	855	LMG	C15-C16-C17-C18
14	B	3031	CLA	CAA-CBA-CGA-O1A
16	B	3044	BCR	C6-C7-C8-C9
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	A	802	CLA	C10-C11-C12-C13
14	A	810	CLA	C5-C6-C7-C8
14	A	844	CLA	O1A-CGA-O2A-C1
14	B	3031	CLA	CAA-CBA-CGA-O2A
14	A	819	CLA	CAA-CBA-CGA-O2A
14	J	101	CLA	CAA-CBA-CGA-O2A
14	B	3042	CLA	C15-C16-C17-C18
14	B	3014	CLA	C8-C10-C11-C12
14	A	844	CLA	CBA-CGA-O2A-C1
14	B	3010	CLA	C4C-C3C-CAC-CBC
18	M	101	LHG	C28-C29-C30-C31
14	B	3027	CLA	C16-C17-C18-C20
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	826	CLA	O1D-CGD-O2D-CED
14	A	835	CLA	O1D-CGD-O2D-CED
18	A	854	LHG	O6-C4-C5-C6
14	A	856	CLA	C16-C17-C18-C19
17	A	852	LMG	O1-C7-C8-O7
14	A	809	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
15	A	846	PQN	C23-C25-C26-C27
14	A	844	CLA	C8-C10-C11-C12
14	B	3018	CLA	C11-C12-C13-C14
14	A	827	CLA	C14-C13-C15-C16
14	B	3007	CLA	C11-C10-C8-C9
14	B	3022	CLA	C4C-C3C-CAC-CBC
22	L	207	DGD	C5D-C6D-O5D-C1E
14	A	827	CLA	C8-C10-C11-C12
14	B	3008	CLA	C2A-CAA-CBA-CGA
14	B	3028	CLA	C2-C1-O2A-CGA
14	A	840	CLA	C2-C1-O2A-CGA
15	B	3043	PQN	C26-C27-C28-C29
13	A	801	CL0	C8-C10-C11-C12
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	3030	CLA	C4-C3-C5-C6
14	B	3034	CLA	C3A-C2A-CAA-CBA
17	A	852	LMG	O10-C28-O8-C9
18	B	3050	LHG	O1-C1-C2-C3
14	B	3023	CLA	C2C-C3C-CAC-CBC
22	L	207	DGD	C2D-C1D-O3G-C3G
14	A	844	CLA	O2A-C1-C2-C3
16	J	104	BCR	C18-C19-C20-C21
14	F	202	CLA	CAA-CBA-CGA-O2A
14	B	3036	CLA	CAA-CBA-CGA-O2A
14	B	3037	CLA	CAA-CBA-CGA-O2A
14	A	843	CLA	C4C-C3C-CAC-CBC
14	J	101	CLA	CAA-CBA-CGA-O1A
22	L	207	DGD	CFB-CGB-CHB-CIB
21	L	202	LMT	C4-C5-C6-C7
14	B	3037	CLA	CAA-CBA-CGA-O1A
18	A	854	LHG	O6-C4-C5-O7
21	L	202	LMT	C6-C7-C8-C9
14	B	3027	CLA	C13-C15-C16-C17
14	A	826	CLA	CBD-CGD-O2D-CED
17	A	852	LMG	C15-C16-C17-C18
14	B	3036	CLA	CAA-CBA-CGA-O1A
14	F	202	CLA	CAA-CBA-CGA-O1A
17	B	3049	LMG	O7-C10-C11-C12
14	A	802	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	B	3011	CLA	C6-C7-C8-C9
14	B	3029	CLA	C6-C7-C8-C9
14	A	808	CLA	CAA-CBA-CGA-O2A
14	M	102	CLA	CAA-CBA-CGA-O1A
16	J	103	BCR	C21-C22-C23-C24
17	A	852	LMG	C19-C20-C21-C22
14	A	803	CLA	C12-C13-C15-C16
14	A	812	CLA	C12-C13-C15-C16
14	A	822	CLA	C12-C13-C15-C16
14	A	827	CLA	C12-C13-C15-C16
14	B	3027	CLA	C11-C10-C8-C7
14	B	3041	CLA	C11-C12-C13-C15
14	B	3041	CLA	C12-C13-C15-C16
18	M	101	LHG	C10-C11-C12-C13
22	L	207	DGD	CBB-CCB-CDB-CEB
14	K	103	CLA	C2C-C3C-CAC-CBC
14	B	3008	CLA	C2B-C3B-CAB-CBB
14	L	205	CLA	C2B-C3B-CAB-CBB
16	A	847	BCR	C5-C6-C7-C8
16	A	848	BCR	C1-C6-C7-C8
16	A	848	BCR	C5-C6-C7-C8
16	A	850	BCR	C5-C6-C7-C8
16	B	3047	BCR	C23-C24-C25-C26
18	M	101	LHG	C5-C4-O6-P
14	A	829	CLA	C16-C17-C18-C20
14	B	3027	CLA	C2A-CAA-CBA-CGA
14	A	809	CLA	C15-C16-C17-C18
18	B	3050	LHG	O7-C7-C8-C9
14	A	843	CLA	C2C-C3C-CAC-CBC
17	A	852	LMG	O8-C28-C29-C30
14	B	3013	CLA	CAA-CBA-CGA-O1A
16	B	3048	BCR	C11-C10-C9-C34
14	B	3040	CLA	C2-C1-O2A-CGA
17	B	3049	LMG	C16-C17-C18-C19
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	3015	CLA	C11-C10-C8-C9
14	B	3006	CLA	C15-C16-C17-C18
14	A	840	CLA	C4B-C3B-CAB-CBB
14	B	3003	CLA	C1A-C2A-CAA-CBA
14	B	3014	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	B	3021	CLA	C4B-C3B-CAB-CBB
14	B	3034	CLA	C1A-C2A-CAA-CBA
14	B	3042	CLA	C4B-C3B-CAB-CBB
14	X	1701	CLA	C4B-C3B-CAB-CBB
14	B	3023	CLA	C4-C3-C5-C6
14	A	807	CLA	CAA-CBA-CGA-O2A
14	A	845	CLA	CAA-CBA-CGA-O2A
14	B	3011	CLA	CAA-CBA-CGA-O2A
14	B	3014	CLA	CAA-CBA-CGA-O2A
14	M	102	CLA	CAA-CBA-CGA-O2A
16	I	101	BCR	C17-C18-C19-C20
16	J	103	BCR	C11-C12-C13-C14
16	L	201	BCR	C7-C8-C9-C10
16	L	208	BCR	C21-C22-C23-C24
14	A	836	CLA	C6-C7-C8-C9
17	A	855	LMG	C19-C20-C21-C22
14	A	803	CLA	CAA-CBA-CGA-O2A
14	B	3006	CLA	CAA-CBA-CGA-O2A
18	A	854	LHG	C8-C7-O7-C5
22	L	207	DGD	C2A-C3A-C4A-C5A
14	B	3015	CLA	C2-C1-O2A-CGA
14	L	205	CLA	C2-C1-O2A-CGA
14	A	820	CLA	C11-C10-C8-C7
14	A	839	CLA	C11-C12-C13-C15
14	B	3014	CLA	C11-C10-C8-C7
14	B	3013	CLA	CAA-CBA-CGA-O2A
14	A	809	CLA	C16-C17-C18-C20
14	B	3027	CLA	C16-C17-C18-C19
14	A	815	CLA	CAA-CBA-CGA-O2A
14	B	3014	CLA	C3A-C2A-CAA-CBA
18	A	853	LHG	C17-C18-C19-C20
14	A	806	CLA	C10-C11-C12-C13
17	B	3049	LMG	C19-C20-C21-C22
14	A	808	CLA	CAA-CBA-CGA-O1A
14	B	3029	CLA	CAA-CBA-CGA-O2A
18	A	853	LHG	O10-C23-C24-C25
14	A	806	CLA	C11-C12-C13-C14
14	A	814	CLA	C11-C10-C8-C9
14	A	830	CLA	C11-C12-C13-C14
14	B	3009	CLA	C11-C10-C8-C9
14	B	3015	CLA	C14-C13-C15-C16
14	B	3020	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	B	3015	CLA	CAA-CBA-CGA-O2A
14	B	3006	CLA	CAA-CBA-CGA-O1A
17	B	3049	LMG	O9-C10-C11-C12
14	A	844	CLA	C13-C15-C16-C17
14	B	3009	CLA	CBD-CGD-O2D-CED
16	A	849	BCR	C7-C8-C9-C10
17	A	852	LMG	O10-C28-C29-C30
17	I	102	LMG	O9-C10-C11-C12
14	A	820	CLA	CAA-CBA-CGA-O2A
22	L	207	DGD	CDB-CEB-CFB-CGB
14	A	845	CLA	CAA-CBA-CGA-O1A
18	M	101	LHG	O9-C7-C8-C9
14	A	856	CLA	C8-C10-C11-C12
14	B	3027	CLA	CAD-CBD-CGD-O2D
14	K	103	CLA	CAD-CBD-CGD-O2D
22	L	207	DGD	CEA-CFA-CGA-CHA
14	B	3007	CLA	CAA-CBA-CGA-O2A
14	B	3021	CLA	CAA-CBA-CGA-O2A
14	A	814	CLA	C3-C5-C6-C7
14	B	3011	CLA	CAA-CBA-CGA-O1A
14	A	803	CLA	CAA-CBA-CGA-O1A
14	A	837	CLA	CAA-CBA-CGA-O1A
14	B	3021	CLA	CAA-CBA-CGA-O1A
17	I	102	LMG	O7-C10-C11-C12
18	A	853	LHG	O7-C7-C8-C9
14	A	815	CLA	CAA-CBA-CGA-O1A
14	B	3029	CLA	CAA-CBA-CGA-O1A
18	A	853	LHG	C28-C29-C30-C31
14	A	809	CLA	CAA-CBA-CGA-O2A
14	B	3014	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

115 monomers are involved in 304 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	833	CLA	1	0
16	J	105	BCR	10	0
14	A	806	CLA	4	0
14	K	101	CLA	5	0
14	B	3027	CLA	2	0
14	B	3019	CLA	3	0
16	A	849	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	3033	CLA	3	0
13	A	801	CL0	1	0
14	B	3003	CLA	4	0
14	B	3004	CLA	5	0
14	A	815	CLA	3	0
14	K	103	CLA	1	0
16	K	102	BCR	5	0
14	B	3017	CLA	2	0
14	B	3024	CLA	3	0
16	J	104	BCR	6	0
14	B	3039	CLA	1	0
14	A	835	CLA	4	0
14	B	3025	CLA	4	0
14	A	841	CLA	5	0
16	L	201	BCR	3	0
14	A	808	CLA	3	0
14	A	814	CLA	1	0
14	B	3032	CLA	2	0
14	L	205	CLA	4	0
14	A	817	CLA	2	0
14	A	838	CLA	1	0
14	B	3013	CLA	2	0
14	M	102	CLA	4	0
16	F	203	BCR	4	0
14	A	834	CLA	2	0
17	I	102	LMG	3	0
14	B	3031	CLA	1	0
14	A	819	CLA	5	0
14	A	823	CLA	2	0
14	B	3020	CLA	2	0
14	A	827	CLA	2	0
14	B	3041	CLA	3	0
14	B	3026	CLA	2	0
16	B	3051	BCR	4	0
14	A	844	CLA	4	0
14	B	3035	CLA	1	0
18	B	3050	LHG	2	0
14	A	804	CLA	7	0
14	A	836	CLA	2	0
14	X	1701	CLA	3	0
14	A	803	CLA	3	0
14	A	828	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	M	101	LHG	3	0
14	B	3030	CLA	1	0
14	B	3042	CLA	1	0
14	A	842	CLA	3	0
16	I	101	BCR	4	0
18	A	854	LHG	1	0
14	B	3011	CLA	1	0
14	L	204	CLA	2	0
14	J	101	CLA	2	0
14	A	845	CLA	2	0
16	J	103	BCR	3	0
17	A	855	LMG	1	0
16	L	208	BCR	2	0
14	A	802	CLA	2	0
16	M	103	BCR	2	0
16	F	201	BCR	4	0
14	A	825	CLA	2	0
15	A	846	PQN	9	0
14	A	820	CLA	5	0
14	B	3021	CLA	2	0
16	A	850	BCR	4	0
14	B	3040	CLA	1	0
14	B	3007	CLA	3	0
14	A	811	CLA	6	0
14	A	829	CLA	8	0
14	B	3010	CLA	7	0
16	B	3045	BCR	8	0
14	A	821	CLA	3	0
16	L	209	BCR	2	0
14	B	3037	CLA	2	0
16	B	3046	BCR	4	0
14	A	830	CLA	3	0
14	A	832	CLA	5	0
14	B	3006	CLA	2	0
15	B	3043	PQN	2	0
14	A	826	CLA	3	0
14	A	843	CLA	4	0
16	B	3047	BCR	4	0
14	A	839	CLA	1	0
14	B	3005	CLA	2	0
14	A	813	CLA	5	0
16	A	851	BCR	8	0

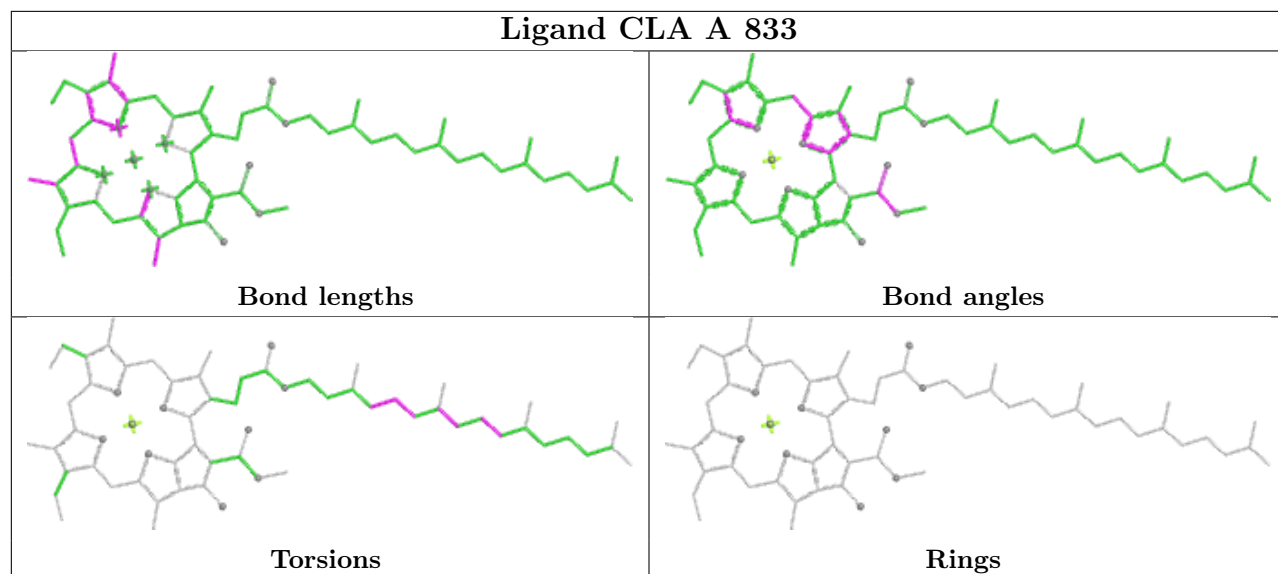
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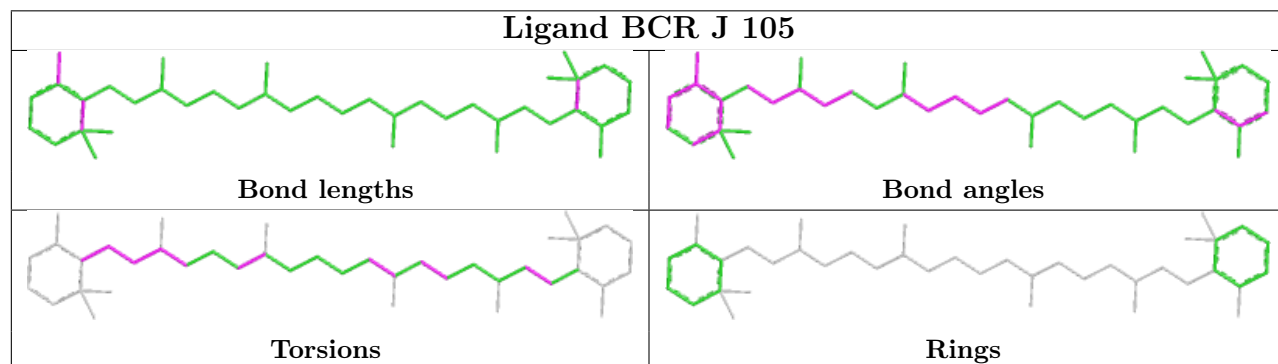
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	3012	CLA	1	0
14	A	831	CLA	5	0
22	L	207	DGD	2	0
14	B	3008	CLA	3	0
14	A	809	CLA	1	0
14	A	818	CLA	3	0
16	B	3044	BCR	1	0
14	A	856	CLA	5	0
14	A	812	CLA	4	0
14	A	810	CLA	1	0
14	B	3034	CLA	3	0
14	B	3018	CLA	6	0
14	J	102	CLA	1	0
14	A	807	CLA	1	0
19	C	101	SF4	1	0
14	B	3015	CLA	1	0
14	B	3028	CLA	3	0
16	A	847	BCR	7	0
18	A	853	LHG	3	0
14	B	3022	CLA	1	0
14	B	3038	CLA	1	0
14	F	202	CLA	9	0
14	B	3016	CLA	2	0
14	B	3014	CLA	4	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.

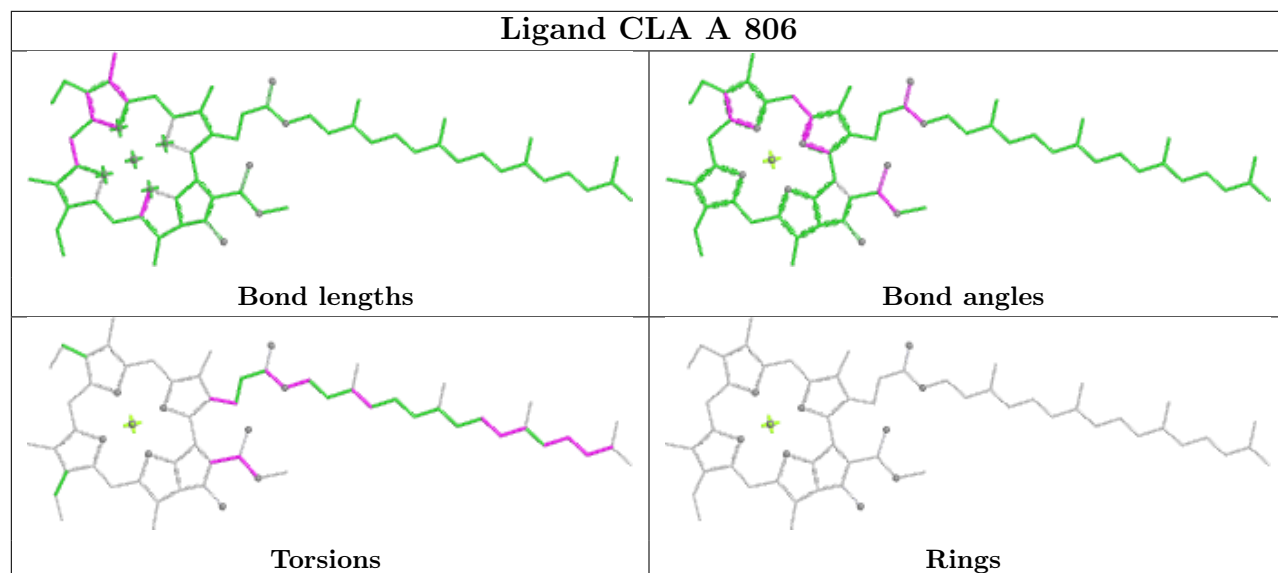
Ligand CLA A 833

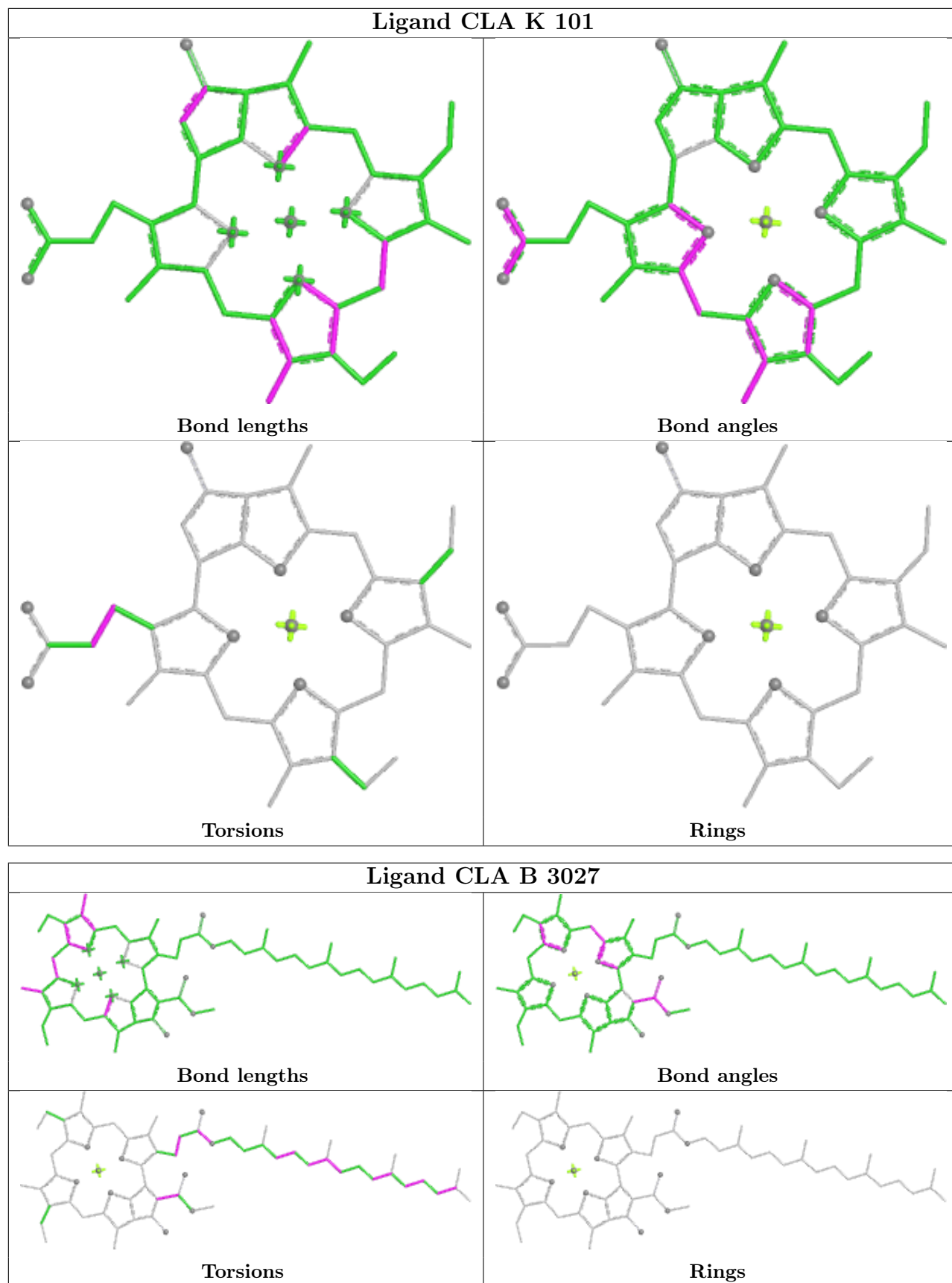


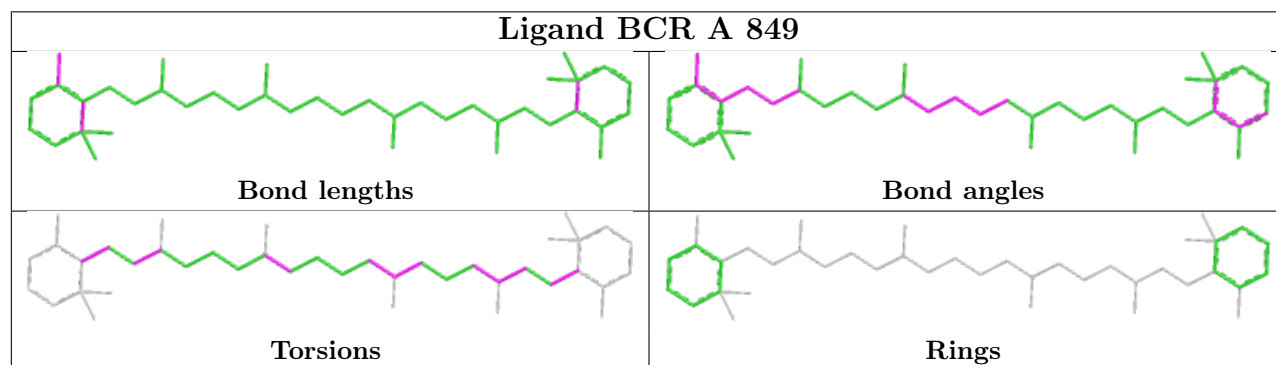
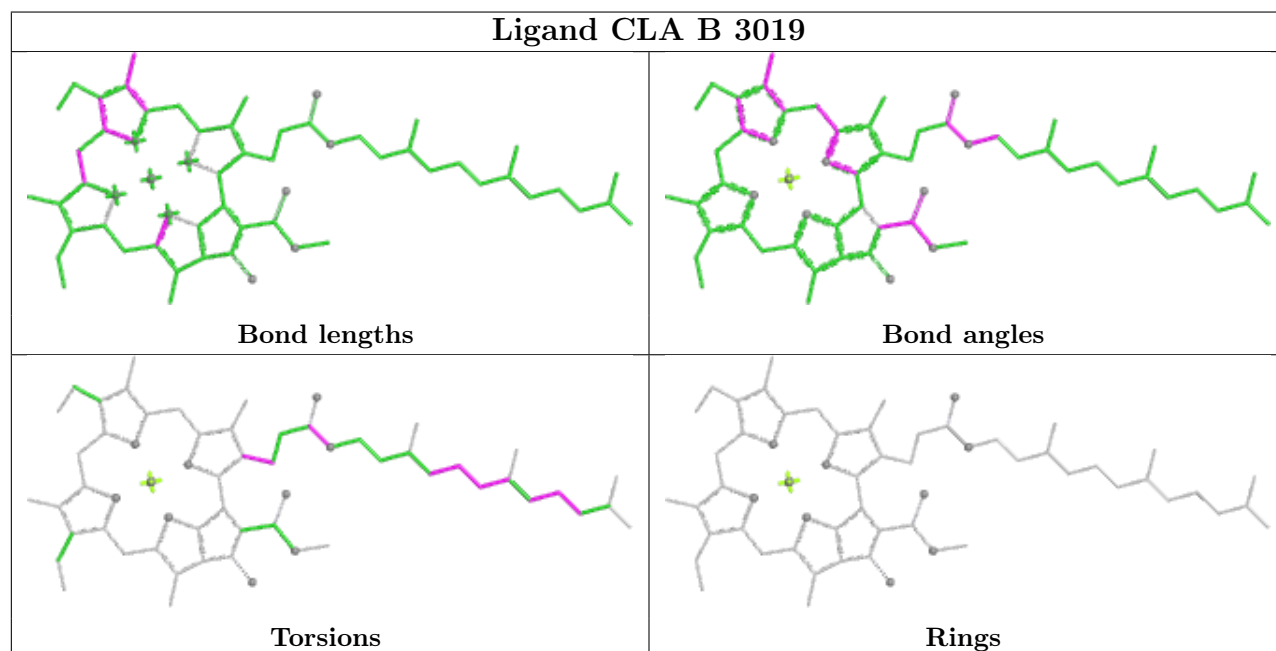
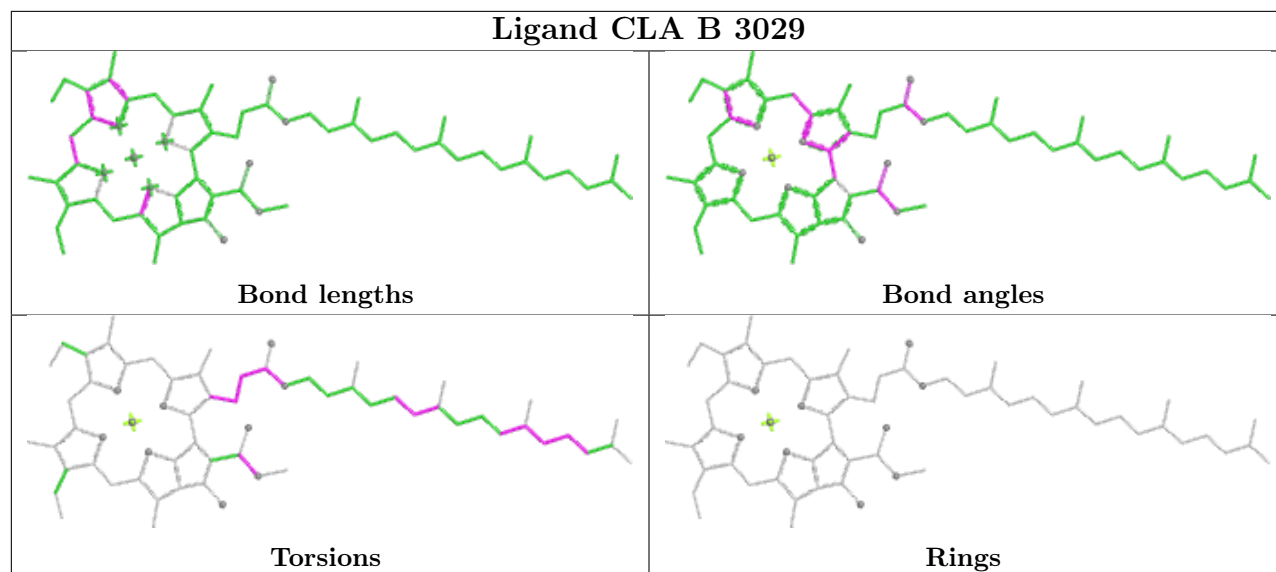
Ligand BCR J 105



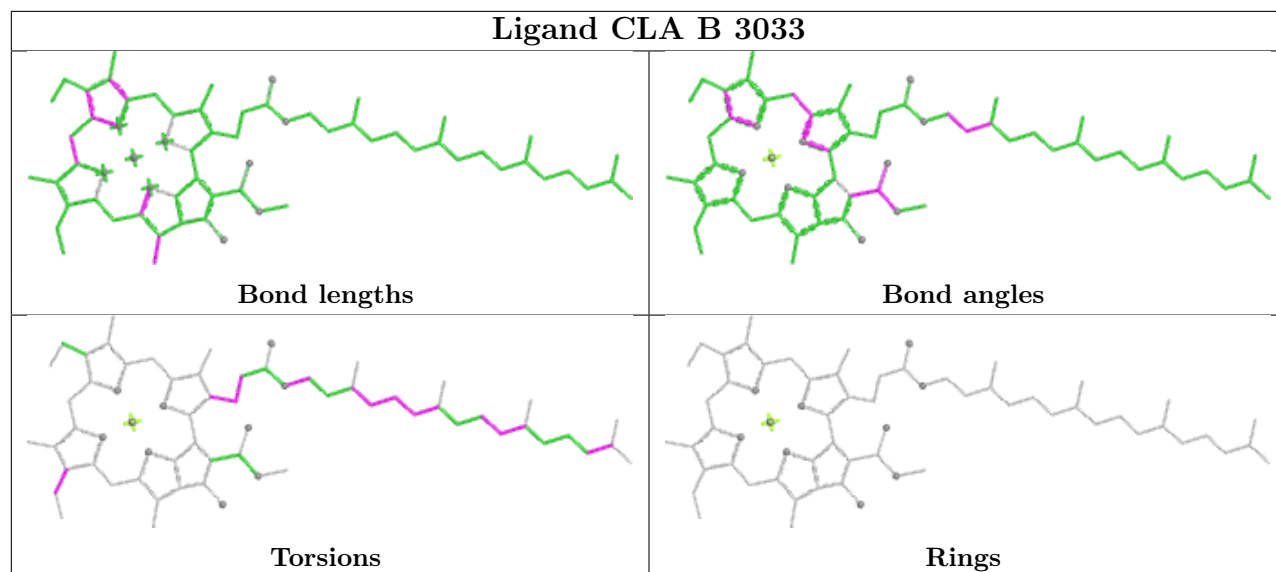
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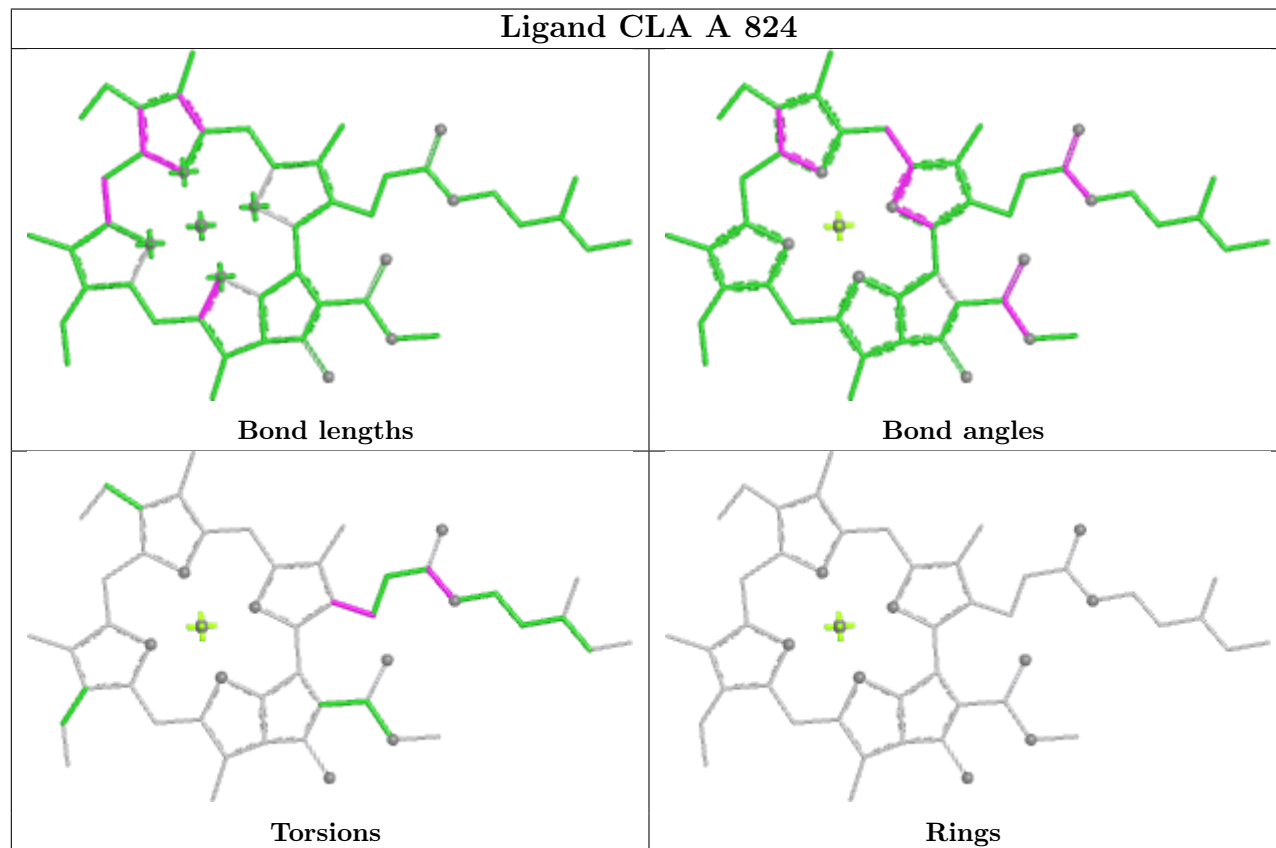




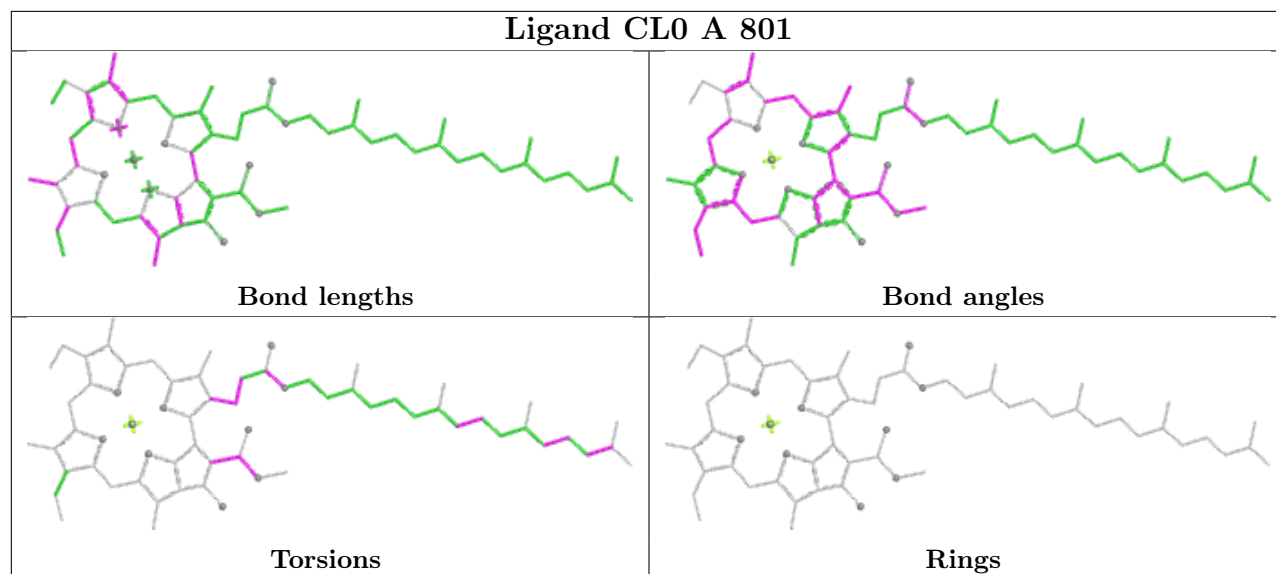
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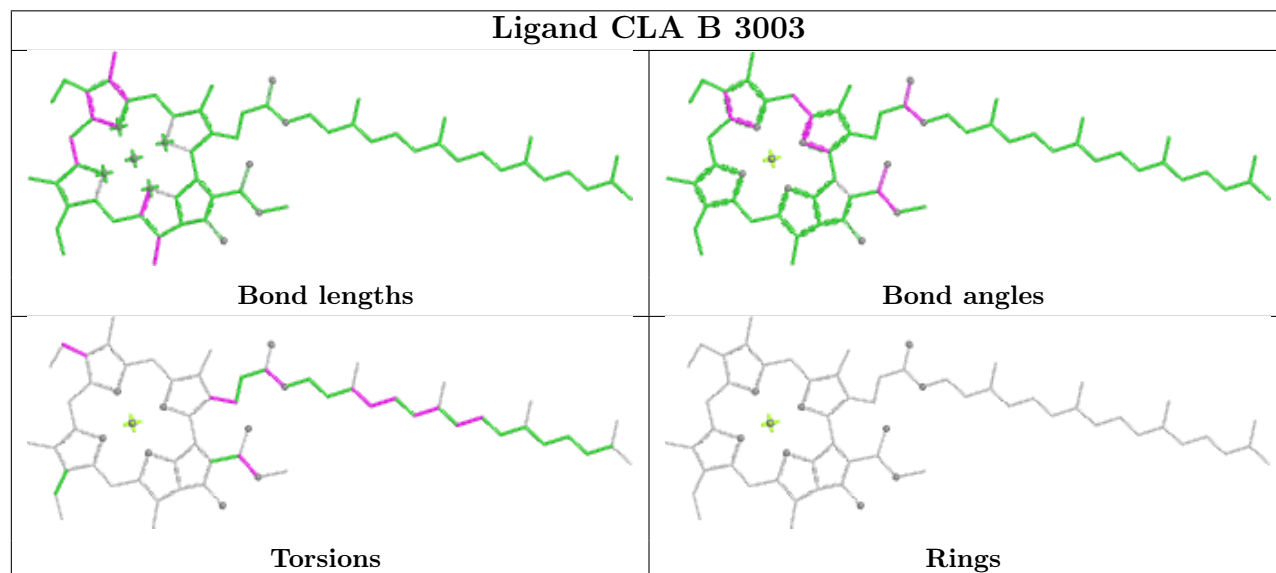
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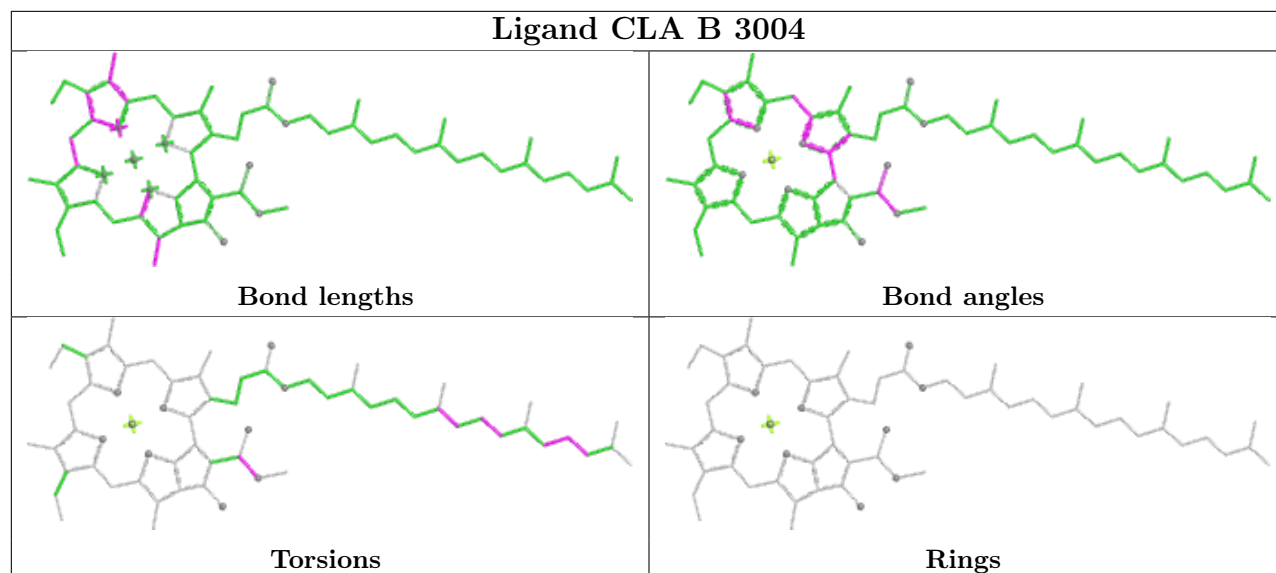
Ligand CL0 A 801



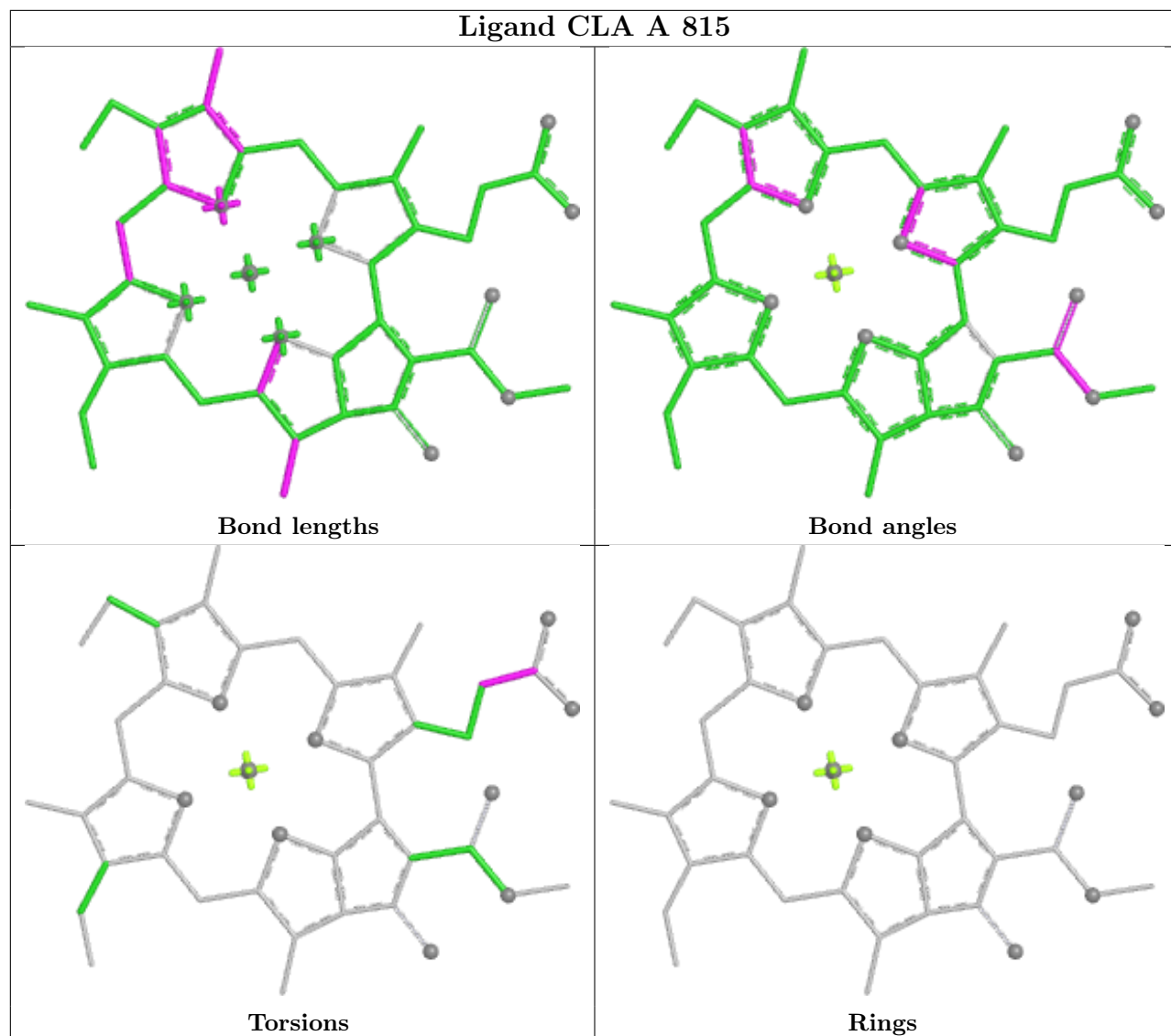
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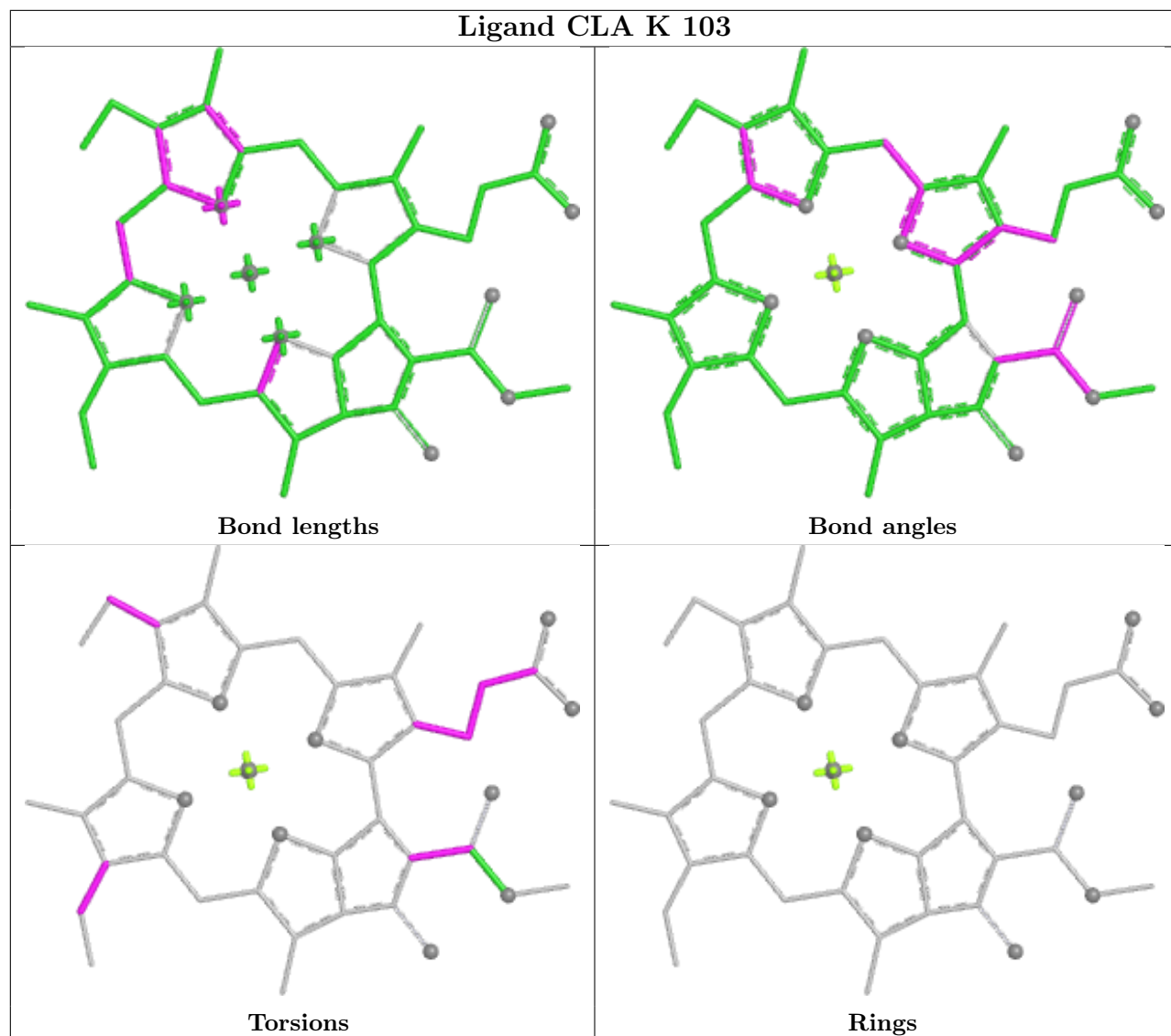
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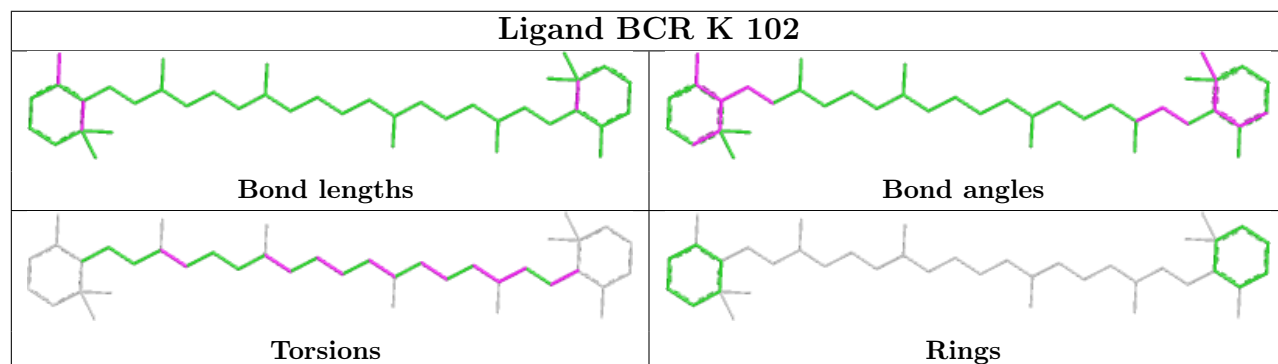
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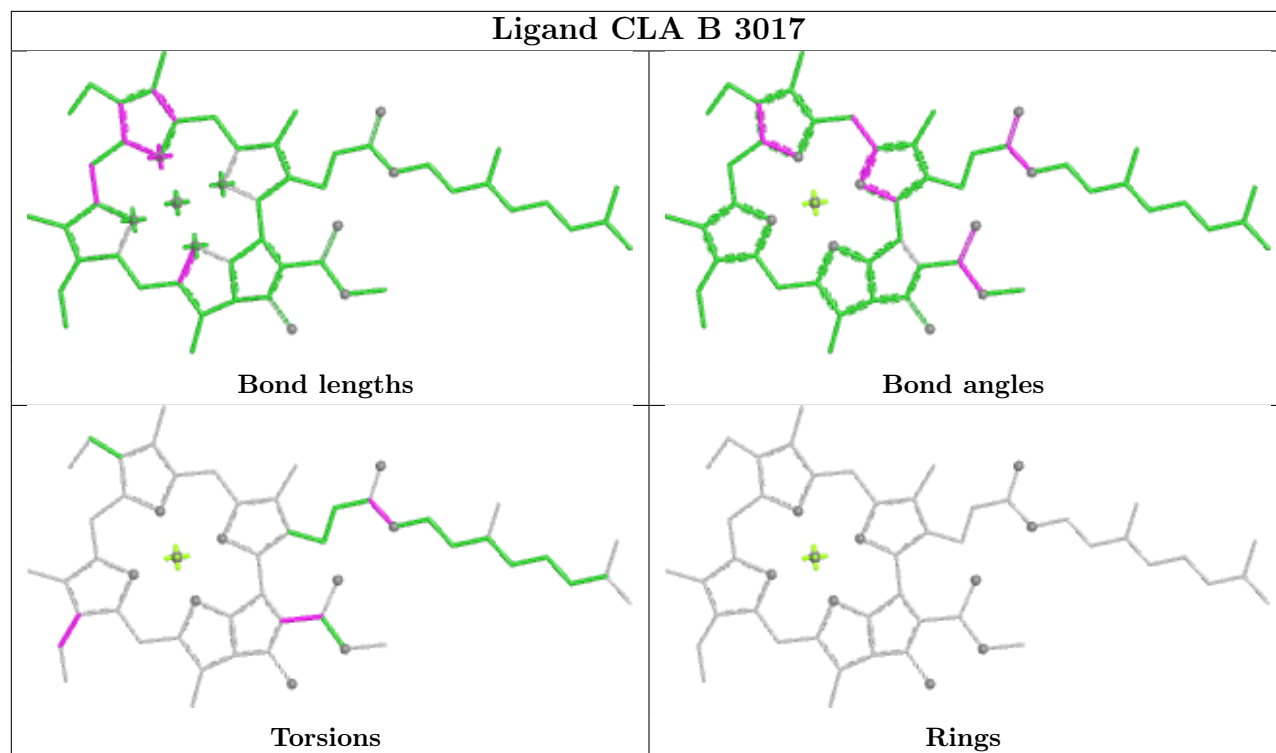


Ligand CLA K 103

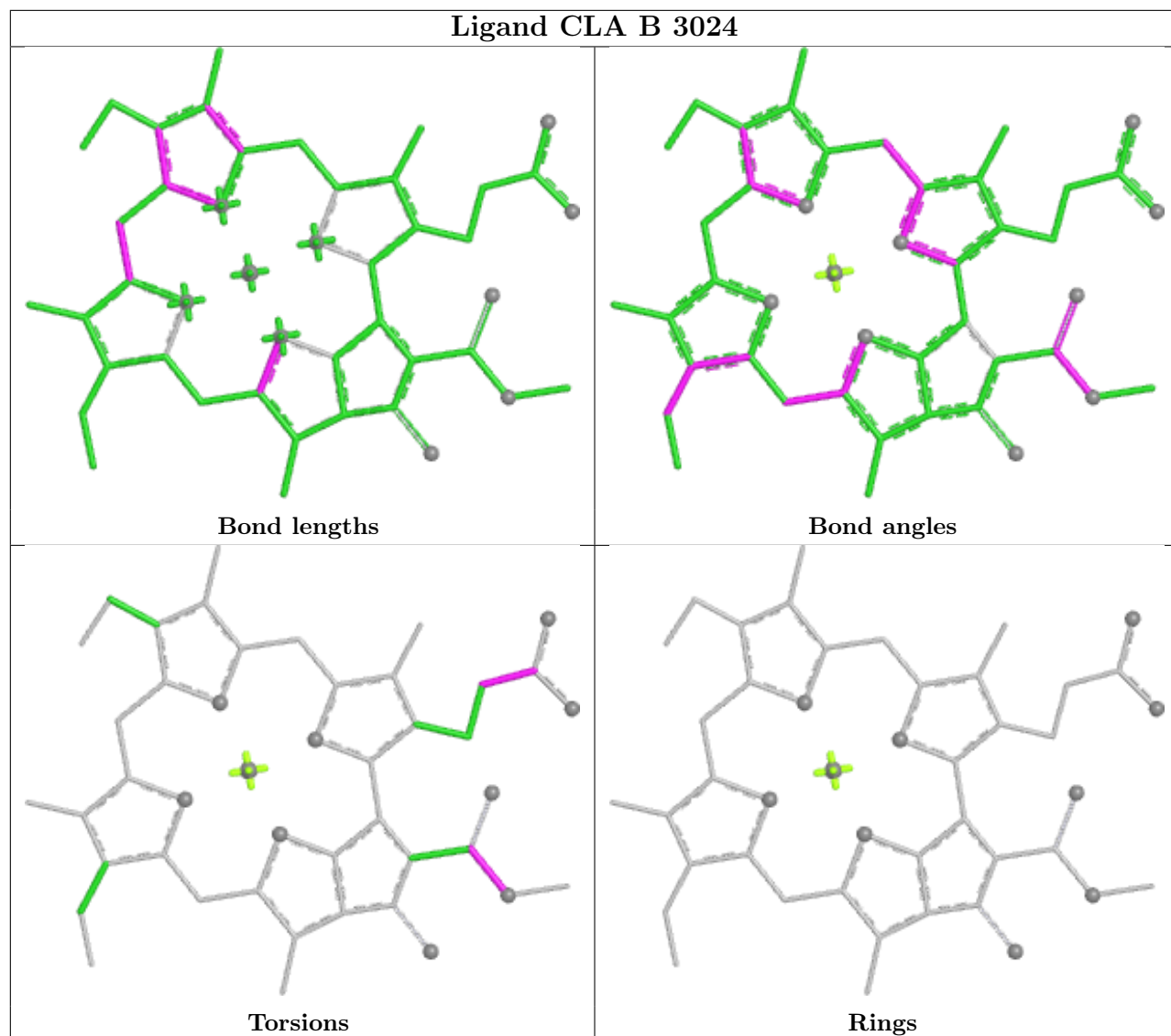


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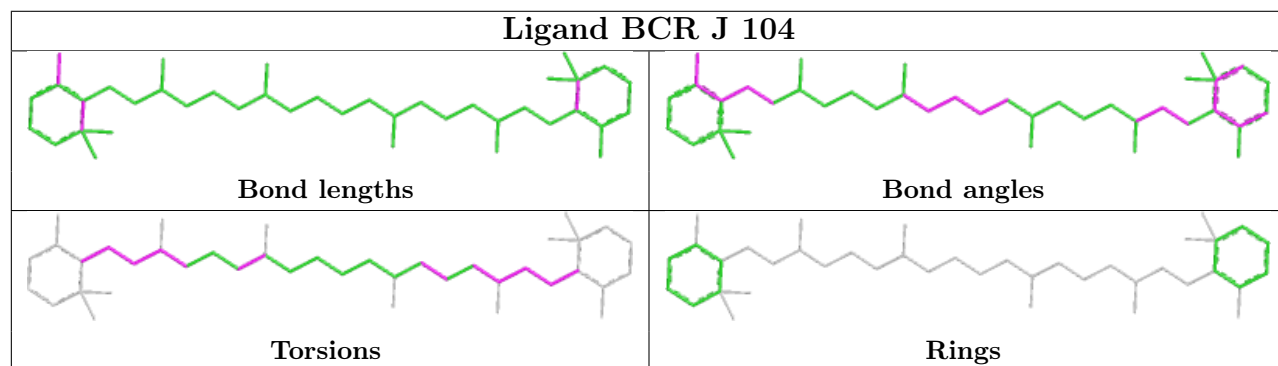


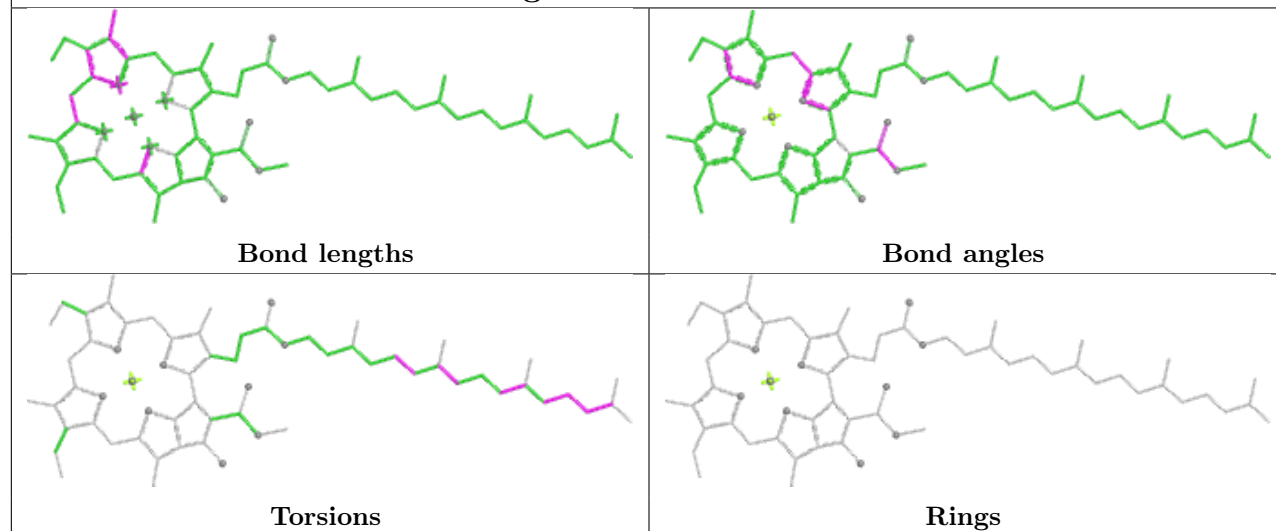
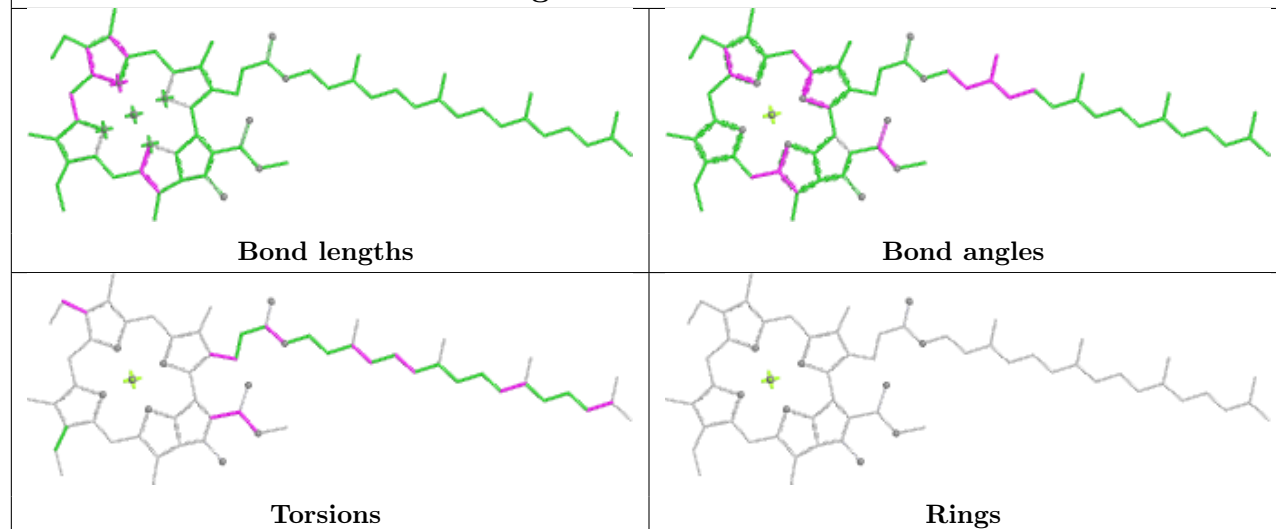


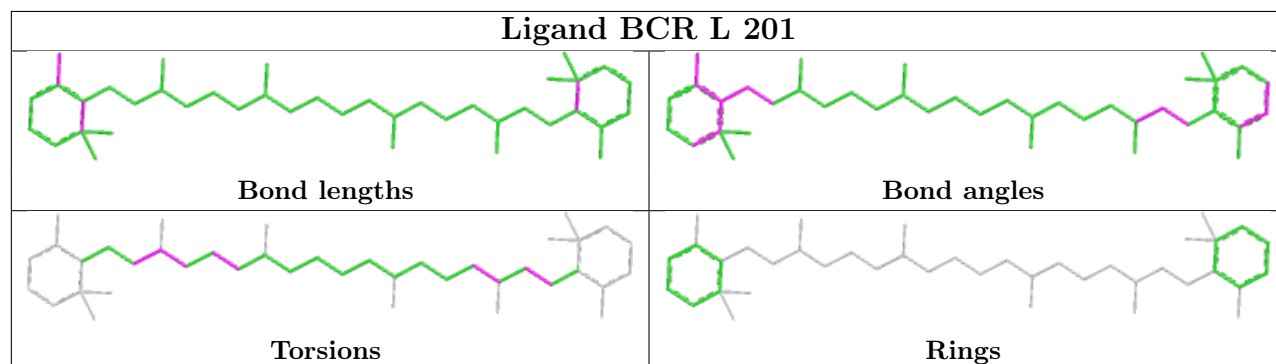
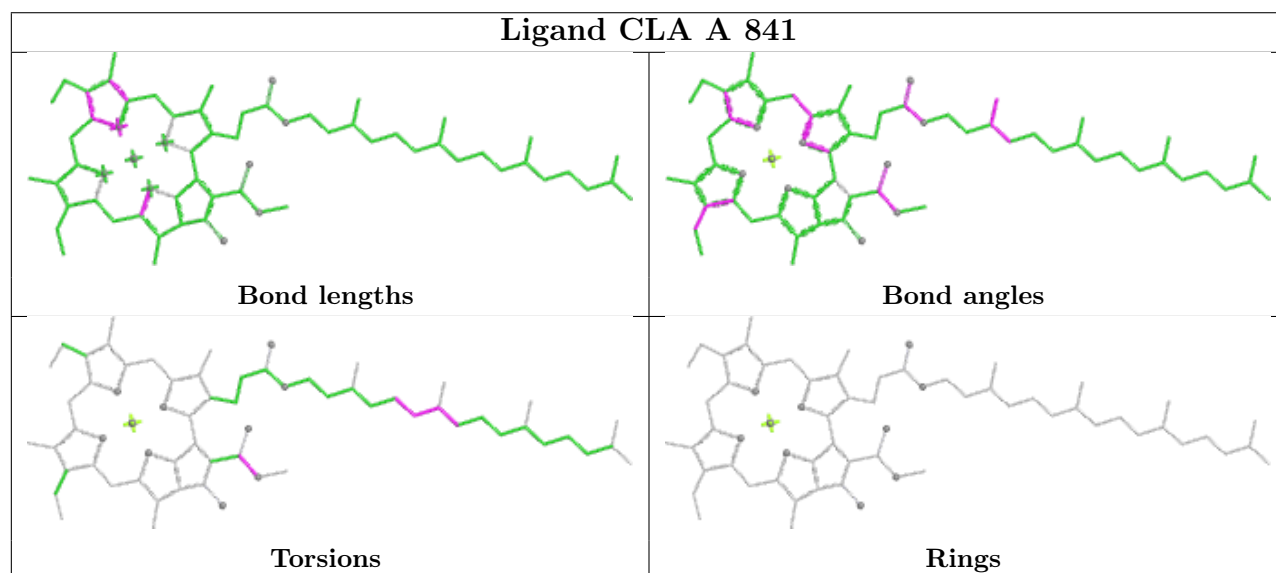
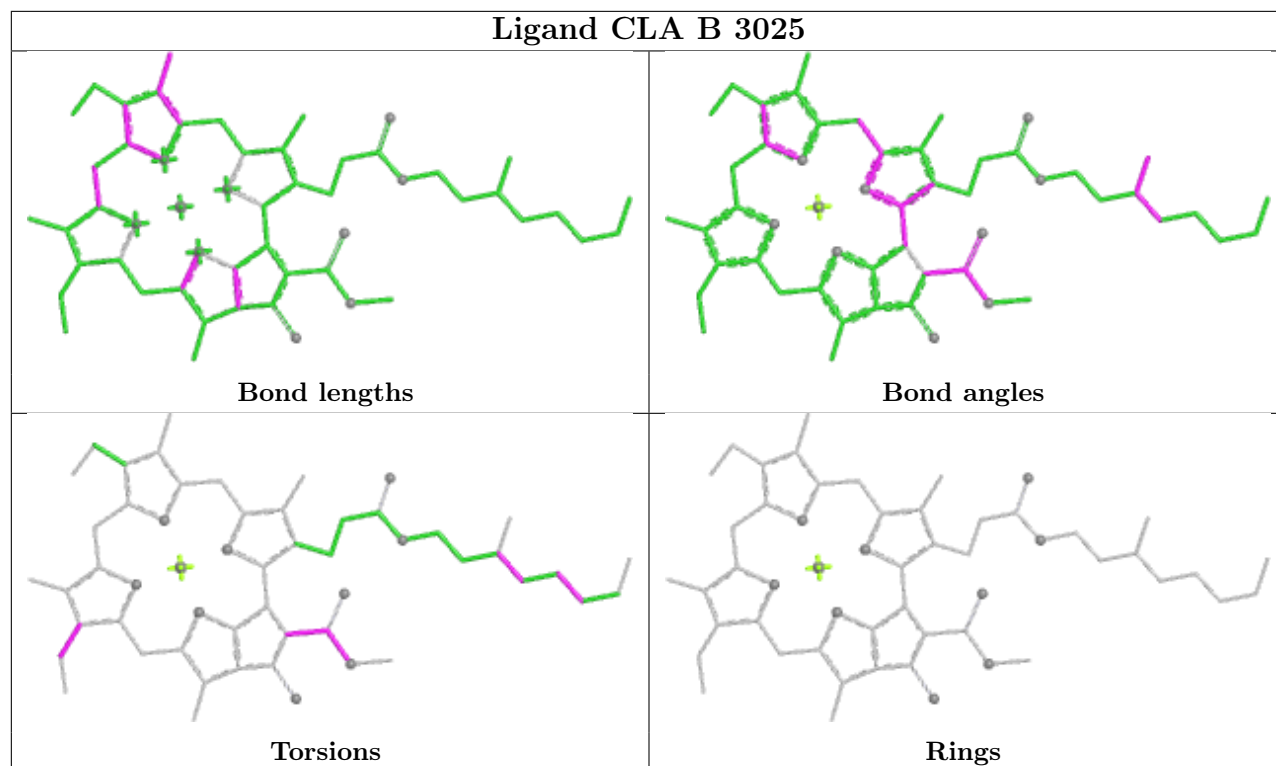
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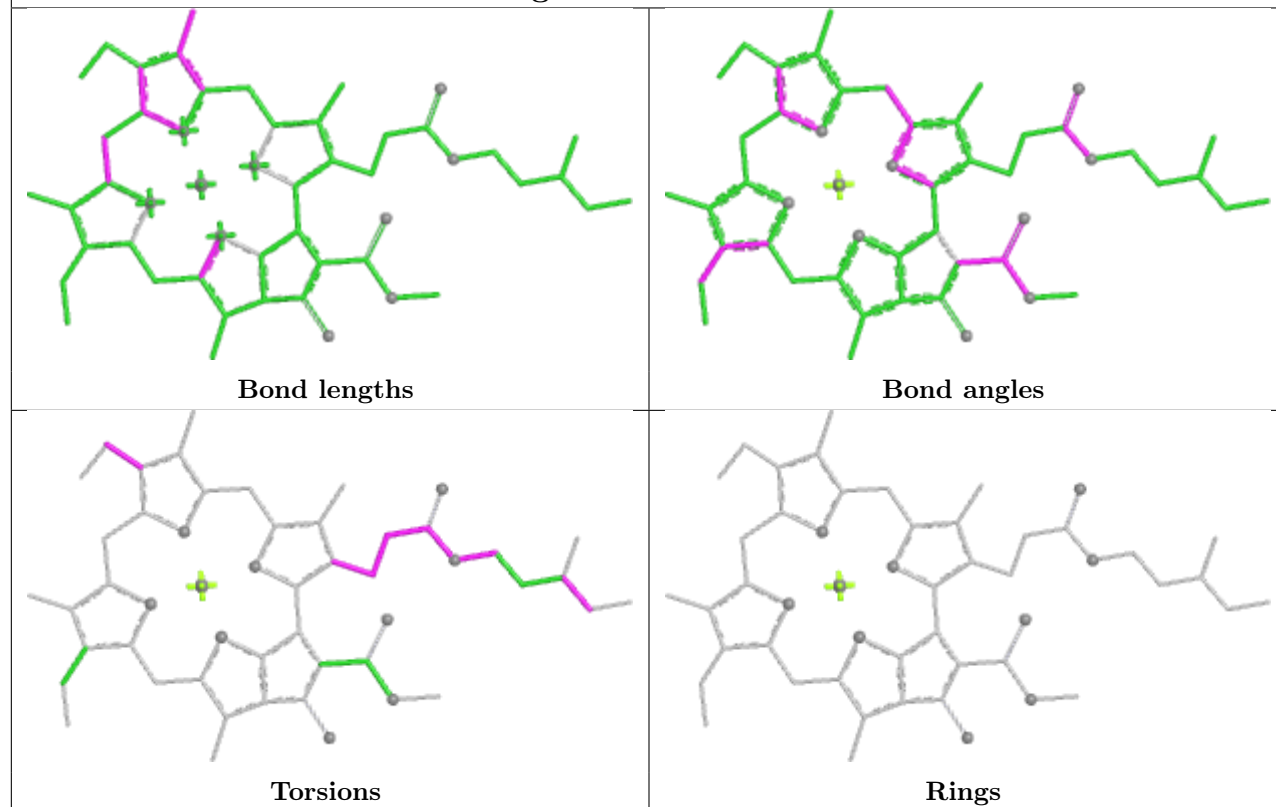
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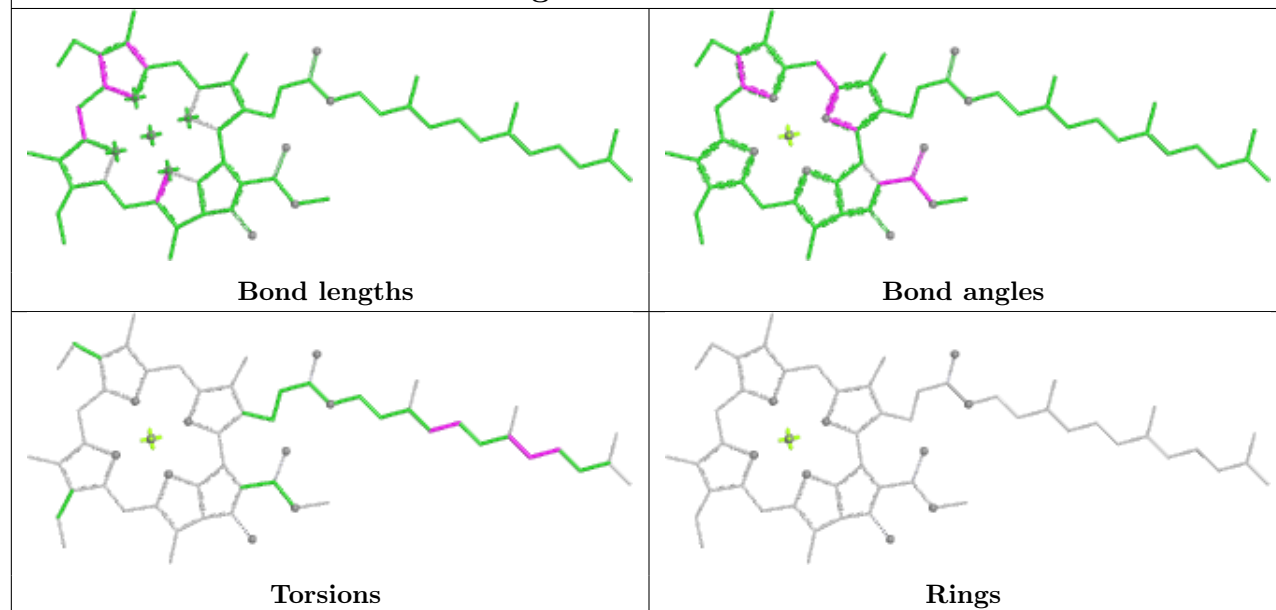
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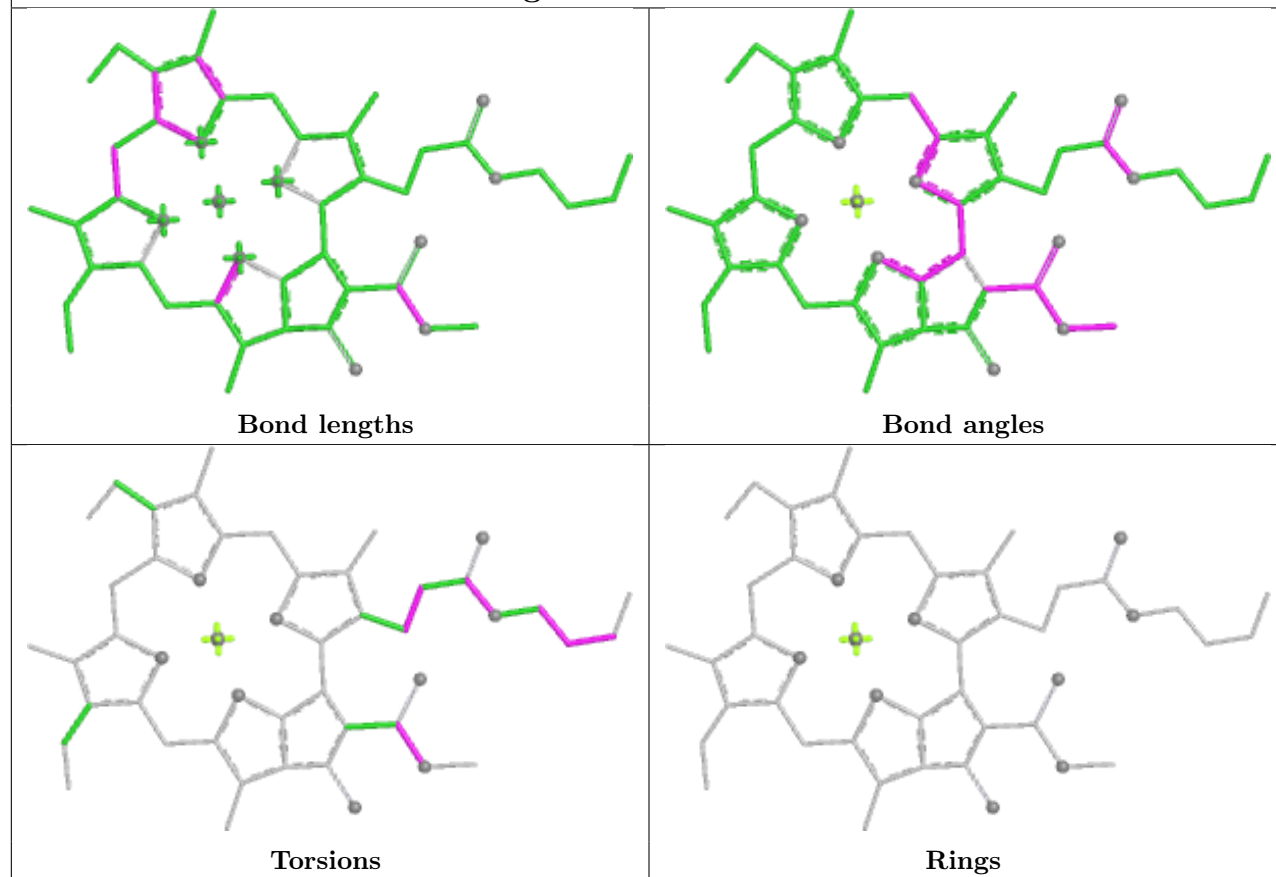
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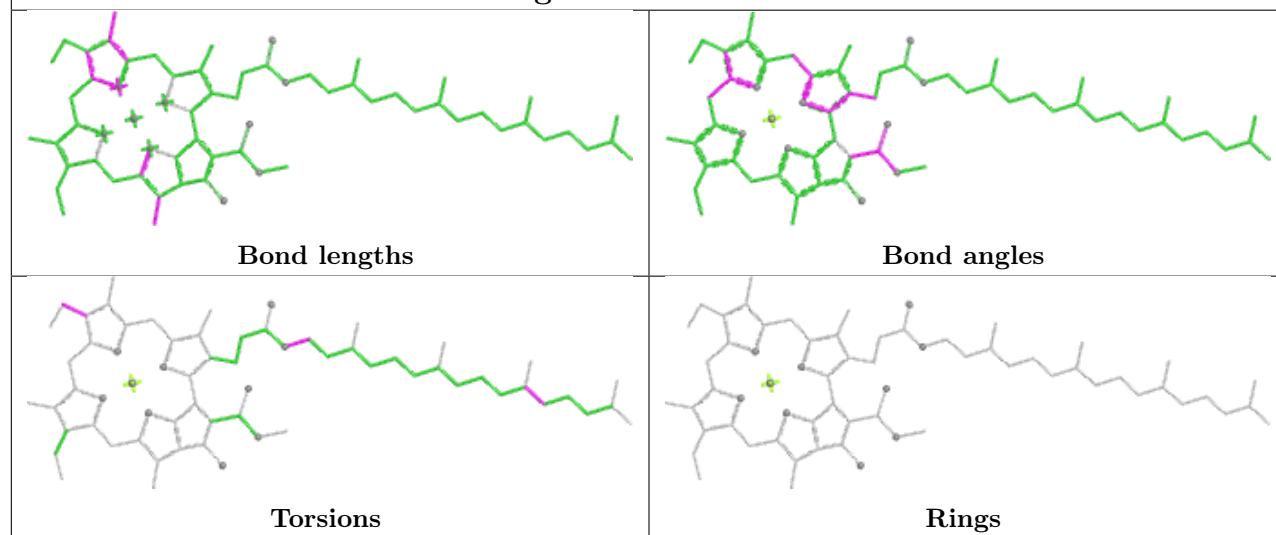
Ligand CLA A 814



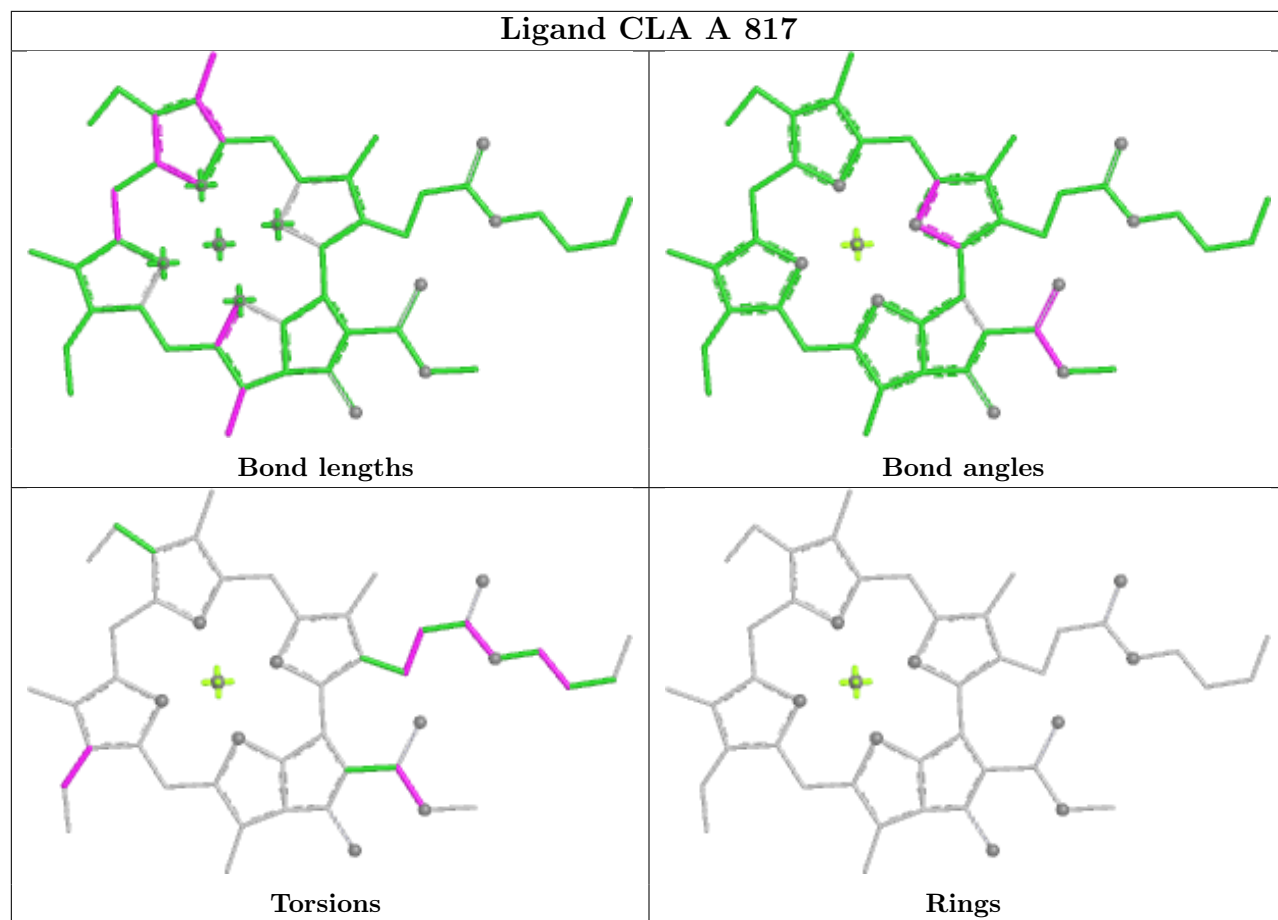
Ligand CLA B 3032



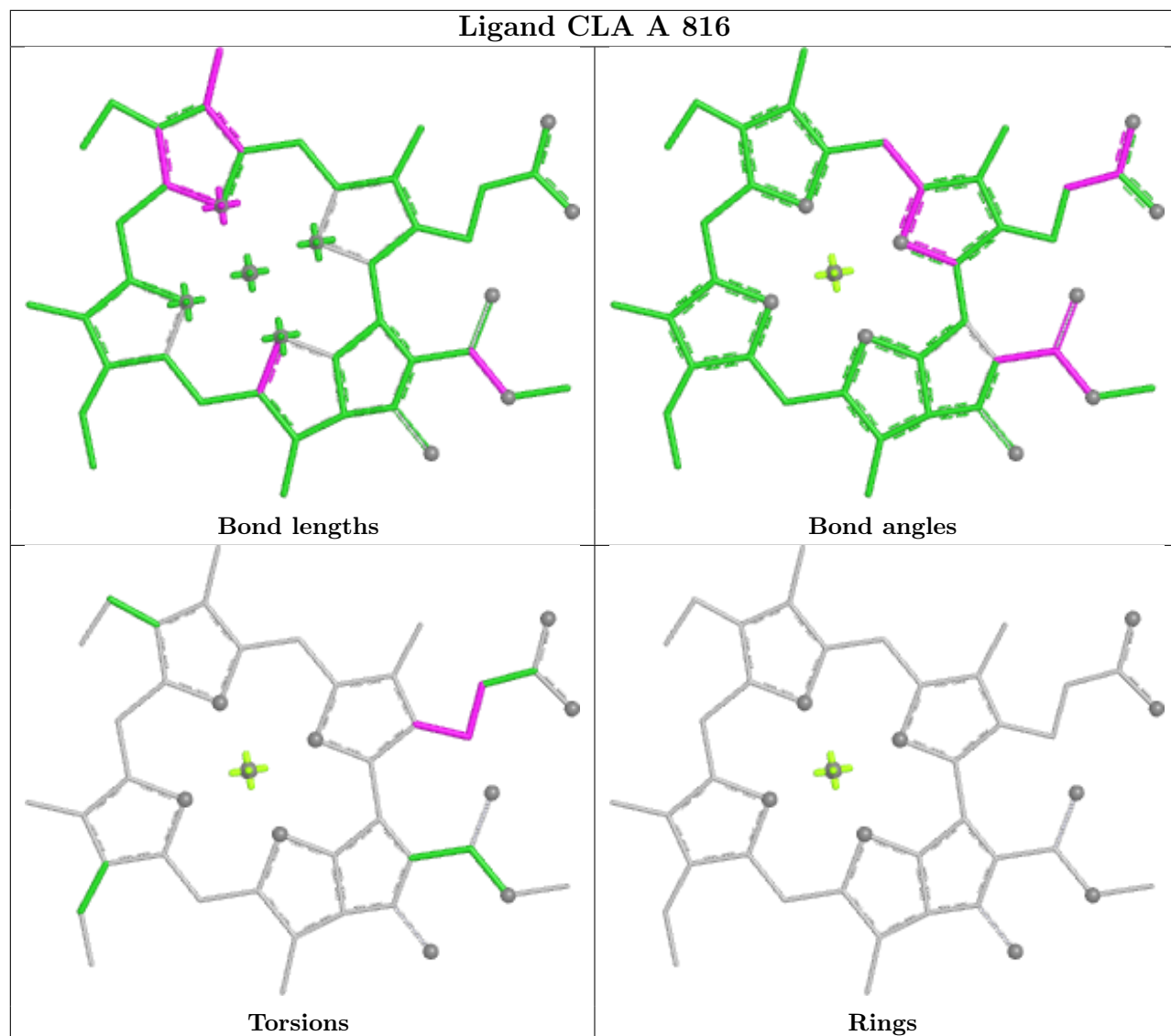
Ligand CLA L 205

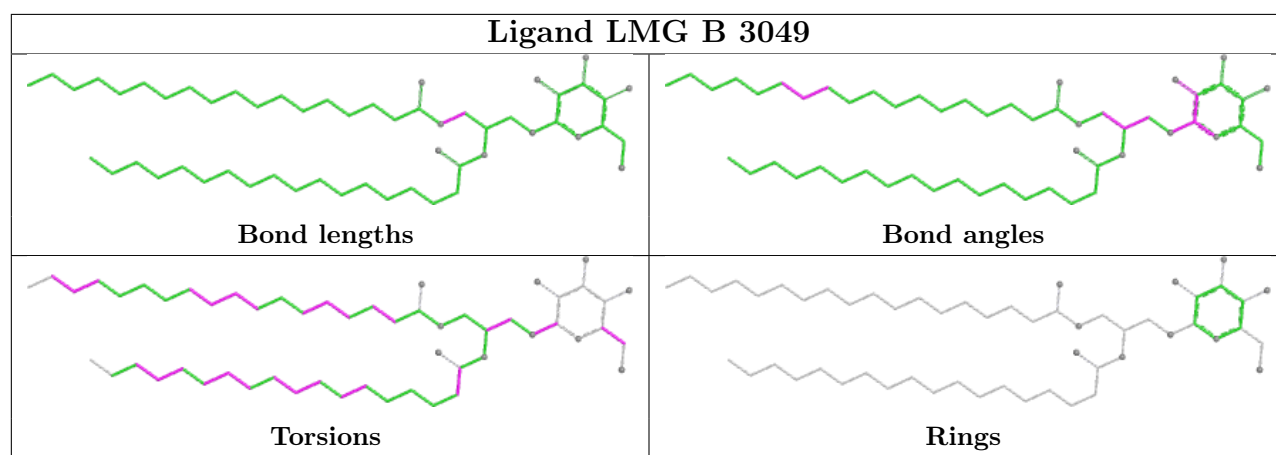
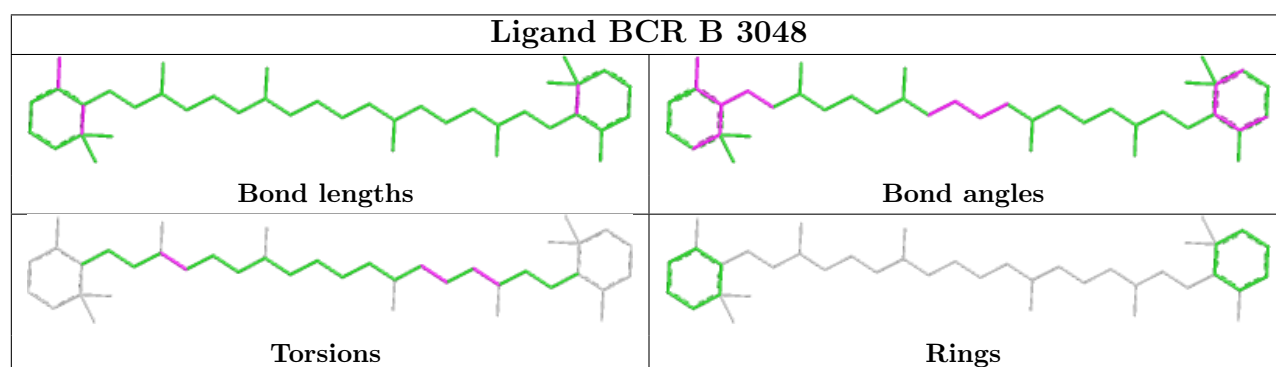
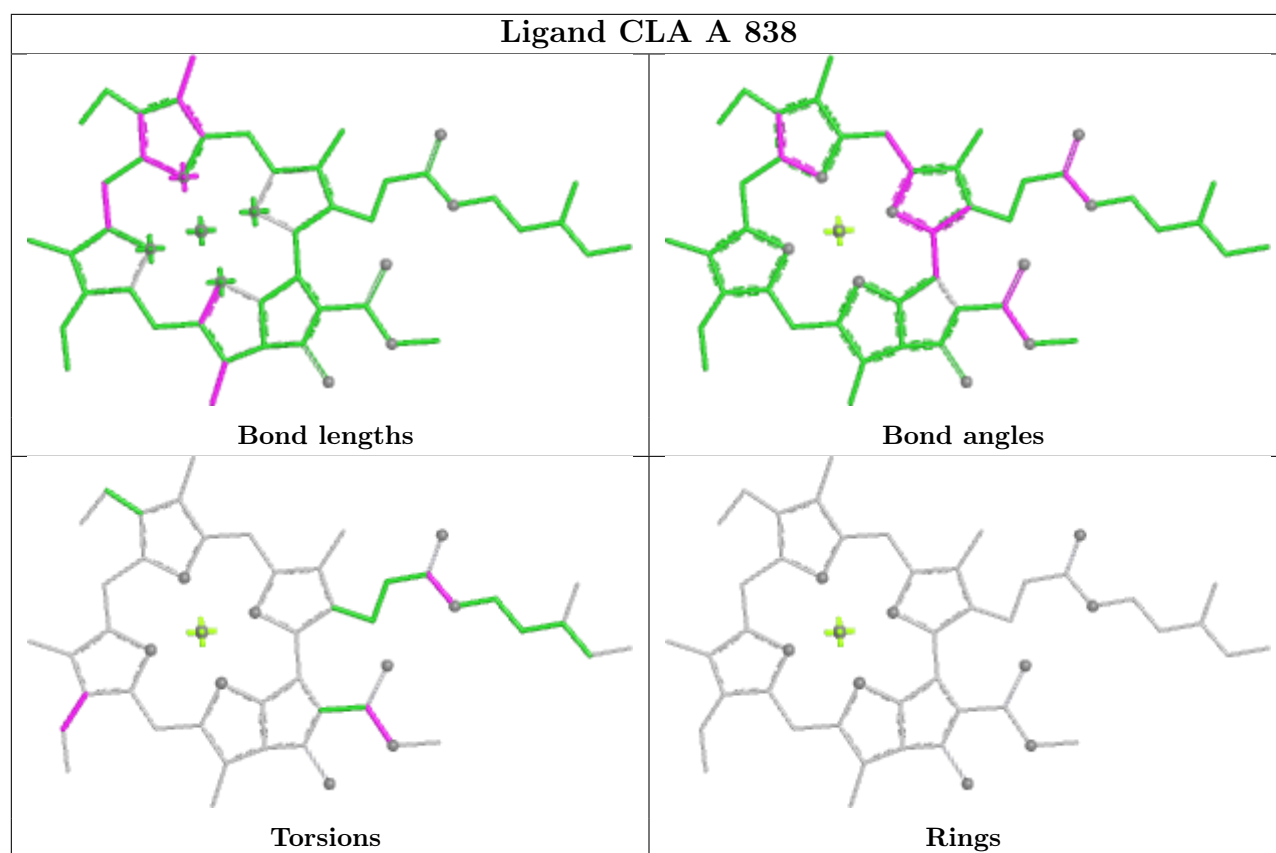


Ligand CLA A 817

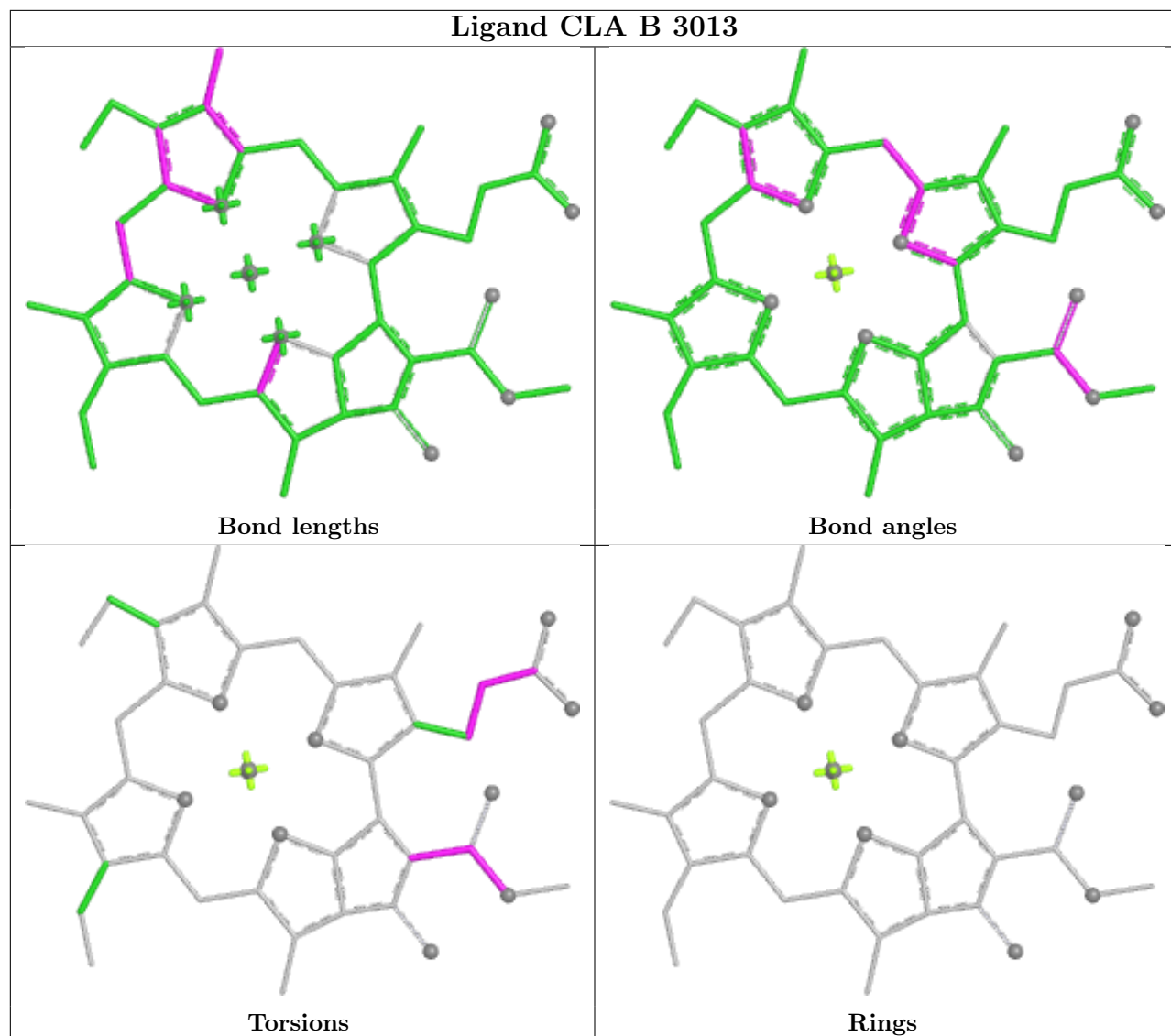


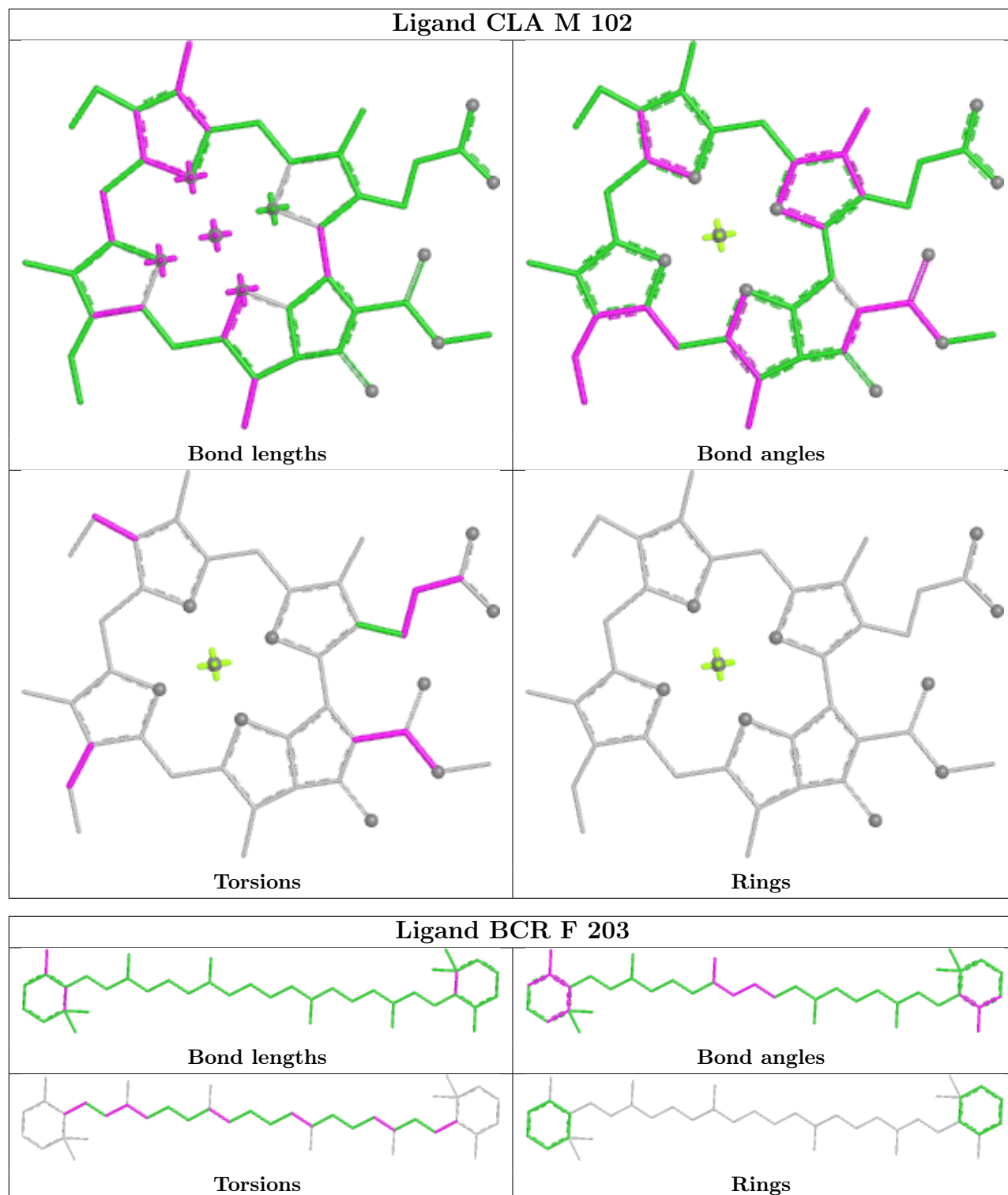
Ligand CLA A 816

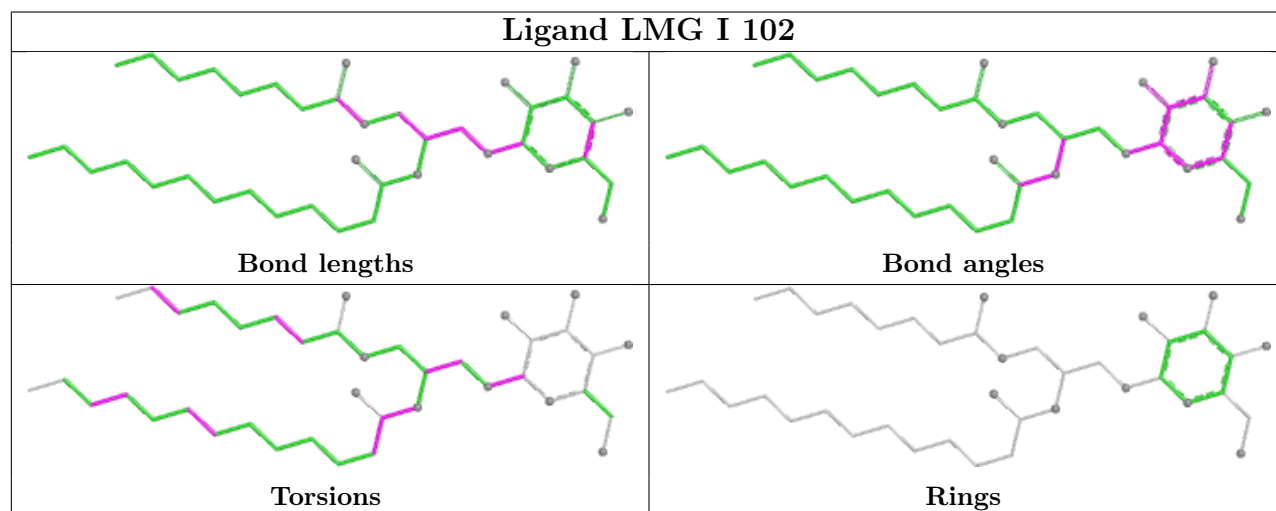
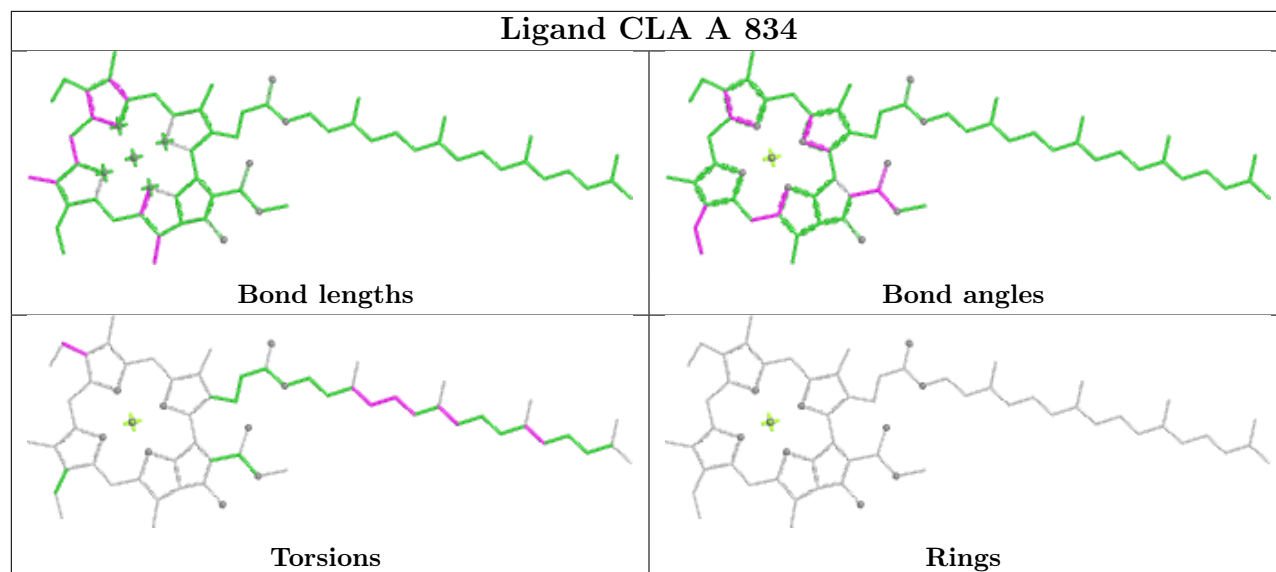




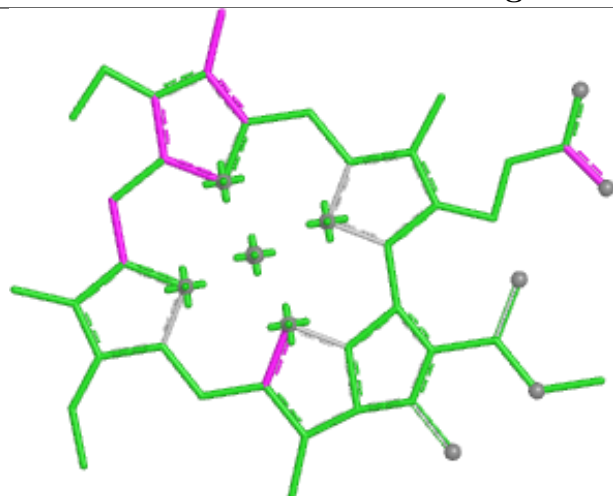
Ligand CLA B 3013



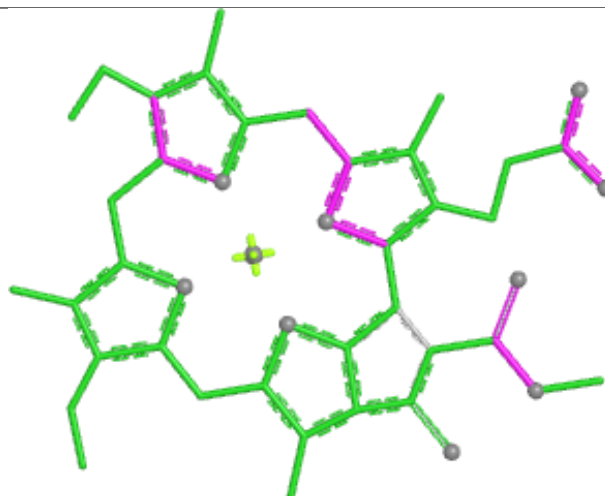




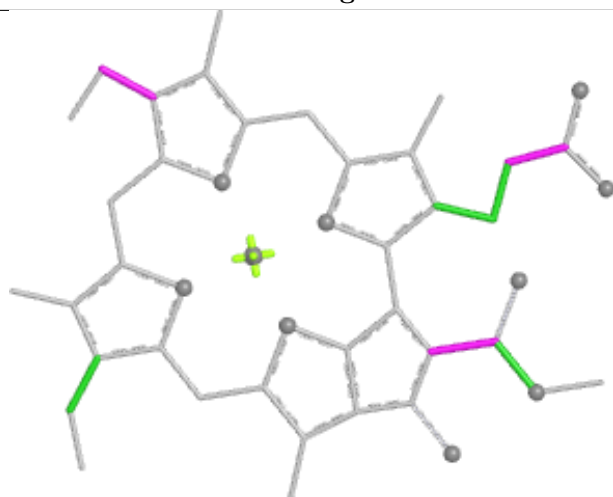
Ligand CLA B 3031



Bond lengths



Bond angles

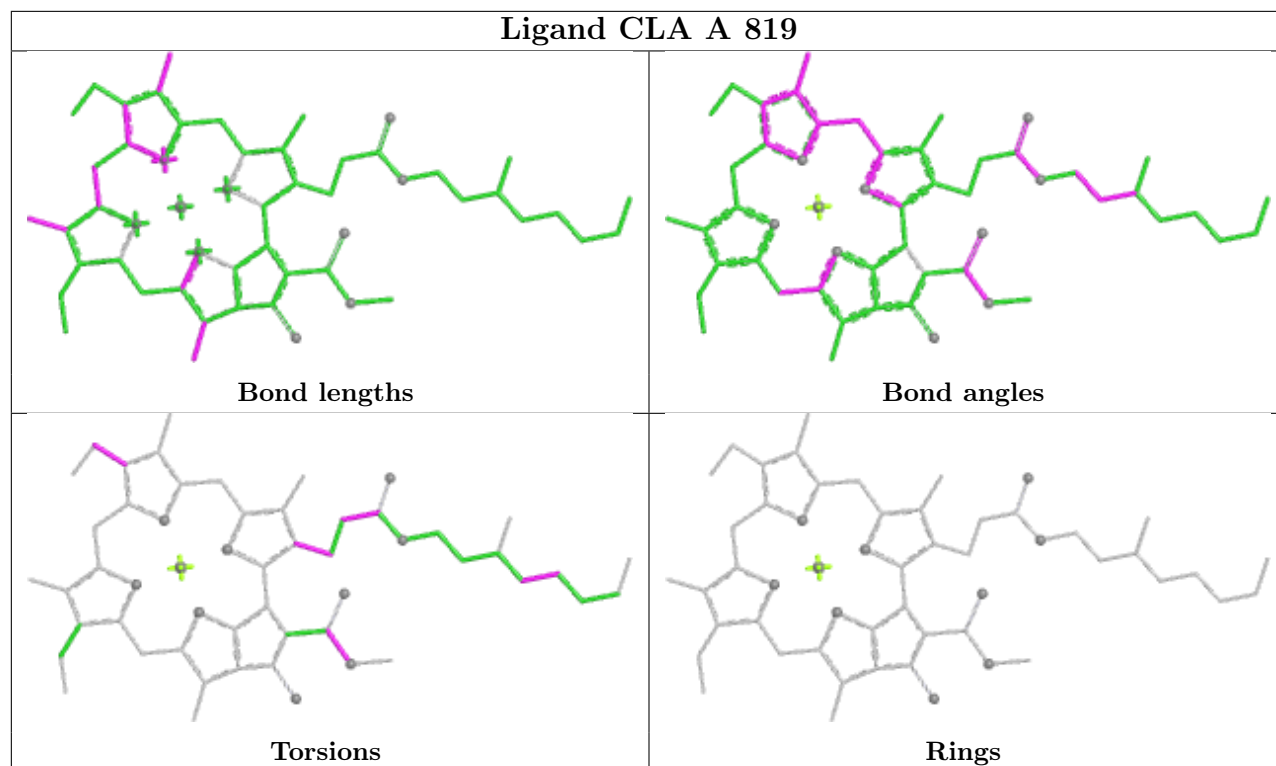


Torsions

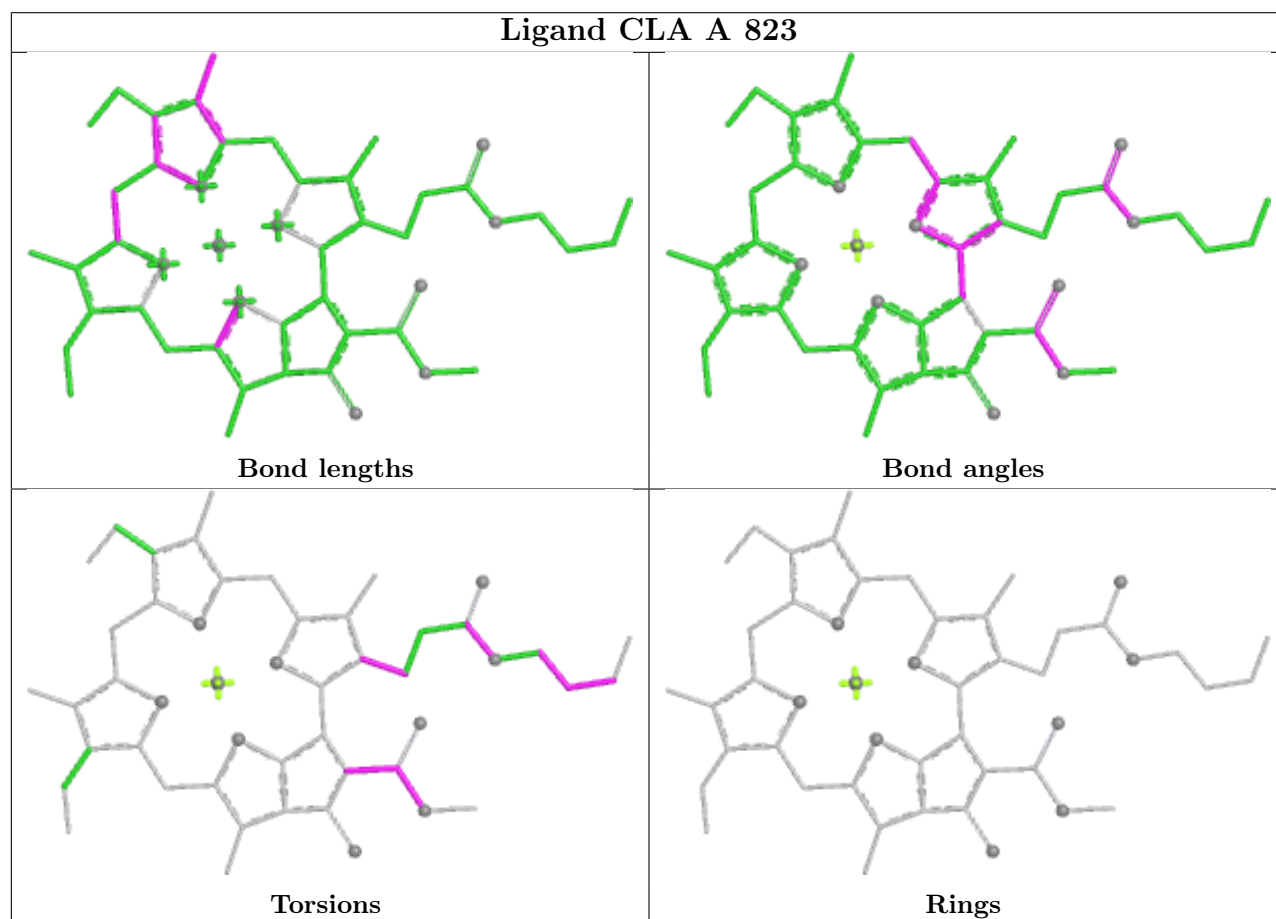


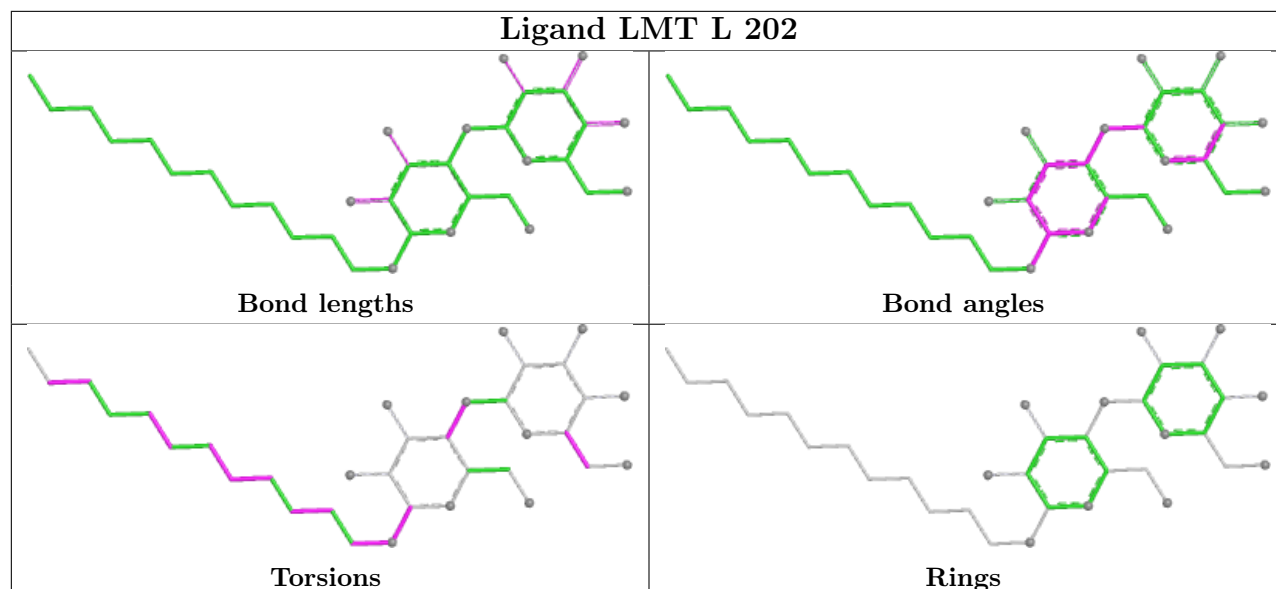
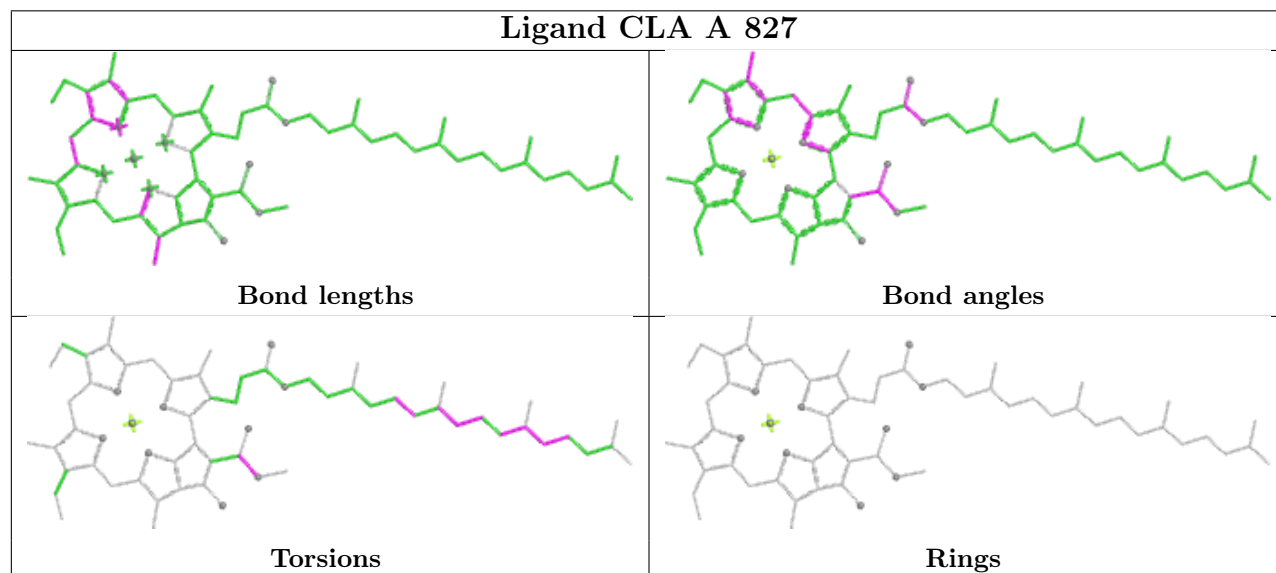
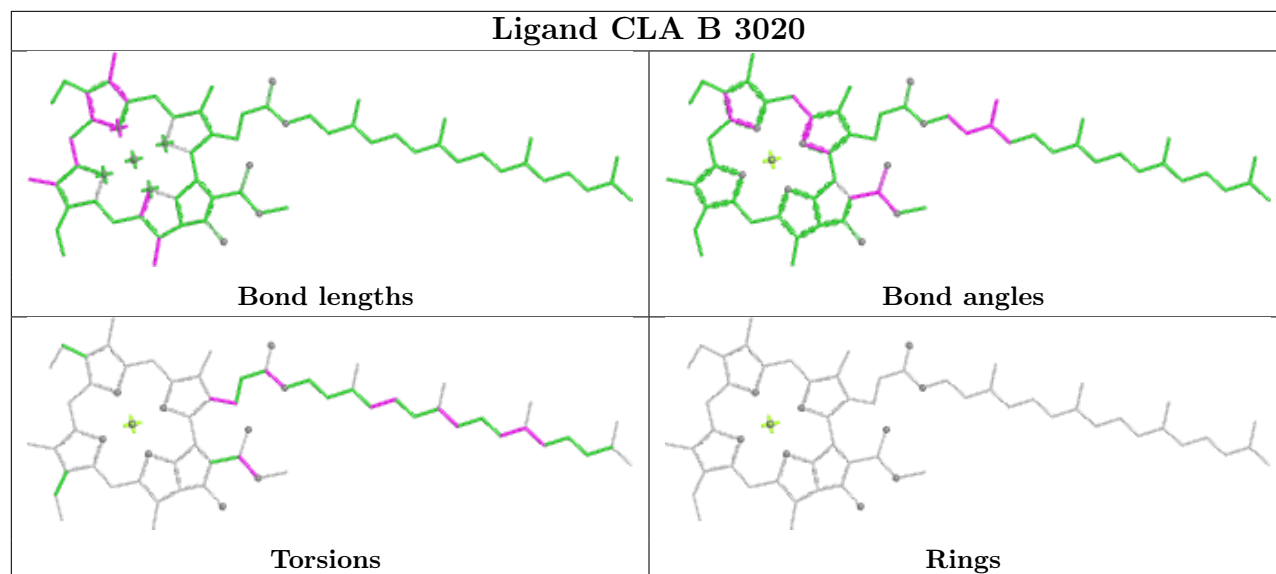
Rings

Ligand CLA A 819

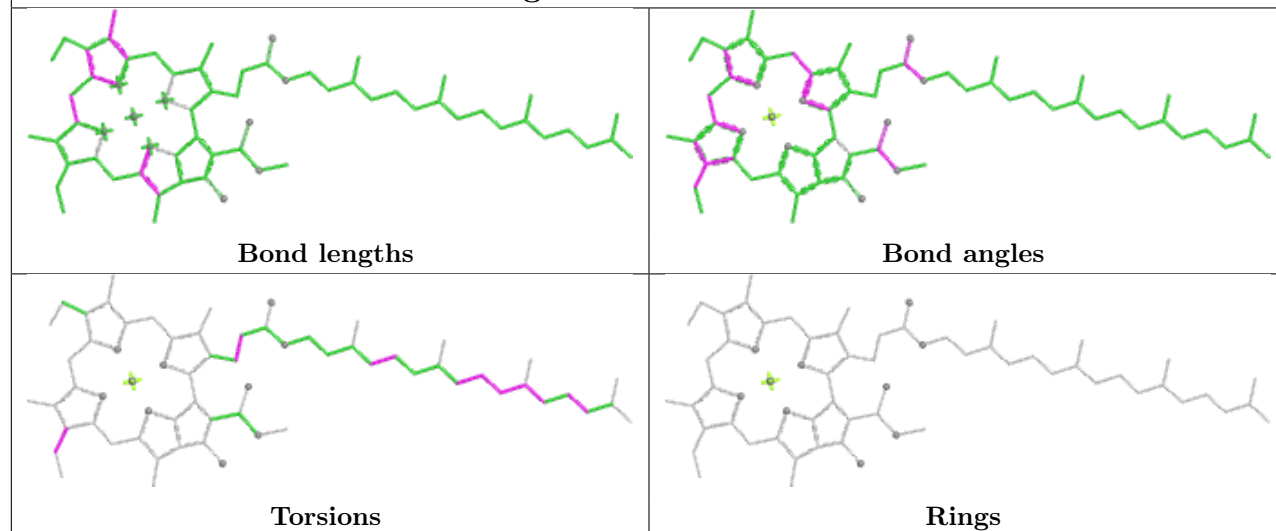


Ligand CLA A 823

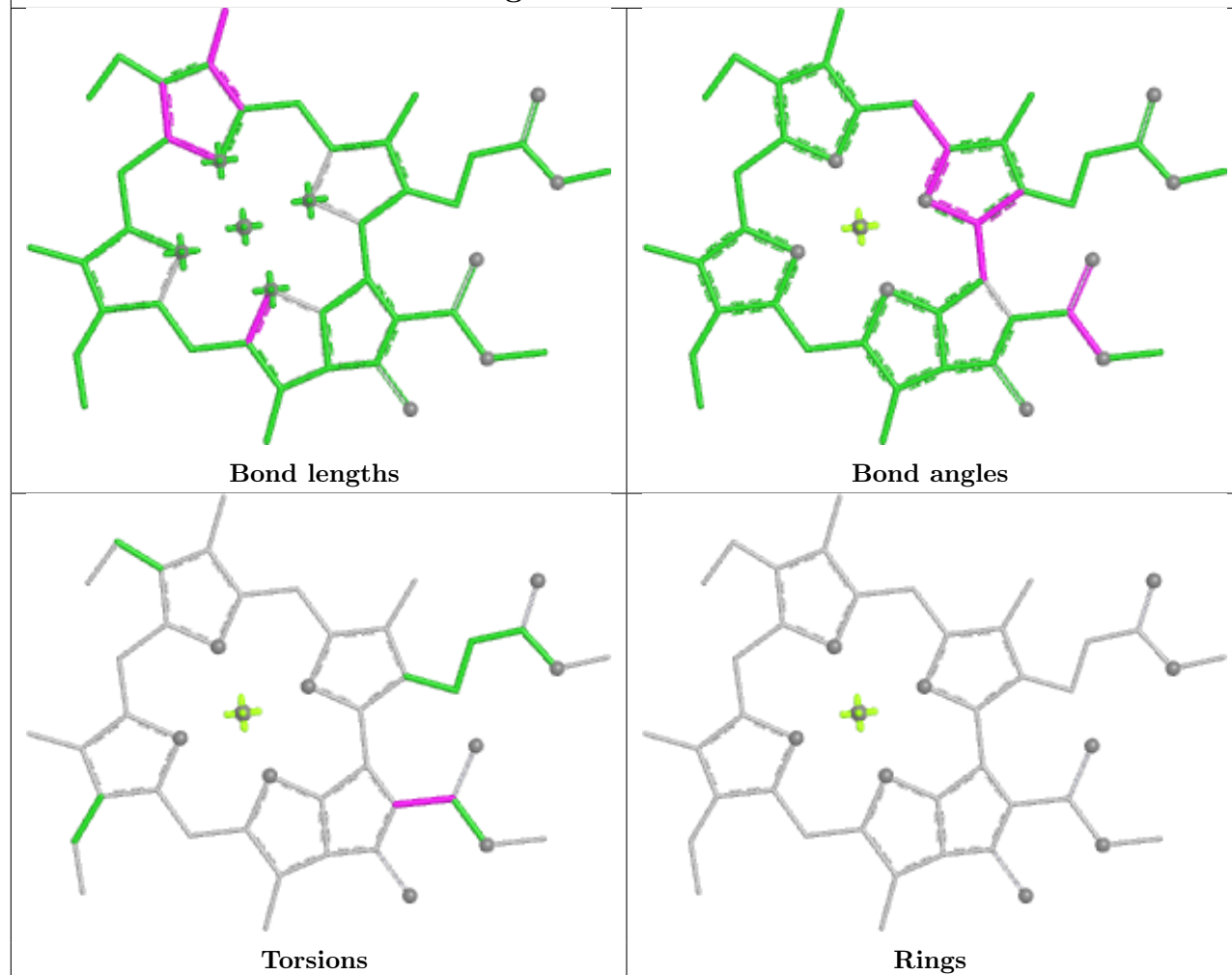




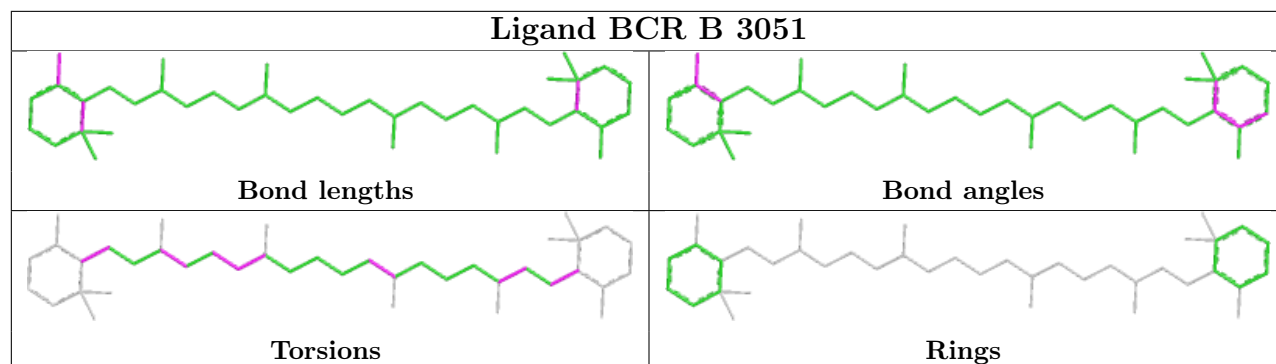
Ligand CLA B 3041



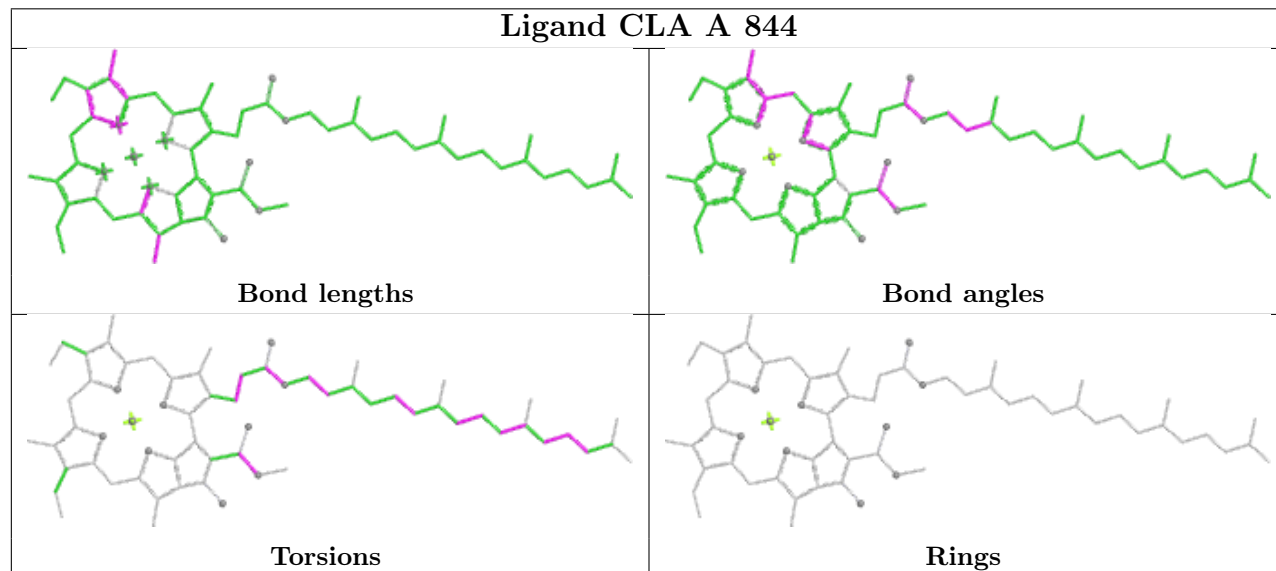
Ligand CLA B 3026



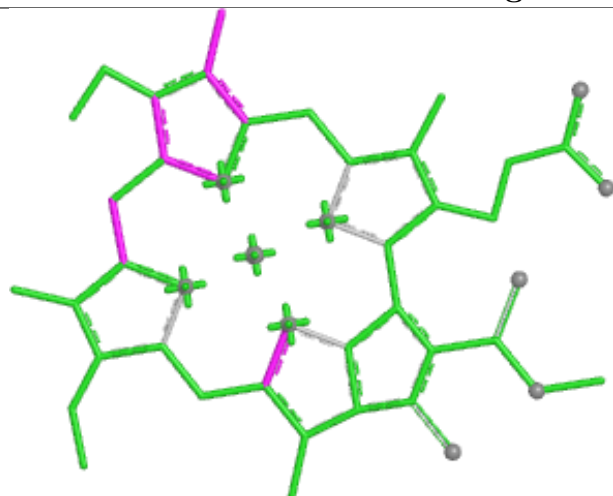
Ligand BCR B 3051



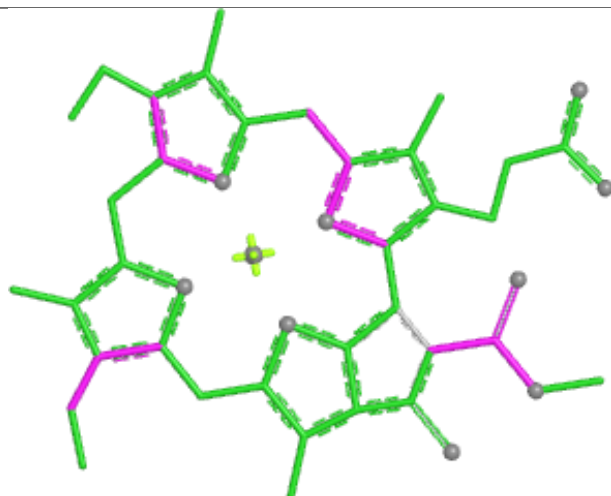
Ligand CLA A 844



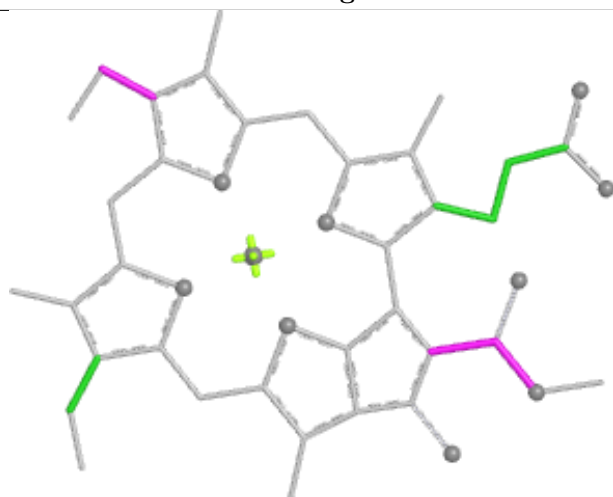
Ligand CLA B 3035



Bond lengths



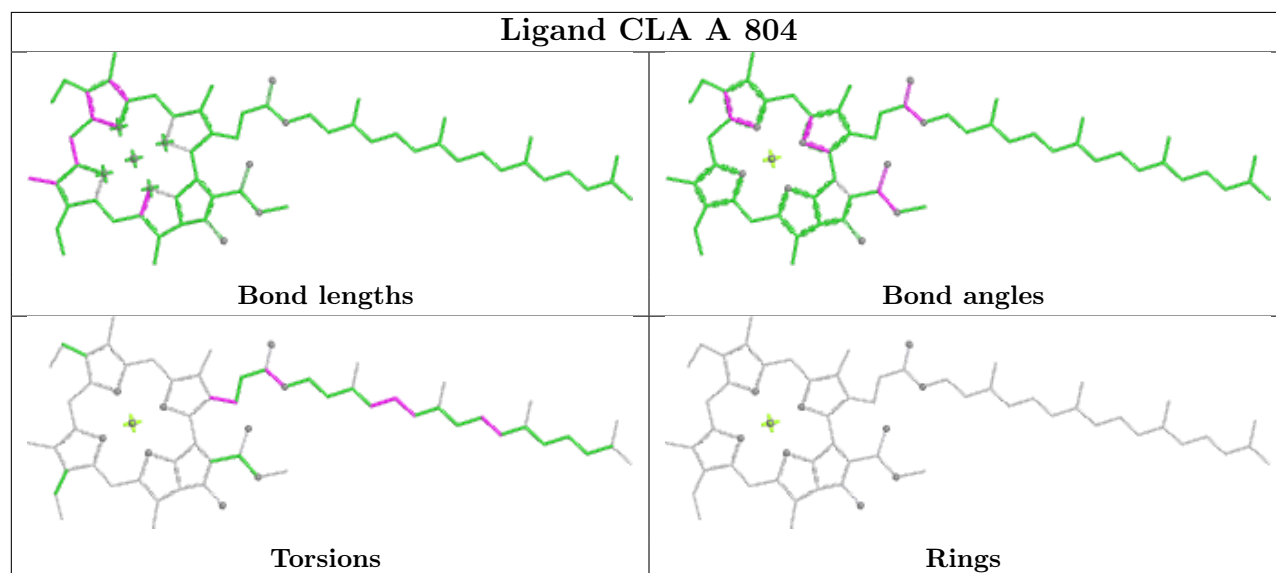
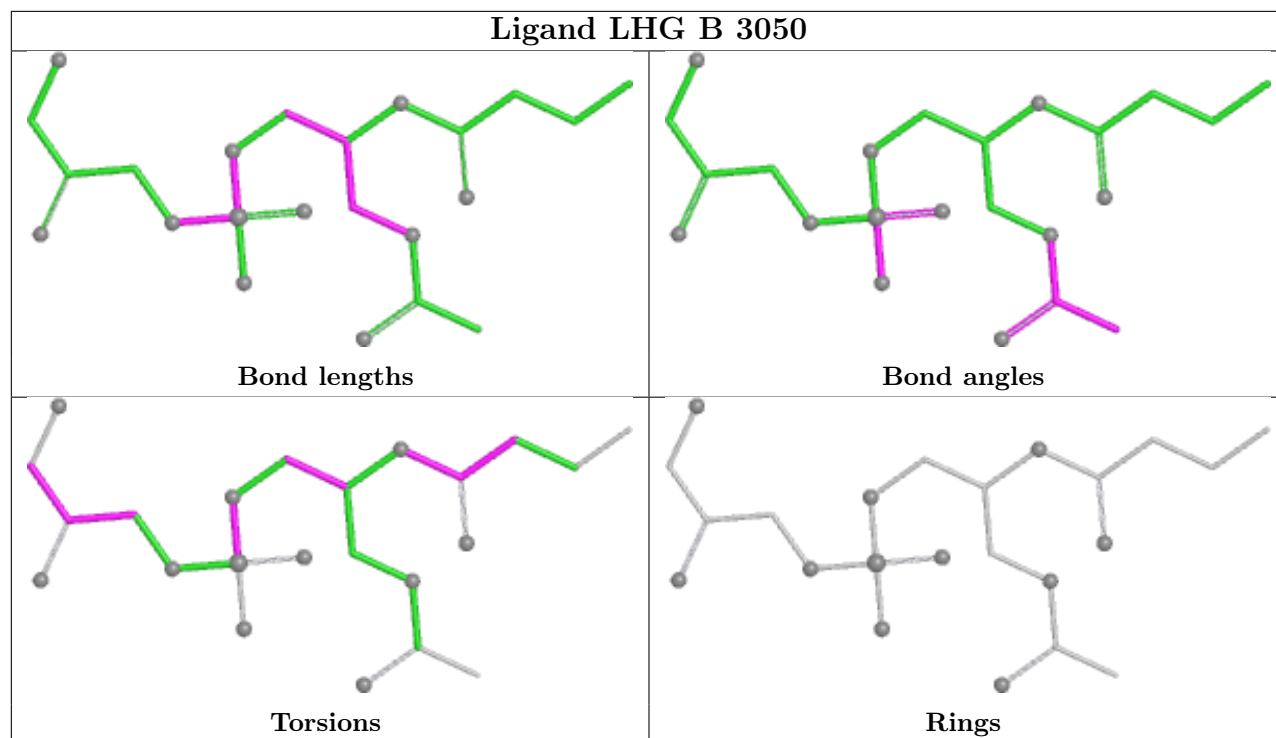
Bond angles

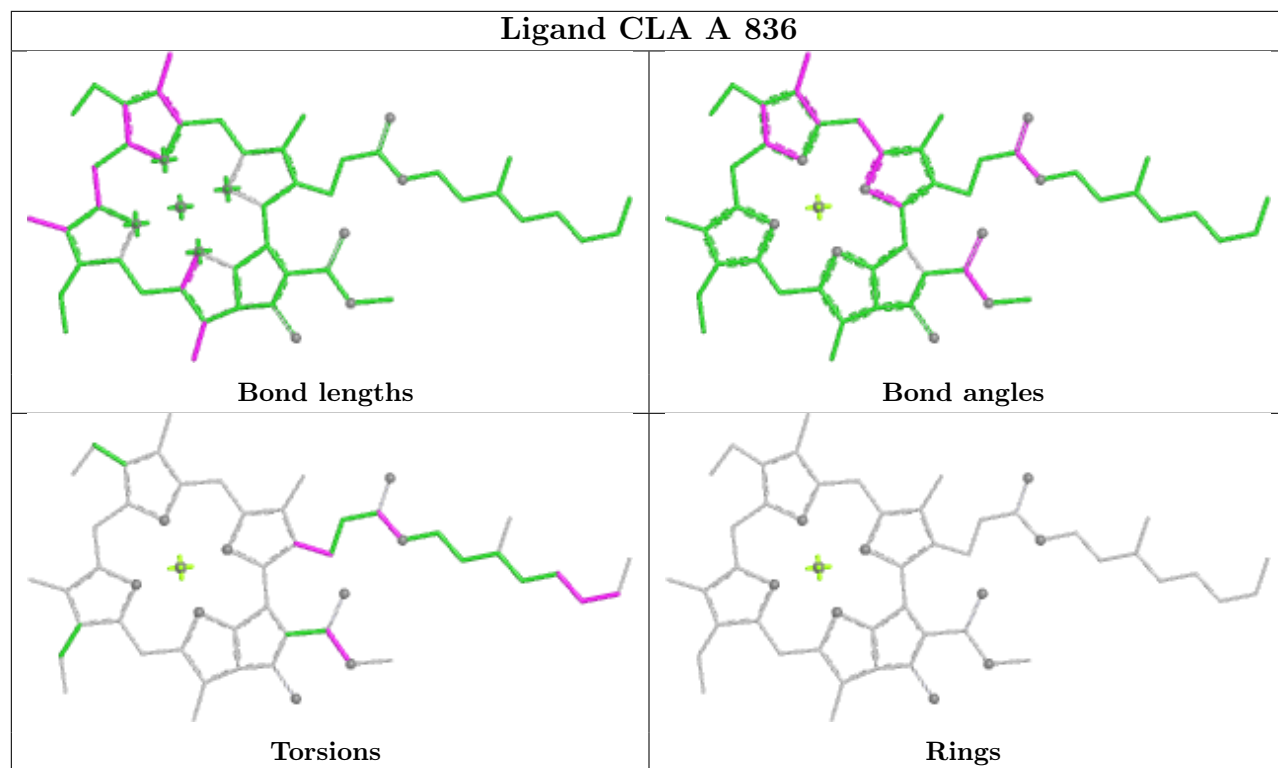


Torsions

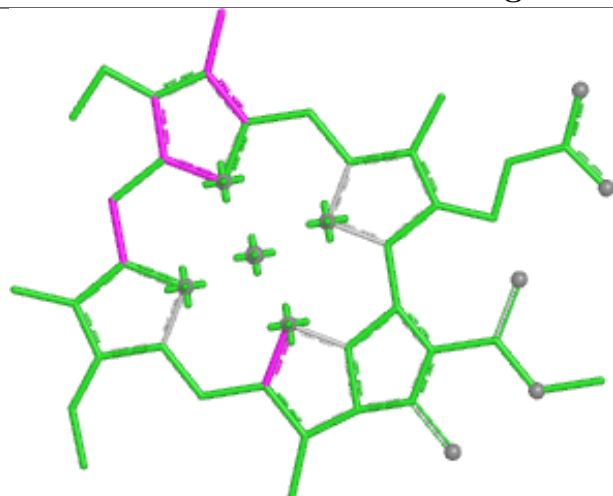


Rings

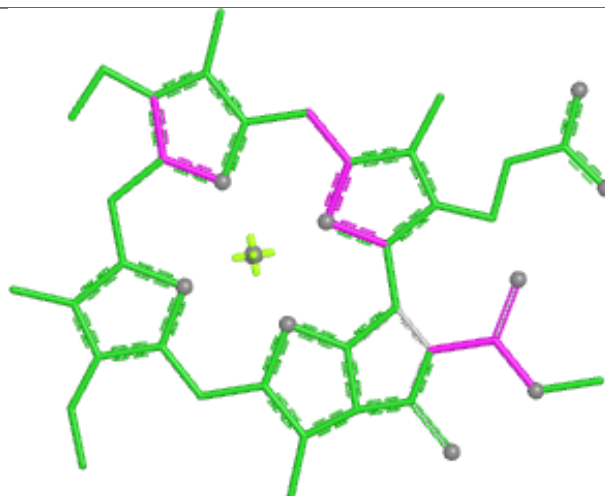




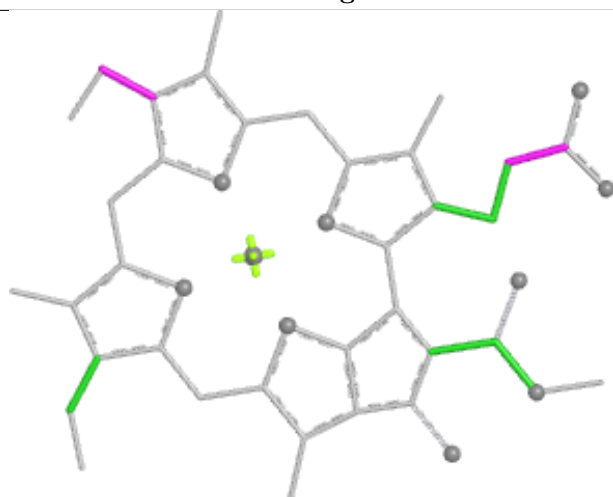
Ligand CLA X 1701



Bond lengths



Bond angles

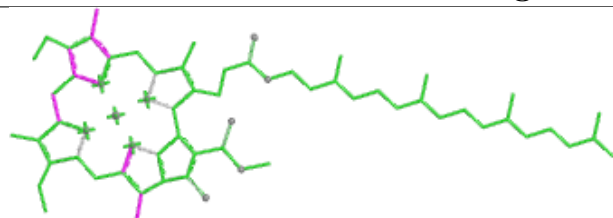


Torsions

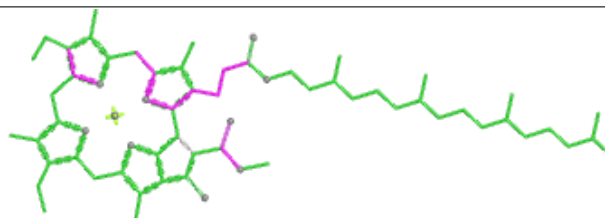


Rings

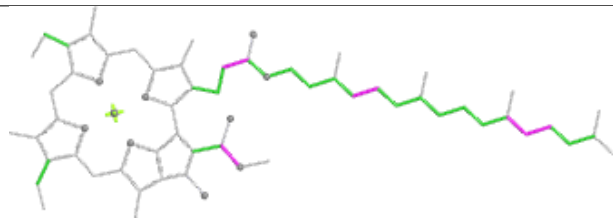
Ligand CLA A 803



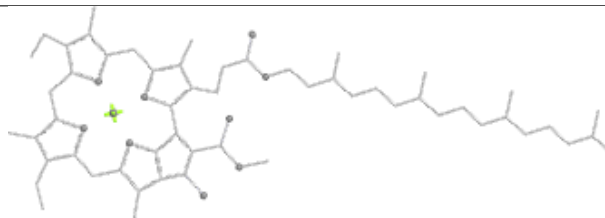
Bond lengths



Bond angles

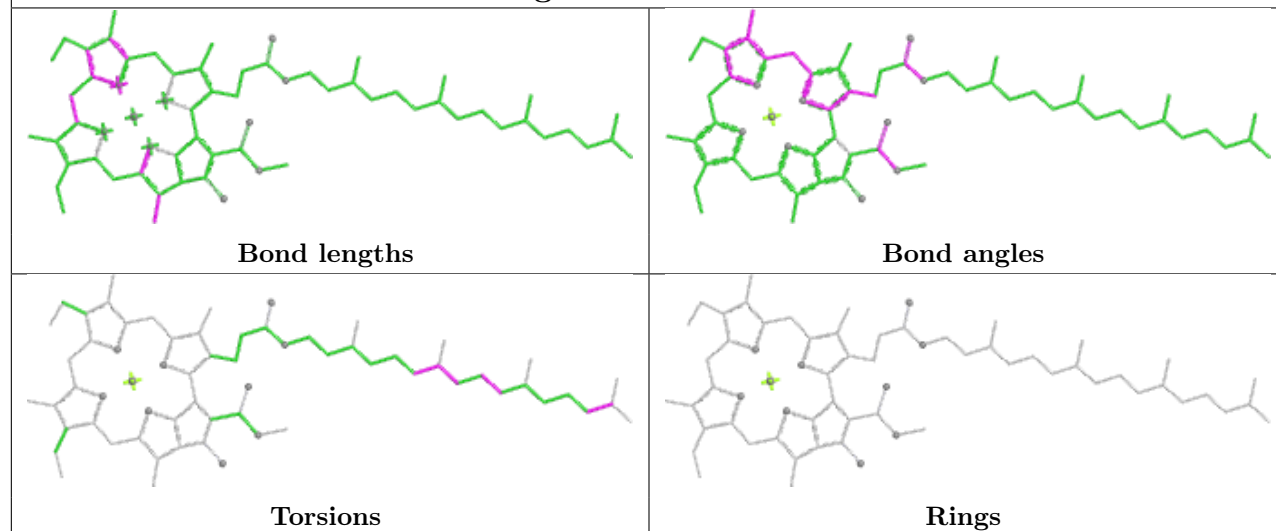


Torsions

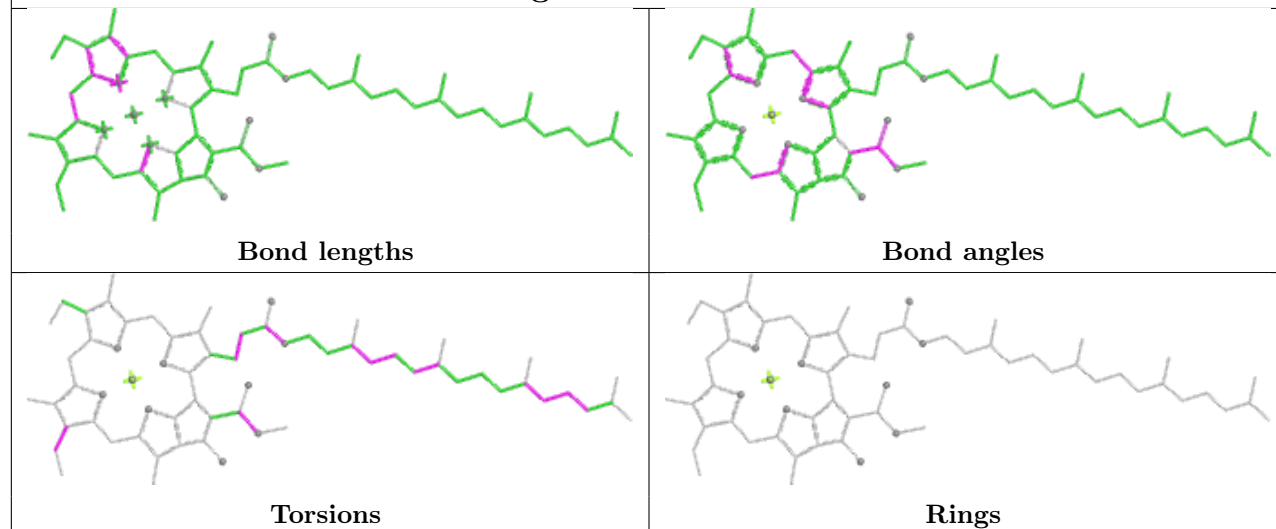


Rings

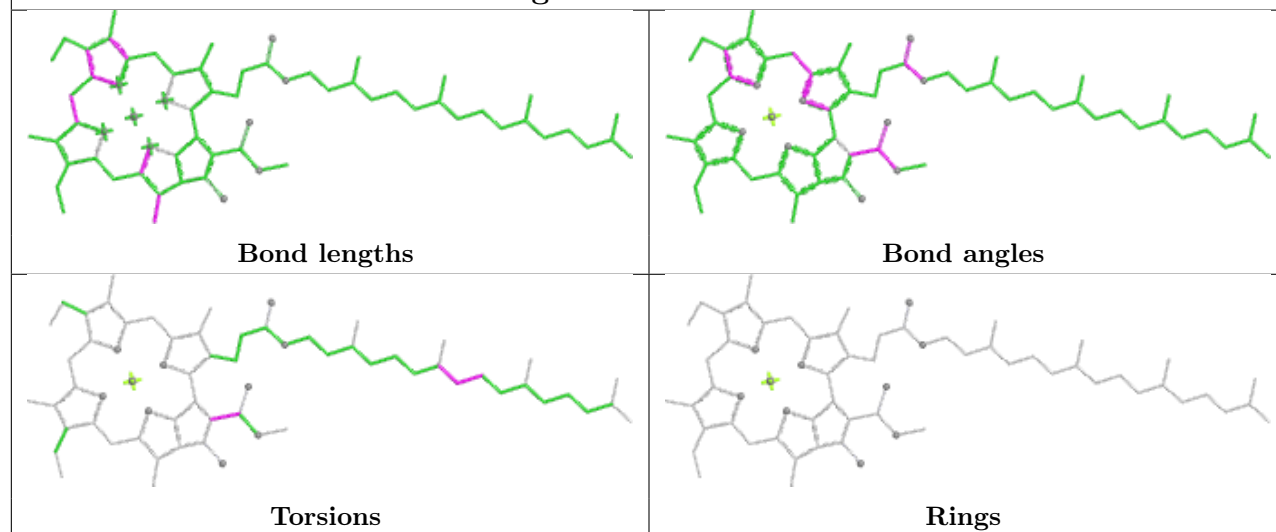
Ligand CLA L 206

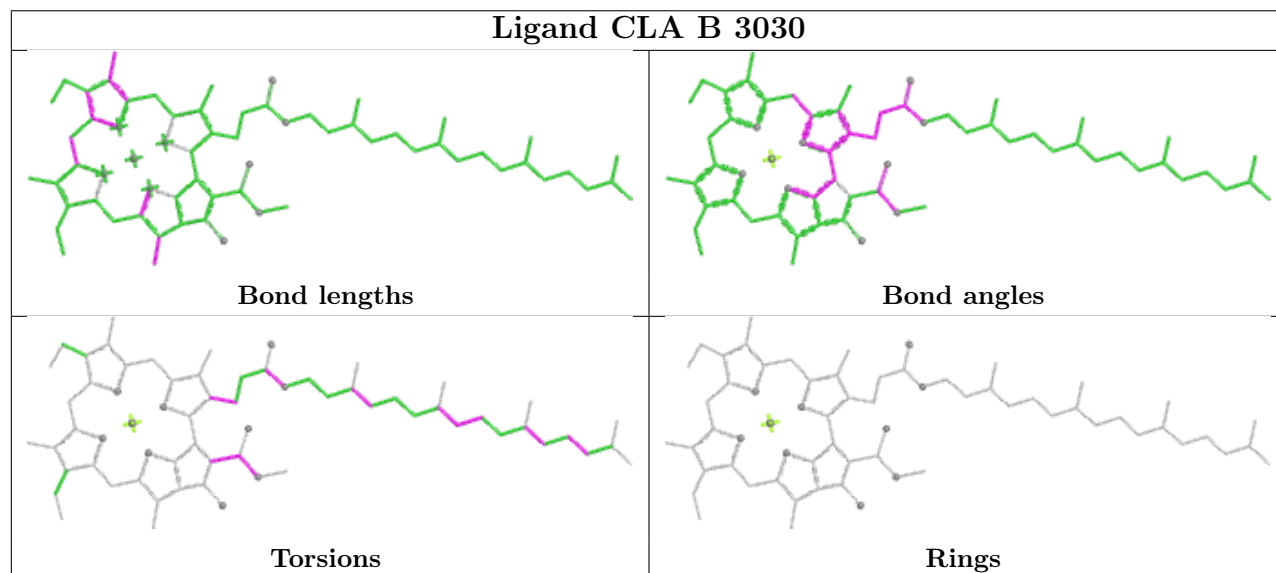
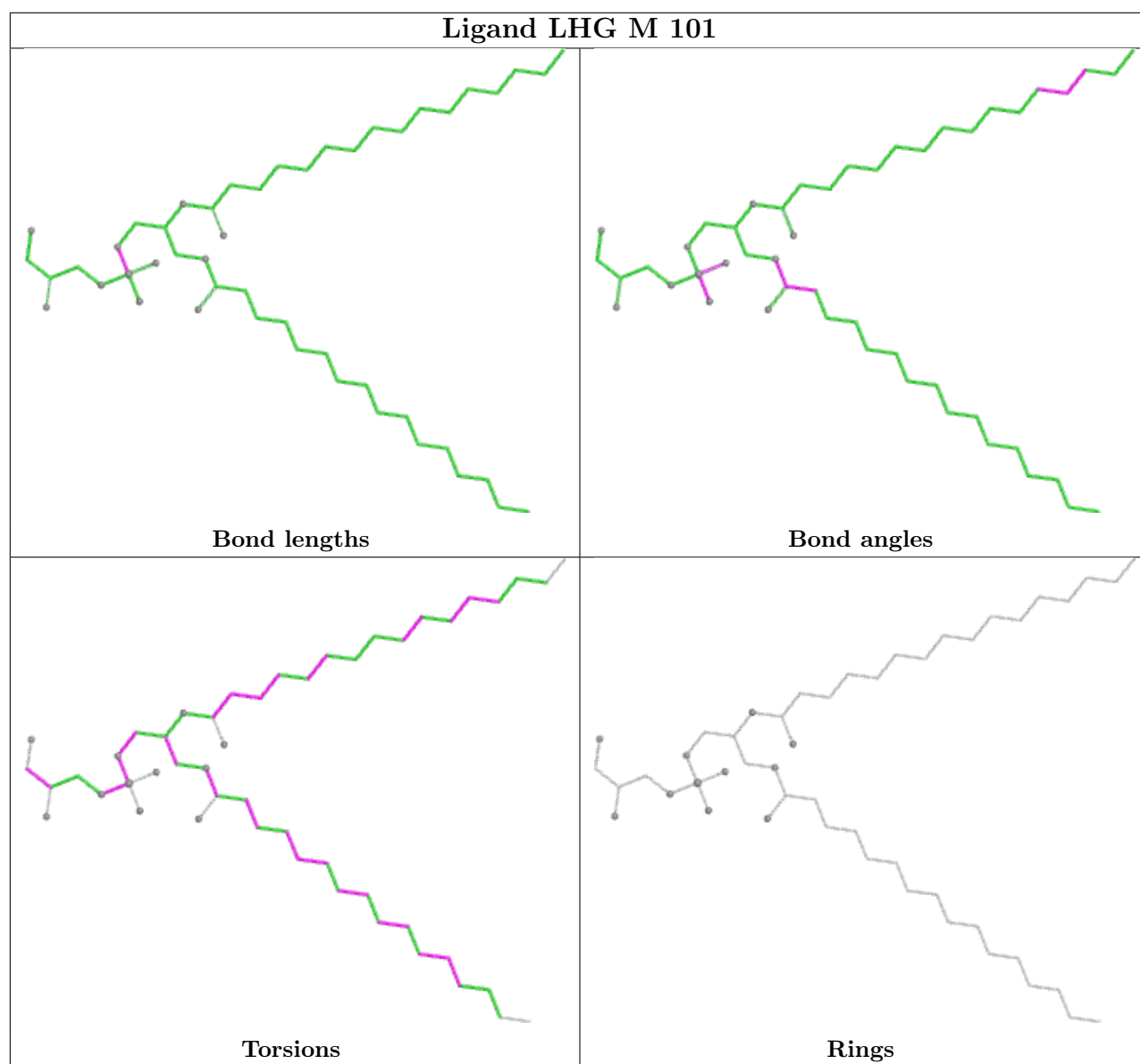


Ligand CLA A 822

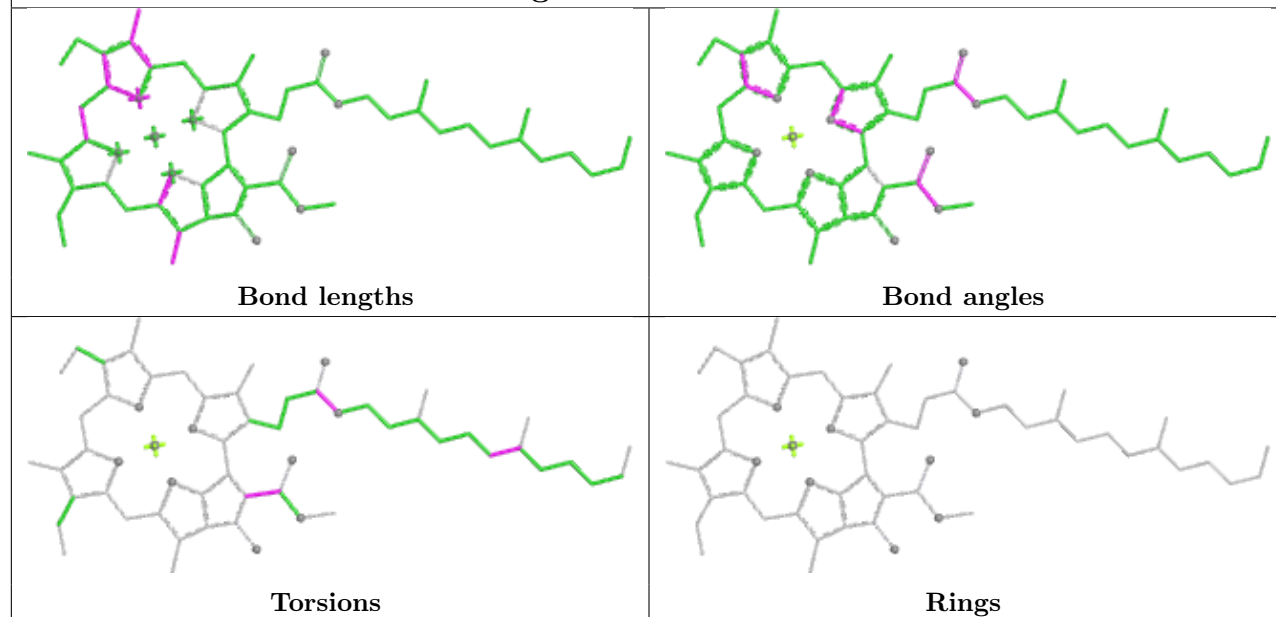


Ligand CLA A 828

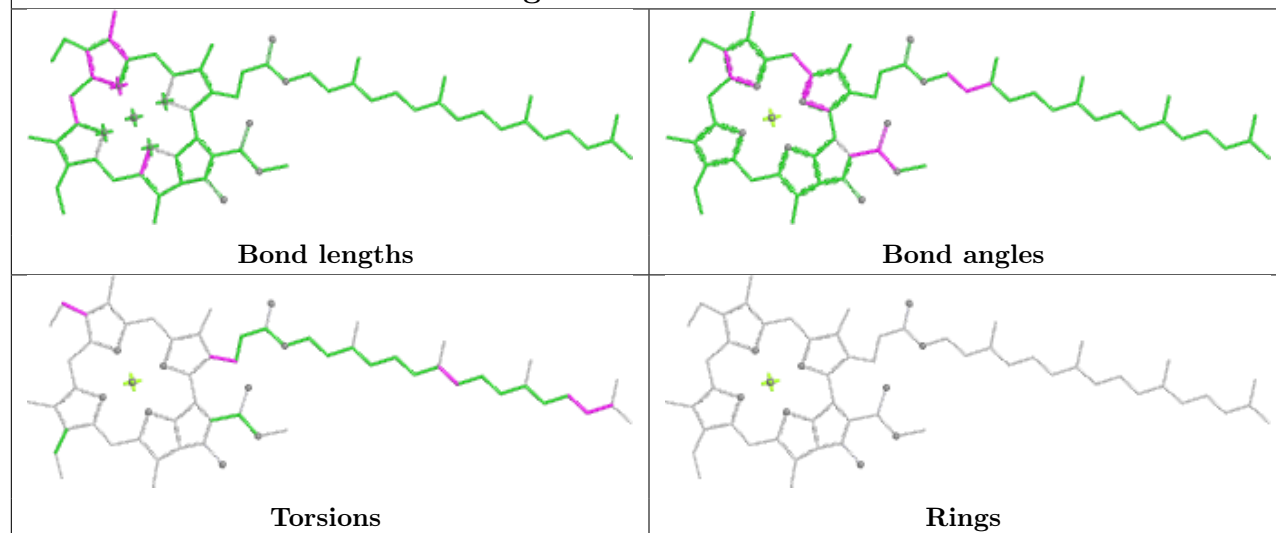




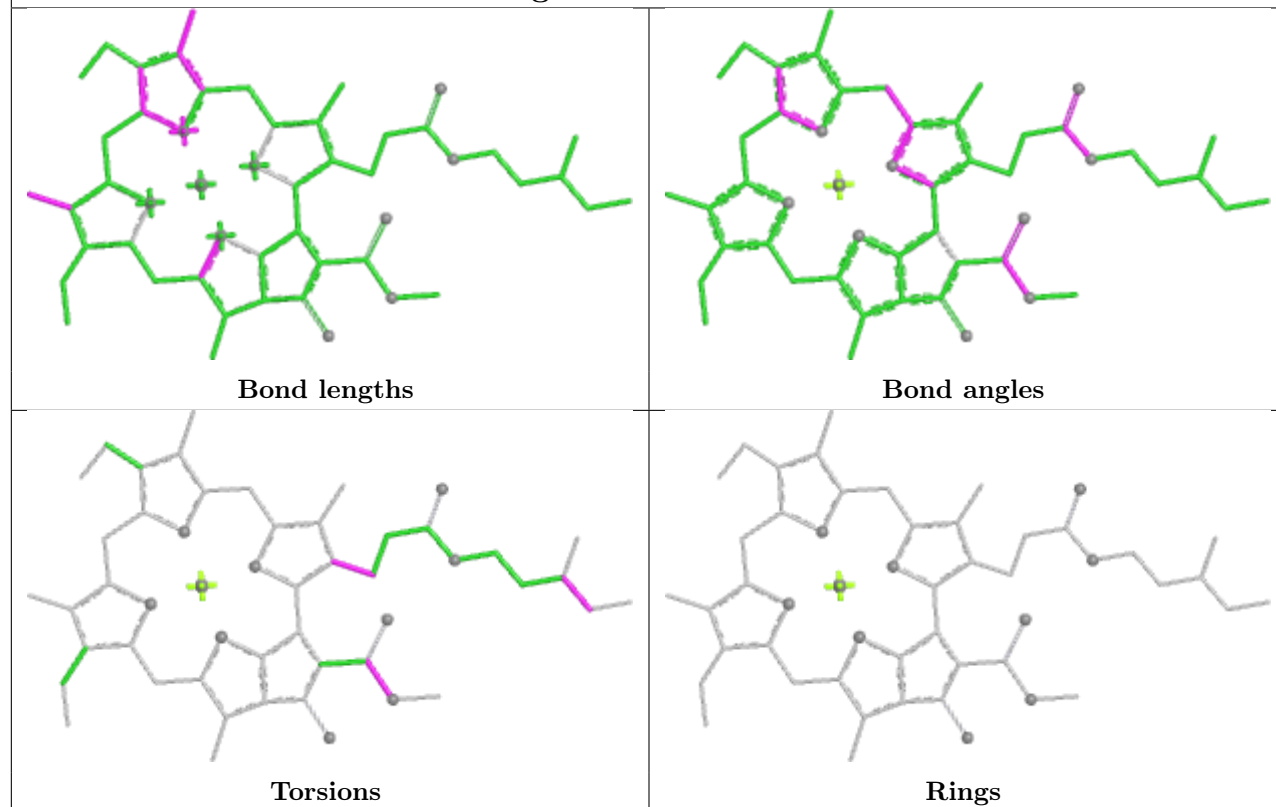
Ligand CLA A 805



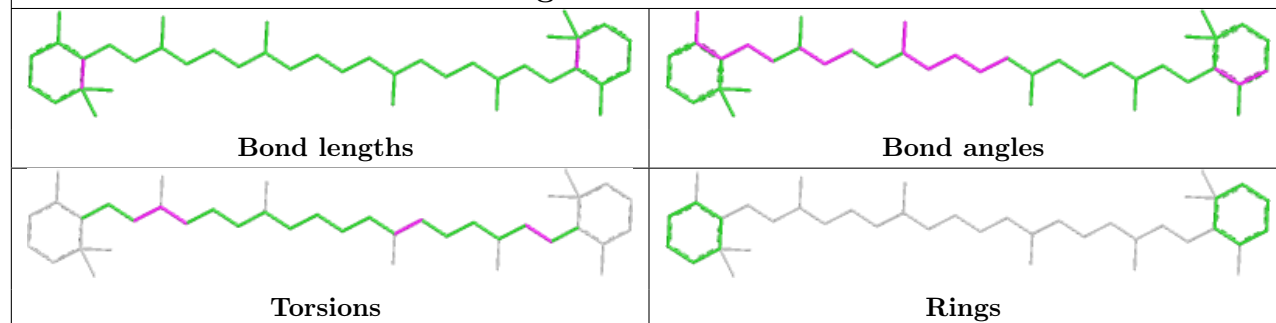
Ligand CLA B 3042

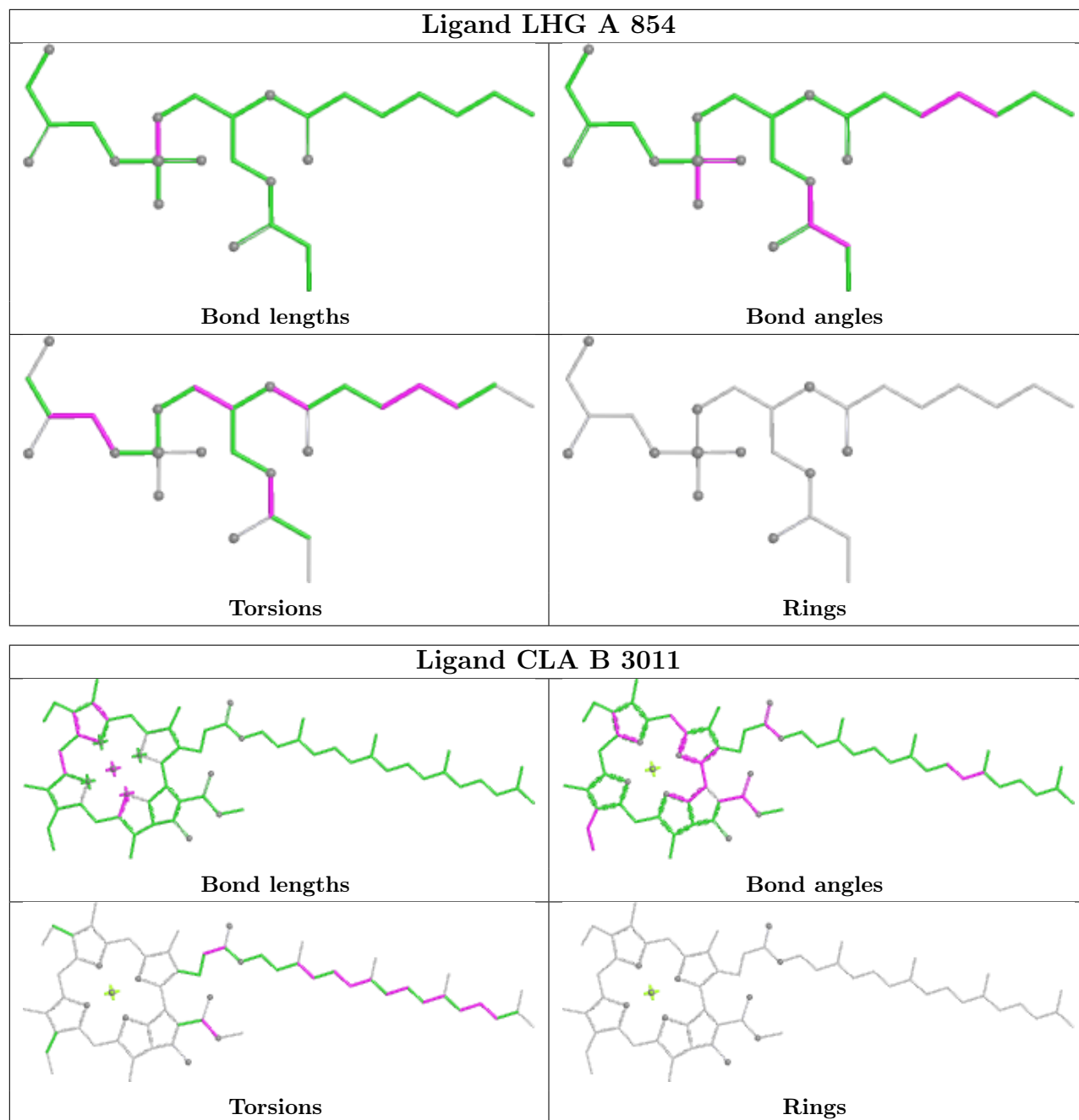


Ligand CLA A 842

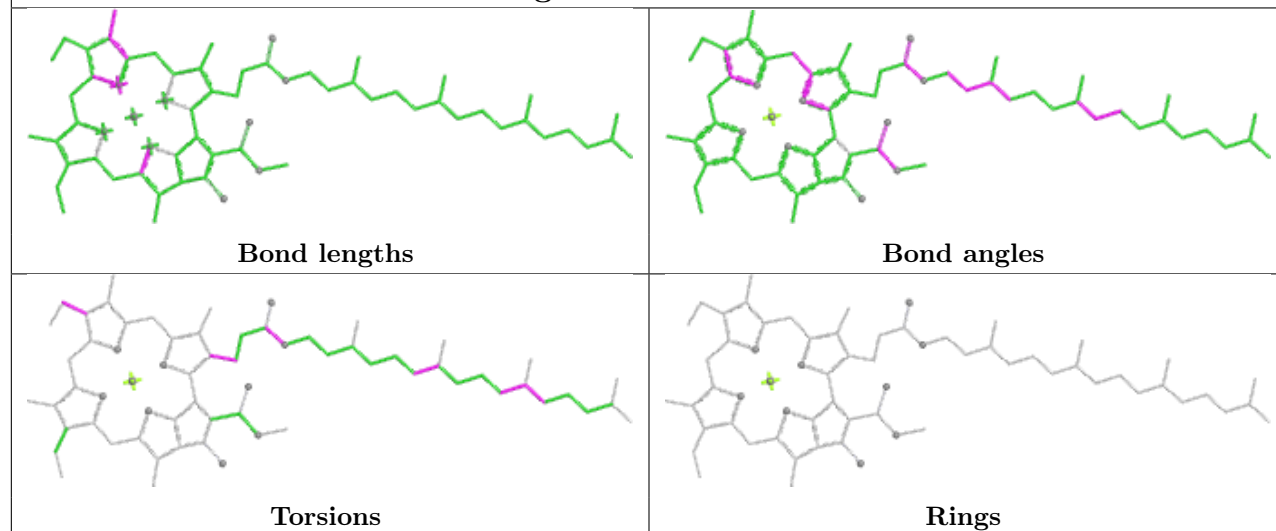


Ligand BCR I 101

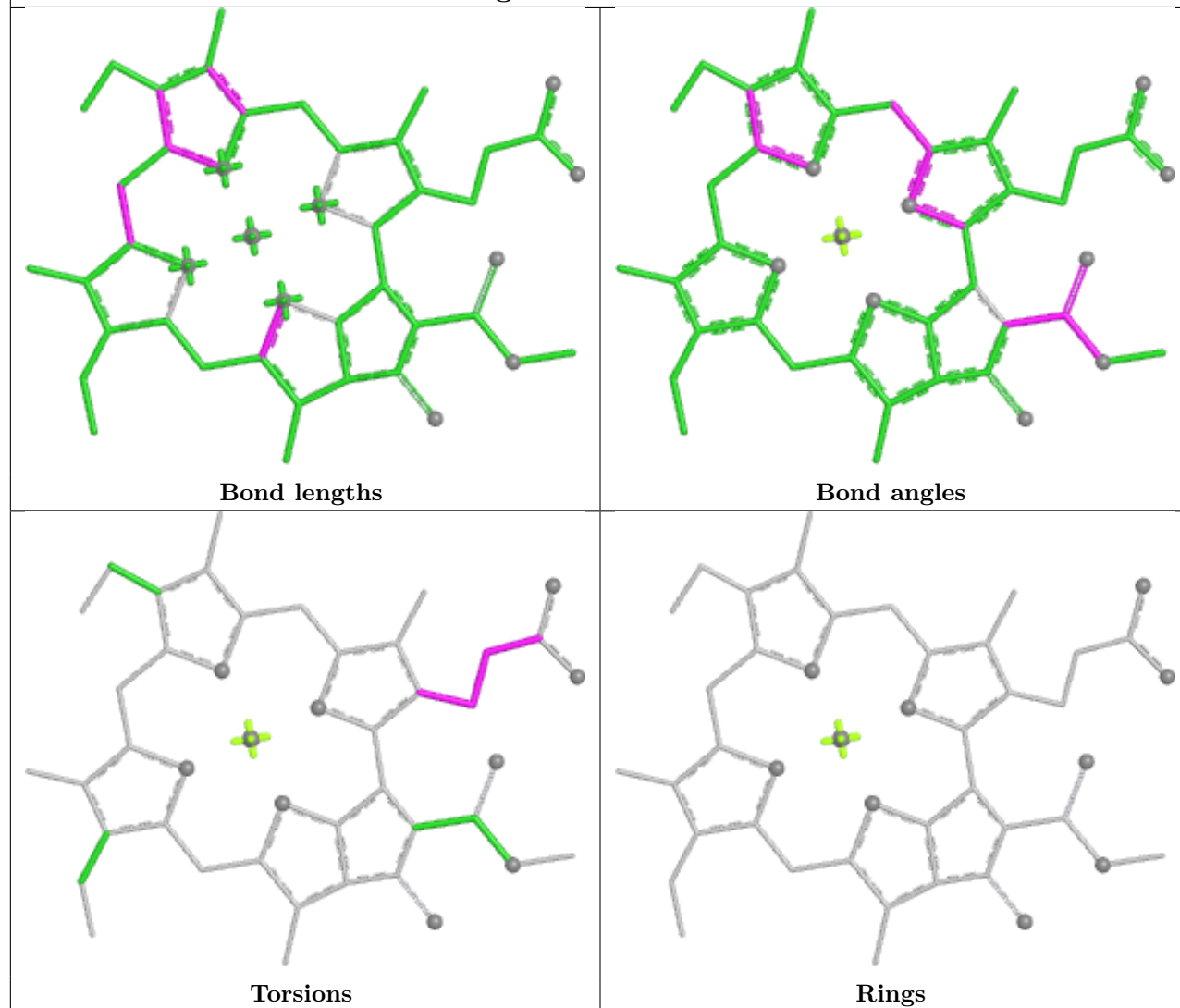


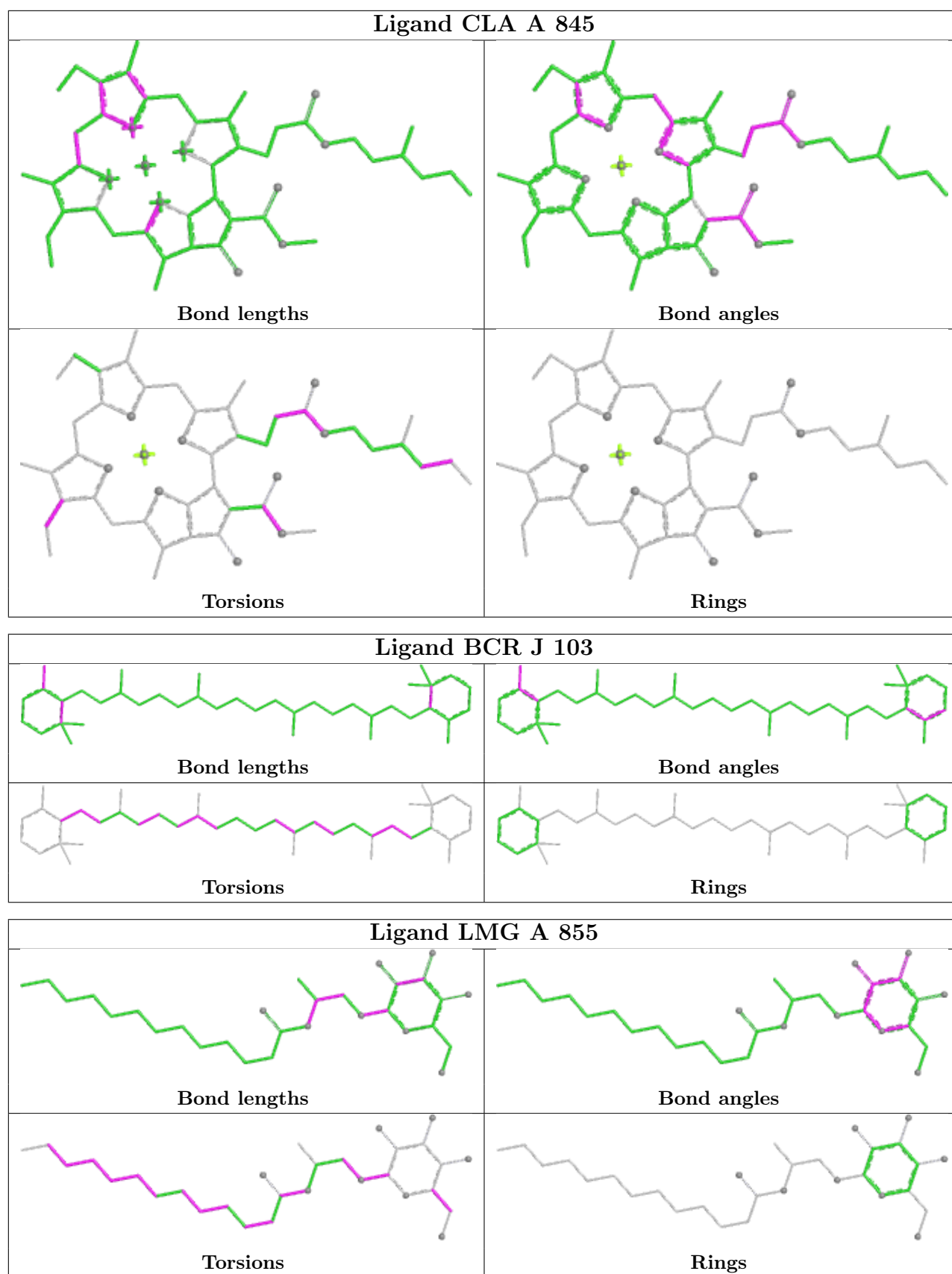


Ligand CLA L 204

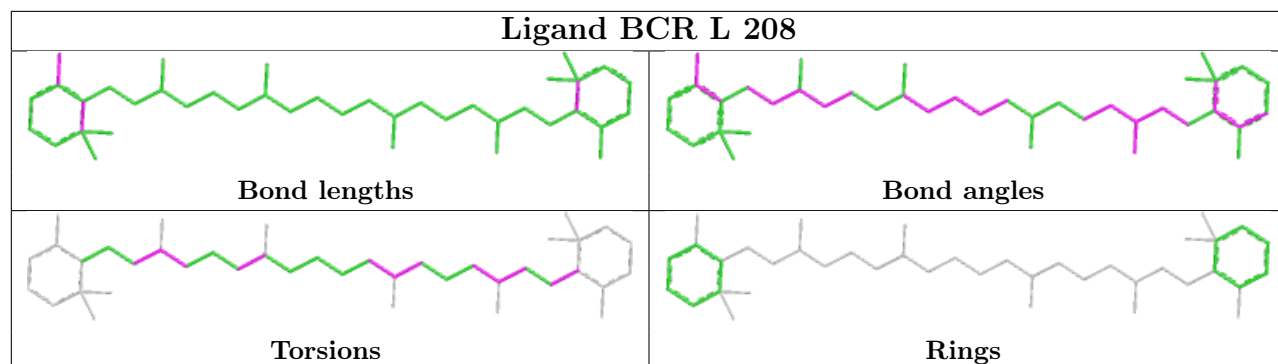


Ligand CLA J 101

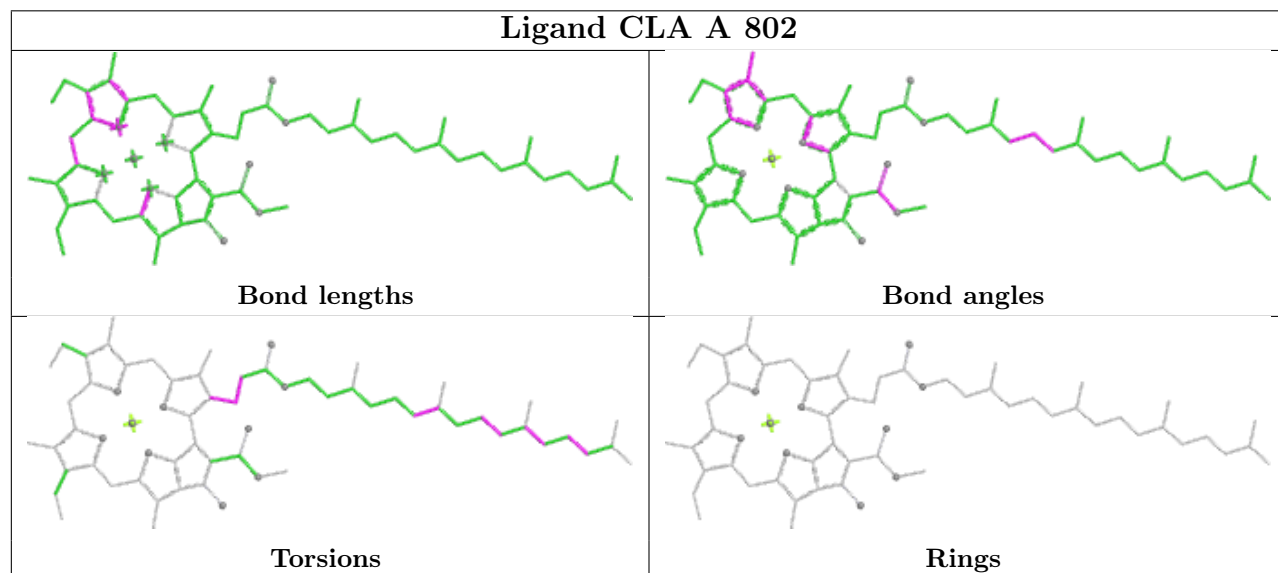




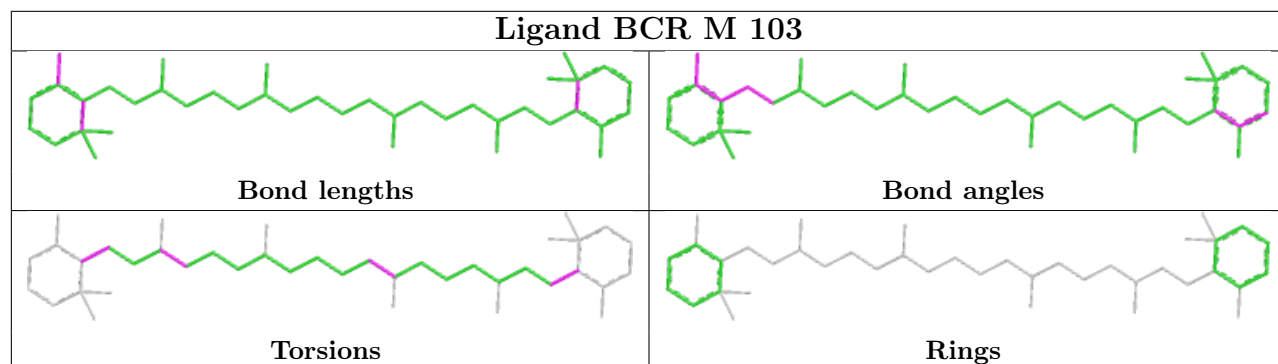
Ligand BCR L 208



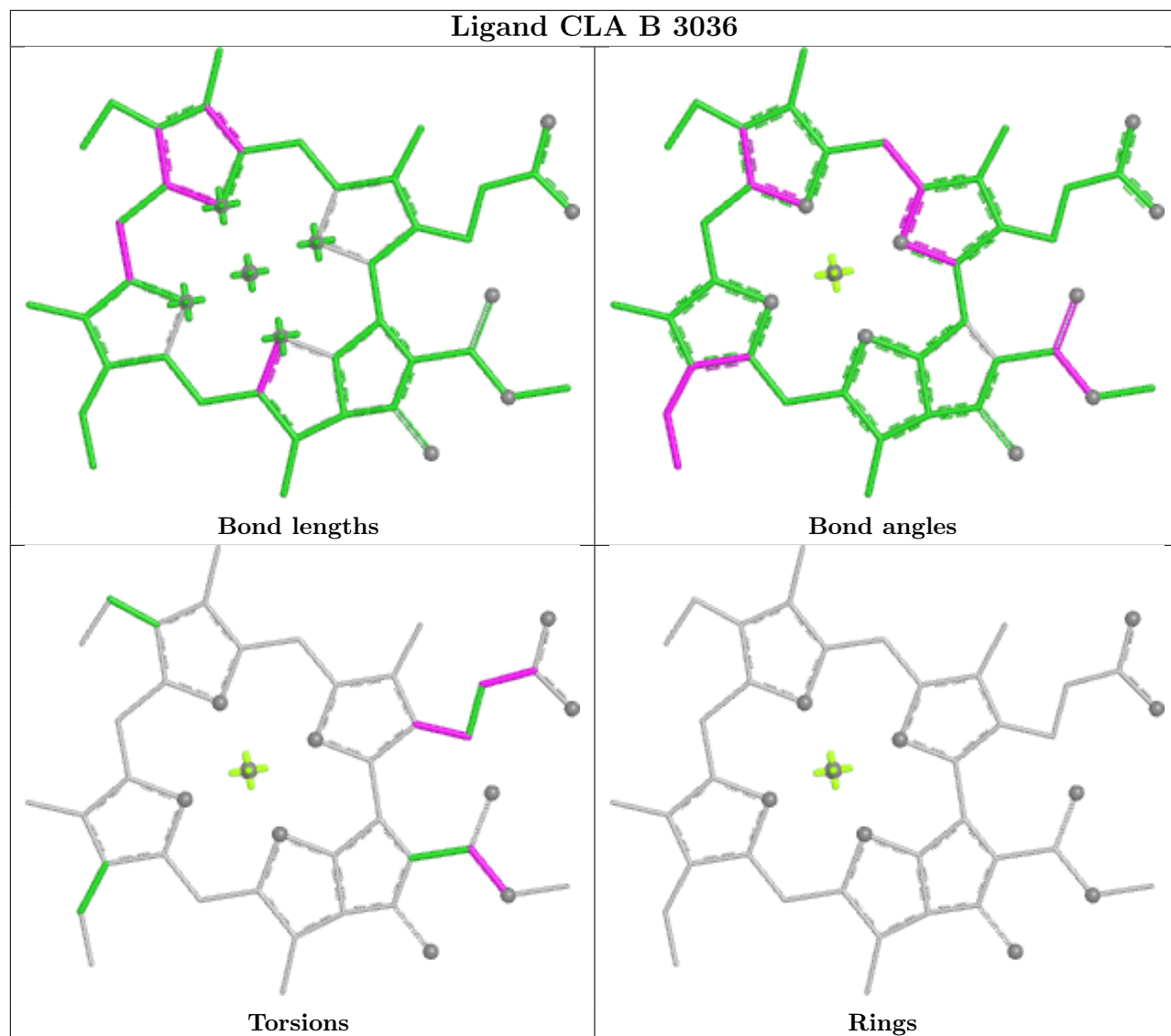
Ligand CLA A 802



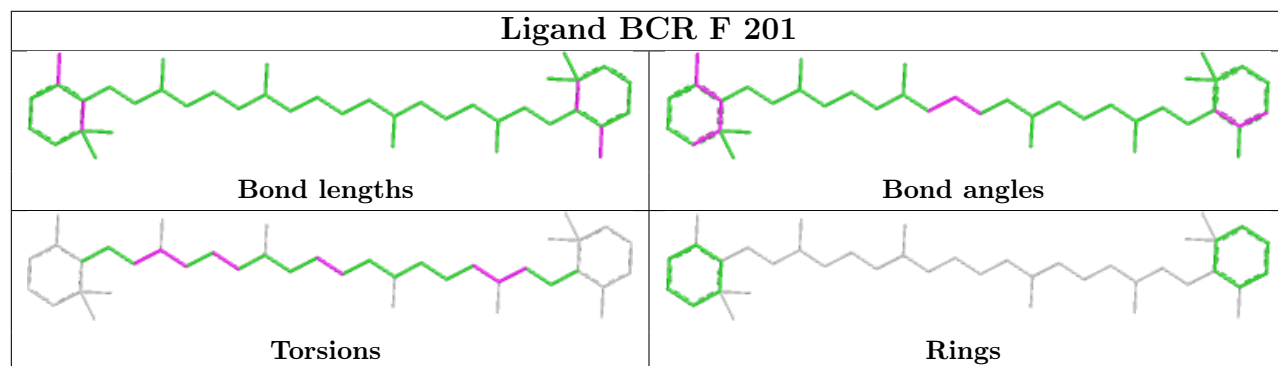
Ligand BCR M 103



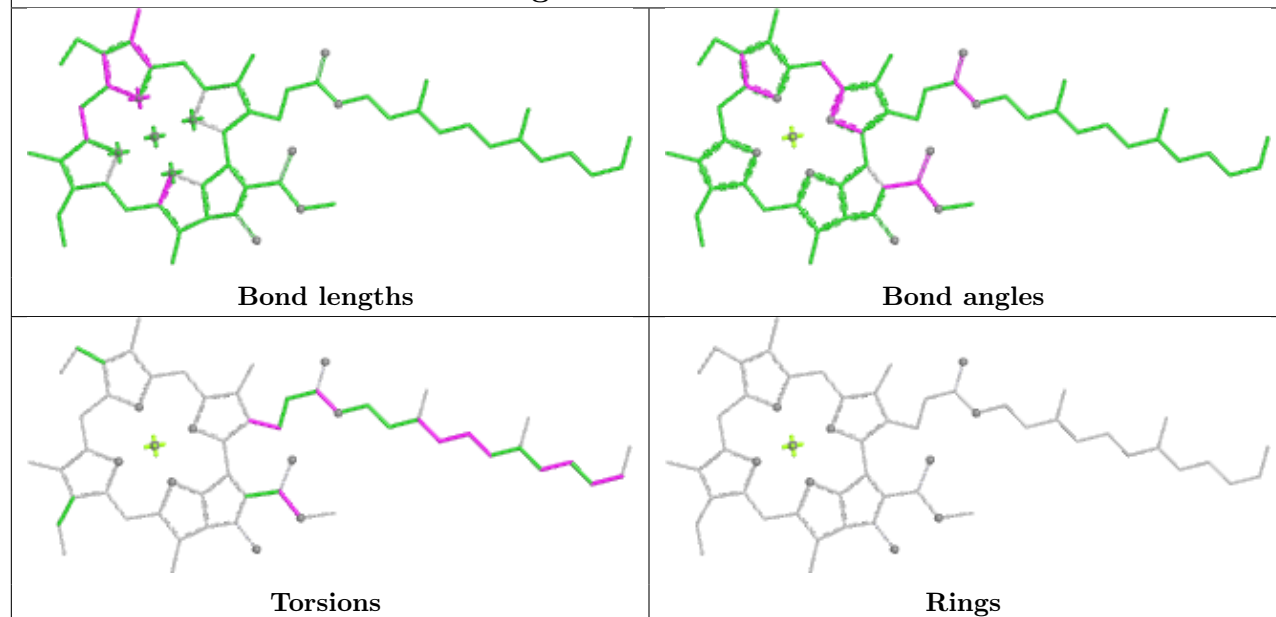
Ligand CLA B 3036



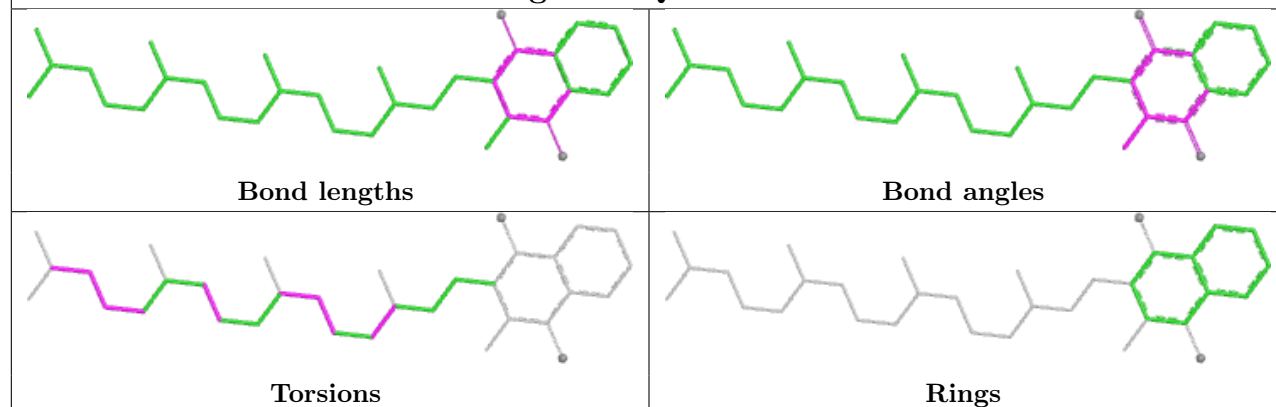
Ligand BCR F 201



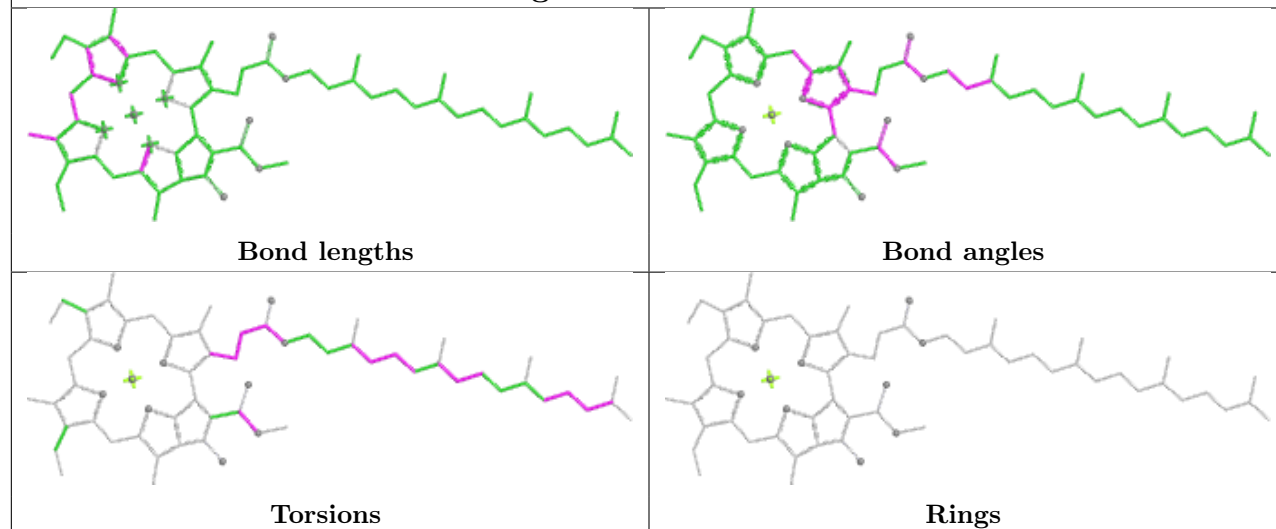
Ligand CLA A 825



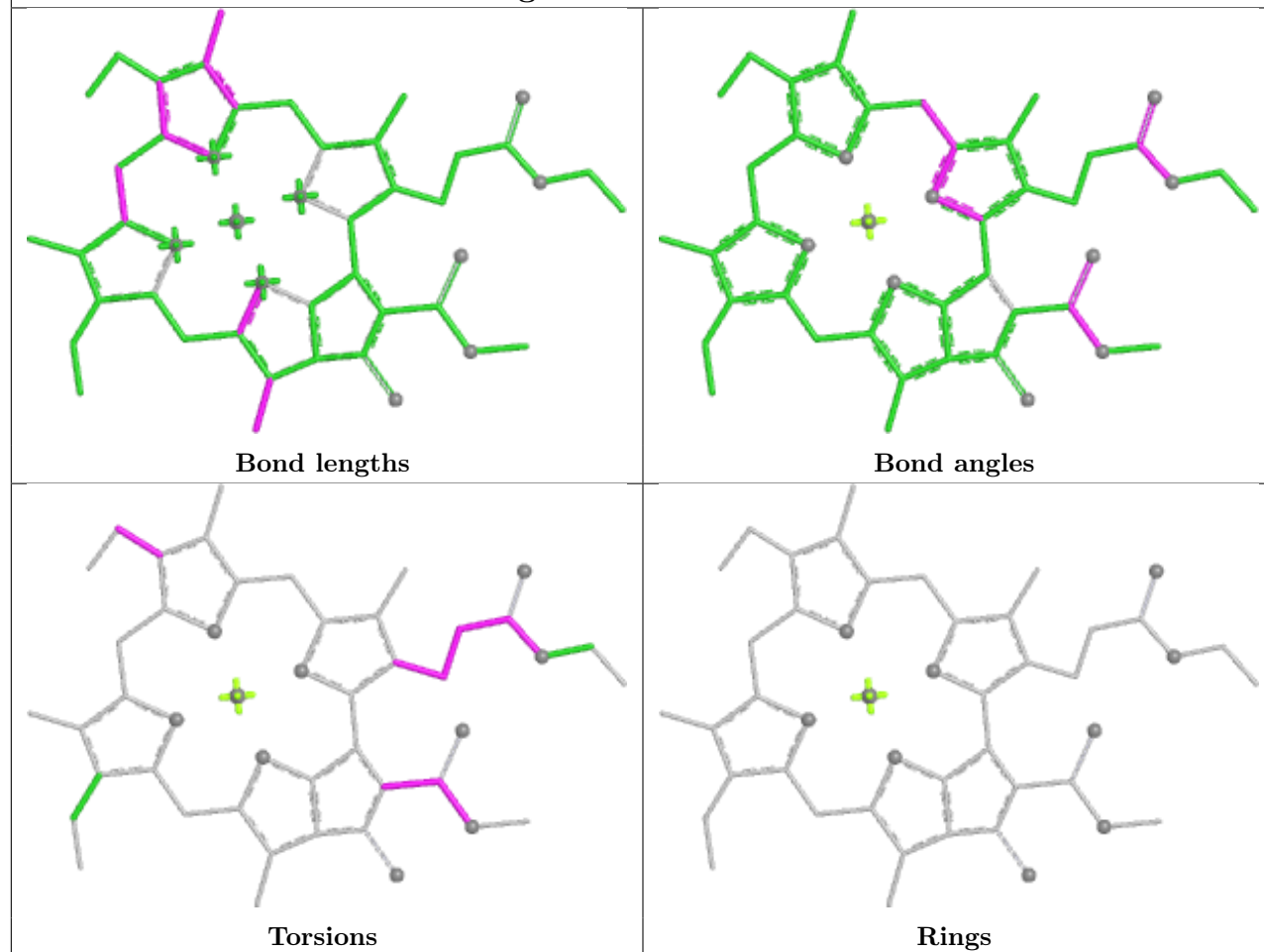
Ligand PQN A 846



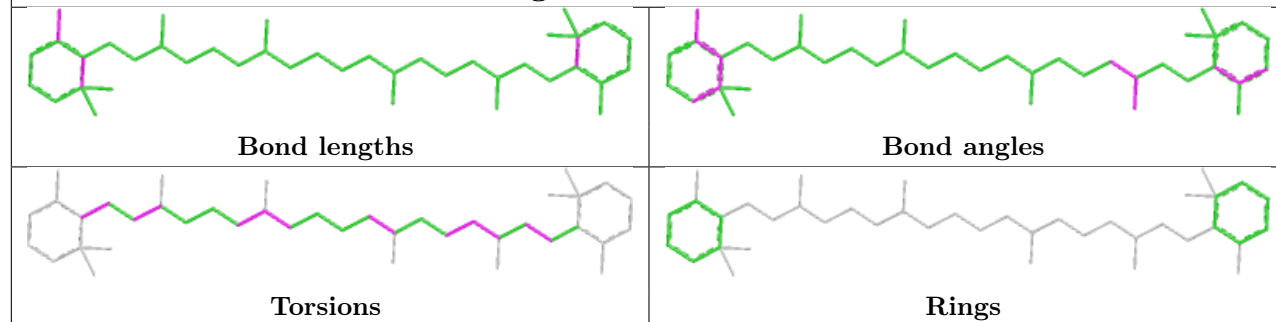
Ligand CLA A 820



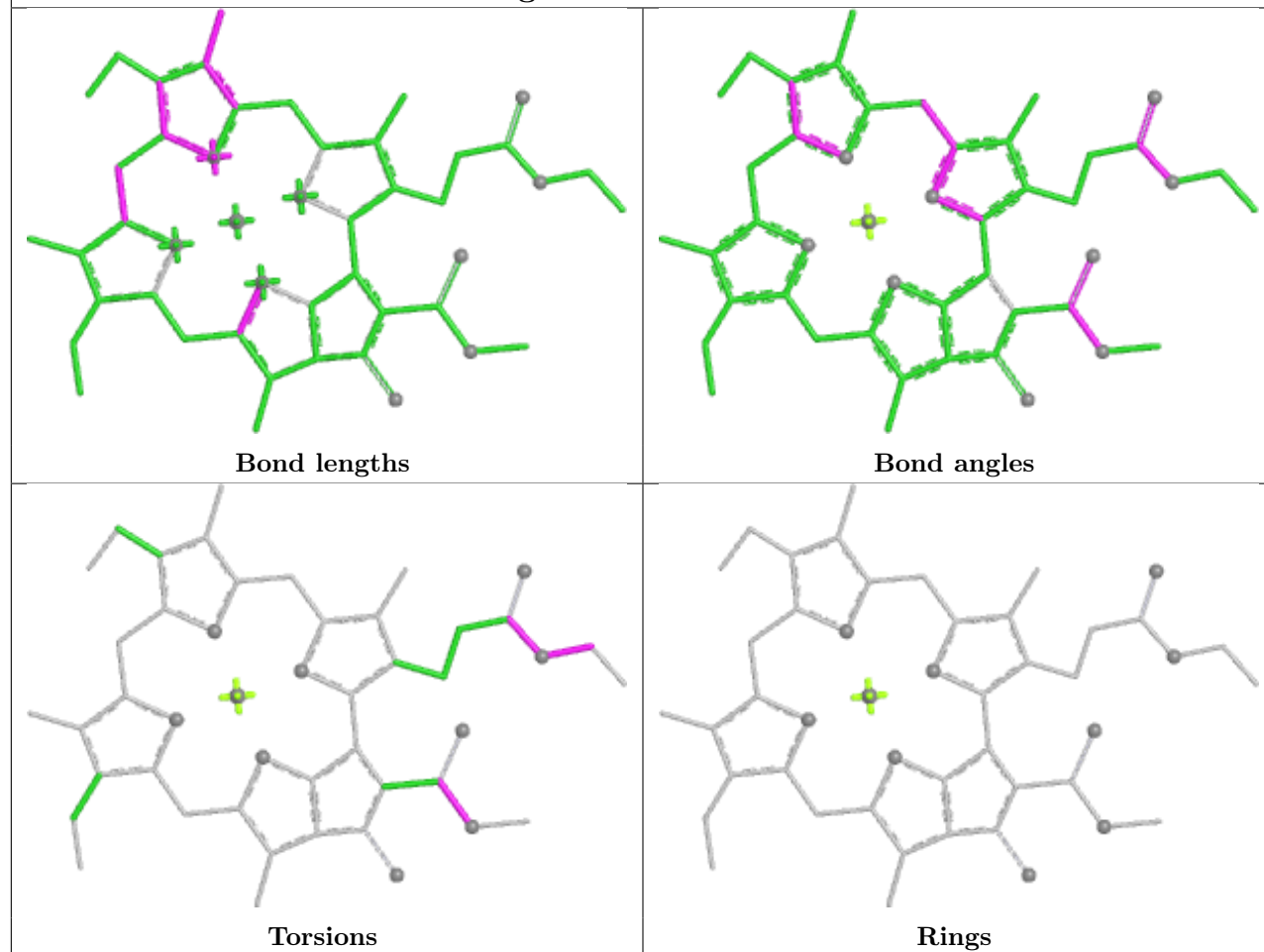
Ligand CLA B 3021



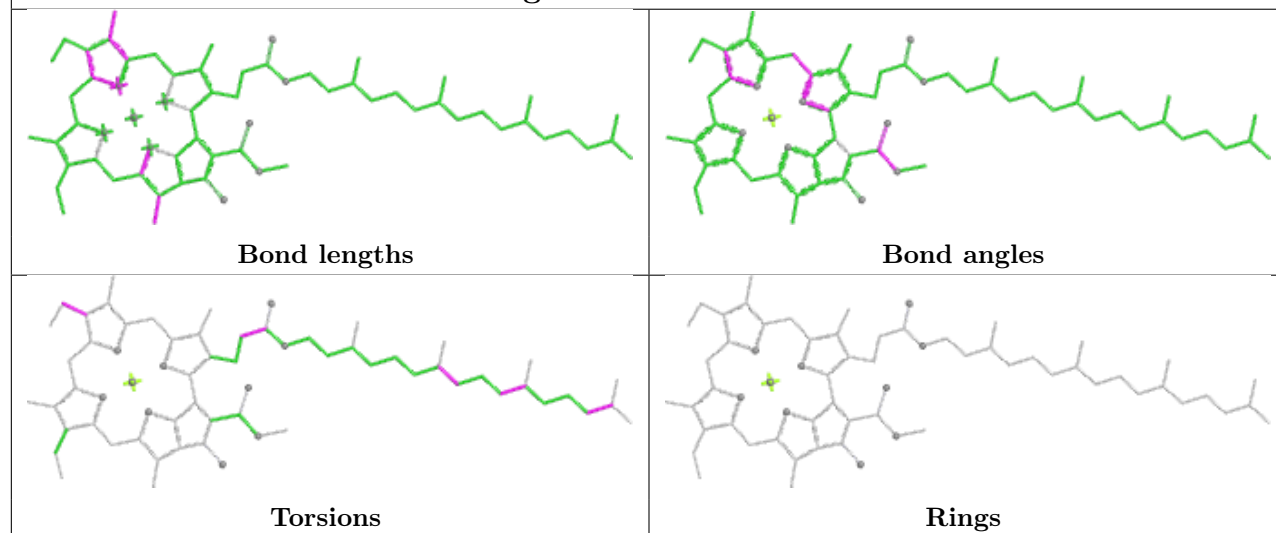
Ligand BCR A 850



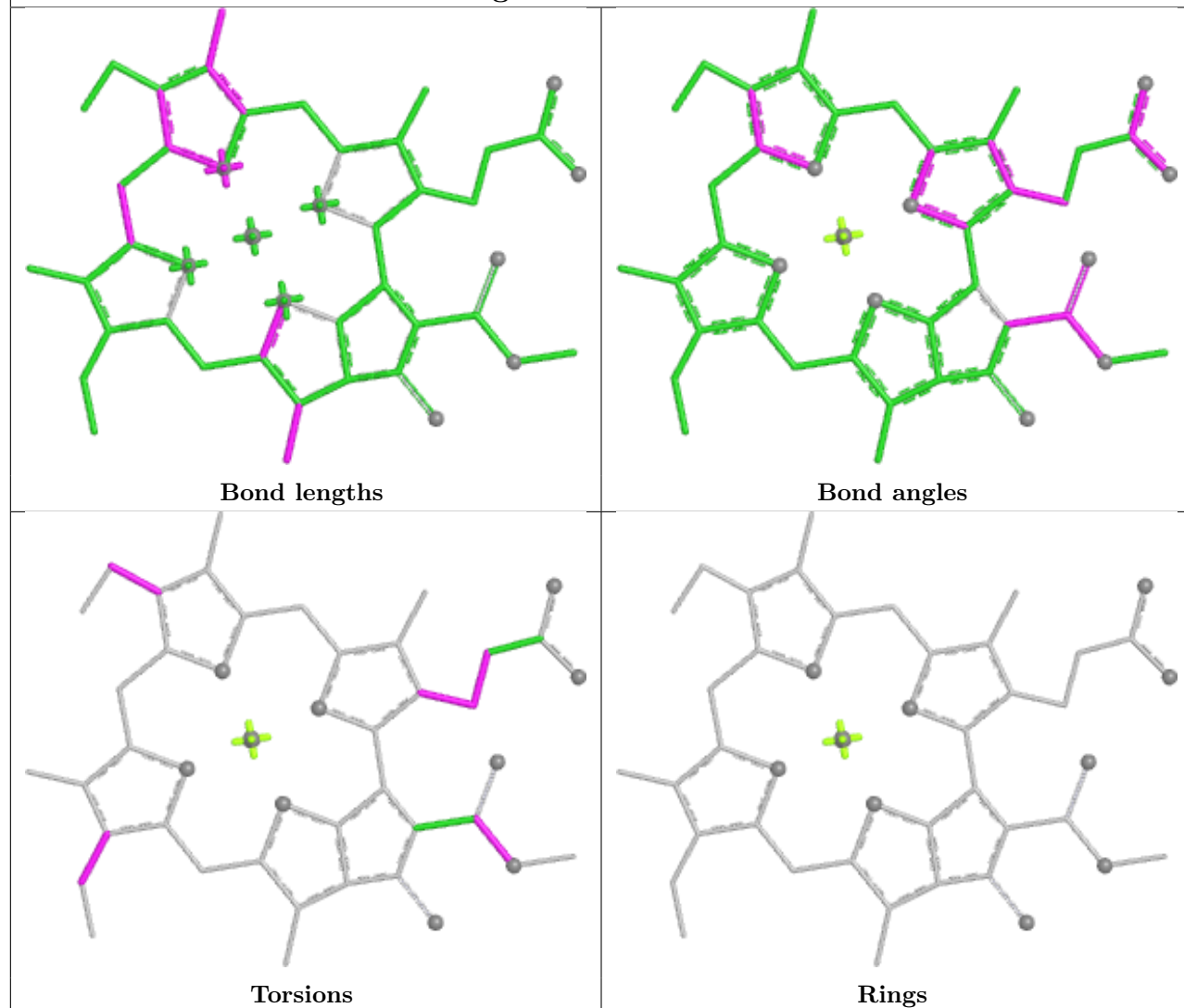
Ligand CLA B 3040



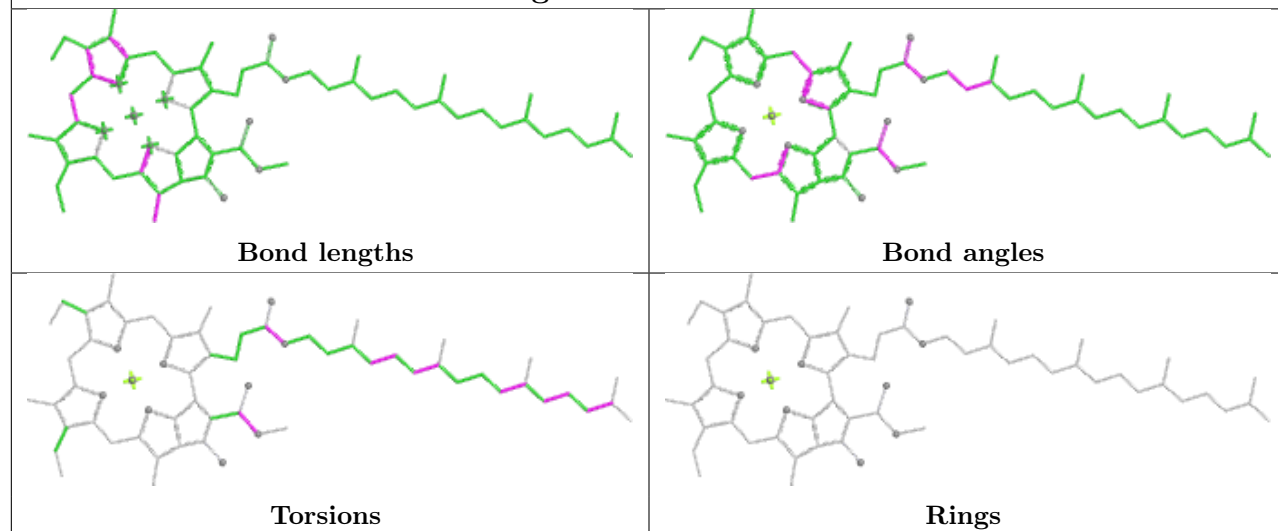
Ligand CLA B 3007

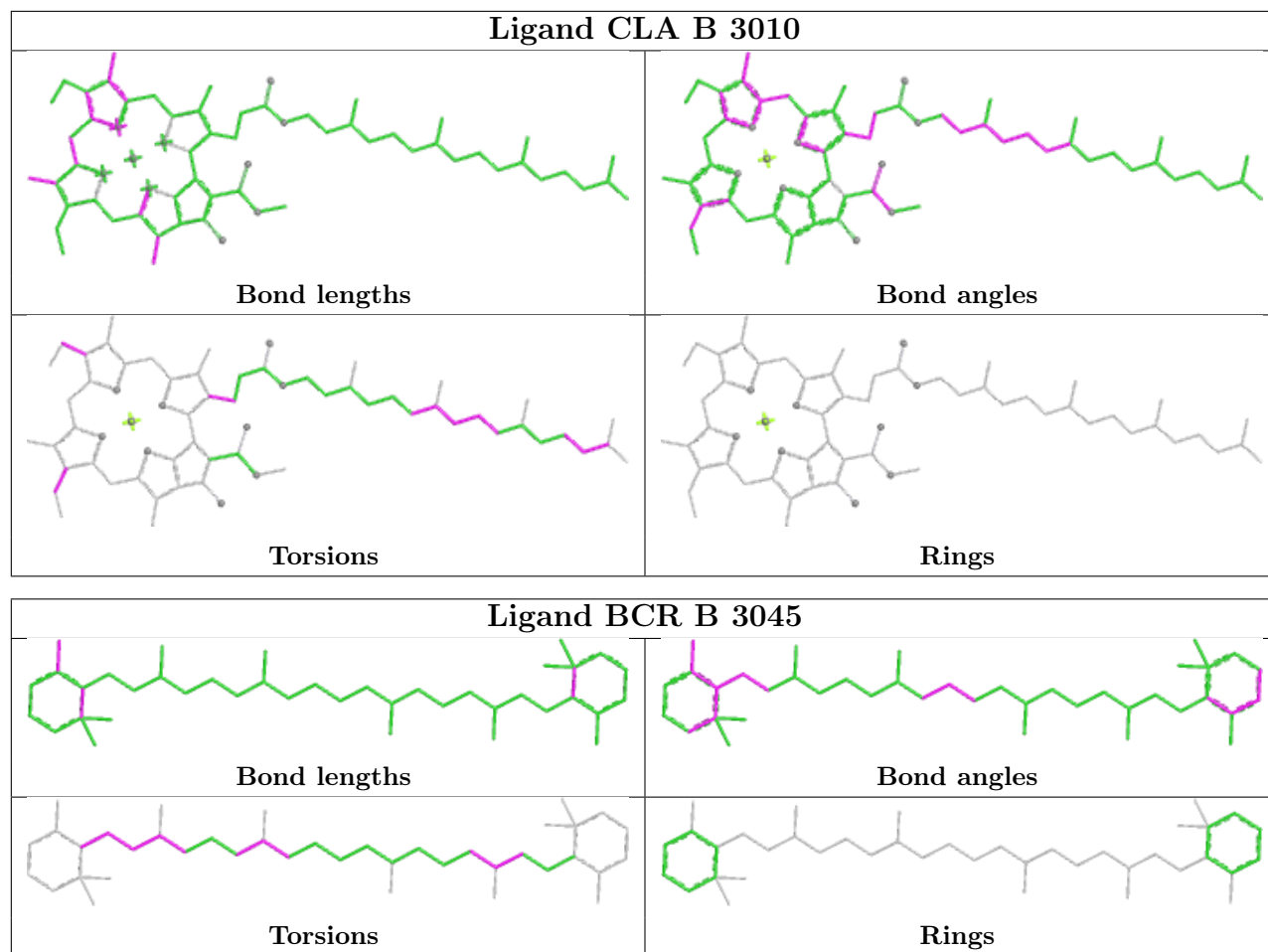


Ligand CLA A 811

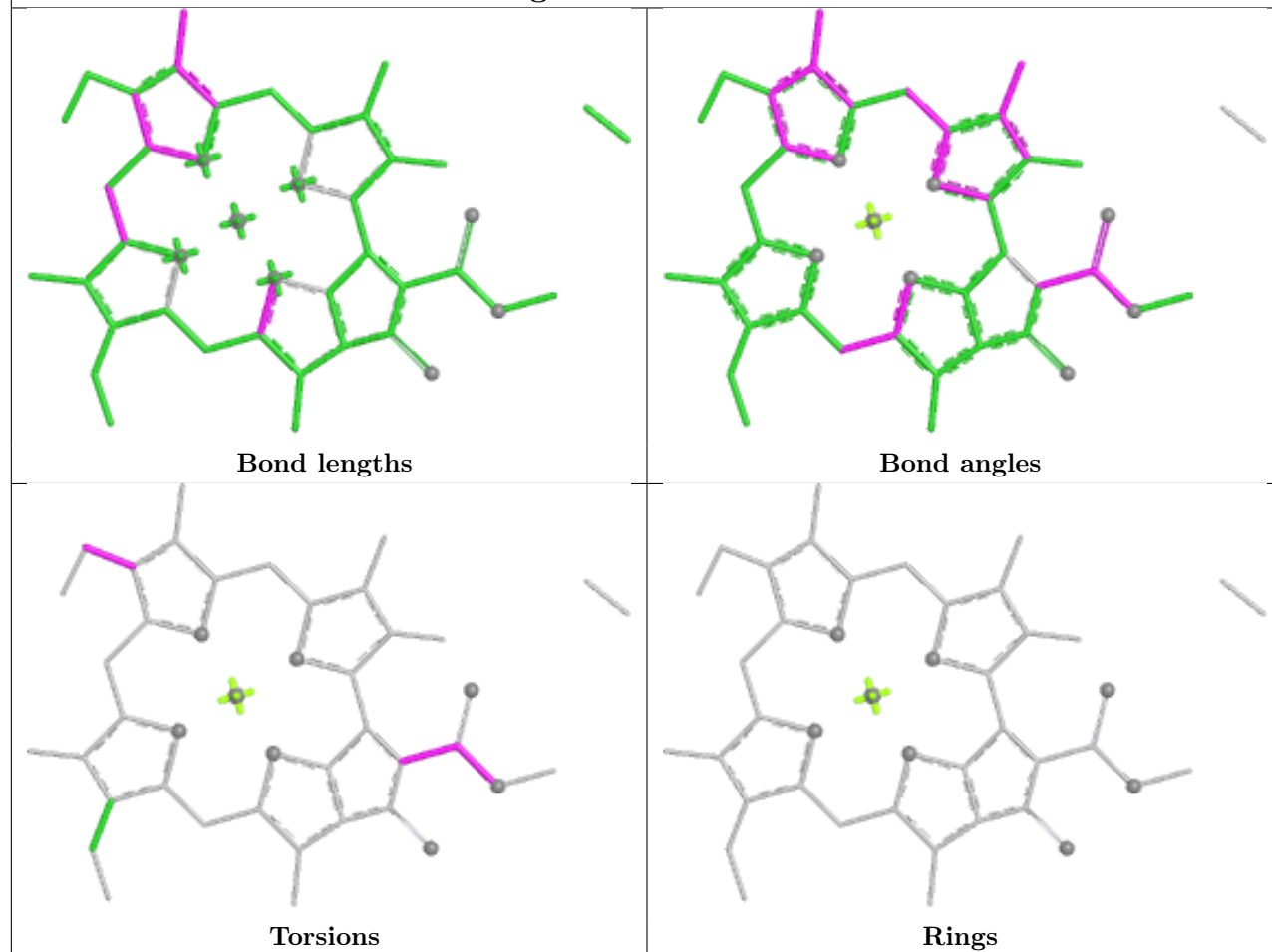


Ligand CLA A 829

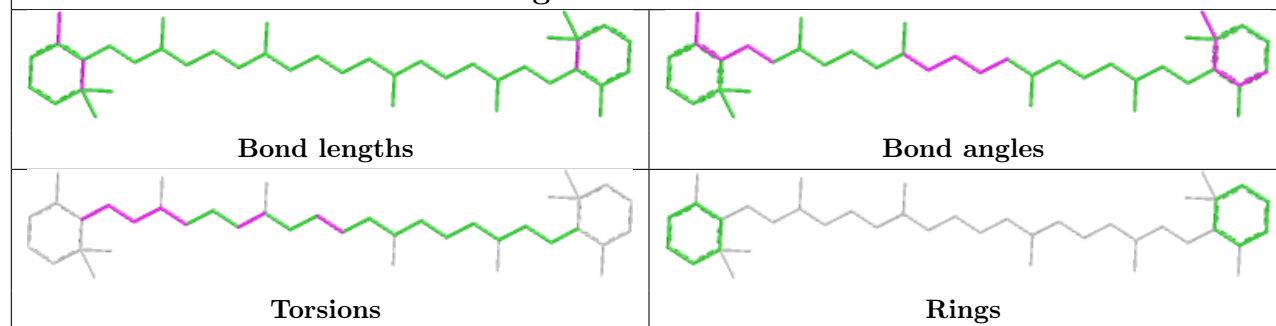




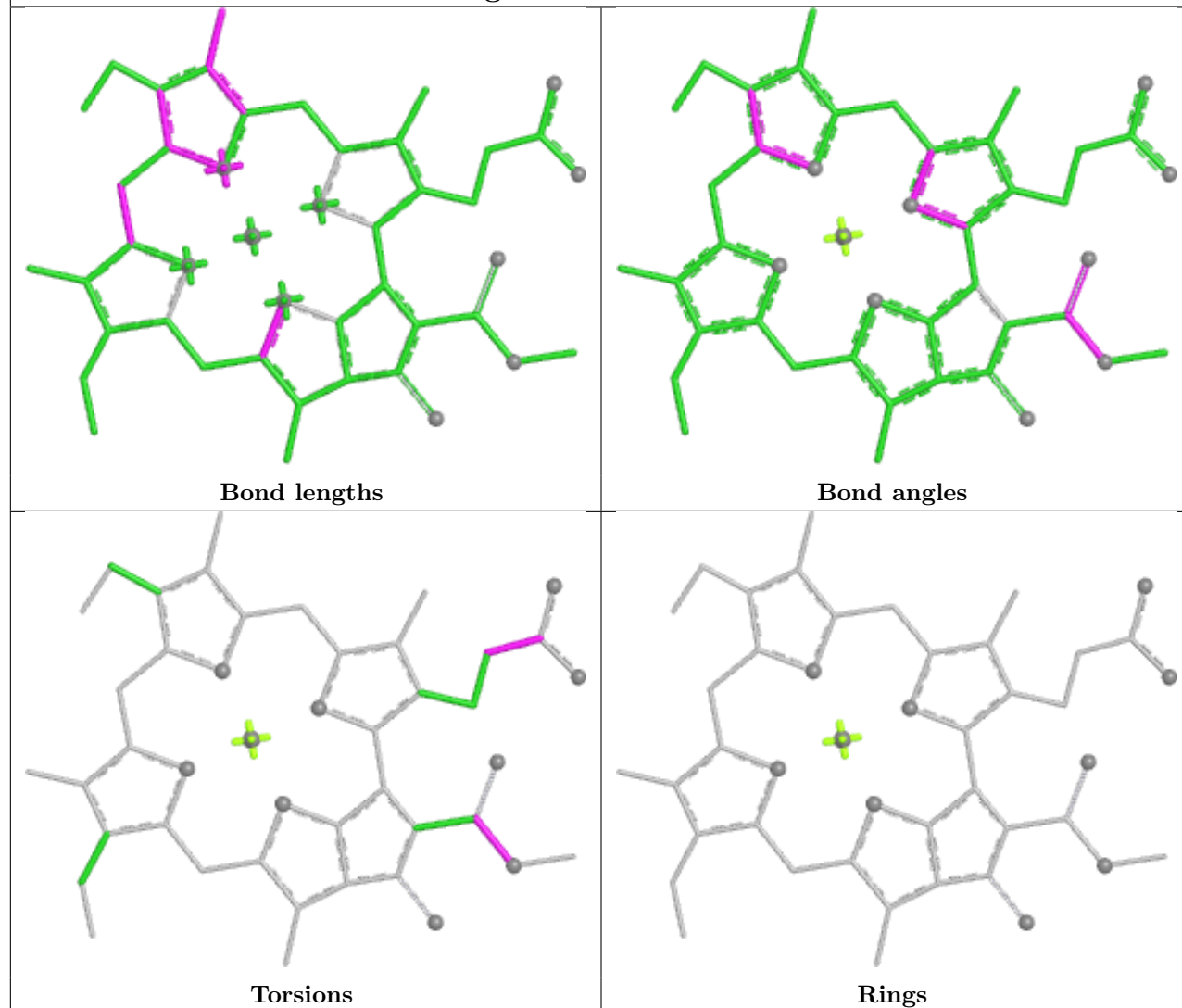
Ligand CLA A 821



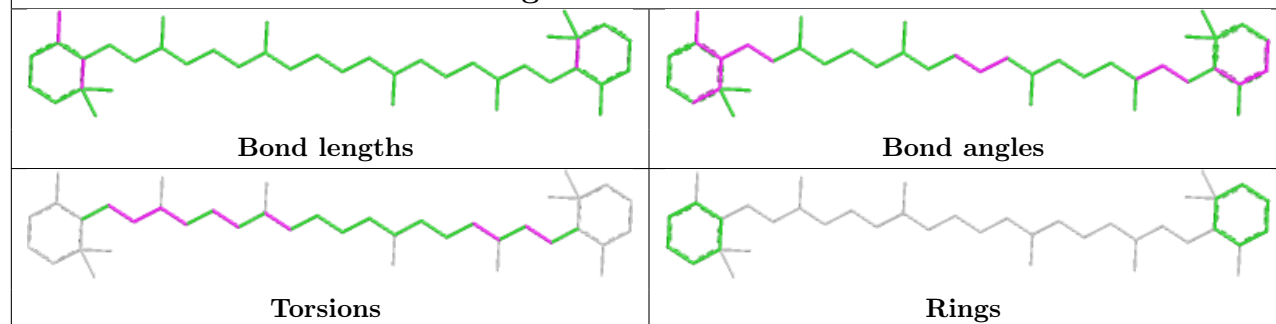
Ligand BCR L 209



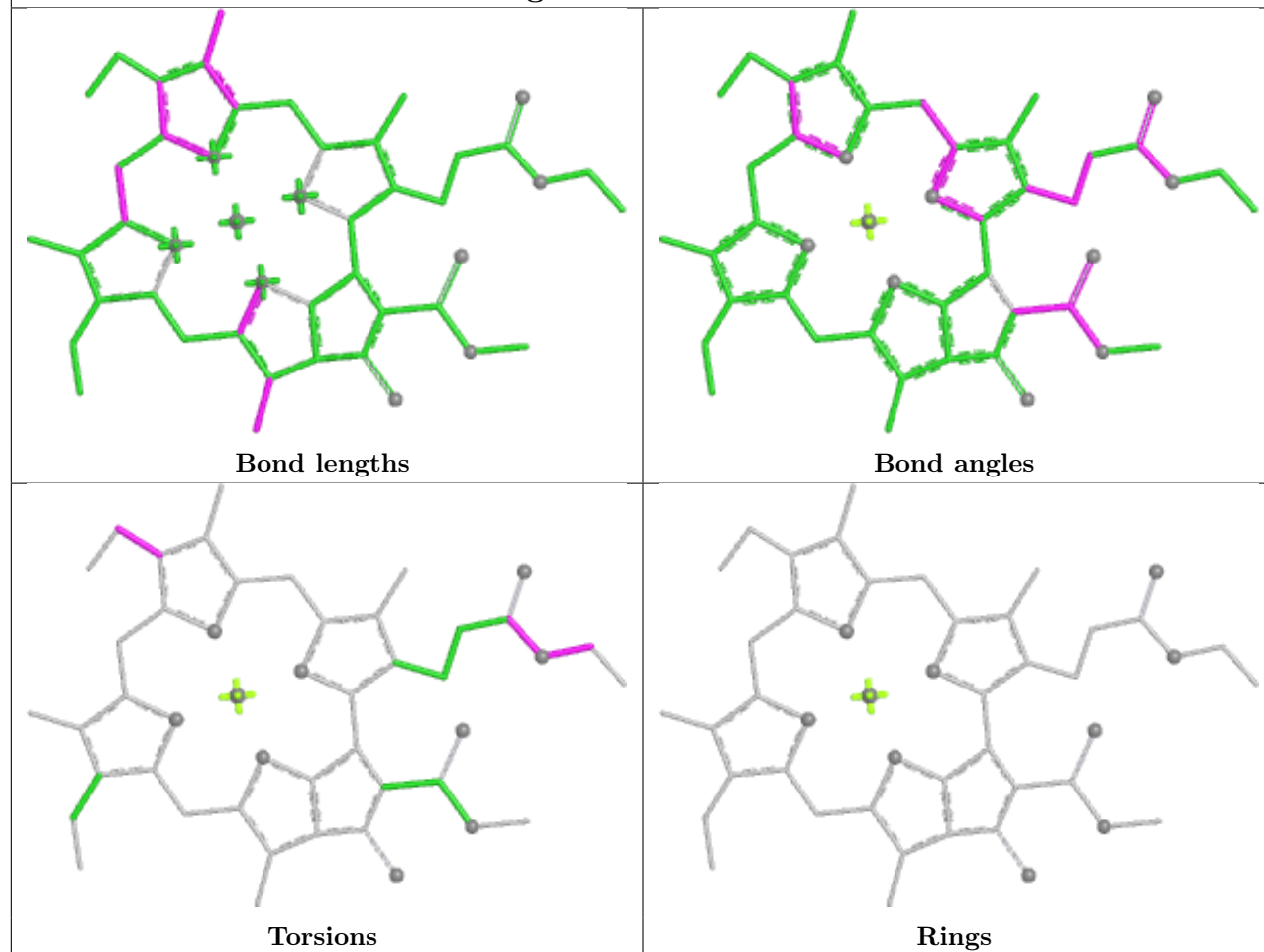
Ligand CLA B 3037



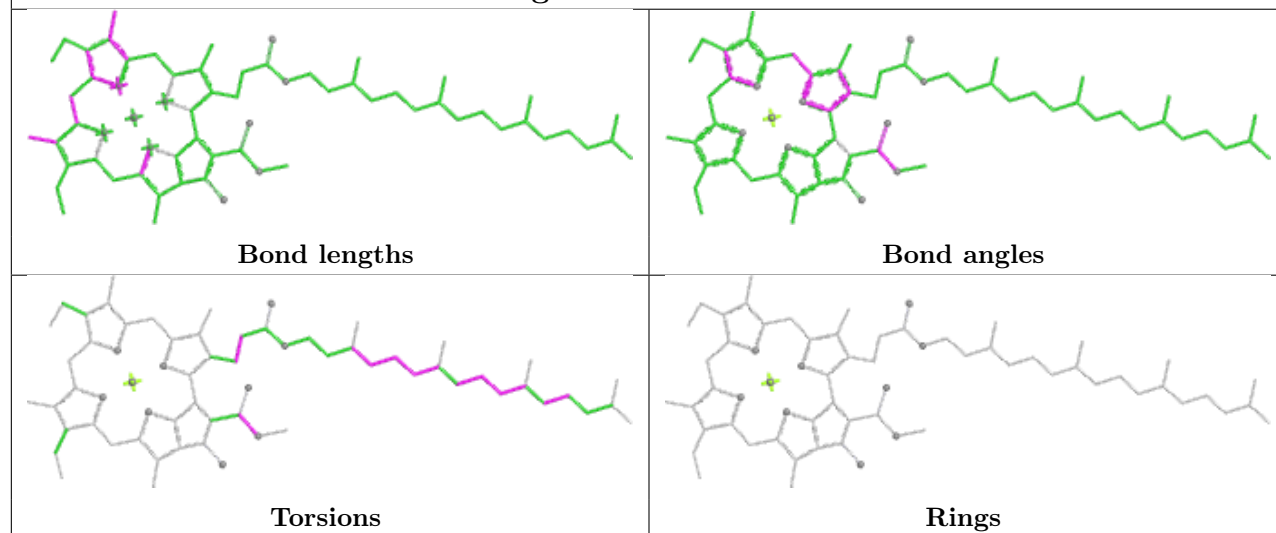
Ligand BCR B 3046



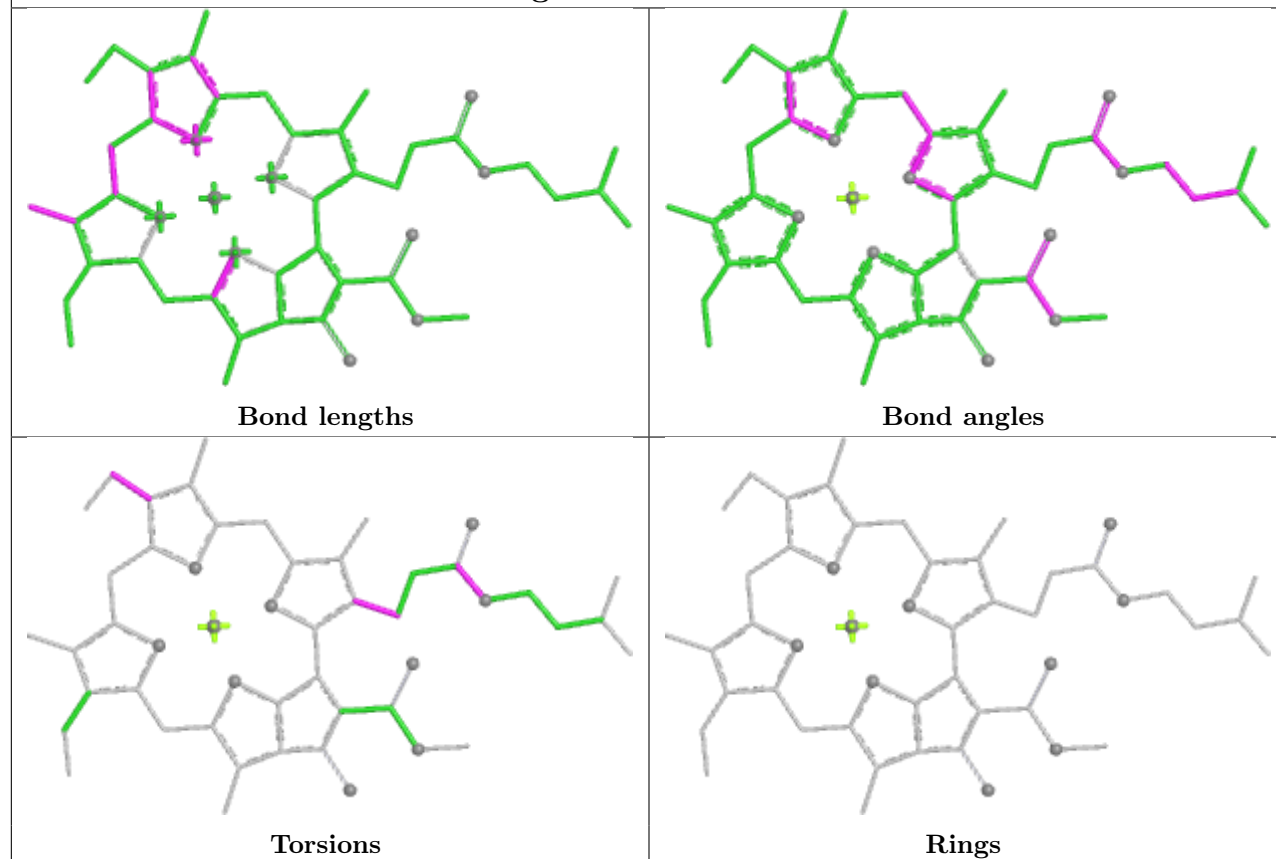
Ligand CLA A 840



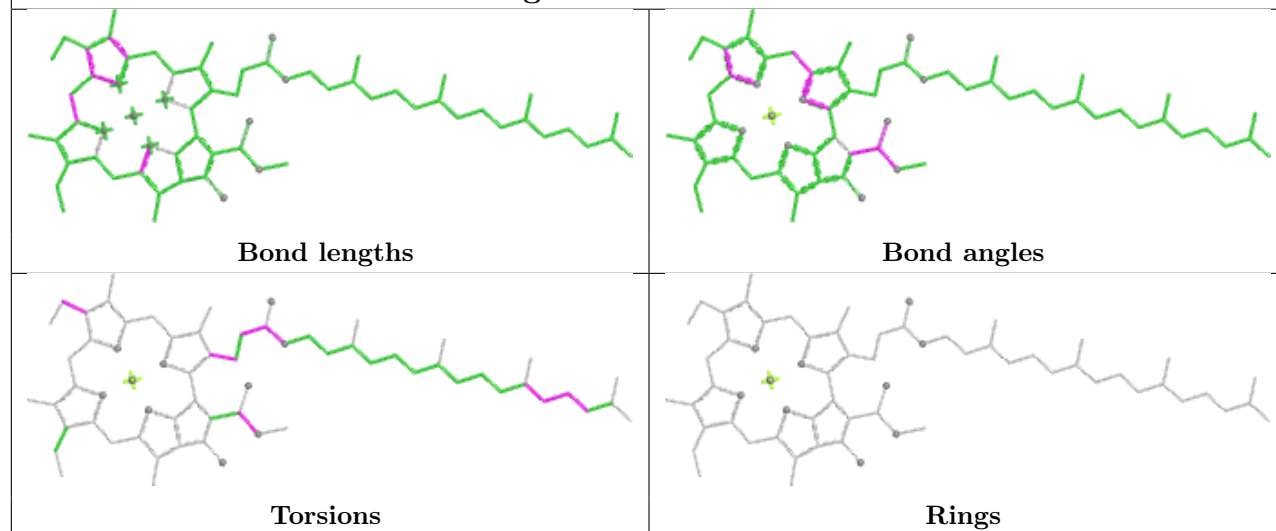
Ligand CLA A 830

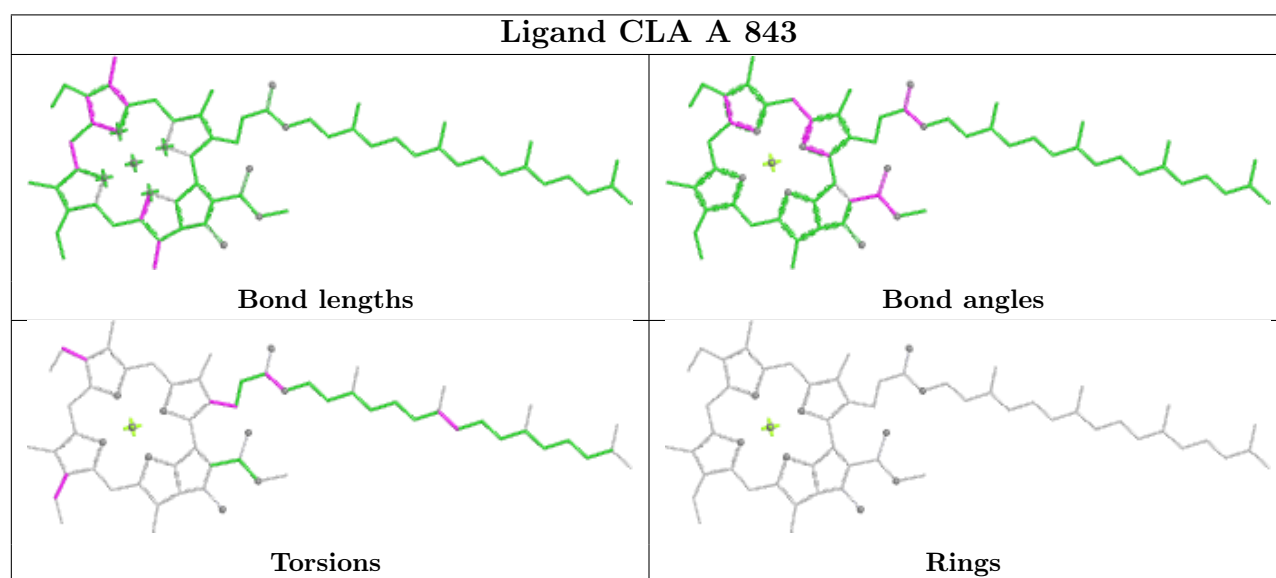
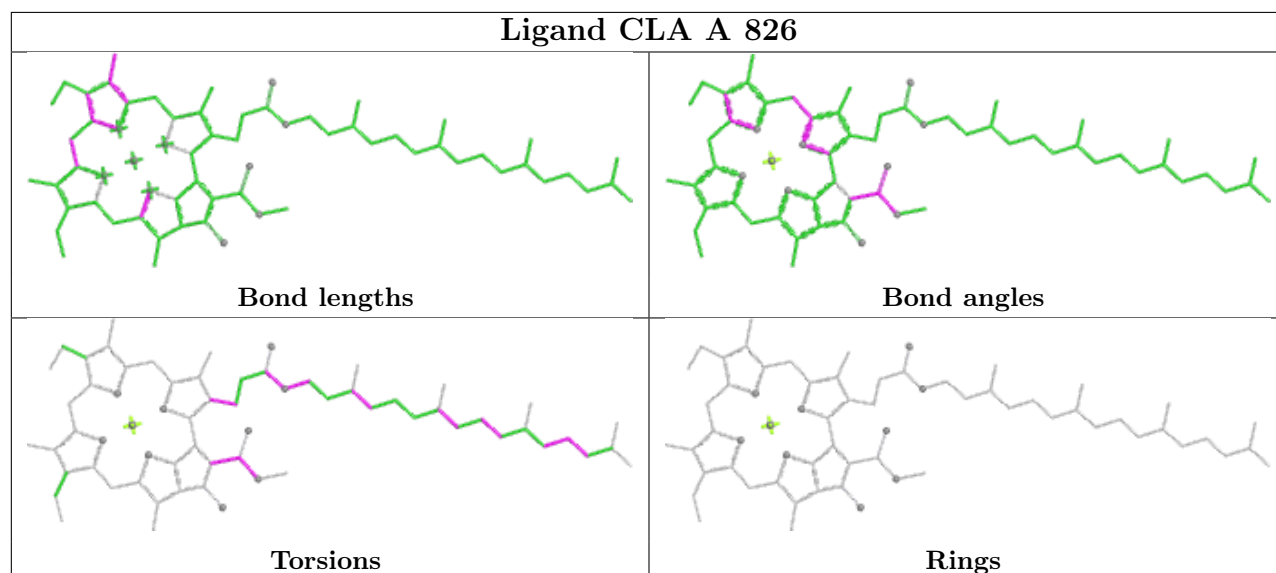
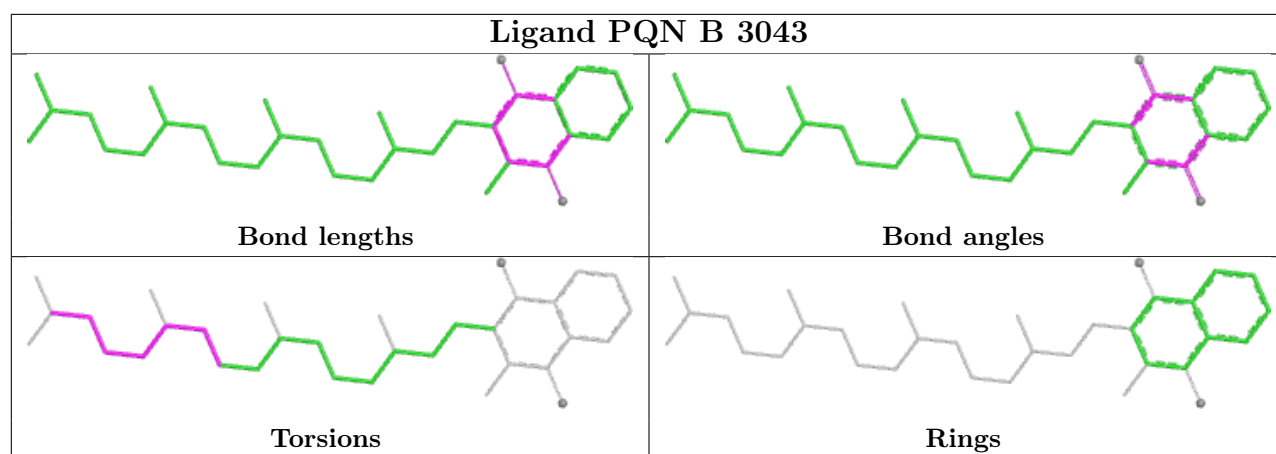


Ligand CLA A 832

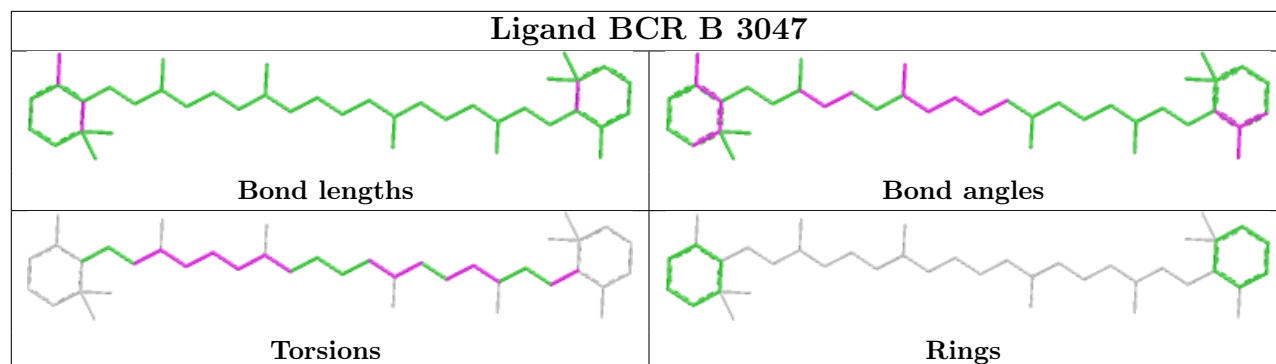


Ligand CLA B 3006

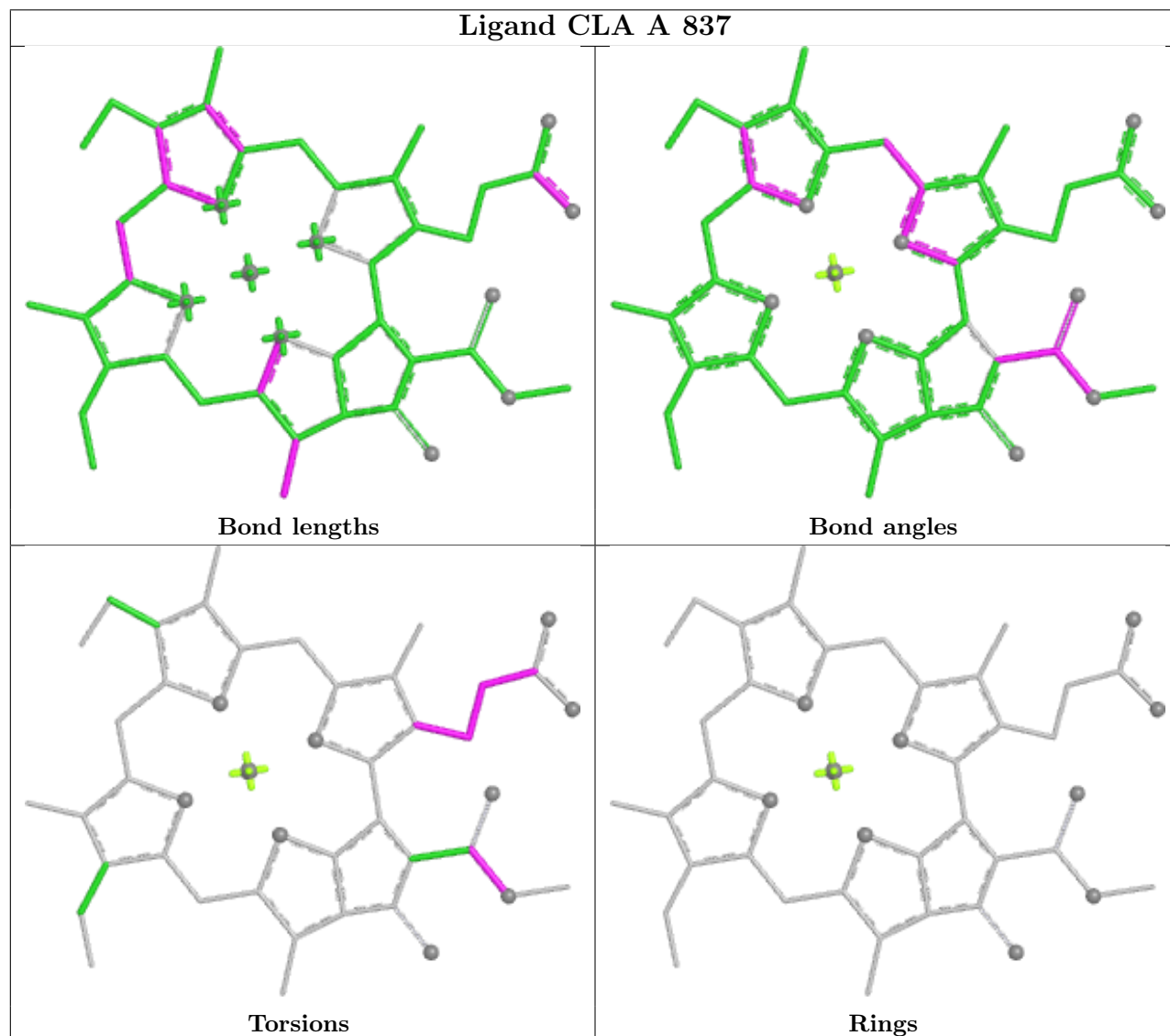


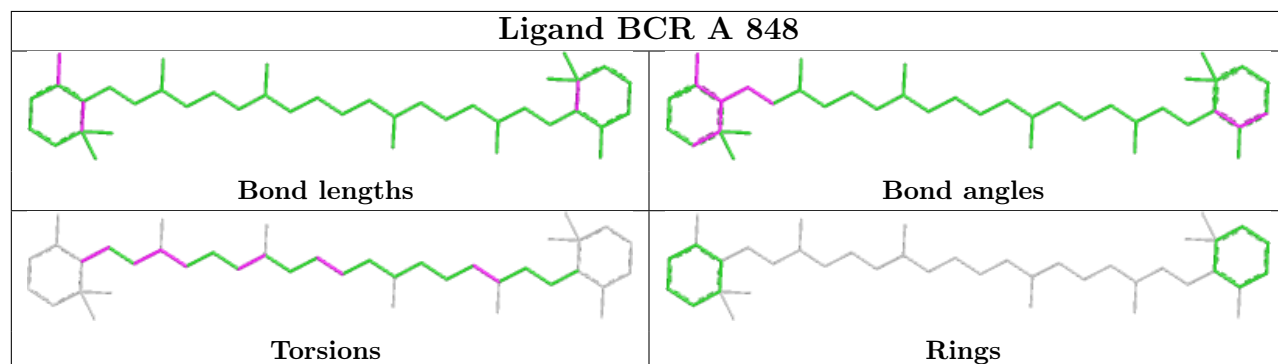
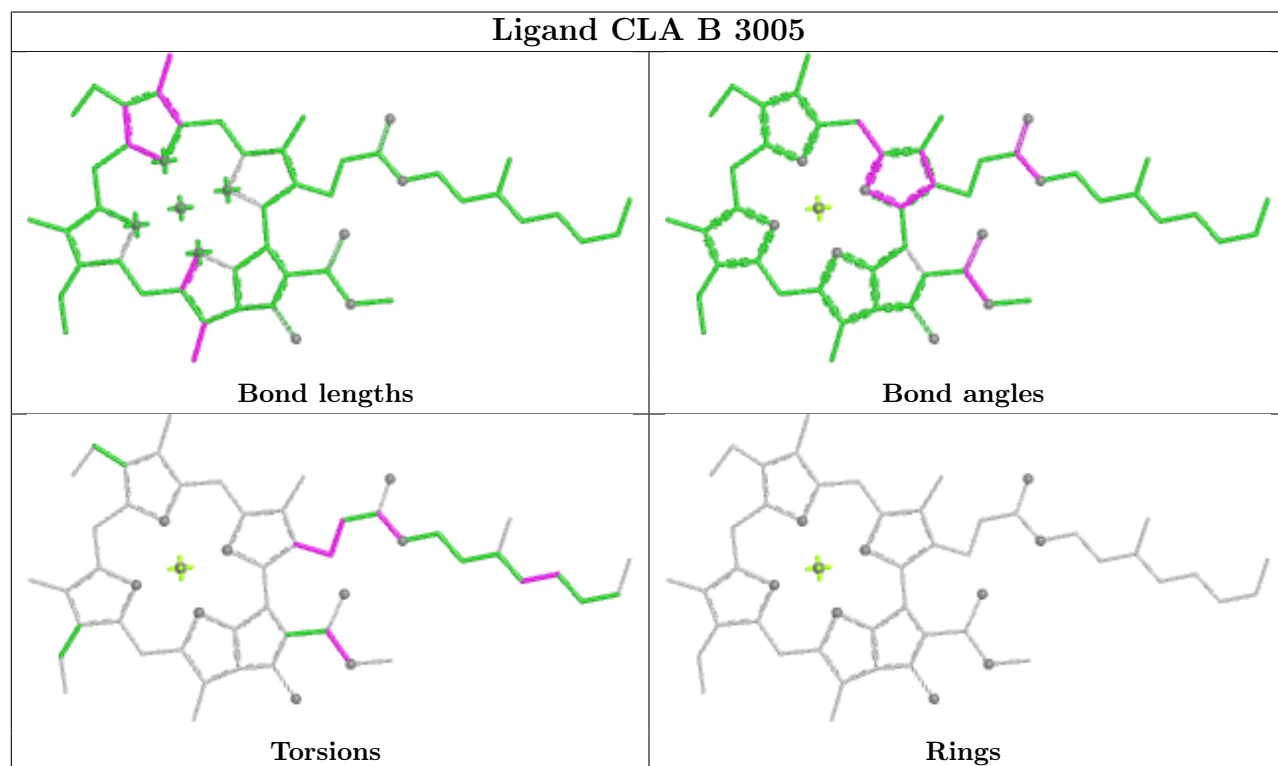
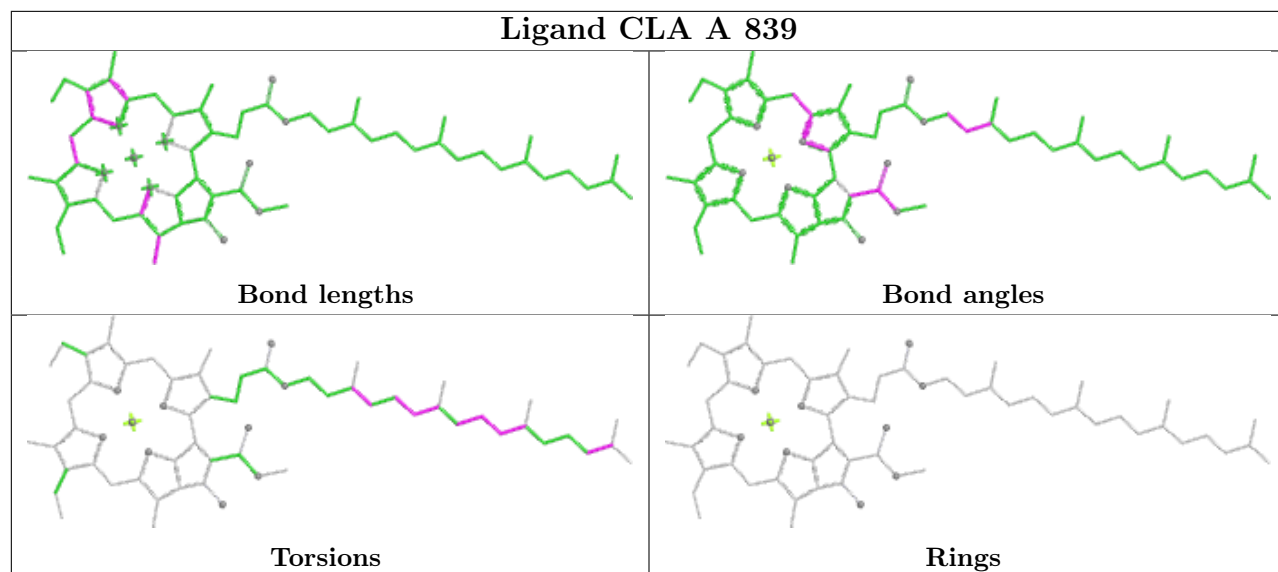


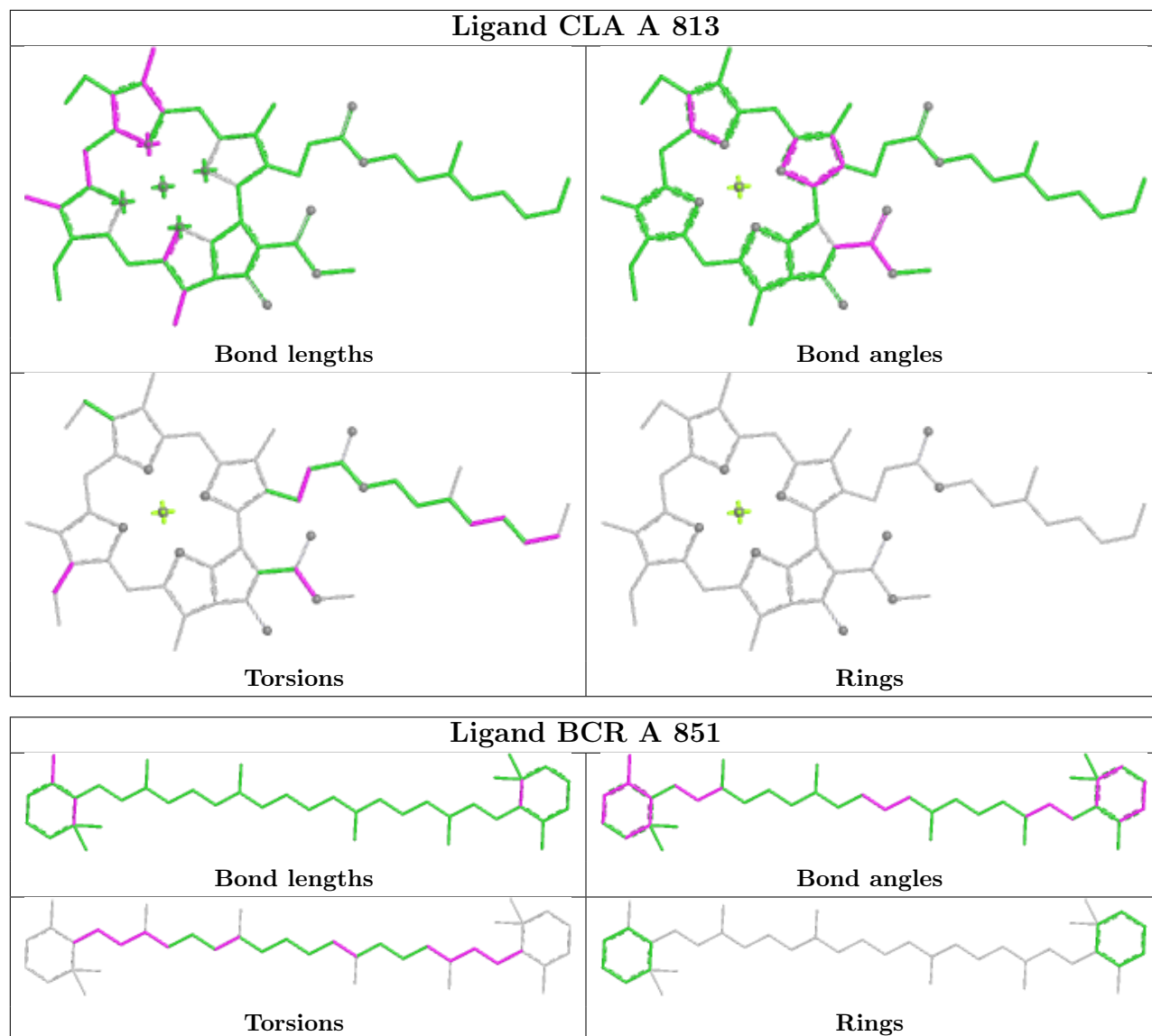
Ligand BCR B 3047



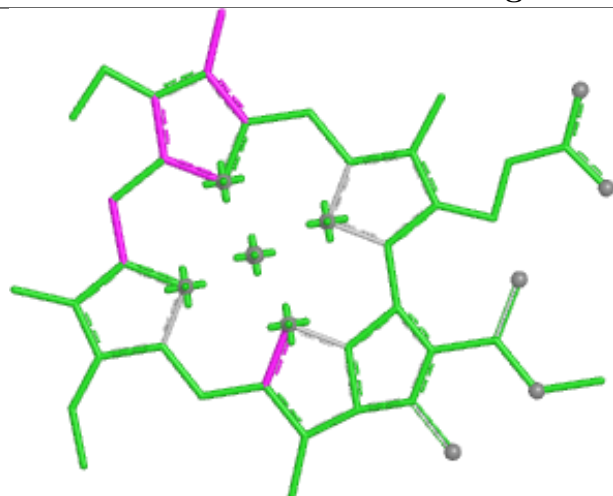
Ligand CLA A 837



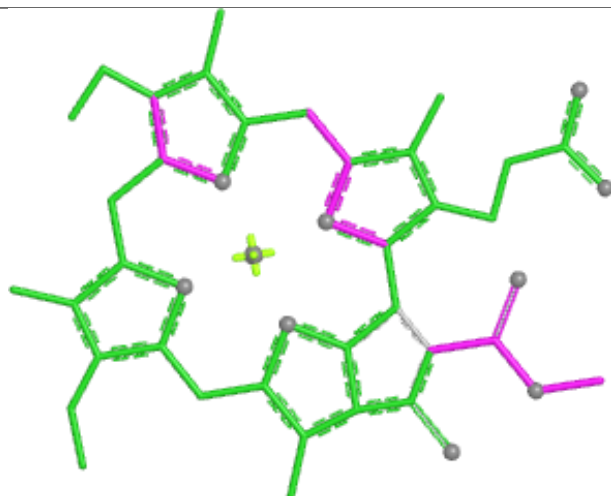




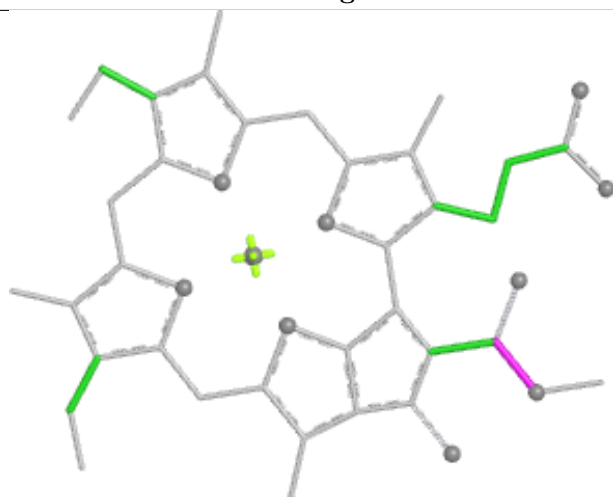
Ligand CLA B 3012



Bond lengths



Bond angles

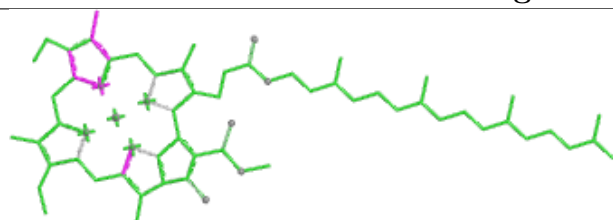


Torsions

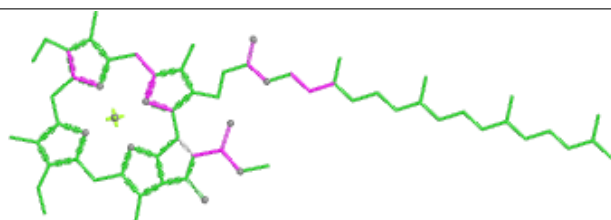


Rings

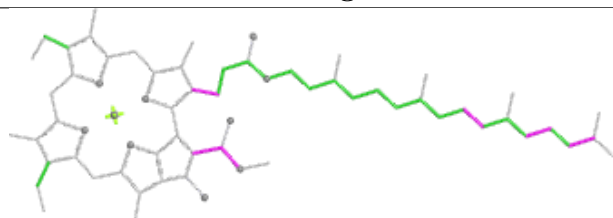
Ligand CLA A 831



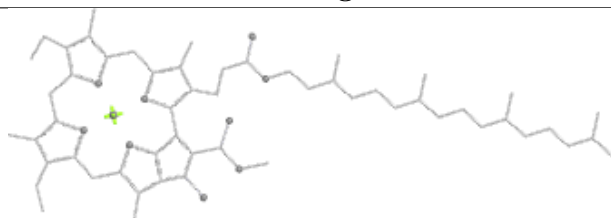
Bond lengths



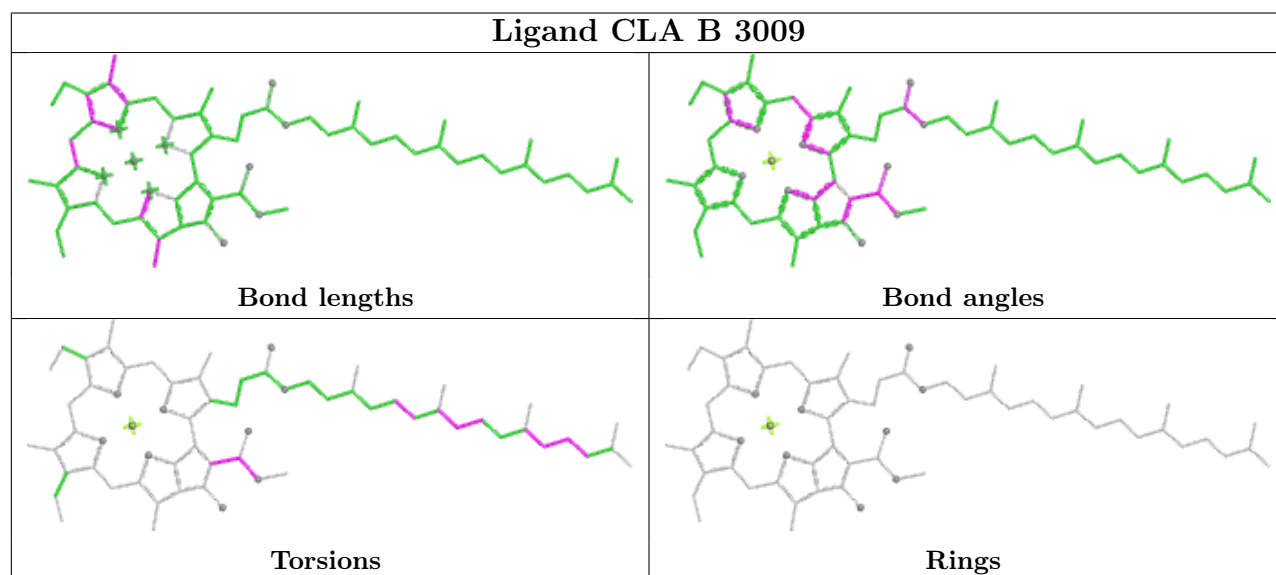
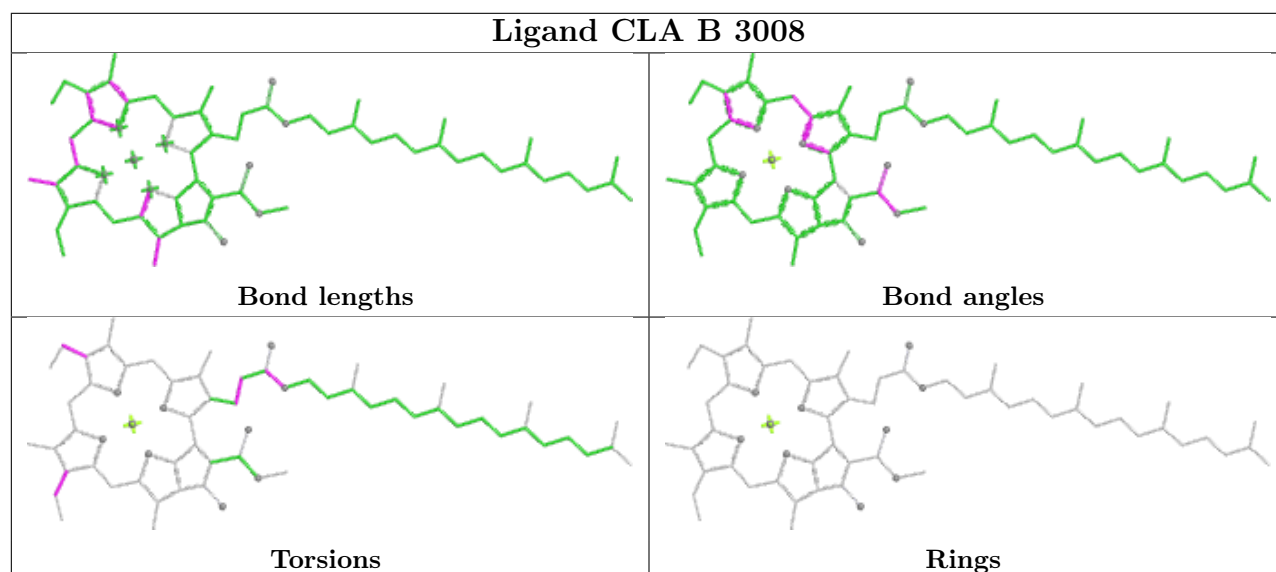
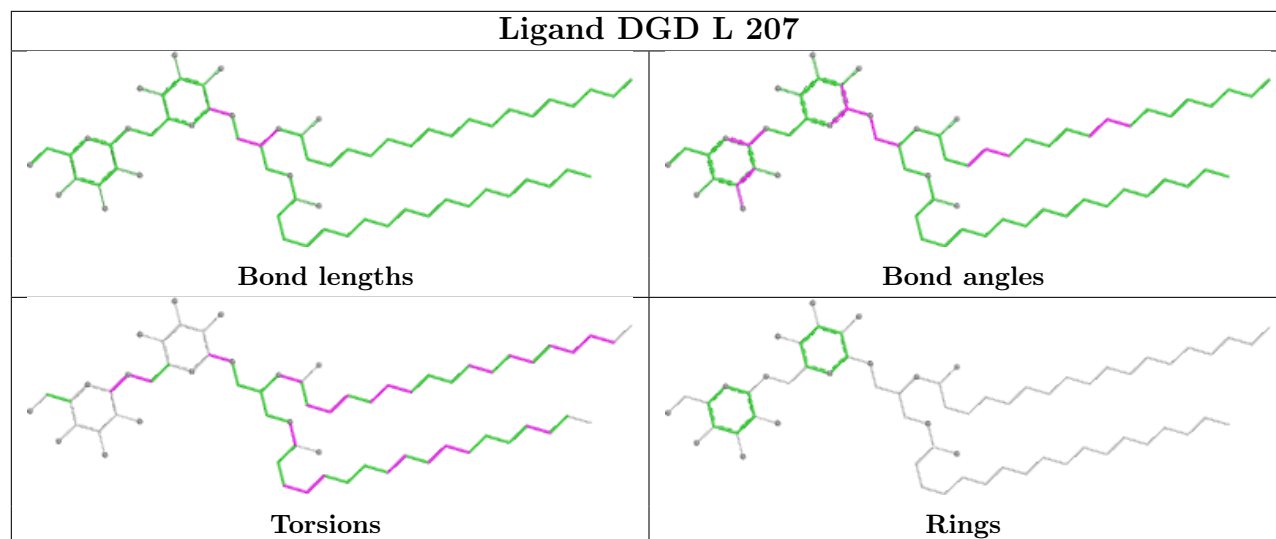
Bond angles

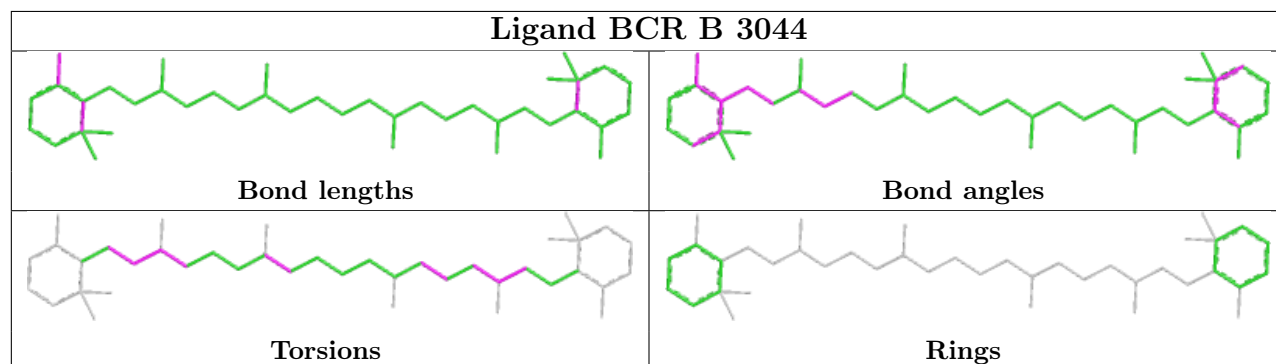
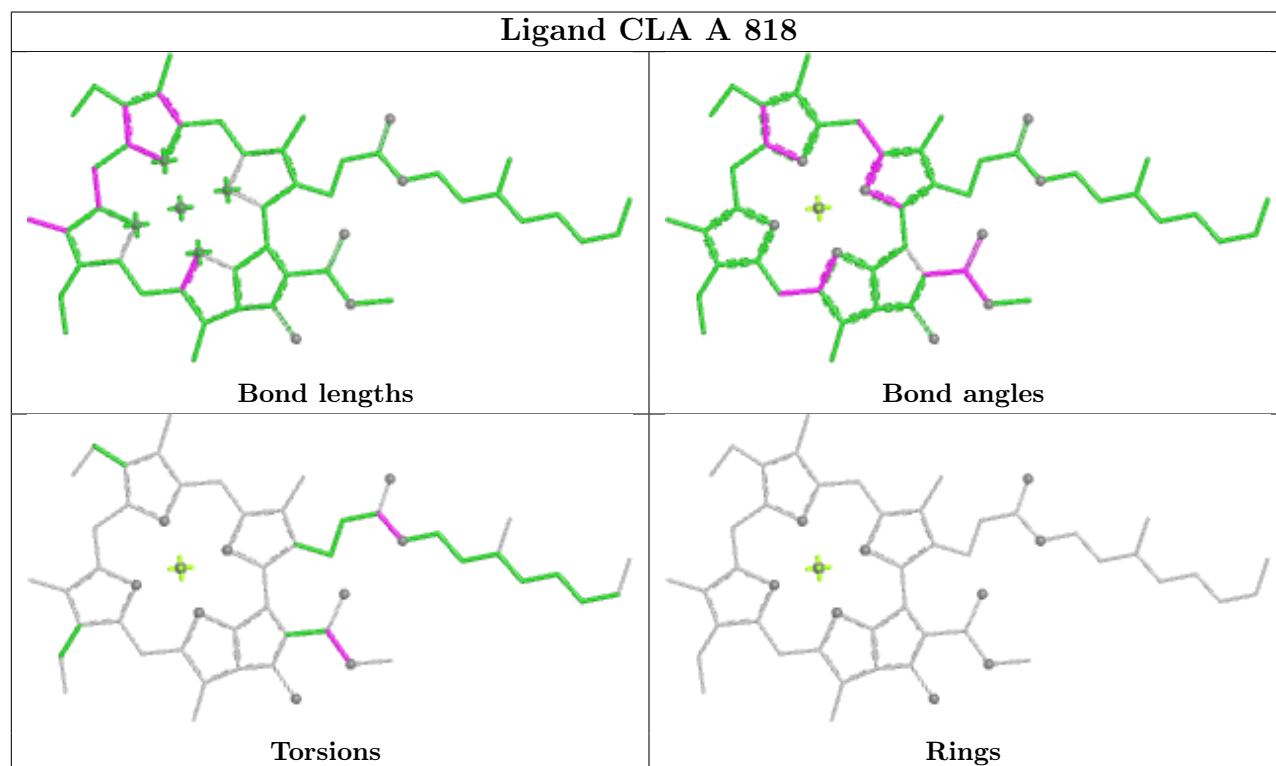
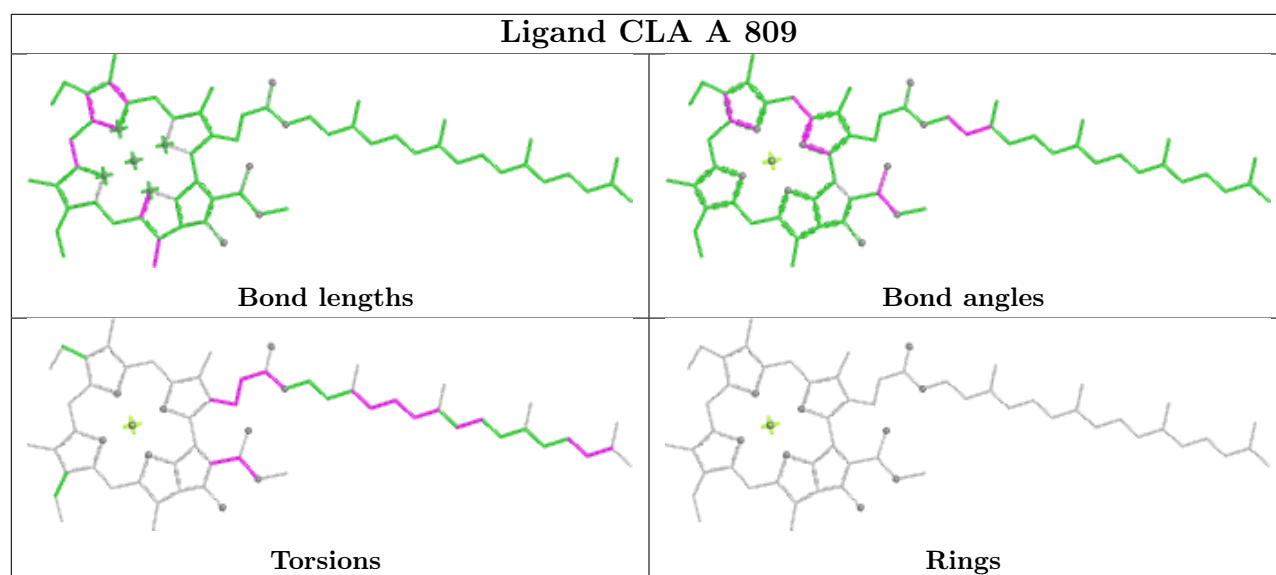


Torsions

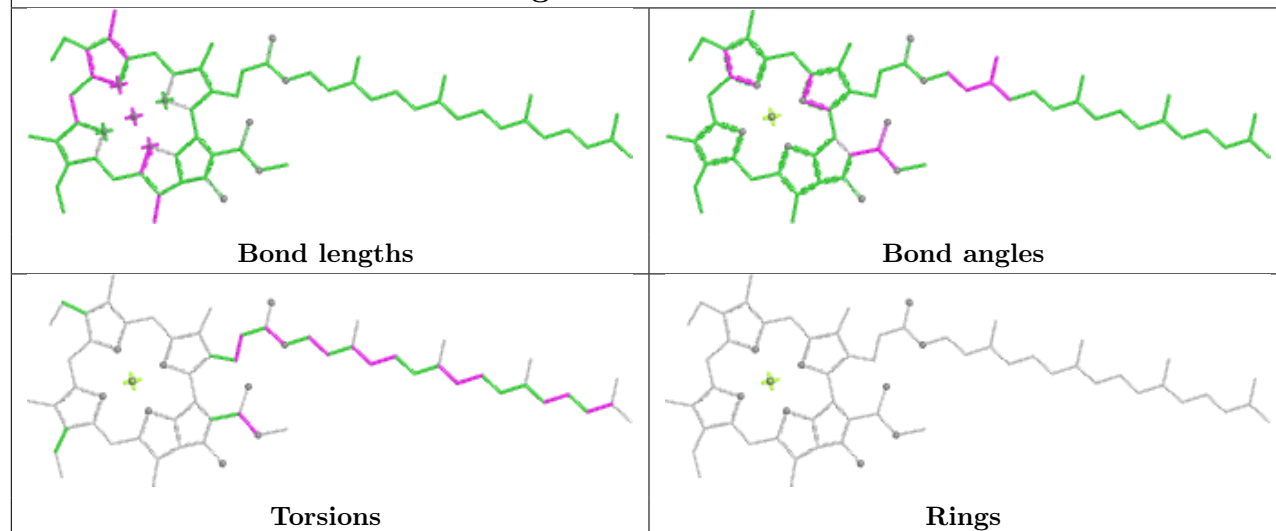


Rings

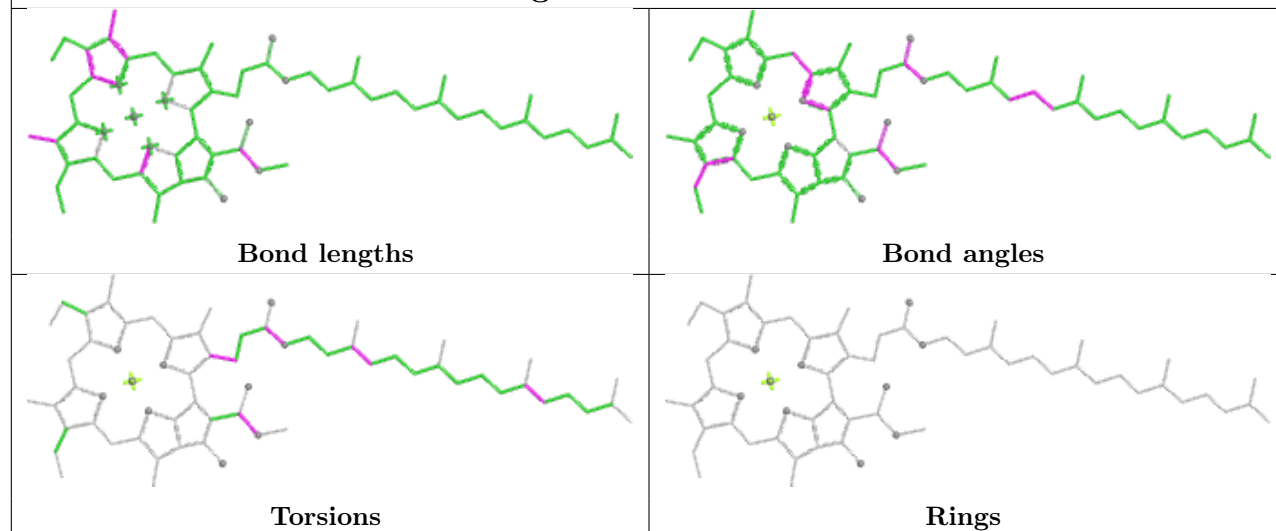




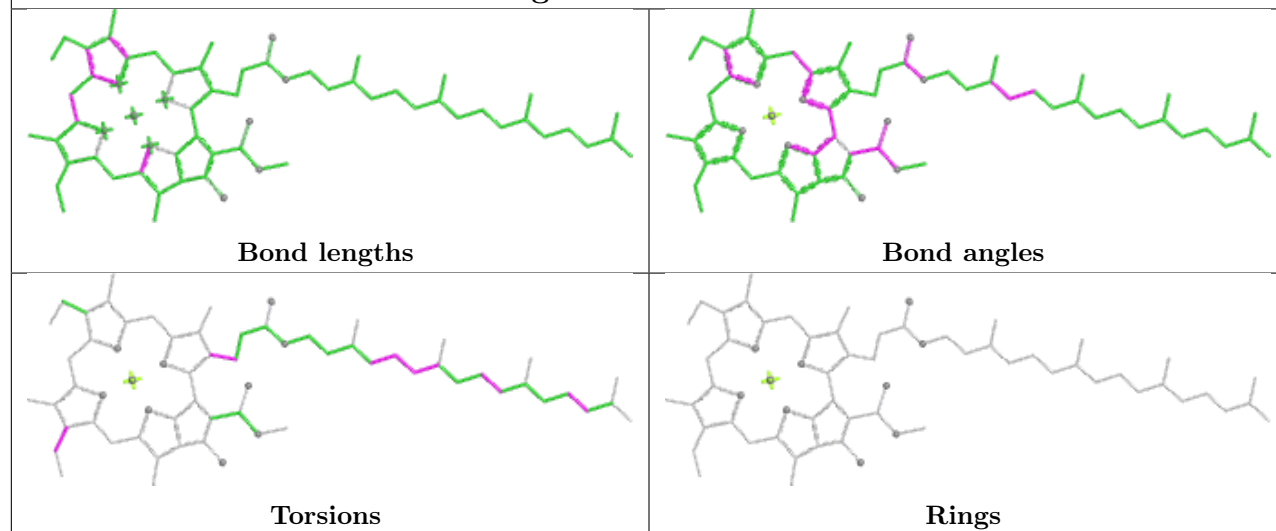
Ligand CLA A 856



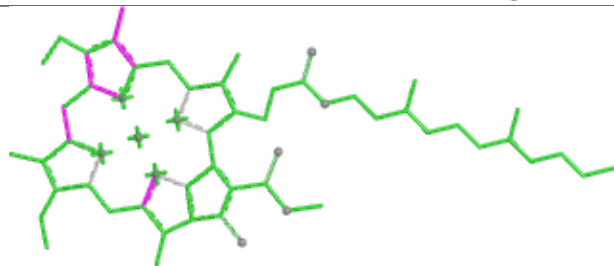
Ligand CLA A 812



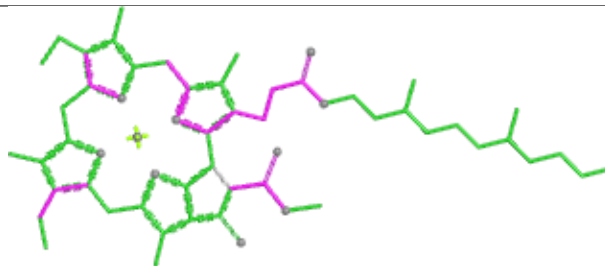
Ligand CLA A 810



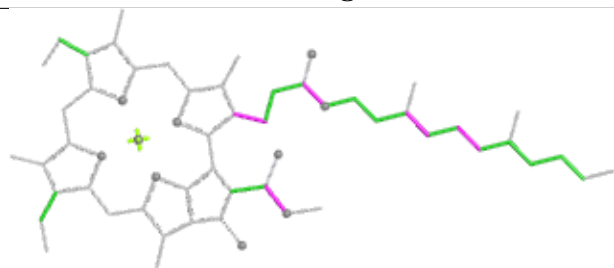
Ligand CLA B 3034



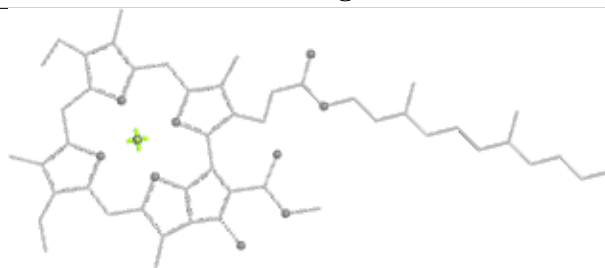
Bond lengths



Bond angles

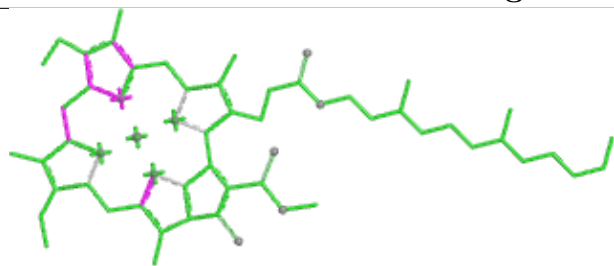


Torsions

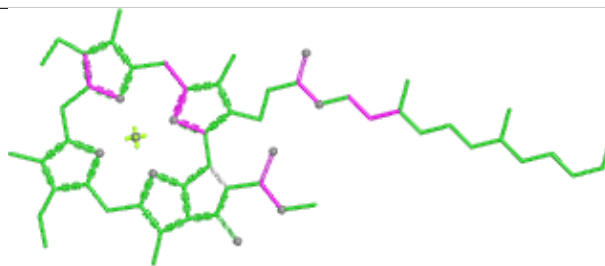


Rings

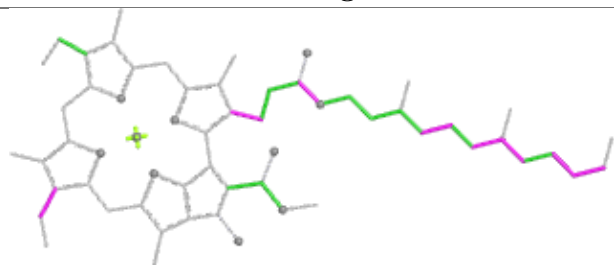
Ligand CLA B 3018



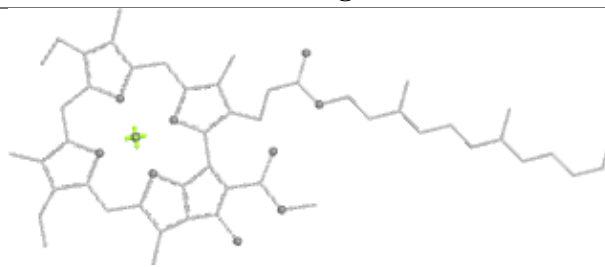
Bond lengths



Bond angles

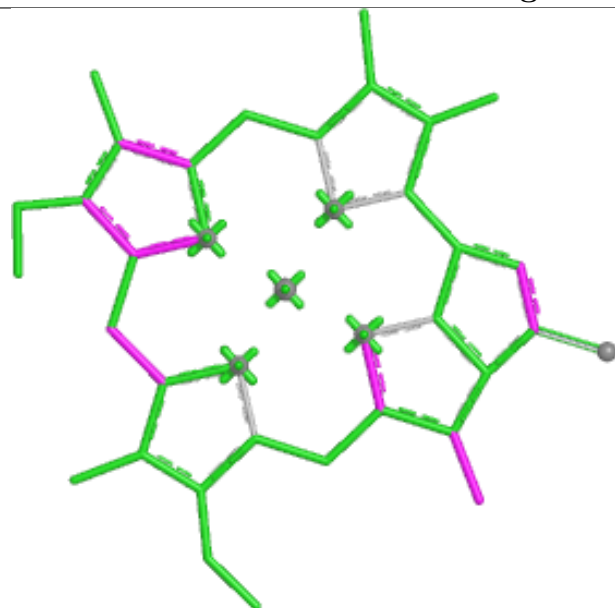


Torsions

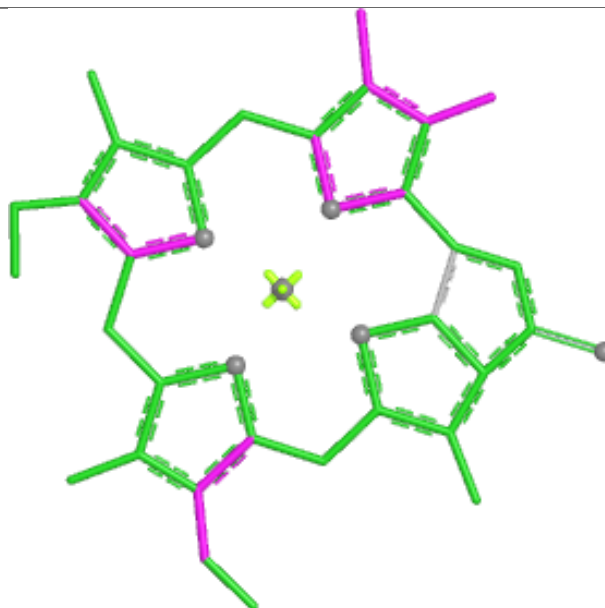


Rings

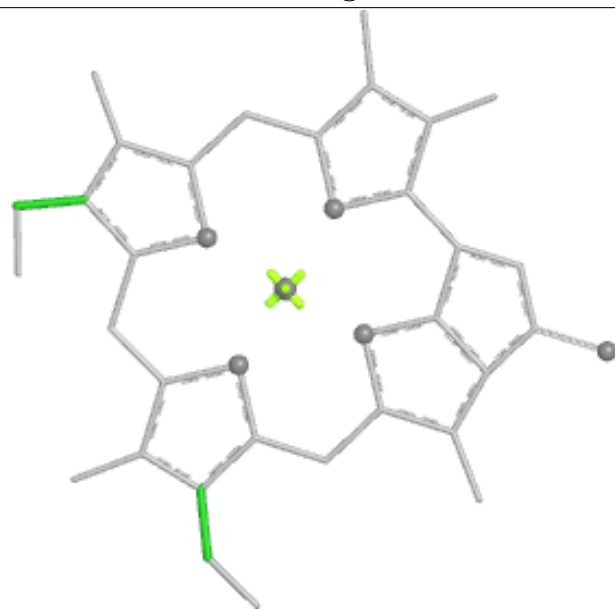
Ligand CLA J 102



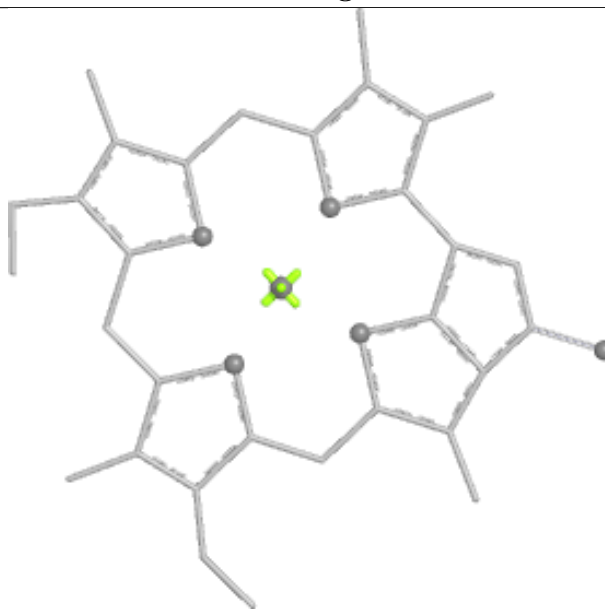
Bond lengths



Bond angles

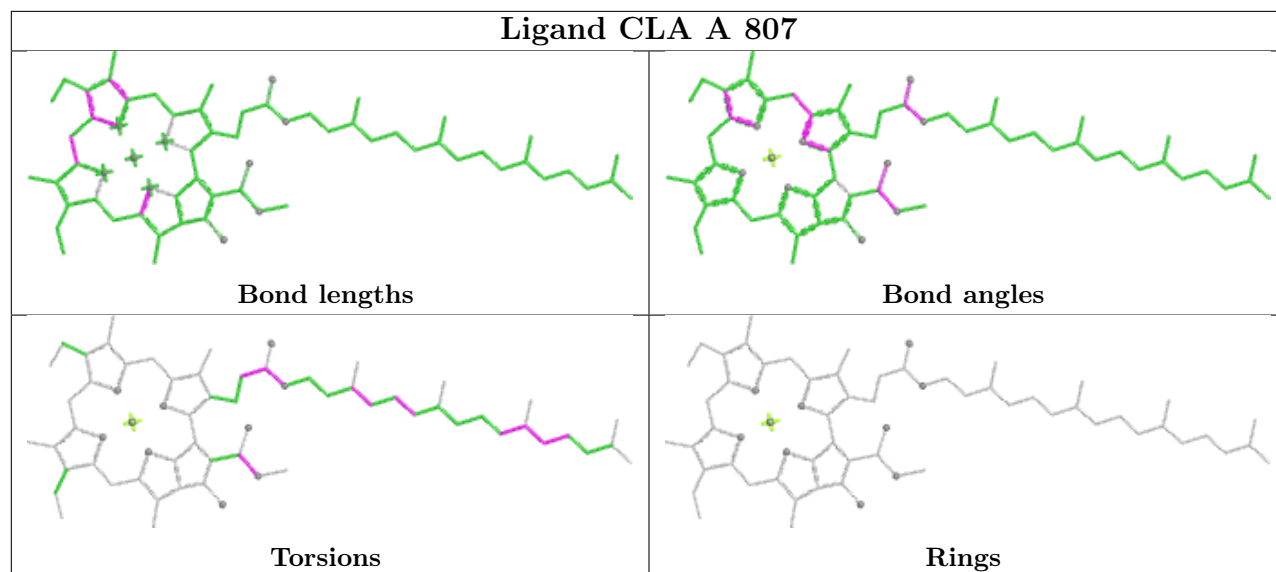


Torsions

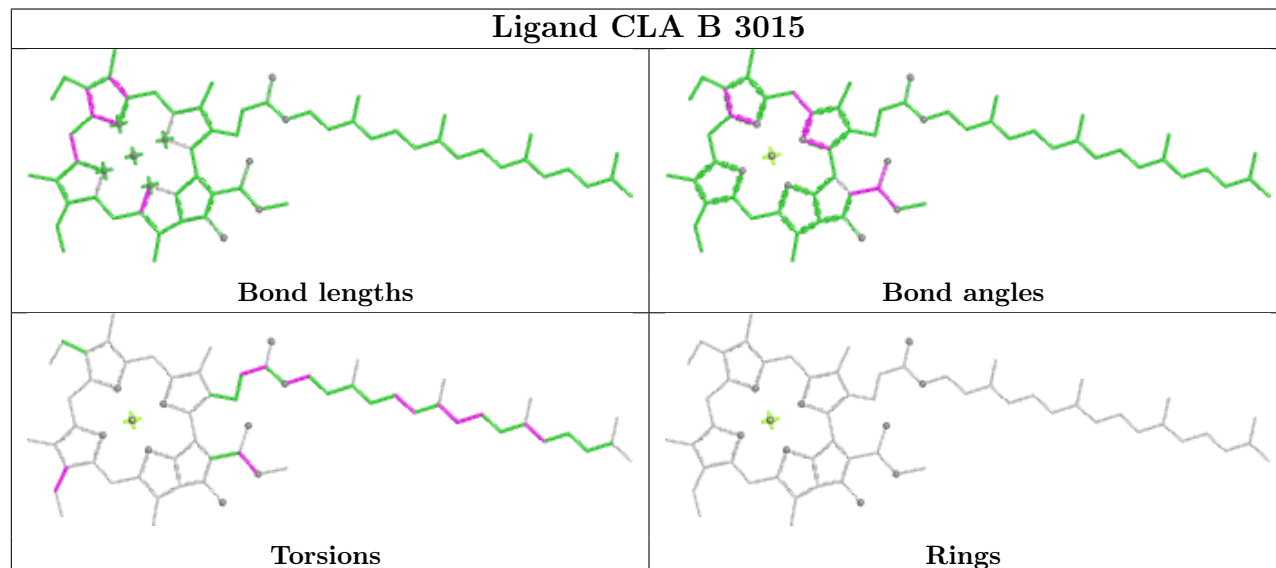


Rings

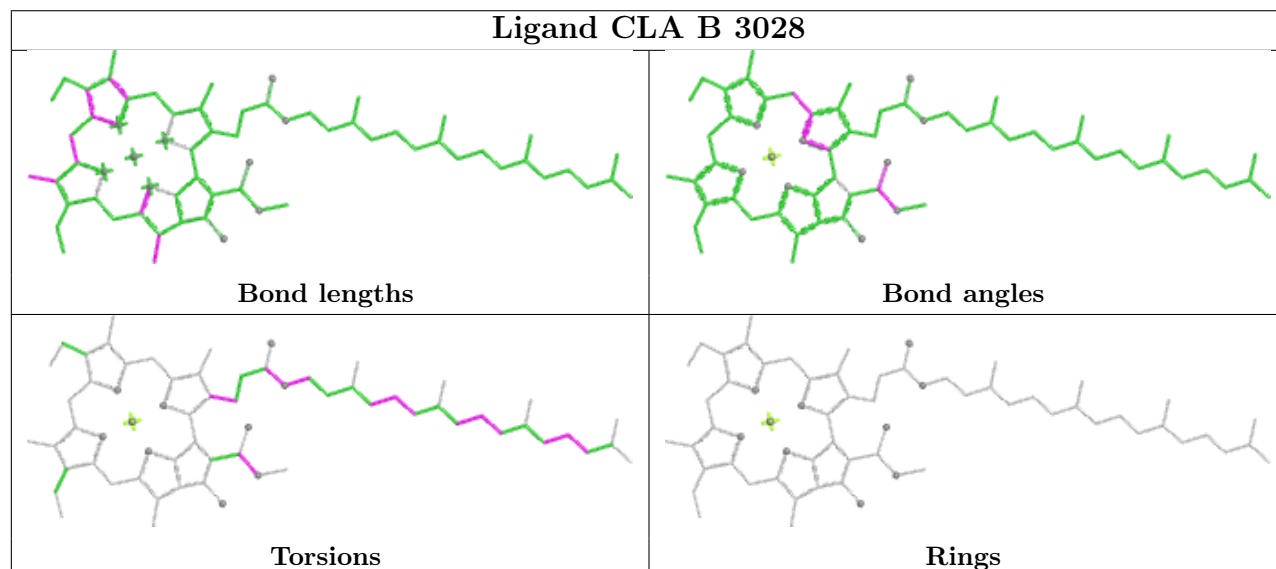
Ligand CLA A 807

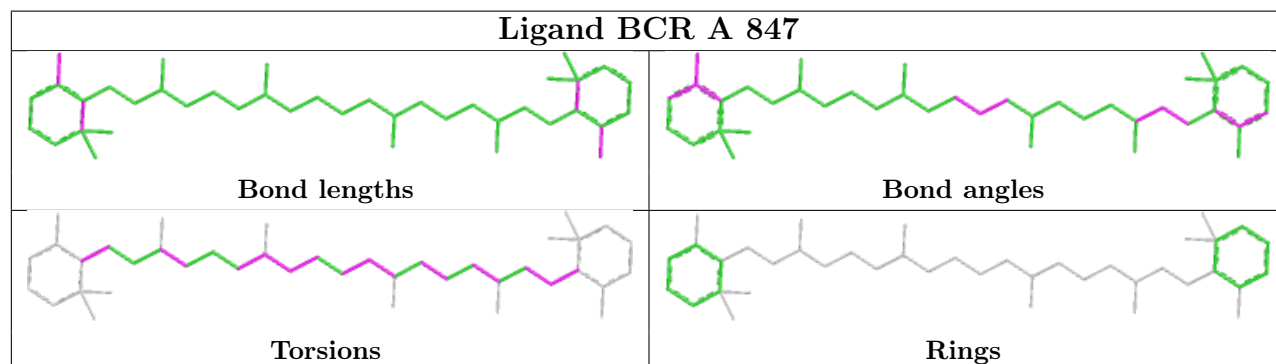
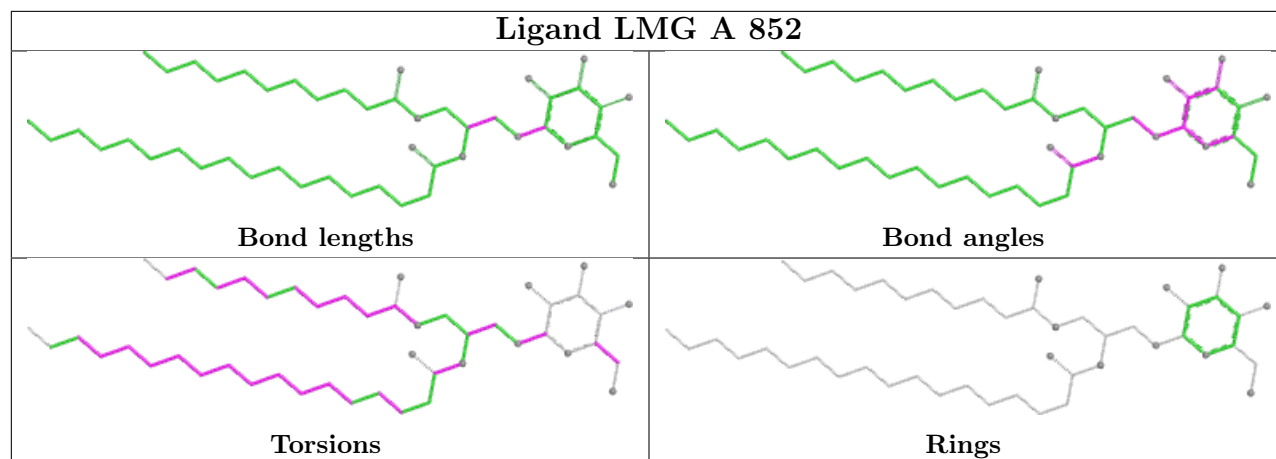


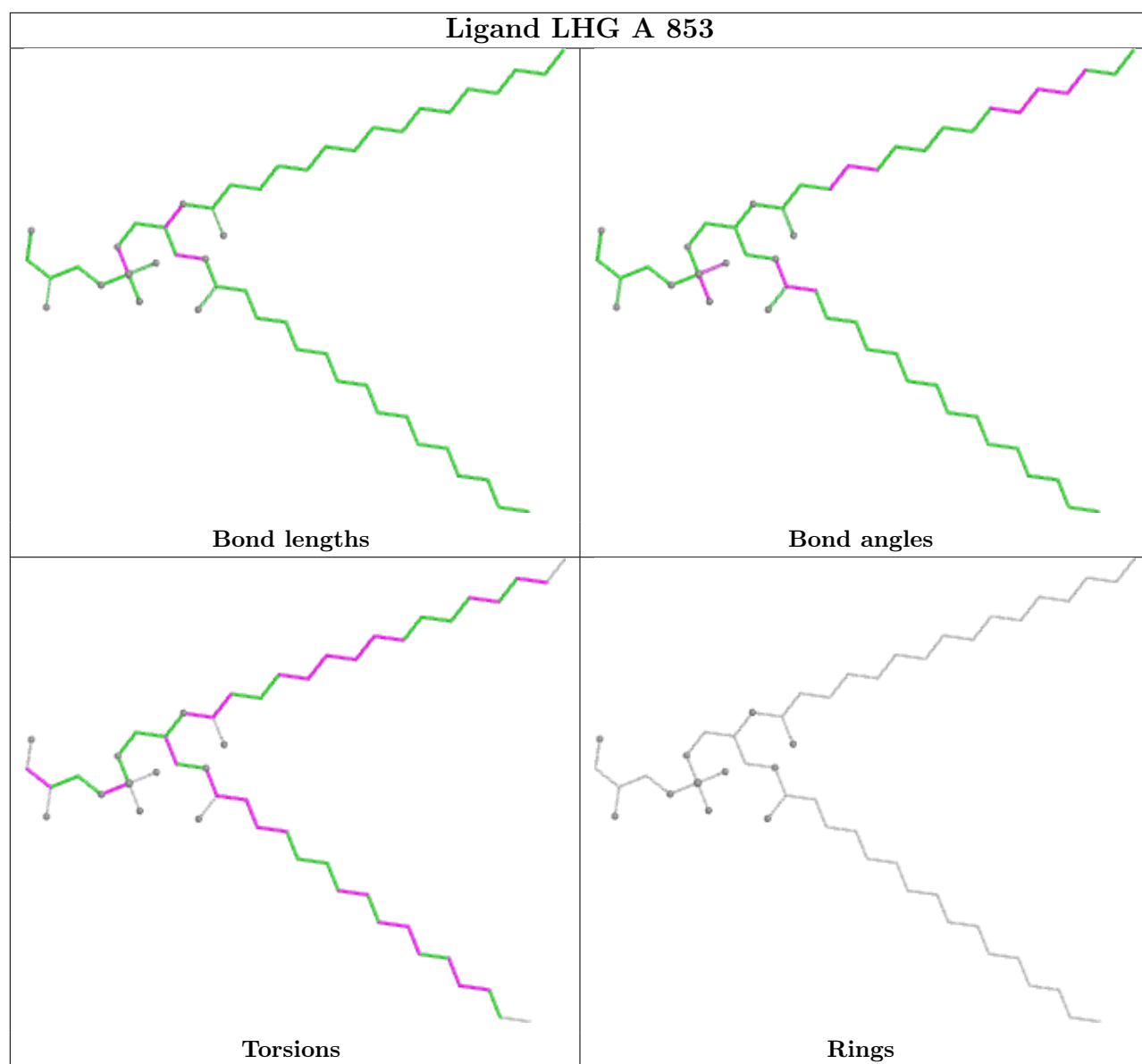
Ligand CLA B 3015



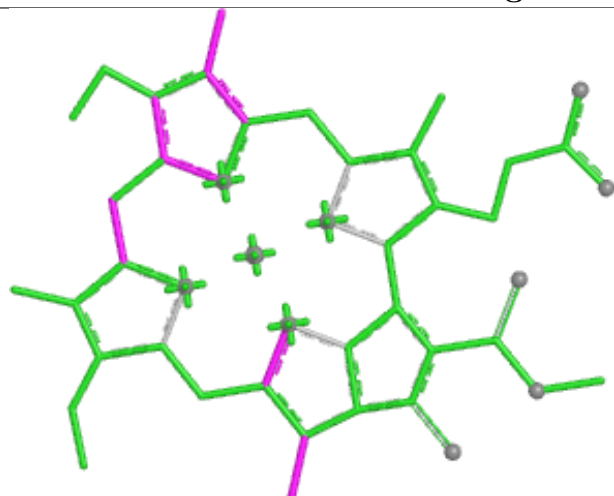
Ligand CLA B 3028



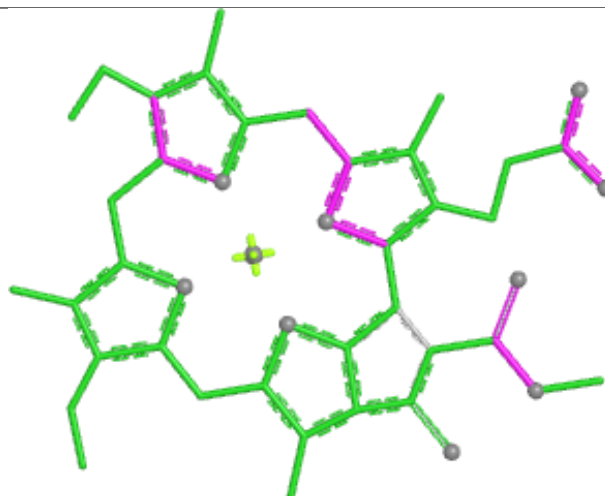




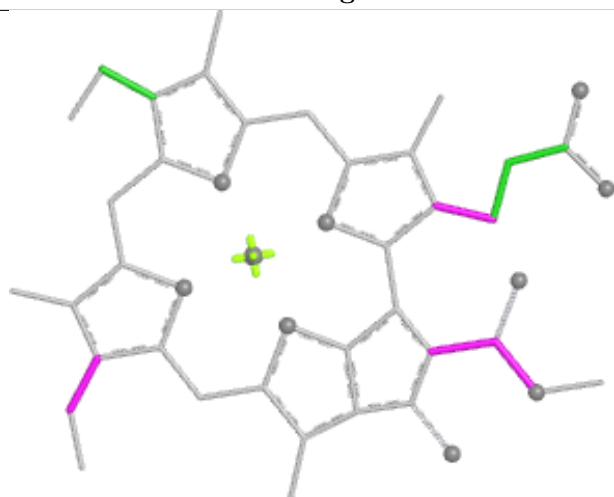
Ligand CLA B 3022



Bond lengths



Bond angles

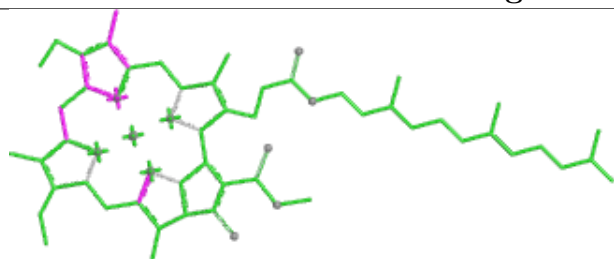


Torsions

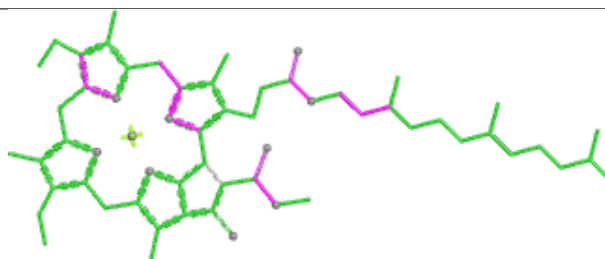


Rings

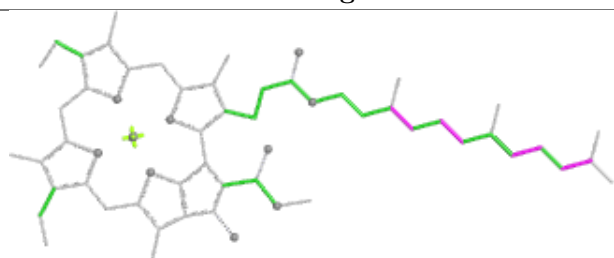
Ligand CLA B 3038



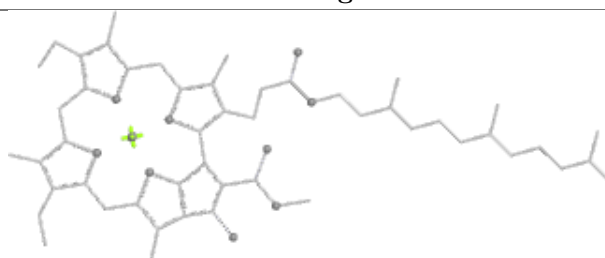
Bond lengths



Bond angles

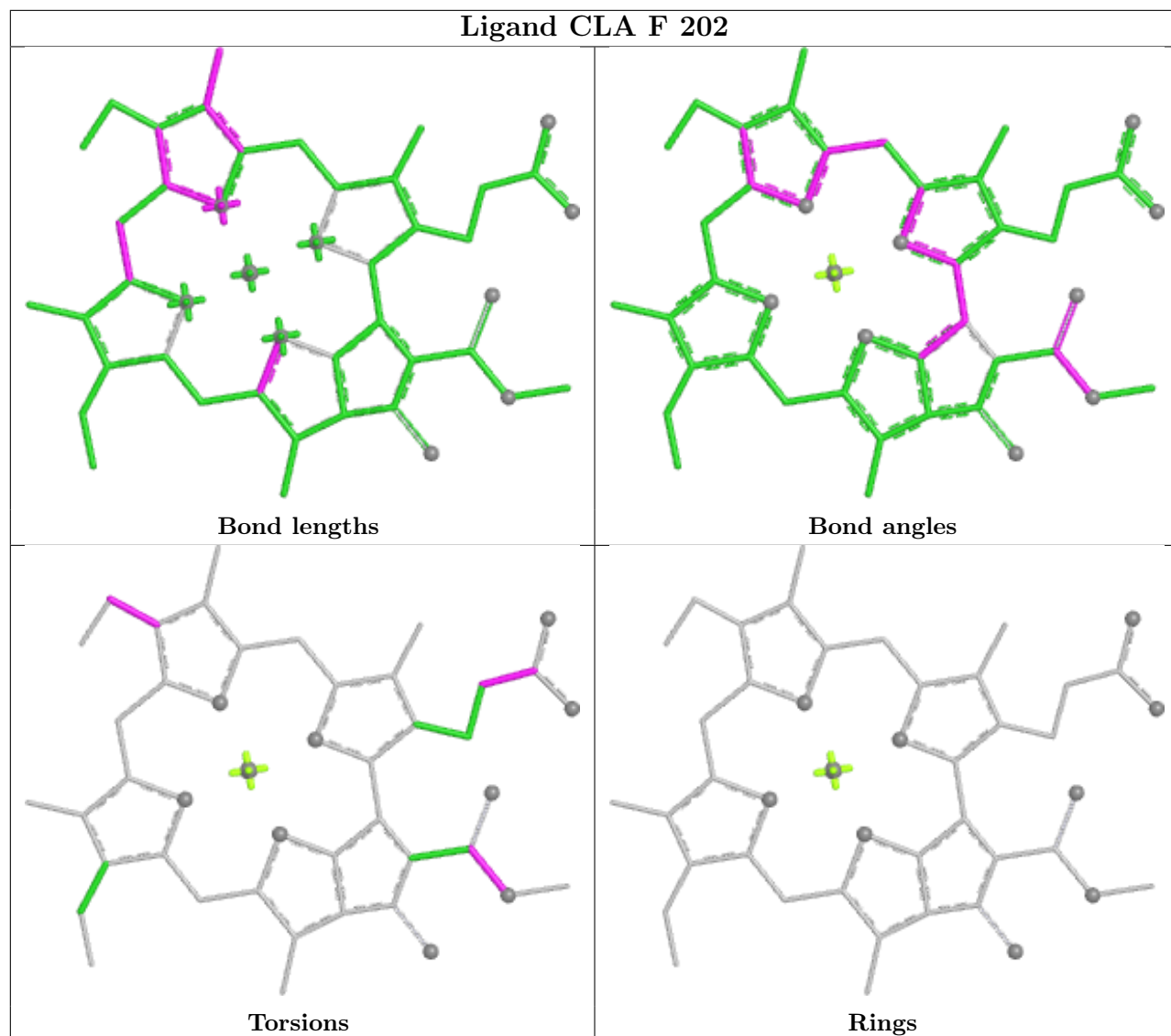


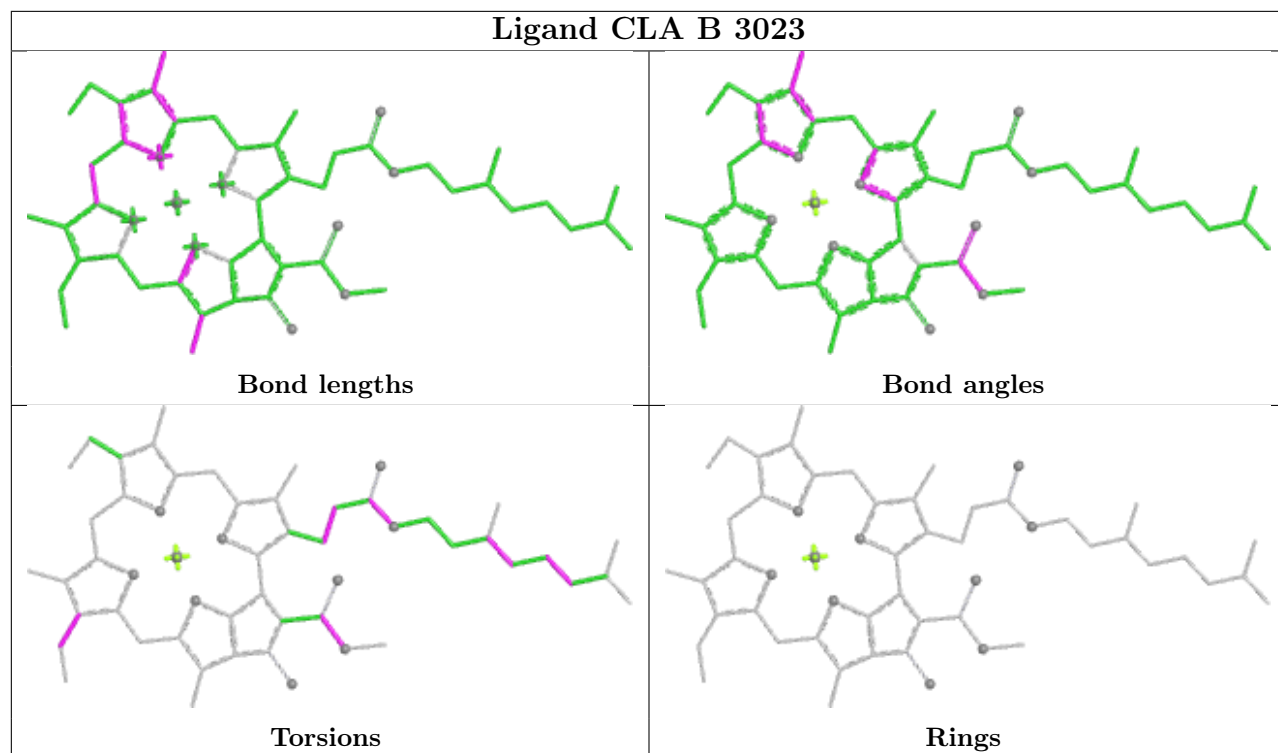
Torsions



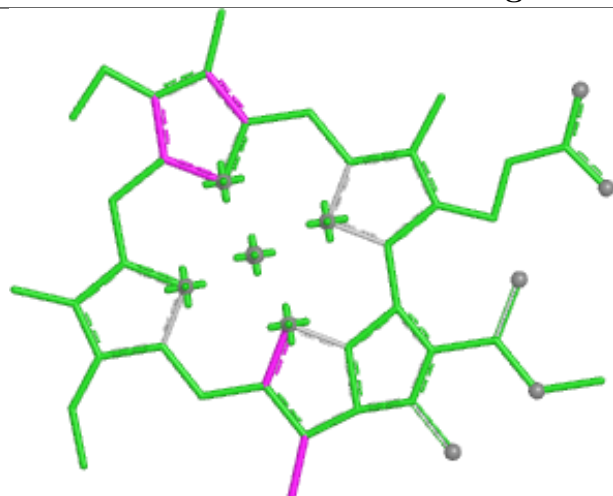
Rings

Ligand CLA F 202

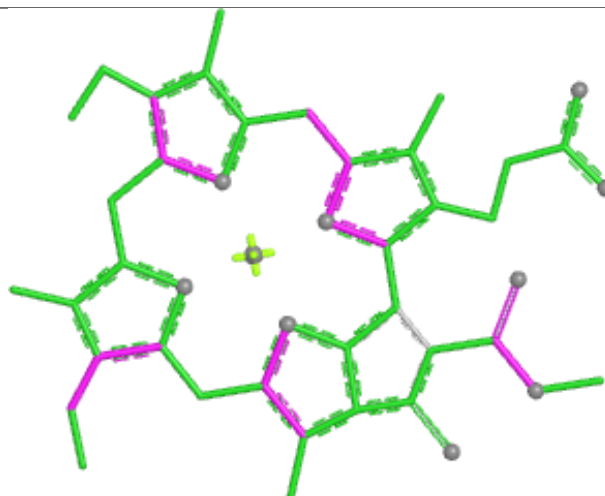




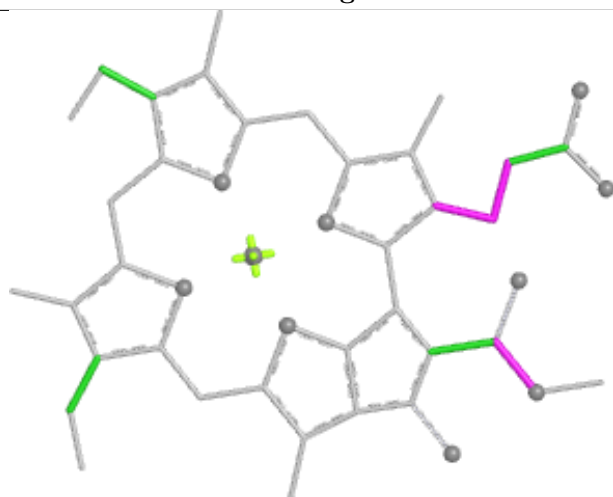
Ligand CLA B 3016



Bond lengths



Bond angles

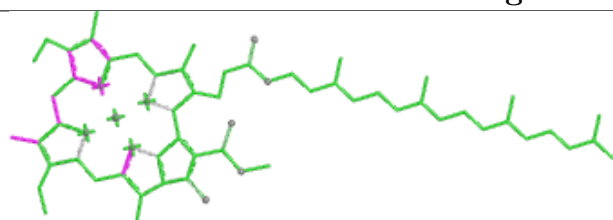


Torsions

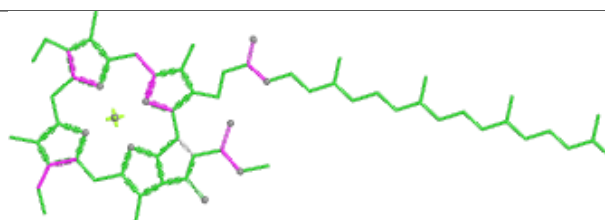


Rings

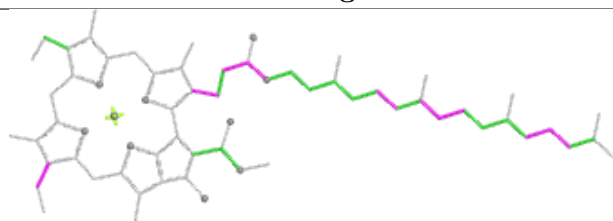
Ligand CLA B 3014



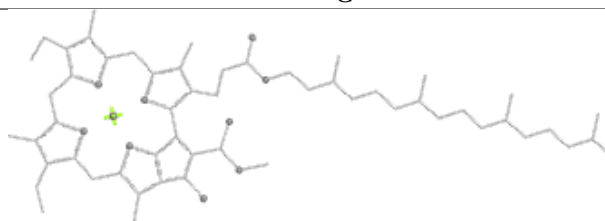
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-1.51	1 (0%) 92 86	21, 87, 139, 184	0
2	B	739/740 (99%)	-1.78	0 100 100	13, 60, 106, 141	0
3	C	80/80 (100%)	-1.79	0 100 100	12, 53, 81, 91	0
4	D	138/138 (100%)	-1.84	0 100 100	30, 65, 92, 147	0
5	E	69/75 (92%)	-1.72	0 100 100	54, 82, 104, 120	0
6	F	141/164 (85%)	-1.53	0 100 100	54, 106, 125, 133	0
7	I	38/38 (100%)	-1.90	0 100 100	17, 34, 62, 96	0
8	J	41/41 (100%)	-1.28	0 100 100	97, 116, 130, 149	0
9	K	47/83 (56%)	-0.69	0 100 100	132, 166, 183, 200	0
10	L	151/154 (98%)	-1.90	0 100 100	13, 33, 72, 120	0
11	M	31/31 (100%)	-1.79	0 100 100	30, 53, 78, 102	0
12	X	29/35 (82%)	-1.64	0 100 100	67, 87, 116, 130	0
All	All	2244/2334 (96%)	-1.65	1 (0%) 100 100	12, 70, 132, 200	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	ALA	2.5

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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
14	CLA	K	101	41/65	0.96	0.10	112,149,185,194	0
14	CLA	A	816	45/65	0.97	0.11	105,143,169,179	0
14	CLA	A	817	49/65	0.97	0.07	63,127,159,160	0
14	CLA	A	821	43/65	0.97	0.10	72,130,170,176	0
14	CLA	A	813	54/65	0.97	0.07	74,100,128,136	0
14	CLA	A	818	54/65	0.98	0.09	95,124,151,161	0
14	CLA	A	812	65/65	0.98	0.09	81,114,144,146	0
14	CLA	A	823	49/65	0.98	0.07	78,116,146,158	0
14	CLA	J	101	45/65	0.98	0.06	118,137,171,176	0
14	CLA	J	102	37/65	0.98	0.05	102,125,149,163	0
14	CLA	A	815	45/65	0.98	0.09	85,114,150,156	0
14	CLA	K	103	45/65	0.98	0.05	101,132,164,166	0
14	CLA	X	1701	45/65	0.98	0.06	75,104,134,140	0
16	BCR	A	847	40/40	0.98	0.06	96,131,161,175	0
16	BCR	J	104	40/40	0.98	0.05	78,116,145,150	0
16	BCR	K	102	40/40	0.98	0.09	107,147,166,175	0
17	LMG	A	852	48/55	0.98	0.06	56,113,152,160	0
18	LHG	B	3050	23/49	0.98	0.05	73,111,139,145	0
21	LMT	L	202	35/35	0.98	0.06	74,142,179,192	0
22	DGD	L	207	66/66	0.98	0.05	45,99,155,168	0
14	CLA	A	829	65/65	0.99	0.05	59,85,110,117	0
14	CLA	A	831	65/65	0.99	0.04	55,87,110,118	0
14	CLA	A	836	54/65	0.99	0.04	47,87,128,136	0
14	CLA	A	837	45/65	0.99	0.05	80,104,127,137	0
14	CLA	B	3012	45/65	0.99	0.03	45,67,88,111	0
14	CLA	B	3013	45/65	0.99	0.04	57,89,115,119	0
14	CLA	B	3017	55/65	0.99	0.04	61,96,133,166	0
14	CLA	B	3020	65/65	0.99	0.04	48,91,121,132	0
14	CLA	B	3021	47/65	0.99	0.04	69,98,129,135	0
14	CLA	B	3022	45/65	0.99	0.04	67,93,119,120	0
14	CLA	B	3023	55/65	0.99	0.04	69,94,122,122	0
14	CLA	B	3036	45/65	0.99	0.03	44,79,107,111	0
14	CLA	B	3037	45/65	0.99	0.04	64,88,120,121	0
14	CLA	F	202	45/65	0.99	0.06	86,115,145,151	0
14	CLA	A	808	51/65	0.99	0.04	81,103,130,133	0
14	CLA	A	810	65/65	0.99	0.04	44,99,148,161	0
14	CLA	A	811	45/65	0.99	0.06	92,125,152,159	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CLA	A	805	59/65	0.99	0.04	75,98,125,141	0
14	CLA	M	102	45/65	0.99	0.09	83,131,166,180	0
14	CLA	A	819	54/65	0.99	0.05	61,94,116,132	0
14	CLA	A	820	65/65	0.99	0.04	65,100,125,134	0
16	BCR	A	848	40/40	0.99	0.06	77,119,171,177	0
16	BCR	A	849	40/40	0.99	0.04	61,91,155,157	0
16	BCR	A	850	40/40	0.99	0.04	41,74,108,125	0
16	BCR	B	3044	40/40	0.99	0.06	75,110,143,161	0
16	BCR	B	3046	40/40	0.99	0.05	43,76,131,143	0
16	BCR	B	3047	40/40	0.99	0.04	54,79,99,106	0
16	BCR	B	3051	40/40	0.99	0.04	46,84,127,134	0
16	BCR	F	201	40/40	0.99	0.07	45,91,124,132	0
16	BCR	F	203	40/40	0.99	0.04	43,94,126,147	0
14	CLA	A	806	65/65	0.99	0.04	67,101,136,142	0
16	BCR	J	105	40/40	0.99	0.06	67,114,154,161	0
14	CLA	A	822	65/65	0.99	0.04	51,87,121,127	0
16	BCR	M	103	40/40	0.99	0.03	21,48,76,82	0
14	CLA	A	814	60/65	0.99	0.08	73,115,140,141	0
17	LMG	A	855	30/55	0.99	0.06	32,83,145,162	0
17	LMG	I	102	40/55	0.99	0.07	49,85,120,144	0
14	CLA	A	824	51/65	0.99	0.05	67,101,132,138	0
18	LHG	M	101	49/49	0.99	0.05	47,89,164,181	0
14	CLA	A	826	65/65	0.99	0.05	71,100,131,134	0
14	CLA	A	828	65/65	0.99	0.05	59,93,128,135	0
14	CLA	B	3018	59/65	1.00	0.04	47,81,109,117	0
14	CLA	B	3019	60/65	1.00	0.03	49,70,100,107	0
14	CLA	A	803	65/65	1.00	0.02	42,67,87,108	0
14	CLA	A	809	65/65	1.00	0.03	38,84,123,129	0
14	CLA	A	830	65/65	1.00	0.04	55,88,118,121	0
14	CLA	A	804	65/65	1.00	0.03	59,98,125,132	0
14	CLA	B	3024	45/65	1.00	0.02	30,61,94,106	0
14	CLA	B	3025	54/65	1.00	0.02	48,64,87,87	0
14	CLA	B	3026	46/65	1.00	0.02	36,64,89,90	0
14	CLA	B	3027	65/65	1.00	0.03	38,65,91,97	0
14	CLA	B	3028	65/65	1.00	0.03	15,48,100,102	0
14	CLA	B	3029	65/65	1.00	0.02	27,61,79,97	0
14	CLA	B	3030	65/65	1.00	0.02	20,47,80,98	0
14	CLA	B	3031	45/65	1.00	0.03	46,73,95,113	0
14	CLA	B	3032	49/65	1.00	0.03	34,69,97,122	0
14	CLA	B	3033	65/65	1.00	0.03	56,86,112,121	0
14	CLA	B	3034	58/65	1.00	0.05	63,98,137,141	0
14	CLA	B	3035	45/65	1.00	0.03	55,73,95,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CLA	A	832	50/65	1.00	0.03	33,61,91,117	0
14	CLA	A	833	65/65	1.00	0.03	24,63,135,140	0
14	CLA	B	3038	60/65	1.00	0.03	41,81,112,122	0
14	CLA	B	3039	65/65	1.00	0.03	42,88,128,143	0
14	CLA	B	3040	47/65	1.00	0.02	49,74,93,105	0
14	CLA	B	3041	65/65	1.00	0.01	2,18,52,58	0
14	CLA	B	3042	65/65	1.00	0.02	4,29,52,55	0
14	CLA	A	834	65/65	1.00	0.02	10,37,65,71	0
14	CLA	A	835	65/65	1.00	0.02	2,32,62,90	0
13	CL0	A	801	65/65	1.00	0.03	2,46,71,74	0
14	CLA	A	802	65/65	1.00	0.02	20,38,54,75	0
14	CLA	A	838	51/65	1.00	0.02	36,59,79,102	0
14	CLA	L	204	65/65	1.00	0.02	11,41,72,93	0
14	CLA	L	205	65/65	1.00	0.02	8,45,117,130	0
14	CLA	L	206	65/65	1.00	0.02	21,46,75,85	0
14	CLA	A	839	65/65	1.00	0.03	21,59,97,120	0
14	CLA	A	840	47/65	1.00	0.03	22,55,75,93	0
15	PQN	A	846	33/33	1.00	0.04	61,89,118,121	0
15	PQN	B	3043	33/33	1.00	0.03	27,47,66,70	0
14	CLA	A	841	65/65	1.00	0.02	32,69,123,132	0
14	CLA	A	842	51/65	1.00	0.04	36,75,124,143	0
14	CLA	A	843	65/65	1.00	0.02	37,73,117,135	0
14	CLA	A	844	65/65	1.00	0.02	2,17,50,59	0
16	BCR	A	851	40/40	1.00	0.03	20,63,90,93	0
14	CLA	A	845	52/65	1.00	0.03	44,84,111,120	0
16	BCR	B	3045	40/40	1.00	0.02	48,74,114,123	0
14	CLA	A	856	65/65	1.00	0.03	38,65,91,102	0
14	CLA	B	3003	65/65	1.00	0.03	16,49,70,76	0
16	BCR	B	3048	40/40	1.00	0.02	14,34,61,61	0
14	CLA	B	3004	65/65	1.00	0.02	9,33,53,64	0
14	CLA	B	3005	54/65	1.00	0.02	23,48,67,74	0
14	CLA	B	3006	65/65	1.00	0.02	26,56,90,101	0
16	BCR	I	101	40/40	1.00	0.02	2,28,50,68	0
16	BCR	J	103	40/40	1.00	0.04	60,102,125,129	0
14	CLA	B	3007	65/65	1.00	0.02	22,50,77,90	0
14	CLA	B	3008	65/65	1.00	0.02	10,35,66,89	0
14	CLA	B	3009	65/65	1.00	0.02	10,39,72,76	0
16	BCR	L	201	40/40	1.00	0.02	2,34,59,61	0
16	BCR	L	208	40/40	1.00	0.02	3,28,48,65	0
16	BCR	L	209	40/40	1.00	0.02	2,38,86,98	0
14	CLA	B	3010	65/65	1.00	0.02	5,38,66,90	0
14	CLA	B	3011	65/65	1.00	0.02	2,24,59,69	0

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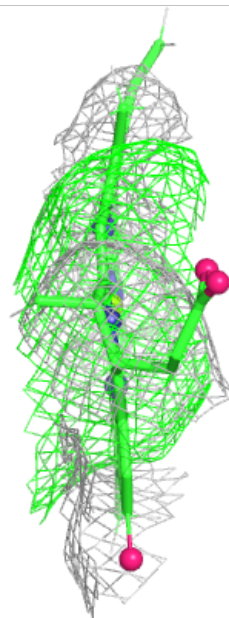
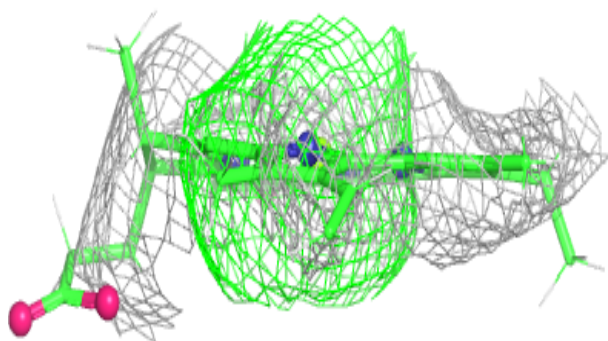
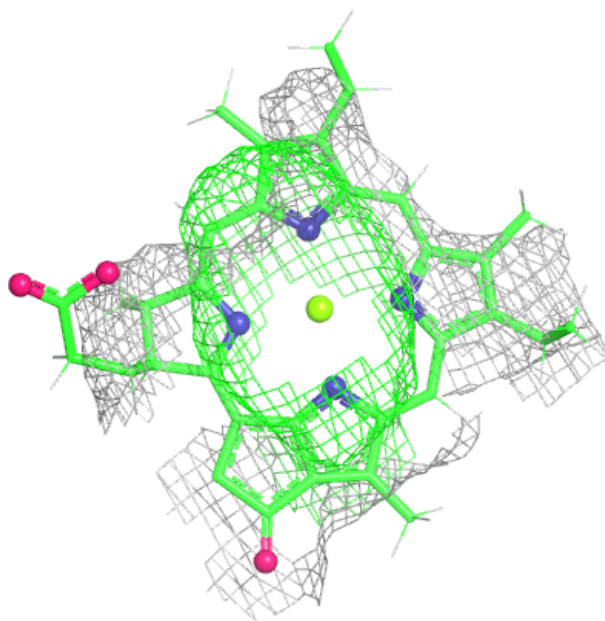
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CLA	A	825	59/65	1.00	0.03	49,83,123,135	0
17	LMG	B	3049	55/55	1.00	0.03	20,58,84,87	0
14	CLA	A	807	65/65	1.00	0.03	56,84,110,116	0
18	LHG	A	853	49/49	1.00	0.04	38,84,108,118	0
18	LHG	A	854	27/49	1.00	0.03	46,79,116,117	0
14	CLA	B	3014	65/65	1.00	0.03	42,72,99,102	0
14	CLA	B	3015	65/65	1.00	0.03	45,77,112,117	0
19	SF4	B	3001	8/8	1.00	0.01	29,46,88,118	0
19	SF4	C	101	8/8	1.00	0.01	23,51,58,71	0
19	SF4	C	102	8/8	1.00	0.01	38,45,62,64	0
20	CA	B	3002	1/1	1.00	0.02	69,69,69,69	0
20	CA	L	203	1/1	1.00	0.00	27,27,27,27	0
14	CLA	B	3016	45/65	1.00	0.03	61,82,115,118	0
14	CLA	A	827	65/65	1.00	0.03	29,68,145,167	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.

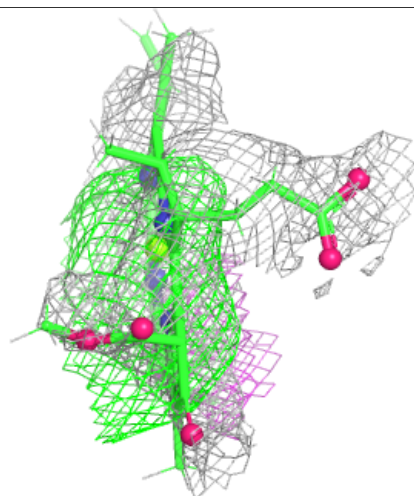
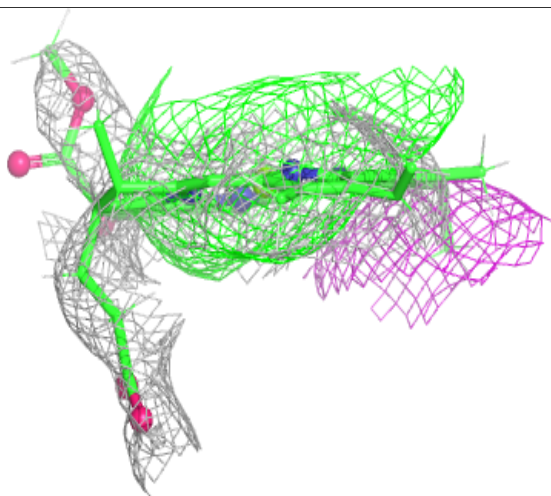
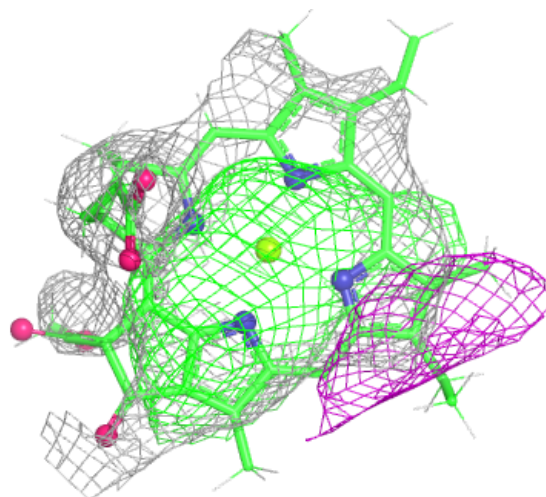
Electron density around CLA K 101:

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



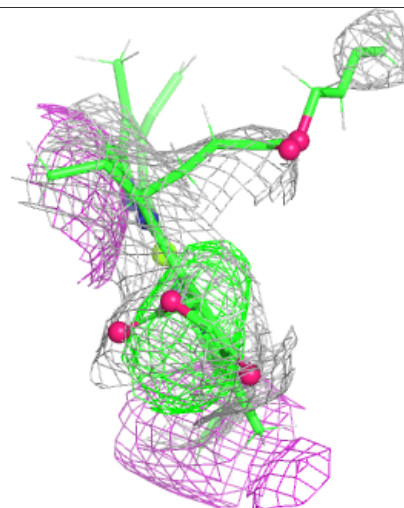
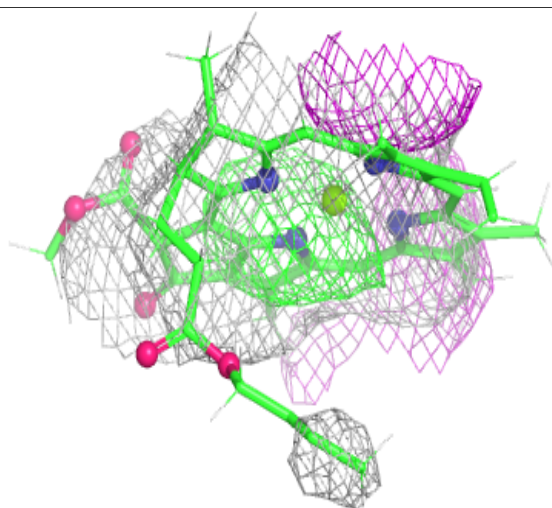
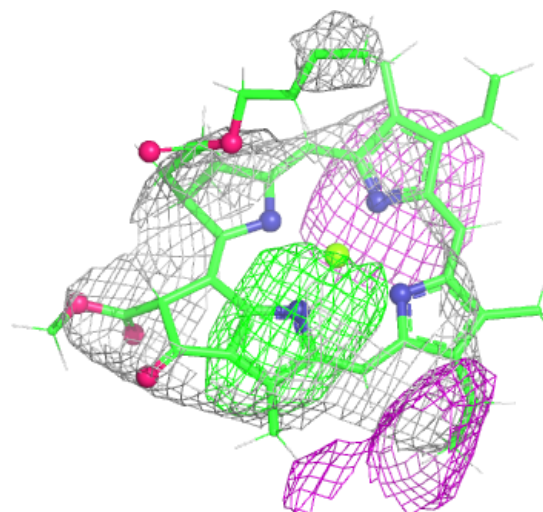
Electron density around CLA A 816:

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and green (positive)



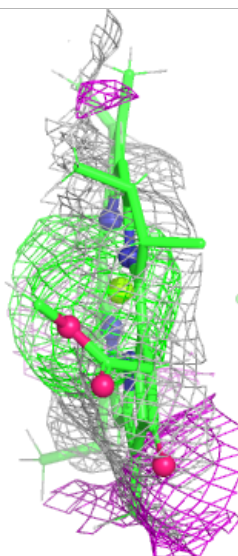
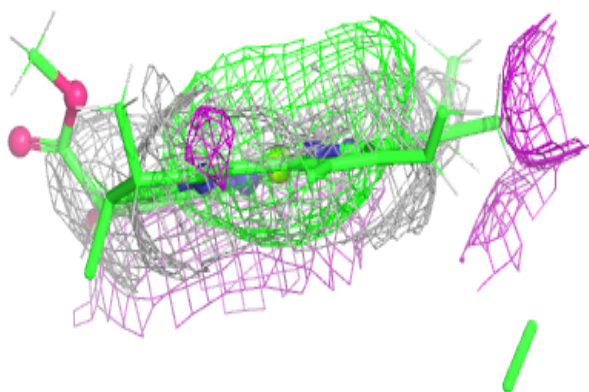
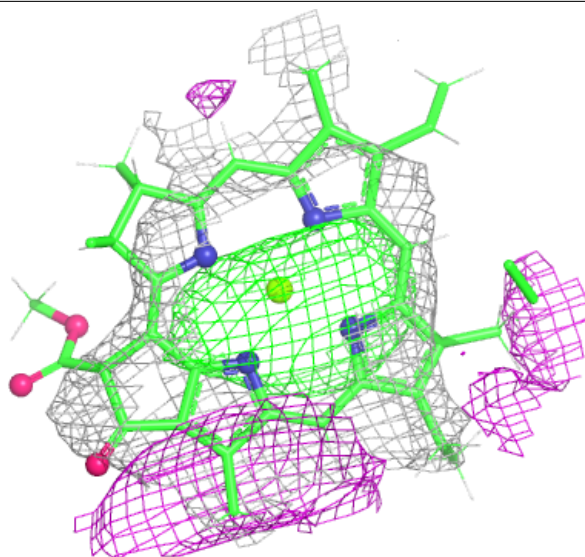
Electron density around CLA A 817:

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and green (positive)



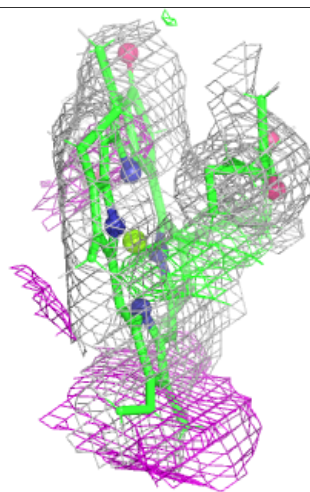
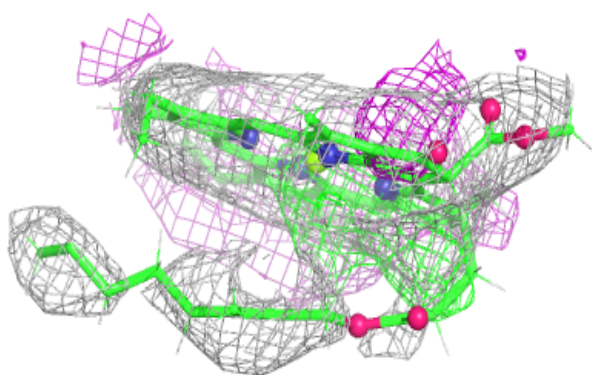
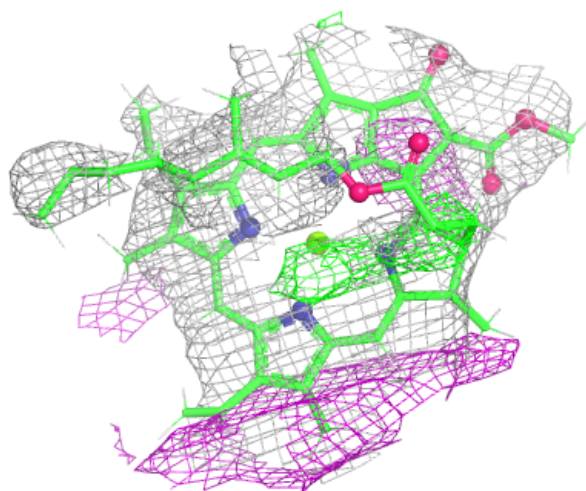
Electron density around CLA A 821:

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



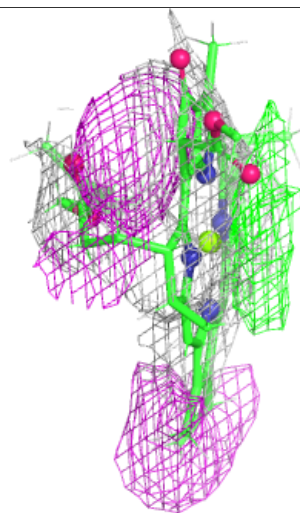
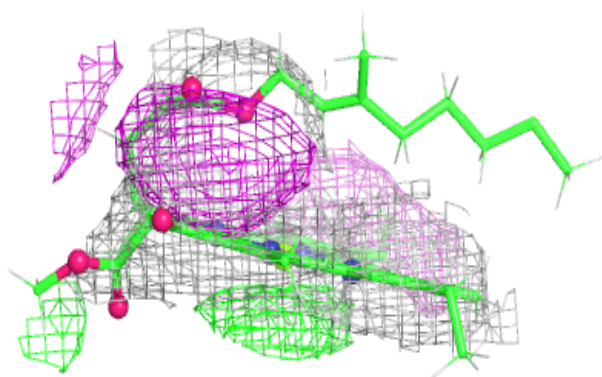
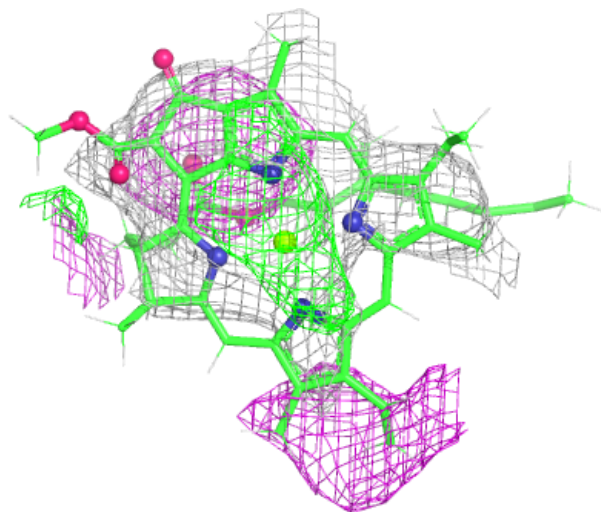
Electron density around CLA A 813:

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



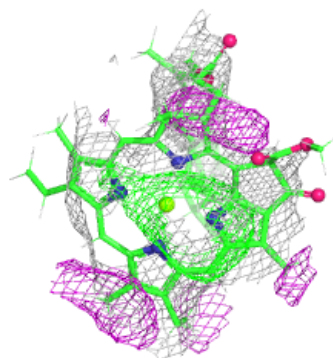
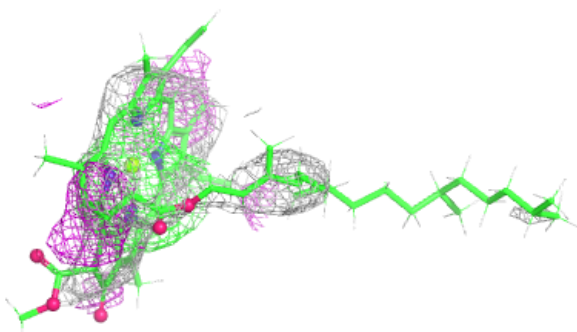
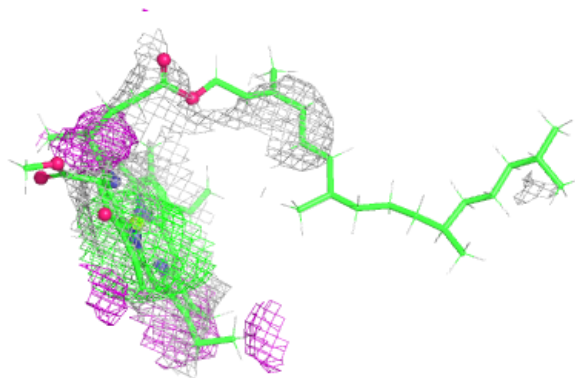
Electron density around CLA A 818:

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and green (positive)



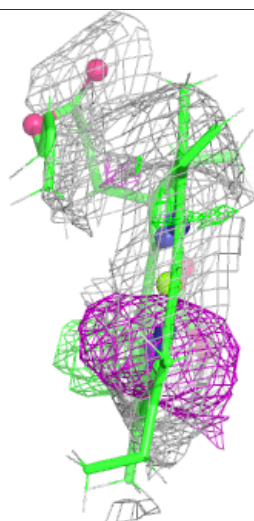
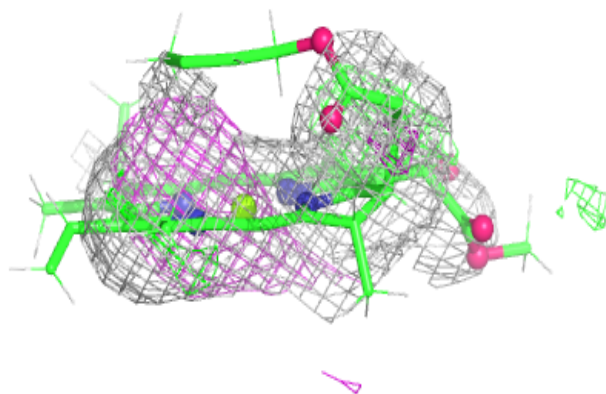
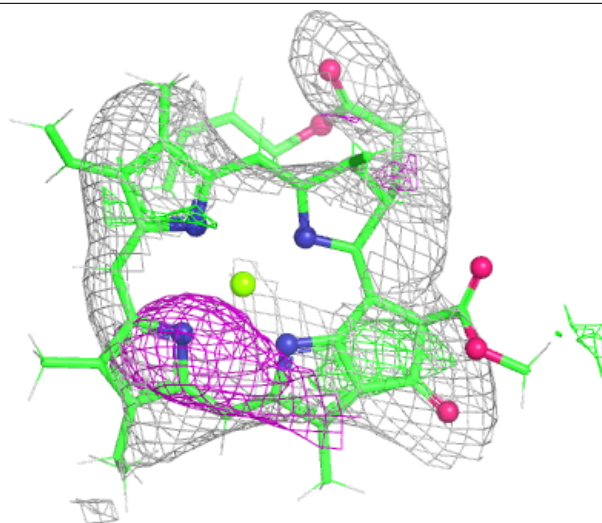
Electron density around CLA A 812:

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and green (positive)



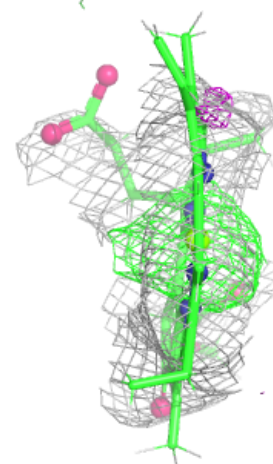
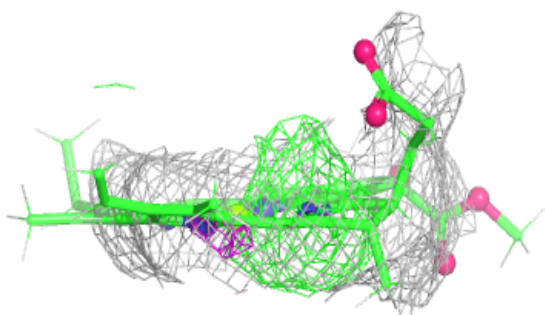
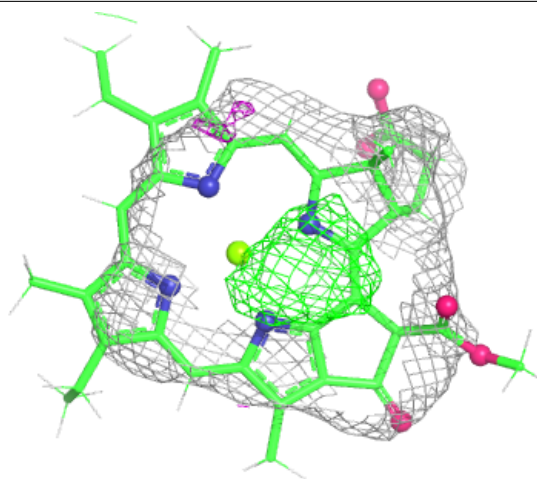
Electron density around CLA A 823:

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and green (positive)



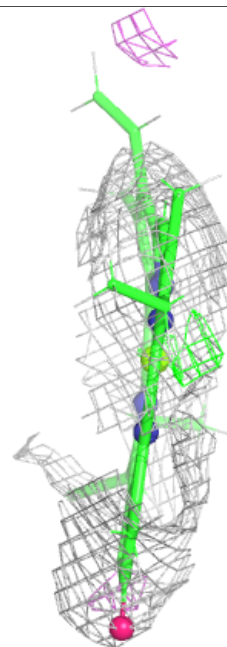
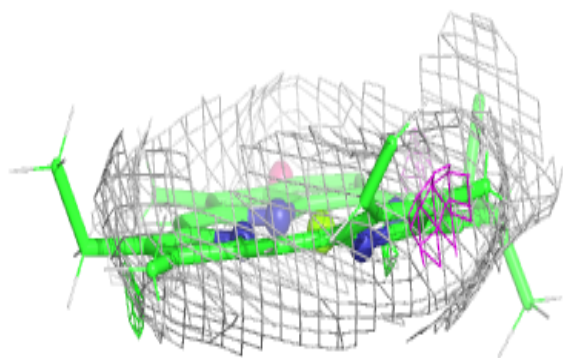
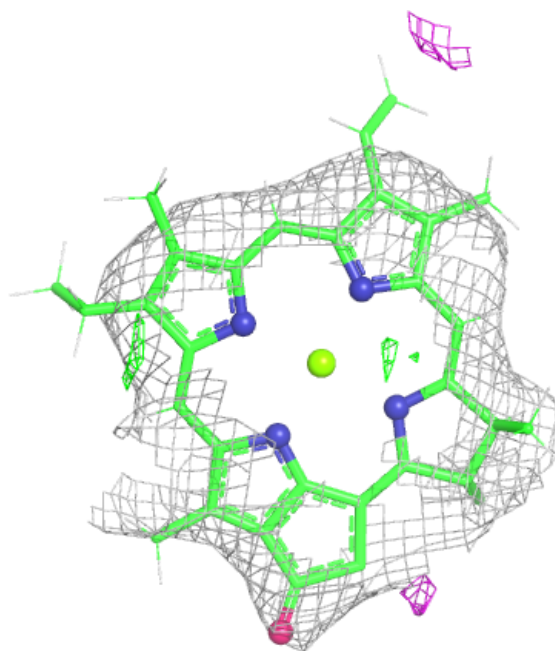
Electron density around CLA J 101:

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and green (positive)



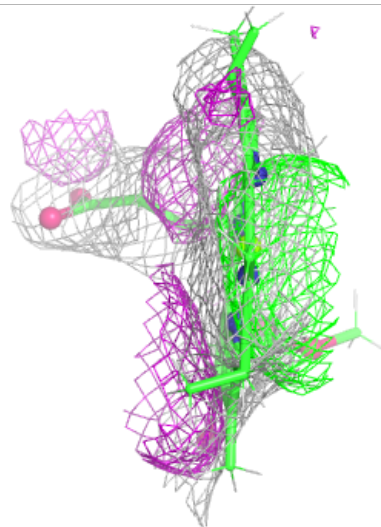
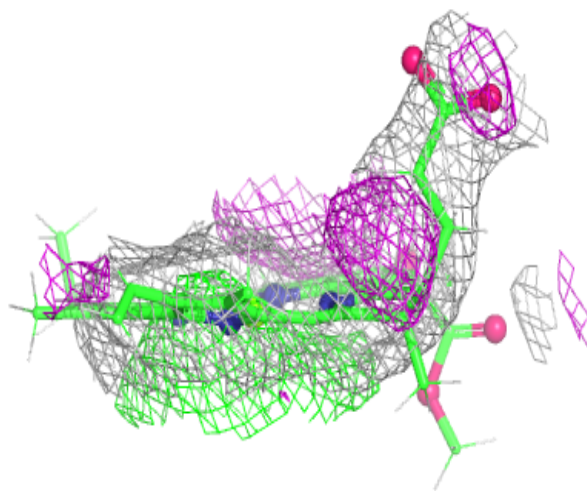
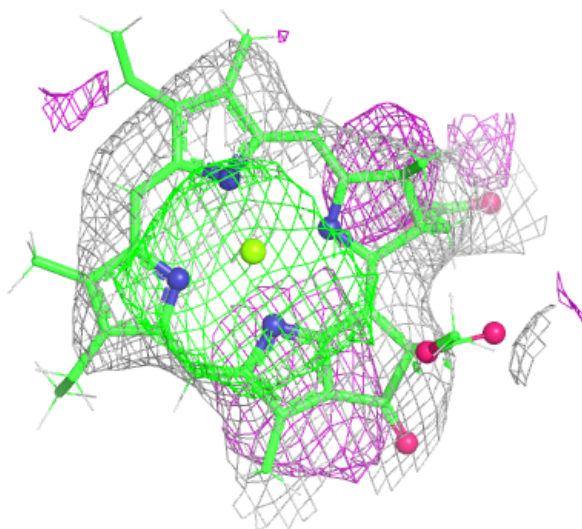
Electron density around CLA J 102:

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and green (positive)



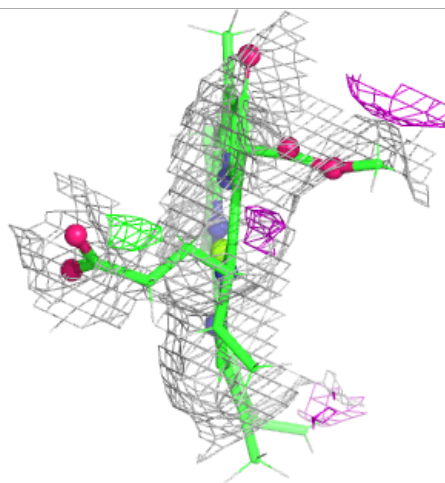
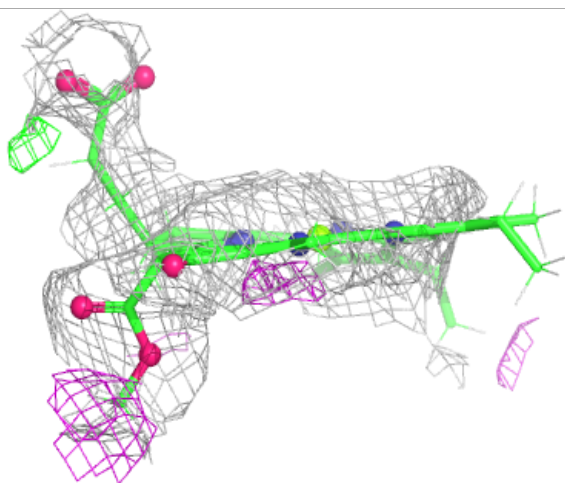
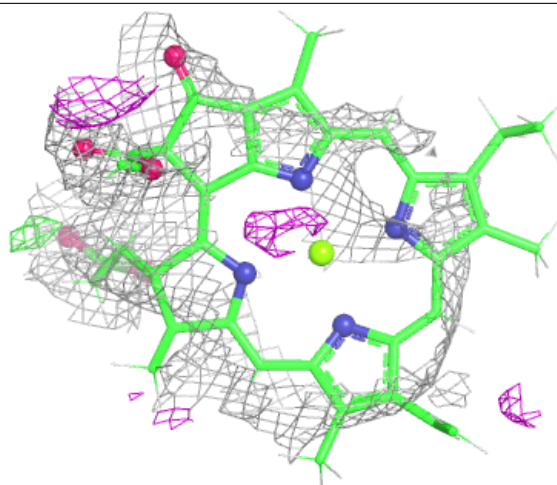
Electron density around CLA A 815:

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and green (positive)



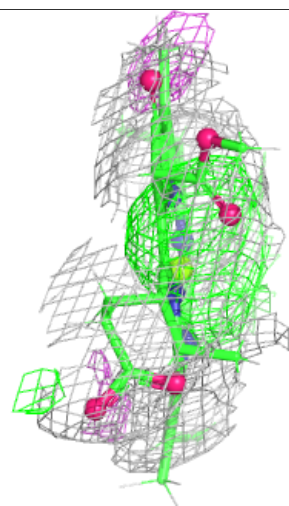
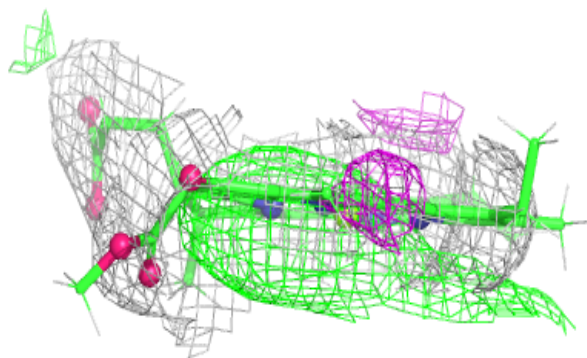
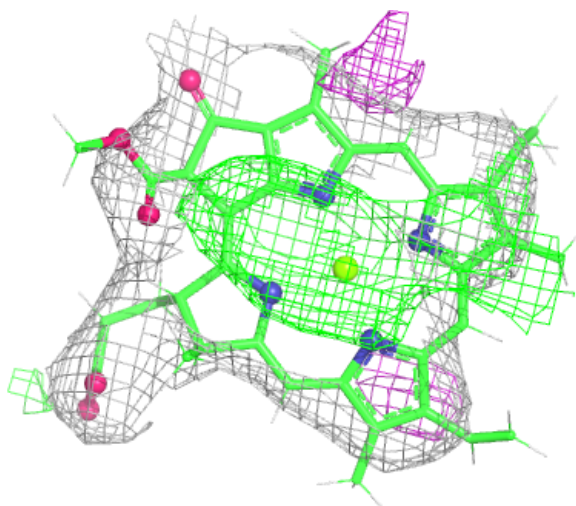
Electron density around CLA K 103:

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and green (positive)



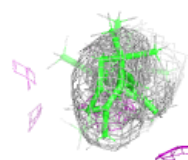
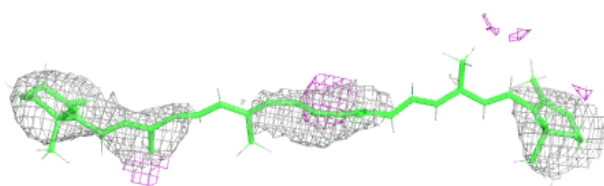
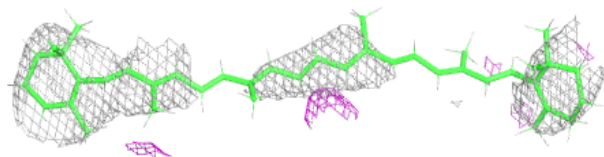
Electron density around CLA X 1701:

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and green (positive)

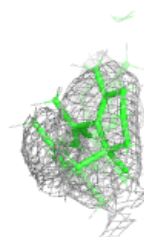
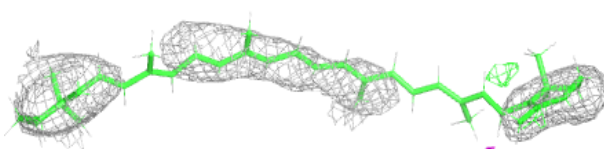
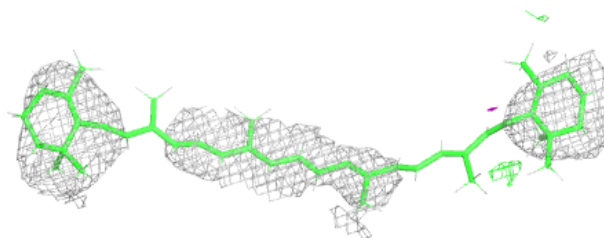


Electron density around BCR A 847:

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

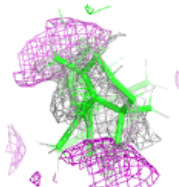
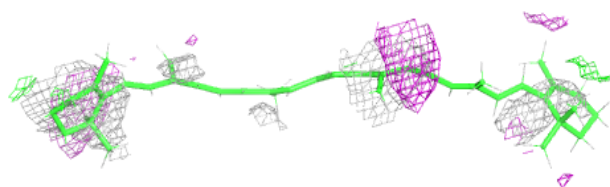
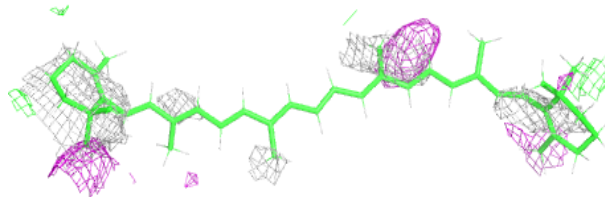
**Electron density around BCR J 104:**

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and green (positive)

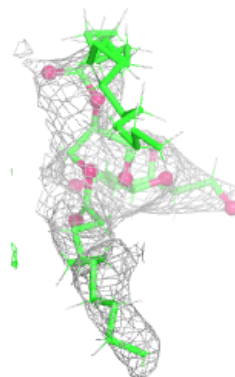
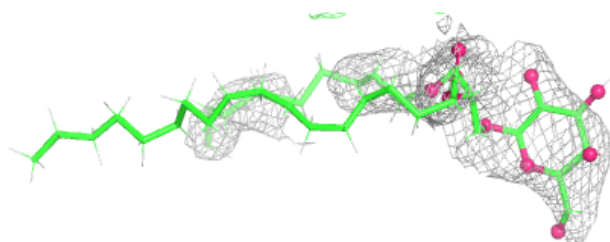
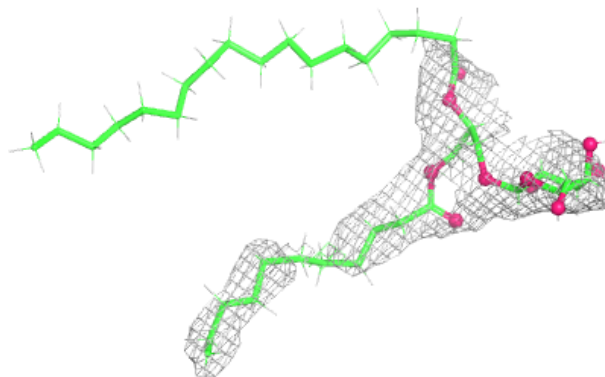


Electron density around BCR K 102:

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and green (positive)

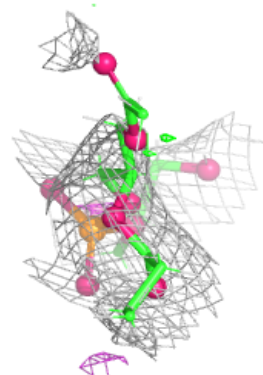
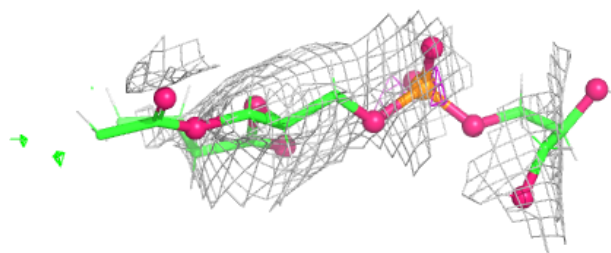
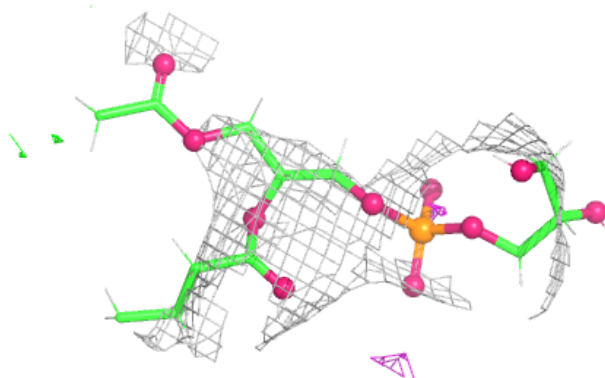
**Electron density around LMG A 852:**

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and green (positive)

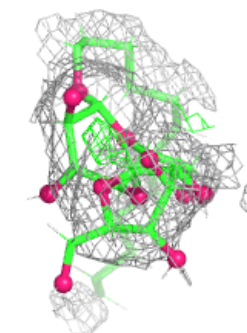
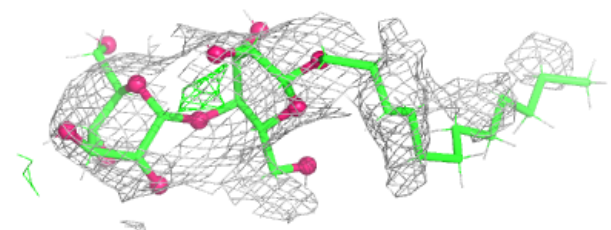
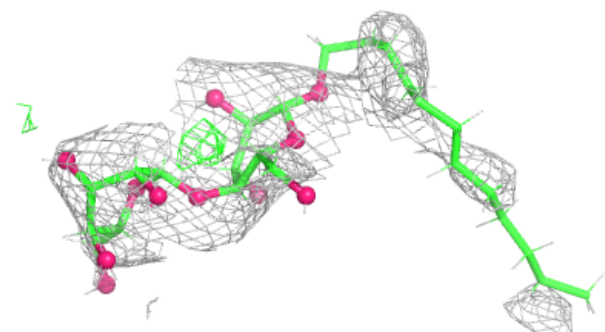


Electron density around LHG B 3050:

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and green (positive)

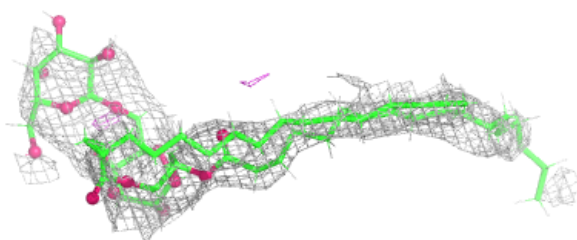
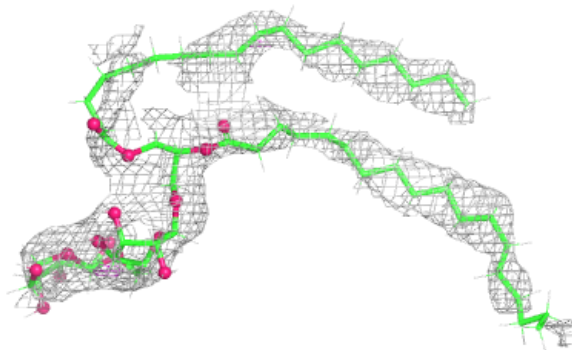
**Electron density around LMT L 202:**

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

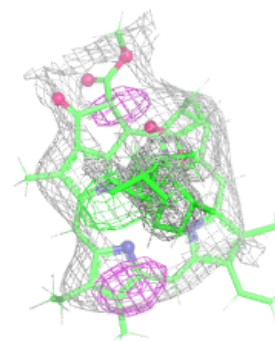
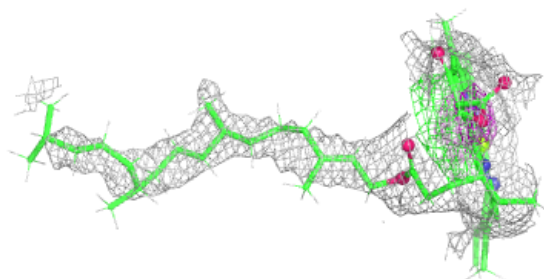
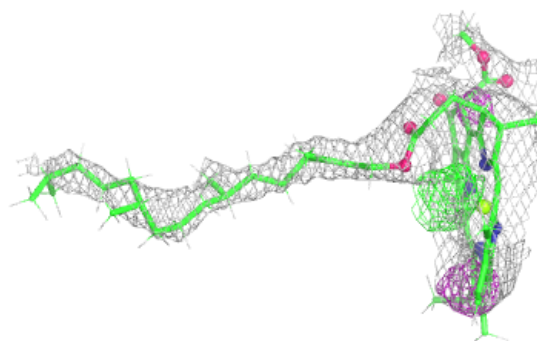


Electron density around DGD L 207:

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and green (positive)

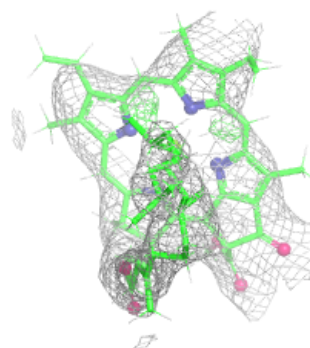
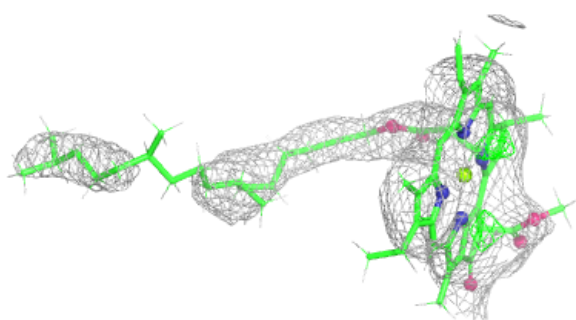
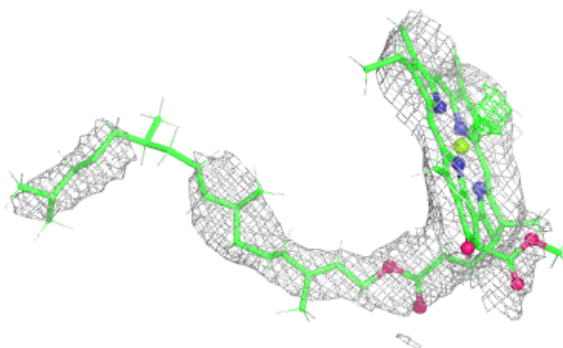
**Electron density around CLA A 829:**

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and green (positive)

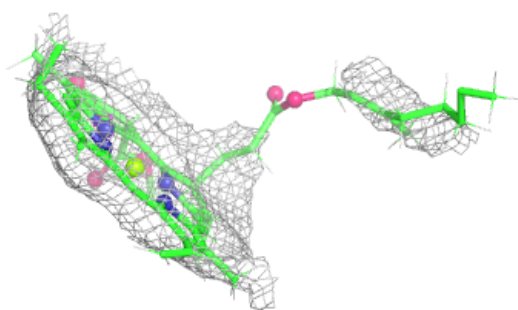
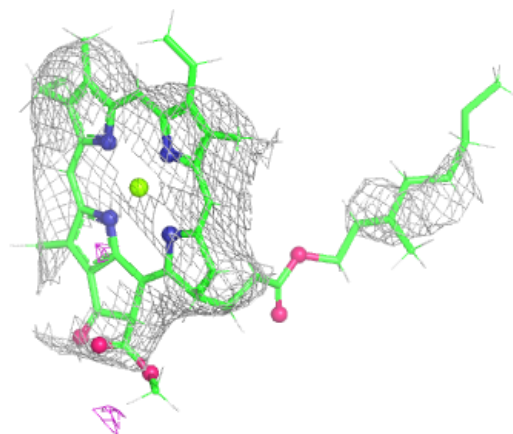


Electron density around CLA A 831:

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and green (positive)

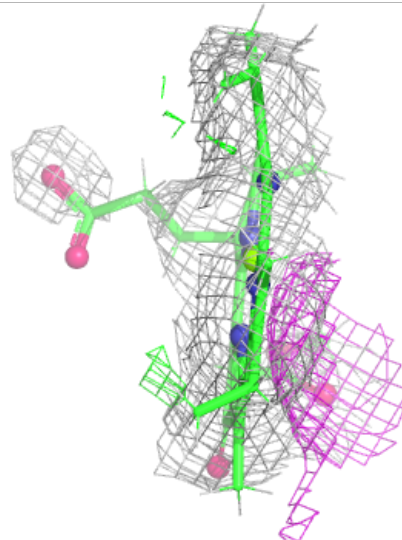
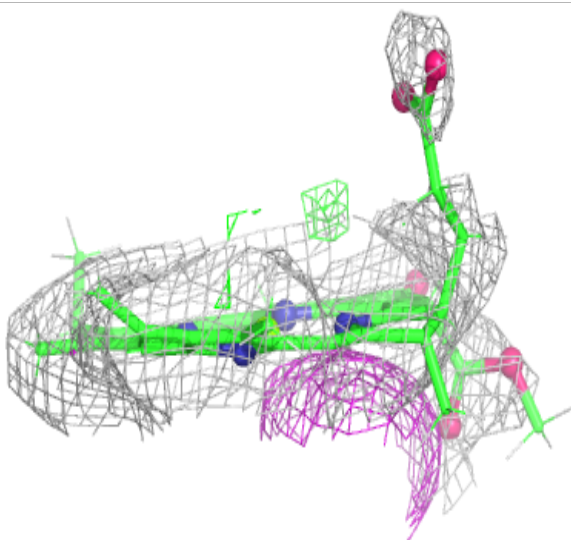
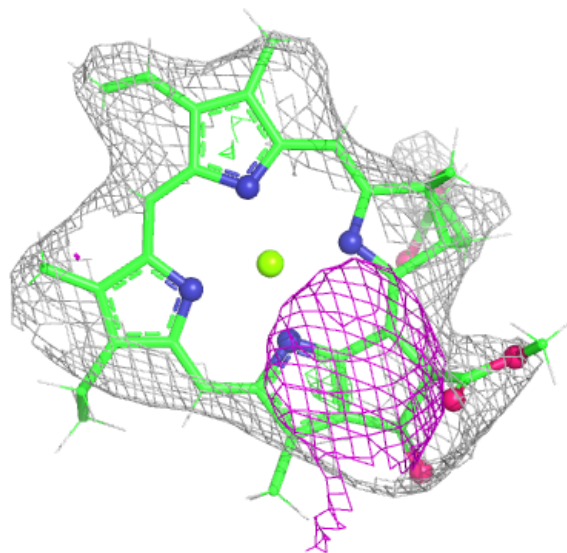
**Electron density around CLA A 836:**

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and green (positive)



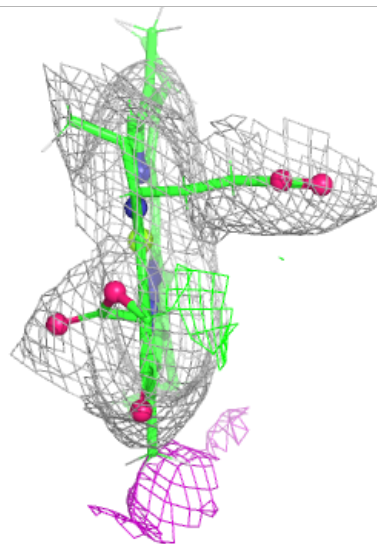
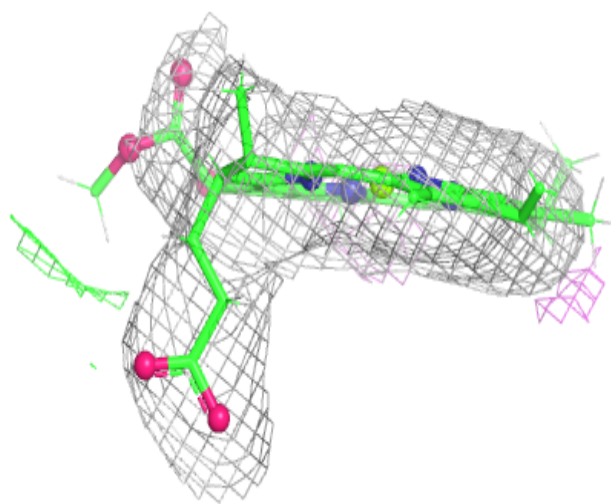
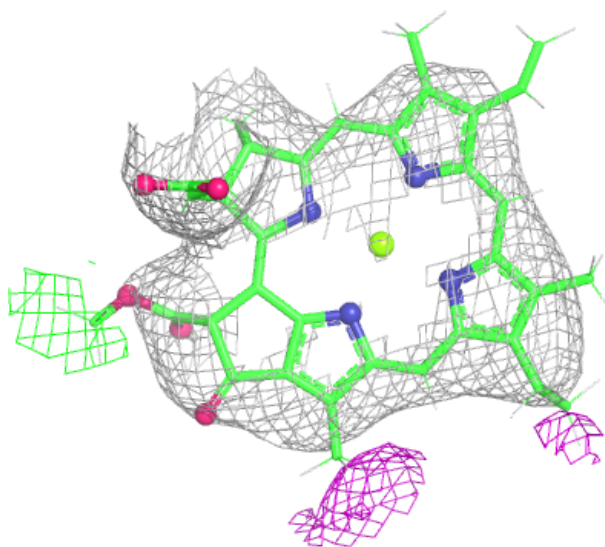
Electron density around CLA A 837:

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



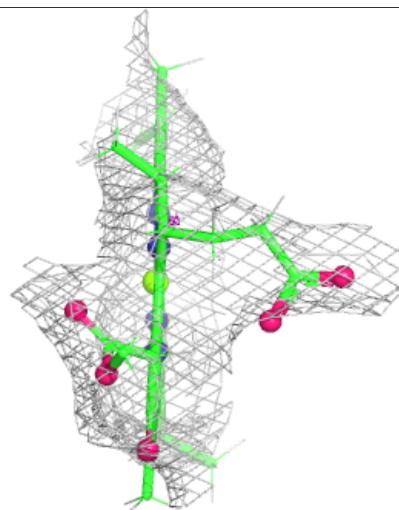
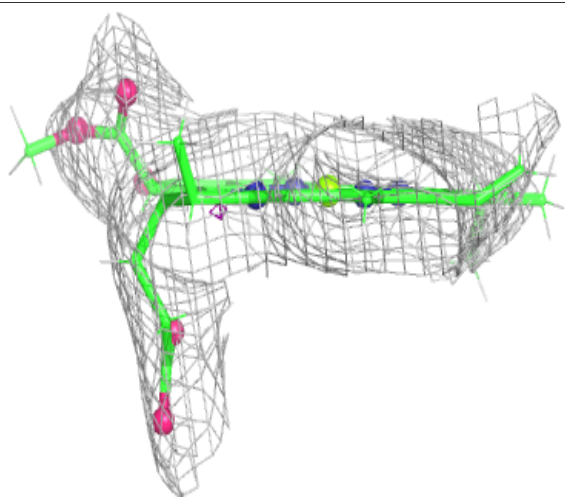
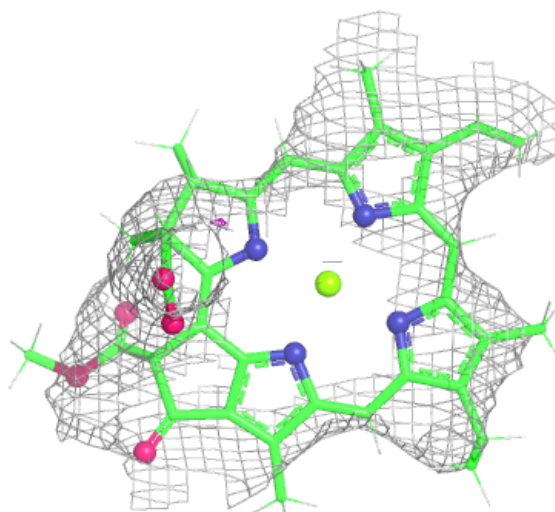
Electron density around CLA B 3012:

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



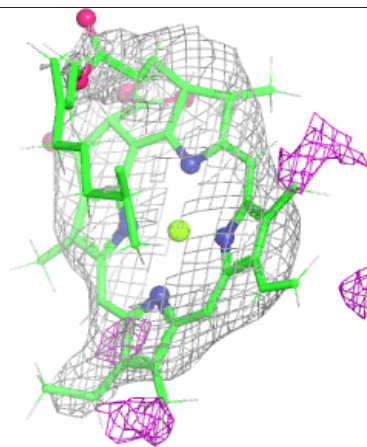
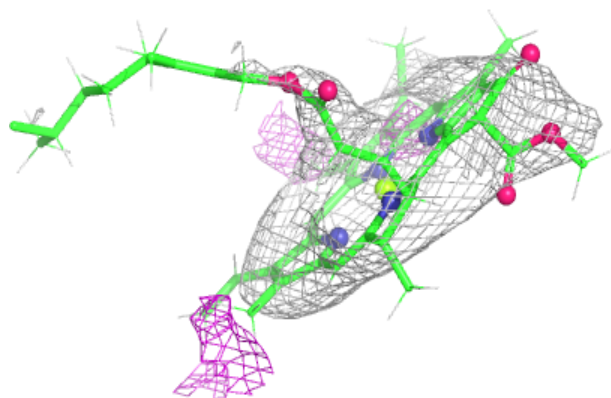
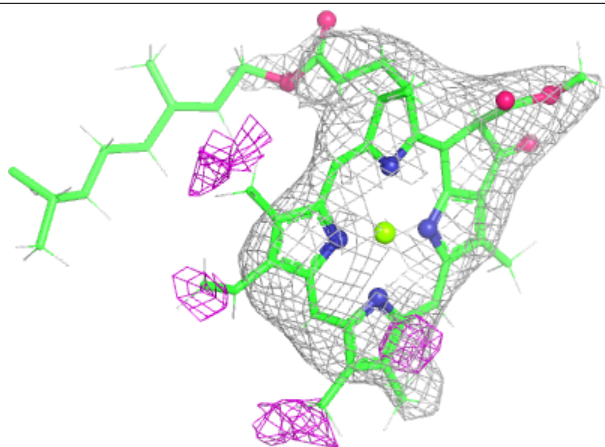
Electron density around CLA B 3013:

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



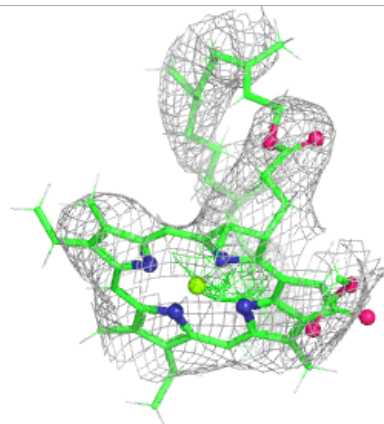
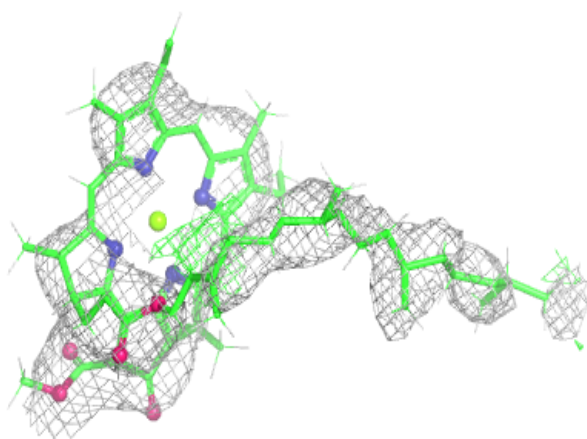
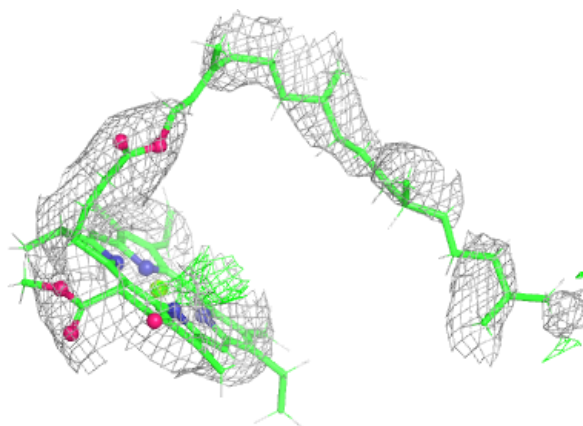
Electron density around CLA B 3017:

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



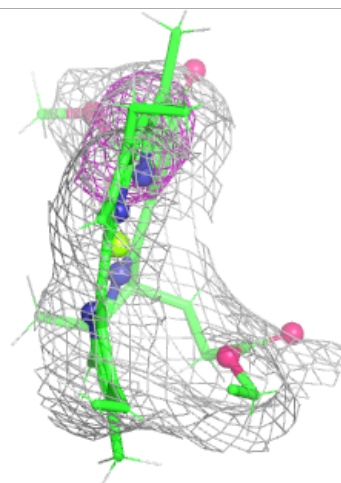
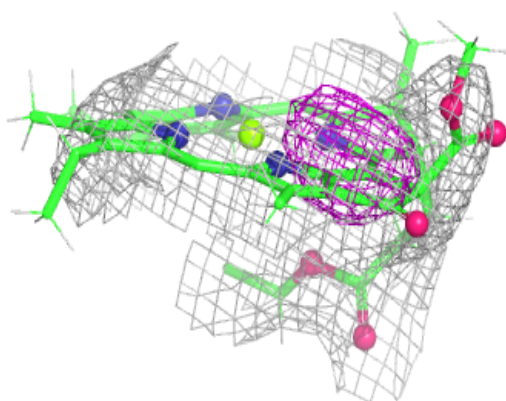
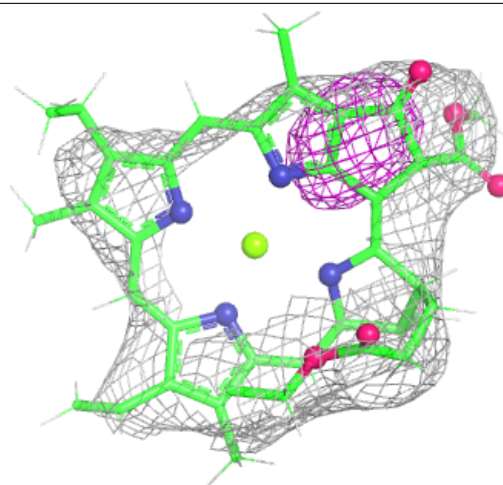
Electron density around CLA B 3020:

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



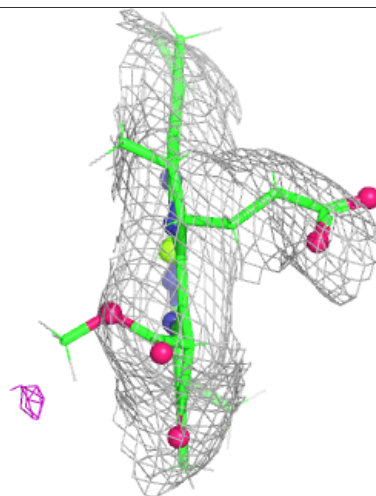
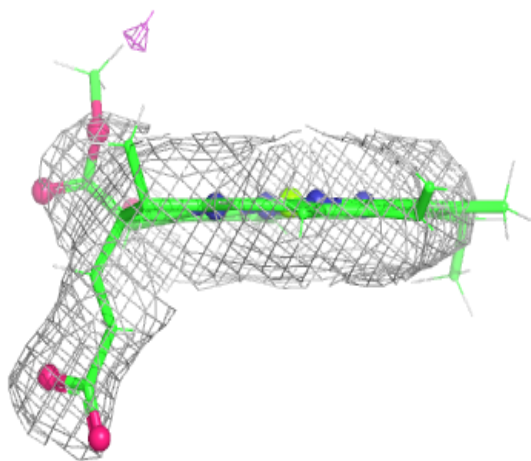
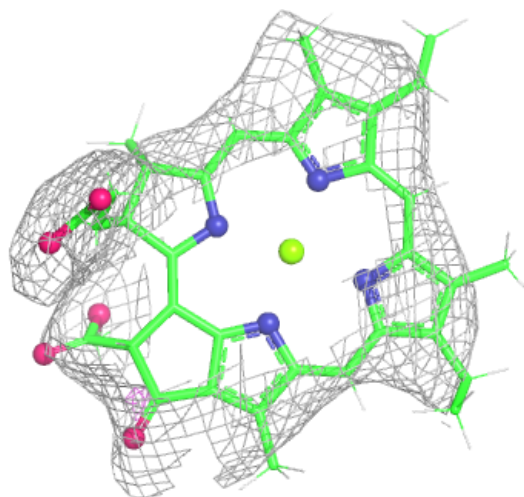
Electron density around CLA B 3021:

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



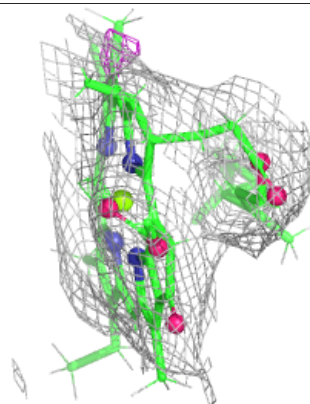
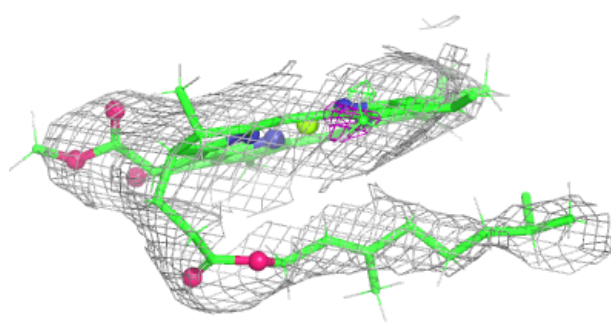
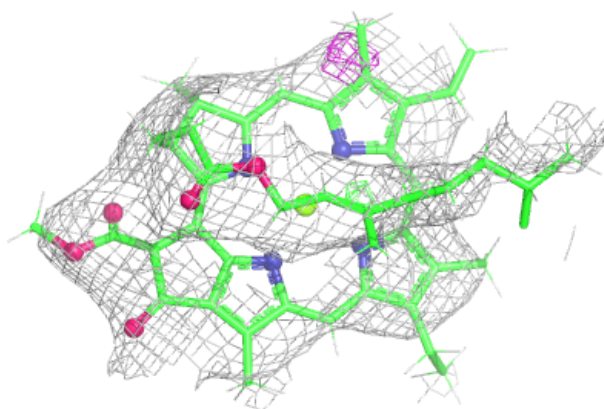
Electron density around CLA B 3022:

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



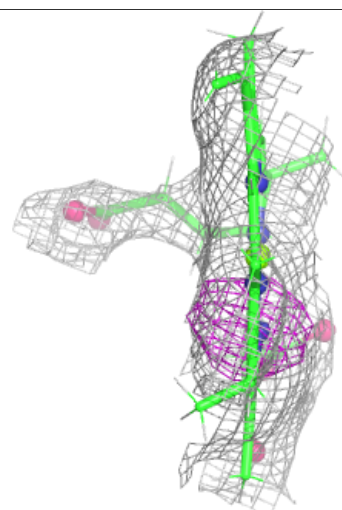
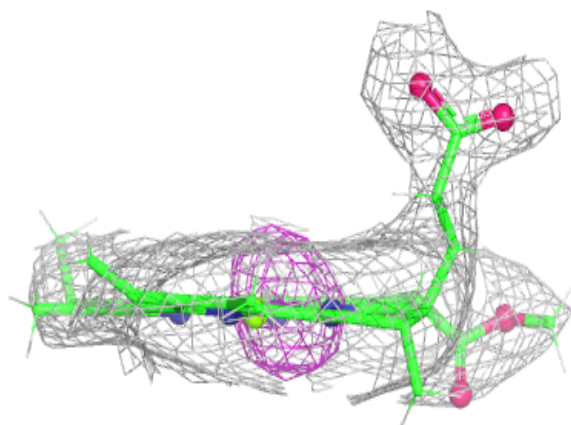
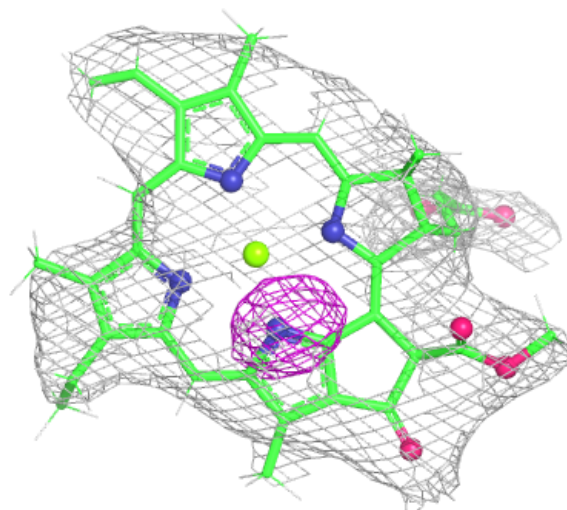
Electron density around CLA B 3023:

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



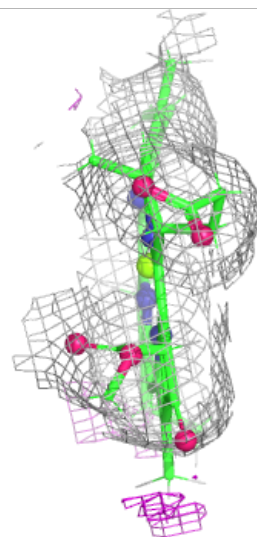
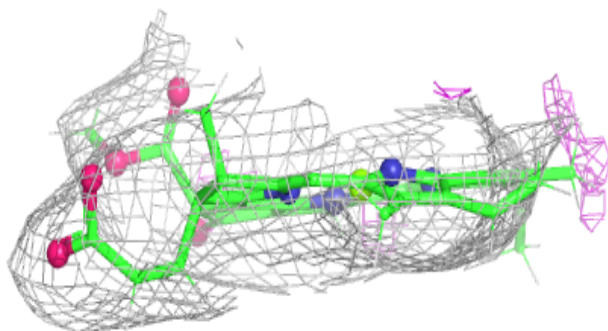
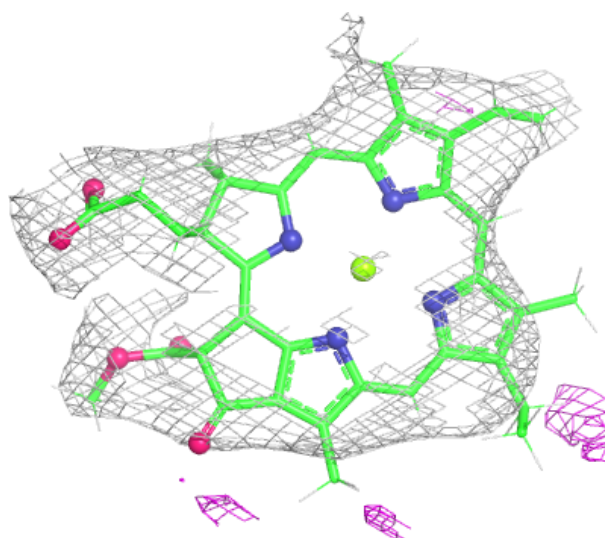
Electron density around CLA B 3036:

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



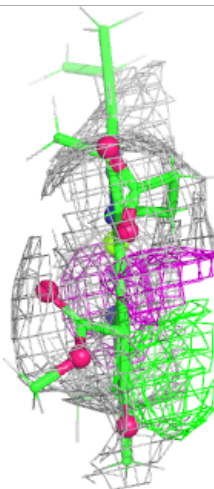
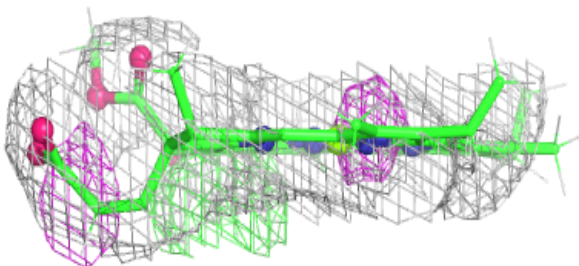
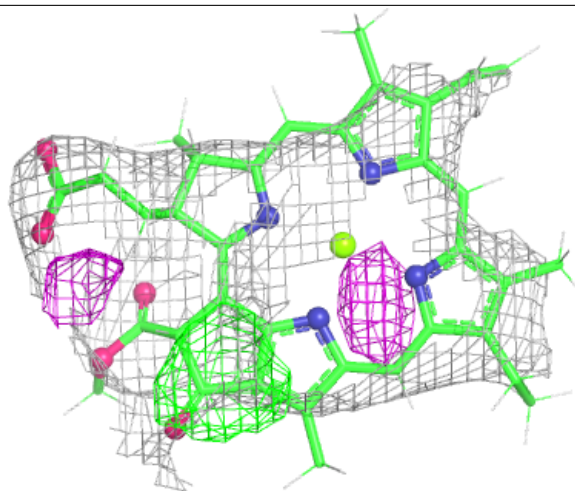
Electron density around CLA B 3037:

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



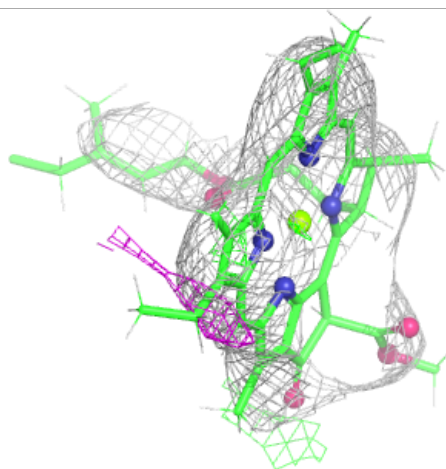
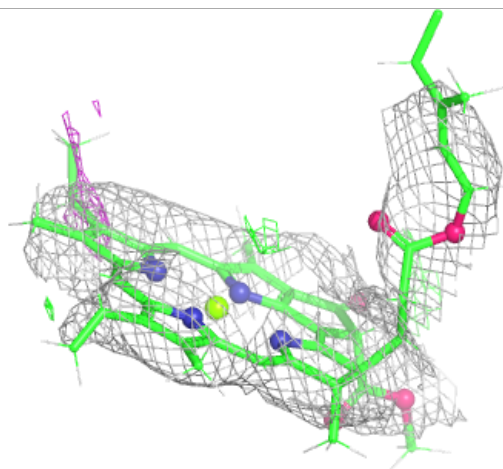
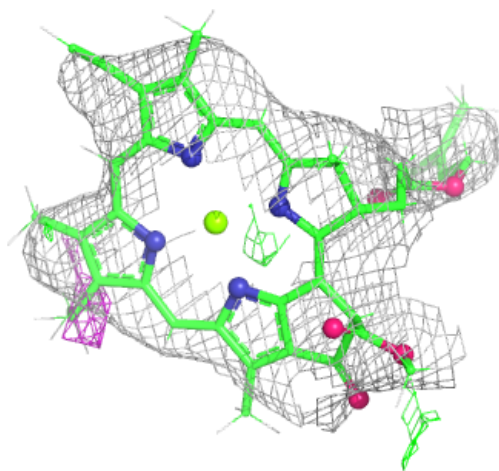
Electron density around CLA F 202:

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



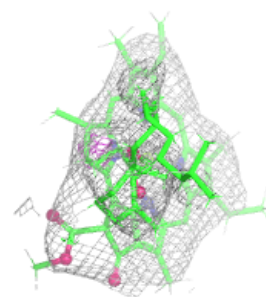
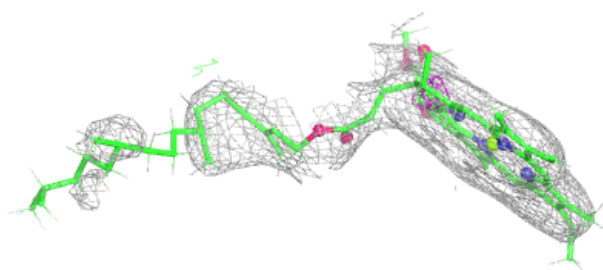
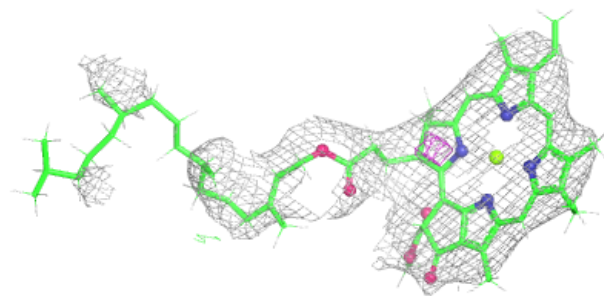
Electron density around CLA A 808:

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



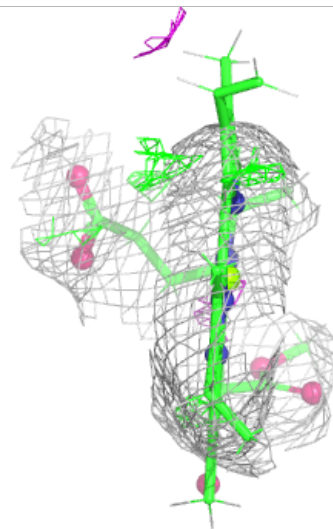
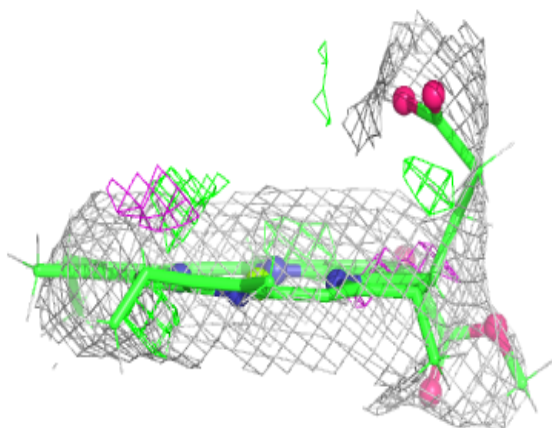
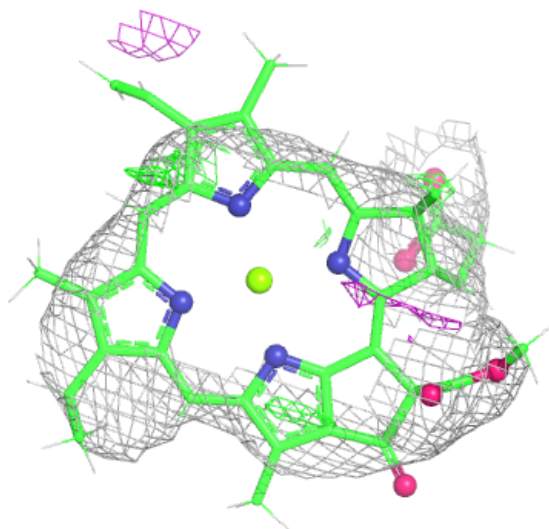
Electron density around CLA A 810:

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



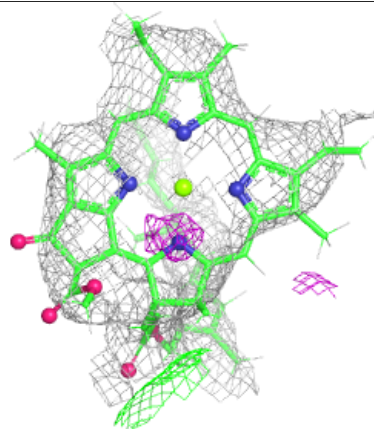
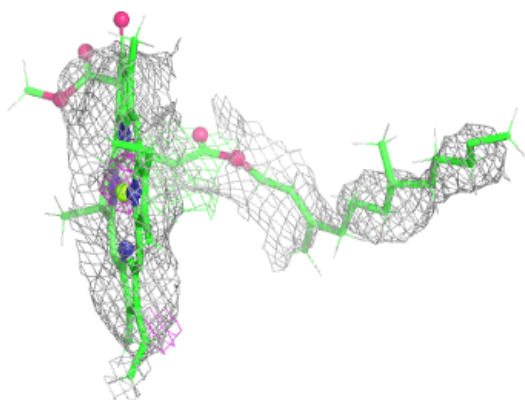
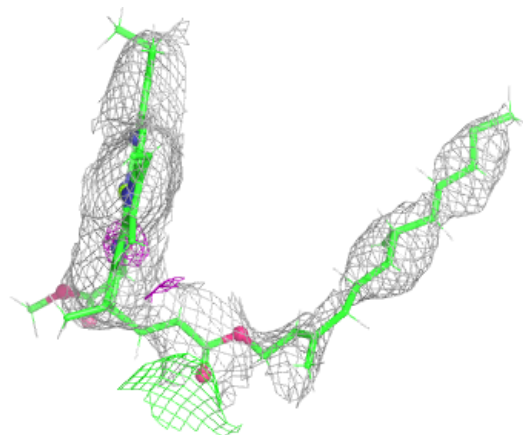
Electron density around CLA A 811:

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



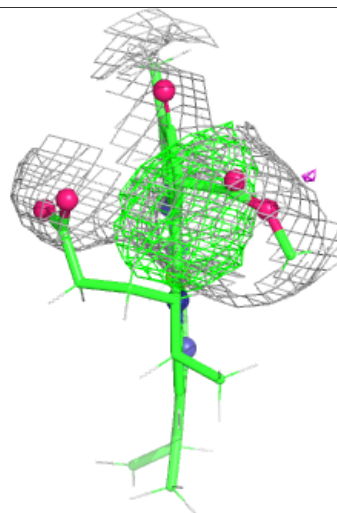
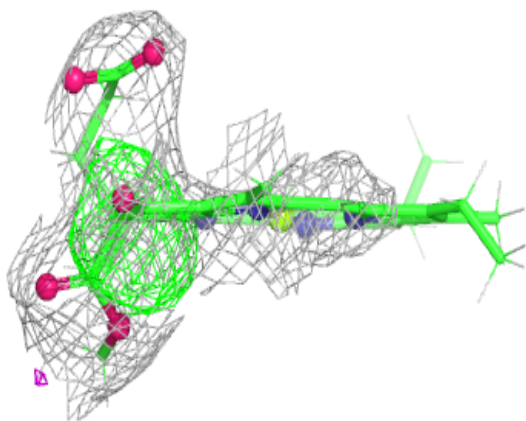
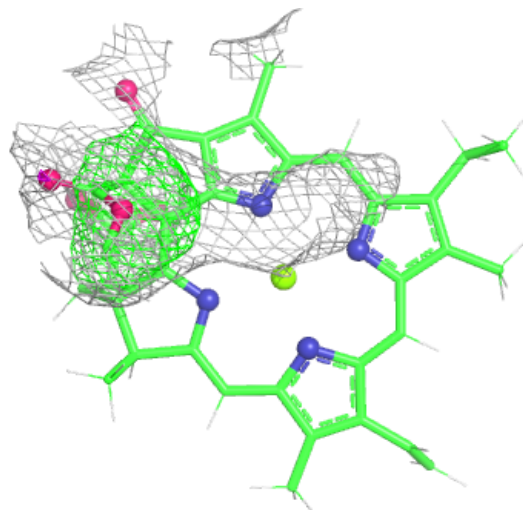
Electron density around CLA A 805:

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



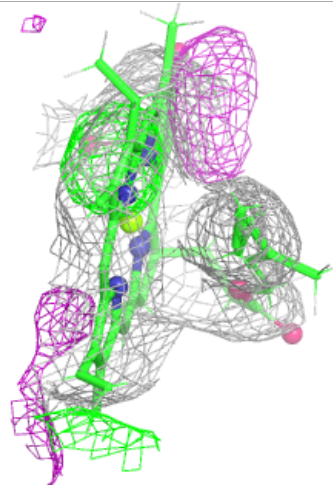
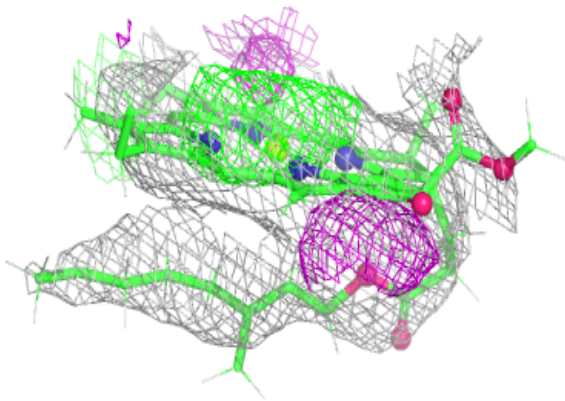
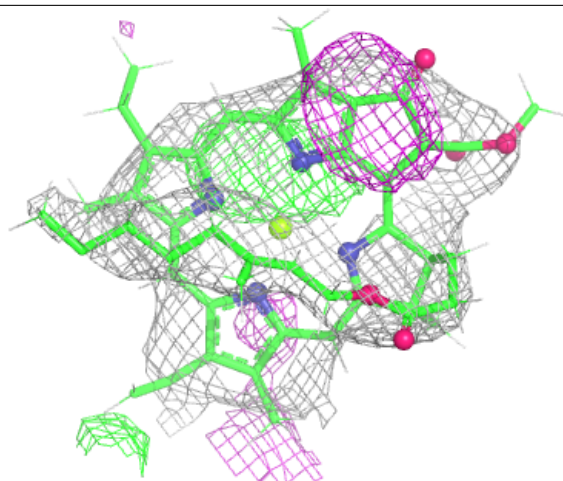
Electron density around CLA M 102:

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



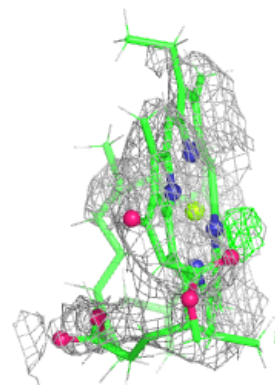
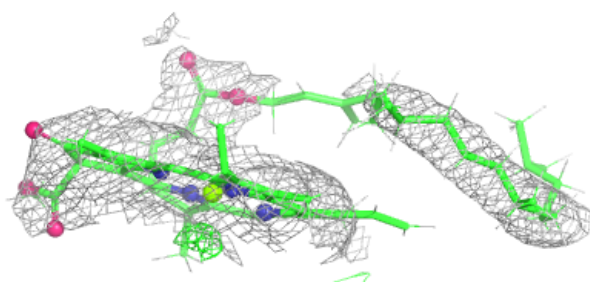
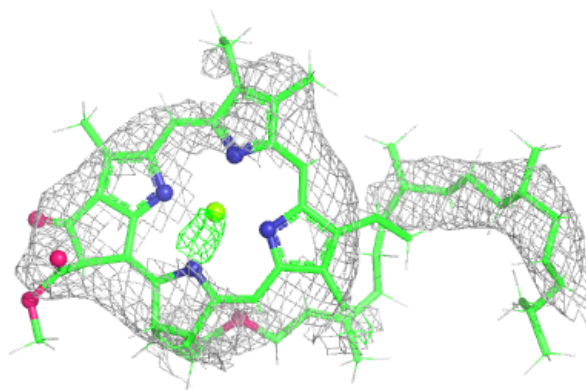
Electron density around CLA A 819:

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

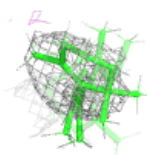
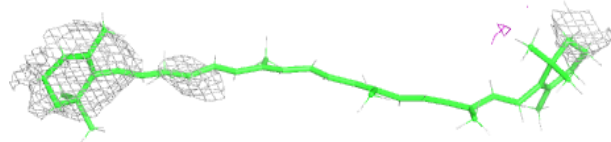
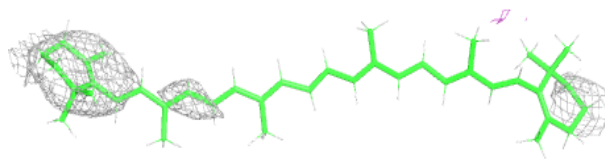


Electron density around CLA A 820:

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

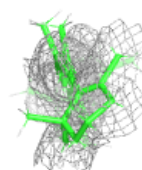
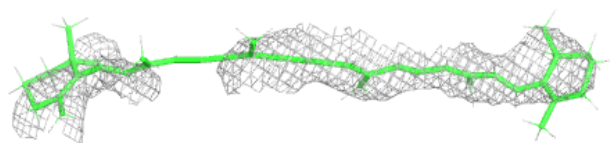
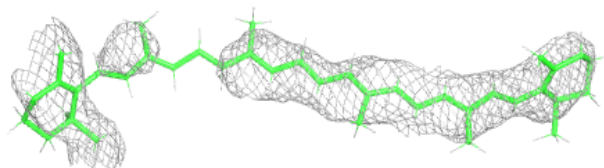
**Electron density around BCR A 848:**

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

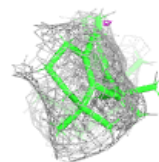
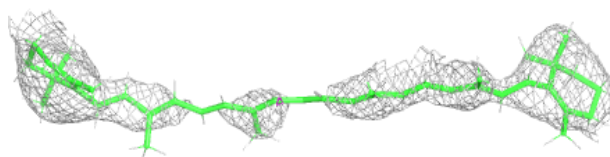
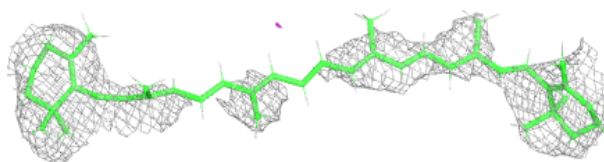


Electron density around BCR A 849:

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

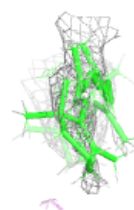
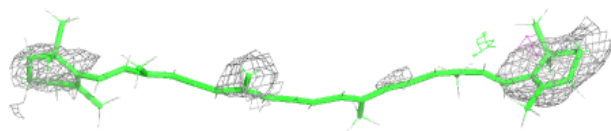
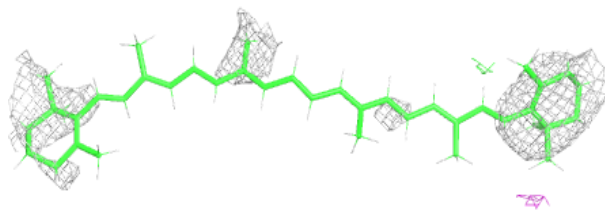
**Electron density around BCR A 850:**

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

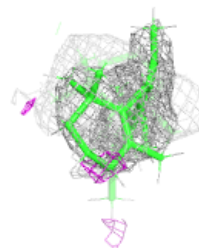
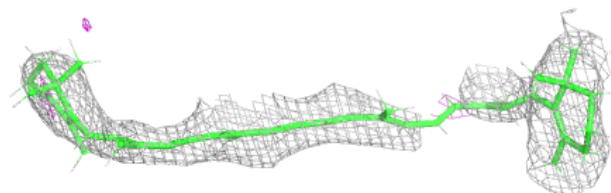
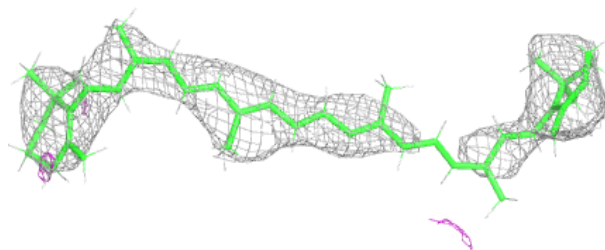


Electron density around BCR B 3044:

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

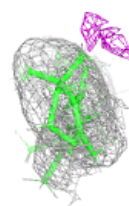
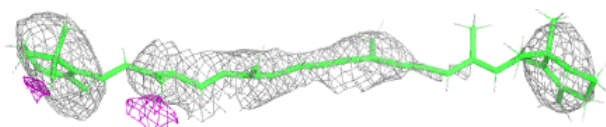
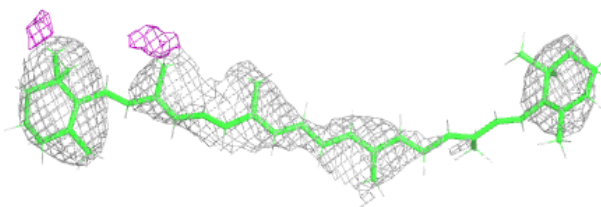
**Electron density around BCR B 3046:**

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

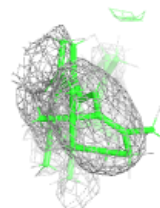
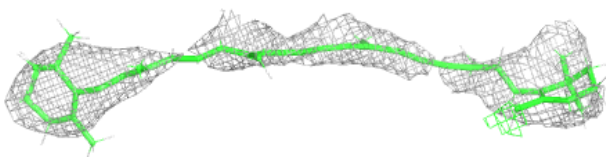
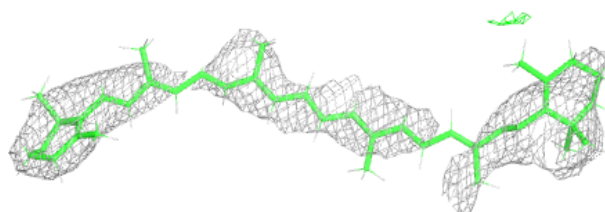


Electron density around BCR B 3047:

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

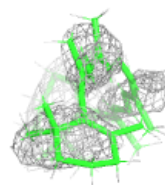
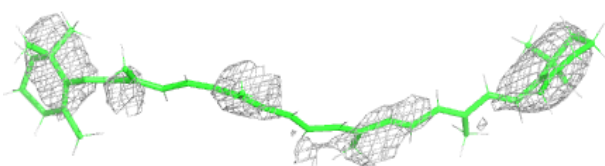
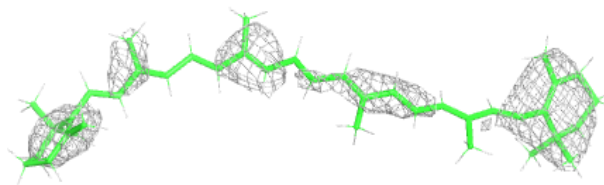
**Electron density around BCR B 3051:**

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

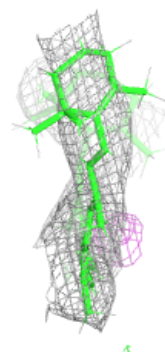
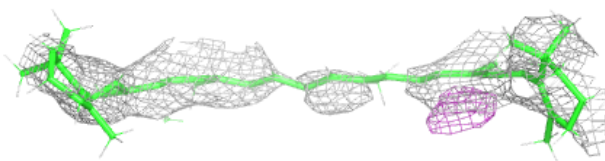
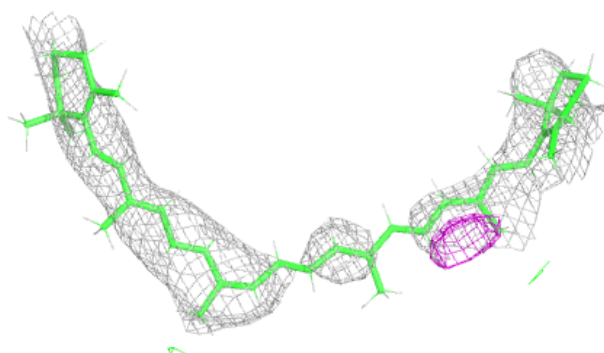


Electron density around BCR F 201:

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

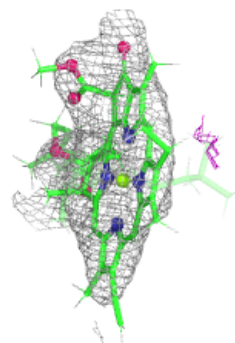
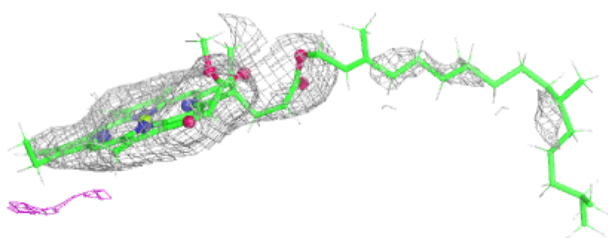
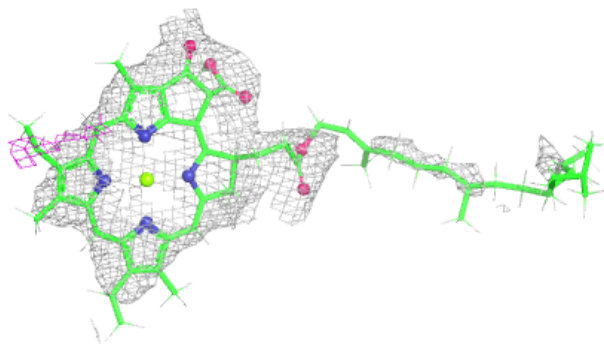
**Electron density around BCR F 203:**

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

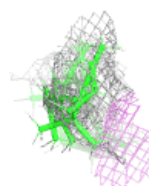
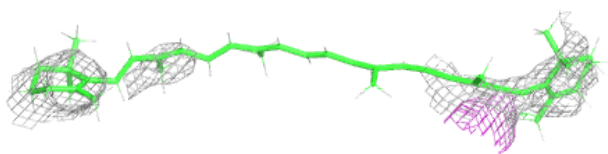
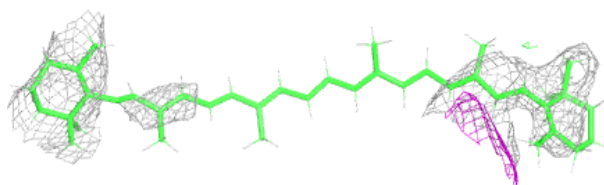


Electron density around CLA A 806:

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

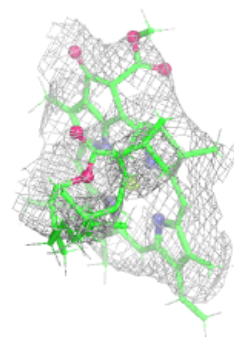
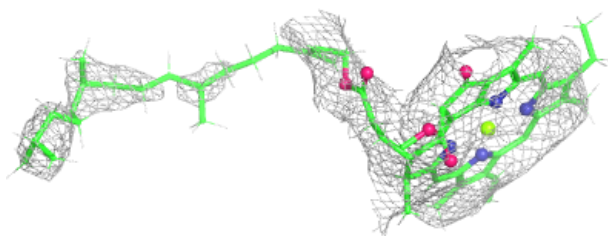
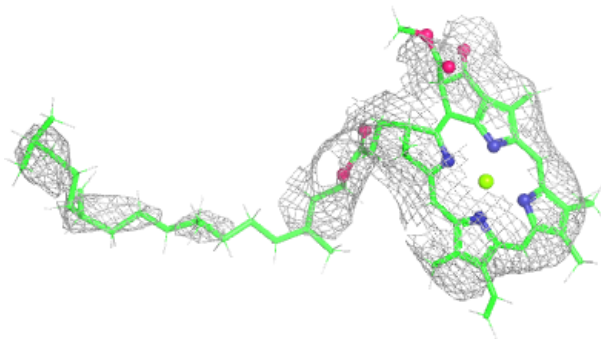
**Electron density around BCR J 105:**

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

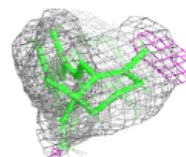
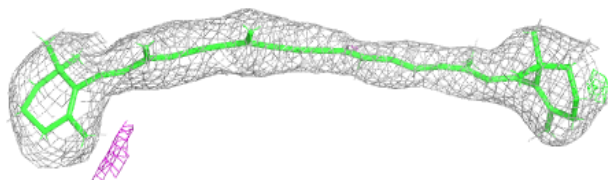
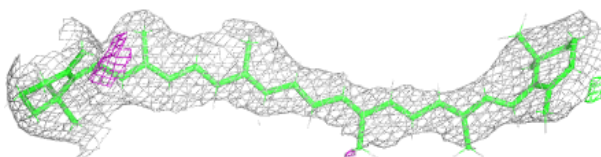


Electron density around CLA A 822:

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

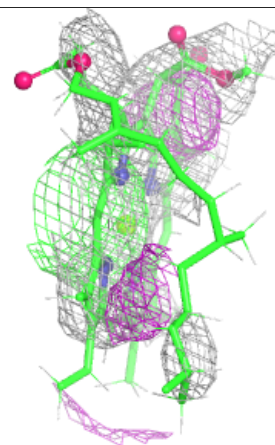
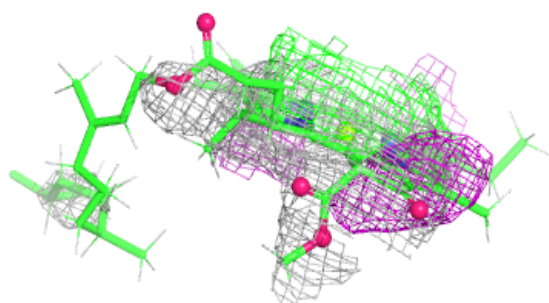
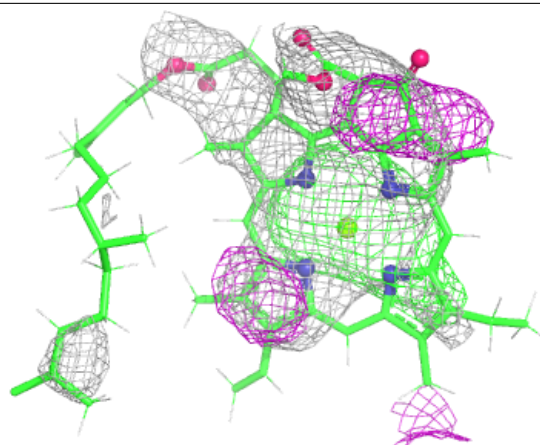
**Electron density around BCR M 103:**

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

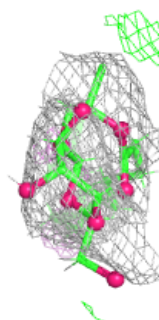
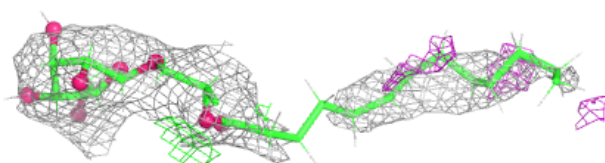
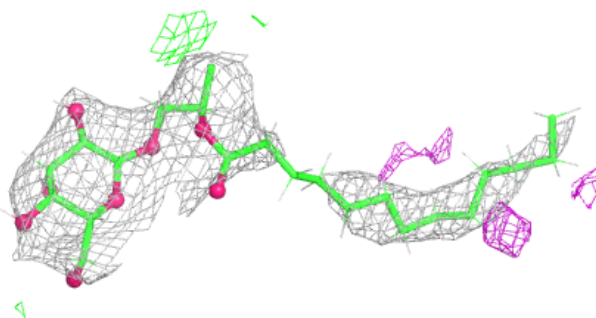


Electron density around CLA A 814:

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

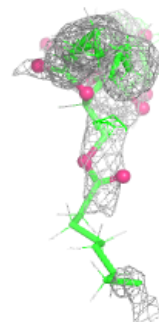
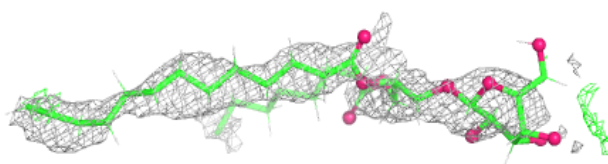
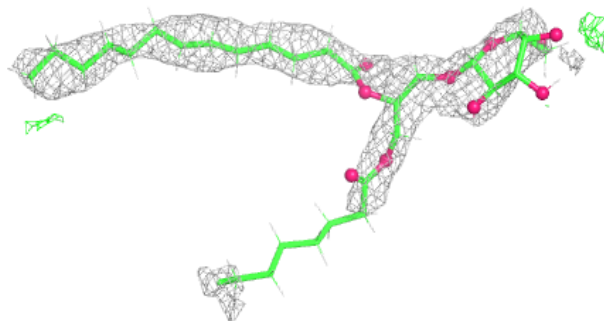
**Electron density around LMG A 855:**

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



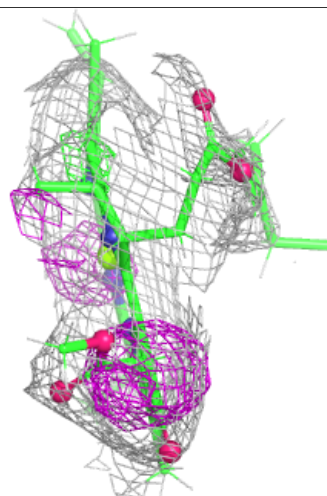
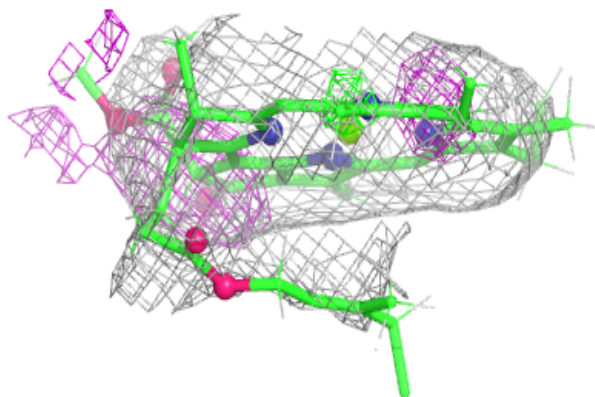
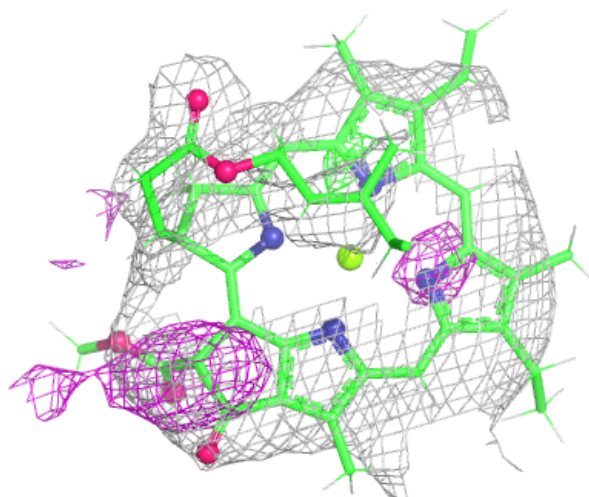
Electron density around LMG I 102:

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



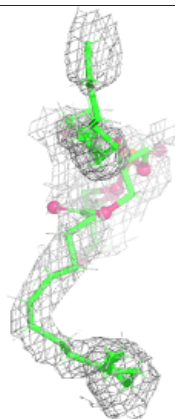
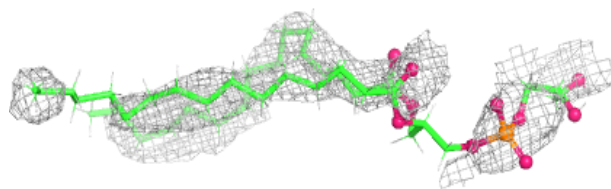
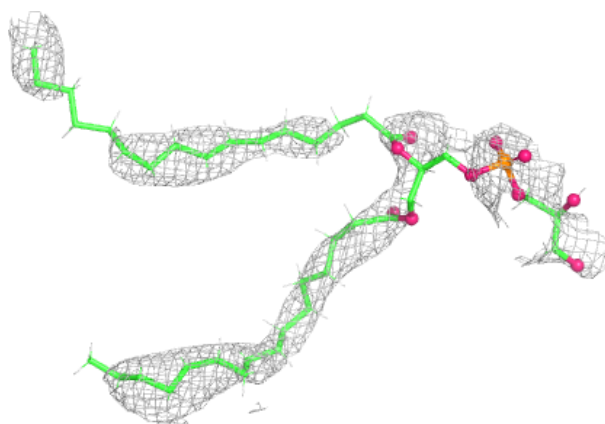
Electron density around CLA A 824:

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



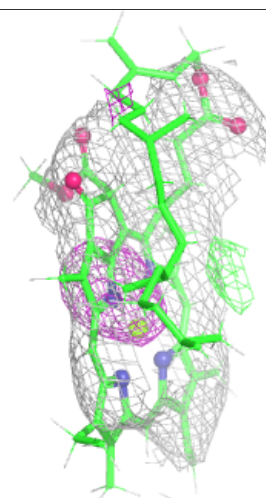
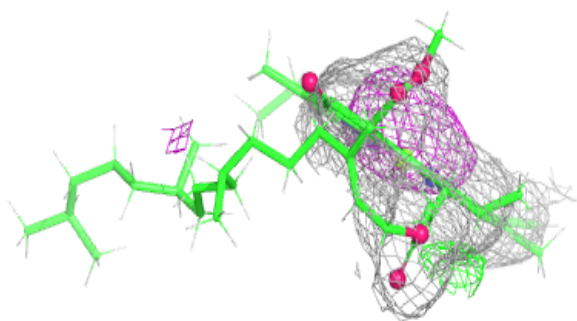
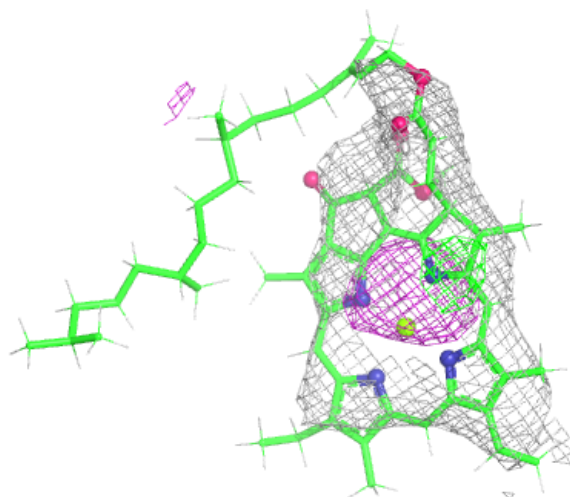
Electron density around LHG M 101:

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



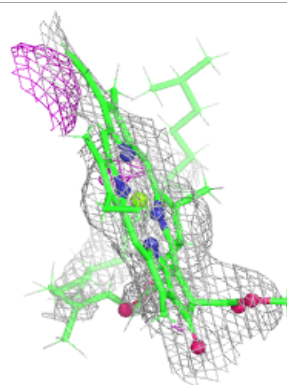
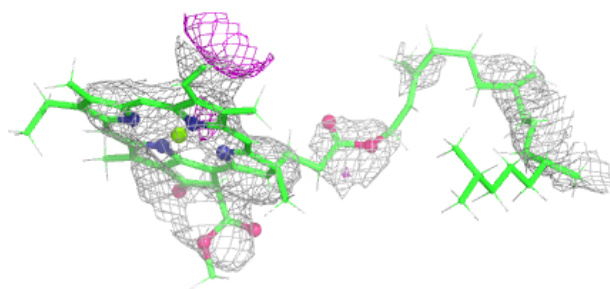
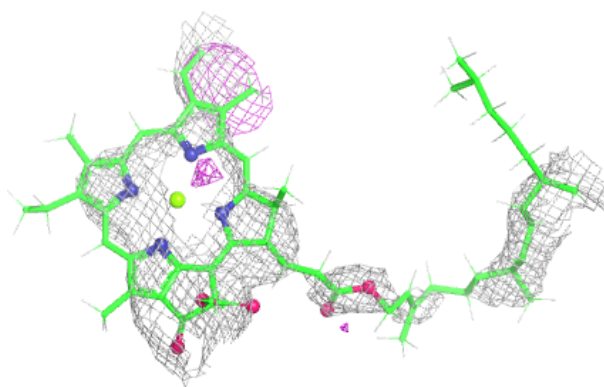
Electron density around CLA A 826:

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

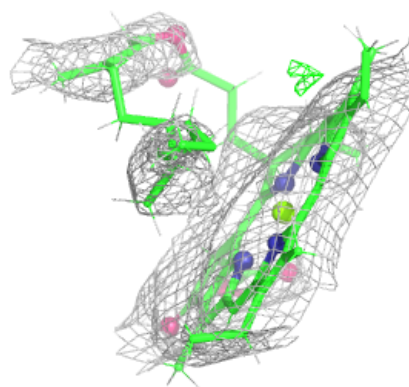
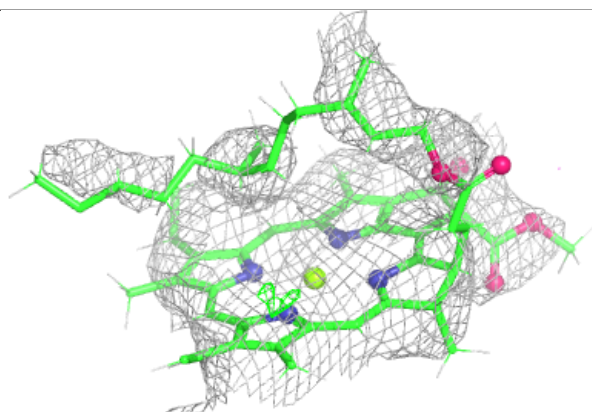
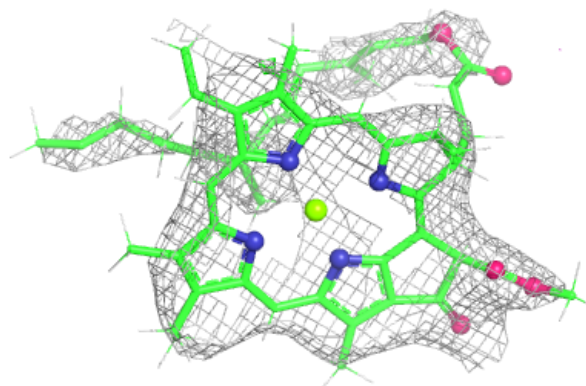


Electron density around CLA A 828:

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

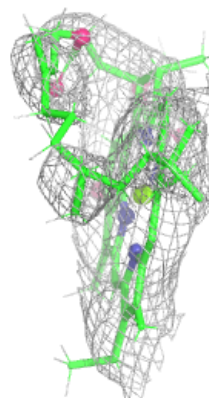
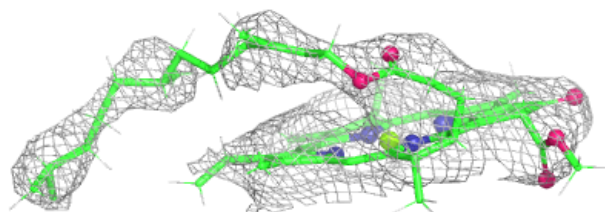
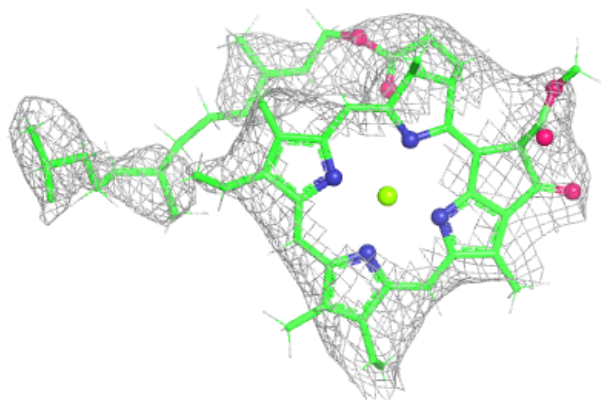
**Electron density around CLA B 3018:**

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

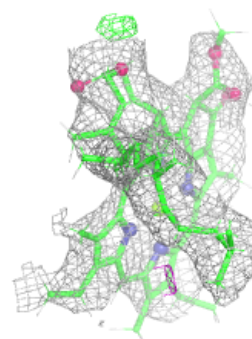
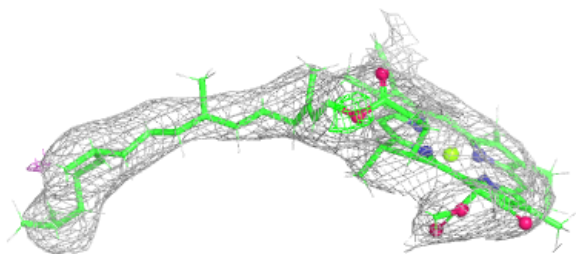
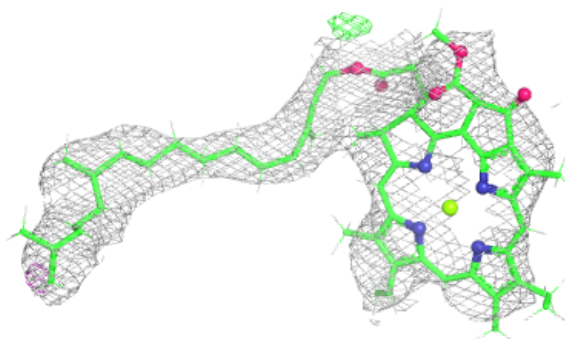


Electron density around CLA B 3019:

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

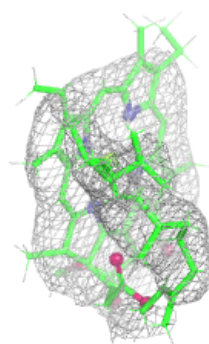
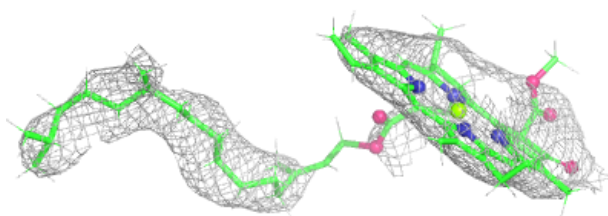
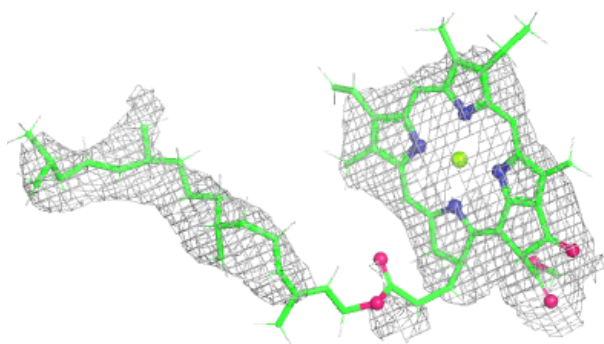
**Electron density around CLA A 803:**

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

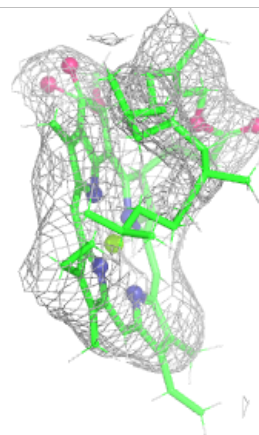
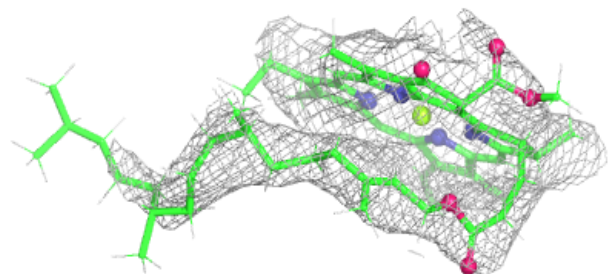
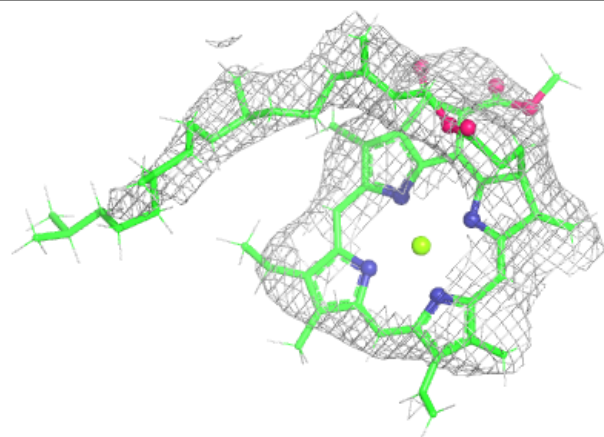


Electron density around CLA A 809:

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

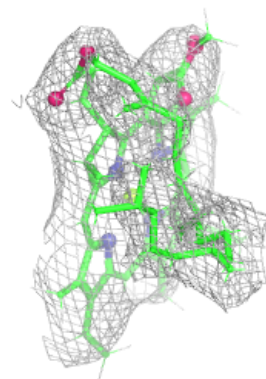
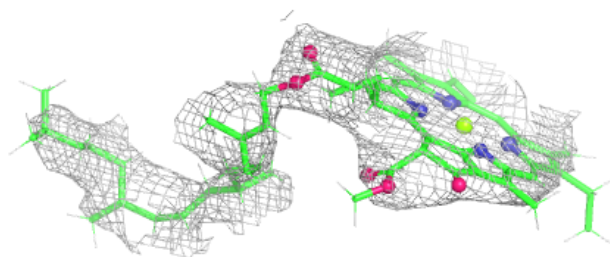
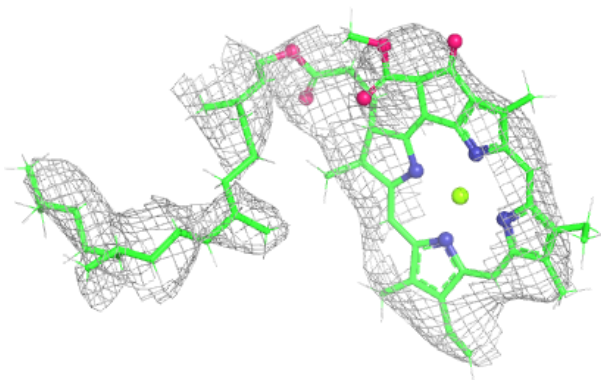
**Electron density around CLA A 830:**

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



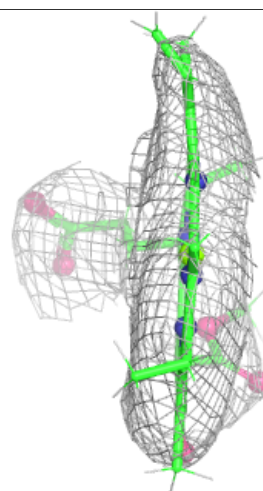
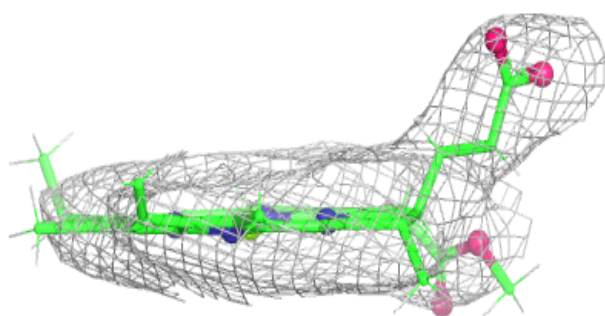
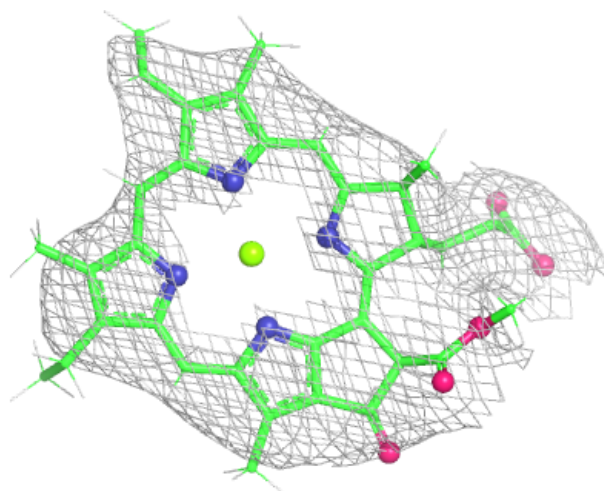
Electron density around CLA A 804:

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



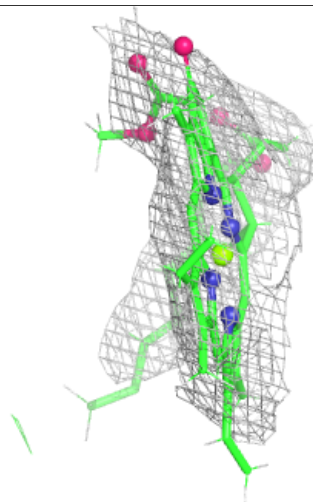
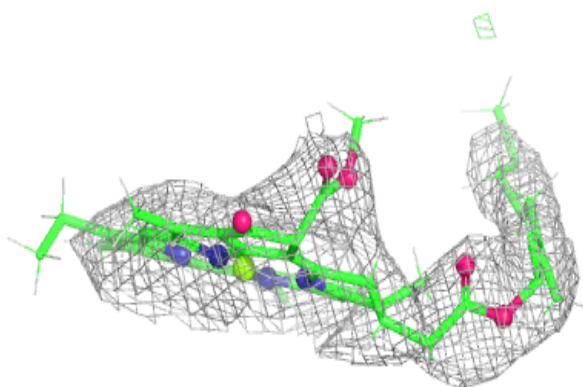
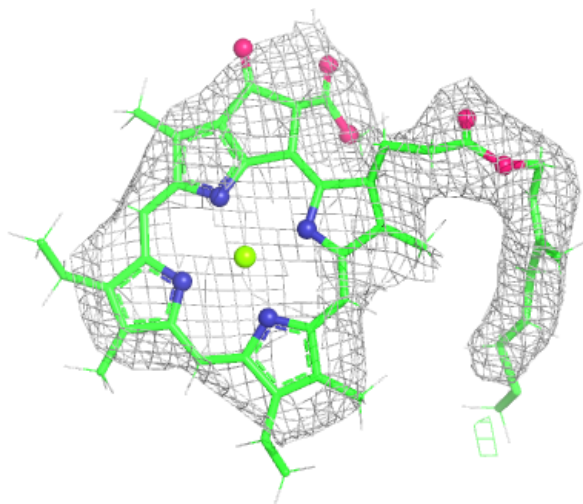
Electron density around CLA B 3024:

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



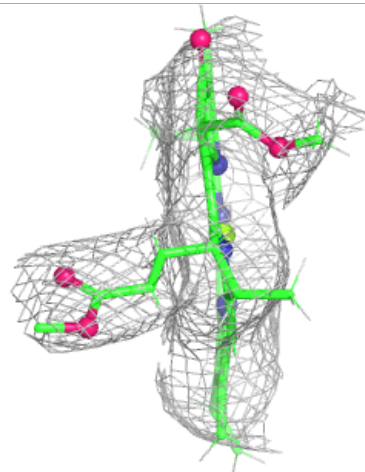
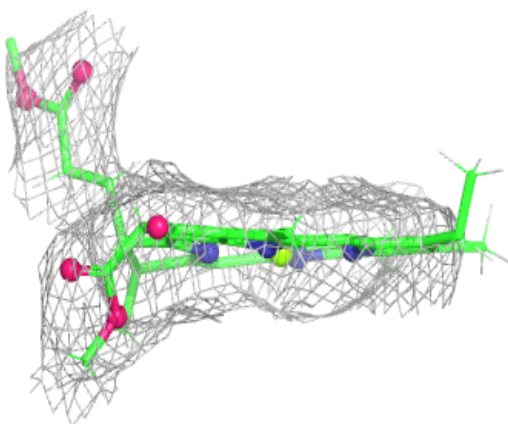
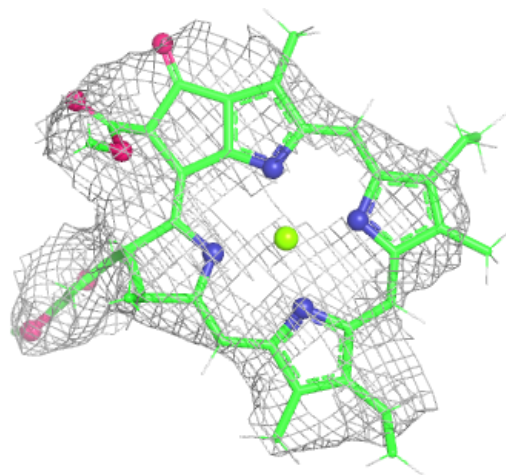
Electron density around CLA B 3025:

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



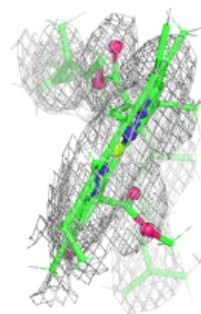
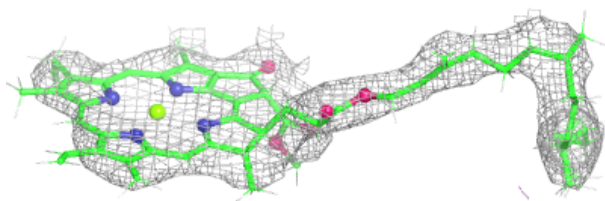
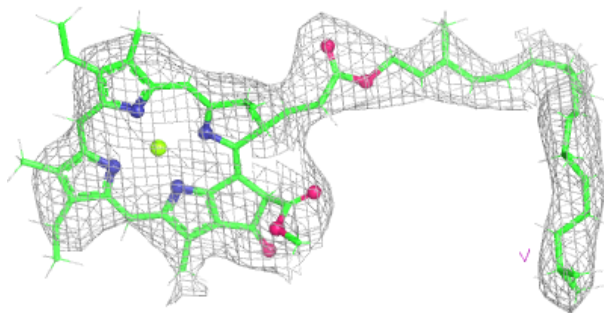
Electron density around CLA B 3026:

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



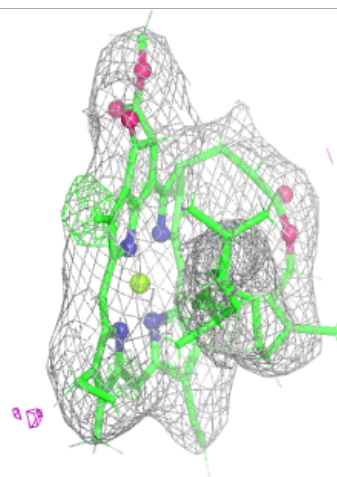
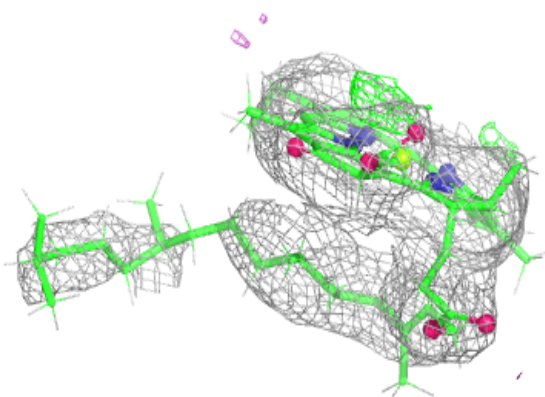
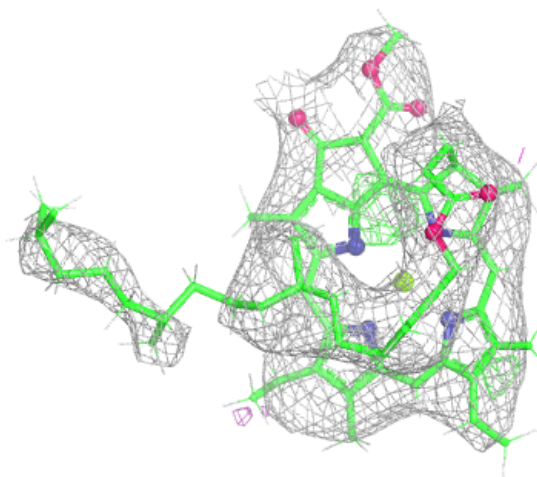
Electron density around CLA B 3027:

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



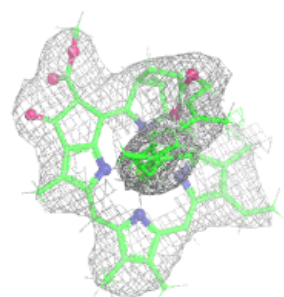
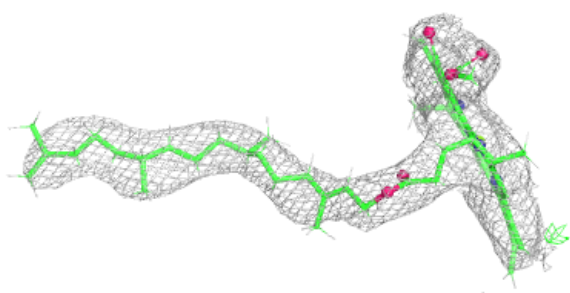
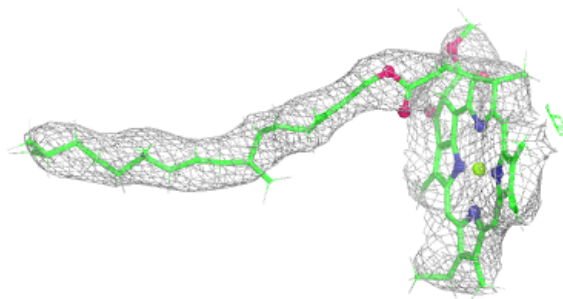
Electron density around CLA B 3028:

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

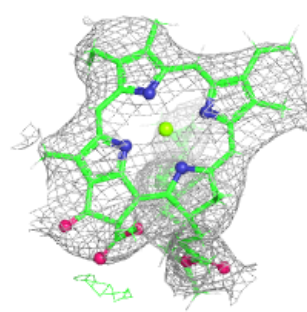
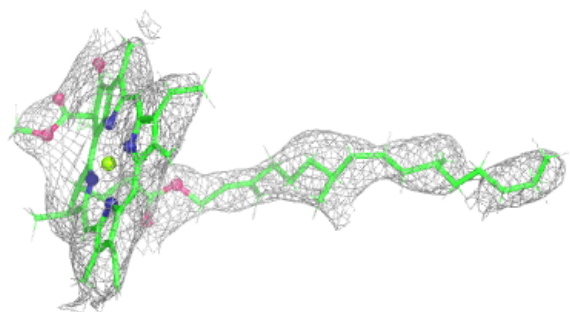
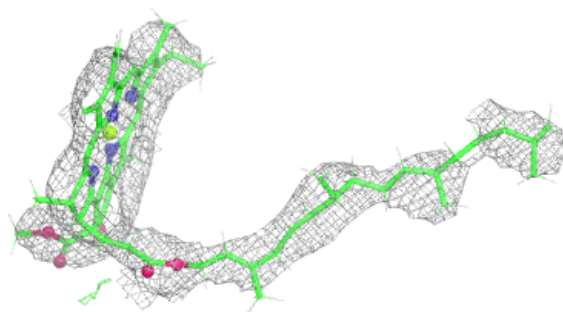


Electron density around CLA B 3029:

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

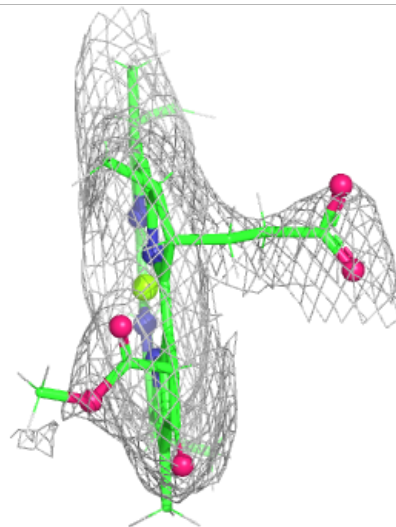
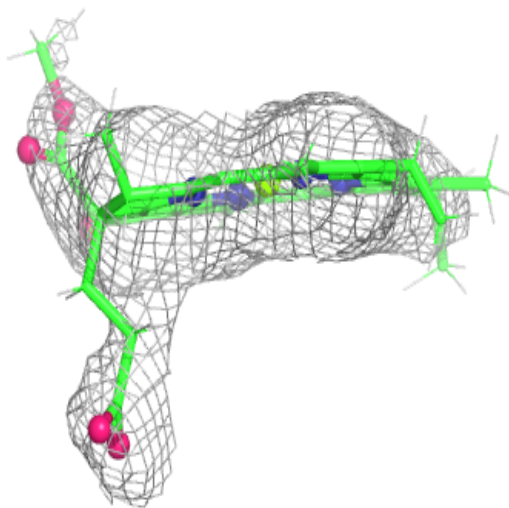
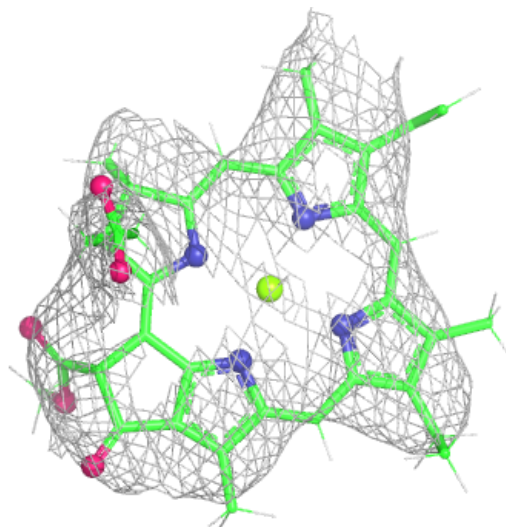
**Electron density around CLA B 3030:**

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



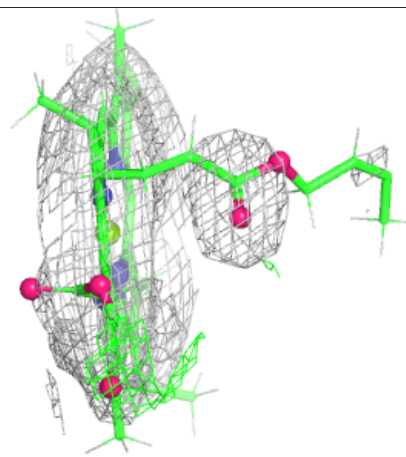
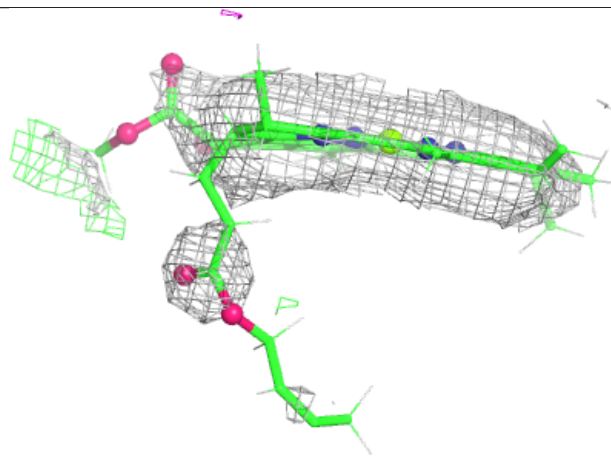
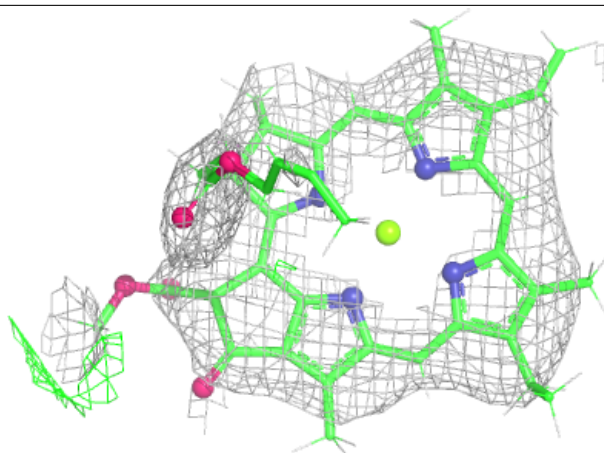
Electron density around CLA B 3031:

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



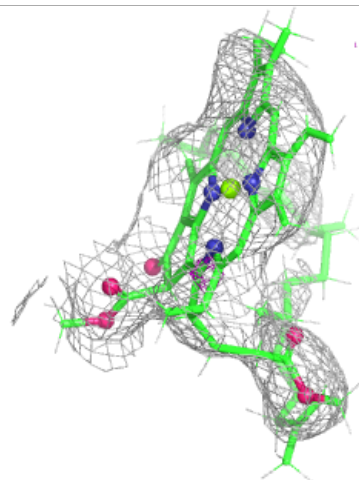
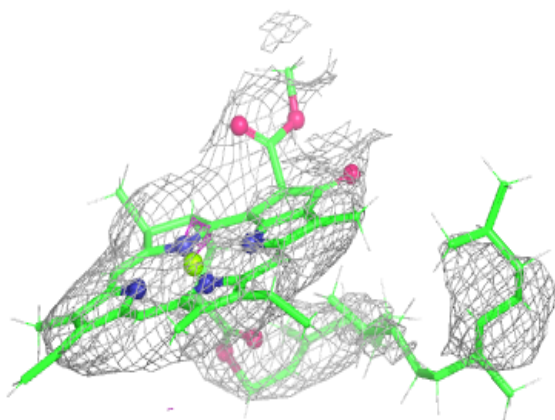
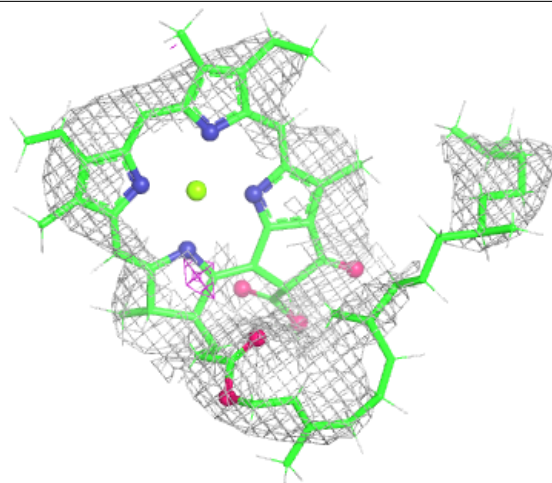
Electron density around CLA B 3032:

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



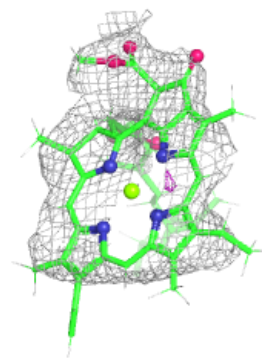
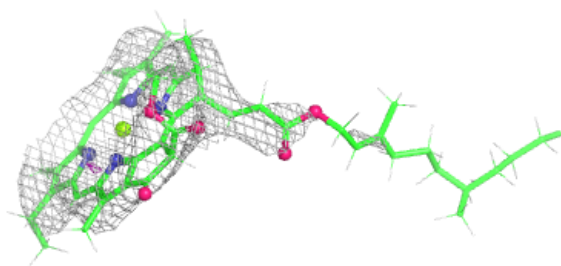
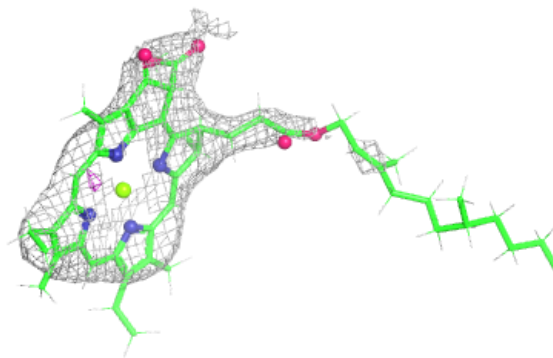
Electron density around CLA B 3033:

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



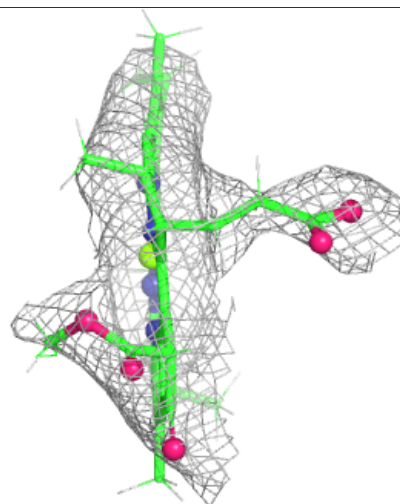
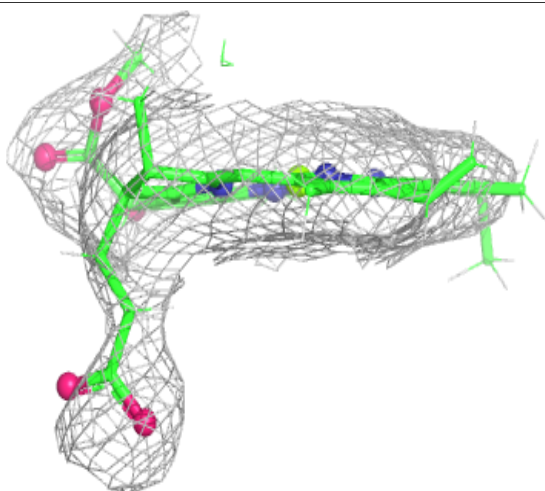
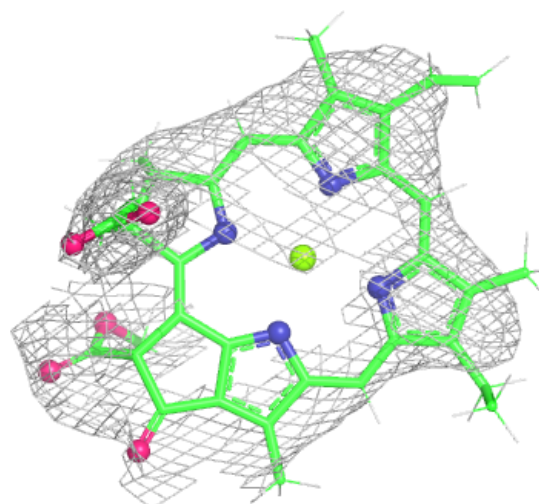
Electron density around CLA B 3034:

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



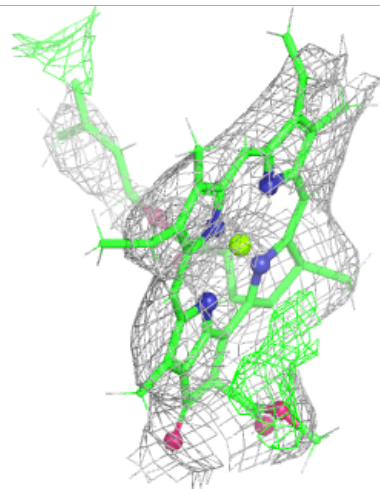
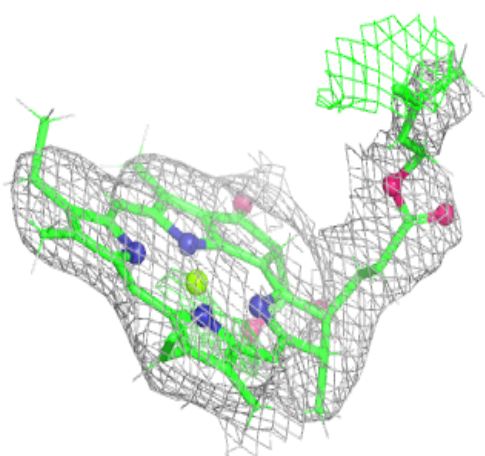
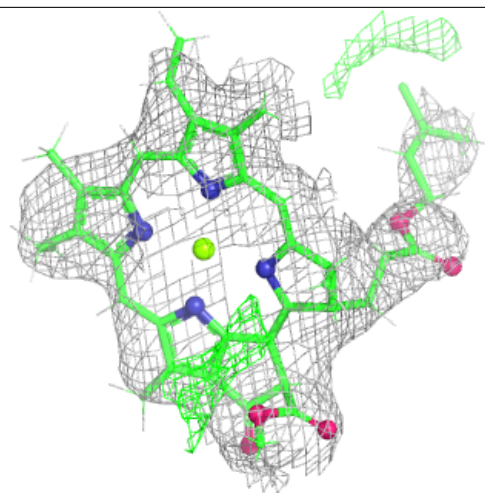
Electron density around CLA B 3035:

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



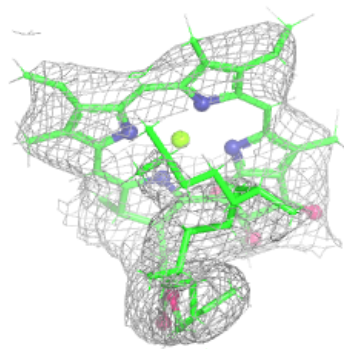
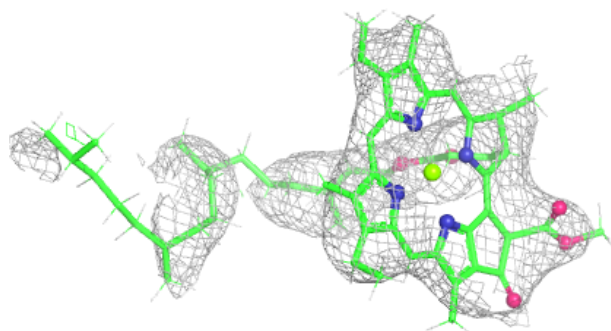
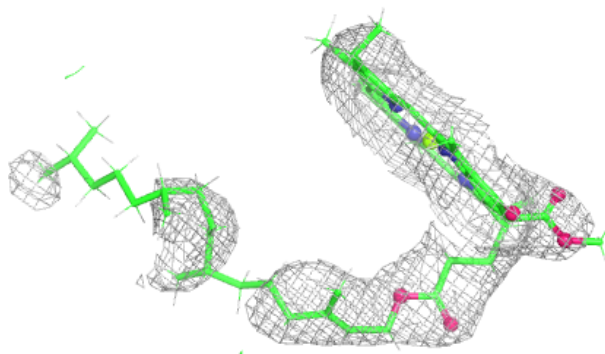
Electron density around CLA A 832:

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

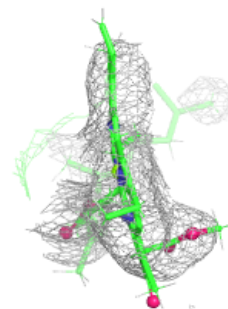
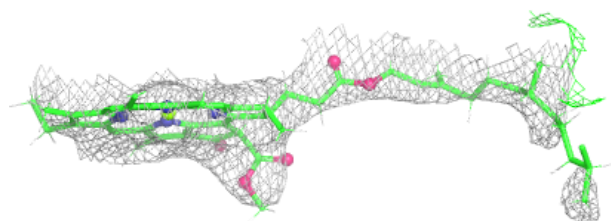
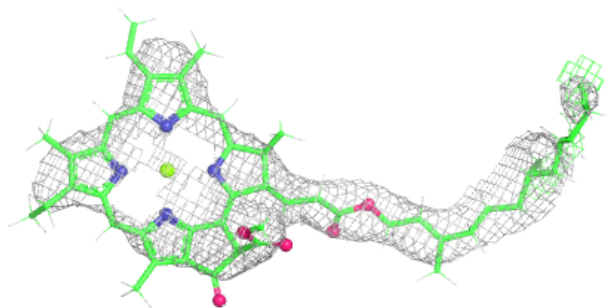


Electron density around CLA A 833:

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

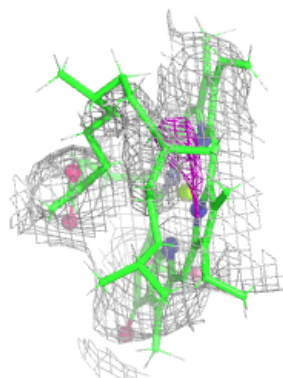
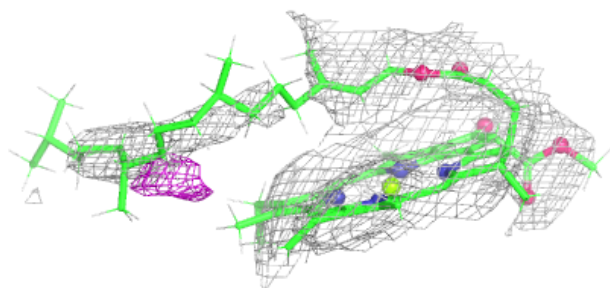
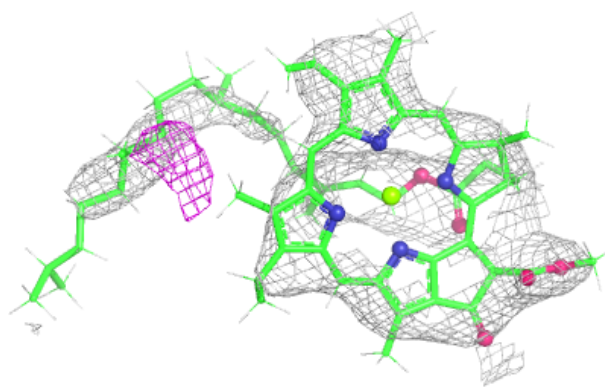
**Electron density around CLA B 3038:**

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



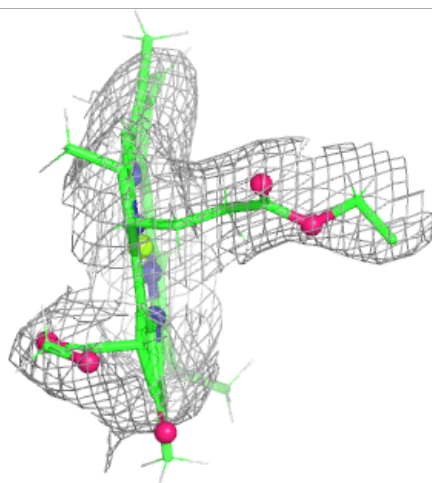
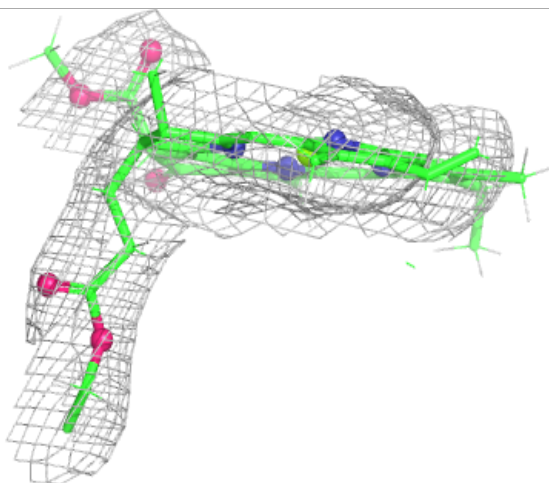
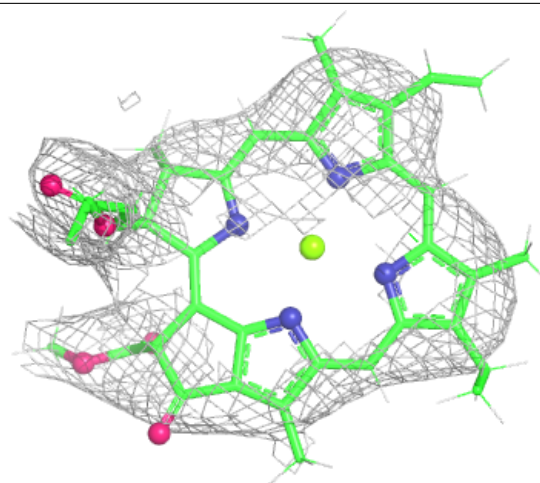
Electron density around CLA B 3039:

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



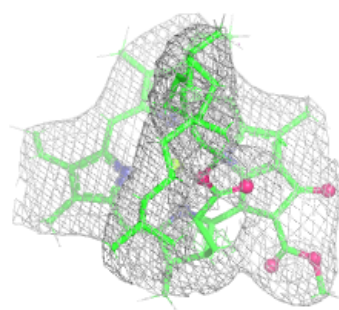
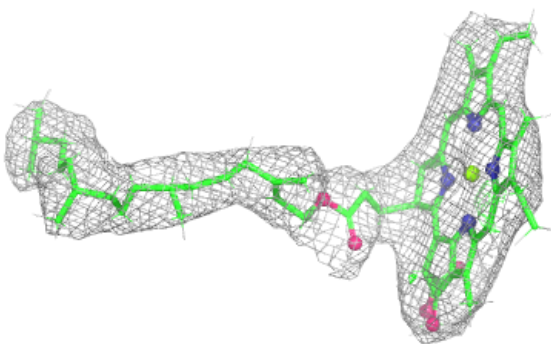
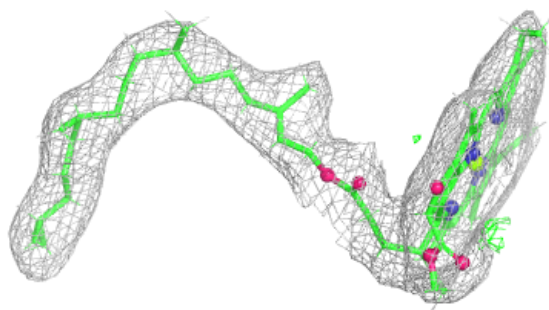
Electron density around CLA B 3040:

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

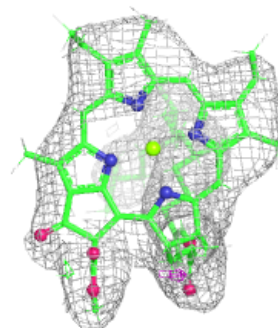
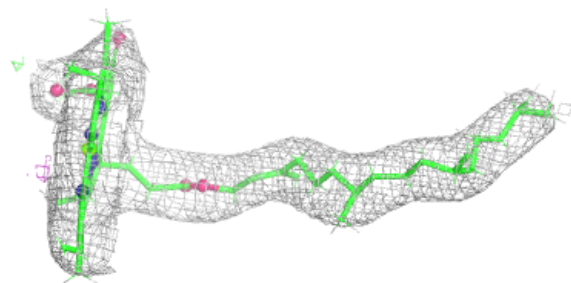
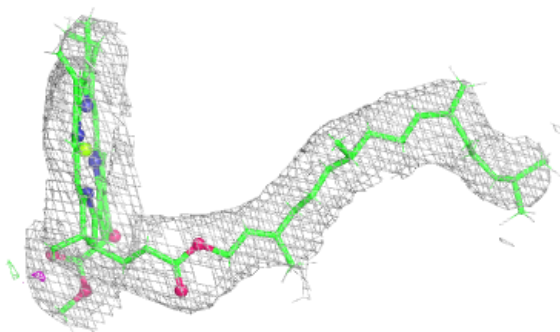


Electron density around CLA B 3041:

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

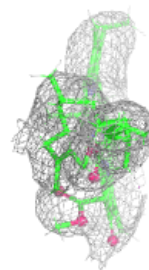
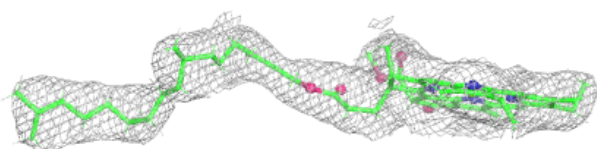
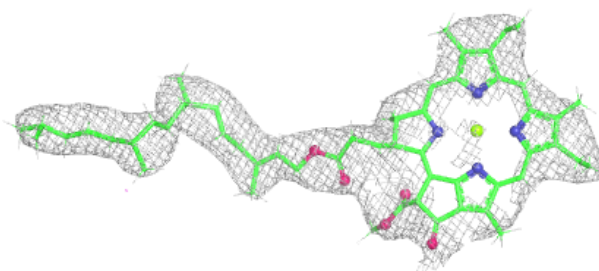
**Electron density around CLA B 3042:**

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

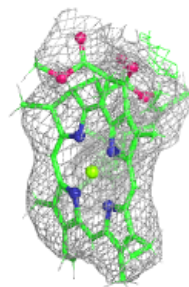
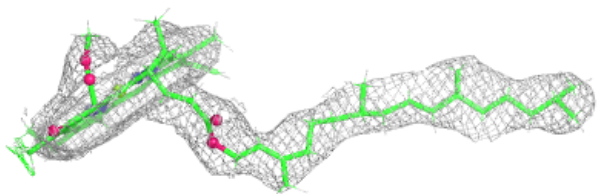
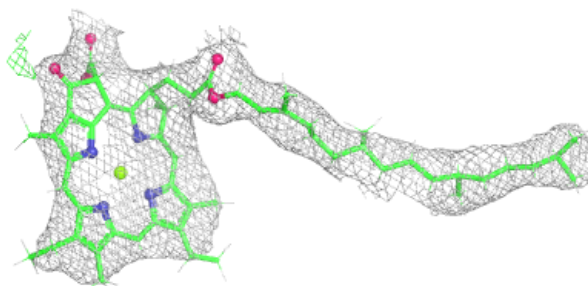


Electron density around CLA A 834:

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

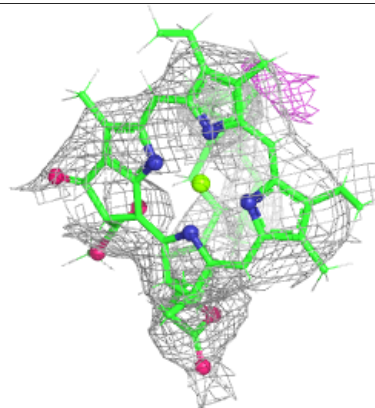
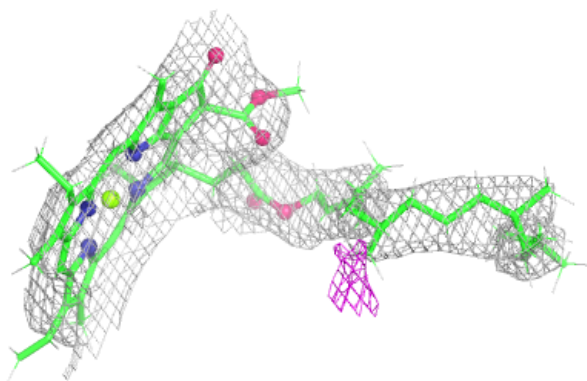
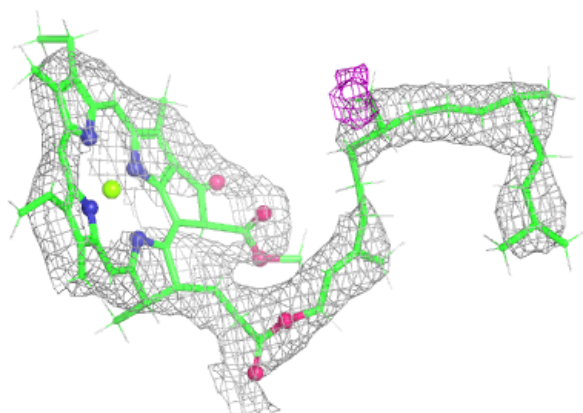
**Electron density around CLA A 835:**

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

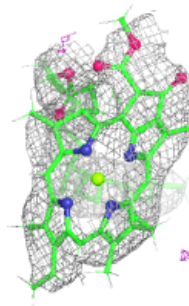
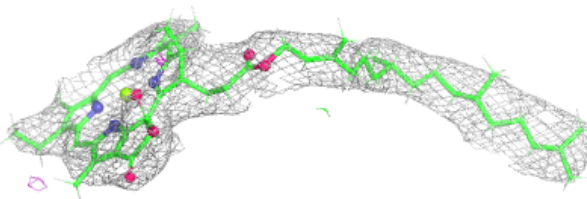
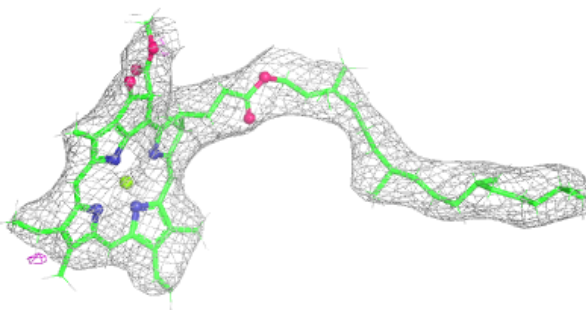


Electron density around CL0 A 801:

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

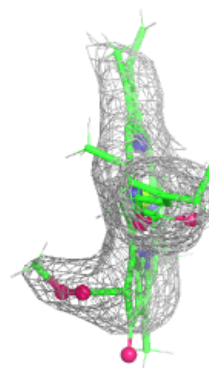
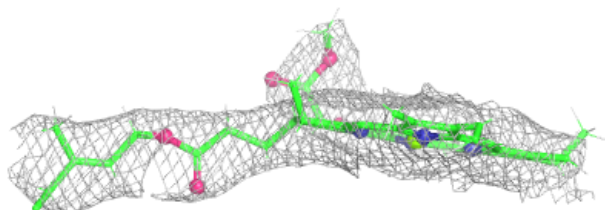
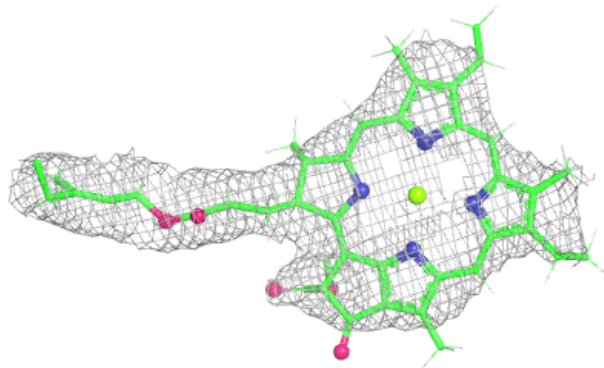
**Electron density around CLA A 802:**

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



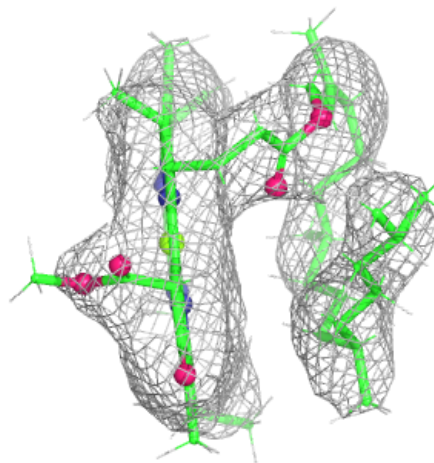
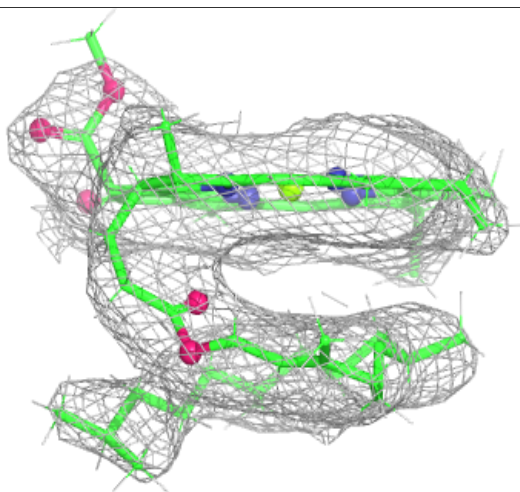
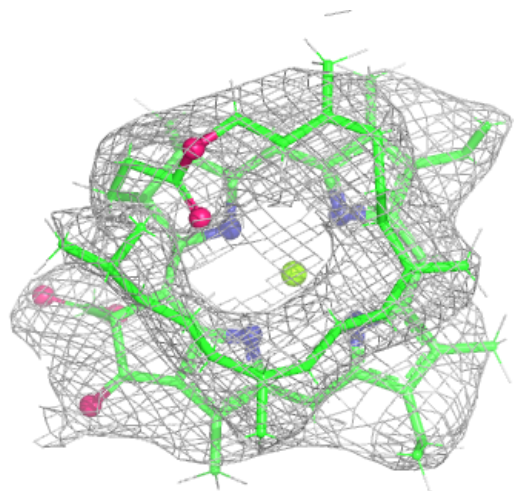
Electron density around CLA A 838:

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



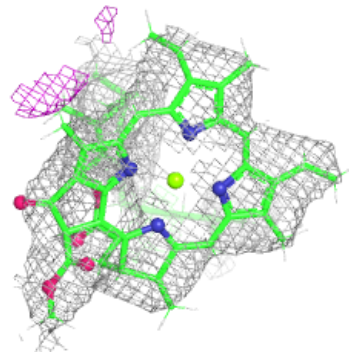
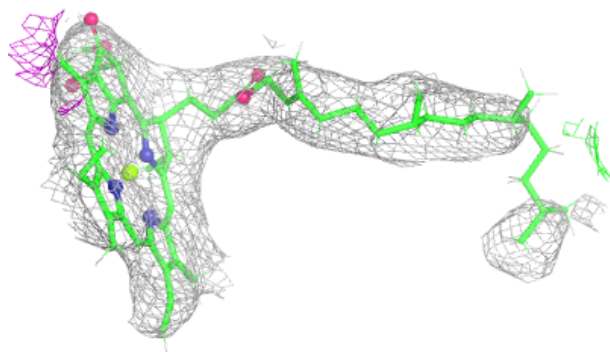
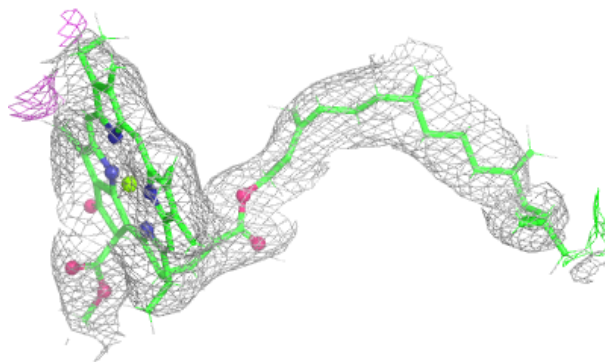
Electron density around CLA L 204:

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

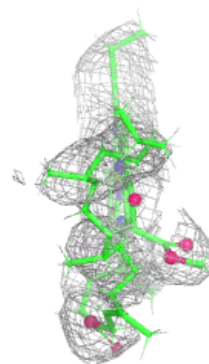
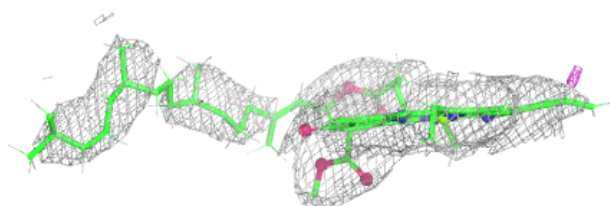
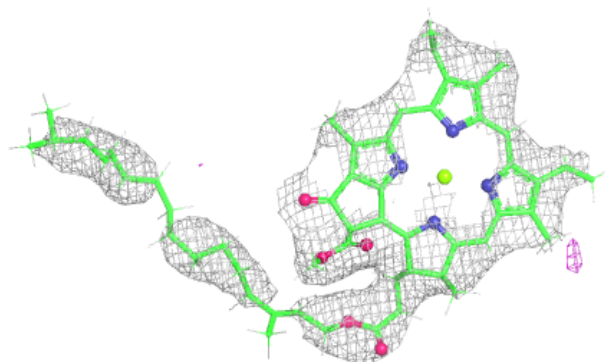


Electron density around CLA L 205:

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

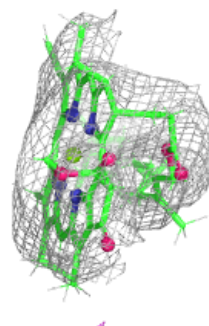
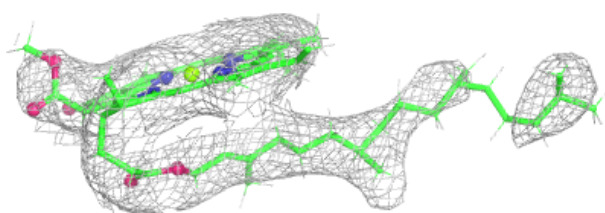
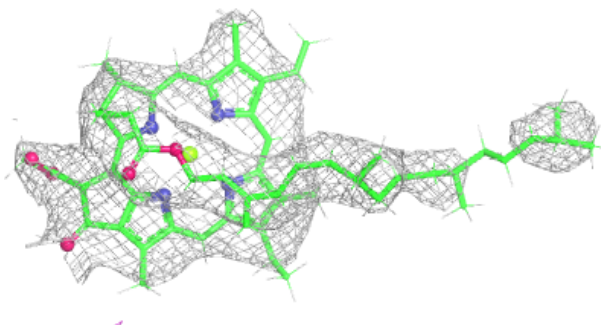
**Electron density around CLA L 206:**

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



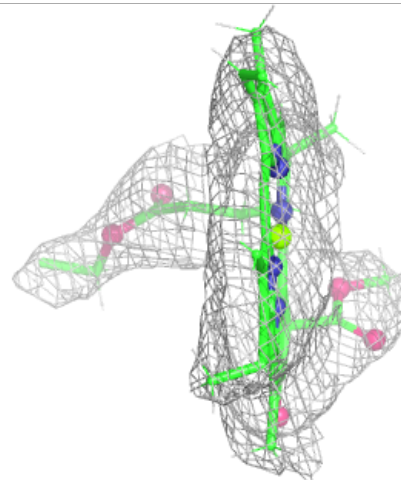
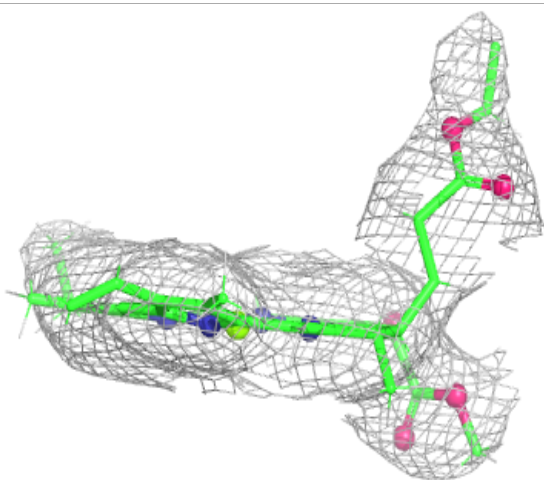
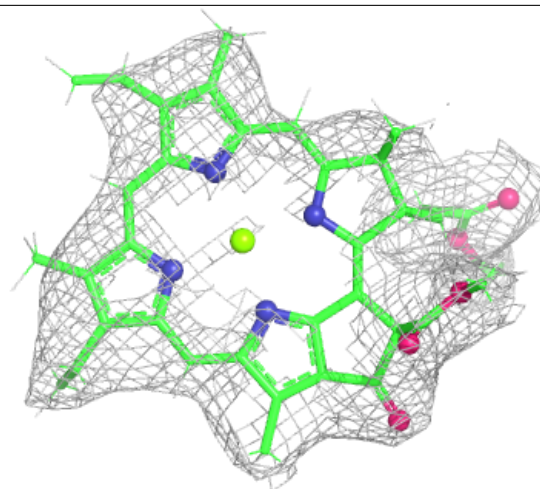
Electron density around CLA A 839:

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



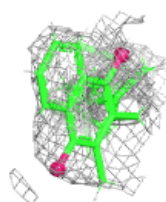
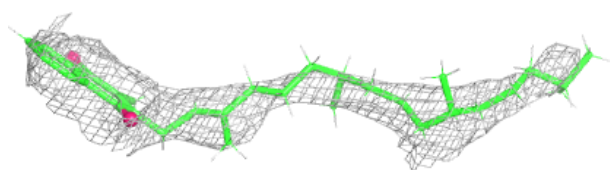
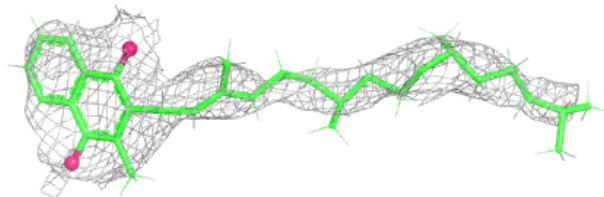
Electron density around CLA A 840:

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

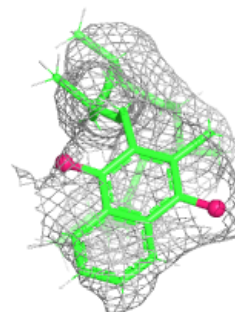
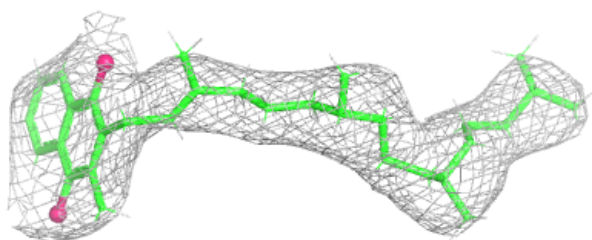
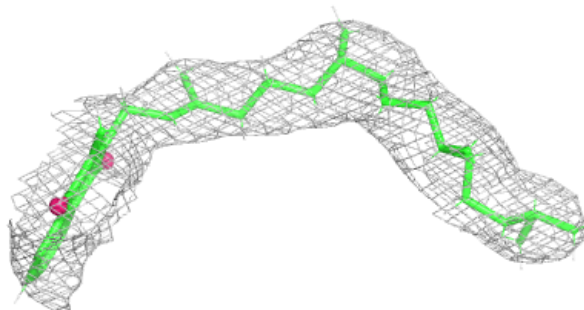


Electron density around PQN A 846:

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

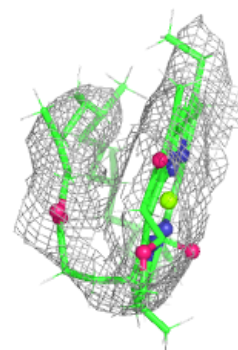
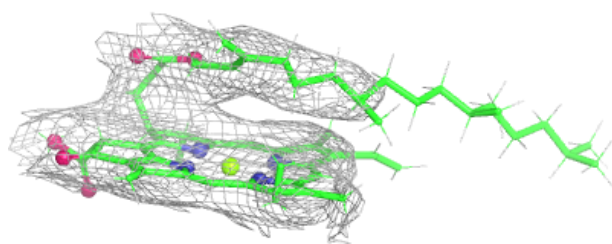
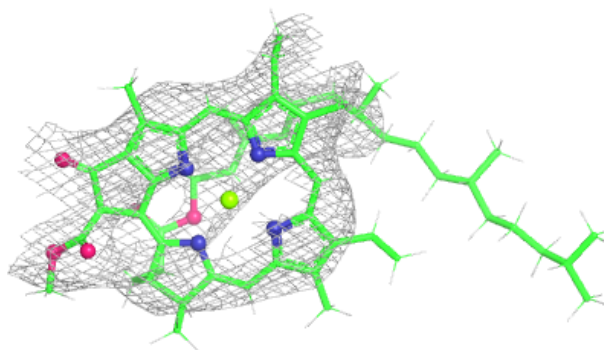
**Electron density around PQN B 3043:**

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

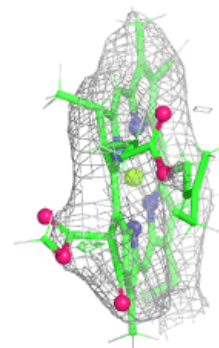
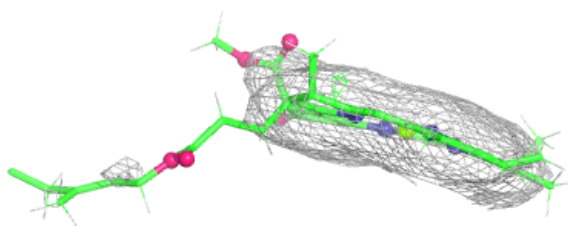
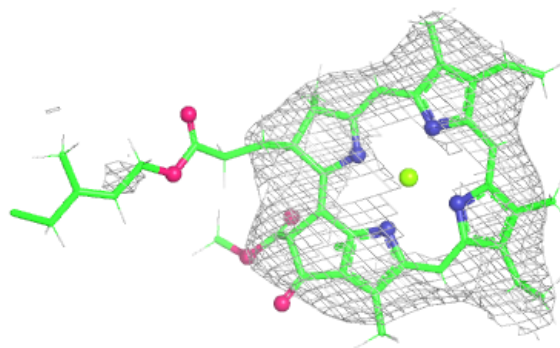


Electron density around CLA A 841:

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

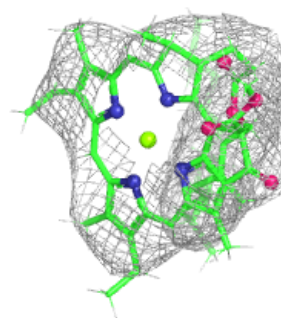
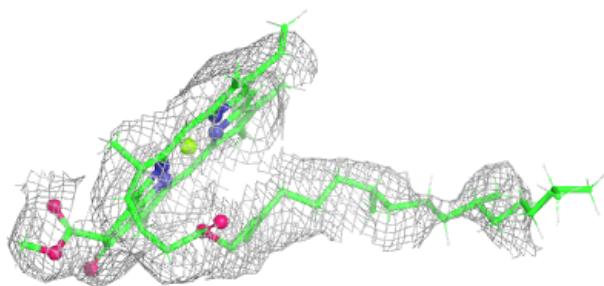
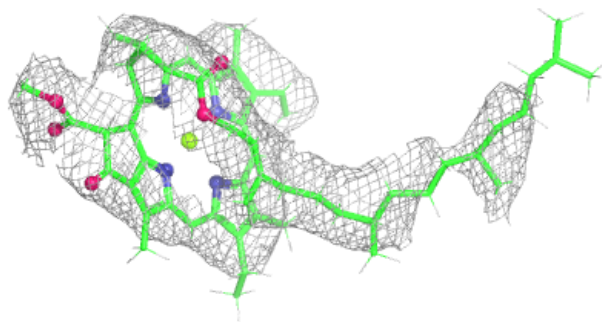
**Electron density around CLA A 842:**

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

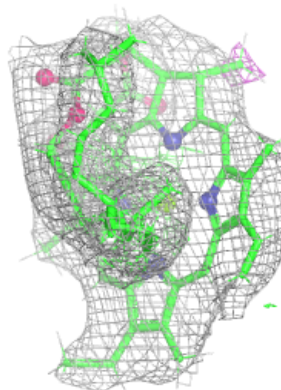
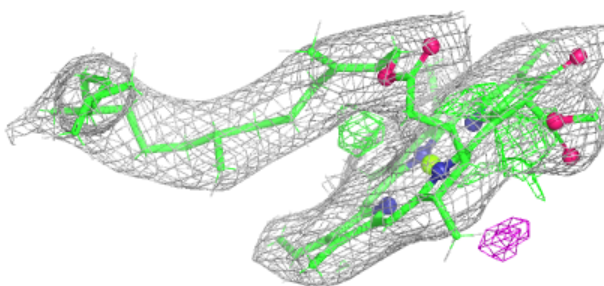
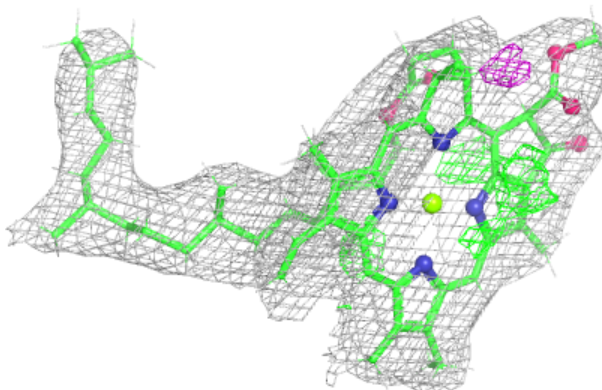


Electron density around CLA A 843:

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

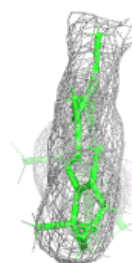
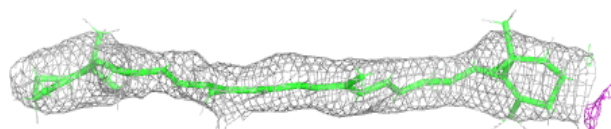
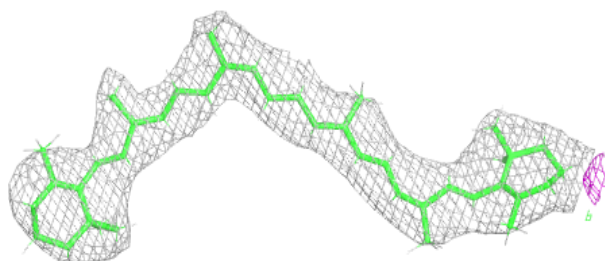
**Electron density around CLA A 844:**

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

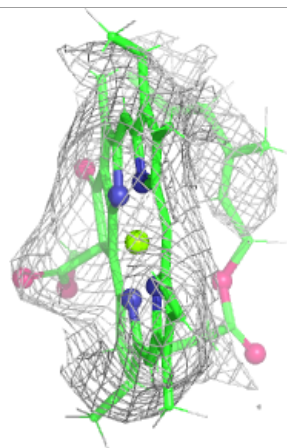
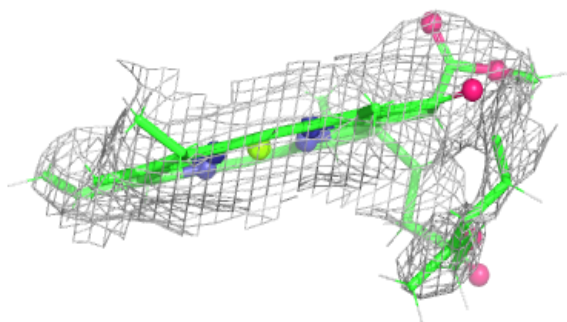
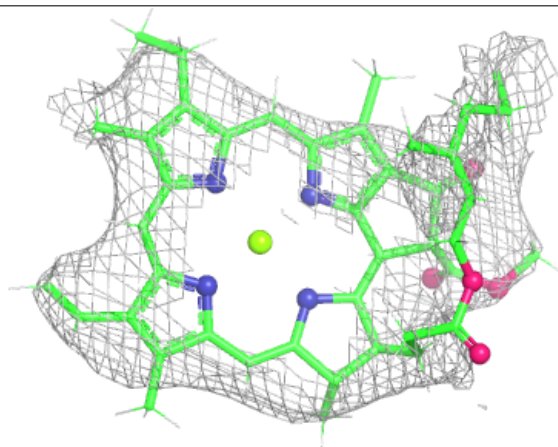


Electron density around BCR A 851:

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

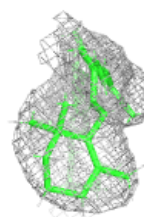
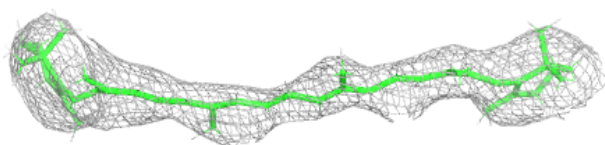
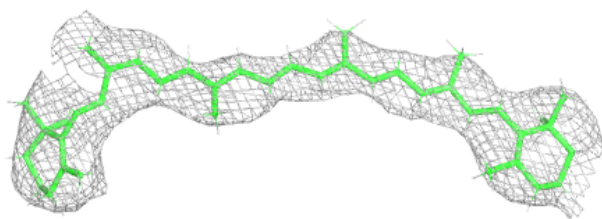
**Electron density around CLA A 845:**

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

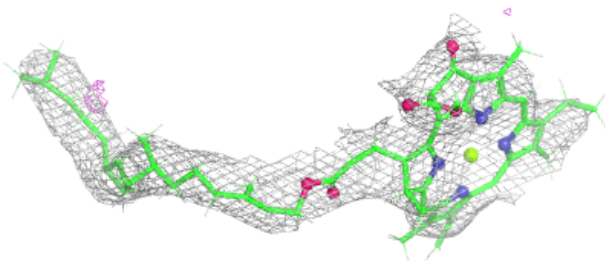
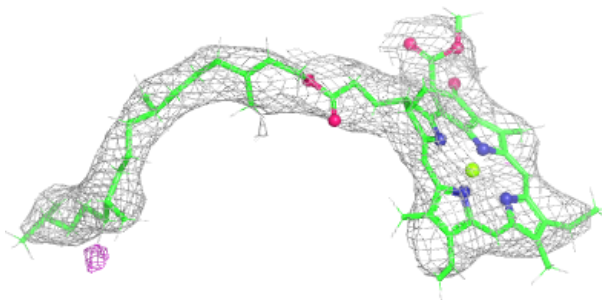


Electron density around BCR B 3045:

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

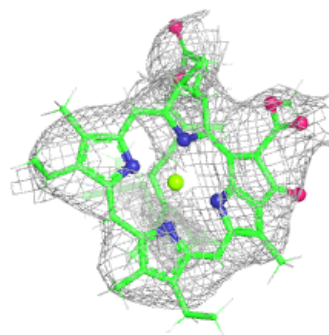
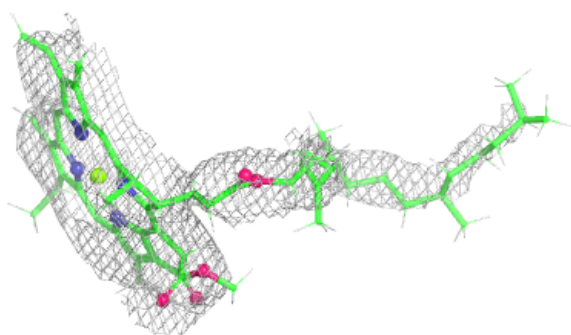
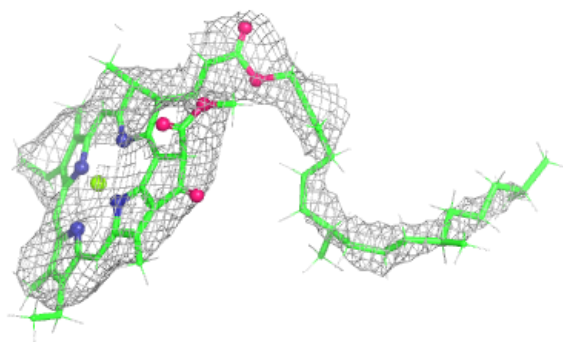
**Electron density around CLA A 856:**

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

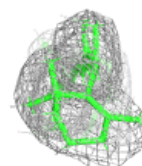
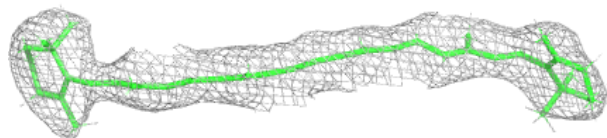
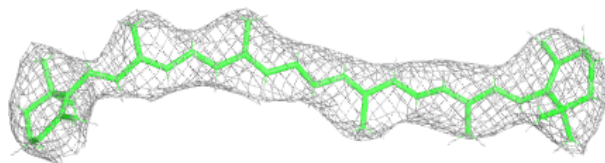


Electron density around CLA B 3003:

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

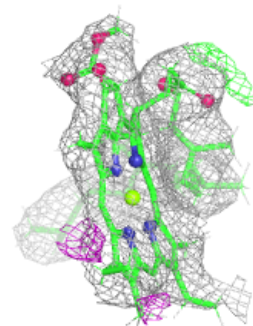
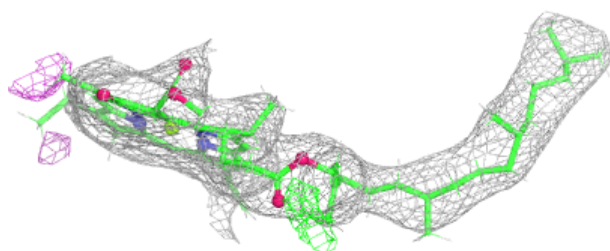
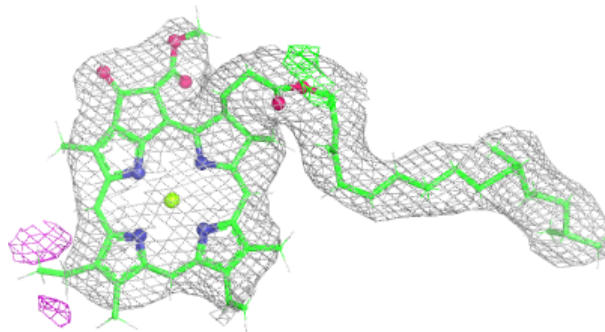
**Electron density around BCR B 3048:**

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

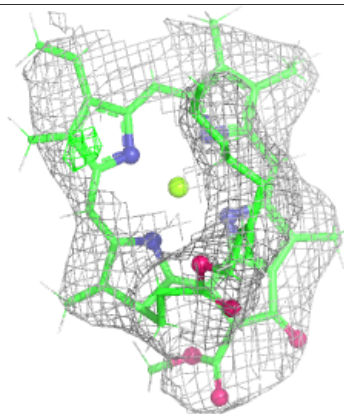
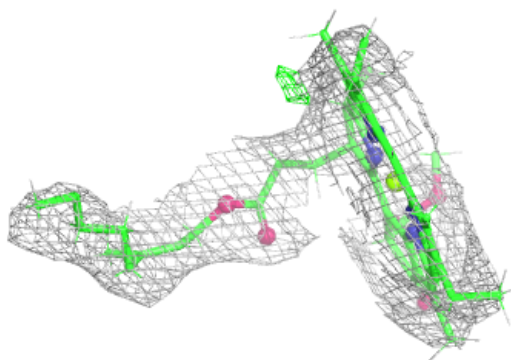
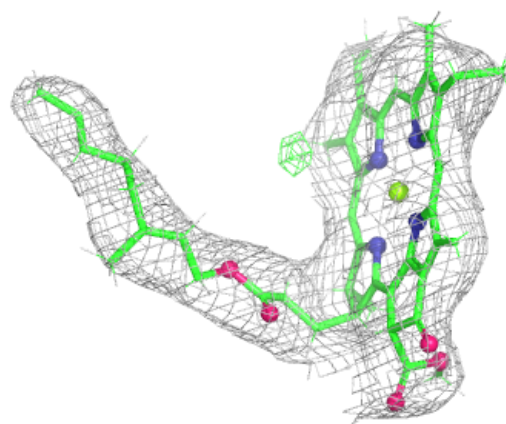


Electron density around CLA B 3004:

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

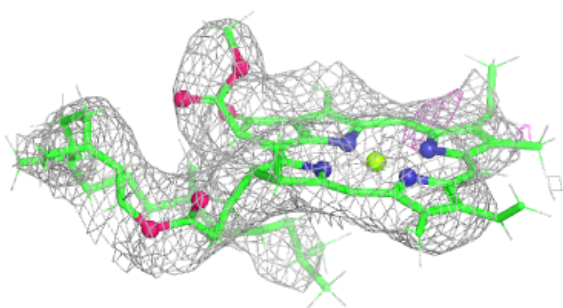
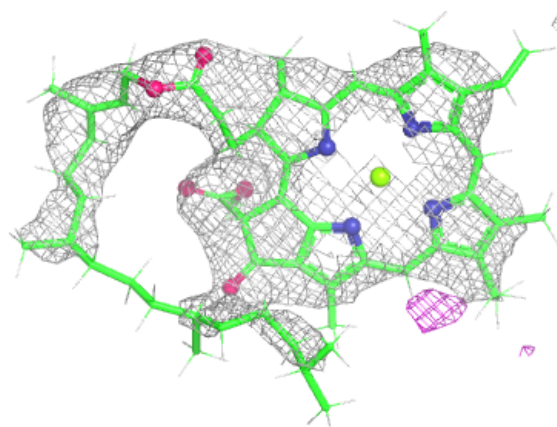
**Electron density around CLA B 3005:**

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

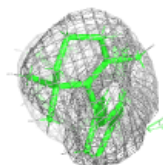
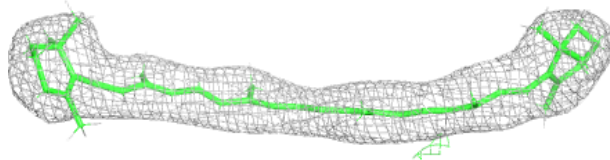
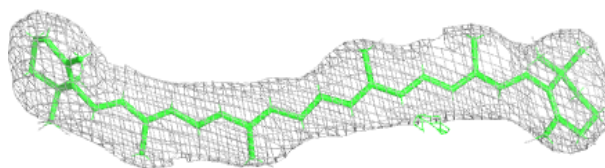


Electron density around CLA B 3006:

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

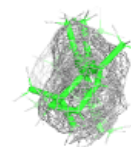
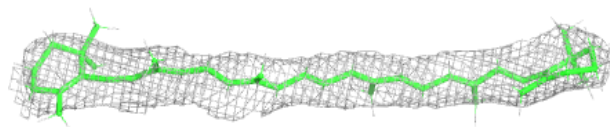
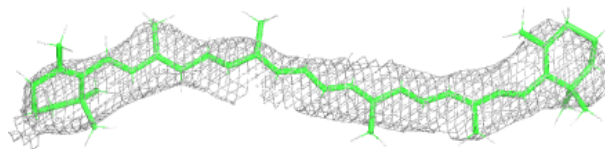
**Electron density around BCR I 101:**

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



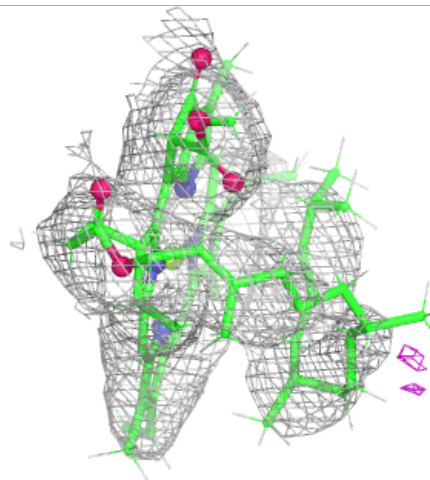
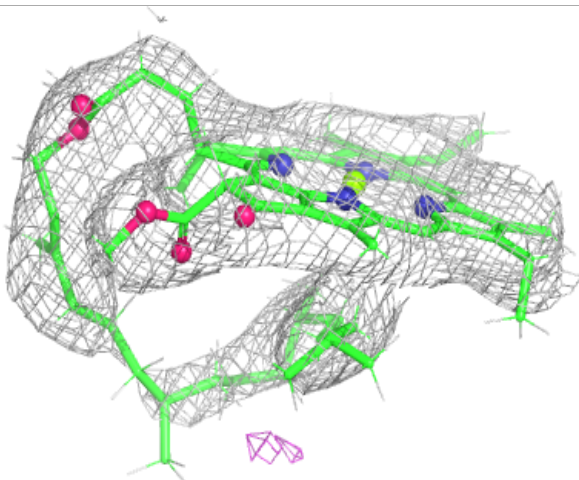
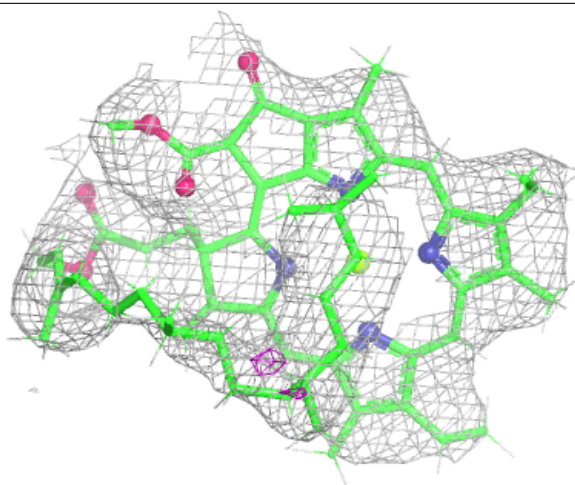
Electron density around BCR J 103:

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



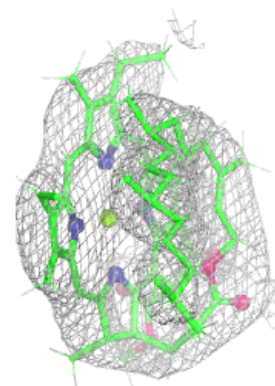
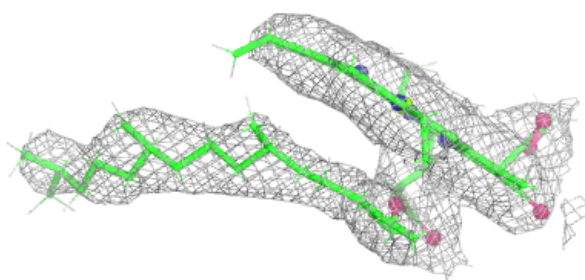
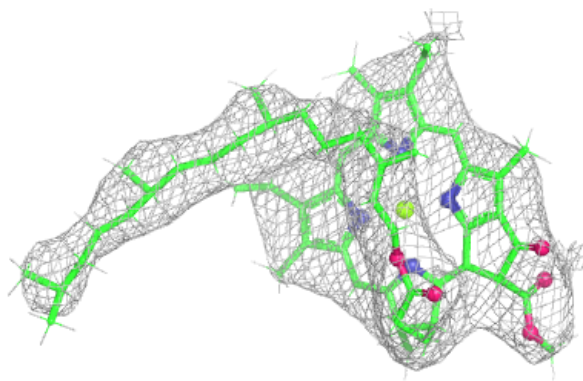
Electron density around CLA B 3007:

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



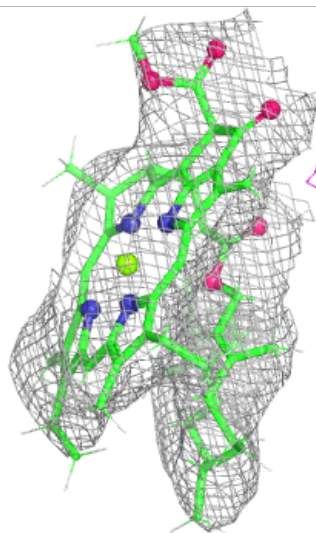
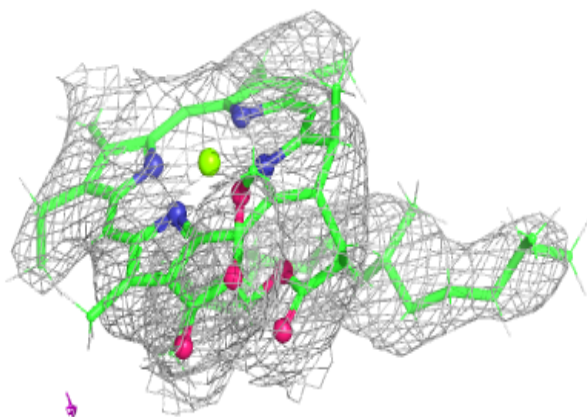
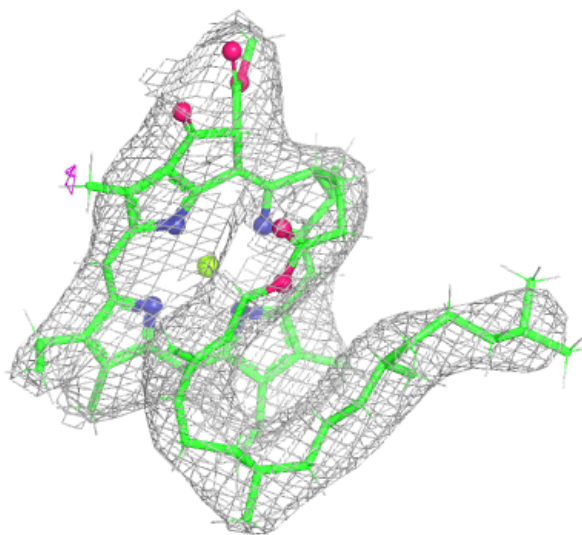
Electron density around CLA B 3008:

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



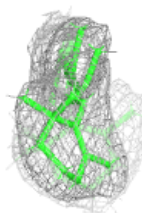
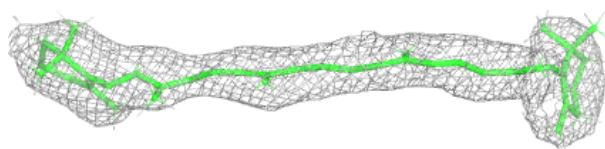
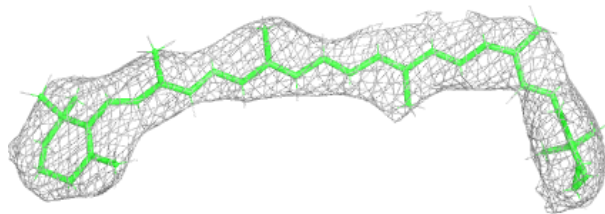
Electron density around CLA B 3009:

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

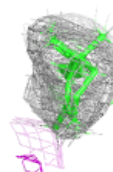
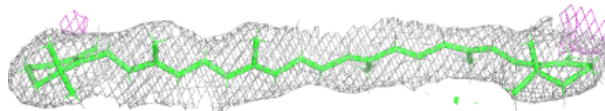
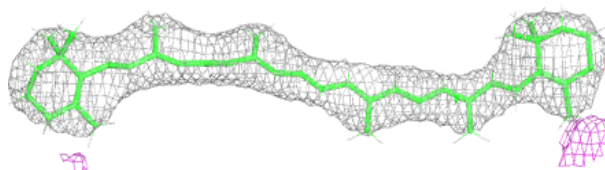


Electron density around BCR L 201:

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

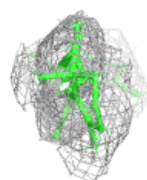
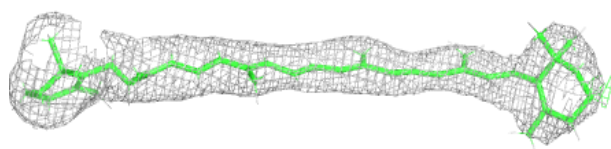
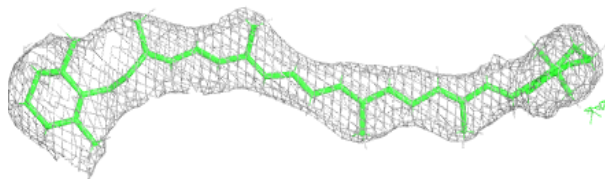
**Electron density around BCR L 208:**

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

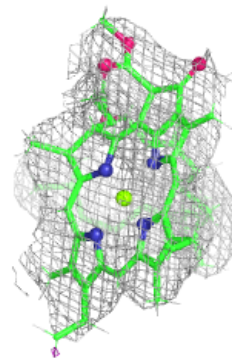
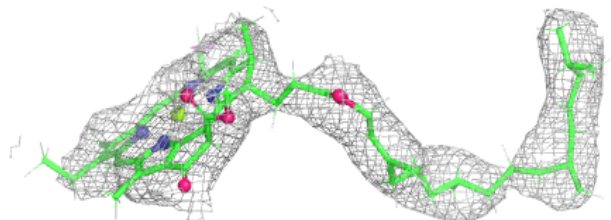
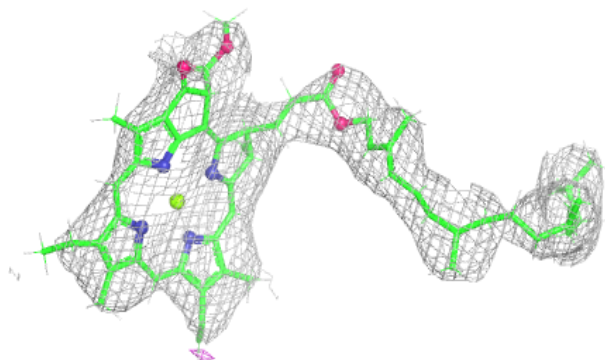


Electron density around BCR L 209:

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

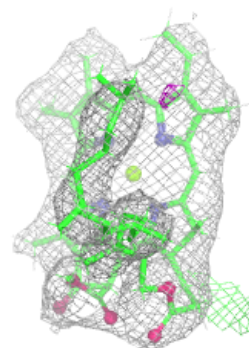
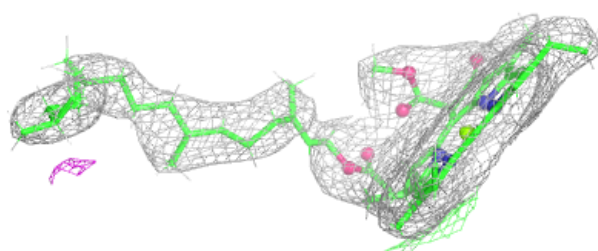
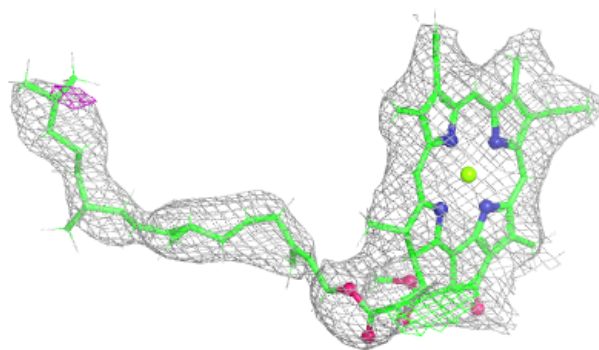
**Electron density around CLA B 3010:**

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



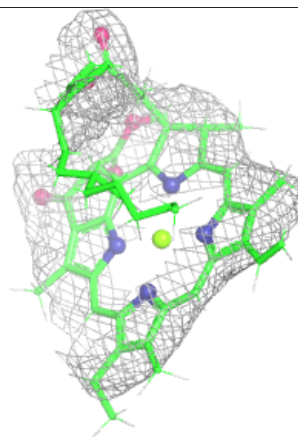
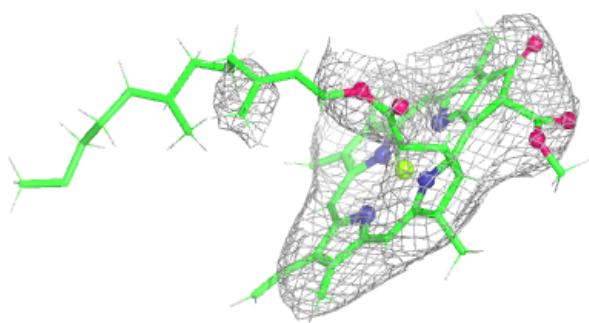
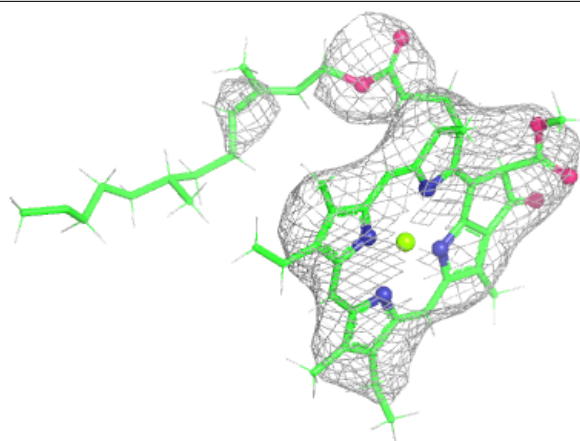
Electron density around CLA B 3011:

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

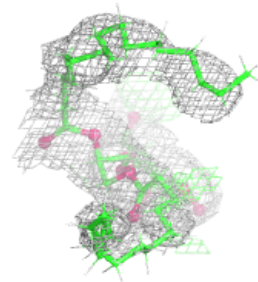
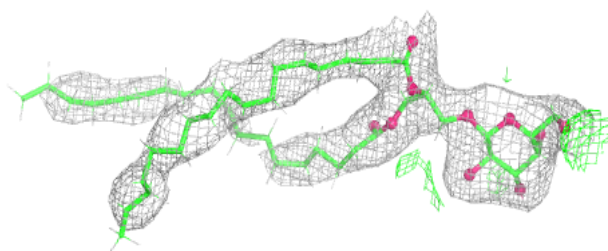
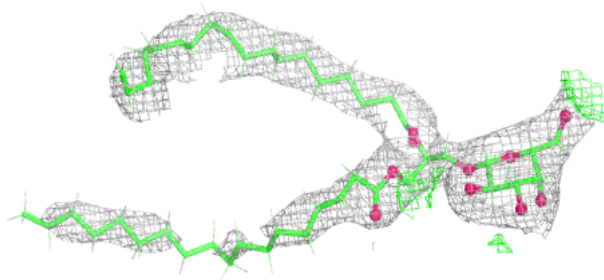


Electron density around CLA A 825:

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

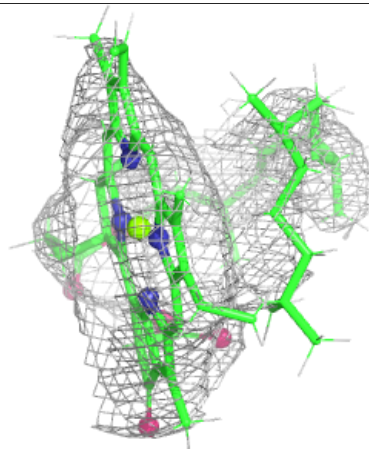
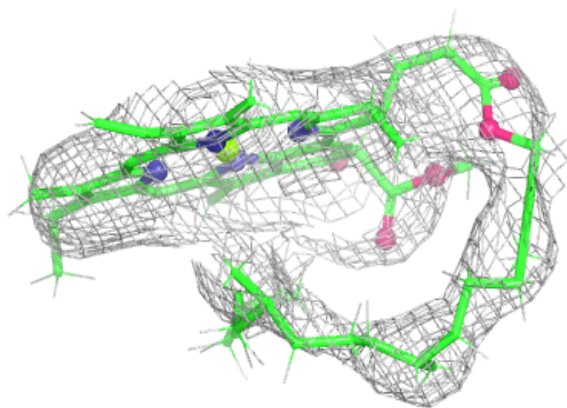
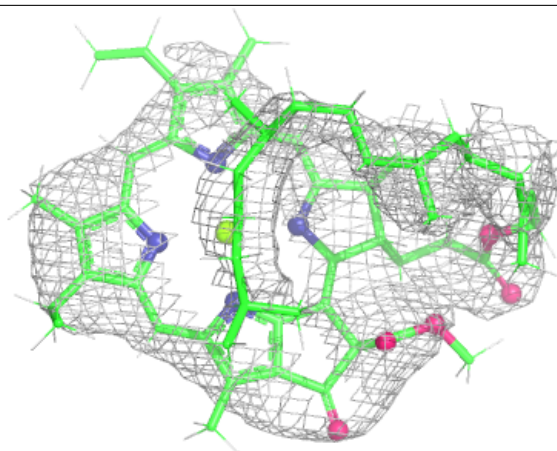
**Electron density around LMG B 3049:**

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



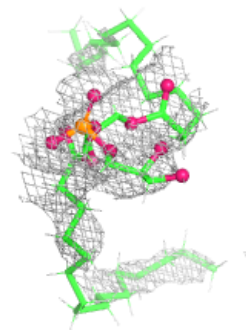
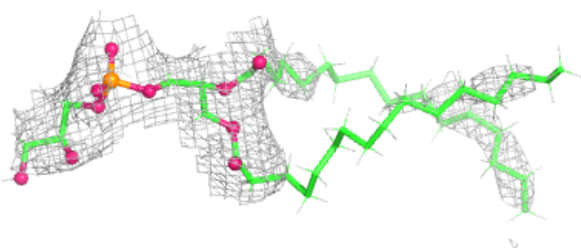
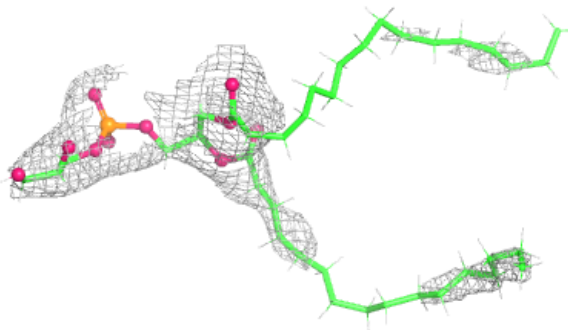
Electron density around CLA A 807:

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

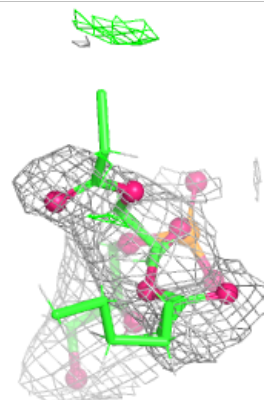
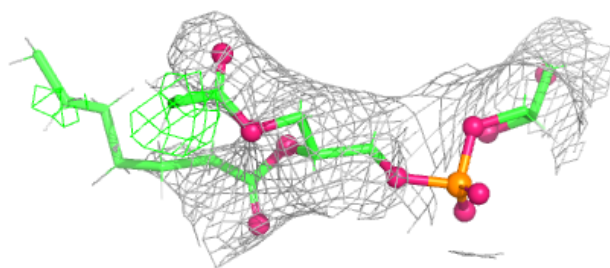
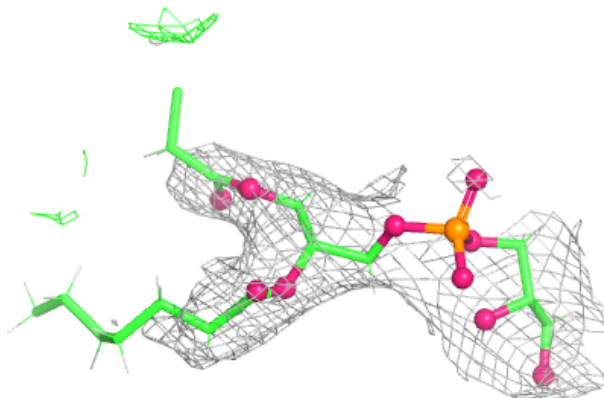


Electron density around LHG A 853:

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

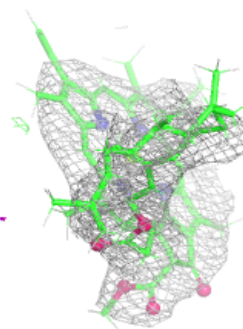
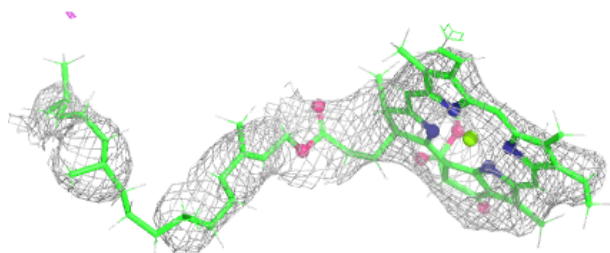
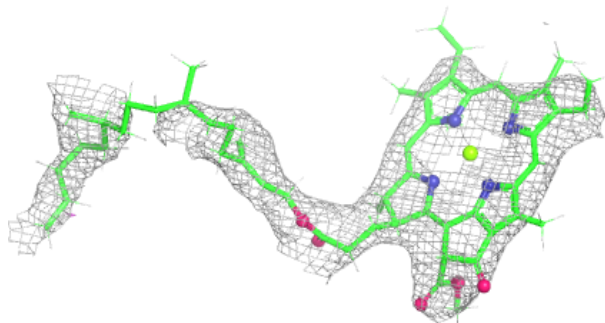
**Electron density around LHG A 854:**

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

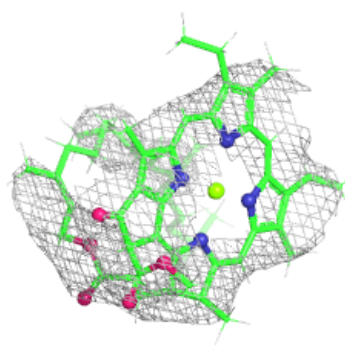
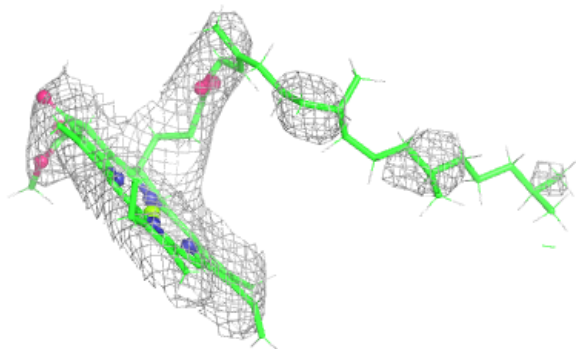
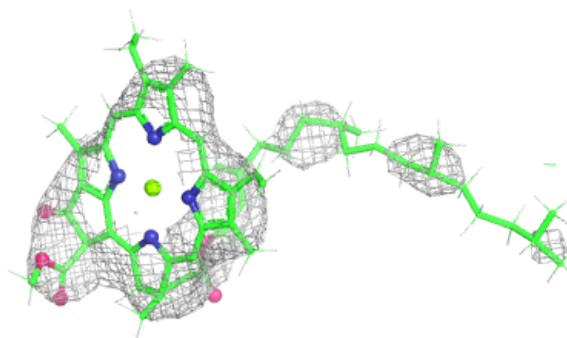


Electron density around CLA B 3014:

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

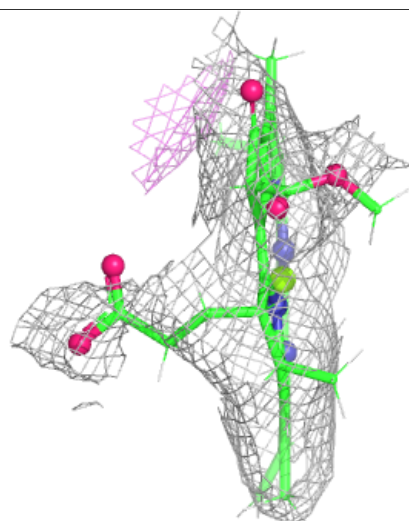
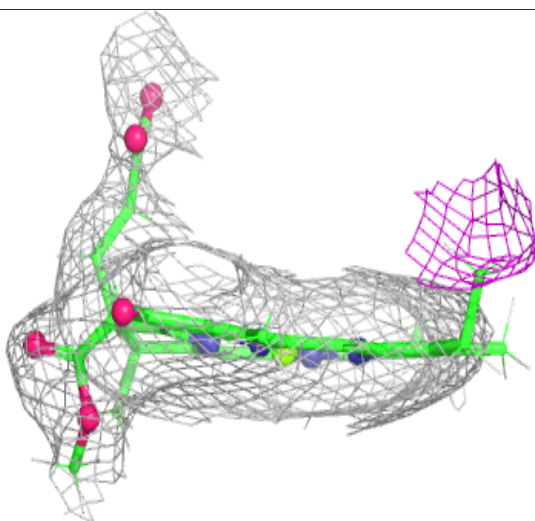
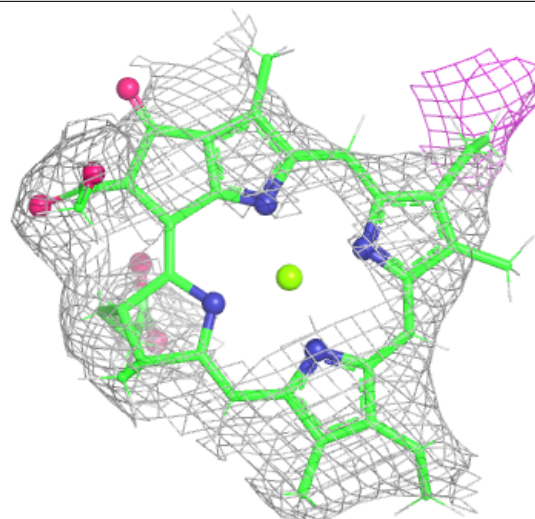
**Electron density around CLA B 3015:**

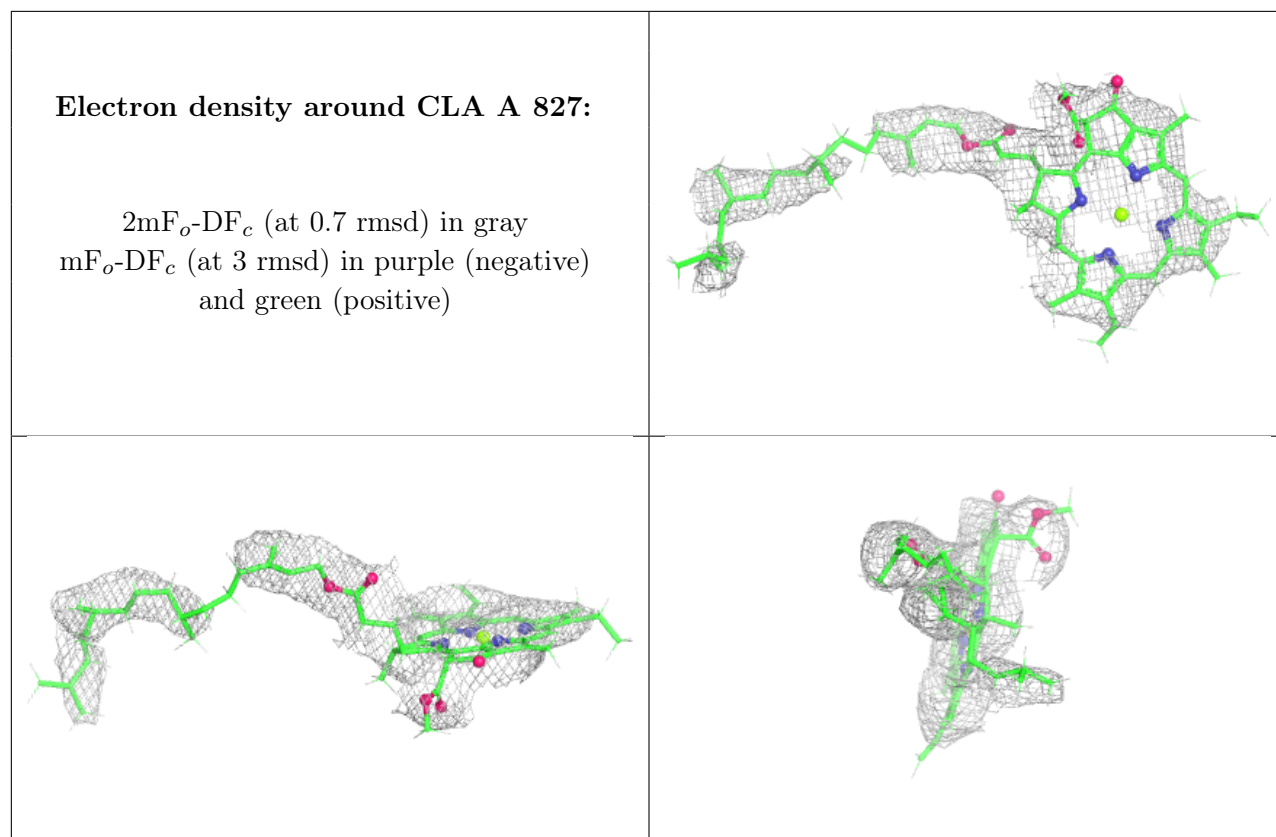
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 3016:

$2mF_o-DF_c$ (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.