



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 07:53 PM EDT

PDB ID : 7M75 / pdb_00007m75
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 : 2.75 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:

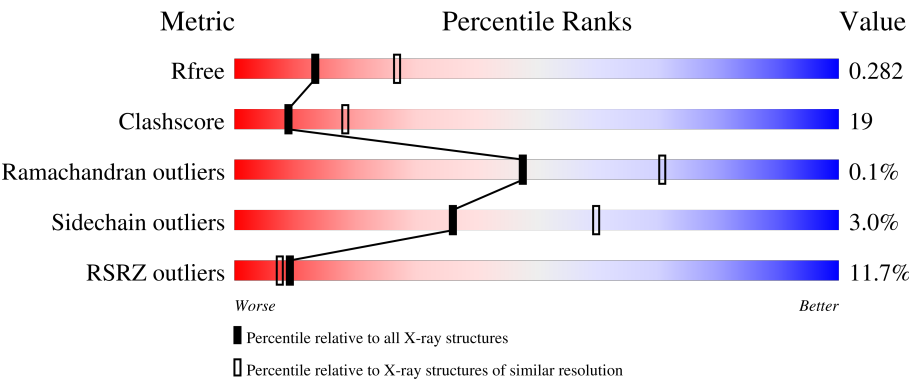
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	16% 62% 35% ..
2	B	740	9% 69% 29% .
3	C	80	2% 56% 42% .
4	D	138	5% 74% 24% .

Continued on next page...

Continued from previous page...

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	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 48896 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

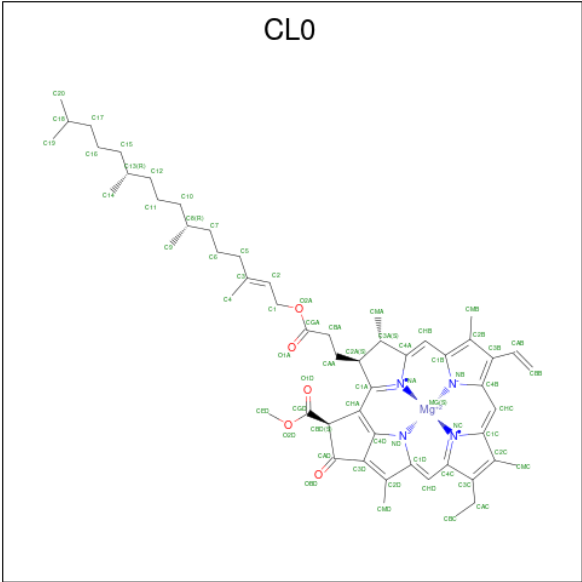
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

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.

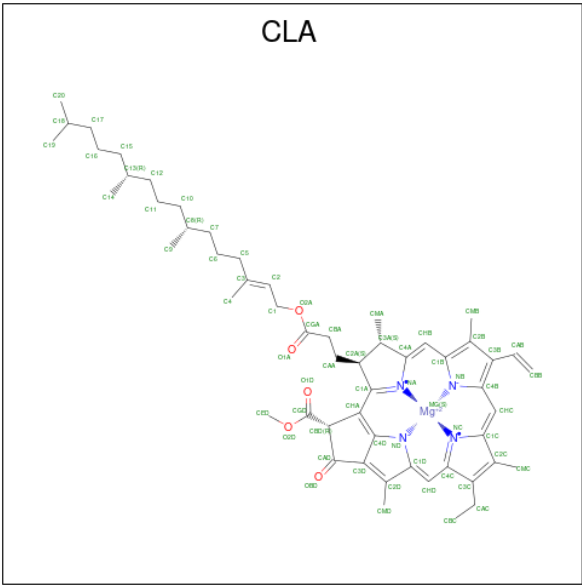
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
12	X	29	Total	C	H	N	O		0	0	0
			459	172	217	35	35				

- 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: $C_{55}H_{72}MgN_4O_5$).



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

Continued on next page...

Continued from previous page...

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
			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		
14	A	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
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		
14	B	1	Total	C	H	Mg	N	O	0	0
			104	45	49	1	4	5		

Continued on next page...

Continued from previous page...

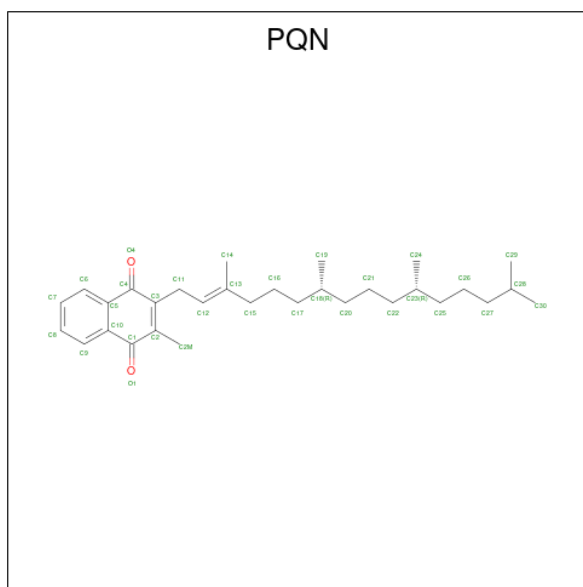
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			79	36	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	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
			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	F	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	I	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	J	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		

Continued on next page...

Continued from previous page...

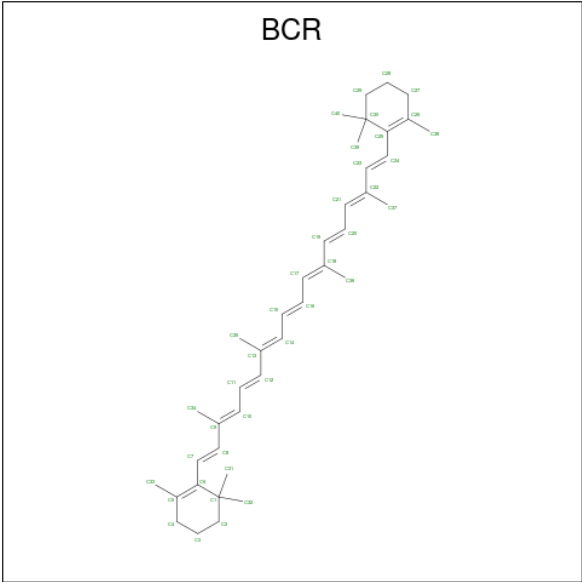
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	J	1	Total	C	H	Mg	N	O	0	0
			62	31	25	1	4	1		
14	K	1	Total	C	H	Mg	N	O	0	0
			70	33	29	1	4	3		
14	K	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	L	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	L	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	L	1	Total	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: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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: $C_{40}H_{56}$).



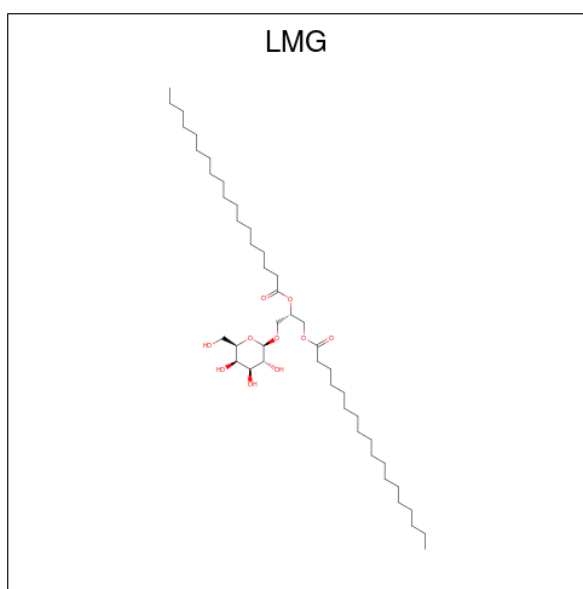
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	A	1	Total	C	H	0	0
			96	40	56		
16	A	1	Total	C	H	0	0
			96	40	56		
16	A	1	Total	C	H	0	0
			96	40	56		
16	A	1	Total	C	H	0	0
			96	40	56		
16	A	1	Total	C	H	0	0
			96	40	56		
16	B	1	Total	C	H	0	0
			96	40	56		
16	B	1	Total	C	H	0	0
			96	40	56		
16	B	1	Total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

Continued on next page...

Continued from previous page...

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

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



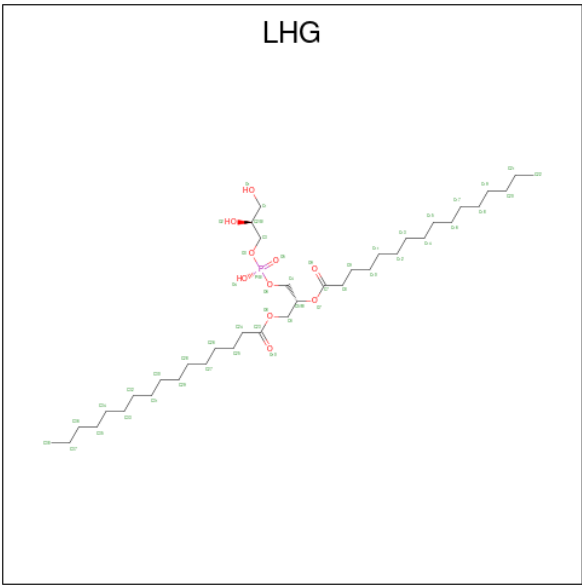
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	H	O	0	0
			118	38	70	10		
17	A	1	Total	C	H	O	0	0
			67	22	37	8		
17	B	1	Total	C	H	O	0	0
			141	45	86	10		

Continued on next page...

Continued from previous page...

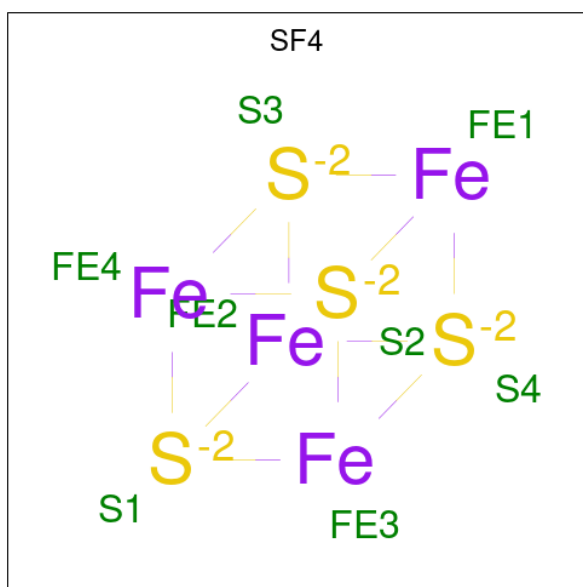
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	I	1	Total	C	H	O	0	0
			91	30	51	10		

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



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: Fe₄S₄).

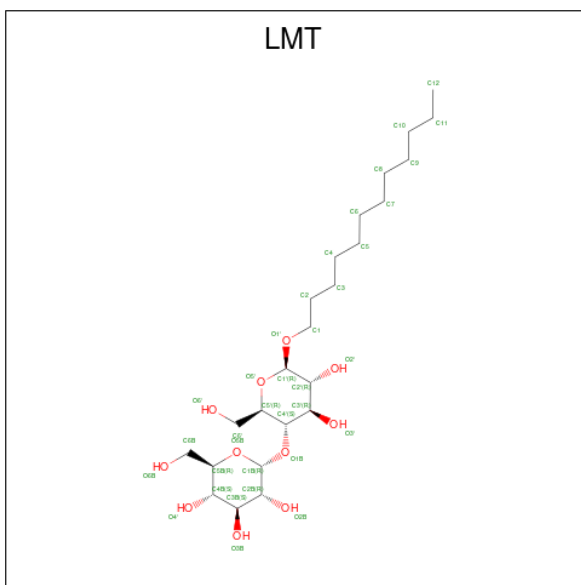


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	B	1	Total	Fe	S	0	0
			8	4	4		
19	C	1	Total	Fe	S	0	0
			8	4	4		
19	C	1	Total	Fe	S	0	0
			8	4	4		

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

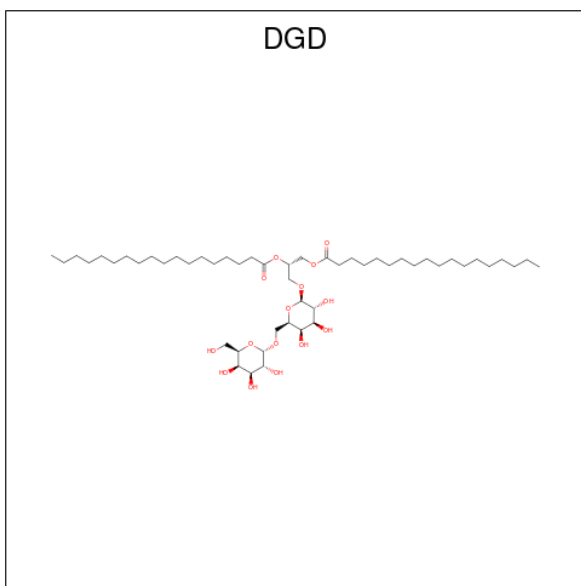
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	B	1	Total	Ca	0	0
			1	1		
20	L	1	Total	Ca	0	0
			1	1		

- 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		

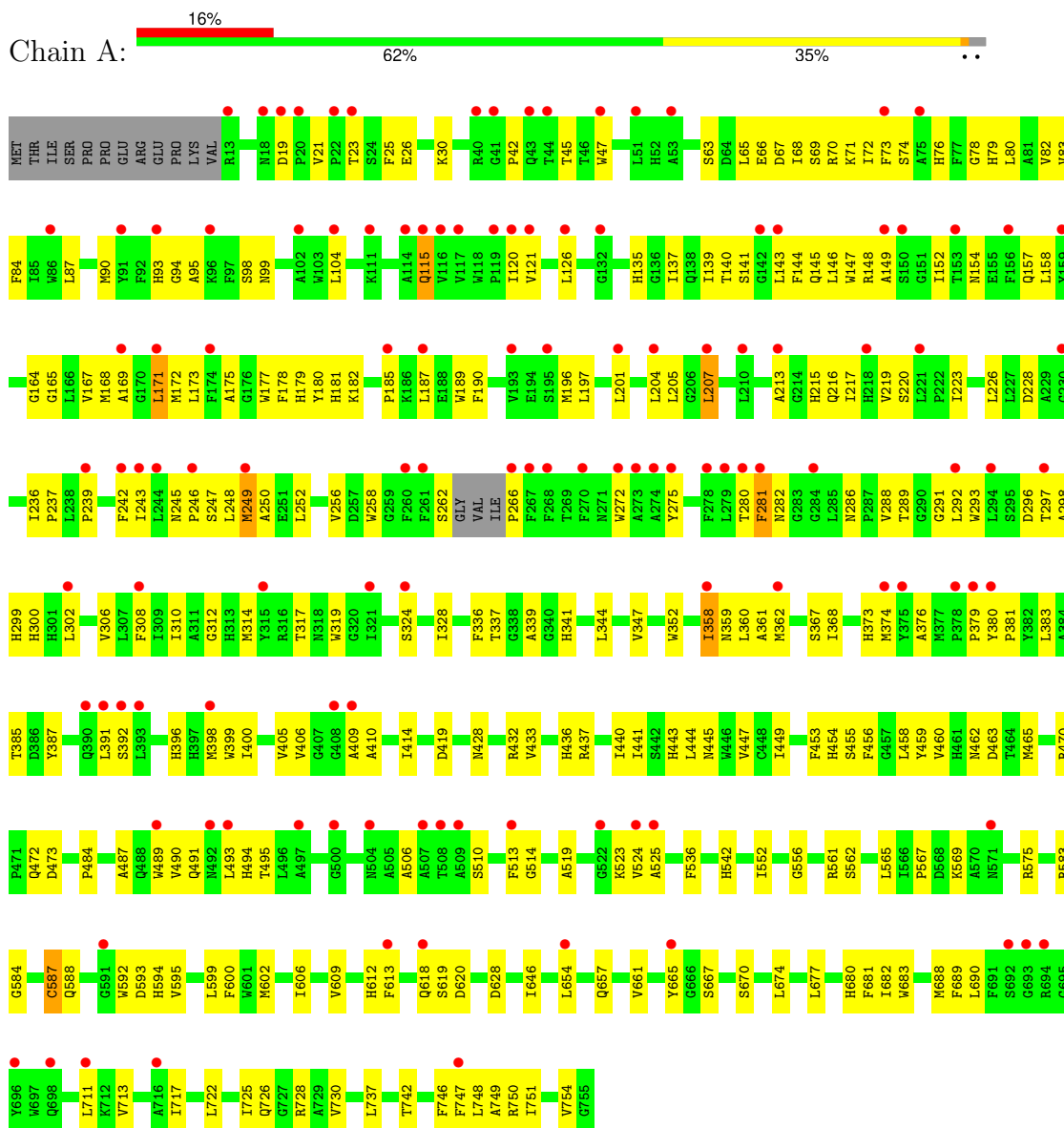
- Molecule 23 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	30	Total 30	O 30	0	0
23	B	41	Total 41	O 41	0	0
23	C	11	Total 11	O 11	0	0
23	D	14	Total 14	O 14	0	0
23	E	1	Total 1	O 1	0	0
23	F	2	Total 2	O 2	0	0
23	I	3	Total 3	O 3	0	0
23	J	1	Total 1	O 1	0	0
23	L	15	Total 15	O 15	0	0
23	M	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

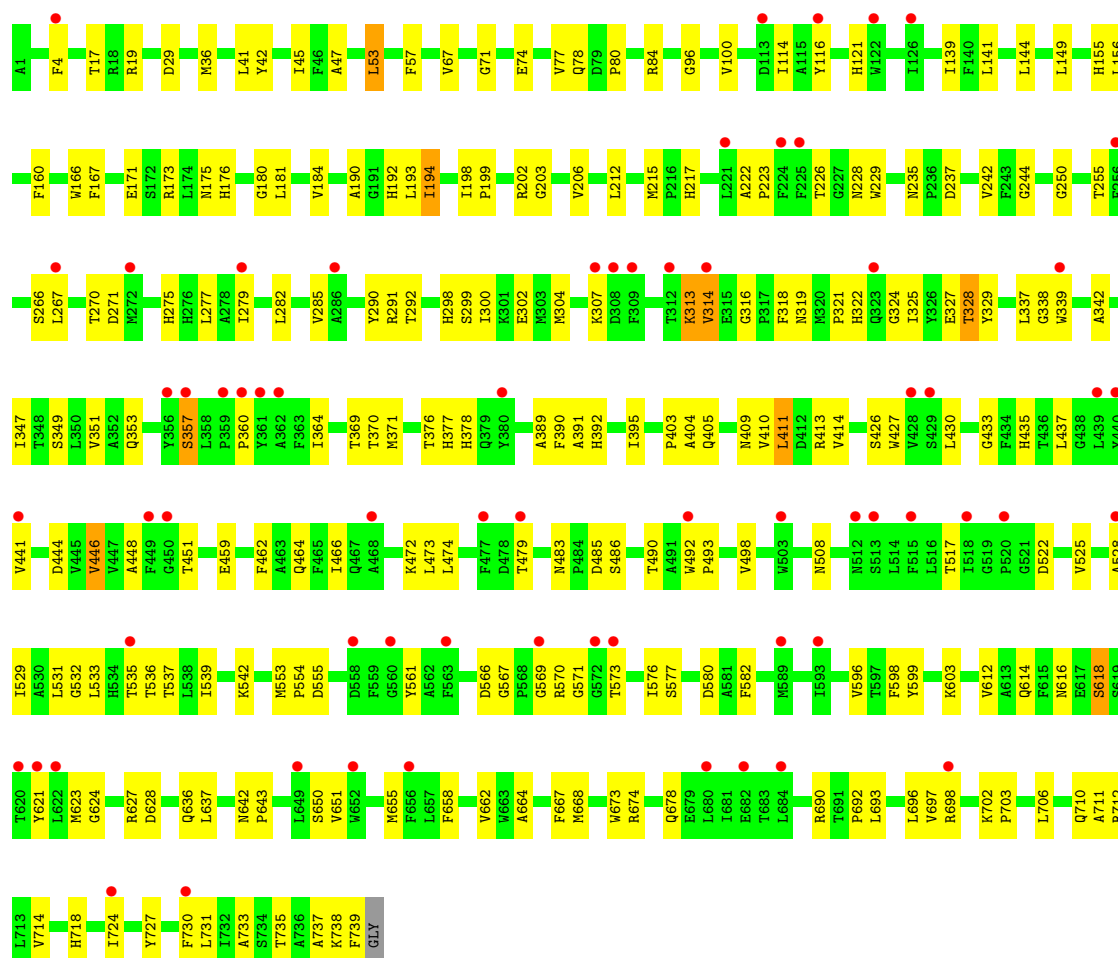
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

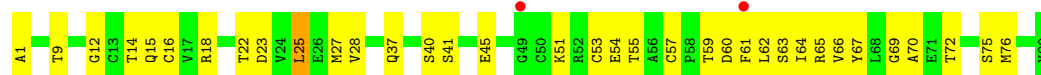


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





• Molecule 3: Photosystem I iron-sulfur center

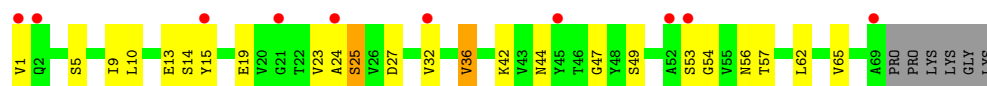


• Molecule 4: Photosystem I reaction center subunit II

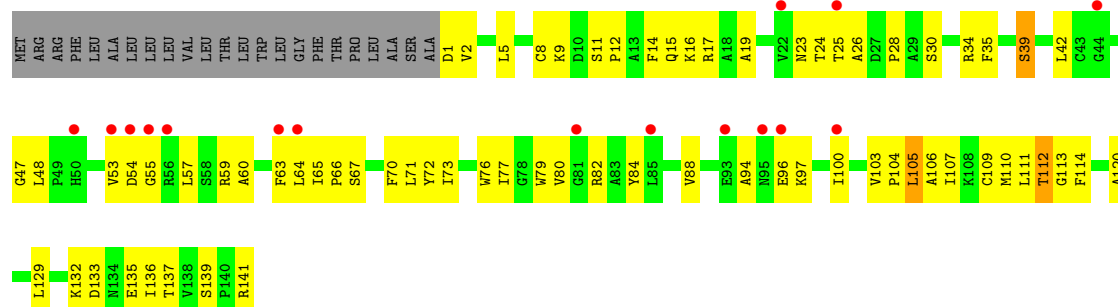


• Molecule 5: Photosystem I reaction center subunit IV

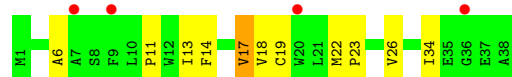




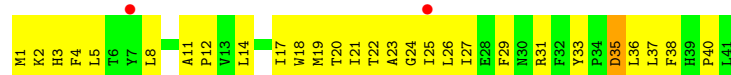
• Molecule 6: Photosystem I reaction center subunit III



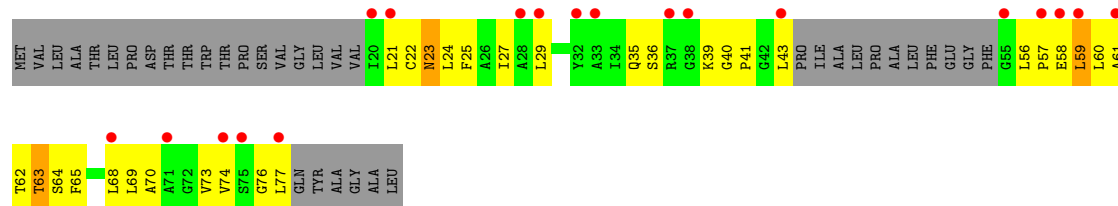
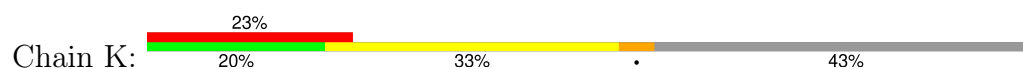
• Molecule 7: Photosystem I reaction center subunit VIII



• Molecule 8: Photosystem I reaction center subunit IX

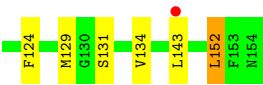


• Molecule 9: Photosystem I reaction center subunit Psak



• Molecule 10: Photosystem I reaction center subunit XI

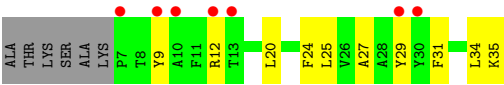




● Molecule 11: Photosystem I reaction center subunit XII



● Molecule 12: Photosystem I 4.8K protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	285.43Å 285.43Å 166.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	56.71 – 2.75 56.71 – 2.75	Depositor EDS
% Data completeness (in resolution range)	95.0 (56.71-2.75) 91.4 (56.71-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.16 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.264 , 0.279 0.268 , 0.282	Depositor DCC
R_{free} test set	2009 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 84.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	48896	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% 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: CLA, LMT, LHG, PQN, CL0, BCR, SF4, DGD, CA, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/5983	0.52	1/8158 (0.0%)
2	B	0.27	0/6107	0.50	0/8345
3	C	0.26	0/608	0.52	0/824
4	D	0.22	0/1101	0.48	0/1492
5	E	0.22	0/551	0.48	0/750
6	F	0.28	0/1087	0.49	0/1476
7	I	0.27	0/312	0.68	0/425
8	J	0.33	0/350	0.58	0/477
9	K	0.28	0/337	0.66	0/454
10	L	0.27	0/1148	0.53	0/1558
11	M	0.32	0/244	0.58	0/332
12	X	0.30	0/251	0.49	0/342
All	All	0.27	0/18079	0.51	1/24633 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	MET	CA-CB-CG	5.33	124.75	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5784	5638	5639	306	0
2	B	5889	5618	5649	216	0
3	C	598	576	580	37	0
4	D	1075	1077	1077	30	0
5	E	539	528	528	18	0
6	F	1065	1076	1077	79	0
7	I	301	306	306	15	0
8	J	338	347	347	53	0
9	K	333	354	354	47	0
10	L	1119	1125	1125	30	0
11	M	241	264	264	12	0
12	X	242	217	249	14	0
13	A	65	72	72	2	0
14	A	2628	2615	2615	99	0
14	B	2219	2160	2160	75	0
14	F	45	33	33	8	0
14	I	65	72	72	8	0
14	J	82	58	58	0	0
14	K	86	62	62	3	0
14	L	195	216	216	4	0
14	M	45	33	33	3	0
14	X	45	33	33	2	0
15	A	33	46	46	7	0
15	B	33	46	46	3	0
16	A	200	280	280	16	0
16	B	240	336	336	13	0
16	F	80	112	112	8	0
16	I	120	168	168	8	0
16	J	120	168	168	13	0
16	K	40	56	56	4	0
16	L	40	56	56	2	0
16	M	40	56	56	2	0
17	A	78	107	105	0	0
17	B	55	86	86	1	0
17	I	40	51	50	0	0
18	A	76	100	98	4	0
18	B	23	20	16	2	0
18	M	49	74	74	1	0
19	B	8	0	0	0	0
19	C	16	0	0	0	0
20	B	1	0	0	0	0
20	L	1	0	0	0	0
21	L	35	46	46	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	L	66	96	96	2	0
23	A	30	0	0	5	0
23	B	41	0	0	5	0
23	C	11	0	0	2	0
23	D	14	0	0	1	0
23	E	1	0	0	0	0
23	F	2	0	0	0	0
23	I	3	0	0	2	0
23	J	1	0	0	0	0
23	L	15	0	0	0	0
23	M	1	0	0	0	0
All	All	24512	24384	24444	905	0

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

All (905) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:32:THR:OG1	4:D:79:ASP:OD2	1.81	0.98
4:D:3:LEU:HD21	4:D:91:THR:HG21	1.47	0.95
2:B:307:LYS:O	2:B:314:VAL:HG23	1.68	0.93
9:K:60:LEU:O	9:K:63:THR:OG1	1.87	0.93
1:A:661:VAL:HG21	1:A:746:PHE:HA	1.51	0.91
1:A:661:VAL:HG22	1:A:749:ALA:HB3	1.51	0.90
6:F:1:ASP:N	6:F:5:LEU:O	2.05	0.89
6:F:76:TRP:CZ3	6:F:114:PHE:N	2.42	0.88
2:B:181:LEU:HD21	14:B:3014:CLA:H43	1.58	0.86
8:J:17:ILE:HD12	8:J:18:TRP:N	1.91	0.86
1:A:120:ILE:HD11	8:J:31:ARG:HB2	1.57	0.84
1:A:336:PHE:O	1:A:432:ARG:NH1	2.11	0.82
1:A:68:ILE:HD12	1:A:69:SER:N	1.94	0.81
1:A:120:ILE:CD1	8:J:31:ARG:HB2	2.10	0.81
2:B:114:ILE:HD11	2:B:116:TYR:CZ	2.15	0.81
1:A:249:MET:HB2	1:A:258:TRP:CH2	2.16	0.81
2:B:627:ARG:NH2	2:B:628:ASP:OD2	2.13	0.81
14:I:101:CLA:MG	23:I:201:HOH:O	1.24	0.79
6:F:53:VAL:HG13	6:F:63:PHE:CD1	2.18	0.78
8:J:23:ALA:O	8:J:27:ILE:HD12	1.83	0.78
8:J:21:ILE:O	8:J:25:ILE:HD12	1.84	0.78
5:E:19:GLU:OE2	5:E:42:LYS:NZ	2.13	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:MET:HB2	1:A:258:TRP:CZ3	2.21	0.75
16:A:851:BCR:H362	14:A:856:CLA:C4	2.17	0.75
1:A:65:LEU:HD12	1:A:68:ILE:HD11	1.69	0.74
2:B:184:VAL:HG21	16:B:3044:BCR:H332	1.69	0.74
2:B:483:ASN:OD1	2:B:486:SER:N	2.21	0.74
4:D:114:SER:OG	23:D:201:HOH:O	2.06	0.74
1:A:489:TRP:O	1:A:493:LEU:HD23	1.87	0.73
1:A:66:GLU:HA	1:A:187:LEU:HD13	1.69	0.73
6:F:76:TRP:CZ3	6:F:113:GLY:C	2.66	0.73
14:F:202:CLA:HBC2	8:J:19:MET:HE3	1.69	0.73
14:M:102:CLA:H2A	14:M:102:CLA:HED2	1.69	0.73
1:A:722:LEU:HD23	1:A:726:GLN:OE1	1.90	0.72
1:A:513:PHE:HE1	14:A:828:CLA:HBC2	1.54	0.71
14:A:821:CLA:HMB2	9:K:64:SER:OG	1.91	0.71
1:A:68:ILE:HD12	1:A:69:SER:H	1.54	0.71
1:A:205:LEU:CD2	1:A:308:PHE:CE2	2.74	0.70
2:B:84:ARG:NH2	23:B:3103:HOH:O	2.23	0.70
4:D:9:LEU:HB2	4:D:48:VAL:HG12	1.71	0.70
1:A:454:HIS:O	1:A:458:LEU:HG	1.91	0.70
15:A:846:PQN:H193	16:F:201:BCR:H382	1.72	0.70
14:B:3008:CLA:H192	18:M:101:LHG:H383	1.74	0.70
6:F:76:TRP:HZ3	6:F:114:PHE:HA	1.56	0.70
9:K:60:LEU:O	9:K:63:THR:N	2.17	0.70
1:A:657:GLN:O	23:A:901:HOH:O	2.08	0.70
3:C:28:VAL:HG12	4:D:109:ARG:HB3	1.74	0.70
5:E:62:LEU:HD23	5:E:62:LEU:H	1.56	0.70
2:B:479:THR:HG21	12:X:29:TYR:O	1.92	0.69
1:A:68:ILE:O	1:A:72:ILE:HG13	1.92	0.69
1:A:661:VAL:HG23	23:A:901:HOH:O	1.92	0.69
1:A:143:LEU:HD22	1:A:146:LEU:HD22	1.75	0.69
1:A:143:LEU:HD22	1:A:146:LEU:CD2	2.22	0.68
2:B:459:GLU:OE1	2:B:464:GLN:NE2	2.26	0.68
8:J:25:ILE:HD12	8:J:25:ILE:H	1.57	0.68
14:B:3033:CLA:H142	16:F:203:BCR:H333	1.75	0.68
6:F:9:LYS:O	6:F:15:GLN:NE2	2.27	0.67
9:K:60:LEU:C	9:K:63:THR:HG1	1.99	0.67
1:A:205:LEU:HG	1:A:308:PHE:CE2	2.30	0.67
1:A:249:MET:CB	1:A:258:TRP:CH2	2.77	0.67
2:B:116:TYR:HA	2:B:370:THR:HG22	1.76	0.66
9:K:21:LEU:HD12	14:K:101:CLA:C3D	2.26	0.66
2:B:337:LEU:HD23	2:B:392:HIS:CG	2.30	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:636:GLN:OE1	2:B:737:ALA:HB1	1.95	0.66
6:F:1:ASP:OD2	6:F:42:LEU:HD21	1.94	0.66
16:A:851:BCR:H362	14:A:856:CLA:H42	1.78	0.66
6:F:35:PHE:O	6:F:39:SER:OG	2.12	0.65
2:B:319:ASN:OD1	2:B:319:ASN:O	2.14	0.65
5:E:56:ASN:OD1	5:E:57:THR:HG23	1.95	0.65
1:A:359:ASN:ND2	14:A:806:CLA:OBD	2.29	0.65
2:B:376:THR:HG21	2:B:731:LEU:HD13	1.79	0.65
1:A:524:VAL:HG12	1:A:525:ALA:N	2.12	0.64
1:A:575:ARG:NH1	14:A:831:CLA:O1D	2.30	0.64
2:B:181:LEU:CD2	14:B:3014:CLA:H43	2.27	0.64
3:C:51:LYS:O	3:C:55:THR:HG23	1.97	0.64
4:D:38:VAL:O	4:D:75:ARG:NH1	2.30	0.64
8:J:1:MET:O	8:J:4:PHE:N	2.30	0.64
1:A:249:MET:O	1:A:252:LEU:N	2.29	0.64
1:A:495:THR:HG21	1:A:514:GLY:HA3	1.78	0.64
1:A:367:SER:OG	1:A:400:ILE:HD11	1.97	0.64
3:C:54:GLU:HG2	3:C:62:LEU:HD13	1.79	0.64
10:L:29:THR:O	10:L:33:ASN:ND2	2.30	0.64
14:A:811:CLA:HBC3	14:A:811:CLA:HHD	1.80	0.63
1:A:306:VAL:HG21	14:A:818:CLA:HMC3	1.80	0.63
9:K:65:PHE:CD2	16:K:102:BCR:H402	2.32	0.63
17:B:3048:LMG:O5	23:B:3101:HOH:O	2.15	0.63
14:A:804:CLA:HED3	15:A:846:PQN:H262	1.81	0.63
9:K:65:PHE:HD2	16:K:102:BCR:H402	1.63	0.63
2:B:180:GLY:O	2:B:184:VAL:HG12	1.99	0.62
1:A:683:TRP:HZ3	14:A:856:CLA:HMD3	1.64	0.62
3:C:51:LYS:HD3	3:C:54:GLU:OE2	2.00	0.62
1:A:250:ALA:N	1:A:258:TRP:CZ3	2.67	0.62
1:A:179:HIS:CE1	14:A:811:CLA:NA	2.67	0.62
1:A:249:MET:CB	1:A:258:TRP:HH2	2.14	0.61
6:F:8:CYS:HB3	6:F:14:PHE:CD2	2.35	0.61
16:I:105:BCR:H392	16:I:105:BCR:H23C	1.82	0.61
1:A:171:LEU:HD12	1:A:172:MET:N	2.16	0.61
3:C:9:THR:OG1	3:C:63:SER:OG	2.14	0.61
2:B:300:ILE:O	2:B:304:MET:HG2	1.99	0.61
2:B:567:GLY:O	2:B:573:THR:HG22	2.00	0.61
1:A:256:VAL:HG12	1:A:258:TRP:CD1	2.35	0.61
2:B:337:LEU:HD23	2:B:392:HIS:ND1	2.16	0.61
9:K:56:LEU:HD12	9:K:59:LEU:HD23	1.82	0.61
2:B:698:ARG:HG2	2:B:698:ARG:HH11	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:F:202:CLA:HBC2	8:J:19:MET:CE	2.30	0.61
2:B:291:ARG:NH2	2:B:302:GLU:OE1	2.34	0.61
2:B:300:ILE:HD12	2:B:300:ILE:H	1.66	0.61
1:A:177:TRP:CE3	1:A:178:PHE:HA	2.35	0.60
2:B:319:ASN:OD1	18:B:3049:LHG:O4	2.19	0.60
2:B:580:ASP:OD1	2:B:712:ARG:NH1	2.34	0.60
1:A:298:ALA:O	1:A:302:LEU:HD23	2.01	0.60
2:B:325:ILE:HA	2:B:328:THR:HG22	1.84	0.60
1:A:73:PHE:CE1	14:A:814:CLA:C3D	2.84	0.60
14:A:804:CLA:H193	14:A:843:CLA:H18	1.82	0.60
1:A:490:VAL:HA	1:A:493:LEU:HD21	1.84	0.60
1:A:143:LEU:O	1:A:146:LEU:N	2.34	0.59
2:B:662:VAL:HG12	2:B:718:HIS:O	2.02	0.59
6:F:76:TRP:CE3	6:F:113:GLY:C	2.80	0.59
2:B:710:GLN:O	2:B:714:VAL:HG23	2.01	0.59
4:D:119:ILE:HD12	4:D:119:ILE:H	1.66	0.59
8:J:23:ALA:C	8:J:27:ILE:HD12	2.27	0.59
12:X:24:PHE:CD1	14:X:1701:CLA:HMA1	2.37	0.59
2:B:190:ALA:O	2:B:194:ILE:HG13	2.02	0.59
7:I:18:VAL:O	7:I:23:PRO:CD	2.51	0.59
1:A:65:LEU:O	1:A:68:ILE:HD11	2.03	0.59
16:A:851:BCR:H23C	16:A:851:BCR:H403	1.83	0.59
2:B:561:TYR:O	2:B:577:SER:OG	2.20	0.59
10:L:16:HIS:O	10:L:17:LEU:HD23	2.02	0.59
11:M:23:PHE:O	11:M:27:THR:HG23	2.02	0.59
2:B:304:MET:HE2	2:B:325:ILE:CG1	2.33	0.59
1:A:90:MET:HE1	14:A:809:CLA:H2A	1.85	0.59
1:A:120:ILE:HD13	16:J:104:BCR:H322	1.84	0.59
1:A:465:MET:HE1	1:A:470:ARG:NH2	2.17	0.59
10:L:20:PRO:O	10:L:24:SER:OG	2.16	0.59
1:A:204:LEU:HD12	14:A:814:CLA:CHB	2.33	0.58
1:A:286:ASN:HB3	1:A:289:THR:OG1	2.01	0.58
1:A:373:HIS:CD2	14:A:828:CLA:NC	2.71	0.58
12:X:9:TYR:HA	12:X:12:ARG:NH1	2.18	0.58
2:B:47:ALA:HB2	2:B:156:LEU:HG	1.85	0.58
16:A:851:BCR:H372	2:B:441:VAL:HG11	1.84	0.58
1:A:65:LEU:HD12	1:A:65:LEU:O	2.03	0.58
1:A:600:PHE:HZ	1:A:690:LEU:HD11	1.68	0.58
2:B:529:ILE:HD13	2:B:596:VAL:HG22	1.85	0.58
6:F:76:TRP:HE1	14:F:202:CLA:CAD	2.16	0.58
6:F:139:SER:O	6:F:141:ARG:NH1	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:21:ILE:O	8:J:24:GLY:N	2.37	0.58
1:A:189:TRP:HZ3	1:A:190:PHE:CE1	2.20	0.58
16:F:201:BCR:H333	8:J:26:LEU:HD11	1.84	0.58
1:A:154:ASN:OD1	1:A:157:GLN:NE2	2.36	0.57
6:F:110:MET:HG2	14:F:202:CLA:OBD	2.04	0.57
1:A:205:LEU:HG	1:A:308:PHE:CZ	2.39	0.57
2:B:202:ARG:NE	2:B:237:ASP:OD1	2.38	0.57
4:D:3:LEU:CD2	4:D:91:THR:HG21	2.26	0.57
10:L:35:PRO:HG3	14:L:204:CLA:HED2	1.86	0.57
2:B:522:ASP:OD2	2:B:603:LYS:NZ	2.33	0.57
14:I:101:CLA:HHD	14:I:101:CLA:HBC3	1.84	0.57
1:A:256:VAL:HB	1:A:258:TRP:HE1	1.68	0.57
8:J:27:ILE:HD12	8:J:27:ILE:H	1.68	0.57
2:B:291:ARG:HE	2:B:299:SER:HB3	1.69	0.57
2:B:17:THR:HG23	2:B:702:LYS:O	2.04	0.57
15:A:846:PQN:C19	16:F:201:BCR:H382	2.34	0.57
2:B:553:MET:HE1	2:B:566:ASP:HB2	1.87	0.57
6:F:132:LYS:HG2	6:F:133:ASP:H	1.69	0.57
1:A:245:ASN:ND2	1:A:247:SER:OG	2.38	0.56
16:I:105:BCR:H24C	10:L:93:LEU:HD21	1.87	0.56
1:A:143:LEU:O	1:A:146:LEU:HB3	2.05	0.56
6:F:96:GLU:OE2	6:F:100:ILE:HD13	2.05	0.56
1:A:71:LYS:NZ	23:A:904:HOH:O	2.37	0.56
1:A:282:ASN:O	1:A:506:ALA:HB3	2.05	0.56
1:A:444:LEU:O	1:A:447:VAL:HG12	2.05	0.56
2:B:304:MET:HE2	2:B:325:ILE:HD11	1.88	0.56
2:B:176:HIS:CE1	14:B:3013:CLA:NA	2.74	0.56
14:A:817:CLA:HBC3	14:A:817:CLA:HHD	1.86	0.56
2:B:304:MET:CE	2:B:325:ILE:HD11	2.36	0.56
8:J:21:ILE:HD12	8:J:22:THR:N	2.21	0.56
5:E:1:VAL:N	5:E:5:SER:OG	2.39	0.56
14:B:3031:CLA:H3A	14:B:3032:CLA:OBD	2.06	0.56
16:I:103:BCR:H331	16:I:103:BCR:C8	2.36	0.56
1:A:205:LEU:HD12	14:A:820:CLA:HMC3	1.87	0.55
6:F:73:ILE:O	6:F:77:ILE:HG12	2.06	0.55
6:F:76:TRP:HZ3	6:F:114:PHE:CA	2.19	0.55
16:J:103:BCR:H321	16:J:103:BCR:HC8	1.88	0.55
1:A:115:GLN:HE22	14:A:809:CLA:C1B	2.19	0.55
4:D:100:VAL:HG23	4:D:109:ARG:NH2	2.20	0.55
8:J:22:THR:O	8:J:26:LEU:HD23	2.07	0.55
1:A:628:ASP:OD1	1:A:628:ASP:N	2.38	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:HIS:HB2	2:B:364:ILE:HD13	1.87	0.55
2:B:614:GLN:O	2:B:618:SER:OG	2.23	0.55
8:J:23:ALA:C	8:J:27:ILE:CD1	2.79	0.55
1:A:750:ARG:O	1:A:754:VAL:HG22	2.07	0.55
1:A:282:ASN:O	1:A:506:ALA:N	2.36	0.55
1:A:168:MET:O	1:A:171:LEU:HG	2.06	0.55
2:B:536:THR:HG21	14:B:3026:CLA:HBC3	1.88	0.55
14:B:3009:CLA:C1A	14:B:3009:CLA:CGA	2.85	0.55
6:F:53:VAL:HG22	6:F:63:PHE:HB2	1.87	0.55
6:F:111:LEU:N	6:F:111:LEU:HD12	2.22	0.55
1:A:337:THR:OG1	18:A:854:LHG:O2	2.05	0.55
14:A:802:CLA:OBD	14:B:3003:CLA:HMB3	2.06	0.55
16:L:207:BCR:H311	16:L:207:BCR:H343	1.88	0.55
1:A:141:SER:HB2	1:A:143:LEU:HG	1.88	0.55
1:A:472:GLN:OE1	1:A:472:GLN:N	2.35	0.54
12:X:24:PHE:CE1	14:X:1701:CLA:HMA1	2.42	0.54
1:A:95:ALA:HA	1:A:158:LEU:HD13	1.89	0.54
9:K:21:LEU:HD11	14:K:101:CLA:HMD2	1.90	0.54
5:E:24:ALA:O	5:E:25:SER:O	2.26	0.54
11:M:27:THR:OG1	14:M:102:CLA:HED3	2.06	0.54
2:B:277:LEU:C	2:B:277:LEU:HD23	2.32	0.54
8:J:22:THR:HA	8:J:25:ILE:HD13	1.89	0.54
14:B:3016:CLA:HMB1	16:B:3045:BCR:H352	1.89	0.54
1:A:362:MET:HE3	14:A:828:CLA:H43	1.90	0.54
1:A:494:HIS:HB3	1:A:513:PHE:HD2	1.73	0.54
5:E:27:ASP:OD2	5:E:32:VAL:HG21	2.08	0.54
2:B:96:GLY:O	2:B:100:VAL:HG23	2.07	0.54
2:B:279:ILE:HD11	14:B:3018:CLA:C3C	2.37	0.54
1:A:682:ILE:HD13	1:A:737:LEU:HD23	1.89	0.54
2:B:175:ASN:ND2	2:B:290:TYR:O	2.41	0.54
2:B:724:ILE:HG23	14:B:3028:CLA:HAB	1.89	0.54
1:A:185:PRO:HB2	1:A:189:TRP:CE3	2.43	0.54
1:A:459:TYR:HB3	1:A:646:ILE:HD11	1.90	0.54
1:A:487:ALA:O	1:A:491:GLN:HG2	2.07	0.54
1:A:565:LEU:HD13	2:B:678:GLN:HG2	1.89	0.53
2:B:318:PHE:HB2	14:B:3024:CLA:HMA3	1.91	0.53
2:B:433:GLY:N	2:B:531:LEU:HD13	2.23	0.53
6:F:54:ASP:OD1	6:F:55:GLY:N	2.41	0.53
7:I:18:VAL:O	7:I:23:PRO:HD3	2.08	0.53
16:I:102:BCR:H382	16:I:102:BCR:H23C	1.90	0.53
1:A:177:TRP:CE3	1:A:177:TRP:C	2.86	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:841:CLA:H93	15:A:846:PQN:H293	1.88	0.53
2:B:255:THR:OG1	2:B:271:ASP:OD1	2.25	0.53
6:F:96:GLU:O	6:F:100:ILE:HD12	2.08	0.53
1:A:72:ILE:HD12	1:A:352:TRP:CE2	2.43	0.53
1:A:219:VAL:HG13	1:A:239:PRO:HB3	1.90	0.53
5:E:56:ASN:OD1	5:E:57:THR:N	2.40	0.53
9:K:65:PHE:CE1	9:K:69:LEU:HD11	2.44	0.53
8:J:17:ILE:HA	8:J:20:THR:HG22	1.90	0.53
1:A:120:ILE:HD12	8:J:31:ARG:HB2	1.90	0.53
2:B:149:LEU:HD22	11:M:22:ALA:HA	1.89	0.53
5:E:53:SER:OG	5:E:54:GLY:N	2.39	0.53
1:A:249:MET:C	1:A:258:TRP:CZ3	2.86	0.53
1:A:256:VAL:HB	1:A:258:TRP:NE1	2.24	0.53
2:B:554:PRO:HD2	3:C:61:PHE:CZ	2.44	0.53
1:A:376:ALA:O	1:A:510:SER:OG	2.27	0.53
2:B:304:MET:HE3	2:B:322:HIS:O	2.08	0.53
6:F:23:ASN:OD1	6:F:30:SER:OG	2.10	0.53
1:A:201:LEU:O	1:A:205:LEU:HB3	2.09	0.53
1:A:243:ILE:HD12	14:A:817:CLA:HBC2	1.91	0.53
1:A:286:ASN:OD1	1:A:288:VAL:HG12	2.09	0.53
2:B:36:MET:HE2	2:B:41:LEU:HA	1.90	0.53
2:B:329:TYR:CZ	14:B:3025:CLA:NC	2.77	0.53
7:I:17:VAL:O	7:I:18:VAL:C	2.52	0.53
2:B:531:LEU:O	2:B:535:THR:HG22	2.09	0.53
14:B:3034:CLA:H2A	14:B:3034:CLA:HED2	1.91	0.53
11:M:14:ILE:O	11:M:18:PRO:HD2	2.08	0.52
1:A:490:VAL:HA	1:A:493:LEU:CD2	2.39	0.52
2:B:637:LEU:HD13	2:B:733:ALA:CB	2.39	0.52
1:A:21:VAL:HG11	1:A:181:HIS:HA	1.90	0.52
10:L:47:GLY:O	10:L:124:PHE:HA	2.10	0.52
1:A:726:GLN:HG3	18:A:853:LHG:C8	2.40	0.52
14:A:844:CLA:HHC	14:A:844:CLA:HBB1	1.91	0.52
7:I:22:MET:N	7:I:23:PRO:HD2	2.25	0.52
6:F:16:LYS:N	6:F:16:LYS:HE2	2.25	0.52
6:F:64:LEU:O	6:F:67:SER:OG	2.26	0.52
1:A:141:SER:OG	14:A:809:CLA:O1D	2.28	0.52
2:B:390:PHE:CE1	16:B:3046:BCR:H373	2.44	0.52
3:C:57:CYS:SG	3:C:59:THR:OG1	2.67	0.52
6:F:76:TRP:CZ3	6:F:114:PHE:CA	2.92	0.52
1:A:139:ILE:C	1:A:139:ILE:HD12	2.35	0.52
1:A:175:ALA:HB2	14:A:811:CLA:HBC2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:HIS:HB3	14:A:819:CLA:HMB2	1.92	0.52
1:A:722:LEU:HD12	15:A:846:PQN:O4	2.10	0.52
7:I:17:VAL:HG12	7:I:18:VAL:N	2.24	0.52
1:A:140:THR:HG21	1:A:748:LEU:HD11	1.92	0.52
2:B:664:ALA:O	2:B:667:PHE:HB2	2.09	0.52
14:A:841:CLA:O1A	2:B:427:TRP:HD1	1.93	0.51
7:I:18:VAL:O	7:I:23:PRO:HD2	2.10	0.51
14:A:810:CLA:HAB	14:B:3034:CLA:HMD2	1.92	0.51
2:B:668:MET:HB2	14:B:3004:CLA:C1C	2.41	0.51
9:K:58:GLU:HA	9:K:60:LEU:HD22	1.93	0.51
8:J:23:ALA:O	8:J:26:LEU:N	2.42	0.51
1:A:286:ASN:OD1	1:A:286:ASN:C	2.53	0.51
1:A:654:LEU:HD22	13:A:801:CL0:H26	1.93	0.51
2:B:690:ARG:HH21	4:D:18:LEU:HD23	1.76	0.51
6:F:80:VAL:HG21	6:F:110:MET:HA	1.92	0.51
2:B:121:HIS:CB	2:B:364:ILE:HD13	2.41	0.51
2:B:255:THR:HG23	2:B:270:THR:HB	1.93	0.51
9:K:41:PRO:HD2	9:K:56:LEU:HD22	1.91	0.51
9:K:58:GLU:HB2	9:K:60:LEU:HD22	1.93	0.51
1:A:201:LEU:C	1:A:201:LEU:HD13	2.36	0.51
2:B:474:LEU:H	2:B:474:LEU:HD22	1.76	0.51
8:J:35:ASP:OD1	8:J:35:ASP:N	2.42	0.51
1:A:246:PRO:O	1:A:258:TRP:CE3	2.64	0.51
7:I:22:MET:HG3	7:I:23:PRO:HD3	1.93	0.51
1:A:67:ASP:OD1	1:A:71:LYS:CE	2.59	0.51
1:A:360:LEU:HD23	14:A:806:CLA:HED1	1.93	0.51
2:B:304:MET:CE	2:B:322:HIS:HB3	2.41	0.51
6:F:53:VAL:HG13	6:F:63:PHE:HD1	1.69	0.51
6:F:105:LEU:HD12	6:F:106:ALA:N	2.26	0.51
1:A:66:GLU:OE2	1:A:70:ARG:NH2	2.44	0.50
1:A:70:ARG:NH1	1:A:185:PRO:O	2.45	0.50
1:A:396:HIS:HE1	14:A:829:CLA:ND	2.07	0.50
1:A:575:ARG:HD2	1:A:725:ILE:HG21	1.93	0.50
2:B:275:HIS:HB2	14:B:3018:CLA:CHB	2.41	0.50
4:D:118:SER:OG	4:D:121:GLN:OE1	2.27	0.50
1:A:280:THR:HG22	1:A:281:PHE:N	2.27	0.50
1:A:437:ARG:HH22	1:A:562:SER:HB2	1.76	0.50
2:B:569:GLY:HA3	3:C:55:THR:HG22	1.92	0.50
5:E:15:TYR:CD2	5:E:44:ASN:HA	2.46	0.50
10:L:33:ASN:O	10:L:38:ARG:HD3	2.10	0.50
4:D:2:THR:HB	4:D:3:LEU:HD22	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:47:GLY:O	6:F:48:LEU:HD23	2.11	0.50
1:A:361:ALA:HB1	16:A:850:BCR:H343	1.92	0.50
6:F:55:GLY:HA2	12:X:31:PHE:CZ	2.47	0.50
1:A:216:GLN:HE22	1:A:297:THR:HG22	1.76	0.50
2:B:313:LYS:O	2:B:313:LYS:HG3	2.06	0.50
3:C:40:SER:OG	4:D:112:VAL:HG12	2.11	0.50
6:F:103:VAL:HG22	6:F:107:ILE:HD12	1.92	0.50
8:J:36:LEU:HD11	16:J:105:BCR:H392	1.94	0.50
1:A:205:LEU:HD21	1:A:308:PHE:CE2	2.46	0.50
4:D:60:ARG:HB2	4:D:63:GLN:HG3	1.94	0.50
6:F:16:LYS:O	6:F:19:ALA:HB3	2.12	0.50
4:D:2:THR:HG22	4:D:3:LEU:H	1.76	0.50
10:L:56:TYR:HB2	10:L:131:SER:HB2	1.94	0.50
1:A:344:LEU:O	1:A:347:VAL:HG22	2.12	0.49
2:B:472:LYS:NZ	2:B:517:THR:OG1	2.45	0.49
2:B:473:LEU:HD12	2:B:508:ASN:OD1	2.12	0.49
7:I:17:VAL:O	7:I:18:VAL:O	2.30	0.49
1:A:216:GLN:HA	1:A:220:SER:H	1.77	0.49
1:A:249:MET:C	1:A:258:TRP:CH2	2.90	0.49
1:A:584:GLY:HA3	3:C:76:MET:HE2	1.95	0.49
1:A:19:ASP:HB2	1:A:182:LYS:HD2	1.93	0.49
6:F:133:ASP:HA	6:F:136:ILE:HD11	1.94	0.49
10:L:41:LEU:HD13	10:L:45:LEU:HD23	1.95	0.49
1:A:201:LEU:O	1:A:201:LEU:HD13	2.11	0.49
1:A:592:TRP:O	1:A:595:VAL:HG22	2.12	0.49
14:A:829:CLA:HBB1	14:A:829:CLA:HMB3	1.94	0.49
2:B:17:THR:CG2	2:B:703:PRO:HA	2.42	0.49
2:B:566:ASP:H	2:B:573:THR:HG23	1.77	0.49
1:A:324:SER:O	1:A:328:ILE:HG13	2.12	0.49
2:B:353:GLN:O	2:B:357:SER:OG	2.29	0.49
8:J:2:LYS:HA	8:J:5:LEU:HD23	1.93	0.49
1:A:94:GLY:O	1:A:98:SER:HB3	2.11	0.49
1:A:688:MET:HB2	14:A:803:CLA:C1C	2.43	0.49
14:I:101:CLA:HHC	14:I:101:CLA:HBB1	1.95	0.49
4:D:101:PHE:HB3	4:D:103:GLU:OE1	2.12	0.49
10:L:152:LEU:HD12	10:L:152:LEU:O	2.12	0.49
1:A:205:LEU:CG	1:A:308:PHE:CE2	2.93	0.49
1:A:207:LEU:HD12	16:A:847:BCR:H361	1.95	0.49
1:A:250:ALA:N	1:A:258:TRP:HZ3	2.09	0.49
1:A:722:LEU:HD12	15:A:846:PQN:C4	2.42	0.49
2:B:637:LEU:HD13	2:B:733:ALA:HB3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:14:PHE:CE1	6:F:35:PHE:HD2	2.31	0.49
9:K:40:GLY:N	9:K:41:PRO:CD	2.76	0.49
1:A:207:LEU:CD1	16:A:847:BCR:H361	2.43	0.49
5:E:15:TYR:CD2	5:E:44:ASN:HB2	2.47	0.49
1:A:215:HIS:O	1:A:219:VAL:N	2.46	0.49
1:A:293:TRP:HB2	1:A:296:ASP:OD2	2.13	0.49
1:A:149:ALA:O	1:A:220:SER:OG	2.31	0.48
2:B:184:VAL:CG2	16:B:3044:BCR:H332	2.39	0.48
2:B:525:VAL:O	2:B:529:ILE:HG13	2.13	0.48
6:F:12:PRO:O	6:F:16:LYS:HG2	2.12	0.48
9:K:65:PHE:HE2	16:K:102:BCR:H272	1.76	0.48
5:E:56:ASN:OD1	5:E:57:THR:CG2	2.61	0.48
1:A:654:LEU:HD22	13:A:801:CL0:CMD	2.43	0.48
2:B:19:ARG:NH2	7:I:34:ILE:O	2.46	0.48
2:B:282:LEU:O	2:B:285:VAL:HG12	2.13	0.48
2:B:342:ALA:HB2	16:B:3046:BCR:H372	1.96	0.48
2:B:462:PHE:O	2:B:466:ILE:HG13	2.13	0.48
1:A:189:TRP:CZ3	1:A:190:PHE:CE1	3.01	0.48
2:B:612:VAL:O	2:B:616:ASN:OD1	2.31	0.48
9:K:24:LEU:HD13	9:K:69:LEU:HB3	1.95	0.48
1:A:220:SER:HA	1:A:223:ILE:HG22	1.96	0.48
1:A:245:ASN:HB3	1:A:248:LEU:HD12	1.96	0.48
14:B:3034:CLA:H43	16:J:105:BCR:H361	1.96	0.48
1:A:383:LEU:HD23	1:A:383:LEU:H	1.78	0.48
1:A:711:LEU:HD11	14:B:3032:CLA:H3A	1.96	0.48
8:J:2:LYS:HD2	8:J:2:LYS:O	2.14	0.48
9:K:22:CYS:HA	9:K:25:PHE:HB2	1.95	0.48
9:K:63:THR:HG21	14:K:101:CLA:HMB2	1.95	0.48
2:B:483:ASN:OD1	2:B:485:ASP:N	2.44	0.48
6:F:76:TRP:NE1	14:F:202:CLA:HBD	2.29	0.48
6:F:105:LEU:HD12	6:F:106:ALA:H	1.78	0.48
1:A:104:LEU:HD12	1:A:104:LEU:O	2.13	0.48
2:B:57:PHE:CD2	2:B:144:LEU:HB3	2.48	0.48
2:B:121:HIS:CG	2:B:364:ILE:CD1	2.96	0.48
4:D:95:HIS:HB3	4:D:96:PRO:CD	2.44	0.48
1:A:26:GLU:OE2	1:A:30:LYS:NZ	2.47	0.48
1:A:213:ALA:O	1:A:217:ILE:HG23	2.14	0.48
14:A:820:CLA:C2D	14:A:830:CLA:H41	2.44	0.48
14:A:829:CLA:H193	16:J:103:BCR:C14	2.44	0.48
6:F:96:GLU:OE2	6:F:100:ILE:CD1	2.61	0.48
10:L:52:MET:HE2	14:L:203:CLA:H2A	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:12:LEU:HB3	16:M:103:BCR:H21C	1.96	0.48
12:X:20:LEU:C	12:X:20:LEU:HD13	2.39	0.48
1:A:76:HIS:CE1	14:A:806:CLA:ND	2.82	0.48
1:A:453:PHE:O	1:A:454:HIS:C	2.55	0.48
1:A:583:ARG:HA	3:C:76:MET:C	2.39	0.48
1:A:583:ARG:HA	3:C:76:MET:HA	1.95	0.48
2:B:325:ILE:HA	2:B:328:THR:CG2	2.43	0.48
2:B:430:LEU:HD21	16:F:201:BCR:C40	2.43	0.48
6:F:76:TRP:CH2	6:F:114:PHE:CD1	3.02	0.48
1:A:78:GLY:O	1:A:82:VAL:HG23	2.14	0.47
1:A:120:ILE:HD11	8:J:31:ARG:CB	2.37	0.47
1:A:249:MET:HB3	1:A:258:TRP:HH2	1.77	0.47
5:E:23:VAL:HG13	5:E:36:VAL:HG23	1.96	0.47
6:F:25:THR:OG1	6:F:26:ALA:N	2.46	0.47
10:L:54:HIS:HA	10:L:57:PHE:CE2	2.49	0.47
1:A:196:MET:HB2	14:A:814:CLA:HBC2	1.96	0.47
1:A:337:THR:HG22	14:A:832:CLA:OBD	2.14	0.47
1:A:152:ILE:HD13	14:A:815:CLA:O1D	2.14	0.47
1:A:689:PHE:CD2	1:A:730:VAL:HG11	2.50	0.47
2:B:42:TYR:CD2	2:B:167:PHE:HB3	2.48	0.47
14:B:3030:CLA:HBB1	14:B:3030:CLA:HMB1	1.96	0.47
9:K:74:VAL:O	9:K:77:LEU:HD21	2.15	0.47
1:A:143:LEU:O	1:A:144:PHE:C	2.58	0.47
1:A:201:LEU:CD1	1:A:308:PHE:O	2.63	0.47
1:A:352:TRP:CD1	14:A:826:CLA:H202	2.49	0.47
14:A:821:CLA:HMA2	9:K:61:ALA:CB	2.44	0.47
2:B:215:MET:HE2	2:B:217:HIS:O	2.14	0.47
6:F:109:CYS:O	6:F:112:THR:HG22	2.15	0.47
1:A:237:PRO:HG2	1:A:242:PHE:CZ	2.49	0.47
1:A:306:VAL:CG2	14:A:818:CLA:HMC3	2.44	0.47
1:A:465:MET:HE3	1:A:473:ASP:CB	2.45	0.47
14:B:3030:CLA:H2A	14:B:3030:CLA:O2D	2.15	0.47
9:K:43:LEU:HD13	9:K:57:PRO:HG3	1.97	0.47
9:K:60:LEU:O	9:K:61:ALA:C	2.58	0.47
1:A:120:ILE:HG23	1:A:121:VAL:HG22	1.97	0.47
1:A:379:PRO:HB2	14:A:820:CLA:HAA2	1.97	0.47
1:A:524:VAL:CG1	1:A:525:ALA:N	2.76	0.47
1:A:670:SER:HB2	2:B:448:ALA:HB1	1.96	0.47
2:B:304:MET:HE3	2:B:304:MET:HA	1.96	0.47
14:B:3028:CLA:H141	14:B:3030:CLA:H152	1.97	0.47
10:L:106:SER:OG	10:L:107:SER:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ARG:NH2	1:A:228:ASP:OD1	2.42	0.47
1:A:164:GLY:O	1:A:167:VAL:HG12	2.14	0.47
1:A:493:LEU:HD23	1:A:493:LEU:H	1.79	0.47
1:A:552:ILE:CD1	14:B:3004:CLA:HMD3	2.44	0.47
1:A:747:PHE:O	1:A:751:ILE:HG22	2.15	0.47
14:A:817:CLA:HBB2	16:A:847:BCR:H352	1.96	0.47
2:B:222:ALA:N	2:B:223:PRO:CD	2.78	0.47
2:B:555:ASP:OD2	3:C:65:ARG:NH1	2.48	0.47
22:L:206:DGD:O6E	22:L:206:DGD:O4D	2.30	0.47
1:A:67:ASP:OD1	1:A:67:ASP:C	2.58	0.47
1:A:681:PHE:CD2	16:A:851:BCR:H363	2.50	0.47
2:B:437:LEU:O	2:B:441:VAL:HG12	2.14	0.47
1:A:593:ASP:OD1	1:A:728:ARG:NH1	2.48	0.47
2:B:155:HIS:HE1	14:B:3012:CLA:ND	2.10	0.47
2:B:435:HIS:CG	16:J:105:BCR:H333	2.50	0.47
2:B:599:TYR:CZ	14:B:3038:CLA:HBC2	2.50	0.47
2:B:655:MET:HA	2:B:658:PHE:HB3	1.97	0.47
3:C:25:LEU:HD23	3:C:41:SER:HA	1.96	0.47
1:A:217:ILE:HG22	1:A:298:ALA:HB1	1.97	0.47
1:A:286:ASN:HA	1:A:293:TRP:CZ2	2.50	0.47
2:B:36:MET:HE2	2:B:41:LEU:CA	2.45	0.47
2:B:395:ILE:HD13	14:B:3030:CLA:HED3	1.96	0.47
6:F:17:ARG:NE	6:F:48:LEU:HD21	2.30	0.47
1:A:262:SER:HA	1:A:266:PRO:HG3	1.98	0.46
1:A:280:THR:HG21	1:A:282:ASN:OD1	2.15	0.46
1:A:399:TRP:CE3	1:A:606:ILE:HG21	2.51	0.46
1:A:726:GLN:HG3	18:A:853:LHG:C7	2.45	0.46
2:B:304:MET:HE2	2:B:325:ILE:CD1	2.45	0.46
2:B:674:ARG:N	23:B:3108:HOH:O	2.45	0.46
10:L:110:PRO:O	10:L:113:THR:HG22	2.15	0.46
2:B:304:MET:HE2	2:B:325:ILE:HG13	1.96	0.46
2:B:618:SER:HA	2:B:621:TYR:CE1	2.50	0.46
6:F:88:VAL:HG12	6:F:94:ALA:HA	1.97	0.46
12:X:12:ARG:HG2	12:X:12:ARG:HH11	1.79	0.46
1:A:84:PHE:O	1:A:87:LEU:HD12	2.15	0.46
1:A:168:MET:HE3	1:A:171:LEU:HD21	1.98	0.46
1:A:300:HIS:HB2	14:A:819:CLA:C1B	2.45	0.46
14:A:814:CLA:OBD	14:A:826:CLA:H92	2.15	0.46
1:A:358:ILE:HG22	16:A:849:BCR:HC7	1.98	0.46
1:A:556:GLY:CA	1:A:594:HIS:ND1	2.78	0.46
14:A:810:CLA:H92	14:A:810:CLA:C3	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:811:CLA:O1A	14:A:813:CLA:H42	2.15	0.46
2:B:466:ILE:HD11	14:B:3038:CLA:H12	1.98	0.46
6:F:8:CYS:SG	6:F:42:LEU:C	2.99	0.46
8:J:38:PHE:O	8:J:40:PRO:HD3	2.15	0.46
10:L:61:PRO:HA	14:L:205:CLA:HMB2	1.97	0.46
2:B:29:ASP:OD1	23:B:3102:HOH:O	2.21	0.46
2:B:36:MET:CE	2:B:41:LEU:N	2.78	0.46
14:B:3008:CLA:CGD	7:I:11:PRO:HG3	2.46	0.46
8:J:21:ILE:O	8:J:22:THR:C	2.57	0.46
12:X:29:TYR:CD1	12:X:34:LEU:HB2	2.51	0.46
1:A:25:PHE:CE1	8:J:4:PHE:HD2	2.33	0.46
1:A:26:GLU:HG2	1:A:30:LYS:NZ	2.30	0.46
1:A:74:SER:HB3	1:A:180:TYR:HB2	1.97	0.46
1:A:178:PHE:O	1:A:182:LYS:O	2.34	0.46
1:A:391:LEU:HD12	1:A:613:PHE:HE1	1.81	0.46
16:A:849:BCR:H333	16:A:850:BCR:H333	1.96	0.46
2:B:555:ASP:OD1	3:C:65:ARG:NH1	2.46	0.46
3:C:12:GLY:O	3:C:14:THR:HG23	2.15	0.46
6:F:111:LEU:HD12	6:F:111:LEU:H	1.80	0.46
8:J:29:PHE:CD1	8:J:29:PHE:C	2.94	0.46
8:J:36:LEU:HD11	16:J:105:BCR:C39	2.46	0.46
14:A:804:CLA:H193	14:A:843:CLA:C18	2.46	0.46
10:L:57:PHE:CD1	10:L:57:PHE:C	2.93	0.46
3:C:72:THR:N	3:C:75:SER:OG	2.48	0.46
1:A:602:MET:HB2	14:A:827:CLA:HBC1	1.98	0.46
6:F:76:TRP:CZ3	6:F:114:PHE:HA	2.44	0.46
10:L:143:LEU:H	10:L:143:LEU:HD22	1.81	0.46
1:A:177:TRP:HE3	1:A:178:PHE:N	2.14	0.46
1:A:405:VAL:HG13	16:A:850:BCR:H342	1.98	0.46
1:A:465:MET:HE3	1:A:473:ASP:HB3	1.98	0.46
1:A:524:VAL:HG12	1:A:525:ALA:H	1.79	0.46
14:B:3005:CLA:HHC	14:B:3007:CLA:OBD	2.16	0.46
6:F:80:VAL:CG2	6:F:110:MET:HA	2.45	0.46
1:A:172:MET:HA	1:A:175:ALA:HB3	1.96	0.45
1:A:177:TRP:CE3	1:A:178:PHE:CA	2.99	0.45
1:A:256:VAL:CG1	1:A:258:TRP:HE1	2.29	0.45
1:A:374:MET:HE1	14:A:830:CLA:O1D	2.15	0.45
2:B:339:TRP:HE1	14:B:3025:CLA:C2B	2.28	0.45
2:B:229:TRP:O	14:B:3017:CLA:H3A	2.16	0.45
1:A:256:VAL:CB	1:A:258:TRP:HE1	2.30	0.45
2:B:364:ILE:HG23	2:B:371:MET:SD	2.56	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:HIS:CE1	14:A:806:CLA:HMA2	2.52	0.45
2:B:498:VAL:HG11	14:B:3017:CLA:HED1	1.97	0.45
3:C:23:ASP:O	3:C:23:ASP:OD2	2.33	0.45
8:J:33:TYR:CE2	16:J:105:BCR:H401	2.52	0.45
9:K:59:LEU:C	9:K:59:LEU:HD12	2.41	0.45
10:L:59:ILE:HG22	10:L:78:GLY:O	2.16	0.45
1:A:310:ILE:O	14:A:823:CLA:HBC1	2.15	0.45
2:B:290:TYR:CD1	2:B:300:ILE:HD11	2.51	0.45
6:F:79:TRP:CH2	6:F:120:ALA:HA	2.52	0.45
1:A:67:ASP:OD1	1:A:71:LYS:HE3	2.16	0.45
1:A:256:VAL:HG12	1:A:258:TRP:HD1	1.78	0.45
2:B:322:HIS:CE1	2:B:410:VAL:HG11	2.52	0.45
14:B:3033:CLA:O1A	14:B:3033:CLA:C2	2.63	0.45
8:J:40:PRO:HD2	16:J:105:BCR:H382	1.99	0.45
1:A:246:PRO:O	1:A:258:TRP:CZ3	2.70	0.45
1:A:314:MET:HE1	14:A:822:CLA:C2D	2.47	0.45
1:A:368:ILE:HG12	1:A:398:MET:HE3	1.98	0.45
1:A:385:THR:O	1:A:523:LYS:NZ	2.45	0.45
1:A:619:SER:OG	1:A:620:ASP:OD1	2.32	0.45
6:F:2:VAL:O	6:F:5:LEU:HD13	2.17	0.45
8:J:4:PHE:HE1	8:J:8:LEU:HD13	1.81	0.45
1:A:358:ILE:HD11	23:A:913:HOH:O	2.16	0.45
2:B:479:THR:HA	12:X:35:LYS:HG2	1.99	0.45
3:C:62:LEU:O	4:D:119:ILE:HD11	2.17	0.45
8:J:17:ILE:HD12	8:J:18:TRP:CA	2.47	0.45
10:L:110:PRO:O	10:L:113:THR:CG2	2.64	0.45
1:A:396:HIS:HB2	14:A:829:CLA:C1B	2.46	0.45
1:A:455:SER:OG	1:A:456:PHE:N	2.50	0.45
2:B:175:ASN:HB3	14:B:3021:CLA:HMD1	1.99	0.45
2:B:298:HIS:CD2	14:B:3022:CLA:ND	2.85	0.45
16:B:3046:BCR:H24C	16:B:3046:BCR:H371	1.84	0.45
3:C:37:GLN:HB3	4:D:105:VAL:HG21	1.99	0.45
6:F:79:TRP:CH2	6:F:120:ALA:CB	2.99	0.45
9:K:65:PHE:CE2	16:K:102:BCR:H292	2.52	0.45
11:M:30:TYR:O	11:M:31:LYS:C	2.60	0.45
1:A:387:TYR:HB3	1:A:751:ILE:HD11	1.99	0.45
1:A:587:CYS:HB2	2:B:673:TRP:HB3	1.99	0.45
3:C:54:GLU:HG2	3:C:62:LEU:HD22	1.99	0.45
6:F:88:VAL:HG11	6:F:97:LYS:HB2	1.99	0.45
9:K:64:SER:HB3	9:K:68:LEU:CD2	2.46	0.45
1:A:80:LEU:HB3	1:A:172:MET:SD	2.56	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:THR:OG1	2:B:228:ASN:ND2	2.50	0.44
2:B:533:LEU:O	2:B:537:THR:HG23	2.18	0.44
18:B:3049:LHG:O1	12:X:12:ARG:NH2	2.50	0.44
3:C:60:ASP:OD2	5:E:14:SER:OG	2.27	0.44
6:F:24:THR:OG1	6:F:34:ARG:NH1	2.50	0.44
6:F:76:TRP:CD2	6:F:113:GLY:HA3	2.53	0.44
6:F:103:VAL:HG22	6:F:107:ILE:CD1	2.46	0.44
1:A:177:TRP:HE3	1:A:178:PHE:CA	2.29	0.44
1:A:341:HIS:HB3	1:A:344:LEU:HD12	1.99	0.44
1:A:462:ASN:O	1:A:463:ASP:C	2.59	0.44
14:A:821:CLA:HMA2	9:K:61:ALA:HB2	1.98	0.44
6:F:84:TYR:CD1	6:F:84:TYR:C	2.94	0.44
9:K:24:LEU:HD11	9:K:70:ALA:HB2	1.98	0.44
1:A:98:SER:OG	1:A:99:ASN:N	2.50	0.44
1:A:175:ALA:HA	14:A:811:CLA:HBC2	1.98	0.44
1:A:289:THR:HG22	1:A:381:PRO:HB3	1.98	0.44
1:A:317:THR:HG22	14:A:821:CLA:O1D	2.17	0.44
14:A:844:CLA:HHC	14:A:844:CLA:CBB	2.48	0.44
2:B:41:LEU:O	2:B:45:ILE:HG12	2.18	0.44
2:B:313:LYS:O	2:B:314:VAL:HG13	2.17	0.44
2:B:473:LEU:HD12	2:B:473:LEU:H	1.82	0.44
2:B:566:ASP:HB3	2:B:573:THR:HG21	1.99	0.44
6:F:77:ILE:CD1	14:F:202:CLA:ND	2.81	0.44
9:K:29:LEU:HD22	9:K:62:THR:CG2	2.47	0.44
1:A:141:SER:CB	1:A:143:LEU:HG	2.48	0.44
1:A:300:HIS:HE1	14:A:819:CLA:ND	2.10	0.44
14:A:810:CLA:CAB	14:B:3034:CLA:HMD2	2.47	0.44
2:B:192:HIS:HB2	14:B:3015:CLA:CHC	2.47	0.44
2:B:266:SER:OG	2:B:267:LEU:N	2.49	0.44
2:B:730:PHE:CD1	14:B:3003:CLA:HMD2	2.52	0.44
3:C:53:CYS:SG	3:C:66:VAL:HG21	2.58	0.44
1:A:23:THR:O	1:A:23:THR:OG1	2.32	0.44
1:A:152:ILE:HD12	1:A:157:GLN:HB3	1.99	0.44
1:A:197:LEU:HD13	14:A:826:CLA:C3D	2.48	0.44
2:B:275:HIS:HB2	14:B:3018:CLA:C1B	2.46	0.44
2:B:360:PRO:HG3	14:B:3019:CLA:HBA2	1.98	0.44
2:B:525:VAL:HG21	2:B:599:TYR:CD1	2.53	0.44
2:B:598:PHE:CE1	2:B:727:TYR:CE1	3.06	0.44
5:E:15:TYR:CE2	5:E:44:ASN:HA	2.52	0.44
16:I:105:BCR:H24C	10:L:93:LEU:CD2	2.47	0.44
1:A:606:ILE:HA	1:A:609:VAL:HG22	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:430:LEU:HD21	16:F:201:BCR:H402	2.00	0.44
2:B:674:ARG:HD2	2:B:706:LEU:O	2.18	0.44
14:B:3031:CLA:H2A	14:B:3031:CLA:O1D	2.18	0.44
1:A:398:MET:CE	14:A:827:CLA:HMD2	2.48	0.44
2:B:277:LEU:HD23	2:B:277:LEU:O	2.18	0.44
4:D:9:LEU:HD23	4:D:48:VAL:HG13	2.00	0.44
9:K:23:ASN:O	9:K:27:ILE:HG12	2.18	0.44
1:A:70:ARG:HB3	1:A:180:TYR:HD1	1.83	0.44
1:A:175:ALA:CA	14:A:811:CLA:HBC2	2.48	0.44
1:A:175:ALA:CB	14:A:811:CLA:HBC2	2.48	0.44
14:A:804:CLA:HHC	14:A:804:CLA:HBB1	1.99	0.44
2:B:324:GLY:HA2	2:B:327:GLU:OE1	2.18	0.44
5:E:1:VAL:HG12	5:E:1:VAL:O	2.17	0.44
6:F:76:TRP:NE1	14:F:202:CLA:CAD	2.79	0.44
16:I:102:BCR:H20C	16:I:102:BCR:H361	1.85	0.44
10:L:86:ILE:HG22	10:L:129:MET:HE2	2.00	0.44
1:A:201:LEU:HD12	1:A:312:GLY:N	2.33	0.44
14:A:813:CLA:HHC	14:A:813:CLA:HBB1	2.00	0.44
2:B:36:MET:CE	2:B:41:LEU:CA	2.96	0.44
2:B:642:ASN:HB2	2:B:643:PRO:CD	2.47	0.44
16:B:3046:BCR:C8	16:B:3046:BCR:H331	2.48	0.44
10:L:72:ASP:N	10:L:72:ASP:OD1	2.50	0.44
1:A:152:ILE:CD1	1:A:157:GLN:HB3	2.48	0.43
1:A:204:LEU:CD1	14:A:814:CLA:CHB	2.95	0.43
1:A:433:VAL:HA	1:A:436:HIS:CE1	2.52	0.43
2:B:171:GLU:HG3	2:B:300:ILE:CD1	2.48	0.43
2:B:292:THR:HG21	14:B:3021:CLA:OBD	2.18	0.43
6:F:73:ILE:HD13	14:F:202:CLA:H3A	1.99	0.43
16:L:207:BCR:H20C	16:L:207:BCR:H361	1.82	0.43
1:A:25:PHE:CE1	8:J:4:PHE:CD2	3.06	0.43
1:A:143:LEU:HD22	1:A:146:LEU:HD23	1.97	0.43
1:A:409:ALA:HA	16:A:850:BCR:HC41	2.00	0.43
2:B:411:LEU:O	2:B:414:VAL:CG2	2.66	0.43
2:B:651:VAL:CG1	14:B:3010:CLA:HHD	2.48	0.43
22:L:206:DGD:O4D	22:L:206:DGD:O5D	2.36	0.43
1:A:76:HIS:C	14:A:814:CLA:HED3	2.43	0.43
1:A:432:ARG:HD3	14:A:832:CLA:OBD	2.17	0.43
14:B:3011:CLA:HHC	14:B:3011:CLA:HBB1	2.00	0.43
3:C:65:ARG:HB3	3:C:67:TYR:CE1	2.53	0.43
10:L:85:LEU:O	10:L:88:VAL:HG22	2.17	0.43
1:A:484:PRO:HG3	1:A:536:PHE:HB2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:HIS:CG	2:B:364:ILE:HD12	2.54	0.43
2:B:291:ARG:N	2:B:298:HIS:O	2.51	0.43
2:B:651:VAL:HG13	14:B:3010:CLA:HAC1	2.01	0.43
14:B:3011:CLA:CBB	7:I:19:CYS:HB3	2.48	0.43
8:J:33:TYR:N	8:J:33:TYR:CD1	2.86	0.43
11:M:4:THR:H	11:M:7:GLN:NE2	2.15	0.43
16:M:103:BCR:H321	16:M:103:BCR:HC8	2.00	0.43
1:A:717:ILE:O	1:A:717:ILE:HG22	2.18	0.43
14:A:829:CLA:H41	14:A:829:CLA:H72	2.00	0.43
14:B:3010:CLA:HMB3	14:B:3011:CLA:CHC	2.48	0.43
3:C:37:GLN:NE2	4:D:105:VAL:CG2	2.82	0.43
6:F:82:ARG:NH2	6:F:129:LEU:HD12	2.34	0.43
9:K:62:THR:HA	9:K:65:PHE:HB3	2.01	0.43
1:A:126:LEU:HB3	1:A:137:ILE:HD11	2.00	0.43
1:A:680:HIS:CE1	1:A:742:THR:HG21	2.54	0.43
2:B:203:GLY:HA2	2:B:244:GLY:O	2.19	0.43
2:B:267:LEU:N	2:B:267:LEU:HD23	2.33	0.43
6:F:23:ASN:OD1	6:F:30:SER:N	2.52	0.43
8:J:1:MET:O	8:J:5:LEU:HD22	2.18	0.43
9:K:65:PHE:CD1	9:K:65:PHE:C	2.95	0.43
9:K:74:VAL:O	9:K:77:LEU:CD2	2.67	0.43
10:L:49:GLU:HB2	14:L:203:CLA:HED1	2.00	0.43
12:X:29:TYR:CE1	12:X:34:LEU:HB2	2.53	0.43
1:A:26:GLU:HG3	8:J:3:HIS:CE1	2.53	0.43
1:A:115:GLN:O	1:A:115:GLN:CG	2.66	0.43
1:A:584:GLY:CA	3:C:76:MET:HE2	2.49	0.43
1:A:688:MET:HB2	14:A:803:CLA:CHC	2.48	0.43
2:B:316:GLY:O	2:B:319:ASN:N	2.51	0.43
6:F:72:TYR:OH	6:F:114:PHE:O	2.30	0.43
12:X:25:LEU:C	12:X:25:LEU:HD23	2.43	0.43
1:A:217:ILE:HD12	1:A:217:ILE:C	2.43	0.43
1:A:433:VAL:HG12	14:A:832:CLA:C1D	2.49	0.43
1:A:440:ILE:HG22	1:A:441:ILE:N	2.34	0.43
14:A:803:CLA:CMD	2:B:539:ILE:HD13	2.48	0.43
14:A:814:CLA:CAD	14:A:826:CLA:H92	2.48	0.43
4:D:9:LEU:N	4:D:9:LEU:HD22	2.34	0.43
6:F:1:ASP:OD2	6:F:42:LEU:CD2	2.64	0.43
8:J:23:ALA:O	8:J:24:GLY:C	2.62	0.43
1:A:204:LEU:HD11	14:A:814:CLA:H3A	2.00	0.43
1:A:339:ALA:HB3	1:A:428:ASN:HA	2.01	0.43
1:A:396:HIS:HB2	14:A:829:CLA:CHB	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:ARG:O	1:A:569:LYS:HB3	2.18	0.43
14:A:829:CLA:H193	16:J:103:BCR:H14C	2.00	0.43
2:B:139:ILE:HG23	11:M:14:ILE:HD13	2.01	0.43
2:B:192:HIS:O	2:B:193:LEU:C	2.62	0.43
6:F:65:ILE:HB	6:F:66:PRO:HD3	1.99	0.43
11:M:13:VAL:O	11:M:16:LEU:HB2	2.19	0.43
2:B:338:GLY:HA2	2:B:389:ALA:HA	2.01	0.43
2:B:357:SER:CB	14:B:3027:CLA:HMC2	2.49	0.43
14:B:3034:CLA:H11	8:J:29:PHE:CE1	2.54	0.43
4:D:95:HIS:HB3	4:D:96:PRO:HD3	1.99	0.43
16:F:203:BCR:H24C	16:F:203:BCR:H371	1.90	0.43
9:K:60:LEU:HB2	9:K:63:THR:OG1	2.19	0.43
1:A:42:PRO:HB3	1:A:47:TRP:CD2	2.54	0.42
1:A:73:PHE:CE2	1:A:189:TRP:HH2	2.37	0.42
1:A:145:GLN:H	1:A:145:GLN:CD	2.26	0.42
2:B:242:VAL:HG23	2:B:242:VAL:O	2.18	0.42
10:L:60:GLY:N	10:L:61:PRO:HD2	2.34	0.42
12:X:20:LEU:HD13	12:X:20:LEU:O	2.19	0.42
14:A:841:CLA:HBC1	15:A:846:PQN:H212	2.01	0.42
14:A:845:CLA:CHC	18:A:854:LHG:HC31	2.49	0.42
2:B:275:HIS:HE1	14:B:3018:CLA:ND	2.15	0.42
2:B:319:ASN:O	2:B:319:ASN:CG	2.62	0.42
2:B:369:THR:HA	2:B:735:THR:HG21	2.01	0.42
2:B:616:ASN:OD1	2:B:616:ASN:N	2.52	0.42
14:B:3010:CLA:H91	14:B:3041:CLA:O1A	2.19	0.42
9:K:65:PHE:C	9:K:65:PHE:HD1	2.26	0.42
1:A:247:SER:O	1:A:248:LEU:C	2.63	0.42
1:A:341:HIS:CD2	14:A:825:CLA:ND	2.86	0.42
1:A:556:GLY:HA2	1:A:594:HIS:ND1	2.34	0.42
2:B:391:ALA:HA	23:B:3141:HOH:O	2.19	0.42
2:B:446:VAL:HG22	2:B:451:THR:OG1	2.18	0.42
2:B:451:THR:OG1	2:B:451:THR:O	2.37	0.42
7:I:22:MET:HG3	7:I:23:PRO:CD	2.49	0.42
10:L:24:SER:O	10:L:28:LYS:HG3	2.18	0.42
1:A:26:GLU:O	1:A:30:LYS:HE3	2.20	0.42
1:A:226:LEU:HB2	1:A:236:ILE:HD12	2.01	0.42
1:A:414:ILE:HD13	14:A:831:CLA:CED	2.50	0.42
14:B:3037:CLA:HHC	14:B:3037:CLA:HBB1	2.01	0.42
14:I:101:CLA:HHC	14:I:101:CLA:CBB	2.49	0.42
9:K:69:LEU:O	9:K:73:VAL:HG23	2.19	0.42
1:A:618:GLN:HE22	1:A:657:GLN:NE2	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:THR:HG21	2:B:703:PRO:HA	2.00	0.42
2:B:570:ARG:N	5:E:47:GLY:O	2.53	0.42
16:B:3045:BCR:H20C	16:B:3045:BCR:H361	1.89	0.42
6:F:67:SER:O	6:F:71:LEU:HG	2.19	0.42
1:A:65:LEU:O	1:A:68:ILE:CD1	2.66	0.42
1:A:519:ALA:HB1	1:A:523:LYS:O	2.18	0.42
14:A:802:CLA:H201	14:B:3010:CLA:H2	2.00	0.42
2:B:173:ARG:CA	14:B:3014:CLA:HBC2	2.50	0.42
2:B:339:TRP:HE1	14:B:3025:CLA:C3B	2.32	0.42
15:B:3042:PQN:H141	14:I:101:CLA:HBB2	2.01	0.42
4:D:36:GLU:HA	4:D:49:MET:O	2.20	0.42
6:F:77:ILE:O	6:F:80:VAL:HG12	2.19	0.42
1:A:567:PRO:O	23:A:903:HOH:O	2.22	0.42
14:A:834:CLA:HMD1	14:A:835:CLA:H143	2.02	0.42
2:B:36:MET:CE	2:B:41:LEU:HA	2.49	0.42
2:B:74:GLU:O	2:B:77:VAL:HG22	2.20	0.42
2:B:321:PRO:O	2:B:409:ASN:HB2	2.19	0.42
2:B:698:ARG:HG2	2:B:698:ARG:NH1	2.33	0.42
3:C:69:GLY:O	3:C:70:ALA:C	2.62	0.42
8:J:17:ILE:HD12	8:J:17:ILE:C	2.44	0.42
11:M:17:LEU:HB3	11:M:18:PRO:CD	2.49	0.42
1:A:272:TRP:O	1:A:275:TYR:HB2	2.20	0.42
1:A:380:TYR:O	1:A:383:LEU:CD2	2.67	0.42
1:A:385:THR:HG22	1:A:524:VAL:O	2.19	0.42
1:A:609:VAL:HG11	14:A:838:CLA:HBB2	2.02	0.42
2:B:692:PRO:O	2:B:693:LEU:HB2	2.20	0.42
2:B:693:LEU:HA	2:B:696:LEU:CD1	2.50	0.42
9:K:29:LEU:HD22	9:K:62:THR:OG1	2.20	0.42
11:M:24:ARG:NH1	14:M:102:CLA:HBB	2.34	0.42
1:A:379:PRO:HD2	1:A:383:LEU:HD11	2.02	0.42
2:B:78:GLN:C	2:B:80:PRO:HD3	2.45	0.42
3:C:15:GLN:HA	3:C:18:ARG:HD2	2.01	0.42
3:C:22:THR:O	4:D:61:LYS:NZ	2.44	0.42
5:E:9:ILE:O	5:E:10:LEU:HD12	2.20	0.42
8:J:24:GLY:HA2	8:J:27:ILE:HD13	2.02	0.42
1:A:319:TRP:HB3	9:K:58:GLU:OE2	2.20	0.42
2:B:351:VAL:HG22	14:B:3019:CLA:H42	2.01	0.42
2:B:493:PRO:HG3	14:B:3037:CLA:C1D	2.49	0.42
2:B:711:ALA:CB	15:B:3042:PQN:C8	2.97	0.42
8:J:1:MET:O	8:J:3:HIS:N	2.53	0.42
8:J:11:ALA:N	8:J:12:PRO:HD2	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LEU:C	1:A:145:GLN:N	2.76	0.41
1:A:495:THR:HG21	1:A:514:GLY:CA	2.47	0.41
14:A:843:CLA:CGA	14:A:843:CLA:C1A	2.97	0.41
2:B:53:LEU:HD21	14:B:3006:CLA:CGA	2.50	0.41
1:A:80:LEU:HA	1:A:83:VAL:HG12	2.03	0.41
1:A:168:MET:O	1:A:172:MET:HG2	2.20	0.41
14:A:821:CLA:CAA	9:K:58:GLU:OE1	2.67	0.41
2:B:535:THR:O	2:B:539:ILE:HG13	2.20	0.41
2:B:668:MET:HB2	14:B:3004:CLA:CHC	2.50	0.41
6:F:79:TRP:CZ3	6:F:120:ALA:HB2	2.55	0.41
9:K:70:ALA:O	9:K:74:VAL:HG23	2.20	0.41
1:A:25:PHE:O	8:J:3:HIS:HB3	2.20	0.41
1:A:135:HIS:ND1	1:A:135:HIS:N	2.68	0.41
1:A:173:LEU:C	1:A:173:LEU:HD23	2.45	0.41
1:A:713:VAL:O	1:A:713:VAL:HG22	2.20	0.41
14:A:844:CLA:HMB2	2:B:697:VAL:HG21	2.03	0.41
2:B:160:PHE:CD1	2:B:160:PHE:N	2.88	0.41
2:B:339:TRP:HH2	16:B:3050:BCR:H341	1.85	0.41
2:B:347:ILE:HG21	14:B:3025:CLA:H43	2.03	0.41
2:B:571:GLY:HA2	5:E:49:SER:HA	2.03	0.41
14:B:3004:CLA:CGA	14:B:3004:CLA:H3A	2.50	0.41
3:C:62:LEU:HB3	3:C:64:ILE:O	2.20	0.41
6:F:17:ARG:CD	6:F:48:LEU:HD21	2.50	0.41
7:I:6:ALA:HB2	11:M:3:LEU:O	2.21	0.41
16:I:102:BCR:H351	16:I:102:BCR:H15C	1.81	0.41
9:K:64:SER:O	9:K:68:LEU:CD2	2.68	0.41
10:L:124:PHE:CD1	10:L:124:PHE:C	2.99	0.41
14:A:845:CLA:HBC2	14:A:845:CLA:CMC	2.50	0.41
16:A:851:BCR:H373	2:B:437:LEU:CD1	2.50	0.41
4:D:41:MET:HE1	4:D:58:PHE:HE1	1.85	0.41
9:K:43:LEU:HB3	9:K:57:PRO:CG	2.51	0.41
1:A:406:VAL:HG11	1:A:599:LEU:CD2	2.51	0.41
1:A:682:ILE:CD1	1:A:737:LEU:HD23	2.49	0.41
2:B:198:ILE:HD13	2:B:270:THR:HG22	2.02	0.41
2:B:321:PRO:HG3	2:B:413:ARG:HH21	1.85	0.41
2:B:490:THR:HG22	2:B:492:TRP:HA	2.02	0.41
2:B:727:TYR:HB2	14:B:3003:CLA:HED3	2.03	0.41
14:B:3004:CLA:H141	14:B:3004:CLA:H161	1.91	0.41
16:B:3044:BCR:H15C	16:B:3044:BCR:H351	1.96	0.41
3:C:60:ASP:OD1	3:C:60:ASP:O	2.38	0.41
6:F:70:PHE:O	6:F:71:LEU:C	2.62	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:103:VAL:N	6:F:104:PRO:CD	2.83	0.41
8:J:17:ILE:O	8:J:21:ILE:HG23	2.19	0.41
9:K:64:SER:O	9:K:68:LEU:HD22	2.21	0.41
1:A:80:LEU:O	1:A:83:VAL:HG12	2.19	0.41
1:A:177:TRP:O	1:A:181:HIS:HB2	2.21	0.41
2:B:67:VAL:O	2:B:71:GLY:N	2.44	0.41
2:B:299:SER:OG	2:B:302:GLU:HG3	2.20	0.41
2:B:569:GLY:CA	3:C:55:THR:HG22	2.50	0.41
15:B:3042:PQN:H141	14:I:101:CLA:CBB	2.51	0.41
4:D:27:TYR:CE2	4:D:61:LYS:HB2	2.55	0.41
6:F:64:LEU:N	6:F:64:LEU:CD1	2.84	0.41
1:A:76:HIS:CE1	14:A:806:CLA:C4D	3.03	0.41
1:A:93:HIS:HE1	14:A:808:CLA:NC	2.18	0.41
1:A:139:ILE:HD12	1:A:139:ILE:O	2.20	0.41
2:B:618:SER:O	2:B:624:GLY:HA3	2.20	0.41
14:B:3014:CLA:H143	14:B:3029:CLA:HMD2	2.01	0.41
6:F:8:CYS:HB3	6:F:14:PHE:CE2	2.54	0.41
6:F:59:ARG:HA	6:F:59:ARG:HD2	1.94	0.41
6:F:64:LEU:N	6:F:64:LEU:HD12	2.35	0.41
9:K:35:GLN:O	9:K:36:SER:HB3	2.20	0.41
10:L:143:LEU:HD22	10:L:143:LEU:N	2.36	0.41
1:A:94:GLY:HA3	1:A:147:TRP:CH2	2.56	0.41
1:A:665:TYR:OH	1:A:674:LEU:HD23	2.21	0.41
2:B:42:TYR:HD2	2:B:167:PHE:HB3	1.83	0.41
14:B:3038:CLA:H11	14:B:3039:CLA:O1A	2.20	0.41
3:C:1:ALA:HB1	23:C:204:HOH:O	2.20	0.41
8:J:38:PHE:CD1	8:J:38:PHE:N	2.89	0.41
16:J:103:BCR:C8	16:J:103:BCR:H311	2.50	0.41
1:A:165:GLY:N	16:A:847:BCR:HC21	2.36	0.41
1:A:314:MET:HE1	14:A:822:CLA:C3D	2.51	0.41
1:A:398:MET:HE2	1:A:398:MET:HB3	1.95	0.41
1:A:443:HIS:CD2	14:A:833:CLA:NC	2.89	0.41
1:A:519:ALA:HA	1:A:524:VAL:HA	2.03	0.41
1:A:677:LEU:HD13	2:B:623:MET:HE2	2.02	0.41
14:A:811:CLA:HBC3	14:A:811:CLA:CHD	2.49	0.41
2:B:277:LEU:HD21	14:B:3017:CLA:CAB	2.50	0.41
2:B:403:PRO:O	2:B:404:ALA:C	2.64	0.41
2:B:528:ALA:CB	14:B:3003:CLA:H192	2.50	0.41
14:B:3010:CLA:H43	16:I:102:BCR:H342	2.02	0.41
14:B:3011:CLA:HHC	14:B:3011:CLA:CBB	2.51	0.41
4:D:61:LYS:HE3	4:D:94:ILE:HD12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:57:LEU:HA	6:F:60:ALA:HB2	2.02	0.41
6:F:84:TYR:CE1	6:F:88:VAL:HG21	2.56	0.41
8:J:21:ILE:HD12	8:J:25:ILE:HD11	2.03	0.41
9:K:39:LYS:HD2	9:K:56:LEU:CD1	2.51	0.41
1:A:149:ALA:HB2	1:A:381:PRO:HD3	2.03	0.41
1:A:444:LEU:HB2	14:A:840:CLA:CBB	2.51	0.41
1:A:588:GLN:CD	2:B:673:TRP:HB2	2.46	0.41
2:B:555:ASP:CG	3:C:65:ARG:NH1	2.79	0.41
6:F:23:ASN:HD21	6:F:28:PRO:C	2.29	0.41
7:I:13:ILE:HG23	7:I:14:PHE:N	2.36	0.41
8:J:14:LEU:HA	8:J:17:ILE:HG13	2.03	0.41
9:K:39:LYS:HD2	9:K:56:LEU:HD13	2.03	0.41
9:K:58:GLU:HB2	9:K:60:LEU:CD2	2.51	0.41
1:A:297:THR:HG23	14:A:820:CLA:HMA3	2.03	0.40
1:A:445:ASN:O	1:A:449:ILE:HG13	2.21	0.40
1:A:493:LEU:HD11	14:A:836:CLA:HAC2	2.02	0.40
16:A:850:BCR:H11C	16:A:850:BCR:H341	1.95	0.40
2:B:4:PHE:CD2	7:I:34:ILE:HG22	2.56	0.40
2:B:235:ASN:OD1	2:B:235:ASN:C	2.63	0.40
2:B:738:LYS:O	2:B:739:PHE:CD2	2.74	0.40
14:B:3024:CLA:HBC2	16:B:3050:BCR:H343	2.02	0.40
3:C:27:MET:HE3	3:C:27:MET:HA	2.02	0.40
6:F:96:GLU:OE2	6:F:96:GLU:HA	2.20	0.40
10:L:111:LEU:HD12	10:L:111:LEU:HA	1.92	0.40
2:B:347:ILE:HD13	14:B:3025:CLA:H43	2.03	0.40
16:B:3046:BCR:H15C	16:B:3046:BCR:H351	1.89	0.40
3:C:23:ASP:OD2	3:C:23:ASP:C	2.65	0.40
4:D:9:LEU:HD22	4:D:50:ARG:HD3	2.03	0.40
6:F:2:VAL:O	6:F:2:VAL:HG13	2.21	0.40
14:I:101:CLA:NB	23:I:201:HOH:O	2.37	0.40
8:J:33:TYR:O	8:J:36:LEU:HD23	2.21	0.40
16:J:104:BCR:H321	16:J:104:BCR:C8	2.51	0.40
1:A:392:SER:HB3	14:A:829:CLA:HBB	2.03	0.40
14:A:803:CLA:HED1	2:B:426:SER:OG	2.22	0.40
2:B:199:PRO:HB2	2:B:206:VAL:HG23	2.04	0.40
2:B:537:THR:HG21	14:B:3026:CLA:HAB	2.04	0.40
16:B:3045:BCR:H24C	16:B:3045:BCR:H371	1.92	0.40
4:D:30:THR:O	4:D:80:TYR:HA	2.21	0.40
1:A:84:PHE:HB3	1:A:169:ALA:HB2	2.03	0.40
1:A:120:ILE:HG23	1:A:121:VAL:N	2.35	0.40
1:A:376:ALA:HB1	1:A:510:SER:OG	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:HIS:HE1	1:A:612:HIS:ND1	2.19	0.40
1:A:565:LEU:HD13	2:B:678:GLN:CG	2.51	0.40
2:B:173:ARG:N	14:B:3014:CLA:HBC2	2.36	0.40
2:B:235:ASN:OD1	2:B:250:GLY:HA2	2.21	0.40
2:B:405:GLN:OE1	2:B:405:GLN:C	2.64	0.40
14:I:101:CLA:H142	10:L:85:LEU:CD1	2.51	0.40
8:J:1:MET:O	8:J:2:LYS:C	2.64	0.40
12:X:27:ALA:O	12:X:31:PHE:HD1	2.05	0.40
1:A:149:ALA:HB2	1:A:381:PRO:CD	2.52	0.40
1:A:291:GLY:HA3	1:A:380:TYR:O	2.22	0.40
1:A:292:LEU:HD12	1:A:379:PRO:HA	2.04	0.40
1:A:410:ALA:O	1:A:414:ILE:HG13	2.22	0.40
2:B:166:TRP:HD1	14:B:3013:CLA:HED1	1.85	0.40
2:B:377:HIS:CD2	2:B:378:HIS:HD1	2.40	0.40
2:B:531:LEU:O	2:B:532:GLY:C	2.63	0.40
2:B:576:ILE:O	2:B:576:ILE:CG1	2.70	0.40
3:C:55:THR:HG21	23:C:207:HOH:O	2.21	0.40
6:F:103:VAL:N	6:F:104:PRO:HD3	2.36	0.40
16:F:203:BCR:H20C	16:F:203:BCR:H361	1.93	0.40
8:J:12:PRO:HB2	16:J:104:BCR:H391	2.03	0.40
8:J:37:LEU:HD23	8:J:37:LEU:O	2.21	0.40
9:K:76:GLY:C	9:K:77:LEU:HD23	2.47	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%)	678 (92%)	58 (8%)	0	100	100
2	B	737/740 (100%)	684 (93%)	52 (7%)	1 (0%)	48	71
3	C	78/80 (98%)	73 (94%)	5 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	136/138 (99%)	123 (90%)	13 (10%)	0	100	100
5	E	67/75 (89%)	55 (82%)	11 (16%)	1 (2%)	8	15
6	F	139/164 (85%)	124 (89%)	15 (11%)	0	100	100
7	I	36/38 (95%)	29 (81%)	7 (19%)	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%)	140 (94%)	9 (6%)	0	100	100
11	M	29/31 (94%)	29 (100%)	0	0	100	100
12	X	27/35 (77%)	26 (96%)	1 (4%)	0	100	100
All	All	2216/2334 (95%)	2031 (92%)	183 (8%)	2 (0%)	48	71

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%)	578 (98%)	11 (2%)	50	70
2	B	597/597 (100%)	582 (98%)	15 (2%)	42	64
3	C	67/67 (100%)	64 (96%)	3 (4%)	24	46
4	D	115/115 (100%)	110 (96%)	5 (4%)	26	47
5	E	59/64 (92%)	56 (95%)	3 (5%)	21	40
6	F	109/128 (85%)	103 (94%)	6 (6%)	19	37
7	I	32/32 (100%)	30 (94%)	2 (6%)	16	30
8	J	36/36 (100%)	35 (97%)	1 (3%)	38	61
9	K	33/61 (54%)	30 (91%)	3 (9%)	9	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	L	117/119 (98%)	112 (96%)	5 (4%)	26	47
11	M	26/26 (100%)	26 (100%)	0	100	100
12	X	23/27 (85%)	23 (100%)	0	100	100
All	All	1803/1875 (96%)	1749 (97%)	54 (3%)	36	60

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR
1	A	63	SER
1	A	115	GLN
1	A	171	LEU
1	A	207	LEU
1	A	281	PHE
1	A	358	ILE
1	A	419	ASP
1	A	460	VAL
1	A	587	CYS
1	A	667	SER
2	B	53	LEU
2	B	141	LEU
2	B	212	LEU
2	B	313	LYS
2	B	314	VAL
2	B	328	THR
2	B	349	SER
2	B	357	SER
2	B	411	LEU
2	B	444	ASP
2	B	446	VAL
2	B	542	LYS
2	B	582	PHE
2	B	618	SER
2	B	650	SER
3	C	16	CYS
3	C	25	LEU
3	C	45	GLU
4	D	3	LEU
4	D	33	SER
4	D	115	VAL
4	D	118	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	119	ILE
5	E	13	GLU
5	E	36	VAL
5	E	65	VAL
6	F	11	SER
6	F	39	SER
6	F	105	LEU
6	F	112	THR
6	F	135	GLU
6	F	137	THR
7	I	17	VAL
7	I	26	VAL
8	J	35	ASP
9	K	23	ASN
9	K	59	LEU
9	K	63	THR
10	L	83	ILE
10	L	106	SER
10	L	113	THR
10	L	134	VAL
10	L	152	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) 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	445	ASN
1	A	542	HIS
1	A	657	GLN
2	B	9	GLN
2	B	13	GLN
2	B	105	GLN
2	B	121	HIS
2	B	204	GLN
2	B	217	HIS
2	B	228	ASN
2	B	319	ASN
2	B	377	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	467	GLN
2	B	591	ASN
2	B	614	GLN
2	B	710	GLN
3	C	37	GLN
4	D	37	GLN
6	F	50	HIS
6	F	134	ASN
8	J	3	HIS
10	L	75	ASN
10	L	102	GLN
10	L	119	GLN
10	L	141	ASN
11	M	7	GLN

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	811	1	49,53,73	1.41	8 (16%)	58,89,113	1.39	6 (10%)
14	CLA	A	805	1,14	63,67,73	1.27	7 (11%)	74,105,113	1.24	5 (6%)
21	LMT	L	201	-	36,36,36	1.08	4 (11%)	47,47,47	1.18	4 (8%)
14	CLA	A	824	1	55,59,73	1.33	5 (9%)	64,96,113	1.31	6 (9%)
14	CLA	B	3032	2	53,57,73	1.34	8 (15%)	61,93,113	1.41	10 (16%)
16	BCR	A	848	-	41,41,41	1.18	3 (7%)	56,56,56	1.29	6 (10%)
14	CLA	B	3012	2	49,53,73	1.42	7 (14%)	58,89,113	1.48	7 (12%)
14	CLA	B	3028	2	69,73,73	1.19	7 (10%)	82,113,113	1.19	5 (6%)
16	BCR	J	103	-	41,41,41	1.17	3 (7%)	56,56,56	1.21	6 (10%)
14	CLA	A	836	1	58,62,73	1.30	7 (12%)	68,99,113	1.32	5 (7%)
14	CLA	B	3035	2	49,53,73	1.42	7 (14%)	58,89,113	1.43	4 (6%)
14	CLA	B	3016	2	49,53,73	1.40	7 (14%)	58,89,113	1.44	5 (8%)
14	CLA	B	3005	2	58,62,73	1.31	5 (8%)	68,99,113	1.41	4 (5%)
14	CLA	A	819	1	58,62,73	1.31	9 (15%)	68,99,113	1.37	9 (13%)
16	BCR	F	203	-	41,41,41	1.16	3 (7%)	56,56,56	1.23	5 (8%)
14	CLA	B	3006	2	69,73,73	1.20	6 (8%)	82,113,113	1.28	5 (6%)
14	CLA	B	3025	2	58,62,73	1.32	6 (10%)	68,99,113	1.38	7 (10%)
14	CLA	A	856	23	69,73,73	1.18	8 (11%)	82,113,113	1.28	6 (7%)
14	CLA	B	3003	2	69,73,73	1.20	8 (11%)	82,113,113	1.34	4 (4%)
16	BCR	A	847	-	41,41,41	1.21	3 (7%)	56,56,56	1.23	6 (10%)
14	CLA	A	815	1	49,53,73	1.40	7 (14%)	58,89,113	1.36	5 (8%)
14	CLA	A	839	1	69,73,73	1.16	7 (10%)	82,113,113	1.37	7 (8%)
14	CLA	B	3022	2	49,53,73	1.41	6 (12%)	58,89,113	1.37	5 (8%)
14	CLA	B	3040	2	51,55,73	1.38	6 (11%)	60,91,113	1.37	4 (6%)
13	CL0	A	801	1	69,73,73	1.19	8 (11%)	82,113,113	1.28	8 (9%)
14	CLA	A	841	1	69,73,73	1.18	5 (7%)	82,113,113	1.31	5 (6%)
14	CLA	I	101	-	69,73,73	1.21	4 (5%)	82,113,113	1.38	6 (7%)
14	CLA	B	3027	2	69,73,73	1.20	5 (7%)	82,113,113	1.20	5 (6%)
14	CLA	L	204	10	69,73,73	1.16	8 (11%)	82,113,113	1.33	5 (6%)
14	CLA	A	842	23	55,59,73	1.32	7 (12%)	64,96,113	1.42	5 (7%)
14	CLA	A	822	23	69,73,73	1.19	6 (8%)	82,113,113	1.19	6 (7%)
14	CLA	A	844	23	69,73,73	1.18	8 (11%)	82,113,113	1.32	7 (8%)
14	CLA	A	834	1	69,73,73	1.21	7 (10%)	82,113,113	1.21	4 (4%)
15	PQN	A	846	-	34,34,34	2.09	7 (20%)	43,45,45	1.30	6 (13%)
14	CLA	B	3018	2	63,67,73	1.23	6 (9%)	74,105,113	1.30	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	3010	2	69,73,73	1.22	7 (10%)	82,113,113	1.38	9 (10%)
22	DGD	L	206	-	67,67,67	0.99	4 (5%)	81,81,81	1.29	8 (9%)
14	CLA	A	809	1	69,73,73	1.17	6 (8%)	82,113,113	1.23	6 (7%)
14	CLA	B	3015	2	69,73,73	1.18	6 (8%)	82,113,113	1.22	4 (4%)
14	CLA	A	838	1	55,59,73	1.36	7 (12%)	64,96,113	1.30	5 (7%)
14	CLA	X	1701	12	49,53,73	1.41	7 (14%)	58,89,113	1.46	5 (8%)
14	CLA	A	827	23	69,73,73	1.17	7 (10%)	82,113,113	1.22	7 (8%)
18	LHG	M	101	-	48,48,48	0.63	1 (2%)	51,54,54	1.19	3 (5%)
16	BCR	A	851	-	41,41,41	1.16	3 (7%)	56,56,56	1.39	5 (8%)
14	CLA	A	837	1	49,53,73	1.42	5 (10%)	58,89,113	1.35	4 (6%)
14	CLA	B	3033	2	69,73,73	1.20	6 (8%)	82,113,113	1.26	5 (6%)
14	CLA	J	102	8	41,45,73	1.51	6 (14%)	50,78,113	1.33	6 (12%)
14	CLA	B	3011	2	69,73,73	1.20	9 (13%)	82,113,113	1.27	7 (8%)
14	CLA	A	833	1	69,73,73	1.18	8 (11%)	82,113,113	1.26	3 (3%)
16	BCR	I	105	-	41,41,41	1.18	3 (7%)	56,56,56	1.44	9 (16%)
14	CLA	B	3014	2	69,73,73	1.22	6 (8%)	82,113,113	1.26	5 (6%)
14	CLA	A	812	1,14	69,73,73	1.20	8 (11%)	82,113,113	1.23	5 (6%)
14	CLA	B	3041	2	69,73,73	1.22	7 (10%)	82,113,113	1.34	5 (6%)
16	BCR	B	3046	-	41,41,41	1.15	3 (7%)	56,56,56	1.30	7 (12%)
16	BCR	B	3050	-	41,41,41	1.23	3 (7%)	56,56,56	1.26	7 (12%)
14	CLA	B	3017	2	59,63,73	1.29	7 (11%)	70,101,113	1.28	5 (7%)
16	BCR	A	850	-	41,41,41	1.13	3 (7%)	56,56,56	1.24	6 (10%)
14	CLA	B	3034	2	62,66,73	1.24	6 (9%)	73,104,113	1.34	7 (9%)
18	LHG	A	853	-	48,48,48	0.62	1 (2%)	51,54,54	1.24	4 (7%)
14	CLA	B	3026	23	50,54,73	1.39	6 (12%)	59,90,113	1.47	6 (10%)
14	CLA	A	831	1	69,73,73	1.19	8 (11%)	82,113,113	1.23	5 (6%)
16	BCR	B	3044	-	41,41,41	1.17	3 (7%)	56,56,56	1.21	6 (10%)
14	CLA	A	830	1	69,73,73	1.20	5 (7%)	82,113,113	1.19	5 (6%)
14	CLA	B	3024	2	49,53,73	1.39	9 (18%)	58,89,113	1.42	6 (10%)
14	CLA	B	3038	2	64,68,73	1.26	6 (9%)	76,107,113	1.23	5 (6%)
14	CLA	B	3030	2	69,73,73	1.19	6 (8%)	82,113,113	1.27	7 (8%)
14	CLA	B	3019	2	64,68,73	1.24	5 (7%)	76,107,113	1.25	6 (7%)
14	CLA	B	3020	23	69,73,73	1.17	9 (13%)	82,113,113	1.28	6 (7%)
14	CLA	A	810	1	69,73,73	1.21	8 (11%)	82,113,113	1.28	6 (7%)
17	LMG	B	3048	-	55,55,55	0.72	0	63,63,63	1.33	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	826	23	69,73,73	1.18	7 (10%)	82,113,113	1.24	6 (7%)
18	LHG	A	854	14	26,26,48	1.00	1 (3%)	29,32,54	1.31	3 (10%)
14	CLA	A	804	1	69,73,73	1.20	7 (10%)	82,113,113	1.15	4 (4%)
19	SF4	C	102	3	0,12,12	-	-	-	-	-
14	CLA	A	817	23	53,57,73	1.35	6 (11%)	61,93,113	1.30	4 (6%)
14	CLA	B	3031	2	49,53,73	1.41	6 (12%)	58,89,113	1.53	6 (10%)
14	CLA	A	821	1	46,50,73	1.42	7 (15%)	54,84,113	1.45	9 (16%)
18	LHG	B	3049	-	22,22,48	1.17	2 (9%)	25,28,54	1.24	1 (4%)
14	CLA	B	3039	2	69,73,73	1.19	6 (8%)	82,113,113	1.25	6 (7%)
14	CLA	A	832	1	54,58,73	1.34	8 (14%)	64,95,113	1.43	8 (12%)
16	BCR	A	849	-	41,41,41	1.13	3 (7%)	56,56,56	1.22	5 (8%)
14	CLA	B	3023	23	59,63,73	1.29	7 (11%)	70,101,113	1.29	4 (5%)
14	CLA	M	102	23	49,53,73	1.49	10 (20%)	58,89,113	1.39	9 (15%)
14	CLA	B	3037	23	49,53,73	1.43	5 (10%)	58,89,113	1.34	4 (6%)
16	BCR	B	3047	-	41,41,41	1.14	3 (7%)	56,56,56	1.29	8 (14%)
14	CLA	A	813	1	58,62,73	1.29	6 (10%)	68,99,113	1.31	5 (7%)
14	CLA	A	823	1	53,57,73	1.35	5 (9%)	61,93,113	1.43	6 (9%)
16	BCR	B	3043	-	41,41,41	1.15	3 (7%)	56,56,56	1.22	6 (10%)
14	CLA	B	3008	2	69,73,73	1.18	6 (8%)	82,113,113	1.32	4 (4%)
14	CLA	A	825	1	63,67,73	1.27	5 (7%)	74,105,113	1.23	5 (6%)
19	SF4	C	101	3	0,12,12	-	-	-	-	-
14	CLA	B	3007	2	69,73,73	1.20	6 (8%)	82,113,113	1.27	4 (4%)
16	BCR	L	207	-	41,41,41	1.17	3 (7%)	56,56,56	1.27	6 (10%)
14	CLA	A	816	1	49,53,73	1.40	5 (10%)	58,89,113	1.51	4 (6%)
14	CLA	A	828	1	69,73,73	1.23	5 (7%)	82,113,113	1.23	6 (7%)
16	BCR	M	103	-	41,41,41	1.19	3 (7%)	56,56,56	1.13	3 (5%)
14	CLA	B	3004	-	69,73,73	1.24	9 (13%)	82,113,113	1.29	8 (9%)
14	CLA	A	840	1	51,55,73	1.42	6 (11%)	60,91,113	1.39	6 (10%)
15	PQN	B	3042	-	34,34,34	1.98	7 (20%)	43,45,45	1.23	5 (11%)
14	CLA	B	3013	2	49,53,73	1.42	5 (10%)	58,89,113	1.40	5 (8%)
17	LMG	A	855	-	30,30,55	1.16	2 (6%)	37,37,63	1.26	4 (10%)
19	SF4	B	3001	1,2	0,12,12	-	-	-	-	-
14	CLA	A	835	1	69,73,73	1.15	6 (8%)	82,113,113	1.23	7 (8%)
17	LMG	A	852	-	48,48,55	0.84	1 (2%)	56,56,63	1.26	5 (8%)
16	BCR	K	102	-	41,41,41	1.11	3 (7%)	56,56,56	1.41	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	3029	2	69,73,73	1.18	7 (10%)	82,113,113	1.28	5 (6%)
14	CLA	A	806	1	69,73,73	1.18	6 (8%)	82,113,113	1.29	6 (7%)
14	CLA	A	829	1	69,73,73	1.18	5 (7%)	82,113,113	1.17	4 (4%)
14	CLA	A	807	1	69,73,73	1.22	6 (8%)	82,113,113	1.18	4 (4%)
16	BCR	J	104	-	41,41,41	1.19	3 (7%)	56,56,56	1.26	6 (10%)
14	CLA	A	808	1	55,59,73	1.36	6 (10%)	64,96,113	1.35	6 (9%)
17	LMG	I	104	-	40,40,55	1.14	4 (10%)	48,48,63	1.16	3 (6%)
14	CLA	F	202	23	49,53,73	1.46	7 (14%)	58,89,113	1.29	5 (8%)
14	CLA	K	101	9	45,49,73	1.42	6 (13%)	54,83,113	1.35	4 (7%)
16	BCR	I	103	-	41,41,41	1.20	3 (7%)	56,56,56	1.40	7 (12%)
14	CLA	A	818	1	58,62,73	1.31	6 (10%)	68,99,113	1.32	4 (5%)
14	CLA	A	814	1	64,68,73	1.24	7 (10%)	76,107,113	1.27	5 (6%)
14	CLA	A	845	18	56,60,73	1.32	5 (8%)	65,97,113	1.47	6 (9%)
14	CLA	B	3021	2	51,55,73	1.36	6 (11%)	60,91,113	1.39	4 (6%)
14	CLA	K	103	-	49,53,73	1.40	6 (12%)	58,89,113	1.37	5 (8%)
14	CLA	A	802	23	69,73,73	1.18	6 (8%)	82,113,113	1.24	6 (7%)
16	BCR	B	3045	-	41,41,41	1.14	3 (7%)	56,56,56	1.23	8 (14%)
16	BCR	I	102	-	41,41,41	1.09	3 (7%)	56,56,56	1.36	8 (14%)
16	BCR	J	105	-	41,41,41	1.14	3 (7%)	56,56,56	1.31	8 (14%)
14	CLA	L	203	10	69,73,73	1.18	5 (7%)	82,113,113	1.47	7 (8%)
16	BCR	F	201	-	41,41,41	1.21	3 (7%)	56,56,56	1.22	5 (8%)
14	CLA	A	803	-	69,73,73	1.20	7 (10%)	82,113,113	1.24	6 (7%)
14	CLA	B	3036	23	49,53,73	1.43	6 (12%)	58,89,113	1.41	4 (6%)
14	CLA	A	820	1	69,73,73	1.17	6 (8%)	82,113,113	1.40	8 (9%)
14	CLA	B	3009	2	69,73,73	1.18	5 (7%)	82,113,113	1.31	5 (6%)
14	CLA	A	843	1	69,73,73	1.20	7 (10%)	82,113,113	1.24	5 (6%)
14	CLA	J	101	8	49,53,73	1.44	5 (10%)	58,89,113	1.33	4 (6%)
14	CLA	L	205	23	69,73,73	1.17	8 (11%)	82,113,113	1.36	8 (9%)

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	811	1	-	8/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	805	1,14	-	9/32/108/115	-
21	LMT	L	201	-	-	11/21/61/61	0/2/2/2
14	CLA	A	824	1	-	2/23/99/115	-
14	CLA	B	3032	2	-	7/20/96/115	-
16	BCR	A	848	-	-	7/29/63/63	0/2/2/2
14	CLA	B	3012	2	-	2/15/91/115	-
14	CLA	B	3028	2	-	12/39/115/115	-
16	BCR	J	103	-	-	12/29/63/63	0/2/2/2
14	CLA	A	836	1	-	7/26/102/115	-
14	CLA	B	3035	2	-	6/15/91/115	-
14	CLA	B	3016	2	-	3/15/91/115	-
14	CLA	B	3005	2	-	5/26/102/115	-
14	CLA	A	819	1	-	10/26/102/115	-
16	BCR	F	203	-	-	12/29/63/63	0/2/2/2
14	CLA	B	3006	2	-	14/39/115/115	-
14	CLA	B	3025	2	-	9/26/102/115	-
14	CLA	A	856	23	-	15/39/115/115	-
14	CLA	B	3003	2	-	14/39/115/115	-
16	BCR	A	847	-	-	13/29/63/63	0/2/2/2
14	CLA	A	815	1	-	2/15/91/115	-
14	CLA	A	839	1	-	8/39/115/115	-
14	CLA	B	3022	2	-	6/15/91/115	-
14	CLA	B	3040	2	-	5/18/94/115	-
13	CL0	A	801	1	-	10/39/115/115	-
14	CLA	A	841	1	-	7/39/115/115	-
14	CLA	I	101	-	-	9/39/115/115	-
14	CLA	B	3027	2	-	8/39/115/115	-
14	CLA	L	204	10	-	5/39/115/115	-
14	CLA	A	842	23	-	4/23/99/115	-
14	CLA	A	822	23	-	14/39/115/115	-
14	CLA	A	844	23	-	10/39/115/115	-
14	CLA	A	834	1	-	9/39/115/115	-
15	PQN	A	846	-	-	10/23/43/43	0/2/2/2
14	CLA	B	3018	2	-	11/32/108/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	3010	2	-	16/39/115/115	-
22	DGD	L	206	-	-	19/55/95/95	0/2/2/2
14	CLA	A	809	1	-	15/39/115/115	-
14	CLA	B	3015	2	-	13/39/115/115	-
14	CLA	A	838	1	-	6/23/99/115	-
14	CLA	X	1701	12	-	4/15/91/115	-
14	CLA	A	827	23	-	10/39/115/115	-
18	LHG	M	101	-	-	26/53/53/53	-
16	BCR	A	851	-	-	17/29/63/63	0/2/2/2
14	CLA	A	837	1	-	6/15/91/115	-
14	CLA	B	3033	2	-	17/39/115/115	-
14	CLA	J	102	8	-	0/4/76/115	-
14	CLA	B	3011	2	-	13/39/115/115	-
14	CLA	A	833	1	-	6/39/115/115	-
16	BCR	I	105	-	-	17/29/63/63	0/2/2/2
14	CLA	B	3014	2	-	12/39/115/115	-
14	CLA	A	812	1,14	-	9/39/115/115	-
14	CLA	B	3041	2	-	7/39/115/115	-
16	BCR	B	3046	-	-	14/29/63/63	0/2/2/2
16	BCR	B	3050	-	-	10/29/63/63	0/2/2/2
14	CLA	B	3017	2	-	5/27/103/115	-
16	BCR	A	850	-	-	9/29/63/63	0/2/2/2
14	CLA	B	3034	2	-	9/31/107/115	-
18	LHG	A	853	-	-	23/53/53/53	-
14	CLA	B	3026	23	-	2/17/93/115	-
14	CLA	A	831	1	-	8/39/115/115	-
16	BCR	B	3044	-	-	11/29/63/63	0/2/2/2
14	CLA	A	830	1	-	14/39/115/115	-
14	CLA	B	3024	2	-	4/15/91/115	-
14	CLA	B	3038	2	-	9/33/109/115	-
14	CLA	B	3030	2	-	13/39/115/115	-
14	CLA	B	3019	2	-	10/33/109/115	-
14	CLA	B	3020	23	-	13/39/115/115	-
14	CLA	A	810	1	-	8/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	LMG	B	3048	-	-	24/50/70/70	0/1/1/1
14	CLA	A	826	23	-	12/39/115/115	-
18	LHG	A	854	14	-	10/31/31/53	-
14	CLA	A	804	1	-	9/39/115/115	-
19	SF4	C	102	3	-	-	0/6/5/5
14	CLA	A	817	23	-	7/20/96/115	-
14	CLA	B	3031	2	-	8/15/91/115	-
14	CLA	A	821	1	-	4/10/86/115	-
18	LHG	B	3049	-	-	11/26/26/53	-
14	CLA	B	3039	2	-	10/39/115/115	-
14	CLA	A	832	1	-	6/21/97/115	-
16	BCR	A	849	-	-	7/29/63/63	0/2/2/2
14	CLA	B	3023	23	-	6/27/103/115	-
14	CLA	M	102	23	-	9/15/91/115	-
14	CLA	B	3037	23	-	4/15/91/115	-
16	BCR	B	3047	-	-	2/29/63/63	0/2/2/2
14	CLA	A	813	1	-	5/26/102/115	-
14	CLA	A	823	1	-	11/20/96/115	-
16	BCR	B	3043	-	-	7/29/63/63	0/2/2/2
14	CLA	B	3008	2	-	9/39/115/115	-
14	CLA	A	825	1	-	11/32/108/115	-
19	SF4	C	101	3	-	-	0/6/5/5
14	CLA	B	3007	2	-	12/39/115/115	-
16	BCR	L	207	-	-	9/29/63/63	0/2/2/2
14	CLA	A	816	1	-	4/15/91/115	-
14	CLA	A	828	1	-	6/39/115/115	-
16	BCR	M	103	-	-	8/29/63/63	0/2/2/2
14	CLA	B	3004	-	-	8/39/115/115	-
14	CLA	A	840	1	-	4/18/94/115	-
15	PQN	B	3042	-	-	8/23/43/43	0/2/2/2
14	CLA	B	3013	2	-	5/15/91/115	-
17	LMG	A	855	-	-	12/23/43/70	0/1/1/1
19	SF4	B	3001	1,2	-	-	0/6/5/5
14	CLA	A	835	1	-	9/39/115/115	-
17	LMG	A	852	-	-	24/43/63/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	K	102	-	-	9/29/63/63	0/2/2/2
14	CLA	B	3029	2	-	16/39/115/115	-
14	CLA	A	806	1	-	17/39/115/115	-
14	CLA	A	829	1	-	9/39/115/115	-
14	CLA	A	807	1	-	13/39/115/115	-
16	BCR	J	104	-	-	15/29/63/63	0/2/2/2
14	CLA	A	808	1	-	12/23/99/115	-
17	LMG	I	104	-	-	17/35/55/70	0/1/1/1
14	CLA	F	202	23	-	6/15/91/115	-
14	CLA	K	101	9	-	1/9/81/115	-
16	BCR	I	103	-	-	5/29/63/63	0/2/2/2
14	CLA	A	818	1	-	3/26/102/115	-
14	CLA	A	814	1	-	4/33/109/115	-
14	CLA	A	845	18	-	7/24/100/115	-
14	CLA	B	3021	2	-	11/18/94/115	-
14	CLA	K	103	-	-	8/15/91/115	-
14	CLA	A	802	23	-	10/39/115/115	-
16	BCR	B	3045	-	-	10/29/63/63	0/2/2/2
16	BCR	I	102	-	-	5/29/63/63	0/2/2/2
16	BCR	J	105	-	-	11/29/63/63	0/2/2/2
14	CLA	L	203	10	-	13/39/115/115	-
16	BCR	F	201	-	-	9/29/63/63	0/2/2/2
14	CLA	A	803	-	-	5/39/115/115	-
14	CLA	B	3036	23	-	6/15/91/115	-
14	CLA	A	820	1	-	18/39/115/115	-
14	CLA	B	3009	2	-	7/39/115/115	-
14	CLA	A	843	1	-	6/39/115/115	-
14	CLA	J	101	8	-	6/15/91/115	-
14	CLA	L	205	23	-	8/39/115/115	-

All (726) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	3042	PQN	O1-C1	5.97	1.35	1.23
15	A	846	PQN	O4-C4	5.93	1.35	1.23
15	B	3042	PQN	O4-C4	5.92	1.35	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	846	PQN	O1-C1	5.83	1.35	1.23
15	A	846	PQN	C10-C1	-4.89	1.38	1.48
14	A	840	CLA	C1D-ND	4.06	1.43	1.37
16	A	847	BCR	C1-C6	-4.05	1.48	1.53
16	M	103	BCR	C1-C6	-4.00	1.48	1.53
16	J	103	BCR	C1-C6	-4.00	1.48	1.53
16	B	3050	BCR	C30-C25	-3.98	1.48	1.53
16	I	103	BCR	C1-C6	-3.98	1.48	1.53
14	I	101	CLA	C1D-ND	3.97	1.43	1.37
16	L	207	BCR	C1-C6	-3.95	1.48	1.53
16	A	851	BCR	C1-C6	-3.87	1.48	1.53
16	J	104	BCR	C1-C6	-3.86	1.48	1.53
14	B	3007	CLA	C1D-ND	3.84	1.42	1.37
14	B	3006	CLA	C1D-ND	3.84	1.42	1.37
14	A	823	CLA	C1D-ND	3.83	1.42	1.37
14	A	828	CLA	C1D-ND	3.83	1.42	1.37
16	B	3044	BCR	C1-C6	-3.82	1.48	1.53
14	B	3014	CLA	C1D-ND	3.81	1.42	1.37
14	A	825	CLA	C1D-ND	3.81	1.42	1.37
16	B	3050	BCR	C1-C6	-3.81	1.48	1.53
16	I	105	BCR	C1-C6	-3.80	1.48	1.53
14	B	3018	CLA	C1D-ND	3.79	1.42	1.37
14	B	3026	CLA	C1D-ND	3.79	1.42	1.37
17	A	855	LMG	O7-C8	-3.78	1.40	1.47
14	A	824	CLA	C1D-ND	3.77	1.42	1.37
14	A	807	CLA	C1D-ND	3.76	1.42	1.37
14	B	3040	CLA	C1D-ND	3.76	1.42	1.37
14	B	3036	CLA	C1D-ND	3.75	1.42	1.37
14	B	3012	CLA	C1D-ND	3.75	1.42	1.37
14	A	816	CLA	C1D-ND	3.75	1.42	1.37
14	B	3021	CLA	C1D-ND	3.74	1.42	1.37
14	B	3027	CLA	C1D-ND	3.74	1.42	1.37
14	A	832	CLA	C1D-ND	3.73	1.42	1.37
14	A	810	CLA	C1D-ND	3.73	1.42	1.37
14	F	202	CLA	C1D-ND	3.72	1.42	1.37
14	J	101	CLA	C1D-ND	3.71	1.42	1.37
16	F	203	BCR	C1-C6	-3.71	1.49	1.53
16	A	848	BCR	C1-C6	-3.70	1.49	1.53
16	F	201	BCR	C1-C6	-3.70	1.49	1.53
14	B	3031	CLA	C1D-ND	3.70	1.42	1.37
14	B	3028	CLA	C1D-ND	3.69	1.42	1.37
14	A	834	CLA	C4B-NB	3.68	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	818	CLA	C1D-ND	3.68	1.42	1.37
14	B	3030	CLA	C1D-ND	3.68	1.42	1.37
16	A	849	BCR	C1-C6	-3.68	1.49	1.53
14	A	829	CLA	C1D-ND	3.68	1.42	1.37
14	B	3035	CLA	C1D-ND	3.67	1.42	1.37
14	A	819	CLA	C1D-ND	3.67	1.42	1.37
14	B	3016	CLA	C1D-ND	3.67	1.42	1.37
14	A	845	CLA	C1D-ND	3.66	1.42	1.37
14	B	3033	CLA	C1D-ND	3.65	1.42	1.37
14	A	806	CLA	C1D-ND	3.65	1.42	1.37
14	A	812	CLA	C1D-ND	3.64	1.42	1.37
14	B	3037	CLA	C4B-NB	3.63	1.42	1.37
14	A	820	CLA	C1D-ND	3.63	1.42	1.37
14	A	802	CLA	C1D-ND	3.62	1.42	1.37
14	B	3038	CLA	C1D-ND	3.62	1.42	1.37
16	B	3047	BCR	C1-C6	-3.61	1.49	1.53
14	A	805	CLA	C4B-NB	3.61	1.42	1.37
14	A	837	CLA	C1D-ND	3.61	1.42	1.37
15	A	846	PQN	C5-C4	-3.61	1.41	1.48
14	B	3025	CLA	C1D-ND	3.61	1.42	1.37
14	A	836	CLA	C1D-ND	3.60	1.42	1.37
14	B	3030	CLA	C4B-NB	3.60	1.42	1.37
14	A	842	CLA	C1D-ND	3.60	1.42	1.37
14	A	843	CLA	C1D-ND	3.60	1.42	1.37
16	B	3043	BCR	C1-C6	-3.60	1.49	1.53
16	F	201	BCR	C30-C25	-3.59	1.49	1.53
14	A	841	CLA	C1D-ND	3.58	1.42	1.37
14	A	839	CLA	C1D-ND	3.58	1.42	1.37
14	A	808	CLA	C1D-ND	3.57	1.42	1.37
16	B	3045	BCR	C1-C6	-3.57	1.49	1.53
14	K	103	CLA	C1D-ND	3.56	1.42	1.37
14	A	822	CLA	C1D-ND	3.56	1.42	1.37
14	B	3039	CLA	C1D-ND	3.56	1.42	1.37
14	B	3013	CLA	C4B-NB	3.55	1.42	1.37
14	B	3017	CLA	C1D-ND	3.55	1.42	1.37
14	B	3003	CLA	C1D-ND	3.55	1.42	1.37
14	B	3022	CLA	C1D-ND	3.55	1.42	1.37
14	B	3013	CLA	C1D-ND	3.54	1.42	1.37
14	B	3015	CLA	C1D-ND	3.54	1.42	1.37
14	A	804	CLA	C1D-ND	3.53	1.42	1.37
14	B	3024	CLA	C1D-ND	3.53	1.42	1.37
16	A	848	BCR	C30-C25	-3.51	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3037	CLA	C1D-ND	3.51	1.42	1.37
14	J	102	CLA	C1D-ND	3.51	1.42	1.37
14	B	3005	CLA	C1D-ND	3.51	1.42	1.37
14	A	831	CLA	C1D-ND	3.50	1.42	1.37
14	A	808	CLA	C4B-NB	3.50	1.42	1.37
14	A	838	CLA	C1D-ND	3.50	1.42	1.37
14	A	840	CLA	C4B-NB	3.50	1.42	1.37
14	A	830	CLA	C1D-ND	3.48	1.42	1.37
14	A	814	CLA	C1D-ND	3.47	1.42	1.37
14	B	3040	CLA	C4B-NB	3.46	1.42	1.37
14	L	203	CLA	C1D-ND	3.46	1.42	1.37
14	X	1701	CLA	C1D-ND	3.46	1.42	1.37
14	A	828	CLA	C4B-NB	3.46	1.42	1.37
14	B	3009	CLA	C1D-ND	3.46	1.42	1.37
14	B	3034	CLA	C1D-ND	3.46	1.42	1.37
14	B	3029	CLA	C1D-ND	3.45	1.42	1.37
14	A	813	CLA	C1D-ND	3.45	1.42	1.37
14	B	3008	CLA	C1D-ND	3.45	1.42	1.37
14	I	101	CLA	C1B-C2B	3.45	1.51	1.43
14	A	804	CLA	C4B-NB	3.45	1.42	1.37
14	A	817	CLA	C4B-NB	3.45	1.42	1.37
14	B	3031	CLA	C4B-NB	3.44	1.42	1.37
14	A	826	CLA	C1D-ND	3.44	1.42	1.37
14	A	803	CLA	C4B-NB	3.44	1.42	1.37
14	B	3019	CLA	C1D-ND	3.44	1.42	1.37
15	B	3042	PQN	C5-C4	-3.43	1.41	1.48
14	B	3011	CLA	C1D-ND	3.43	1.42	1.37
14	F	202	CLA	C4B-NB	3.42	1.42	1.37
14	A	833	CLA	C1D-ND	3.42	1.42	1.37
14	A	821	CLA	C1D-ND	3.41	1.42	1.37
14	L	205	CLA	C1D-ND	3.39	1.42	1.37
14	A	815	CLA	C1D-ND	3.39	1.42	1.37
14	B	3032	CLA	C1D-ND	3.39	1.42	1.37
17	I	104	LMG	C7-C8	3.39	1.61	1.50
14	A	837	CLA	C4B-NB	3.38	1.42	1.37
14	A	805	CLA	C1D-ND	3.37	1.42	1.37
14	A	817	CLA	C1D-ND	3.37	1.42	1.37
14	A	830	CLA	C4B-NB	3.35	1.42	1.37
16	J	104	BCR	C30-C25	-3.34	1.49	1.53
14	A	807	CLA	C4B-NB	3.34	1.42	1.37
14	B	3020	CLA	C1D-ND	3.33	1.42	1.37
14	B	3023	CLA	C1D-ND	3.33	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	102	BCR	C1-C6	-3.33	1.49	1.53
14	A	844	CLA	C4B-NB	3.33	1.42	1.37
14	B	3003	CLA	C4B-NB	3.33	1.42	1.37
14	X	1701	CLA	C4B-NB	3.32	1.42	1.37
16	J	105	BCR	C1-C6	-3.32	1.49	1.53
16	M	103	BCR	C30-C25	-3.31	1.49	1.53
14	J	102	CLA	C4B-NB	3.31	1.42	1.37
16	J	105	BCR	C30-C25	-3.31	1.49	1.53
14	B	3036	CLA	C4B-NB	3.30	1.42	1.37
14	A	838	CLA	C4B-NB	3.30	1.42	1.37
14	K	101	CLA	C1D-ND	3.30	1.42	1.37
14	J	101	CLA	C4B-NB	3.30	1.42	1.37
14	A	829	CLA	C4B-NB	3.30	1.42	1.37
14	A	809	CLA	C1D-ND	3.30	1.42	1.37
14	A	835	CLA	C1D-ND	3.30	1.42	1.37
14	B	3027	CLA	C4B-NB	3.30	1.42	1.37
14	B	3041	CLA	C4B-NB	3.30	1.42	1.37
14	B	3038	CLA	C4B-NB	3.29	1.42	1.37
14	B	3017	CLA	C4B-NB	3.29	1.42	1.37
14	B	3019	CLA	C4B-NB	3.29	1.42	1.37
14	A	827	CLA	C1D-ND	3.29	1.42	1.37
14	B	3039	CLA	C4B-NB	3.28	1.42	1.37
14	A	803	CLA	C1D-ND	3.27	1.42	1.37
14	A	843	CLA	C4B-NB	3.27	1.42	1.37
14	A	844	CLA	C1D-ND	3.27	1.42	1.37
14	A	811	CLA	C1D-ND	3.27	1.42	1.37
14	A	823	CLA	C4B-NB	3.27	1.42	1.37
14	A	813	CLA	C4B-NB	3.26	1.42	1.37
15	A	846	PQN	C3-C2	3.25	1.41	1.35
14	A	834	CLA	C1D-ND	3.25	1.42	1.37
16	B	3046	BCR	C1-C6	-3.24	1.49	1.53
16	B	3046	BCR	C30-C25	-3.24	1.49	1.53
14	B	3041	CLA	C1D-ND	3.24	1.42	1.37
14	A	836	CLA	C4B-NB	3.23	1.42	1.37
15	B	3042	PQN	C10-C1	-3.23	1.41	1.48
14	B	3005	CLA	C1B-C2B	3.23	1.50	1.43
16	A	850	BCR	C1-C6	-3.23	1.49	1.53
14	B	3029	CLA	C4B-NB	3.23	1.42	1.37
14	B	3009	CLA	C4B-NB	3.22	1.42	1.37
16	A	847	BCR	C30-C25	-3.22	1.49	1.53
14	B	3026	CLA	C4B-NB	3.22	1.42	1.37
14	B	3021	CLA	C4B-NB	3.21	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	L	203	CLA	C1B-C2B	3.20	1.50	1.43
14	L	204	CLA	C4B-NB	3.20	1.42	1.37
14	A	812	CLA	C4B-NB	3.20	1.42	1.37
14	B	3022	CLA	C4B-NB	3.20	1.42	1.37
16	F	203	BCR	C30-C25	-3.20	1.49	1.53
13	A	801	CL0	C1D-ND	3.19	1.42	1.37
14	A	818	CLA	C4B-NB	3.19	1.42	1.37
14	A	824	CLA	C4B-NB	3.18	1.42	1.37
13	A	801	CL0	C4B-NB	3.17	1.42	1.37
14	A	809	CLA	C4B-NB	3.17	1.42	1.37
16	I	105	BCR	C30-C25	-3.17	1.49	1.53
14	A	841	CLA	C1B-C2B	3.17	1.50	1.43
14	B	3004	CLA	C1D-ND	3.16	1.42	1.37
14	B	3025	CLA	C4B-NB	3.16	1.42	1.37
14	B	3033	CLA	C4B-NB	3.16	1.42	1.37
14	M	102	CLA	C4B-NB	3.15	1.42	1.37
14	B	3033	CLA	C1B-C2B	3.15	1.50	1.43
14	A	806	CLA	C4B-NB	3.15	1.42	1.37
14	B	3005	CLA	C4B-NB	3.15	1.42	1.37
14	B	3006	CLA	C4B-NB	3.15	1.42	1.37
14	J	102	CLA	C1B-C2B	3.14	1.50	1.43
16	I	103	BCR	C30-C25	-3.14	1.49	1.53
16	A	850	BCR	C30-C25	-3.14	1.49	1.53
14	B	3004	CLA	C4B-NB	3.14	1.42	1.37
16	L	207	BCR	C30-C25	-3.13	1.49	1.53
14	A	826	CLA	C4B-NB	3.13	1.42	1.37
14	A	825	CLA	C4B-NB	3.13	1.42	1.37
14	A	856	CLA	C4B-NB	3.13	1.42	1.37
14	B	3035	CLA	C4B-NB	3.13	1.42	1.37
14	A	815	CLA	C4B-NB	3.12	1.42	1.37
14	A	841	CLA	C4B-NB	3.12	1.42	1.37
14	A	856	CLA	C1D-ND	3.11	1.41	1.37
14	B	3012	CLA	C4B-NB	3.09	1.41	1.37
15	B	3042	PQN	C3-C2	3.09	1.40	1.35
14	A	816	CLA	C4B-NB	3.09	1.41	1.37
14	B	3032	CLA	C4B-NB	3.09	1.41	1.37
14	B	3009	CLA	C1B-C2B	3.09	1.50	1.43
14	A	840	CLA	C1B-C2B	3.08	1.50	1.43
14	B	3027	CLA	C1B-C2B	3.08	1.50	1.43
14	A	821	CLA	C4B-NB	3.08	1.41	1.37
14	A	820	CLA	C4B-NB	3.08	1.41	1.37
14	B	3006	CLA	C1B-C2B	3.07	1.50	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	811	CLA	C4B-NB	3.07	1.41	1.37
16	I	102	BCR	C30-C25	-3.07	1.49	1.53
16	J	103	BCR	C30-C25	-3.06	1.49	1.53
14	B	3016	CLA	C4B-NB	3.06	1.41	1.37
14	A	810	CLA	C4B-NB	3.06	1.41	1.37
14	A	845	CLA	C4B-NB	3.05	1.41	1.37
14	A	814	CLA	C4B-NB	3.05	1.41	1.37
14	A	805	CLA	C1B-C2B	3.05	1.50	1.43
14	M	102	CLA	C1B-C2B	3.05	1.50	1.43
14	A	812	CLA	C1B-C2B	3.04	1.50	1.43
14	K	101	CLA	C4B-NB	3.04	1.41	1.37
14	A	831	CLA	C4B-NB	3.04	1.41	1.37
14	B	3007	CLA	C1B-C2B	3.04	1.50	1.43
14	B	3041	CLA	C1B-C2B	3.03	1.50	1.43
14	B	3007	CLA	C4B-NB	3.03	1.41	1.37
14	A	832	CLA	C4B-NB	3.03	1.41	1.37
14	B	3034	CLA	C4B-NB	3.03	1.41	1.37
16	B	3044	BCR	C30-C25	-3.02	1.49	1.53
14	B	3018	CLA	C4B-NB	3.01	1.41	1.37
14	B	3028	CLA	C1B-C2B	3.01	1.50	1.43
18	B	3049	LHG	P-O6	3.01	1.71	1.59
14	M	102	CLA	C1D-ND	3.00	1.41	1.37
14	A	819	CLA	C4B-NB	3.00	1.41	1.37
14	A	842	CLA	C4B-NB	2.99	1.41	1.37
14	B	3015	CLA	C1B-C2B	2.99	1.50	1.43
14	B	3020	CLA	C4B-NB	2.99	1.41	1.37
16	I	102	BCR	C1-C6	-2.99	1.50	1.53
14	A	839	CLA	C4B-NB	2.99	1.41	1.37
14	A	816	CLA	C1B-C2B	2.98	1.50	1.43
14	B	3038	CLA	C1B-C2B	2.98	1.50	1.43
14	B	3014	CLA	C4B-NB	2.98	1.41	1.37
14	L	204	CLA	C1B-C2B	2.97	1.50	1.43
14	A	802	CLA	C4B-NB	2.97	1.41	1.37
14	B	3008	CLA	C1B-C2B	2.97	1.50	1.43
14	B	3023	CLA	C4B-NB	2.97	1.41	1.37
14	B	3010	CLA	C4B-NB	2.96	1.41	1.37
14	A	808	CLA	C1B-C2B	2.96	1.50	1.43
14	B	3035	CLA	C1B-C2B	2.95	1.50	1.43
14	A	834	CLA	C1B-C2B	2.95	1.50	1.43
14	B	3017	CLA	C1B-C2B	2.95	1.50	1.43
16	B	3043	BCR	C30-C25	-2.95	1.50	1.53
16	B	3045	BCR	C30-C25	-2.94	1.50	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	830	CLA	C1B-C2B	2.94	1.50	1.43
14	L	205	CLA	C4B-NB	2.94	1.41	1.37
14	B	3015	CLA	C4B-NB	2.94	1.41	1.37
14	A	827	CLA	C4B-NB	2.94	1.41	1.37
14	K	103	CLA	C4B-NB	2.94	1.41	1.37
14	B	3024	CLA	C4B-NB	2.94	1.41	1.37
14	A	835	CLA	C1B-C2B	2.93	1.50	1.43
14	B	3022	CLA	C1B-C2B	2.93	1.50	1.43
14	I	101	CLA	C4B-NB	2.93	1.41	1.37
14	A	811	CLA	C1B-C2B	2.93	1.50	1.43
15	A	846	PQN	C3-C4	-2.93	1.39	1.47
14	A	829	CLA	C1B-C2B	2.93	1.50	1.43
14	A	833	CLA	C1B-C2B	2.93	1.50	1.43
18	A	854	LHG	P-O6	2.93	1.70	1.59
14	B	3016	CLA	C1B-C2B	2.92	1.50	1.43
15	B	3042	PQN	C3-C4	-2.92	1.39	1.47
14	B	3011	CLA	C4B-NB	2.91	1.41	1.37
15	A	846	PQN	C2-C1	-2.91	1.40	1.47
14	A	818	CLA	C1B-C2B	2.90	1.49	1.43
14	A	828	CLA	C1B-C2B	2.90	1.49	1.43
14	A	822	CLA	C4B-NB	2.90	1.41	1.37
14	A	845	CLA	C1B-C2B	2.89	1.49	1.43
14	B	3029	CLA	C1B-C2B	2.89	1.49	1.43
14	A	832	CLA	C1B-C2B	2.89	1.49	1.43
14	A	833	CLA	C4B-NB	2.89	1.41	1.37
14	B	3003	CLA	C1B-C2B	2.89	1.49	1.43
14	J	101	CLA	C1B-C2B	2.88	1.49	1.43
14	A	842	CLA	C1B-C2B	2.87	1.49	1.43
14	B	3014	CLA	C1B-C2B	2.87	1.49	1.43
14	B	3028	CLA	C4B-NB	2.87	1.41	1.37
14	A	813	CLA	C1B-C2B	2.87	1.49	1.43
14	A	806	CLA	C1B-C2B	2.87	1.49	1.43
14	B	3034	CLA	C1B-C2B	2.86	1.49	1.43
14	B	3031	CLA	C1B-C2B	2.86	1.49	1.43
14	B	3026	CLA	C1B-C2B	2.86	1.49	1.43
14	A	824	CLA	C1B-C2B	2.85	1.49	1.43
14	A	809	CLA	C1B-C2B	2.85	1.49	1.43
14	B	3019	CLA	C1B-C2B	2.85	1.49	1.43
14	A	826	CLA	C1B-C2B	2.84	1.49	1.43
14	A	815	CLA	C1B-C2B	2.83	1.49	1.43
14	B	3010	CLA	C1D-ND	2.82	1.41	1.37
14	A	814	CLA	C1B-C2B	2.82	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3024	CLA	C1B-C2B	2.82	1.49	1.43
14	A	817	CLA	C1B-C2B	2.81	1.49	1.43
13	A	801	CL0	C1B-C2B	2.81	1.49	1.43
14	A	839	CLA	C1B-C2B	2.81	1.49	1.43
14	X	1701	CLA	C1B-C2B	2.80	1.49	1.43
14	A	810	CLA	C1B-C2B	2.79	1.49	1.43
16	K	102	BCR	C30-C25	-2.79	1.50	1.53
14	B	3010	CLA	CMB-C2B	-2.79	1.45	1.50
14	B	3020	CLA	C1B-C2B	2.79	1.49	1.43
14	A	828	CLA	CHC-C1C	2.79	1.44	1.38
14	A	823	CLA	C1B-C2B	2.79	1.49	1.43
14	B	3008	CLA	C4B-NB	2.78	1.41	1.37
14	A	843	CLA	C1B-C2B	2.78	1.49	1.43
14	A	809	CLA	CHC-C1C	2.78	1.44	1.38
14	A	856	CLA	C1B-C2B	2.77	1.49	1.43
14	B	3039	CLA	C1B-C2B	2.77	1.49	1.43
14	A	825	CLA	C1B-C2B	2.77	1.49	1.43
14	B	3023	CLA	C1B-C2B	2.76	1.49	1.43
16	A	849	BCR	C30-C25	-2.75	1.50	1.53
14	B	3036	CLA	C1B-C2B	2.75	1.49	1.43
14	B	3004	CLA	CHC-C1C	2.75	1.44	1.38
14	B	3011	CLA	C1B-C2B	2.74	1.49	1.43
14	L	203	CLA	C4B-NB	2.74	1.41	1.37
14	A	837	CLA	C1B-C2B	2.73	1.49	1.43
14	B	3030	CLA	C1B-C2B	2.72	1.49	1.43
14	B	3037	CLA	C3B-C4B	2.72	1.50	1.42
14	K	101	CLA	C1B-C2B	2.72	1.49	1.43
14	A	836	CLA	C1B-C2B	2.70	1.49	1.43
15	B	3042	PQN	C2-C1	-2.70	1.41	1.47
14	A	825	CLA	C3B-C4B	2.70	1.50	1.42
14	B	3040	CLA	C1B-C2B	2.69	1.49	1.43
14	B	3010	CLA	MG-NB	-2.68	2.00	2.05
14	A	827	CLA	C1B-C2B	2.68	1.49	1.43
14	B	3013	CLA	C1B-C2B	2.68	1.49	1.43
14	A	803	CLA	CHC-C1C	2.68	1.43	1.38
14	B	3025	CLA	C1B-C2B	2.67	1.49	1.43
14	B	3013	CLA	C3B-C4B	2.67	1.50	1.42
14	A	804	CLA	C3B-C4B	2.67	1.50	1.42
14	B	3011	CLA	C3B-C4B	2.67	1.50	1.42
14	A	804	CLA	C1B-C2B	2.67	1.49	1.43
14	A	820	CLA	CMC-C2C	-2.66	1.45	1.50
14	A	807	CLA	C1B-C2B	2.66	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	835	CLA	C4B-NB	2.66	1.41	1.37
14	K	101	CLA	C3B-C4B	2.65	1.50	1.42
14	B	3021	CLA	C1B-C2B	2.65	1.49	1.43
14	A	803	CLA	C1B-C2B	2.65	1.49	1.43
14	A	821	CLA	CHC-C1C	2.65	1.43	1.38
14	F	202	CLA	C1B-C2B	2.65	1.49	1.43
14	B	3030	CLA	C3B-C4B	2.65	1.50	1.42
14	A	825	CLA	CHC-C1C	2.64	1.43	1.38
14	A	820	CLA	C1B-C2B	2.64	1.49	1.43
14	A	828	CLA	C3B-C4B	2.64	1.50	1.42
14	J	101	CLA	C3B-C4B	2.62	1.50	1.42
14	A	831	CLA	C1B-C2B	2.62	1.49	1.43
16	B	3047	BCR	C30-C25	-2.62	1.50	1.53
17	I	104	LMG	O1-C1	2.62	1.44	1.40
14	A	809	CLA	C3B-C4B	2.61	1.50	1.42
14	B	3011	CLA	CHC-C1C	2.60	1.43	1.38
14	K	103	CLA	C1B-C2B	2.60	1.49	1.43
14	B	3037	CLA	C1B-C2B	2.60	1.49	1.43
14	B	3012	CLA	C1B-C2B	2.60	1.49	1.43
17	I	104	LMG	C4-C5	2.60	1.58	1.53
14	A	838	CLA	C1B-C2B	2.59	1.49	1.43
14	K	101	CLA	CHC-C1C	2.59	1.43	1.38
14	A	821	CLA	C3B-C4B	2.58	1.50	1.42
14	A	830	CLA	C3B-C4B	2.58	1.50	1.42
14	A	807	CLA	C3B-C4B	2.58	1.50	1.42
14	A	829	CLA	C3B-C4B	2.58	1.50	1.42
14	A	844	CLA	C3B-C4B	2.57	1.50	1.42
14	A	822	CLA	C1B-C2B	2.57	1.49	1.43
14	A	819	CLA	CHC-C1C	2.57	1.43	1.38
14	B	3013	CLA	CHC-C1C	2.57	1.43	1.38
14	L	204	CLA	C1D-ND	2.57	1.41	1.37
14	A	844	CLA	C1B-C2B	2.57	1.49	1.43
22	L	206	DGD	O2G-C2G	-2.55	1.40	1.46
14	B	3018	CLA	C3B-C4B	2.55	1.50	1.42
14	A	822	CLA	C3B-C4B	2.53	1.50	1.42
14	B	3032	CLA	C1B-C2B	2.53	1.49	1.43
14	B	3025	CLA	C3B-C4B	2.53	1.50	1.42
14	B	3037	CLA	CHC-C1C	2.53	1.43	1.38
14	M	102	CLA	MG-NB	-2.52	2.00	2.05
14	J	101	CLA	CHC-C1C	2.52	1.43	1.38
14	A	802	CLA	C1B-C2B	2.52	1.49	1.43
13	A	801	CL0	CMD-C2D	-2.52	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3039	CLA	CHC-C1C	2.51	1.43	1.38
14	A	813	CLA	C3B-C4B	2.51	1.50	1.42
14	A	839	CLA	CHC-C1C	2.51	1.43	1.38
14	B	3018	CLA	CHC-C1C	2.51	1.43	1.38
14	A	837	CLA	C3B-C4B	2.50	1.50	1.42
14	A	821	CLA	C1B-C2B	2.50	1.49	1.43
14	A	803	CLA	C3B-C4B	2.50	1.50	1.42
14	A	824	CLA	C3B-C4B	2.50	1.50	1.42
14	A	822	CLA	CHC-C1C	2.50	1.43	1.38
14	B	3027	CLA	CHC-C1C	2.50	1.43	1.38
14	A	827	CLA	CHC-C1C	2.50	1.43	1.38
16	A	851	BCR	C30-C25	-2.49	1.50	1.53
14	A	820	CLA	C3B-C4B	2.48	1.50	1.42
14	A	824	CLA	CHC-C1C	2.48	1.43	1.38
14	A	843	CLA	CHC-C1C	2.48	1.43	1.38
14	L	205	CLA	C3B-C4B	2.48	1.50	1.42
14	A	831	CLA	CMB-C2B	-2.48	1.45	1.50
14	A	839	CLA	C3B-C4B	2.47	1.49	1.42
14	A	817	CLA	C3B-C4B	2.47	1.49	1.42
14	A	819	CLA	C3B-C4B	2.47	1.49	1.42
14	B	3039	CLA	C3B-C4B	2.47	1.49	1.42
14	J	102	CLA	C3B-C4B	2.47	1.49	1.42
14	B	3036	CLA	C3B-C4B	2.46	1.49	1.42
14	A	818	CLA	CHC-C1C	2.46	1.43	1.38
14	A	836	CLA	C3B-C4B	2.46	1.49	1.42
14	B	3024	CLA	CHC-C1C	2.46	1.43	1.38
14	B	3004	CLA	C3B-C4B	2.46	1.49	1.42
14	B	3027	CLA	C3B-C4B	2.45	1.49	1.42
14	B	3041	CLA	C3B-C4B	2.45	1.49	1.42
14	A	843	CLA	C3B-C4B	2.45	1.49	1.42
14	B	3040	CLA	C3B-C4B	2.45	1.49	1.42
14	L	205	CLA	C1B-C2B	2.45	1.48	1.43
14	B	3019	CLA	CHC-C1C	2.45	1.43	1.38
14	B	3031	CLA	C3B-C4B	2.45	1.49	1.42
14	B	3038	CLA	C3B-C4B	2.44	1.49	1.42
14	F	202	CLA	CHC-C1C	2.44	1.43	1.38
14	B	3030	CLA	CHC-C1C	2.44	1.43	1.38
14	A	817	CLA	CHC-C1C	2.44	1.43	1.38
16	B	3044	BCR	C33-C5	-2.43	1.47	1.50
14	B	3018	CLA	C1B-C2B	2.43	1.48	1.43
14	A	837	CLA	CHC-C1C	2.43	1.43	1.38
14	B	3014	CLA	C3B-C4B	2.43	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3019	CLA	C3B-C4B	2.43	1.49	1.42
14	A	830	CLA	CHC-C1C	2.42	1.43	1.38
14	I	101	CLA	C3B-C4B	2.42	1.49	1.42
14	B	3025	CLA	CHC-C1C	2.42	1.43	1.38
13	A	801	CL0	CMB-C2B	-2.42	1.45	1.50
14	A	823	CLA	C3B-C4B	2.42	1.49	1.42
17	A	852	LMG	C7-C8	2.42	1.58	1.50
14	F	202	CLA	C3B-C4B	2.42	1.49	1.42
14	A	818	CLA	C3B-C4B	2.42	1.49	1.42
14	B	3014	CLA	CHC-C1C	2.41	1.43	1.38
14	X	1701	CLA	C3B-C4B	2.41	1.49	1.42
14	A	804	CLA	CHC-C1C	2.41	1.43	1.38
14	A	835	CLA	CHC-C1C	2.41	1.43	1.38
14	A	827	CLA	CMD-C2D	-2.40	1.45	1.50
16	F	203	BCR	C33-C5	-2.40	1.47	1.50
14	A	805	CLA	CHC-C1C	2.40	1.43	1.38
14	A	842	CLA	C3B-C4B	2.40	1.49	1.42
14	B	3004	CLA	C1B-C2B	2.39	1.48	1.43
16	I	105	BCR	C33-C5	-2.39	1.47	1.50
14	A	808	CLA	CHC-C1C	2.39	1.43	1.38
14	A	838	CLA	MG-NB	-2.39	2.01	2.05
14	B	3017	CLA	C3B-C4B	2.38	1.49	1.42
14	B	3029	CLA	C3B-C4B	2.38	1.49	1.42
14	A	834	CLA	C3B-C4B	2.38	1.49	1.42
14	A	826	CLA	C3B-C4B	2.37	1.49	1.42
16	J	104	BCR	C33-C5	-2.37	1.47	1.50
16	B	3043	BCR	C33-C5	-2.37	1.47	1.50
14	A	819	CLA	MG-NB	-2.36	2.01	2.05
14	B	3022	CLA	C3B-C4B	2.36	1.49	1.42
16	J	105	BCR	C33-C5	-2.36	1.47	1.50
14	B	3012	CLA	C3B-C4B	2.36	1.49	1.42
14	B	3031	CLA	CHC-C1C	2.36	1.43	1.38
14	B	3036	CLA	CHC-C1C	2.35	1.43	1.38
14	A	840	CLA	C3B-C4B	2.35	1.49	1.42
14	B	3003	CLA	C3B-C4B	2.35	1.49	1.42
14	B	3021	CLA	C3B-C4B	2.35	1.49	1.42
14	A	814	CLA	CHC-C1C	2.35	1.43	1.38
14	A	827	CLA	C3B-C4B	2.35	1.49	1.42
14	B	3034	CLA	C3B-C4B	2.35	1.49	1.42
14	B	3041	CLA	CHC-C1C	2.35	1.43	1.38
14	A	812	CLA	C3B-C4B	2.34	1.49	1.42
14	M	102	CLA	CMD-C2D	-2.34	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	810	CLA	C3B-C4B	2.34	1.49	1.42
16	M	103	BCR	C33-C5	-2.34	1.47	1.50
14	B	3023	CLA	MG-NB	-2.34	2.01	2.05
14	A	838	CLA	C3B-C4B	2.34	1.49	1.42
14	K	103	CLA	CHC-C1C	2.34	1.43	1.38
16	A	851	BCR	C33-C5	-2.33	1.47	1.50
14	L	205	CLA	CHC-C1C	2.33	1.43	1.38
14	A	807	CLA	CHC-C1C	2.33	1.43	1.38
14	A	838	CLA	CHC-C1C	2.33	1.43	1.38
14	J	102	CLA	CHC-C1C	2.33	1.43	1.38
16	F	201	BCR	C33-C5	-2.32	1.47	1.50
16	A	847	BCR	C33-C5	-2.32	1.47	1.50
14	A	836	CLA	CHC-C1C	2.32	1.43	1.38
16	A	849	BCR	C33-C5	-2.32	1.47	1.50
14	A	841	CLA	CHC-C1C	2.32	1.43	1.38
14	A	814	CLA	C3B-C4B	2.32	1.49	1.42
14	L	204	CLA	MG-NB	-2.31	2.01	2.05
14	B	3004	CLA	MG-NB	-2.31	2.01	2.05
14	A	845	CLA	C3B-C4B	2.31	1.49	1.42
21	L	201	LMT	O3B-C3B	-2.31	1.37	1.43
14	A	835	CLA	C3B-C4B	2.30	1.49	1.42
14	B	3038	CLA	CHC-C1C	2.30	1.43	1.38
14	A	816	CLA	C3B-C4B	2.30	1.49	1.42
14	K	103	CLA	C3B-C4B	2.30	1.49	1.42
14	B	3004	CLA	CMD-C2D	-2.29	1.46	1.50
14	L	204	CLA	CHC-C1C	2.29	1.43	1.38
14	B	3024	CLA	C3B-C4B	2.29	1.49	1.42
14	B	3003	CLA	CMD-C2D	-2.29	1.46	1.50
16	A	850	BCR	C33-C5	-2.29	1.47	1.50
14	A	831	CLA	C3B-C4B	2.29	1.49	1.42
14	A	802	CLA	C3B-C4B	2.28	1.49	1.42
14	A	806	CLA	C3B-C4B	2.28	1.49	1.42
14	B	3010	CLA	C1B-C2B	2.28	1.48	1.43
16	J	103	BCR	C33-C5	-2.28	1.47	1.50
16	L	207	BCR	C33-C5	-2.28	1.47	1.50
16	B	3046	BCR	C33-C5	-2.28	1.47	1.50
16	A	848	BCR	C33-C5	-2.28	1.47	1.50
14	B	3026	CLA	C3B-C4B	2.27	1.49	1.42
14	A	833	CLA	CHC-C1C	2.27	1.43	1.38
16	B	3045	BCR	C33-C5	-2.27	1.47	1.50
14	B	3009	CLA	C3B-C4B	2.27	1.49	1.42
14	A	826	CLA	CHC-C1C	2.27	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	102	CLA	CHC-C1C	2.27	1.43	1.38
14	A	805	CLA	C3B-C4B	2.27	1.49	1.42
14	B	3032	CLA	C3B-C4B	2.27	1.49	1.42
14	B	3017	CLA	CHC-C1C	2.26	1.43	1.38
16	I	102	BCR	C33-C5	-2.26	1.47	1.50
14	A	808	CLA	C3B-C4B	2.26	1.49	1.42
14	A	841	CLA	C3B-C4B	2.26	1.49	1.42
14	A	842	CLA	CHC-C1C	2.26	1.43	1.38
14	B	3041	CLA	MG-NB	-2.26	2.01	2.05
14	B	3003	CLA	CHC-C1C	2.26	1.43	1.38
13	A	801	CL0	CHC-C1C	2.25	1.43	1.38
14	B	3033	CLA	C3B-C4B	2.25	1.49	1.42
14	F	202	CLA	CMB-C2B	-2.25	1.46	1.50
14	B	3011	CLA	MG-ND	-2.25	2.01	2.05
14	B	3016	CLA	C3B-C4B	2.25	1.49	1.42
16	B	3050	BCR	C33-C5	-2.25	1.47	1.50
14	B	3003	CLA	CMB-C2B	-2.25	1.46	1.50
14	B	3008	CLA	C3B-C4B	2.25	1.49	1.42
16	B	3047	BCR	C33-C5	-2.25	1.47	1.50
14	A	820	CLA	CHC-C1C	2.24	1.43	1.38
14	A	803	CLA	CMD-C2D	-2.24	1.46	1.50
14	A	856	CLA	MG-NB	-2.24	2.01	2.05
14	A	829	CLA	CHC-C1C	2.24	1.43	1.38
16	K	102	BCR	C33-C5	-2.24	1.47	1.50
22	L	206	DGD	O5D-C6D	-2.24	1.39	1.43
14	A	856	CLA	C3B-C4B	2.24	1.49	1.42
14	B	3022	CLA	CHC-C1C	2.24	1.43	1.38
14	M	102	CLA	MG-ND	-2.24	2.01	2.05
14	B	3035	CLA	C3B-C4B	2.24	1.49	1.42
17	A	855	LMG	C7-C8	2.24	1.55	1.50
14	B	3020	CLA	CMC-C2C	-2.23	1.46	1.50
14	A	815	CLA	CHC-C1C	2.23	1.43	1.38
14	B	3008	CLA	CMD-C2D	-2.23	1.46	1.50
14	L	204	CLA	C3B-C4B	2.22	1.49	1.42
14	B	3015	CLA	CHC-C1C	2.22	1.42	1.38
14	L	203	CLA	MG-NB	-2.22	2.01	2.05
14	A	834	CLA	CHC-C1C	2.22	1.42	1.38
14	B	3023	CLA	CMD-C2D	-2.22	1.46	1.50
14	A	811	CLA	C3B-C4B	2.22	1.49	1.42
14	B	3034	CLA	CHC-C1C	2.22	1.42	1.38
14	B	3011	CLA	MG-NB	-2.21	2.01	2.05
14	B	3009	CLA	CMD-C2D	-2.21	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	K	101	CLA	CBD-CAD	2.21	1.56	1.51
16	I	103	BCR	C33-C5	-2.21	1.47	1.50
14	B	3023	CLA	CMB-C2B	-2.20	1.46	1.50
14	X	1701	CLA	CHC-C1C	2.20	1.42	1.38
14	A	806	CLA	CHC-C1C	2.20	1.42	1.38
14	B	3032	CLA	MG-NB	-2.20	2.01	2.05
14	B	3040	CLA	CHC-C1C	2.19	1.42	1.38
14	A	823	CLA	CHC-C1C	2.19	1.42	1.38
14	A	819	CLA	CMB-C2B	-2.19	1.46	1.50
13	A	801	CL0	MG-NB	-2.19	2.01	2.05
21	L	201	LMT	O2B-C2B	-2.19	1.37	1.43
14	A	815	CLA	MG-NB	-2.18	2.01	2.05
14	A	813	CLA	CHC-C1C	2.18	1.42	1.38
14	A	840	CLA	CHC-C1C	2.18	1.42	1.38
14	A	802	CLA	CHC-C1C	2.18	1.42	1.38
14	B	3020	CLA	CMB-C2B	-2.18	1.46	1.50
14	B	3007	CLA	CMB-C2B	-2.18	1.46	1.50
14	B	3023	CLA	C3B-C4B	2.18	1.49	1.42
14	B	3032	CLA	CMB-C2B	-2.17	1.46	1.50
22	L	206	DGD	C6D-C5D	2.17	1.58	1.51
14	B	3007	CLA	C3B-C4B	2.17	1.49	1.42
14	J	102	CLA	CBD-CAD	2.17	1.56	1.51
14	F	202	CLA	MG-NB	-2.17	2.01	2.05
14	A	805	CLA	CMD-C2D	-2.17	1.46	1.50
14	B	3020	CLA	MG-NB	-2.17	2.01	2.05
14	B	3028	CLA	MG-NB	-2.17	2.01	2.05
14	A	833	CLA	C3B-C4B	2.16	1.49	1.42
14	B	3005	CLA	CMD-C2D	-2.16	1.46	1.50
13	A	801	CL0	C3B-C4B	2.16	1.49	1.42
14	A	844	CLA	MG-NB	-2.16	2.01	2.05
14	A	814	CLA	MG-NB	-2.16	2.01	2.05
14	A	834	CLA	CMB-C2B	-2.15	1.46	1.50
14	K	103	CLA	MG-NB	-2.15	2.01	2.05
14	B	3006	CLA	C3B-C4B	2.15	1.49	1.42
14	B	3014	CLA	MG-NB	-2.15	2.01	2.05
14	A	822	CLA	MG-NB	-2.15	2.01	2.05
14	A	842	CLA	CMC-C2C	-2.15	1.46	1.50
14	L	205	CLA	CMB-C2B	-2.15	1.46	1.50
18	A	853	LHG	P-O6	2.15	1.67	1.59
14	L	203	CLA	CMB-C2B	-2.14	1.46	1.50
14	B	3010	CLA	MG-ND	-2.14	2.01	2.05
14	A	856	CLA	CHC-C1C	2.14	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	L	204	CLA	CMB-C2B	-2.14	1.46	1.50
14	A	833	CLA	MG-NB	-2.14	2.01	2.05
14	A	839	CLA	CMC-C2C	-2.14	1.46	1.50
14	B	3041	CLA	CMD-C2D	-2.14	1.46	1.50
14	B	3004	CLA	MG-ND	-2.14	2.01	2.05
14	A	813	CLA	CMD-C2D	-2.14	1.46	1.50
14	A	810	CLA	MG-NB	-2.14	2.01	2.05
14	B	3012	CLA	CHC-C1C	2.14	1.42	1.38
14	A	811	CLA	CHC-C1C	2.14	1.42	1.38
14	A	815	CLA	C3B-C4B	2.13	1.49	1.42
14	A	802	CLA	MG-NB	-2.13	2.01	2.05
14	B	3035	CLA	CHC-C1C	2.13	1.42	1.38
14	B	3005	CLA	C3B-C4B	2.13	1.48	1.42
14	A	819	CLA	C1B-C2B	2.13	1.48	1.43
14	B	3021	CLA	CMB-C2B	-2.13	1.46	1.50
14	M	102	CLA	C3B-C4B	2.13	1.48	1.42
14	B	3032	CLA	CHC-C1C	2.12	1.42	1.38
14	B	3024	CLA	CMC-C2C	-2.12	1.46	1.50
14	A	831	CLA	CHC-C1C	2.12	1.42	1.38
14	A	811	CLA	CMD-C2D	-2.12	1.46	1.50
14	B	3025	CLA	CMB-C2B	-2.12	1.46	1.50
17	I	104	LMG	C9-C8	2.12	1.57	1.50
14	M	102	CLA	MG-NC	2.12	2.11	2.06
14	A	832	CLA	C3B-C4B	2.12	1.48	1.42
14	A	831	CLA	MG-NB	-2.12	2.01	2.05
14	B	3020	CLA	CMD-C2D	-2.12	1.46	1.50
14	X	1701	CLA	CMB-C2B	-2.11	1.46	1.50
14	A	821	CLA	CMB-C2B	-2.11	1.46	1.50
14	A	811	CLA	MG-NB	-2.11	2.01	2.05
14	B	3026	CLA	CMB-C2B	-2.11	1.46	1.50
14	B	3015	CLA	C3B-C4B	2.11	1.48	1.42
14	A	814	CLA	CMD-C2D	-2.11	1.46	1.50
14	B	3020	CLA	CHC-C1C	2.11	1.42	1.38
14	L	205	CLA	MG-NB	-2.11	2.01	2.05
14	B	3015	CLA	MG-NB	-2.11	2.01	2.05
14	A	844	CLA	CHC-C1C	2.11	1.42	1.38
14	B	3020	CLA	C3B-C4B	2.10	1.48	1.42
14	A	817	CLA	CMB-C2B	-2.10	1.46	1.50
14	A	843	CLA	MG-NB	-2.10	2.01	2.05
14	B	3040	CLA	MG-NB	-2.10	2.01	2.05
14	A	819	CLA	CMD-C2D	-2.10	1.46	1.50
14	B	3012	CLA	CMD-C2D	-2.10	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3006	CLA	CHC-C1C	2.10	1.42	1.38
14	B	3028	CLA	CMD-C2D	-2.10	1.46	1.50
14	B	3024	CLA	MG-NB	-2.10	2.01	2.05
14	A	827	CLA	MG-NB	-2.10	2.01	2.05
14	A	836	CLA	CMB-C2B	-2.09	1.46	1.50
14	B	3029	CLA	CHC-C1C	2.09	1.42	1.38
14	A	811	CLA	CMB-C2B	-2.09	1.46	1.50
14	A	821	CLA	MG-NB	-2.09	2.01	2.05
14	X	1701	CLA	CMD-C2D	-2.09	1.46	1.50
14	A	819	CLA	CMC-C2C	-2.09	1.46	1.50
14	A	815	CLA	CMB-C2B	-2.09	1.46	1.50
14	A	832	CLA	MG-NB	-2.09	2.01	2.05
21	L	201	LMT	O3'-C3'	-2.09	1.37	1.43
14	A	838	CLA	CMD-C2D	-2.09	1.46	1.50
14	A	856	CLA	CMD-C2D	-2.09	1.46	1.50
14	A	832	CLA	CHC-C1C	2.09	1.42	1.38
14	A	844	CLA	CMD-C2D	-2.08	1.46	1.50
14	A	844	CLA	CMB-C2B	-2.08	1.46	1.50
14	B	3029	CLA	CMD-C2D	-2.08	1.46	1.50
14	B	3028	CLA	C3B-C4B	2.08	1.48	1.42
14	B	3018	CLA	MG-NB	-2.08	2.01	2.05
14	A	839	CLA	CMD-C2D	-2.08	1.46	1.50
14	M	102	CLA	CMB-C2B	-2.08	1.46	1.50
14	A	818	CLA	MG-NB	-2.08	2.01	2.05
14	B	3026	CLA	CHC-C1C	2.08	1.42	1.38
14	A	804	CLA	CMC-C2C	-2.08	1.46	1.50
14	A	833	CLA	CMC-C2C	-2.07	1.46	1.50
14	B	3035	CLA	CMB-C2B	-2.07	1.46	1.50
14	B	3011	CLA	CMD-C2D	-2.07	1.46	1.50
18	M	101	LHG	P-O6	2.07	1.67	1.59
14	A	832	CLA	CMC-C2C	-2.07	1.46	1.50
14	A	833	CLA	CMB-C2B	-2.07	1.46	1.50
14	A	810	CLA	CMD-C2D	-2.06	1.46	1.50
14	A	816	CLA	CHC-C1C	2.06	1.42	1.38
14	B	3012	CLA	CMB-C2B	-2.06	1.46	1.50
14	A	812	CLA	CHC-C1C	2.06	1.42	1.38
14	A	812	CLA	CMD-C2D	-2.06	1.46	1.50
14	A	807	CLA	CMB-C2B	-2.06	1.46	1.50
14	B	3006	CLA	CMB-C2B	-2.05	1.46	1.50
14	A	810	CLA	CHC-C1C	2.05	1.42	1.38
14	B	3010	CLA	CMD-C2D	-2.05	1.46	1.50
14	B	3034	CLA	CMB-C2B	-2.05	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3008	CLA	CHC-C1C	2.05	1.42	1.38
14	A	832	CLA	CMD-C2D	-2.05	1.46	1.50
22	L	206	DGD	C3D-C2D	2.05	1.57	1.52
14	B	3039	CLA	MG-NB	-2.04	2.01	2.05
14	A	812	CLA	CMB-C2B	-2.04	1.46	1.50
14	B	3033	CLA	CMB-C2B	-2.04	1.46	1.50
14	L	204	CLA	CMD-C2D	-2.04	1.46	1.50
14	A	845	CLA	CMB-C2B	-2.04	1.46	1.50
14	A	805	CLA	CMB-C2B	-2.04	1.46	1.50
14	B	3004	CLA	CMB-C2B	-2.04	1.46	1.50
14	A	831	CLA	CMD-C2D	-2.04	1.46	1.50
14	A	826	CLA	CMB-C2B	-2.04	1.46	1.50
14	A	835	CLA	MG-NB	-2.04	2.01	2.05
14	A	803	CLA	CMB-C2B	-2.03	1.46	1.50
14	A	834	CLA	CMD-C2D	-2.03	1.46	1.50
18	B	3049	LHG	C6-C5	2.03	1.57	1.50
14	A	810	CLA	CMB-C2B	-2.03	1.46	1.50
14	B	3030	CLA	CMB-C2B	-2.03	1.46	1.50
14	B	3022	CLA	CMB-C2B	-2.03	1.46	1.50
14	B	3024	CLA	O2A-CGA	2.02	1.37	1.30
14	A	809	CLA	CMD-C2D	-2.02	1.46	1.50
14	A	836	CLA	CMC-C2C	-2.02	1.46	1.50
14	A	856	CLA	CMB-C2B	-2.02	1.46	1.50
14	A	842	CLA	CMD-C2D	-2.02	1.46	1.50
14	B	3032	CLA	CMD-C2D	-2.02	1.46	1.50
14	B	3021	CLA	CHC-C1C	2.02	1.42	1.38
14	B	3017	CLA	MG-NB	-2.02	2.01	2.05
14	A	804	CLA	CMD-C2D	-2.02	1.46	1.50
14	B	3028	CLA	CMC-C2C	-2.01	1.46	1.50
14	B	3016	CLA	CHC-C1C	2.01	1.42	1.38
14	L	205	CLA	CMC-C2C	-2.01	1.46	1.50
14	B	3035	CLA	O2A-CGA	2.01	1.37	1.30
14	B	3003	CLA	MG-NB	-2.01	2.01	2.05
14	A	826	CLA	CMD-C2D	-2.01	1.46	1.50
14	B	3011	CLA	CMC-C2C	-2.01	1.46	1.50
14	B	3029	CLA	MG-ND	-2.01	2.01	2.05
14	B	3033	CLA	CMD-C2D	-2.01	1.46	1.50
14	B	3038	CLA	CMB-C2B	-2.01	1.46	1.50
14	B	3007	CLA	MG-NB	-2.01	2.01	2.05
14	A	806	CLA	CMB-C2B	-2.01	1.46	1.50
14	A	808	CLA	CMB-C2B	-2.01	1.46	1.50
21	L	201	LMT	O2'-C2'	-2.01	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3031	CLA	O2A-CGA	2.00	1.37	1.30
14	A	840	CLA	CMB-C2B	-2.00	1.46	1.50
14	A	843	CLA	CMD-C2D	-2.00	1.46	1.50
14	B	3016	CLA	CMB-C2B	-2.00	1.46	1.50
14	B	3017	CLA	CMD-C2D	-2.00	1.46	1.50
14	B	3016	CLA	O2A-CGA	2.00	1.37	1.30
14	B	3036	CLA	MG-NB	-2.00	2.01	2.05
14	B	3024	CLA	CMB-C2B	-2.00	1.46	1.50
14	A	812	CLA	CMC-C2C	-2.00	1.46	1.50

All (731) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3033	CLA	C4A-NA-C1A	7.67	110.18	106.68
14	A	842	CLA	C4A-NA-C1A	7.65	110.17	106.68
14	I	101	CLA	C4A-NA-C1A	7.56	110.13	106.68
14	A	816	CLA	C4A-NA-C1A	7.50	110.10	106.68
14	B	3005	CLA	C4A-NA-C1A	7.45	110.08	106.68
14	A	820	CLA	C4A-NA-C1A	7.42	110.07	106.68
14	B	3031	CLA	C4A-NA-C1A	7.38	110.05	106.68
14	L	204	CLA	C4A-NA-C1A	7.35	110.03	106.68
14	B	3041	CLA	C4A-NA-C1A	7.33	110.03	106.68
14	B	3003	CLA	C4A-NA-C1A	7.30	110.01	106.68
14	L	205	CLA	C4A-NA-C1A	7.29	110.00	106.68
14	L	203	CLA	C4A-NA-C1A	7.28	110.00	106.68
14	A	845	CLA	C4A-NA-C1A	7.26	109.99	106.68
14	A	806	CLA	C4A-NA-C1A	7.14	109.94	106.68
14	B	3006	CLA	C4A-NA-C1A	7.13	109.93	106.68
14	B	3009	CLA	C4A-NA-C1A	7.08	109.91	106.68
14	A	832	CLA	C4A-NA-C1A	6.92	109.83	106.68
14	A	840	CLA	C4A-NA-C1A	6.90	109.83	106.68
14	B	3008	CLA	C4A-NA-C1A	6.85	109.81	106.68
14	A	833	CLA	C4A-NA-C1A	6.81	109.79	106.68
14	A	834	CLA	C4A-NA-C1A	6.81	109.79	106.68
14	A	831	CLA	C4A-NA-C1A	6.74	109.75	106.68
14	B	3007	CLA	C4A-NA-C1A	6.73	109.75	106.68
14	B	3016	CLA	C4A-NA-C1A	6.67	109.72	106.68
14	B	3029	CLA	C4A-NA-C1A	6.67	109.72	106.68
14	A	836	CLA	C4A-NA-C1A	6.65	109.71	106.68
14	A	841	CLA	C4A-NA-C1A	6.62	109.70	106.68
14	B	3040	CLA	C4A-NA-C1A	6.62	109.70	106.68
14	A	813	CLA	C4A-NA-C1A	6.60	109.69	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	829	CLA	C4A-NA-C1A	6.60	109.69	106.68
14	B	3017	CLA	C4A-NA-C1A	6.58	109.68	106.68
14	B	3025	CLA	C4A-NA-C1A	6.58	109.68	106.68
14	B	3013	CLA	C4A-NA-C1A	6.54	109.66	106.68
14	B	3012	CLA	C4A-NA-C1A	6.53	109.66	106.68
14	B	3035	CLA	C4A-NA-C1A	6.53	109.66	106.68
14	B	3022	CLA	C4A-NA-C1A	6.51	109.65	106.68
14	B	3036	CLA	C4A-NA-C1A	6.51	109.65	106.68
14	A	839	CLA	C4A-NA-C1A	6.49	109.64	106.68
14	B	3015	CLA	C4A-NA-C1A	6.49	109.64	106.68
14	X	1701	CLA	C4A-NA-C1A	6.49	109.64	106.68
14	A	808	CLA	C4A-NA-C1A	6.49	109.64	106.68
14	A	817	CLA	C4A-NA-C1A	6.48	109.64	106.68
13	A	801	CL0	C4A-NA-C1A	6.45	109.62	106.68
14	B	3026	CLA	C4A-NA-C1A	6.45	109.62	106.68
14	A	828	CLA	C4A-NA-C1A	6.43	109.61	106.68
14	B	3028	CLA	C4A-NA-C1A	6.42	109.61	106.68
14	B	3027	CLA	C4A-NA-C1A	6.37	109.59	106.68
14	A	823	CLA	C4A-NA-C1A	6.36	109.58	106.68
14	B	3020	CLA	C4A-NA-C1A	6.33	109.57	106.68
14	B	3038	CLA	C4A-NA-C1A	6.31	109.56	106.68
14	A	809	CLA	C4A-NA-C1A	6.30	109.55	106.68
14	A	843	CLA	C4A-NA-C1A	6.28	109.54	106.68
14	B	3039	CLA	C4A-NA-C1A	6.27	109.54	106.68
14	B	3034	CLA	C4A-NA-C1A	6.26	109.53	106.68
14	A	826	CLA	C4A-NA-C1A	6.26	109.53	106.68
14	A	812	CLA	C4A-NA-C1A	6.21	109.51	106.68
14	A	830	CLA	C4A-NA-C1A	6.21	109.51	106.68
14	A	837	CLA	C4A-NA-C1A	6.19	109.50	106.68
14	A	802	CLA	C4A-NA-C1A	6.17	109.49	106.68
14	B	3021	CLA	C4A-NA-C1A	6.08	109.45	106.68
14	A	805	CLA	C4A-NA-C1A	6.06	109.44	106.68
14	B	3037	CLA	C4A-NA-C1A	6.05	109.44	106.68
14	A	811	CLA	C4A-NA-C1A	6.02	109.42	106.68
14	B	3019	CLA	C4A-NA-C1A	5.99	109.41	106.68
14	B	3023	CLA	C4A-NA-C1A	5.99	109.41	106.68
14	A	803	CLA	C4A-NA-C1A	5.95	109.39	106.68
14	A	824	CLA	C4A-NA-C1A	5.95	109.39	106.68
14	A	810	CLA	C4A-NA-C1A	5.88	109.36	106.68
14	K	101	CLA	C4A-NA-C1A	5.88	109.36	106.68
14	A	856	CLA	C4A-NA-C1A	5.83	109.34	106.68
14	B	3011	CLA	C4A-NA-C1A	5.82	109.33	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	818	CLA	C4A-NA-C1A	5.81	109.33	106.68
14	A	815	CLA	C4A-NA-C1A	5.78	109.32	106.68
14	J	102	CLA	C4A-NA-C1A	5.77	109.31	106.68
14	B	3018	CLA	C4A-NA-C1A	5.75	109.30	106.68
14	A	825	CLA	C4A-NA-C1A	5.73	109.29	106.68
14	B	3024	CLA	C4A-NA-C1A	5.72	109.29	106.68
14	B	3010	CLA	C4A-NA-C1A	5.70	109.28	106.68
14	B	3032	CLA	C4A-NA-C1A	5.63	109.25	106.68
14	A	844	CLA	C4A-NA-C1A	5.55	109.21	106.68
14	A	827	CLA	C4A-NA-C1A	5.51	109.19	106.68
14	J	101	CLA	C4A-NA-C1A	5.51	109.19	106.68
14	A	814	CLA	C4A-NA-C1A	5.50	109.19	106.68
14	B	3030	CLA	C4A-NA-C1A	5.50	109.19	106.68
14	A	821	CLA	C4A-NA-C1A	5.50	109.19	106.68
14	A	807	CLA	C4A-NA-C1A	5.40	109.14	106.68
14	B	3014	CLA	C4A-NA-C1A	5.34	109.12	106.68
14	A	838	CLA	C4A-NA-C1A	5.24	109.07	106.68
14	A	804	CLA	C4A-NA-C1A	5.20	109.05	106.68
14	A	819	CLA	C4A-NA-C1A	4.94	108.94	106.68
14	A	822	CLA	C4A-NA-C1A	4.90	108.92	106.68
14	K	103	CLA	C4A-NA-C1A	4.61	108.78	106.68
18	A	854	LHG	O4-P-O5	4.51	133.44	112.44
14	B	3004	CLA	C4A-NA-C1A	4.51	108.74	106.68
18	A	853	LHG	O4-P-O5	4.46	133.17	112.44
18	M	101	LHG	O4-P-O5	4.43	133.06	112.44
14	L	203	CLA	C1-C2-C3	-4.42	118.96	126.20
14	A	835	CLA	C4A-NA-C1A	4.35	108.66	106.68
14	F	202	CLA	C4A-NA-C1A	4.31	108.65	106.68
16	A	851	BCR	C2-C1-C6	4.29	116.67	110.44
16	K	102	BCR	C2-C1-C6	4.26	116.63	110.44
18	B	3049	LHG	O4-P-O5	4.23	132.12	112.44
14	A	819	CLA	C3B-C4B-NB	-4.14	106.83	110.53
14	A	839	CLA	O2D-CGD-CBD	4.14	118.46	111.23
14	A	839	CLA	O2D-CGD-O1D	-4.08	115.90	123.85
14	B	3030	CLA	CAA-C2A-C3A	-3.97	102.27	113.00
14	B	3004	CLA	C3B-C4B-NB	-3.80	107.14	110.53
14	M	102	CLA	C4A-NA-C1A	3.67	108.35	106.68
14	A	827	CLA	C3B-C4B-NB	-3.65	107.27	110.53
14	A	856	CLA	O2D-CGD-O1D	-3.62	116.79	123.85
14	X	1701	CLA	O2D-CGD-O1D	-3.62	116.80	123.85
16	I	105	BCR	C27-C26-C25	3.57	127.53	122.70
14	B	3031	CLA	O2D-CGD-O1D	-3.57	116.90	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	103	BCR	C15-C16-C17	-3.55	116.25	123.52
14	A	838	CLA	C3B-C4B-NB	-3.54	107.37	110.53
14	A	818	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
22	L	206	DGD	O3G-C3G-C2G	-3.52	102.26	110.82
14	A	828	CLA	C3B-C4B-NB	-3.47	107.43	110.53
14	B	3005	CLA	O2D-CGD-O1D	-3.45	117.12	123.85
14	B	3024	CLA	C3B-C4B-NB	-3.43	107.47	110.53
14	K	103	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
14	B	3010	CLA	C1-C2-C3	-3.41	120.61	126.20
14	B	3014	CLA	CAC-C3C-C4C	3.38	129.19	124.79
14	F	202	CLA	C3B-C4B-NB	-3.38	107.52	110.53
14	B	3025	CLA	C3B-C4B-NB	-3.38	107.52	110.53
14	A	835	CLA	C1-C2-C3	-3.37	120.67	126.20
18	A	854	LHG	O8-C23-C24	3.34	121.30	111.15
14	K	103	CLA	O2D-CGD-CBD	3.33	117.05	111.23
16	B	3046	BCR	C15-C16-C17	-3.33	116.71	123.52
14	A	816	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
14	A	844	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
14	B	3020	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
14	B	3032	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
14	A	816	CLA	O2D-CGD-CBD	3.31	117.01	111.23
14	B	3006	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
14	B	3017	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
16	I	105	BCR	C30-C25-C26	-3.29	118.14	122.64
16	A	847	BCR	C33-C5-C6	-3.28	120.90	124.48
14	A	843	CLA	C3B-C4B-NB	-3.28	107.61	110.53
14	A	804	CLA	C3B-C4B-NB	-3.27	107.61	110.53
16	K	102	BCR	C27-C26-C25	3.27	127.12	122.70
14	A	813	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
14	B	3011	CLA	C3B-C4B-NB	-3.26	107.62	110.53
14	B	3014	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
14	A	809	CLA	C3B-C4B-NB	-3.23	107.64	110.53
14	A	814	CLA	C3B-C4B-NB	-3.23	107.64	110.53
16	F	201	BCR	C27-C26-C25	3.23	127.06	122.70
14	B	3018	CLA	C3B-C4B-NB	-3.22	107.65	110.53
14	A	833	CLA	C3B-C4B-NB	-3.21	107.66	110.53
14	B	3037	CLA	C3B-C4B-NB	-3.20	107.67	110.53
16	F	203	BCR	C35-C13-C14	-3.20	117.63	122.82
14	A	805	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
14	A	818	CLA	C3B-C4B-NB	-3.20	107.67	110.53
14	L	204	CLA	C3B-C4B-NB	-3.18	107.69	110.53
14	A	821	CLA	O2D-CGD-O1D	-3.17	117.68	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	830	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
14	A	803	CLA	C3B-C4B-NB	-3.15	107.72	110.53
14	A	818	CLA	O2D-CGD-CBD	3.15	116.73	111.23
16	A	851	BCR	C33-C5-C6	-3.12	121.08	124.48
14	A	832	CLA	C3B-C4B-NB	-3.11	107.75	110.53
14	B	3003	CLA	C3B-C4B-NB	-3.10	107.76	110.53
14	A	822	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
16	F	201	BCR	C2-C1-C6	3.10	114.94	110.44
14	A	826	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
16	B	3050	BCR	C27-C26-C25	3.10	126.89	122.70
14	B	3013	CLA	C3B-C4B-NB	-3.09	107.78	110.53
14	J	101	CLA	O2D-CGD-O1D	-3.08	117.84	123.85
14	M	102	CLA	O2D-CGD-O1D	-3.08	117.84	123.85
14	B	3039	CLA	C3B-C4B-NB	-3.08	107.78	110.53
17	B	3048	LMG	O6-C1-O1	-3.08	102.77	110.04
14	A	814	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
14	B	3016	CLA	O2D-CGD-O1D	-3.06	117.88	123.85
16	J	105	BCR	C7-C8-C9	-3.06	121.70	126.23
16	J	105	BCR	C2-C1-C6	3.06	114.89	110.44
14	B	3005	CLA	O2D-CGD-CBD	3.06	116.58	111.23
14	B	3010	CLA	C3B-C4B-NB	-3.06	107.80	110.53
14	B	3014	CLA	C3B-C4B-NB	-3.05	107.81	110.53
14	B	3021	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
14	I	101	CLA	CAC-C3C-C4C	3.05	128.75	124.79
14	B	3031	CLA	C3B-C4B-NB	-3.04	107.81	110.53
14	A	841	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
14	B	3032	CLA	C3B-C4B-NB	-3.02	107.83	110.53
14	A	825	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
16	B	3050	BCR	C33-C5-C6	-3.01	121.20	124.48
14	B	3035	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
14	A	806	CLA	C3B-C4B-NB	-3.00	107.85	110.53
14	A	844	CLA	C3B-C4B-NB	-3.00	107.85	110.53
14	K	101	CLA	C3B-C4B-NB	-2.99	107.86	110.53
14	A	811	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
16	L	207	BCR	C15-C16-C17	-2.99	117.40	123.52
14	A	814	CLA	O2D-CGD-CBD	2.99	116.46	111.23
16	I	103	BCR	C15-C14-C13	-2.99	123.09	127.28
14	A	820	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
14	A	807	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
14	B	3030	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
14	A	812	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
16	I	103	BCR	C11-C10-C9	-2.97	123.11	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3003	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
14	B	3030	CLA	CHB-C4A-NA	2.97	128.69	124.40
14	B	3029	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
14	A	836	CLA	C3B-C4B-NB	-2.97	107.88	110.53
14	A	822	CLA	C3B-C4B-NB	-2.97	107.88	110.53
14	A	825	CLA	C3B-C4B-NB	-2.96	107.89	110.53
16	F	203	BCR	C27-C26-C25	2.96	126.70	122.70
14	A	839	CLA	C3B-C4B-NB	-2.95	107.90	110.53
14	A	804	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
16	F	203	BCR	C2-C1-C6	2.95	114.72	110.44
14	B	3036	CLA	C3B-C4B-NB	-2.94	107.90	110.53
14	A	817	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
14	A	821	CLA	C3B-C4B-NB	-2.94	107.91	110.53
18	M	101	LHG	O8-C23-C24	2.94	120.78	111.83
16	B	3043	BCR	C29-C30-C25	2.93	114.70	110.44
14	F	202	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
14	A	820	CLA	CAA-C2A-C1A	-2.92	102.40	111.97
15	A	846	PQN	O1-C1-C10	-2.92	116.90	121.57
14	L	204	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
14	B	3008	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
14	A	808	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
16	J	103	BCR	C33-C5-C6	-2.92	121.30	124.48
14	A	823	CLA	CHB-C4A-NA	2.91	128.60	124.40
14	A	845	CLA	CHB-C4A-NA	2.91	128.60	124.40
21	L	201	LMT	C2'-C3'-C4'	2.90	116.27	109.68
14	A	839	CLA	CHB-C4A-NA	2.90	128.58	124.40
14	B	3023	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
13	A	801	CL0	C3B-C4B-NB	-2.89	107.95	110.53
14	B	3003	CLA	CHB-C4A-NA	2.89	128.57	124.40
14	B	3027	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
14	B	3026	CLA	C2A-C1A-CHA	2.88	128.87	123.87
14	A	823	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
14	B	3034	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
14	A	807	CLA	C3B-C4B-NB	-2.88	107.96	110.53
16	M	103	BCR	C33-C5-C6	-2.86	121.36	124.48
16	I	105	BCR	C11-C10-C9	-2.86	123.27	127.28
16	I	102	BCR	C27-C26-C25	2.85	126.56	122.70
14	B	3009	CLA	CHB-C4A-NA	2.84	128.50	124.40
14	B	3026	CLA	CHB-C4A-NA	2.84	128.50	124.40
14	B	3025	CLA	CHB-C4A-NA	2.84	128.50	124.40
14	B	3026	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
16	A	849	BCR	C27-C26-C25	2.83	126.53	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	842	CLA	C3B-C4B-NB	-2.83	108.00	110.53
16	J	105	BCR	C27-C26-C25	2.83	126.53	122.70
14	A	829	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
14	X	1701	CLA	CHB-C4A-NA	2.83	128.48	124.40
15	B	3042	PQN	O1-C1-C10	-2.83	117.05	121.57
14	A	803	CLA	CAA-C2A-C1A	-2.83	102.71	111.97
16	B	3045	BCR	C24-C23-C22	-2.82	122.06	126.23
14	A	802	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
14	B	3019	CLA	C3B-C4B-NB	-2.82	108.01	110.53
14	A	837	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
14	L	205	CLA	C3B-C4B-NB	-2.81	108.02	110.53
14	I	101	CLA	O2A-CGA-O1A	-2.81	116.60	123.63
21	L	201	LMT	C1'-O5'-C5'	-2.81	108.23	113.72
14	A	805	CLA	C3B-C4B-NB	-2.81	108.02	110.53
16	I	105	BCR	C33-C5-C6	-2.81	121.42	124.48
14	A	806	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
14	B	3041	CLA	C3B-C4B-NB	-2.80	108.03	110.53
14	B	3018	CLA	CHB-C4A-NA	2.80	128.44	124.40
16	B	3046	BCR	C2-C1-C6	2.80	114.50	110.44
14	L	205	CLA	CHB-C4A-NA	2.79	128.43	124.40
14	A	836	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
14	A	837	CLA	C3B-C4B-NB	-2.79	108.04	110.53
16	A	849	BCR	C15-C16-C17	-2.79	117.82	123.52
14	B	3025	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
14	J	101	CLA	C3B-C4B-NB	-2.78	108.05	110.53
16	B	3043	BCR	C2-C1-C6	2.78	114.47	110.44
14	B	3040	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
16	A	848	BCR	C27-C26-C25	2.77	126.45	122.70
14	A	820	CLA	CHB-C4A-NA	2.77	128.40	124.40
14	M	102	CLA	C3B-C4B-NB	-2.77	108.06	110.53
14	A	838	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
14	B	3008	CLA	CHB-C4A-NA	2.76	128.38	124.40
16	F	203	BCR	C33-C5-C6	-2.75	121.48	124.48
14	B	3027	CLA	C3B-C4B-NB	-2.75	108.08	110.53
14	A	819	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
14	B	3015	CLA	C3B-C4B-NB	-2.75	108.08	110.53
14	A	835	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
14	A	824	CLA	C3B-C4B-NB	-2.75	108.08	110.53
14	A	826	CLA	C3B-C4B-NB	-2.74	108.08	110.53
14	B	3005	CLA	CHB-C4A-NA	2.74	128.35	124.40
17	A	855	LMG	O6-C1-O1	-2.74	103.57	110.04
14	B	3036	CLA	O2D-CGD-O1D	-2.74	118.52	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	840	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
15	A	846	PQN	C2M-C2-C3	-2.73	119.96	124.45
14	L	205	CLA	CAA-C2A-C1A	-2.73	103.03	111.97
14	B	3020	CLA	C3B-C4B-NB	-2.73	108.09	110.53
14	A	813	CLA	C3B-C4B-NB	-2.73	108.09	110.53
16	A	850	BCR	C27-C26-C25	2.72	126.38	122.70
16	B	3047	BCR	C28-C27-C26	-2.72	109.20	114.06
16	A	848	BCR	C33-C5-C6	-2.72	121.51	124.48
14	B	3029	CLA	CHB-C4A-NA	2.72	128.32	124.40
16	I	102	BCR	C15-C16-C17	-2.72	117.96	123.52
14	B	3033	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
14	B	3011	CLA	CHB-C4A-NA	2.72	128.32	124.40
14	B	3009	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
14	A	824	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
14	B	3027	CLA	CHB-C4A-NA	2.71	128.31	124.40
17	I	104	LMG	O6-C1-O1	-2.71	103.64	110.04
14	A	809	CLA	CHB-C4A-NA	2.71	128.31	124.40
14	A	841	CLA	O2A-CGA-O1A	-2.71	116.85	123.63
14	A	832	CLA	CHB-C4A-NA	2.71	128.31	124.40
14	A	843	CLA	CHB-C4A-NA	2.71	128.31	124.40
16	I	102	BCR	C15-C14-C13	-2.71	123.48	127.28
14	L	203	CLA	O2A-CGA-O1A	-2.70	116.87	123.63
14	L	203	CLA	CHB-C4A-NA	2.70	128.30	124.40
14	X	1701	CLA	O2D-CGD-CBD	2.70	115.95	111.23
14	K	103	CLA	C3B-C4B-NB	-2.69	108.12	110.53
14	B	3015	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
14	A	842	CLA	CHB-C4A-NA	2.68	128.27	124.40
14	B	3016	CLA	CHB-C4A-NA	2.68	128.27	124.40
14	B	3022	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
14	B	3013	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
14	A	809	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
14	A	808	CLA	C3B-C4B-NB	-2.68	108.14	110.53
14	A	810	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
14	A	835	CLA	C3B-C4B-NB	-2.68	108.14	110.53
14	A	845	CLA	C1-C2-C3	-2.67	121.82	126.20
14	B	3010	CLA	C6-C5-C3	-2.67	106.97	113.47
14	B	3012	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
14	A	815	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
14	A	834	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
14	M	102	CLA	C2D-C1D-ND	-2.65	107.50	110.13
14	B	3007	CLA	CHB-C4A-NA	2.65	128.22	124.40
16	I	102	BCR	C33-C5-C6	-2.65	121.60	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3010	CLA	C6-C7-C8	-2.65	107.17	115.97
14	B	3008	CLA	O2D-CGD-CBD	2.64	115.85	111.23
14	A	815	CLA	C3B-C4B-NB	-2.63	108.18	110.53
16	I	103	BCR	C2-C1-C6	2.63	114.26	110.44
16	K	102	BCR	C24-C23-C22	-2.62	122.36	126.23
13	A	801	CL0	O2D-CGD-O1D	-2.62	118.75	123.85
16	L	207	BCR	C8-C7-C6	-2.62	120.00	127.00
14	A	831	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
14	B	3004	CLA	CAC-C3C-C4C	2.61	128.19	124.79
14	A	827	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
16	I	102	BCR	C24-C23-C22	-2.61	122.37	126.23
14	B	3038	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
16	B	3044	BCR	C2-C1-C6	2.61	114.22	110.44
14	B	3015	CLA	CHB-C4A-NA	2.61	128.16	124.40
14	A	845	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
14	A	816	CLA	CHB-C4A-NA	2.59	128.14	124.40
14	A	825	CLA	CHB-C4A-NA	2.59	128.13	124.40
14	A	803	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
14	B	3037	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
16	B	3047	BCR	C15-C16-C17	-2.58	118.24	123.52
14	A	856	CLA	C4-C3-C5	2.58	119.71	115.23
16	J	104	BCR	C15-C16-C17	-2.58	118.25	123.52
13	A	801	CL0	O1D-CGD-CBD	2.58	129.60	124.52
14	B	3031	CLA	O2D-CGD-CBD	2.58	115.73	111.23
16	A	848	BCR	C15-C16-C17	-2.57	118.26	123.52
16	A	847	BCR	C27-C26-C25	2.57	126.17	122.70
14	A	856	CLA	O2D-CGD-CBD	2.56	115.71	111.23
16	I	105	BCR	C15-C16-C17	-2.56	118.28	123.52
16	J	103	BCR	C27-C26-C25	2.56	126.16	122.70
16	B	3047	BCR	C2-C1-C6	2.55	114.14	110.44
14	B	3011	CLA	C2A-C1A-CHA	2.55	128.29	123.87
14	A	844	CLA	CMB-C2B-C1B	-2.55	121.54	125.42
14	B	3036	CLA	CHB-C4A-NA	2.55	128.07	124.40
16	J	104	BCR	C24-C23-C22	-2.54	122.47	126.23
14	A	843	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
14	A	830	CLA	C3B-C4B-NB	-2.54	108.26	110.53
14	B	3004	CLA	O2A-CGA-O1A	-2.54	117.28	123.63
14	A	808	CLA	O2D-CGD-CBD	2.54	115.67	111.23
14	B	3009	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
14	A	810	CLA	CHB-C4A-NA	2.53	128.05	124.40
14	K	101	CLA	CHB-C4A-NA	2.52	128.04	124.40
14	A	842	CLA	C1-C2-C3	-2.52	122.06	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	206	DGD	O3G-C1D-C2D	-2.52	104.45	108.27
13	A	801	CL0	CHB-C4A-NA	2.52	128.03	124.40
14	L	203	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
14	B	3031	CLA	CHB-C4A-NA	2.52	128.03	124.40
14	B	3024	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
14	B	3040	CLA	C3B-C4B-NB	-2.51	108.29	110.53
14	A	807	CLA	CHB-C4A-NA	2.51	128.03	124.40
14	B	3006	CLA	O2D-CGD-CBD	2.51	115.62	111.23
14	B	3004	CLA	C2D-C1D-ND	-2.51	107.64	110.13
14	A	811	CLA	C3B-C4B-NB	-2.51	108.29	110.53
17	A	852	LMG	C1-O6-C5	-2.50	108.83	113.72
14	B	3006	CLA	C3B-C4B-NB	-2.50	108.30	110.53
14	A	821	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
14	A	806	CLA	CHB-C4A-NA	2.50	128.00	124.40
16	A	851	BCR	C28-C27-C26	-2.49	109.61	114.06
14	A	819	CLA	C1-C2-C3	-2.49	122.12	126.20
14	B	3018	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
14	A	810	CLA	C3B-C4B-NB	-2.49	108.31	110.53
14	B	3025	CLA	C2A-C1A-CHA	2.49	128.18	123.87
14	B	3035	CLA	C3B-C4B-NB	-2.49	108.31	110.53
14	B	3032	CLA	CMB-C2B-C1B	-2.48	121.64	125.42
18	A	853	LHG	O8-C23-C24	2.48	119.40	111.83
14	B	3012	CLA	CHB-C4A-NA	2.48	127.98	124.40
14	A	831	CLA	CHB-C4A-NA	2.48	127.98	124.40
16	J	104	BCR	C27-C26-C25	2.47	126.05	122.70
22	L	206	DGD	O6E-C1E-O5D	-2.47	104.20	110.04
16	L	207	BCR	C33-C5-C6	-2.47	121.79	124.48
21	L	201	LMT	C1'-C2'-C3'	2.47	115.20	110.01
14	A	809	CLA	C1-C2-C3	-2.47	122.16	126.20
14	B	3034	CLA	CAA-CBA-CGA	-2.46	106.21	113.21
14	B	3012	CLA	C3B-C4B-NB	-2.46	108.33	110.53
14	B	3041	CLA	C7-C6-C5	-2.46	106.70	113.26
16	A	849	BCR	C33-C5-C6	-2.46	121.80	124.48
14	A	803	CLA	CHB-C4A-NA	2.46	127.95	124.40
14	A	812	CLA	CHB-C4A-NA	2.46	127.95	124.40
14	A	836	CLA	CHB-C4A-NA	2.46	127.95	124.40
16	B	3044	BCR	C33-C5-C6	-2.46	121.81	124.48
14	B	3038	CLA	CHB-C4A-NA	2.46	127.94	124.40
22	L	206	DGD	O6D-C1D-O3G	-2.45	104.24	110.04
16	B	3043	BCR	C33-C5-C6	-2.45	121.81	124.48
14	A	832	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
17	A	852	LMG	C7-O1-C1	2.45	119.05	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	849	BCR	C15-C14-C13	-2.45	123.84	127.28
14	A	806	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
14	B	3030	CLA	C3B-C4B-NB	-2.44	108.35	110.53
16	J	104	BCR	C33-C5-C6	-2.44	121.83	124.48
14	B	3023	CLA	C3B-C4B-NB	-2.43	108.36	110.53
14	B	3018	CLA	O2A-CGA-O1A	-2.43	117.54	123.63
14	B	3033	CLA	CHB-C4A-NA	2.43	127.91	124.40
14	B	3037	CLA	CHB-C4A-NA	2.43	127.91	124.40
14	A	823	CLA	C3B-C4B-NB	-2.43	108.36	110.53
14	B	3034	CLA	CAA-C2A-C1A	-2.43	104.01	111.97
14	B	3035	CLA	CHB-C4A-NA	2.43	127.91	124.40
14	B	3011	CLA	C4-C3-C5	2.43	119.45	115.23
16	F	201	BCR	C16-C15-C14	-2.43	118.55	123.52
14	A	828	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
16	A	850	BCR	C33-C5-C6	-2.42	121.84	124.48
14	A	826	CLA	CHB-C4A-NA	2.42	127.89	124.40
16	A	850	BCR	C2-C1-C6	2.42	113.95	110.44
16	A	848	BCR	C2-C1-C6	2.42	113.95	110.44
16	A	847	BCR	C15-C16-C17	-2.42	118.57	123.52
14	X	1701	CLA	C3B-C4B-NB	-2.41	108.38	110.53
14	M	102	CLA	CMA-C3A-C4A	2.41	118.26	111.77
16	J	105	BCR	C15-C16-C17	-2.41	118.59	123.52
16	A	850	BCR	C37-C22-C21	-2.41	118.92	122.82
14	B	3009	CLA	C3B-C4B-NB	-2.41	108.38	110.53
16	L	207	BCR	C38-C26-C25	-2.41	121.86	124.48
16	B	3047	BCR	C27-C26-C25	2.40	125.95	122.70
16	J	105	BCR	C11-C10-C9	-2.40	123.91	127.28
14	I	101	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
14	A	827	CLA	CHB-C4A-NA	2.39	127.85	124.40
14	B	3020	CLA	O2D-CGD-CBD	2.39	115.41	111.23
14	B	3007	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
14	B	3022	CLA	CHB-C4A-NA	2.39	127.85	124.40
16	I	103	BCR	C7-C8-C9	-2.39	122.71	126.23
14	B	3010	CLA	CBA-CAA-C2A	-2.38	106.71	113.79
14	A	819	CLA	CHB-C4A-NA	2.38	127.83	124.40
14	A	835	CLA	CHB-C4A-NA	2.38	127.83	124.40
14	A	822	CLA	CHB-C4A-NA	2.38	127.83	124.40
14	B	3010	CLA	CMB-C2B-C1B	-2.37	121.80	125.42
14	B	3026	CLA	C3B-C4B-NB	-2.37	108.41	110.53
14	J	101	CLA	CHB-C4A-NA	2.37	127.82	124.40
14	B	3017	CLA	CHB-C4A-NA	2.37	127.82	124.40
14	A	819	CLA	O2A-CGA-O1A	-2.37	117.71	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	3045	BCR	C33-C5-C6	-2.36	121.91	124.48
16	J	105	BCR	C3-C4-C5	-2.36	109.84	114.06
14	B	3021	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
16	B	3047	BCR	C8-C7-C6	-2.36	120.70	127.00
14	A	819	CLA	CHB-C1B-NB	2.36	127.59	124.05
16	B	3047	BCR	C33-C5-C6	-2.36	121.91	124.48
14	B	3041	CLA	C4-C3-C5	2.36	119.32	115.23
14	B	3006	CLA	CHB-C4A-NA	2.35	127.79	124.40
16	J	103	BCR	C15-C14-C13	-2.35	123.98	127.28
14	B	3029	CLA	C1-C2-C3	-2.35	122.35	126.20
14	A	813	CLA	O2D-CGD-CBD	2.35	115.34	111.23
15	A	846	PQN	C10-C1-C2	2.35	122.23	118.97
14	A	841	CLA	CHB-C4A-NA	2.34	127.78	124.40
14	B	3013	CLA	CHB-C4A-NA	2.34	127.78	124.40
14	B	3030	CLA	C2A-C1A-CHA	2.34	127.93	123.87
14	A	808	CLA	CHB-C4A-NA	2.34	127.78	124.40
14	B	3011	CLA	CHA-C1A-NA	-2.34	121.09	126.39
16	A	847	BCR	C8-C7-C6	-2.34	120.76	127.00
14	A	828	CLA	CHB-C4A-NA	2.33	127.77	124.40
14	L	205	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
14	B	3028	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
16	I	103	BCR	C27-C26-C25	2.33	125.85	122.70
14	B	3041	CLA	CAA-CBA-CGA	-2.33	106.60	113.21
14	B	3007	CLA	C3B-C4B-NB	-2.32	108.46	110.53
16	B	3046	BCR	C27-C26-C25	2.32	125.84	122.70
14	I	101	CLA	CHB-C4A-NA	2.32	127.75	124.40
14	B	3039	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
14	A	822	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
15	B	3042	PQN	O4-C4-C3	-2.31	116.95	120.67
14	B	3019	CLA	O2D-CGD-O1D	-2.31	119.34	123.85
14	B	3022	CLA	C3B-C4B-NB	-2.31	108.47	110.53
14	A	830	CLA	C1-C2-C3	-2.31	122.42	126.20
14	B	3032	CLA	CHB-C4A-NA	2.31	127.73	124.40
14	B	3017	CLA	C3B-C4B-NB	-2.30	108.47	110.53
14	A	827	CLA	CAA-C2A-C1A	-2.30	104.44	111.97
16	I	102	BCR	C35-C13-C14	-2.30	119.09	122.82
17	A	852	LMG	C1-C2-C3	-2.30	105.18	110.01
16	M	103	BCR	C27-C26-C25	2.30	125.81	122.70
17	B	3048	LMG	C4-C3-C2	-2.30	106.80	110.83
17	B	3048	LMG	C40-C39-C38	-2.29	102.77	114.37
14	B	3012	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
14	A	814	CLA	CHB-C4A-NA	2.29	127.71	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3028	CLA	C4-C3-C5	2.29	119.21	115.23
16	I	103	BCR	C33-C5-C6	-2.29	121.98	124.48
14	A	829	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
16	K	102	BCR	C35-C13-C12	2.29	121.58	118.09
14	L	203	CLA	C5-C3-C2	2.29	126.30	121.17
16	A	851	BCR	C15-C16-C17	-2.29	118.84	123.52
16	B	3045	BCR	C27-C26-C25	2.29	125.79	122.70
14	A	813	CLA	CHB-C4A-NA	2.28	127.70	124.40
14	B	3020	CLA	CHB-C4A-NA	2.28	127.69	124.40
14	A	821	CLA	CMA-C3A-C2A	-2.28	111.00	116.23
16	K	102	BCR	C15-C16-C17	-2.28	118.86	123.52
14	B	3019	CLA	CHB-C4A-NA	2.28	127.68	124.40
14	A	821	CLA	O2D-CGD-CBD	2.28	115.21	111.23
14	B	3021	CLA	CHB-C4A-NA	2.27	127.68	124.40
14	L	204	CLA	CHB-C4A-NA	2.27	127.68	124.40
16	F	201	BCR	C8-C7-C6	-2.27	120.94	127.00
14	I	101	CLA	C4D-CHA-C1A	2.27	123.95	121.24
14	A	806	CLA	O1D-CGD-CBD	2.27	128.99	124.52
14	A	810	CLA	C6-C5-C3	2.27	118.99	113.47
16	L	207	BCR	C27-C26-C25	2.27	125.77	122.70
16	B	3046	BCR	C24-C23-C22	-2.26	122.89	126.23
17	B	3048	LMG	C3-C4-C5	-2.26	106.13	110.23
14	A	811	CLA	CAA-C2A-C3A	2.26	119.11	113.00
14	A	810	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
14	A	837	CLA	CHB-C4A-NA	2.25	127.65	124.40
14	A	838	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
17	A	855	LMG	O3-C3-C2	-2.25	105.06	110.38
15	B	3042	PQN	C5-C4-C3	2.25	122.40	118.27
15	A	846	PQN	O4-C4-C3	-2.25	117.06	120.67
16	B	3044	BCR	C27-C26-C25	2.25	125.74	122.70
14	B	3038	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
16	F	201	BCR	C33-C5-C6	-2.25	122.03	124.48
14	A	840	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
14	A	823	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
14	A	842	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
22	L	206	DGD	CDB-CCB-CBB	-2.25	103.01	114.37
14	A	820	CLA	C1-C2-C3	-2.24	122.52	126.20
14	L	204	CLA	O2D-CGD-CBD	2.24	115.15	111.23
13	A	801	CL0	C1-O2A-CGA	2.24	122.07	116.65
14	A	809	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
14	B	3024	CLA	CHB-C4A-NA	2.23	127.62	124.40
14	B	3040	CLA	CHB-C4A-NA	2.23	127.62	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	802	CLA	CHD-C1D-ND	-2.23	121.66	124.80
14	B	3004	CLA	CHB-C4A-NA	2.23	127.62	124.40
14	B	3032	CLA	O1D-CGD-CBD	2.23	128.92	124.52
16	B	3045	BCR	C15-C16-C17	-2.23	118.96	123.52
14	A	844	CLA	CHB-C4A-NA	2.23	127.62	124.40
16	B	3047	BCR	C16-C15-C14	-2.23	118.96	123.52
14	B	3011	CLA	O2D-CGD-O1D	-2.23	119.51	123.85
14	B	3030	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
14	A	825	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
14	B	3033	CLA	C1-C2-C3	-2.22	122.56	126.20
16	B	3043	BCR	C28-C27-C26	-2.22	110.09	114.06
14	A	822	CLA	CMB-C2B-C3B	2.22	131.77	126.55
16	B	3045	BCR	C15-C14-C13	-2.22	124.17	127.28
14	B	3025	CLA	C1-O2A-CGA	2.21	122.01	116.65
18	A	853	LHG	C18-C17-C16	-2.21	103.18	114.37
14	A	802	CLA	O1D-CGD-CBD	2.21	128.88	124.52
16	B	3046	BCR	C11-C10-C9	-2.21	124.18	127.28
14	A	843	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
14	A	830	CLA	CHB-C4A-NA	2.21	127.59	124.40
14	A	840	CLA	O2D-CGD-CBD	2.21	115.09	111.23
14	A	802	CLA	C3B-C4B-NB	-2.21	108.56	110.53
17	I	104	LMG	O2-C2-C1	-2.20	104.82	110.08
14	A	826	CLA	C11-C10-C8	-2.20	108.64	115.97
17	A	855	LMG	C1-O6-C5	-2.20	109.42	113.72
14	B	3019	CLA	C1-O2A-CGA	2.20	121.97	116.65
22	L	206	DGD	C5B-C4B-C3B	-2.20	103.26	114.37
16	A	847	BCR	C38-C26-C25	-2.20	122.09	124.48
14	A	812	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
14	A	832	CLA	C1-C2-C3	-2.20	123.21	126.76
14	A	836	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
14	B	3039	CLA	C1-C2-C3	-2.20	122.60	126.20
16	A	849	BCR	C7-C8-C9	-2.19	122.99	126.23
14	A	832	CLA	C2A-C1A-CHA	2.19	127.67	123.87
14	B	3018	CLA	C2A-C1A-CHA	2.19	127.67	123.87
16	J	103	BCR	C24-C23-C22	-2.19	122.99	126.23
14	A	820	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
16	J	105	BCR	C15-C14-C13	-2.19	124.21	127.28
14	M	102	CLA	CHC-C4B-NB	2.19	127.33	124.05
14	A	827	CLA	O2D-CGD-CBD	2.19	115.05	111.23
14	A	838	CLA	CHB-C4A-NA	2.18	127.55	124.40
14	A	803	CLA	CAA-CBA-CGA	-2.18	107.02	113.21
14	M	102	CLA	O2D-CGD-CBD	2.18	115.04	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	J	102	CLA	CHB-C4A-NA	2.18	127.54	124.40
14	B	3010	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
14	B	3023	CLA	CHB-C4A-NA	2.18	127.54	124.40
16	A	851	BCR	C24-C23-C22	-2.18	123.02	126.23
14	A	819	CLA	CMB-C2B-C1B	-2.18	122.11	125.42
16	B	3044	BCR	C16-C15-C14	-2.17	119.07	123.52
15	A	846	PQN	C5-C4-C3	2.17	122.25	118.27
22	L	206	DGD	CBB-CAB-C9B	-2.17	103.40	114.37
14	A	829	CLA	C1-C2-C3	-2.17	122.64	126.20
16	I	105	BCR	C37-C22-C21	-2.17	119.30	122.82
14	A	831	CLA	C3B-C4B-NB	-2.17	108.59	110.53
14	A	826	CLA	O2D-CGD-CBD	2.17	115.02	111.23
16	A	850	BCR	C15-C16-C17	-2.17	119.09	123.52
16	J	103	BCR	C15-C16-C17	-2.17	119.09	123.52
16	A	847	BCR	C24-C23-C22	-2.16	123.03	126.23
14	A	828	CLA	C1-C2-C3	-2.16	122.65	126.20
17	I	104	LMG	O8-C28-O10	-2.16	118.22	123.63
16	A	848	BCR	C15-C14-C13	-2.16	124.25	127.28
17	A	852	LMG	O7-C10-O9	-2.16	118.66	123.70
14	A	845	CLA	C3B-C4B-NB	-2.16	108.60	110.53
16	B	3050	BCR	C11-C10-C9	-2.16	124.25	127.28
14	B	3004	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
14	B	3014	CLA	O2D-CGD-CBD	2.15	114.99	111.23
14	A	834	CLA	C1-O2A-CGA	2.15	121.85	116.65
14	A	844	CLA	O2D-CGD-CBD	2.15	114.98	111.23
16	F	203	BCR	C38-C26-C25	-2.15	122.14	124.48
22	L	206	DGD	CFB-CEB-CDB	-2.15	103.52	114.37
14	B	3034	CLA	CHB-C4A-NA	2.15	127.50	124.40
16	J	104	BCR	C15-C14-C13	-2.15	124.27	127.28
16	K	102	BCR	C40-C30-C25	2.15	113.61	110.24
14	B	3032	CLA	CED-O2D-CGD	2.15	120.78	115.92
14	A	812	CLA	CAC-C3C-C4C	2.14	127.58	124.79
14	B	3033	CLA	O2D-CGD-CBD	2.14	114.98	111.23
13	A	801	CL0	O2A-CGA-O1A	-2.14	118.27	123.63
14	A	821	CLA	CHB-C4A-NA	2.14	127.49	124.40
16	B	3043	BCR	C24-C23-C22	-2.14	123.07	126.23
14	K	101	CLA	O2A-CGA-O1A	-2.14	117.83	123.33
16	I	105	BCR	C38-C26-C27	-2.14	109.04	113.60
16	B	3046	BCR	C15-C14-C13	-2.14	124.28	127.28
14	A	824	CLA	CHB-C4A-NA	2.14	127.48	124.40
14	A	828	CLA	O1D-CGD-CBD	2.14	128.73	124.52
14	J	102	CLA	CAC-C3C-C4C	2.13	127.57	124.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3031	CLA	C3A-C2A-C1A	2.13	104.53	101.34
14	B	3032	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
14	A	805	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
14	B	3004	CLA	O2D-CGD-O1D	-2.13	119.70	123.85
16	B	3045	BCR	C2-C1-C6	2.13	113.53	110.44
15	A	846	PQN	C2M-C2-C1	2.13	120.59	116.68
14	B	3016	CLA	C3B-C4B-NB	-2.13	108.63	110.53
17	A	852	LMG	O3-C3-C2	-2.13	105.37	110.38
14	A	856	CLA	C3B-C4B-NB	-2.12	108.63	110.53
14	A	841	CLA	C3B-C4B-NB	-2.12	108.64	110.53
16	I	102	BCR	C30-C25-C26	-2.12	119.74	122.64
16	K	102	BCR	C33-C5-C6	-2.12	122.17	124.48
16	B	3050	BCR	C7-C8-C9	-2.12	123.10	126.23
14	A	815	CLA	CHB-C4A-NA	2.12	127.45	124.40
14	B	3024	CLA	O1D-CGD-CBD	2.12	128.69	124.52
14	A	856	CLA	O2A-CGA-O1A	-2.12	118.34	123.63
16	B	3050	BCR	C16-C15-C14	-2.11	119.19	123.52
14	A	840	CLA	CHB-C4A-NA	2.11	127.45	124.40
14	L	203	CLA	C6-C7-C8	-2.11	108.94	115.97
14	B	3034	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
16	B	3043	BCR	C15-C16-C17	-2.11	119.20	123.52
14	B	3028	CLA	CHC-C4B-NB	2.11	127.21	124.05
14	L	205	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
14	B	3012	CLA	C3A-C2A-C1A	2.11	104.50	101.34
14	A	821	CLA	CMB-C2B-C3B	2.11	131.51	126.55
14	A	835	CLA	C5-C3-C2	2.11	125.90	121.17
14	F	202	CLA	CHB-C1B-NB	2.11	127.21	124.05
14	A	845	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
16	B	3045	BCR	C8-C7-C6	-2.10	121.38	127.00
14	B	3039	CLA	CHB-C4A-NA	2.10	127.43	124.40
14	B	3029	CLA	C3B-C4B-NB	-2.10	108.66	110.53
14	B	3022	CLA	O2A-CGA-O1A	-2.10	117.94	123.33
16	J	105	BCR	C33-C5-C6	-2.10	122.20	124.48
14	A	811	CLA	O2A-CGA-O1A	-2.09	117.94	123.33
14	A	833	CLA	CHB-C4A-NA	2.09	127.42	124.40
14	A	804	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
14	A	820	CLA	C2A-C1A-CHA	2.09	127.50	123.87
14	A	824	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
14	A	839	CLA	CMB-C2B-C3B	2.09	131.46	126.55
16	K	102	BCR	C16-C15-C14	-2.09	119.25	123.52
14	A	805	CLA	CHB-C4A-NA	2.09	127.41	124.40
16	J	103	BCR	C38-C26-C25	-2.09	122.21	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L	205	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
14	B	3016	CLA	O2D-CGD-CBD	2.09	114.88	111.23
14	A	815	CLA	O2A-CGA-O1A	-2.08	117.97	123.33
14	B	3027	CLA	O2A-CGA-O1A	-2.08	118.41	123.63
14	J	102	CLA	CMA-C3A-C2A	-2.08	111.45	116.23
16	B	3044	BCR	C8-C7-C6	-2.08	121.43	127.00
14	A	832	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
16	I	105	BCR	C36-C18-C17	-2.08	119.44	122.82
14	A	811	CLA	O2D-CGD-CBD	2.08	114.86	111.23
15	B	3042	PQN	C10-C1-C2	2.08	121.86	118.97
16	B	3050	BCR	C35-C13-C12	2.08	121.26	118.09
15	B	3042	PQN	C2M-C2-C3	-2.08	121.04	124.45
14	A	844	CLA	C6-C7-C8	-2.08	109.06	115.97
14	M	102	CLA	CAC-C3C-C4C	2.08	127.49	124.79
18	A	853	LHG	C20-C19-C18	-2.07	103.91	114.37
14	J	102	CLA	C3B-C4B-NB	-2.07	108.68	110.53
14	A	827	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
14	B	3028	CLA	CBC-CAC-C3C	-2.06	106.82	112.42
16	B	3047	BCR	C30-C25-C26	-2.06	119.82	122.64
14	J	102	CLA	CAA-C2A-C3A	-2.06	111.51	116.23
21	L	201	LMT	O1B-C4'-C3'	2.06	112.46	107.23
14	A	834	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
14	A	824	CLA	CHD-C1D-ND	-2.06	121.91	124.80
14	A	839	CLA	C1-C2-C3	-2.06	122.83	126.20
16	A	848	BCR	C35-C13-C14	-2.06	119.49	122.82
14	A	832	CLA	O1D-CGD-CBD	2.05	128.57	124.52
14	B	3024	CLA	CAC-C3C-C4C	2.05	127.46	124.79
14	A	835	CLA	C4-C3-C2	-2.05	118.36	123.63
14	A	808	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
16	J	104	BCR	C38-C26-C25	-2.05	122.25	124.48
16	B	3050	BCR	C30-C25-C26	-2.05	119.84	122.64
14	A	840	CLA	CAC-C3C-C4C	2.05	127.45	124.79
14	A	817	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
16	I	105	BCR	C15-C14-C13	-2.05	124.41	127.28
14	L	205	CLA	CMB-C2B-C3B	2.05	131.36	126.55
16	B	3045	BCR	C7-C8-C9	-2.04	123.21	126.23
14	B	3012	CLA	CMB-C2B-C3B	2.04	131.36	126.55
14	A	819	CLA	CMB-C2B-C3B	2.04	131.35	126.55
14	A	802	CLA	CHB-C4A-NA	2.04	127.34	124.40
14	B	3026	CLA	CHA-C1A-NA	-2.04	121.77	126.39
14	A	823	CLA	C2A-C1A-CHA	2.04	127.40	123.87
16	A	850	BCR	C8-C7-C6	-2.04	121.56	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3025	CLA	CHA-C1A-NA	-2.03	121.78	126.39
14	B	3010	CLA	O1D-CGD-CBD	2.03	128.53	124.52
14	B	3017	CLA	O2D-CGD-CBD	2.03	114.78	111.23
14	B	3032	CLA	CMB-C2B-C3B	2.03	131.33	126.55
17	B	3048	LMG	C38-C37-C36	-2.03	104.11	114.37
14	K	103	CLA	CHB-C4A-NA	2.03	127.32	124.40
16	B	3044	BCR	C28-C27-C26	-2.03	110.44	114.06
14	A	820	CLA	CAA-CBA-CGA	-2.02	107.46	113.21
14	A	821	CLA	CHD-C1D-ND	-2.02	121.95	124.80
16	I	102	BCR	C8-C7-C6	-2.02	121.59	127.00
14	A	817	CLA	CHB-C4A-NA	2.02	127.32	124.40
16	L	207	BCR	C16-C15-C14	-2.02	119.38	123.52
14	B	3019	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
14	B	3038	CLA	C3B-C4B-NB	-2.02	108.73	110.53
17	A	855	LMG	O1-C7-C8	-2.02	105.92	110.82
14	B	3013	CLA	C3A-C2A-C1A	2.02	104.36	101.34
14	B	3039	CLA	O2D-CGD-O1D	-2.02	119.92	123.85
14	B	3034	CLA	C3B-C4B-NB	-2.01	108.73	110.53
14	A	831	CLA	O1D-CGD-CBD	2.01	128.49	124.52
14	F	202	CLA	CHA-C1A-NA	-2.01	121.84	126.39
16	K	102	BCR	C3-C4-C5	-2.01	110.47	114.06
18	M	101	LHG	C20-C19-C18	-2.01	104.21	114.37
14	B	3032	CLA	CHB-C1B-NB	2.01	127.06	124.05
14	M	102	CLA	CGD-CBD-CAD	2.01	117.35	110.85
14	B	3020	CLA	C1-C2-C3	-2.01	122.91	126.20
16	M	103	BCR	C28-C27-C26	-2.01	110.48	114.06
17	B	3048	LMG	C42-C41-C40	-2.01	104.23	114.37
16	B	3046	BCR	C33-C5-C6	-2.00	122.30	124.48
18	A	854	LHG	C11-C10-C9	-2.00	104.24	114.37
13	A	801	CL0	CED-O2D-CGD	2.00	120.45	115.92

There are no chirality outliers.

All (1219) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	801	CL0	C1A-C2A-CAA-CBA
13	A	801	CL0	C3A-C2A-CAA-CBA
14	A	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	806	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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
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	C3A-C2A-CAA-CBA
14	A	821	CLA	CHA-CBD-CGD-O1D
14	A	821	CLA	CHA-CBD-CGD-O2D
14	A	823	CLA	C1A-C2A-CAA-CBA
14	A	823	CLA	C3A-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	830	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	834	CLA	C2B-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	835	CLA	CHA-CBD-CGD-O1D
14	A	835	CLA	CHA-CBD-CGD-O2D
14	A	837	CLA	C1A-C2A-CAA-CBA
14	A	838	CLA	CBD-CGD-O2D-CED
14	A	843	CLA	C1A-C2A-CAA-CBA
14	A	845	CLA	CBD-CGD-O2D-CED
14	B	3003	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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	3009	CLA	CHA-CBD-CGD-O1D
14	B	3009	CLA	CHA-CBD-CGD-O2D
14	B	3012	CLA	CBD-CGD-O2D-CED
14	B	3016	CLA	CBD-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	CHA-CBD-CGD-O1D
14	B	3022	CLA	CHA-CBD-CGD-O2D
14	B	3022	CLA	CBD-CGD-O2D-CED
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	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	F	202	CLA	C2B-C3B-CAB-CBB
14	F	202	CLA	C4B-C3B-CAB-CBB
14	J	101	CLA	C1A-C2A-CAA-CBA
14	J	101	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	K	103	CLA	C1A-C2A-CAA-CBA
14	K	103	CLA	C3A-C2A-CAA-CBA
14	K	103	CLA	C4B-C3B-CAB-CBB
14	L	203	CLA	C1A-C2A-CAA-CBA
14	L	203	CLA	C3A-C2A-CAA-CBA
14	M	102	CLA	CBD-CGD-O2D-CED
16	A	847	BCR	C7-C8-C9-C10
16	A	847	BCR	C16-C17-C18-C36
16	A	847	BCR	C22-C23-C24-C25
16	A	848	BCR	C11-C10-C9-C8
16	A	849	BCR	C21-C22-C23-C24
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	C18-C19-C20-C21
16	A	851	BCR	C20-C21-C22-C23
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	3043	BCR	C21-C22-C23-C24
16	B	3044	BCR	C6-C7-C8-C9
16	B	3044	BCR	C7-C8-C9-C34
16	B	3044	BCR	C11-C10-C9-C8
16	B	3044	BCR	C21-C22-C23-C24
16	B	3045	BCR	C11-C10-C9-C8
16	B	3045	BCR	C11-C10-C9-C34
16	B	3045	BCR	C10-C11-C12-C13
16	B	3046	BCR	C7-C8-C9-C10
16	B	3046	BCR	C7-C8-C9-C34
16	B	3046	BCR	C10-C11-C12-C13
16	B	3046	BCR	C11-C12-C13-C35
16	B	3046	BCR	C16-C17-C18-C36
16	B	3046	BCR	C20-C21-C22-C37
16	B	3047	BCR	C18-C19-C20-C21
16	B	3050	BCR	C11-C12-C13-C14
16	B	3050	BCR	C11-C12-C13-C35
16	F	201	BCR	C37-C22-C23-C24
16	F	203	BCR	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	I	102	BCR	C7-C8-C9-C34
16	I	102	BCR	C20-C21-C22-C23
16	I	103	BCR	C7-C8-C9-C34
16	I	103	BCR	C11-C10-C9-C8
16	I	103	BCR	C20-C21-C22-C23
16	I	103	BCR	C20-C21-C22-C37
16	I	105	BCR	C7-C8-C9-C34
16	I	105	BCR	C11-C10-C9-C34
16	I	105	BCR	C11-C12-C13-C14
16	I	105	BCR	C36-C18-C19-C20
16	I	105	BCR	C20-C21-C22-C37
16	J	103	BCR	C1-C6-C7-C8
16	J	103	BCR	C5-C6-C7-C8
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	C21-C22-C23-C24
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	C16-C17-C18-C36
16	K	102	BCR	C18-C19-C20-C21
16	K	102	BCR	C21-C22-C23-C24
16	K	102	BCR	C37-C22-C23-C24
16	L	207	BCR	C6-C7-C8-C9
16	L	207	BCR	C7-C8-C9-C10
16	L	207	BCR	C7-C8-C9-C34
16	L	207	BCR	C11-C10-C9-C8
16	L	207	BCR	C11-C10-C9-C34
16	M	103	BCR	C1-C6-C7-C8
16	M	103	BCR	C5-C6-C7-C8
16	M	103	BCR	C11-C10-C9-C8
17	A	852	LMG	O9-C10-O7-C8
17	A	855	LMG	O6-C1-O1-C7
17	A	855	LMG	O9-C10-O7-C8
17	B	3048	LMG	C2-C1-O1-C7
17	I	104	LMG	O6-C1-O1-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	A	853	LHG	C3-O3-P-O5
18	A	854	LHG	C1-C2-C3-O3
18	B	3049	LHG	C1-C2-C3-O3
18	B	3049	LHG	C3-O3-P-O4
18	B	3049	LHG	C4-O6-P-O3
18	B	3049	LHG	C4-O6-P-O4
18	B	3049	LHG	C4-O6-P-O5
18	B	3049	LHG	C8-C7-O7-C5
18	M	101	LHG	C3-O3-P-O4
18	M	101	LHG	C3-O3-P-O6
18	M	101	LHG	C4-O6-P-O3
22	L	206	DGD	O6D-C1D-O3G-C3G
14	A	807	CLA	O1D-CGD-O2D-CED
14	A	817	CLA	O1D-CGD-O2D-CED
14	A	820	CLA	O1D-CGD-O2D-CED
14	A	845	CLA	O1D-CGD-O2D-CED
14	B	3003	CLA	O1D-CGD-O2D-CED
14	B	3012	CLA	O1D-CGD-O2D-CED
14	B	3013	CLA	O1D-CGD-O2D-CED
14	B	3032	CLA	O1D-CGD-O2D-CED
14	B	3035	CLA	O1D-CGD-O2D-CED
14	A	807	CLA	CBD-CGD-O2D-CED
14	A	820	CLA	CBD-CGD-O2D-CED
14	A	822	CLA	CBD-CGD-O2D-CED
14	A	823	CLA	CBD-CGD-O2D-CED
14	A	836	CLA	CBD-CGD-O2D-CED
14	A	841	CLA	CBD-CGD-O2D-CED
14	A	842	CLA	CBD-CGD-O2D-CED
14	B	3006	CLA	CBD-CGD-O2D-CED
14	B	3013	CLA	CBD-CGD-O2D-CED
14	B	3020	CLA	CBD-CGD-O2D-CED
14	B	3034	CLA	CBD-CGD-O2D-CED
14	B	3036	CLA	CBD-CGD-O2D-CED
14	B	3037	CLA	CBD-CGD-O2D-CED
14	F	202	CLA	CBD-CGD-O2D-CED
14	A	829	CLA	O1D-CGD-O2D-CED
14	B	3004	CLA	O1D-CGD-O2D-CED
14	A	822	CLA	O1D-CGD-O2D-CED
14	A	823	CLA	O1D-CGD-O2D-CED
14	B	3006	CLA	O1D-CGD-O2D-CED
14	B	3036	CLA	O1D-CGD-O2D-CED
14	B	3037	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	A	801	CL0	O1A-CGA-O2A-C1
14	A	806	CLA	O1A-CGA-O2A-C1
14	A	820	CLA	O1A-CGA-O2A-C1
14	A	845	CLA	O1A-CGA-O2A-C1
18	M	101	LHG	O10-C23-O8-C6
14	B	3022	CLA	O1D-CGD-O2D-CED
14	A	838	CLA	O1D-CGD-O2D-CED
14	B	3005	CLA	O1D-CGD-O2D-CED
14	B	3016	CLA	O1D-CGD-O2D-CED
14	M	102	CLA	O1D-CGD-O2D-CED
14	A	820	CLA	C3-C5-C6-C7
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	3027	CLA	C3-C5-C6-C7
14	B	3033	CLA	C3-C5-C6-C7
14	I	101	CLA	C3-C5-C6-C7
13	A	801	CL0	CBA-CGA-O2A-C1
14	A	820	CLA	CBA-CGA-O2A-C1
14	B	3032	CLA	CBA-CGA-O2A-C1
18	M	101	LHG	C24-C23-O8-C6
21	L	201	LMT	C3'-C4'-O1B-C1B
14	A	812	CLA	CBD-CGD-O2D-CED
14	A	844	CLA	CBD-CGD-O2D-CED
14	B	3015	CLA	CBD-CGD-O2D-CED
14	B	3021	CLA	CBD-CGD-O2D-CED
14	B	3025	CLA	CBD-CGD-O2D-CED
17	A	855	LMG	C11-C10-O7-C8
14	A	806	CLA	O1D-CGD-O2D-CED
14	A	819	CLA	O1D-CGD-O2D-CED
14	B	3034	CLA	O1D-CGD-O2D-CED
14	I	101	CLA	C2C-C3C-CAC-CBC
14	A	830	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	A	806	CLA	C2-C3-C5-C6
14	A	856	CLA	C2-C3-C5-C6
13	A	801	CL0	CBD-CGD-O2D-CED
14	B	3020	CLA	O1D-CGD-O2D-CED
14	A	820	CLA	C2A-CAA-CBA-CGA
14	A	830	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	806	CLA	CBA-CGA-O2A-C1
14	A	817	CLA	CBA-CGA-O2A-C1
14	A	825	CLA	CBA-CGA-O2A-C1
14	A	838	CLA	CBA-CGA-O2A-C1
14	A	845	CLA	CBA-CGA-O2A-C1
14	L	203	CLA	CBA-CGA-O2A-C1
22	L	206	DGD	C2A-C1A-O1G-C1G
14	A	825	CLA	O1A-CGA-O2A-C1
14	A	829	CLA	O1A-CGA-O2A-C1
14	A	838	CLA	O1A-CGA-O2A-C1
14	L	203	CLA	O1A-CGA-O2A-C1
18	B	3049	LHG	O9-C7-O7-C5
14	F	202	CLA	O1D-CGD-O2D-CED
14	A	856	CLA	C3-C5-C6-C7
14	B	3018	CLA	C3-C5-C6-C7
14	A	856	CLA	CBD-CGD-O2D-CED
14	B	3023	CLA	CBD-CGD-O2D-CED
14	B	3031	CLA	CBD-CGD-O2D-CED
18	A	854	LHG	O2-C2-C3-O3
14	A	842	CLA	O1D-CGD-O2D-CED
14	A	812	CLA	CBA-CGA-O2A-C1
14	A	829	CLA	CBA-CGA-O2A-C1
14	B	3032	CLA	O1A-CGA-O2A-C1
14	B	3029	CLA	CBD-CGD-O2D-CED
14	A	845	CLA	C2C-C3C-CAC-CBC
14	A	841	CLA	O1D-CGD-O2D-CED
14	A	836	CLA	O1D-CGD-O2D-CED
14	B	3040	CLA	CBD-CGD-O2D-CED
15	A	846	PQN	C14-C13-C15-C16
14	B	3025	CLA	C2-C3-C5-C6
15	A	846	PQN	C12-C13-C15-C16
14	A	817	CLA	O1A-CGA-O2A-C1
22	L	206	DGD	O1A-C1A-O1G-C1G
17	B	3048	LMG	O6-C5-C6-O5
17	B	3048	LMG	C4-C5-C6-O5
14	B	3016	CLA	C2A-CAA-CBA-CGA
14	I	101	CLA	C2A-CAA-CBA-CGA
17	B	3048	LMG	O6-C1-O1-C7
21	L	201	LMT	O5'-C1'-O1'-C1
22	L	206	DGD	O6E-C1E-O5D-C6D
14	A	808	CLA	CBA-CGA-O2A-C1
14	A	809	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	3021	CLA	CBA-CGA-O2A-C1
14	A	804	CLA	CBD-CGD-O2D-CED
14	A	813	CLA	CBD-CGD-O2D-CED
14	A	816	CLA	CBD-CGD-O2D-CED
14	A	831	CLA	CBD-CGD-O2D-CED
14	A	837	CLA	CBD-CGD-O2D-CED
14	B	3011	CLA	CBD-CGD-O2D-CED
14	B	3030	CLA	CBD-CGD-O2D-CED
14	J	101	CLA	CBD-CGD-O2D-CED
14	A	812	CLA	O1A-CGA-O2A-C1
21	L	201	LMT	O5B-C5B-C6B-O6B
14	A	825	CLA	CBD-CGD-O2D-CED
14	A	808	CLA	O1A-CGA-O2A-C1
14	A	805	CLA	CBA-CGA-O2A-C1
14	A	823	CLA	CBA-CGA-O2A-C1
14	A	836	CLA	CBA-CGA-O2A-C1
14	A	840	CLA	CBA-CGA-O2A-C1
14	A	843	CLA	CBA-CGA-O2A-C1
14	B	3017	CLA	CBA-CGA-O2A-C1
14	B	3021	CLA	O1A-CGA-O2A-C1
14	A	809	CLA	C3-C5-C6-C7
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	3009	CLA	C14-C13-C15-C16
14	B	3020	CLA	C11-C12-C13-C14
14	B	3027	CLA	C11-C10-C8-C9
14	I	101	CLA	C14-C13-C15-C16
15	A	846	PQN	C16-C17-C18-C19
14	A	812	CLA	O1D-CGD-O2D-CED
17	I	104	LMG	C2-C1-O1-C7
21	L	201	LMT	C2'-C1'-O1'-C1
22	L	206	DGD	C2E-C1E-O5D-C6D
14	A	844	CLA	O1D-CGD-O2D-CED
18	A	853	LHG	O10-C23-O8-C6
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	3043	BCR	C7-C8-C9-C34
16	B	3043	BCR	C37-C22-C23-C24
16	B	3044	BCR	C11-C12-C13-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	F	203	BCR	C7-C8-C9-C34
16	I	102	BCR	C37-C22-C23-C24
16	I	105	BCR	C11-C12-C13-C35
16	I	105	BCR	C37-C22-C23-C24
16	J	103	BCR	C11-C12-C13-C35
16	J	104	BCR	C37-C22-C23-C24
16	J	105	BCR	C7-C8-C9-C34
16	L	207	BCR	C11-C12-C13-C35
17	I	104	LMG	O6-C5-C6-O5
16	A	847	BCR	C11-C12-C13-C14
16	B	3050	BCR	C21-C22-C23-C24
14	A	823	CLA	O1A-CGA-O2A-C1
14	A	840	CLA	O1A-CGA-O2A-C1
14	B	3015	CLA	O1D-CGD-O2D-CED
14	A	826	CLA	CBA-CGA-O2A-C1
14	B	3019	CLA	CBA-CGA-O2A-C1
14	A	806	CLA	C2-C1-O2A-CGA
14	B	3030	CLA	C15-C16-C17-C18
14	B	3021	CLA	O1D-CGD-O2D-CED
14	A	843	CLA	O1A-CGA-O2A-C1
14	A	829	CLA	C13-C15-C16-C17
14	B	3004	CLA	C15-C16-C17-C18
14	I	101	CLA	C8-C10-C11-C12
21	L	201	LMT	C4B-C5B-C6B-O6B
14	A	856	CLA	CBA-CGA-O2A-C1
14	B	3018	CLA	CBA-CGA-O2A-C1
14	I	101	CLA	C4C-C3C-CAC-CBC
17	A	852	LMG	C28-C29-C30-C31
14	A	805	CLA	O1A-CGA-O2A-C1
14	A	811	CLA	CBD-CGD-O2D-CED
14	A	807	CLA	C5-C6-C7-C8
14	B	3003	CLA	C8-C10-C11-C12
14	B	3023	CLA	C5-C6-C7-C8
15	B	3042	PQN	C20-C21-C22-C23
13	A	801	CL0	C2A-CAA-CBA-CGA
14	A	808	CLA	C2A-CAA-CBA-CGA
14	B	3013	CLA	C2A-CAA-CBA-CGA
14	B	3029	CLA	C2A-CAA-CBA-CGA
14	B	3033	CLA	C2A-CAA-CBA-CGA
16	A	847	BCR	C18-C19-C20-C21
16	J	104	BCR	C18-C19-C20-C21
15	B	3042	PQN	C23-C25-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	3017	CLA	O1A-CGA-O2A-C1
14	B	3019	CLA	O1A-CGA-O2A-C1
13	A	801	CL0	C13-C15-C16-C17
14	A	802	CLA	C15-C16-C17-C18
14	A	825	CLA	C8-C10-C11-C12
14	A	830	CLA	C8-C10-C11-C12
14	A	834	CLA	C5-C6-C7-C8
18	B	3049	LHG	O2-C2-C3-O3
14	A	809	CLA	O1A-CGA-O2A-C1
17	I	104	LMG	O10-C28-O8-C9
17	A	855	LMG	C10-C11-C12-C13
14	A	845	CLA	C4C-C3C-CAC-CBC
14	A	831	CLA	C10-C11-C12-C13
14	B	3028	CLA	C8-C10-C11-C12
14	A	802	CLA	C3-C5-C6-C7
13	A	801	CL0	O1D-CGD-O2D-CED
14	B	3004	CLA	C10-C11-C12-C13
14	B	3017	CLA	CBD-CGD-O2D-CED
14	A	826	CLA	O1A-CGA-O2A-C1
14	A	836	CLA	O1A-CGA-O2A-C1
14	B	3023	CLA	O1D-CGD-O2D-CED
14	B	3025	CLA	O1D-CGD-O2D-CED
14	A	804	CLA	CBA-CGA-O2A-C1
18	A	853	LHG	C24-C23-O8-C6
14	B	3010	CLA	CBD-CGD-O2D-CED
14	B	3018	CLA	O1A-CGA-O2A-C1
14	A	833	CLA	C10-C11-C12-C13
17	I	104	LMG	O9-C10-O7-C8
14	B	3005	CLA	C2A-CAA-CBA-CGA
14	M	102	CLA	C2A-CAA-CBA-CGA
14	B	3031	CLA	O1D-CGD-O2D-CED
14	A	809	CLA	C5-C6-C7-C8
14	A	810	CLA	C15-C16-C17-C18
14	A	833	CLA	C5-C6-C7-C8
14	B	3004	CLA	C13-C15-C16-C17
14	B	3006	CLA	C13-C15-C16-C17
14	B	3029	CLA	C15-C16-C17-C18
14	L	205	CLA	CBD-CGD-O2D-CED
14	A	856	CLA	O1D-CGD-O2D-CED
14	A	822	CLA	C15-C16-C17-C18
14	A	826	CLA	C15-C16-C17-C18
14	B	3010	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	3014	CLA	C13-C15-C16-C17
15	A	846	PQN	C25-C26-C27-C28
14	B	3040	CLA	O1D-CGD-O2D-CED
14	A	803	CLA	C13-C15-C16-C17
14	A	804	CLA	C10-C11-C12-C13
14	B	3011	CLA	C13-C15-C16-C17
14	B	3034	CLA	C5-C6-C7-C8
14	A	856	CLA	O1A-CGA-O2A-C1
17	A	855	LMG	C2-C1-O1-C7
14	B	3029	CLA	O1D-CGD-O2D-CED
14	A	806	CLA	C16-C17-C18-C20
16	A	847	BCR	C20-C21-C22-C37
16	A	848	BCR	C20-C21-C22-C37
16	A	849	BCR	C16-C17-C18-C36
16	A	850	BCR	C16-C17-C18-C36
16	B	3043	BCR	C20-C21-C22-C37
16	B	3044	BCR	C20-C21-C22-C37
16	B	3046	BCR	C11-C10-C9-C34
16	B	3047	BCR	C11-C10-C9-C34
16	B	3050	BCR	C16-C17-C18-C36
16	F	201	BCR	C20-C21-C22-C37
16	F	203	BCR	C35-C13-C14-C15
16	F	203	BCR	C16-C17-C18-C36
16	F	203	BCR	C20-C21-C22-C37
16	I	105	BCR	C16-C17-C18-C36
16	J	103	BCR	C16-C17-C18-C36
16	J	104	BCR	C11-C10-C9-C34
16	K	102	BCR	C11-C10-C9-C34
16	L	207	BCR	C35-C13-C14-C15
16	M	103	BCR	C11-C10-C9-C34
16	A	847	BCR	C11-C12-C13-C35
16	A	849	BCR	C36-C18-C19-C20
16	B	3050	BCR	C37-C22-C23-C24
16	F	201	BCR	C7-C8-C9-C34
16	J	105	BCR	C11-C12-C13-C35
14	A	814	CLA	C8-C10-C11-C12
18	B	3049	LHG	O1-C1-C2-C3
14	A	803	CLA	CBD-CGD-O2D-CED
14	A	820	CLA	C16-C17-C18-C19
14	A	804	CLA	C3-C5-C6-C7
14	A	833	CLA	C3-C5-C6-C7
14	B	3020	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	A	847	BCR	C16-C17-C18-C19
16	A	850	BCR	C20-C21-C22-C23
16	B	3045	BCR	C12-C13-C14-C15
16	B	3050	BCR	C11-C10-C9-C8
16	B	3050	BCR	C16-C17-C18-C19
16	I	102	BCR	C11-C10-C9-C8
16	I	105	BCR	C11-C10-C9-C8
16	I	105	BCR	C20-C21-C22-C23
16	J	103	BCR	C12-C13-C14-C15
16	J	103	BCR	C16-C17-C18-C19
16	J	105	BCR	C16-C17-C18-C19
16	K	102	BCR	C11-C10-C9-C8
17	A	852	LMG	C11-C10-O7-C8
17	I	104	LMG	C11-C10-O7-C8
18	A	853	LHG	C8-C7-O7-C5
14	A	811	CLA	C2C-C3C-CAC-CBC
14	B	3009	CLA	C13-C15-C16-C17
14	A	826	CLA	C2-C1-O2A-CGA
14	B	3033	CLA	C2-C1-O2A-CGA
14	A	806	CLA	C16-C17-C18-C19
14	A	820	CLA	C16-C17-C18-C20
14	A	839	CLA	C16-C17-C18-C20
14	B	3007	CLA	C16-C17-C18-C20
14	L	205	CLA	C16-C17-C18-C19
15	A	846	PQN	C26-C27-C28-C29
14	A	804	CLA	O1A-CGA-O2A-C1
14	A	816	CLA	O1D-CGD-O2D-CED
17	A	855	LMG	C16-C17-C18-C19
18	M	101	LHG	C32-C33-C34-C35
22	L	206	DGD	C4B-C5B-C6B-C7B
14	A	813	CLA	C3-C5-C6-C7
14	J	101	CLA	O1D-CGD-O2D-CED
14	A	808	CLA	C4B-C3B-CAB-CBB
14	A	832	CLA	C4B-C3B-CAB-CBB
14	B	3006	CLA	C4B-C3B-CAB-CBB
14	B	3008	CLA	C4B-C3B-CAB-CBB
14	M	102	CLA	C4B-C3B-CAB-CBB
14	B	3033	CLA	C16-C17-C18-C20
15	A	846	PQN	C26-C27-C28-C30
14	A	856	CLA	C2A-CAA-CBA-CGA
14	K	101	CLA	C2A-CAA-CBA-CGA
14	K	103	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	820	CLA	C13-C15-C16-C17
18	A	853	LHG	O2-C2-C3-O3
15	A	846	PQN	C15-C16-C17-C18
14	A	836	CLA	C5-C6-C7-C8
14	A	804	CLA	C3A-C2A-CAA-CBA
14	A	806	CLA	C3A-C2A-CAA-CBA
14	A	826	CLA	C3A-C2A-CAA-CBA
14	A	842	CLA	C3A-C2A-CAA-CBA
14	A	843	CLA	C3A-C2A-CAA-CBA
21	L	201	LMT	C1-C2-C3-C4
15	A	846	PQN	C20-C21-C22-C23
14	A	804	CLA	O1D-CGD-O2D-CED
14	B	3030	CLA	O1D-CGD-O2D-CED
16	A	847	BCR	C15-C16-C17-C18
13	A	801	CL0	C16-C17-C18-C20
14	A	813	CLA	O1D-CGD-O2D-CED
14	B	3024	CLA	CBD-CGD-O2D-CED
17	B	3048	LMG	C17-C18-C19-C20
14	A	831	CLA	O1D-CGD-O2D-CED
14	A	837	CLA	O1D-CGD-O2D-CED
14	A	818	CLA	CBA-CGA-O2A-C1
17	I	104	LMG	C29-C28-O8-C9
17	A	852	LMG	C17-C18-C19-C20
14	A	829	CLA	C3-C5-C6-C7
18	M	101	LHG	C7-C8-C9-C10
22	L	206	DGD	C1B-C2B-C3B-C4B
18	A	853	LHG	C12-C13-C14-C15
17	A	852	LMG	C20-C21-C22-C23
14	A	825	CLA	O1D-CGD-O2D-CED
14	B	3011	CLA	C8-C10-C11-C12
17	A	852	LMG	C30-C31-C32-C33
18	M	101	LHG	C14-C15-C16-C17
14	K	103	CLA	C2B-C3B-CAB-CBB
16	A	847	BCR	C23-C24-C25-C30
16	A	849	BCR	C1-C6-C7-C8
16	A	849	BCR	C5-C6-C7-C8
16	A	849	BCR	C23-C24-C25-C26
16	A	849	BCR	C23-C24-C25-C30
16	A	851	BCR	C1-C6-C7-C8
16	B	3044	BCR	C1-C6-C7-C8
16	B	3050	BCR	C1-C6-C7-C8
16	F	203	BCR	C23-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	I	105	BCR	C23-C24-C25-C30
16	J	104	BCR	C23-C24-C25-C30
16	J	105	BCR	C1-C6-C7-C8
16	J	105	BCR	C5-C6-C7-C8
16	K	102	BCR	C23-C24-C25-C26
16	K	102	BCR	C23-C24-C25-C30
16	L	207	BCR	C1-C6-C7-C8
16	M	103	BCR	C23-C24-C25-C26
16	M	103	BCR	C23-C24-C25-C30
17	A	855	LMG	C18-C19-C20-C21
14	A	844	CLA	CBA-CGA-O2A-C1
17	A	852	LMG	C33-C34-C35-C36
14	A	844	CLA	C2A-CAA-CBA-CGA
14	B	3019	CLA	C8-C10-C11-C12
17	A	852	LMG	C23-C24-C25-C26
16	B	3043	BCR	C18-C19-C20-C21
16	B	3044	BCR	C10-C11-C12-C13
16	B	3050	BCR	C10-C11-C12-C13
16	F	201	BCR	C18-C19-C20-C21
16	J	105	BCR	C18-C19-C20-C21
14	L	205	CLA	C16-C17-C18-C20
17	B	3048	LMG	C14-C15-C16-C17
14	B	3034	CLA	CBA-CGA-O2A-C1
14	A	805	CLA	C6-C7-C8-C9
17	B	3048	LMG	C35-C36-C37-C38
14	B	3011	CLA	O1D-CGD-O2D-CED
22	L	206	DGD	C2D-C1D-O3G-C3G
14	A	844	CLA	C5-C6-C7-C8
22	L	206	DGD	C5B-C6B-C7B-C8B
17	A	855	LMG	C13-C14-C15-C16
17	I	104	LMG	C18-C19-C20-C21
18	M	101	LHG	C25-C26-C27-C28
17	B	3048	LMG	C34-C35-C36-C37
14	A	822	CLA	C3-C5-C6-C7
16	J	103	BCR	C11-C12-C13-C14
13	A	801	CL0	C16-C17-C18-C19
14	A	839	CLA	C16-C17-C18-C19
14	B	3010	CLA	C16-C17-C18-C19
14	B	3010	CLA	C16-C17-C18-C20
14	B	3033	CLA	C16-C17-C18-C19
14	B	3033	CLA	C4-C3-C5-C6
14	B	3030	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	818	CLA	O1A-CGA-O2A-C1
14	A	844	CLA	O1A-CGA-O2A-C1
14	A	839	CLA	C8-C10-C11-C12
14	B	3019	CLA	C5-C6-C7-C8
14	B	3039	CLA	C13-C15-C16-C17
18	M	101	LHG	C23-C24-C25-C26
17	A	852	LMG	C11-C12-C13-C14
17	A	852	LMG	C18-C19-C20-C21
18	A	853	LHG	O7-C5-C6-O8
14	B	3014	CLA	CBA-CGA-O2A-C1
18	A	854	LHG	C11-C10-C9-C8
14	A	820	CLA	C15-C16-C17-C18
14	B	3038	CLA	C5-C6-C7-C8
22	L	206	DGD	C9B-CAB-CBB-CCB
17	A	855	LMG	O6-C5-C6-O5
14	A	830	CLA	C5-C6-C7-C8
14	B	3025	CLA	C3-C5-C6-C7
14	B	3028	CLA	C3-C5-C6-C7
14	B	3033	CLA	C2-C3-C5-C6
17	B	3048	LMG	C23-C24-C25-C26
17	A	852	LMG	C16-C17-C18-C19
18	M	101	LHG	C33-C34-C35-C36
14	A	830	CLA	C10-C11-C12-C13
14	B	3010	CLA	O1D-CGD-O2D-CED
17	A	852	LMG	O10-C28-O8-C9
14	A	819	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	820	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	3020	CLA	C1A-C2A-CAA-CBA
14	A	807	CLA	C11-C12-C13-C15
14	A	833	CLA	C11-C10-C8-C7
14	A	834	CLA	C11-C10-C8-C7
14	A	841	CLA	C6-C7-C8-C10
14	A	856	CLA	C11-C10-C8-C7
14	B	3007	CLA	C11-C12-C13-C15
14	B	3027	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	3039	CLA	C11-C10-C8-C7
14	B	3008	CLA	C2C-C3C-CAC-CBC
14	B	3034	CLA	O1A-CGA-O2A-C1
17	I	104	LMG	C15-C16-C17-C18
22	L	206	DGD	C2B-C3B-C4B-C5B
14	A	841	CLA	C5-C6-C7-C8
14	A	807	CLA	C11-C12-C13-C14
14	A	828	CLA	C11-C10-C8-C9
14	B	3007	CLA	C11-C12-C13-C14
14	B	3019	CLA	C6-C7-C8-C9
14	B	3029	CLA	C14-C13-C15-C16
14	B	3039	CLA	C11-C10-C8-C9
14	B	3039	CLA	C11-C12-C13-C14
14	L	203	CLA	C14-C13-C15-C16
18	A	854	LHG	O9-C7-O7-C5
17	A	852	LMG	C2-C1-O1-C7
17	I	104	LMG	O1-C7-C8-C9
18	A	853	LHG	C4-C5-C6-O8
18	M	101	LHG	C4-C5-C6-O8
14	A	839	CLA	C10-C11-C12-C13
17	B	3048	LMG	C31-C32-C33-C34
18	A	853	LHG	C30-C31-C32-C33
16	A	851	BCR	C16-C17-C18-C36
16	B	3043	BCR	C11-C10-C9-C34
14	B	3033	CLA	C5-C6-C7-C8
17	A	852	LMG	C22-C23-C24-C25
14	A	810	CLA	C10-C11-C12-C13
14	B	3015	CLA	C8-C10-C11-C12
14	B	3018	CLA	C10-C11-C12-C13
14	B	3008	CLA	CBA-CGA-O2A-C1
14	A	844	CLA	O2A-C1-C2-C3
14	A	822	CLA	C13-C15-C16-C17
18	M	101	LHG	C26-C27-C28-C29
18	M	101	LHG	C30-C31-C32-C33
14	B	3010	CLA	C2C-C3C-CAC-CBC
14	B	3014	CLA	O1A-CGA-O2A-C1
16	A	847	BCR	C11-C10-C9-C8
14	A	817	CLA	C2C-C3C-CAC-CBC
16	J	104	BCR	C6-C7-C8-C9
14	A	826	CLA	C10-C11-C12-C13
14	L	205	CLA	C10-C11-C12-C13
14	B	3006	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	3029	CLA	CBA-CGA-O2A-C1
14	A	825	CLA	C11-C12-C13-C14
17	B	3048	LMG	C41-C42-C43-C44
18	A	854	LHG	C9-C10-C11-C12
18	M	101	LHG	C11-C10-C9-C8
18	M	101	LHG	O7-C5-C6-O8
22	L	206	DGD	C7A-C8A-C9A-CAA
14	B	3010	CLA	C10-C11-C12-C13
14	A	808	CLA	C2-C1-O2A-CGA
14	B	3007	CLA	C16-C17-C18-C19
14	A	827	CLA	CBA-CGA-O2A-C1
14	B	3029	CLA	C5-C6-C7-C8
16	B	3043	BCR	C14-C15-C16-C17
14	I	101	CLA	C15-C16-C17-C18
14	A	822	CLA	C4-C3-C5-C6
17	A	852	LMG	C35-C36-C37-C38
14	B	3028	CLA	CBA-CGA-O2A-C1
14	B	3040	CLA	CBA-CGA-O2A-C1
21	L	201	LMT	C5'-C4'-O1B-C1B
18	M	101	LHG	C17-C18-C19-C20
21	L	201	LMT	C2-C1-O1'-C1'
14	A	822	CLA	C14-C13-C15-C16
14	A	834	CLA	C11-C10-C8-C9
14	A	841	CLA	C6-C7-C8-C9
14	A	856	CLA	C11-C10-C8-C9
14	B	3004	CLA	C11-C10-C8-C9
14	B	3020	CLA	C11-C10-C8-C9
14	B	3030	CLA	C11-C10-C8-C9
14	B	3033	CLA	C11-C12-C13-C14
14	A	803	CLA	O1D-CGD-O2D-CED
14	A	811	CLA	O1D-CGD-O2D-CED
14	B	3028	CLA	C10-C11-C12-C13
14	B	3010	CLA	C4B-C3B-CAB-CBB
14	L	203	CLA	C4B-C3B-CAB-CBB
17	B	3048	LMG	C30-C31-C32-C33
14	A	803	CLA	C3-C5-C6-C7
14	B	3025	CLA	C5-C6-C7-C8
14	A	813	CLA	C6-C7-C8-C9
14	A	822	CLA	C6-C7-C8-C10
14	A	828	CLA	C11-C10-C8-C7
14	A	830	CLA	C6-C7-C8-C10
14	B	3003	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	3004	CLA	C11-C10-C8-C7
14	B	3010	CLA	C11-C10-C8-C7
14	B	3011	CLA	C11-C12-C13-C15
14	B	3019	CLA	C6-C7-C8-C10
14	B	3029	CLA	C12-C13-C15-C16
14	B	3030	CLA	C11-C10-C8-C7
14	B	3030	CLA	C12-C13-C15-C16
14	B	3033	CLA	C11-C12-C13-C15
14	B	3039	CLA	C11-C12-C13-C15
14	L	203	CLA	C12-C13-C15-C16
14	L	204	CLA	C12-C13-C15-C16
14	B	3039	CLA	C5-C6-C7-C8
15	B	3042	PQN	C18-C20-C21-C22
14	B	3041	CLA	C16-C17-C18-C20
17	A	852	LMG	C14-C15-C16-C17
14	A	808	CLA	C3A-C2A-CAA-CBA
14	A	837	CLA	C3A-C2A-CAA-CBA
14	B	3020	CLA	C3A-C2A-CAA-CBA
14	B	3022	CLA	C3A-C2A-CAA-CBA
14	B	3033	CLA	C3A-C2A-CAA-CBA
14	A	827	CLA	C5-C6-C7-C8
14	B	3033	CLA	C10-C11-C12-C13
14	B	3015	CLA	CBA-CGA-O2A-C1
16	A	850	BCR	C19-C20-C21-C22
14	B	3017	CLA	O1D-CGD-O2D-CED
16	A	848	BCR	C37-C22-C23-C24
22	L	206	DGD	CDB-CEB-CFB-CGB
18	A	853	LHG	C24-C25-C26-C27
14	B	3032	CLA	O2A-C1-C2-C3
14	A	810	CLA	C3-C5-C6-C7
14	B	3008	CLA	O1A-CGA-O2A-C1
22	L	206	DGD	CAA-CBA-CCA-CDA
14	B	3011	CLA	C5-C6-C7-C8
14	B	3008	CLA	C4-C3-C5-C6
14	B	3029	CLA	O1A-CGA-O2A-C1
17	A	852	LMG	C21-C22-C23-C24
14	A	825	CLA	C5-C6-C7-C8
16	A	847	BCR	C23-C24-C25-C26
16	A	851	BCR	C5-C6-C7-C8
16	B	3044	BCR	C5-C6-C7-C8
16	B	3046	BCR	C23-C24-C25-C30
16	B	3050	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	F	201	BCR	C23-C24-C25-C30
16	I	105	BCR	C23-C24-C25-C26
22	L	206	DGD	C3A-C4A-C5A-C6A
14	A	806	CLA	C13-C15-C16-C17
14	A	820	CLA	C8-C10-C11-C12
14	B	3015	CLA	C5-C6-C7-C8
17	I	104	LMG	C4-C5-C6-O5
14	A	811	CLA	C4C-C3C-CAC-CBC
16	I	103	BCR	C10-C11-C12-C13
14	A	839	CLA	C5-C6-C7-C8
14	A	822	CLA	C2-C3-C5-C6
17	A	852	LMG	C19-C20-C21-C22
14	A	822	CLA	C6-C7-C8-C9
14	A	833	CLA	C11-C10-C8-C9
14	B	3003	CLA	C6-C7-C8-C9
14	L	204	CLA	C14-C13-C15-C16
18	A	853	LHG	C9-C10-C11-C12
17	A	852	LMG	C29-C30-C31-C32
16	A	851	BCR	C6-C7-C8-C9
14	B	3006	CLA	O1A-CGA-O2A-C1
21	L	201	LMT	C3-C4-C5-C6
18	M	101	LHG	O1-C1-C2-O2
14	B	3008	CLA	C2-C3-C5-C6
14	B	3041	CLA	C16-C17-C18-C19
18	A	853	LHG	C35-C36-C37-C38
14	B	3028	CLA	C13-C15-C16-C17
16	I	102	BCR	C20-C21-C22-C37
16	J	104	BCR	C35-C13-C14-C15
16	M	103	BCR	C16-C17-C18-C36
14	B	3028	CLA	O1A-CGA-O2A-C1
14	A	826	CLA	C13-C15-C16-C17
18	A	853	LHG	C19-C20-C21-C22
14	A	802	CLA	C6-C7-C8-C10
14	A	827	CLA	C11-C10-C8-C7
14	A	829	CLA	C6-C7-C8-C10
14	A	839	CLA	C6-C7-C8-C10
14	B	3007	CLA	C11-C10-C8-C7
14	B	3020	CLA	C11-C10-C8-C7
14	B	3020	CLA	C11-C12-C13-C15
14	B	3027	CLA	C11-C10-C8-C7
14	B	3041	CLA	C11-C10-C8-C7
14	L	203	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	M	101	LHG	C16-C17-C18-C19
18	M	101	LHG	C28-C29-C30-C31
16	A	850	BCR	C7-C8-C9-C10
16	B	3044	BCR	C7-C8-C9-C10
16	I	105	BCR	C7-C8-C9-C10
16	J	103	BCR	C21-C22-C23-C24
16	J	104	BCR	C7-C8-C9-C10
14	B	3015	CLA	O1A-CGA-O2A-C1
14	B	3040	CLA	O1A-CGA-O2A-C1
14	B	3014	CLA	C15-C16-C17-C18
14	B	3032	CLA	C2A-CAA-CBA-CGA
14	B	3024	CLA	O1D-CGD-O2D-CED
18	M	101	LHG	O1-C1-C2-C3
14	B	3038	CLA	C8-C10-C11-C12
14	A	827	CLA	O1A-CGA-O2A-C1
14	B	3028	CLA	C5-C6-C7-C8
16	B	3046	BCR	C16-C17-C18-C19
16	K	102	BCR	C16-C17-C18-C19
14	A	817	CLA	O2A-C1-C2-C3
14	A	823	CLA	O2A-C1-C2-C3
17	B	3048	LMG	O1-C7-C8-C9
14	A	826	CLA	C4-C3-C5-C6
14	B	3014	CLA	C2C-C3C-CAC-CBC
17	A	852	LMG	O1-C7-C8-O7
17	I	104	LMG	O1-C7-C8-O7
14	A	802	CLA	C6-C7-C8-C9
14	A	809	CLA	C6-C7-C8-C9
14	A	827	CLA	C11-C12-C13-C14
14	A	839	CLA	C6-C7-C8-C9
14	B	3011	CLA	C11-C12-C13-C14
15	B	3042	PQN	C24-C23-C25-C26
14	A	817	CLA	C4C-C3C-CAC-CBC
14	B	3041	CLA	CBA-CGA-O2A-C1
18	A	853	LHG	C10-C11-C12-C13
14	B	3009	CLA	C15-C16-C17-C18
14	A	843	CLA	C13-C15-C16-C17
14	A	828	CLA	C8-C10-C11-C12
14	A	814	CLA	C3-C5-C6-C7
14	B	3028	CLA	C15-C16-C17-C18
14	A	825	CLA	C3-C5-C6-C7
14	B	3007	CLA	C4B-C3B-CAB-CBB
14	B	3028	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	3030	CLA	C1A-C2A-CAA-CBA
14	B	3035	CLA	C4B-C3B-CAB-CBB
14	A	822	CLA	C2A-CAA-CBA-CGA
17	B	3048	LMG	C38-C39-C40-C41
14	B	3014	CLA	C5-C6-C7-C8
14	A	802	CLA	C12-C13-C15-C16
14	A	810	CLA	C6-C7-C8-C10
14	A	814	CLA	C11-C10-C8-C7
14	B	3006	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
14	L	205	CLA	C6-C7-C8-C10
15	B	3042	PQN	C22-C23-C25-C26
14	B	3028	CLA	O1D-CGD-O2D-CED
14	A	822	CLA	CBA-CGA-O2A-C1
17	A	852	LMG	C32-C33-C34-C35
17	B	3048	LMG	C36-C37-C38-C39
14	B	3038	CLA	C4-C3-C5-C6
14	B	3038	CLA	C11-C12-C13-C15
17	A	855	LMG	C12-C13-C14-C15
14	B	3023	CLA	O1A-CGA-O2A-C1
14	B	3019	CLA	C3-C5-C6-C7
14	A	827	CLA	C11-C10-C8-C9
14	A	830	CLA	C6-C7-C8-C9
14	B	3030	CLA	C14-C13-C15-C16
14	B	3041	CLA	C11-C10-C8-C9
14	B	3009	CLA	C8-C10-C11-C12
16	B	3046	BCR	C19-C20-C21-C22
14	B	3029	CLA	C13-C15-C16-C17
14	A	823	CLA	C1-C2-C3-C4
14	B	3032	CLA	C1-C2-C3-C4
14	L	205	CLA	O1D-CGD-O2D-CED
17	B	3048	LMG	O1-C7-C8-O7
14	A	812	CLA	C10-C11-C12-C13
14	B	3011	CLA	CAD-CBD-CGD-O2D
14	A	809	CLA	C15-C16-C17-C18
14	B	3023	CLA	CBA-CGA-O2A-C1
17	I	104	LMG	C28-C29-C30-C31
14	A	822	CLA	O1A-CGA-O2A-C1
14	B	3041	CLA	O1A-CGA-O2A-C1
14	A	805	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	826	CLA	CHA-CBD-CGD-O2D
14	B	3011	CLA	CAD-CBD-CGD-O1D
14	M	102	CLA	CHA-CBD-CGD-O1D
14	M	102	CLA	CHA-CBD-CGD-O2D
16	I	105	BCR	C9-C10-C11-C12
18	A	854	LHG	C3-O3-P-O5
18	B	3049	LHG	C3-O3-P-O6
18	M	101	LHG	C3-O3-P-O5
18	M	101	LHG	C4-O6-P-O5
14	B	3039	CLA	C16-C17-C18-C20
16	I	105	BCR	C14-C15-C16-C17
14	I	101	CLA	C10-C11-C12-C13
14	A	820	CLA	C4-C3-C5-C6
14	A	808	CLA	C2B-C3B-CAB-CBB
14	A	832	CLA	C2B-C3B-CAB-CBB
14	B	3006	CLA	C2B-C3B-CAB-CBB
14	B	3008	CLA	C2B-C3B-CAB-CBB
14	B	3035	CLA	C2B-C3B-CAB-CBB
16	F	203	BCR	C1-C6-C7-C8
22	L	206	DGD	C9A-CAA-CBA-CCA
14	A	826	CLA	C2-C3-C5-C6
18	A	854	LHG	C2-C3-O3-P
14	A	831	CLA	C13-C15-C16-C17
17	I	104	LMG	C32-C33-C34-C35
14	A	844	CLA	C15-C16-C17-C18
16	J	103	BCR	C9-C10-C11-C12
14	A	829	CLA	C6-C7-C8-C9
14	A	834	CLA	C14-C13-C15-C16
14	B	3010	CLA	C6-C7-C8-C9
14	B	3010	CLA	C11-C10-C8-C9
14	L	203	CLA	C6-C7-C8-C9
14	A	806	CLA	C11-C12-C13-C15
14	A	807	CLA	C12-C13-C15-C16
14	A	829	CLA	C11-C12-C13-C15
14	B	3027	CLA	C6-C7-C8-C10
16	A	847	BCR	C12-C13-C14-C15
16	J	105	BCR	C11-C10-C9-C8
18	A	853	LHG	C11-C12-C13-C14
18	A	853	LHG	C28-C29-C30-C31
16	B	3045	BCR	C22-C23-C24-C25
16	F	203	BCR	C22-C23-C24-C25
14	A	856	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	3039	CLA	C16-C17-C18-C19
14	A	807	CLA	O1A-CGA-O2A-C1
14	B	3015	CLA	C16-C17-C18-C19
14	A	806	CLA	C15-C16-C17-C18
18	A	853	LHG	C13-C14-C15-C16
14	B	3028	CLA	CBD-CGD-O2D-CED
17	A	852	LMG	C4-C5-C6-O5
14	A	809	CLA	C2A-CAA-CBA-CGA
14	B	3023	CLA	C2A-CAA-CBA-CGA
16	B	3045	BCR	C19-C20-C21-C22
16	B	3046	BCR	C9-C10-C11-C12
14	B	3014	CLA	C4C-C3C-CAC-CBC
14	B	3003	CLA	C4-C3-C5-C6
14	A	820	CLA	C2-C3-C5-C6
14	B	3018	CLA	C11-C10-C8-C9
14	B	3029	CLA	C6-C7-C8-C9
14	L	203	CLA	C11-C12-C13-C14
14	A	807	CLA	CBA-CGA-O2A-C1
14	B	3003	CLA	C4B-C3B-CAB-CBB
17	B	3048	LMG	C16-C17-C18-C19
14	B	3025	CLA	C6-C7-C8-C9
14	A	837	CLA	CAA-CBA-CGA-O2A
18	A	853	LHG	C27-C28-C29-C30
22	L	206	DGD	C2A-C3A-C4A-C5A
14	B	3010	CLA	C6-C7-C8-C10
14	L	203	CLA	C11-C12-C13-C15
17	B	3048	LMG	C40-C41-C42-C43
14	A	856	CLA	C16-C17-C18-C19
14	A	825	CLA	C3A-C2A-CAA-CBA
14	A	830	CLA	C4-C3-C5-C6
14	A	836	CLA	C3A-C2A-CAA-CBA
14	B	3030	CLA	C3A-C2A-CAA-CBA
16	J	104	BCR	C22-C23-C24-C25
14	B	3007	CLA	O1D-CGD-O2D-CED
14	B	3028	CLA	C2-C1-O2A-CGA
14	A	827	CLA	C13-C15-C16-C17
16	B	3046	BCR	C11-C12-C13-C14
14	A	809	CLA	C4-C3-C5-C6
14	A	834	CLA	C4-C3-C5-C6
14	B	3038	CLA	C2-C3-C5-C6
14	B	3010	CLA	C15-C16-C17-C18
14	B	3019	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	3008	CLA	C2A-CAA-CBA-CGA
14	A	837	CLA	CAA-CBA-CGA-O1A
14	B	3013	CLA	CAA-CBA-CGA-O2A
14	A	810	CLA	C5-C6-C7-C8
14	B	3031	CLA	CAA-CBA-CGA-O2A
14	K	103	CLA	CAA-CBA-CGA-O1A
14	A	809	CLA	C14-C13-C15-C16
14	A	827	CLA	C14-C13-C15-C16
14	A	835	CLA	C11-C10-C8-C9
14	A	841	CLA	C11-C10-C8-C9
14	B	3006	CLA	C14-C13-C15-C16
15	A	846	PQN	C21-C22-C23-C24
17	B	3048	LMG	C19-C20-C21-C22
17	I	104	LMG	C7-C8-O7-C10
17	I	104	LMG	C9-C8-O7-C10
21	L	201	LMT	C9-C10-C11-C12
18	A	853	LHG	C34-C35-C36-C37
14	B	3013	CLA	CAA-CBA-CGA-O1A
14	A	841	CLA	C2A-CAA-CBA-CGA
14	A	836	CLA	C1A-C2A-CAA-CBA
14	B	3014	CLA	C1A-C2A-CAA-CBA
14	B	3034	CLA	C1A-C2A-CAA-CBA
16	B	3045	BCR	C20-C21-C22-C23
16	B	3046	BCR	C20-C21-C22-C23
16	F	201	BCR	C16-C17-C18-C19
17	B	3048	LMG	C22-C23-C24-C25
14	A	838	CLA	C4C-C3C-CAC-CBC
14	B	3010	CLA	C2B-C3B-CAB-CBB
14	L	203	CLA	C2B-C3B-CAB-CBB
14	M	102	CLA	C2B-C3B-CAB-CBB
16	A	850	BCR	C1-C6-C7-C8
16	B	3046	BCR	C23-C24-C25-C26
16	F	203	BCR	C5-C6-C7-C8
16	F	203	BCR	C23-C24-C25-C26
16	L	207	BCR	C5-C6-C7-C8
14	A	810	CLA	C2C-C3C-CAC-CBC
14	A	807	CLA	C4-C3-C5-C6
14	B	3034	CLA	C4-C3-C5-C6
18	A	854	LHG	O6-C4-C5-C6
14	B	3003	CLA	C2-C3-C5-C6
14	B	3037	CLA	CAA-CBA-CGA-O1A
14	B	3037	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	831	CLA	C11-C10-C8-C7
14	A	834	CLA	C12-C13-C15-C16
14	B	3015	CLA	C11-C10-C8-C7
14	B	3018	CLA	C11-C10-C8-C7
14	I	101	CLA	C12-C13-C15-C16
14	A	840	CLA	C2-C1-O2A-CGA
14	A	802	CLA	C2A-CAA-CBA-CGA
14	B	3021	CLA	C2A-CAA-CBA-CGA
17	B	3048	LMG	C18-C19-C20-C21
14	B	3017	CLA	C2C-C3C-CAC-CBC
14	K	103	CLA	CAA-CBA-CGA-O2A
14	B	3007	CLA	CBD-CGD-O2D-CED
14	A	818	CLA	C6-C7-C8-C9
14	A	815	CLA	CAA-CBA-CGA-O2A
14	A	805	CLA	C11-C12-C13-C14
14	A	809	CLA	C2-C3-C5-C6
14	A	830	CLA	C2-C3-C5-C6
14	A	834	CLA	C2-C3-C5-C6
14	M	102	CLA	CAA-CBA-CGA-O1A
14	A	827	CLA	C8-C10-C11-C12
17	B	3048	LMG	C42-C43-C44-C45
14	A	825	CLA	C4-C3-C5-C6
14	B	3030	CLA	C4-C3-C5-C6
14	B	3031	CLA	CAA-CBA-CGA-O1A
16	A	848	BCR	C14-C15-C16-C17
17	A	855	LMG	C19-C20-C21-C22
15	B	3042	PQN	C25-C26-C27-C28
14	M	102	CLA	CAA-CBA-CGA-O2A
14	A	813	CLA	C2A-CAA-CBA-CGA
14	F	202	CLA	CAA-CBA-CGA-O2A
14	X	1701	CLA	CAA-CBA-CGA-O1A
14	B	3011	CLA	C4-C3-C5-C6
14	J	101	CLA	CAA-CBA-CGA-O2A
14	A	835	CLA	C5-C6-C7-C8
14	B	3014	CLA	C8-C10-C11-C12
14	A	821	CLA	C4B-C3B-CAB-CBB
14	A	823	CLA	C4B-C3B-CAB-CBB
14	B	3005	CLA	C4B-C3B-CAB-CBB
14	B	3006	CLA	C15-C16-C17-C18
14	B	3024	CLA	CAA-CBA-CGA-O2A
14	X	1701	CLA	CAA-CBA-CGA-O2A
14	A	815	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	3015	CLA	C16-C17-C18-C20
16	B	3044	BCR	C11-C10-C9-C34
16	B	3045	BCR	C20-C21-C22-C37
14	A	839	CLA	C4-C3-C5-C6
18	A	853	LHG	C23-C24-C25-C26
14	A	819	CLA	CAA-CBA-CGA-O2A
14	B	3036	CLA	CAA-CBA-CGA-O2A
14	B	3010	CLA	C4C-C3C-CAC-CBC
17	A	852	LMG	C13-C14-C15-C16
14	B	3024	CLA	CAA-CBA-CGA-O1A
14	A	828	CLA	C14-C13-C15-C16
14	A	830	CLA	C11-C12-C13-C14
14	B	3033	CLA	C6-C7-C8-C9
14	L	205	CLA	C6-C7-C8-C9
14	A	838	CLA	C2C-C3C-CAC-CBC
14	A	816	CLA	C2A-CAA-CBA-CGA
14	B	3029	CLA	C2-C1-O2A-CGA
14	A	816	CLA	C3A-C2A-CAA-CBA
14	B	3014	CLA	C3A-C2A-CAA-CBA
14	B	3034	CLA	C3A-C2A-CAA-CBA
14	L	204	CLA	C3A-C2A-CAA-CBA
14	A	832	CLA	CBA-CGA-O2A-C1
14	A	833	CLA	O2A-C1-C2-C3
14	A	856	CLA	O2A-C1-C2-C3
17	A	855	LMG	C17-C18-C19-C20
16	F	201	BCR	C10-C11-C12-C13
16	F	203	BCR	C18-C19-C20-C21
14	F	202	CLA	CAA-CBA-CGA-O1A
16	A	851	BCR	C16-C17-C18-C19
16	F	203	BCR	C20-C21-C22-C23
14	J	101	CLA	CAA-CBA-CGA-O1A
22	L	206	DGD	CEB-CFB-CGB-CHB
18	A	854	LHG	O6-C4-C5-O7
16	J	103	BCR	C6-C7-C8-C9
14	B	3036	CLA	CAA-CBA-CGA-O1A
18	A	853	LHG	C16-C17-C18-C19
14	B	3003	CLA	CBA-CGA-O2A-C1
17	A	852	LMG	O8-C28-C29-C30
14	B	3003	CLA	O1A-CGA-O2A-C1
14	A	810	CLA	C6-C7-C8-C9
14	A	814	CLA	C11-C10-C8-C9
14	B	3007	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	3018	CLA	C6-C7-C8-C9
14	B	3029	CLA	C11-C12-C13-C14
14	A	835	CLA	C16-C17-C18-C20
14	A	808	CLA	CAA-CBA-CGA-O2A
14	B	3006	CLA	CAA-CBA-CGA-O2A
14	A	820	CLA	C5-C6-C7-C8
14	A	810	CLA	C4C-C3C-CAC-CBC
14	A	812	CLA	C12-C13-C15-C16
14	A	822	CLA	C12-C13-C15-C16
14	A	826	CLA	C11-C10-C8-C7
14	A	827	CLA	C12-C13-C15-C16
14	A	830	CLA	C11-C12-C13-C15
14	B	3003	CLA	C11-C10-C8-C7
14	B	3011	CLA	C6-C7-C8-C10
14	L	204	CLA	C11-C10-C8-C7
15	B	3042	PQN	C21-C22-C23-C25
14	A	821	CLA	C2B-C3B-CAB-CBB
14	B	3003	CLA	C2B-C3B-CAB-CBB
14	B	3007	CLA	C2B-C3B-CAB-CBB
16	A	848	BCR	C1-C6-C7-C8
16	A	850	BCR	C5-C6-C7-C8
16	F	201	BCR	C23-C24-C25-C26
18	A	854	LHG	O8-C23-C24-C25
14	A	828	CLA	C2-C1-O2A-CGA
14	B	3015	CLA	C2-C1-O2A-CGA
14	B	3011	CLA	CAA-CBA-CGA-O2A
17	B	3048	LMG	O7-C10-C11-C12
14	B	3040	CLA	C2-C1-O2A-CGA
14	B	3014	CLA	CAA-CBA-CGA-O2A
14	A	805	CLA	C2-C3-C5-C6
14	B	3018	CLA	C11-C12-C13-C14
18	M	101	LHG	C5-C6-O8-C23
14	A	807	CLA	CAA-CBA-CGA-O2A
17	B	3048	LMG	C20-C21-C22-C23
14	B	3007	CLA	CAA-CBA-CGA-O2A
17	I	104	LMG	O7-C10-C11-C12
16	B	3045	BCR	C35-C13-C14-C15
21	L	201	LMT	C6-C7-C8-C9
14	A	831	CLA	C11-C10-C8-C9
14	B	3020	CLA	C14-C13-C15-C16
14	B	3027	CLA	C6-C7-C8-C9
14	L	205	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	830	CLA	C13-C15-C16-C17
14	A	802	CLA	C1A-C2A-CAA-CBA
14	A	825	CLA	C1A-C2A-CAA-CBA
14	A	840	CLA	C4B-C3B-CAB-CBB
14	B	3010	CLA	C1A-C2A-CAA-CBA
14	B	3021	CLA	C4B-C3B-CAB-CBB
14	B	3027	CLA	C1A-C2A-CAA-CBA
14	B	3038	CLA	C1A-C2A-CAA-CBA
14	B	3039	CLA	C4B-C3B-CAB-CBB
14	X	1701	CLA	C1A-C2A-CAA-CBA
16	B	3045	BCR	C6-C7-C8-C9
18	B	3049	LHG	O7-C7-C8-C9
14	B	3034	CLA	C2-C3-C5-C6
16	A	851	BCR	C11-C12-C13-C14
16	F	201	BCR	C21-C22-C23-C24
16	I	105	BCR	C17-C18-C19-C20
16	J	104	BCR	C11-C12-C13-C14
14	B	3015	CLA	C10-C11-C12-C13
14	B	3041	CLA	C15-C16-C17-C18
14	B	3018	CLA	O1D-CGD-O2D-CED
14	B	3004	CLA	C2A-CAA-CBA-CGA
14	A	844	CLA	C16-C17-C18-C19
14	B	3020	CLA	C16-C17-C18-C20
14	A	802	CLA	C10-C11-C12-C13
15	A	846	PQN	C23-C25-C26-C27
14	A	805	CLA	C4-C3-C5-C6
14	A	820	CLA	C11-C10-C8-C7
14	A	828	CLA	C12-C13-C15-C16
14	A	835	CLA	C11-C12-C13-C15
14	A	843	CLA	C11-C10-C8-C7
14	A	844	CLA	C11-C12-C13-C15
14	B	3015	CLA	C12-C13-C15-C16
14	B	3038	CLA	C6-C7-C8-C10
14	B	3039	CLA	C15-C16-C17-C18
15	B	3042	PQN	C26-C27-C28-C29
14	B	3015	CLA	C2A-CAA-CBA-CGA
14	B	3038	CLA	O1A-CGA-O2A-C1
14	B	3009	CLA	C5-C6-C7-C8
14	A	802	CLA	C3A-C2A-CAA-CBA
14	X	1701	CLA	C3A-C2A-CAA-CBA
16	M	103	BCR	C20-C21-C22-C23
14	L	204	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	3038	CLA	CBA-CGA-O2A-C1
14	B	3014	CLA	CAA-CBA-CGA-O1A
14	A	819	CLA	CBA-CGA-O2A-C1
14	B	3027	CLA	CBA-CGA-O2A-C1
14	A	806	CLA	C11-C12-C13-C14
14	A	807	CLA	C14-C13-C15-C16
14	B	3003	CLA	C11-C10-C8-C9
14	A	807	CLA	CAA-CBA-CGA-O1A
14	A	808	CLA	CAA-CBA-CGA-O1A
14	A	804	CLA	C5-C6-C7-C8
16	I	105	BCR	C15-C16-C17-C18
14	A	856	CLA	C10-C11-C12-C13
14	B	3007	CLA	CAA-CBA-CGA-O1A
18	A	853	LHG	O10-C23-C24-C25
18	M	101	LHG	O9-C7-C8-C9
14	A	832	CLA	O1A-CGA-O2A-C1
14	B	3006	CLA	CAA-CBA-CGA-O1A
14	A	819	CLA	O1A-CGA-O2A-C1
14	B	3011	CLA	CAA-CBA-CGA-O1A
14	A	807	CLA	C8-C10-C11-C12
22	L	206	DGD	CFB-CGB-CHB-CIB
14	A	835	CLA	C16-C17-C18-C19
18	M	101	LHG	O7-C7-C8-C9
14	A	856	CLA	CAD-CBD-CGD-O2D
14	K	103	CLA	CAD-CBD-CGD-O2D
14	L	203	CLA	CAD-CBD-CGD-O2D
14	B	3008	CLA	CAA-CBA-CGA-O2A
14	B	3021	CLA	CAA-CBA-CGA-O2A
18	A	853	LHG	O7-C7-C8-C9
14	B	3020	CLA	C13-C15-C16-C17
14	A	805	CLA	O1D-CGD-O2D-CED
14	A	809	CLA	CAA-CBA-CGA-O2A
14	A	820	CLA	CAA-CBA-CGA-O2A
14	B	3033	CLA	CAA-CBA-CGA-O2A
14	A	845	CLA	C2-C3-C5-C6
14	B	3033	CLA	C2C-C3C-CAC-CBC

There are no ring outliers.

107 monomers are involved in 267 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	811	CLA	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	3032	CLA	2	0
14	B	3012	CLA	1	0
14	B	3028	CLA	2	0
16	J	103	BCR	4	0
14	A	836	CLA	1	0
14	B	3016	CLA	1	0
14	B	3005	CLA	1	0
14	A	819	CLA	3	0
16	F	203	BCR	3	0
14	B	3006	CLA	1	0
14	B	3025	CLA	5	0
14	A	856	CLA	3	0
14	B	3003	CLA	4	0
16	A	847	BCR	4	0
14	A	815	CLA	1	0
14	B	3022	CLA	1	0
13	A	801	CL0	2	0
14	A	841	CLA	3	0
14	I	101	CLA	8	0
14	B	3027	CLA	1	0
14	L	204	CLA	1	0
14	A	822	CLA	2	0
14	A	844	CLA	3	0
14	A	834	CLA	1	0
15	A	846	PQN	7	0
14	B	3018	CLA	4	0
14	B	3010	CLA	6	0
22	L	206	DGD	2	0
14	A	809	CLA	3	0
14	B	3015	CLA	1	0
14	A	838	CLA	1	0
14	X	1701	CLA	2	0
14	A	827	CLA	2	0
18	M	101	LHG	1	0
16	A	851	BCR	6	0
14	B	3033	CLA	2	0
14	B	3011	CLA	4	0
14	A	833	CLA	1	0
16	I	105	BCR	3	0
14	B	3014	CLA	5	0
14	B	3041	CLA	1	0
16	B	3046	BCR	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	3050	BCR	2	0
14	B	3017	CLA	3	0
16	A	850	BCR	5	0
14	B	3034	CLA	5	0
18	A	853	LHG	2	0
14	B	3026	CLA	2	0
14	A	831	CLA	2	0
16	B	3044	BCR	3	0
14	A	830	CLA	2	0
14	B	3024	CLA	2	0
14	B	3038	CLA	3	0
14	B	3030	CLA	4	0
14	B	3019	CLA	2	0
14	A	810	CLA	3	0
17	B	3048	LMG	1	0
14	A	826	CLA	4	0
18	A	854	LHG	2	0
14	A	804	CLA	4	0
14	A	817	CLA	3	0
14	B	3031	CLA	2	0
14	A	821	CLA	5	0
18	B	3049	LHG	2	0
14	B	3039	CLA	1	0
14	A	832	CLA	3	0
16	A	849	BCR	2	0
14	M	102	CLA	3	0
14	B	3037	CLA	2	0
14	A	813	CLA	2	0
14	A	823	CLA	1	0
14	B	3008	CLA	2	0
14	A	825	CLA	1	0
14	B	3007	CLA	1	0
16	L	207	BCR	2	0
14	A	828	CLA	3	0
16	M	103	BCR	2	0
14	B	3004	CLA	5	0
14	A	840	CLA	1	0
15	B	3042	PQN	3	0
14	B	3013	CLA	2	0
14	A	835	CLA	1	0
16	K	102	BCR	4	0
14	B	3029	CLA	1	0

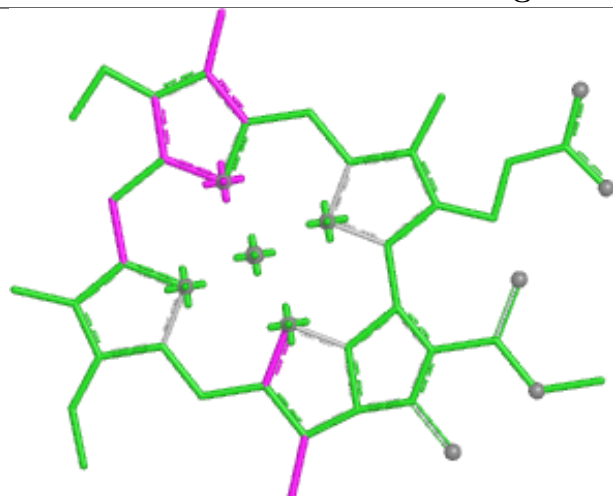
Continued on next page...

Continued from previous page...

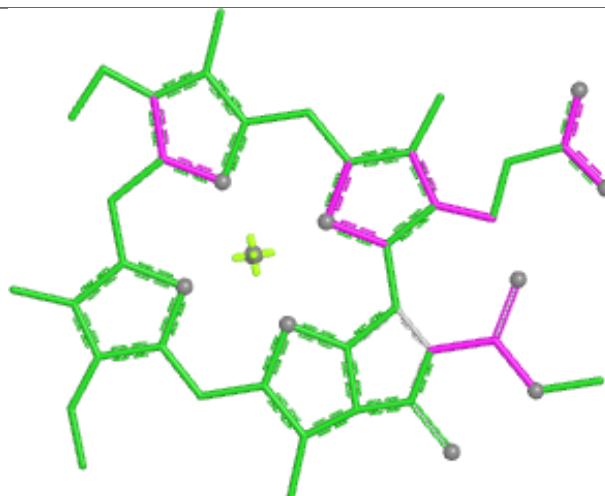
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	806	CLA	5	0
14	A	829	CLA	8	0
16	J	104	BCR	3	0
14	A	808	CLA	1	0
14	F	202	CLA	8	0
14	K	101	CLA	3	0
16	I	103	BCR	1	0
14	A	818	CLA	2	0
14	A	814	CLA	8	0
14	A	845	CLA	2	0
14	B	3021	CLA	2	0
14	A	802	CLA	2	0
16	B	3045	BCR	3	0
16	I	102	BCR	4	0
16	J	105	BCR	6	0
14	L	203	CLA	2	0
16	F	201	BCR	5	0
14	A	803	CLA	4	0
14	A	820	CLA	4	0
14	B	3009	CLA	1	0
14	A	843	CLA	3	0
14	L	205	CLA	1	0

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

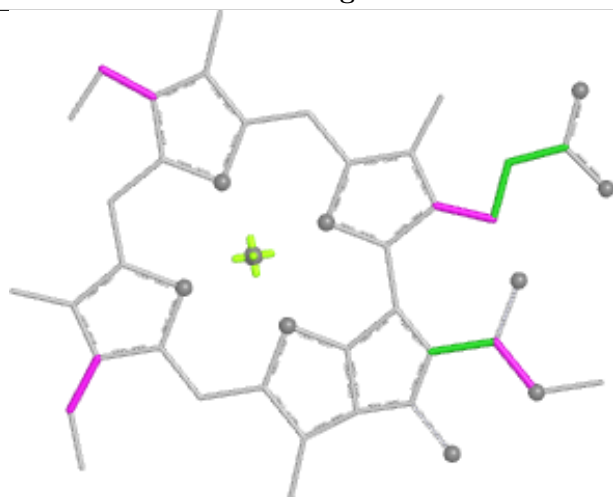
Ligand CLA A 811



Bond lengths



Bond angles

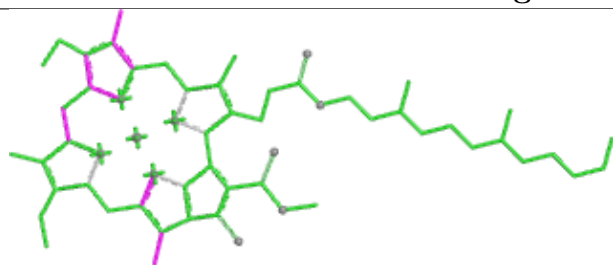


Torsions

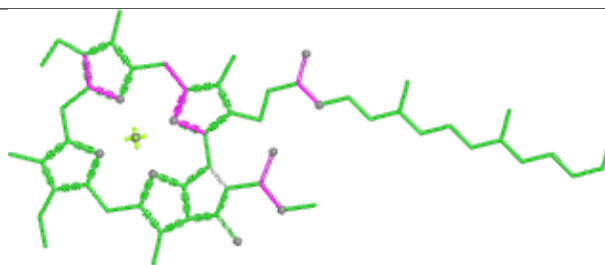


Rings

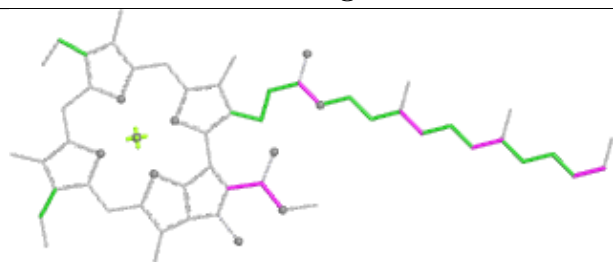
Ligand CLA A 805



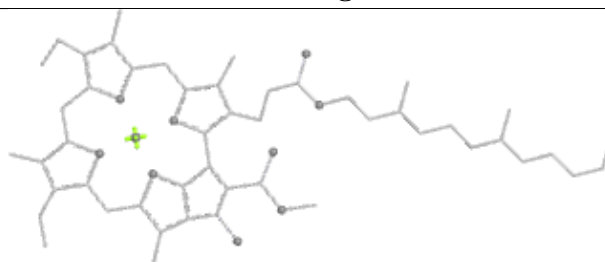
Bond lengths



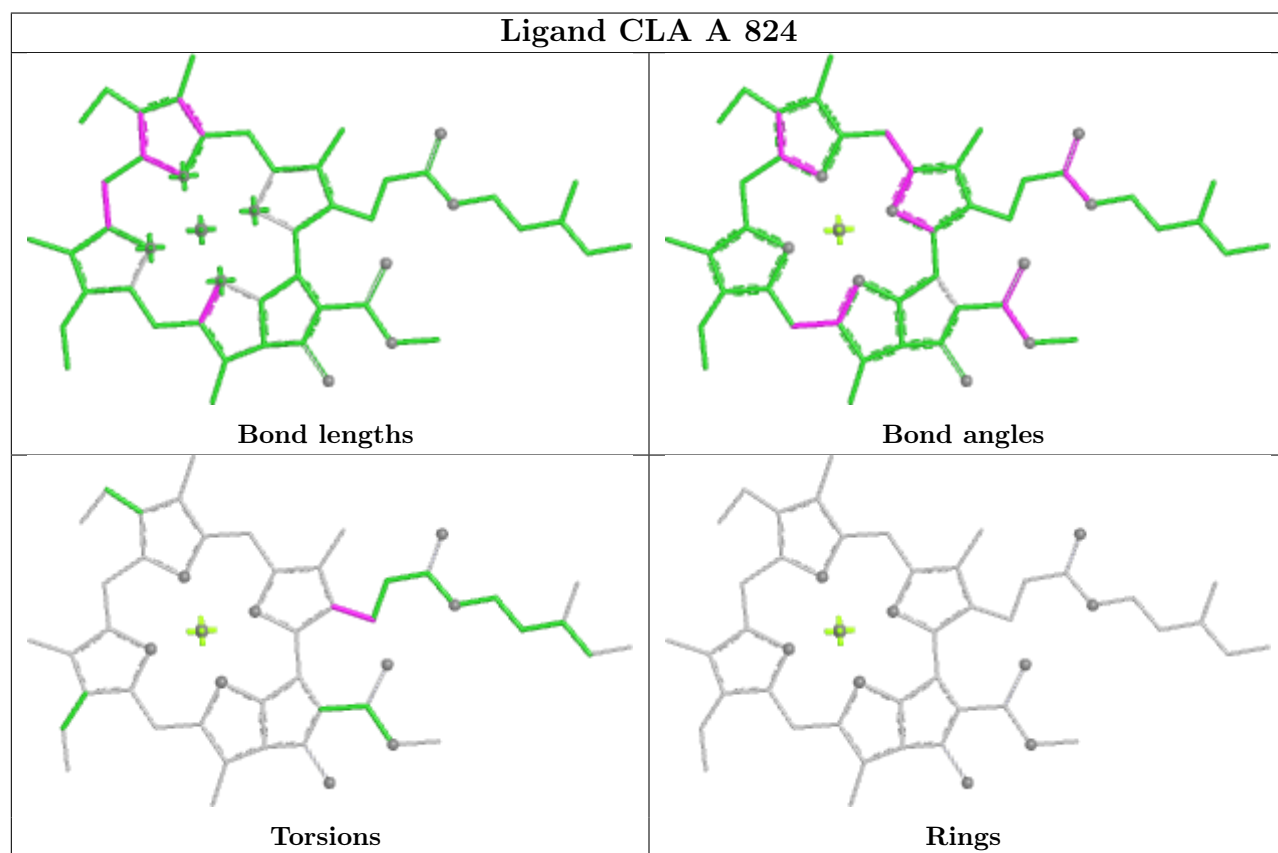
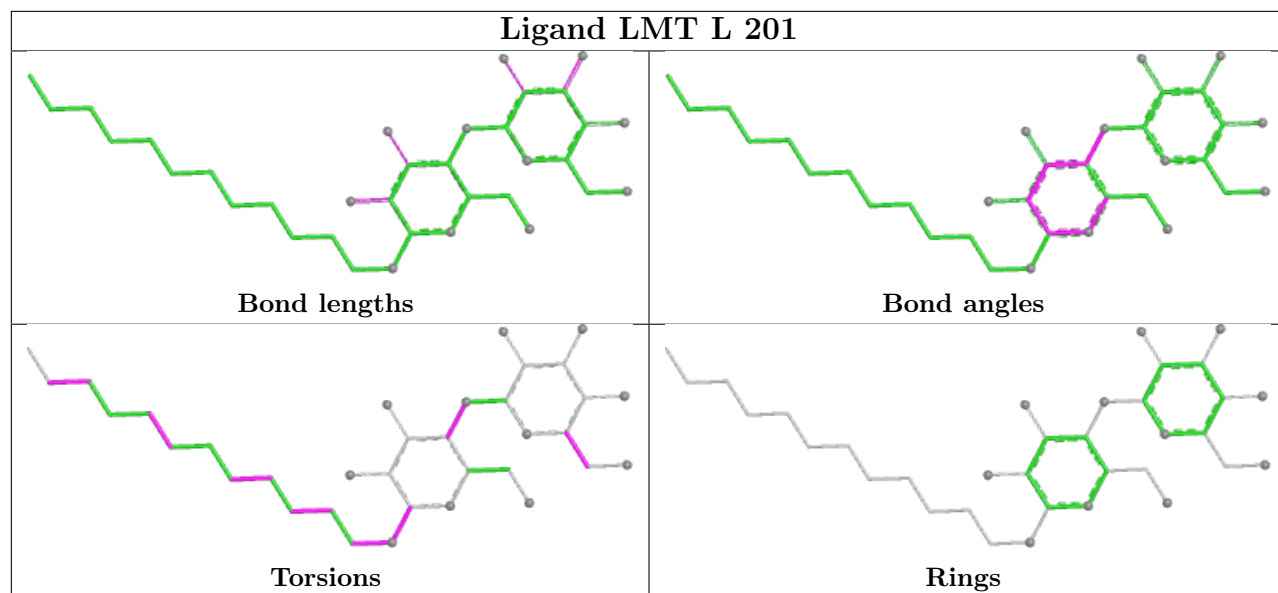
Bond angles



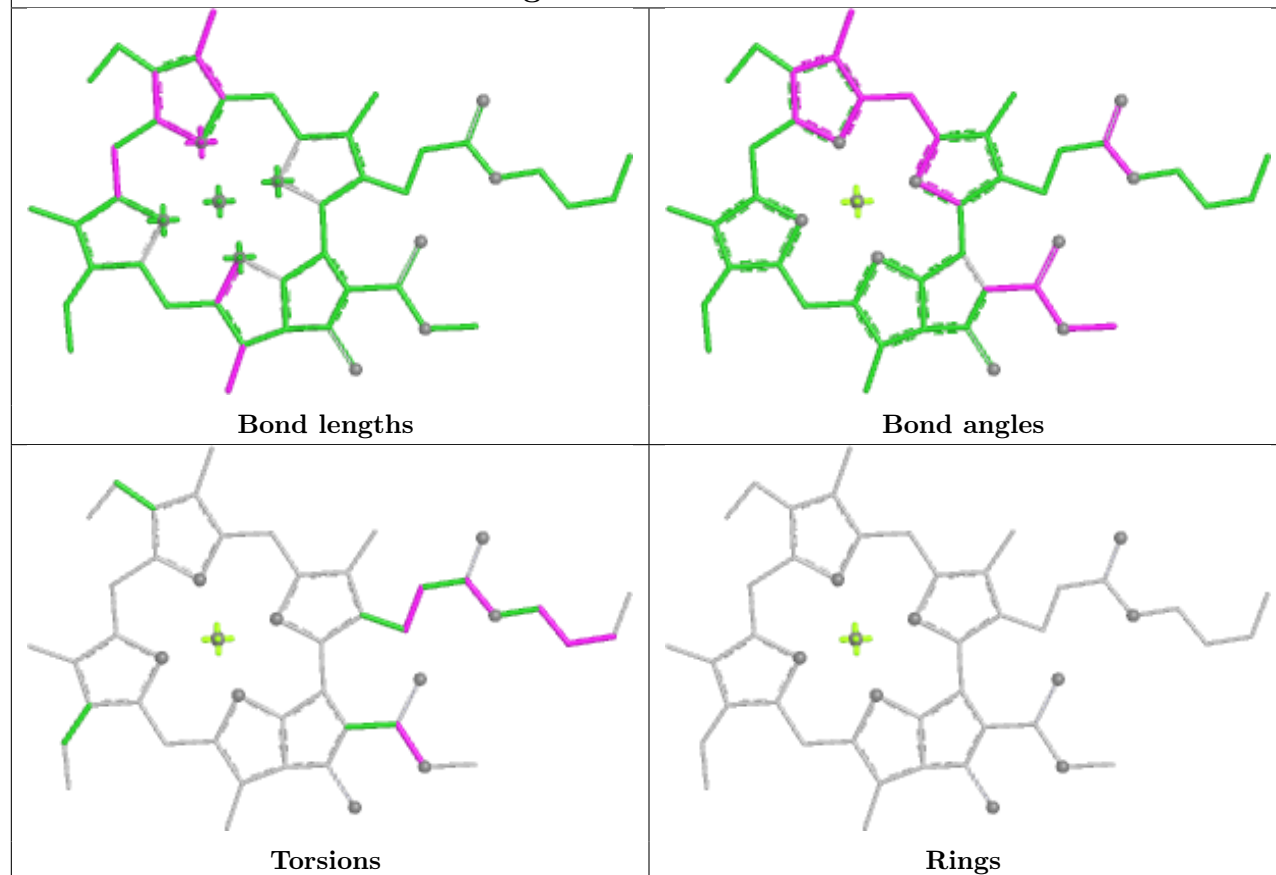
Torsions



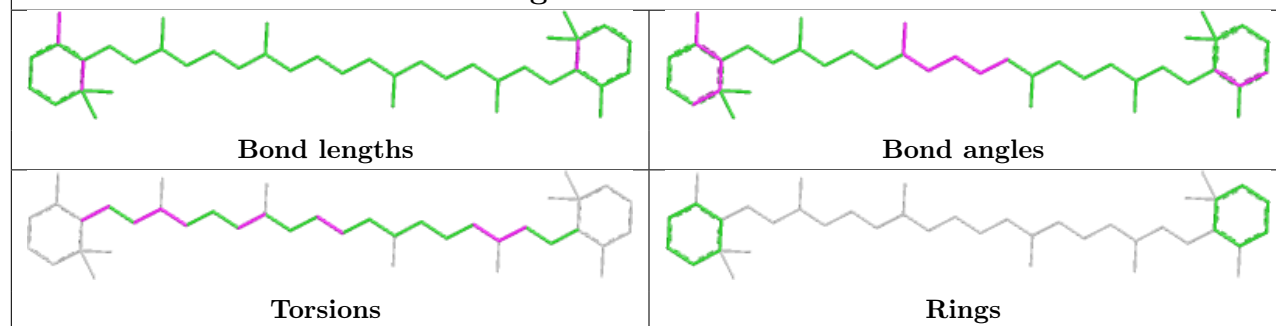
Rings



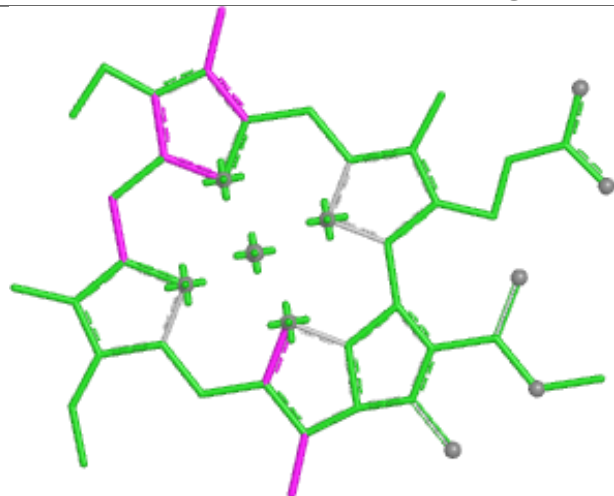
Ligand CLA B 3032



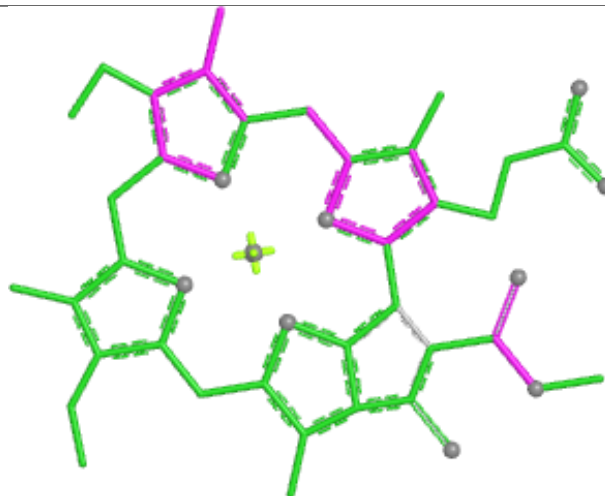
Ligand BCR A 848



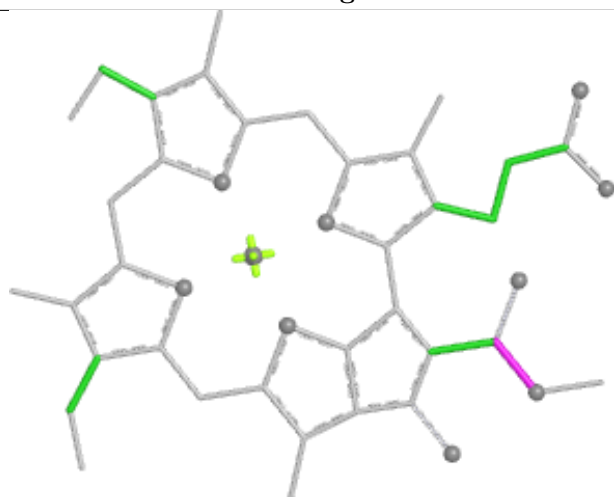
Ligand CLA B 3012



Bond lengths



Bond angles

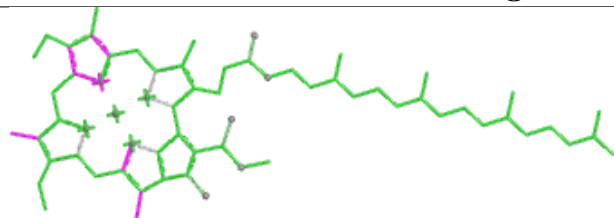


Torsions

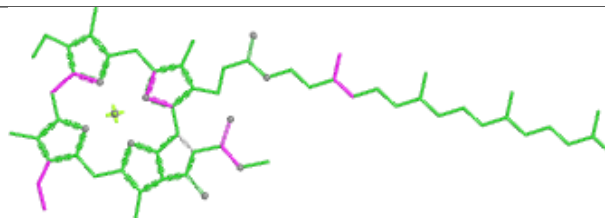


Rings

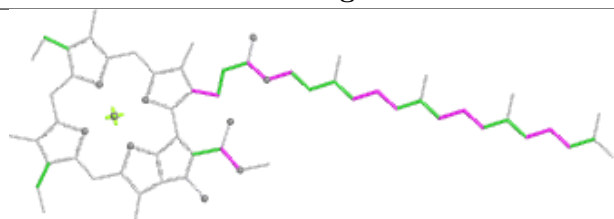
Ligand CLA B 3028



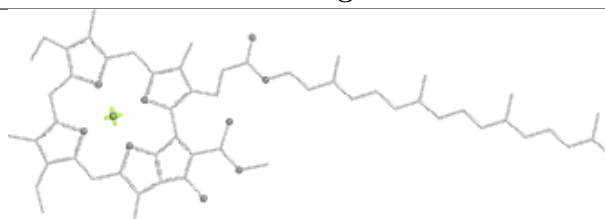
Bond lengths



Bond angles

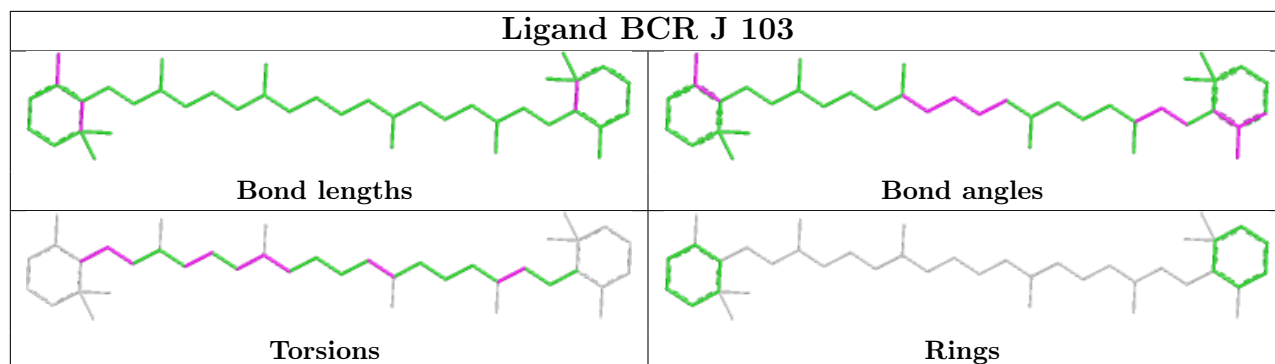


Torsions

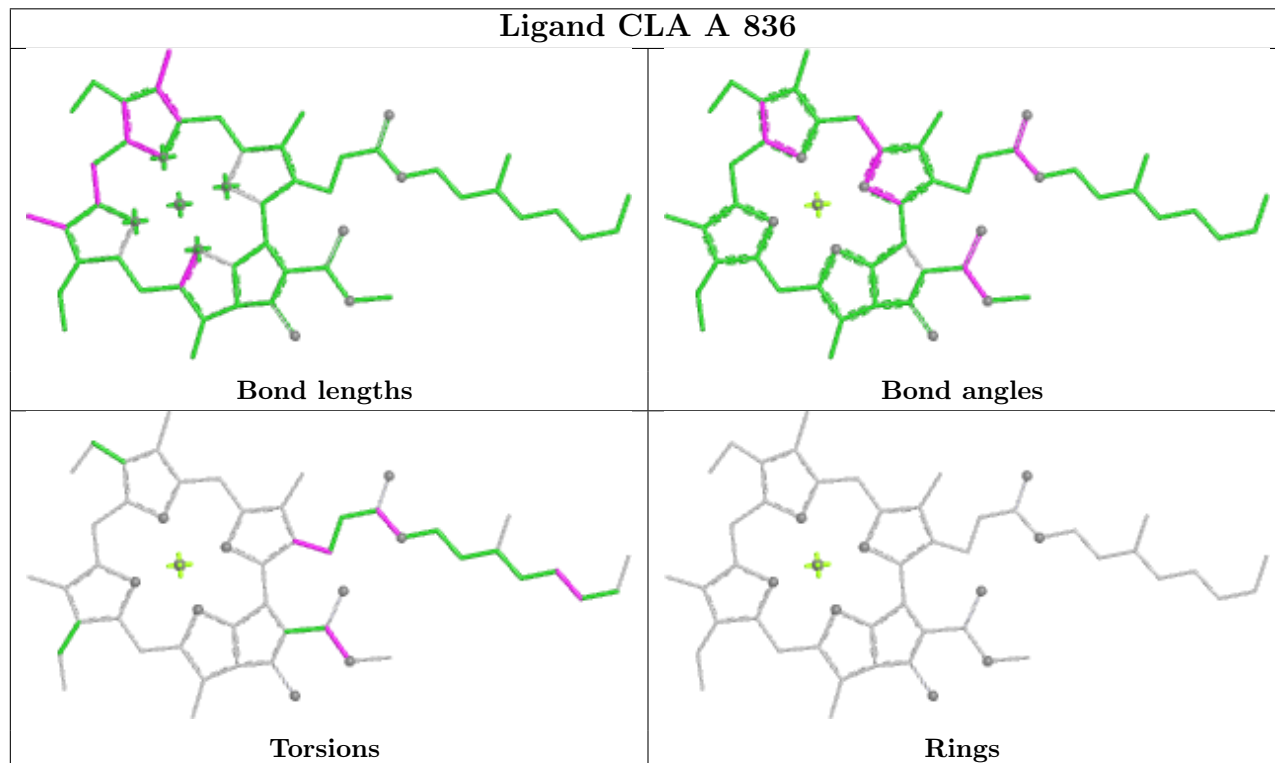


Rings

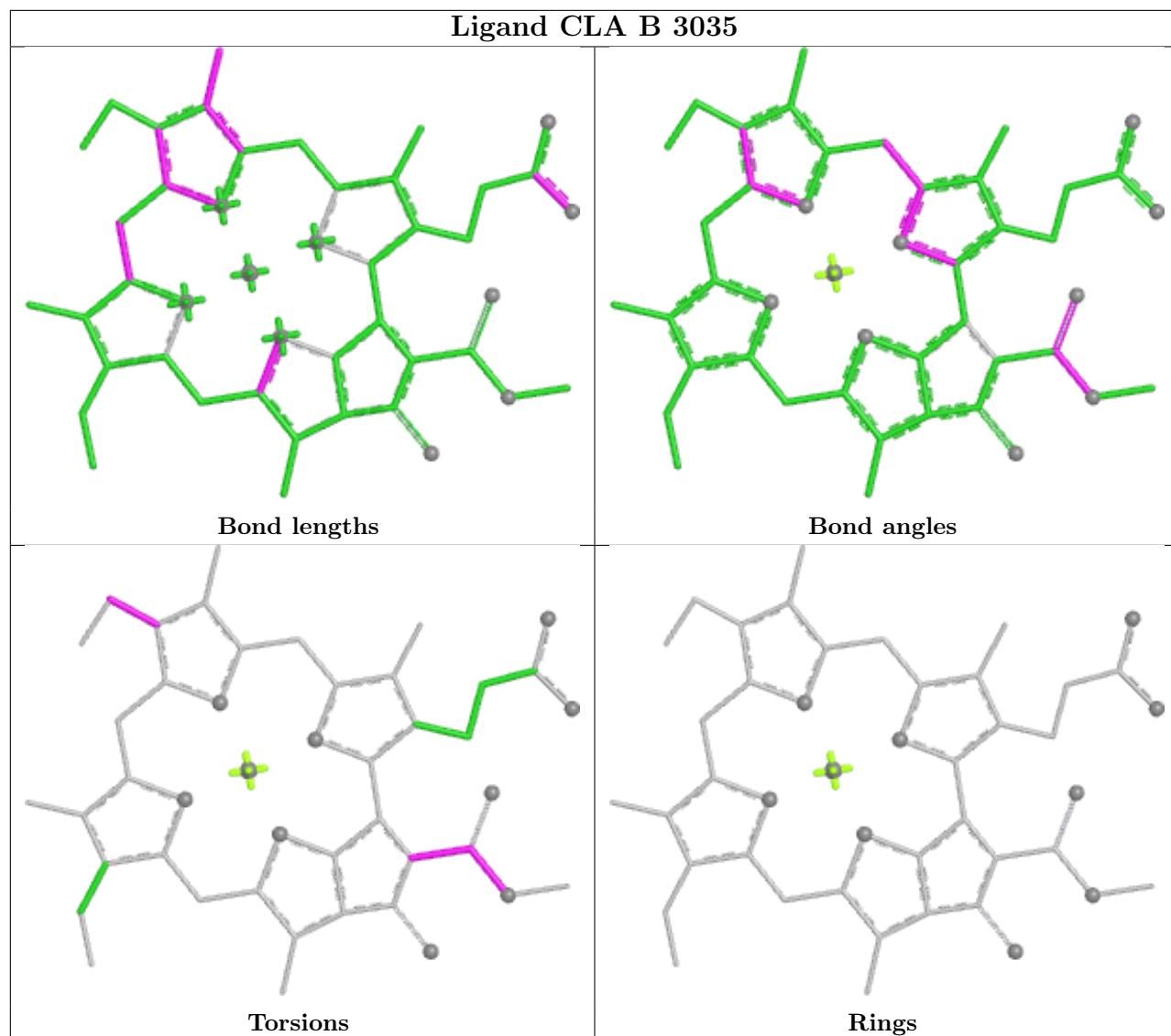
Ligand BCR J 103



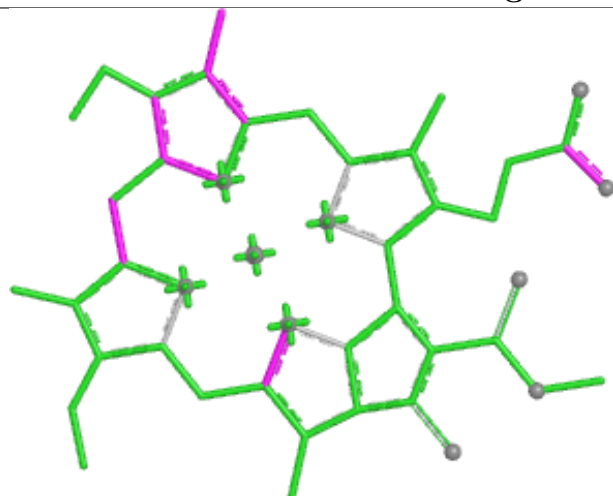
Ligand CLA A 836



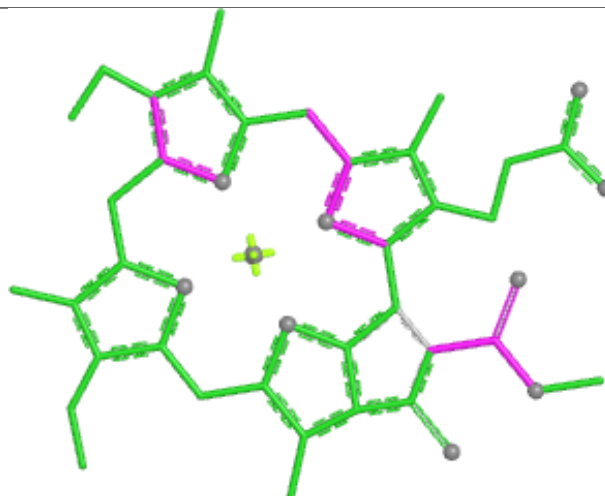
Ligand CLA B 3035



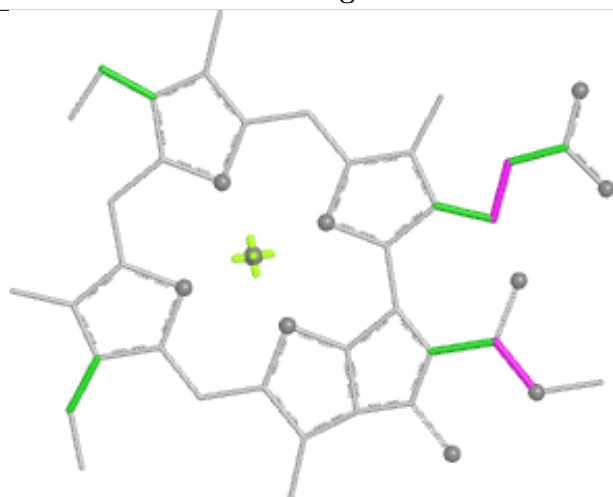
Ligand CLA B 3016



Bond lengths



Bond angles

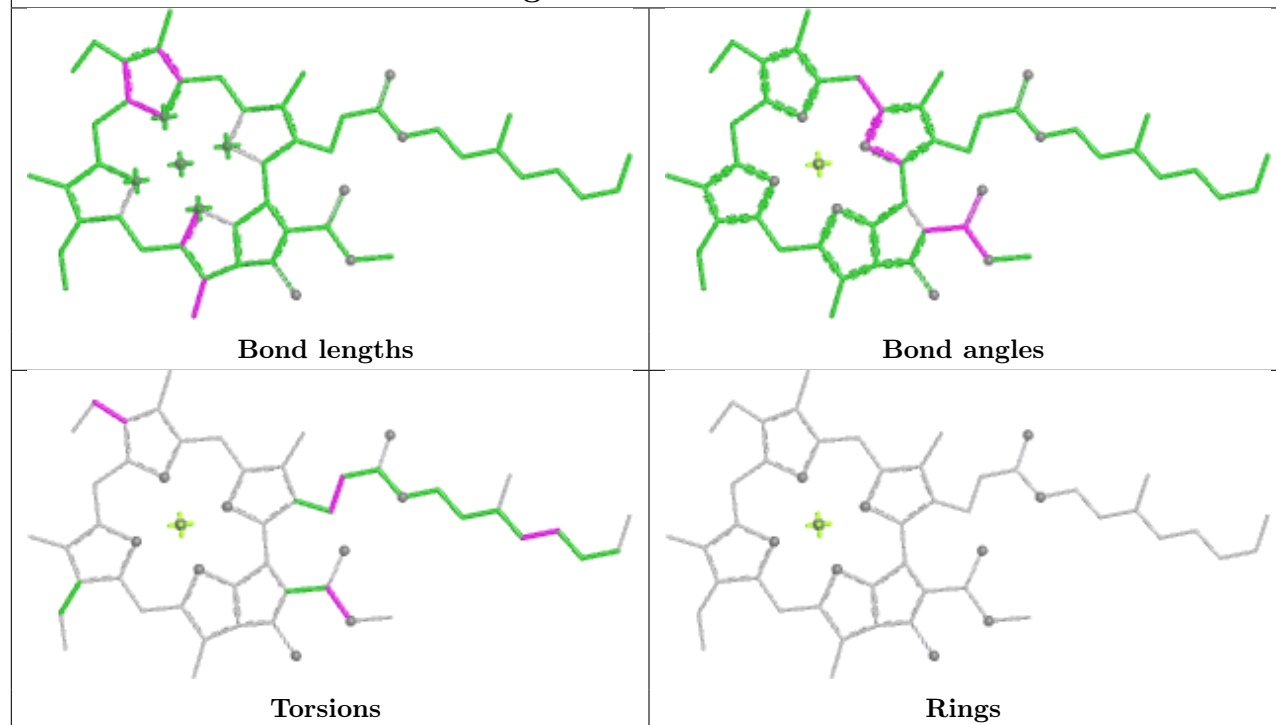


Torsions

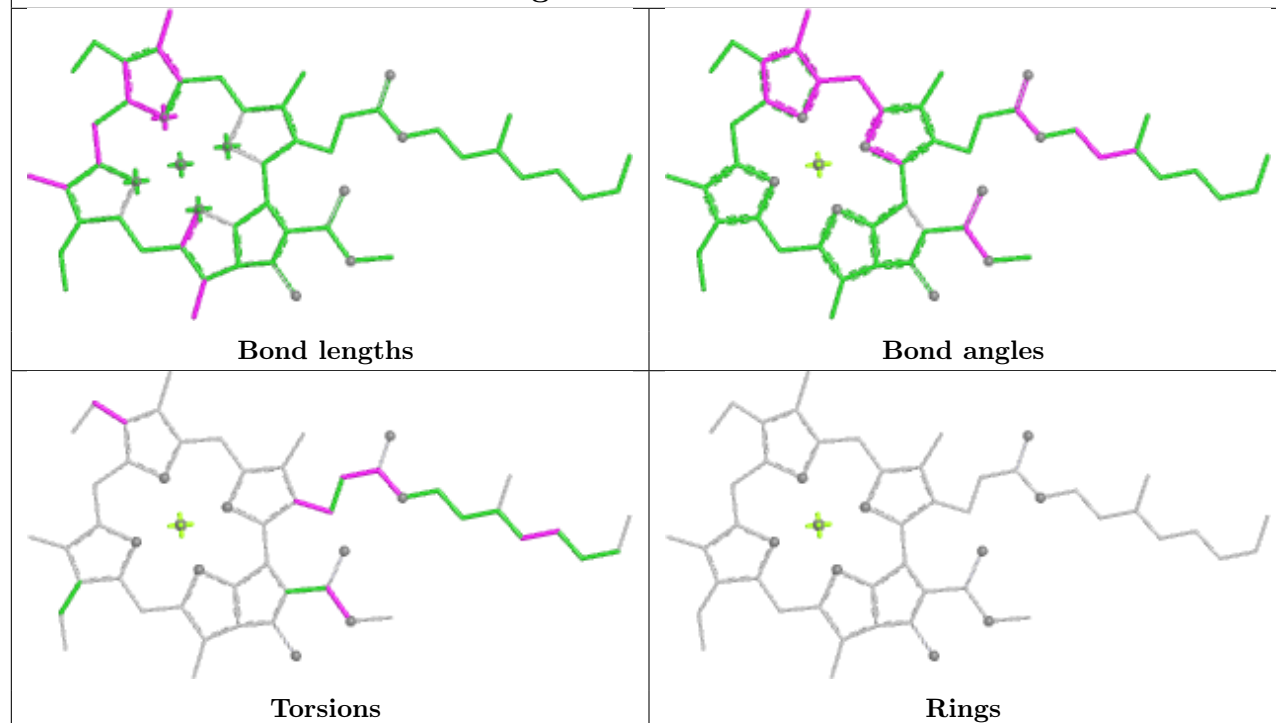


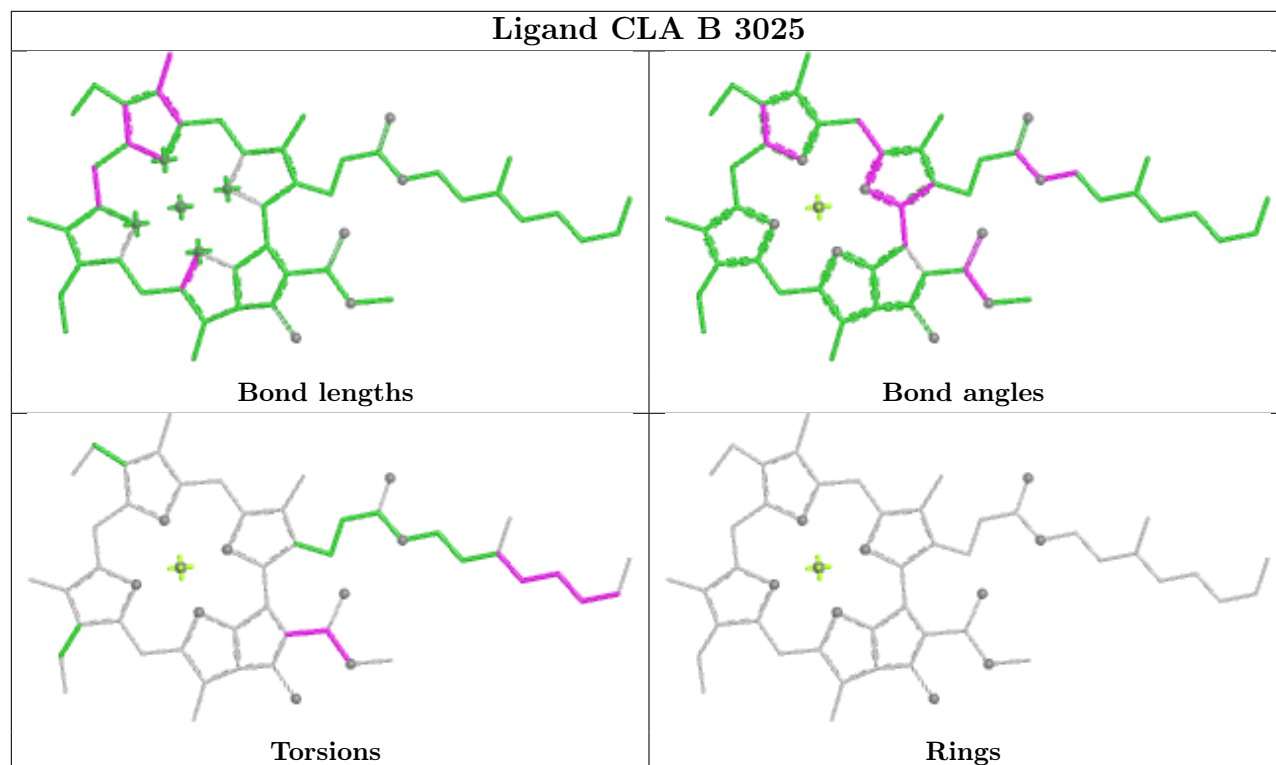
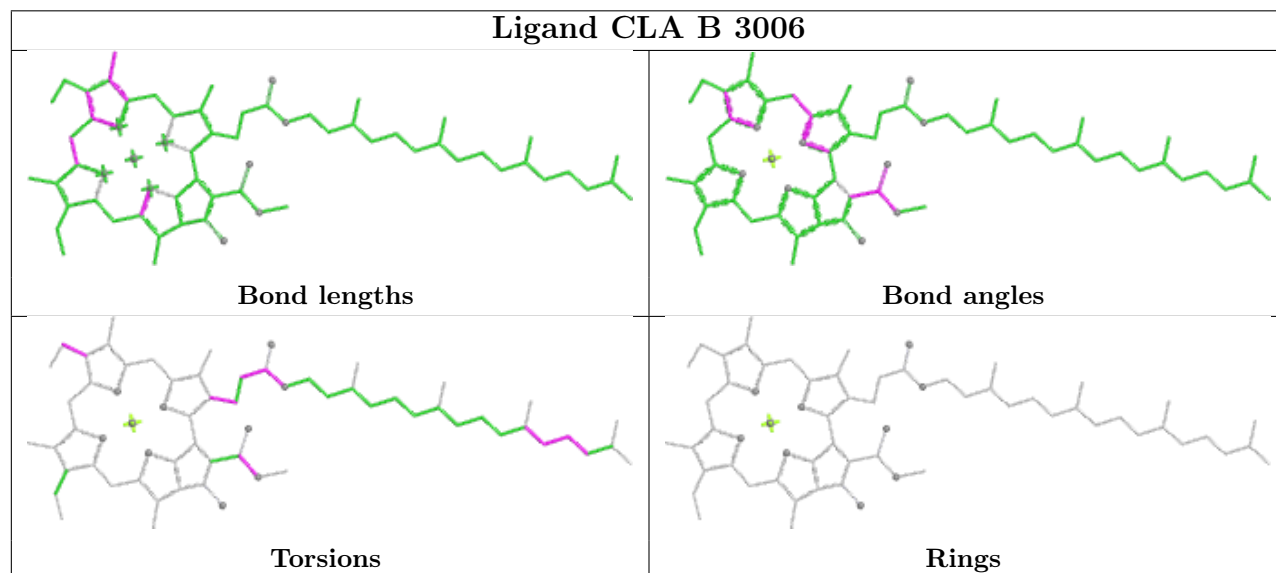
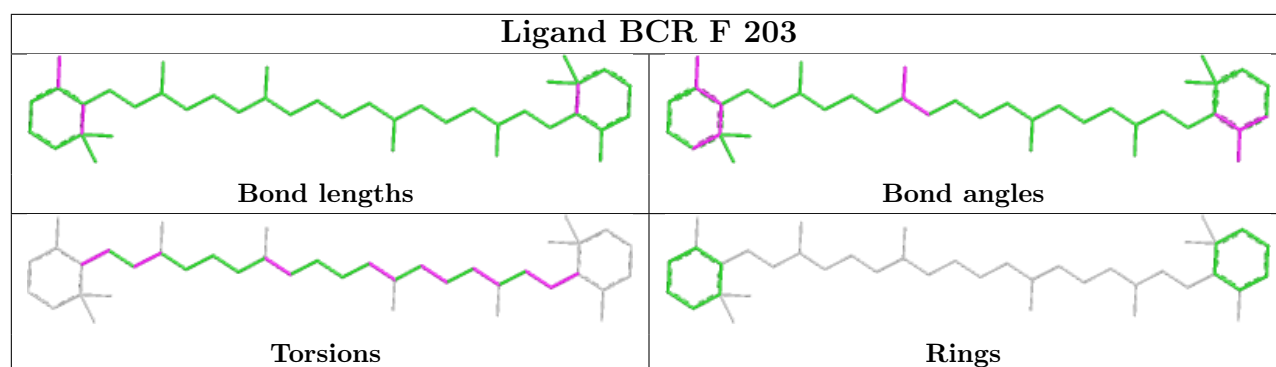
Rings

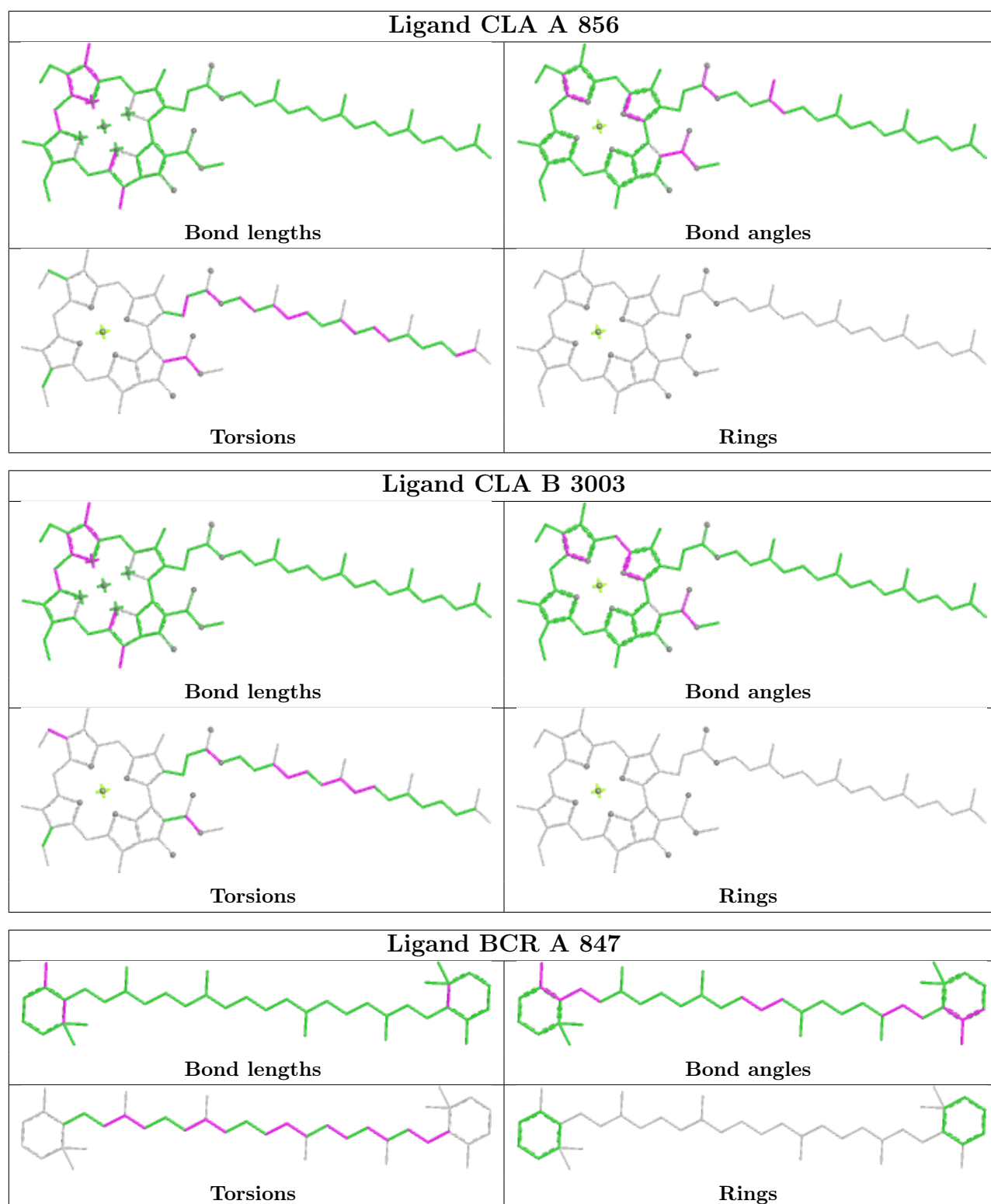
Ligand CLA B 3005



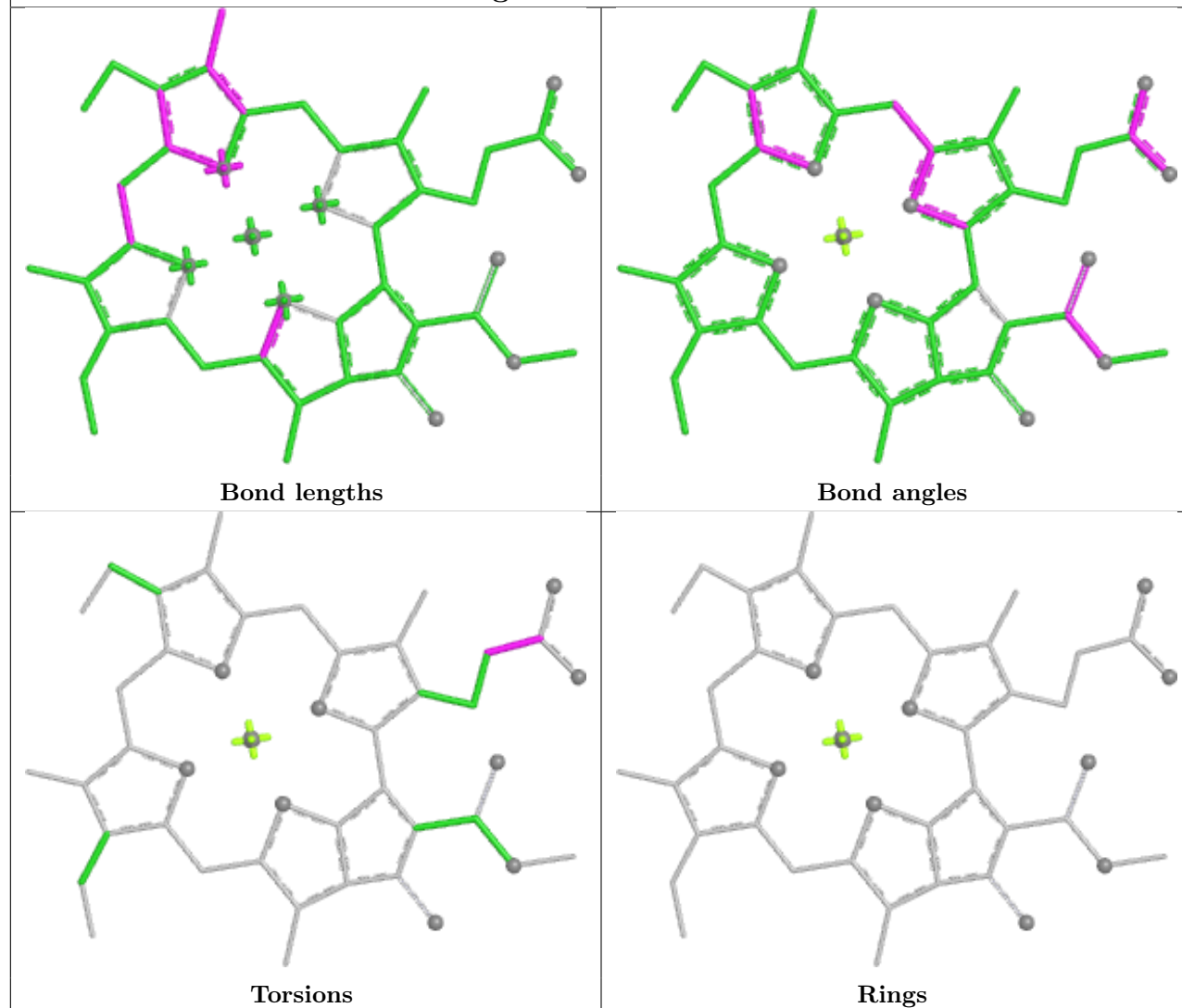
Ligand CLA A 819



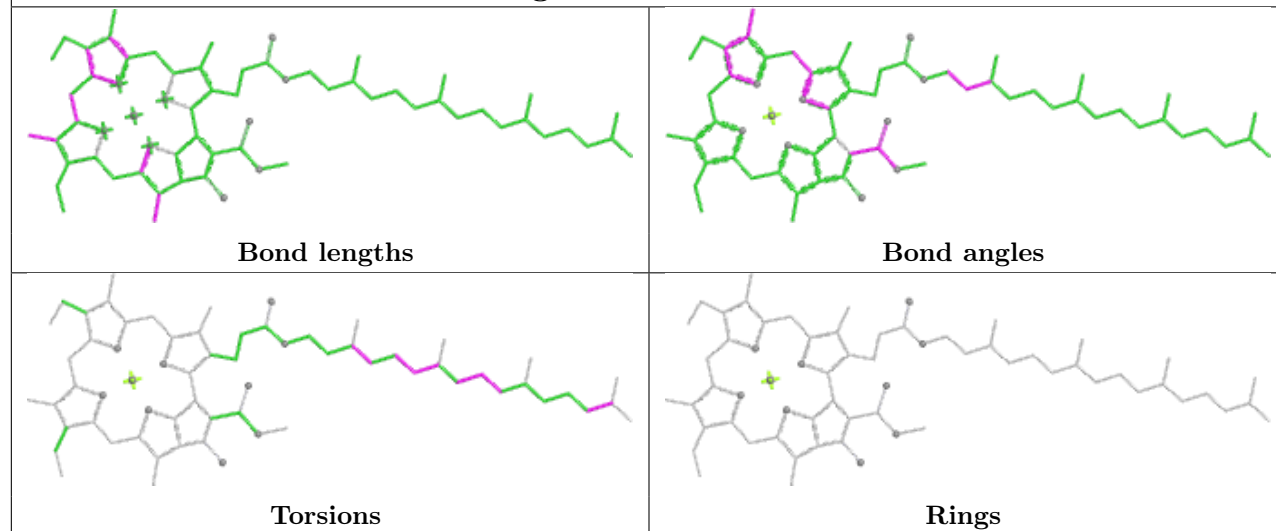




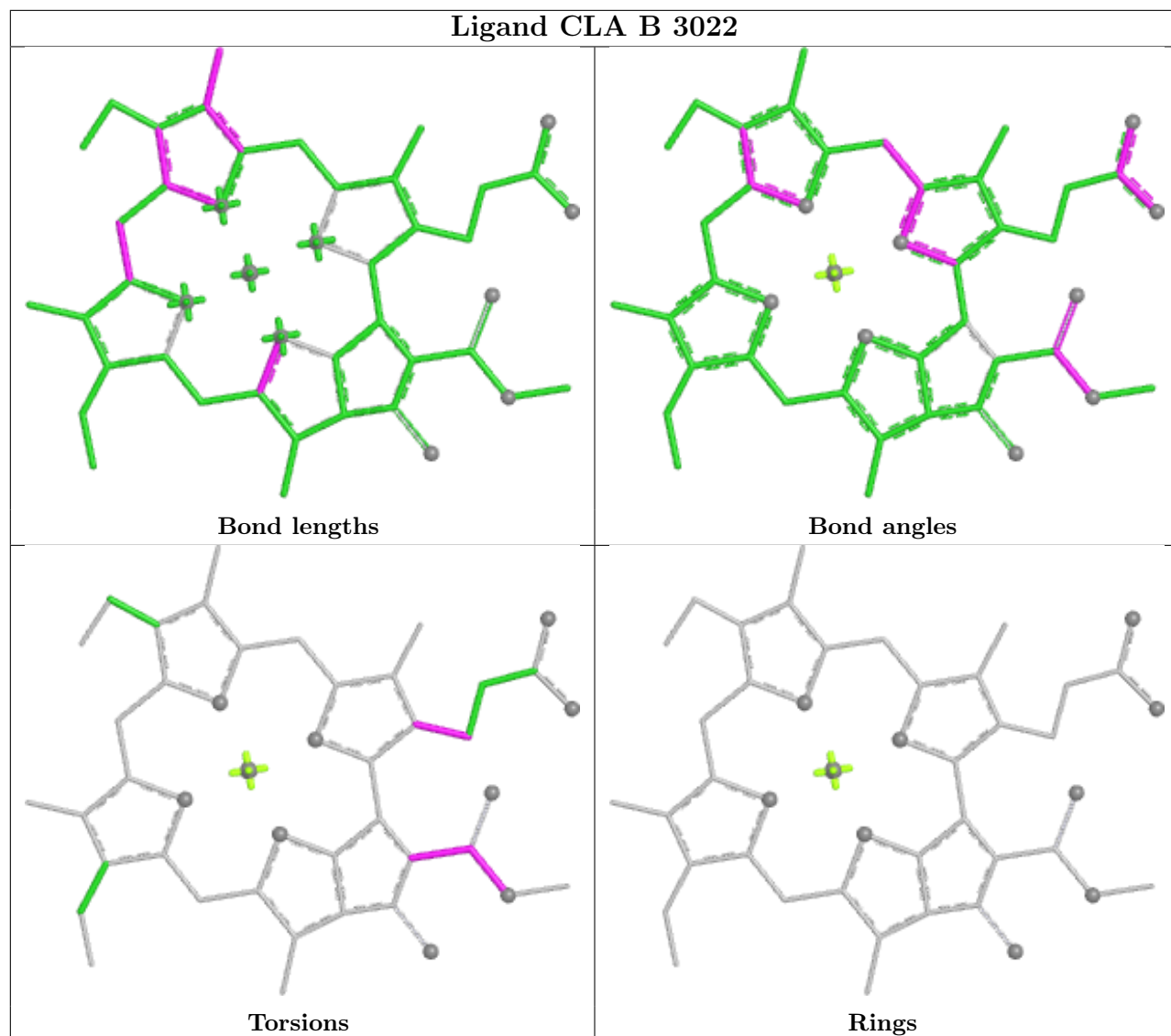
Ligand CLA A 815



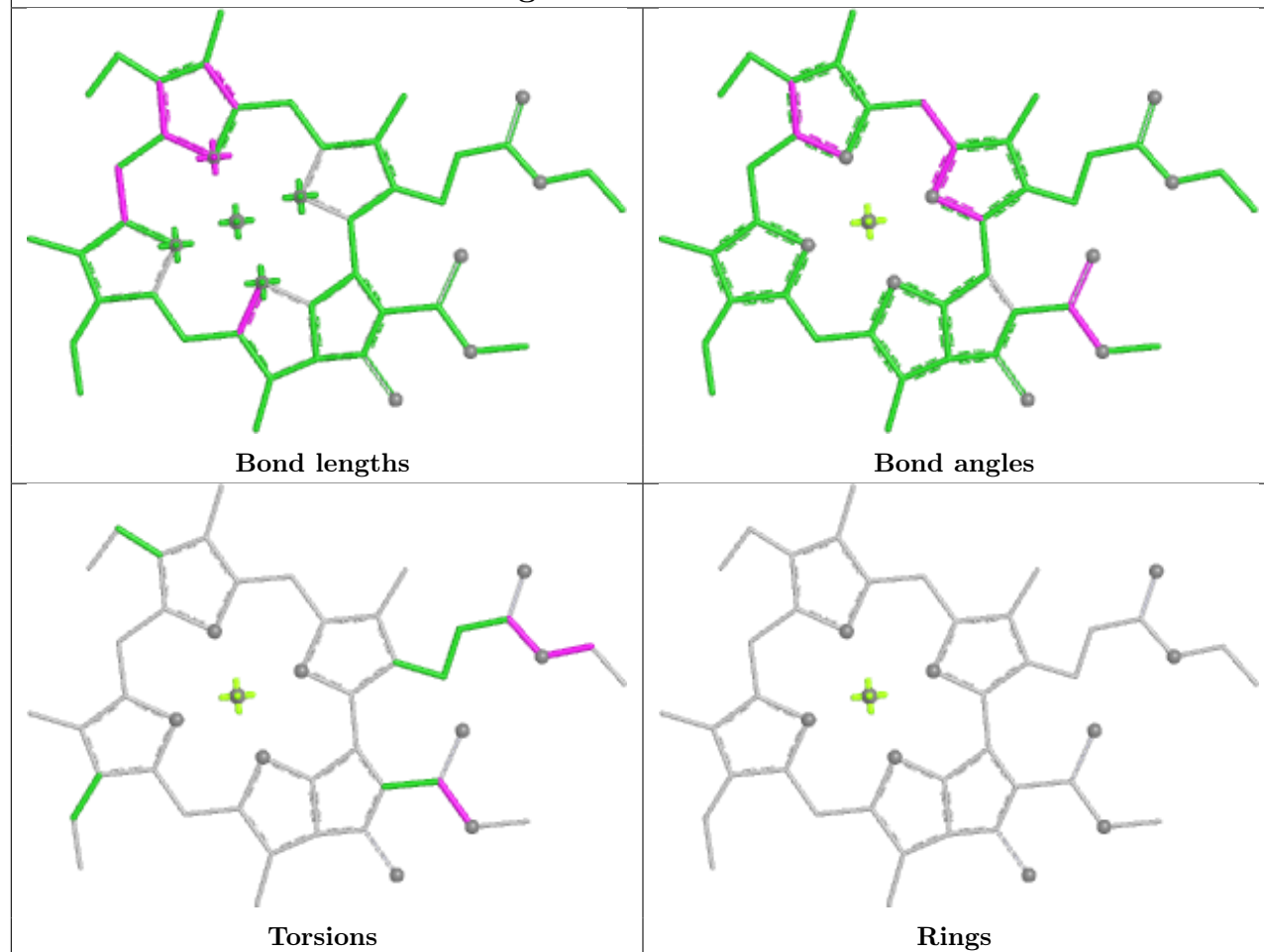
Ligand CLA A 839



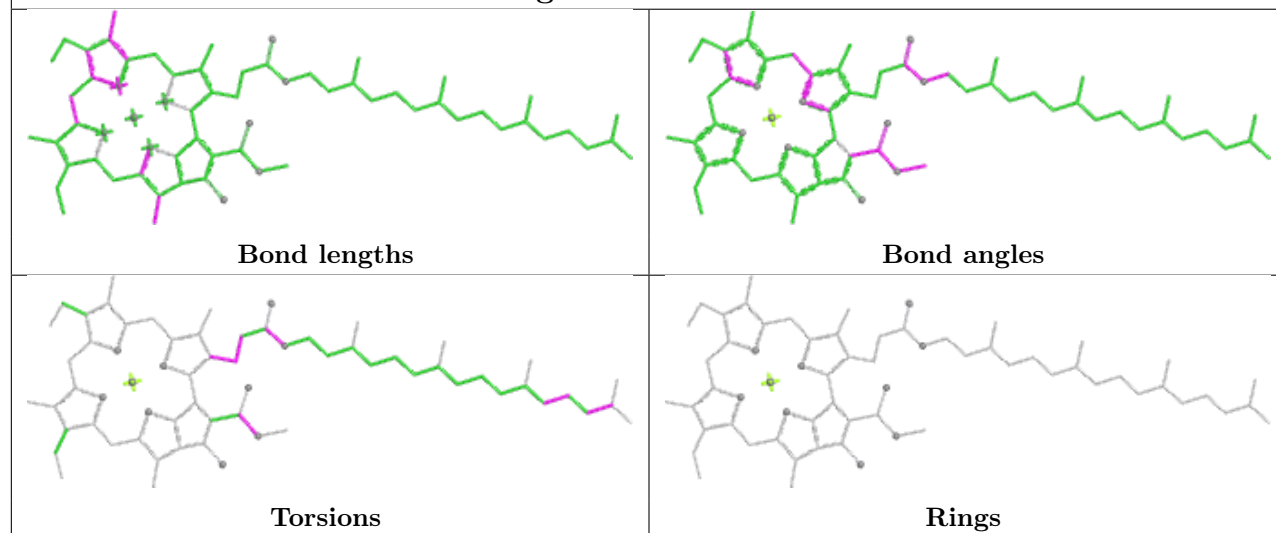
Ligand CLA B 3022



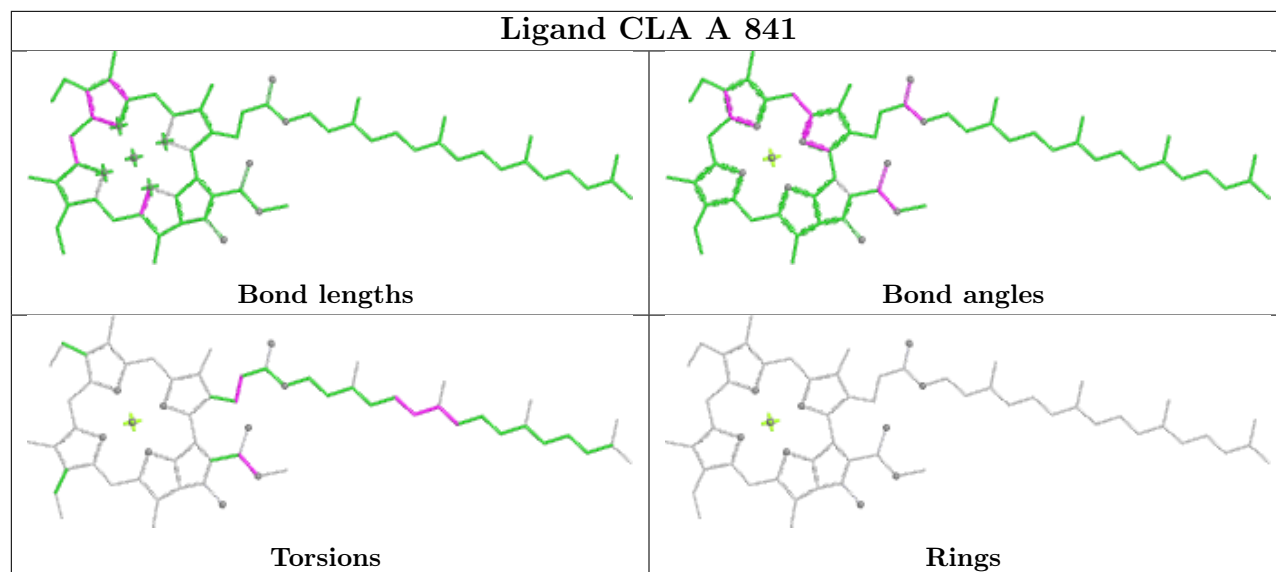
Ligand CLA B 3040



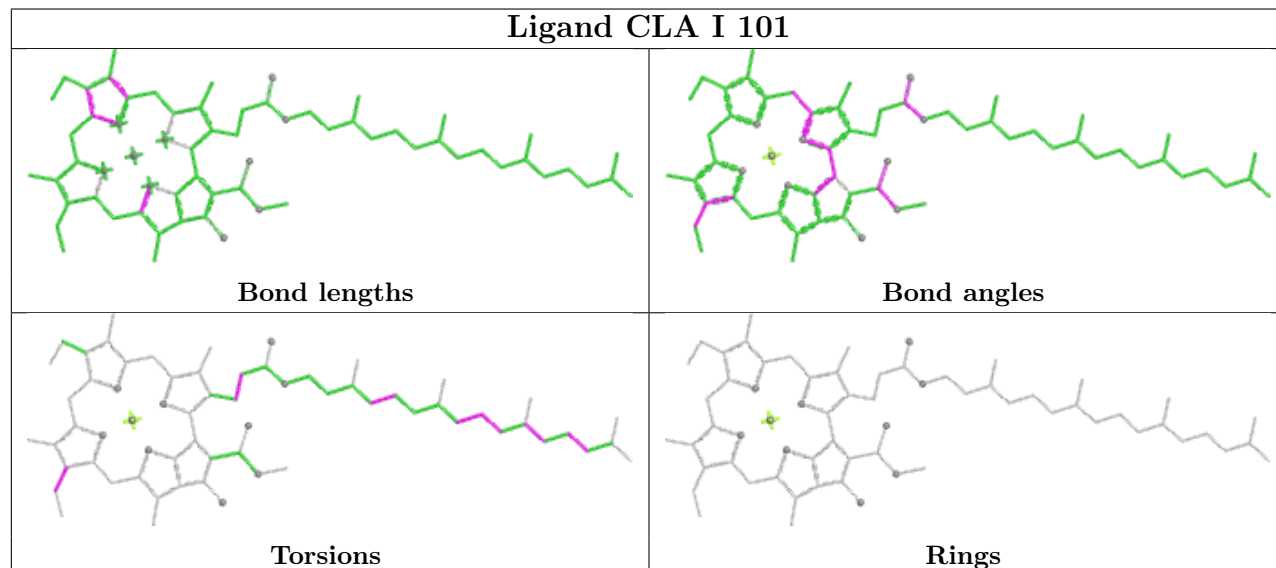
Ligand CL0 A 801



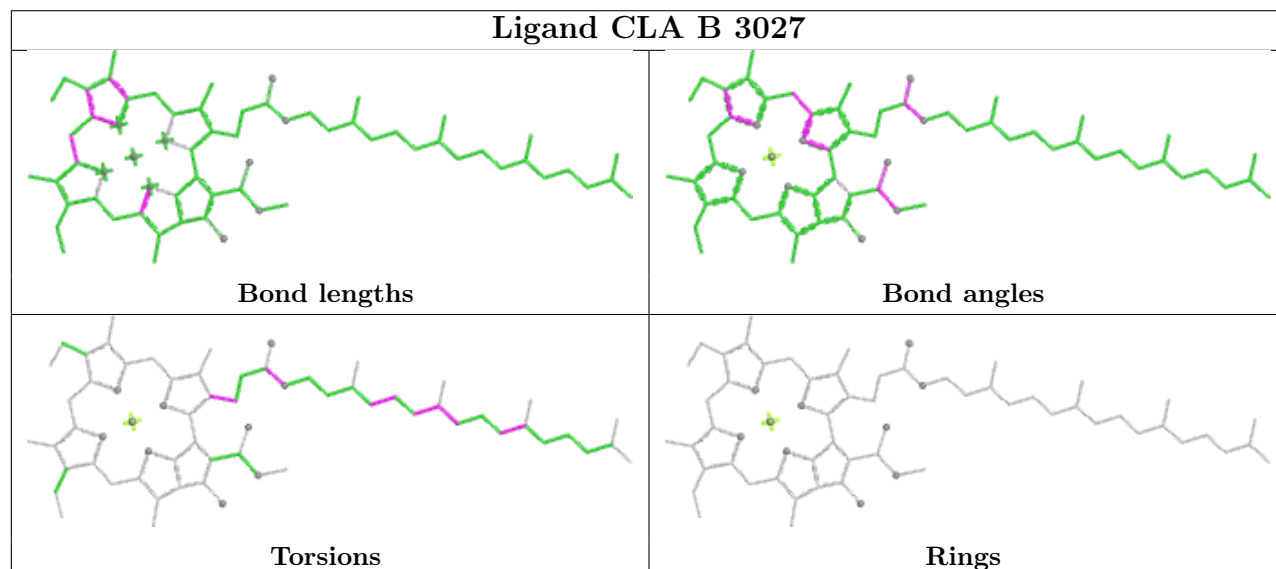
Ligand CLA A 841



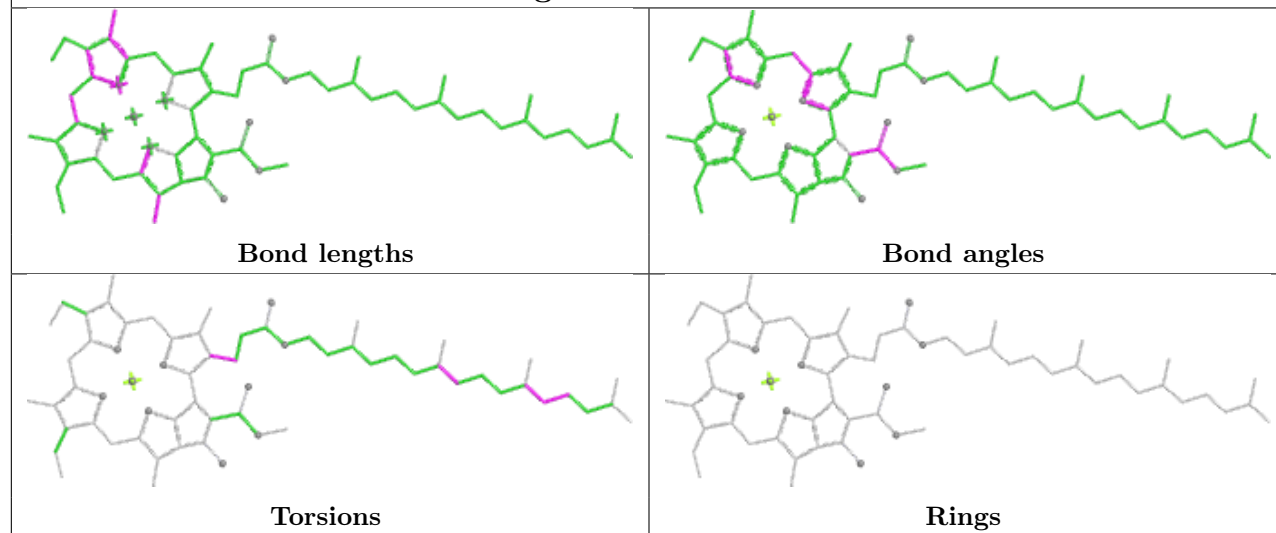
Ligand CLA I 101



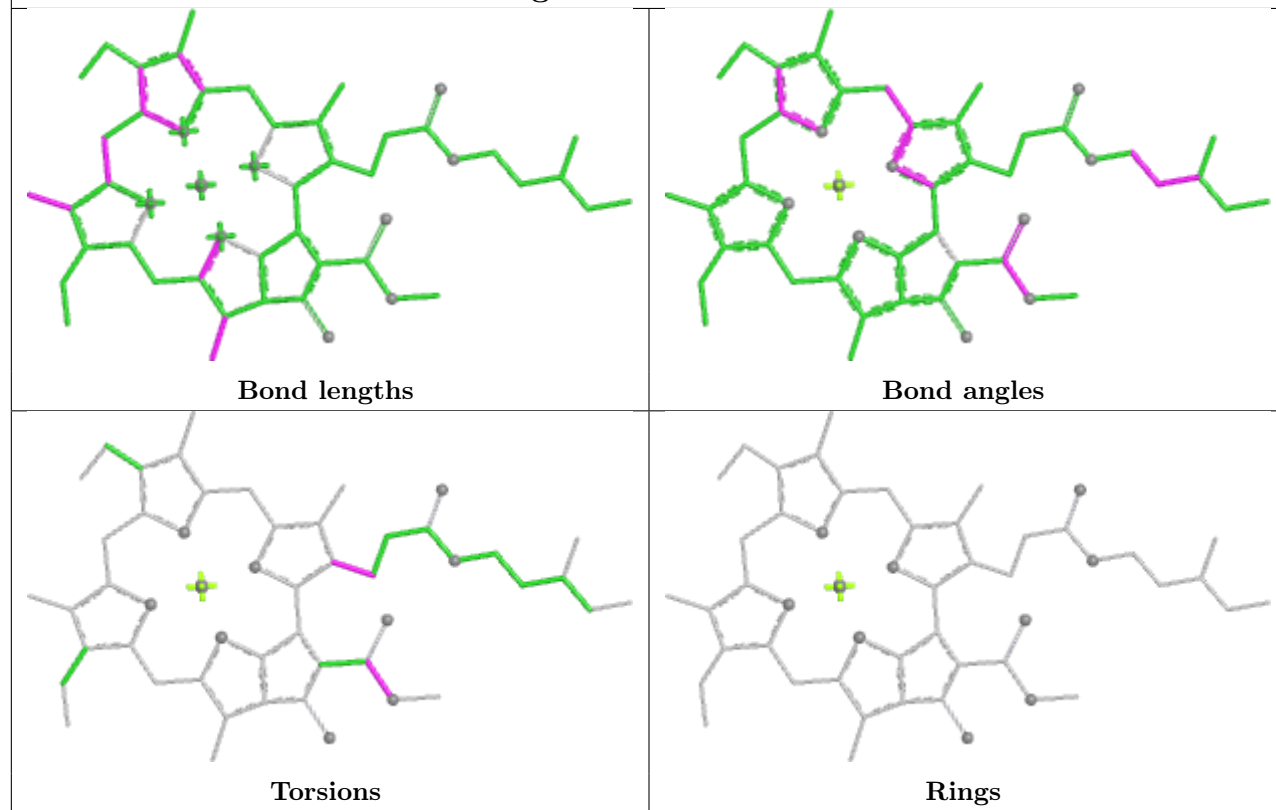
Ligand CLA B 3027



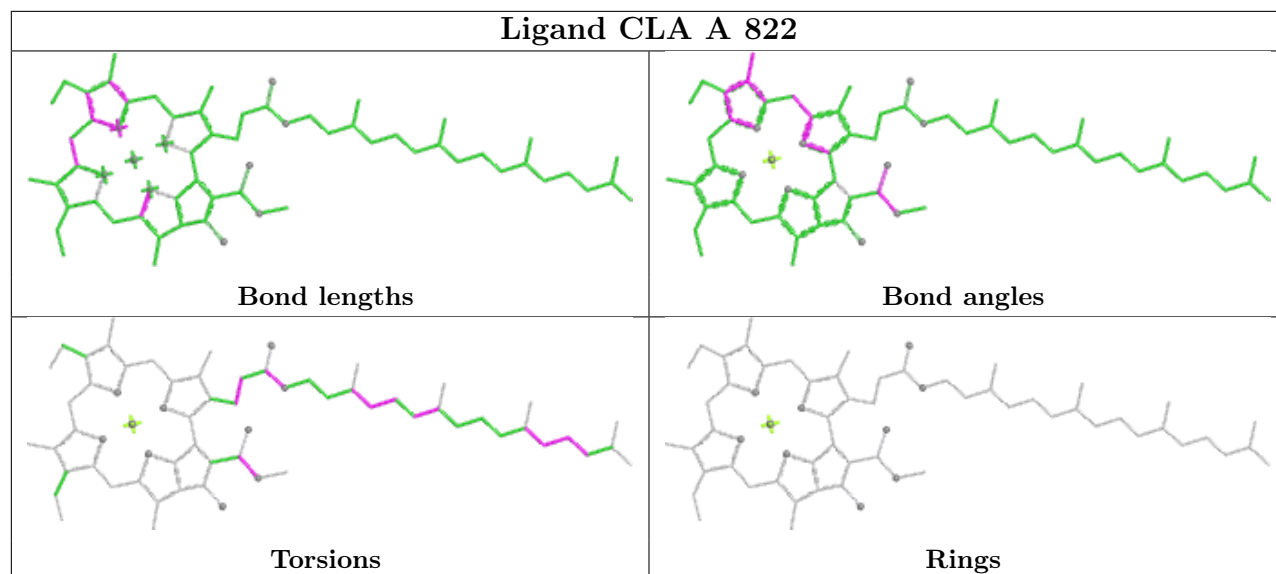
Ligand CLA L 204



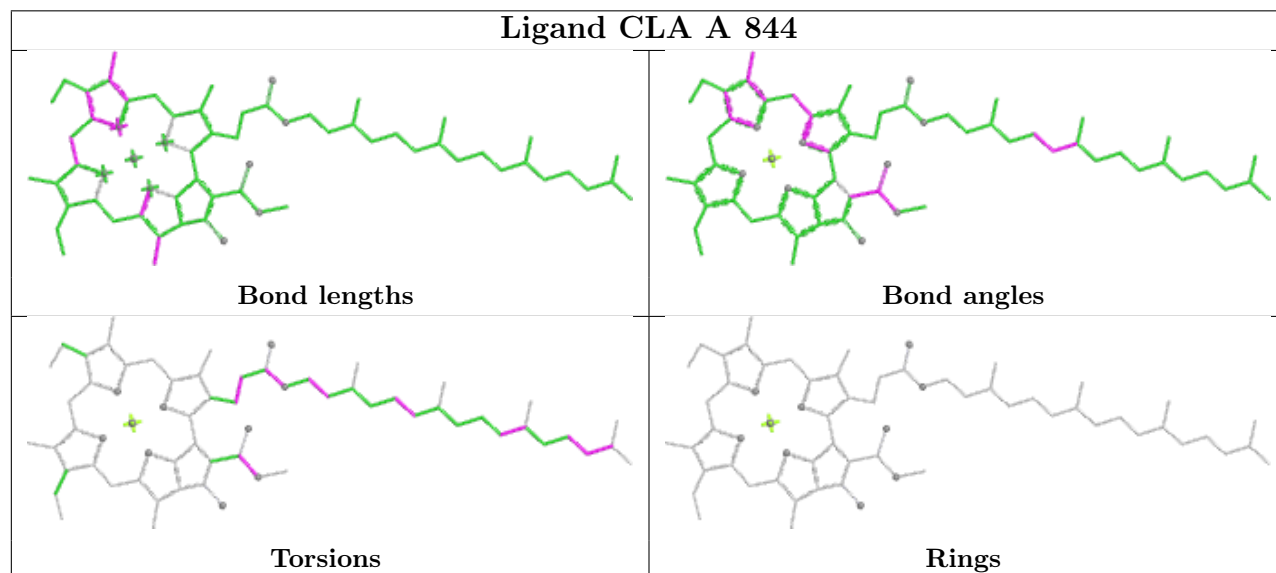
Ligand CLA A 842



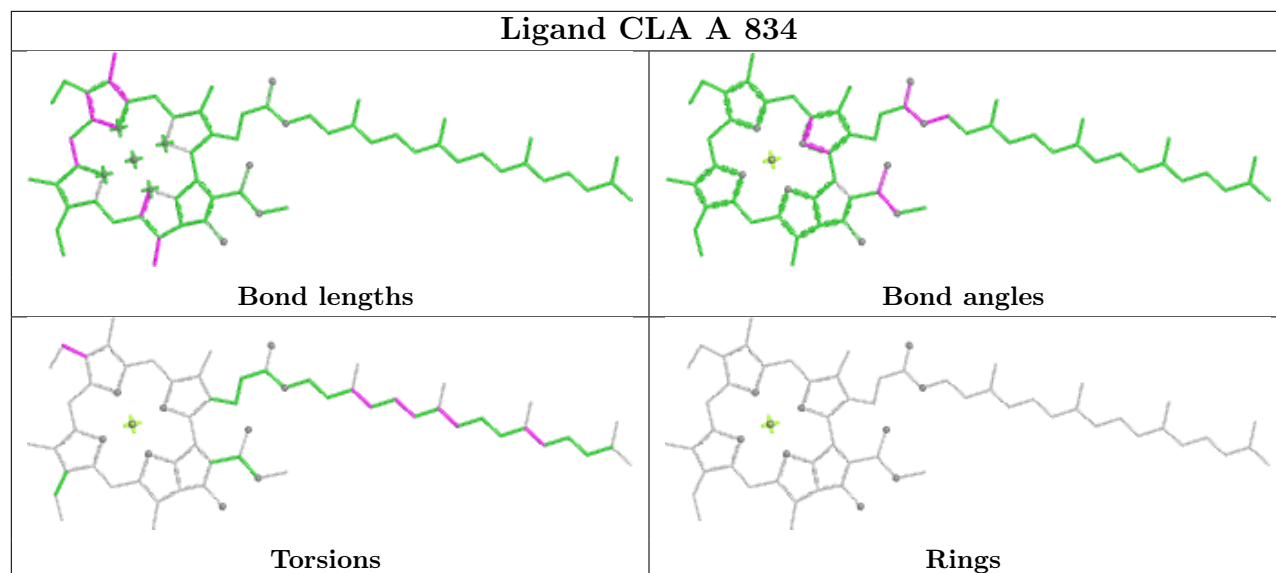
Ligand CLA A 822

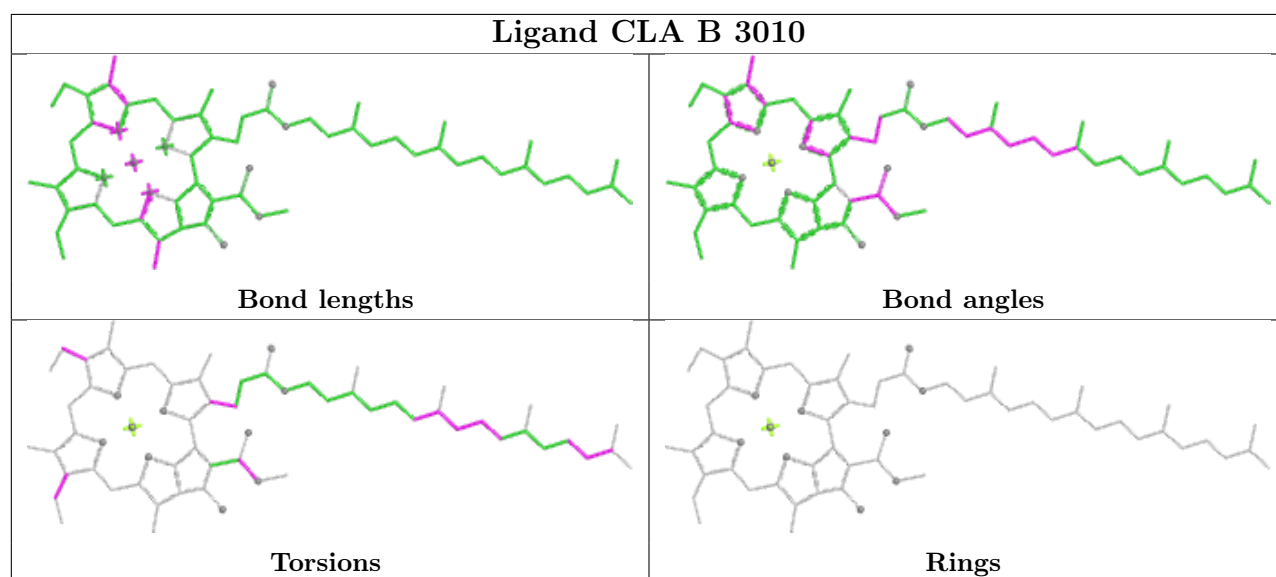
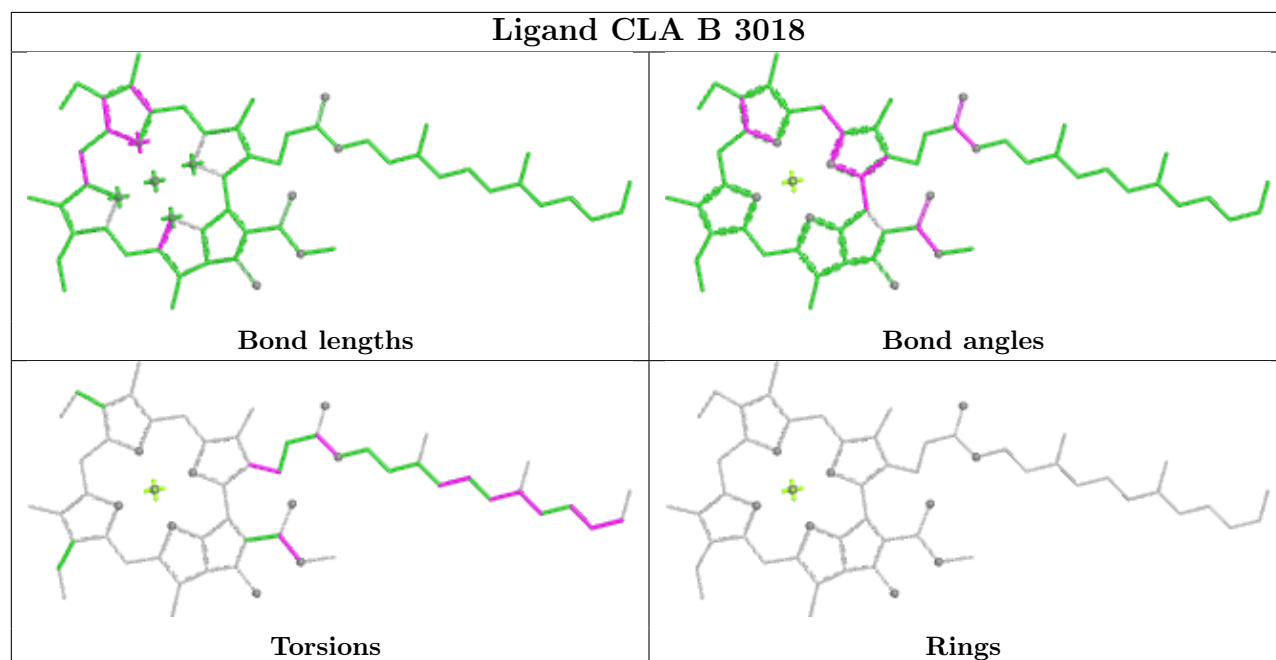
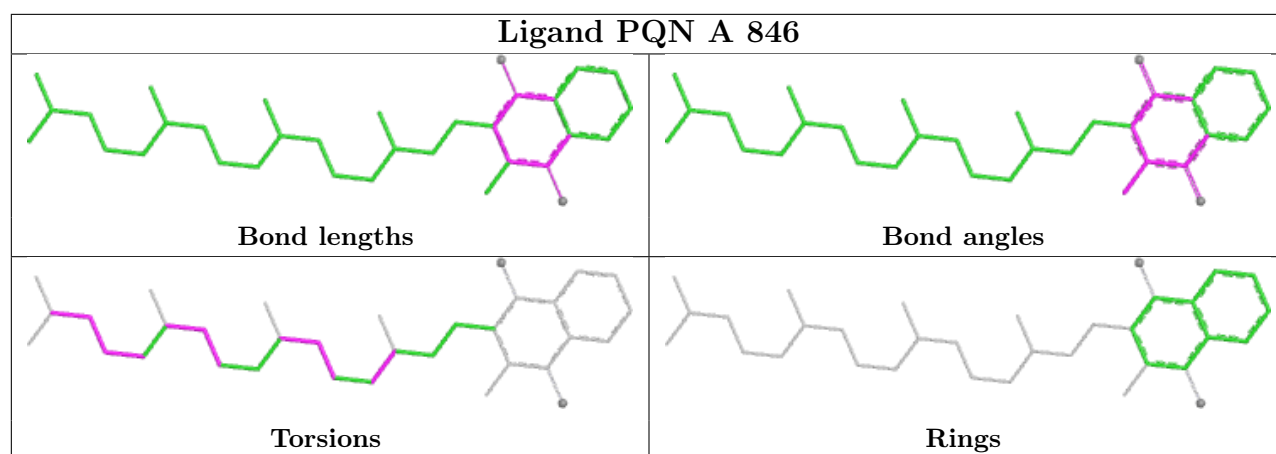


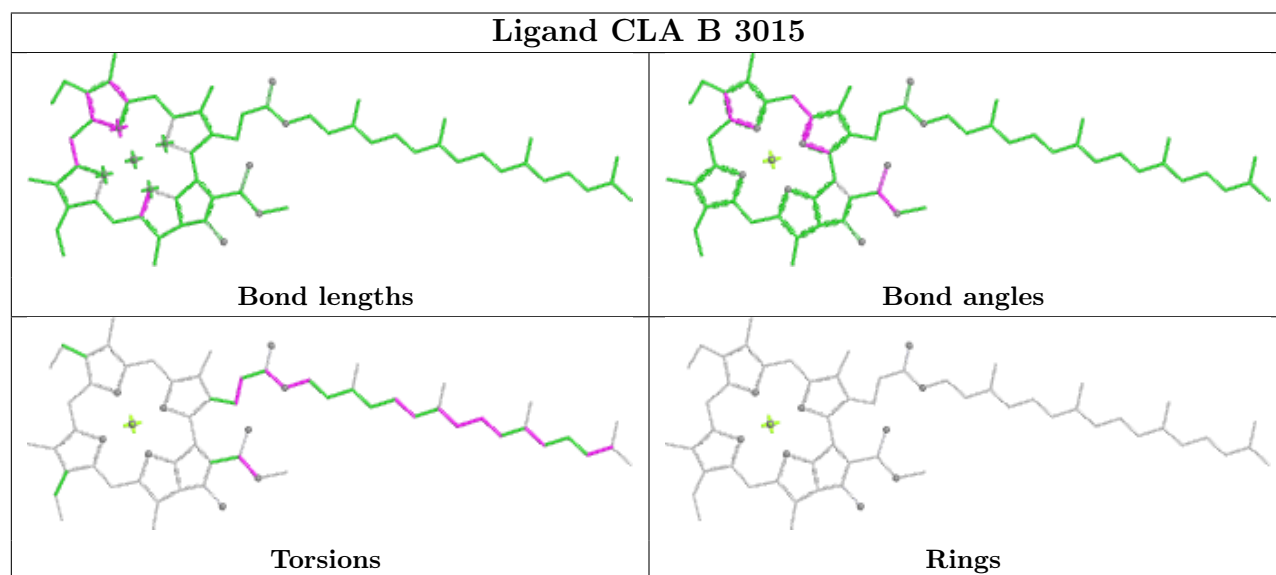
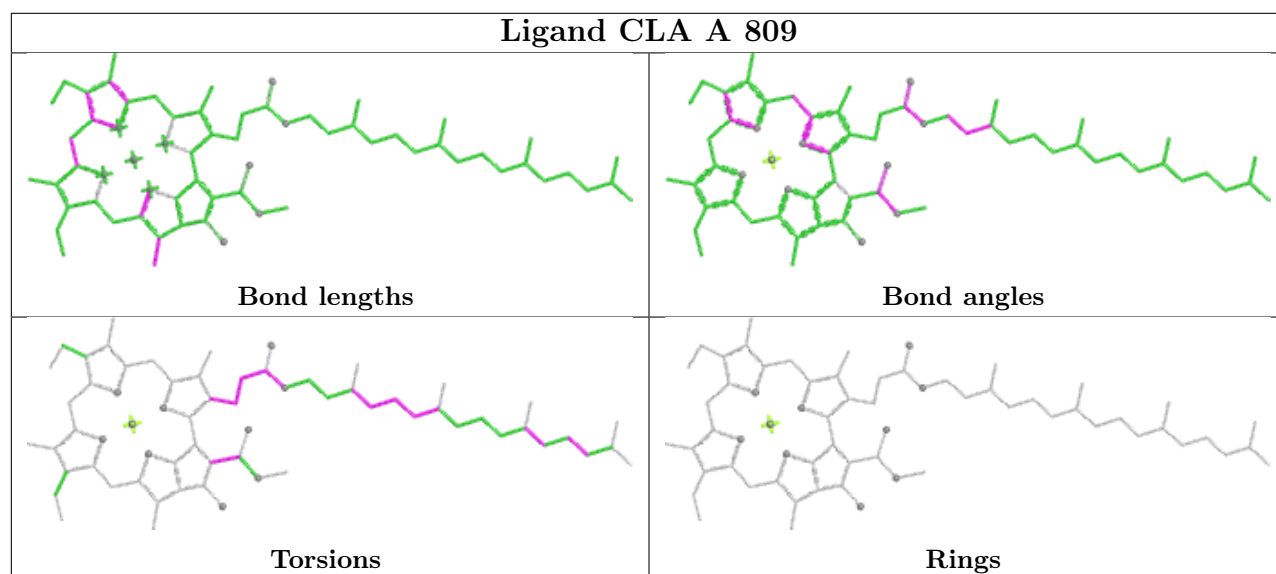
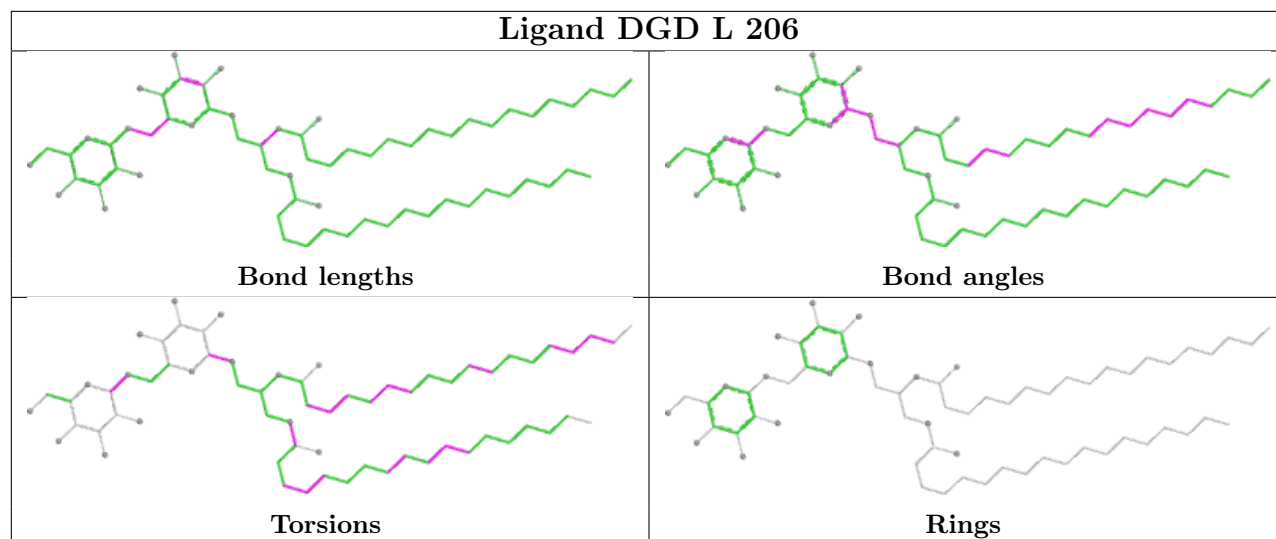
Ligand CLA A 844

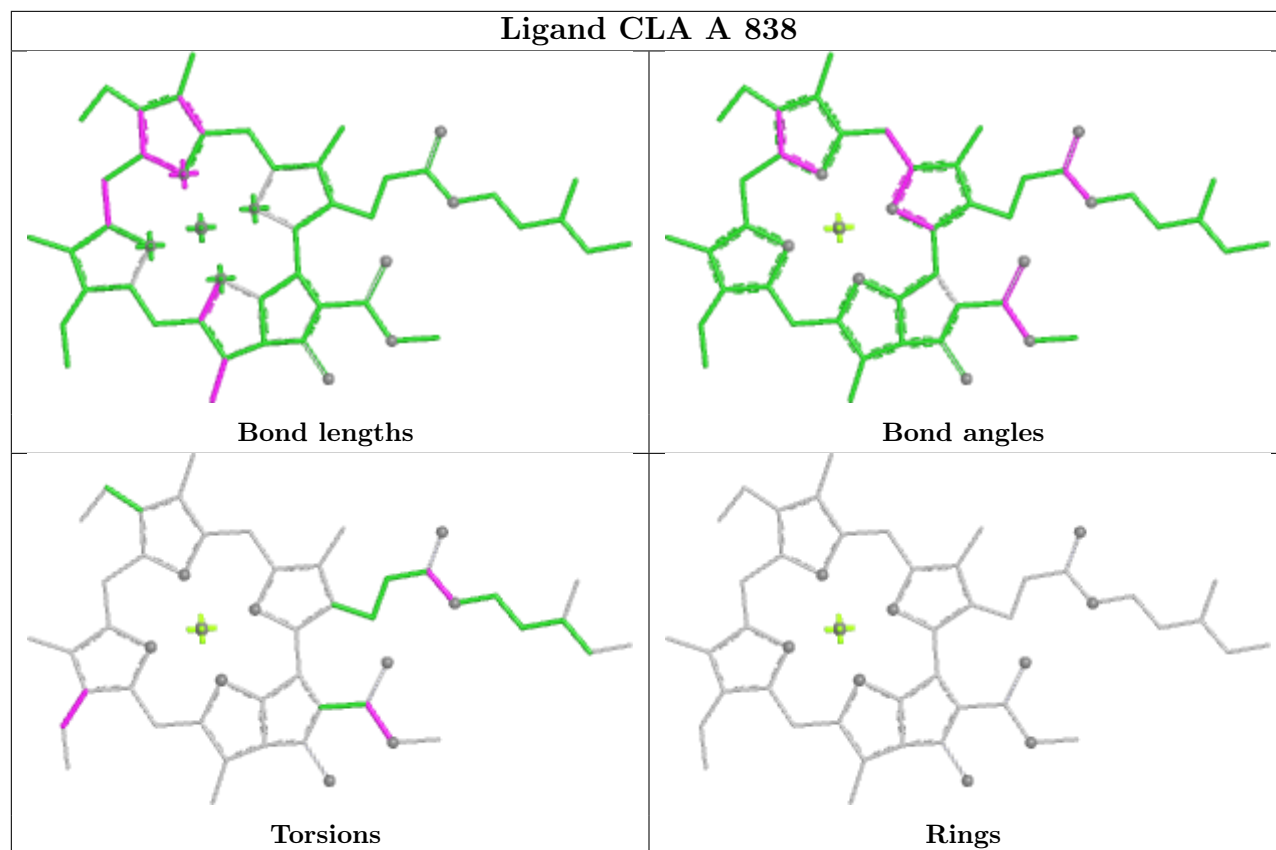


Ligand CLA A 834

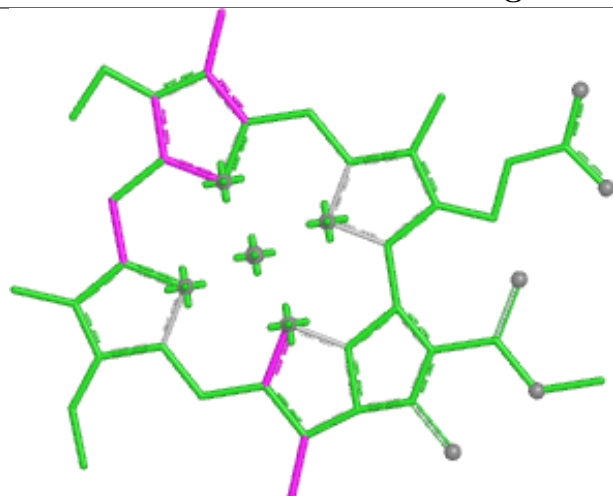




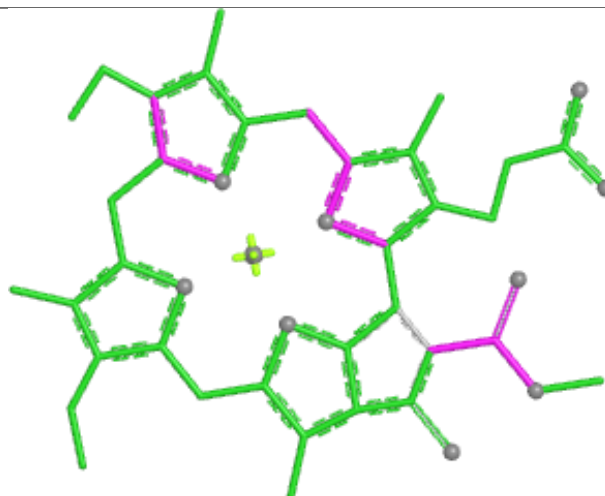




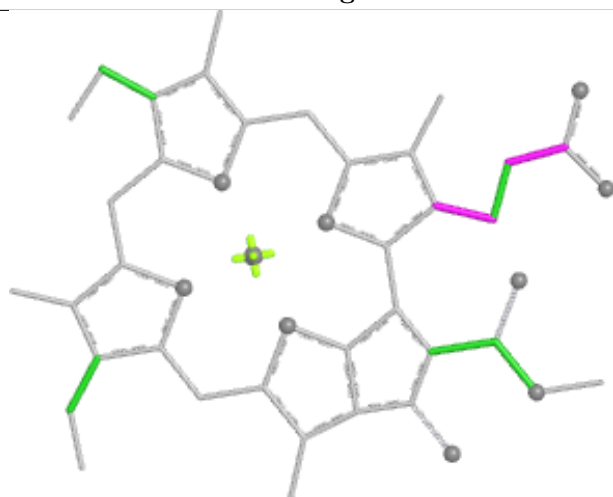
Ligand CLA X 1701



Bond lengths



Bond angles

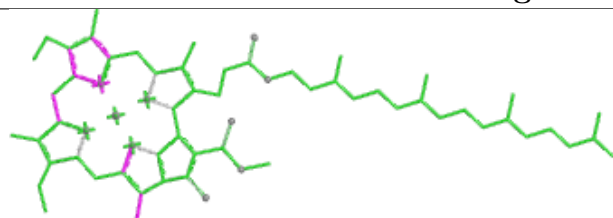


Torsions

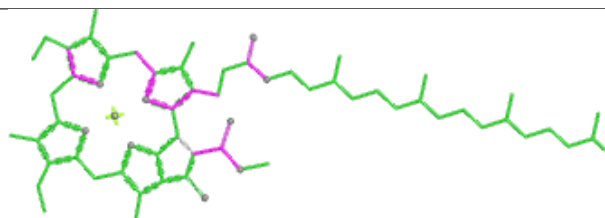


Rings

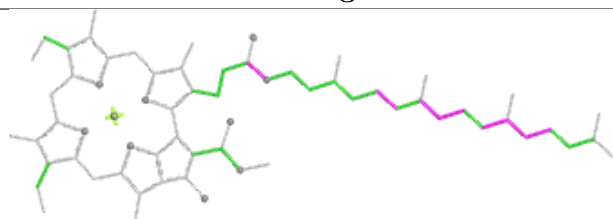
Ligand CLA A 827



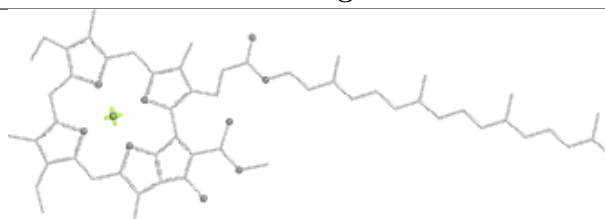
Bond lengths



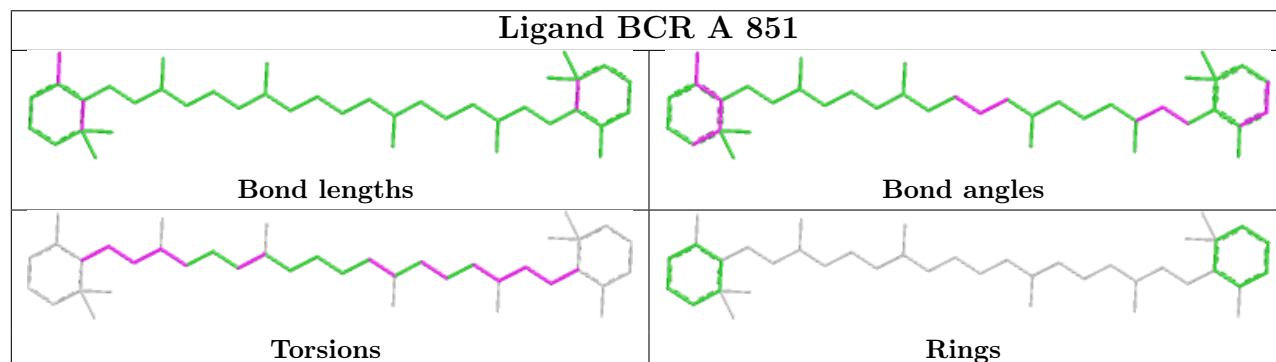
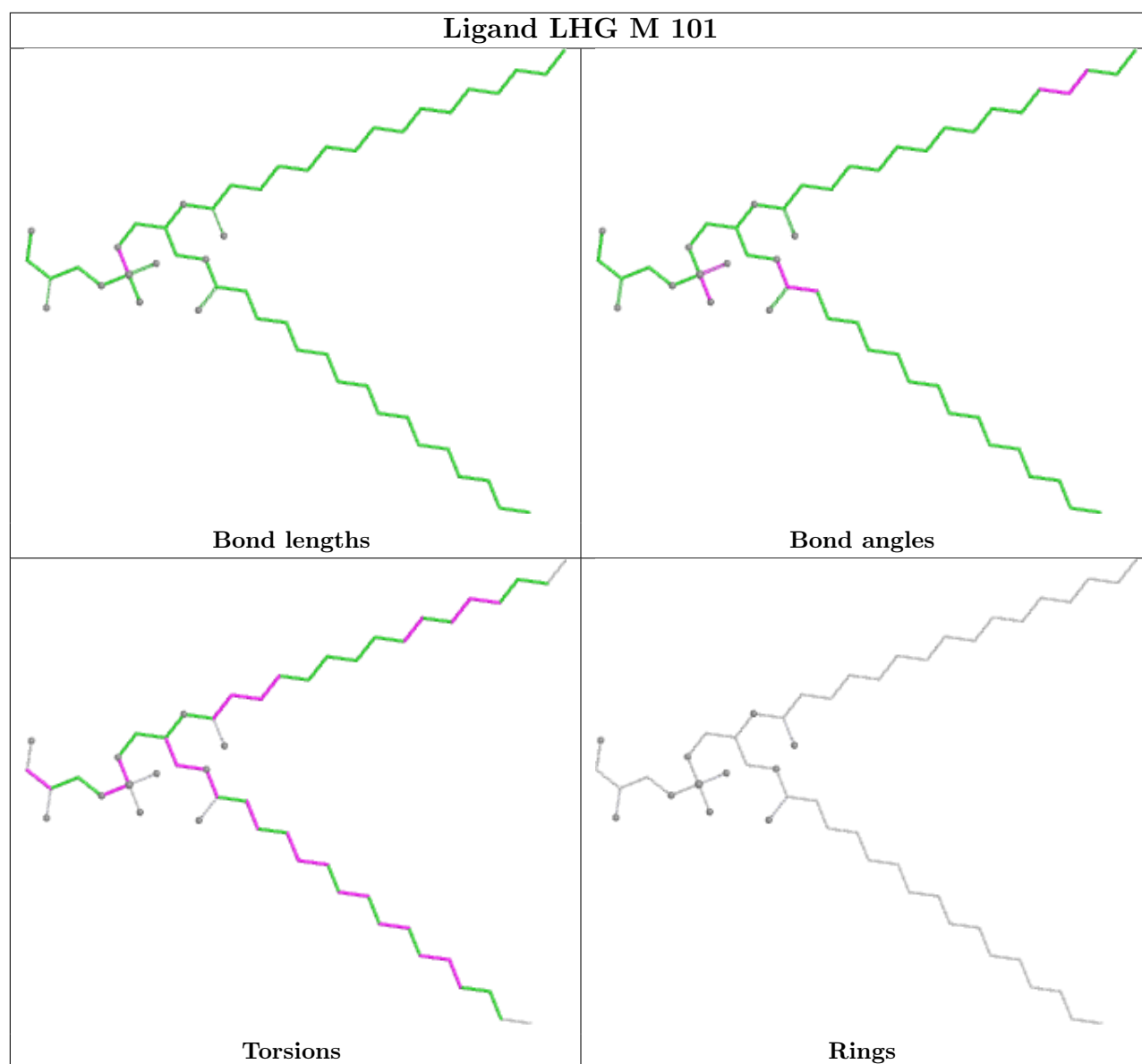
Bond angles



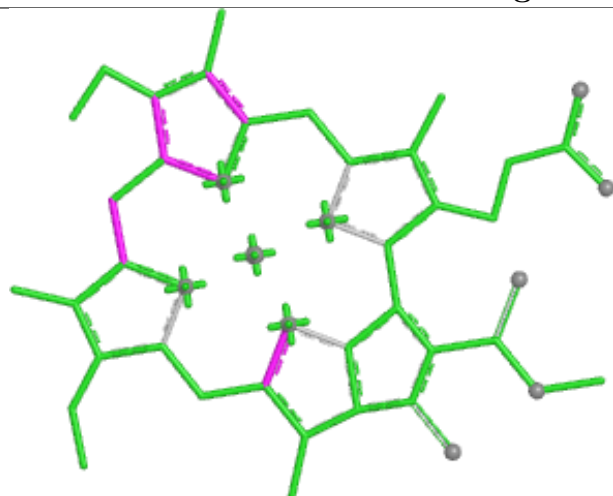
Torsions



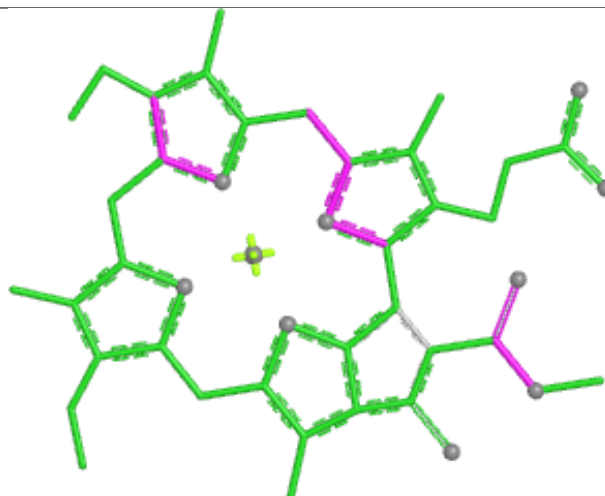
Rings



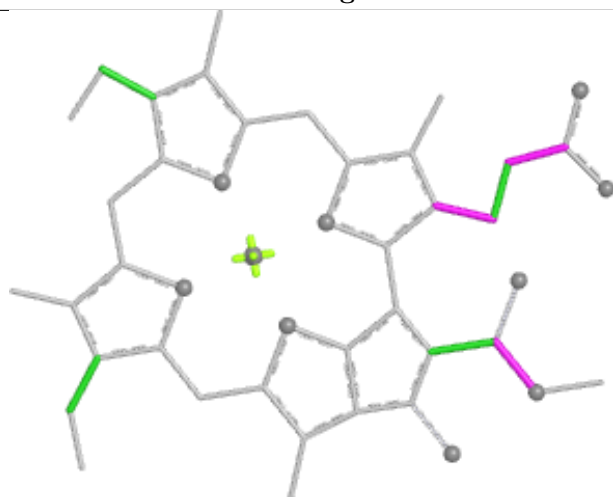
Ligand CLA A 837



Bond lengths



Bond angles

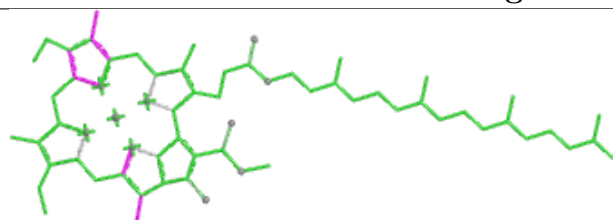


Torsions

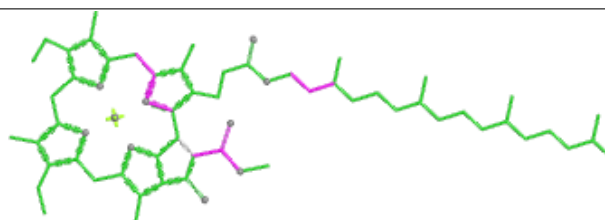


Rings

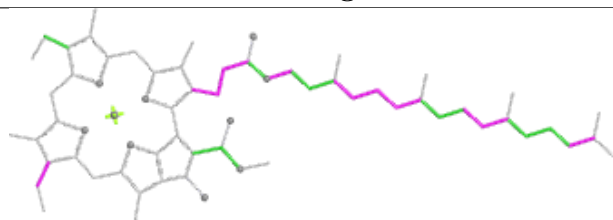
Ligand CLA B 3033



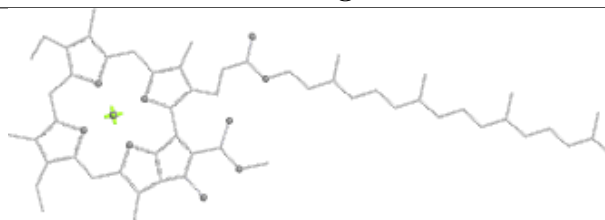
Bond lengths



Bond angles

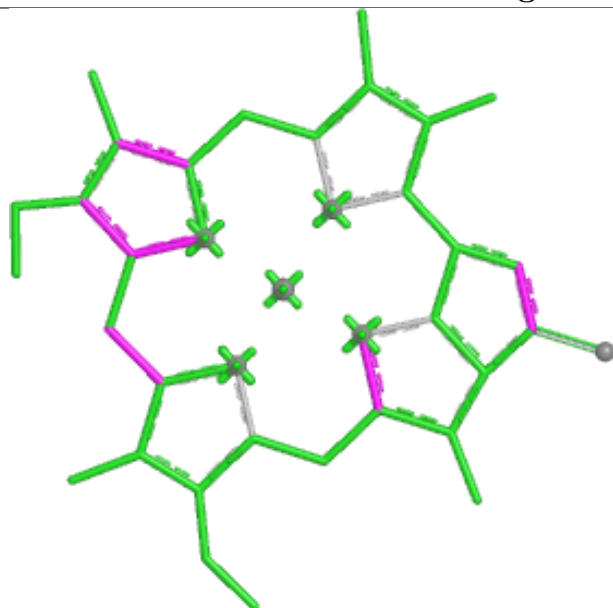


Torsions

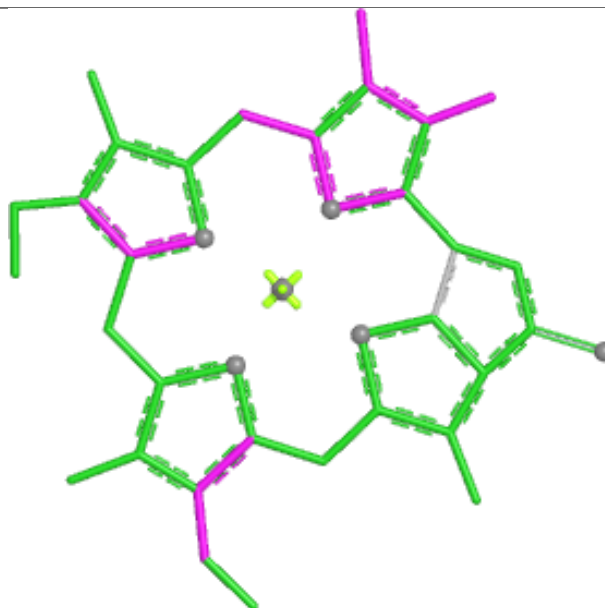


Rings

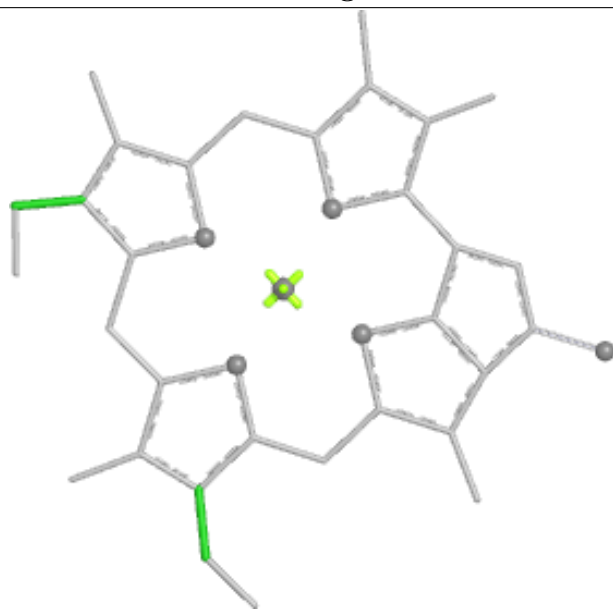
Ligand CLA J 102



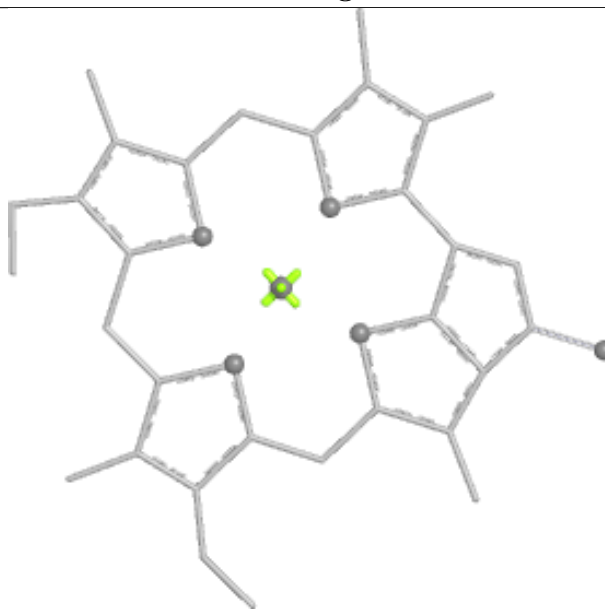
Bond lengths



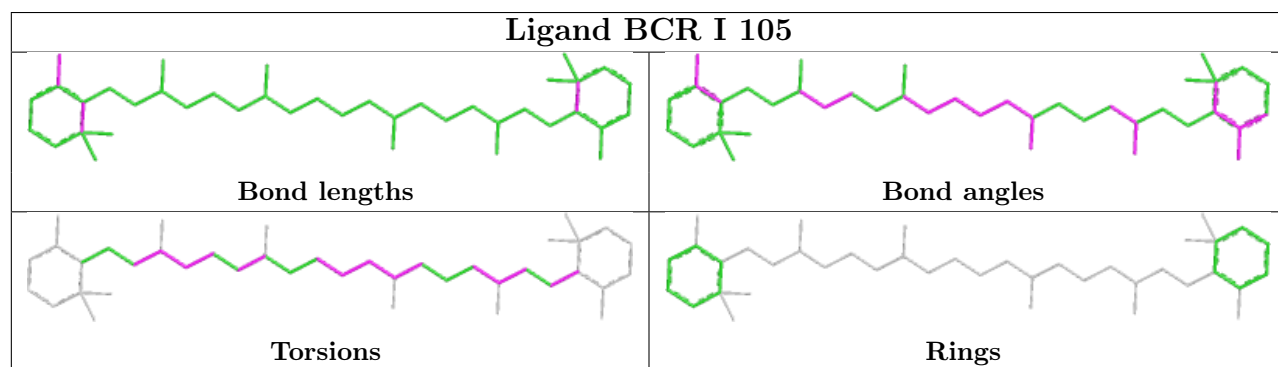
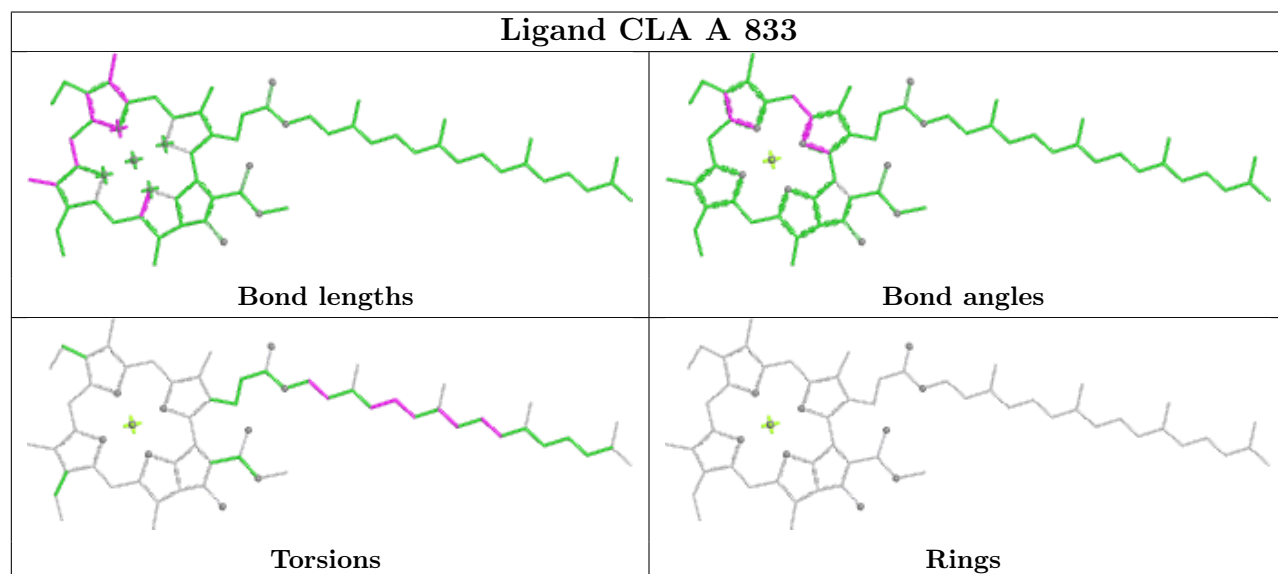
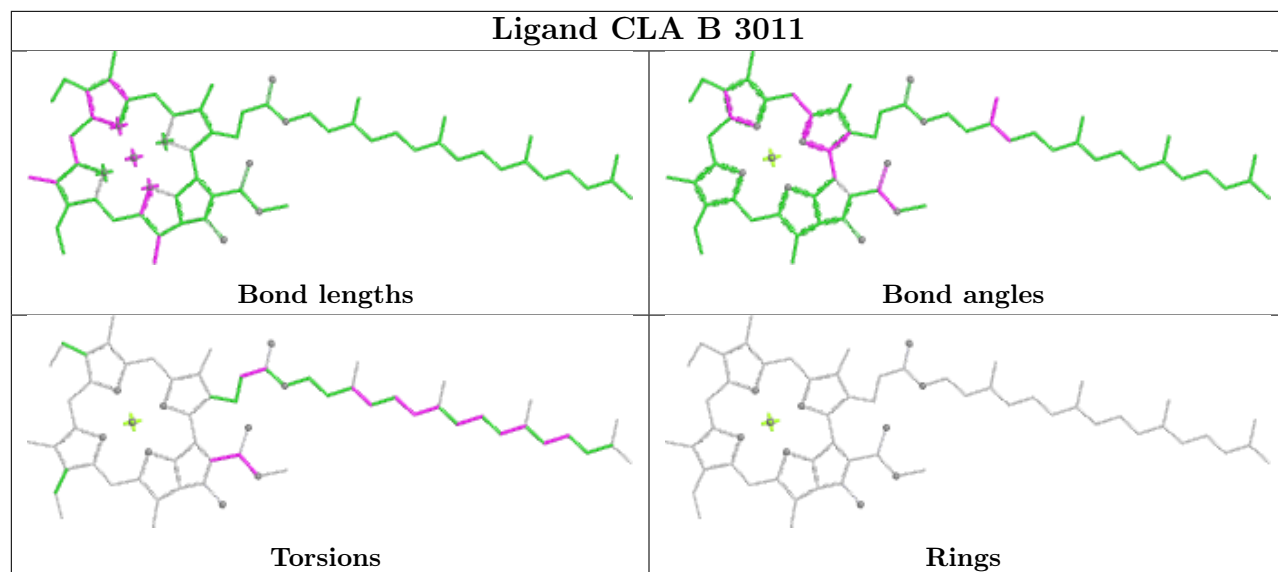
Bond angles

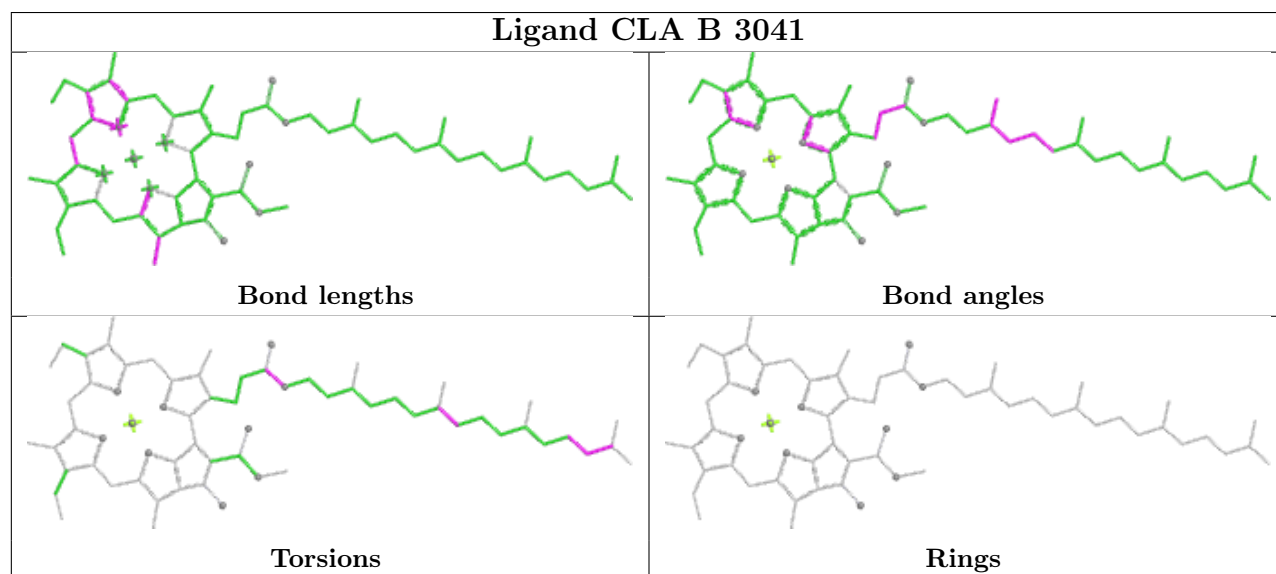
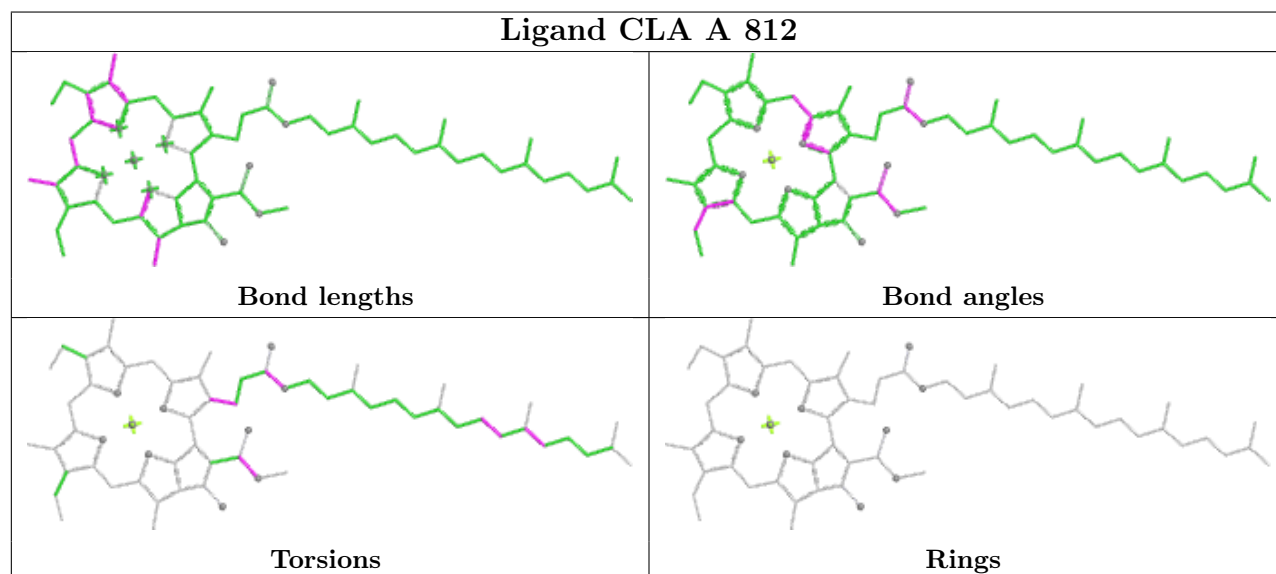
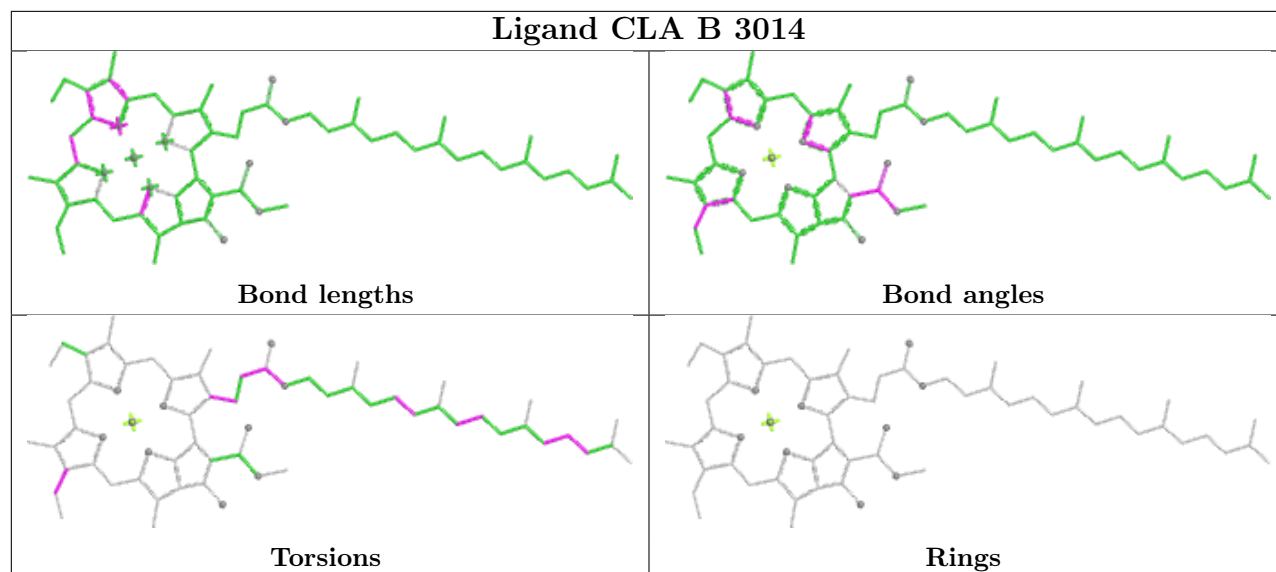


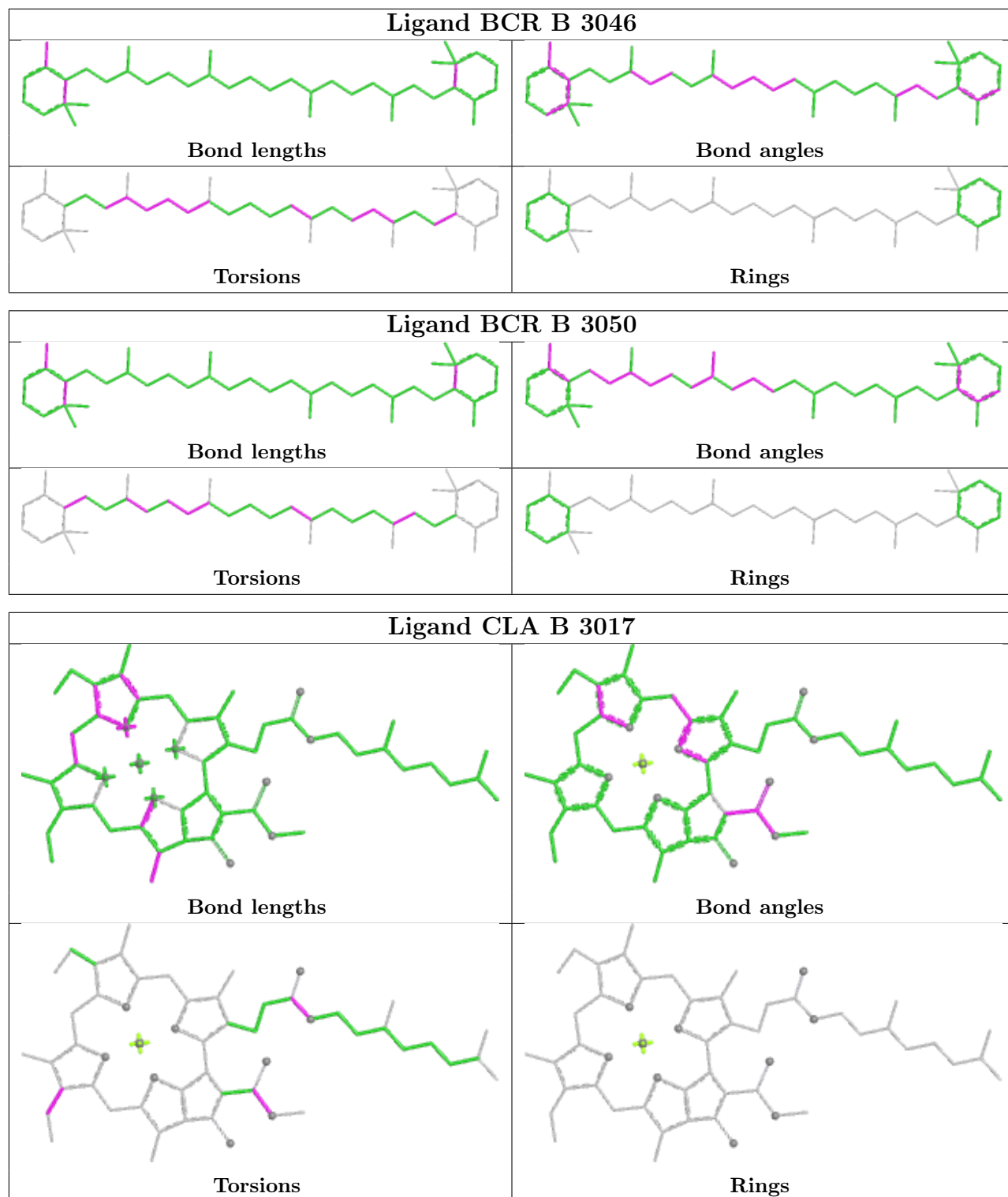
Torsions

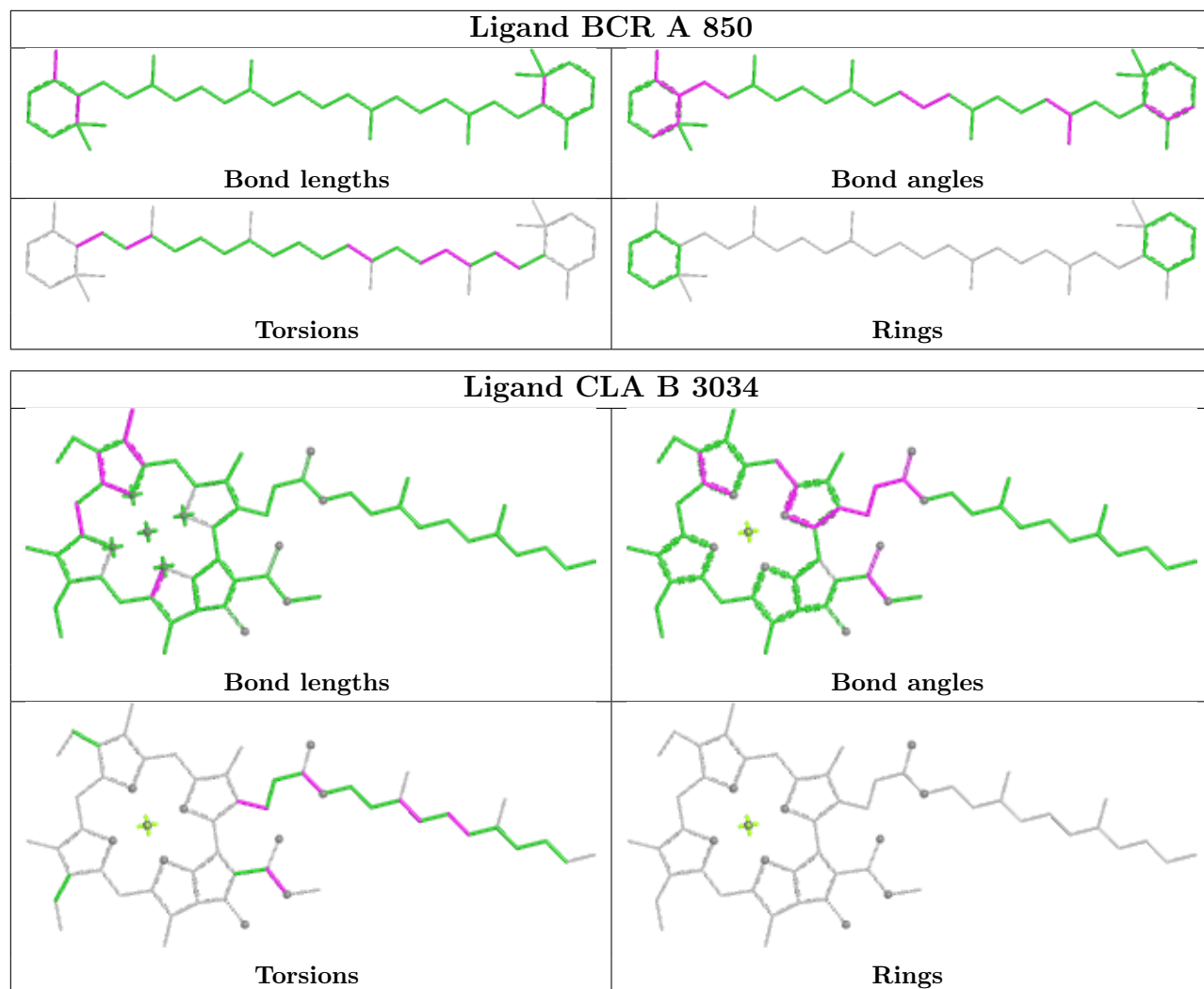


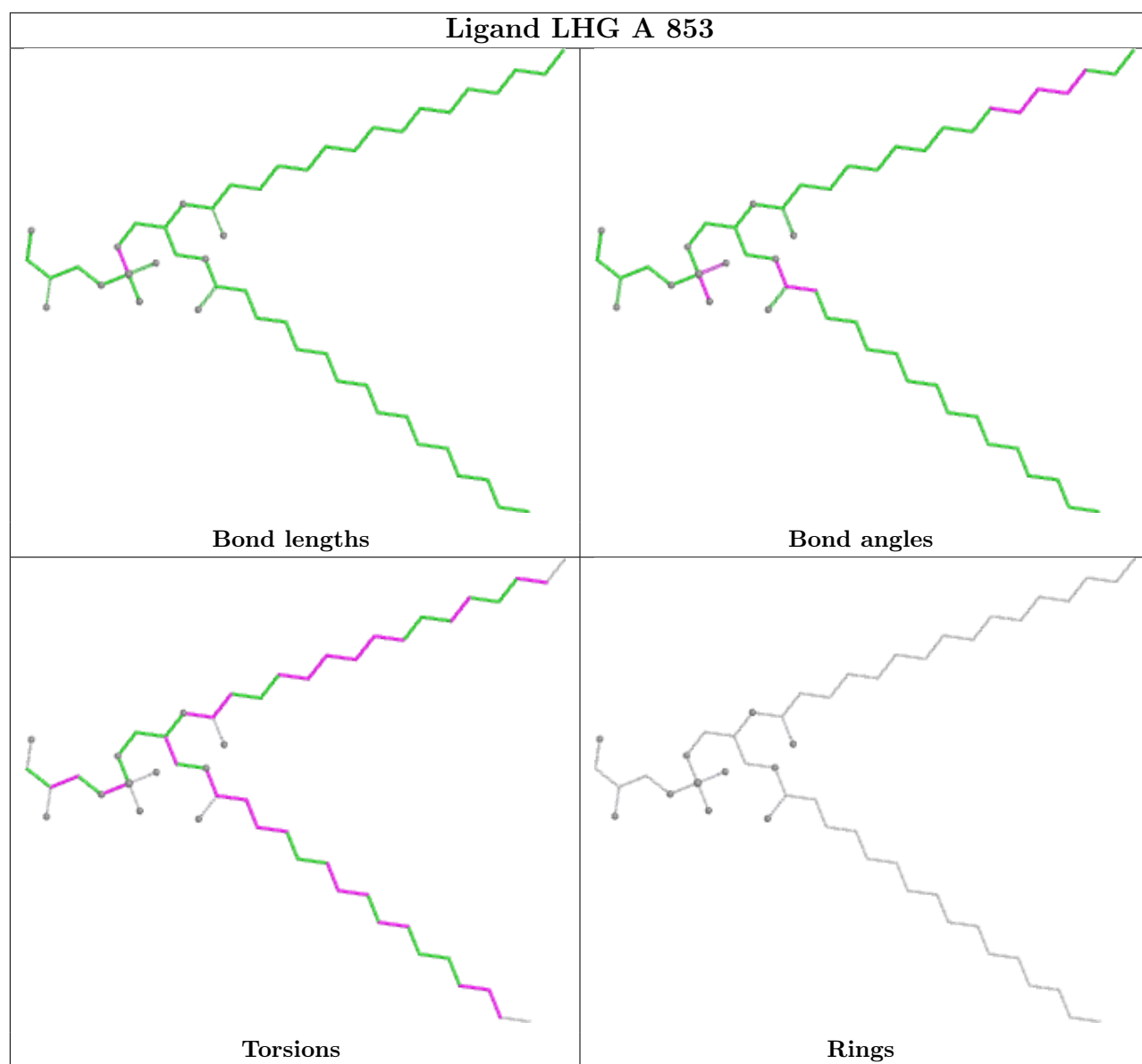
Rings



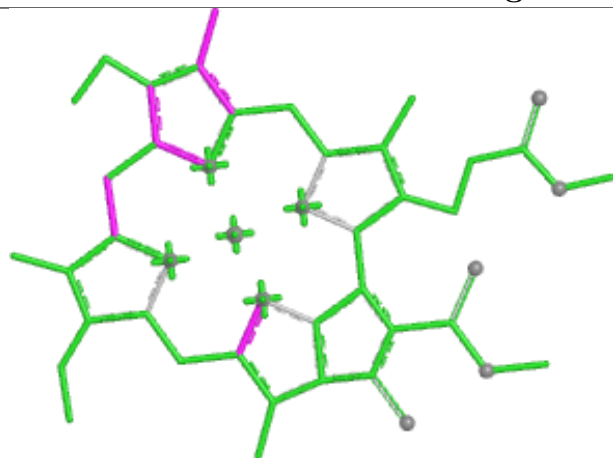




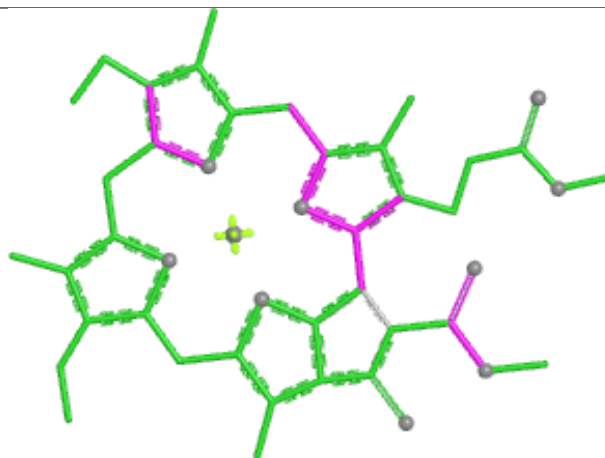




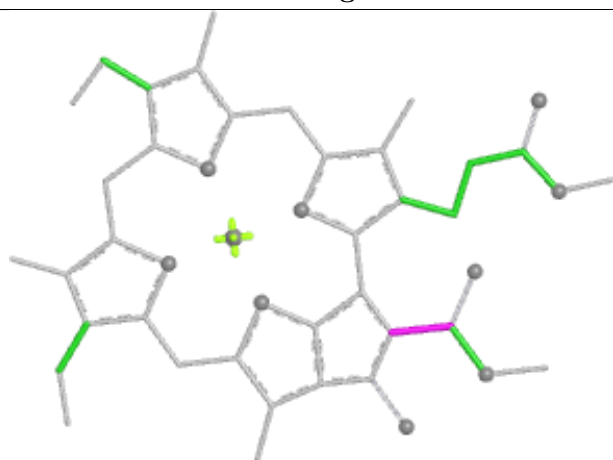
Ligand CLA B 3026



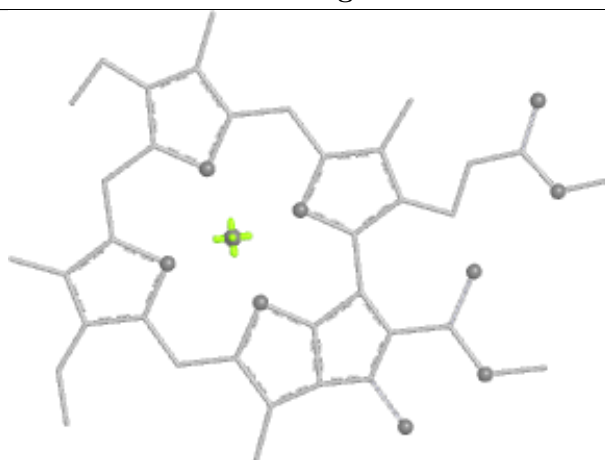
Bond lengths



Bond angles

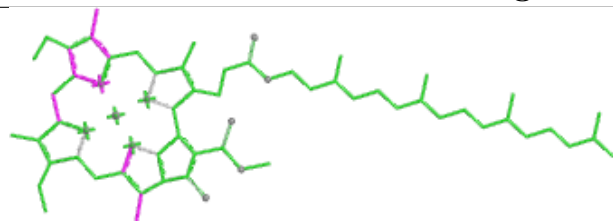


Torsions

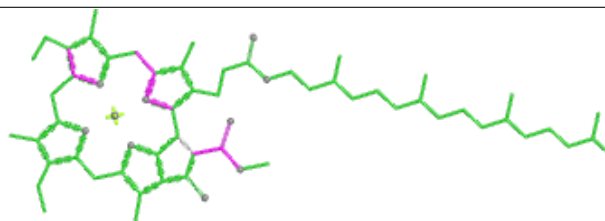


Rings

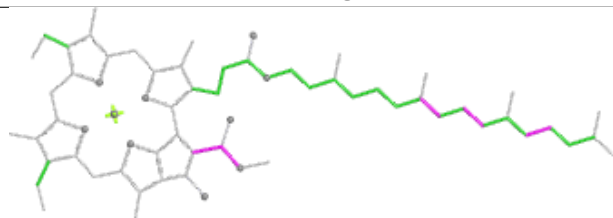
Ligand CLA A 831



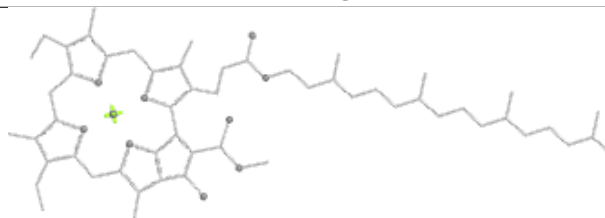
Bond lengths



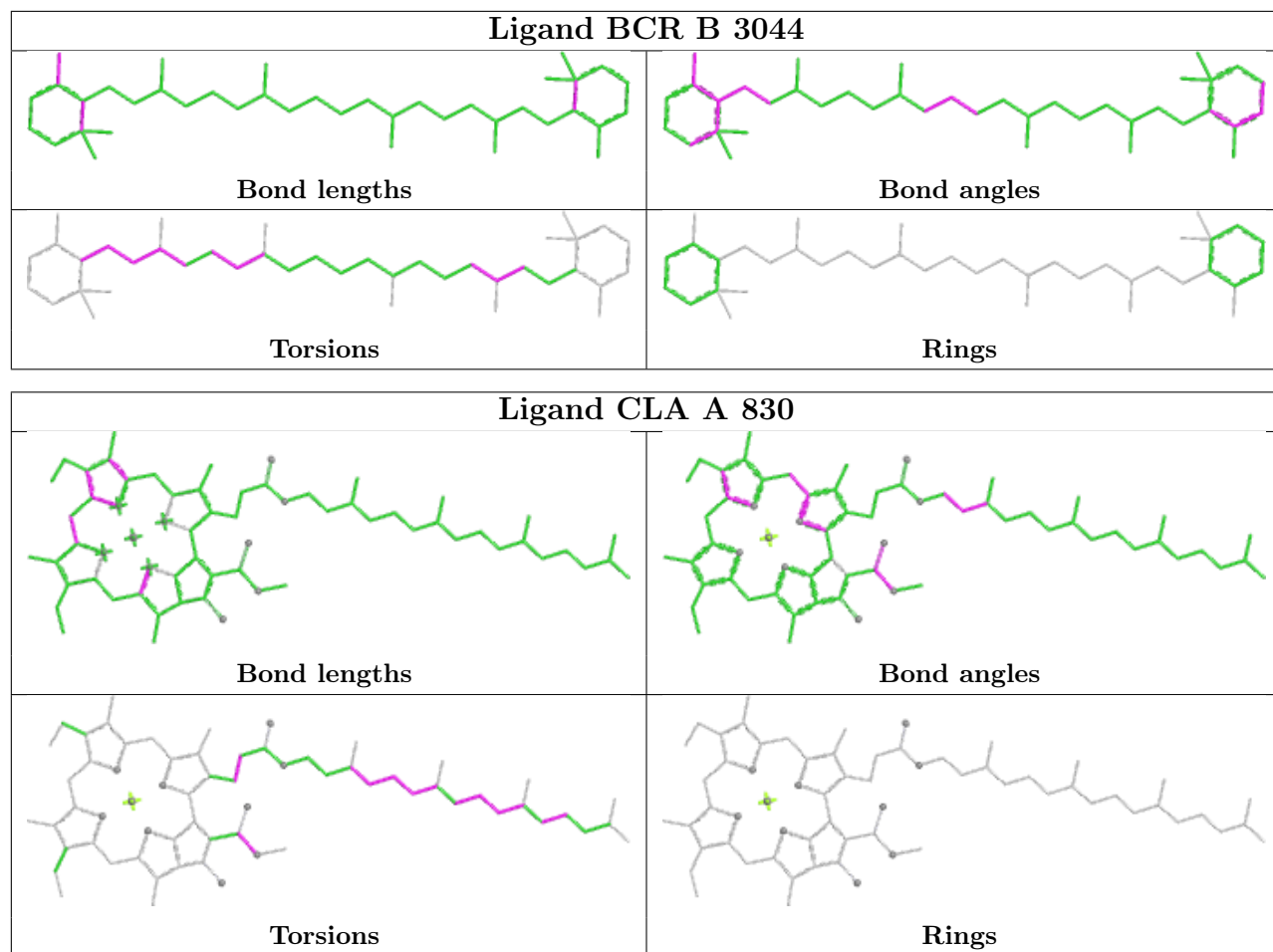
Bond angles



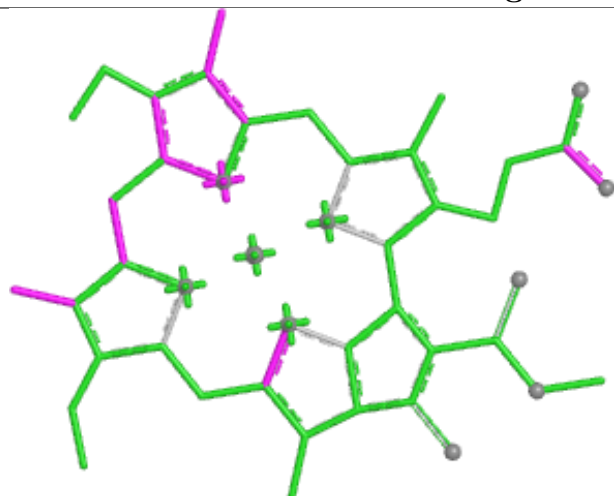
Torsions



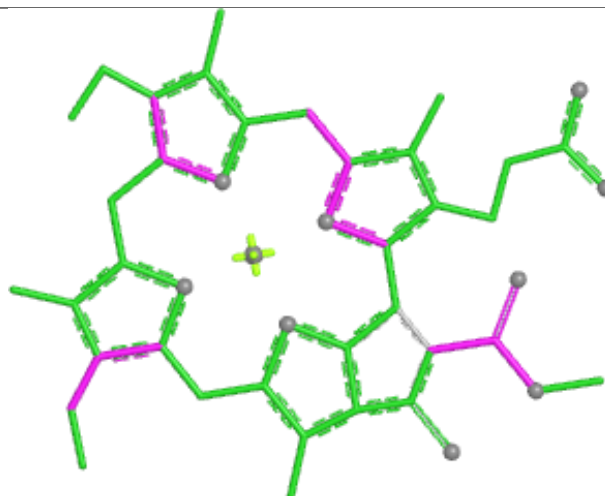
Rings



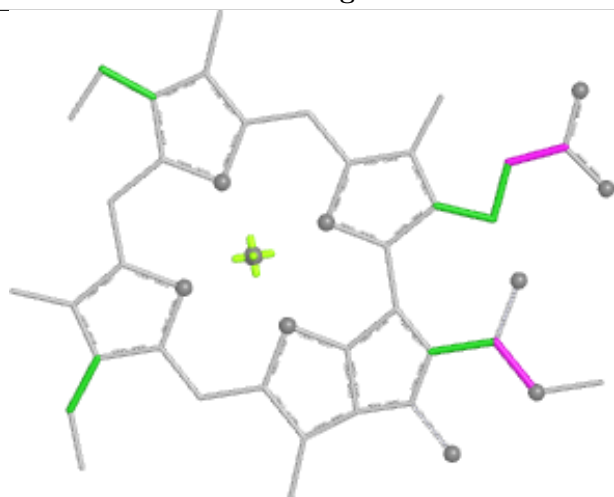
Ligand CLA B 3024



Bond lengths



Bond angles

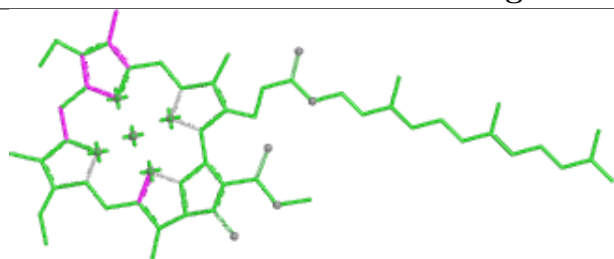


Torsions

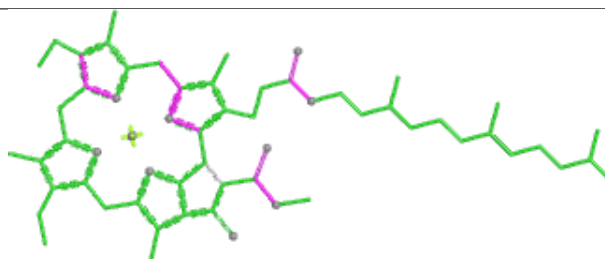


Rings

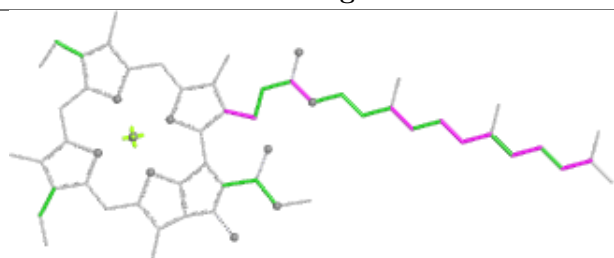
Ligand CLA B 3038



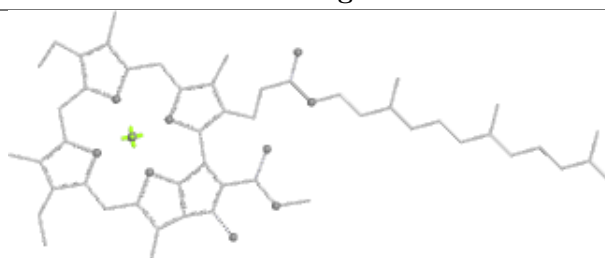
Bond lengths



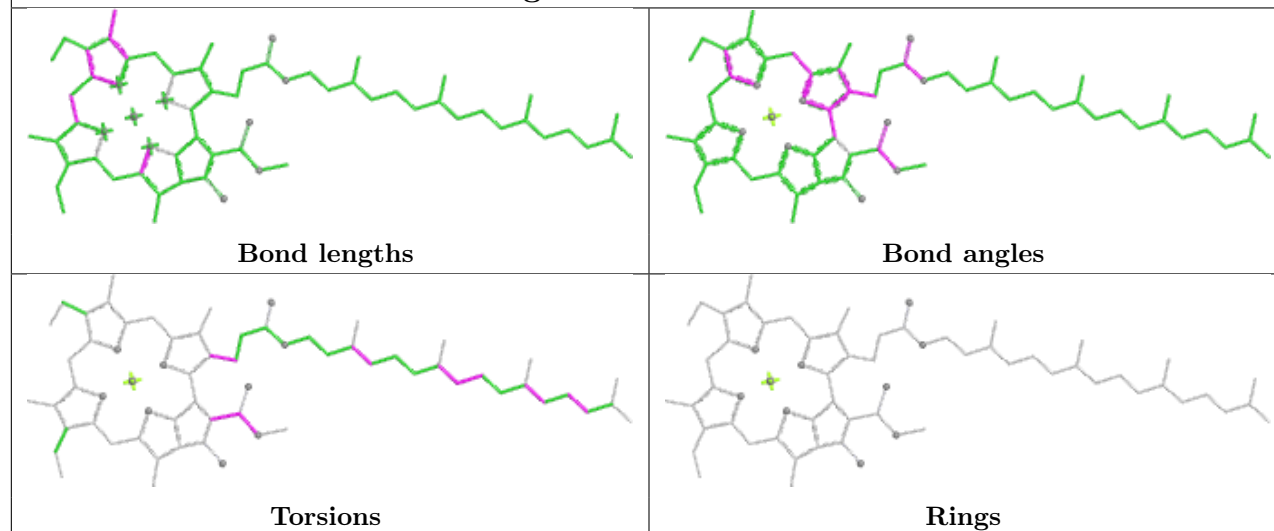
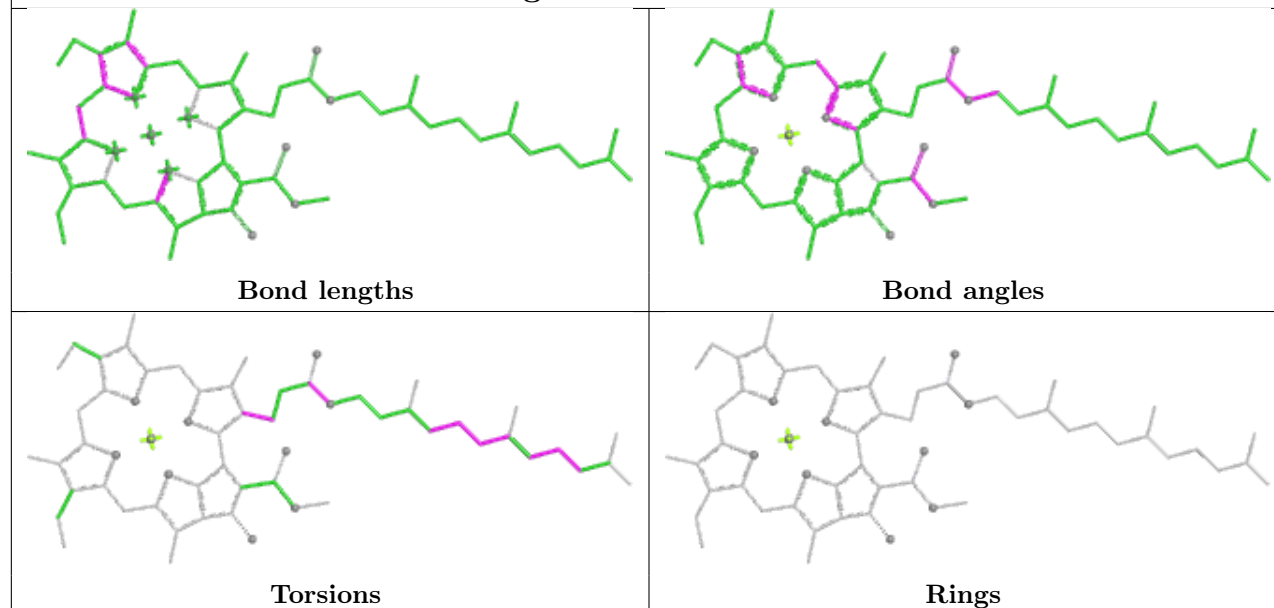
Bond angles

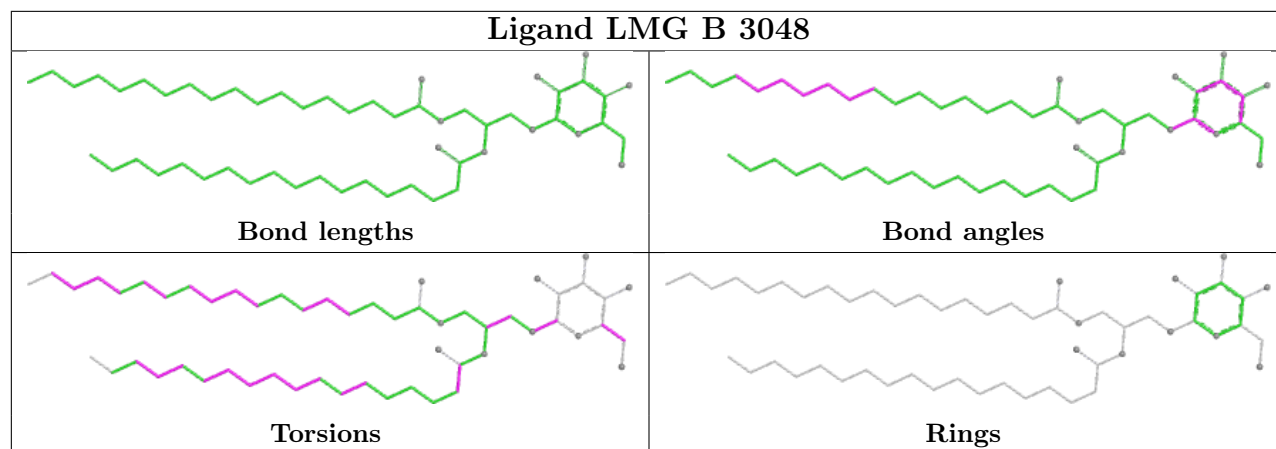
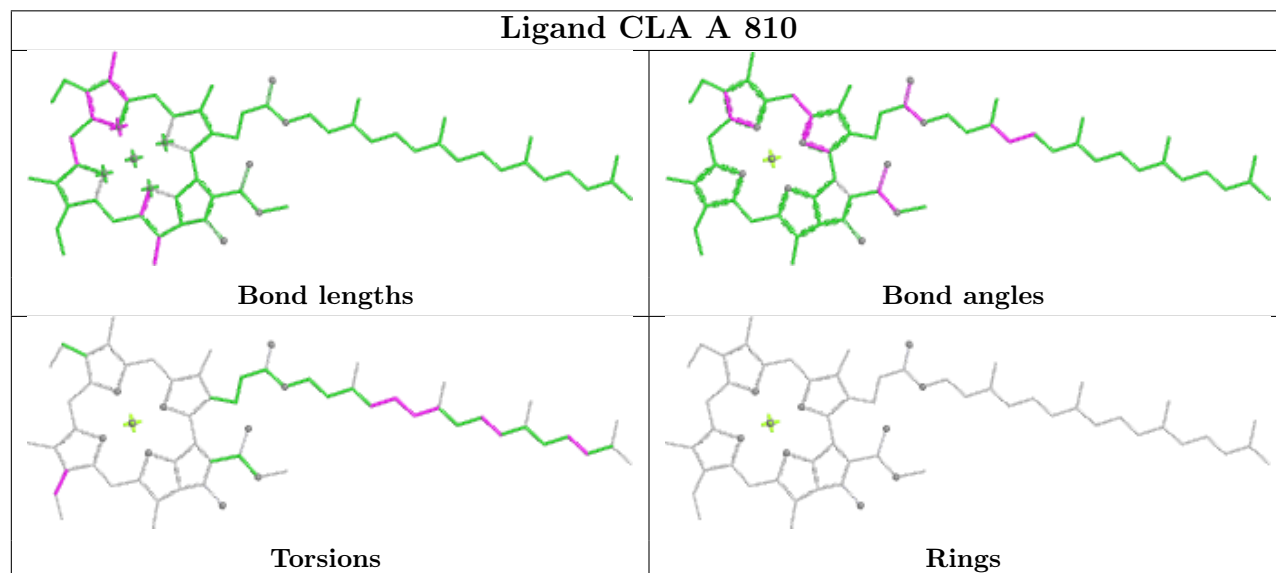
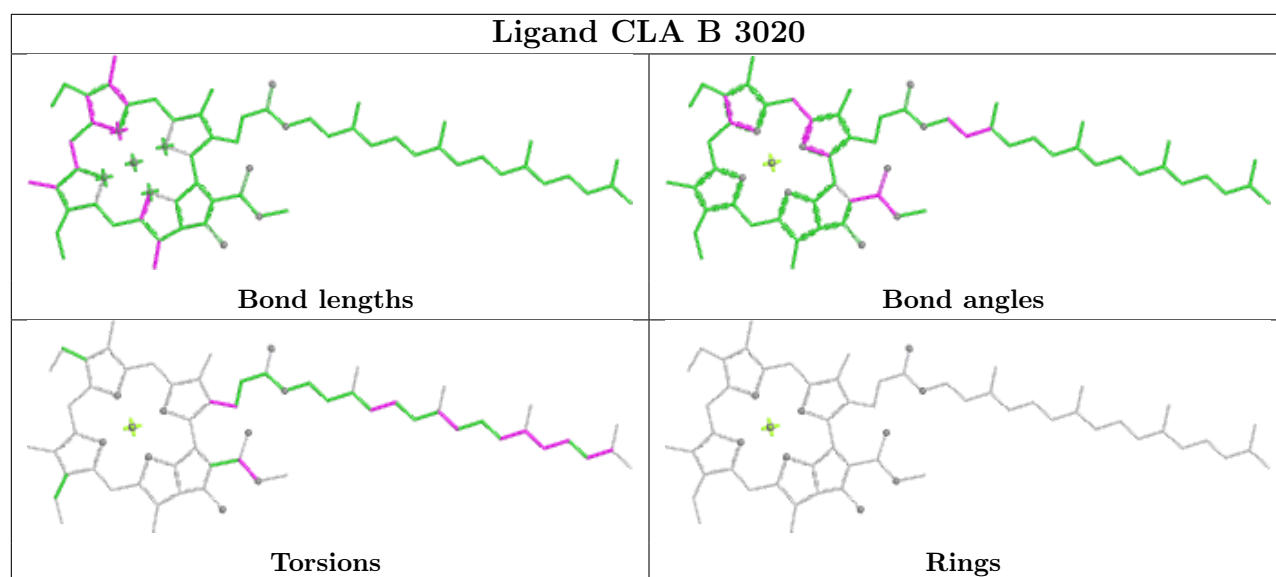


Torsions

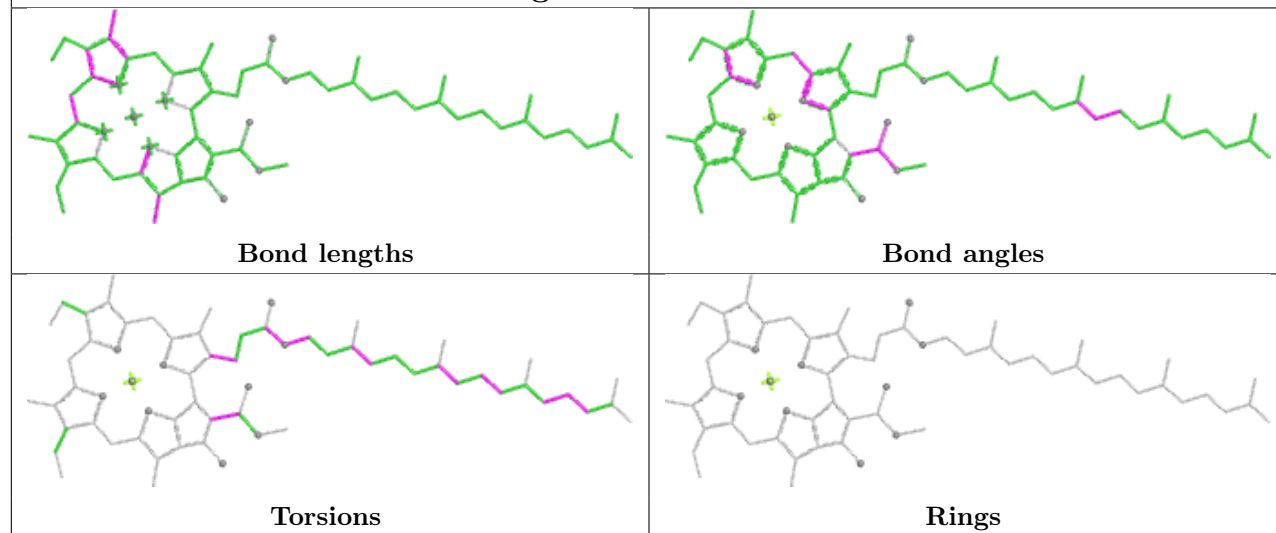


Rings

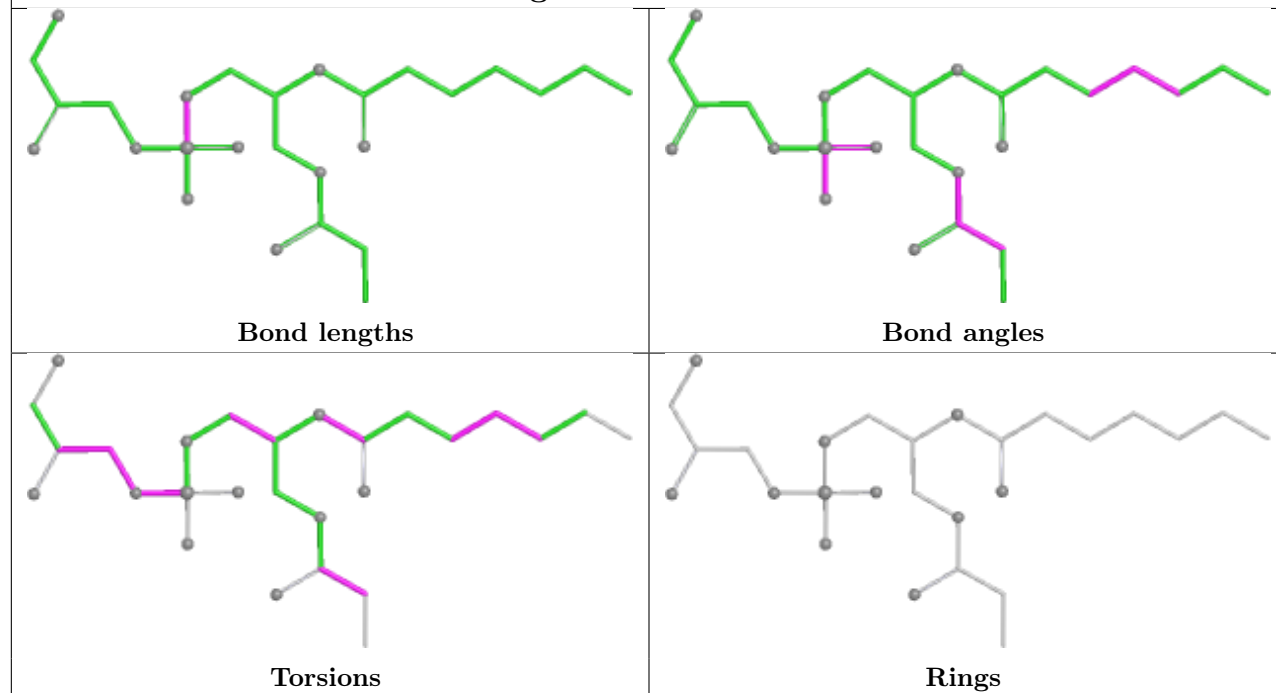
Ligand CLA B 3030**Ligand CLA B 3019**



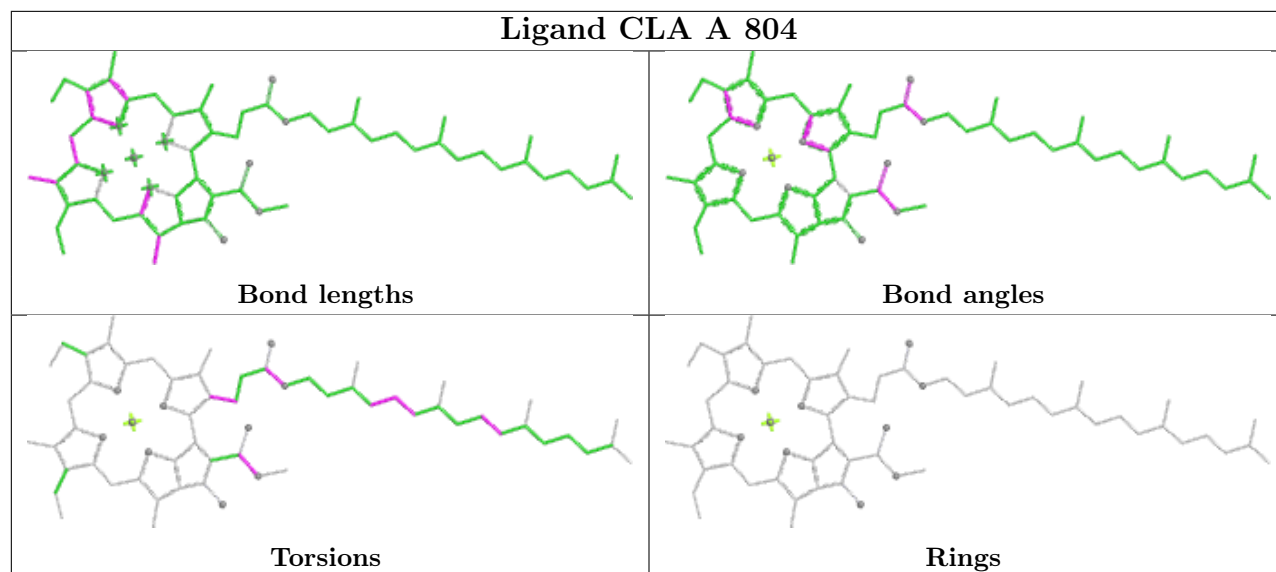
Ligand CLA A 826



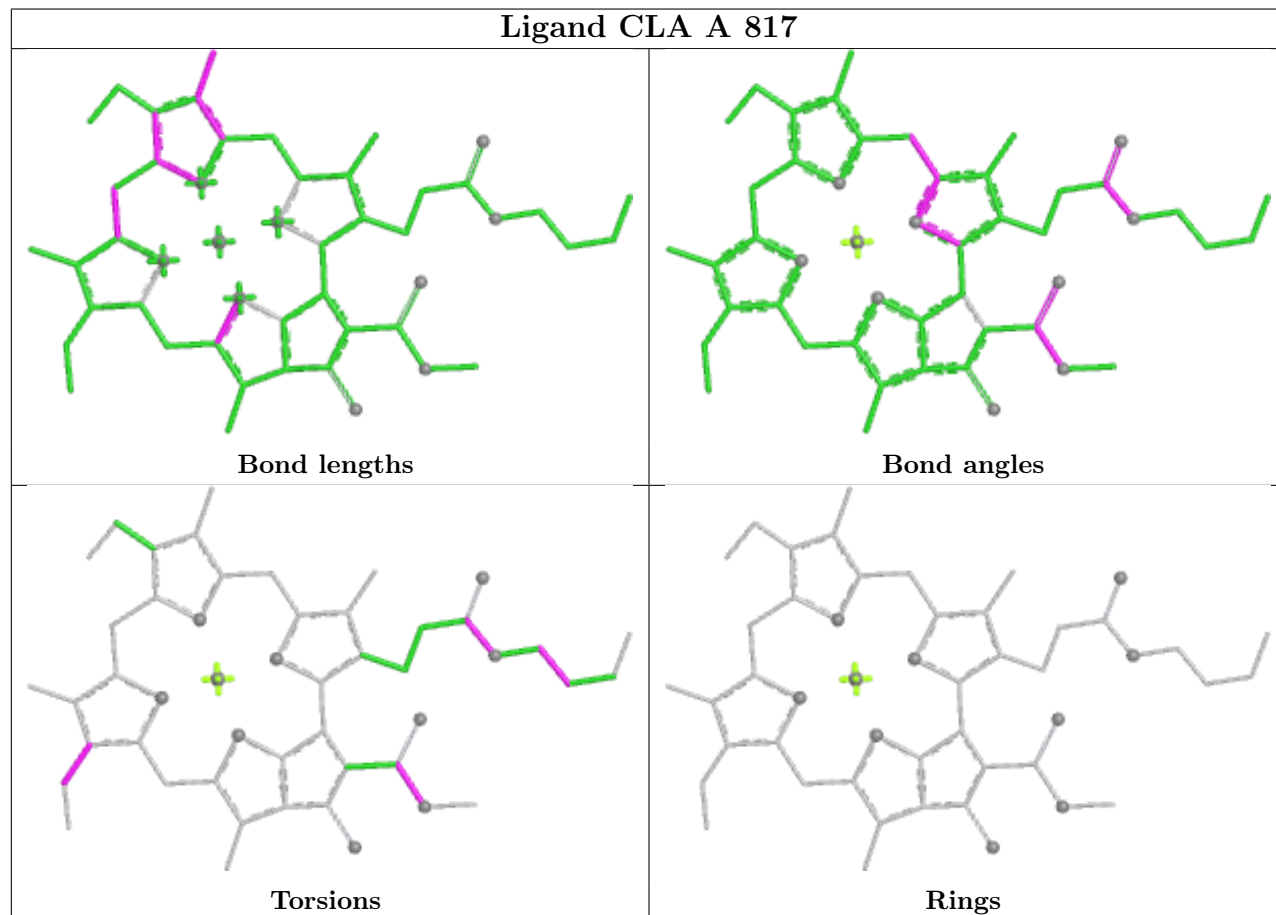
Ligand LHG A 854



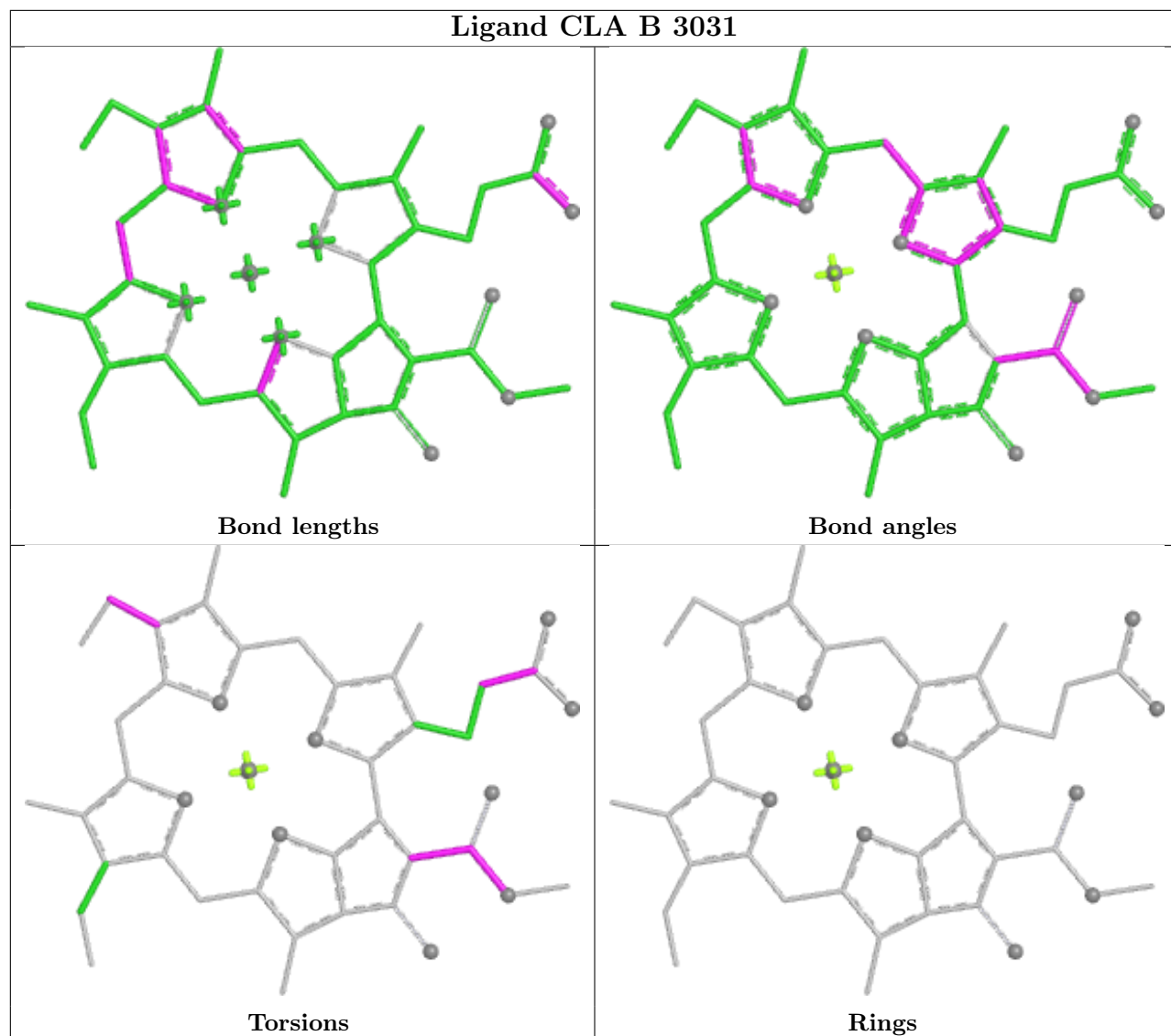
Ligand CLA A 804



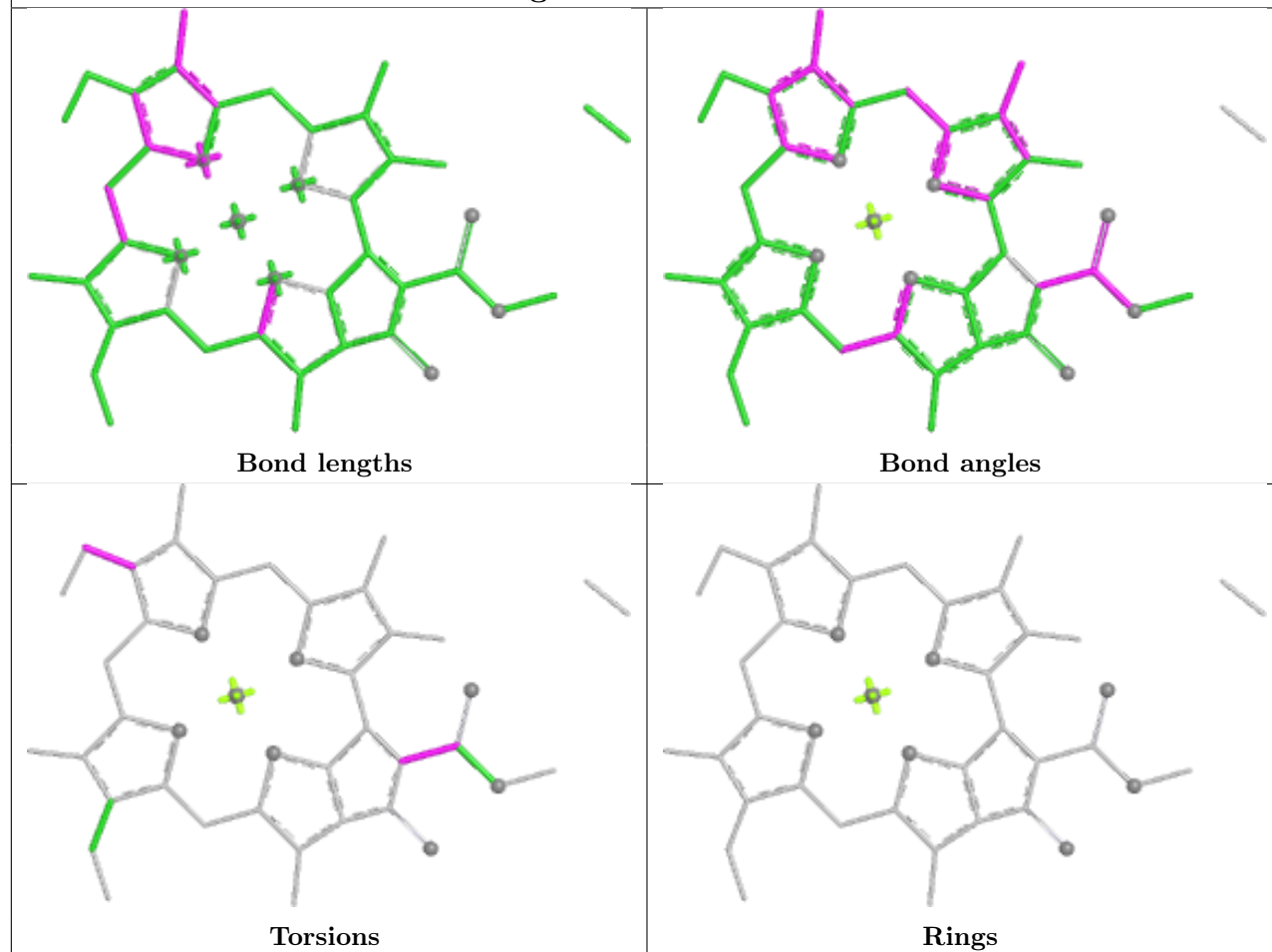
Ligand CLA A 817



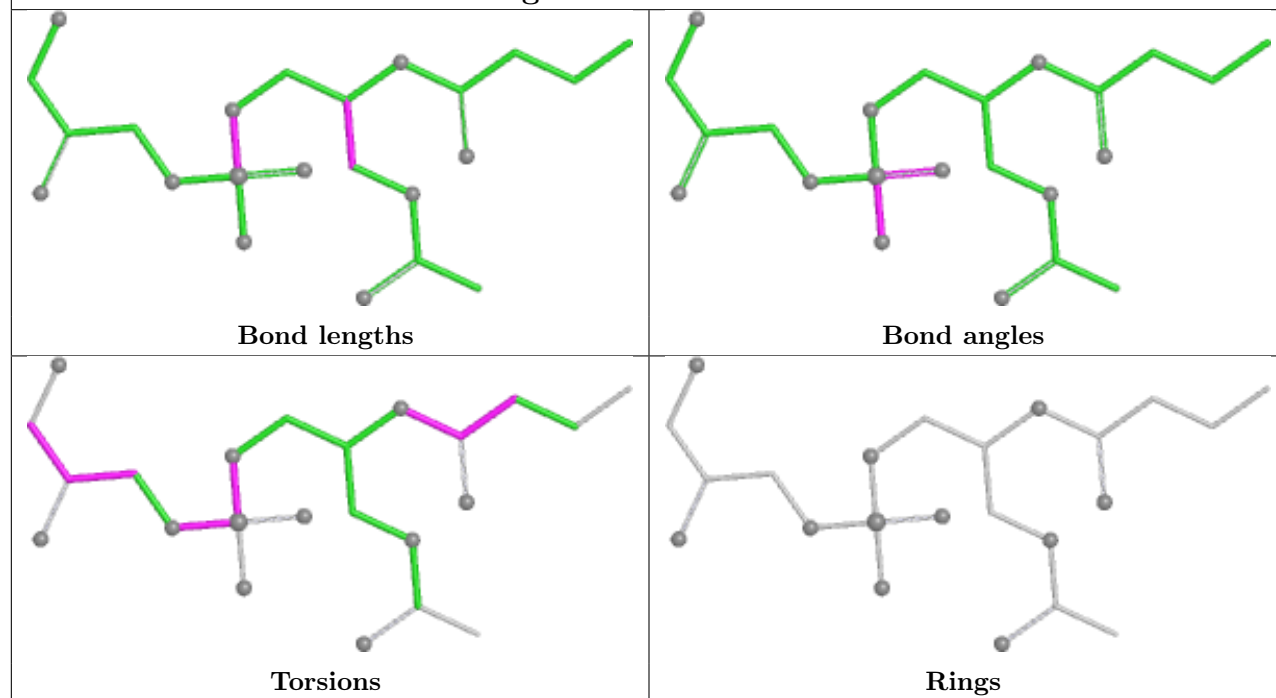
Ligand CLA B 3031



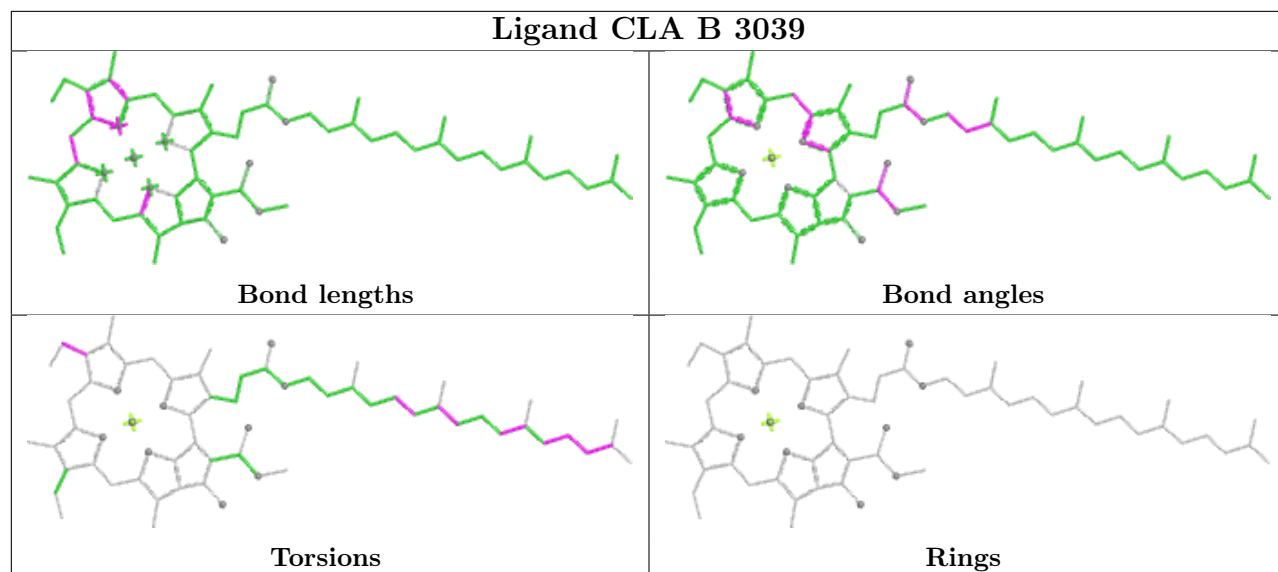
Ligand CLA A 821



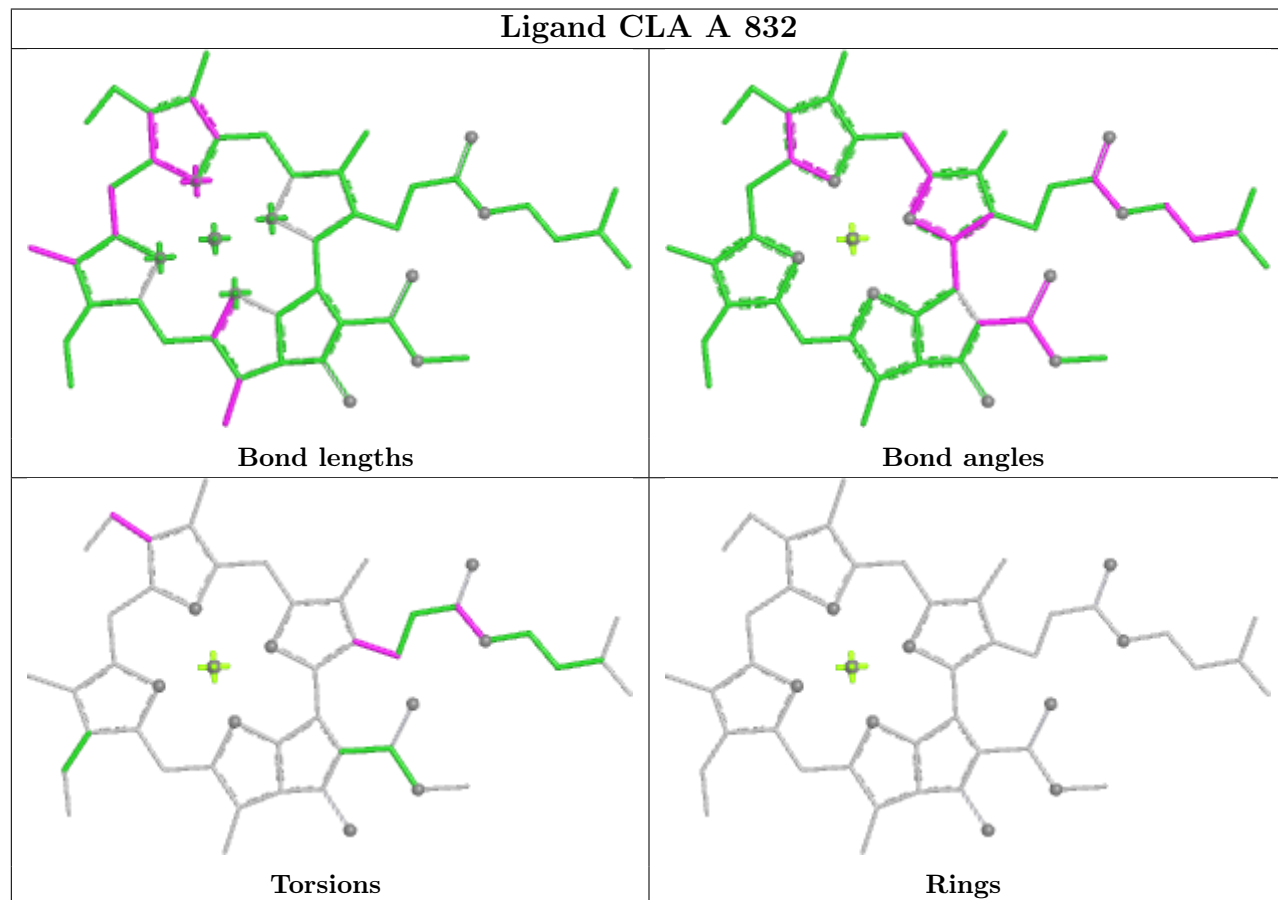
Ligand LHG B 3049

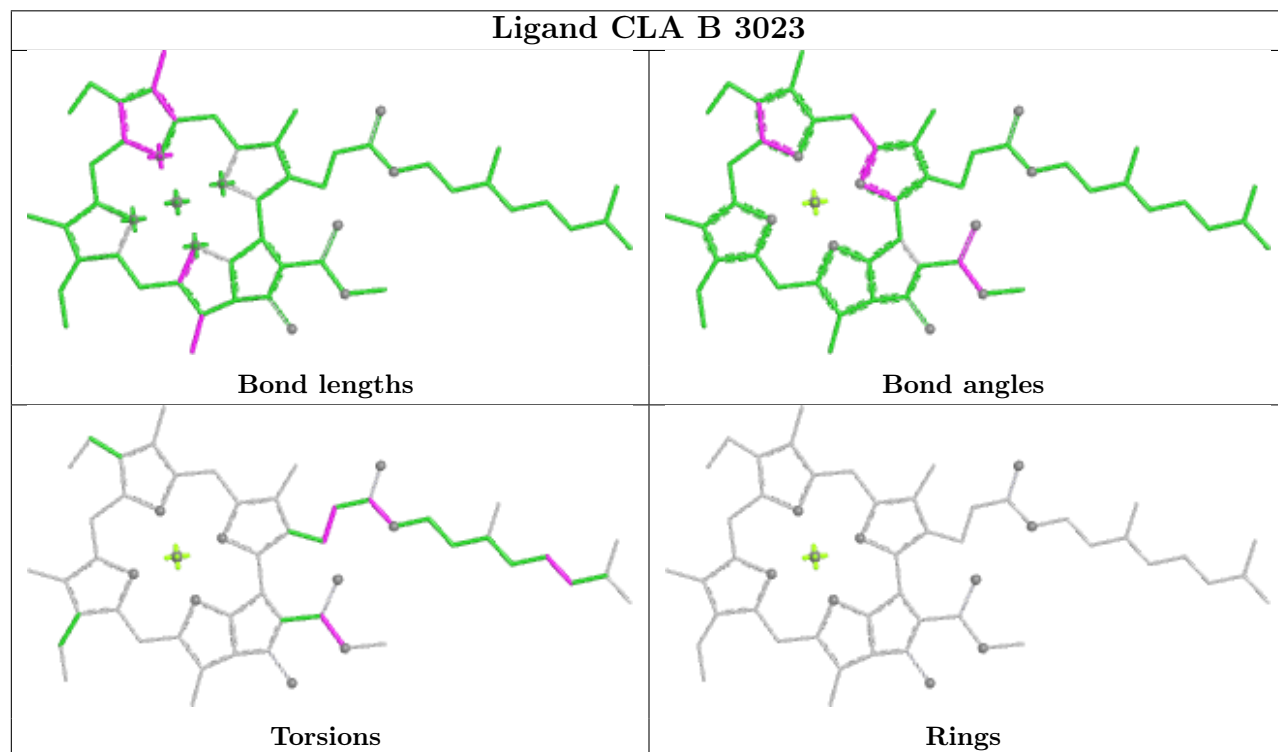
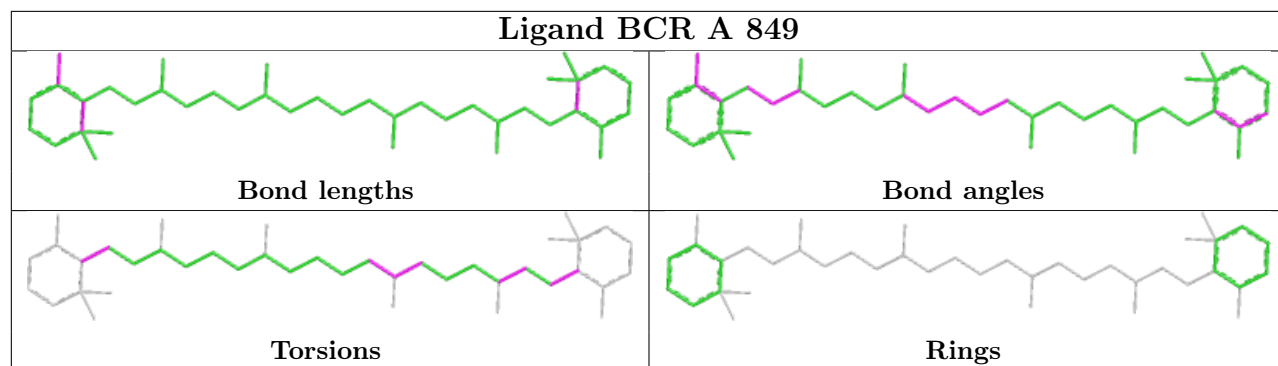


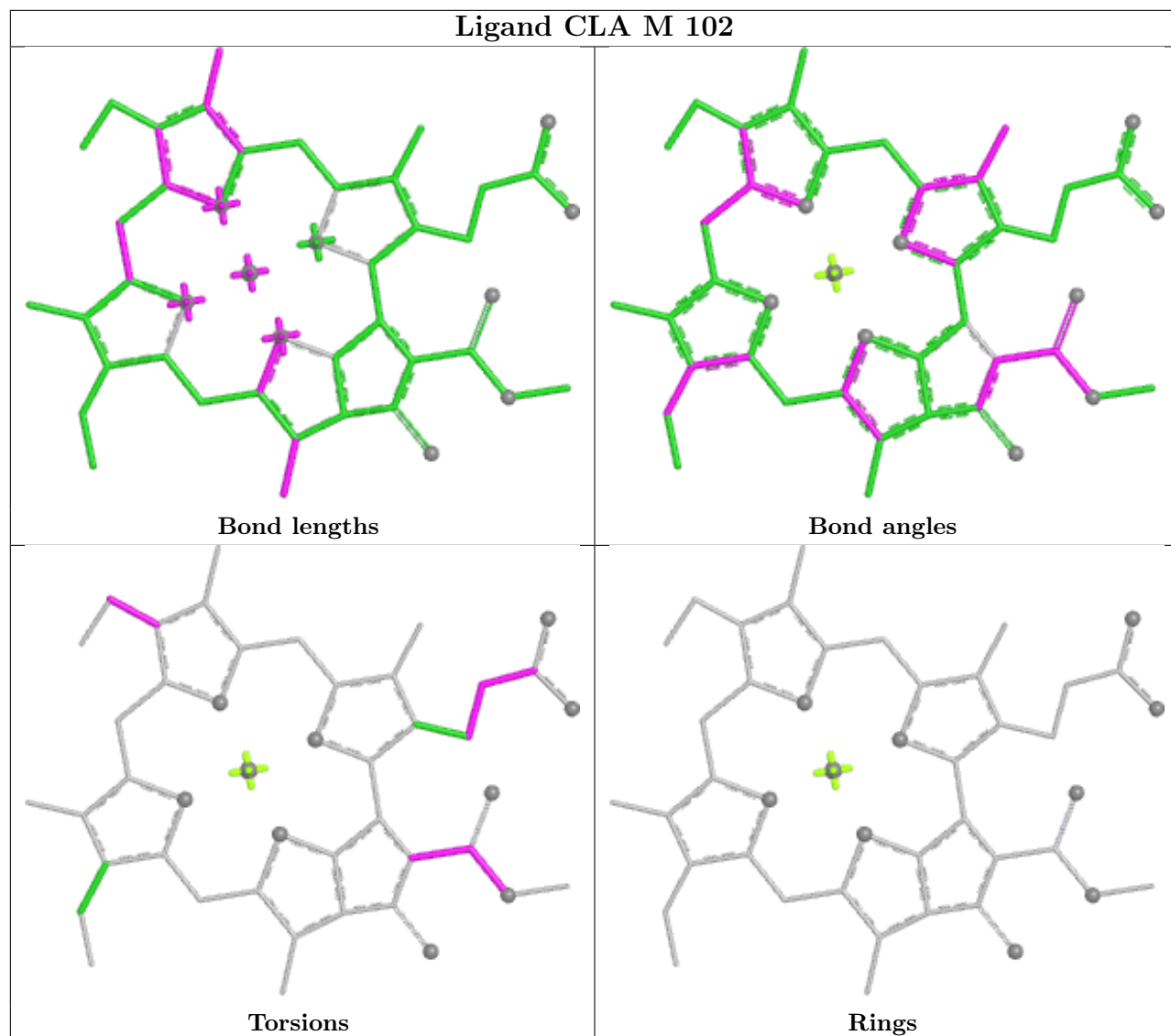
Ligand CLA B 3039



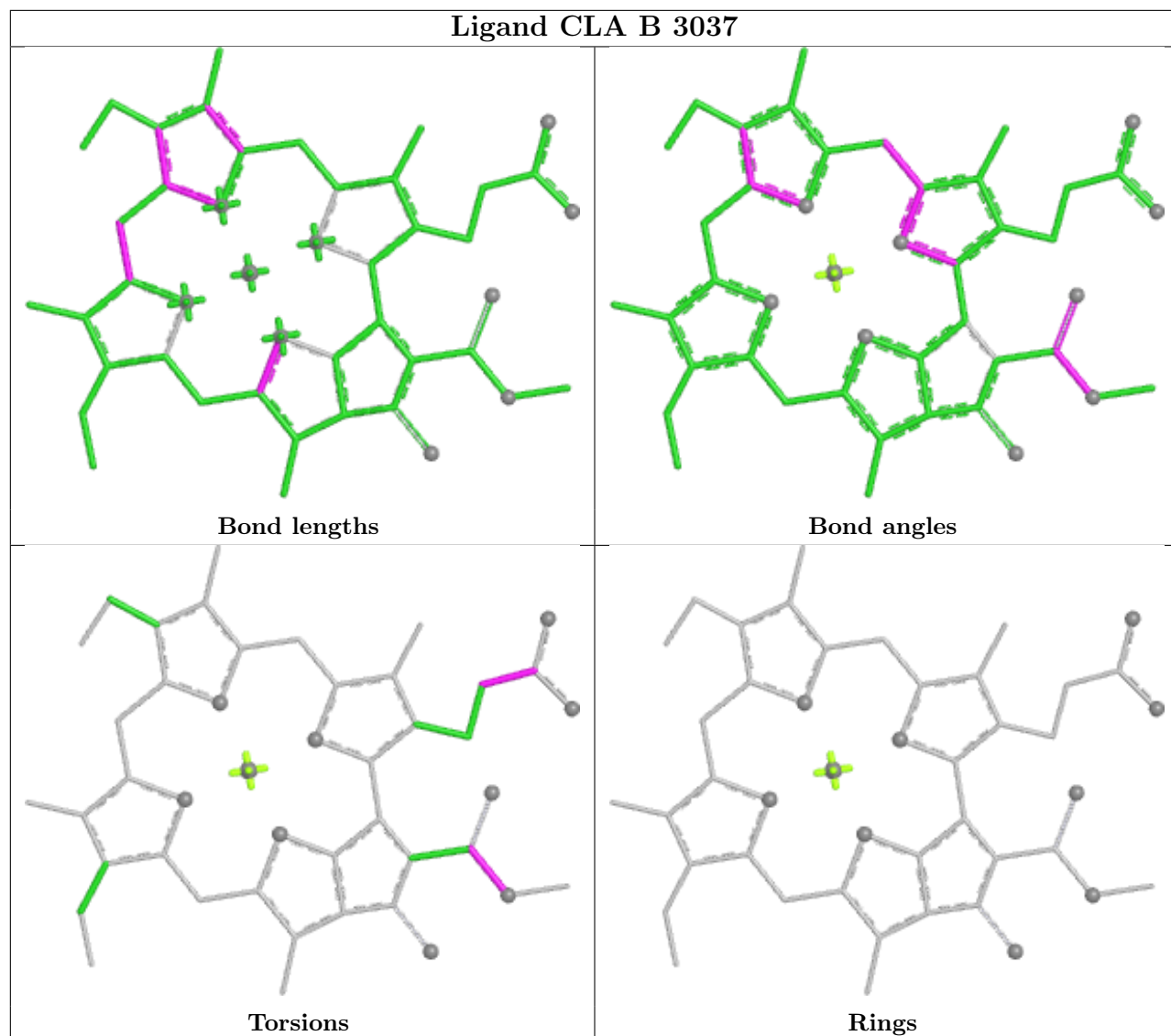
Ligand CLA A 832



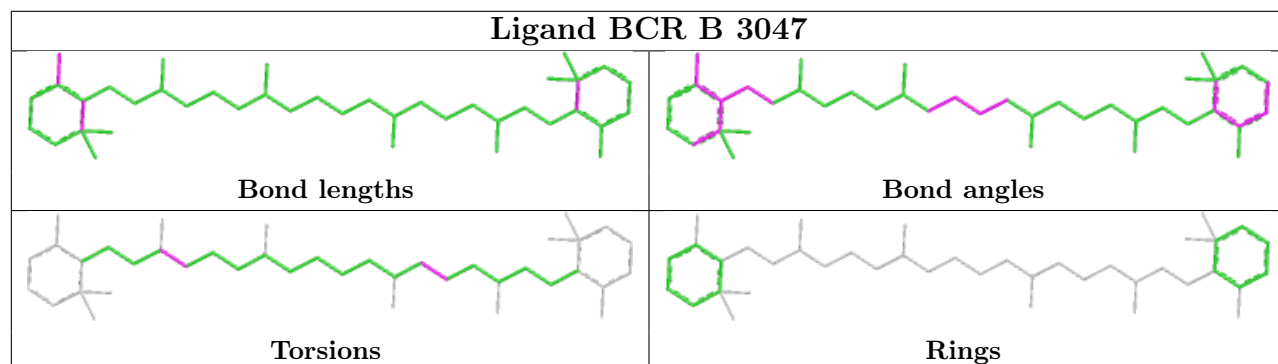




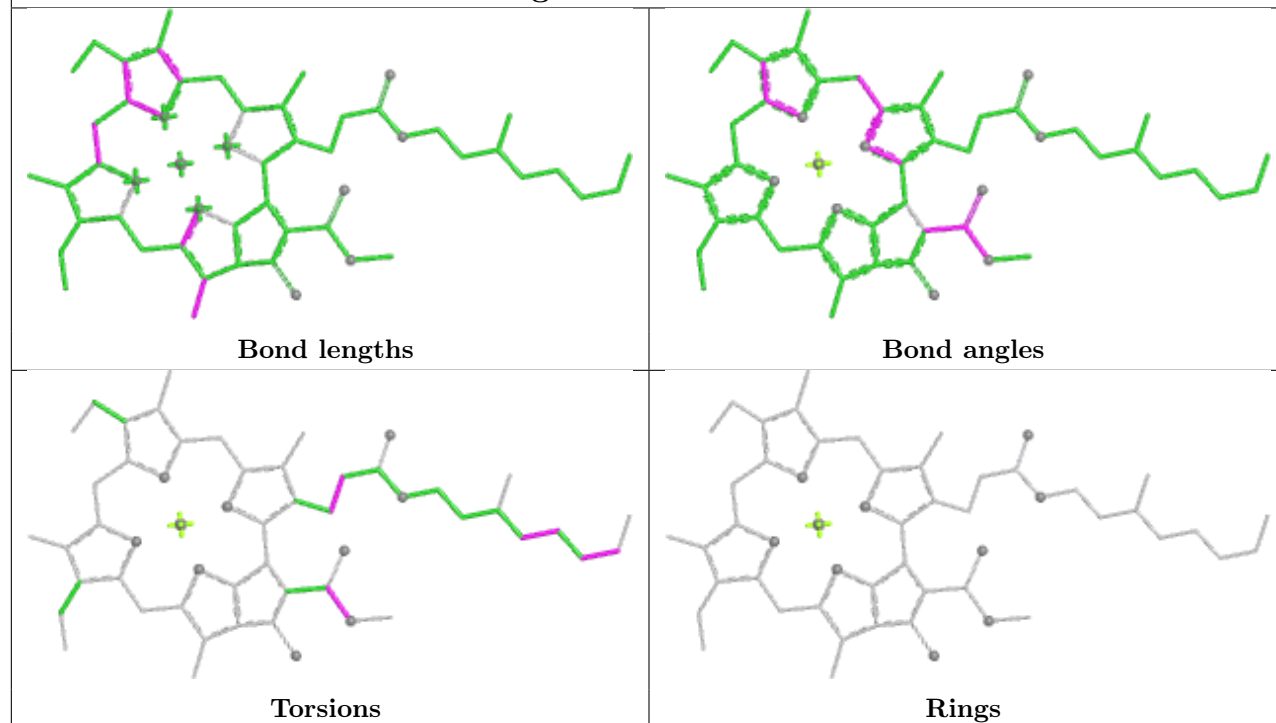
Ligand CLA B 3037



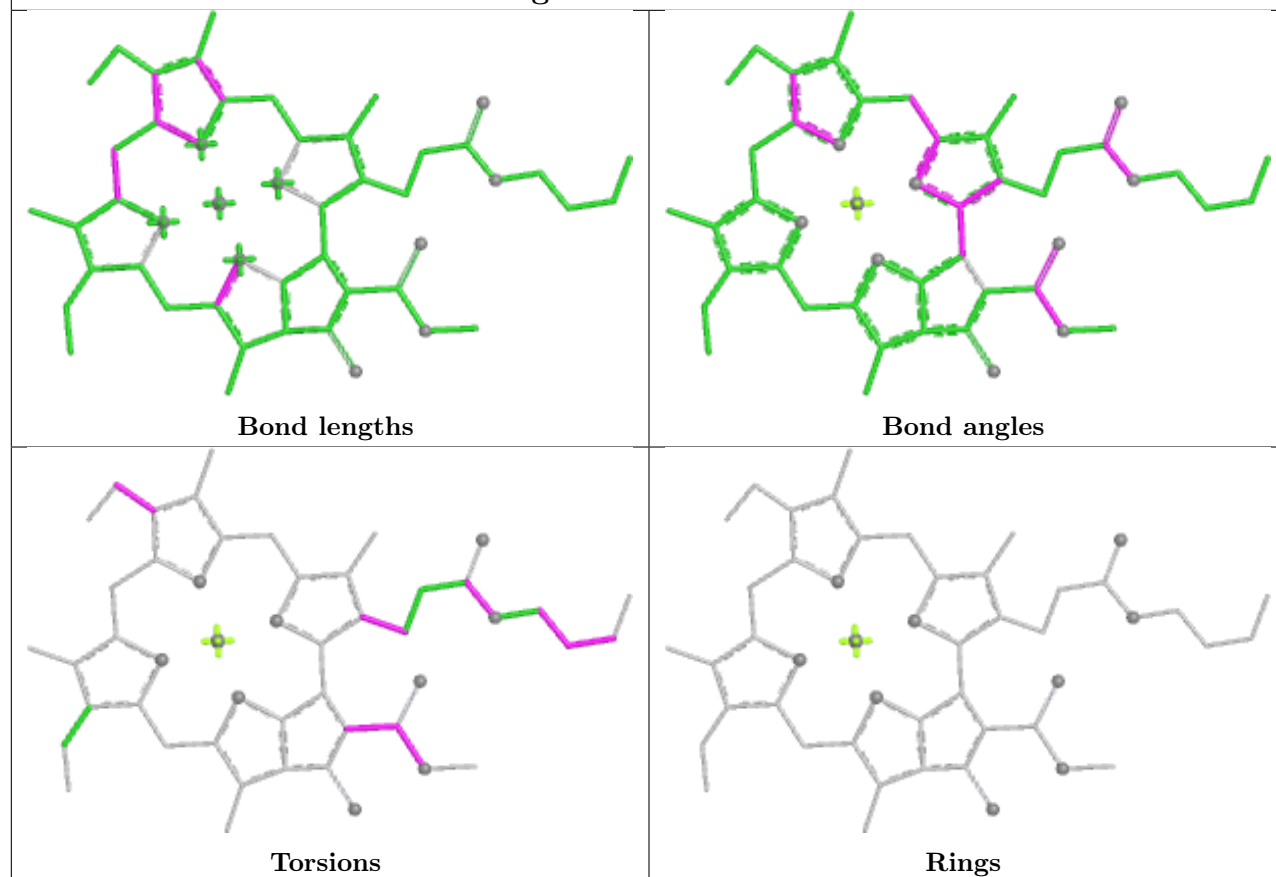
Ligand BCR B 3047



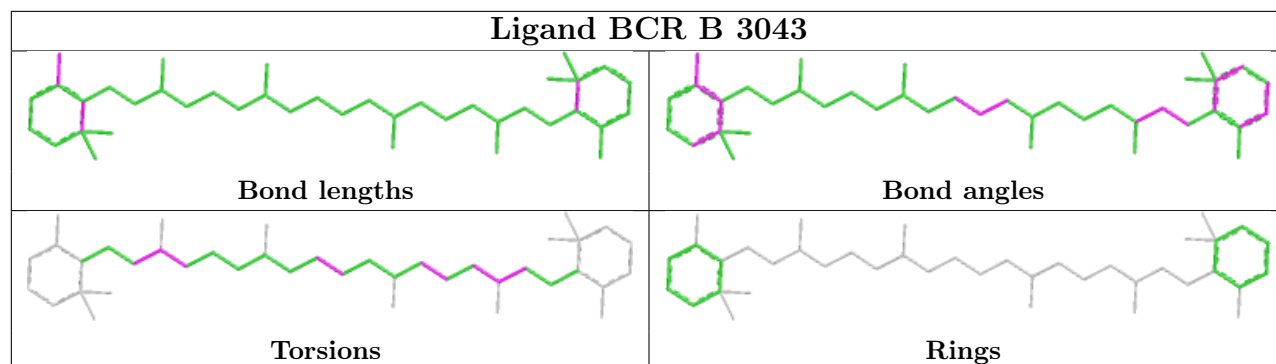
Ligand CLA A 813



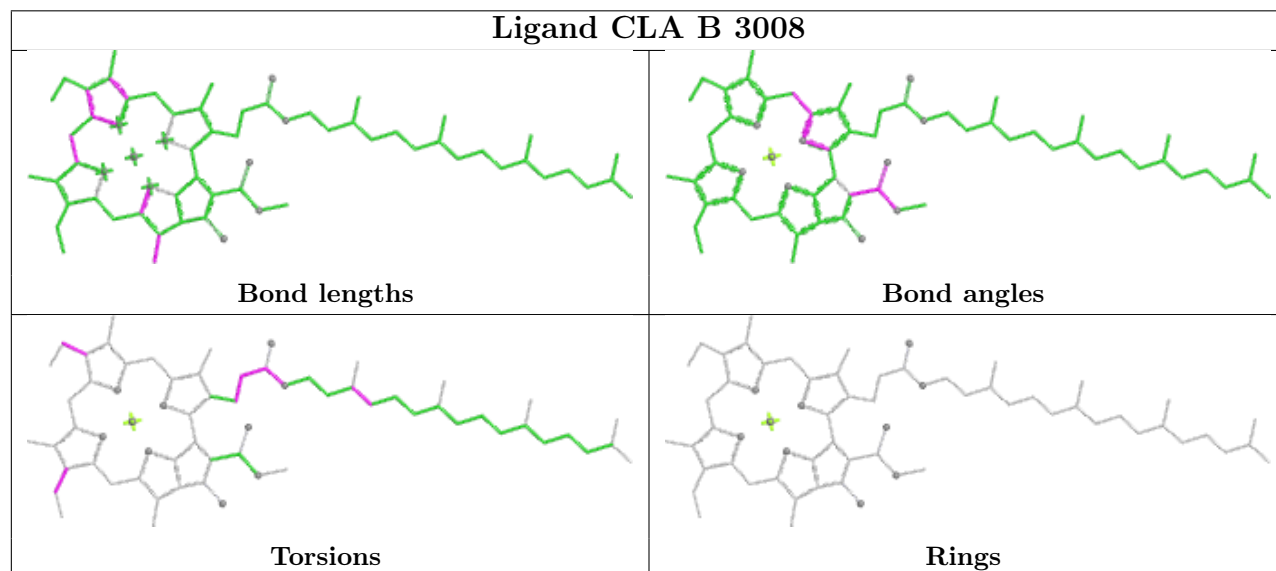
Ligand CLA A 823



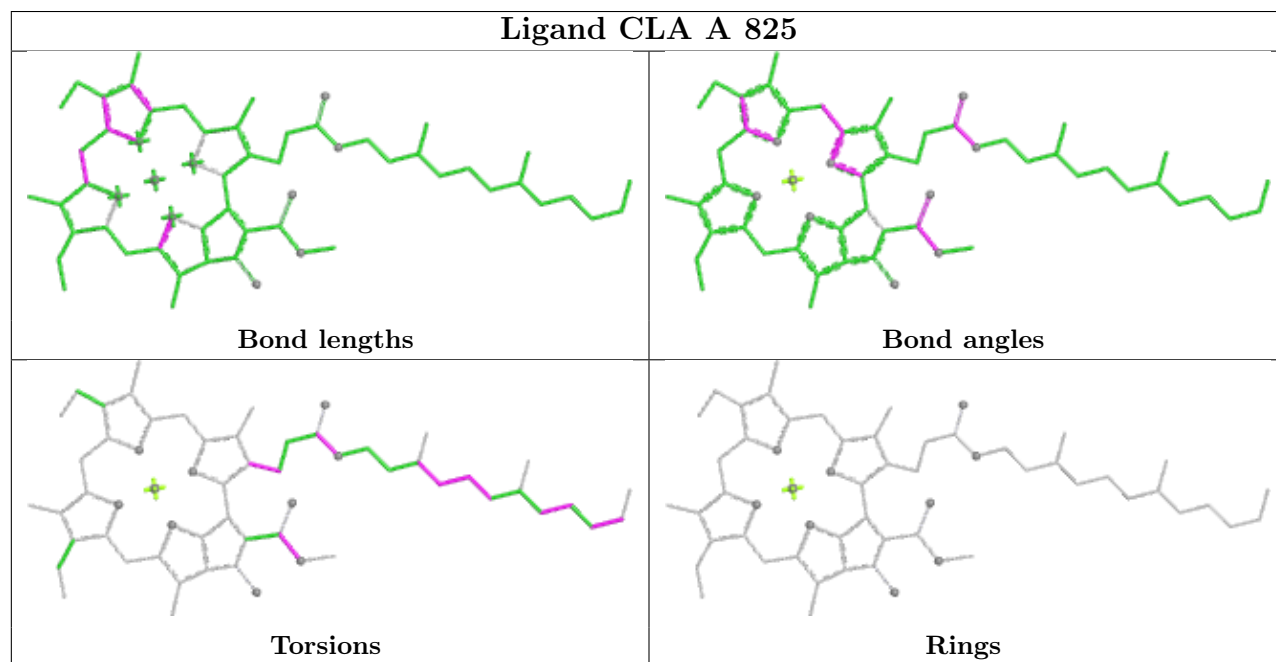
Ligand BCR B 3043

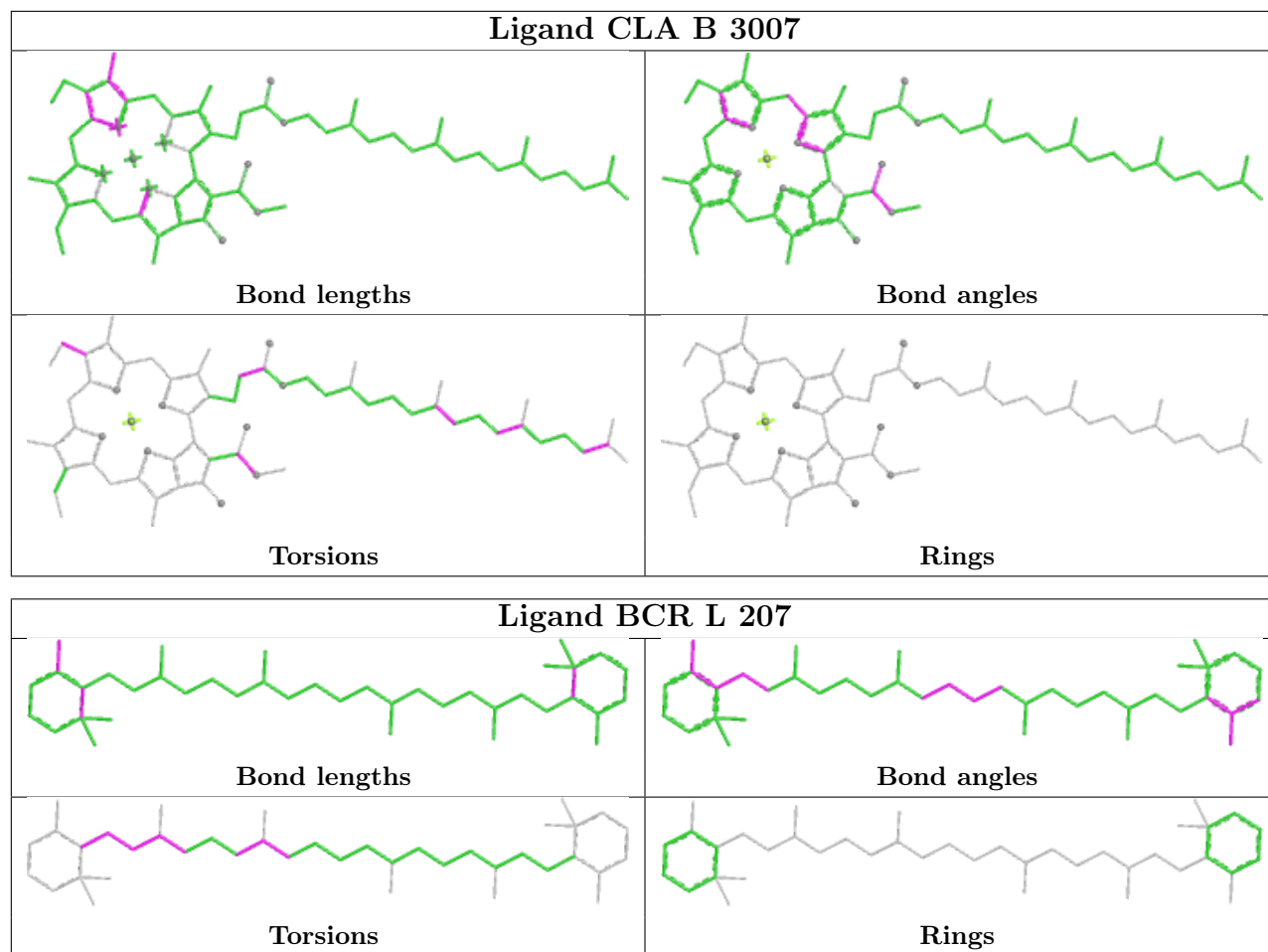


Ligand CLA B 3008

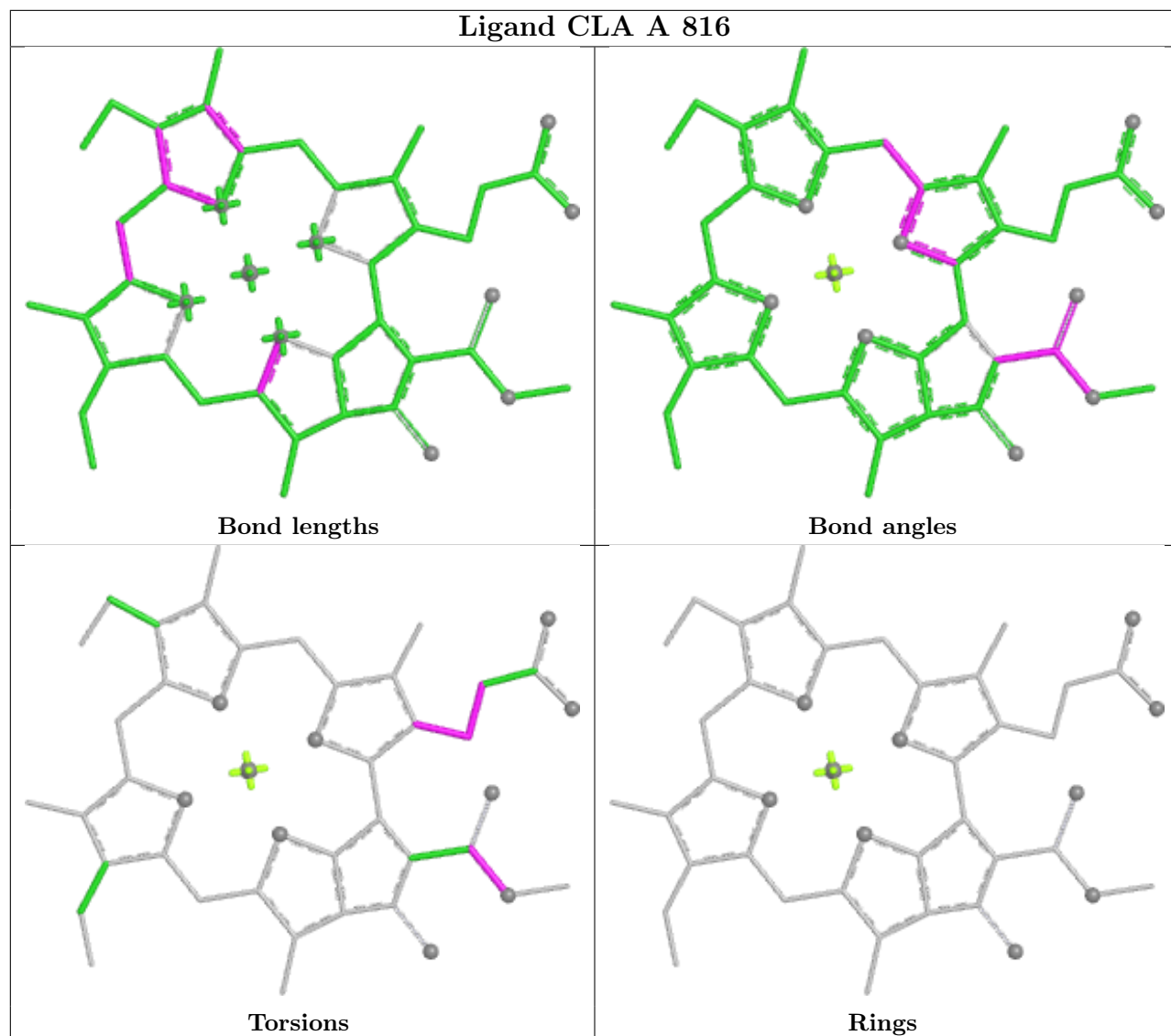


Ligand CLA A 825

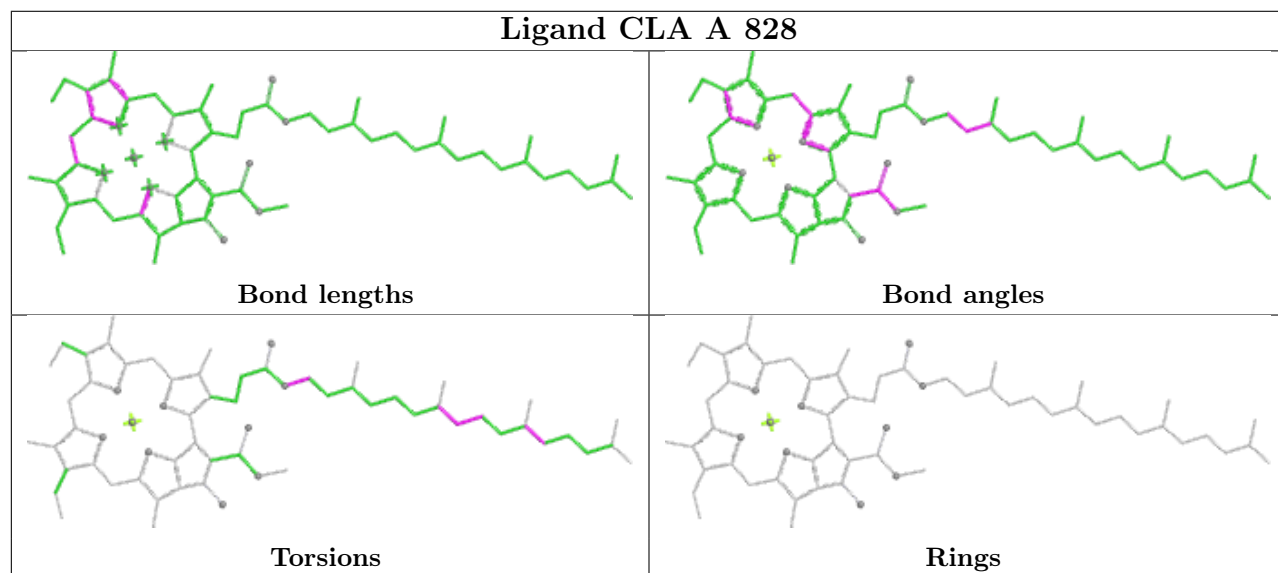


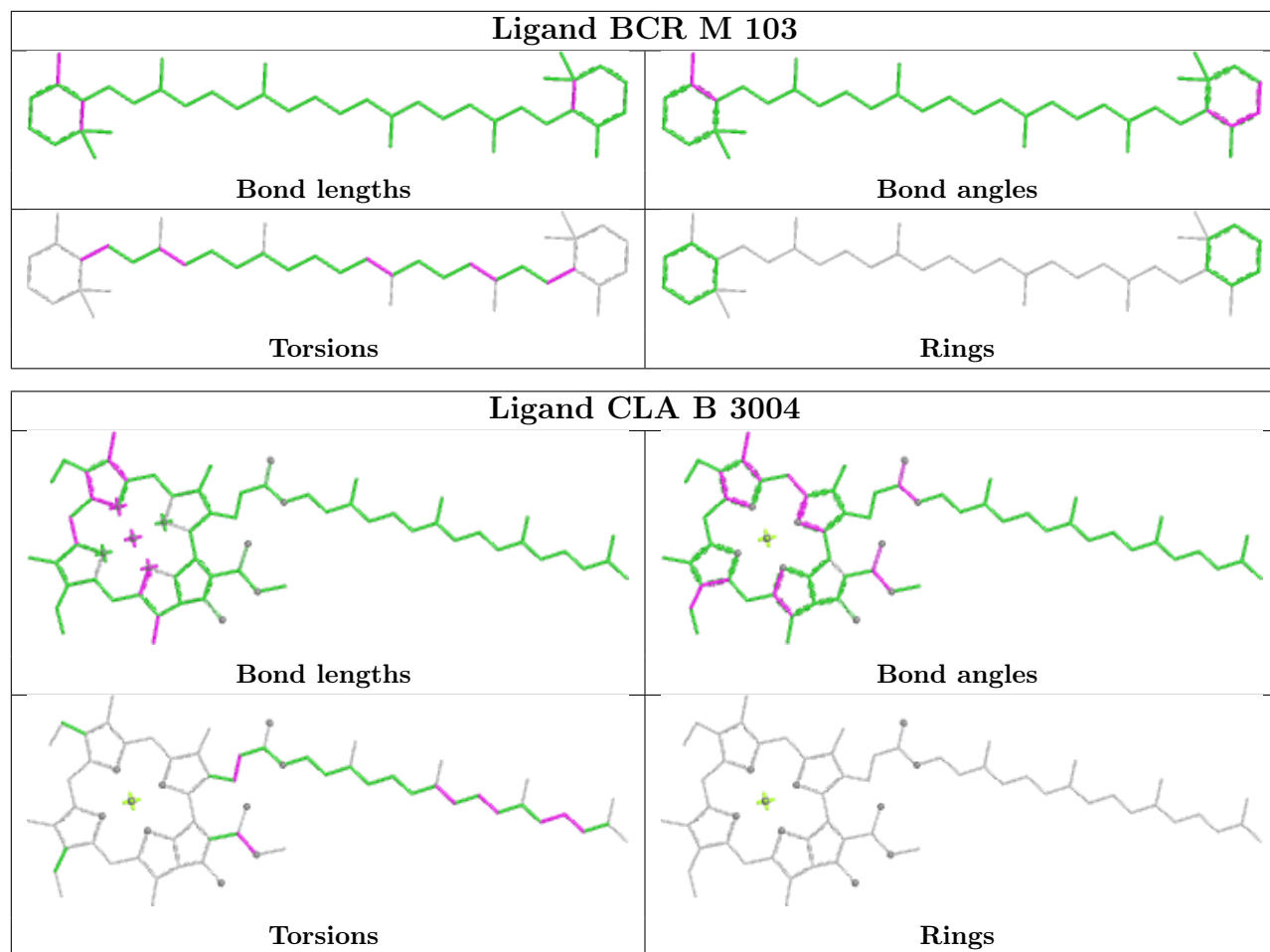


Ligand CLA A 816

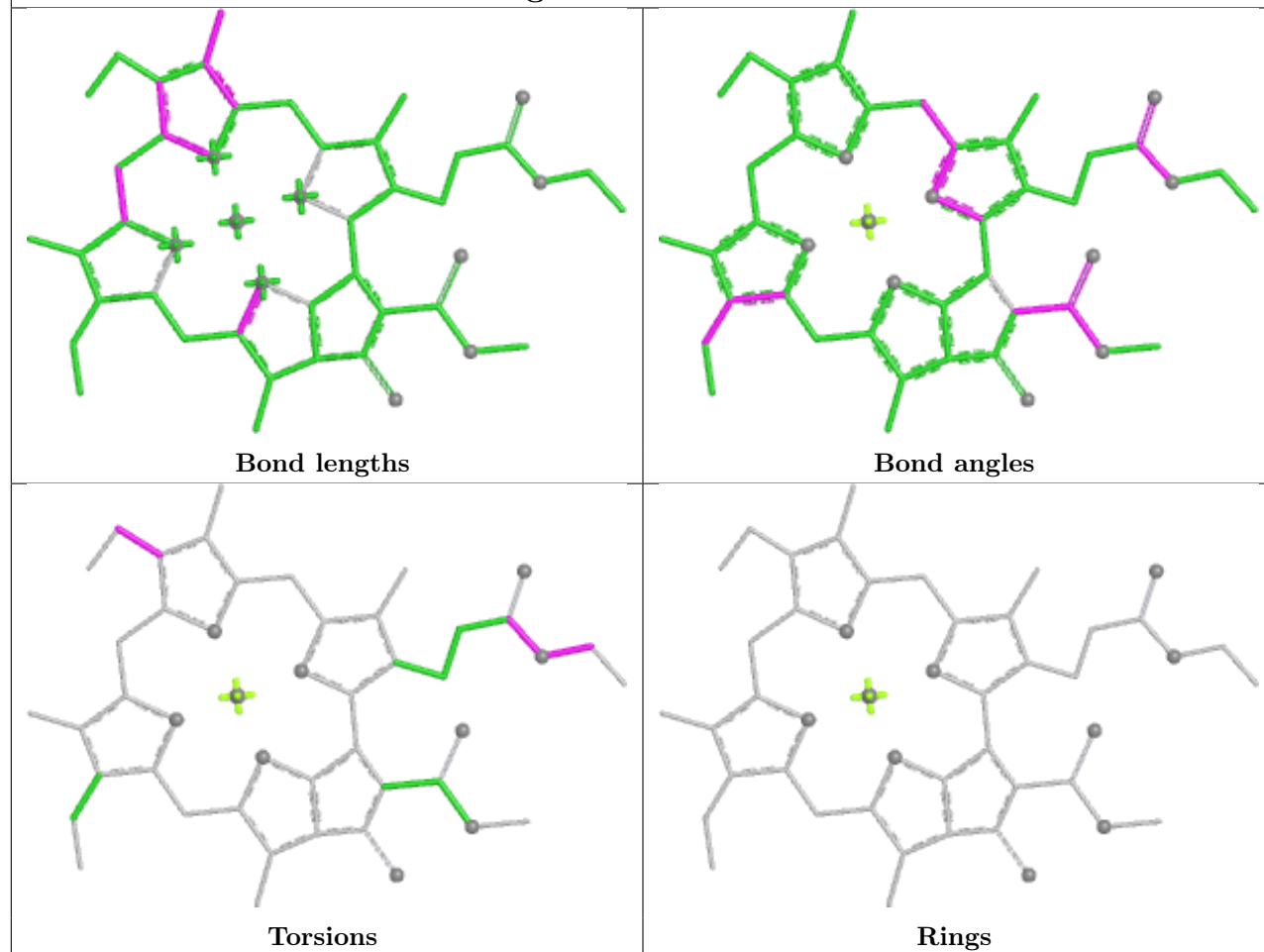


Ligand CLA A 828

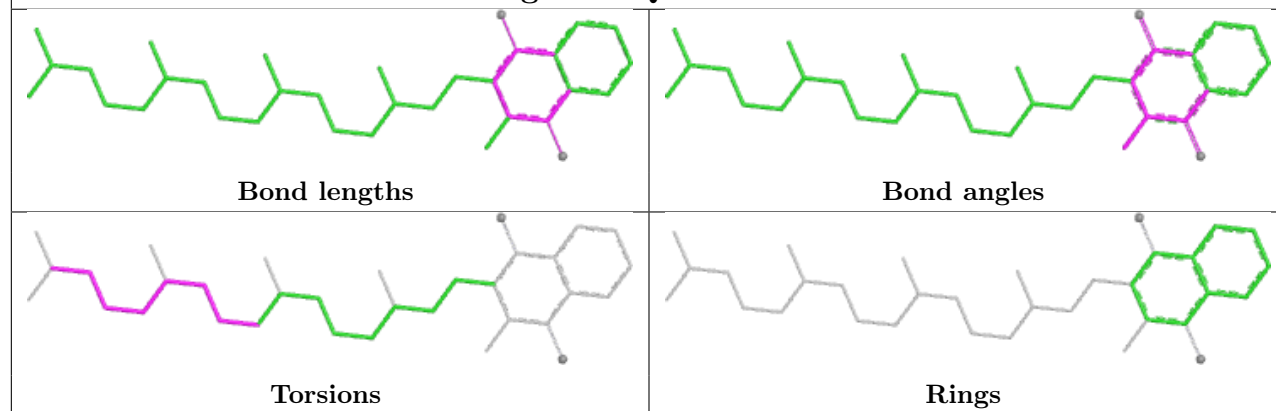




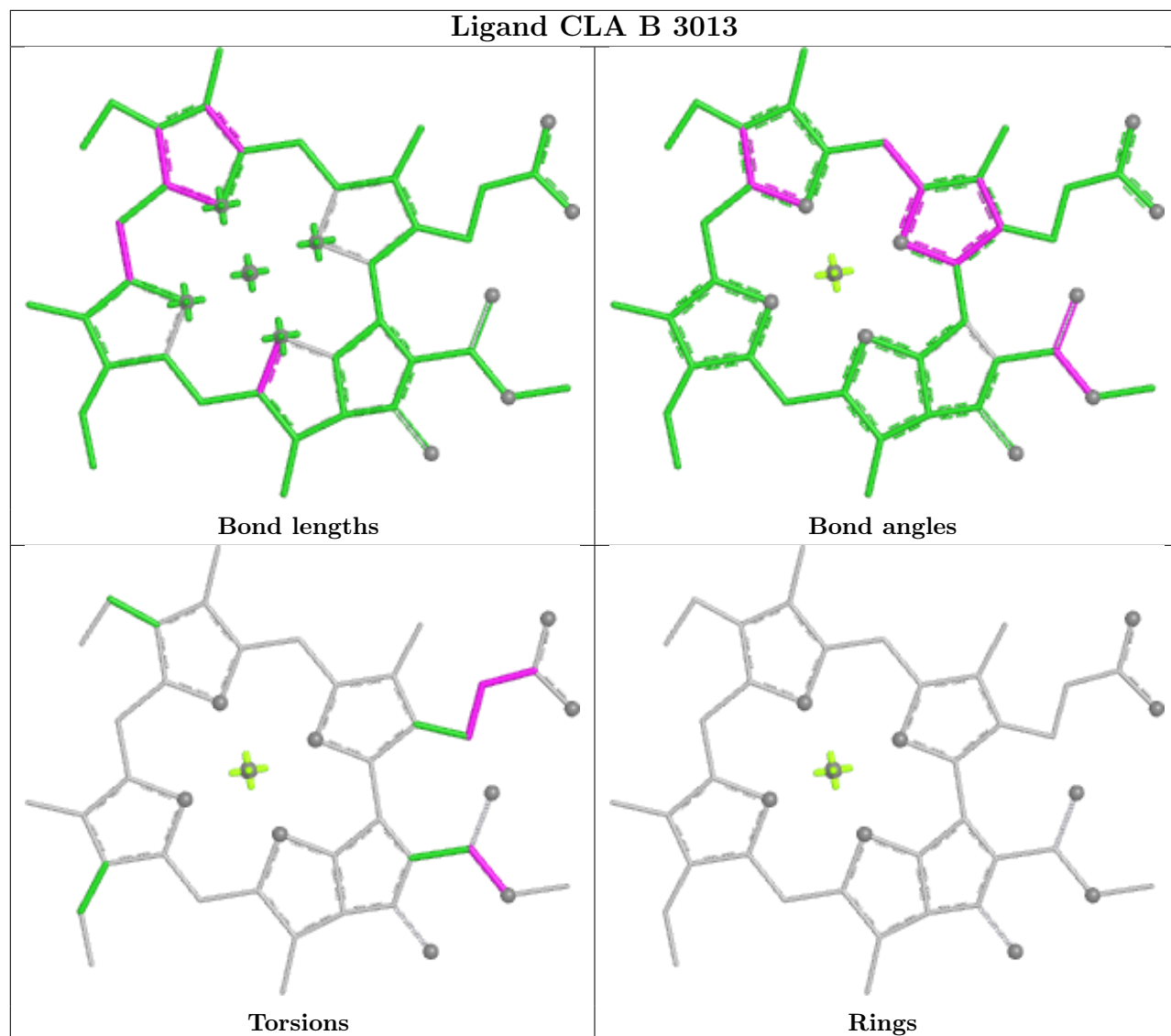
Ligand CLA A 840



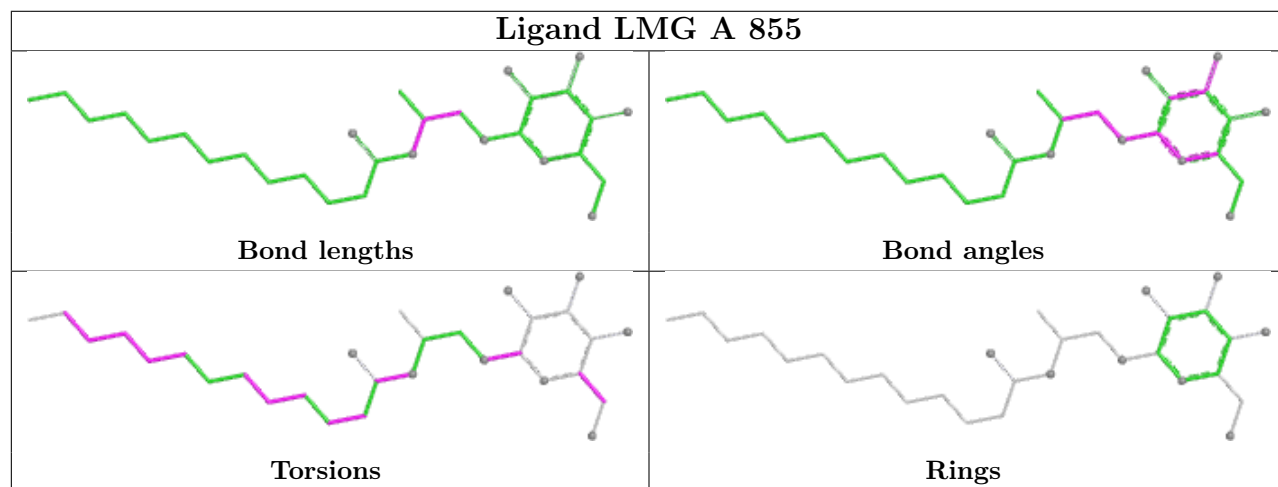
Ligand PQN B 3042

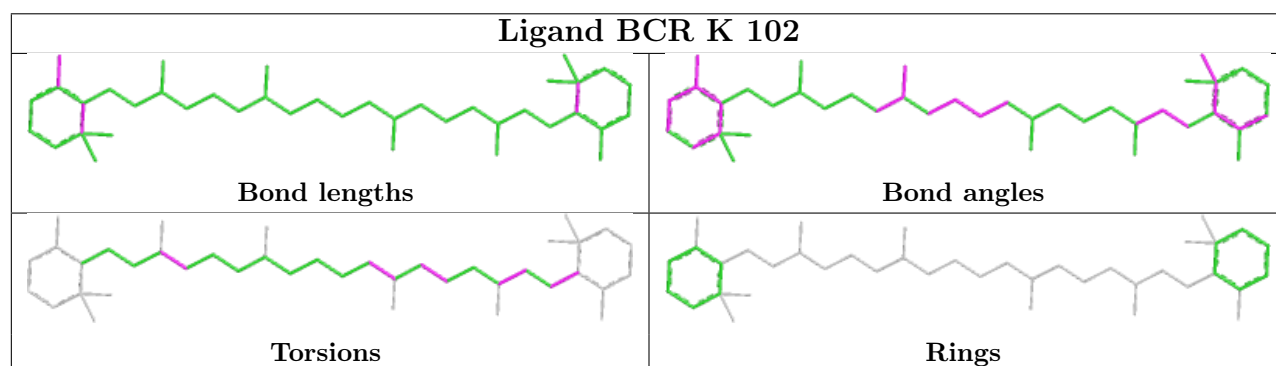
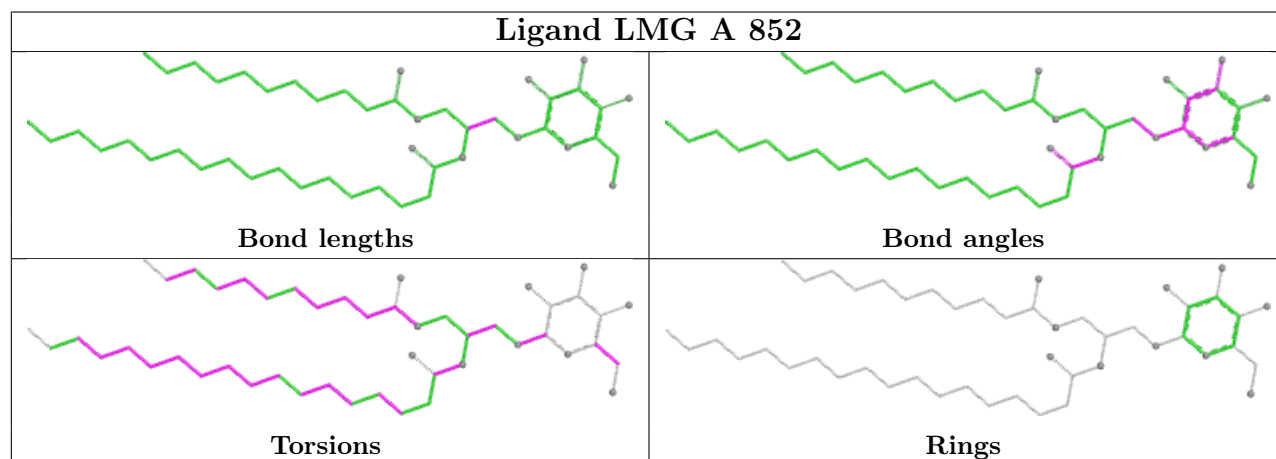
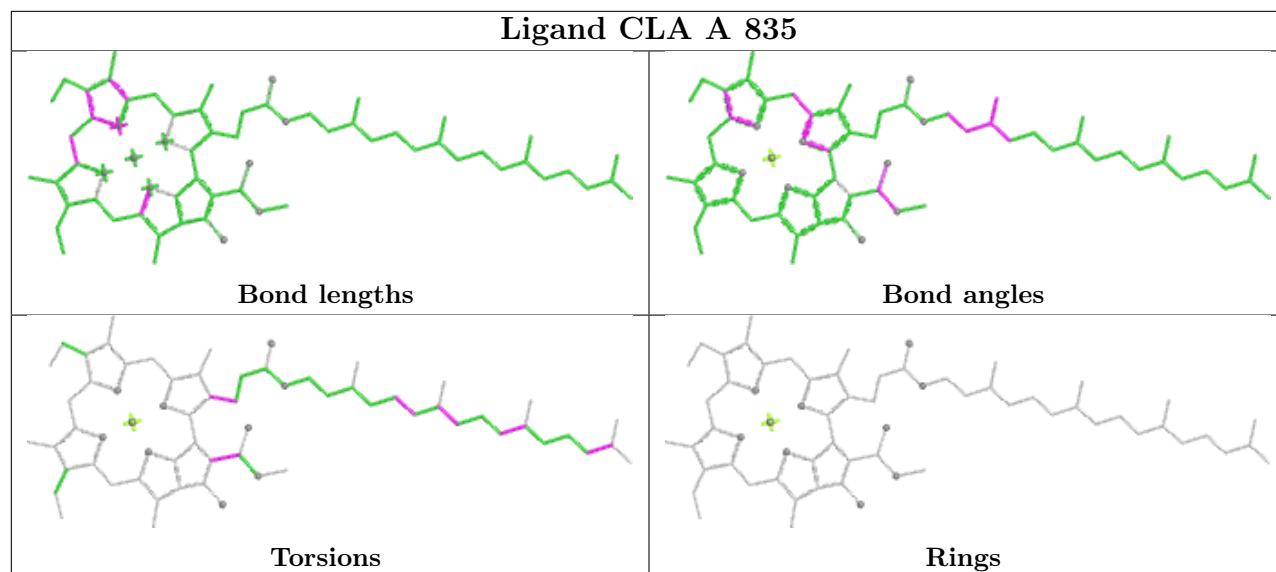


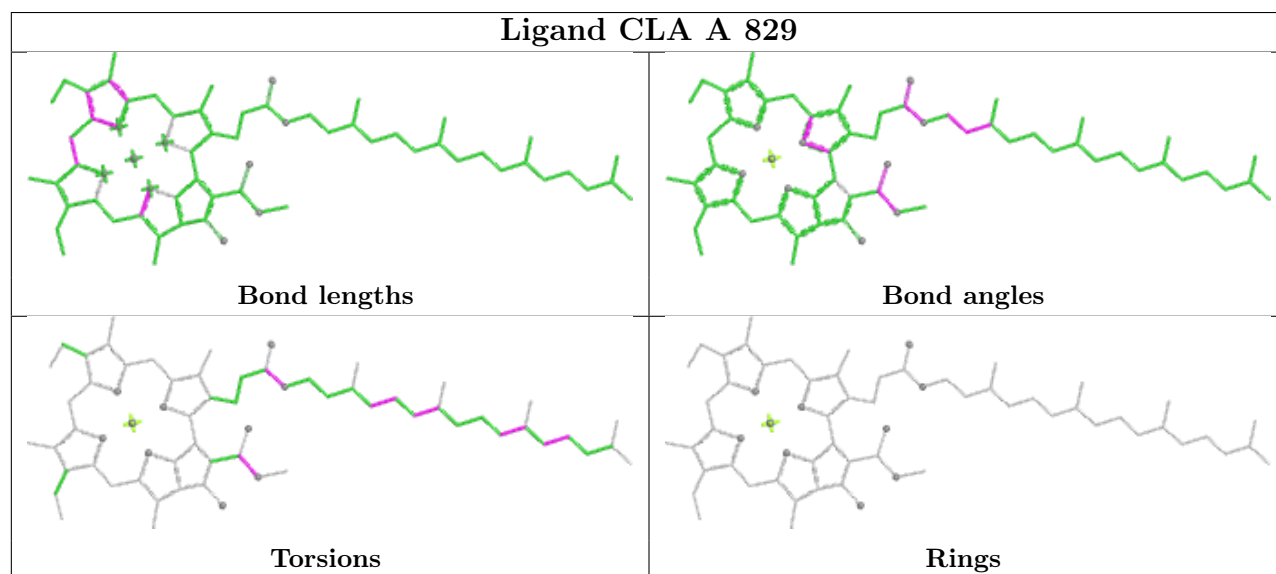
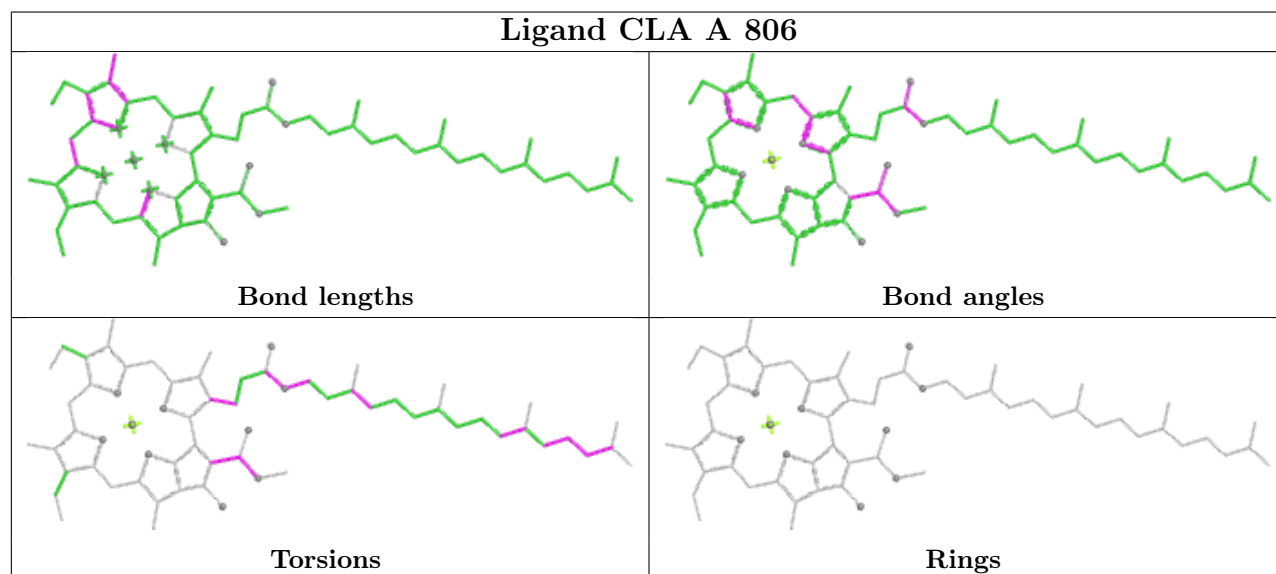
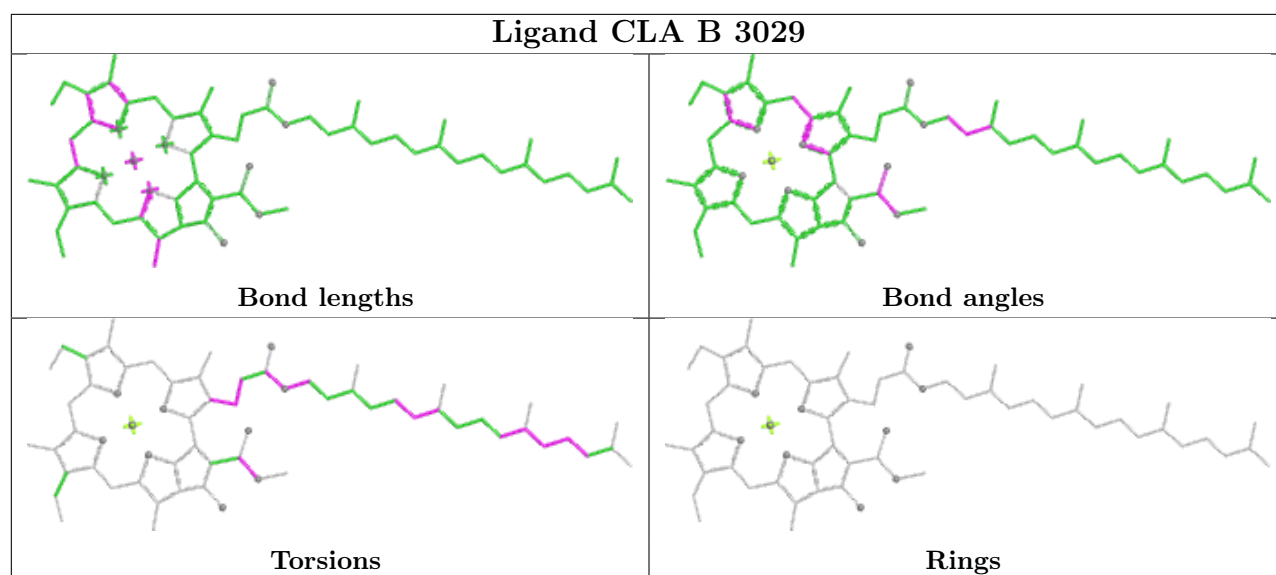
Ligand CLA B 3013

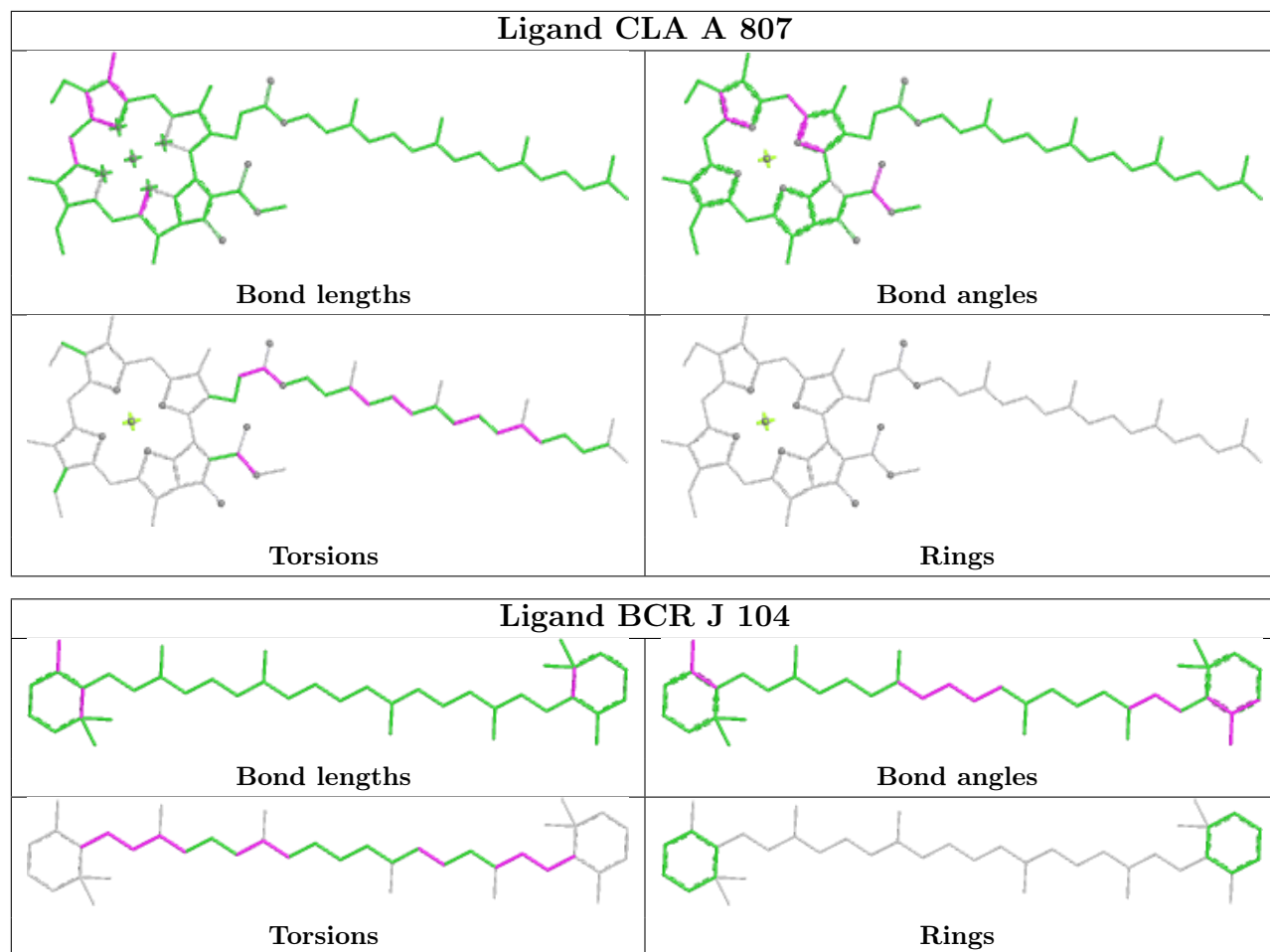


Ligand LMG A 855

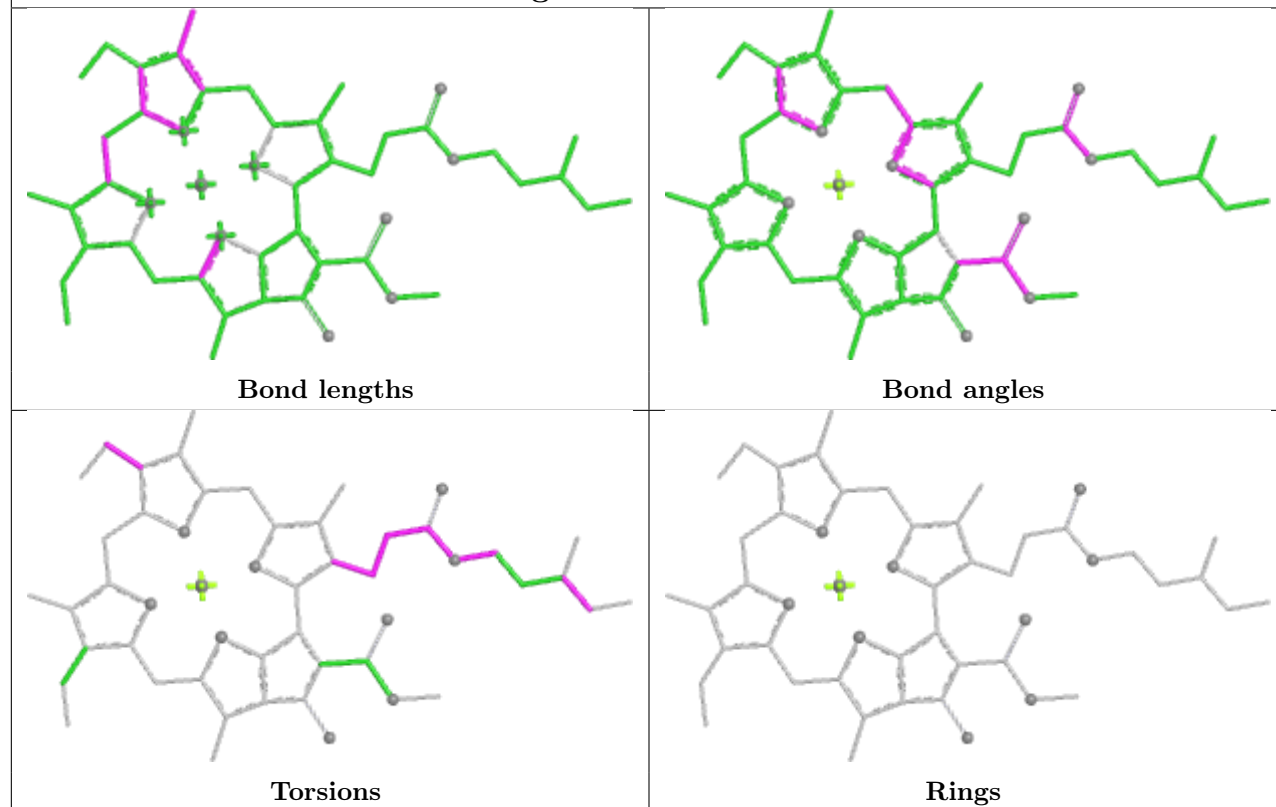




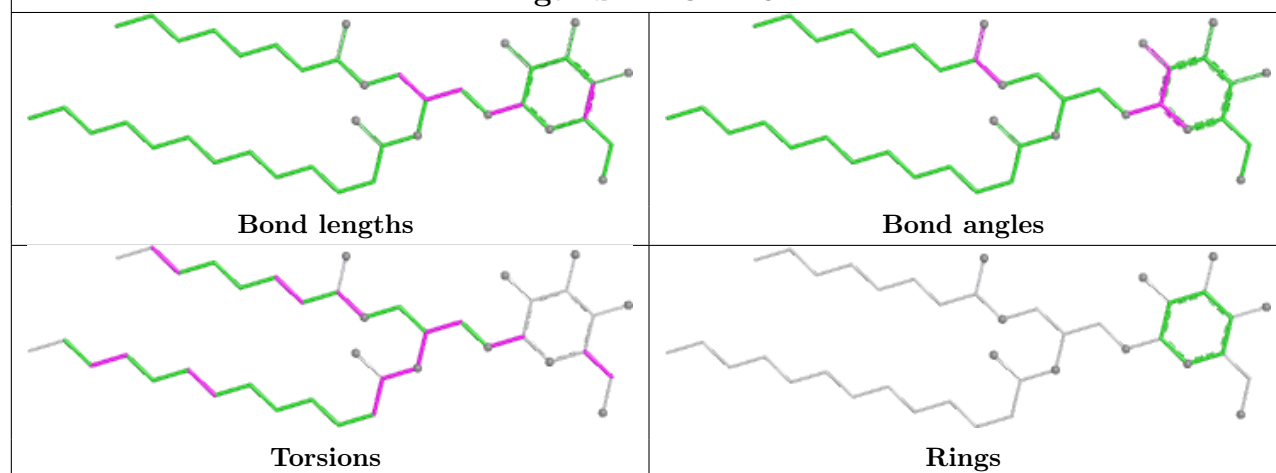




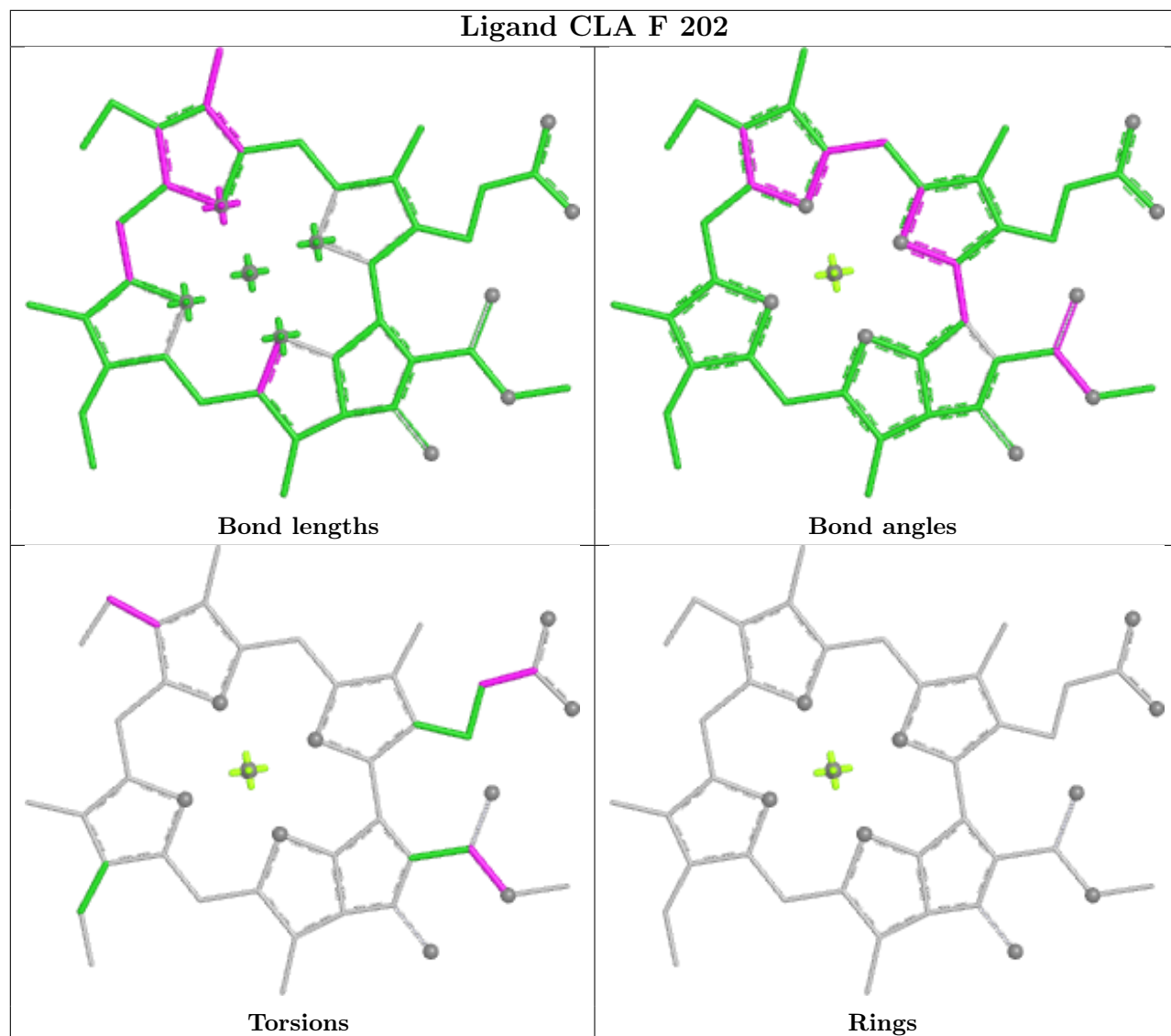
Ligand CLA A 808

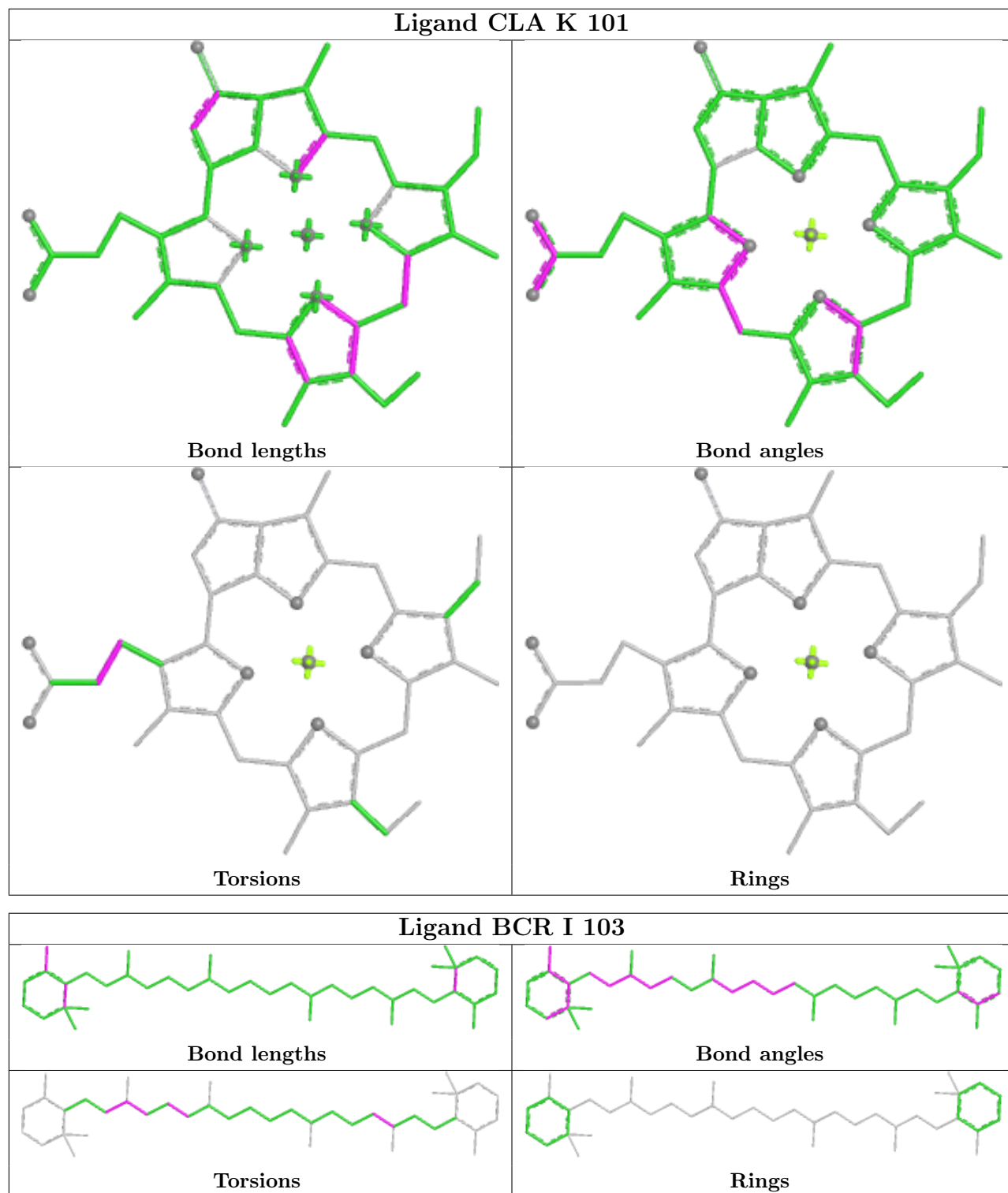


Ligand LMG I 104

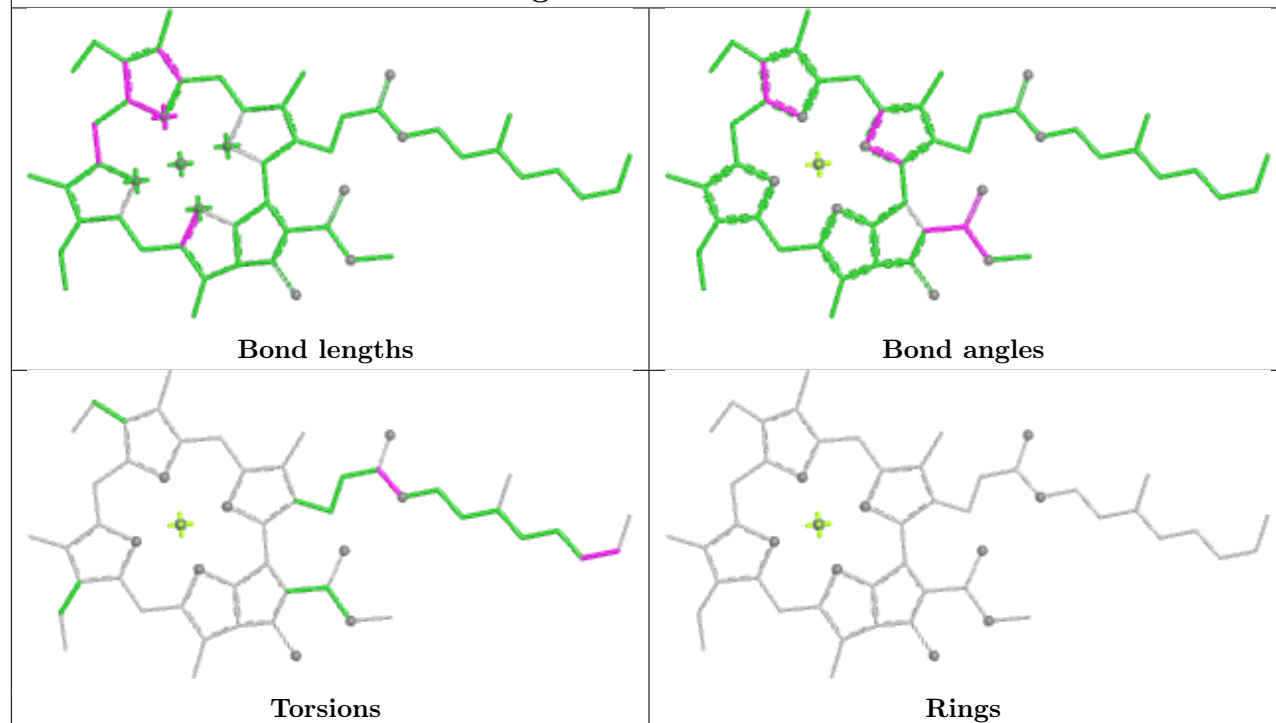


Ligand CLA F 202

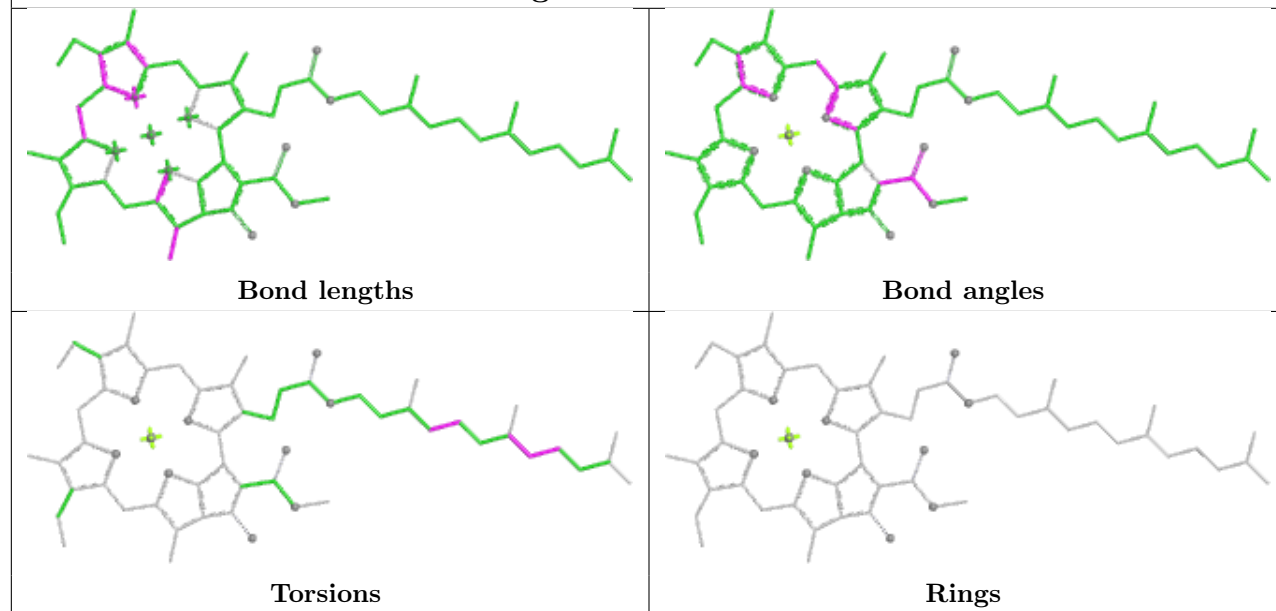


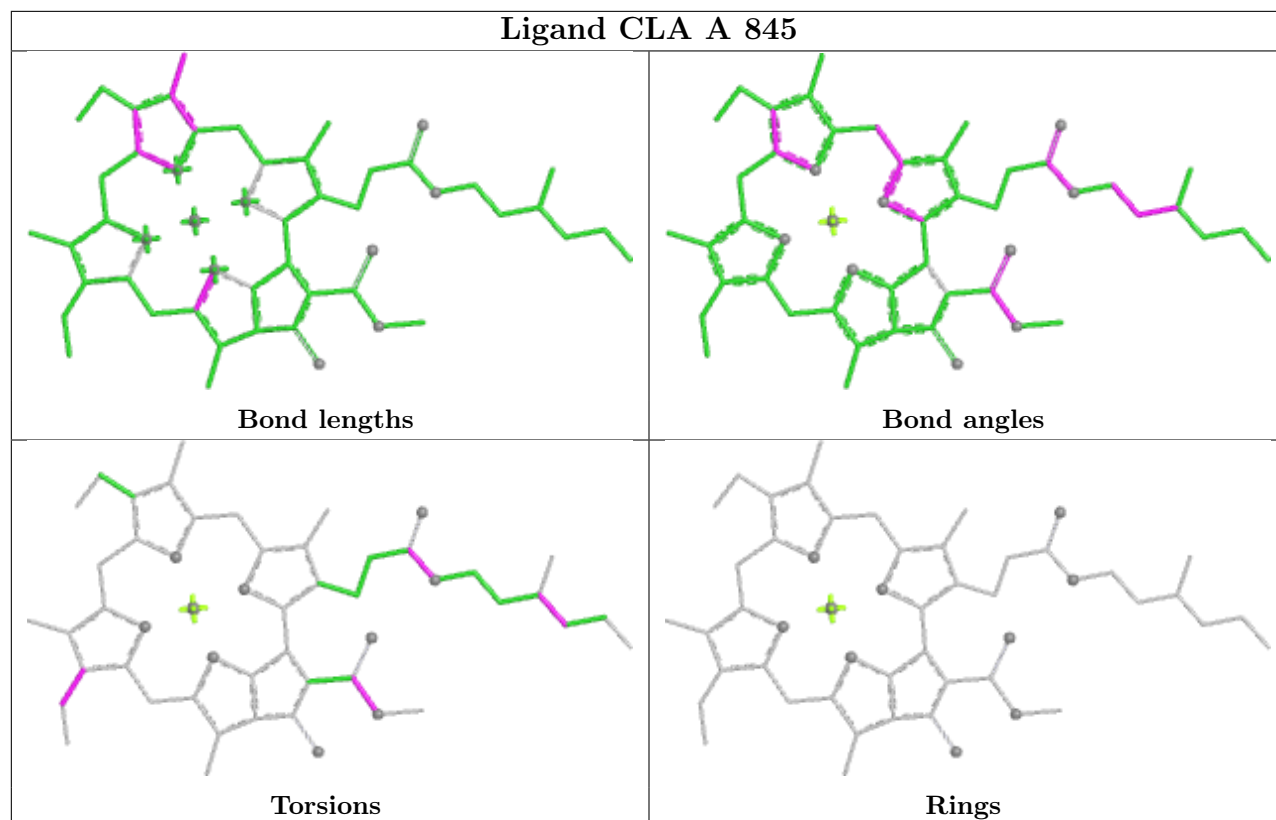


Ligand CLA A 818

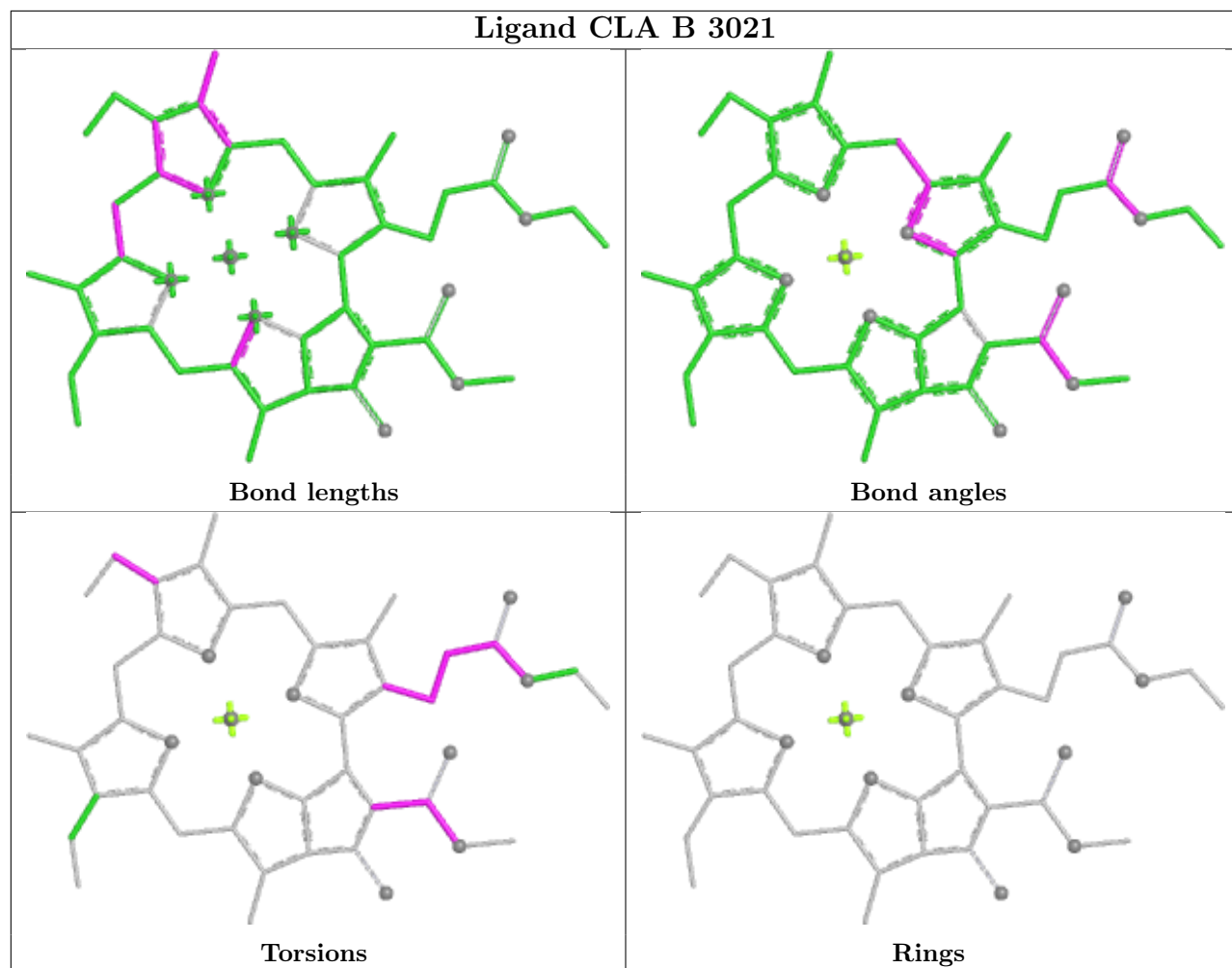


Ligand CLA A 814

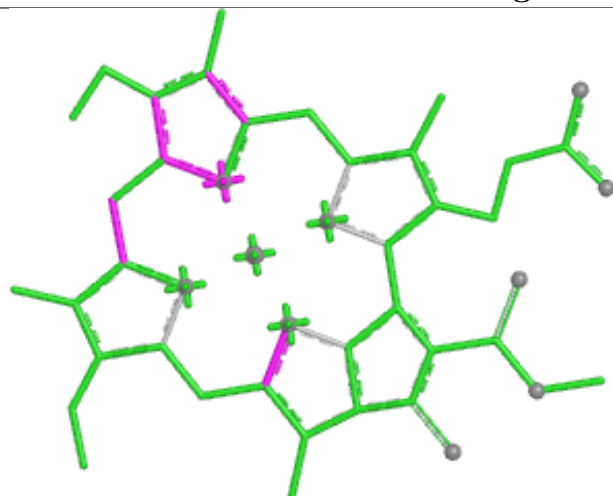




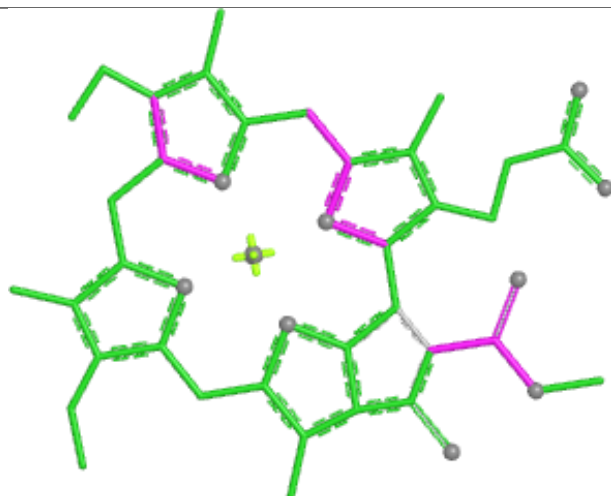
Ligand CLA B 3021



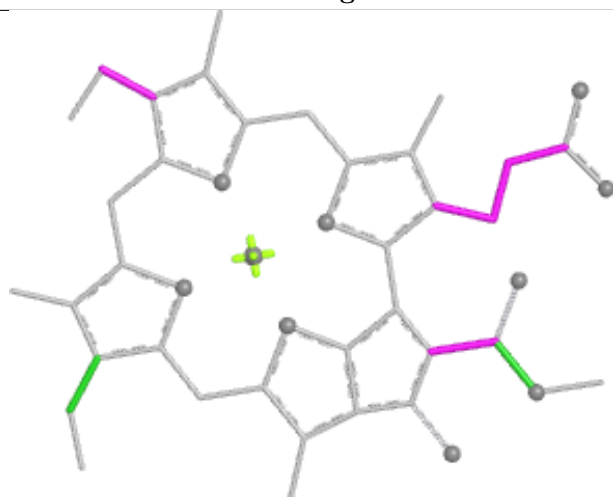
Ligand CLA K 103



Bond lengths



Bond angles

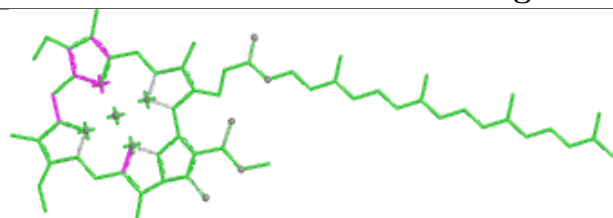


Torsions

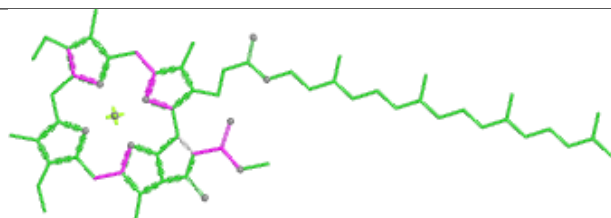


Rings

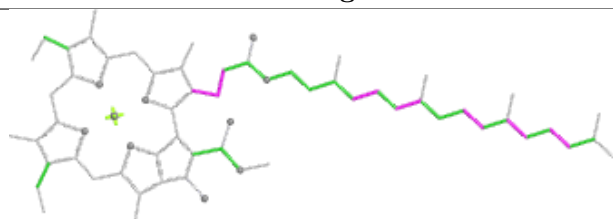
Ligand CLA A 802



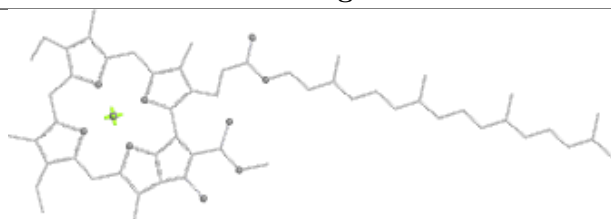
Bond lengths



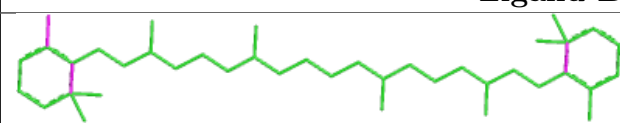
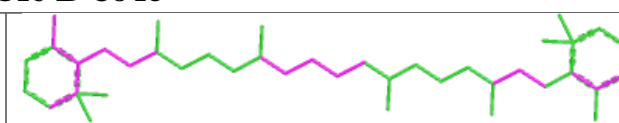
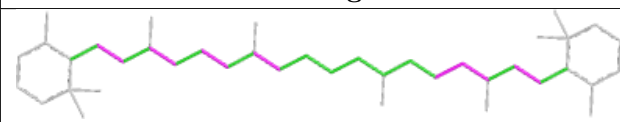
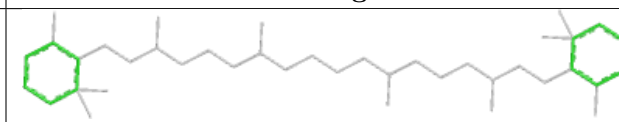
Bond angles

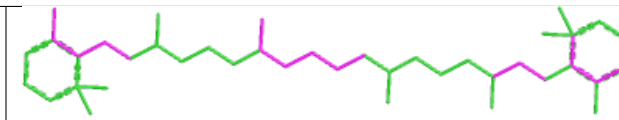
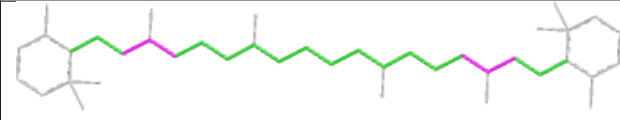
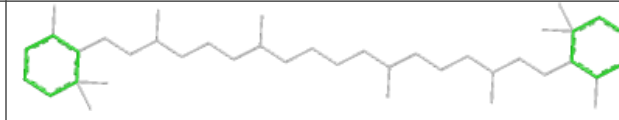


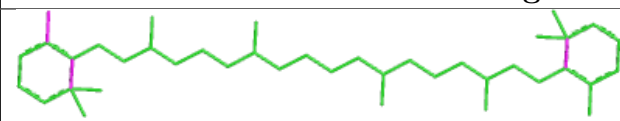
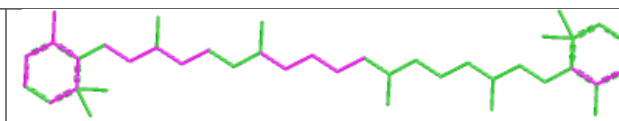
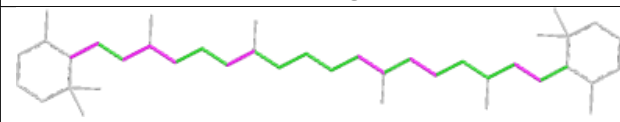
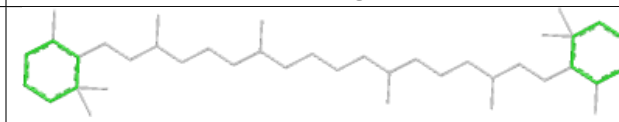
Torsions

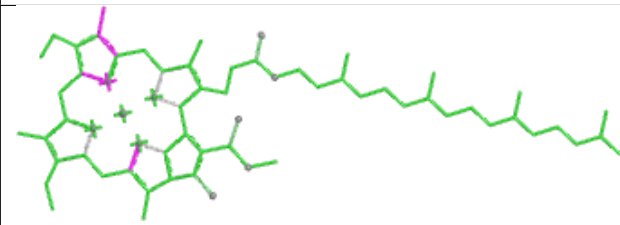
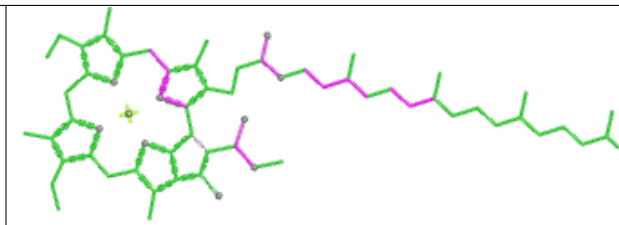
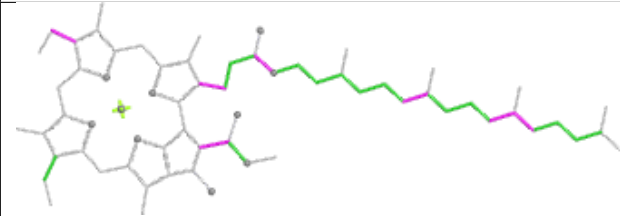
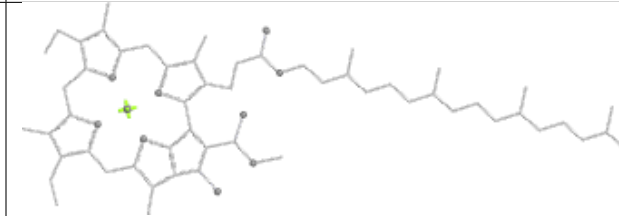


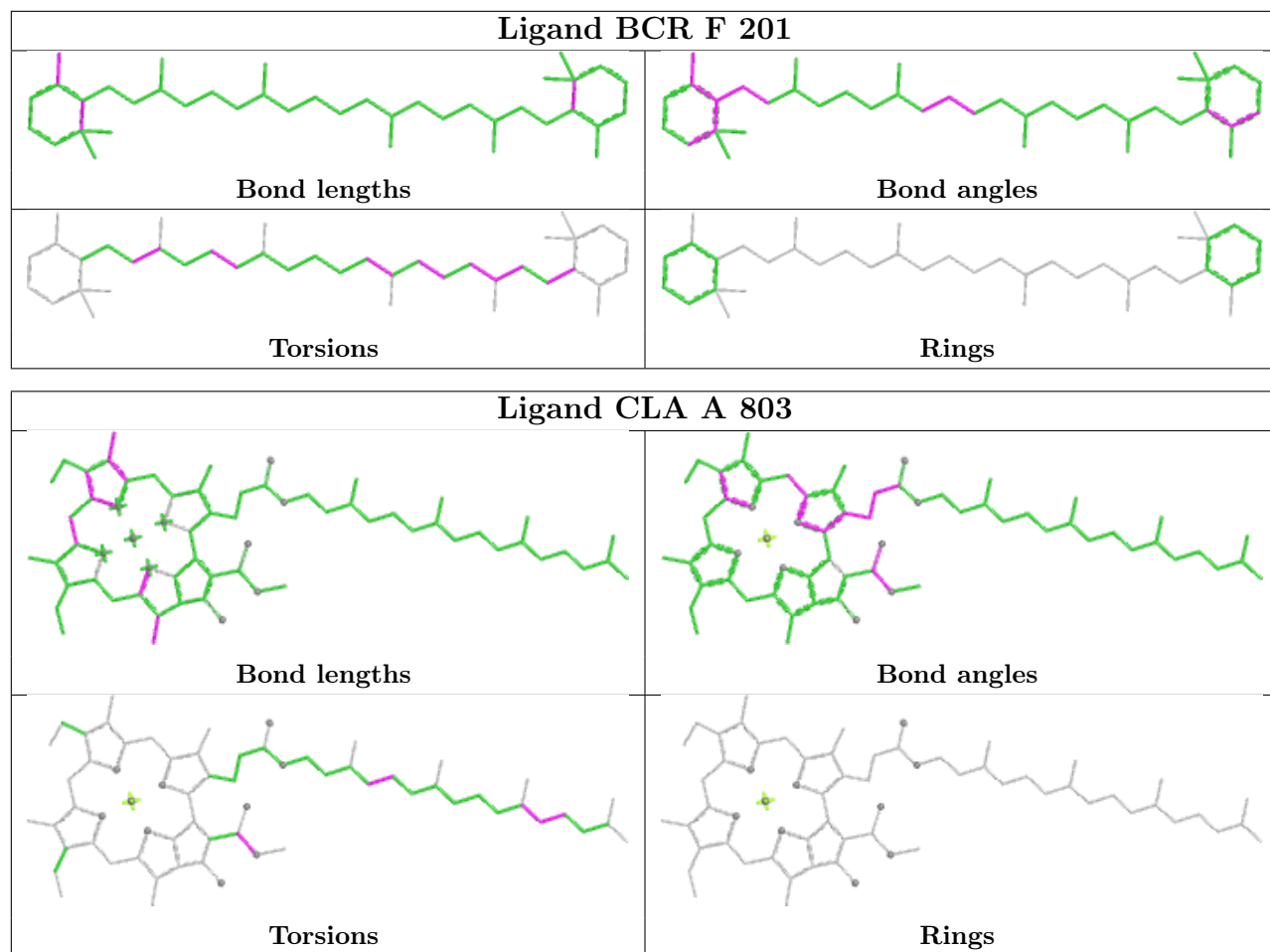
Rings

Ligand BCR B 3045	
	
Bond lengths	Bond angles
	
Torsions	Rings

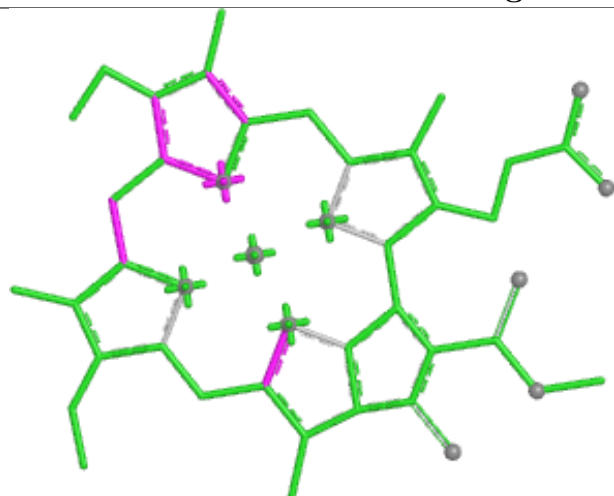
Ligand BCR I 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR J 105	
	
Bond lengths	Bond angles
	
Torsions	Rings

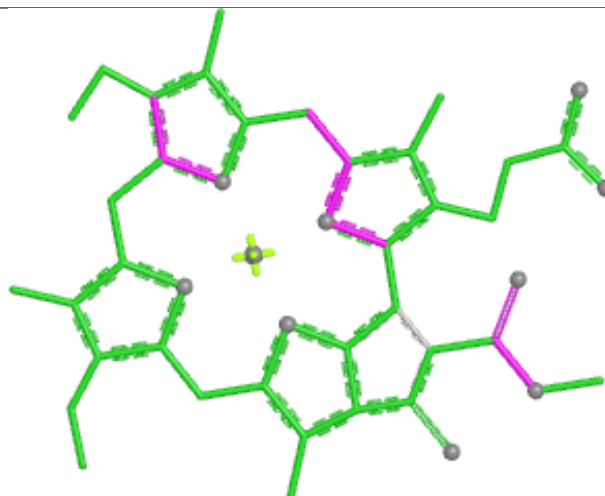
Ligand CLA L 203	
	
Bond lengths	Bond angles
	
Torsions	Rings



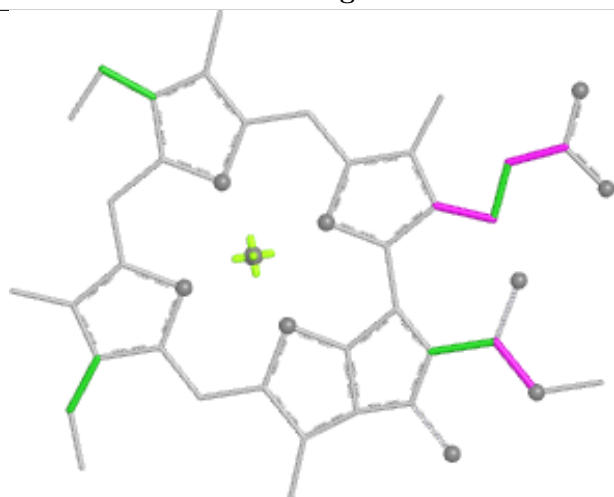
Ligand CLA B 3036



Bond lengths



Bond angles

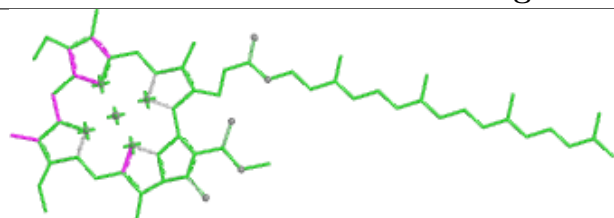


Torsions

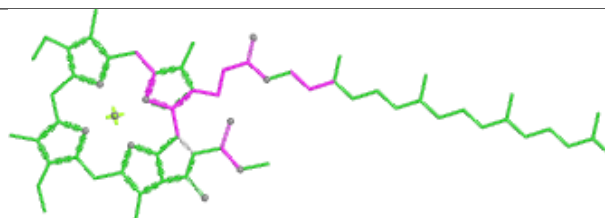


Rings

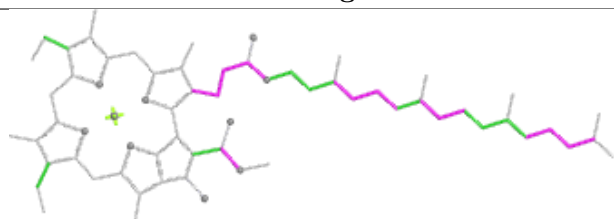
Ligand CLA A 820



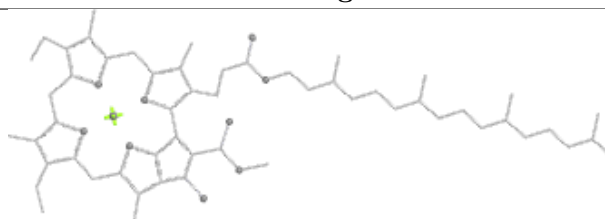
Bond lengths



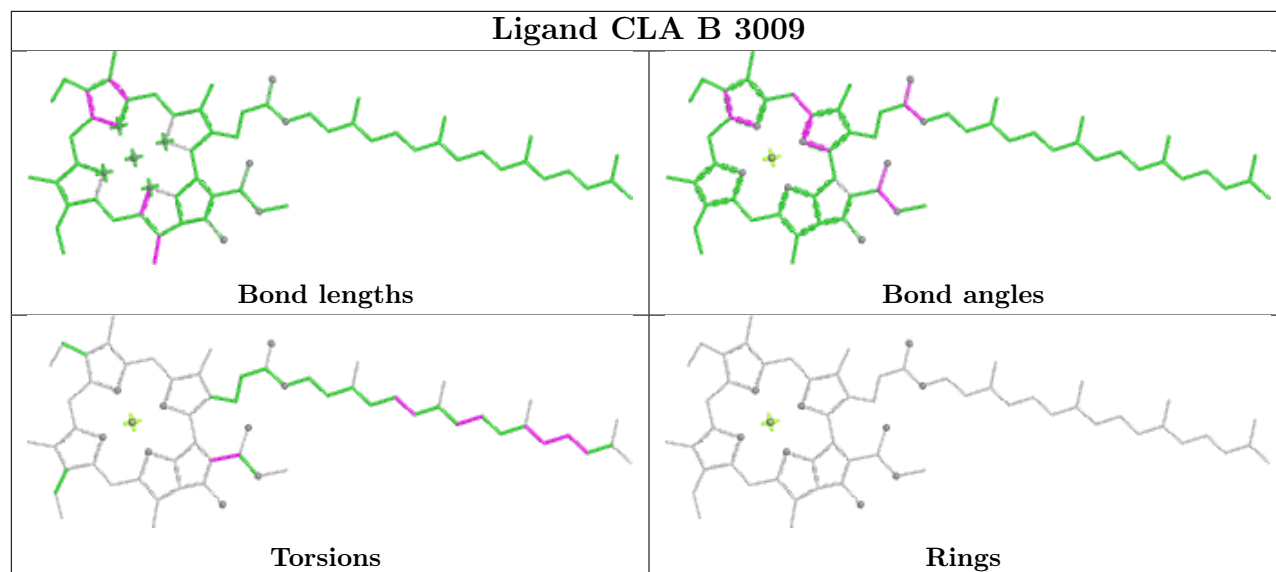
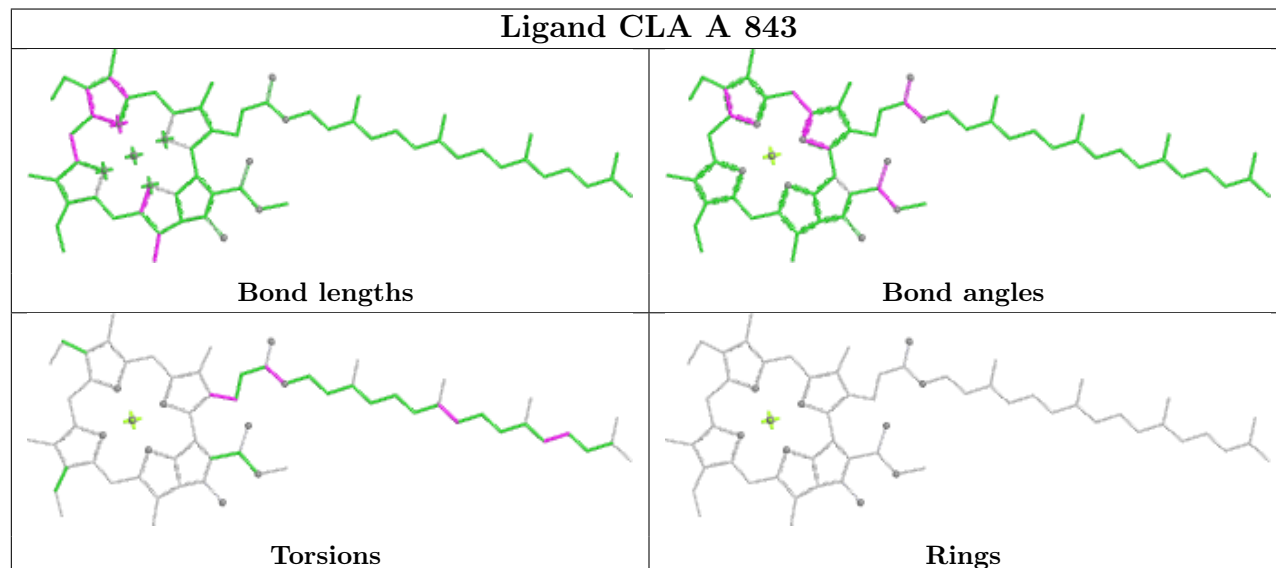
Bond angles



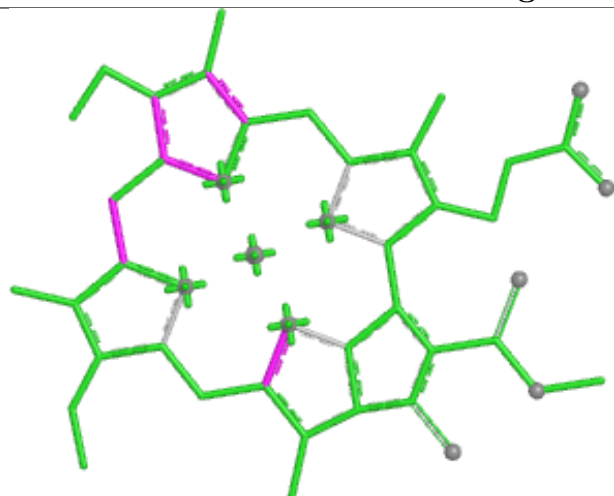
Torsions



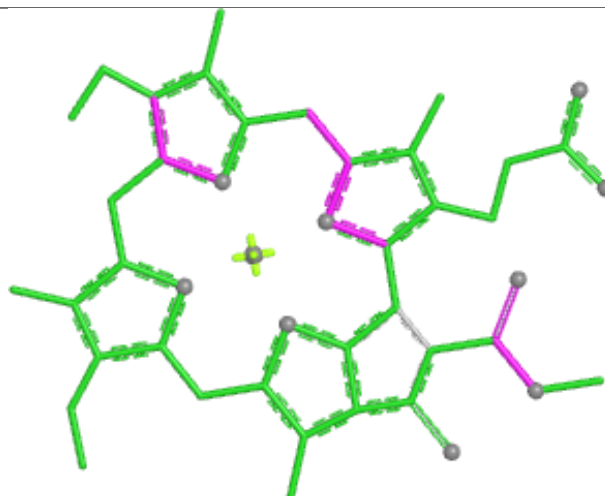
Rings

Ligand CLA B 3009**Ligand CLA A 843**

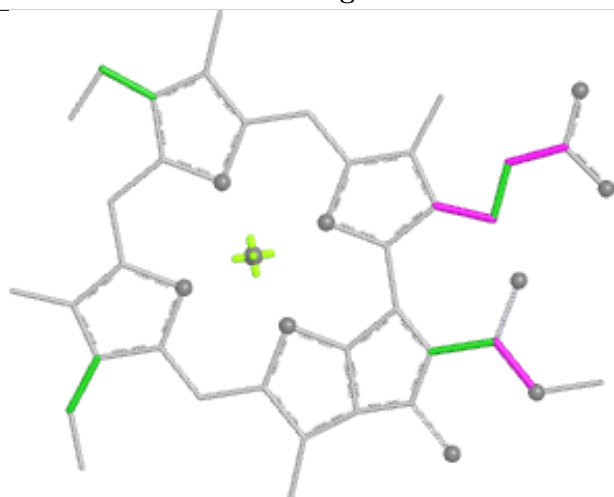
Ligand CLA J 101



Bond lengths



Bond angles

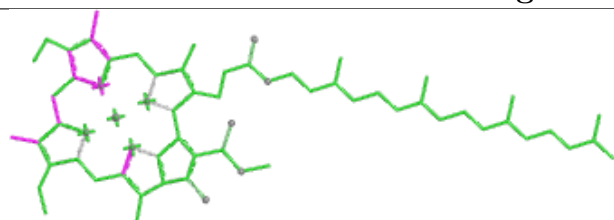


Torsions

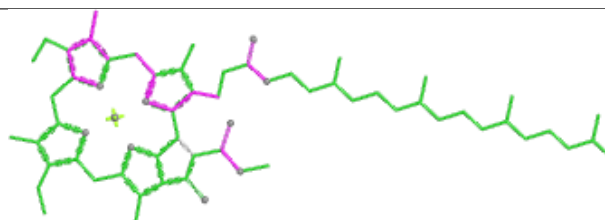


Rings

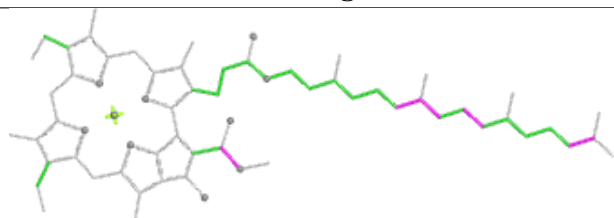
Ligand CLA L 205



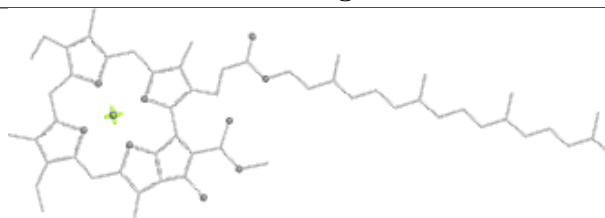
Bond lengths



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%)	1.05	123 (16%) 4 4	32, 97, 149, 195	0
2	B	739/740 (99%)	0.68	66 (8%) 15 15	23, 70, 117, 151	0
3	C	80/80 (100%)	0.36	2 (2%) 58 56	22, 63, 91, 101	0
4	D	138/138 (100%)	0.35	7 (5%) 33 33	40, 75, 102, 157	0
5	E	69/75 (92%)	1.05	10 (14%) 6 5	64, 92, 114, 130	0
6	F	141/164 (85%)	0.83	16 (11%) 10 8	64, 116, 135, 143	0
7	I	38/38 (100%)	0.67	4 (10%) 11 11	27, 44, 72, 106	0
8	J	41/41 (100%)	0.85	2 (4%) 35 34	107, 126, 140, 160	0
9	K	47/83 (56%)	2.06	19 (40%) 0 0	142, 176, 193, 210	0
10	L	151/154 (98%)	0.29	3 (1%) 65 63	24, 43, 82, 131	0
11	M	31/31 (100%)	0.57	4 (12%) 7 6	40, 63, 88, 113	0
12	X	29/35 (82%)	1.23	7 (24%) 2 1	73, 97, 127, 140	0
All	All	2244/2334 (96%)	0.80	263 (11%) 9 7	22, 81, 142, 210	0

All (263) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	ALA	14.7
1	A	379	PRO	6.4
1	A	281	PHE	6.3
1	A	43	GLN	5.7
1	A	278	PHE	5.5
1	A	716	ALA	5.4
6	F	95	ASN	5.3
1	A	40	ARG	5.3
9	K	55	GLY	5.1
9	K	71	ALA	5.1
9	K	68	LEU	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	2	GLN	5.0
1	A	174	PHE	5.0
1	A	268	PHE	5.0
2	B	314	VAL	5.0
9	K	57	PRO	4.9
1	A	261	PHE	4.7
1	A	267	PHE	4.7
2	B	360	PRO	4.7
1	A	693	GLY	4.6
10	L	143	LEU	4.4
1	A	613	PHE	4.4
1	A	279	LEU	4.3
6	F	53	VAL	4.3
1	A	120	ILE	4.3
1	A	169	ALA	4.3
2	B	503	TRP	4.2
1	A	18	ASN	4.2
6	F	63	PHE	4.1
12	X	10	ALA	4.0
9	K	21	LEU	4.0
3	C	49	GLY	3.9
1	A	273	ALA	3.9
1	A	260	PHE	3.8
1	A	275	TYR	3.8
1	A	119	PRO	3.8
2	B	359	PRO	3.8
6	F	96	GLU	3.8
6	F	54	ASP	3.7
9	K	20	ILE	3.7
1	A	149	ALA	3.7
2	B	513	SER	3.7
4	D	44	ALA	3.6
1	A	694	ARG	3.6
12	X	12	ARG	3.6
12	X	13	THR	3.5
1	A	270	PHE	3.5
2	B	589	MET	3.5
5	E	53	SER	3.5
1	A	153	THR	3.4
9	K	28	ALA	3.4
2	B	573	THR	3.3
1	A	116	VAL	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	69	ALA	3.3
1	A	19	ASP	3.3
2	B	312	THR	3.3
1	A	524	VAL	3.3
11	M	31	LYS	3.2
1	A	53	ALA	3.2
1	A	321	ILE	3.2
9	K	74	VAL	3.2
1	A	218	HIS	3.2
9	K	38	GLY	3.2
1	A	358	ILE	3.2
6	F	100	ILE	3.2
1	A	102	ALA	3.1
9	K	77	LEU	3.1
1	A	522	GLY	3.1
1	A	375	TYR	3.1
11	M	30	TYR	3.1
2	B	221	LEU	3.1
2	B	267	LEU	3.1
2	B	680	LEU	3.1
1	A	280	THR	3.1
2	B	620	THR	3.1
1	A	272	TRP	3.1
2	B	256	PHE	3.1
1	A	91	TYR	3.0
5	E	45	TYR	3.0
1	A	22	PRO	3.0
1	A	239	PRO	3.0
1	A	747	PHE	3.0
2	B	656	PHE	3.0
1	A	292	LEU	3.0
5	E	52	ALA	3.0
9	K	59	LEU	3.0
1	A	44	THR	3.0
2	B	622	LEU	2.9
1	A	244	LEU	2.9
1	A	374	MET	2.9
4	D	1	THR	2.9
7	I	36	GLY	2.9
1	A	294	LEU	2.9
1	A	497	ALA	2.9
2	B	477	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	117	VAL	2.8
1	A	193	VAL	2.8
5	E	1	VAL	2.8
1	A	266	PRO	2.8
2	B	113	ASP	2.8
9	K	43	LEU	2.8
2	B	309	PHE	2.8
2	B	515	PHE	2.8
1	A	121	VAL	2.8
2	B	224	PHE	2.8
9	K	32	TYR	2.8
2	B	307	LYS	2.7
1	A	324	SER	2.7
1	A	297	THR	2.7
1	A	513	PHE	2.7
1	A	20	PRO	2.7
1	A	380	TYR	2.7
2	B	323	GLN	2.7
1	A	591	GLY	2.7
6	F	55	GLY	2.7
1	A	509	ALA	2.7
1	A	698	GLN	2.7
2	B	560	GLY	2.7
2	B	652	TRP	2.7
1	A	393	LEU	2.6
6	F	93	GLU	2.6
1	A	111	LYS	2.6
1	A	75	ALA	2.6
1	A	409	ALA	2.6
2	B	122	TRP	2.6
1	A	315	TYR	2.6
2	B	520	PRO	2.6
1	A	104	LEU	2.6
2	B	380	TYR	2.6
1	A	210	LEU	2.5
10	L	4	LEU	2.5
2	B	361	TYR	2.5
2	B	621	TYR	2.5
2	B	569	GLY	2.5
1	A	246	PRO	2.5
1	A	114	ALA	2.5
1	A	492	ASN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	692	SER	2.5
1	A	284	GLY	2.5
2	B	450	GLY	2.5
2	B	449	PHE	2.5
2	B	339	TRP	2.5
2	B	518	ILE	2.5
2	B	116	TYR	2.5
2	B	440	TYR	2.5
1	A	13	ARG	2.5
1	A	204	LEU	2.5
2	B	724	ILE	2.5
1	A	93	HIS	2.5
1	A	571	ASN	2.4
1	A	493	LEU	2.4
2	B	535	THR	2.4
1	A	711	LEU	2.4
9	K	29	LEU	2.4
1	A	73	PHE	2.4
1	A	171	LEU	2.4
1	A	221	LEU	2.4
2	B	439	LEU	2.4
4	D	94	ILE	2.4
5	E	32	VAL	2.4
2	B	528	ALA	2.4
1	A	391	LEU	2.4
2	B	649	LEU	2.4
1	A	378	PRO	2.4
12	X	7	PRO	2.4
5	E	21	GLY	2.4
1	A	115	GLN	2.4
2	B	698	ARG	2.4
1	A	242	PHE	2.4
1	A	126	LEU	2.3
4	D	136	TYR	2.3
2	B	479	THR	2.3
1	A	150	SER	2.3
1	A	390	GLN	2.3
6	F	44	GLY	2.3
6	F	81	GLY	2.3
1	A	143	LEU	2.3
1	A	159	TYR	2.3
2	B	308	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	41	GLY	2.3
6	F	85	LEU	2.3
2	B	279	ILE	2.3
2	B	356	TYR	2.3
8	J	7	TYR	2.3
1	A	504	ASN	2.3
1	A	302	LEU	2.3
4	D	138	PRO	2.3
1	A	142	GLY	2.3
1	A	507	ALA	2.2
7	I	7	ALA	2.2
9	K	33	ALA	2.2
2	B	512	ASN	2.2
9	K	37	ARG	2.2
1	A	132	GLY	2.2
1	A	500	GLY	2.2
1	A	51	LEU	2.2
1	A	201	LEU	2.2
2	B	492	TRP	2.2
2	B	4	PHE	2.2
3	C	61	PHE	2.2
9	K	61	ALA	2.2
1	A	23	THR	2.2
1	A	665	TYR	2.2
12	X	9	TYR	2.2
12	X	29	TYR	2.2
1	A	185	PRO	2.2
2	B	441	VAL	2.2
1	A	249	MET	2.2
8	J	25	ILE	2.2
2	B	468	ALA	2.2
1	A	508	THR	2.2
1	A	696	TYR	2.2
5	E	15	TYR	2.2
12	X	30	TYR	2.2
6	F	50	HIS	2.2
1	A	213	ALA	2.2
6	F	25	THR	2.2
11	M	9	TYR	2.2
2	B	572	GLY	2.2
1	A	392	SER	2.2
1	A	86	TRP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	I	20	TRP	2.1
1	A	96	LYS	2.1
10	L	111	LEU	2.1
2	B	558	ASP	2.1
2	B	429	SER	2.1
6	F	22	VAL	2.1
9	K	75	SER	2.1
2	B	225	PHE	2.1
1	A	47	TRP	2.1
6	F	56	ARG	2.1
1	A	362	MET	2.1
6	F	64	LEU	2.1
1	A	195	SER	2.1
2	B	362	ALA	2.1
5	E	24	ALA	2.1
9	K	58	GLU	2.1
2	B	272	MET	2.1
2	B	563	PHE	2.1
2	B	730	PHE	2.1
1	A	654	LEU	2.1
2	B	684	LEU	2.1
1	A	230	GLY	2.1
4	D	45	GLY	2.1
1	A	243	ILE	2.1
1	A	156	PHE	2.1
7	I	9	PHE	2.1
1	A	525	ALA	2.0
2	B	286	ALA	2.0
2	B	357	SER	2.0
1	A	489	TRP	2.0
1	A	398	MET	2.0
1	A	408	GLY	2.0
2	B	428	VAL	2.0
1	A	308	PHE	2.0
2	B	682	GLU	2.0
4	D	81	LYS	2.0
1	A	187	LEU	2.0
1	A	207	LEU	2.0
1	A	618	GLN	2.0
11	M	3	LEU	2.0
2	B	126	ILE	2.0
2	B	593	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	DGD	L	206	66/66	0.62	0.21	55,109,166,179	0
14	CLA	M	102	45/65	0.65	0.26	93,141,177,190	0
21	LMT	L	201	35/35	0.66	0.19	84,152,189,202	0
17	LMG	I	104	40/55	0.70	0.29	59,95,131,154	0
17	LMG	A	852	48/55	0.71	0.20	66,123,163,170	0
14	CLA	J	101	45/65	0.72	0.16	128,147,182,186	0
18	LHG	B	3049	23/49	0.72	0.22	83,121,149,155	0
14	CLA	A	816	45/65	0.78	0.21	116,153,179,189	0
14	CLA	K	103	45/65	0.78	0.19	111,142,174,176	0
16	BCR	K	102	40/40	0.79	0.29	117,157,176,186	0
18	LHG	M	101	49/49	0.79	0.23	57,99,174,191	0
14	CLA	J	102	37/65	0.79	0.17	112,135,160,173	0
16	BCR	B	3043	40/40	0.79	0.24	85,120,154,171	0
14	CLA	A	817	49/65	0.81	0.16	73,138,169,170	0
17	LMG	A	855	30/55	0.82	0.17	42,93,155,172	0
14	CLA	A	845	52/65	0.82	0.16	54,94,121,130	0
14	CLA	A	818	54/65	0.82	0.19	106,134,161,172	0
14	CLA	F	202	45/65	0.83	0.15	96,125,156,161	0
14	CLA	K	101	41/65	0.83	0.17	122,159,195,204	0
16	BCR	A	847	40/40	0.83	0.29	106,141,172,186	0
14	CLA	A	828	65/65	0.85	0.21	69,103,138,145	0
16	BCR	J	104	40/40	0.85	0.22	88,126,155,160	0
16	BCR	B	3046	40/40	0.86	0.26	64,90,110,116	0
14	CLA	A	811	45/65	0.86	0.16	102,135,162,170	0
16	BCR	A	848	40/40	0.87	0.30	88,129,181,187	0
14	CLA	A	813	54/65	0.87	0.14	84,111,138,146	0
14	CLA	A	823	49/65	0.88	0.13	88,126,156,168	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CLA	B	3021	47/65	0.88	0.14	79,108,139,145	0
16	BCR	B	3050	40/40	0.88	0.20	56,94,138,144	0
16	BCR	A	849	40/40	0.88	0.22	71,101,165,167	0
16	BCR	J	105	40/40	0.88	0.22	77,124,164,171	0
16	BCR	A	850	40/40	0.88	0.19	51,84,118,135	0
16	BCR	M	103	40/40	0.88	0.14	31,58,86,92	0
14	CLA	A	837	45/65	0.89	0.14	90,114,137,148	0
14	CLA	A	808	51/65	0.89	0.15	91,113,140,144	0
14	CLA	B	3018	59/65	0.89	0.19	57,91,119,127	0
14	CLA	A	824	51/65	0.89	0.14	77,111,142,148	0
16	BCR	F	203	40/40	0.89	0.22	53,104,137,157	0
14	CLA	B	3032	49/65	0.89	0.15	44,79,107,132	0
14	CLA	A	821	43/65	0.89	0.16	82,140,180,186	0
14	CLA	A	836	54/65	0.89	0.20	57,97,138,146	0
14	CLA	A	820	65/65	0.90	0.17	76,110,135,144	0
14	CLA	A	815	45/65	0.90	0.15	96,124,160,166	0
16	BCR	F	201	40/40	0.90	0.23	55,101,134,142	0
14	CLA	A	814	60/65	0.90	0.19	83,125,150,151	0
14	CLA	B	3034	58/65	0.90	0.16	73,108,147,151	0
14	CLA	A	819	54/65	0.90	0.15	71,104,126,142	0
16	BCR	B	3044	40/40	0.90	0.19	58,84,124,133	0
16	BCR	L	207	40/40	0.90	0.14	7,48,96,108	0
14	CLA	B	3027	65/65	0.91	0.17	48,75,102,107	0
14	CLA	B	3015	65/65	0.91	0.15	56,87,122,127	0
16	BCR	B	3045	40/40	0.91	0.15	53,86,141,153	0
14	CLA	B	3017	55/65	0.91	0.14	71,107,143,176	0
14	CLA	X	1701	45/65	0.91	0.14	85,114,144,150	0
14	CLA	B	3038	60/65	0.91	0.17	51,91,123,132	0
14	CLA	A	838	51/65	0.91	0.14	46,69,90,112	0
16	BCR	J	103	40/40	0.91	0.21	71,112,135,139	0
20	CA	B	3002	1/1	0.91	0.12	80,80,80,80	0
14	CLA	B	3013	45/65	0.91	0.11	67,99,126,129	0
14	CLA	B	3023	55/65	0.91	0.15	79,105,132,133	0
14	CLA	B	3022	45/65	0.92	0.11	77,103,130,130	0
14	CLA	B	3012	45/65	0.92	0.10	55,77,98,121	0
16	BCR	A	851	40/40	0.92	0.19	30,73,100,103	0
14	CLA	B	3025	54/65	0.92	0.15	58,75,97,98	0
14	CLA	A	822	65/65	0.92	0.18	61,97,131,137	0
14	CLA	B	3031	45/65	0.92	0.13	56,83,106,123	0
14	CLA	L	205	65/65	0.92	0.15	31,56,85,95	0
14	CLA	B	3019	60/65	0.92	0.16	60,81,110,117	0
14	CLA	B	3020	65/65	0.92	0.20	58,101,131,143	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CLA	A	812	65/65	0.92	0.17	91,124,154,157	0
16	BCR	I	103	40/40	0.92	0.13	12,44,69,71	0
16	BCR	I	105	40/40	0.92	0.13	13,38,58,75	0
14	CLA	B	3039	65/65	0.92	0.17	52,98,138,154	0
14	CLA	I	101	65/65	0.93	0.12	2,28,62,68	0
14	CLA	A	839	65/65	0.93	0.12	31,69,107,130	0
14	CLA	A	842	51/65	0.93	0.15	46,85,134,153	0
14	CLA	A	803	65/65	0.93	0.17	52,77,98,118	0
14	CLA	B	3003	65/65	0.93	0.15	26,59,80,87	0
14	CLA	B	3026	46/65	0.93	0.15	46,74,99,100	0
14	CLA	A	826	65/65	0.93	0.17	81,111,141,144	0
14	CLA	B	3029	65/65	0.93	0.15	37,71,89,107	0
15	PQN	A	846	33/33	0.93	0.19	61,89,118,121	0
14	CLA	A	810	65/65	0.93	0.15	54,109,158,171	0
14	CLA	A	833	65/65	0.93	0.15	34,73,145,150	0
14	CLA	B	3033	65/65	0.93	0.15	66,96,122,131	0
14	CLA	A	834	65/65	0.93	0.12	20,47,75,81	0
14	CLA	B	3036	45/65	0.93	0.14	54,90,117,121	0
18	LHG	A	853	49/49	0.93	0.20	48,94,118,128	0
14	CLA	A	804	65/65	0.93	0.17	69,108,135,142	0
14	CLA	A	805	59/65	0.93	0.16	85,108,135,151	0
14	CLA	B	3040	47/65	0.93	0.14	59,84,103,115	0
14	CLA	A	807	65/65	0.93	0.17	66,94,120,127	0
16	BCR	B	3047	40/40	0.93	0.13	25,44,71,71	0
14	CLA	A	829	65/65	0.94	0.17	69,96,120,127	0
14	CLA	A	843	65/65	0.94	0.15	47,83,127,146	0
14	CLA	A	830	65/65	0.94	0.14	65,98,128,131	0
14	CLA	A	856	65/65	0.94	0.17	48,75,101,112	0
16	BCR	I	102	40/40	0.94	0.11	8,39,60,78	0
14	CLA	A	832	50/65	0.94	0.12	43,71,101,127	0
14	CLA	L	203	65/65	0.94	0.12	21,51,82,104	0
14	CLA	L	204	65/65	0.94	0.12	18,55,127,140	0
14	CLA	B	3004	65/65	0.94	0.12	20,43,63,75	0
14	CLA	B	3008	65/65	0.94	0.12	20,45,77,99	0
14	CLA	B	3030	65/65	0.94	0.14	30,57,90,108	0
14	CLA	A	802	65/65	0.94	0.12	30,49,65,85	0
15	PQN	B	3042	33/33	0.94	0.13	27,47,66,70	0
13	CL0	A	801	65/65	0.94	0.14	11,56,81,84	0
14	CLA	B	3014	65/65	0.94	0.13	52,82,109,112	0
17	LMG	B	3048	55/55	0.94	0.14	30,68,94,97	0
14	CLA	A	825	59/65	0.94	0.18	60,93,133,145	0
14	CLA	B	3035	45/65	0.94	0.11	65,83,105,108	0

Continued on next page...

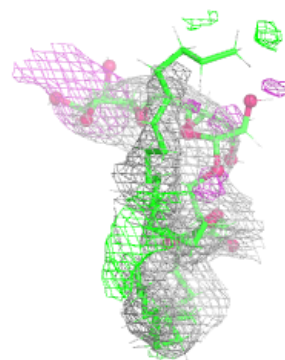
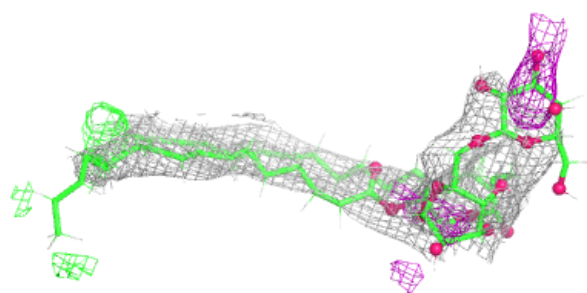
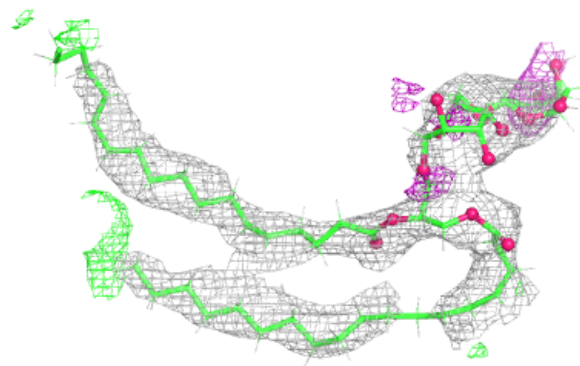
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	LHG	A	854	27/49	0.94	0.13	56,89,126,128	0
14	CLA	B	3016	45/65	0.94	0.10	71,92,125,128	0
14	CLA	A	809	65/65	0.94	0.16	48,94,134,139	0
14	CLA	A	827	65/65	0.94	0.17	40,78,156,177	0
14	CLA	A	806	65/65	0.94	0.18	77,111,146,152	0
14	CLA	A	840	47/65	0.94	0.12	32,65,86,103	0
14	CLA	B	3010	65/65	0.95	0.10	16,48,76,100	0
14	CLA	A	844	65/65	0.95	0.10	2,28,60,69	0
14	CLA	A	831	65/65	0.95	0.18	66,97,120,129	0
14	CLA	B	3041	65/65	0.95	0.12	14,39,62,65	0
14	CLA	B	3005	54/65	0.95	0.12	33,58,77,85	0
14	CLA	B	3006	65/65	0.95	0.12	37,66,100,111	0
14	CLA	B	3007	65/65	0.95	0.12	32,61,87,100	0
14	CLA	A	841	65/65	0.95	0.13	42,79,133,142	0
20	CA	L	202	1/1	0.95	0.06	37,37,37,37	0
14	CLA	B	3009	65/65	0.95	0.10	20,49,82,86	0
14	CLA	B	3037	45/65	0.95	0.10	74,99,130,131	0
19	SF4	B	3001	8/8	0.96	0.09	40,56,98,128	0
19	SF4	C	101	8/8	0.96	0.08	33,61,68,81	0
14	CLA	A	835	65/65	0.96	0.10	11,42,72,100	0
14	CLA	B	3011	65/65	0.96	0.09	4,34,70,79	0
14	CLA	B	3024	45/65	0.96	0.09	40,71,104,116	0
14	CLA	B	3028	65/65	0.96	0.14	25,58,110,112	0
19	SF4	C	102	8/8	0.99	0.03	48,55,72,74	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.

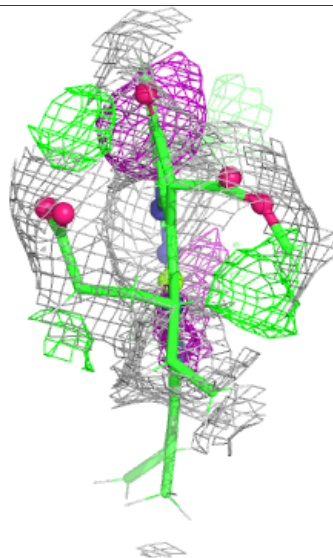
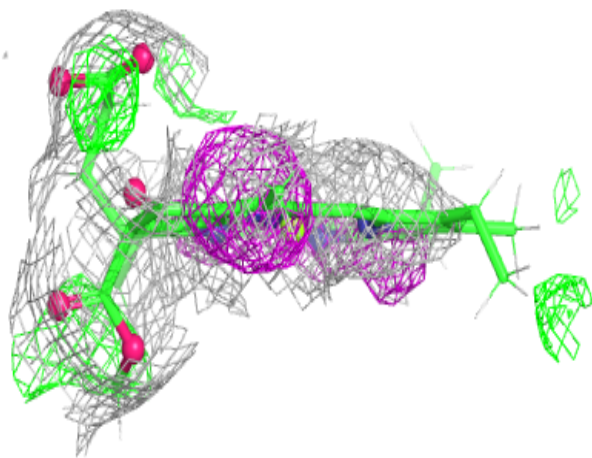
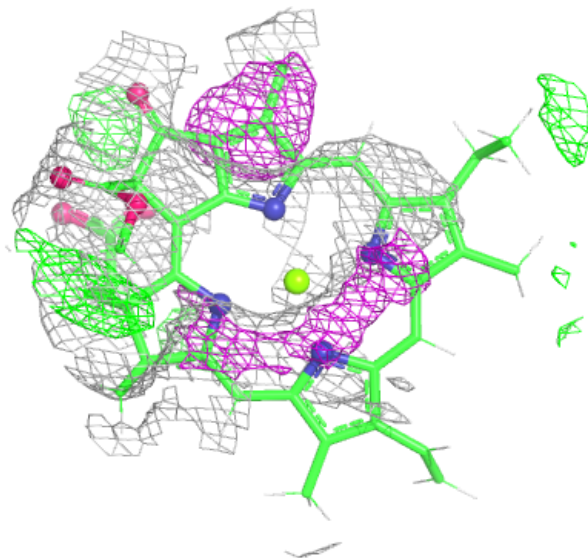
Electron density around DGD L 206:

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



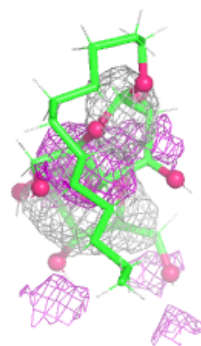
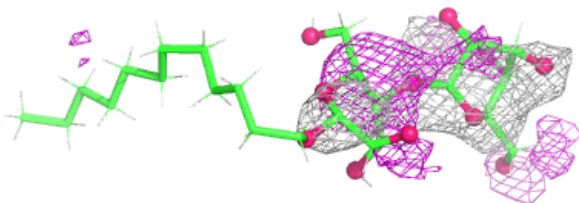
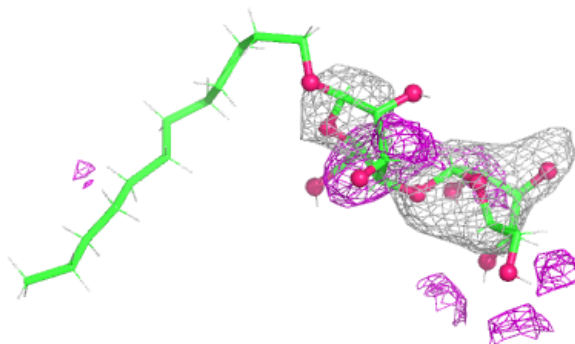
Electron density around CLA M 102:

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

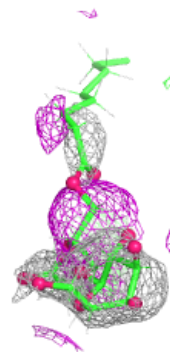
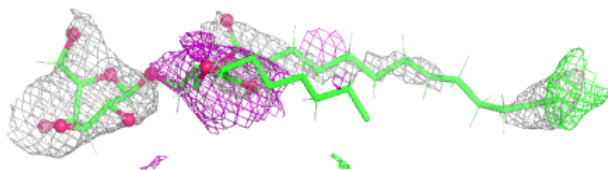
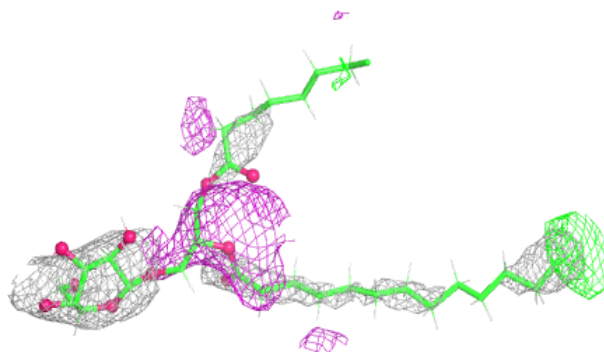


Electron density around LMT L 201:

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

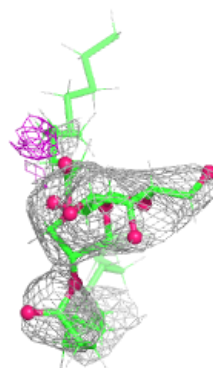
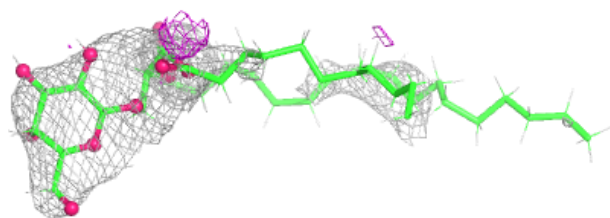
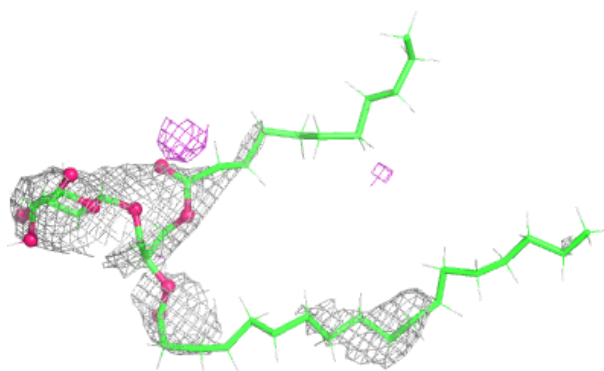
**Electron density around LMG I 104:**

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



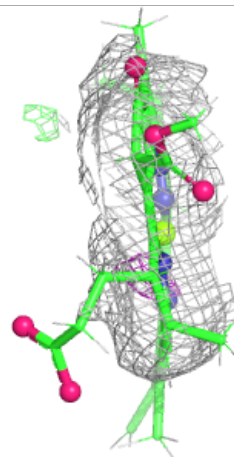
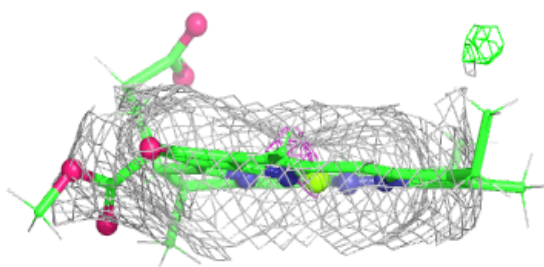
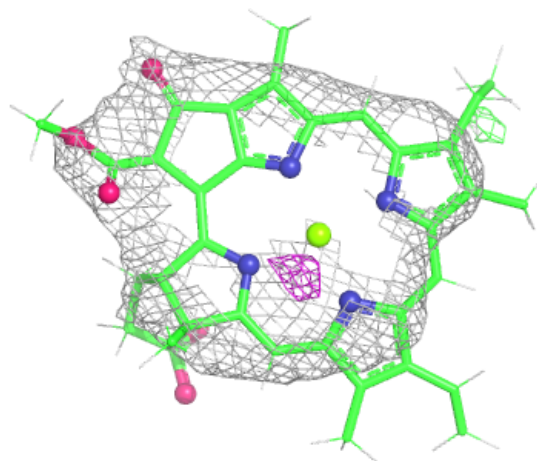
Electron density around LMG A 852:

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



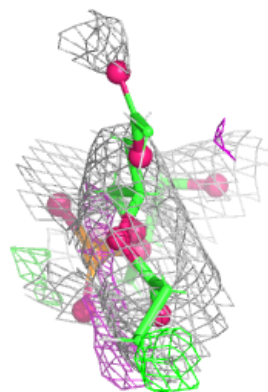
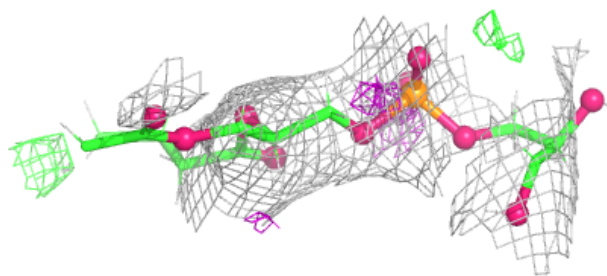
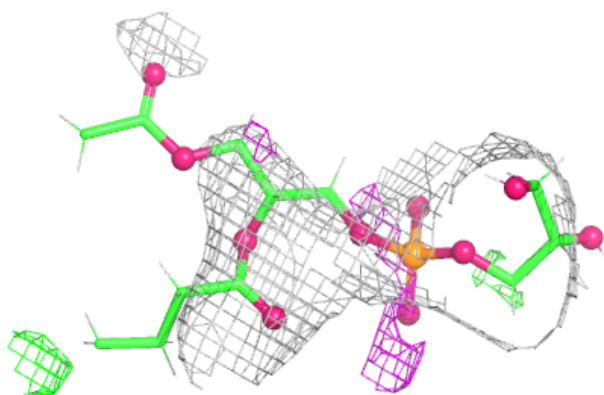
Electron density around CLA J 101:

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



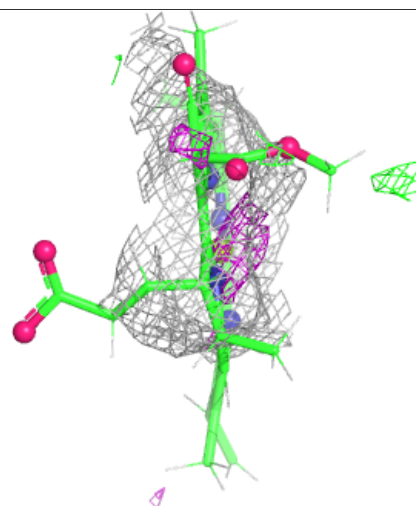
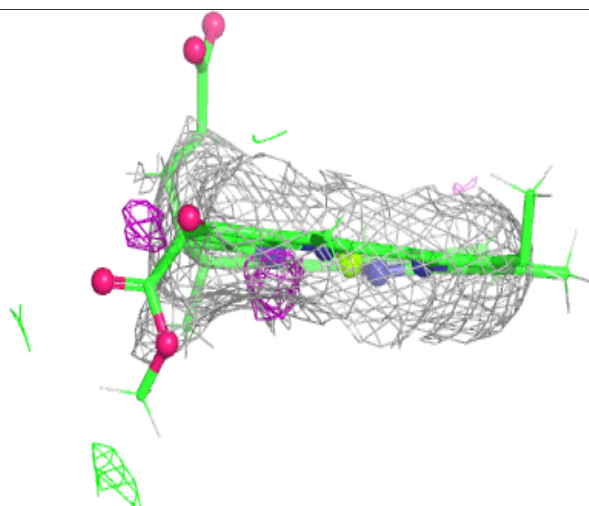
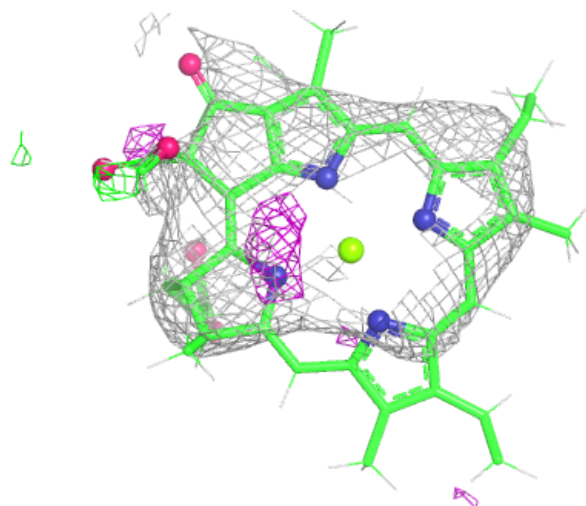
Electron density around LHG B 3049:

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



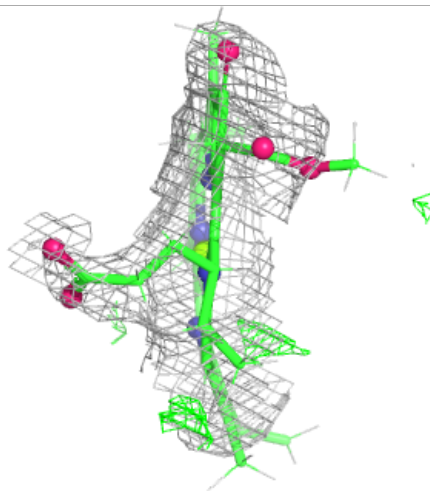
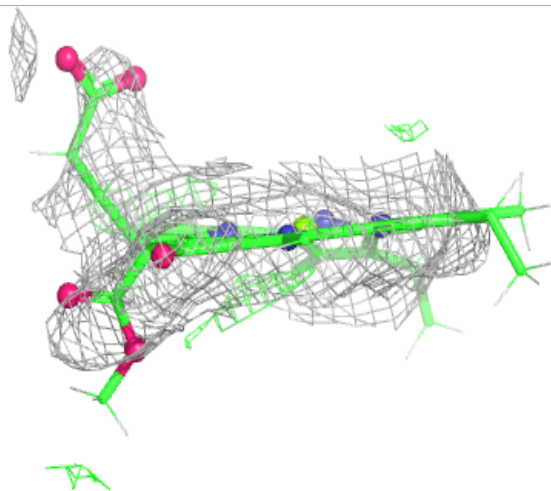
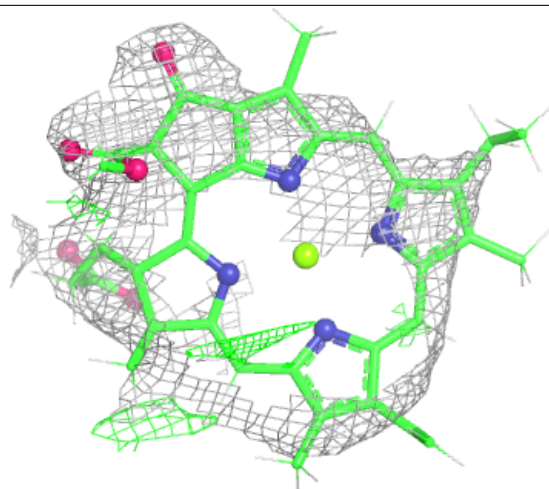
Electron density around CLA A 816:

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



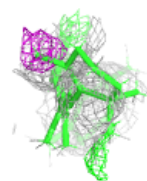
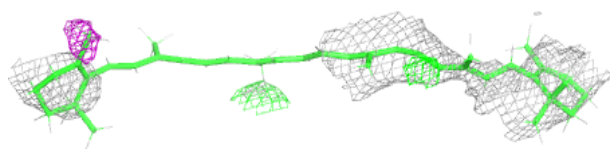
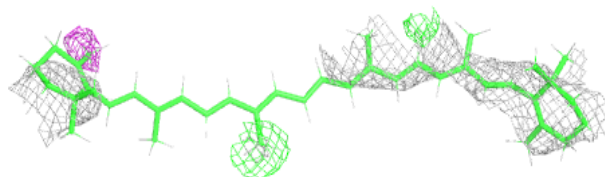
Electron density around CLA K 103:

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

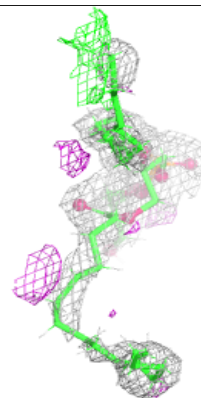
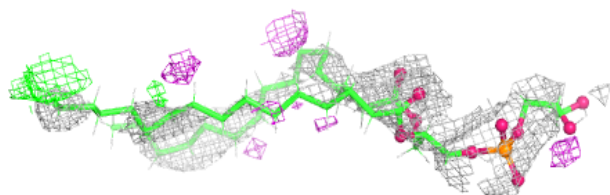
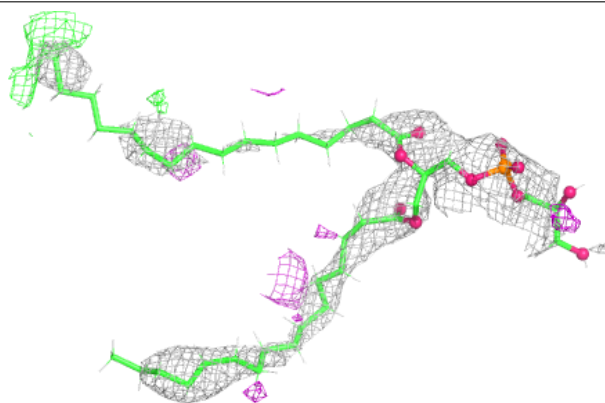


Electron density around BCR K 102:

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

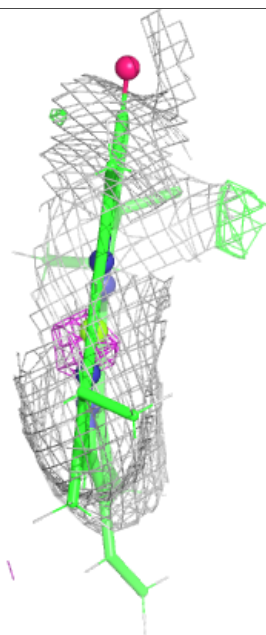
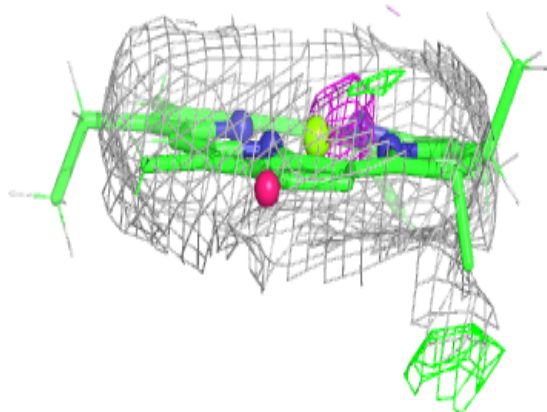
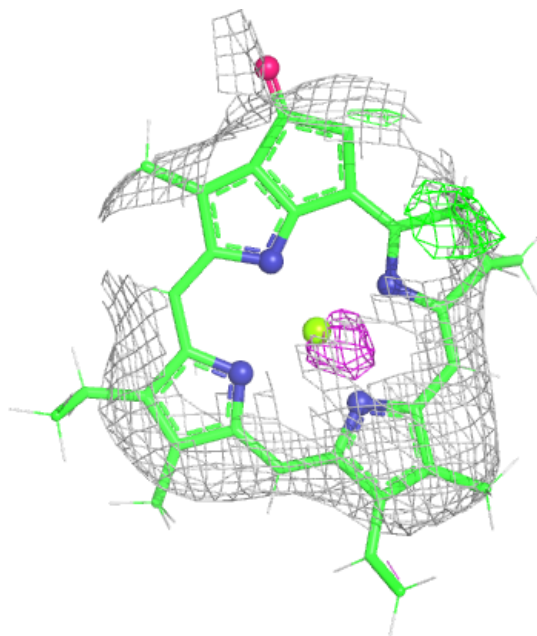
**Electron density around LHG M 101:**

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



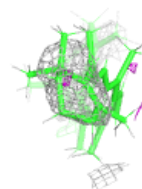
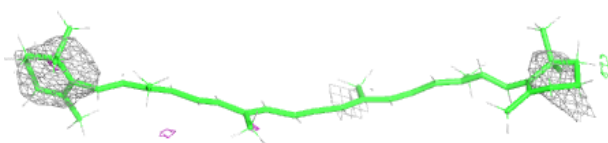
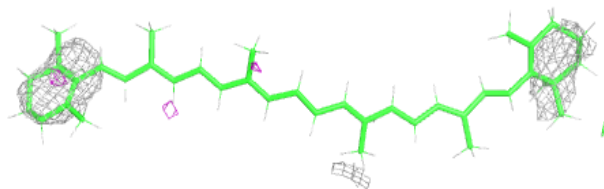
Electron density around CLA J 102:

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



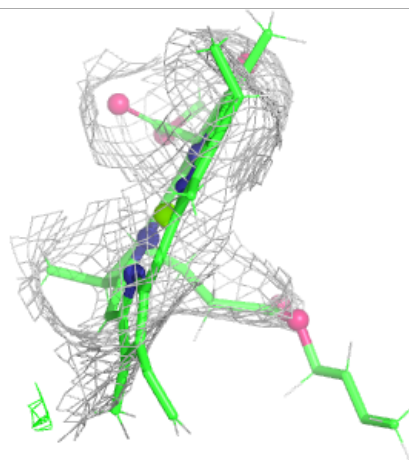
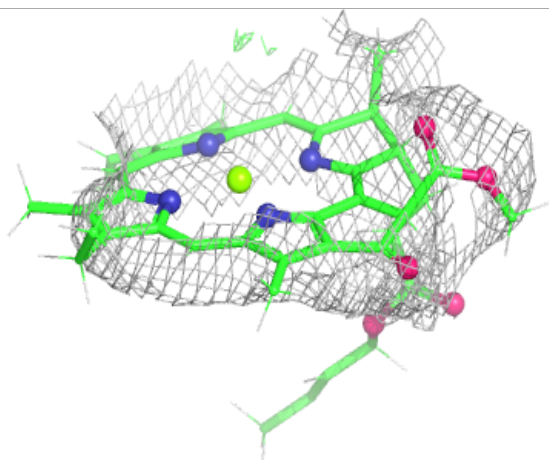
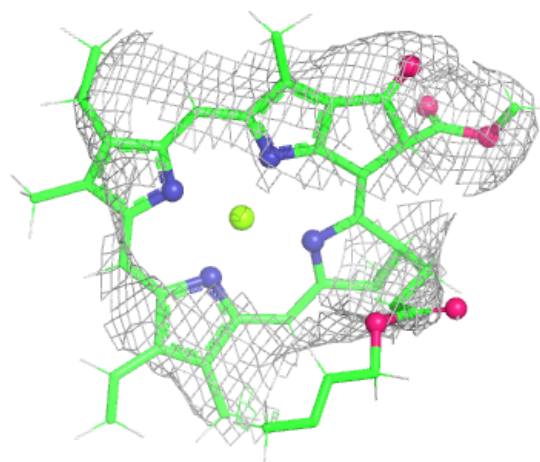
Electron density around BCR B 3043:

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



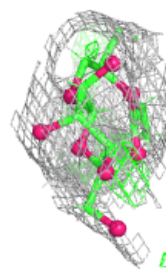
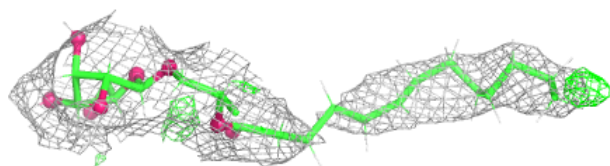
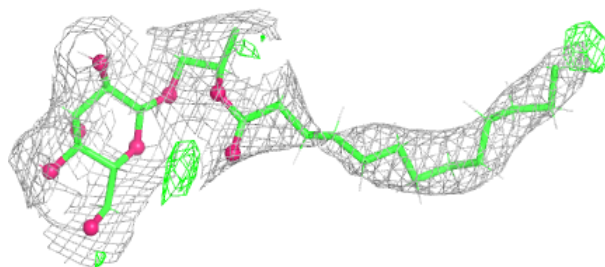
Electron density around CLA A 817:

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



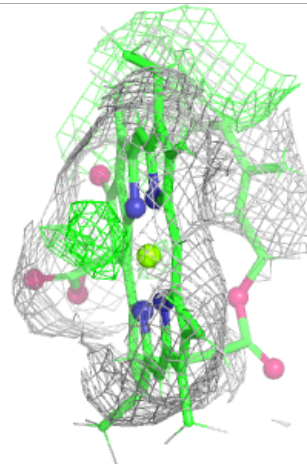
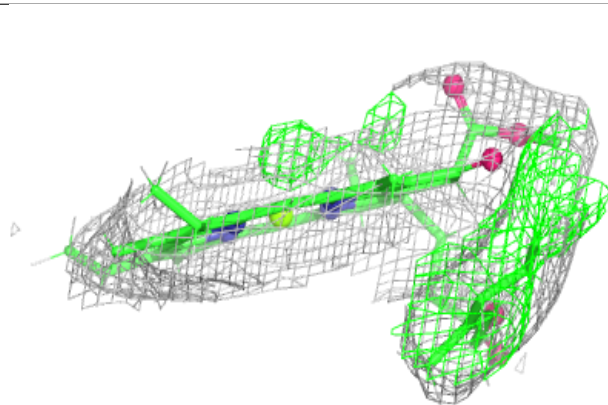
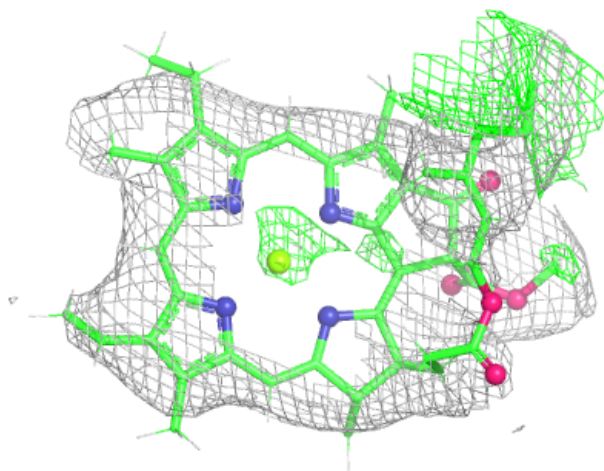
Electron density around LMG A 855:

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



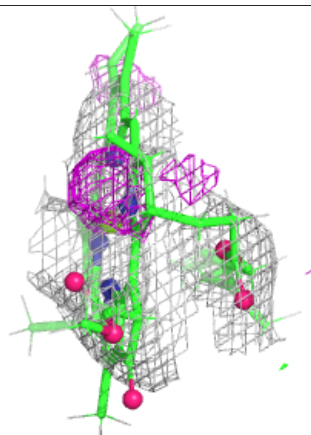
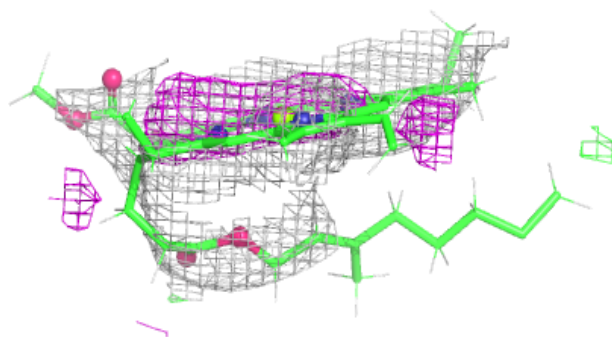
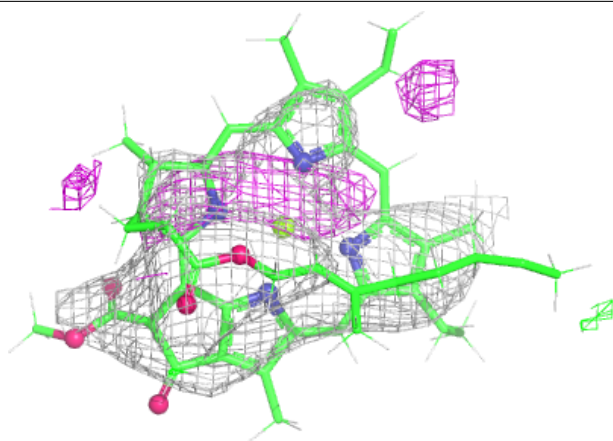
Electron density around CLA A 845:

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



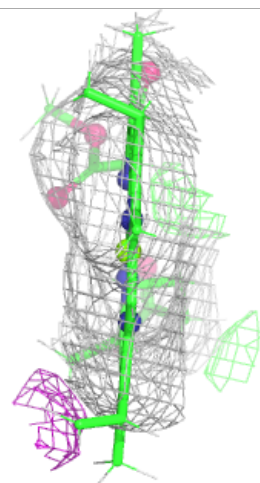
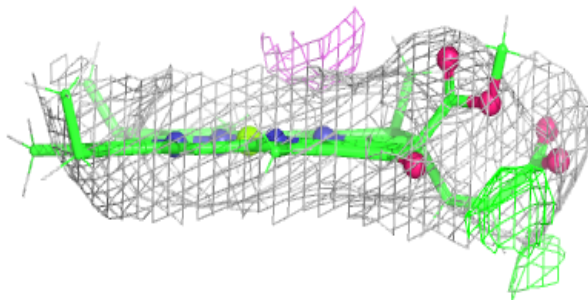
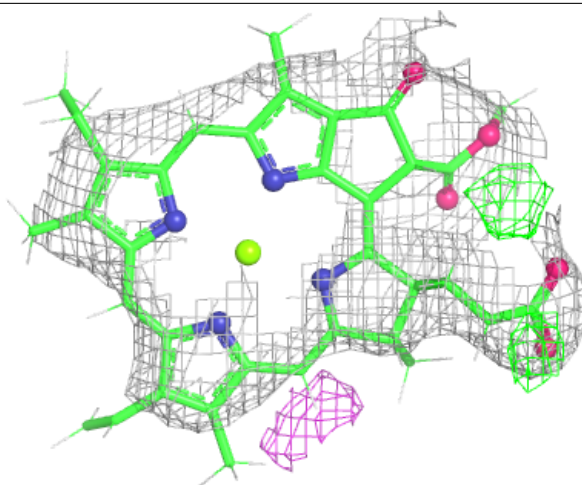
Electron density around CLA A 818:

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



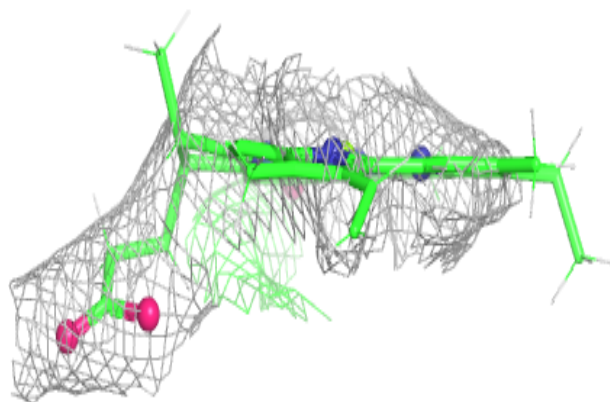
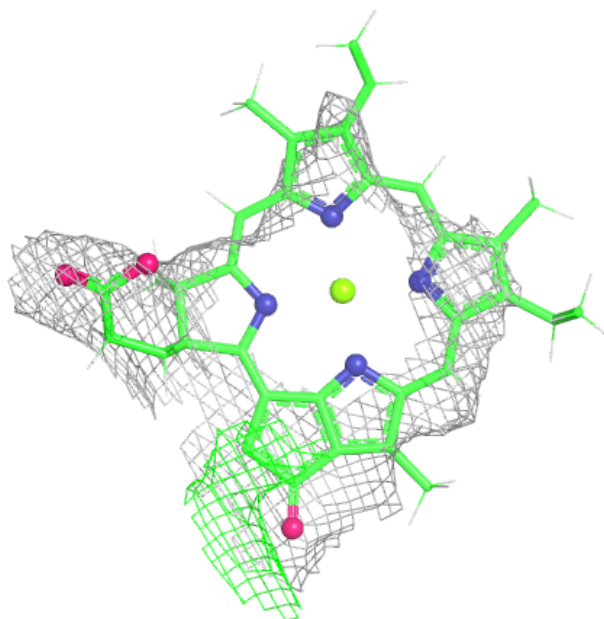
Electron density around CLA F 202:

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



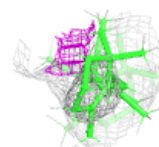
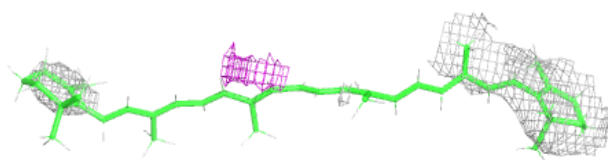
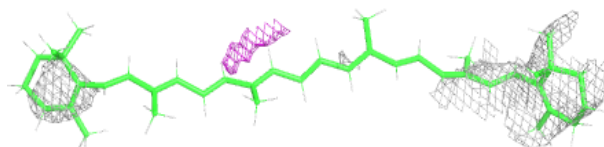
Electron density around CLA K 101:

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

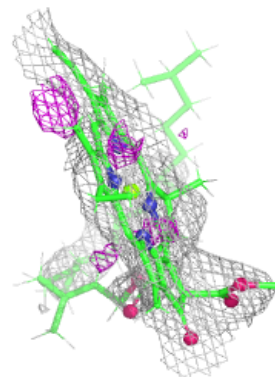
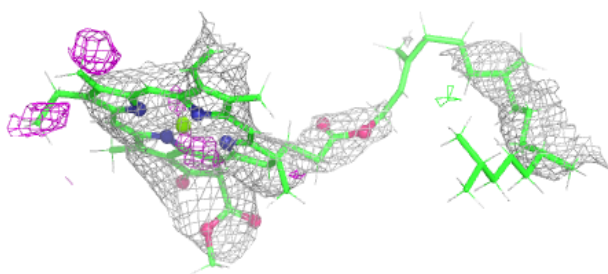
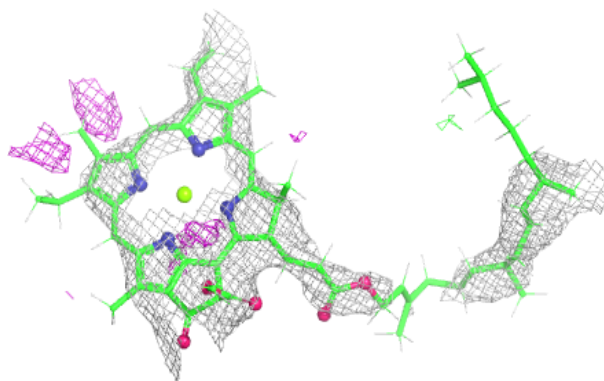


Electron density around BCR A 847:

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

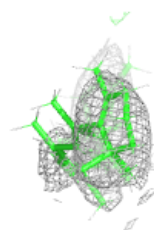
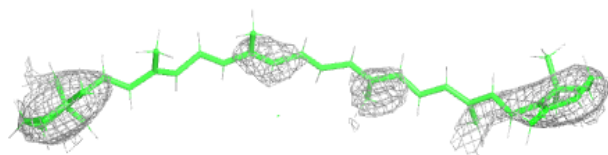
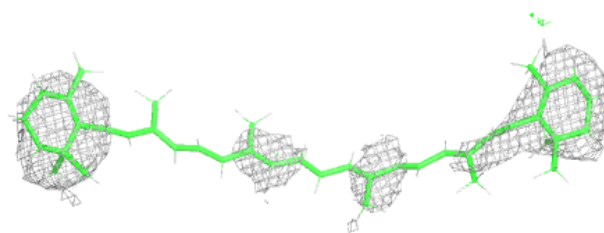
**Electron density around CLA A 828:**

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

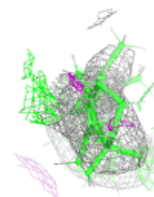
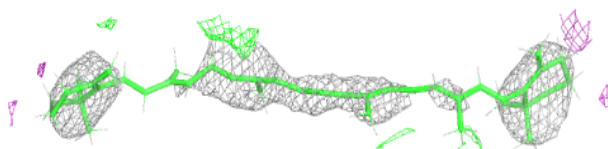
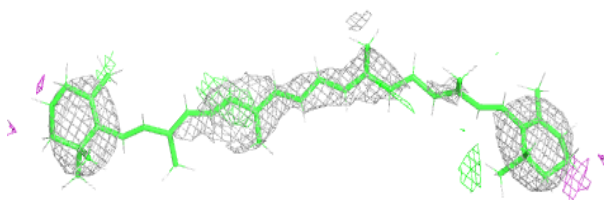


Electron density around BCR J 104:

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

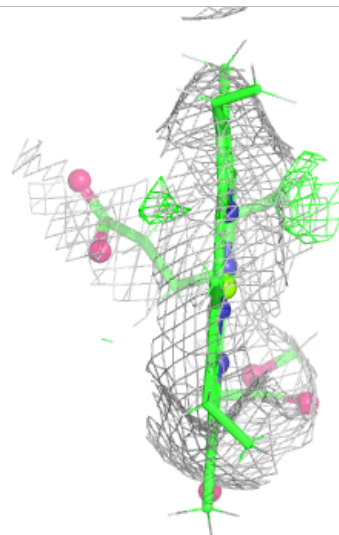
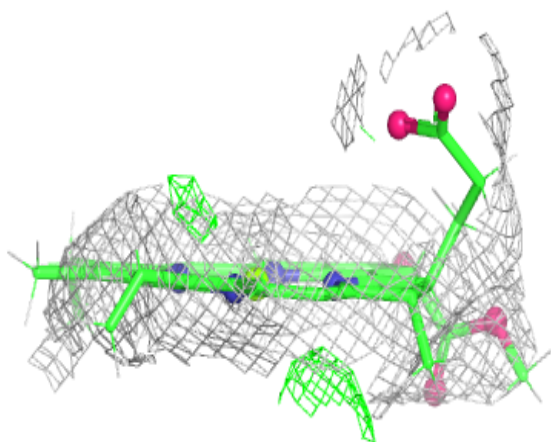
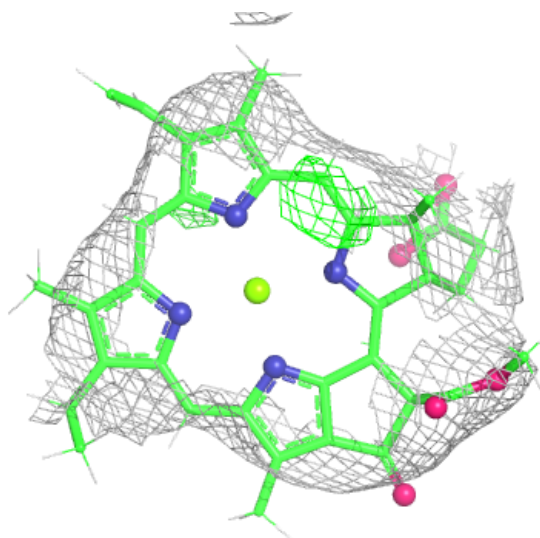
**Electron density around BCR B 3046:**

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



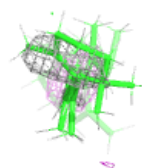
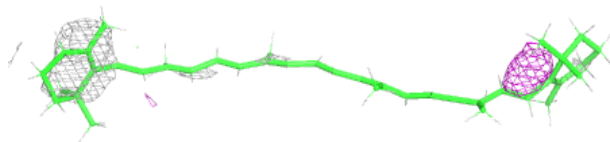
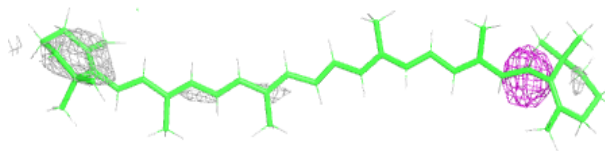
Electron density around CLA A 811:

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



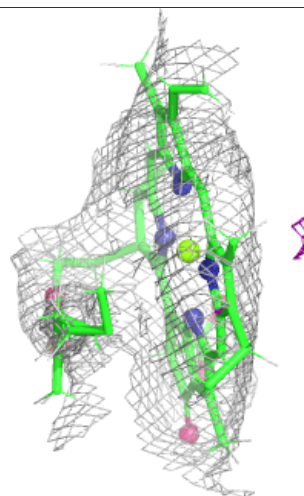
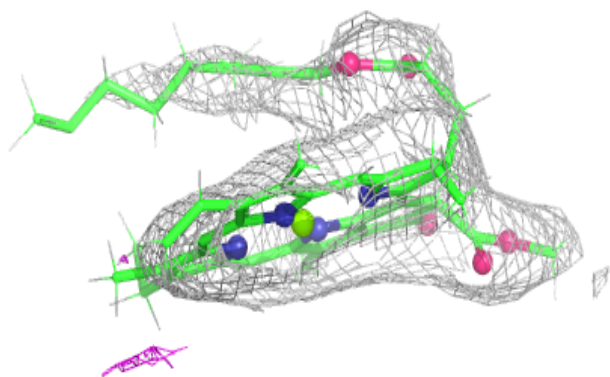
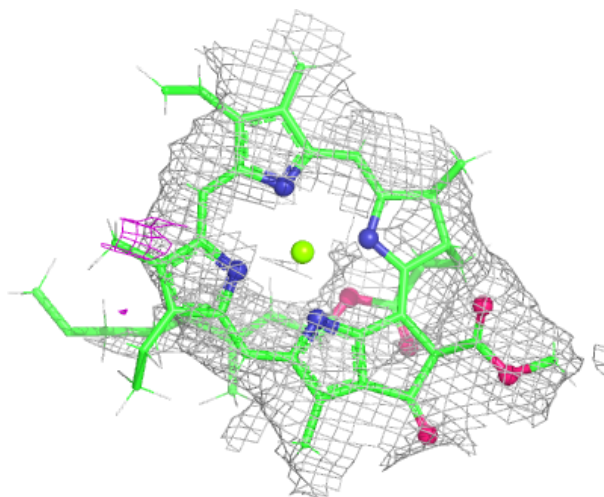
Electron density around BCR A 848:

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



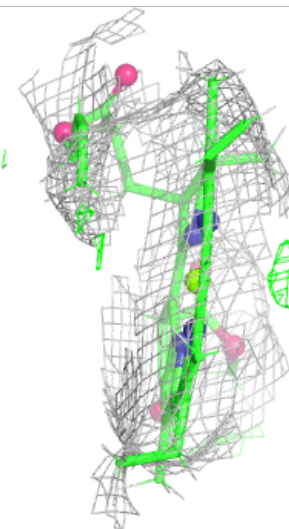
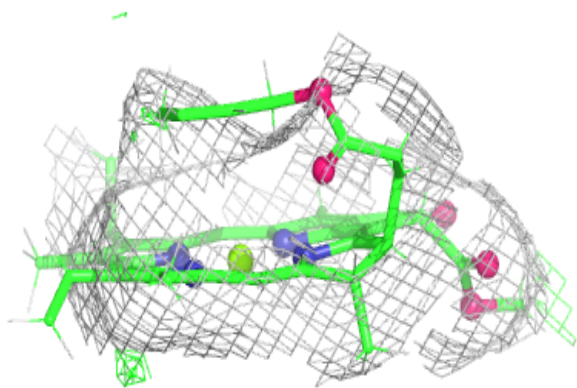
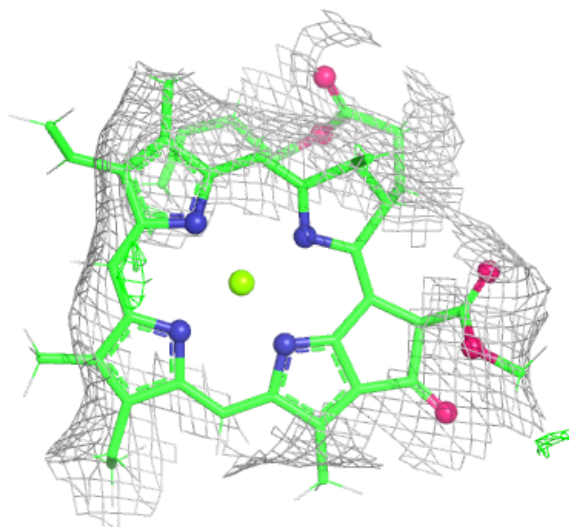
Electron density around CLA A 813:

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



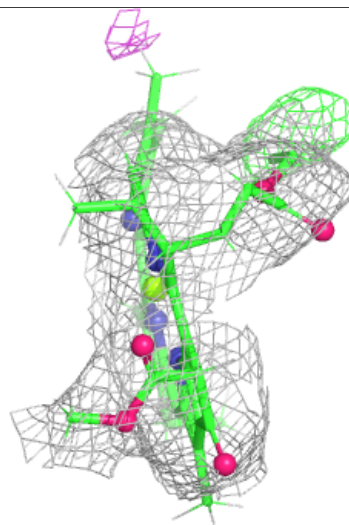
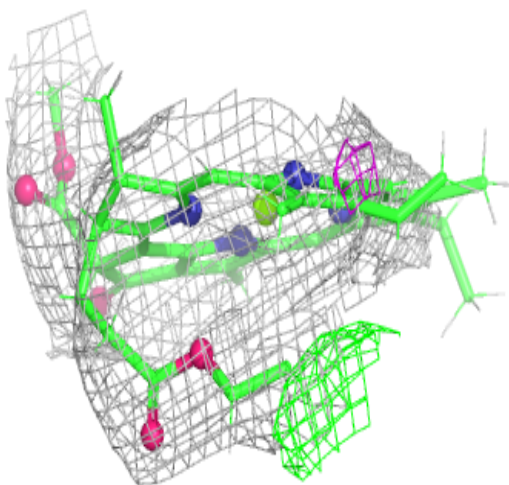
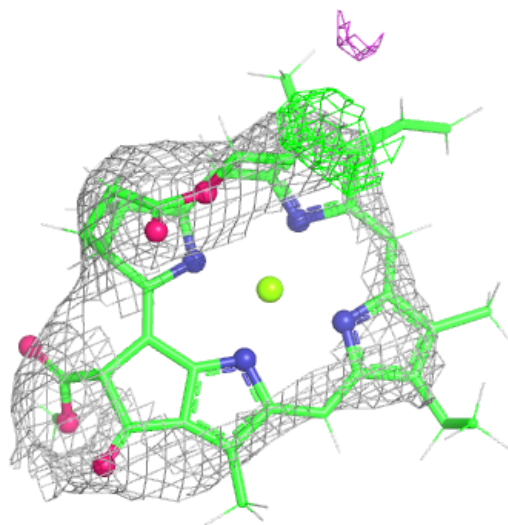
Electron density around CLA A 823:

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



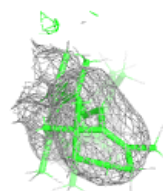
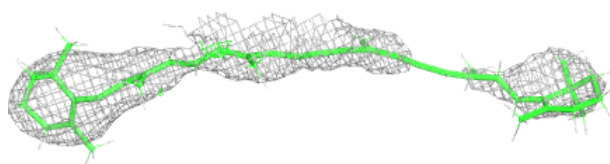
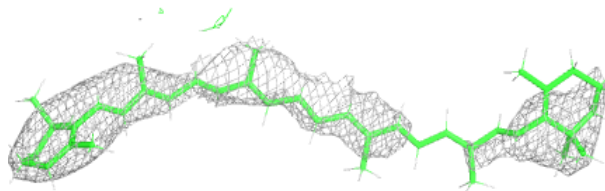
Electron density around CLA B 3021:

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

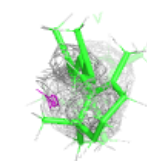
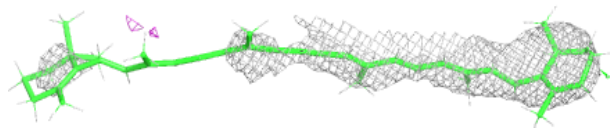
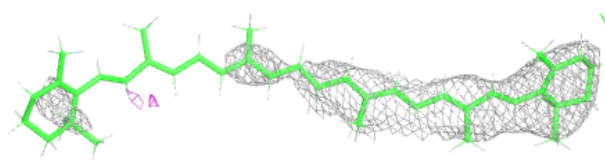


Electron density around BCR B 3050:

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

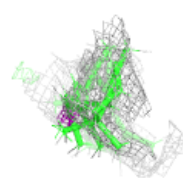
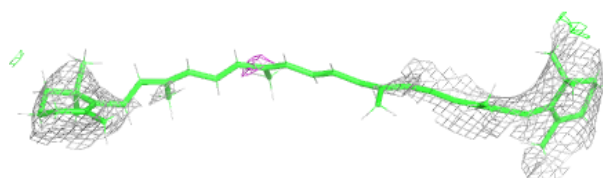
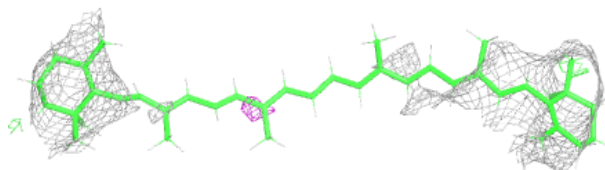
**Electron density around BCR A 849:**

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

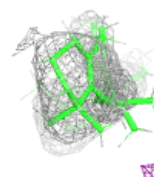
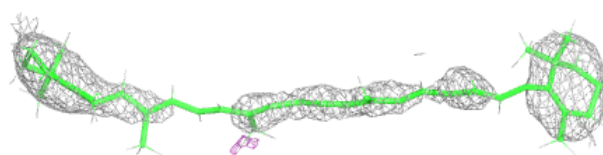
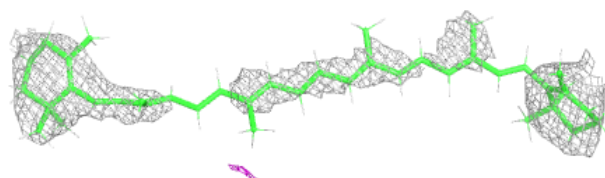


Electron density around BCR J 105:

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

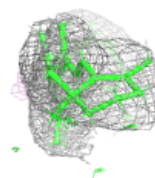
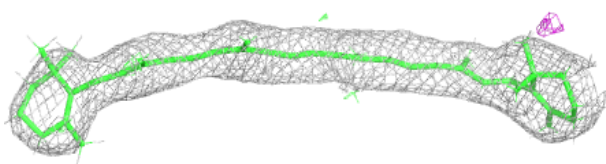
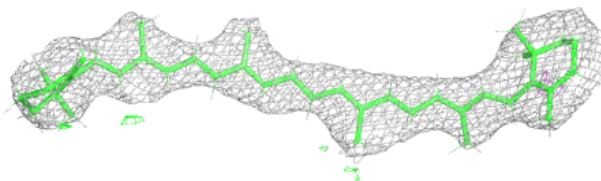
**Electron density around BCR A 850:**

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



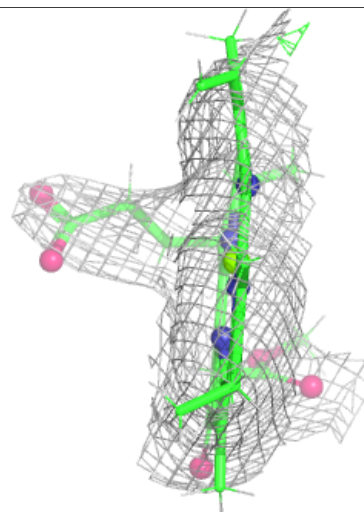
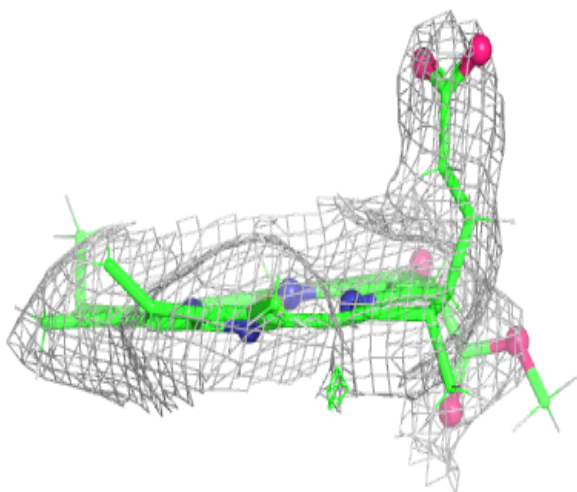
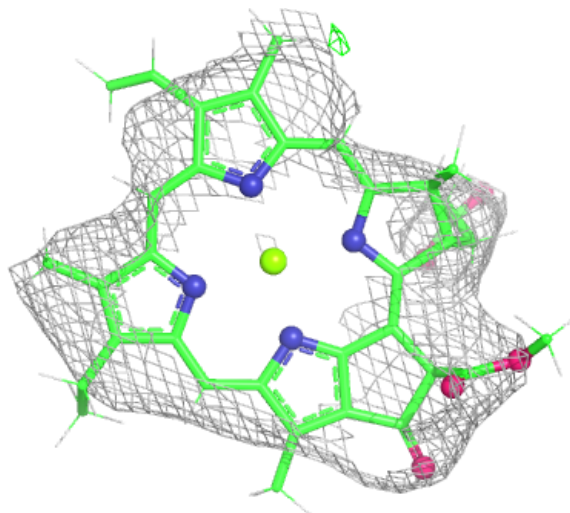
Electron density around BCR M 103:

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



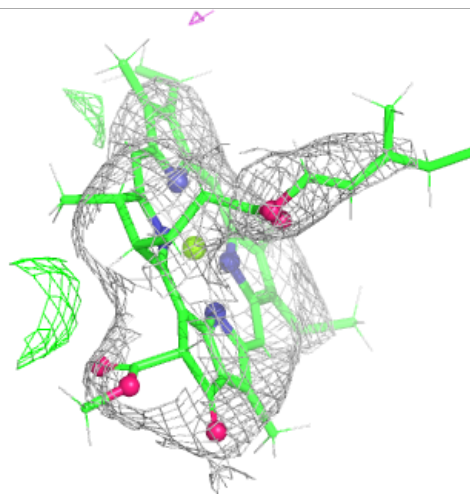
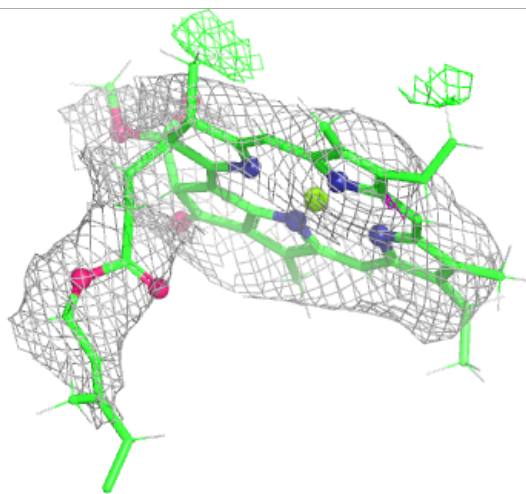
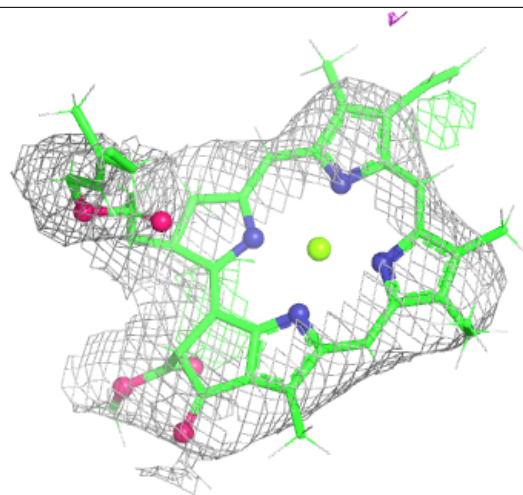
Electron density around CLA A 837:

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



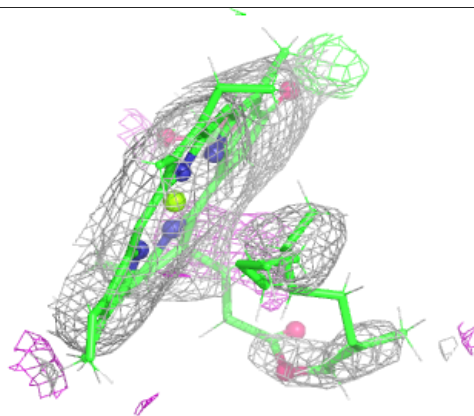
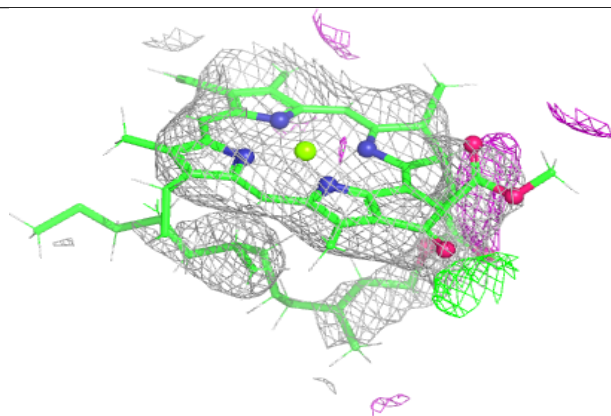
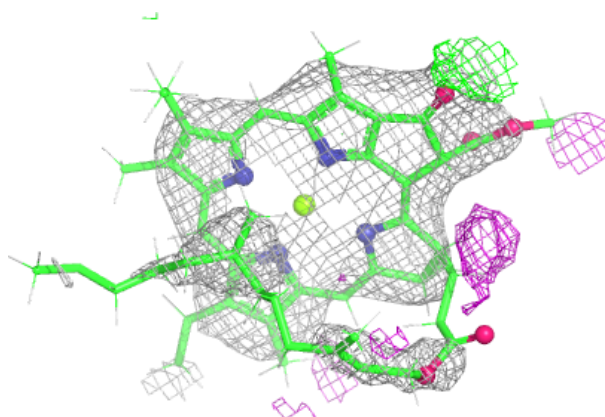
Electron density around CLA A 808:

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



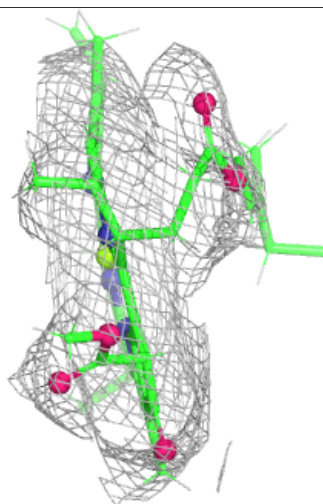
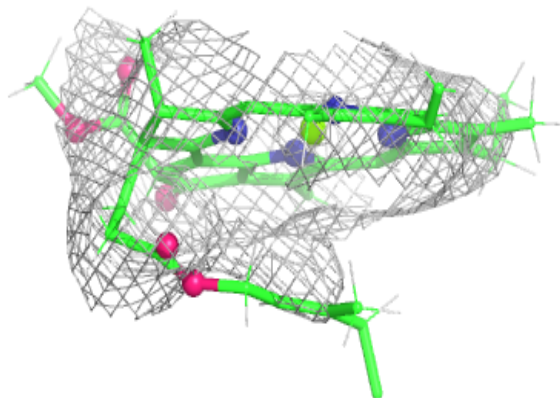
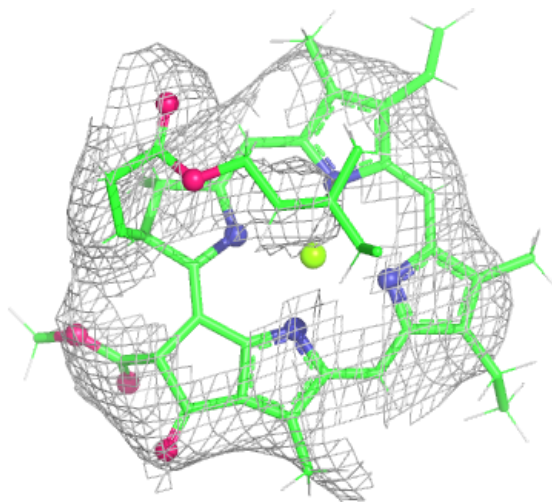
Electron density around CLA B 3018:

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



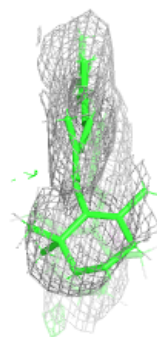
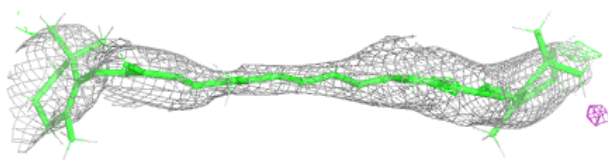
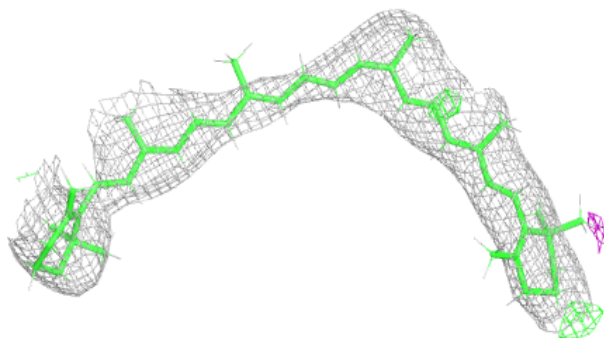
Electron density around CLA A 824:

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



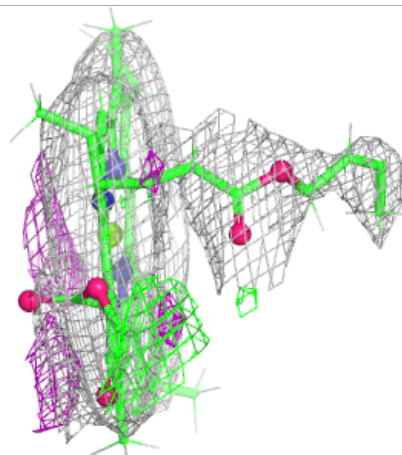
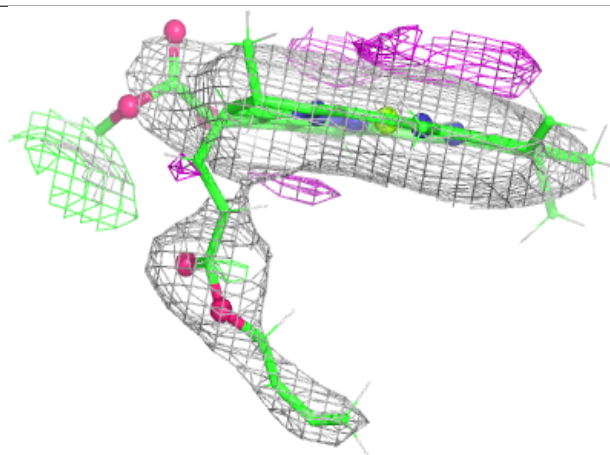
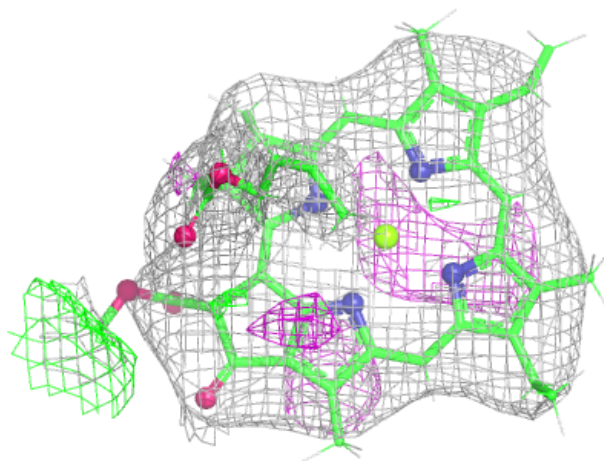
Electron density around BCR F 203:

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



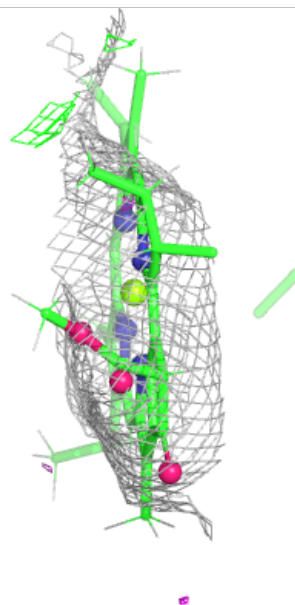
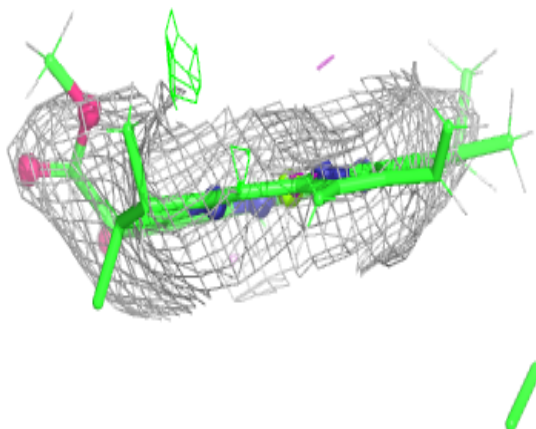
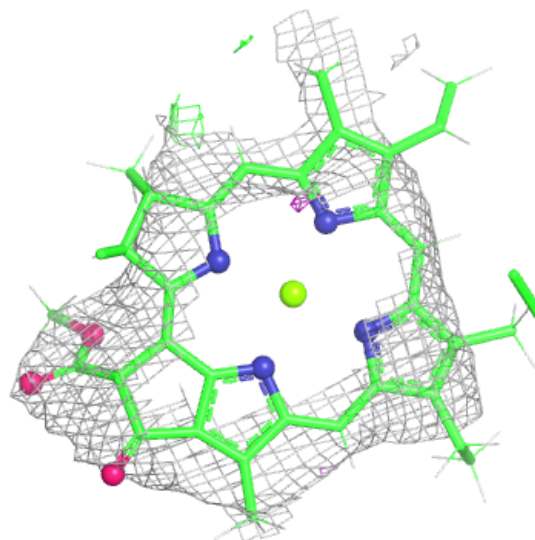
Electron density around CLA B 3032:

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



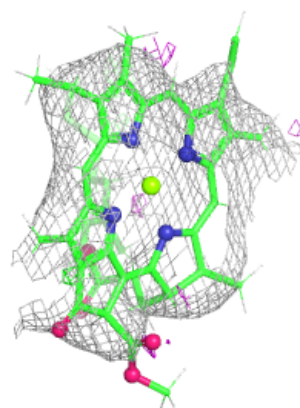
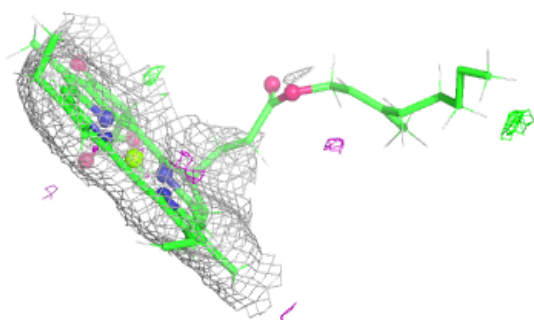
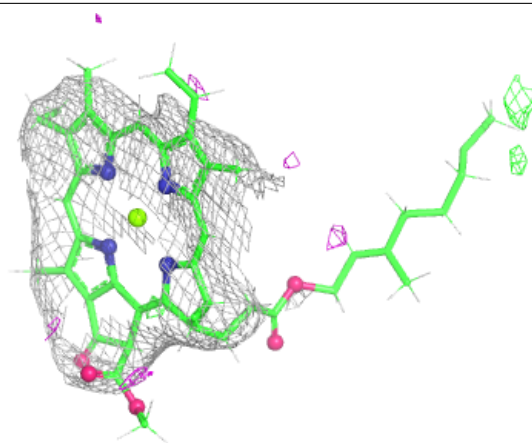
Electron density around CLA A 821:

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

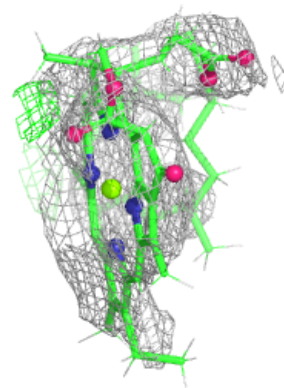
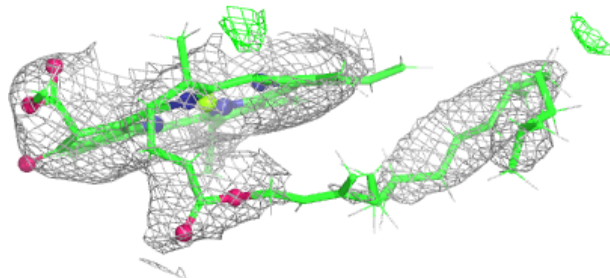
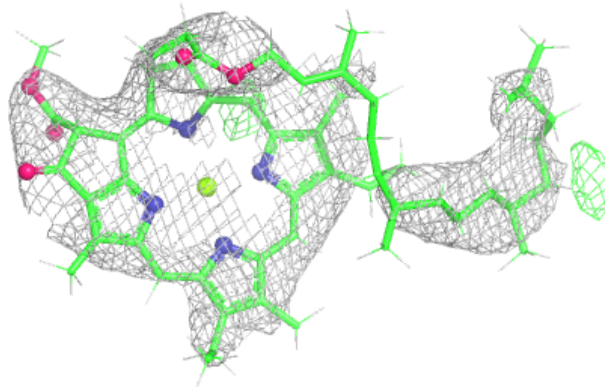


Electron density around CLA A 836:

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

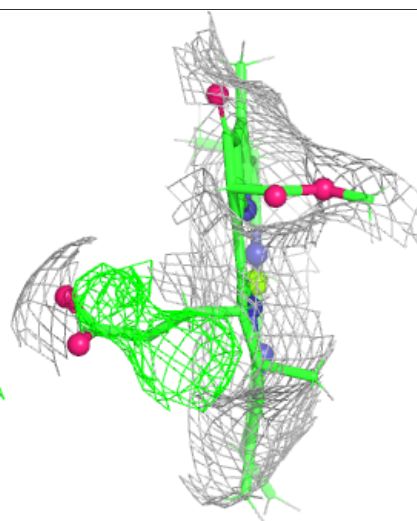
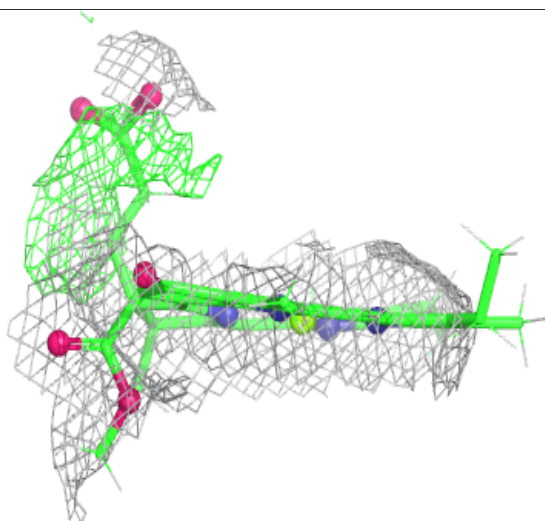
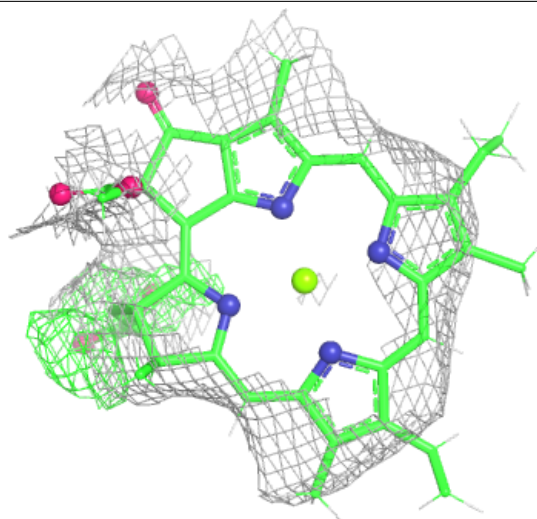
**Electron density around CLA A 820:**

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



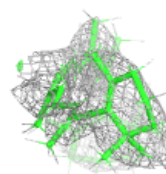
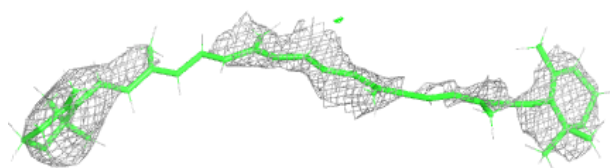
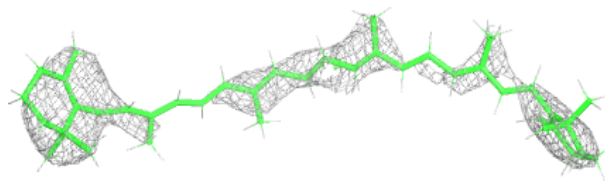
Electron density around CLA A 815:

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



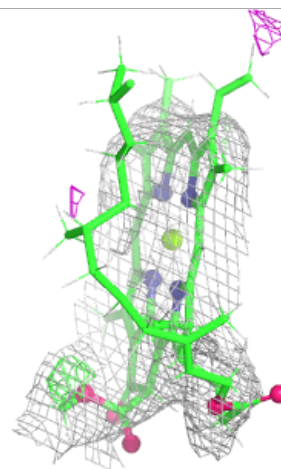
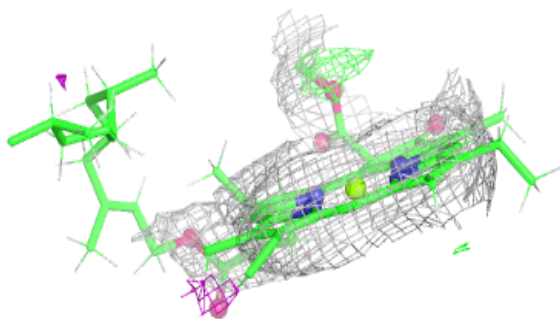
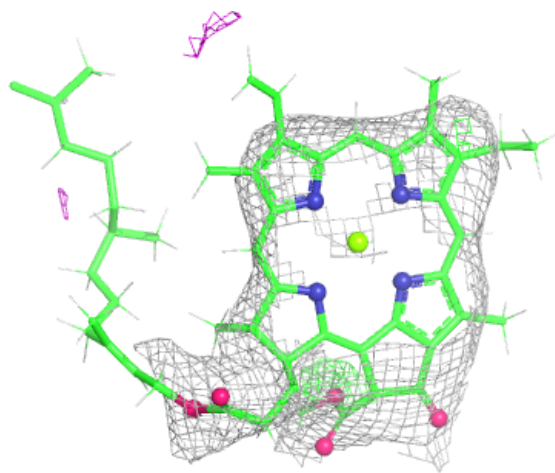
Electron density around BCR F 201:

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



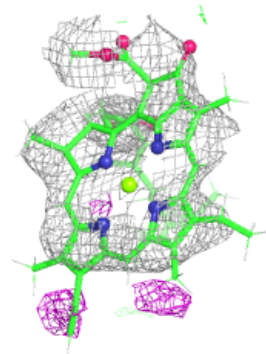
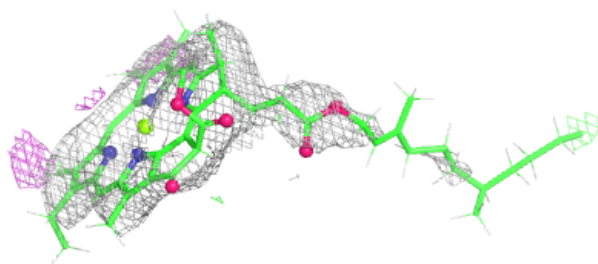
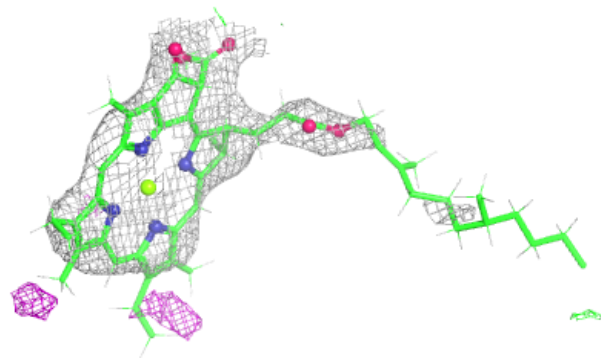
Electron density around CLA A 814:

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



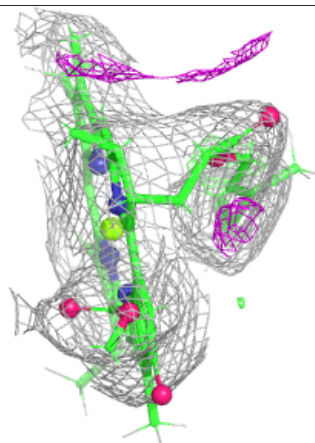
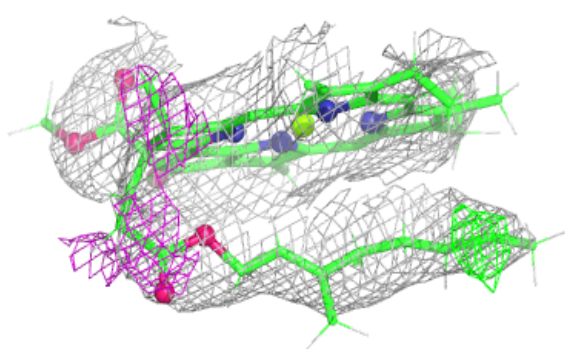
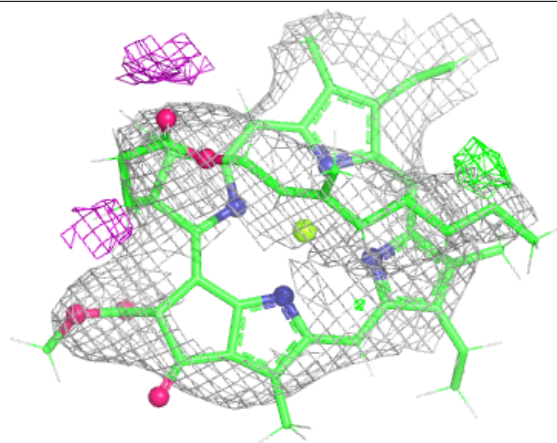
Electron density around CLA B 3034:

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

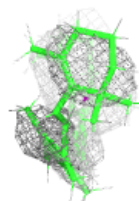
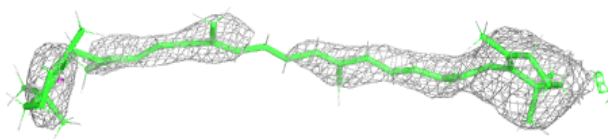
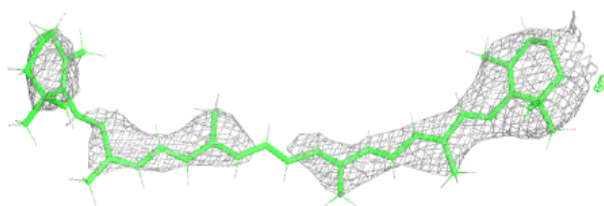


Electron density around CLA A 819:

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

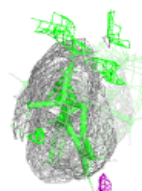
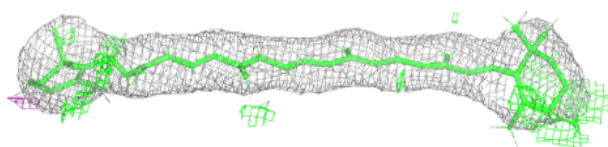
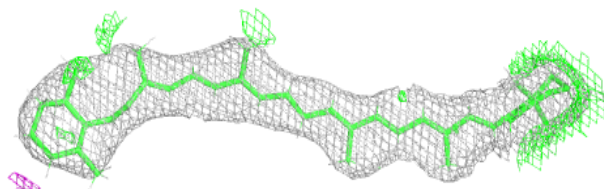
**Electron density around BCR B 3044:**

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

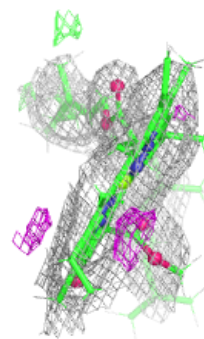
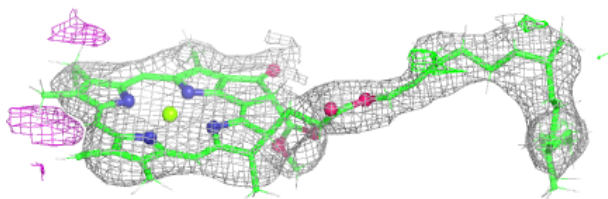
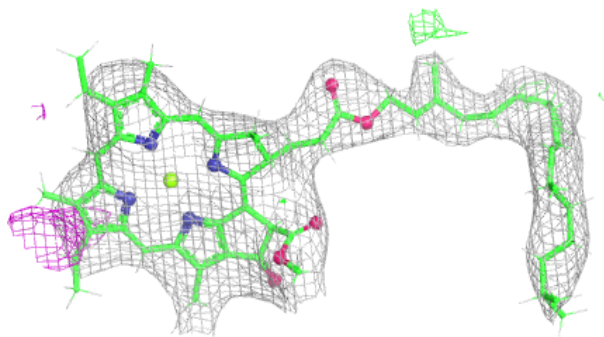


Electron density around BCR L 207:

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

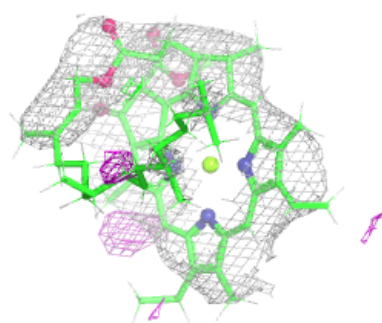
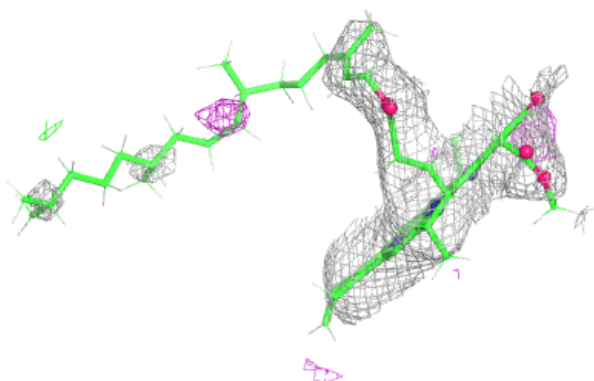
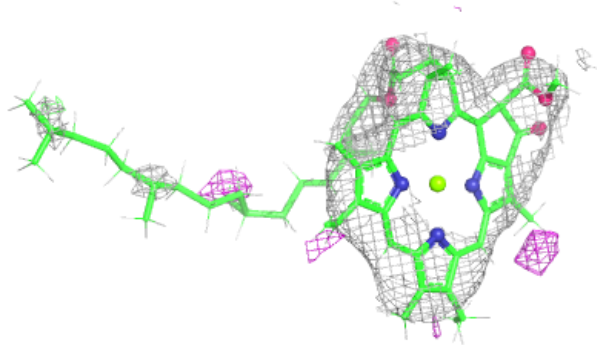
**Electron density around CLA B 3027:**

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

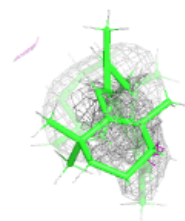
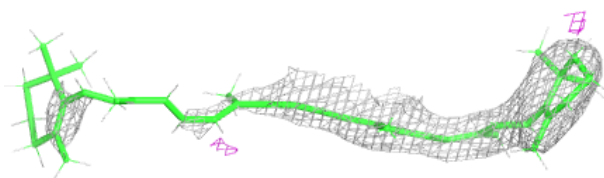
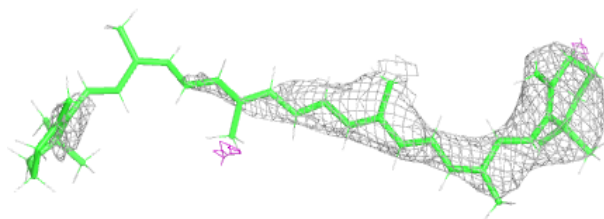


Electron density around CLA B 3015:

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

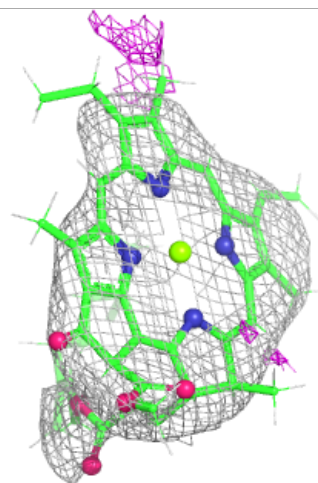
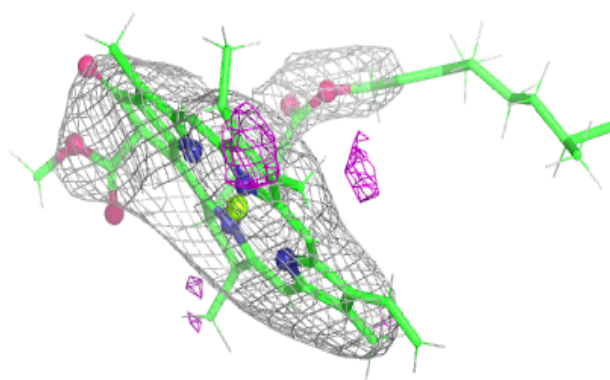
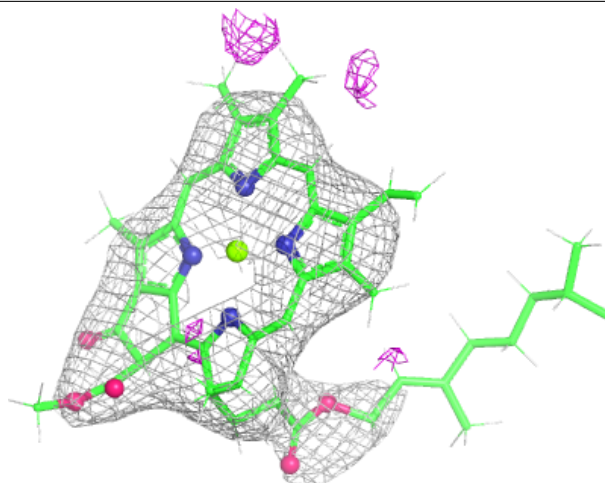
**Electron density around BCR B 3045:**

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



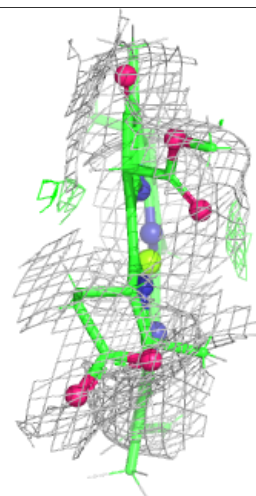
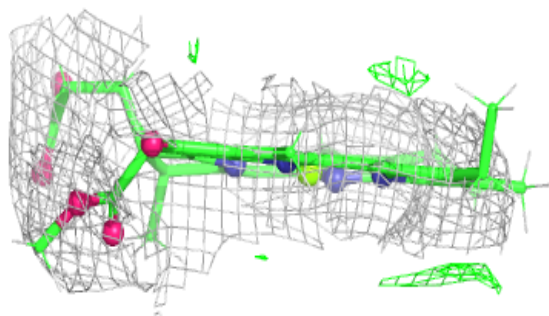
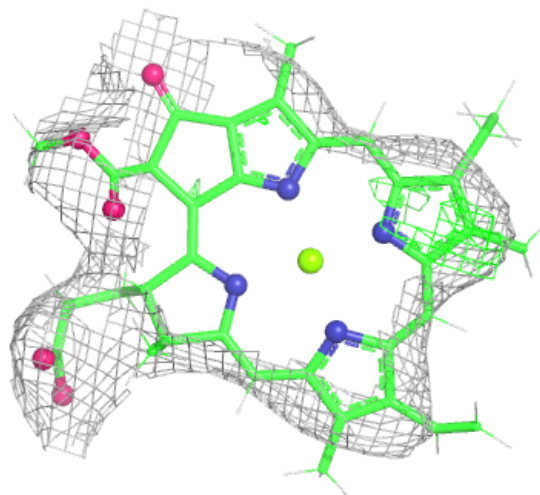
Electron density around CLA B 3017:

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



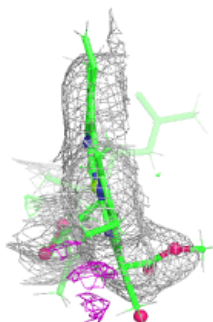
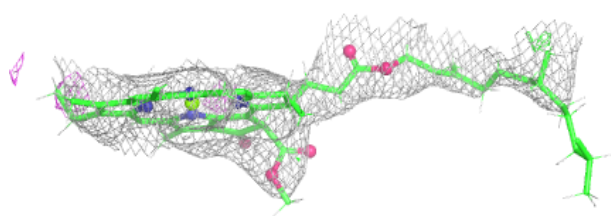
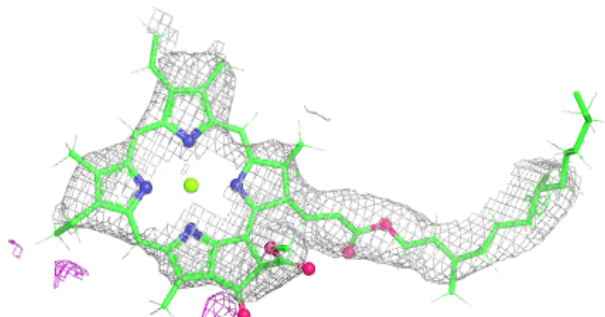
Electron density around CLA X 1701:

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

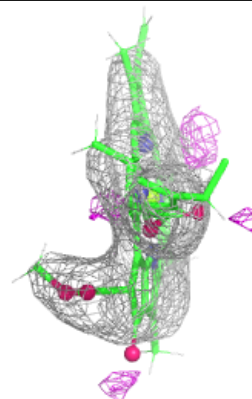
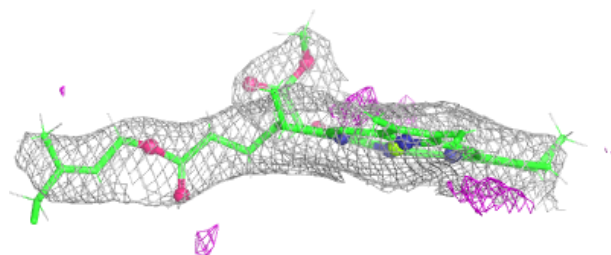
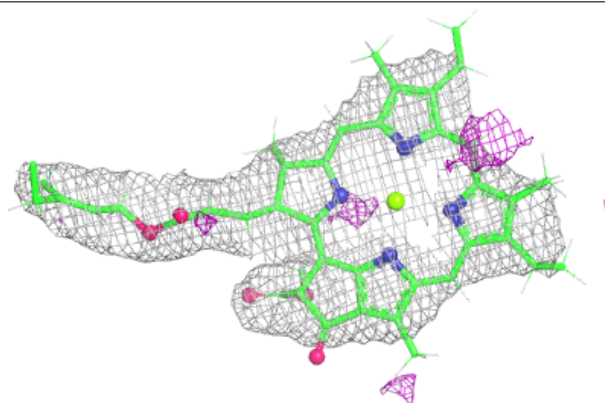


Electron density around CLA B 3038:

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

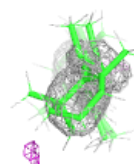
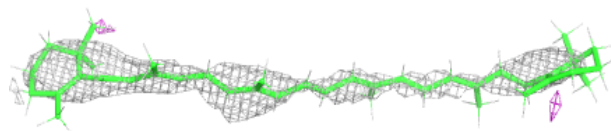
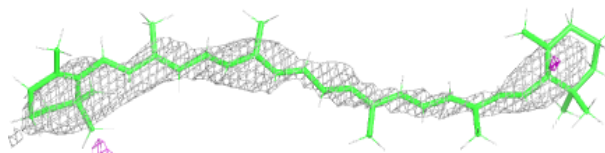
**Electron density around CLA A 838:**

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



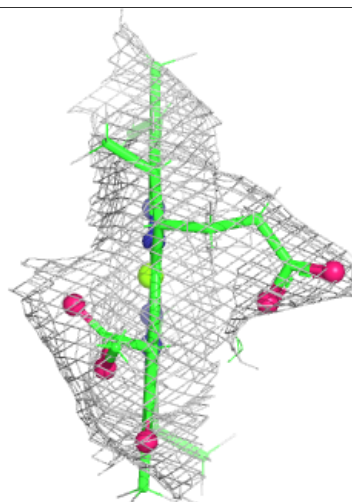
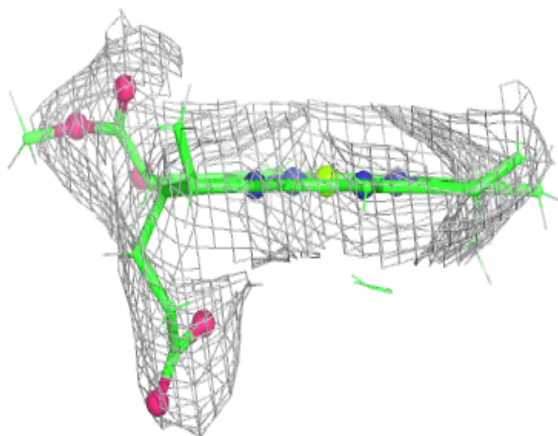
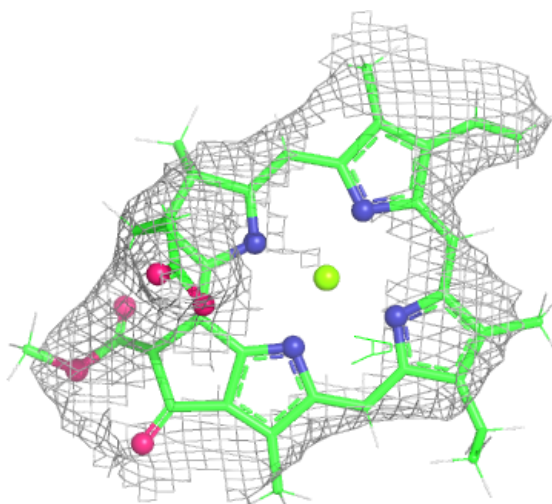
Electron density around BCR J 103:

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



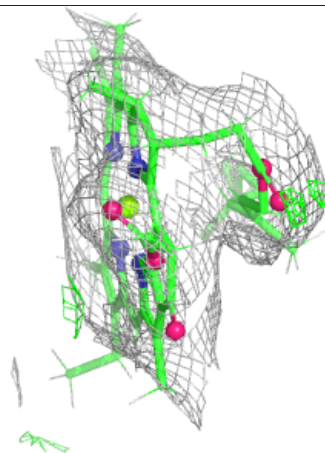
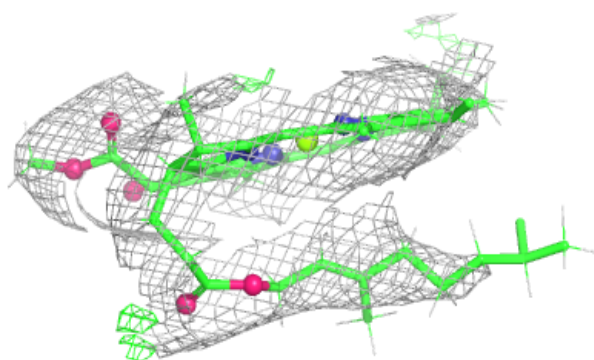
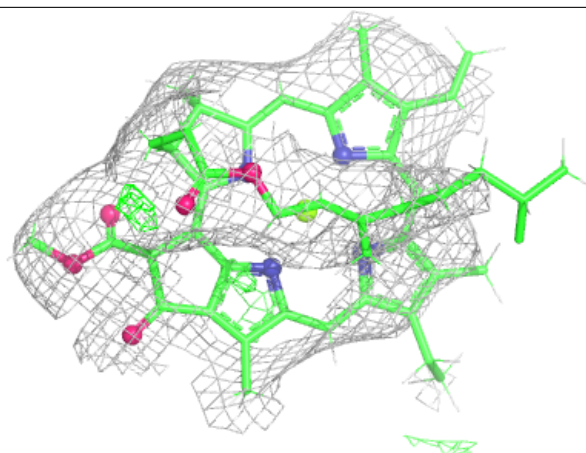
Electron density around CLA B 3013:

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



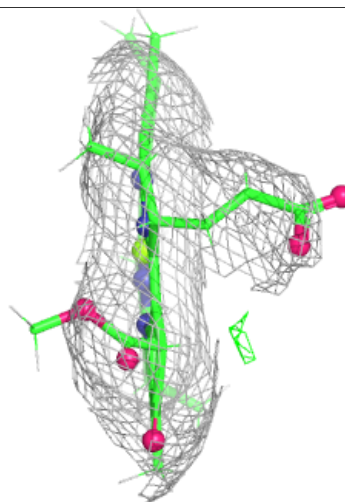
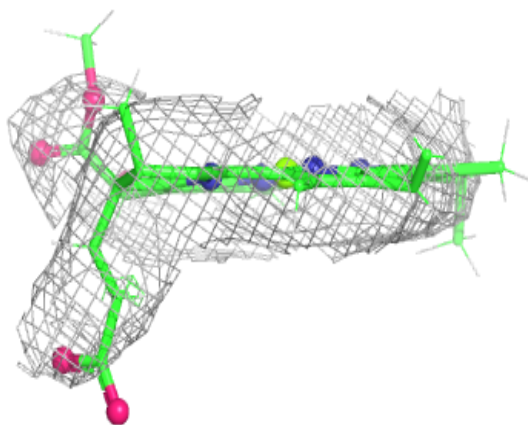
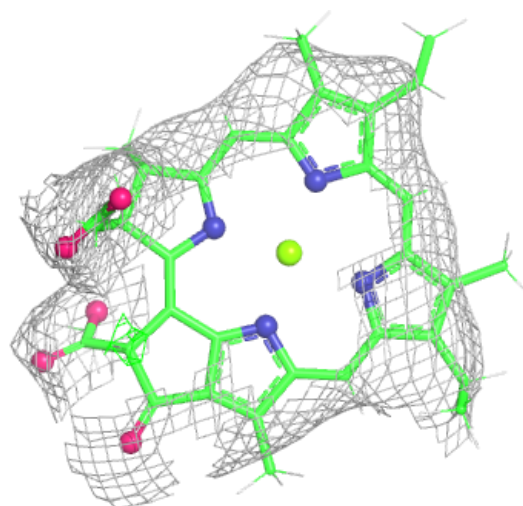
Electron density around CLA B 3023:

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



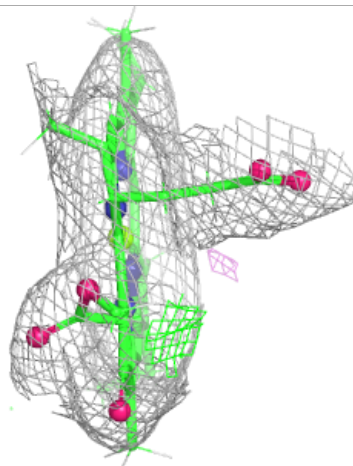
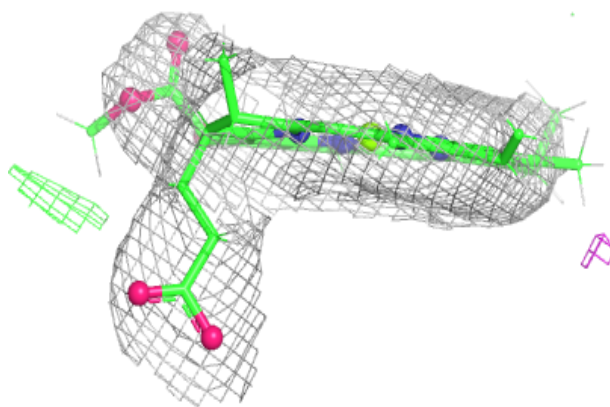
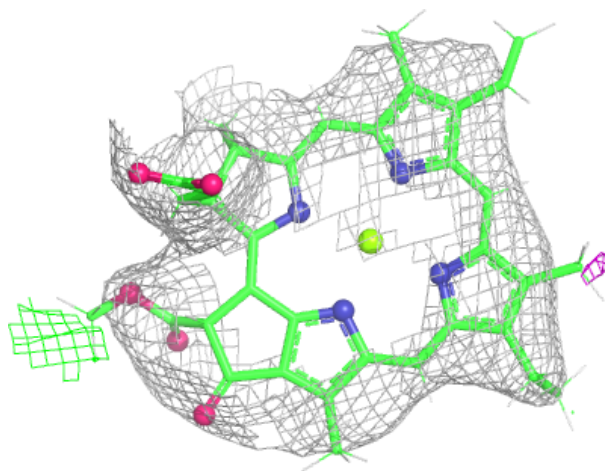
Electron density around CLA B 3022:

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



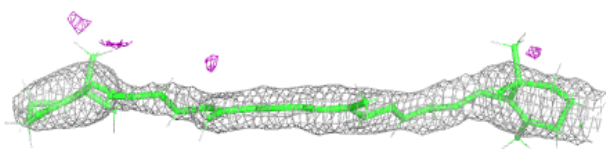
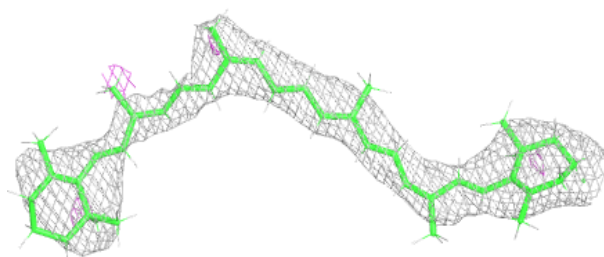
Electron density around CLA B 3012:

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



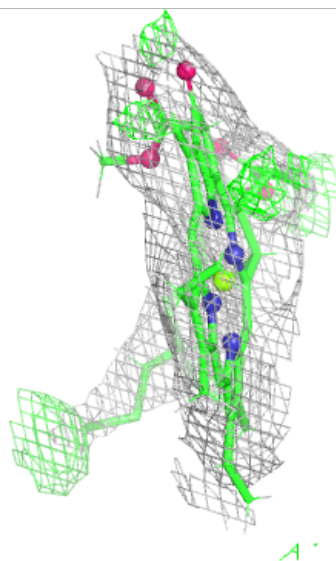
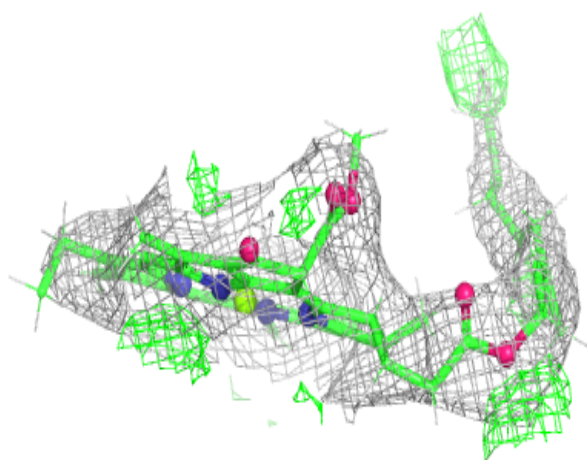
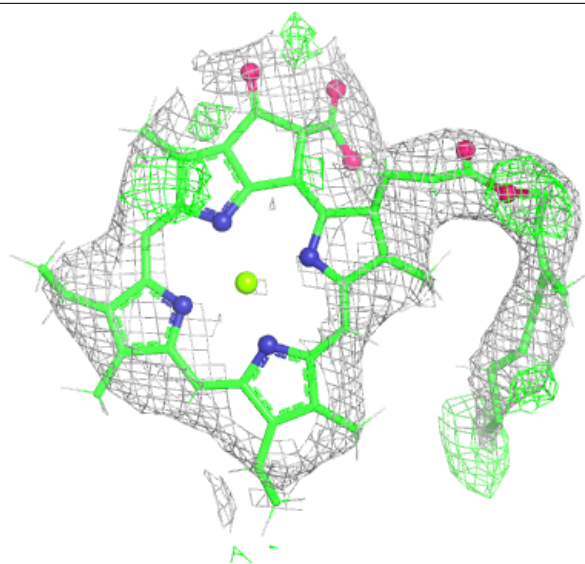
Electron density around BCR A 851:

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



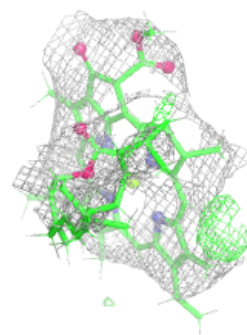
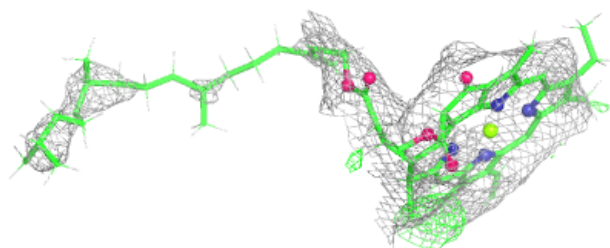
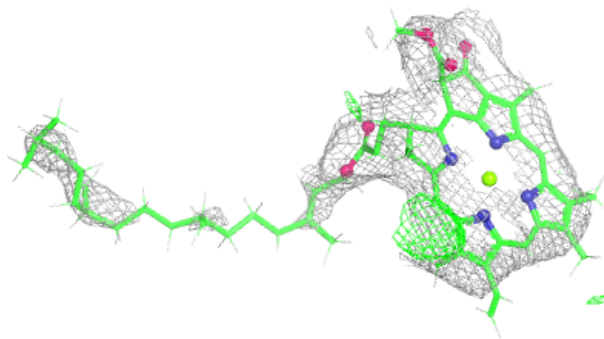
Electron density around CLA B 3025:

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



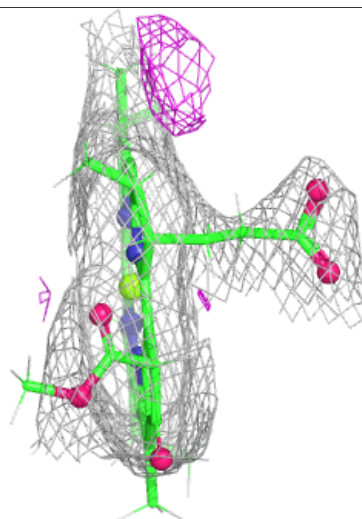
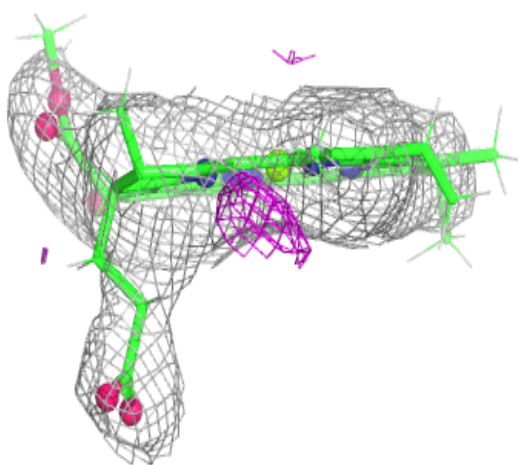
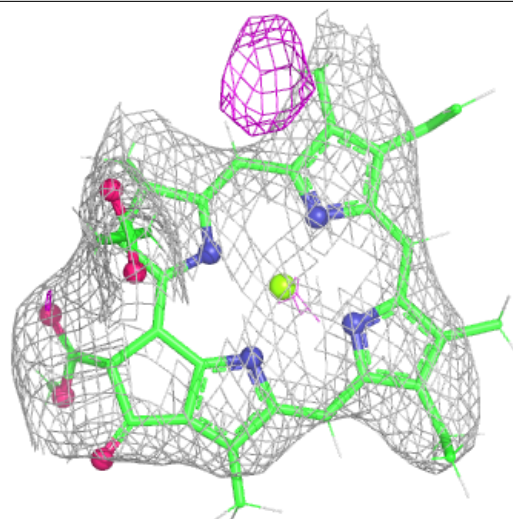
Electron density around CLA A 822:

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



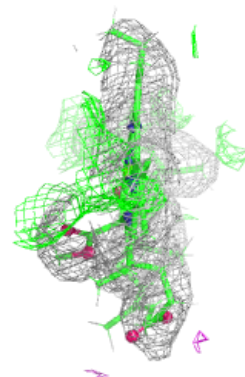
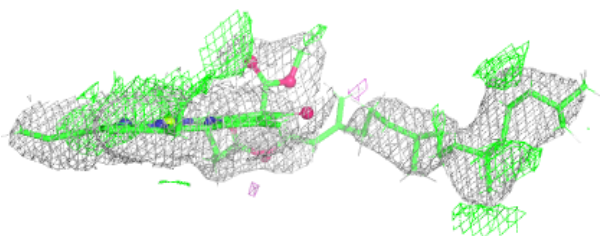
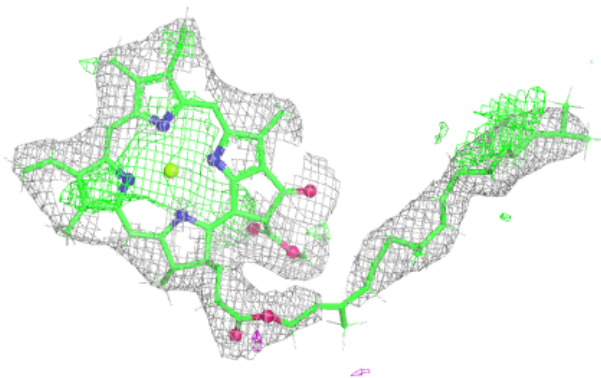
Electron density around CLA B 3031:

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

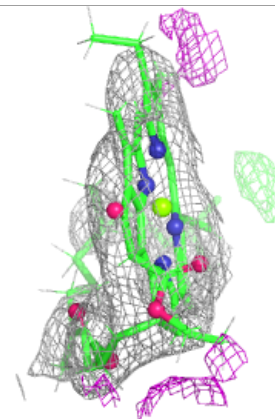
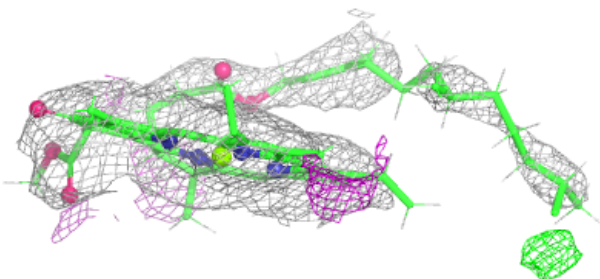
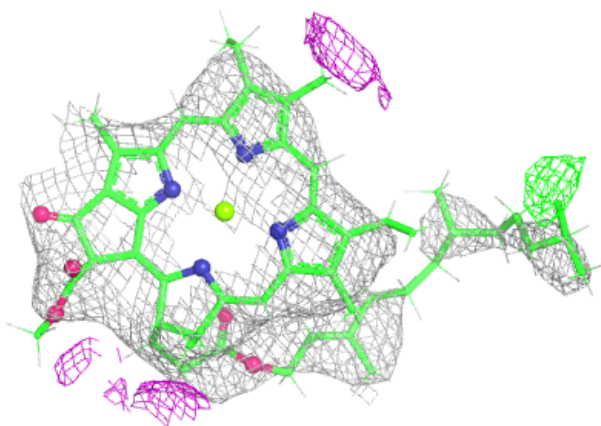


Electron density around CLA L 205:

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

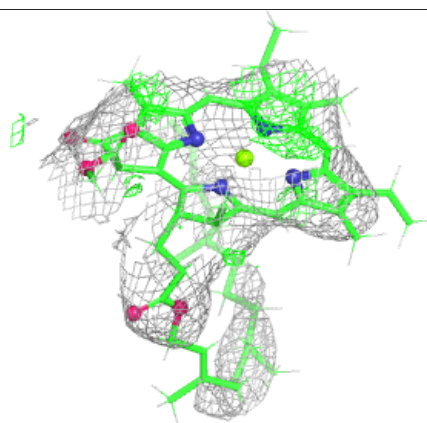
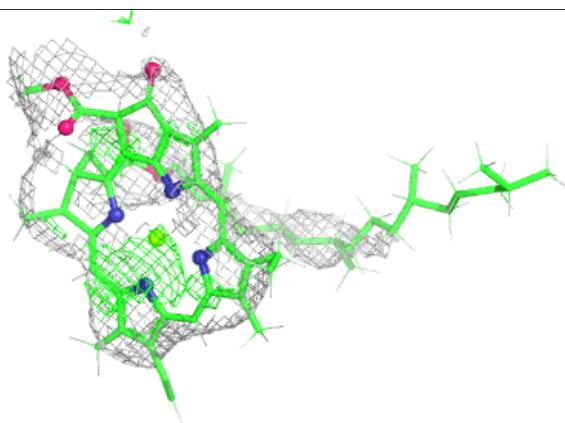
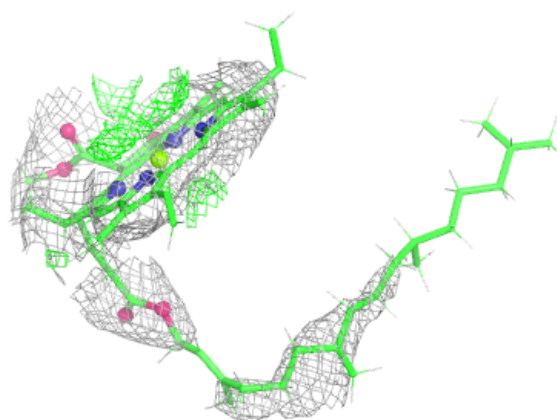
**Electron density around CLA B 3019:**

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

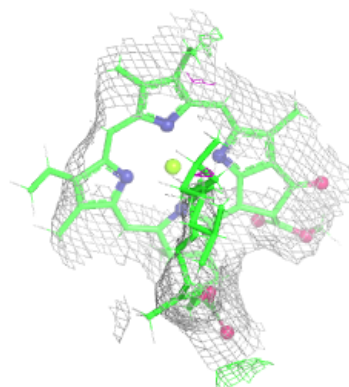
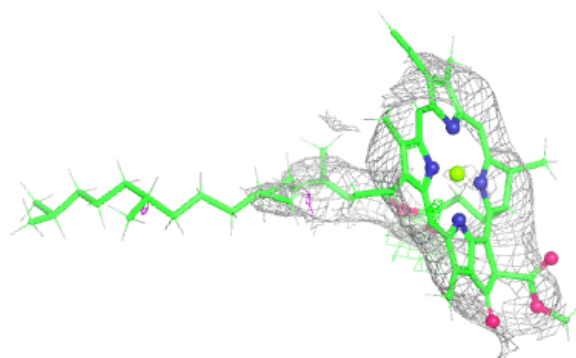
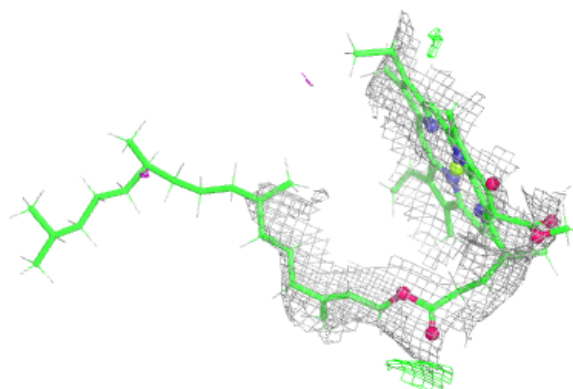


Electron density around CLA B 3020:

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

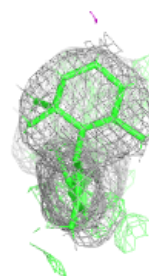
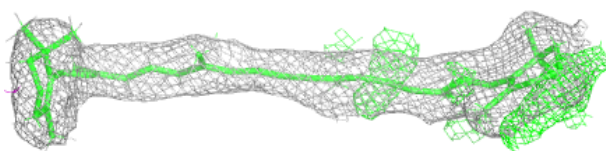
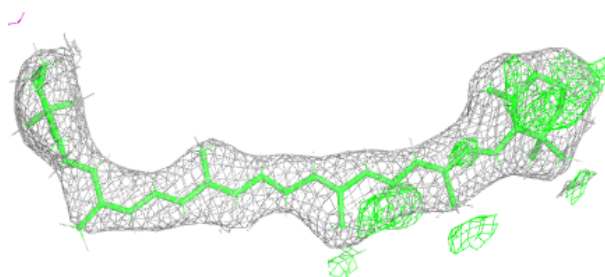
**Electron density around CLA A 812:**

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

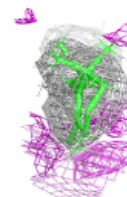
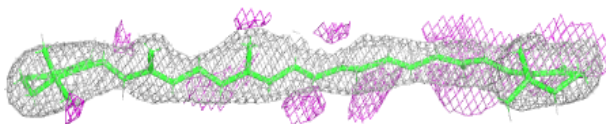
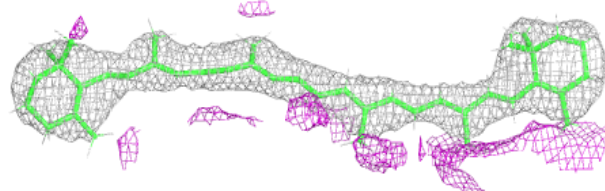


Electron density around BCR I 103:

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

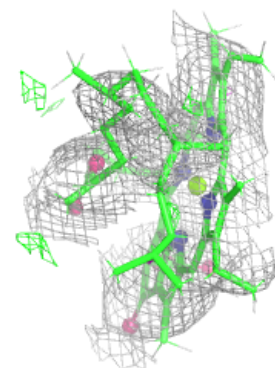
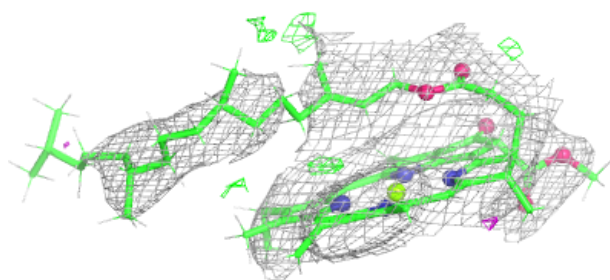
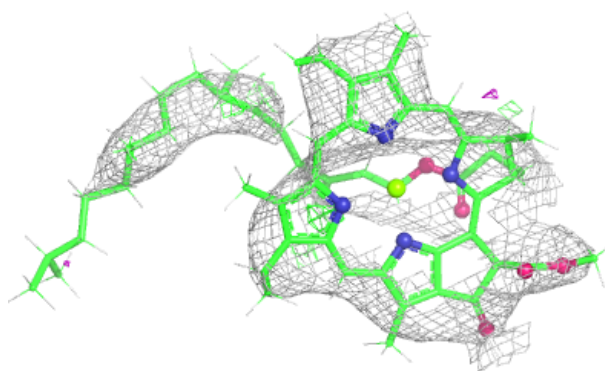
**Electron density around BCR I 105:**

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

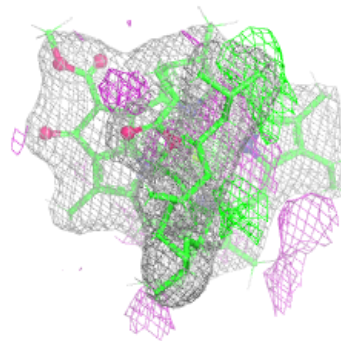
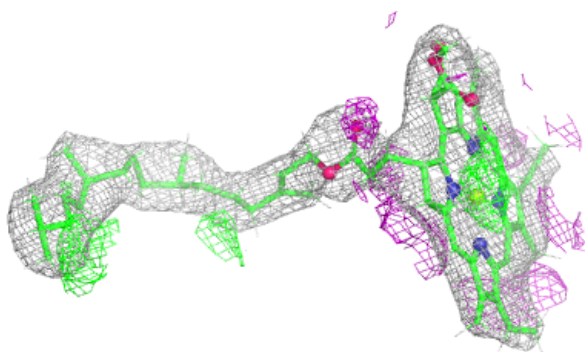
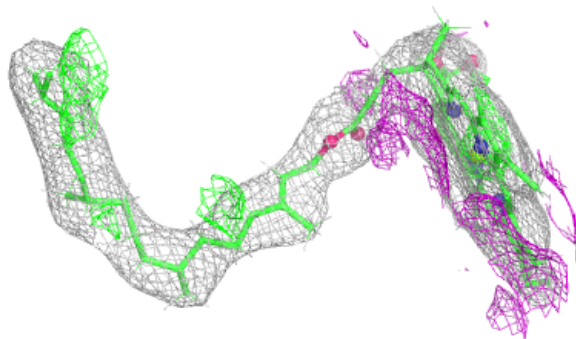


Electron density around CLA B 3039:

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

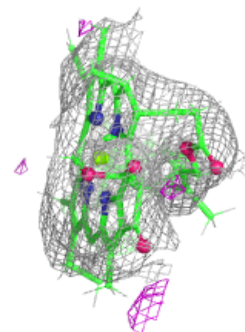
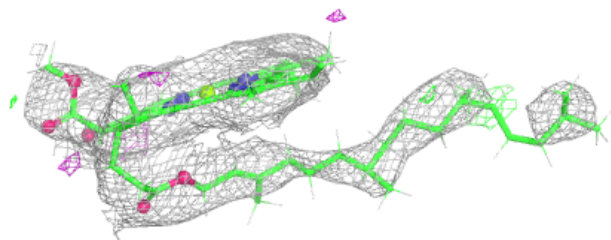
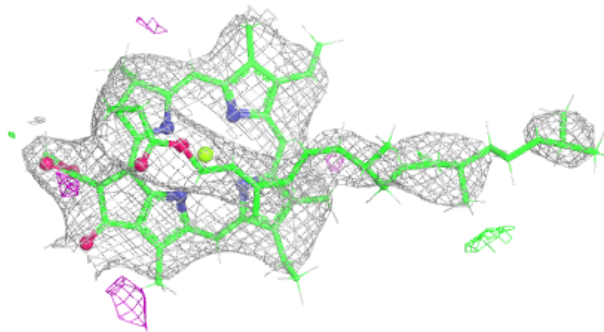
**Electron density around CLA I 101:**

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

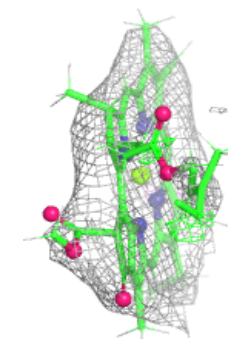
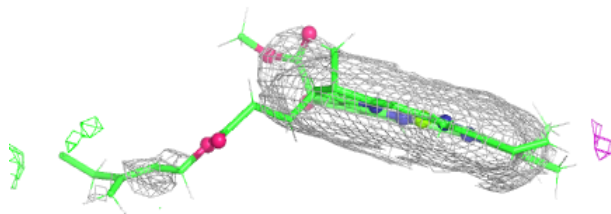
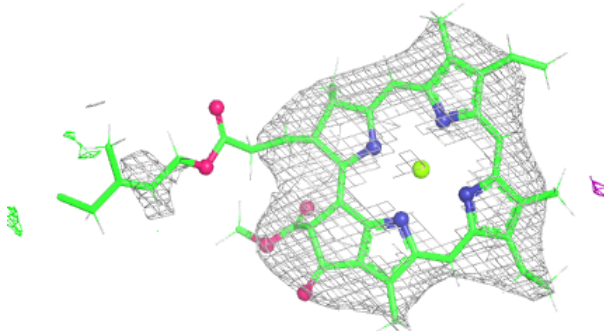


Electron density around CLA A 839:

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

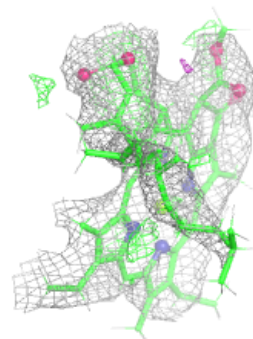
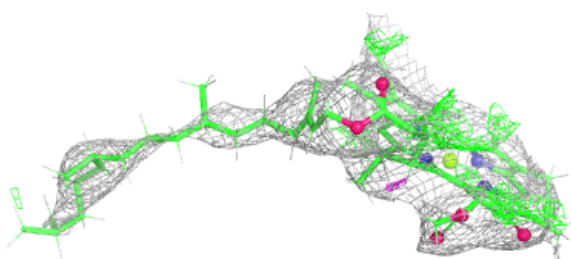
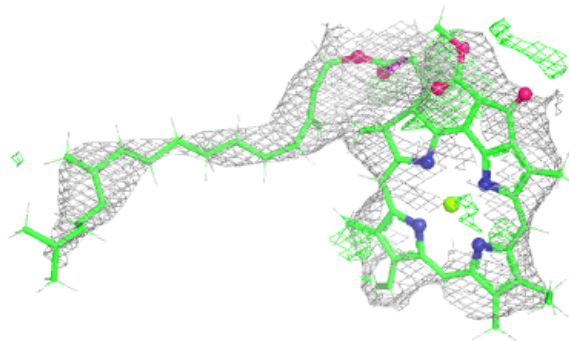
**Electron density around CLA A 842:**

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

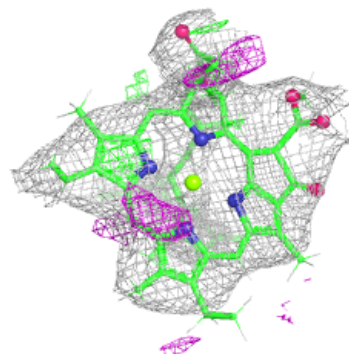
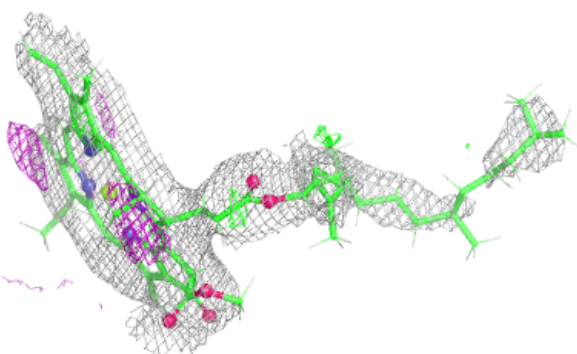
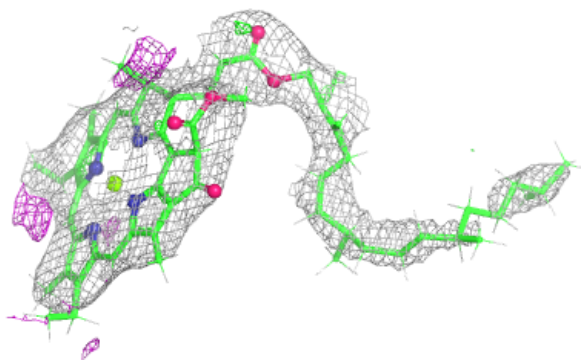


Electron density around CLA A 803:

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

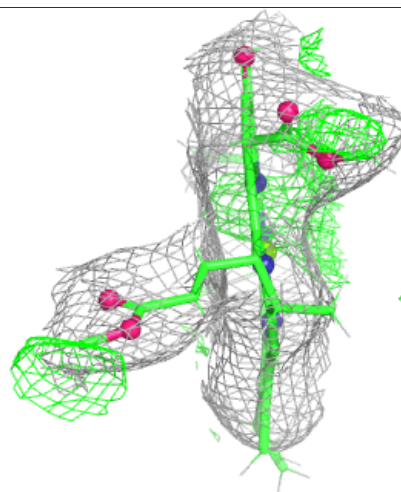
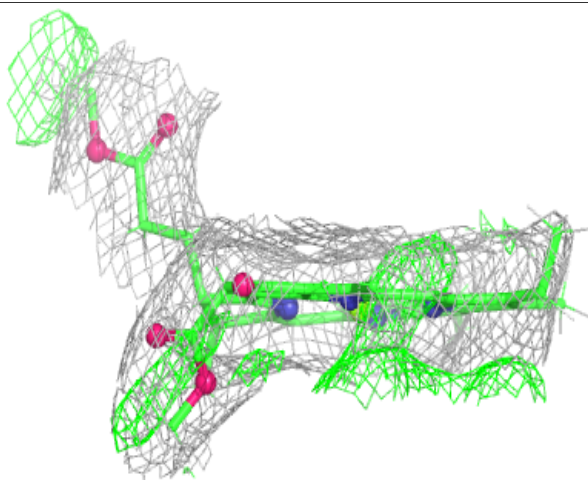
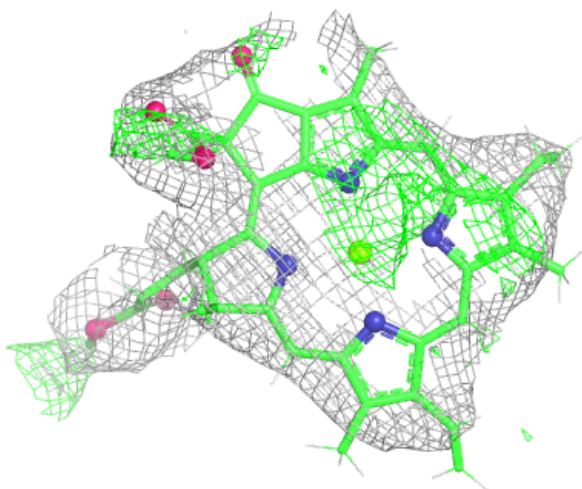
**Electron density around CLA B 3003:**

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



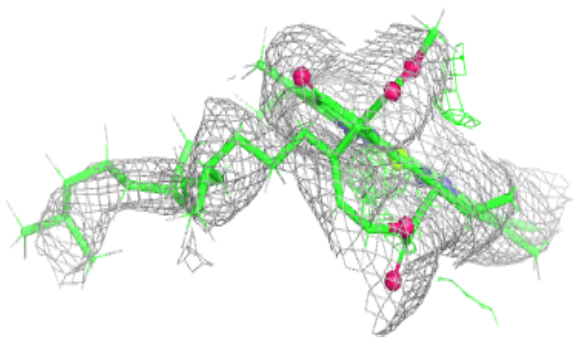
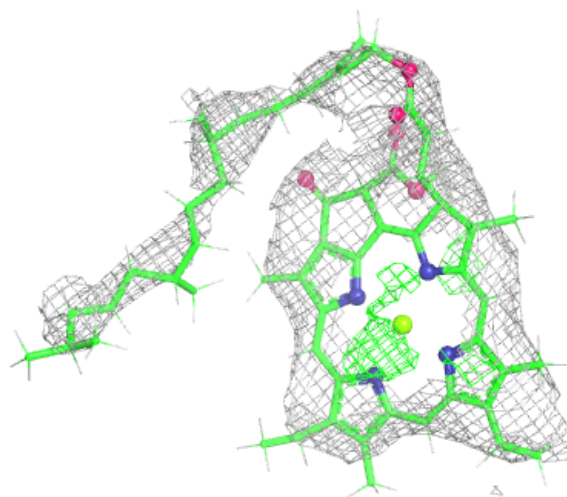
Electron density around CLA B 3026:

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



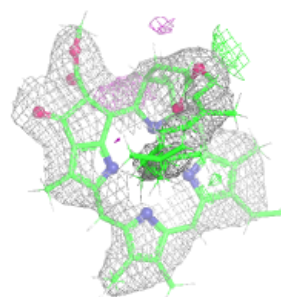
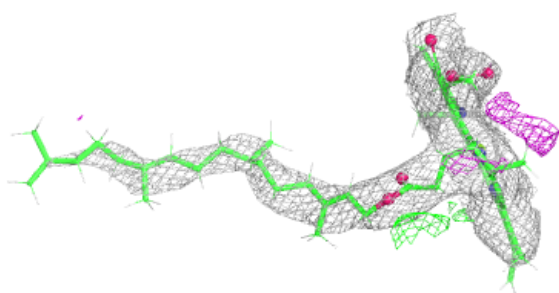
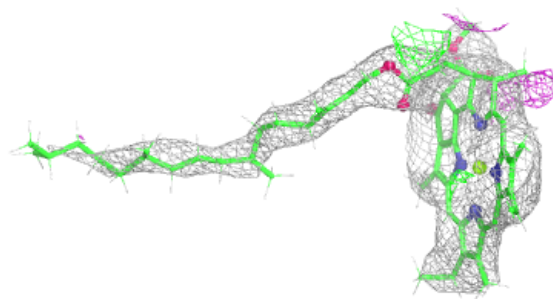
Electron density around CLA A 826:

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

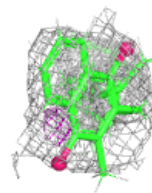
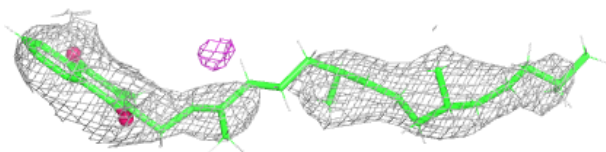
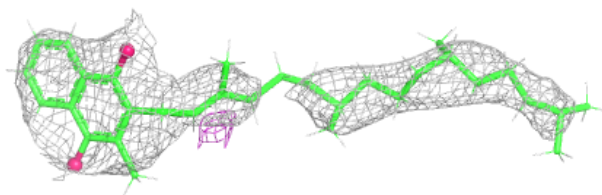


Electron density around CLA B 3029:

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

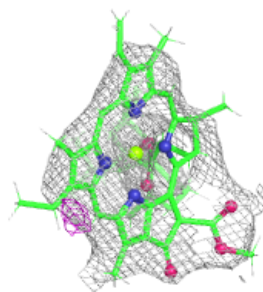
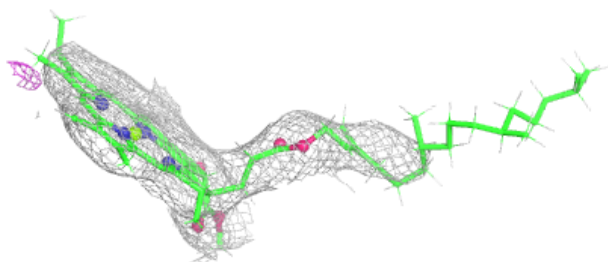
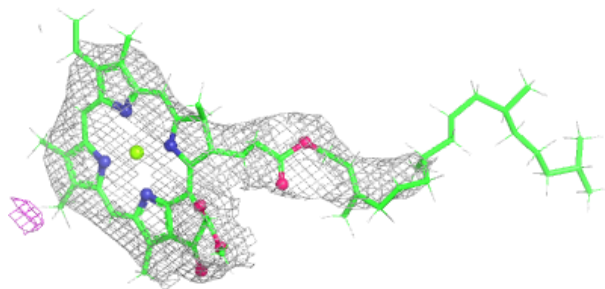
**Electron density around PQN A 846:**

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

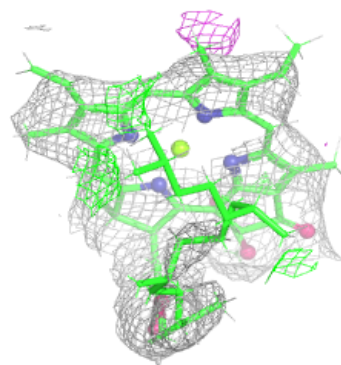
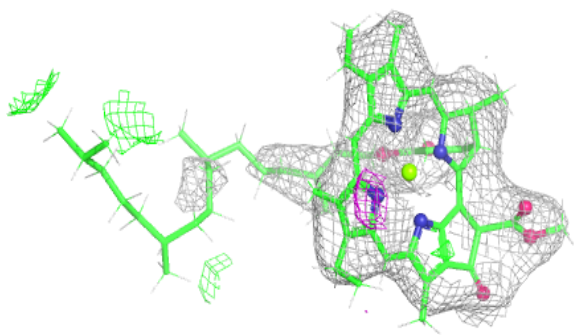
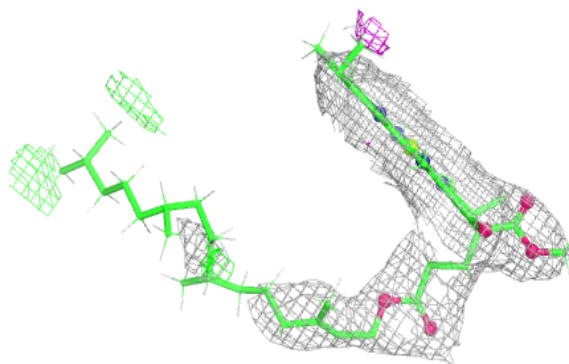


Electron density around CLA A 810:

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

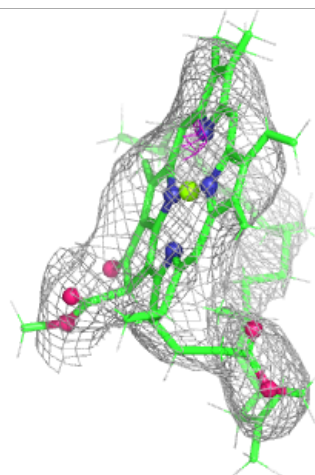
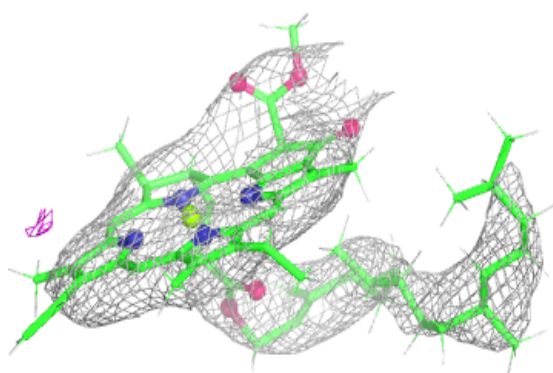
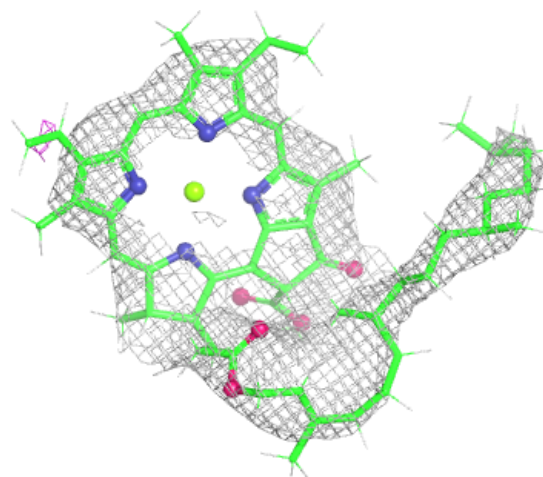
**Electron density around CLA A 833:**

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



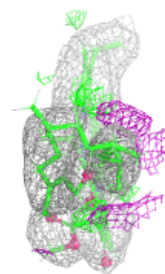
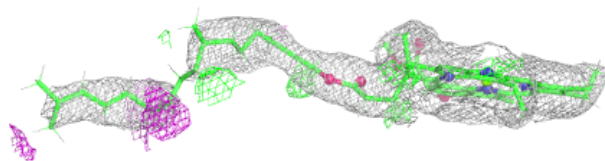
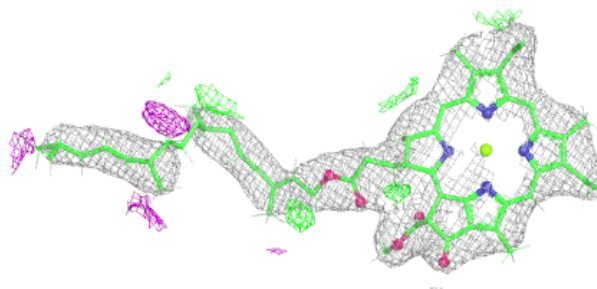
Electron density around CLA B 3033:

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



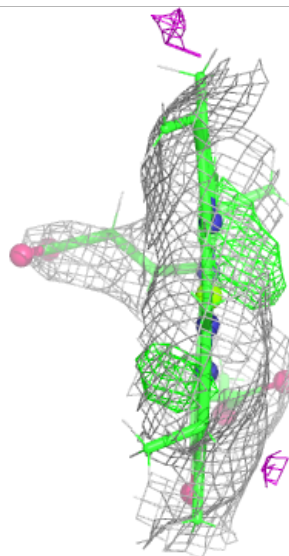
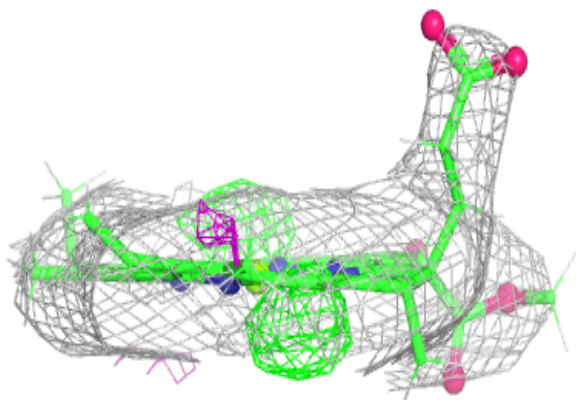
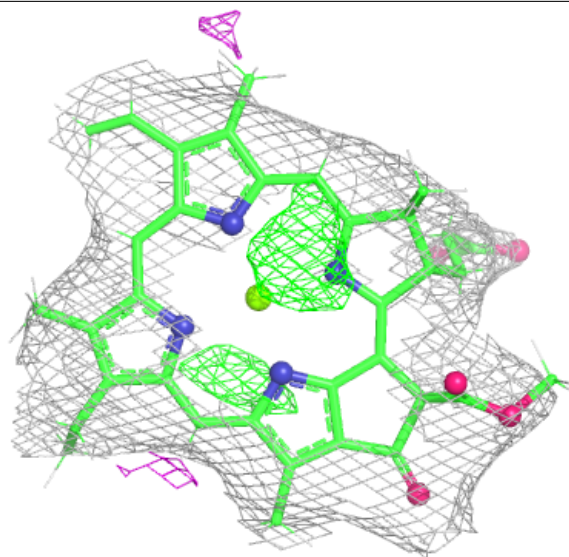
Electron density around CLA A 834:

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



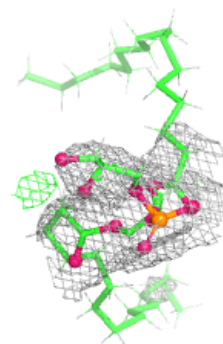
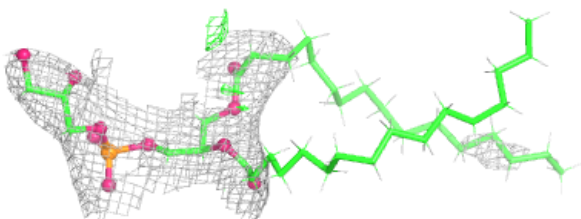
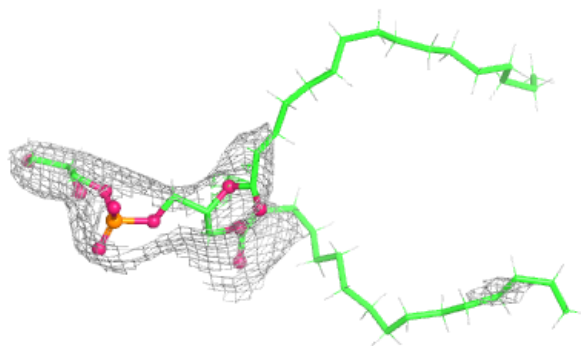
Electron density around CLA B 3036:

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

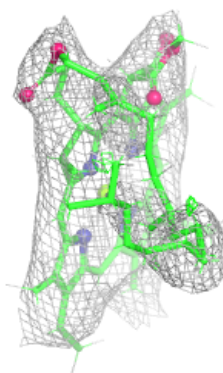
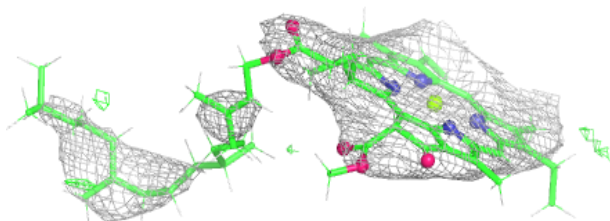
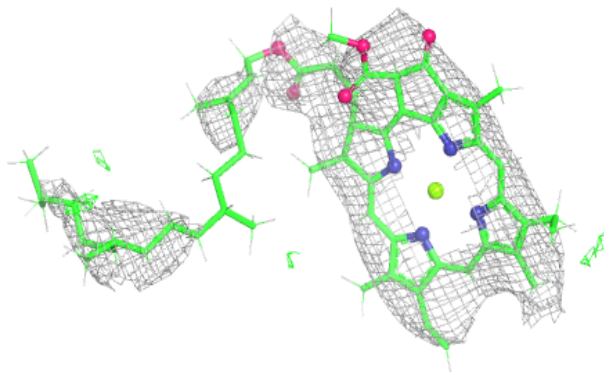


Electron density around LHG A 853:

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

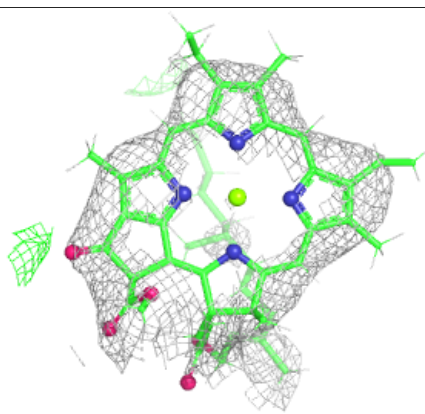
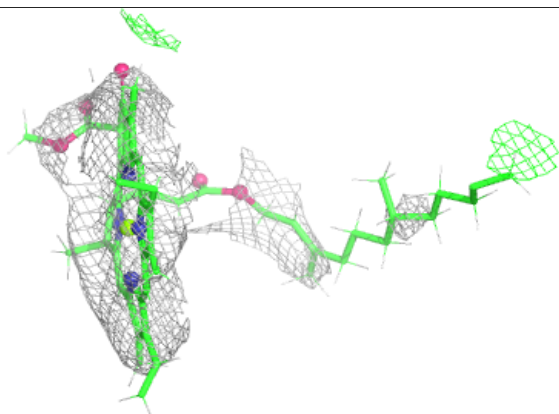
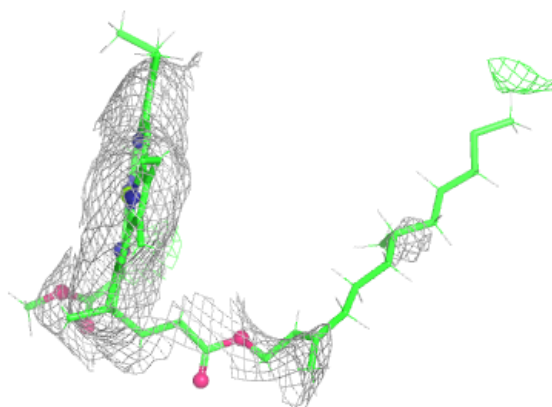
**Electron density around CLA A 804:**

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



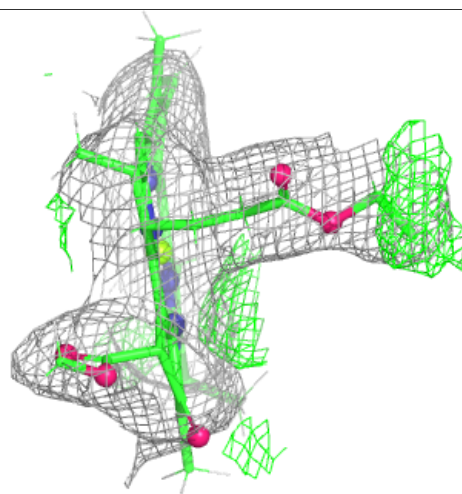
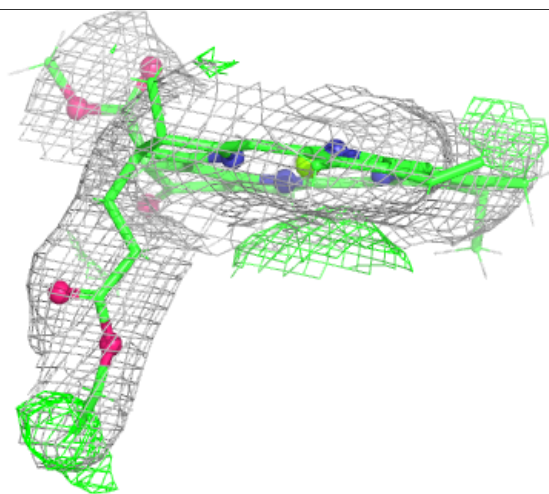
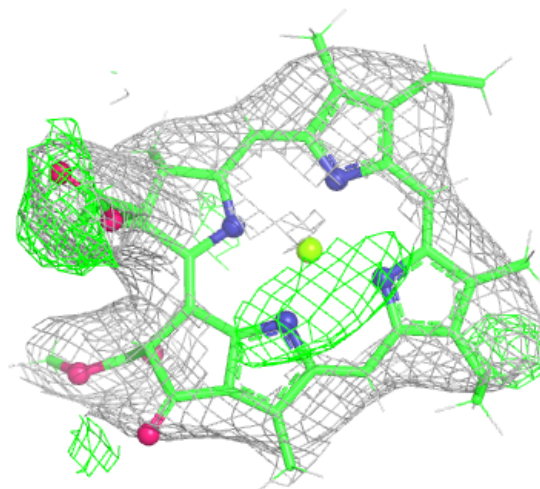
Electron density around CLA A 805:

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



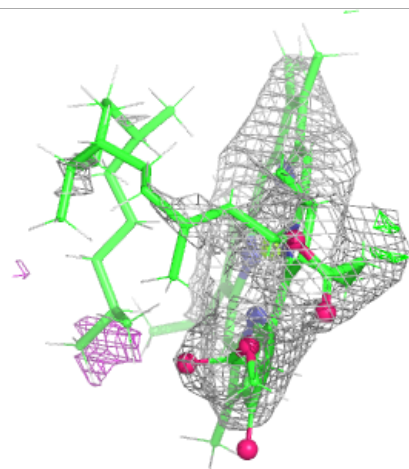
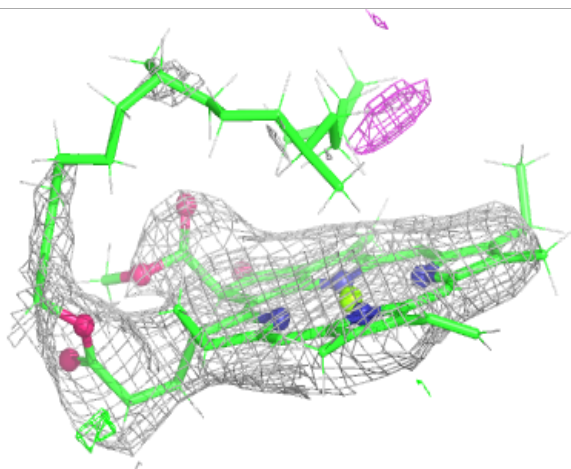
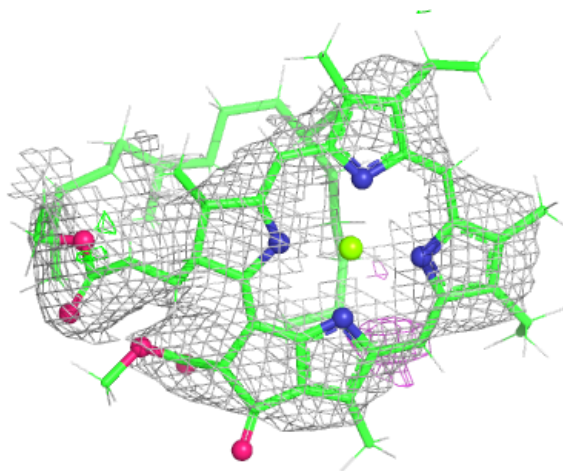
Electron density around CLA B 3040:

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



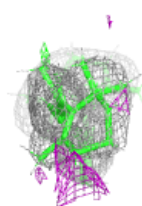
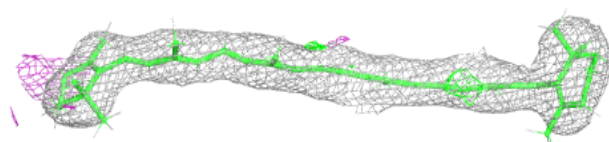
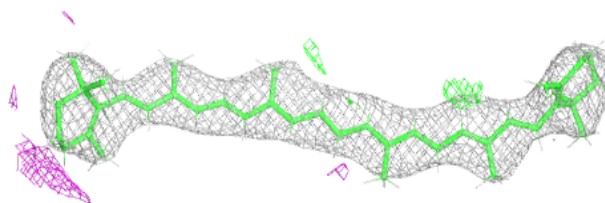
Electron density around CLA A 807:

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

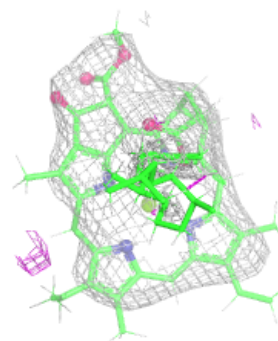
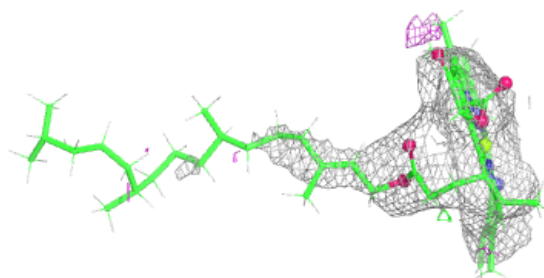
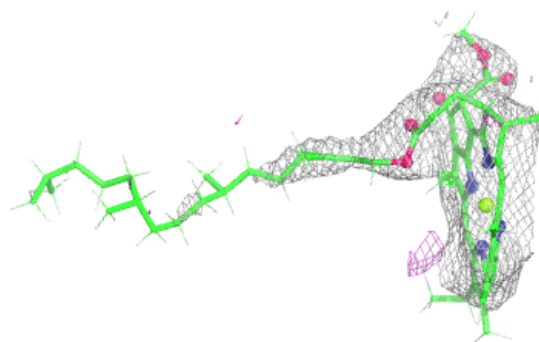


Electron density around BCR B 3047:

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

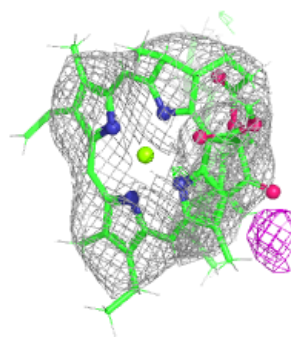
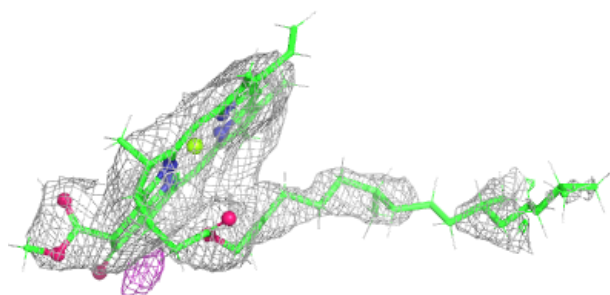
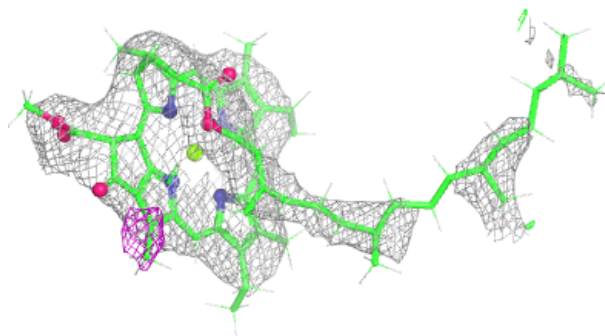
**Electron density around CLA A 829:**

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



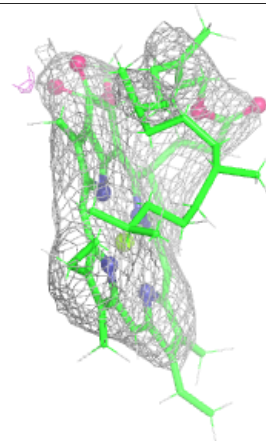
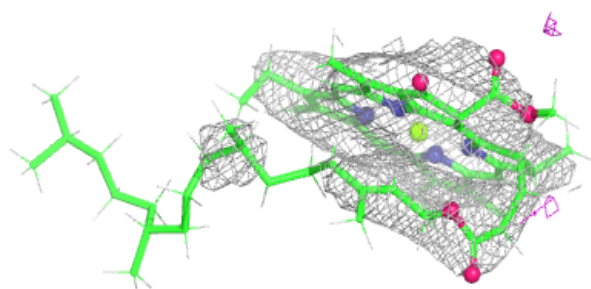
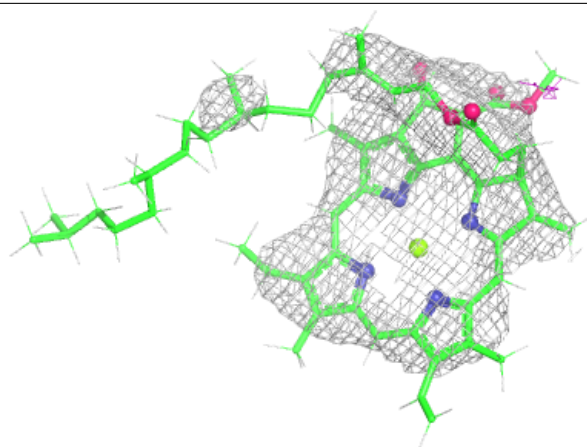
Electron density around CLA A 843:

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



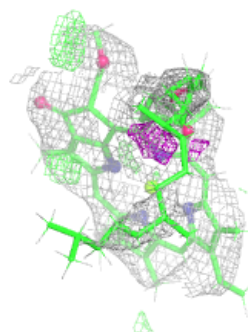
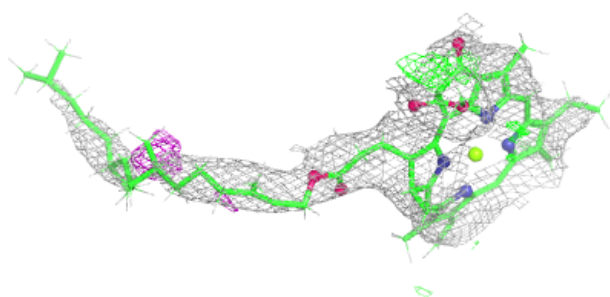
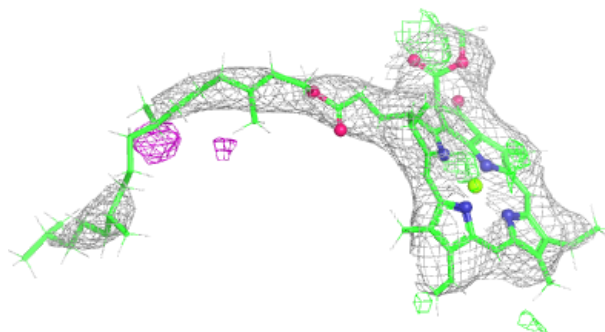
Electron density around CLA A 830:

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

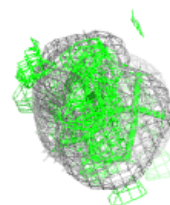
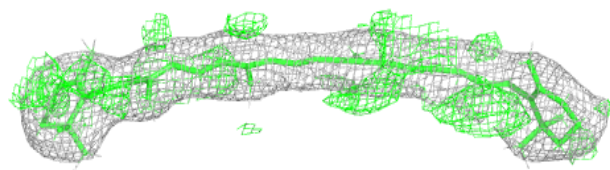
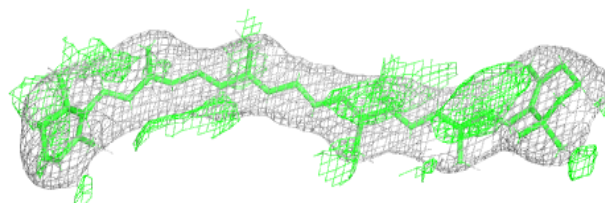


Electron density around CLA A 856:

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

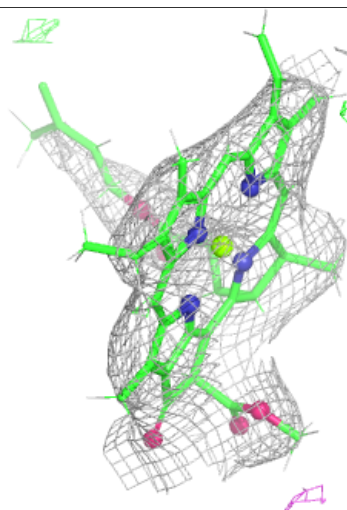
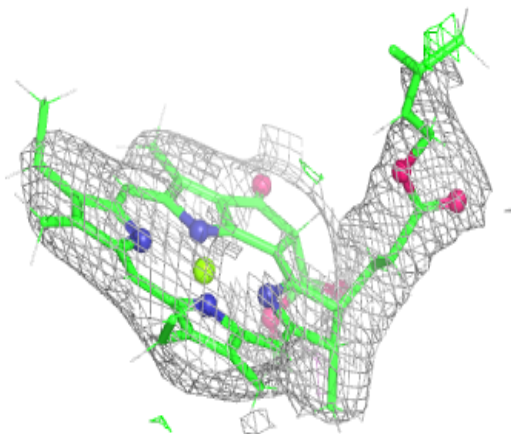
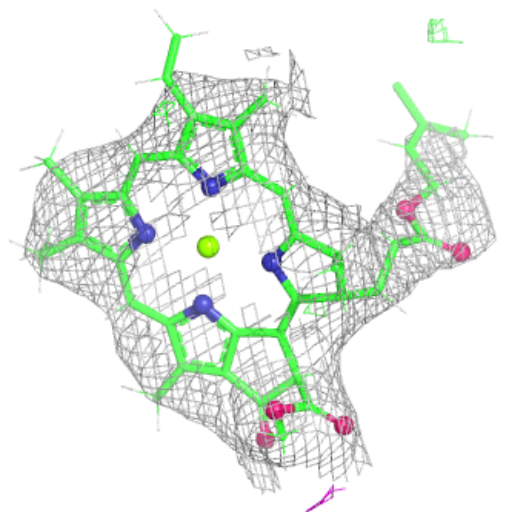
**Electron density around BCR I 102:**

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



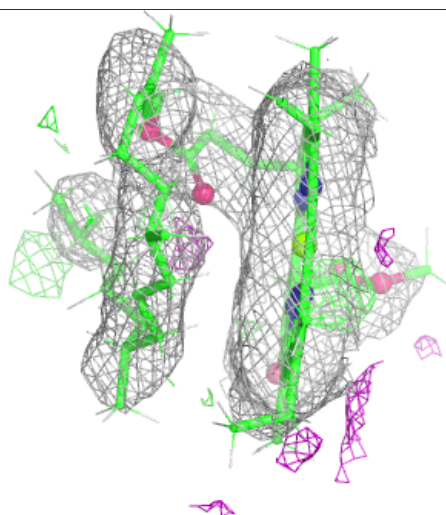
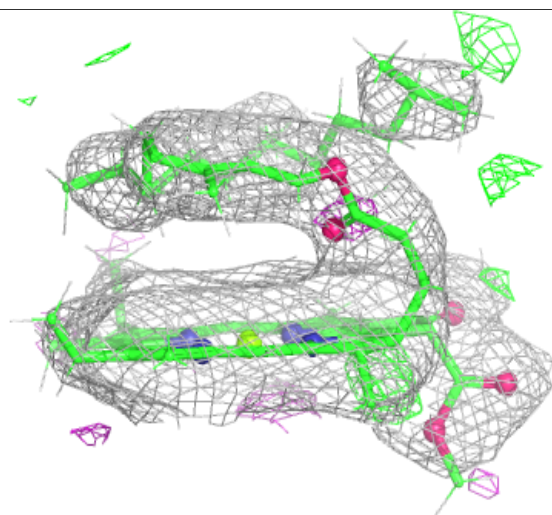
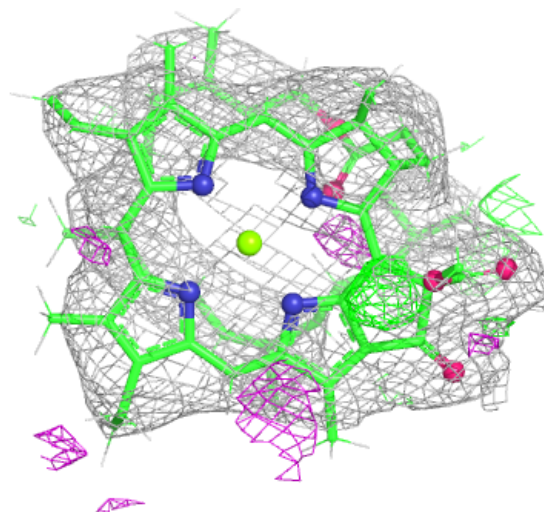
Electron density around CLA A 832:

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



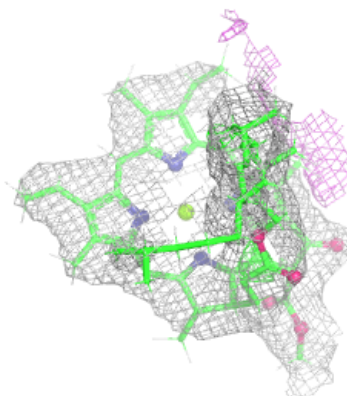
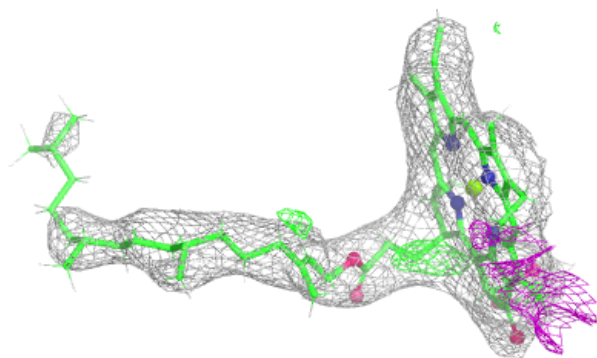
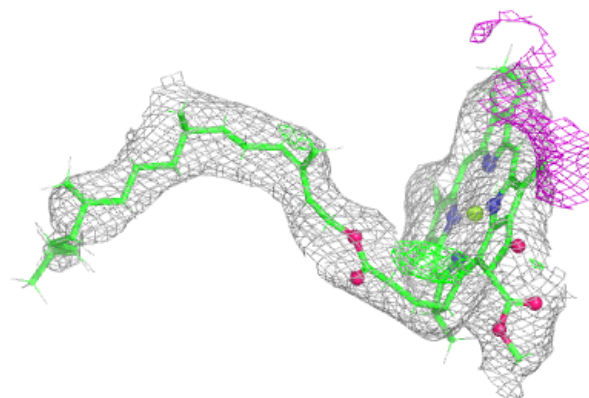
Electron density around CLA L 203:

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

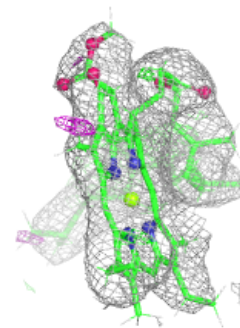
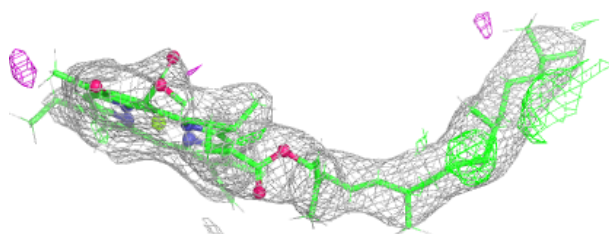
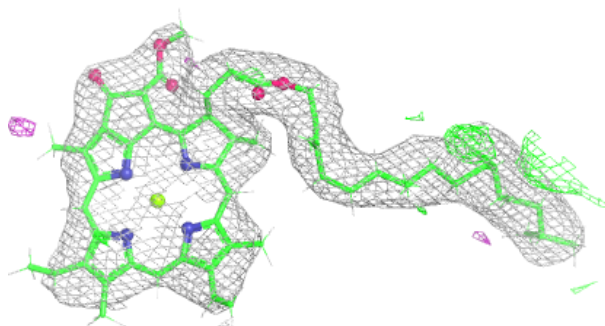


Electron density around CLA L 204:

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

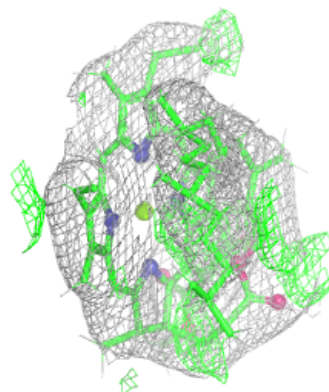
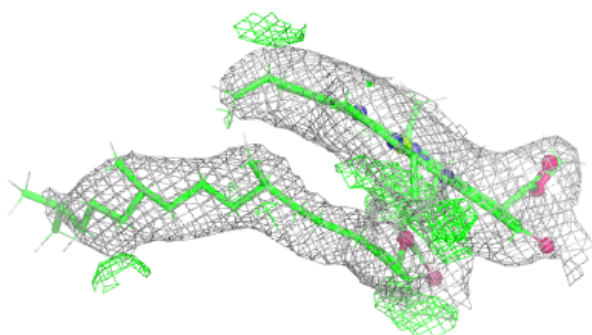
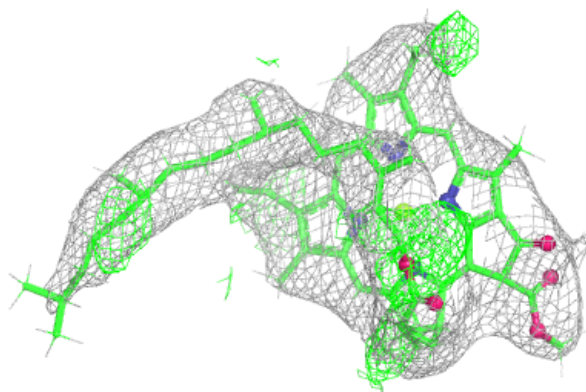
**Electron density around CLA B 3004:**

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

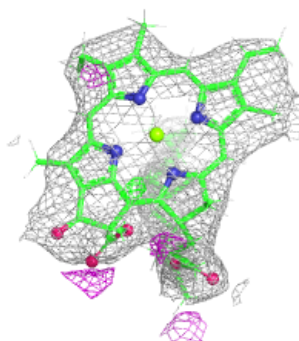
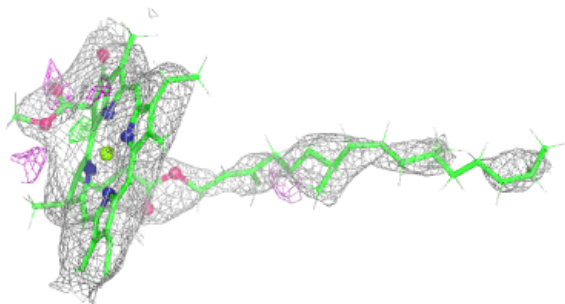
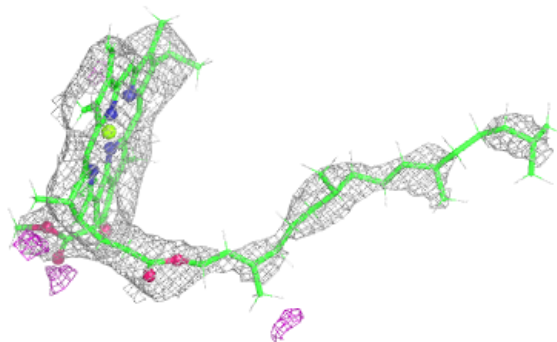


Electron density around CLA B 3008:

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

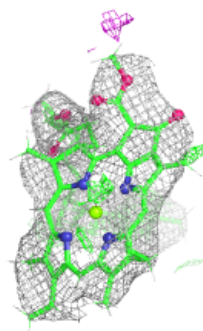
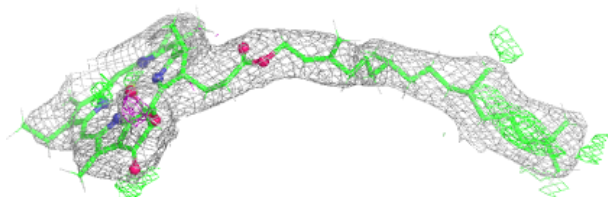
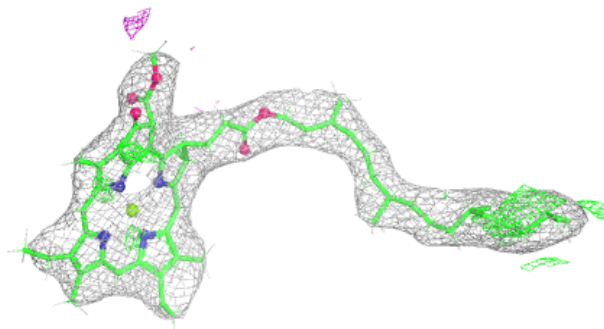
**Electron density around CLA B 3030:**

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

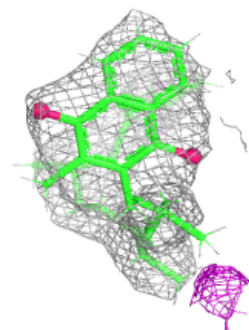
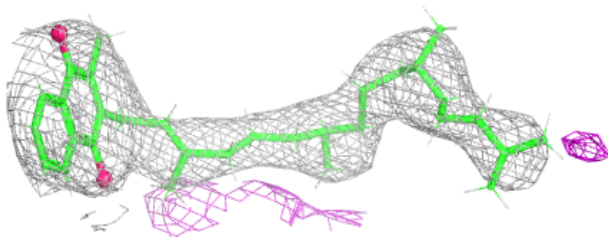
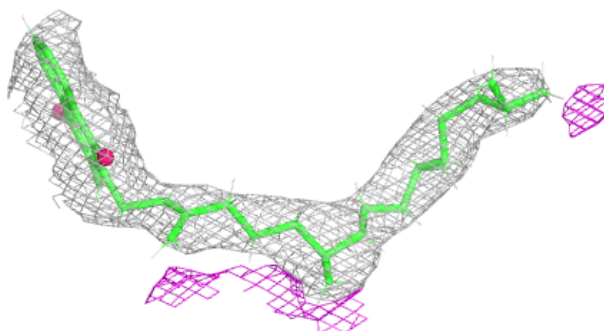


Electron density around CLA A 802:

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

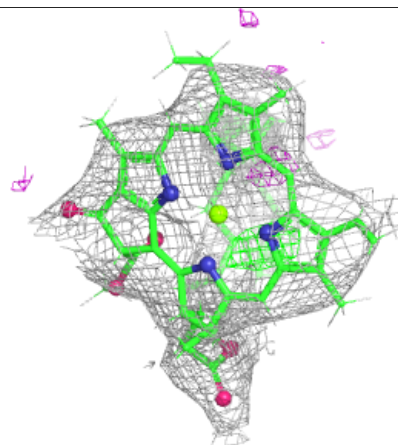
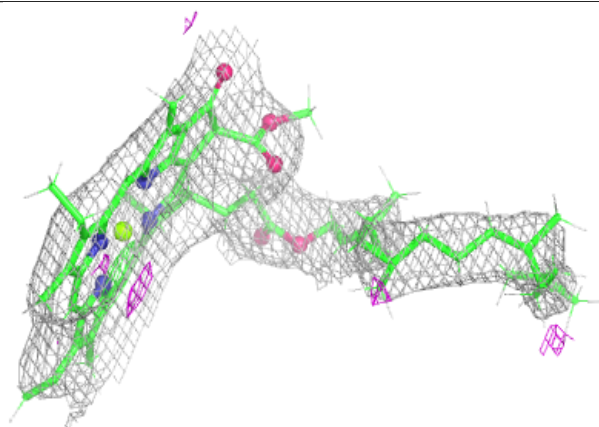
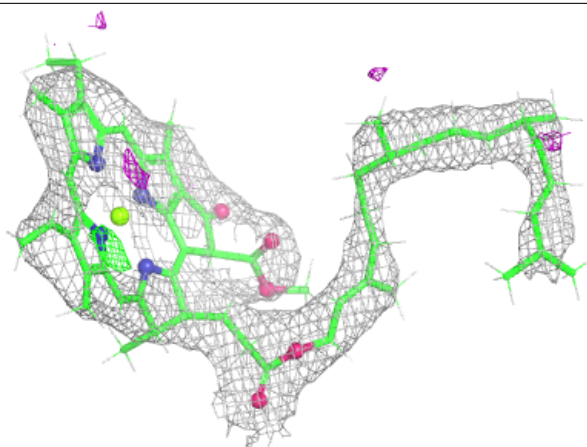
**Electron density around PQN B 3042:**

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

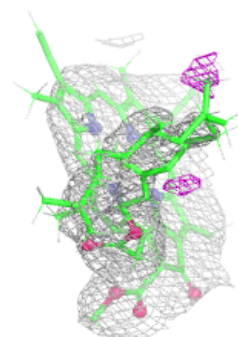
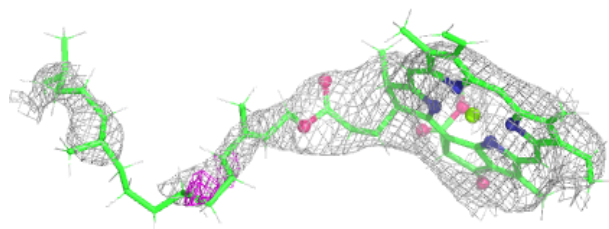
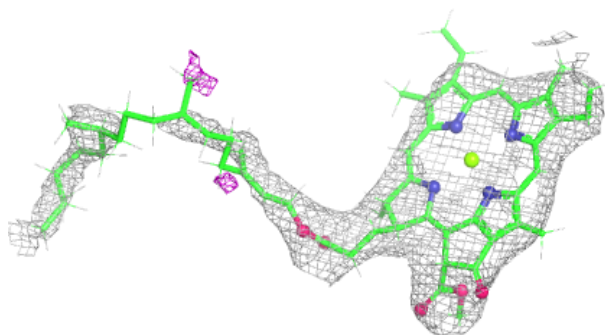


Electron density around CL0 A 801:

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

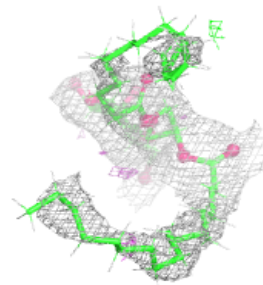
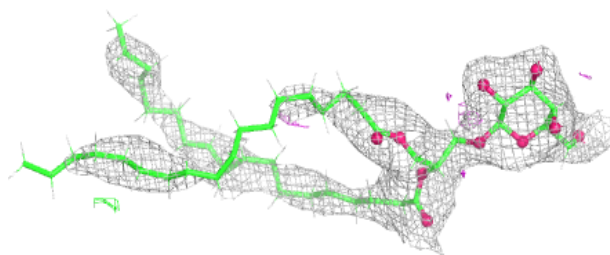
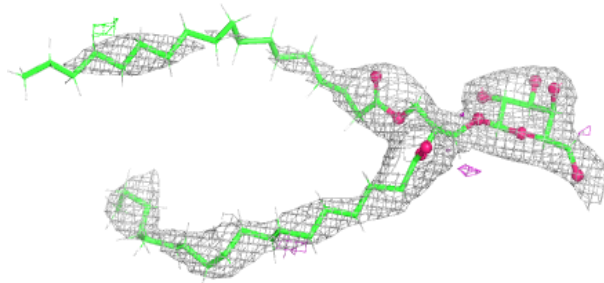
**Electron density around CLA B 3014:**

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

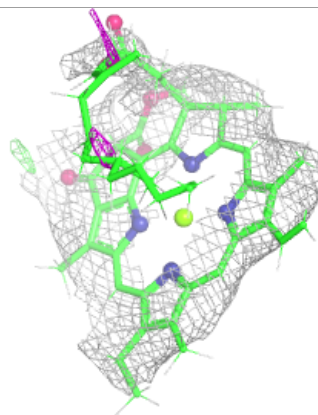
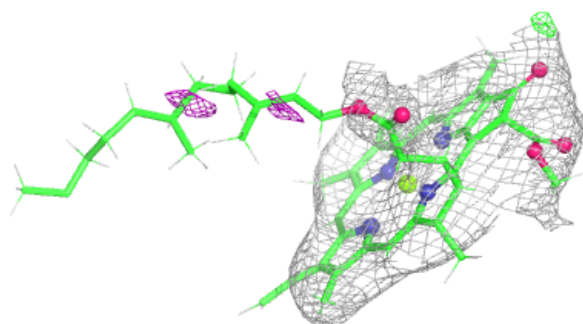
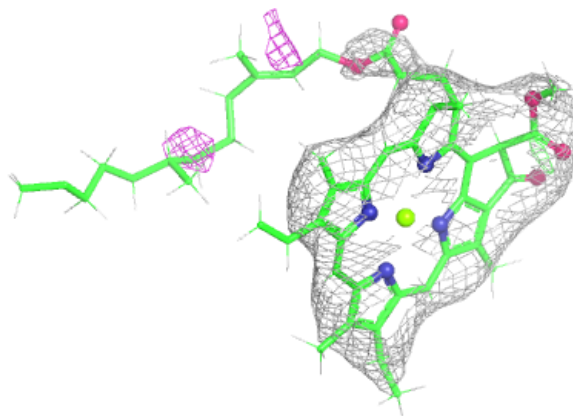


Electron density around LMG B 3048:

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

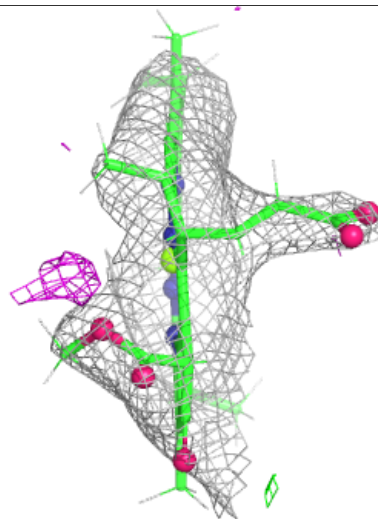
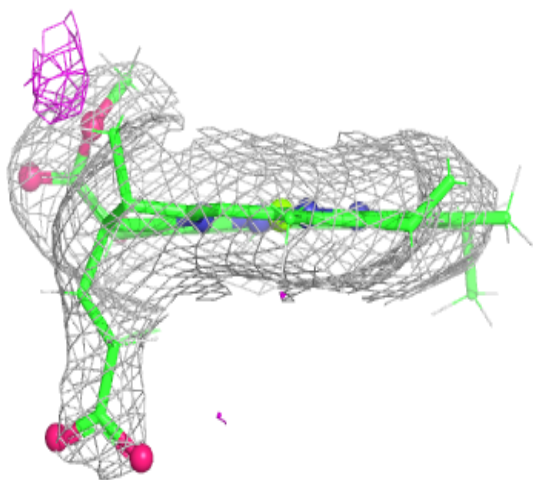
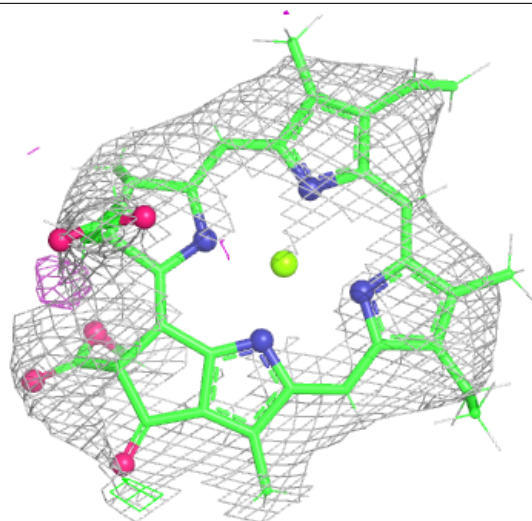
**Electron density around CLA A 825:**

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



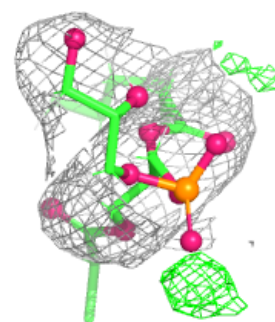
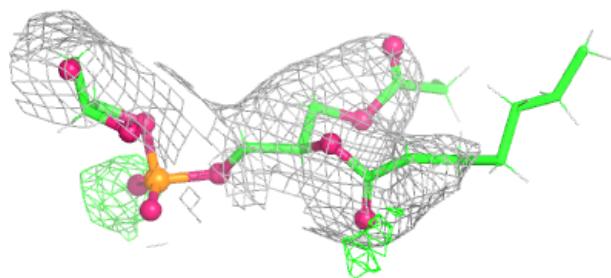
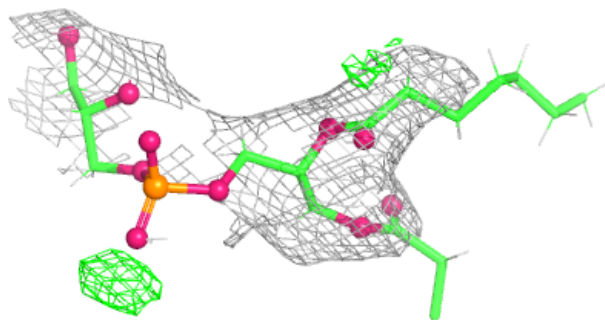
Electron density around CLA B 3035:

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



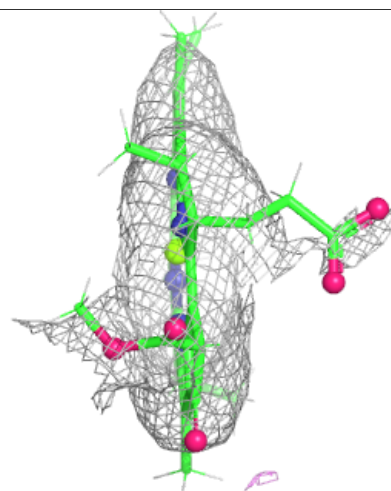
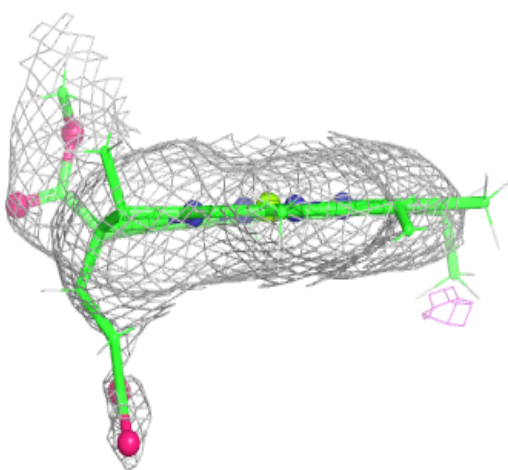
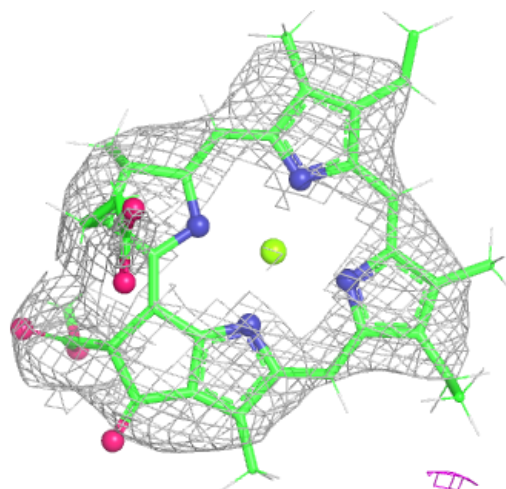
Electron density around LHG A 854:

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



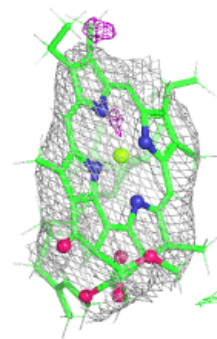
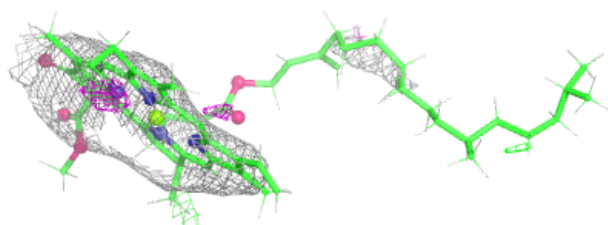
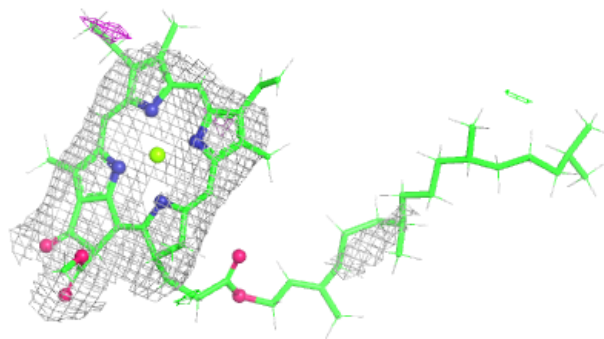
Electron density around CLA B 3016:

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

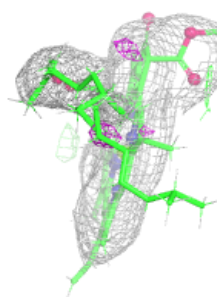
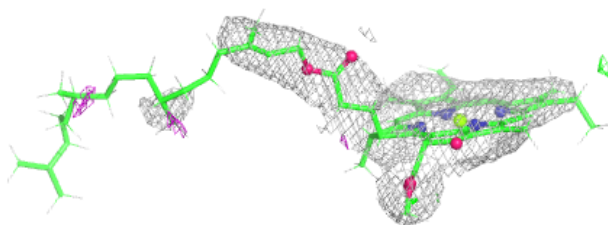
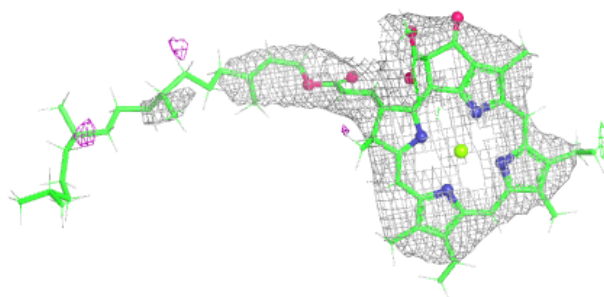


Electron density around CLA A 809:

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

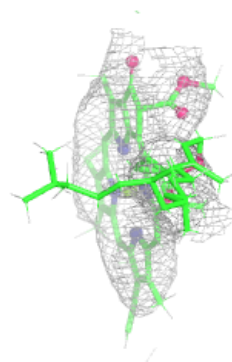
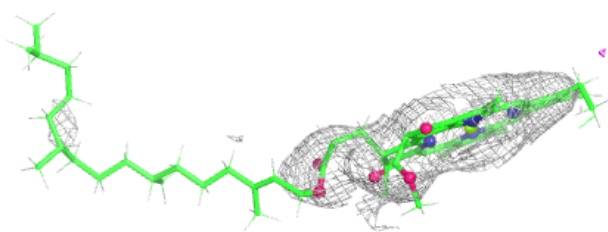
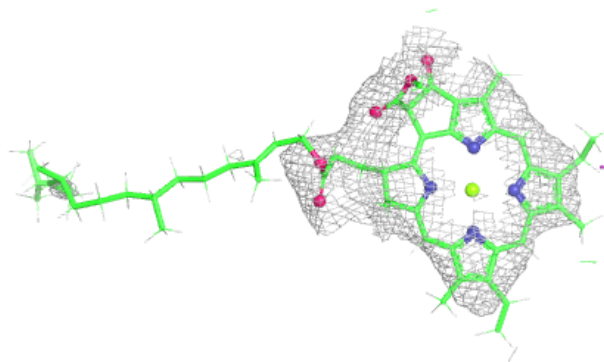
**Electron density around CLA A 827:**

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



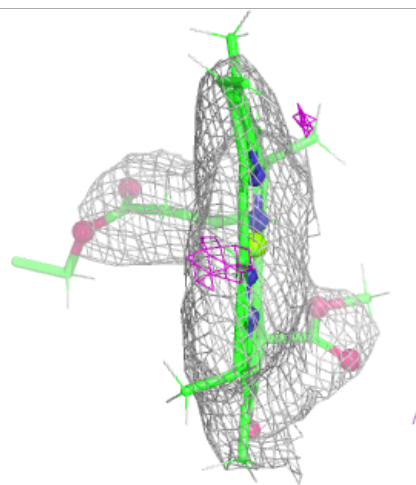
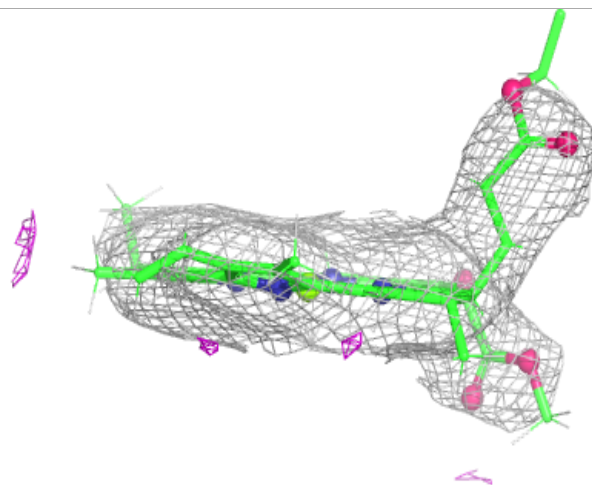
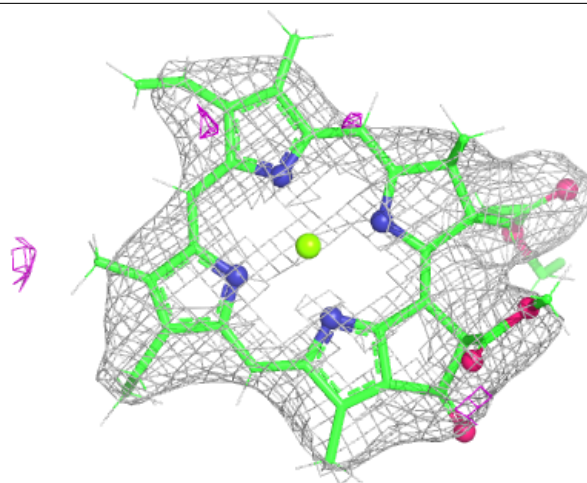
Electron density around CLA A 806:

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



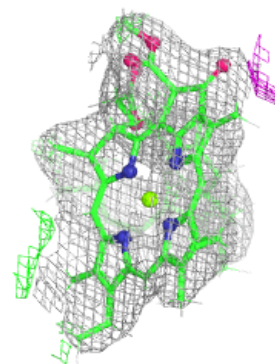
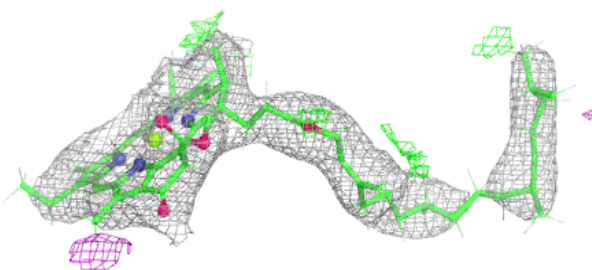
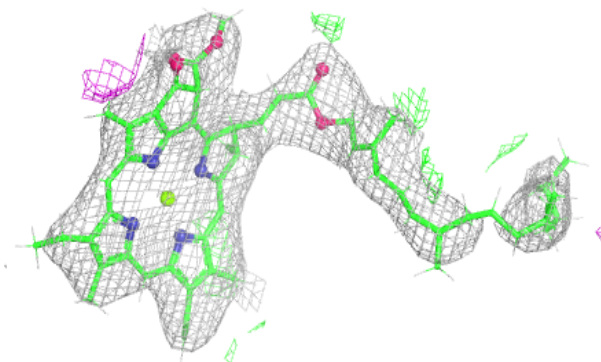
Electron density around CLA A 840:

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

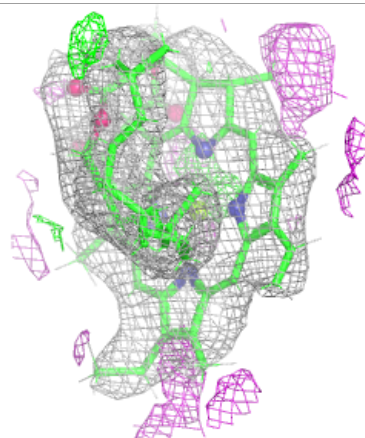
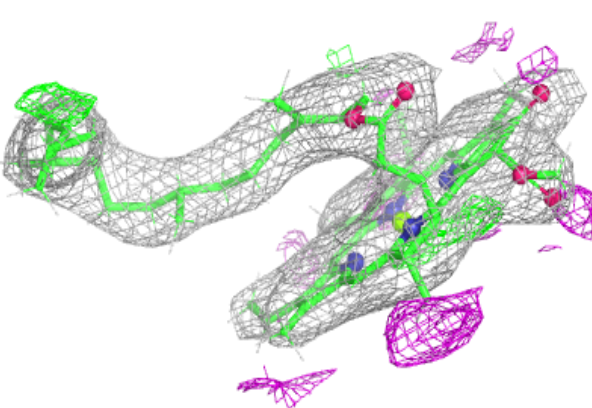
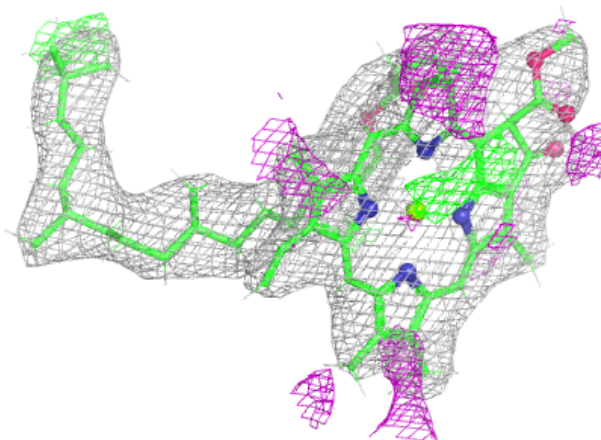


Electron density around CLA B 3010:

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

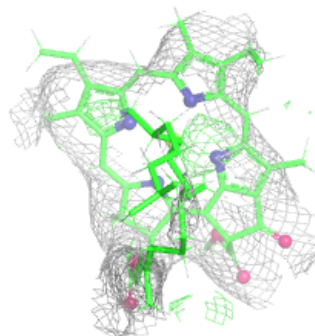
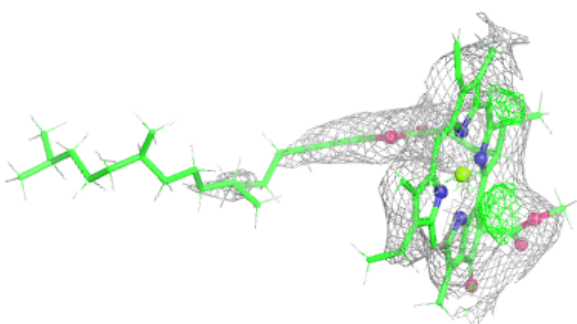
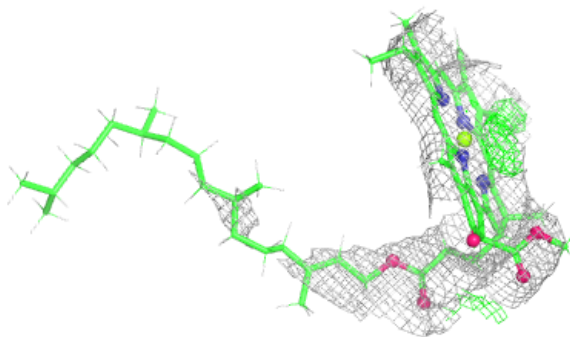
**Electron density around CLA A 844:**

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

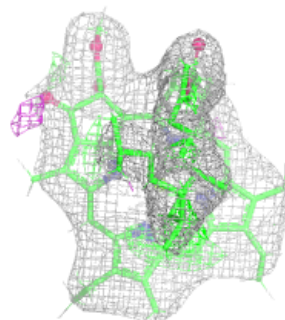
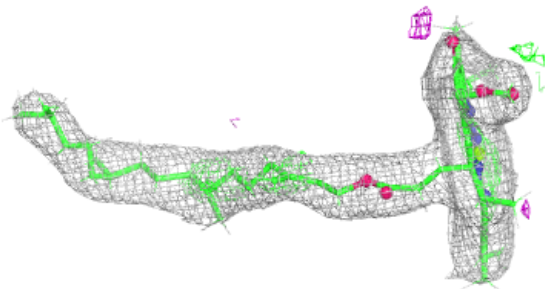
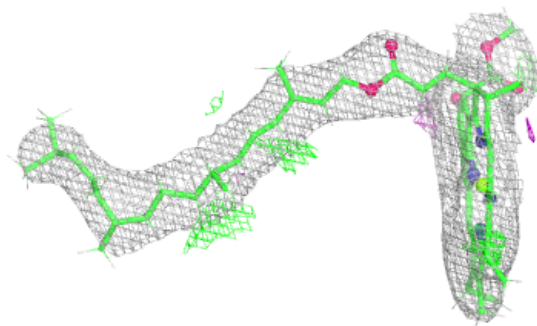


Electron density around CLA A 831:

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

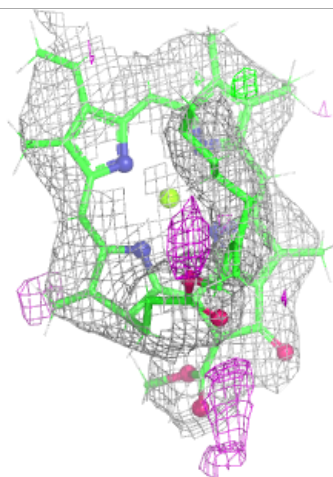
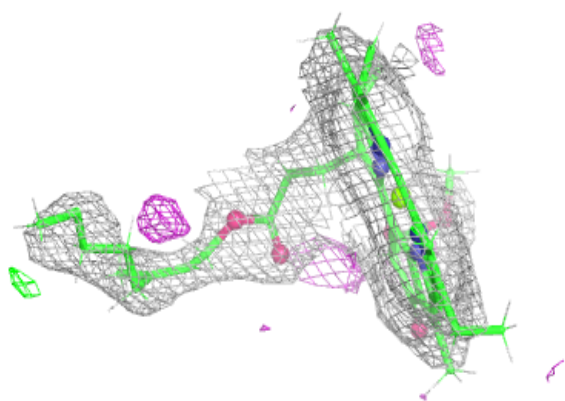
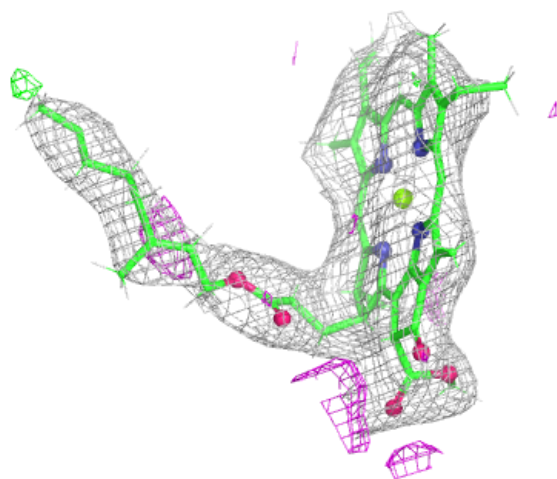
**Electron density around CLA B 3041:**

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



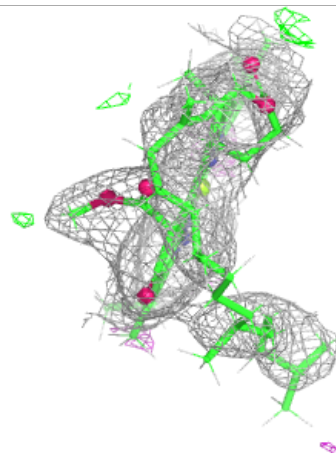
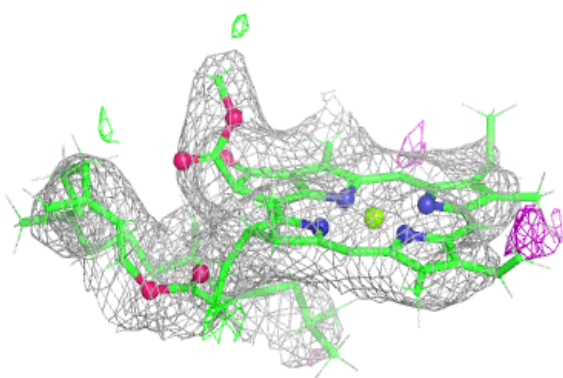
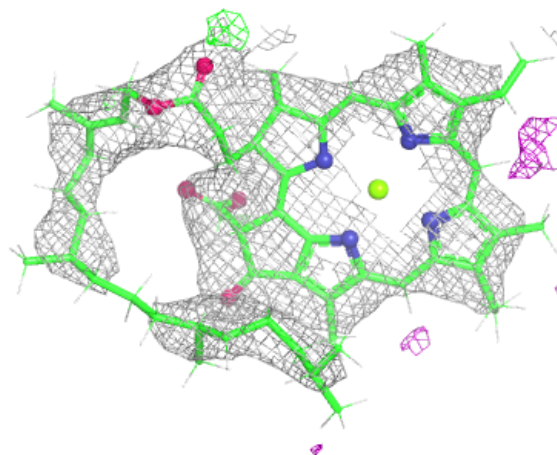
Electron density around CLA B 3005:

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



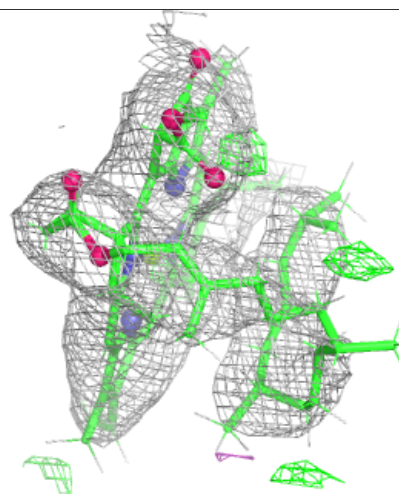
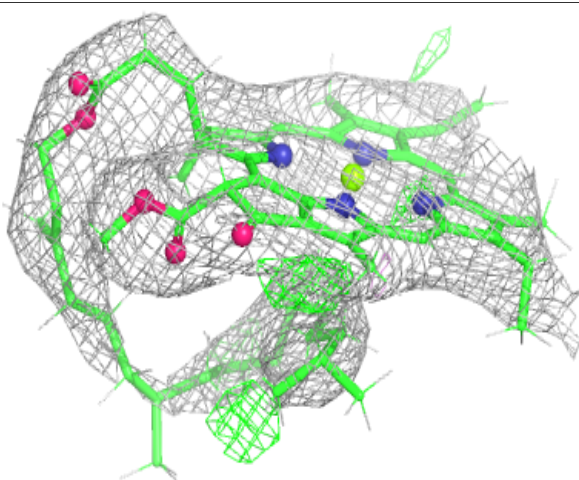
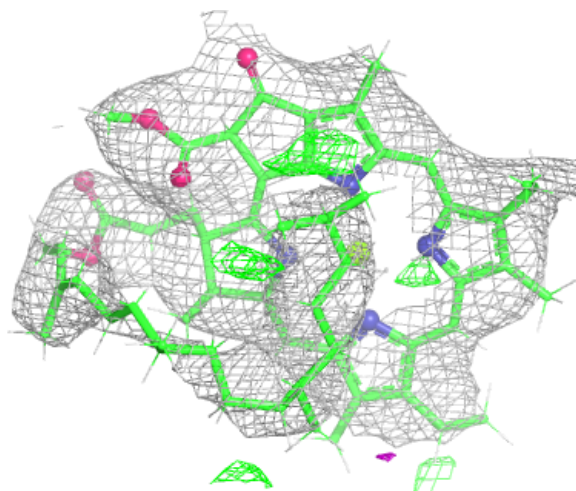
Electron density around CLA B 3006:

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



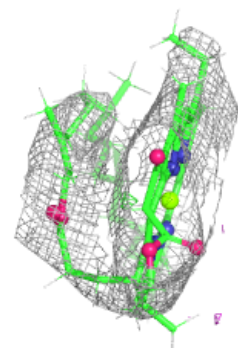
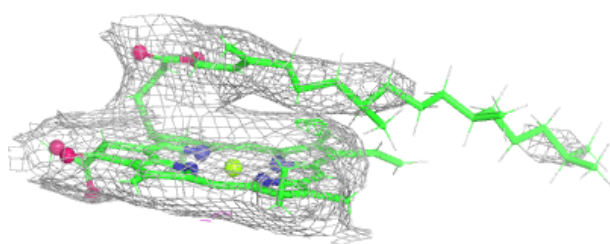
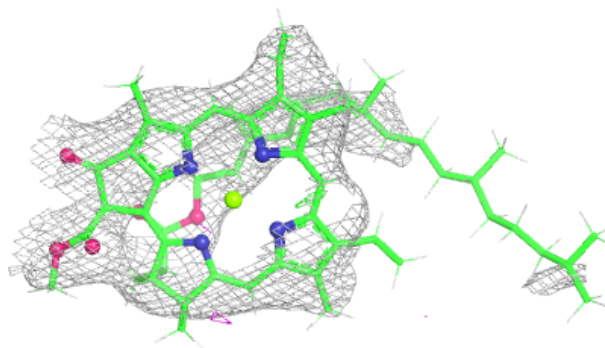
Electron density around CLA B 3007:

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



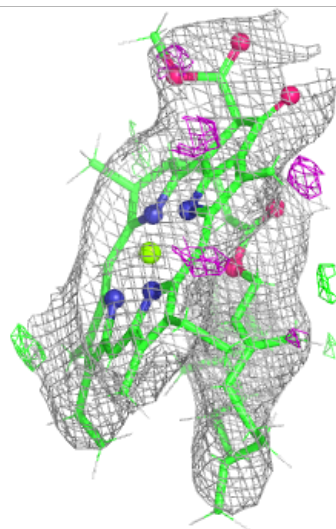
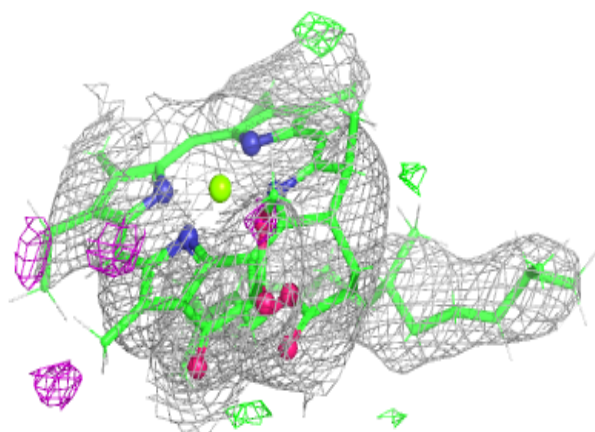
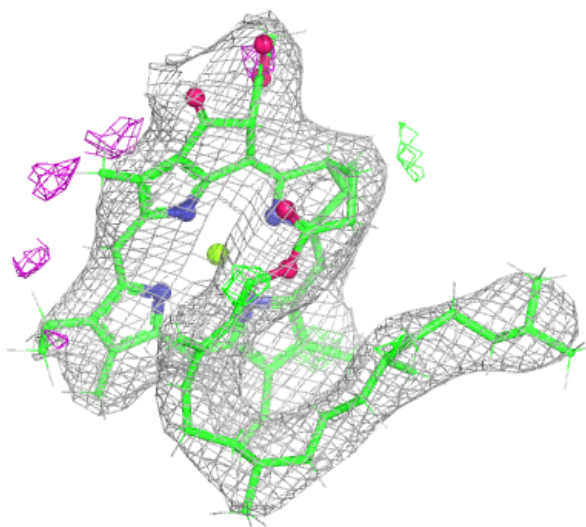
Electron density around CLA A 841:

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



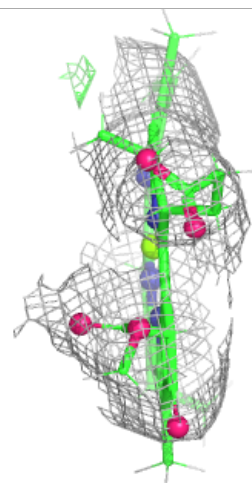
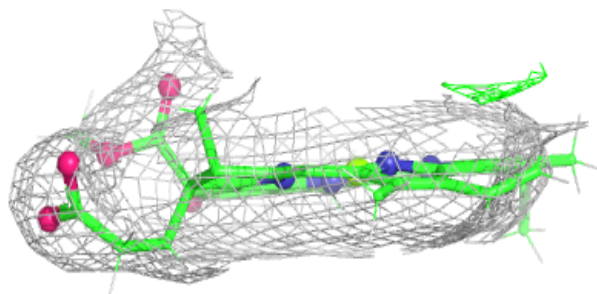
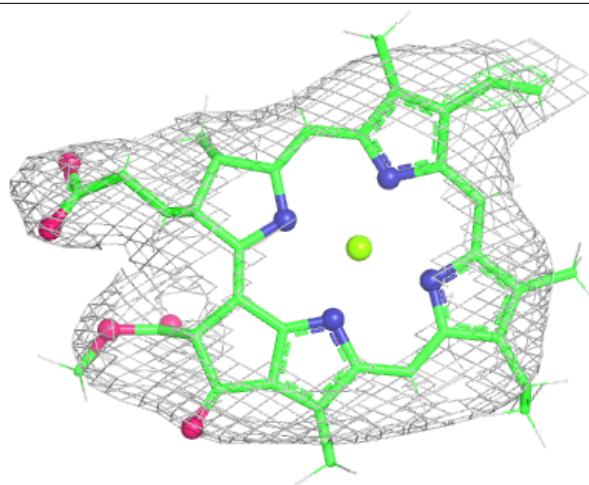
Electron density around CLA B 3009:

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



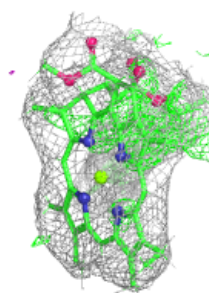
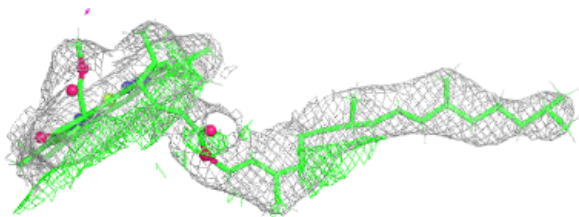
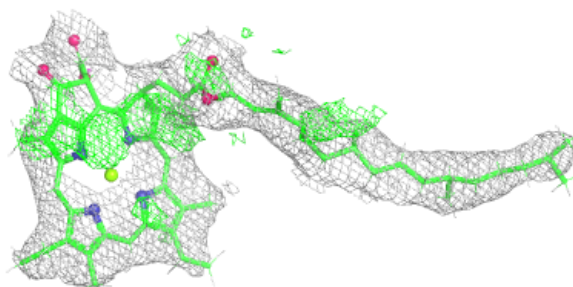
Electron density around CLA B 3037:

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

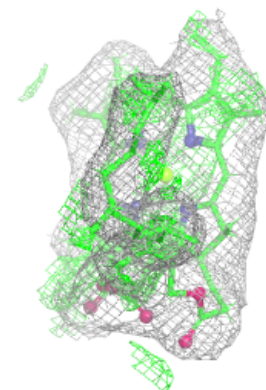
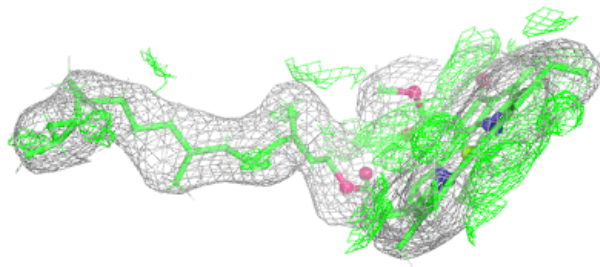
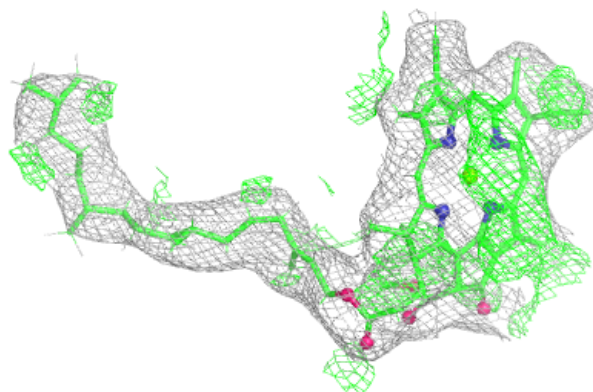


Electron density around CLA A 835:

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

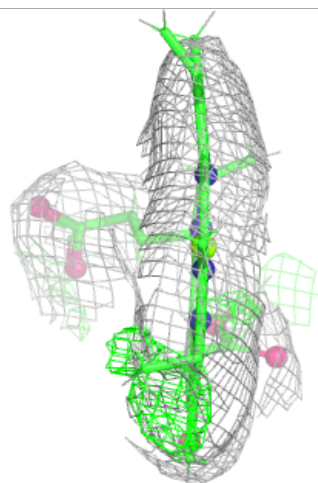
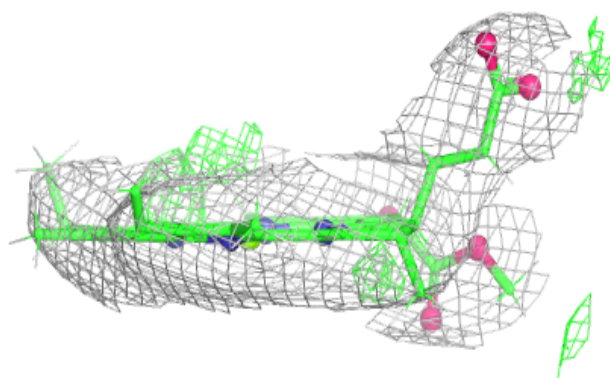
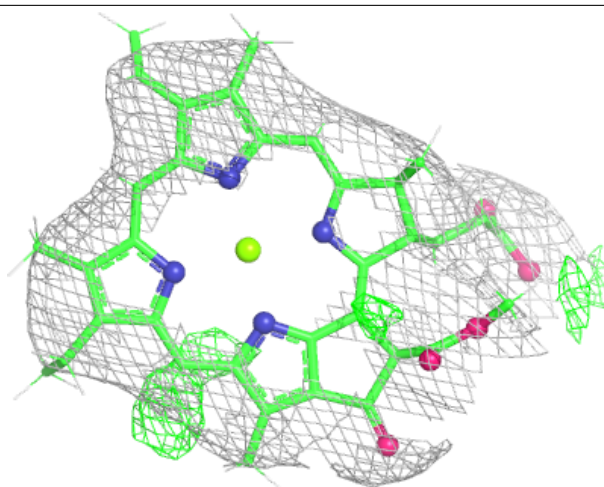
**Electron density around CLA B 3011:**

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



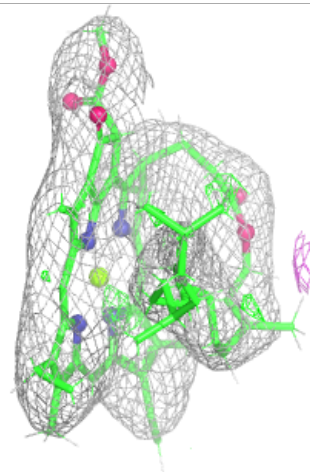
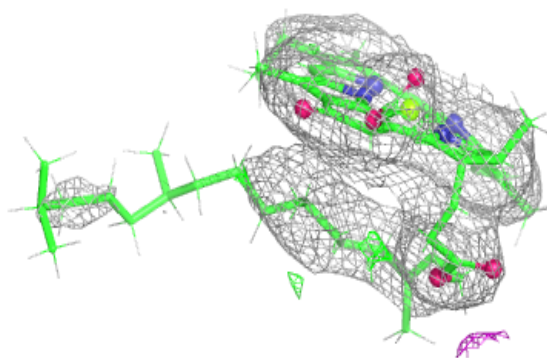
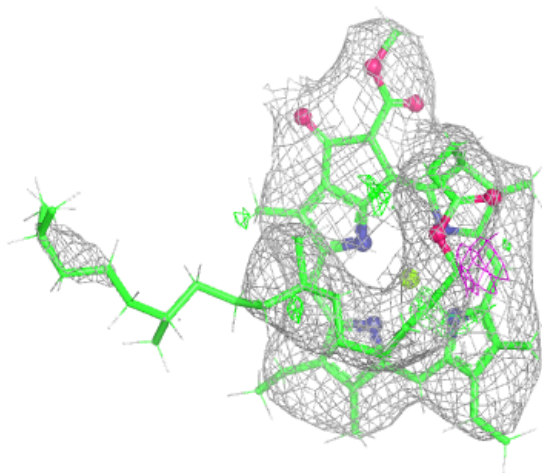
Electron density around CLA B 3024:

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



Electron density around CLA B 3028:

$2mF_o-DF_c$ (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.