



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 06:26 AM UTC

PDB ID : 7DKZ / pdb_00007dkz
Title : Structure of plant photosystem I-light harvesting complex I supercomplex
Authors : Wang, J.; Yu, L.J.; Wang, W.
Deposited on : 2020-11-25
Resolution : 2.39 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

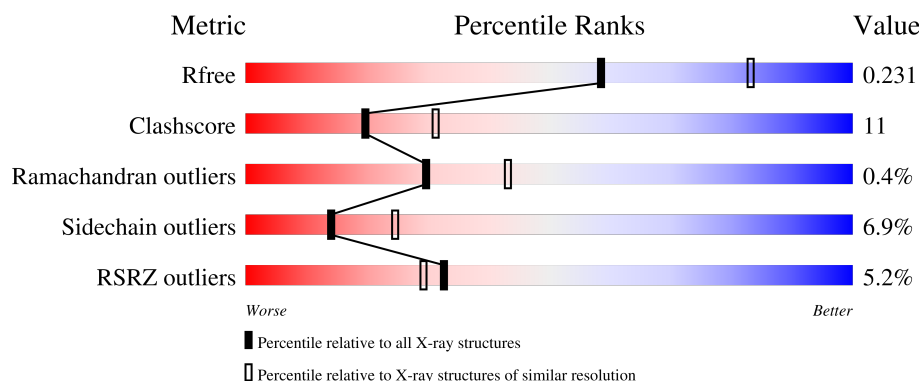
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	1	195	8% 74% 22% .
2	2	269	6% 54% 19% . 24%
3	3	275	8% 63% 14% . 21%
4	4	198	2% 76% 19% . .
5	A	758	3% 77% 19% . .

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Mol	Chain	Length	Quality of chain
6	B	734	
7	C	81	
8	D	143	
9	E	66	
10	F	154	
11	G	97	
12	H	88	
13	I	40	
14	J	42	
15	L	157	
16	K	80	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	1	301	X	-	-	-
17	CLA	1	302	X	-	-	-
17	CLA	1	303	X	-	-	-
17	CLA	1	304	X	-	-	-
17	CLA	1	306	X	-	-	-
17	CLA	1	307	X	-	-	-
17	CLA	1	308	X	-	-	-
17	CLA	1	309	X	-	-	-
17	CLA	1	310	X	-	-	-
17	CLA	1	311	X	-	-	-
17	CLA	1	312	X	-	-	-
17	CLA	1	313	X	-	-	-
17	CLA	2	301	X	-	-	-
17	CLA	2	302	X	-	-	-
17	CLA	2	303	X	-	-	-
17	CLA	2	307	X	-	-	-
17	CLA	2	308	X	-	-	-
17	CLA	2	309	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	2	310	X	-	-	-
17	CLA	2	311	X	-	-	-
17	CLA	2	312	X	-	-	-
17	CLA	2	319	X	-	-	-
17	CLA	3	602	X	-	-	-
17	CLA	3	603	X	-	-	-
17	CLA	3	604	X	-	-	-
17	CLA	3	605	X	-	-	-
17	CLA	3	606	X	-	-	-
17	CLA	3	608	X	-	-	-
17	CLA	3	609	X	-	-	-
17	CLA	3	610	X	-	-	-
17	CLA	3	611	X	-	-	-
17	CLA	3	612	X	-	-	-
17	CLA	3	613	X	-	-	-
17	CLA	4	302	X	-	-	-
17	CLA	4	304	X	-	-	-
17	CLA	4	308	X	-	-	-
17	CLA	4	309	X	-	-	-
17	CLA	4	310	X	-	-	-
17	CLA	4	312	X	-	-	-
17	CLA	4	313	X	-	-	-
17	CLA	4	314	X	-	-	-
17	CLA	A	801	X	-	-	-
17	CLA	A	802	X	-	-	-
17	CLA	A	803	X	-	-	-
17	CLA	A	804	X	-	-	-
17	CLA	A	805	X	-	-	-
17	CLA	A	806	X	-	-	-
17	CLA	A	807	X	-	-	-
17	CLA	A	808	X	-	-	-
17	CLA	A	809	X	-	-	-
17	CLA	A	810	X	-	-	-
17	CLA	A	811	X	-	-	-
17	CLA	A	812	X	-	-	-
17	CLA	A	813	X	-	-	-
17	CLA	A	814	X	-	-	-
17	CLA	A	815	X	-	-	-
17	CLA	A	816	X	-	-	-
17	CLA	A	817	X	-	-	-
17	CLA	A	818	X	-	-	-
17	CLA	A	819	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	A	820	X	-	-	-
17	CLA	A	821	X	-	-	-
17	CLA	A	822	X	-	-	-
17	CLA	A	823	X	-	-	-
17	CLA	A	824	X	-	-	-
17	CLA	A	825	X	-	-	-
17	CLA	A	826	X	-	-	-
17	CLA	A	827	X	-	-	-
17	CLA	A	828	X	-	-	-
17	CLA	A	829	X	-	-	-
17	CLA	A	830	X	-	-	-
17	CLA	A	831	X	-	-	-
17	CLA	A	832	X	-	-	-
17	CLA	A	833	X	-	-	-
17	CLA	A	834	X	-	-	-
17	CLA	A	835	X	-	-	-
17	CLA	A	836	X	-	-	-
17	CLA	A	837	X	-	-	-
17	CLA	A	838	X	-	-	-
17	CLA	A	839	X	-	-	-
17	CLA	A	840	X	-	-	-
17	CLA	A	841	X	-	-	-
17	CLA	A	843	X	-	-	-
17	CLA	A	853	X	-	-	-
17	CLA	B	802	X	-	-	-
17	CLA	B	803	X	-	-	-
17	CLA	B	804	X	-	-	-
17	CLA	B	805	X	-	-	-
17	CLA	B	806	X	-	-	-
17	CLA	B	807	X	-	-	-
17	CLA	B	808	X	-	-	-
17	CLA	B	809	X	-	-	-
17	CLA	B	810	X	-	-	-
17	CLA	B	811	X	-	-	-
17	CLA	B	813	X	-	-	-
17	CLA	B	814	X	-	-	-
17	CLA	B	815	X	-	-	-
17	CLA	B	816	X	-	-	-
17	CLA	B	817	X	-	-	-
17	CLA	B	818	X	-	-	-
17	CLA	B	819	X	-	-	-
17	CLA	B	820	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	B	821	X	-	-	-
17	CLA	B	822	X	-	-	-
17	CLA	B	823	X	-	-	-
17	CLA	B	824	X	-	-	-
17	CLA	B	825	X	-	-	-
17	CLA	B	826	X	-	-	-
17	CLA	B	827	X	-	-	-
17	CLA	B	828	X	-	-	-
17	CLA	B	829	X	-	-	-
17	CLA	B	830	X	-	-	-
17	CLA	B	831	X	-	-	-
17	CLA	B	832	X	-	-	-
17	CLA	B	833	X	-	-	-
17	CLA	B	834	X	-	-	-
17	CLA	B	835	X	-	-	-
17	CLA	B	836	X	-	-	-
17	CLA	B	837	X	-	-	-
17	CLA	B	838	X	-	-	-
17	CLA	B	839	X	-	-	-
17	CLA	B	840	X	-	-	-
17	CLA	B	841	X	-	-	-
17	CLA	B	842	X	-	-	-
17	CLA	F	304	X	-	-	-
17	CLA	F	306	X	-	-	-
17	CLA	F	307	X	-	-	-
17	CLA	G	103	X	-	-	-
17	CLA	G	104	X	-	-	-
17	CLA	G	105	X	-	-	-
17	CLA	J	101	X	-	-	-
17	CLA	J	103	X	-	-	-
17	CLA	K	201	X	-	-	-
17	CLA	K	202	X	-	-	-
17	CLA	L	202	X	-	-	-
17	CLA	L	203	X	-	-	-
18	CHL	1	305	X	-	-	-
18	CHL	2	304	X	-	-	-
18	CHL	2	305	X	-	-	-
18	CHL	2	306	X	-	-	-
18	CHL	2	313	X	-	-	-
18	CHL	3	601	X	-	-	-
18	CHL	3	607	X	-	-	-
18	CHL	4	301	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CHL	4	305	X	-	-	-
18	CHL	4	306	X	-	-	-
18	CHL	4	307	X	-	-	-
18	CHL	4	315	X	-	-	-
19	LUT	4	316	-	X	-	-
20	XAT	4	317	X	-	-	-
26	DGD	4	323	-	-	X	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 36093 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lhca1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	195	Total	C	N	O	S	0	0	0
			1507	979	252	271	5			

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	204	Total	C	N	O	S	0	0	0
			1592	1042	261	285	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	216	Total	C	N	O	S	0	0	0
			1661	1088	268	300	5			

- Molecule 4 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	195	Total	C	N	O	S	0	0	0
			1535	1006	249	277	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	89	LYS	ARG	conflict	UNP Q9SQL2
4	128	ASP	ALA	conflict	UNP Q9SQL2
4	149	PHE	SER	conflict	UNP Q9SQL2

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	742	Total	C	N	O	S	0	0	0
			5852	3835	997	1002	18			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	ILE	VAL	conflict	UNP A0A0F6NFW5

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	733	Total	C	N	O	S	0	0	0
			5856	3848	998	996	14			

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

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

- Molecule 8 is a protein called PsaD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	D	140	Total	C	N	O	S	0	0	0
			1110	716	191	200	3			

- Molecule 9 is a protein called PsaE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	E	63	Total	C	N	O	0	0	0
			505	320	89	96			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	PRO	-	expression tag	UNP E1C9K6
E	0	PRO	-	expression tag	UNP E1C9K6
E	14	GLN	LYS	conflict	UNP E1C9K6
E	60	VAL	-	expression tag	UNP E1C9K6
E	61	GLU	-	expression tag	UNP E1C9K6
E	62	GLU	-	expression tag	UNP E1C9K6
E	63	VAL	-	expression tag	UNP E1C9K6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	64	LYS	-	expression tag	UNP E1C9K6

- Molecule 10 is a protein called PSI-F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	F	152	Total	C	N	O	S	0	0	0
			1198	777	208	211	2			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	79	ALA	SER	conflict	UNP A0A0M3KL12
F	86	ASP	GLU	conflict	UNP A0A0M3KL12
F	107	LEU	ILE	conflict	UNP A0A0M3KL12
F	110	PRO	ALA	conflict	UNP A0A0M3KL12
F	133	GLY	ALA	conflict	UNP A0A0M3KL12
F	187	ASP	GLU	conflict	UNP A0A0M3KL12
F	203	THR	SER	conflict	UNP A0A0M3KL12

- Molecule 11 is a protein called PsaG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	G	95	Total	C	N	O		0	0	0
			737	477	122	138				

- Molecule 12 is a protein called PsaH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	H	88	Total	C	N	O		0	0	0
			673	442	106	125				

- Molecule 13 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	I	30	Total	C	N	O	S	0	0	0
			226	156	34	35	1			

- Molecule 14 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	J	39	Total	C	N	O	S	0	0	0
			309	208	48	52	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	32	PHE	LEU	conflict	UNP D5MAL3

- Molecule 15 is a protein called PsaL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	L	151	Total	C	N	O	S	0	0	0
			1122	737	182	202	1			

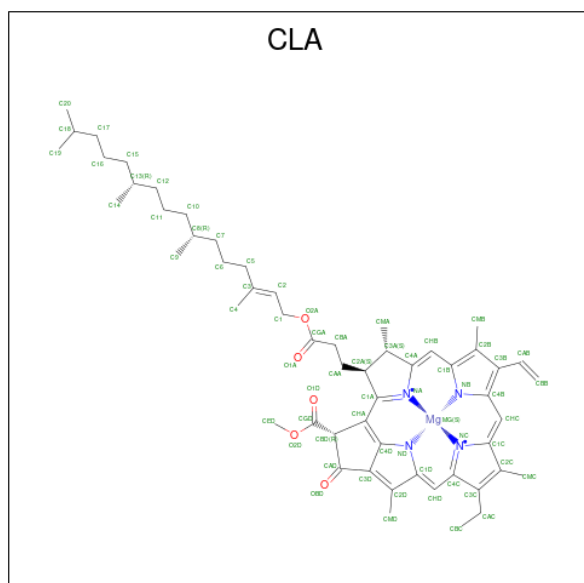
- Molecule 16 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	K	77	Total	C	N	O	S	0	0	0
			515	326	86	100	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	85	ALA	VAL	conflict	UNP E1C9L3

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	2	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			43	35	1	4	3		
17	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	3	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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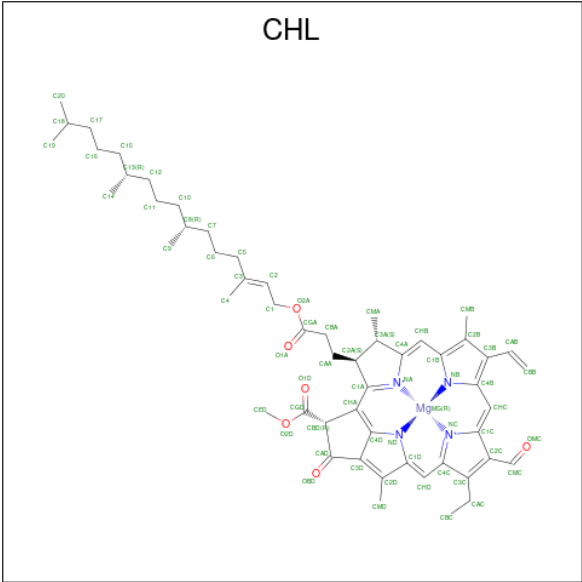
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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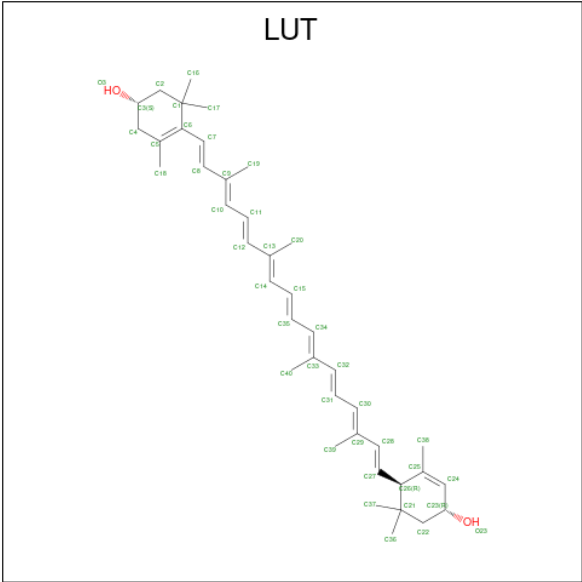
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	F	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	G	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	G	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	G	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	J	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	J	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	K	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		

- Molecule 18 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



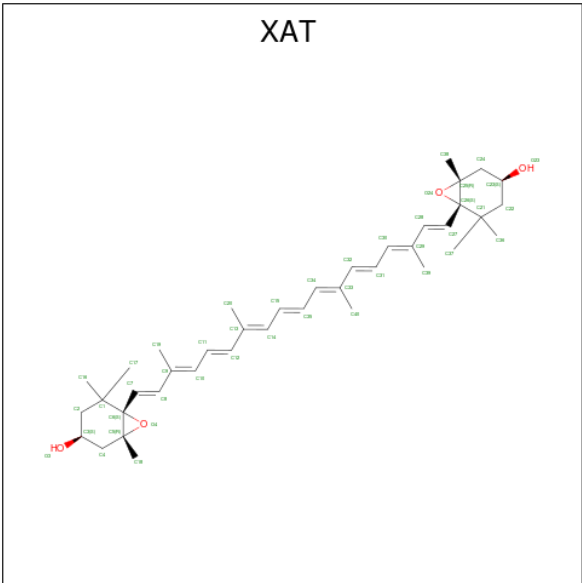
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	1	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
18	2	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
18	2	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
18	2	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
18	2	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
18	3	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
18	3	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
18	4	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
18	4	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
18	4	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
18	4	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
18	4	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		

- Molecule 19 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



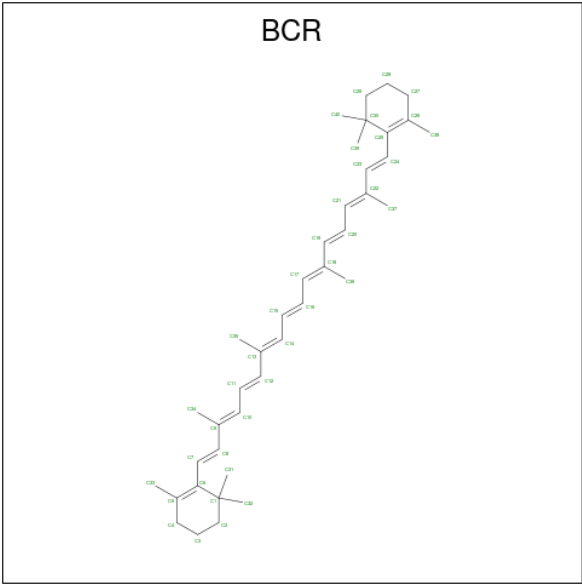
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	1	1	Total	C	O	0	0
			42	40	2		
19	2	1	Total	C	O	0	0
			42	40	2		
19	3	1	Total	C	O	0	0
			42	40	2		
19	4	1	Total	C	O	0	0
			42	40	2		

- Molecule 20 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	1	1	Total	C	O	0	0
			44	40	4		
20	2	1	Total	C	O	0	0
			44	40	4		
20	3	1	Total	C	O	0	0
			44	40	4		
20	4	1	Total	C	O	0	0
			44	40	4		

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



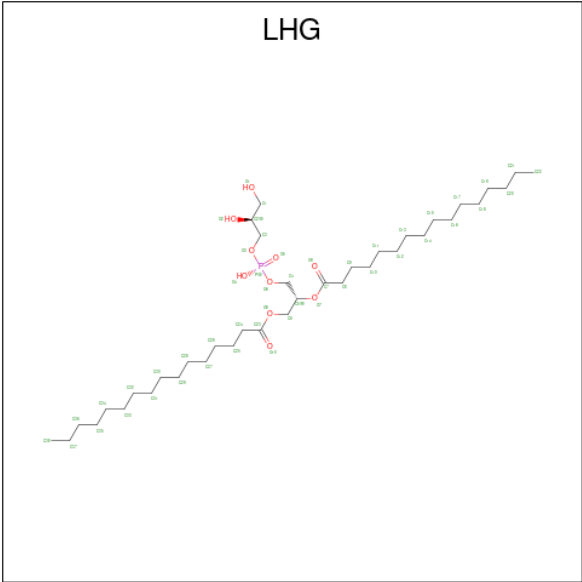
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	1	1	Total	C	0	0
			40	40		
21	2	1	Total	C	0	0
			40	40		
21	3	1	Total	C	0	0
			40	40		
21	4	1	Total	C	0	0
			40	40		
21	A	1	Total	C	0	0
			40	40		
21	A	1	Total	C	0	0
			40	40		
21	A	1	Total	C	0	0
			40	40		
21	A	1	Total	C	0	0
			40	40		

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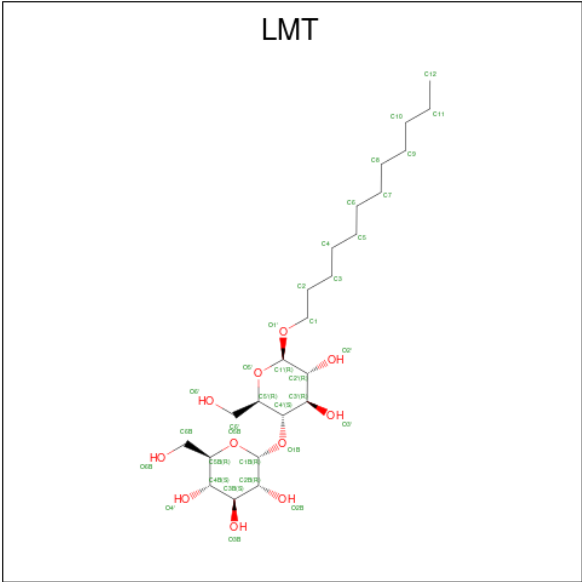
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	F	1	Total C 40 40	0	0
21	F	1	Total C 40 40	0	0
21	G	1	Total C 40 40	0	0
21	I	1	Total C 40 40	0	0
21	J	1	Total C 40 40	0	0
21	J	1	Total C 40 40	0	0
21	L	1	Total C 40 40	0	0
21	L	1	Total C 40 40	0	0
21	L	1	Total C 40 40	0	0
21	K	1	Total C 40 40	0	0

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



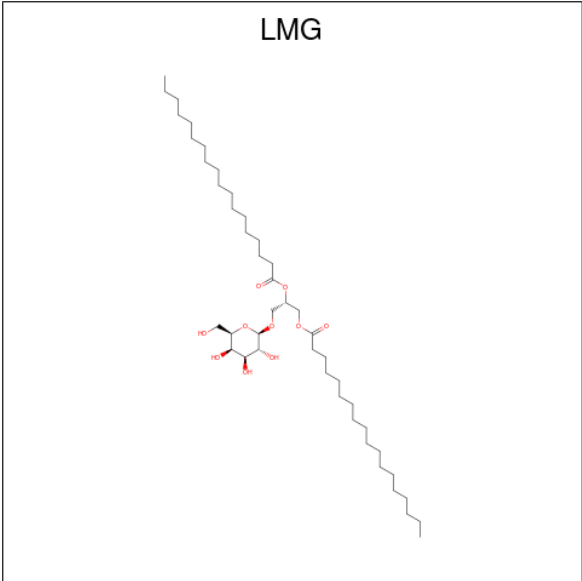
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	1	1	Total	C	O	P	0	0
			49	38	10	1		
22	2	1	Total	C	O	P	0	0
			37	26	10	1		
22	A	1	Total	C	O	P	0	0
			49	38	10	1		
22	A	1	Total	C	O	P	0	0
			27	16	10	1		
22	B	1	Total	C	O	P	0	0
			23	12	10	1		
22	F	1	Total	C	O	P	0	0
			40	29	10	1		
22	G	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 23 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	2	1	Total	C	O	0	0
			35	24	11		
23	A	1	Total	C	O	0	0
			35	24	11		

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



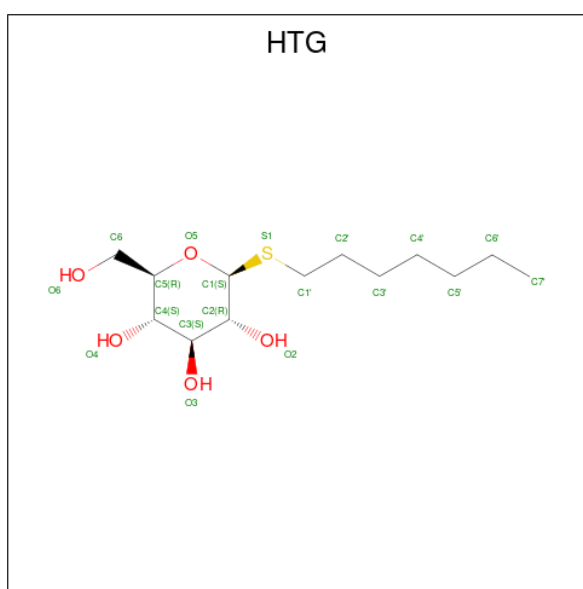
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	4	1	Total	C	O	0	0
			50	40	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	4	1	Total	C	O	0	0
			49	39	10		
24	B	1	Total	C	O	0	0
			52	42	10		
24	F	1	Total	C	O	0	0
			55	45	10		
24	G	1	Total	C	O	0	0
			40	30	10		

- Molecule 25 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



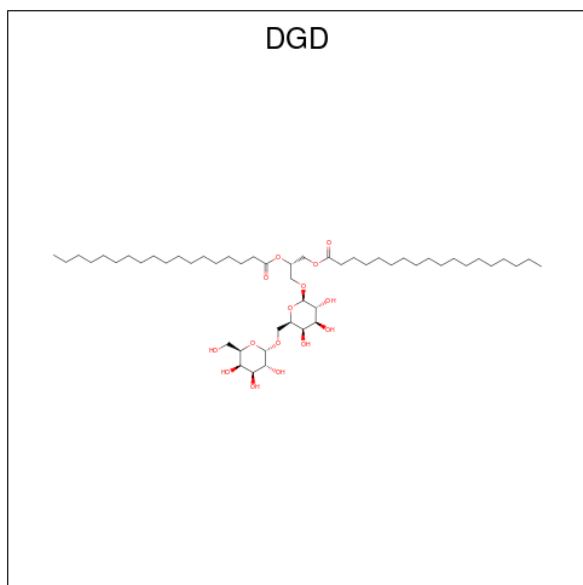
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	4	1	Total	C	O	S	0	0
			19	13	5	1		
25	4	1	Total	C	O	S	0	0
			19	13	5	1		
25	A	1	Total	C	O	S	0	0
			19	13	5	1		
25	B	1	Total	C	O	S	0	0
			19	13	5	1		
25	F	1	Total	C	O	S	0	0
			17	11	5	1		
25	F	1	Total	C	O	S	0	0
			19	13	5	1		
25	F	1	Total	C	O	S	0	0
			16	10	5	1		

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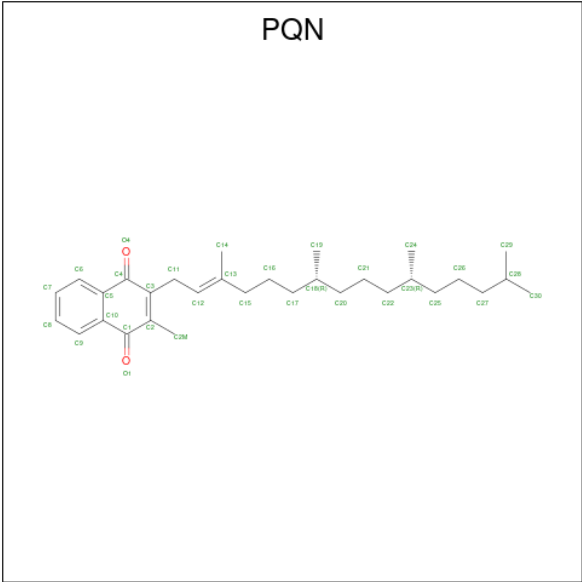
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	J	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



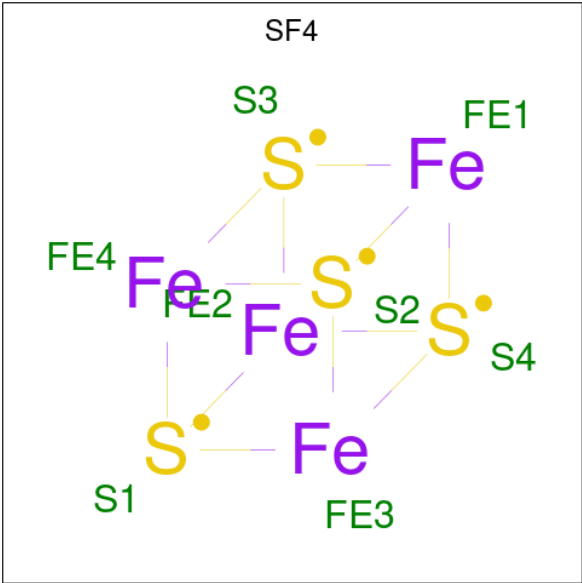
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	4	1	Total	C	O	0	0
			60	45	15		
26	B	1	Total	C	O	0	0
			66	51	15		

- Molecule 27 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 28 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	Fe	S	0	0
			8	4	4		
28	C	1	Total	Fe	S	0	0
			8	4	4		

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

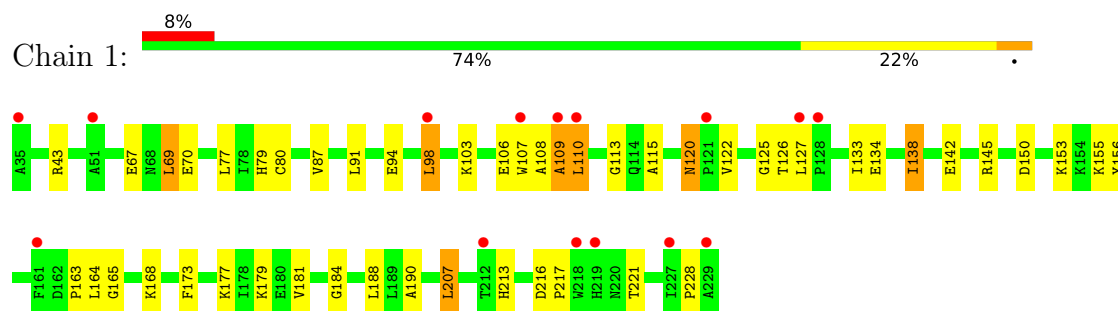
- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	1	3	Total	O	0	0
			3	3		
29	2	5	Total	O	0	0
			5	5		
29	3	3	Total	O	0	0
			3	3		
29	4	7	Total	O	0	0
			7	7		
29	A	25	Total	O	0	0
			25	25		
29	B	39	Total	O	0	0
			39	39		
29	C	3	Total	O	0	0
			3	3		
29	F	5	Total	O	0	0
			5	5		
29	G	1	Total	O	0	0
			1	1		
29	J	1	Total	O	0	0
			1	1		
29	L	1	Total	O	0	0
			1	1		

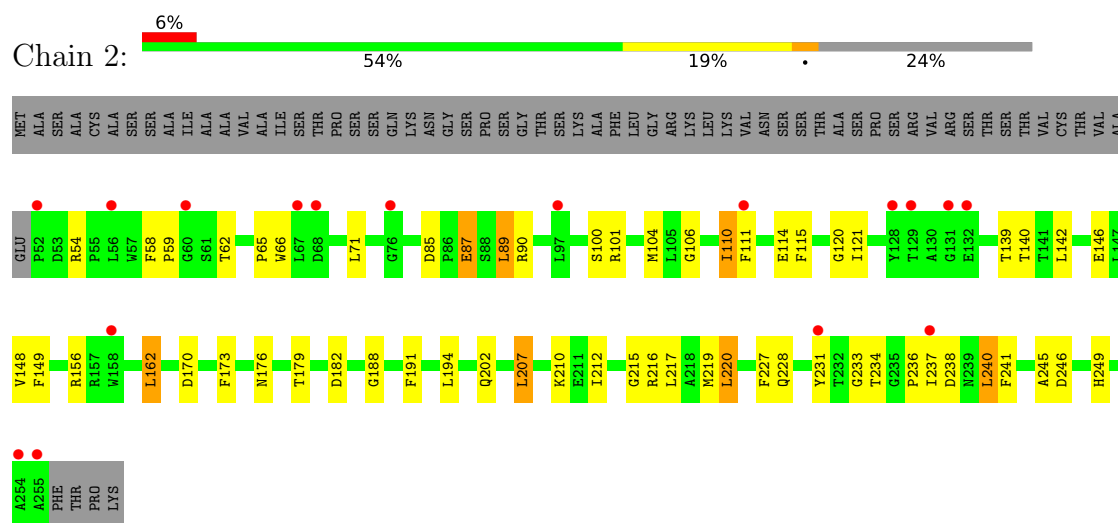
3 Residue-property plots [i](#)

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.

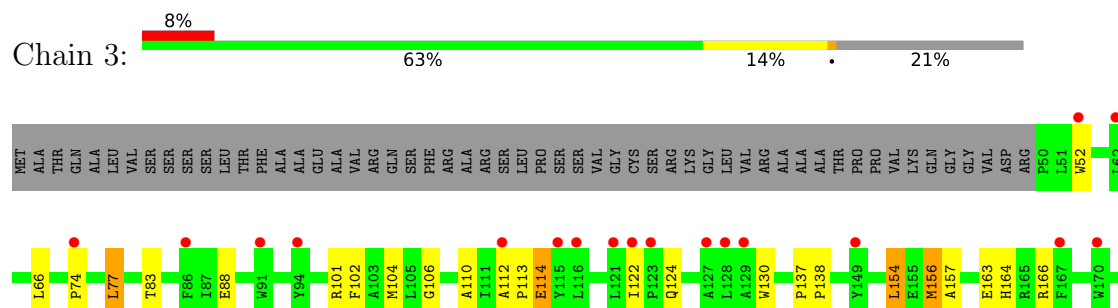
- Molecule 1: Lhca1



- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

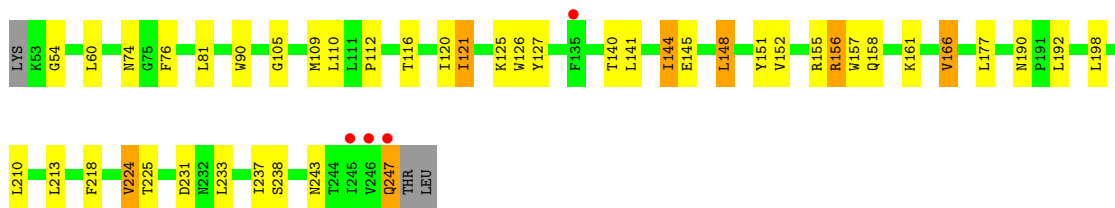
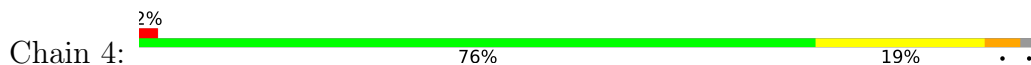


- Molecule 3: Chlorophyll a-b binding protein 3, chloroplastic

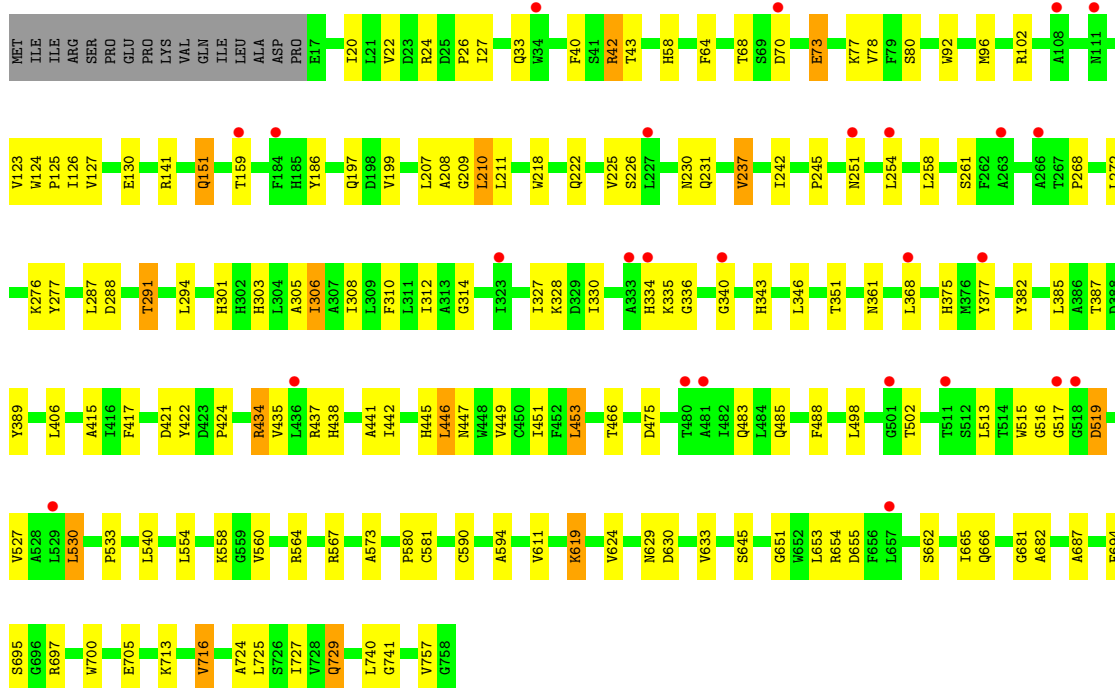
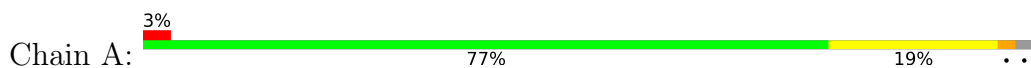




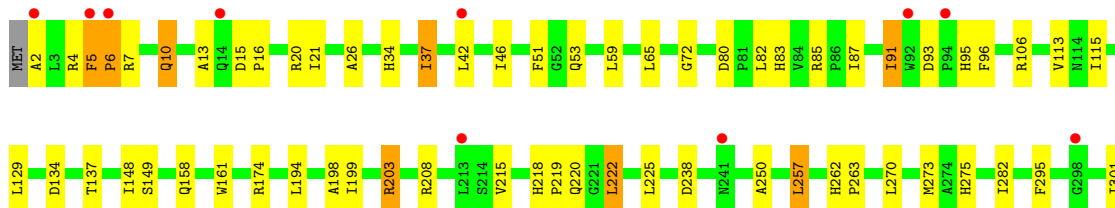
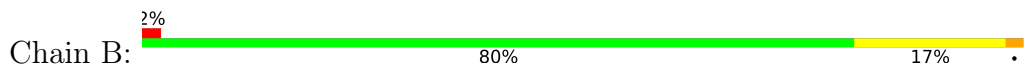
- Molecule 4: Chlorophyll a-b binding protein P4, chloroplastic

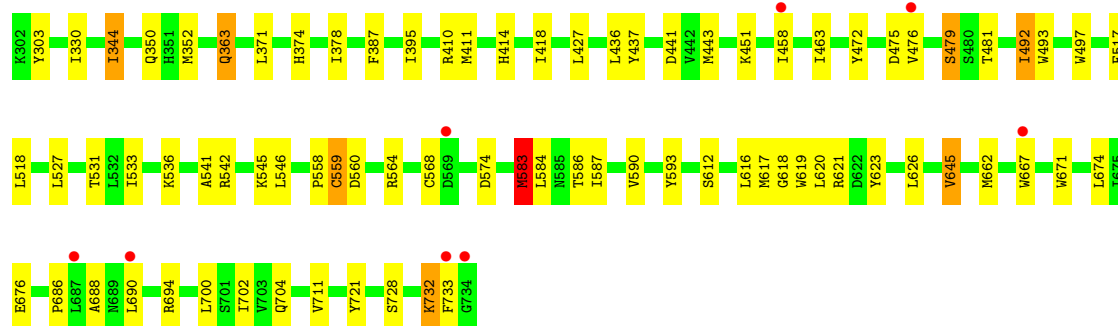


- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

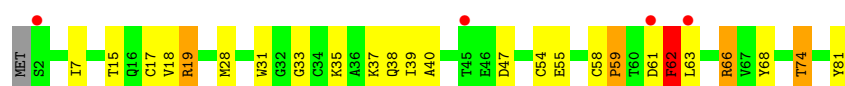


- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

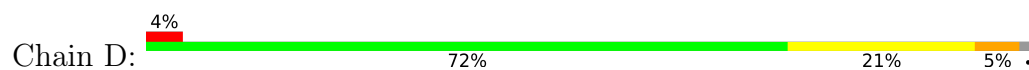




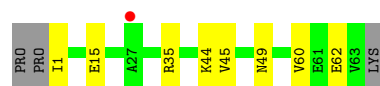
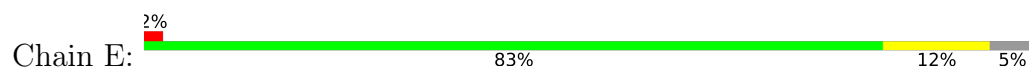
• Molecule 7: Photosystem I iron-sulfur center



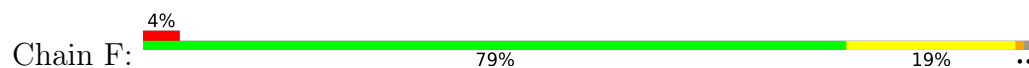
• Molecule 8: PsaD



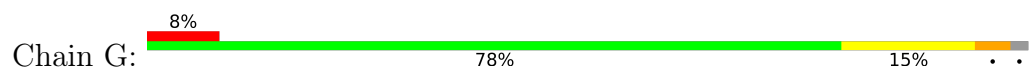
• Molecule 9: PsaE

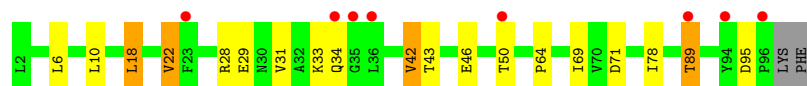


• Molecule 10: PSI-F

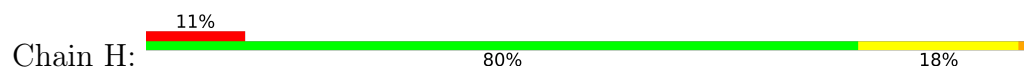


• Molecule 11: PsaG

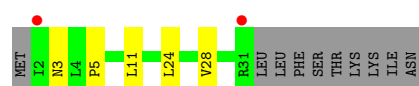




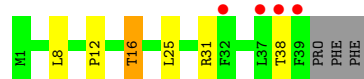
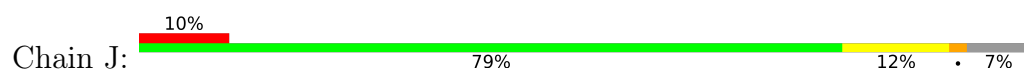
• Molecule 12: PsaH



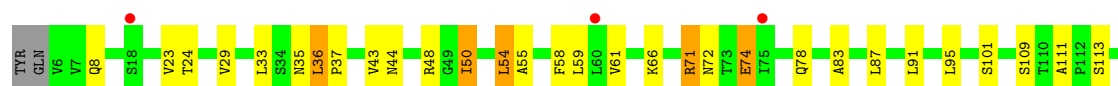
• Molecule 13: Photosystem I reaction center subunit VIII



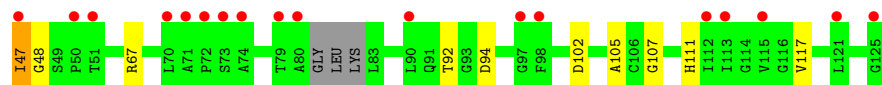
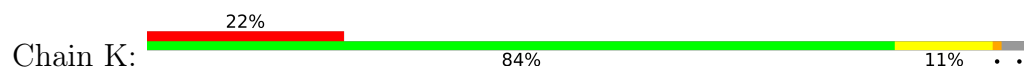
• Molecule 14: Photosystem I reaction center subunit IX



• Molecule 15: PsaL



• Molecule 16: PSI-K



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	225.65Å 168.95Å 185.22Å 90.00° 121.39° 90.00°	Depositor
Resolution (Å)	44.41 – 2.39 44.41 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.9 (44.41-2.39) 98.9 (44.41-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.189 , 0.227 0.195 , 0.231	Depositor DCC
R_{free} test set	11616 reflections (4.10%)	wwPDB-VP
Wilson B-factor (Å ²)	65.4	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 70.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	36093	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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: LMT, CHL, LUT, HTG, PQN, XAT, LHG, LMG, CLA, BCR, SF4, DGD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.28	0/1557	0.45	0/2127
2	2	0.21	0/1651	0.40	0/2262
3	3	0.14	0/1713	0.32	0/2326
4	4	0.45	0/1584	0.65	0/2159
5	A	0.30	0/6050	0.47	0/8254
6	B	0.46	1/6068 (0.0%)	0.65	1/8286 (0.0%)
7	C	0.99	2/624 (0.3%)	1.30	10/846 (1.2%)
8	D	0.31	0/1140	0.54	0/1540
9	E	0.39	0/515	0.56	0/700
10	F	0.46	0/1226	0.68	0/1658
11	G	0.54	0/755	0.70	0/1027
12	H	0.19	0/693	0.34	0/942
13	I	0.39	0/232	0.42	0/317
14	J	0.40	0/317	0.57	0/432
15	L	0.19	0/1153	0.36	0/1576
16	K	0.12	0/520	0.30	0/707
All	All	0.39	3/25798 (0.0%)	0.56	11/35159 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	C	1	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	59	PRO	N-CA	17.60	1.69	1.47
7	C	58	CYS	C-N	9.29	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	6	PRO	C-O	-5.05	1.17	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	58	CYS	CA-C-N	16.34	137.69	120.04
7	C	58	CYS	C-N-CA	16.34	137.69	120.04
7	C	62	PHE	CB-CA-C	11.20	132.72	110.42
7	C	62	PHE	CA-CB-CG	-6.52	107.28	113.80
7	C	59	PRO	CA-N-CD	-6.52	102.88	112.00
7	C	62	PHE	N-CA-CB	6.00	120.63	110.49
7	C	61	ASP	N-CA-CB	5.99	119.42	109.60
7	C	61	ASP	CA-C-N	5.28	131.62	121.54
7	C	61	ASP	C-N-CA	5.28	131.62	121.54
7	C	61	ASP	CA-CB-CG	-5.22	107.38	112.60
6	B	583	MET	CG-SD-CE	5.02	111.94	100.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	C	62	PHE	CA

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	1	1507	0	1468	35	0
2	2	1592	0	1531	52	0
3	3	1661	0	1620	37	0
4	4	1535	0	1496	41	0
5	A	5852	0	5713	102	0
6	B	5856	0	5653	113	0
7	C	611	0	591	19	0
8	D	1110	0	1123	19	0
9	E	505	0	503	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	F	1198	0	1228	19	0
11	G	737	0	721	13	0
12	H	673	0	667	12	0
13	I	226	0	242	3	0
14	J	309	0	320	5	0
15	L	1122	0	1133	27	0
16	K	515	0	513	5	0
17	1	672	0	636	29	0
17	2	533	0	480	18	0
17	3	542	0	433	16	0
17	4	540	0	476	22	0
17	A	2582	0	2646	114	0
17	B	2493	0	2566	109	0
17	F	165	0	154	8	0
17	G	137	0	101	5	0
17	J	107	0	103	5	0
17	K	105	0	92	5	0
17	L	180	0	183	12	0
18	1	48	0	33	4	0
18	2	185	0	128	14	0
18	3	103	0	72	20	0
18	4	262	0	207	29	0
19	1	42	0	56	7	0
19	2	42	0	56	4	0
19	3	42	0	56	4	0
19	4	42	0	56	3	0
20	1	44	0	56	3	0
20	2	44	0	56	9	0
20	3	44	0	56	12	0
20	4	44	0	56	9	0
21	1	40	0	56	0	0
21	2	40	0	56	9	0
21	3	40	0	56	4	0
21	4	40	0	56	14	0
21	A	240	0	336	25	0
21	B	240	0	336	25	0
21	F	80	0	112	3	0
21	G	40	0	56	2	0
21	I	40	0	56	4	0
21	J	80	0	112	7	0
21	K	40	0	56	5	0
21	L	120	0	168	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	1	49	0	74	6	0
22	2	37	0	44	6	0
22	A	76	0	98	3	0
22	B	23	0	16	1	0
22	F	40	0	53	2	0
22	G	49	0	74	2	0
23	2	35	0	46	3	0
23	A	35	0	45	2	0
24	4	99	0	143	7	0
24	B	52	0	77	4	0
24	F	55	0	86	1	0
24	G	40	0	53	3	0
25	4	38	0	52	4	0
25	A	19	0	26	0	0
25	B	19	0	26	1	0
25	F	52	0	62	2	0
25	J	19	0	26	3	0
26	4	60	0	81	29	0
26	B	66	0	96	7	0
27	A	33	0	46	6	0
27	B	33	0	46	3	0
28	A	8	0	0	0	0
28	C	16	0	0	0	0
29	1	3	0	0	0	0
29	2	5	0	0	0	0
29	3	3	0	0	0	0
29	4	7	0	0	0	0
29	A	25	0	0	1	0
29	B	39	0	0	2	0
29	C	3	0	0	0	0
29	F	5	0	0	0	0
29	G	1	0	0	0	0
29	J	1	0	0	0	0
29	L	1	0	0	0	0
All	All	36093	0	36006	826	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 11.

All (826) 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)
7:C:59:PRO:N	7:C:59:PRO:CA	1.69	1.32
6:B:303:TYR:CD2	11:G:34:GLN:HB3	1.94	1.03
3:3:74:PRO:HD2	20:3:615:XAT:O23	1.57	1.02
3:3:229:MET:HB3	20:3:615:XAT:H402	1.42	1.02
17:3:602:CLA:HAB	20:3:615:XAT:H32	1.44	0.99
26:4:323:DGD:C6B	26:4:323:DGD:HBE1	1.96	0.96
26:4:323:DGD:HBE1	26:4:323:DGD:HB61	1.48	0.95
2:2:219:MET:HB3	20:2:315:XAT:H402	1.46	0.95
6:B:303:TYR:CG	11:G:34:GLN:HB3	2.03	0.94
18:3:601:CHL:C10	18:3:601:CHL:C7	2.49	0.91
26:4:323:DGD:HBT1	26:4:323:DGD:HBF1	1.50	0.91
26:4:323:DGD:HD1	26:4:323:DGD:HG12	1.53	0.90
3:3:101:ARG:NH1	3:3:221:GLU:OE2	2.07	0.88
18:3:601:CHL:C7	18:3:601:CHL:C9	2.52	0.88
21:A:851:BCR:H362	17:A:853:CLA:H42	1.58	0.86
6:B:5:PHE:HB3	6:B:6:PRO:HD3	1.58	0.86
24:4:320:LMG:H191	24:4:320:LMG:H331	1.56	0.85
18:3:601:CHL:C10	18:3:601:CHL:C9	2.54	0.85
4:4:155:ARG:HG3	18:4:301:CHL:HED3	1.58	0.85
5:A:725:LEU:HB2	27:A:842:PQN:H6	1.59	0.83
16:K:117:VAL:HG22	17:K:202:CLA:HAB	1.62	0.82
4:4:156:ARG:NH1	17:4:308:CLA:O1D	2.13	0.81
17:A:803:CLA:HAB	17:A:810:CLA:H142	1.62	0.81
6:B:574:ASP:OD2	29:B:901:HOH:O	1.96	0.81
26:4:323:DGD:O5E	26:4:323:DGD:O4E	1.93	0.80
7:C:66:ARG:HG2	7:C:68:TYR:CZ	2.16	0.80
26:4:323:DGD:HBT1	26:4:323:DGD:CEB	2.12	0.80
17:A:840:CLA:H42	17:B:802:CLA:H193	1.64	0.79
17:3:603:CLA:HBB1	20:3:615:XAT:H35	1.64	0.79
18:3:607:CHL:HHC	18:3:607:CHL:HBB1	1.64	0.78
17:4:302:CLA:H72	20:4:317:XAT:H30	1.65	0.77
18:4:306:CHL:H12	24:4:320:LMG:H212	1.67	0.76
17:A:838:CLA:H111	17:A:838:CLA:HAB	1.67	0.76
6:B:517:PHE:HA	17:B:838:CLA:HED1	1.67	0.75
5:A:222:GLN:HA	5:A:226:SER:HB3	1.66	0.75
6:B:533:ILE:HD12	17:B:802:CLA:HMD3	1.69	0.74
18:4:301:CHL:H71	21:4:318:BCR:HC7	1.69	0.74
17:A:804:CLA:H61	21:A:848:BCR:HC8	1.70	0.74
17:B:830:CLA:HHC	17:B:830:CLA:HBB1	1.67	0.74
17:A:815:CLA:HHC	17:A:815:CLA:HBB1	1.70	0.73
6:B:583:MET:HE2	6:B:584:LEU:HA	1.69	0.73
14:J:31:ARG:HD3	21:J:105:BCR:H312	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1:303:CLA:H2A	17:1:303:CLA:HED3	1.71	0.73
5:A:725:LEU:HB3	5:A:729:GLN:HG2	1.71	0.72
26:4:323:DGD:HBE2	26:4:323:DGD:HBN1	1.71	0.72
10:F:160:ILE:HD11	21:F:308:BCR:H282	1.71	0.72
5:A:533:PRO:O	5:A:619:LYS:NZ	2.23	0.71
17:B:809:CLA:HHC	17:B:809:CLA:HBB1	1.72	0.71
17:1:311:CLA:HAB	17:1:311:CLA:H122	1.70	0.71
4:4:144:ILE:HD12	4:4:148:LEU:HD22	1.72	0.71
6:B:16:PRO:HG3	7:C:74:THR:HG22	1.72	0.71
6:B:531:THR:HG21	17:B:827:CLA:HAB	1.73	0.71
12:H:89:PHE:HB3	15:L:50:ILE:HD13	1.73	0.71
17:A:853:CLA:H11	6:B:616:LEU:HD12	1.72	0.70
5:A:42:ARG:H	5:A:42:ARG:HD2	1.56	0.70
3:3:74:PRO:CD	20:3:615:XAT:O23	2.39	0.70
1:1:98:LEU:HD13	1:1:103:LYS:HE2	1.73	0.70
2:2:87:GLU:OE1	2:2:90:ARG:NH2	2.23	0.70
10:F:178:ARG:NH2	10:F:219:GLU:OE1	2.23	0.69
5:A:488:PHE:HB3	17:A:835:CLA:H11	1.74	0.69
6:B:711:VAL:HG22	26:B:850:DGD:HBW2	1.76	0.68
18:3:601:CHL:C9	18:3:601:CHL:C6	2.71	0.68
6:B:463:ILE:HD11	17:B:837:CLA:H2	1.75	0.68
6:B:546:LEU:O	6:B:564:ARG:NH1	2.27	0.68
6:B:158:GLN:HB2	6:B:161:TRP:HD1	1.58	0.68
15:L:35:ASN:HB3	17:L:202:CLA:HAC1	1.77	0.67
22:1:317:LHG:HC81	21:4:318:BCR:HC42	1.76	0.67
5:A:26:PRO:HB2	5:A:27:ILE:HD12	1.76	0.67
17:A:805:CLA:H151	17:A:828:CLA:HBB2	1.77	0.67
6:B:700:LEU:HD22	6:B:704:GLN:NE2	2.10	0.67
2:2:110:ILE:HG22	20:2:315:XAT:H41	1.76	0.66
6:B:129:LEU:HD12	6:B:134:ASP:HB3	1.76	0.66
11:G:78:ILE:HG12	24:G:101:LMG:H262	1.76	0.66
1:1:109:ALA:HB2	18:1:305:CHL:HMD3	1.76	0.66
17:A:828:CLA:H61	21:A:848:BCR:H342	1.77	0.66
17:B:810:CLA:H92	21:B:849:BCR:HC7	1.77	0.66
1:1:87:VAL:HG11	19:1:314:LUT:H10	1.77	0.66
26:4:323:DGD:HBN2	26:4:323:DGD:HB91	1.78	0.66
2:2:148:VAL:HG23	2:2:149:PHE:HD1	1.59	0.66
17:2:301:CLA:H72	20:2:315:XAT:H28	1.78	0.65
11:G:42:VAL:HG13	11:G:46:GLU:HB2	1.79	0.65
24:B:852:LMG:H111	24:B:852:LMG:H182	1.77	0.65
22:2:317:LHG:HC82	22:2:317:LHG:H262	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:846:BCR:H353	21:K:203:BCR:H323	1.77	0.65
1:1:79:HIS:HD2	20:1:315:XAT:H15	1.62	0.65
4:4:166:VAL:HG13	18:4:307:CHL:HMC	1.78	0.64
11:G:64:PRO:HG2	17:G:105:CLA:HBC2	1.79	0.64
16:K:67:ARG:NH1	16:K:94:ASP:OD2	2.31	0.64
26:4:323:DGD:HBE1	26:4:323:DGD:C7B	2.28	0.64
22:2:317:LHG:H132	18:3:601:CHL:H2	1.80	0.64
5:A:33:GLN:HB2	17:A:810:CLA:HAA2	1.80	0.64
6:B:583:MET:HE3	6:B:587:ILE:HG13	1.80	0.63
17:A:839:CLA:HHC	17:A:839:CLA:HBB1	1.81	0.63
6:B:222:LEU:HB2	24:B:852:LMG:HC4	1.80	0.63
6:B:617:MET:HE1	6:B:620:LEU:HD23	1.80	0.63
6:B:5:PHE:CB	6:B:6:PRO:HD3	2.29	0.63
17:3:609:CLA:HAB	19:3:614:LUT:H32	1.80	0.63
8:D:210:LEU:HD22	8:D:210:LEU:H	1.63	0.63
5:A:231:GLN:HG2	5:A:258:LEU:HD22	1.81	0.62
17:B:835:CLA:H18	17:B:836:CLA:HBC3	1.81	0.62
22:1:317:LHG:HC42	18:4:301:CHL:HAC2	1.82	0.62
14:J:8:LEU:HB3	25:J:102:HTG:H7'2	1.81	0.62
6:B:527:LEU:O	6:B:531:THR:HG23	2.00	0.62
17:F:306:CLA:HHC	17:F:306:CLA:HBB1	1.80	0.62
1:1:179:LYS:HD3	17:1:310:CLA:HBA1	1.79	0.62
2:2:149:PHE:CD2	21:2:316:BCR:H15C	2.35	0.62
24:4:320:LMG:O5	24:4:320:LMG:O4	2.18	0.62
18:2:306:CHL:HBB2	18:2:313:CHL:C2C	2.30	0.62
4:4:60:LEU:HD21	25:4:321:HTG:S1	2.40	0.62
1:1:145:ARG:NH1	17:1:307:CLA:O1D	2.26	0.62
17:1:304:CLA:H2A	17:1:304:CLA:HED3	1.82	0.61
5:A:335:LYS:H	17:A:843:CLA:HBC3	1.64	0.61
17:A:838:CLA:H91	17:F:306:CLA:HAC2	1.82	0.61
6:B:208:ARG:NE	17:B:816:CLA:HED2	2.15	0.61
18:4:301:CHL:H8	21:4:318:BCR:H311	1.82	0.61
4:4:247:GLN:HE21	4:4:247:GLN:N	1.98	0.61
5:A:716:VAL:HG13	10:F:178:ARG:HG3	1.82	0.61
2:2:149:PHE:HB3	21:2:316:BCR:H17C	1.82	0.61
26:4:323:DGD:HD5	26:4:323:DGD:O2E	2.01	0.61
2:2:106:GLY:HA2	20:2:315:XAT:H181	1.82	0.61
5:A:564:ARG:HA	5:A:573:ALA:HB2	1.82	0.61
22:2:317:LHG:H141	18:3:601:CHL:H52	1.82	0.61
17:K:201:CLA:HMC3	21:K:203:BCR:H311	1.83	0.61
17:A:853:CLA:HHB	17:B:804:CLA:H202	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:443:MET:HA	6:B:443:MET:HE2	1.83	0.61
2:2:149:PHE:HA	21:2:316:BCR:H351	1.83	0.60
18:2:305:CHL:HBB1	18:2:305:CHL:HHC	1.82	0.60
4:4:155:ARG:CG	18:4:301:CHL:HED3	2.29	0.60
24:4:320:LMG:H171	24:4:320:LMG:H311	1.83	0.60
26:4:323:DGD:O2D	26:4:323:DGD:HG2	2.01	0.60
1:1:77:LEU:HD12	1:1:155:LYS:HB2	1.84	0.60
3:3:77:LEU:HD23	17:3:602:CLA:H11	1.83	0.60
18:2:306:CHL:H12	17:2:308:CLA:HBC2	1.83	0.59
26:4:323:DGD:O1B	26:4:323:DGD:HA32	2.01	0.59
12:H:73:TYR:OH	15:L:24:THR:O	2.17	0.59
17:B:809:CLA:H2	21:I:101:BCR:HC42	1.83	0.59
5:A:662:SER:O	5:A:666:GLN:HG2	2.02	0.59
5:A:64:PHE:CD2	17:A:804:CLA:HMC2	2.37	0.59
6:B:91:ILE:HD11	6:B:96:PHE:CE2	2.38	0.59
1:1:120:ASN:N	1:1:120:ASN:OD1	2.36	0.59
11:G:43:THR:OG1	11:G:46:GLU:HG3	2.02	0.59
21:L:205:BCR:H403	21:L:205:BCR:H23C	1.83	0.59
17:A:837:CLA:H111	21:A:849:BCR:H10C	1.85	0.59
6:B:560:ASP:OD2	6:B:564:ARG:NH2	2.36	0.59
17:B:822:CLA:HBC3	21:B:845:BCR:H332	1.85	0.59
4:4:192:LEU:HD12	19:4:316:LUT:H222	1.84	0.58
17:B:803:CLA:HAA1	15:L:24:THR:HG22	1.85	0.58
5:A:558:LYS:HE3	6:B:674:LEU:HB2	1.84	0.58
17:G:104:CLA:HHC	17:G:104:CLA:HBB1	1.83	0.58
26:4:323:DGD:HD1	26:4:323:DGD:C1G	2.24	0.58
18:2:313:CHL:HHC	18:2:313:CHL:HBB1	1.86	0.58
10:F:172:TRP:CD1	10:F:209:GLY:HA3	2.38	0.58
18:4:315:CHL:HHC	18:4:315:CHL:HBB1	1.84	0.58
13:I:24:LEU:HD13	21:L:205:BCR:HC8	1.85	0.58
6:B:65:LEU:HD11	21:B:846:BCR:HC42	1.85	0.58
17:4:303:CLA:HBB1	20:4:317:XAT:H35	1.85	0.58
17:A:841:CLA:H161	15:L:91:LEU:HD21	1.86	0.58
15:L:109:SER:HB3	15:L:123:PRO:HB2	1.85	0.58
12:H:76:ASP:OD1	12:H:76:ASP:N	2.36	0.57
5:A:141:ARG:HG3	10:F:114:PRO:HB3	1.85	0.57
6:B:667:TRP:HA	27:B:843:PQN:H8	1.86	0.57
5:A:124:TRP:CD2	17:A:808:CLA:HED3	2.40	0.57
2:2:110:ILE:HG22	20:2:315:XAT:C4	2.33	0.57
5:A:375:HIS:ND1	17:A:817:CLA:OBD	2.38	0.57
17:A:825:CLA:HMB2	17:A:837:CLA:HBA1	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:204:ARG:HD3	22:F:302:LHG:H272	1.87	0.57
3:3:232:ILE:HG21	20:3:615:XAT:H14	1.87	0.57
4:4:233:LEU:O	4:4:237:ILE:HG13	2.05	0.57
17:A:819:CLA:HBB2	21:A:847:BCR:H333	1.87	0.57
26:4:323:DGD:O1B	26:4:323:DGD:HA41	2.05	0.57
6:B:733:PHE:HD2	12:H:141:ARG:HH21	1.52	0.57
17:B:838:CLA:HMB3	17:B:838:CLA:HBB1	1.86	0.57
17:A:805:CLA:H92	22:A:844:LHG:H351	1.87	0.57
18:4:305:CHL:H2	21:4:318:BCR:H19C	1.86	0.56
6:B:583:MET:HE3	6:B:587:ILE:CG1	2.35	0.56
17:B:812:CLA:H52	15:L:83:ALA:HB2	1.86	0.56
18:4:305:CHL:C2	21:4:318:BCR:H19C	2.35	0.56
17:A:825:CLA:H51	17:A:835:CLA:H51	1.86	0.56
17:A:829:CLA:HBB1	17:A:829:CLA:HMB1	1.87	0.56
17:B:809:CLA:H111	21:I:101:BCR:HC31	1.87	0.56
17:B:828:CLA:H122	21:B:847:BCR:H373	1.87	0.56
8:D:173:TYR:HB3	8:D:175:GLU:OE2	2.04	0.56
3:3:101:ARG:HA	3:3:104:MET:HE3	1.86	0.56
17:B:827:CLA:H43	17:B:835:CLA:HBB2	1.87	0.56
17:1:303:CLA:H2	17:1:304:CLA:HBD	1.87	0.56
17:4:303:CLA:C2C	20:4:317:XAT:H203	2.36	0.56
5:A:268:PRO:HB3	5:A:276:LYS:HD2	1.88	0.56
17:A:801:CLA:HED1	29:A:923:HOH:O	2.04	0.56
6:B:411:MET:HE2	21:B:847:BCR:H402	1.87	0.56
8:D:144:LEU:HB3	8:D:150:ILE:HG12	1.88	0.56
17:G:104:CLA:H3A	21:G:106:BCR:H363	1.87	0.56
17:B:828:CLA:HED1	17:B:835:CLA:HAB	1.88	0.56
7:C:35:LYS:O	7:C:37:LYS:HD3	2.06	0.56
17:B:806:CLA:HBC1	26:B:850:DGD:HAT1	1.87	0.56
22:1:317:LHG:H372	22:1:317:LHG:H192	1.88	0.56
5:A:40:PHE:HB3	17:A:803:CLA:HED2	1.86	0.56
5:A:251:ASN:HB3	5:A:254:LEU:HD13	1.87	0.56
6:B:26:ALA:HB2	26:B:850:DGD:HA32	1.88	0.56
6:B:374:HIS:HB2	17:B:829:CLA:C1B	2.36	0.56
17:B:806:CLA:HBC3	17:B:831:CLA:H41	1.88	0.56
8:D:76:PRO:HG2	8:D:78:THR:HG22	1.87	0.56
5:A:312:ILE:HG22	21:A:846:BCR:H17C	1.87	0.55
17:B:805:CLA:H111	21:B:849:BCR:H362	1.88	0.55
1:1:115:ALA:HB3	1:1:125:GLY:HA3	1.89	0.55
17:3:608:CLA:H12	17:3:613:CLA:HAB	1.88	0.55
4:4:125:LYS:HD2	4:4:127:TYR:OH	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:475:ASP:OD1	15:L:71:ARG:NH2	2.40	0.55
26:4:323:DGD:CBB	26:4:323:DGD:CFB	2.85	0.55
6:B:295:PHE:HB2	17:B:822:CLA:HED1	1.88	0.55
5:A:700:TRP:CZ2	27:A:842:PQN:H2M3	2.42	0.55
15:L:111:ALA:HB2	15:L:127:GLN:HG3	1.88	0.55
5:A:261:SER:HB3	5:A:277:TYR:HD1	1.71	0.55
26:4:323:DGD:CFB	26:4:323:DGD:CAB	2.85	0.54
17:A:836:CLA:HBB1	17:A:836:CLA:HMB3	1.89	0.54
17:B:834:CLA:HHB	25:F:305:HTG:H61	1.88	0.54
24:B:852:LMG:H222	24:B:852:LMG:H291	1.88	0.54
5:A:368:LEU:HD11	17:A:818:CLA:H71	1.89	0.54
6:B:203:ARG:HD2	6:B:250:ALA:HB1	1.89	0.54
17:4:311:CLA:HED3	17:4:311:CLA:H51	1.89	0.54
5:A:209:GLY:HA2	17:A:819:CLA:HBC1	1.88	0.54
17:B:809:CLA:H102	21:I:101:BCR:HC41	1.90	0.54
2:2:100:SER:HB3	2:2:215:GLY:HA3	1.89	0.54
6:B:5:PHE:CD1	6:B:5:PHE:C	2.83	0.54
17:2:301:CLA:HAB	20:2:315:XAT:H32	1.90	0.54
1:1:142:GLU:OE2	1:1:145:ARG:NH2	2.41	0.54
26:4:323:DGD:HBN2	26:4:323:DGD:C9B	2.38	0.54
6:B:671:TRP:CZ2	27:B:843:PQN:H2M3	2.43	0.54
5:A:645:SER:O	5:A:651:GLY:HA3	2.07	0.53
4:4:125:LYS:HE3	4:4:231:ASP:OD2	2.07	0.53
4:4:151:TYR:HB2	18:4:301:CHL:H11	1.89	0.53
4:4:190:ASN:HA	19:4:316:LUT:H24	1.89	0.53
17:B:811:CLA:HMB1	17:B:811:CLA:HBB1	1.90	0.53
16:K:107:GLY:O	16:K:111:HIS:ND1	2.41	0.53
6:B:303:TYR:CG	11:G:34:GLN:CB	2.87	0.53
17:4:302:CLA:HBB1	17:4:302:CLA:HMB3	1.89	0.53
6:B:257:LEU:HG	17:B:819:CLA:HMB2	1.89	0.53
7:C:17:CYS:HB2	7:C:54:CYS:HB2	1.89	0.53
2:2:101:ARG:NH1	18:2:306:CHL:OBD	2.35	0.53
2:2:146:GLU:OE2	18:2:305:CHL:HMC	2.09	0.53
17:4:304:CLA:HBB1	17:4:304:CLA:HMB3	1.90	0.53
5:A:406:LEU:HD21	17:A:805:CLA:H142	1.90	0.53
5:A:441:ALA:O	5:A:445:HIS:ND1	2.41	0.53
21:A:851:BCR:H382	21:A:851:BCR:H23C	1.90	0.53
6:B:443:MET:SD	6:B:451:LYS:HE3	2.49	0.53
15:L:33:LEU:HA	15:L:36:LEU:HD22	1.91	0.53
17:A:818:CLA:H112	17:A:820:CLA:HBB2	1.91	0.53
6:B:15:ASP:HB3	6:B:20:ARG:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:95:LEU:HD21	21:L:205:BCR:H383	1.91	0.53
17:1:304:CLA:HBB2	18:1:305:CHL:HBB2	1.91	0.53
4:4:155:ARG:CG	18:4:301:CHL:CED	2.87	0.53
24:4:320:LMG:H162	24:4:320:LMG:H292	1.89	0.53
6:B:350:GLN:HG3	17:B:827:CLA:HED1	1.90	0.53
17:2:312:CLA:HAA2	3:3:154:LEU:HG	1.91	0.53
4:4:144:ILE:HG13	4:4:145:GLU:N	2.23	0.53
22:1:317:LHG:H132	18:4:301:CHL:H2	1.90	0.52
4:4:247:GLN:N	4:4:247:GLN:NE2	2.57	0.52
5:A:124:TRP:HD1	23:A:855:LMT:H6'2	1.75	0.52
2:2:58:PHE:HE1	18:3:601:CHL:HED3	1.74	0.52
4:4:247:GLN:HE21	4:4:247:GLN:CA	2.21	0.52
5:A:654:ARG:HD2	5:A:655:ASP:OD1	2.10	0.52
17:B:838:CLA:H152	21:F:308:BCR:H23C	1.91	0.52
17:1:304:CLA:HBB2	18:1:305:CHL:CBB	2.39	0.52
17:4:303:CLA:C1C	20:4:317:XAT:H203	2.40	0.52
6:B:497:TRP:CE3	17:B:819:CLA:H11	2.44	0.52
6:B:583:MET:HE2	6:B:584:LEU:CA	2.38	0.52
5:A:530:LEU:HD11	5:A:624:VAL:HA	1.91	0.52
5:A:483:GLN:HB3	5:A:485:GLN:HE21	1.74	0.52
10:F:195:ILE:HG13	10:F:196:ILE:HG13	1.91	0.52
2:2:71:LEU:HD11	2:2:89:LEU:HD11	1.91	0.52
3:3:74:PRO:HD2	20:3:615:XAT:C23	2.40	0.52
4:4:145:GLU:OE1	18:4:306:CHL:HMC	2.10	0.52
26:4:323:DGD:HBE2	26:4:323:DGD:CFB	2.39	0.52
4:4:112:PRO:O	4:4:116:THR:HG23	2.10	0.52
25:4:321:HTG:H7'3	22:F:302:LHG:H141	1.92	0.52
17:A:823:CLA:HBB	17:A:843:CLA:CBB	2.40	0.52
17:4:302:CLA:HAB	20:4:317:XAT:H32	1.91	0.51
17:A:816:CLA:CHD	17:A:817:CLA:HBB2	2.40	0.51
17:B:827:CLA:CHB	17:B:839:CLA:HBA2	2.40	0.51
1:1:70:GLU:OE2	1:1:155:LYS:NZ	2.33	0.51
5:A:434:ARG:HH11	5:A:437:ARG:HH12	1.56	0.51
6:B:2:ALA:N	6:B:10:GLN:HB2	2.24	0.51
17:B:803:CLA:H92	21:L:206:BCR:H402	1.92	0.51
17:B:837:CLA:C4	17:F:307:CLA:HBB2	2.39	0.51
7:C:47:ASP:OD2	8:D:134:LYS:NZ	2.28	0.51
8:D:188:PHE:HB3	9:E:35:ARG:HH12	1.75	0.51
11:G:89:THR:HG22	24:G:101:LMG:HC72	1.91	0.51
5:A:519:ASP:N	5:A:519:ASP:OD1	2.43	0.51
17:A:814:CLA:H43	21:A:846:BCR:HC41	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:201:CLA:H3A	21:K:203:BCR:H363	1.92	0.51
17:2:303:CLA:HMB2	18:2:304:CHL:HBB1	1.92	0.51
2:2:219:MET:HB3	20:2:315:XAT:C40	2.30	0.51
11:G:34:GLN:O	11:G:34:GLN:HG3	2.10	0.51
5:A:68:THR:HG22	5:A:70:ASP:H	1.76	0.51
6:B:282:ILE:HG21	17:B:818:CLA:H92	1.93	0.51
2:2:176:ASN:HB3	18:2:313:CHL:C2D	2.41	0.51
11:G:18:LEU:HA	11:G:22:VAL:HG13	1.93	0.51
5:A:446:LEU:HD13	5:A:554:LEU:HA	1.92	0.51
21:A:851:BCR:H21C	17:A:853:CLA:H143	1.93	0.51
4:4:155:ARG:NH1	18:4:315:CHL:HMC	2.26	0.50
17:K:201:CLA:H3A	21:K:203:BCR:C36	2.41	0.50
2:2:114:GLU:HG2	2:2:236:PRO:HD2	1.93	0.50
26:4:323:DGD:HBN2	26:4:323:DGD:CAB	2.41	0.50
26:4:323:DGD:C7B	26:4:323:DGD:CBB	2.85	0.50
15:L:71:ARG:NH1	15:L:72:ASN:OD1	2.44	0.50
4:4:90:TRP:NE1	26:4:323:DGD:HE4	2.26	0.50
10:F:199:VAL:O	10:F:203:THR:HG23	2.12	0.50
1:1:91:LEU:HD21	19:1:314:LUT:H173	1.93	0.50
22:1:317:LHG:H301	17:4:314:CLA:HED1	1.94	0.50
17:4:304:CLA:H2	21:4:318:BCR:H272	1.94	0.50
17:1:308:CLA:HHC	19:1:314:LUT:H32	1.93	0.50
17:A:839:CLA:HBB2	27:A:842:PQN:H141	1.94	0.50
6:B:82:LEU:HD22	6:B:363:GLN:HG3	1.94	0.50
21:B:844:BCR:H362	21:G:106:BCR:H312	1.94	0.50
1:1:188:LEU:HB3	20:1:315:XAT:H402	1.94	0.49
5:A:335:LYS:O	17:A:843:CLA:HBC3	2.11	0.49
6:B:411:MET:HG3	21:B:847:BCR:H402	1.94	0.49
17:A:834:CLA:HMB3	21:A:850:BCR:H281	1.93	0.49
6:B:194:LEU:HA	6:B:198:ALA:HB3	1.94	0.49
6:B:593:TYR:CE1	17:B:837:CLA:HBC2	2.47	0.49
14:J:31:ARG:HD3	21:J:105:BCR:C31	2.41	0.49
1:1:190:ALA:HA	17:1:311:CLA:HBB1	1.95	0.49
17:A:806:CLA:H102	17:A:808:CLA:H92	1.94	0.49
1:1:165:GLY:HA3	1:1:168:LYS:HE3	1.93	0.49
2:2:207:LEU:HD22	17:2:308:CLA:HHB	1.93	0.49
26:4:323:DGD:HBT1	26:4:323:DGD:CFB	2.41	0.49
1:1:107:TRP:CZ2	1:1:115:ALA:HB2	2.47	0.49
1:1:177:LYS:O	1:1:181:VAL:HG23	2.13	0.49
3:3:238:GLN:OE1	19:3:614:LUT:H42	2.12	0.49
5:A:125:PRO:HA	5:A:130:GLU:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:819:CLA:HAC2	17:B:826:CLA:H202	1.94	0.49
1:1:216:ASP:OD1	1:1:216:ASP:N	2.43	0.49
15:L:54:LEU:HB3	17:L:202:CLA:HMA1	1.94	0.49
2:2:148:VAL:HG23	2:2:149:PHE:CD1	2.45	0.49
5:A:415:ALA:HB1	5:A:594:ALA:HB1	1.95	0.49
6:B:344:ILE:HD11	17:B:830:CLA:HBC1	1.95	0.49
17:B:837:CLA:H41	17:F:307:CLA:HBB2	1.94	0.49
4:4:140:THR:O	4:4:144:ILE:HG23	2.13	0.49
4:4:155:ARG:NH1	4:4:166:VAL:HG22	2.28	0.49
5:A:665:ILE:HD12	6:B:621:ARG:HG3	1.94	0.49
17:A:832:CLA:H191	17:B:803:CLA:H93	1.93	0.49
2:2:59:PRO:HB2	3:3:176:MET:HE1	1.94	0.49
17:4:314:CLA:HBC2	26:4:323:DGD:HA81	1.95	0.49
17:B:811:CLA:H102	17:B:829:CLA:H193	1.93	0.49
7:C:15:THR:HG22	7:C:28:MET:HG3	1.95	0.49
18:4:307:CHL:CGA	17:4:309:CLA:HMD2	2.43	0.48
5:A:80:SER:OG	5:A:186:TYR:HB2	2.12	0.48
17:A:819:CLA:HBB1	21:A:846:BCR:H14C	1.94	0.48
7:C:31:TRP:HB2	7:C:39:ILE:HG22	1.94	0.48
8:D:200:VAL:HG11	8:D:210:LEU:HD21	1.94	0.48
1:1:155:LYS:HG3	1:1:156:TYR:CD2	2.48	0.48
18:3:601:CHL:HHC	18:3:601:CHL:HBB1	1.95	0.48
5:A:208:ALA:HB2	5:A:314:GLY:HA3	1.95	0.48
17:A:841:CLA:H151	21:L:201:BCR:H351	1.95	0.48
17:3:602:CLA:CAB	20:3:615:XAT:H32	2.30	0.48
6:B:34:HIS:O	6:B:37:ILE:HG13	2.13	0.48
18:4:306:CHL:H3A	18:4:306:CHL:HBA2	1.55	0.48
6:B:218:HIS:HE1	6:B:220:GLN:HG3	1.79	0.48
17:B:821:CLA:H203	17:B:826:CLA:H171	1.95	0.48
21:B:847:BCR:H393	21:B:848:BCR:H383	1.93	0.48
12:H:130:LYS:HE3	12:H:133:GLN:NE2	2.29	0.48
15:L:66:LYS:HE3	17:L:204:CLA:H11	1.96	0.48
5:A:336:GLY:N	22:A:845:LHG:HC32	2.29	0.48
17:B:816:CLA:H141	21:B:845:BCR:H16C	1.95	0.48
5:A:308:ILE:HD12	21:K:203:BCR:HC31	1.94	0.48
17:B:825:CLA:H42	17:B:826:CLA:H112	1.94	0.48
17:B:832:CLA:HBA2	17:B:842:CLA:H41	1.96	0.48
11:G:28:ARG:NH2	11:G:71:ASP:OD2	2.46	0.48
17:1:308:CLA:H92	17:1:308:CLA:H61	1.66	0.48
2:2:106:GLY:O	2:2:110:ILE:HG23	2.13	0.48
17:A:807:CLA:HBA2	17:A:807:CLA:H3A	1.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:164:LEU:HD12	19:1:314:LUT:H222	1.94	0.48
3:3:250:LEU:HB2	19:3:614:LUT:H22	1.96	0.48
6:B:542:ARG:NH2	29:B:906:HOH:O	2.47	0.48
2:2:139:THR:HA	2:2:142:LEU:HD12	1.96	0.48
4:4:224:VAL:HG12	4:4:225:THR:HG23	1.96	0.48
17:A:811:CLA:HHC	17:A:811:CLA:HBB1	1.95	0.48
6:B:106:ARG:NH2	6:B:113:VAL:O	2.41	0.48
17:2:311:CLA:H101	22:2:317:LHG:H311	1.96	0.47
17:A:825:CLA:H3A	17:A:837:CLA:O1A	2.14	0.47
2:2:110:ILE:HG22	20:2:315:XAT:C5	2.44	0.47
17:B:837:CLA:HBB1	17:B:837:CLA:HMB1	1.97	0.47
12:H:65:ASN:OD1	12:H:70:TRP:NE1	2.42	0.47
12:H:82:ASN:HD22	12:H:82:ASN:HA	1.52	0.47
17:1:309:CLA:HBB2	21:4:318:BCR:H322	1.95	0.47
3:3:229:MET:HB3	20:3:615:XAT:C40	2.30	0.47
18:4:306:CHL:HBB1	20:4:317:XAT:H161	1.97	0.47
17:A:809:CLA:H12	17:A:811:CLA:H43	1.95	0.47
17:A:823:CLA:C2	21:A:849:BCR:H16C	2.44	0.47
18:2:306:CHL:HMB3	21:2:316:BCR:H16C	1.95	0.47
3:3:112:ALA:HB3	3:3:113:PRO:HD3	1.96	0.47
4:4:157:TRP:CE2	4:4:161:LYS:HD2	2.50	0.47
11:G:69:ILE:HD12	11:G:69:ILE:H	1.79	0.47
12:H:85:GLN:HE22	17:L:202:CLA:H202	1.79	0.47
4:4:151:TYR:HE2	18:4:307:CHL:CBB	2.27	0.47
6:B:80:ASP:OD2	6:B:83:HIS:HB2	2.13	0.47
17:B:808:CLA:H52	26:B:850:DGD:HB71	1.97	0.47
17:B:833:CLA:HBC2	17:B:839:CLA:HMC2	1.95	0.47
25:J:102:HTG:H4'2	25:J:102:HTG:H1'1	1.60	0.47
17:1:309:CLA:HBC2	17:1:311:CLA:H141	1.96	0.47
2:2:111:PHE:CE2	19:2:314:LUT:H8	2.50	0.47
23:2:318:LMT:O6B	23:2:318:LMT:O4'	2.18	0.47
3:3:106:GLY:HA2	20:3:615:XAT:H181	1.96	0.47
4:4:76:PHE:HB3	17:4:302:CLA:CAD	2.45	0.47
17:A:817:CLA:H3A	17:A:817:CLA:HBA2	1.52	0.47
6:B:174:ARG:HD2	17:B:826:CLA:OBD	2.13	0.47
8:D:111:ILE:HG12	8:D:121:ILE:HG12	1.96	0.47
12:H:94:ALA:O	12:H:97:THR:OG1	2.23	0.47
16:K:47:ILE:HG23	16:K:48:GLY:H	1.79	0.47
2:2:104:MET:SD	17:2:308:CLA:HAB	2.55	0.47
4:4:105:GLY:HA3	20:4:317:XAT:C9	2.45	0.47
17:A:810:CLA:H102	17:A:810:CLA:H61	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:834:CLA:H3A	17:A:834:CLA:HBA2	1.67	0.47
6:B:662:MET:HB2	17:B:805:CLA:C1C	2.44	0.47
1:1:134:GLU:O	1:1:138:ILE:HB	2.15	0.47
6:B:59:LEU:HD21	17:B:809:CLA:H112	1.95	0.47
17:A:829:CLA:H62	17:A:829:CLA:H41	1.69	0.47
8:D:102:ILE:HG23	8:D:104:TRP:HZ3	1.80	0.47
17:1:309:CLA:CBB	21:4:318:BCR:H322	2.45	0.46
22:2:317:LHG:H142	22:2:317:LHG:H112	1.72	0.46
10:F:112:SER:HB2	10:F:114:PRO:HD2	1.97	0.46
17:B:838:CLA:C1A	17:B:838:CLA:CGA	2.93	0.46
3:3:113:PRO:HA	3:3:122:ILE:HD11	1.97	0.46
17:A:814:CLA:H12	21:A:846:BCR:HC31	1.97	0.46
7:C:7:ILE:HG12	7:C:40:ALA:HB3	1.97	0.46
10:F:78:ILE:HD11	10:F:154:ARG:NH1	2.30	0.46
10:F:99:LYS:HA	10:F:99:LYS:HD3	1.69	0.46
17:1:312:CLA:H3A	17:1:312:CLA:HBA2	1.50	0.46
2:2:194:LEU:HD12	19:2:314:LUT:H222	1.97	0.46
17:2:301:CLA:CAB	20:2:315:XAT:H32	2.45	0.46
6:B:676:GLU:HG2	7:C:81:TYR:HE2	1.80	0.46
17:1:307:CLA:H51	21:B:847:BCR:HC31	1.97	0.46
17:3:605:CLA:H3A	21:3:616:BCR:C21	2.45	0.46
21:2:316:BCR:HC31	17:4:310:CLA:CAB	2.45	0.46
17:4:304:CLA:HBA2	25:4:322:HTG:S1	2.56	0.46
5:A:567:ARG:NH2	8:D:89:GLY:O	2.42	0.46
17:A:820:CLA:H2	17:A:820:CLA:H62	1.68	0.46
6:B:593:TYR:CZ	17:B:837:CLA:HBC2	2.50	0.46
17:B:831:CLA:H13	26:B:850:DGD:HAF1	1.96	0.46
17:K:202:CLA:H41	17:K:202:CLA:H61	1.50	0.46
5:A:92:TRP:CZ2	17:A:827:CLA:HED2	2.51	0.46
17:A:803:CLA:H43	17:A:810:CLA:HMC2	1.98	0.46
17:A:820:CLA:H192	17:A:820:CLA:H162	1.71	0.46
17:A:831:CLA:H111	17:A:831:CLA:H72	1.54	0.46
17:A:835:CLA:HBB1	17:A:835:CLA:HMB3	1.98	0.46
6:B:437:TYR:CZ	6:B:518:LEU:HB3	2.51	0.46
2:2:241:PHE:O	2:2:245:ALA:N	2.45	0.46
17:2:307:CLA:HHC	17:2:307:CLA:HBB1	1.96	0.46
3:3:110:ALA:HB1	3:3:130:TRP:HB3	1.97	0.46
18:4:305:CHL:HBB2	18:4:306:CHL:CBB	2.45	0.46
18:4:315:CHL:HBB2	21:4:318:BCR:HC8	1.98	0.46
17:A:821:CLA:HMD2	21:A:846:BCR:H23C	1.98	0.46
17:B:825:CLA:H51	17:B:826:CLA:H142	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:189:ARG:HG2	8:D:190:SER:O	2.15	0.46
17:L:202:CLA:H151	17:L:202:CLA:H18	1.77	0.46
2:2:121:ILE:HD12	2:2:121:ILE:H	1.80	0.46
6:B:218:HIS:CD2	6:B:219:PRO:HD2	2.50	0.46
6:B:275:HIS:CD2	17:B:819:CLA:HAB	2.51	0.46
17:B:809:CLA:HED2	13:I:5:PRO:HB3	1.97	0.46
7:C:62:PHE:HD2	8:D:191:ILE:HG21	1.81	0.46
21:J:104:BCR:H20C	21:J:104:BCR:H361	1.75	0.46
15:L:95:LEU:HB3	15:L:136:THR:CG2	2.46	0.46
17:1:307:CLA:HBA2	17:1:307:CLA:H12	1.72	0.46
17:1:308:CLA:H92	19:1:314:LUT:H371	1.97	0.46
2:2:228:GLN:OE1	19:2:314:LUT:H42	2.16	0.46
4:4:81:LEU:HD13	17:4:302:CLA:H42	1.98	0.46
5:A:199:VAL:HG23	5:A:327:ILE:HD12	1.97	0.46
5:A:218:TRP:HD1	5:A:303:HIS:CD2	2.34	0.46
21:A:846:BCR:H20C	21:A:846:BCR:H361	1.74	0.46
17:B:823:CLA:CMD	21:B:844:BCR:HC7	2.46	0.46
10:F:212:TRP:CG	10:F:213:PRO:HD3	2.50	0.46
5:A:449:VAL:HG22	5:A:453:LEU:HD22	1.98	0.45
17:A:803:CLA:H2	17:A:810:CLA:H71	1.97	0.45
17:B:824:CLA:H43	22:G:102:LHG:H112	1.98	0.45
18:4:315:CHL:H2A	18:4:315:CHL:HED3	1.99	0.45
6:B:303:TYR:HE2	17:B:824:CLA:HED2	1.80	0.45
21:B:844:BCR:H15C	21:B:844:BCR:H351	1.81	0.45
17:1:302:CLA:H142	17:1:302:CLA:H111	1.81	0.45
17:B:810:CLA:H8	17:B:810:CLA:HBB1	1.99	0.45
17:B:834:CLA:H41	17:B:834:CLA:H61	1.81	0.45
3:3:66:LEU:HG	17:3:602:CLA:HED2	1.97	0.45
5:A:422:TYR:CE1	5:A:424:PRO:HD3	2.52	0.45
23:A:855:LMT:H6E	21:J:105:BCR:HC42	1.98	0.45
6:B:218:HIS:CG	6:B:219:PRO:HD2	2.52	0.45
17:2:311:CLA:H61	17:2:311:CLA:H2	1.62	0.45
17:A:832:CLA:HBC3	17:A:832:CLA:HHD	1.98	0.45
6:B:612:SER:O	6:B:618:GLY:HA3	2.17	0.45
17:B:827:CLA:H142	17:B:842:CLA:H203	1.98	0.45
10:F:156:TRP:CZ3	25:F:310:HTG:H2'1	2.51	0.45
17:L:202:CLA:HBA2	17:L:202:CLA:H3A	1.42	0.45
17:3:602:CLA:H71	20:3:615:XAT:H28	1.99	0.45
5:A:446:LEU:HB3	5:A:554:LEU:HD13	1.99	0.45
5:A:498:LEU:O	5:A:502:THR:OG1	2.29	0.45
17:A:820:CLA:H122	17:A:823:CLA:H93	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:851:BCR:H371	21:A:851:BCR:H24C	1.72	0.45
6:B:4:ARG:HD3	6:B:13:ALA:O	2.16	0.45
6:B:275:HIS:HB3	17:B:819:CLA:HMB1	1.98	0.45
17:B:810:CLA:H62	17:B:810:CLA:H102	1.74	0.45
18:2:313:CHL:HBB2	21:2:316:BCR:C8	2.47	0.45
26:4:323:DGD:HBN1	26:4:323:DGD:CBB	2.39	0.45
5:A:92:TRP:O	5:A:96:MET:HG2	2.17	0.45
5:A:151:GLN:H	5:A:151:GLN:HG2	1.44	0.45
5:A:417:PHE:CD1	5:A:421:ASP:HB2	2.52	0.45
6:B:257:LEU:HD22	6:B:493:TRP:HB3	1.99	0.45
17:B:836:CLA:HBB1	17:B:836:CLA:HMB3	1.99	0.45
2:2:202:GLN:N	2:2:202:GLN:OE1	2.47	0.45
3:3:83:THR:OG1	5:A:24:ARG:NH2	2.40	0.45
6:B:374:HIS:HB2	17:B:829:CLA:CHB	2.47	0.45
17:B:823:CLA:H92	17:B:823:CLA:H62	1.79	0.45
7:C:38:GLN:OE1	8:D:177:VAL:HG22	2.17	0.45
4:4:156:ARG:HG3	18:4:307:CHL:C1D	2.47	0.45
6:B:301:ILE:HG21	17:B:826:CLA:HAC1	1.99	0.45
6:B:694:ARG:NH2	15:L:101:SER:O	2.50	0.45
8:D:101:VAL:HB	8:D:128:LEU:HD11	1.97	0.45
6:B:531:THR:CG2	17:B:827:CLA:HAB	2.46	0.44
3:3:164:HIS:ND1	18:3:601:CHL:HBA1	2.32	0.44
17:4:311:CLA:H51	17:4:311:CLA:H12	1.80	0.44
5:A:225:VAL:HG13	5:A:245:PRO:HB3	1.99	0.44
5:A:740:LEU:HD11	21:A:851:BCR:HC8	2.00	0.44
17:A:836:CLA:H41	17:A:836:CLA:H62	1.58	0.44
17:A:836:CLA:H91	17:L:203:CLA:H201	1.98	0.44
17:A:840:CLA:H41	17:A:840:CLA:H61	1.25	0.44
21:A:848:BCR:H20C	21:A:848:BCR:H361	1.74	0.44
2:2:170:ASP:HB3	2:2:173:PHE:O	2.17	0.44
17:3:608:CLA:HBB1	17:3:608:CLA:HMB3	2.00	0.44
5:A:208:ALA:HB1	17:A:819:CLA:HBC3	1.99	0.44
5:A:237:VAL:HG22	5:A:242:ILE:HG12	1.99	0.44
17:A:817:CLA:H91	17:A:817:CLA:H111	1.74	0.44
17:B:826:CLA:H161	17:B:826:CLA:H122	1.65	0.44
17:B:829:CLA:H142	17:B:829:CLA:H111	1.76	0.44
8:D:95:GLN:OE1	12:H:69:GLN:HG3	2.17	0.44
15:L:48:ARG:NH2	15:L:124:ASP:OD1	2.36	0.44
6:B:93:ASP:OD1	6:B:95:HIS:ND1	2.24	0.44
17:B:803:CLA:C4B	17:L:203:CLA:H93	2.47	0.44
24:F:309:LMG:H142	24:F:309:LMG:H171	1.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:L:206:BCR:H11C	21:L:206:BCR:H341	1.88	0.44
4:4:116:THR:HA	4:4:121:ILE:O	2.18	0.44
21:4:318:BCR:H20C	21:4:318:BCR:H361	1.79	0.44
5:A:580:PRO:HB3	5:A:727:ILE:HB	2.00	0.44
5:A:697:ARG:HB3	27:A:842:PQN:H7	1.99	0.44
17:A:841:CLA:H101	17:A:841:CLA:H13	1.77	0.44
27:A:842:PQN:H143	27:A:842:PQN:H112	1.91	0.44
22:B:801:LHG:HC62	17:B:842:CLA:HBA1	1.98	0.44
1:1:80:CYS:HB3	1:1:184:GLY:HA3	2.00	0.44
22:2:317:LHG:HC2	18:3:601:CHL:HBC1	1.99	0.44
18:3:601:CHL:HBA2	17:3:613:CLA:O1D	2.18	0.44
4:4:155:ARG:CZ	4:4:166:VAL:HG22	2.47	0.44
5:A:288:ASP:HB3	5:A:291:THR:HG22	1.99	0.44
17:A:803:CLA:HBA2	17:A:803:CLA:H3A	1.73	0.44
17:B:803:CLA:H112	17:B:803:CLA:H91	1.73	0.44
7:C:31:TRP:CH2	7:C:33:GLY:HA3	2.53	0.44
2:2:59:PRO:HG3	3:3:179:GLN:CD	2.42	0.44
6:B:475:ASP:HA	6:B:479:SER:HB3	1.99	0.44
17:B:841:CLA:H111	17:B:841:CLA:H152	1.73	0.44
8:D:103:THR:HA	8:D:127:ASN:O	2.18	0.44
8:D:156:ARG:HB2	8:D:166:LEU:HD11	1.99	0.44
1:1:173:PHE:CZ	17:1:308:CLA:HED3	2.53	0.44
1:1:217:PRO:O	1:1:221:THR:HG22	2.18	0.44
5:A:197:GLN:NE2	5:A:351:THR:O	2.44	0.44
6:B:199:ILE:O	6:B:203:ARG:HG3	2.18	0.44
6:B:218:HIS:CE1	6:B:220:GLN:HG3	2.53	0.44
6:B:350:GLN:HG3	17:B:827:CLA:CED	2.48	0.44
6:B:395:ILE:HD11	6:B:541:ALA:HB1	1.99	0.44
17:J:101:CLA:H62	17:J:101:CLA:H102	1.53	0.44
2:2:227:PHE:O	2:2:231:TYR:HD2	2.01	0.44
4:4:81:LEU:HD22	10:F:211:SER:HB3	1.99	0.44
5:A:515:TRP:O	5:A:517:GLY:N	2.51	0.44
17:A:838:CLA:H2	17:A:838:CLA:H61	1.82	0.44
6:B:619:TRP:O	6:B:623:TYR:HB3	2.17	0.44
6:B:645:VAL:CG1	17:B:811:CLA:HHD	2.48	0.44
17:L:203:CLA:H62	17:L:203:CLA:H41	1.71	0.44
1:1:94:GLU:CD	1:1:207:LEU:HB2	2.43	0.43
5:A:334:HIS:HA	17:A:843:CLA:HBC2	2.00	0.43
17:A:838:CLA:C9	17:F:306:CLA:HAC2	2.47	0.43
6:B:330:ILE:HG22	17:B:807:CLA:HHD	2.00	0.43
6:B:410:ARG:HD3	17:B:832:CLA:OBD	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:810:CLA:H192	17:B:810:CLA:H162	1.79	0.43
15:L:61:VAL:HG21	15:L:150:ALA:HB3	1.99	0.43
2:2:156:ARG:NE	18:2:306:CHL:OMC	2.43	0.43
3:3:250:LEU:HD13	19:3:614:LUT:H163	2.00	0.43
17:4:304:CLA:C4B	20:4:317:XAT:H183	2.48	0.43
26:4:323:DGD:HBT2	26:4:323:DGD:HB72	1.61	0.43
5:A:210:LEU:HD11	17:A:812:CLA:H3A	2.00	0.43
5:A:305:ALA:HB1	17:A:816:CLA:HBC2	1.99	0.43
5:A:389:TYR:OH	5:A:527:VAL:O	2.31	0.43
6:B:721:TYR:HB2	17:B:804:CLA:HED2	2.00	0.43
17:B:821:CLA:HBA2	17:B:825:CLA:H43	2.00	0.43
17:1:301:CLA:HAB	20:1:315:XAT:H32	2.01	0.43
5:A:58:HIS:HB2	22:A:844:LHG:H102	2.01	0.43
5:A:697:ARG:NH1	5:A:724:ALA:HB3	2.33	0.43
17:A:816:CLA:CED	17:A:816:CLA:H2A	2.48	0.43
17:A:837:CLA:H91	17:A:837:CLA:H112	1.82	0.43
17:2:308:CLA:H61	17:2:308:CLA:H101	1.69	0.43
3:3:214:LEU:HG	3:3:218:LYS:HE3	2.00	0.43
5:A:207:LEU:O	5:A:310:PHE:HB3	2.18	0.43
5:A:466:THR:HG23	17:B:811:CLA:HMC3	2.00	0.43
17:A:810:CLA:H121	17:J:101:CLA:HBB2	2.01	0.43
17:A:839:CLA:H92	17:A:839:CLA:H61	1.75	0.43
15:L:58:PHE:CD1	15:L:150:ALA:HB2	2.53	0.43
3:3:226:ARG:HH22	17:3:602:CLA:HED3	1.83	0.43
5:A:343:HIS:HB3	5:A:346:LEU:HD12	2.00	0.43
5:A:705:GLU:CD	6:B:545:LYS:HB2	2.43	0.43
17:A:840:CLA:H101	17:J:101:CLA:H43	2.00	0.43
6:B:387:PHE:CZ	21:B:848:BCR:H373	2.53	0.43
6:B:527:LEU:HD23	6:B:586:THR:HG21	2.00	0.43
17:B:810:CLA:C1A	17:B:810:CLA:CGA	2.96	0.43
2:2:115:PHE:HA	2:2:237:ILE:HG13	1.99	0.43
5:A:694:PHE:HB2	17:B:802:CLA:HBC2	2.00	0.43
21:A:849:BCR:H24C	21:A:849:BCR:H371	1.82	0.43
21:B:845:BCR:H361	21:B:845:BCR:H20C	1.72	0.43
1:1:108:ALA:O	1:1:110:LEU:N	2.52	0.43
1:1:213:HIS:CG	17:1:311:CLA:HAA2	2.54	0.43
17:1:309:CLA:NA	22:1:317:LHG:O4	2.51	0.43
17:1:311:CLA:H2	17:1:312:CLA:OBD	2.19	0.43
2:2:59:PRO:HD2	18:3:601:CHL:O1D	2.19	0.43
2:2:162:LEU:HD21	23:2:318:LMT:H22	2.00	0.43
2:2:210:LYS:HD3	17:2:310:CLA:HBD	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:157:ALA:HA	18:3:601:CHL:H12	2.00	0.43
6:B:411:MET:CE	21:B:847:BCR:H292	2.49	0.43
21:I:101:BCR:H20C	21:I:101:BCR:H361	1.85	0.43
14:J:16:THR:HG21	21:J:105:BCR:H403	2.00	0.43
2:2:220:LEU:HD21	17:2:301:CLA:HAC1	2.01	0.43
2:2:246:ASP:OD2	2:2:249:HIS:HB2	2.17	0.43
5:A:335:LYS:HB2	5:A:340:GLY:O	2.18	0.43
17:A:811:CLA:H2	17:A:811:CLA:H61	1.77	0.43
6:B:472:TYR:HB3	10:F:79:ALA:HA	2.01	0.43
17:B:811:CLA:H143	17:B:811:CLA:H162	1.76	0.43
8:D:205:LYS:HD2	8:D:209:ASP:HB3	2.01	0.43
10:F:199:VAL:HB	25:J:102:HTG:H1'2	2.01	0.43
2:2:65:PRO:HD2	2:2:66:TRP:CZ3	2.53	0.43
4:4:155:ARG:HG3	18:4:301:CHL:CED	2.36	0.43
17:A:803:CLA:H61	17:A:803:CLA:H93	1.73	0.43
17:A:807:CLA:H93	17:A:807:CLA:H61	1.80	0.43
17:A:818:CLA:H122	17:A:818:CLA:H162	1.43	0.43
6:B:72:GLY:HA2	6:B:87:ILE:HB	2.01	0.43
7:C:31:TRP:CZ2	7:C:33:GLY:HA3	2.54	0.43
15:L:55:ALA:HA	21:L:206:BCR:H16C	2.00	0.43
1:1:150:ASP:OD2	1:1:153:LYS:HG2	2.19	0.43
18:1:305:CHL:HMD3	17:G:103:CLA:HBC1	1.99	0.43
3:3:240:LEU:HG	17:A:814:CLA:HBA1	2.00	0.43
17:4:303:CLA:H101	17:4:303:CLA:H61	1.72	0.43
17:A:831:CLA:H61	17:A:831:CLA:H41	1.75	0.43
6:B:378:ILE:HD11	17:B:829:CLA:C3C	2.48	0.43
6:B:704:GLN:HG3	26:B:850:DGD:HA22	2.01	0.43
17:1:308:CLA:HBB1	17:1:310:CLA:H3A	2.01	0.42
5:A:126:ILE:HG13	5:A:127:VAL:HG13	2.01	0.42
5:A:306:ILE:HD13	5:A:306:ILE:HA	1.90	0.42
5:A:442:ILE:HG23	17:A:837:CLA:HBB2	2.01	0.42
17:A:822:CLA:HAB	17:A:843:CLA:CAB	2.49	0.42
6:B:671:TRP:CE2	27:B:843:PQN:H2M3	2.54	0.42
21:L:201:BCR:H333	17:L:203:CLA:NB	2.34	0.42
3:3:164:HIS:C	18:3:601:CHL:HED1	2.43	0.42
21:A:846:BCR:H372	16:K:105:ALA:HA	2.01	0.42
6:B:21:ILE:HG12	13:I:28:VAL:CG1	2.49	0.42
17:B:807:CLA:HBA1	17:B:807:CLA:H3A	1.87	0.42
17:B:823:CLA:H41	17:B:823:CLA:H61	1.46	0.42
1:1:69:LEU:HD23	1:1:69:LEU:HA	1.88	0.42
17:4:304:CLA:CAD	25:4:322:HTG:H1'1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:85:ARG:HD2	6:B:115:ILE:HD13	2.02	0.42
17:B:803:CLA:H122	17:L:203:CLA:H172	2.01	0.42
26:B:850:DGD:HAH1	26:B:850:DGD:HAS2	1.67	0.42
7:C:15:THR:O	7:C:19:ARG:HG2	2.18	0.42
17:1:302:CLA:H11	17:1:302:CLA:H51	1.83	0.42
3:3:101:ARG:HD3	17:3:609:CLA:C4C	2.49	0.42
26:4:323:DGD:HB2	26:4:323:DGD:HBV1	1.70	0.42
5:A:513:LEU:HD13	5:A:513:LEU:HA	1.92	0.42
17:A:820:CLA:H61	17:A:823:CLA:H2	2.01	0.42
18:4:301:CHL:C8	21:4:318:BCR:H311	2.48	0.42
17:4:302:CLA:H3A	17:4:302:CLA:CGA	2.50	0.42
21:B:847:BCR:H24C	21:B:847:BCR:H371	1.88	0.42
7:C:62:PHE:HB3	9:E:15:GLU:HG3	2.01	0.42
1:1:110:LEU:HD23	1:1:110:LEU:O	2.20	0.42
21:3:616:BCR:H15C	21:3:616:BCR:H351	1.88	0.42
17:A:810:CLA:H121	17:J:101:CLA:CBB	2.49	0.42
2:2:179:THR:HG23	2:2:188:GLY:HA2	2.01	0.42
2:2:216:ARG:HA	2:2:219:MET:HE3	2.00	0.42
5:A:218:TRP:HA	17:A:813:CLA:HAB	2.01	0.42
5:A:515:TRP:HA	5:A:515:TRP:CE3	2.54	0.42
17:B:815:CLA:H192	17:B:815:CLA:H161	1.83	0.42
17:B:837:CLA:H92	25:B:851:HTG:H6'2	2.02	0.42
17:1:308:CLA:CAB	19:1:314:LUT:H32	2.50	0.42
2:2:191:PHE:HB3	17:2:308:CLA:HMD1	2.01	0.42
3:3:163:GLU:CD	3:3:166:ARG:HH21	2.28	0.42
26:4:323:DGD:HB22	10:F:221:LEU:CD2	2.50	0.42
5:A:301:HIS:CE1	17:A:817:CLA:HAB	2.54	0.42
5:A:330:ILE:O	5:A:334:HIS:ND1	2.53	0.42
5:A:435:VAL:HA	5:A:438:HIS:CE1	2.55	0.42
17:A:820:CLA:C4C	17:A:826:CLA:H152	2.50	0.42
17:A:825:CLA:H141	17:A:825:CLA:H161	1.86	0.42
21:A:850:BCR:H20C	21:A:850:BCR:H361	1.79	0.42
15:L:37:PRO:O	15:L:48:ARG:HD3	2.20	0.42
15:L:132:TRP:O	15:L:136:THR:HG23	2.19	0.42
17:2:311:CLA:H92	17:2:311:CLA:HMC1	2.02	0.42
18:3:601:CHL:HMD1	21:3:616:BCR:H323	2.02	0.42
24:4:320:LMG:H141	24:4:320:LMG:H111	1.48	0.42
17:A:804:CLA:H3A	17:A:804:CLA:HBA1	1.77	0.42
17:B:818:CLA:C1D	17:B:819:CLA:HBB2	2.50	0.42
7:C:17:CYS:SG	7:C:18:VAL:N	2.93	0.42
9:E:45:VAL:HB	9:E:49:ASN:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:92:LYS:HE2	10:F:92:LYS:HB3	1.53	0.42
17:F:304:CLA:H112	17:F:304:CLA:H152	1.69	0.42
17:L:204:CLA:H3A	17:L:204:CLA:HBA1	1.22	0.42
3:3:226:ARG:HA	3:3:229:MET:HE3	2.02	0.42
4:4:54:GLY:HA3	4:4:74:ASN:OD1	2.20	0.42
4:4:109:MET:HE2	4:4:218:PHE:HD2	1.85	0.42
5:A:629:ASN:HD22	5:A:633:VAL:HB	1.83	0.42
6:B:558:PRO:HB3	6:B:702:ILE:HB	2.02	0.42
17:B:812:CLA:H161	17:B:812:CLA:H141	1.78	0.42
21:B:846:BCR:H361	21:B:846:BCR:H20C	1.75	0.42
1:1:108:ALA:HB1	1:1:127:LEU:HD12	2.01	0.41
23:2:318:LMT:O3'	23:2:318:LMT:O2B	2.28	0.41
3:3:156:MET:HG3	17:3:608:CLA:HBB2	2.01	0.41
3:3:241:VAL:HG13	3:3:242:THR:HG23	2.02	0.41
17:3:603:CLA:HBB1	20:3:615:XAT:C35	2.43	0.41
4:4:158:GLN:OE1	4:4:161:LYS:HE2	2.20	0.41
5:A:382:TYR:HD2	5:A:385:LEU:HD22	1.84	0.41
17:A:814:CLA:C3B	21:A:846:BCR:H333	2.50	0.41
17:B:820:CLA:H62	17:B:820:CLA:H41	1.71	0.41
18:2:304:CHL:H3A	21:2:316:BCR:H21C	2.02	0.41
18:4:305:CHL:HBB2	18:4:306:CHL:HBB1	2.02	0.41
21:4:318:BCR:H24C	21:4:318:BCR:H371	1.88	0.41
5:A:73:GLU:O	5:A:77:LYS:HG3	2.20	0.41
17:A:808:CLA:HMB3	17:A:808:CLA:HBB1	2.02	0.41
6:B:203:ARG:HD3	6:B:238:ASP:OD1	2.20	0.41
15:L:44:ASN:O	15:L:48:ARG:HG3	2.19	0.41
1:1:133:ILE:HD13	1:1:133:ILE:HA	1.93	0.41
2:2:104:MET:HB3	19:2:314:LUT:H402	2.02	0.41
5:A:20:ILE:HD13	17:A:809:CLA:HAA2	2.01	0.41
5:A:682:ALA:HB1	5:A:741:GLY:O	2.19	0.41
17:A:841:CLA:H62	17:A:841:CLA:H41	1.55	0.41
6:B:51:PHE:HB3	6:B:149:SER:O	2.20	0.41
21:L:205:BCR:H20C	21:L:205:BCR:H361	1.85	0.41
18:4:305:CHL:H2	21:4:318:BCR:H17C	2.02	0.41
5:A:361:ASN:ND2	17:A:804:CLA:OBD	2.48	0.41
6:B:262:HIS:HA	6:B:263:PRO:HD3	1.91	0.41
17:B:827:CLA:H141	17:B:827:CLA:H161	1.83	0.41
21:F:308:BCR:H361	21:F:308:BCR:H20C	1.83	0.41
2:2:217:LEU:HD13	17:2:309:CLA:HBC1	2.02	0.41
4:4:213:LEU:HD23	4:4:213:LEU:HA	1.80	0.41
19:4:316:LUT:H31	19:4:316:LUT:H391	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:287:LEU:HD23	5:A:294:LEU:HD23	2.02	0.41
17:A:816:CLA:H143	17:A:816:CLA:H111	1.77	0.41
17:B:805:CLA:H111	17:B:805:CLA:H143	1.80	0.41
17:B:823:CLA:H143	17:B:823:CLA:H161	1.76	0.41
11:G:42:VAL:HG13	11:G:46:GLU:CB	2.49	0.41
2:2:58:PHE:CE1	18:3:601:CHL:HED3	2.55	0.41
2:2:100:SER:CB	2:2:215:GLY:HA3	2.49	0.41
5:A:434:ARG:NH1	5:A:437:ARG:HH12	2.17	0.41
6:B:82:LEU:CD2	6:B:363:GLN:HG3	2.49	0.41
17:B:817:CLA:HMA3	21:B:846:BCR:H372	2.01	0.41
2:2:240:LEU:HD23	17:2:311:CLA:HMA2	2.03	0.41
3:3:137:PRO:N	3:3:138:PRO:HD2	2.36	0.41
4:4:126:TRP:HB2	20:4:317:XAT:H3	2.03	0.41
5:A:687:ALA:HB2	17:A:853:CLA:C3D	2.51	0.41
5:A:695:SER:OG	27:A:842:PQN:H9	2.21	0.41
17:A:804:CLA:H61	17:A:804:CLA:H101	1.88	0.41
17:A:808:CLA:H102	21:J:104:BCR:H332	2.01	0.41
17:A:824:CLA:HBA1	17:A:828:CLA:H193	2.01	0.41
6:B:728:SER:O	6:B:732:LYS:HD3	2.21	0.41
17:B:810:CLA:H193	17:B:829:CLA:H18	2.03	0.41
7:C:55:GLU:HB3	7:C:63:LEU:HD13	2.03	0.41
8:D:168:PRO:HG3	8:D:173:TYR:CE1	2.55	0.41
12:H:130:LYS:HE3	12:H:133:GLN:HE21	1.85	0.41
2:2:238:ASP:OD1	2:2:238:ASP:N	2.54	0.41
3:3:114:GLU:CD	3:3:247:TYR:HB3	2.45	0.41
17:A:840:CLA:H12	17:A:840:CLA:NA	2.35	0.41
10:F:92:LYS:O	10:F:96:GLN:HG2	2.21	0.41
1:1:103:LYS:HG3	1:1:106:GLU:OE2	2.21	0.41
1:1:163:PRO:HD2	19:1:314:LUT:H23	2.03	0.41
2:2:170:ASP:HB2	2:2:176:ASN:HB2	2.03	0.41
4:4:116:THR:HG22	4:4:121:ILE:HD12	2.03	0.41
4:4:155:ARG:CD	18:4:301:CHL:CED	2.98	0.41
18:4:306:CHL:HBC2	24:4:320:LMG:H312	2.03	0.41
21:4:318:BCR:H15C	21:4:318:BCR:H351	1.93	0.41
26:4:323:DGD:O2D	26:4:323:DGD:C3G	2.69	0.41
5:A:335:LYS:H	17:A:843:CLA:CBC	2.32	0.41
5:A:681:GLY:HA2	17:A:853:CLA:H41	2.03	0.41
17:A:803:CLA:H2	17:A:803:CLA:H62	1.71	0.41
17:A:804:CLA:H141	17:A:804:CLA:H161	1.69	0.41
6:B:42:LEU:O	6:B:46:ILE:HG13	2.21	0.41
6:B:53:GLN:HG2	17:B:807:CLA:H3A	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:129:LEU:HD13	17:B:816:CLA:HED3	2.03	0.41
6:B:270:LEU:HD23	6:B:273:MET:HE3	2.02	0.41
6:B:352:MET:HE3	17:B:820:CLA:HBA1	2.02	0.41
6:B:387:PHE:CE2	21:B:848:BCR:H373	2.56	0.41
21:B:844:BCR:H20C	21:B:844:BCR:H361	1.85	0.41
21:B:848:BCR:H15C	21:B:848:BCR:H351	1.88	0.41
21:B:849:BCR:H361	21:B:849:BCR:H20C	1.78	0.41
7:C:19:ARG:HG2	7:C:19:ARG:H	1.55	0.41
24:G:101:LMG:H132	24:G:101:LMG:H161	1.83	0.41
5:A:77:LYS:HE2	5:A:186:TYR:OH	2.21	0.41
17:A:837:CLA:H112	17:A:837:CLA:H143	1.89	0.41
17:F:304:CLA:H161	17:F:304:CLA:H193	1.80	0.41
17:F:306:CLA:O1A	17:F:306:CLA:H2A	2.21	0.41
17:J:101:CLA:H193	17:J:101:CLA:H161	1.81	0.41
21:J:105:BCR:H20C	21:J:105:BCR:H361	1.89	0.41
15:L:113:SER:OG	15:L:123:PRO:HG3	2.21	0.41
15:L:145:SER:HB2	21:L:206:BCR:C5	2.51	0.41
2:2:216:ARG:O	2:2:220:LEU:HD22	2.21	0.40
3:3:164:HIS:HB3	18:3:601:CHL:HED1	2.03	0.40
3:3:182:LEU:HD21	21:3:616:BCR:H343	2.02	0.40
6:B:414:HIS:CE1	6:B:418:ILE:HD11	2.56	0.40
15:L:23:VAL:O	15:L:29:VAL:HG11	2.21	0.40
15:L:74:GLU:CD	15:L:74:GLU:H	2.28	0.40
1:1:179:LYS:HD3	17:1:310:CLA:CBA	2.46	0.40
6:B:686:PRO:O	6:B:688:ALA:N	2.52	0.40
17:B:812:CLA:H101	12:H:117:PHE:HD2	1.86	0.40
17:1:309:CLA:CBC	17:1:311:CLA:H141	2.51	0.40
18:2:313:CHL:CBB	21:2:316:BCR:H10C	2.52	0.40
3:3:102:PHE:CZ	18:3:607:CHL:HED2	2.55	0.40
17:3:610:CLA:H62	17:3:610:CLA:H41	1.77	0.40
5:A:447:ASN:O	5:A:451:ILE:HG13	2.22	0.40
17:A:809:CLA:H8	17:A:812:CLA:H202	2.02	0.40
6:B:558:PRO:O	6:B:559:CYS:HB3	2.22	0.40
17:B:815:CLA:H122	21:B:845:BCR:H381	2.04	0.40
17:B:832:CLA:HBA1	17:B:832:CLA:C4A	2.52	0.40
14:J:12:PRO:O	14:J:16:THR:HG23	2.21	0.40
18:3:601:CHL:C9	18:3:601:CHL:H62	2.51	0.40
17:A:808:CLA:H122	17:A:808:CLA:H8	1.83	0.40
21:A:846:BCR:H15C	21:A:846:BCR:H351	1.76	0.40
17:A:853:CLA:H41	17:A:853:CLA:H61	1.14	0.40
24:B:852:LMG:H251	17:G:104:CLA:C1B	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:306:CHL:HMB3	21:2:316:BCR:H363	2.03	0.40
26:4:323:DGD:HBT1	26:4:323:DGD:HBN2	2.03	0.40
21:A:850:BCR:H15C	21:A:850:BCR:H351	1.92	0.40
6:B:531:THR:HG22	17:B:827:CLA:HHC	2.03	0.40
21:B:847:BCR:H332	22:G:102:LHG:H341	2.04	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	1	193/195 (99%)	178 (92%)	12 (6%)	3 (2%)	7	11
2	2	202/269 (75%)	191 (95%)	9 (4%)	2 (1%)	12	20
3	3	214/275 (78%)	197 (92%)	17 (8%)	0	100	100
4	4	193/198 (98%)	179 (93%)	13 (7%)	1 (0%)	24	37
5	A	740/758 (98%)	707 (96%)	30 (4%)	3 (0%)	30	43
6	B	731/734 (100%)	709 (97%)	19 (3%)	3 (0%)	30	43
7	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
8	D	138/143 (96%)	127 (92%)	9 (6%)	2 (1%)	9	13
9	E	61/66 (92%)	59 (97%)	2 (3%)	0	100	100
10	F	150/154 (97%)	148 (99%)	2 (1%)	0	100	100
11	G	93/97 (96%)	88 (95%)	5 (5%)	0	100	100
12	H	86/88 (98%)	80 (93%)	6 (7%)	0	100	100
13	I	28/40 (70%)	26 (93%)	2 (7%)	0	100	100
14	J	37/42 (88%)	37 (100%)	0	0	100	100
15	L	149/157 (95%)	145 (97%)	4 (3%)	0	100	100
16	K	73/80 (91%)	67 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3166/3377 (94%)	3012 (95%)	140 (4%)	14 (0%)	30	43

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	516	GLY
6	B	5	PHE
8	D	76	PRO
1	1	109	ALA
6	B	559	CYS
1	1	113	GLY
1	1	228	PRO
5	A	581	CYS
2	2	120	GLY
4	4	238	SER
5	A	519	ASP
8	D	169	LYS
6	B	492	ILE
2	2	233	GLY

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	1	155/158 (98%)	145 (94%)	10 (6%)	15	27
2	2	164/216 (76%)	150 (92%)	14 (8%)	10	16
3	3	167/213 (78%)	158 (95%)	9 (5%)	20	35
4	4	161/164 (98%)	146 (91%)	15 (9%)	8	14
5	A	603/618 (98%)	569 (94%)	34 (6%)	19	33
6	B	598/599 (100%)	568 (95%)	30 (5%)	22	38
7	C	69/70 (99%)	65 (94%)	4 (6%)	18	32
8	D	120/122 (98%)	107 (89%)	13 (11%)	6	9
9	E	55/58 (95%)	51 (93%)	4 (7%)	13	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	F	124/127 (98%)	115 (93%)	9 (7%)	13	22
11	G	80/82 (98%)	69 (86%)	11 (14%)	3	4
12	H	71/71 (100%)	65 (92%)	6 (8%)	10	16
13	I	25/36 (69%)	23 (92%)	2 (8%)	11	19
14	J	32/35 (91%)	29 (91%)	3 (9%)	8	13
15	L	118/124 (95%)	106 (90%)	12 (10%)	7	11
16	K	51/58 (88%)	48 (94%)	3 (6%)	18	31
All	All	2593/2751 (94%)	2414 (93%)	179 (7%)	14	24

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	43	ARG
1	1	67	GLU
1	1	69	LEU
1	1	98	LEU
1	1	110	LEU
1	1	120	ASN
1	1	122	VAL
1	1	126	THR
1	1	138	ILE
1	1	207	LEU
2	2	54	ARG
2	2	62	THR
2	2	85	ASP
2	2	87	GLU
2	2	89	LEU
2	2	110	ILE
2	2	140	THR
2	2	162	LEU
2	2	182	ASP
2	2	207	LEU
2	2	212	ILE
2	2	220	LEU
2	2	234	THR
2	2	240	LEU
3	3	52	TRP
3	3	77	LEU
3	3	88	GLU
3	3	114	GLU

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Mol	Chain	Res	Type
3	3	124	GLN
3	3	154	LEU
3	3	156	MET
3	3	224	ASN
3	3	244	VAL
4	4	110	LEU
4	4	120	ILE
4	4	121	ILE
4	4	141	LEU
4	4	144	ILE
4	4	148	LEU
4	4	152	VAL
4	4	156	ARG
4	4	166	VAL
4	4	177	LEU
4	4	198	LEU
4	4	210	LEU
4	4	224	VAL
4	4	243	ASN
4	4	247	GLN
5	A	22	VAL
5	A	42	ARG
5	A	43	THR
5	A	73	GLU
5	A	78	VAL
5	A	102	ARG
5	A	123	VAL
5	A	151	GLN
5	A	159	THR
5	A	210	LEU
5	A	211	LEU
5	A	230	ASN
5	A	237	VAL
5	A	272	LEU
5	A	291	THR
5	A	306	ILE
5	A	328	LYS
5	A	377	TYR
5	A	387	THR
5	A	434	ARG
5	A	446	LEU
5	A	453	LEU

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Mol	Chain	Res	Type
5	A	530	LEU
5	A	540	LEU
5	A	560	VAL
5	A	590	CYS
5	A	611	VAL
5	A	619	LYS
5	A	630	ASP
5	A	653	LEU
5	A	713	LYS
5	A	716	VAL
5	A	729	GLN
5	A	757	VAL
6	B	7	ARG
6	B	10	GLN
6	B	37	ILE
6	B	91	ILE
6	B	137	THR
6	B	148	ILE
6	B	203	ARG
6	B	215	VAL
6	B	222	LEU
6	B	225	LEU
6	B	257	LEU
6	B	344	ILE
6	B	363	GLN
6	B	371	LEU
6	B	427	LEU
6	B	436	LEU
6	B	441	ASP
6	B	458	ILE
6	B	476	VAL
6	B	479	SER
6	B	481	THR
6	B	492	ILE
6	B	536	LYS
6	B	568	CYS
6	B	583	MET
6	B	590	VAL
6	B	626	LEU
6	B	645	VAL
6	B	690	LEU
6	B	732	LYS

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Mol	Chain	Res	Type
7	C	19	ARG
7	C	62	PHE
7	C	66	ARG
7	C	74	THR
8	D	73	GLU
8	D	74	LEU
8	D	78	THR
8	D	96	VAL
8	D	105	GLU
8	D	147	LYS
8	D	150	ILE
8	D	151	LYS
8	D	177	VAL
8	D	189	ARG
8	D	190	SER
8	D	201	LYS
8	D	210	LEU
9	E	1	ILE
9	E	44	LYS
9	E	60	VAL
9	E	62	GLU
10	F	103	SER
10	F	123	GLU
10	F	131	ASN
10	F	134	LYS
10	F	160	ILE
10	F	187	ASP
10	F	201	LEU
10	F	206	VAL
10	F	226	VAL
11	G	6	LEU
11	G	10	LEU
11	G	18	LEU
11	G	22	VAL
11	G	29	GLU
11	G	31	VAL
11	G	33	LYS
11	G	42	VAL
11	G	50	THR
11	G	89	THR
11	G	95	ASP
12	H	61	GLU

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Mol	Chain	Res	Type
12	H	63	LEU
12	H	76	ASP
12	H	82	ASN
12	H	101	LEU
12	H	138	LEU
13	I	3	ASN
13	I	11	LEU
14	J	16	THR
14	J	25	LEU
14	J	38	THR
15	L	8	GLN
15	L	36	LEU
15	L	43	VAL
15	L	50	ILE
15	L	54	LEU
15	L	59	LEU
15	L	71	ARG
15	L	74	GLU
15	L	78	GLN
15	L	87	LEU
15	L	121	LYS
15	L	125	GLN
16	K	47	ILE
16	K	92	THR
16	K	102	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	174	HIS
1	1	220	ASN
2	2	249	HIS
3	3	248	GLN
4	4	98	ASN
4	4	247	GLN
5	A	185	HIS
5	A	483	GLN
5	A	485	GLN
5	A	490	GLN
5	A	729	GLN
6	B	158	GLN
6	B	218	HIS

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Mol	Chain	Res	Type
6	B	229	GLN
6	B	236	ASN
6	B	266	GLN
6	B	504	ASN
6	B	608	GLN
9	E	49	ASN
10	F	89	GLN
12	H	82	ASN
16	K	52	ASN
16	K	123	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

215 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
17	CLA	3	602	3	64,68,73	1.24	6 (9%)	76,107,113	1.25	5 (6%)
17	CLA	A	824	29	69,73,73	1.22	7 (10%)	82,113,113	1.26	7 (8%)
17	CLA	A	823	-	59,63,73	1.31	6 (10%)	70,101,113	1.33	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	F	304	-	69,73,73	1.19	6 (8%)	82,113,113	1.47	10 (12%)
20	XAT	2	315	-	41,47,47	3.71	18 (43%)	54,74,74	5.38	32 (59%)
21	BCR	A	851	-	41,41,41	0.92	2 (4%)	56,56,56	1.23	5 (8%)
17	CLA	3	605	-	46,50,73	1.48	6 (13%)	53,85,113	1.33	4 (7%)
17	CLA	B	837	-	64,68,73	1.08	5 (7%)	76,107,113	1.56	11 (14%)
17	CLA	2	319	4	50,54,73	1.38	6 (12%)	59,90,113	1.43	7 (11%)
21	BCR	3	616	-	41,41,41	1.10	2 (4%)	56,56,56	1.33	6 (10%)
17	CLA	A	826	-	69,73,73	1.15	8 (11%)	82,113,113	1.28	5 (6%)
18	CHL	2	306	29	45,59,74	3.91	20 (44%)	40,96,114	2.55	10 (25%)
25	HTG	4	322	-	19,19,19	0.98	2 (10%)	23,24,24	1.13	3 (13%)
17	CLA	1	303	29	55,59,73	1.30	7 (12%)	64,96,113	1.38	5 (7%)
17	CLA	A	841	29	69,73,73	1.18	8 (11%)	82,113,113	1.30	7 (8%)
17	CLA	F	307	10	59,63,73	1.28	8 (13%)	70,101,113	1.38	8 (11%)
17	CLA	A	814	-	54,58,73	1.32	6 (11%)	64,95,113	1.35	6 (9%)
17	CLA	L	204	-	54,58,73	1.36	5 (9%)	64,95,113	1.34	6 (9%)
17	CLA	B	836	29	49,53,73	1.42	6 (12%)	58,89,113	1.56	10 (17%)
20	XAT	3	615	-	41,47,47	3.71	18 (43%)	54,74,74	5.39	32 (59%)
17	CLA	2	311	2	69,73,73	1.21	7 (10%)	82,113,113	1.30	7 (8%)
17	CLA	2	312	-	47,51,73	1.42	7 (14%)	55,86,113	1.39	5 (9%)
17	CLA	A	839	29	69,73,73	1.21	7 (10%)	82,113,113	1.30	7 (8%)
17	CLA	A	806	-	69,73,73	1.22	8 (11%)	82,113,113	1.21	5 (6%)
17	CLA	A	811	-	58,62,73	1.30	6 (10%)	68,99,113	1.29	4 (5%)
17	CLA	1	312	-	59,63,73	1.30	6 (10%)	70,101,113	1.29	7 (10%)
25	HTG	F	305	-	19,19,19	0.98	2 (10%)	23,24,24	1.60	4 (17%)
17	CLA	1	307	1	69,73,73	1.24	8 (11%)	82,113,113	1.29	6 (7%)
17	CLA	3	610	-	56,60,73	1.34	7 (12%)	65,97,113	1.44	6 (9%)
21	BCR	A	848	-	41,41,41	1.07	2 (4%)	56,56,56	1.23	6 (10%)
17	CLA	A	809	-	69,73,73	1.16	7 (10%)	82,113,113	1.28	9 (10%)
17	CLA	2	307	2	54,58,73	1.34	7 (12%)	64,95,113	1.32	8 (12%)
18	CHL	2	304	29	37,51,74	4.24	18 (48%)	30,86,114	3.03	10 (33%)
17	CLA	B	841	-	69,73,73	1.20	9 (13%)	82,113,113	1.30	8 (9%)
17	CLA	2	302	-	55,59,73	1.34	8 (14%)	64,96,113	1.36	3 (4%)
17	CLA	1	302	-	69,73,73	1.20	7 (10%)	82,113,113	1.26	8 (9%)
17	CLA	A	843	22	56,60,73	1.34	5 (8%)	65,97,113	1.39	6 (9%)
28	SF4	C	102	7	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	2	310	2	56,60,73	1.39	9 (16%)	65,97,113	1.27	4 (6%)
17	CLA	3	608	3	54,58,73	1.36	7 (12%)	64,95,113	1.35	6 (9%)
17	CLA	B	825	-	64,68,73	1.15	7 (10%)	76,107,113	1.54	11 (14%)
17	CLA	A	802	29	69,73,73	1.13	7 (10%)	82,113,113	1.30	7 (8%)
17	CLA	1	301	1	69,73,73	1.25	6 (8%)	82,113,113	1.22	8 (9%)
17	CLA	1	311	1	64,68,73	1.21	8 (12%)	76,107,113	1.27	6 (7%)
18	CHL	4	307	29	45,59,74	3.95	20 (44%)	40,96,114	2.44	10 (25%)
19	LUT	1	314	-	42,43,43	4.67	20 (47%)	51,60,60	5.86	33 (64%)
21	BCR	J	105	-	41,41,41	1.20	4 (9%)	56,56,56	1.46	9 (16%)
17	CLA	1	310	1	56,60,73	1.32	9 (16%)	65,97,113	1.31	6 (9%)
18	CHL	1	305	1	42,56,74	4.14	19 (45%)	36,92,114	2.37	10 (27%)
17	CLA	B	818	-	59,63,73	1.26	6 (10%)	70,101,113	1.49	8 (11%)
25	HTG	J	102	-	19,19,19	1.10	2 (10%)	23,24,24	1.22	3 (13%)
21	BCR	A	846	-	41,41,41	1.05	2 (4%)	56,56,56	1.34	6 (10%)
17	CLA	A	832	-	69,73,73	1.22	6 (8%)	82,113,113	1.34	7 (8%)
21	BCR	L	206	-	41,41,41	1.11	2 (4%)	56,56,56	1.30	7 (12%)
17	CLA	B	828	-	69,73,73	1.23	8 (11%)	82,113,113	1.44	13 (15%)
17	CLA	F	306	29	49,53,73	1.36	6 (12%)	58,89,113	1.39	6 (10%)
17	CLA	A	834	5	49,53,73	1.40	8 (16%)	58,89,113	1.40	5 (8%)
17	CLA	A	830	-	54,58,73	1.33	7 (12%)	64,95,113	1.37	7 (10%)
25	HTG	B	851	-	19,19,19	0.99	1 (5%)	23,24,24	1.76	6 (26%)
17	CLA	3	606	3	51,55,73	1.38	7 (13%)	60,91,113	1.36	5 (8%)
17	CLA	B	833	-	64,68,73	1.22	7 (10%)	76,107,113	1.35	11 (14%)
24	LMG	4	320	-	49,49,55	1.03	4 (8%)	57,57,63	1.46	6 (10%)
17	CLA	B	838	-	69,73,73	1.15	7 (10%)	82,113,113	1.45	7 (8%)
21	BCR	A	850	-	41,41,41	1.17	2 (4%)	56,56,56	1.36	8 (14%)
17	CLA	A	810	17	69,73,73	1.17	6 (8%)	82,113,113	1.25	6 (7%)
17	CLA	A	827	-	69,73,73	1.17	8 (11%)	82,113,113	1.44	11 (13%)
17	CLA	3	611	3	59,63,73	1.29	7 (11%)	70,101,113	1.32	4 (5%)
17	CLA	A	836	-	69,73,73	1.15	6 (8%)	82,113,113	1.34	6 (7%)
17	CLA	B	803	-	69,73,73	1.20	7 (10%)	82,113,113	1.24	5 (6%)
21	BCR	A	847	-	41,41,41	1.11	4 (9%)	56,56,56	1.24	6 (10%)
18	CHL	4	315	4	37,51,74	4.28	18 (48%)	30,86,114	2.68	10 (33%)
17	CLA	G	105	11	50,54,73	1.36	6 (12%)	59,90,113	1.39	6 (10%)
21	BCR	I	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	B	829	-	69,73,73	1.23	8 (11%)	82,113,113	1.22	7 (8%)
17	CLA	3	612	-	49,53,73	1.41	5 (10%)	58,89,113	1.40	4 (6%)
17	CLA	K	201	-	49,53,73	1.39	7 (14%)	58,89,113	1.43	5 (8%)
17	CLA	K	202	-	64,68,73	1.24	7 (10%)	76,107,113	1.30	5 (6%)
22	LHG	A	845	17	26,26,48	0.89	1 (3%)	29,32,54	1.32	3 (10%)
24	LMG	F	309	-	55,55,55	0.84	2 (3%)	63,63,63	1.45	8 (12%)
17	CLA	4	310	-	64,68,73	1.19	7 (10%)	76,107,113	1.53	11 (14%)
17	CLA	A	812	-	69,73,73	1.20	7 (10%)	82,113,113	1.25	6 (7%)
17	CLA	A	815	29	49,53,73	1.43	8 (16%)	58,89,113	1.41	5 (8%)
17	CLA	A	820	29	69,73,73	1.20	7 (10%)	82,113,113	1.19	6 (7%)
17	CLA	B	815	-	69,73,73	1.25	6 (8%)	82,113,113	1.30	8 (9%)
17	CLA	B	816	-	69,73,73	1.21	7 (10%)	82,113,113	1.29	8 (9%)
17	CLA	B	824	-	59,63,73	1.30	8 (13%)	70,101,113	1.36	7 (10%)
17	CLA	B	839	-	51,55,73	1.32	4 (7%)	60,91,113	1.85	15 (25%)
23	LMT	A	855	-	36,36,36	1.09	2 (5%)	47,47,47	0.93	1 (2%)
17	CLA	B	804	-	69,73,73	1.29	9 (13%)	82,113,113	1.17	5 (6%)
17	CLA	A	805	5	69,73,73	1.18	6 (8%)	82,113,113	1.36	8 (9%)
17	CLA	3	603	3	54,58,73	1.32	6 (11%)	64,95,113	1.34	5 (7%)
17	CLA	A	819	-	49,53,73	1.40	5 (10%)	58,89,113	1.45	5 (8%)
17	CLA	B	834	-	62,66,73	1.30	9 (14%)	73,104,113	1.43	10 (13%)
18	CHL	2	313	2	37,51,74	4.27	18 (48%)	30,86,114	2.97	12 (40%)
18	CHL	3	601	2	47,61,74	3.82	19 (40%)	41,98,114	3.09	15 (36%)
21	BCR	L	205	-	41,41,41	1.01	2 (4%)	56,56,56	1.13	4 (7%)
24	LMG	B	852	-	52,52,55	1.07	4 (7%)	60,60,63	1.50	7 (11%)
17	CLA	B	814	-	59,63,73	1.31	6 (10%)	70,101,113	1.42	9 (12%)
17	CLA	B	810	-	69,73,73	1.26	8 (11%)	82,113,113	1.21	10 (12%)
25	HTG	4	321	-	19,19,19	1.04	2 (10%)	23,24,24	1.03	1 (4%)
18	CHL	3	607	29	41,55,74	4.08	20 (48%)	35,91,114	2.59	10 (28%)
17	CLA	B	811	6	69,73,73	1.19	6 (8%)	82,113,113	1.33	7 (8%)
27	PQN	B	843	-	34,34,34	4.72	14 (41%)	43,45,45	4.53	24 (55%)
17	CLA	4	313	-	49,53,73	1.42	6 (12%)	58,89,113	1.47	5 (8%)
21	BCR	A	849	-	41,41,41	1.13	2 (4%)	56,56,56	1.27	7 (12%)
17	CLA	A	807	5	69,73,73	1.18	9 (13%)	82,113,113	1.23	6 (7%)
17	CLA	4	304	29	54,58,73	1.33	6 (11%)	64,95,113	1.57	10 (15%)
17	CLA	A	840	-	69,73,73	1.21	8 (11%)	82,113,113	1.43	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	B	812	-	69,73,73	1.21	7 (10%)	82,113,113	1.16	6 (7%)
25	HTG	A	854	-	19,19,19	0.76	1 (5%)	23,24,24	0.91	0
17	CLA	A	801	-	69,73,73	1.14	6 (8%)	82,113,113	1.60	13 (15%)
17	CLA	1	306	29	50,54,73	1.39	7 (14%)	59,90,113	1.36	5 (8%)
17	CLA	2	308	2	64,68,73	1.21	7 (10%)	76,107,113	1.22	6 (7%)
17	CLA	A	853	29	69,73,73	1.24	8 (11%)	82,113,113	1.83	17 (20%)
17	CLA	1	304	-	46,50,73	1.44	7 (15%)	53,85,113	1.36	4 (7%)
17	CLA	G	103	29	45,49,73	1.48	8 (17%)	54,84,113	1.48	5 (9%)
17	CLA	A	825	29	69,73,73	1.19	6 (8%)	82,113,113	1.34	10 (12%)
17	CLA	B	802	-	69,73,73	1.19	8 (11%)	82,113,113	1.32	13 (15%)
20	XAT	4	317	-	41,47,47	3.80	18 (43%)	54,74,74	5.22	33 (61%)
21	BCR	B	844	-	41,41,41	1.01	2 (4%)	56,56,56	1.28	7 (12%)
21	BCR	B	848	-	41,41,41	1.10	2 (4%)	56,56,56	1.23	7 (12%)
24	LMG	4	319	-	50,50,55	0.87	3 (6%)	58,58,63	1.47	8 (13%)
17	CLA	A	817	-	69,73,73	1.19	7 (10%)	82,113,113	1.30	6 (7%)
23	LMT	2	318	-	36,36,36	1.06	4 (11%)	47,47,47	1.13	3 (6%)
21	BCR	B	847	-	41,41,41	1.13	3 (7%)	56,56,56	1.48	9 (16%)
18	CHL	4	301	1	55,69,74	3.11	25 (45%)	52,108,114	2.52	18 (34%)
17	CLA	B	826	29	69,73,73	1.24	8 (11%)	82,113,113	1.28	9 (10%)
17	CLA	B	806	-	49,53,73	1.26	5 (10%)	58,89,113	1.66	11 (18%)
17	CLA	A	835	-	55,59,73	1.33	8 (14%)	64,96,113	1.40	7 (10%)
17	CLA	1	309	22	69,73,73	1.21	6 (8%)	82,113,113	1.22	8 (9%)
17	CLA	J	101	-	69,73,73	1.24	7 (10%)	82,113,113	1.39	8 (9%)
17	CLA	3	609	3	54,58,73	1.34	5 (9%)	64,95,113	1.32	6 (9%)
17	CLA	G	104	-	54,58,73	1.37	6 (11%)	64,95,113	1.47	7 (10%)
17	CLA	A	821	-	53,57,73	1.32	8 (15%)	61,93,113	1.44	8 (13%)
17	CLA	B	820	-	64,68,73	1.23	6 (9%)	76,107,113	1.46	17 (22%)
17	CLA	B	835	-	69,73,73	1.28	6 (8%)	82,113,113	1.18	6 (7%)
28	SF4	C	101	7	0,12,12	-	-	-	-	-
17	CLA	4	309	4	64,68,73	1.32	6 (9%)	76,107,113	1.21	6 (7%)
17	CLA	2	309	-	45,49,73	1.43	5 (11%)	54,84,113	1.52	7 (12%)
17	CLA	4	312	4	60,64,73	1.26	8 (13%)	71,102,113	1.35	7 (9%)
17	CLA	1	308	1	64,68,73	1.22	6 (9%)	76,107,113	1.21	5 (6%)
17	CLA	1	313	1	50,54,73	1.34	7 (14%)	59,90,113	1.37	6 (10%)
28	SF4	A	852	5,6	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	BCR	2	316	-	41,41,41	1.21	3 (7%)	56,56,56	1.26	7 (12%)
17	CLA	B	831	-	69,73,73	1.18	6 (8%)	82,113,113	1.59	11 (13%)
17	CLA	A	818	-	69,73,73	1.19	8 (11%)	82,113,113	1.31	9 (10%)
21	BCR	L	201	-	41,41,41	1.04	2 (4%)	56,56,56	1.22	6 (10%)
17	CLA	B	805	-	69,73,73	1.19	7 (10%)	82,113,113	1.27	9 (10%)
17	CLA	4	303	4	64,68,73	1.34	7 (10%)	76,107,113	1.36	9 (11%)
17	CLA	L	202	15	69,73,73	1.19	6 (8%)	82,113,113	1.26	5 (6%)
27	PQN	A	842	-	34,34,34	4.86	15 (44%)	43,45,45	4.09	20 (46%)
17	CLA	B	809	-	69,73,73	1.20	7 (10%)	82,113,113	1.20	6 (7%)
18	CHL	2	305	29	42,56,74	4.04	18 (42%)	36,92,114	2.67	13 (36%)
17	CLA	A	822	-	55,59,73	1.32	6 (10%)	64,96,113	1.35	5 (7%)
17	CLA	A	828	-	69,73,73	1.19	4 (5%)	82,113,113	1.26	7 (8%)
17	CLA	B	821	29	69,73,73	1.17	5 (7%)	82,113,113	1.40	6 (7%)
17	CLA	J	103	14	46,50,73	1.40	7 (15%)	53,85,113	1.50	4 (7%)
17	CLA	4	311	4	56,60,73	1.34	6 (10%)	65,97,113	1.36	5 (7%)
17	CLA	A	833	-	54,58,73	1.32	7 (12%)	64,95,113	1.39	6 (9%)
17	CLA	B	832	-	54,58,73	1.33	6 (11%)	64,95,113	1.47	8 (12%)
20	XAT	1	315	-	41,47,47	3.71	18 (43%)	54,74,74	5.39	32 (59%)
18	CHL	4	305	29	50,64,74	3.53	19 (38%)	46,102,114	2.86	15 (32%)
21	BCR	B	849	-	41,41,41	0.98	3 (7%)	56,56,56	1.21	2 (3%)
21	BCR	G	106	-	41,41,41	1.08	2 (4%)	56,56,56	1.15	5 (8%)
26	DGD	B	850	-	67,67,67	1.13	5 (7%)	81,81,81	1.48	11 (13%)
17	CLA	L	203	-	69,73,73	1.18	6 (8%)	82,113,113	1.31	5 (6%)
17	CLA	B	842	22	69,73,73	1.19	6 (8%)	82,113,113	1.46	10 (12%)
17	CLA	A	803	17	59,63,73	1.31	8 (13%)	70,101,113	1.29	5 (7%)
17	CLA	B	808	6	69,73,73	1.21	10 (14%)	82,113,113	1.36	8 (9%)
17	CLA	B	807	-	69,73,73	1.19	10 (14%)	82,113,113	1.31	9 (10%)
21	BCR	J	104	-	41,41,41	1.02	3 (7%)	56,56,56	1.26	4 (7%)
24	LMG	G	101	-	40,40,55	0.86	2 (5%)	48,48,63	1.28	3 (6%)
17	CLA	B	823	-	69,73,73	1.10	5 (7%)	82,113,113	1.40	7 (8%)
17	CLA	B	830	-	69,73,73	1.25	8 (11%)	82,113,113	1.34	11 (13%)
17	CLA	A	829	-	69,73,73	1.15	7 (10%)	82,113,113	1.36	5 (6%)
19	LUT	3	614	-	42,43,43	4.75	20 (47%)	51,60,60	5.68	32 (62%)
17	CLA	B	822	-	54,58,73	1.29	4 (7%)	64,95,113	1.55	8 (12%)
21	BCR	B	846	-	41,41,41	1.06	2 (4%)	56,56,56	1.25	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	2	301	2	69,73,73	1.19	10 (14%)	82,113,113	1.24	7 (8%)
25	HTG	F	301	-	17,17,19	0.88	1 (5%)	21,22,24	0.68	0
17	CLA	A	816	-	69,73,73	1.19	7 (10%)	82,113,113	1.21	5 (6%)
22	LHG	B	801	17	22,22,48	1.10	2 (9%)	25,28,54	1.14	2 (8%)
17	CLA	A	804	-	69,73,73	1.23	5 (7%)	82,113,113	1.29	9 (10%)
25	HTG	F	310	-	16,16,19	1.06	2 (12%)	20,21,24	1.38	4 (20%)
26	DGD	4	323	-	61,61,67	0.89	2 (3%)	75,75,81	1.76	20 (26%)
22	LHG	1	317	17	48,48,48	0.69	1 (2%)	51,54,54	1.25	6 (11%)
17	CLA	2	303	-	64,68,73	1.22	7 (10%)	76,107,113	1.25	5 (6%)
21	BCR	B	845	-	41,41,41	0.94	1 (2%)	56,56,56	1.37	8 (14%)
17	CLA	3	613	-	50,54,73	1.39	8 (16%)	59,90,113	1.39	4 (6%)
17	CLA	B	817	-	59,63,73	1.27	7 (11%)	70,101,113	1.41	8 (11%)
17	CLA	B	827	29	69,73,73	1.16	5 (7%)	82,113,113	1.45	8 (9%)
22	LHG	2	317	-	36,36,48	0.72	1 (2%)	39,42,54	1.26	4 (10%)
17	CLA	4	314	-	51,55,73	1.26	5 (9%)	60,91,113	1.58	9 (15%)
21	BCR	1	316	-	41,41,41	1.08	2 (4%)	56,56,56	1.26	7 (12%)
19	LUT	4	316	-	42,43,43	4.64	22 (52%)	51,60,60	5.88	35 (68%)
17	CLA	A	831	-	69,73,73	1.19	7 (10%)	82,113,113	1.35	8 (9%)
17	CLA	A	808	5	69,73,73	1.13	4 (5%)	82,113,113	1.51	11 (13%)
21	BCR	F	308	-	41,41,41	1.09	2 (4%)	56,56,56	1.28	7 (12%)
17	CLA	A	813	-	49,53,73	1.43	6 (12%)	58,89,113	1.30	4 (6%)
17	CLA	B	813	-	58,62,73	1.32	7 (12%)	71,100,113	1.36	6 (8%)
22	LHG	A	844	-	48,48,48	0.68	1 (2%)	51,54,54	1.31	6 (11%)
18	CHL	4	306	29	45,59,74	3.92	19 (42%)	40,96,114	2.44	13 (32%)
17	CLA	4	308	4	54,58,73	1.34	8 (14%)	64,95,113	1.51	7 (10%)
21	BCR	K	203	-	41,41,41	1.10	2 (4%)	56,56,56	1.23	6 (10%)
17	CLA	A	838	-	69,73,73	1.19	7 (10%)	82,113,113	1.51	12 (14%)
22	LHG	F	302	-	39,39,48	0.65	0	42,45,54	1.28	6 (14%)
22	LHG	G	102	-	48,48,48	0.67	1 (2%)	51,54,54	1.25	6 (11%)
17	CLA	A	837	-	69,73,73	1.20	6 (8%)	82,113,113	1.30	9 (10%)
17	CLA	B	819	-	63,67,73	1.24	6 (9%)	74,105,113	1.37	8 (10%)
21	BCR	4	318	-	41,41,41	0.99	2 (4%)	56,56,56	1.29	8 (14%)
21	BCR	F	303	-	41,41,41	0.95	2 (4%)	56,56,56	1.41	12 (21%)
19	LUT	2	314	-	42,43,43	4.72	20 (47%)	51,60,60	5.81	33 (64%)
17	CLA	B	840	29	69,73,73	1.14	6 (8%)	82,113,113	1.28	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	3	604	-	49,53,73	1.39	8 (16%)	58,89,113	1.38	6 (10%)
17	CLA	4	302	4	64,68,73	1.30	8 (12%)	76,107,113	1.37	8 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	3	602	3	1/1/14/20	5/33/109/115	-
17	CLA	A	824	29	1/1/15/20	10/39/115/115	-
17	CLA	A	823	-	1/1/13/20	7/27/103/115	-
17	CLA	F	304	-	1/1/15/20	8/39/115/115	-
20	XAT	2	315	-	-	13/31/93/93	0/4/4/4
21	BCR	A	851	-	-	7/29/63/63	0/2/2/2
17	CLA	3	605	-	1/1/10/20	2/12/88/115	-
17	CLA	B	837	-	1/1/14/20	10/33/109/115	-
17	CLA	2	319	4	1/1/11/20	2/17/93/115	-
21	BCR	3	616	-	-	7/29/63/63	0/2/2/2
17	CLA	A	826	-	1/1/15/20	8/39/115/115	-
18	CHL	2	306	29	3/3/17/26	5/21/119/137	-
25	HTG	4	322	-	-	1/10/30/30	0/1/1/1
17	CLA	1	303	29	1/1/12/20	8/23/99/115	-
17	CLA	A	841	29	1/1/15/20	12/39/115/115	-
17	CLA	F	307	10	1/1/13/20	8/27/103/115	-
17	CLA	A	814	-	1/1/12/20	9/21/97/115	-
17	CLA	L	204	-	-	7/21/97/115	-
17	CLA	B	836	29	1/1/11/20	4/15/91/115	-
20	XAT	3	615	-	-	13/31/93/93	0/4/4/4
17	CLA	2	311	2	1/1/15/20	14/39/115/115	-
17	CLA	2	312	-	1/1/10/20	0/13/89/115	-
17	CLA	A	839	29	1/1/15/20	16/39/115/115	-
17	CLA	A	806	-	1/1/15/20	8/39/115/115	-
17	CLA	A	811	-	1/1/12/20	5/26/102/115	-
17	CLA	1	312	-	1/1/13/20	9/27/103/115	-
25	HTG	F	305	-	-	3/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	1	307	1	1/1/15/20	13/39/115/115	-
17	CLA	3	610	-	1/1/12/20	10/24/100/115	-
21	BCR	A	848	-	-	6/29/63/63	0/2/2/2
17	CLA	A	809	-	1/1/15/20	14/39/115/115	-
17	CLA	2	307	2	1/1/12/20	1/21/97/115	-
18	CHL	2	304	29	3/3/15/26	5/12/110/137	-
17	CLA	B	841	-	1/1/15/20	13/39/115/115	-
17	CLA	2	302	-	1/1/12/20	2/23/99/115	-
17	CLA	1	302	-	1/1/15/20	18/39/115/115	-
17	CLA	A	843	22	1/1/12/20	11/24/100/115	-
28	SF4	C	102	7	-	-	0/6/5/5
17	CLA	2	310	2	1/1/12/20	6/24/100/115	-
17	CLA	3	608	3	1/1/12/20	4/21/97/115	-
17	CLA	B	825	-	1/1/14/20	8/33/109/115	-
17	CLA	A	802	29	1/1/15/20	6/39/115/115	-
17	CLA	1	301	1	1/1/15/20	9/39/115/115	-
17	CLA	1	311	1	1/1/14/20	8/33/109/115	-
18	CHL	4	307	29	3/3/17/26	2/21/119/137	-
19	LUT	1	314	-	-	12/29/67/67	0/2/2/2
21	BCR	J	105	-	-	7/29/63/63	0/2/2/2
17	CLA	1	310	1	1/1/12/20	9/24/100/115	-
18	CHL	1	305	1	3/3/16/26	5/18/116/137	-
17	CLA	B	818	-	1/1/13/20	5/27/103/115	-
25	HTG	J	102	-	-	6/10/30/30	0/1/1/1
21	BCR	A	846	-	-	2/29/63/63	0/2/2/2
17	CLA	A	832	-	1/1/15/20	13/39/115/115	-
21	BCR	L	206	-	-	4/29/63/63	0/2/2/2
17	CLA	B	828	-	1/1/15/20	7/39/115/115	-
17	CLA	F	306	29	1/1/11/20	0/15/91/115	-
17	CLA	A	834	5	1/1/11/20	6/15/91/115	-
17	CLA	A	830	-	1/1/12/20	5/21/97/115	-
25	HTG	B	851	-	-	7/10/30/30	0/1/1/1
17	CLA	3	606	3	1/1/11/20	8/18/94/115	-
17	CLA	B	833	-	1/1/14/20	5/33/109/115	-
24	LMG	4	320	-	-	21/44/64/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	838	-	1/1/15/20	9/39/115/115	-
21	BCR	A	850	-	-	8/29/63/63	0/2/2/2
17	CLA	A	810	17	1/1/15/20	13/39/115/115	-
17	CLA	A	827	-	1/1/15/20	9/39/115/115	-
17	CLA	3	611	3	1/1/13/20	10/27/103/115	-
17	CLA	A	836	-	1/1/15/20	14/39/115/115	-
17	CLA	B	803	-	1/1/15/20	15/39/115/115	-
21	BCR	A	847	-	-	6/29/63/63	0/2/2/2
18	CHL	4	315	4	3/3/15/26	4/12/110/137	-
17	CLA	G	105	11	1/1/11/20	6/17/93/115	-
21	BCR	I	101	-	-	4/29/63/63	0/2/2/2
17	CLA	B	829	-	1/1/15/20	14/39/115/115	-
17	CLA	3	612	-	1/1/11/20	6/15/91/115	-
17	CLA	K	201	-	1/1/11/20	3/15/91/115	-
17	CLA	K	202	-	1/1/14/20	14/33/109/115	-
22	LHG	A	845	17	-	14/31/31/53	-
24	LMG	F	309	-	-	20/50/70/70	0/1/1/1
17	CLA	4	310	-	1/1/14/20	15/33/109/115	-
17	CLA	A	812	-	1/1/15/20	9/39/115/115	-
17	CLA	A	815	29	1/1/11/20	4/15/91/115	-
17	CLA	A	820	29	1/1/15/20	8/39/115/115	-
17	CLA	B	815	-	1/1/15/20	14/39/115/115	-
17	CLA	B	816	-	1/1/15/20	8/39/115/115	-
17	CLA	B	824	-	1/1/13/20	10/27/103/115	-
17	CLA	B	839	-	1/1/11/20	2/18/94/115	-
23	LMT	A	855	-	-	14/21/61/61	0/2/2/2
17	CLA	B	804	-	1/1/15/20	4/39/115/115	-
17	CLA	A	805	5	1/1/15/20	21/39/115/115	-
17	CLA	3	603	3	1/1/12/20	2/21/97/115	-
17	CLA	A	819	-	1/1/11/20	6/15/91/115	-
17	CLA	B	834	-	1/1/13/20	13/31/107/115	-
18	CHL	2	313	2	3/3/15/26	2/12/110/137	-
18	CHL	3	601	2	3/3/17/26	5/24/122/137	-
21	BCR	L	205	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LMG	B	852	-	-	21/47/67/70	0/1/1/1
17	CLA	B	814	-	1/1/13/20	6/27/103/115	-
17	CLA	B	810	-	1/1/15/20	8/39/115/115	-
25	HTG	4	321	-	-	3/10/30/30	0/1/1/1
18	CHL	3	607	29	3/3/16/26	4/17/115/137	-
17	CLA	B	811	6	1/1/15/20	9/39/115/115	-
27	PQN	B	843	-	-	3/23/43/43	0/2/2/2
17	CLA	4	313	-	1/1/11/20	8/15/91/115	-
21	BCR	A	849	-	-	7/29/63/63	0/2/2/2
17	CLA	A	807	5	1/1/15/20	18/39/115/115	-
17	CLA	4	304	29	1/1/12/20	6/21/97/115	-
17	CLA	A	840	-	1/1/15/20	16/39/115/115	-
17	CLA	B	812	-	-	17/39/115/115	-
25	HTG	A	854	-	-	2/10/30/30	0/1/1/1
17	CLA	A	801	-	2/2/15/20	8/39/115/115	-
17	CLA	1	306	29	1/1/11/20	1/17/93/115	-
17	CLA	2	308	2	1/1/14/20	10/33/109/115	-
17	CLA	A	853	29	1/1/15/20	13/39/115/115	-
17	CLA	1	304	-	1/1/10/20	4/12/88/115	-
17	CLA	G	103	29	1/1/10/20	4/10/86/115	-
17	CLA	A	825	29	1/1/15/20	5/39/115/115	-
17	CLA	B	802	-	1/1/15/20	2/39/115/115	-
20	XAT	4	317	-	3/3/12/26	11/31/93/93	0/4/4/4
21	BCR	B	844	-	-	6/29/63/63	0/2/2/2
21	BCR	B	848	-	-	3/29/63/63	0/2/2/2
24	LMG	4	319	-	-	15/45/65/70	0/1/1/1
17	CLA	A	817	-	1/1/15/20	12/39/115/115	-
23	LMT	2	318	-	-	11/21/61/61	0/2/2/2
21	BCR	B	847	-	-	3/29/63/63	0/2/2/2
18	CHL	4	301	1	4/4/19/26	16/33/131/137	-
17	CLA	B	826	29	1/1/15/20	16/39/115/115	-
17	CLA	B	806	-	1/1/11/20	1/15/91/115	-
17	CLA	A	835	-	1/1/12/20	9/23/99/115	-
17	CLA	1	309	22	1/1/15/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	J	101	-	1/1/15/20	8/39/115/115	-
17	CLA	3	609	3	1/1/12/20	3/21/97/115	-
17	CLA	G	104	-	1/1/12/20	4/21/97/115	-
17	CLA	A	821	-	1/1/11/20	8/20/96/115	-
17	CLA	B	820	-	1/1/14/20	14/33/109/115	-
17	CLA	B	835	-	1/1/15/20	11/39/115/115	-
28	SF4	C	101	7	-	-	0/6/5/5
17	CLA	4	309	4	1/1/14/20	8/33/109/115	-
17	CLA	2	309	-	1/1/10/20	2/10/86/115	-
17	CLA	4	312	4	1/1/13/20	7/29/105/115	-
17	CLA	1	308	1	1/1/14/20	9/33/109/115	-
17	CLA	1	313	1	1/1/11/20	4/17/93/115	-
28	SF4	A	852	5,6	-	-	0/6/5/5
21	BCR	2	316	-	-	17/29/63/63	0/2/2/2
17	CLA	B	831	-	1/1/15/20	10/39/115/115	-
17	CLA	A	818	-	1/1/15/20	15/39/115/115	-
21	BCR	L	201	-	-	11/29/63/63	0/2/2/2
17	CLA	B	805	-	1/1/15/20	10/39/115/115	-
17	CLA	4	303	4	-	15/33/109/115	-
17	CLA	L	202	15	1/1/15/20	14/39/115/115	-
27	PQN	A	842	-	-	6/23/43/43	0/2/2/2
17	CLA	B	809	-	1/1/15/20	13/39/115/115	-
18	CHL	2	305	29	3/3/16/26	3/18/116/137	-
17	CLA	A	822	-	1/1/12/20	11/23/99/115	-
17	CLA	A	828	-	1/1/15/20	8/39/115/115	-
17	CLA	B	821	29	1/1/15/20	5/39/115/115	-
17	CLA	J	103	14	1/1/10/20	6/12/88/115	-
17	CLA	4	311	4	-	4/24/100/115	-
17	CLA	A	833	-	1/1/12/20	4/21/97/115	-
17	CLA	B	832	-	1/1/12/20	2/21/97/115	-
20	XAT	1	315	-	-	13/31/93/93	0/4/4/4
18	CHL	4	305	29	4/4/18/26	9/27/125/137	-
21	BCR	B	849	-	-	8/29/63/63	0/2/2/2
21	BCR	G	106	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	DGD	B	850	-	-	24/55/95/95	0/2/2/2
17	CLA	L	203	-	1/1/15/20	9/39/115/115	-
17	CLA	B	842	22	1/1/15/20	5/39/115/115	-
17	CLA	A	803	17	1/1/13/20	9/27/103/115	-
17	CLA	B	808	6	1/1/15/20	12/39/115/115	-
17	CLA	B	807	-	1/1/15/20	12/39/115/115	-
21	BCR	J	104	-	-	2/29/63/63	0/2/2/2
24	LMG	G	101	-	-	16/35/55/70	0/1/1/1
17	CLA	B	823	-	1/1/15/20	12/39/115/115	-
17	CLA	B	830	-	1/1/15/20	5/39/115/115	-
17	CLA	A	829	-	1/1/15/20	13/39/115/115	-
19	LUT	3	614	-	-	12/29/67/67	0/2/2/2
17	CLA	B	822	-	1/1/12/20	4/21/97/115	-
21	BCR	B	846	-	-	7/29/63/63	0/2/2/2
17	CLA	2	301	2	1/1/15/20	5/39/115/115	-
25	HTG	F	301	-	-	4/8/28/30	0/1/1/1
17	CLA	A	816	-	1/1/15/20	16/39/115/115	-
22	LHG	B	801	17	-	10/26/26/53	-
17	CLA	A	804	-	1/1/15/20	10/39/115/115	-
25	HTG	F	310	-	-	3/7/27/30	0/1/1/1
26	DGD	4	323	-	-	27/49/89/95	0/2/2/2
22	LHG	1	317	17	-	20/53/53/53	-
17	CLA	2	303	-	1/1/14/20	15/33/109/115	-
21	BCR	B	845	-	-	5/29/63/63	0/2/2/2
17	CLA	3	613	-	1/1/11/20	2/17/93/115	-
17	CLA	B	817	-	1/1/13/20	10/27/103/115	-
17	CLA	B	827	29	1/1/15/20	8/39/115/115	-
22	LHG	2	317	-	-	19/41/41/53	-
17	CLA	4	314	-	1/1/11/20	4/18/94/115	-
21	BCR	1	316	-	-	11/29/63/63	0/2/2/2
19	LUT	4	316	-	-	13/29/67/67	0/2/2/2
17	CLA	A	831	-	1/1/15/20	17/39/115/115	-
17	CLA	A	808	5	1/1/15/20	8/39/115/115	-
21	BCR	F	308	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	813	-	1/1/11/20	2/15/91/115	-
17	CLA	B	813	-	1/1/13/20	9/25/101/115	-
22	LHG	A	844	-	-	27/53/53/53	-
18	CHL	4	306	29	3/3/17/26	9/21/119/137	-
17	CLA	4	308	4	1/1/12/20	3/21/97/115	-
21	BCR	K	203	-	-	12/29/63/63	0/2/2/2
17	CLA	A	838	-	1/1/15/20	12/39/115/115	-
22	LHG	F	302	-	-	30/44/44/53	-
22	LHG	G	102	-	-	26/53/53/53	-
17	CLA	A	837	-	1/1/15/20	12/39/115/115	-
17	CLA	B	819	-	1/1/13/20	6/32/108/115	-
21	BCR	4	318	-	-	7/29/63/63	0/2/2/2
21	BCR	F	303	-	-	5/29/63/63	0/2/2/2
19	LUT	2	314	-	-	13/29/67/67	0/2/2/2
17	CLA	B	840	29	1/1/15/20	14/39/115/115	-
17	CLA	3	604	-	1/1/11/20	2/15/91/115	-
17	CLA	4	302	4	1/1/14/20	6/33/109/115	-

All (1473) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	314	LUT	C24-C25	16.50	1.52	1.33
19	2	314	LUT	C24-C25	16.25	1.52	1.33
19	3	614	LUT	C24-C25	16.14	1.52	1.33
19	4	316	LUT	C24-C25	15.71	1.51	1.33
19	3	614	LUT	C5-C6	11.31	1.53	1.34
19	4	316	LUT	C5-C6	11.19	1.53	1.34
19	2	314	LUT	C5-C6	11.12	1.53	1.34
18	4	307	CHL	C2C-C3C	10.99	1.47	1.36
18	1	305	CHL	C2C-C3C	10.92	1.46	1.36
19	1	314	LUT	C5-C6	10.91	1.52	1.34
18	4	306	CHL	C2C-C3C	10.80	1.46	1.36
18	4	305	CHL	C1D-C2D	10.79	1.51	1.39
18	3	601	CHL	C2C-C3C	10.64	1.46	1.36
27	B	843	PQN	C3-C2	10.62	1.54	1.35
27	A	842	PQN	C3-C2	10.51	1.54	1.35
18	2	313	CHL	C2C-C3C	10.48	1.46	1.36
18	2	306	CHL	C2C-C3C	10.33	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	607	CHL	C2C-C3C	10.28	1.46	1.36
18	2	305	CHL	C1D-C2D	10.24	1.51	1.39
18	2	305	CHL	C2C-C3C	10.23	1.46	1.36
27	A	842	PQN	O4-C4	10.10	1.44	1.23
18	4	315	CHL	C2C-C3C	10.09	1.46	1.36
18	3	601	CHL	C1D-C2D	10.09	1.51	1.39
18	4	306	CHL	C1D-C2D	10.07	1.51	1.39
18	2	313	CHL	C1D-C2D	10.03	1.51	1.39
18	4	307	CHL	C1D-C2D	9.95	1.50	1.39
18	2	304	CHL	C1D-C2D	9.95	1.50	1.39
27	A	842	PQN	O1-C1	9.92	1.43	1.23
18	3	607	CHL	C1D-C2D	9.90	1.50	1.39
18	2	304	CHL	C2C-C3C	9.90	1.46	1.36
18	1	305	CHL	C1D-C2D	9.84	1.50	1.39
18	2	306	CHL	C1D-C2D	9.82	1.50	1.39
27	B	843	PQN	O1-C1	9.76	1.43	1.23
27	B	843	PQN	O4-C4	9.27	1.42	1.23
18	4	315	CHL	C1D-C2D	9.26	1.50	1.39
20	4	317	XAT	C8-C7	9.18	1.52	1.32
20	3	615	XAT	C28-C27	9.14	1.52	1.32
20	1	315	XAT	C28-C27	9.10	1.52	1.32
20	2	315	XAT	C28-C27	9.08	1.52	1.32
19	1	314	LUT	C28-C27	9.06	1.52	1.32
19	3	614	LUT	C28-C27	9.06	1.52	1.32
20	4	317	XAT	C28-C27	9.02	1.52	1.32
18	4	315	CHL	C3B-C4B	9.01	1.50	1.41
18	1	305	CHL	C1B-C2B	8.96	1.49	1.39
20	1	315	XAT	C8-C7	8.95	1.52	1.32
20	3	615	XAT	C8-C7	8.94	1.52	1.32
20	2	315	XAT	C8-C7	8.92	1.52	1.32
19	2	314	LUT	C28-C27	8.91	1.52	1.32
27	B	843	PQN	C9-C10	8.84	1.53	1.39
18	4	315	CHL	C1B-C2B	8.78	1.49	1.39
19	4	316	LUT	C28-C27	8.77	1.52	1.32
18	4	305	CHL	C2C-C3C	8.68	1.44	1.36
27	A	842	PQN	C12-C13	8.67	1.53	1.33
18	4	307	CHL	C3B-C4B	8.64	1.49	1.41
18	2	306	CHL	C1B-C2B	8.59	1.49	1.39
27	A	842	PQN	C9-C10	8.55	1.52	1.39
18	1	305	CHL	C3B-C4B	8.52	1.49	1.41
18	2	305	CHL	C1B-C2B	8.48	1.49	1.39
27	A	842	PQN	C8-C9	8.46	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	304	CHL	C1B-C2B	8.42	1.49	1.39
18	2	313	CHL	C1B-C2B	8.37	1.49	1.39
27	A	842	PQN	C7-C6	8.35	1.53	1.38
18	4	305	CHL	C1B-C2B	8.29	1.49	1.39
18	2	313	CHL	C3B-C4B	8.25	1.49	1.41
18	4	301	CHL	C3D-C4D	-8.23	1.29	1.41
18	4	306	CHL	C1B-C2B	8.22	1.48	1.39
18	3	607	CHL	C1B-C2B	8.17	1.48	1.39
27	B	843	PQN	C12-C13	8.15	1.51	1.33
18	4	306	CHL	C3B-C4B	8.09	1.49	1.41
27	B	843	PQN	C6-C5	7.97	1.52	1.39
27	B	843	PQN	C8-C9	7.96	1.52	1.38
18	3	601	CHL	C1B-C2B	7.93	1.48	1.39
18	3	601	CHL	C3B-C4B	7.91	1.49	1.41
18	3	607	CHL	C3B-C4B	7.89	1.49	1.41
27	B	843	PQN	C7-C6	7.85	1.52	1.38
18	2	304	CHL	C3B-C4B	7.84	1.49	1.41
18	2	305	CHL	C3B-C4B	7.81	1.49	1.41
18	4	307	CHL	C1B-C2B	7.79	1.48	1.39
18	4	301	CHL	C3A-C2A	-7.79	1.48	1.54
27	A	842	PQN	C6-C5	7.68	1.51	1.39
18	2	313	CHL	C1A-CHA	7.48	1.48	1.40
18	2	304	CHL	C1A-CHA	7.45	1.48	1.40
19	3	614	LUT	C14-C13	7.40	1.52	1.35
20	4	317	XAT	C34-C33	7.35	1.52	1.35
19	2	314	LUT	C34-C33	7.33	1.52	1.35
18	2	306	CHL	C3B-C4B	7.31	1.48	1.41
19	3	614	LUT	C10-C9	7.31	1.52	1.35
18	3	607	CHL	C1A-CHA	7.30	1.48	1.40
19	2	314	LUT	C10-C9	7.29	1.52	1.35
19	4	316	LUT	C10-C9	7.26	1.52	1.35
18	4	315	CHL	C1A-CHA	7.26	1.48	1.40
18	4	305	CHL	C1A-CHA	7.21	1.48	1.40
19	4	316	LUT	C14-C13	7.17	1.52	1.35
20	1	315	XAT	C14-C13	7.17	1.52	1.35
20	2	315	XAT	C14-C13	7.17	1.52	1.35
19	1	314	LUT	C14-C13	7.17	1.52	1.35
19	3	614	LUT	C30-C29	7.16	1.52	1.35
20	2	315	XAT	C34-C33	7.16	1.52	1.35
18	3	601	CHL	C1A-CHA	7.16	1.48	1.40
20	1	315	XAT	C34-C33	7.16	1.52	1.35
19	2	314	LUT	C14-C13	7.15	1.52	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	615	XAT	C34-C33	7.15	1.52	1.35
20	3	615	XAT	C14-C13	7.14	1.52	1.35
19	3	614	LUT	C34-C33	7.13	1.52	1.35
20	4	317	XAT	C11-C12	7.11	1.53	1.34
19	2	314	LUT	C30-C29	7.04	1.52	1.35
20	2	315	XAT	C10-C9	7.03	1.52	1.35
19	1	314	LUT	C30-C29	7.03	1.52	1.35
20	1	315	XAT	C10-C9	7.02	1.52	1.35
20	3	615	XAT	C10-C9	7.01	1.52	1.35
19	4	316	LUT	C30-C29	7.01	1.52	1.35
18	4	305	CHL	C3B-C4B	7.00	1.48	1.41
18	4	306	CHL	C1A-CHA	7.00	1.48	1.40
19	1	314	LUT	C34-C33	6.98	1.51	1.35
18	4	301	CHL	C2C-C3C	6.96	1.43	1.36
19	4	316	LUT	C34-C33	6.96	1.51	1.35
19	3	614	LUT	C11-C12	6.93	1.52	1.34
19	1	314	LUT	C10-C9	6.92	1.51	1.35
20	4	317	XAT	C10-C9	6.91	1.51	1.35
20	4	317	XAT	C30-C29	6.82	1.51	1.35
20	4	317	XAT	C14-C13	6.81	1.51	1.35
18	2	306	CHL	C1A-CHA	6.79	1.47	1.40
19	2	314	LUT	C11-C12	6.79	1.52	1.34
18	4	301	CHL	C1D-C2D	6.77	1.47	1.39
20	4	317	XAT	C31-C32	6.76	1.52	1.34
19	3	614	LUT	C31-C32	6.75	1.52	1.34
27	B	843	PQN	C10-C5	6.74	1.51	1.40
20	1	315	XAT	C30-C29	6.73	1.51	1.35
20	2	315	XAT	C30-C29	6.72	1.51	1.35
20	3	615	XAT	C30-C29	6.72	1.51	1.35
18	4	307	CHL	C1A-CHA	6.69	1.47	1.40
18	4	301	CHL	C1B-C2B	6.68	1.47	1.39
27	B	843	PQN	C8-C7	6.68	1.52	1.38
18	2	305	CHL	C1A-CHA	6.64	1.47	1.40
19	2	314	LUT	C31-C32	6.64	1.52	1.34
20	3	615	XAT	C11-C12	6.63	1.52	1.34
20	1	315	XAT	C11-C12	6.62	1.52	1.34
20	2	315	XAT	C11-C12	6.60	1.51	1.34
20	1	315	XAT	C31-C32	6.58	1.51	1.34
20	2	315	XAT	C31-C32	6.58	1.51	1.34
20	3	615	XAT	C31-C32	6.57	1.51	1.34
19	4	316	LUT	C31-C32	6.57	1.51	1.34
27	A	842	PQN	C8-C7	6.56	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	314	LUT	C11-C12	6.56	1.51	1.34
19	4	316	LUT	C11-C12	6.55	1.51	1.34
19	1	314	LUT	C31-C32	6.53	1.51	1.34
19	3	614	LUT	C8-C7	6.51	1.52	1.33
19	4	316	LUT	C8-C7	6.49	1.52	1.33
27	A	842	PQN	C10-C5	6.46	1.51	1.40
19	2	314	LUT	C8-C7	6.42	1.52	1.33
19	1	314	LUT	C8-C7	6.25	1.51	1.33
18	4	301	CHL	CHB-C4A	-6.21	1.31	1.38
18	1	305	CHL	C1A-CHA	6.20	1.47	1.40
19	1	314	LUT	C35-C15	6.02	1.52	1.36
19	3	614	LUT	C35-C15	5.98	1.52	1.36
19	2	314	LUT	C35-C15	5.95	1.52	1.36
20	3	615	XAT	C35-C15	5.83	1.52	1.36
20	1	315	XAT	C35-C15	5.82	1.52	1.36
20	2	315	XAT	C35-C15	5.82	1.52	1.36
19	4	316	LUT	C35-C15	5.78	1.52	1.36
20	4	317	XAT	C35-C15	5.67	1.51	1.36
18	1	305	CHL	CHB-C1B	5.55	1.48	1.39
18	4	307	CHL	C3D-C2D	5.52	1.49	1.39
18	2	306	CHL	C3A-C2A	-5.43	1.50	1.54
18	1	305	CHL	CHC-C4B	5.39	1.48	1.39
18	2	313	CHL	O2D-CGD	5.39	1.46	1.33
18	1	305	CHL	O2D-CGD	5.39	1.46	1.33
18	2	304	CHL	OBD-CAD	5.39	1.29	1.22
18	4	306	CHL	CHC-C4B	5.38	1.48	1.39
18	4	301	CHL	CBD-CGD	-5.32	1.45	1.52
18	2	304	CHL	C3A-C2A	-5.30	1.50	1.54
18	3	607	CHL	O2D-CGD	5.23	1.46	1.33
18	3	601	CHL	C3D-C4D	-5.23	1.33	1.41
18	4	315	CHL	CHC-C4B	5.22	1.48	1.39
18	2	306	CHL	OBD-CAD	5.21	1.29	1.22
18	4	315	CHL	C3D-C4D	-5.16	1.33	1.41
18	1	305	CHL	C3D-C4D	-5.15	1.33	1.41
18	4	307	CHL	CHC-C4B	5.15	1.48	1.39
18	2	305	CHL	C3D-C4D	-5.15	1.33	1.41
18	2	313	CHL	CHC-C4B	5.13	1.47	1.39
18	4	306	CHL	O2D-CGD	5.11	1.45	1.33
18	2	305	CHL	O2D-CGD	5.07	1.45	1.33
18	2	304	CHL	C3D-C4D	-5.05	1.33	1.41
18	4	315	CHL	O2D-CGD	5.04	1.45	1.33
18	3	601	CHL	OBD-CAD	5.00	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	305	CHL	C3D-C4D	-4.99	1.33	1.41
18	3	607	CHL	OBD-CAD	4.96	1.28	1.22
18	3	607	CHL	CHB-C4A	-4.96	1.32	1.38
18	3	601	CHL	C3B-C2B	4.96	1.47	1.40
18	4	307	CHL	OBD-CAD	4.95	1.28	1.22
18	2	306	CHL	O2D-CGD	4.93	1.45	1.33
18	4	307	CHL	CHB-C4A	-4.93	1.32	1.38
18	2	313	CHL	C3D-C4D	-4.92	1.34	1.41
18	3	607	CHL	C3D-C4D	-4.91	1.34	1.41
18	2	305	CHL	CHC-C4B	4.90	1.47	1.39
18	3	607	CHL	C3B-C2B	4.90	1.47	1.40
18	1	305	CHL	C3D-C2D	4.89	1.48	1.39
18	1	305	CHL	C3B-C2B	4.89	1.47	1.40
18	1	305	CHL	CHC-C1C	4.89	1.48	1.39
18	2	305	CHL	OBD-CAD	4.88	1.28	1.22
18	4	307	CHL	CHC-C1C	4.87	1.48	1.39
18	4	315	CHL	C3D-C2D	4.87	1.48	1.39
18	2	305	CHL	C3B-C2B	4.87	1.47	1.40
18	2	306	CHL	CHB-C4A	-4.87	1.32	1.38
18	4	315	CHL	CHB-C4A	-4.84	1.32	1.38
18	3	601	CHL	CHC-C4B	4.84	1.47	1.39
18	4	306	CHL	CHD-C4C	4.84	1.48	1.39
18	4	306	CHL	CHC-C1C	4.83	1.48	1.39
18	2	304	CHL	CHC-C4B	4.82	1.47	1.39
18	2	304	CHL	O2D-CGD	4.81	1.45	1.33
18	2	313	CHL	OBD-CAD	4.77	1.28	1.22
18	4	305	CHL	CHC-C4B	4.77	1.47	1.39
18	2	306	CHL	CHD-C4C	4.75	1.48	1.39
18	4	306	CHL	C3B-C2B	4.74	1.46	1.40
18	4	305	CHL	O2D-CGD	4.74	1.44	1.33
18	4	307	CHL	C3D-C4D	-4.73	1.34	1.41
18	4	307	CHL	O2D-CGD	4.73	1.44	1.33
18	2	306	CHL	CHC-C4B	4.72	1.47	1.39
18	2	306	CHL	C3D-C4D	-4.72	1.34	1.41
18	4	305	CHL	CHB-C4A	-4.71	1.32	1.38
18	2	313	CHL	CHB-C1B	4.71	1.47	1.39
18	4	315	CHL	OBD-CAD	4.70	1.28	1.22
18	2	304	CHL	CHB-C4A	-4.70	1.33	1.38
18	4	301	CHL	CHA-CBD	-4.70	1.46	1.51
18	3	607	CHL	C3D-C2D	4.70	1.47	1.39
18	2	306	CHL	CHB-C1B	4.70	1.47	1.39
18	2	313	CHL	C3B-C2B	4.70	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	601	CHL	O2D-CGD	4.69	1.44	1.33
18	4	315	CHL	CHD-C4C	4.68	1.48	1.39
18	2	305	CHL	CHD-C1D	4.66	1.47	1.39
18	4	306	CHL	O2A-CGA	4.65	1.46	1.33
18	2	304	CHL	CHD-C4C	4.61	1.48	1.39
18	2	313	CHL	C3D-C2D	4.61	1.47	1.39
18	2	306	CHL	C3D-C2D	4.61	1.47	1.39
18	3	601	CHL	C3A-C2A	-4.59	1.50	1.54
18	2	305	CHL	CHB-C1B	4.59	1.47	1.39
17	4	309	CLA	C1D-ND	4.58	1.43	1.37
18	2	304	CHL	CHC-C1C	4.58	1.48	1.39
18	3	601	CHL	CHB-C1B	4.58	1.47	1.39
18	4	307	CHL	CHD-C4C	4.56	1.48	1.39
18	1	305	CHL	OBD-CAD	4.56	1.28	1.22
18	4	305	CHL	C3B-C2B	4.55	1.46	1.40
18	4	315	CHL	CHC-C1C	4.54	1.48	1.39
18	4	306	CHL	CHB-C1B	4.54	1.47	1.39
18	4	306	CHL	C3D-C4D	-4.53	1.34	1.41
18	2	305	CHL	O2A-CGA	4.52	1.46	1.33
18	1	305	CHL	O2A-CGA	4.52	1.46	1.33
18	2	305	CHL	C3D-C2D	4.51	1.47	1.39
18	3	607	CHL	CHC-C4B	4.51	1.46	1.39
18	2	305	CHL	CHD-C4C	4.50	1.48	1.39
18	3	601	CHL	CHB-C4A	-4.49	1.33	1.38
21	J	105	BCR	C1-C6	-4.49	1.48	1.53
18	2	304	CHL	CHD-C1D	4.45	1.46	1.39
18	4	306	CHL	OBD-CAD	4.45	1.28	1.22
18	2	313	CHL	CHC-C1C	4.45	1.47	1.39
18	3	607	CHL	CHD-C4C	4.45	1.47	1.39
18	2	306	CHL	CHD-C1D	4.44	1.46	1.39
18	2	305	CHL	CHC-C1C	4.43	1.47	1.39
18	4	315	CHL	CHD-C1D	4.43	1.46	1.39
18	4	306	CHL	C3D-C2D	4.42	1.47	1.39
18	2	304	CHL	CHB-C1B	4.42	1.46	1.39
18	1	305	CHL	CHD-C1D	4.40	1.46	1.39
18	3	601	CHL	CHD-C4C	4.39	1.47	1.39
18	3	601	CHL	C3D-C2D	4.39	1.47	1.39
18	4	305	CHL	O2A-CGA	4.39	1.46	1.33
18	3	607	CHL	C3A-C2A	-4.39	1.50	1.54
21	2	316	BCR	C1-C6	-4.37	1.48	1.53
18	1	305	CHL	CHD-C4C	4.36	1.47	1.39
18	4	305	CHL	CHB-C1B	4.36	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	607	CHL	CHD-C1D	4.34	1.46	1.39
18	2	306	CHL	O2A-CGA	4.32	1.45	1.33
18	3	601	CHL	O2A-CGA	4.32	1.45	1.33
18	2	305	CHL	CHB-C4A	-4.31	1.33	1.38
18	4	307	CHL	O2A-CGA	4.30	1.45	1.33
18	2	313	CHL	CHB-C4A	-4.28	1.33	1.38
18	3	607	CHL	CHB-C1B	4.26	1.46	1.39
18	4	315	CHL	C3B-C2B	4.23	1.46	1.40
18	2	306	CHL	CHC-C1C	4.23	1.47	1.39
18	2	313	CHL	CHD-C4C	4.23	1.47	1.39
18	3	601	CHL	CHC-C1C	4.22	1.47	1.39
17	B	827	CLA	C1D-ND	4.20	1.43	1.37
18	2	305	CHL	C3A-C2A	-4.20	1.51	1.54
17	J	101	CLA	C1D-ND	4.20	1.43	1.37
18	4	305	CHL	C3D-C2D	4.18	1.46	1.39
17	4	303	CLA	C1D-ND	4.18	1.43	1.37
17	A	806	CLA	C1D-ND	4.18	1.43	1.37
18	2	313	CHL	C3A-C2A	-4.18	1.51	1.54
18	4	307	CHL	CHD-C1D	4.17	1.46	1.39
18	2	304	CHL	C3D-C2D	4.17	1.46	1.39
20	4	317	XAT	C8-C9	4.17	1.54	1.46
26	4	323	DGD	O2G-C1B	4.17	1.46	1.34
18	4	315	CHL	C3A-C2A	-4.16	1.51	1.54
18	3	607	CHL	CHC-C1C	4.16	1.47	1.39
18	4	307	CHL	C3B-C2B	4.16	1.46	1.40
18	2	304	CHL	C3B-C2B	4.15	1.46	1.40
18	4	301	CHL	CHB-C1B	4.14	1.46	1.39
17	G	104	CLA	C1D-ND	4.14	1.43	1.37
18	3	607	CHL	O2A-CGA	4.12	1.45	1.33
18	4	315	CHL	CHB-C1B	4.12	1.46	1.39
18	4	301	CHL	CHC-C4B	4.11	1.46	1.39
17	4	311	CLA	C1D-ND	4.10	1.43	1.37
18	3	601	CHL	CHD-C1D	4.09	1.46	1.39
18	4	306	CHL	C3A-C2A	-4.06	1.51	1.54
18	4	307	CHL	CHB-C1B	4.06	1.46	1.39
17	B	828	CLA	C4B-NB	4.04	1.43	1.37
18	4	306	CHL	CHD-C1D	4.03	1.46	1.39
17	3	605	CLA	C1D-ND	4.03	1.43	1.37
18	2	306	CHL	C3B-C2B	4.01	1.45	1.40
17	B	815	CLA	C1D-ND	3.99	1.43	1.37
17	1	301	CLA	C1D-ND	3.97	1.43	1.37
18	2	313	CHL	CHD-C1D	3.97	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	828	CLA	C1D-ND	3.97	1.43	1.37
17	4	312	CLA	C1D-ND	3.95	1.43	1.37
17	1	307	CLA	C1D-ND	3.95	1.43	1.37
17	4	303	CLA	C4B-NB	3.93	1.43	1.37
17	A	804	CLA	C1D-ND	3.92	1.43	1.37
17	3	609	CLA	C1D-ND	3.92	1.43	1.37
17	A	823	CLA	C1D-ND	3.91	1.43	1.37
21	B	847	BCR	C1-C6	-3.90	1.48	1.53
21	A	850	BCR	C30-C25	-3.90	1.48	1.53
18	4	305	CHL	CHD-C1D	3.87	1.45	1.39
18	4	305	CHL	CHC-C1C	3.87	1.46	1.39
18	4	305	CHL	C3A-C2A	-3.86	1.51	1.54
18	4	305	CHL	OBD-CAD	3.85	1.27	1.22
17	B	803	CLA	C1D-ND	3.85	1.42	1.37
18	4	301	CHL	C3B-C4B	3.85	1.45	1.41
18	4	305	CHL	CHD-C4C	3.85	1.46	1.39
17	2	312	CLA	C1D-ND	3.85	1.42	1.37
17	B	808	CLA	C1D-ND	3.85	1.42	1.37
17	B	809	CLA	C1D-ND	3.84	1.42	1.37
18	4	306	CHL	CHB-C4A	-3.83	1.34	1.38
17	B	813	CLA	C1D-ND	3.83	1.42	1.37
17	A	801	CLA	C1D-ND	3.82	1.42	1.37
17	4	304	CLA	C1D-ND	3.82	1.42	1.37
17	B	834	CLA	MG-ND	-3.82	1.98	2.05
17	B	805	CLA	C1D-ND	3.81	1.42	1.37
17	1	306	CLA	C1D-ND	3.81	1.42	1.37
17	2	319	CLA	C1D-ND	3.81	1.42	1.37
17	A	837	CLA	C1D-ND	3.80	1.42	1.37
17	B	810	CLA	C1D-ND	3.80	1.42	1.37
17	A	815	CLA	C1D-ND	3.79	1.42	1.37
21	B	848	BCR	C30-C25	-3.79	1.48	1.53
17	B	839	CLA	C1D-ND	3.78	1.42	1.37
17	B	822	CLA	C1D-ND	3.77	1.42	1.37
17	B	821	CLA	C1D-ND	3.77	1.42	1.37
17	4	310	CLA	C1D-ND	3.76	1.42	1.37
17	2	302	CLA	C1D-ND	3.76	1.42	1.37
17	2	311	CLA	C1D-ND	3.76	1.42	1.37
18	4	307	CHL	C3A-C2A	-3.75	1.51	1.54
17	L	204	CLA	C1D-ND	3.74	1.42	1.37
17	2	310	CLA	C4B-NB	3.74	1.42	1.37
17	3	608	CLA	C1D-ND	3.73	1.42	1.37
17	B	817	CLA	C1D-ND	3.72	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	203	CLA	C1D-ND	3.71	1.42	1.37
17	L	202	CLA	C1D-ND	3.71	1.42	1.37
17	A	843	CLA	C1D-ND	3.71	1.42	1.37
18	1	305	CHL	C3A-C2A	-3.71	1.51	1.54
17	2	309	CLA	C1D-ND	3.71	1.42	1.37
17	3	610	CLA	C1D-ND	3.70	1.42	1.37
17	B	810	CLA	C4B-NB	3.70	1.42	1.37
17	B	804	CLA	C4B-NB	3.70	1.42	1.37
17	B	835	CLA	C4B-NB	3.70	1.42	1.37
24	4	320	LMG	C4-C5	3.70	1.60	1.53
17	3	612	CLA	C1D-ND	3.70	1.42	1.37
17	B	804	CLA	C1D-ND	3.70	1.42	1.37
17	3	611	CLA	C1D-ND	3.70	1.42	1.37
17	2	310	CLA	C1D-ND	3.69	1.42	1.37
17	B	830	CLA	C1D-ND	3.68	1.42	1.37
17	A	831	CLA	C1D-ND	3.67	1.42	1.37
17	4	308	CLA	C1D-ND	3.67	1.42	1.37
17	B	824	CLA	C1D-ND	3.67	1.42	1.37
17	F	307	CLA	C1D-ND	3.66	1.42	1.37
21	B	846	BCR	C30-C25	-3.66	1.49	1.53
21	F	308	BCR	C30-C25	-3.65	1.49	1.53
17	3	602	CLA	C1D-ND	3.64	1.42	1.37
17	A	835	CLA	C1D-ND	3.64	1.42	1.37
17	1	301	CLA	C4B-NB	3.64	1.42	1.37
17	A	812	CLA	C1D-ND	3.64	1.42	1.37
17	3	606	CLA	C1D-ND	3.63	1.42	1.37
27	A	842	PQN	C3-C4	3.63	1.56	1.47
17	G	103	CLA	C1D-ND	3.62	1.42	1.37
17	3	613	CLA	C1D-ND	3.62	1.42	1.37
25	4	321	HTG	C1'-S1	-3.61	1.76	1.81
17	3	604	CLA	C1D-ND	3.61	1.42	1.37
17	1	310	CLA	C1D-ND	3.60	1.42	1.37
17	1	313	CLA	C1D-ND	3.60	1.42	1.37
17	B	829	CLA	C1D-ND	3.60	1.42	1.37
17	A	832	CLA	C1D-ND	3.60	1.42	1.37
17	A	820	CLA	C1D-ND	3.60	1.42	1.37
17	A	833	CLA	C1D-ND	3.59	1.42	1.37
18	1	305	CHL	CHB-C4A	-3.59	1.34	1.38
20	4	317	XAT	C28-C29	3.59	1.53	1.46
17	K	202	CLA	C1D-ND	3.59	1.42	1.37
17	A	813	CLA	C1D-ND	3.59	1.42	1.37
17	2	301	CLA	C4B-NB	3.59	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	814	CLA	C1D-ND	3.58	1.42	1.37
17	3	603	CLA	C1D-ND	3.58	1.42	1.37
17	F	304	CLA	C1D-ND	3.58	1.42	1.37
17	1	309	CLA	C1D-ND	3.58	1.42	1.37
17	B	806	CLA	C1D-ND	3.58	1.42	1.37
17	2	307	CLA	C1D-ND	3.57	1.42	1.37
17	1	309	CLA	C4B-NB	3.56	1.42	1.37
17	A	814	CLA	C1D-ND	3.56	1.42	1.37
17	G	105	CLA	C1D-ND	3.56	1.42	1.37
17	B	834	CLA	C1D-ND	3.56	1.42	1.37
17	A	811	CLA	C1D-ND	3.55	1.42	1.37
17	A	824	CLA	C1D-ND	3.55	1.42	1.37
21	A	850	BCR	C1-C6	-3.55	1.49	1.53
17	B	804	CLA	C1B-C2B	3.55	1.51	1.43
17	A	834	CLA	C1D-ND	3.55	1.42	1.37
17	A	803	CLA	C1D-ND	3.54	1.42	1.37
25	J	102	HTG	C1'-S1	-3.54	1.76	1.81
17	A	809	CLA	C1D-ND	3.54	1.42	1.37
17	A	825	CLA	C1D-ND	3.54	1.42	1.37
17	A	821	CLA	C1D-ND	3.54	1.42	1.37
17	J	103	CLA	C1D-ND	3.54	1.42	1.37
17	1	303	CLA	C1D-ND	3.53	1.42	1.37
18	4	301	CHL	CHC-C1C	3.53	1.46	1.39
17	4	302	CLA	C4B-NB	3.53	1.42	1.37
17	B	812	CLA	C4B-NB	3.53	1.42	1.37
17	A	819	CLA	C1D-ND	3.53	1.42	1.37
17	B	816	CLA	C1D-ND	3.52	1.42	1.37
17	F	306	CLA	C4B-NB	3.51	1.42	1.37
17	B	826	CLA	C1D-ND	3.51	1.42	1.37
21	G	106	BCR	C1-C6	-3.50	1.49	1.53
17	1	312	CLA	C4B-NB	3.50	1.42	1.37
17	A	818	CLA	C1D-ND	3.50	1.42	1.37
17	A	805	CLA	C1D-ND	3.49	1.42	1.37
26	4	323	DGD	O1G-C1A	3.49	1.43	1.33
17	B	836	CLA	C1D-ND	3.48	1.42	1.37
17	2	303	CLA	C1D-ND	3.48	1.42	1.37
17	A	817	CLA	C4B-NB	3.48	1.42	1.37
17	B	826	CLA	C4B-NB	3.48	1.42	1.37
24	B	852	LMG	C4-C3	3.47	1.61	1.52
17	A	843	CLA	C4B-NB	3.47	1.42	1.37
17	B	813	CLA	C4B-C3B	3.47	1.51	1.43
21	2	316	BCR	C30-C25	-3.47	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	317	XAT	C12-C13	3.47	1.53	1.46
17	B	842	CLA	C1D-ND	3.46	1.42	1.37
21	A	849	BCR	C30-C25	-3.45	1.49	1.53
17	A	807	CLA	C1D-ND	3.45	1.42	1.37
26	B	850	DGD	C3D-C2D	3.45	1.61	1.52
25	4	322	HTG	C1'-S1	-3.45	1.76	1.81
17	B	835	CLA	C1D-ND	3.44	1.42	1.37
17	B	815	CLA	C1B-C2B	3.44	1.51	1.43
21	L	205	BCR	C1-C6	-3.43	1.49	1.53
17	A	804	CLA	C4B-NB	3.43	1.42	1.37
17	A	827	CLA	C1D-ND	3.43	1.42	1.37
21	L	201	BCR	C1-C6	-3.43	1.49	1.53
17	G	103	CLA	C4B-NB	3.42	1.42	1.37
27	A	842	PQN	C2-C1	3.42	1.55	1.47
17	A	816	CLA	C1D-ND	3.42	1.42	1.37
17	4	309	CLA	C4B-NB	3.42	1.42	1.37
17	A	822	CLA	C1D-ND	3.42	1.42	1.37
17	A	830	CLA	C1D-ND	3.42	1.42	1.37
21	I	101	BCR	C1-C6	-3.42	1.49	1.53
17	3	605	CLA	C4B-NB	3.41	1.42	1.37
17	1	308	CLA	C1D-ND	3.40	1.42	1.37
17	A	810	CLA	C1D-ND	3.40	1.42	1.37
17	B	841	CLA	C4B-NB	3.40	1.42	1.37
17	L	204	CLA	C4B-NB	3.40	1.42	1.37
17	A	839	CLA	C1D-ND	3.40	1.42	1.37
17	A	841	CLA	C1D-ND	3.40	1.42	1.37
21	J	104	BCR	C1-C6	-3.39	1.49	1.53
17	G	104	CLA	C4B-NB	3.38	1.42	1.37
17	2	308	CLA	C1D-ND	3.37	1.42	1.37
17	A	810	CLA	C4B-NB	3.37	1.42	1.37
17	A	808	CLA	MG-ND	-3.37	1.99	2.05
21	F	308	BCR	C1-C6	-3.37	1.49	1.53
17	B	807	CLA	C1D-ND	3.37	1.42	1.37
17	B	811	CLA	C4B-NB	3.37	1.42	1.37
17	1	304	CLA	C4B-NB	3.37	1.42	1.37
17	B	812	CLA	C1D-ND	3.36	1.42	1.37
17	B	809	CLA	C4B-NB	3.34	1.42	1.37
21	L	206	BCR	C30-C25	-3.34	1.49	1.53
17	1	312	CLA	C1D-ND	3.33	1.42	1.37
21	1	316	BCR	C1-C6	-3.33	1.49	1.53
17	4	313	CLA	C4B-NB	3.33	1.42	1.37
17	A	853	CLA	C1D-ND	3.33	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	851	HTG	C1'-S1	-3.32	1.76	1.81
21	A	849	BCR	C1-C6	-3.31	1.49	1.53
17	1	304	CLA	C1D-ND	3.31	1.42	1.37
17	A	838	CLA	C4B-NB	3.31	1.42	1.37
17	A	817	CLA	C1D-ND	3.31	1.42	1.37
17	2	312	CLA	C4B-NB	3.31	1.42	1.37
17	B	832	CLA	C1D-ND	3.31	1.42	1.37
17	B	818	CLA	C1D-ND	3.30	1.42	1.37
21	L	206	BCR	C1-C6	-3.30	1.49	1.53
17	4	313	CLA	C1D-ND	3.30	1.42	1.37
17	A	837	CLA	C4B-NB	3.30	1.42	1.37
17	K	201	CLA	C1D-ND	3.29	1.42	1.37
17	4	302	CLA	C1D-ND	3.29	1.42	1.37
21	A	847	BCR	C1-C6	-3.29	1.49	1.53
17	B	830	CLA	C4B-NB	3.29	1.42	1.37
17	2	311	CLA	C4B-NB	3.29	1.42	1.37
17	1	311	CLA	C1D-ND	3.28	1.42	1.37
17	A	825	CLA	C4B-NB	3.28	1.42	1.37
17	A	830	CLA	C4B-NB	3.28	1.42	1.37
17	A	836	CLA	C1D-ND	3.28	1.42	1.37
21	A	848	BCR	C30-C25	-3.28	1.49	1.53
17	B	802	CLA	C4B-NB	3.27	1.42	1.37
18	4	301	CHL	C1A-CHA	3.27	1.43	1.40
17	B	838	CLA	C1D-ND	3.27	1.42	1.37
17	A	832	CLA	C4B-NB	3.27	1.42	1.37
17	3	610	CLA	C4B-NB	3.26	1.42	1.37
17	1	302	CLA	C1D-ND	3.25	1.42	1.37
17	1	302	CLA	C4B-NB	3.25	1.42	1.37
17	A	840	CLA	C4B-NB	3.23	1.42	1.37
21	K	203	BCR	C30-C25	-3.23	1.49	1.53
21	B	847	BCR	C38-C26	-3.23	1.45	1.50
17	3	608	CLA	C4B-NB	3.23	1.42	1.37
17	B	836	CLA	MG-ND	-3.23	1.99	2.05
17	A	816	CLA	C4B-NB	3.22	1.42	1.37
17	1	307	CLA	C4B-NB	3.21	1.42	1.37
17	A	826	CLA	C1D-ND	3.21	1.42	1.37
17	3	606	CLA	C4B-NB	3.21	1.42	1.37
17	A	812	CLA	C4B-NB	3.21	1.42	1.37
17	2	309	CLA	C4B-NB	3.21	1.42	1.37
17	B	842	CLA	C1B-C2B	3.20	1.50	1.43
19	2	314	LUT	C12-C13	3.19	1.52	1.46
20	4	317	XAT	C32-C33	3.19	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	819	CLA	C4B-NB	3.19	1.42	1.37
27	B	843	PQN	C10-C1	3.19	1.54	1.48
21	B	848	BCR	C1-C6	-3.18	1.49	1.53
17	2	303	CLA	C4B-NB	3.17	1.42	1.37
17	B	816	CLA	C4B-NB	3.16	1.42	1.37
17	F	304	CLA	C1B-C2B	3.16	1.50	1.43
17	A	820	CLA	C4B-NB	3.16	1.42	1.37
17	3	604	CLA	C4B-NB	3.16	1.42	1.37
17	3	611	CLA	C4B-NB	3.16	1.42	1.37
17	K	202	CLA	C4B-NB	3.16	1.42	1.37
17	A	815	CLA	C4B-NB	3.15	1.42	1.37
19	4	316	LUT	C28-C29	3.15	1.52	1.46
17	1	308	CLA	C4B-NB	3.15	1.42	1.37
17	A	822	CLA	C4B-NB	3.15	1.42	1.37
17	B	840	CLA	C1D-ND	3.15	1.42	1.37
17	A	823	CLA	C4B-NB	3.15	1.42	1.37
17	A	831	CLA	C4B-NB	3.15	1.42	1.37
21	1	316	BCR	C30-C25	-3.15	1.49	1.53
25	F	310	HTG	C1'-S1	-3.15	1.77	1.81
17	B	802	CLA	C1D-ND	3.15	1.42	1.37
17	B	831	CLA	C1D-ND	3.14	1.42	1.37
17	B	802	CLA	CHC-C1C	3.14	1.44	1.38
21	3	616	BCR	C1-C6	-3.14	1.49	1.53
17	2	307	CLA	C4B-NB	3.14	1.42	1.37
17	B	832	CLA	MG-ND	-3.14	1.99	2.05
17	3	612	CLA	C4B-NB	3.14	1.42	1.37
17	B	815	CLA	C4B-NB	3.13	1.42	1.37
21	A	848	BCR	C1-C6	-3.13	1.49	1.53
17	3	603	CLA	C4B-NB	3.13	1.42	1.37
26	B	850	DGD	O5D-C6D	-3.13	1.38	1.43
17	A	803	CLA	C4B-NB	3.13	1.42	1.37
17	A	824	CLA	C4B-NB	3.12	1.42	1.37
17	B	820	CLA	C1D-ND	3.12	1.42	1.37
17	B	814	CLA	C3B-C4B	3.12	1.51	1.42
17	L	203	CLA	C4B-NB	3.12	1.42	1.37
17	A	834	CLA	C4B-NB	3.11	1.42	1.37
17	B	803	CLA	C4B-NB	3.11	1.42	1.37
17	L	202	CLA	C4B-NB	3.11	1.41	1.37
17	A	829	CLA	C1D-ND	3.11	1.41	1.37
17	B	828	CLA	C1D-ND	3.10	1.41	1.37
21	J	105	BCR	C30-C25	-3.10	1.49	1.53
17	G	105	CLA	C4B-NB	3.10	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	602	CLA	C4B-NB	3.10	1.41	1.37
17	A	840	CLA	C1B-C2B	3.10	1.50	1.43
17	2	319	CLA	C4B-NB	3.10	1.41	1.37
17	A	853	CLA	C4B-NB	3.09	1.41	1.37
21	K	203	BCR	C1-C6	-3.09	1.49	1.53
20	3	615	XAT	C32-C33	3.08	1.52	1.46
27	A	842	PQN	C5-C4	3.07	1.54	1.48
17	B	818	CLA	C4B-NB	3.07	1.41	1.37
17	B	830	CLA	MG-ND	-3.07	1.99	2.05
27	A	842	PQN	C10-C1	3.07	1.54	1.48
21	A	846	BCR	C1-C6	-3.07	1.49	1.53
17	B	819	CLA	C1D-ND	3.07	1.41	1.37
19	3	614	LUT	C11-C10	3.06	1.52	1.43
18	4	307	CHL	CBD-CGD	-3.06	1.48	1.52
20	1	315	XAT	C32-C33	3.06	1.52	1.46
17	B	818	CLA	CHC-C1C	3.06	1.44	1.38
17	J	101	CLA	C1B-C2B	3.05	1.50	1.43
19	2	314	LUT	C35-C34	3.05	1.52	1.43
19	3	614	LUT	C31-C30	3.05	1.52	1.43
17	A	810	CLA	C1B-C2B	3.05	1.50	1.43
17	B	829	CLA	C4B-NB	3.05	1.41	1.37
17	B	835	CLA	C3B-C4B	3.04	1.51	1.42
17	A	828	CLA	C1B-C2B	3.04	1.50	1.43
19	3	614	LUT	C28-C29	3.04	1.52	1.46
17	A	813	CLA	C4B-NB	3.04	1.41	1.37
17	A	853	CLA	C1B-C2B	3.03	1.50	1.43
17	B	811	CLA	CMB-C2B	-3.03	1.44	1.50
20	2	315	XAT	C32-C33	3.03	1.52	1.46
17	A	838	CLA	C1B-C2B	3.03	1.50	1.43
19	1	314	LUT	C31-C30	3.03	1.52	1.43
17	A	802	CLA	C1D-ND	3.02	1.41	1.37
17	K	201	CLA	C4B-NB	3.02	1.41	1.37
19	3	614	LUT	C12-C13	3.01	1.52	1.46
17	B	810	CLA	CHC-C1C	3.01	1.44	1.38
17	2	308	CLA	C4B-NB	3.01	1.41	1.37
17	B	835	CLA	CHC-C1C	3.00	1.44	1.38
17	4	311	CLA	C4B-NB	3.00	1.41	1.37
17	B	828	CLA	C1B-C2B	3.00	1.50	1.43
17	B	841	CLA	C1D-ND	3.00	1.41	1.37
21	A	847	BCR	C30-C25	-3.00	1.49	1.53
19	4	316	LUT	C15-C14	3.00	1.52	1.43
19	2	314	LUT	C11-C10	2.99	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	308	CLA	C1B-C2B	2.99	1.50	1.43
17	A	835	CLA	C4B-NB	2.99	1.41	1.37
17	B	810	CLA	C1B-C2B	2.98	1.50	1.43
19	3	614	LUT	C15-C14	2.98	1.52	1.43
17	A	839	CLA	C4B-NB	2.98	1.41	1.37
20	1	315	XAT	C28-C29	2.98	1.52	1.46
17	A	813	CLA	C1B-C2B	2.98	1.50	1.43
17	4	303	CLA	C1B-C2B	2.98	1.50	1.43
17	B	838	CLA	C1B-C2B	2.97	1.50	1.43
24	4	320	LMG	O1-C1	2.97	1.45	1.40
21	I	101	BCR	C30-C25	-2.97	1.50	1.53
17	A	829	CLA	C4B-NB	2.97	1.41	1.37
21	3	616	BCR	C30-C25	-2.97	1.50	1.53
17	3	609	CLA	C4B-NB	2.97	1.41	1.37
17	B	842	CLA	C4B-NB	2.97	1.41	1.37
20	2	315	XAT	C28-C29	2.97	1.52	1.46
17	A	808	CLA	C1D-ND	2.96	1.41	1.37
18	2	306	CHL	CBD-CGD	-2.96	1.48	1.52
17	A	806	CLA	C1B-C2B	2.96	1.50	1.43
17	A	803	CLA	C1B-C2B	2.96	1.50	1.43
17	B	835	CLA	C1B-C2B	2.96	1.50	1.43
17	A	838	CLA	C1D-ND	2.96	1.41	1.37
17	B	829	CLA	MG-NB	-2.96	1.99	2.05
17	4	314	CLA	C1D-ND	2.95	1.41	1.37
21	F	303	BCR	C30-C25	-2.95	1.50	1.53
17	1	306	CLA	C4B-NB	2.95	1.41	1.37
19	1	314	LUT	C28-C29	2.95	1.52	1.46
17	A	824	CLA	C1B-C2B	2.95	1.50	1.43
20	3	615	XAT	C28-C29	2.95	1.52	1.46
21	B	849	BCR	C30-C25	-2.95	1.50	1.53
19	3	614	LUT	C35-C34	2.95	1.52	1.43
17	B	836	CLA	C4B-NB	2.93	1.41	1.37
17	2	301	CLA	C1D-ND	2.93	1.41	1.37
17	B	819	CLA	C4B-NB	2.93	1.41	1.37
17	A	837	CLA	C1B-C2B	2.93	1.50	1.43
27	B	843	PQN	C2-C1	2.93	1.54	1.47
19	4	316	LUT	C31-C30	2.93	1.52	1.43
17	A	827	CLA	C1B-C2B	2.93	1.50	1.43
17	G	105	CLA	C1B-C2B	2.93	1.50	1.43
17	B	825	CLA	C3B-C4B	2.93	1.51	1.42
18	4	301	CHL	CHD-C4C	2.93	1.45	1.39
17	J	101	CLA	CHC-C1C	2.92	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	811	CLA	C4B-NB	2.92	1.41	1.37
17	A	814	CLA	C4B-NB	2.92	1.41	1.37
17	B	822	CLA	C1B-C2B	2.92	1.50	1.43
17	3	613	CLA	C4B-NB	2.91	1.41	1.37
17	1	304	CLA	CHC-C1C	2.91	1.44	1.38
20	1	315	XAT	C11-C10	2.91	1.52	1.43
20	3	615	XAT	C11-C10	2.91	1.52	1.43
17	A	821	CLA	C4B-NB	2.91	1.41	1.37
17	A	841	CLA	C4B-NB	2.91	1.41	1.37
19	4	316	LUT	C32-C33	2.90	1.52	1.46
17	A	804	CLA	CHC-C1C	2.90	1.44	1.38
21	A	851	BCR	C1-C6	-2.90	1.50	1.53
17	B	840	CLA	C1B-C2B	2.90	1.49	1.43
17	1	301	CLA	C1B-C2B	2.90	1.49	1.43
17	F	306	CLA	C1D-ND	2.90	1.41	1.37
17	1	307	CLA	C1B-C2B	2.89	1.49	1.43
17	2	302	CLA	C1B-C2B	2.89	1.49	1.43
17	A	836	CLA	C4B-NB	2.89	1.41	1.37
17	2	302	CLA	C4B-NB	2.89	1.41	1.37
19	2	314	LUT	C8-C9	2.89	1.52	1.46
21	B	844	BCR	C1-C6	-2.89	1.50	1.53
17	G	103	CLA	C1B-C2B	2.89	1.49	1.43
20	2	315	XAT	C11-C10	2.88	1.52	1.43
17	B	823	CLA	C1B-C2B	2.88	1.49	1.43
20	3	615	XAT	C31-C30	2.88	1.52	1.43
20	2	315	XAT	C31-C30	2.88	1.52	1.43
20	1	315	XAT	C31-C30	2.88	1.52	1.43
17	B	841	CLA	MG-NB	-2.88	2.00	2.05
17	A	818	CLA	C4B-NB	2.88	1.41	1.37
17	1	303	CLA	C4B-NB	2.87	1.41	1.37
17	A	841	CLA	C1B-C2B	2.87	1.49	1.43
19	2	314	LUT	C28-C29	2.87	1.52	1.46
17	A	806	CLA	C4B-NB	2.87	1.41	1.37
17	2	303	CLA	C1B-C2B	2.87	1.49	1.43
17	2	312	CLA	C1B-C2B	2.87	1.49	1.43
17	3	609	CLA	C1B-C2B	2.86	1.49	1.43
17	B	805	CLA	C3B-C4B	2.86	1.51	1.42
17	J	101	CLA	C4B-NB	2.86	1.41	1.37
17	4	302	CLA	C3B-C4B	2.86	1.51	1.42
17	B	831	CLA	MG-ND	-2.86	2.00	2.05
17	4	309	CLA	C1B-C2B	2.85	1.49	1.43
17	A	814	CLA	C1B-C2B	2.85	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	801	CLA	C4B-NB	2.85	1.41	1.37
19	1	314	LUT	C15-C14	2.85	1.52	1.43
17	B	815	CLA	CHC-C1C	2.85	1.44	1.38
18	4	301	CHL	O2A-CGA	2.84	1.41	1.33
17	A	803	CLA	CHC-C1C	2.84	1.44	1.38
17	B	807	CLA	MG-NA	2.84	2.13	2.06
17	1	310	CLA	C4B-NB	2.84	1.41	1.37
20	2	315	XAT	C15-C14	2.84	1.52	1.43
26	B	850	DGD	O6D-C5D	-2.84	1.37	1.44
17	4	314	CLA	C4B-NB	2.84	1.41	1.37
20	3	615	XAT	C15-C14	2.84	1.52	1.43
20	2	315	XAT	C35-C34	2.83	1.52	1.43
20	4	317	XAT	C11-C10	2.83	1.52	1.43
20	1	315	XAT	C15-C14	2.83	1.52	1.43
25	F	301	HTG	C1'-S1	-2.83	1.77	1.81
17	L	204	CLA	C1B-C2B	2.83	1.49	1.43
21	G	106	BCR	C30-C25	-2.83	1.50	1.53
17	4	313	CLA	C1B-C2B	2.83	1.49	1.43
17	A	825	CLA	CHC-C1C	2.83	1.44	1.38
27	B	843	PQN	C3-C4	2.83	1.54	1.47
20	1	315	XAT	C35-C34	2.82	1.51	1.43
21	B	846	BCR	C1-C6	-2.82	1.50	1.53
19	2	314	LUT	C15-C14	2.82	1.51	1.43
19	2	314	LUT	C32-C33	2.82	1.52	1.46
19	4	316	LUT	C8-C9	2.82	1.52	1.46
19	3	614	LUT	C32-C33	2.82	1.52	1.46
17	K	202	CLA	C1B-C2B	2.82	1.49	1.43
17	A	819	CLA	C1B-C2B	2.82	1.49	1.43
17	A	802	CLA	C4B-NB	2.81	1.41	1.37
17	B	812	CLA	C1B-C2B	2.81	1.49	1.43
20	3	615	XAT	C35-C34	2.81	1.51	1.43
17	A	822	CLA	C1B-C2B	2.81	1.49	1.43
19	1	314	LUT	C8-C9	2.81	1.52	1.46
17	4	310	CLA	C4B-NB	2.81	1.41	1.37
19	4	316	LUT	C12-C13	2.80	1.52	1.46
17	4	311	CLA	C1B-C2B	2.80	1.49	1.43
19	2	314	LUT	C31-C30	2.80	1.51	1.43
17	1	304	CLA	C1B-C2B	2.80	1.49	1.43
18	4	301	CHL	MG-ND	-2.80	2.00	2.05
17	3	612	CLA	C1B-C2B	2.80	1.49	1.43
19	1	314	LUT	C35-C34	2.80	1.51	1.43
17	B	831	CLA	C1B-C2B	2.79	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	828	CLA	C4B-NB	2.79	1.41	1.37
17	B	827	CLA	C1B-C2B	2.79	1.49	1.43
17	G	104	CLA	C3B-C4B	2.79	1.50	1.42
17	A	833	CLA	C4B-NB	2.78	1.41	1.37
17	B	826	CLA	MG-NA	2.78	2.12	2.06
17	F	306	CLA	C1B-C2B	2.78	1.49	1.43
17	B	814	CLA	CHC-C1C	2.78	1.44	1.38
17	1	309	CLA	C3B-C4B	2.77	1.50	1.42
17	1	302	CLA	C1B-C2B	2.77	1.49	1.43
20	1	315	XAT	C8-C9	2.77	1.51	1.46
20	2	315	XAT	C8-C9	2.77	1.51	1.46
20	3	615	XAT	C8-C9	2.77	1.51	1.46
17	A	812	CLA	C1B-C2B	2.77	1.49	1.43
17	3	605	CLA	C3B-C4B	2.76	1.50	1.42
22	B	801	LHG	P-O6	2.76	1.70	1.59
19	3	614	LUT	C8-C9	2.76	1.51	1.46
17	A	840	CLA	CHC-C1C	2.76	1.44	1.38
17	4	308	CLA	C1B-C2B	2.75	1.49	1.43
17	B	816	CLA	C3B-C4B	2.75	1.50	1.42
17	B	804	CLA	C3B-C4B	2.75	1.50	1.42
17	3	611	CLA	C1B-C2B	2.75	1.49	1.43
17	A	825	CLA	C1B-C2B	2.75	1.49	1.43
17	B	827	CLA	C3B-C4B	2.75	1.50	1.42
25	A	854	HTG	C1'-S1	-2.75	1.77	1.81
17	3	608	CLA	C1B-C2B	2.74	1.49	1.43
17	1	313	CLA	C1B-C2B	2.74	1.49	1.43
17	B	824	CLA	C1B-C2B	2.74	1.49	1.43
17	2	310	CLA	C3B-C4B	2.74	1.50	1.42
17	4	308	CLA	MG-NC	2.74	2.12	2.06
17	B	811	CLA	C1D-ND	2.74	1.41	1.37
17	A	802	CLA	C1B-C2B	2.74	1.49	1.43
17	B	817	CLA	C4B-NB	2.73	1.41	1.37
19	1	314	LUT	C12-C13	2.73	1.51	1.46
17	B	823	CLA	C1D-ND	2.73	1.41	1.37
17	2	310	CLA	C1B-C2B	2.73	1.49	1.43
24	B	852	LMG	C4-C5	2.73	1.58	1.53
17	A	823	CLA	C1B-C2B	2.73	1.49	1.43
17	B	820	CLA	CMD-C2D	-2.73	1.45	1.50
17	B	830	CLA	C1B-C2B	2.72	1.49	1.43
17	A	826	CLA	C1B-C2B	2.72	1.49	1.43
17	1	311	CLA	C1B-C2B	2.72	1.49	1.43
17	B	825	CLA	MG-ND	-2.72	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	317	XAT	C31-C30	2.72	1.51	1.43
17	4	302	CLA	C1B-C2B	2.72	1.49	1.43
17	A	815	CLA	C3B-C4B	2.71	1.50	1.42
17	A	804	CLA	C3B-C4B	2.71	1.50	1.42
17	F	307	CLA	C3B-C4B	2.71	1.50	1.42
17	A	832	CLA	C1B-C2B	2.70	1.49	1.43
17	L	202	CLA	C1B-C2B	2.70	1.49	1.43
17	B	841	CLA	C1B-C2B	2.70	1.49	1.43
17	A	809	CLA	C4B-NB	2.70	1.41	1.37
17	A	831	CLA	C1B-C2B	2.70	1.49	1.43
17	3	605	CLA	C1B-C2B	2.70	1.49	1.43
17	B	808	CLA	C1B-C2B	2.70	1.49	1.43
21	B	844	BCR	C30-C25	-2.69	1.50	1.53
25	J	102	HTG	C1-S1	-2.69	1.76	1.80
17	B	836	CLA	C1B-C2B	2.69	1.49	1.43
17	L	203	CLA	C1B-C2B	2.69	1.49	1.43
17	B	804	CLA	CHC-C1C	2.69	1.43	1.38
17	A	811	CLA	C3B-C4B	2.68	1.50	1.42
17	1	307	CLA	C3B-C4B	2.68	1.50	1.42
17	A	839	CLA	C3B-C4B	2.68	1.50	1.42
17	3	603	CLA	C1B-C2B	2.68	1.49	1.43
17	3	613	CLA	C1B-C2B	2.68	1.49	1.43
17	A	826	CLA	C4B-NB	2.68	1.41	1.37
17	A	820	CLA	C1B-C2B	2.68	1.49	1.43
17	A	801	CLA	C1B-C2B	2.68	1.49	1.43
21	4	318	BCR	C1-C6	-2.67	1.50	1.53
17	K	201	CLA	C1B-C2B	2.67	1.49	1.43
17	A	808	CLA	C1B-C2B	2.67	1.49	1.43
18	4	301	CHL	C4A-C3A	-2.67	1.45	1.51
17	1	306	CLA	C1B-C2B	2.67	1.49	1.43
17	A	840	CLA	C1D-C2D	2.66	1.50	1.45
17	3	604	CLA	C1B-C2B	2.66	1.49	1.43
17	A	843	CLA	C1B-C2B	2.66	1.49	1.43
17	B	830	CLA	CHC-C1C	2.66	1.43	1.38
17	2	311	CLA	C1B-C2B	2.66	1.49	1.43
17	B	834	CLA	CMB-C2B	-2.66	1.45	1.50
17	B	805	CLA	MG-ND	-2.66	2.00	2.05
17	B	842	CLA	MG-ND	-2.65	2.00	2.05
17	2	307	CLA	C3B-C4B	2.65	1.50	1.42
17	B	809	CLA	C3B-C4B	2.65	1.50	1.42
17	1	309	CLA	C1B-C2B	2.65	1.49	1.43
17	B	839	CLA	C1B-C2B	2.65	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	313	CLA	C3B-C4B	2.64	1.50	1.42
17	A	830	CLA	C1B-C2B	2.64	1.49	1.43
17	A	817	CLA	CHC-C1C	2.64	1.43	1.38
17	G	104	CLA	C1B-C2B	2.64	1.49	1.43
17	B	803	CLA	C1B-C2B	2.64	1.49	1.43
17	B	815	CLA	C3B-C4B	2.64	1.50	1.42
17	3	606	CLA	C1B-C2B	2.63	1.49	1.43
17	A	801	CLA	C3D-C4D	2.63	1.50	1.44
17	A	835	CLA	C1B-C2B	2.63	1.49	1.43
17	F	306	CLA	C3B-C4B	2.63	1.50	1.42
17	F	304	CLA	C4B-NB	2.63	1.41	1.37
27	B	843	PQN	C5-C4	2.63	1.53	1.48
17	4	304	CLA	C1B-C2B	2.63	1.49	1.43
19	1	314	LUT	C32-C33	2.62	1.51	1.46
17	1	312	CLA	C1B-C2B	2.62	1.49	1.43
26	B	850	DGD	C3G-C2G	2.62	1.59	1.50
17	B	818	CLA	C1B-C2B	2.62	1.49	1.43
17	B	816	CLA	CHC-C1C	2.61	1.43	1.38
21	L	201	BCR	C30-C25	-2.61	1.50	1.53
17	J	103	CLA	C3B-C4B	2.61	1.50	1.42
17	B	826	CLA	C1B-C2B	2.61	1.49	1.43
17	A	829	CLA	C1B-C2B	2.61	1.49	1.43
17	A	840	CLA	C1D-ND	2.61	1.41	1.37
17	2	308	CLA	C1B-C2B	2.61	1.49	1.43
17	A	836	CLA	C1B-C2B	2.61	1.49	1.43
17	3	610	CLA	C1B-C2B	2.60	1.49	1.43
17	B	806	CLA	C1B-C2B	2.60	1.49	1.43
17	1	302	CLA	CHC-C1C	2.60	1.43	1.38
17	B	820	CLA	CHC-C1C	2.60	1.43	1.38
17	F	307	CLA	C4B-NB	2.59	1.41	1.37
17	B	821	CLA	C1B-C2B	2.59	1.49	1.43
17	F	306	CLA	CHC-C1C	2.59	1.43	1.38
17	B	811	CLA	C1B-C2B	2.59	1.49	1.43
19	4	316	LUT	C11-C10	2.59	1.51	1.43
17	A	816	CLA	C1B-C2B	2.59	1.49	1.43
17	G	103	CLA	C3B-C4B	2.59	1.50	1.42
17	4	312	CLA	C3B-C4B	2.58	1.50	1.42
17	2	309	CLA	C1B-C2B	2.58	1.49	1.43
20	4	317	XAT	C35-C34	2.58	1.51	1.43
17	A	838	CLA	C3B-C4B	2.58	1.50	1.42
17	B	818	CLA	C3B-C4B	2.58	1.50	1.42
17	A	811	CLA	C1B-C2B	2.58	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	605	CLA	CHC-C1C	2.58	1.43	1.38
17	B	833	CLA	C1D-ND	2.58	1.41	1.37
20	3	615	XAT	C12-C13	2.58	1.51	1.46
23	A	855	LMT	O4'-C4B	-2.58	1.36	1.43
17	1	310	CLA	C1B-C2B	2.58	1.49	1.43
24	B	852	LMG	O1-C1	2.57	1.44	1.40
17	B	838	CLA	CHC-C1C	2.57	1.43	1.38
17	1	313	CLA	CHC-C1C	2.57	1.43	1.38
17	B	808	CLA	C3B-C4B	2.57	1.50	1.42
17	A	839	CLA	C1B-C2B	2.56	1.49	1.43
17	B	805	CLA	C4B-NB	2.56	1.41	1.37
20	2	315	XAT	C12-C13	2.56	1.51	1.46
22	1	317	LHG	O7-C5	-2.56	1.40	1.46
17	B	819	CLA	C3B-C4B	2.56	1.50	1.42
17	B	807	CLA	MG-NB	-2.56	2.00	2.05
17	1	312	CLA	CHC-C1C	2.55	1.43	1.38
17	A	815	CLA	C1B-C2B	2.55	1.49	1.43
21	A	846	BCR	C30-C25	-2.55	1.50	1.53
21	B	845	BCR	C30-C25	-2.55	1.50	1.53
17	A	817	CLA	C1B-C2B	2.55	1.49	1.43
20	1	315	XAT	C12-C13	2.55	1.51	1.46
17	A	843	CLA	C3B-C4B	2.55	1.50	1.42
17	4	311	CLA	C3B-C4B	2.55	1.50	1.42
17	A	816	CLA	C3B-C4B	2.55	1.50	1.42
17	4	314	CLA	C1B-C2B	2.55	1.49	1.43
17	A	833	CLA	C1B-C2B	2.55	1.49	1.43
17	2	312	CLA	C3B-C4B	2.54	1.50	1.42
17	B	826	CLA	MG-ND	-2.54	2.00	2.05
17	B	812	CLA	CHC-C1C	2.54	1.43	1.38
17	B	807	CLA	C3B-C4B	2.54	1.50	1.42
17	B	812	CLA	C3B-C4B	2.54	1.50	1.42
17	4	309	CLA	C3B-C4B	2.54	1.50	1.42
24	B	852	LMG	C3-C2	2.54	1.58	1.52
17	A	807	CLA	C4B-NB	2.54	1.41	1.37
17	1	304	CLA	C3B-C4B	2.54	1.50	1.42
17	4	309	CLA	CHC-C1C	2.54	1.43	1.38
17	B	842	CLA	CMB-C2B	-2.53	1.45	1.50
17	B	825	CLA	CHC-C1C	2.53	1.43	1.38
17	A	834	CLA	C1B-C2B	2.53	1.49	1.43
17	2	301	CLA	CHC-C1C	2.53	1.43	1.38
17	B	832	CLA	C1B-C2B	2.53	1.49	1.43
17	4	314	CLA	MG-NB	-2.53	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	827	CLA	C4B-NB	2.53	1.41	1.37
17	L	203	CLA	CHC-C1C	2.53	1.43	1.38
25	F	305	HTG	C1'-S1	-2.52	1.77	1.81
17	2	310	CLA	CHC-C1C	2.52	1.43	1.38
17	B	819	CLA	C1B-C2B	2.52	1.49	1.43
17	A	803	CLA	C3B-C4B	2.52	1.50	1.42
17	J	103	CLA	C4B-NB	2.51	1.41	1.37
17	B	803	CLA	C3B-C4B	2.51	1.50	1.42
17	B	821	CLA	C3B-C4B	2.51	1.50	1.42
17	A	843	CLA	CHC-C1C	2.51	1.43	1.38
17	A	831	CLA	C3B-C4B	2.51	1.50	1.42
17	3	602	CLA	C1B-C2B	2.51	1.49	1.43
22	A	844	LHG	O7-C5	-2.50	1.40	1.46
21	A	851	BCR	C30-C25	-2.50	1.50	1.53
17	B	816	CLA	C1B-C2B	2.50	1.49	1.43
17	A	821	CLA	C1B-C2B	2.50	1.49	1.43
17	1	313	CLA	C4B-NB	2.49	1.41	1.37
17	B	814	CLA	C4B-NB	2.49	1.41	1.37
17	B	833	CLA	MG-NB	-2.49	2.00	2.05
17	2	303	CLA	C3B-C4B	2.49	1.50	1.42
17	A	832	CLA	CHC-C1C	2.49	1.43	1.38
17	A	809	CLA	C3B-C4B	2.49	1.50	1.42
17	B	833	CLA	MG-ND	-2.48	2.00	2.05
18	4	301	CHL	OBD-CAD	2.48	1.25	1.22
17	A	804	CLA	C1B-C2B	2.48	1.49	1.43
17	B	827	CLA	C3C-C2C	2.48	1.42	1.36
17	A	805	CLA	C1B-C2B	2.48	1.49	1.43
17	B	839	CLA	C1D-C2D	2.48	1.50	1.45
17	B	826	CLA	C3B-C4B	2.48	1.50	1.42
22	G	102	LHG	P-O6	2.48	1.69	1.59
17	B	824	CLA	CHC-C1C	2.48	1.43	1.38
17	B	834	CLA	C4B-NB	2.48	1.41	1.37
17	A	853	CLA	CHC-C1C	2.48	1.43	1.38
17	A	838	CLA	CMC-C2C	-2.48	1.45	1.50
17	B	820	CLA	C3C-C2C	2.47	1.42	1.36
25	4	321	HTG	C1-S1	-2.47	1.76	1.80
17	A	812	CLA	CHC-C1C	2.47	1.43	1.38
17	1	303	CLA	C1B-C2B	2.47	1.48	1.43
17	A	809	CLA	C1B-C2B	2.47	1.48	1.43
17	B	830	CLA	C3B-C4B	2.47	1.49	1.42
17	A	818	CLA	C1B-C2B	2.47	1.48	1.43
17	1	312	CLA	MG-NB	-2.47	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	301	CLA	CHC-C1C	2.47	1.43	1.38
17	1	309	CLA	CHC-C1C	2.47	1.43	1.38
20	4	317	XAT	C15-C14	2.47	1.50	1.43
17	2	309	CLA	C3B-C4B	2.46	1.49	1.42
17	B	829	CLA	C3B-C4B	2.46	1.49	1.42
17	4	302	CLA	CHC-C1C	2.46	1.43	1.38
17	A	816	CLA	CHC-C1C	2.46	1.43	1.38
17	4	302	CLA	CMD-C2D	-2.46	1.45	1.50
17	B	825	CLA	C4B-NB	2.46	1.41	1.37
17	A	806	CLA	C3B-C4B	2.46	1.49	1.42
17	A	834	CLA	C3B-C4B	2.46	1.49	1.42
17	B	825	CLA	C1D-ND	2.46	1.41	1.37
17	3	606	CLA	C3B-C4B	2.46	1.49	1.42
17	F	304	CLA	MG-NA	2.46	2.12	2.06
17	F	304	CLA	C3B-C4B	2.46	1.49	1.42
17	4	308	CLA	C4B-NB	2.46	1.41	1.37
17	A	819	CLA	CHC-C1C	2.45	1.43	1.38
17	B	802	CLA	MG-NB	-2.45	2.00	2.05
17	B	823	CLA	C4B-NB	2.45	1.41	1.37
17	4	310	CLA	C1B-C2B	2.45	1.48	1.43
17	B	810	CLA	C3B-C4B	2.45	1.49	1.42
17	3	602	CLA	CHC-C1C	2.45	1.43	1.38
17	3	606	CLA	CHC-C1C	2.45	1.43	1.38
17	3	603	CLA	C3B-C4B	2.45	1.49	1.42
17	B	828	CLA	CMC-C2C	-2.45	1.45	1.50
17	1	302	CLA	C3B-C4B	2.45	1.49	1.42
17	2	311	CLA	C3B-C4B	2.44	1.49	1.42
17	A	802	CLA	MG-ND	-2.44	2.00	2.05
17	B	829	CLA	CHC-C1C	2.44	1.43	1.38
19	3	614	LUT	C7-C6	2.44	1.53	1.45
17	B	838	CLA	C3B-C4B	2.44	1.49	1.42
17	1	306	CLA	CHC-C1C	2.44	1.43	1.38
17	4	303	CLA	C3B-C4B	2.44	1.49	1.42
17	1	311	CLA	C3B-C4B	2.44	1.49	1.42
17	A	831	CLA	MG-NB	-2.44	2.01	2.05
17	4	302	CLA	MG-ND	-2.44	2.01	2.05
17	1	306	CLA	C3B-C4B	2.44	1.49	1.42
17	A	805	CLA	C3B-C4B	2.44	1.49	1.42
24	F	309	LMG	C7-C8	2.44	1.58	1.50
17	A	822	CLA	CHC-C1C	2.44	1.43	1.38
17	B	807	CLA	C1B-C2B	2.44	1.48	1.43
17	K	202	CLA	C3B-C4B	2.44	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	319	CLA	CHC-C1C	2.43	1.43	1.38
17	1	310	CLA	C3B-C4B	2.43	1.49	1.42
17	L	204	CLA	C3B-C4B	2.43	1.49	1.42
17	A	822	CLA	C3B-C4B	2.43	1.49	1.42
17	2	307	CLA	CHC-C1C	2.43	1.43	1.38
17	A	823	CLA	C3B-C4B	2.43	1.49	1.42
17	2	319	CLA	C1B-C2B	2.43	1.48	1.43
17	2	319	CLA	C3B-C4B	2.43	1.49	1.42
17	4	304	CLA	C4B-NB	2.43	1.41	1.37
17	A	839	CLA	CHC-C1C	2.43	1.43	1.38
17	2	308	CLA	C3B-C4B	2.43	1.49	1.42
17	B	822	CLA	C4B-NB	2.43	1.41	1.37
17	A	812	CLA	C3B-C4B	2.43	1.49	1.42
17	A	837	CLA	C3B-C4B	2.42	1.49	1.42
17	B	830	CLA	C2-C3	2.42	1.38	1.33
17	A	823	CLA	CHC-C1C	2.42	1.43	1.38
18	2	313	CHL	CBD-CGD	-2.42	1.49	1.52
17	1	301	CLA	C3B-C4B	2.42	1.49	1.42
17	A	805	CLA	C4B-NB	2.42	1.41	1.37
17	3	608	CLA	C3B-C4B	2.41	1.49	1.42
17	A	819	CLA	C3B-C4B	2.41	1.49	1.42
17	B	817	CLA	C3B-C4B	2.41	1.49	1.42
17	B	817	CLA	CHC-C1C	2.41	1.43	1.38
17	J	101	CLA	MG-NA	2.41	2.12	2.06
17	A	809	CLA	CHC-C1C	2.41	1.43	1.38
17	2	302	CLA	CMC-C2C	-2.41	1.45	1.50
25	F	305	HTG	C1-S1	-2.41	1.76	1.80
18	4	301	CHL	C1A-C2A	-2.41	1.46	1.51
17	A	835	CLA	CHC-C1C	2.41	1.43	1.38
18	4	301	CHL	C3B-C2B	2.41	1.43	1.40
17	B	809	CLA	CHC-C1C	2.41	1.43	1.38
17	A	821	CLA	C3B-C4B	2.40	1.49	1.42
17	3	609	CLA	C3B-C4B	2.40	1.49	1.42
17	A	827	CLA	CHC-C1C	2.40	1.43	1.38
17	B	820	CLA	C3B-C4B	2.40	1.49	1.42
17	A	814	CLA	CHC-C1C	2.40	1.43	1.38
17	B	807	CLA	CMD-C2D	-2.40	1.45	1.50
22	A	845	LHG	P-O6	2.40	1.68	1.59
17	B	823	CLA	CHC-C1C	2.40	1.43	1.38
17	1	308	CLA	C3B-C4B	2.39	1.49	1.42
17	A	820	CLA	C3B-C4B	2.39	1.49	1.42
17	3	608	CLA	CHC-C1C	2.39	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	817	CLA	C3B-C4B	2.39	1.49	1.42
17	3	604	CLA	C3B-C4B	2.39	1.49	1.42
17	A	807	CLA	CHC-C1C	2.39	1.43	1.38
17	1	303	CLA	C3B-C4B	2.39	1.49	1.42
17	K	201	CLA	CHC-C1C	2.39	1.43	1.38
17	2	311	CLA	CHC-C1C	2.39	1.43	1.38
17	A	833	CLA	C3B-C4B	2.39	1.49	1.42
17	B	824	CLA	C4B-NB	2.38	1.41	1.37
17	3	612	CLA	C3B-C4B	2.38	1.49	1.42
17	3	610	CLA	C3B-C4B	2.38	1.49	1.42
17	2	303	CLA	CHC-C1C	2.38	1.43	1.38
17	B	806	CLA	C3B-C4B	2.38	1.49	1.42
17	B	841	CLA	C1D-C2D	2.38	1.50	1.45
17	1	311	CLA	C4B-NB	2.38	1.41	1.37
17	B	834	CLA	C1B-C2B	2.38	1.48	1.43
17	A	825	CLA	C3B-C4B	2.38	1.49	1.42
17	A	853	CLA	CMC-C2C	-2.38	1.45	1.50
17	A	820	CLA	CHC-C1C	2.38	1.43	1.38
17	B	829	CLA	C1B-C2B	2.38	1.48	1.43
17	3	611	CLA	C3B-C4B	2.38	1.49	1.42
17	B	808	CLA	C4B-NB	2.38	1.41	1.37
17	1	312	CLA	C3B-C4B	2.38	1.49	1.42
17	A	801	CLA	C3B-C4B	2.37	1.49	1.42
17	K	201	CLA	C3B-C4B	2.37	1.49	1.42
17	A	827	CLA	C3B-C4B	2.37	1.49	1.42
17	B	805	CLA	CHC-C1C	2.37	1.43	1.38
17	3	609	CLA	CHC-C1C	2.37	1.43	1.38
18	3	607	CHL	CBD-CGD	-2.37	1.49	1.52
17	2	301	CLA	C1B-C2B	2.37	1.48	1.43
17	G	105	CLA	CHC-C1C	2.37	1.43	1.38
17	J	103	CLA	C1B-C2B	2.37	1.48	1.43
17	A	813	CLA	C3B-C4B	2.36	1.49	1.42
17	1	313	CLA	C3B-C4B	2.36	1.49	1.42
23	2	318	LMT	O3B-C3B	-2.36	1.37	1.43
17	B	802	CLA	MG-ND	-2.36	2.01	2.05
17	L	202	CLA	CHC-C1C	2.36	1.43	1.38
17	B	837	CLA	C4B-NB	2.36	1.41	1.37
17	A	818	CLA	C3B-C4B	2.36	1.49	1.42
17	A	836	CLA	CHC-C1C	2.36	1.43	1.38
17	3	613	CLA	CMD-C2D	-2.36	1.45	1.50
17	A	824	CLA	CHC-C1C	2.35	1.43	1.38
17	A	806	CLA	CHC-C1C	2.35	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	310	CLA	MG-ND	-2.35	2.01	2.05
24	4	320	LMG	C4-C3	2.35	1.58	1.52
17	A	818	CLA	CHC-C1C	2.35	1.43	1.38
17	A	821	CLA	MG-NB	-2.35	2.01	2.05
17	2	309	CLA	CHC-C1C	2.35	1.43	1.38
17	A	813	CLA	O2A-CGA	2.35	1.38	1.30
19	4	316	LUT	C35-C34	2.35	1.50	1.43
17	A	810	CLA	C3B-C4B	2.35	1.49	1.42
17	A	840	CLA	CMD-C2D	-2.34	1.46	1.50
17	A	835	CLA	C3B-C4B	2.34	1.49	1.42
18	4	301	CHL	CHD-C1D	2.34	1.43	1.39
17	2	312	CLA	CHC-C1C	2.34	1.43	1.38
23	2	318	LMT	O3'-C3'	-2.34	1.37	1.43
17	J	101	CLA	C3B-C4B	2.34	1.49	1.42
21	J	104	BCR	C30-C25	-2.34	1.50	1.53
17	2	308	CLA	CHC-C1C	2.34	1.43	1.38
17	B	803	CLA	MG-NB	-2.34	2.01	2.05
17	B	837	CLA	C1B-NB	-2.34	1.34	1.37
17	A	802	CLA	CHC-C1C	2.34	1.43	1.38
17	B	805	CLA	C1B-C2B	2.34	1.48	1.43
17	B	822	CLA	C3B-C4B	2.33	1.49	1.42
17	A	813	CLA	CHC-C1C	2.33	1.43	1.38
17	B	837	CLA	C1B-C2B	2.33	1.48	1.43
17	3	602	CLA	C3B-C4B	2.33	1.49	1.42
17	B	819	CLA	MG-ND	-2.33	2.01	2.05
17	B	808	CLA	C1B-NB	-2.33	1.34	1.37
17	A	821	CLA	CHC-C1C	2.33	1.43	1.38
18	3	601	CHL	CBD-CGD	-2.33	1.49	1.52
17	4	304	CLA	C3B-C4B	2.33	1.49	1.42
17	4	312	CLA	C4B-NB	2.32	1.40	1.37
17	F	307	CLA	CMD-C2D	-2.32	1.46	1.50
17	B	842	CLA	C3B-C4B	2.32	1.49	1.42
17	K	202	CLA	CHC-C1C	2.32	1.43	1.38
17	L	203	CLA	C3B-C4B	2.32	1.49	1.42
17	A	830	CLA	C3B-C4B	2.32	1.49	1.42
17	A	839	CLA	CMC-C2C	-2.32	1.46	1.50
17	B	803	CLA	CHC-C1C	2.32	1.43	1.38
17	A	832	CLA	C3B-C4B	2.32	1.49	1.42
17	3	613	CLA	CHC-C1C	2.32	1.43	1.38
17	B	839	CLA	MG-ND	-2.31	2.01	2.05
18	4	315	CHL	CBD-CGD	-2.31	1.49	1.52
17	3	611	CLA	CHC-C1C	2.31	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	J	103	CLA	MG-ND	-2.31	2.01	2.05
17	1	307	CLA	C1D-C2D	2.31	1.49	1.45
17	1	313	CLA	MG-ND	-2.31	2.01	2.05
17	3	612	CLA	CHC-C1C	2.30	1.43	1.38
17	B	825	CLA	C1B-C2B	2.30	1.48	1.43
17	A	806	CLA	MG-ND	-2.30	2.01	2.05
17	B	838	CLA	C3C-C2C	2.30	1.41	1.36
17	B	817	CLA	MG-ND	-2.30	2.01	2.05
17	B	833	CLA	C1B-C2B	2.30	1.48	1.43
17	B	824	CLA	CMD-C2D	-2.30	1.46	1.50
17	4	310	CLA	CHC-C1C	2.29	1.43	1.38
17	1	303	CLA	CHC-C1C	2.29	1.43	1.38
17	A	834	CLA	CHC-C1C	2.29	1.43	1.38
19	4	316	LUT	C7-C6	2.29	1.52	1.45
19	2	314	LUT	C7-C6	2.29	1.52	1.45
17	A	839	CLA	MG-NB	-2.29	2.01	2.05
19	1	314	LUT	C11-C10	2.29	1.50	1.43
17	B	804	CLA	C3D-C4D	2.29	1.49	1.44
17	2	302	CLA	CHC-C1C	2.28	1.43	1.38
17	A	840	CLA	C3B-C4B	2.28	1.49	1.42
17	F	307	CLA	MG-ND	-2.28	2.01	2.05
17	B	831	CLA	MG-NC	2.28	2.11	2.06
17	B	808	CLA	MG-NC	2.28	2.11	2.06
17	4	303	CLA	CHC-C1C	2.28	1.43	1.38
17	B	840	CLA	CMD-C2D	-2.28	1.46	1.50
17	B	834	CLA	C3B-C4B	2.28	1.49	1.42
17	L	204	CLA	CHC-C1C	2.27	1.43	1.38
17	B	832	CLA	CMD-C2D	-2.27	1.46	1.50
17	A	830	CLA	MG-NB	-2.27	2.01	2.05
21	F	303	BCR	C1-C6	-2.27	1.50	1.53
17	2	302	CLA	C3B-C4B	2.27	1.49	1.42
17	4	308	CLA	C3B-C4B	2.27	1.49	1.42
17	A	815	CLA	CHC-C1C	2.27	1.43	1.38
17	A	808	CLA	CMC-C2C	-2.27	1.46	1.50
17	B	820	CLA	C4B-NB	2.27	1.40	1.37
17	B	813	CLA	CMC-C2C	-2.27	1.46	1.50
18	4	305	CHL	CBD-CGD	-2.27	1.49	1.52
17	B	802	CLA	C3B-C4B	2.27	1.49	1.42
17	4	311	CLA	CHC-C1C	2.27	1.43	1.38
17	B	837	CLA	CHC-C1C	2.27	1.43	1.38
17	A	841	CLA	CHC-C1C	2.26	1.43	1.38
17	A	824	CLA	C3B-C4B	2.26	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	310	CLA	CHC-C1C	2.26	1.43	1.38
17	B	838	CLA	C4B-NB	2.26	1.40	1.37
18	4	306	CHL	CMC-C2C	2.26	1.49	1.44
17	J	101	CLA	MG-ND	-2.26	2.01	2.05
17	3	613	CLA	C3B-C4B	2.26	1.49	1.42
17	A	807	CLA	C3B-C4B	2.26	1.49	1.42
17	A	831	CLA	CHC-C1C	2.26	1.43	1.38
17	B	809	CLA	CMD-C2D	-2.26	1.46	1.50
17	A	853	CLA	C3B-C4B	2.25	1.49	1.42
17	2	310	CLA	CMC-C2C	-2.25	1.46	1.50
17	4	313	CLA	MG-NB	-2.25	2.01	2.05
21	J	104	BCR	C38-C26	-2.25	1.47	1.50
17	A	810	CLA	CHC-C1C	2.25	1.43	1.38
17	B	810	CLA	MG-ND	-2.25	2.01	2.05
17	1	307	CLA	CHC-C1C	2.25	1.43	1.38
17	B	804	CLA	MG-NC	2.25	2.11	2.06
17	A	829	CLA	CMB-C2B	-2.25	1.46	1.50
17	B	809	CLA	C1B-C2B	2.25	1.48	1.43
17	3	613	CLA	MG-NB	-2.24	2.01	2.05
17	1	308	CLA	CHC-C1C	2.24	1.43	1.38
18	2	306	CHL	CMC-C2C	2.24	1.49	1.44
17	A	826	CLA	C3B-C4B	2.24	1.49	1.42
17	4	313	CLA	CHC-C1C	2.24	1.43	1.38
17	B	819	CLA	CMB-C2B	-2.24	1.46	1.50
17	A	805	CLA	CHC-C1C	2.24	1.43	1.38
17	J	103	CLA	CHC-C1C	2.24	1.43	1.38
17	B	824	CLA	C3B-C4B	2.23	1.49	1.42
17	B	833	CLA	MG-NA	2.23	2.11	2.06
17	A	807	CLA	C1B-C2B	2.23	1.48	1.43
17	G	104	CLA	CMB-C2B	-2.23	1.46	1.50
21	2	316	BCR	C33-C5	-2.23	1.47	1.50
17	B	803	CLA	CMB-C2B	-2.23	1.46	1.50
17	4	310	CLA	C3B-C4B	2.23	1.49	1.42
17	B	808	CLA	MG-ND	-2.23	2.01	2.05
17	A	805	CLA	MG-NB	-2.23	2.01	2.05
17	2	302	CLA	CMD-C2D	-2.23	1.46	1.50
17	1	302	CLA	C1D-C2D	2.22	1.49	1.45
17	3	613	CLA	CMB-C2B	-2.22	1.46	1.50
17	G	103	CLA	CMD-C2D	-2.22	1.46	1.50
17	A	820	CLA	CMB-C2B	-2.22	1.46	1.50
17	A	814	CLA	C3B-C4B	2.22	1.49	1.42
17	A	807	CLA	CMC-C2C	-2.22	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	802	CLA	C3B-C4B	2.22	1.49	1.42
17	1	311	CLA	CHC-C1C	2.22	1.42	1.38
17	B	817	CLA	C1B-C2B	2.22	1.48	1.43
17	A	811	CLA	CHC-C1C	2.21	1.42	1.38
17	A	853	CLA	MG-NC	2.21	2.11	2.06
17	K	202	CLA	CMD-C2D	-2.21	1.46	1.50
17	B	802	CLA	C1B-C2B	2.21	1.48	1.43
17	B	811	CLA	C3B-C4B	2.21	1.49	1.42
17	4	312	CLA	CMB-C2B	-2.21	1.46	1.50
17	A	826	CLA	CMB-C2B	-2.21	1.46	1.50
17	B	804	CLA	MG-NB	-2.21	2.01	2.05
24	G	101	LMG	O7-C8	-2.20	1.41	1.46
17	B	807	CLA	CHC-C1C	2.20	1.42	1.38
17	2	301	CLA	C3B-C4B	2.20	1.49	1.42
24	4	319	LMG	O6-C5	-2.20	1.39	1.44
17	B	824	CLA	MG-NC	2.20	2.11	2.06
17	3	604	CLA	CHC-C1C	2.20	1.42	1.38
17	A	833	CLA	CMB-C2B	-2.20	1.46	1.50
20	4	317	XAT	O24-C25	-2.20	1.43	1.46
17	4	309	CLA	MG-ND	-2.20	2.01	2.05
17	A	835	CLA	CMB-C2B	-2.20	1.46	1.50
27	A	842	PQN	C2M-C2	2.20	1.55	1.50
17	2	307	CLA	C1B-C2B	2.19	1.48	1.43
17	F	304	CLA	C1D-C2D	2.19	1.49	1.45
17	F	307	CLA	CHC-C1C	2.19	1.42	1.38
17	A	806	CLA	CMC-C2C	-2.19	1.46	1.50
17	B	841	CLA	CMB-C2B	-2.19	1.46	1.50
17	G	103	CLA	CHC-C1C	2.19	1.42	1.38
17	A	801	CLA	C4D-CHA	2.19	1.45	1.38
18	3	607	CHL	CMC-C2C	2.19	1.49	1.44
17	3	603	CLA	CHC-C1C	2.19	1.42	1.38
25	4	322	HTG	C1-S1	-2.19	1.77	1.80
17	G	105	CLA	C3B-C4B	2.19	1.49	1.42
17	A	807	CLA	CMB-C2B	-2.19	1.46	1.50
17	B	828	CLA	MG-NB	-2.19	2.01	2.05
17	A	827	CLA	CMD-C2D	-2.19	1.46	1.50
17	4	303	CLA	MG-NB	-2.19	2.01	2.05
17	B	828	CLA	CHC-C1C	2.18	1.42	1.38
17	B	829	CLA	C4D-CHA	2.18	1.45	1.38
23	A	855	LMT	O3'-C3'	-2.18	1.37	1.43
17	B	836	CLA	C3B-C4B	2.18	1.49	1.42
17	A	833	CLA	CHC-C1C	2.18	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	824	CLA	MG-NB	-2.18	2.01	2.05
17	A	815	CLA	CMB-C2B	-2.18	1.46	1.50
17	B	813	CLA	C4B-NB	2.18	1.40	1.37
17	4	312	CLA	C1B-C2B	2.18	1.48	1.43
17	4	303	CLA	C3D-C4D	2.18	1.49	1.44
17	B	835	CLA	C1D-C2D	2.17	1.49	1.45
17	A	828	CLA	CHC-C1C	2.17	1.42	1.38
17	2	308	CLA	CMD-C2D	-2.17	1.46	1.50
17	A	829	CLA	CMD-C2D	-2.17	1.46	1.50
17	A	830	CLA	CMB-C2B	-2.17	1.46	1.50
17	B	828	CLA	C3B-C4B	2.17	1.49	1.42
17	A	816	CLA	CMD-C2D	-2.17	1.46	1.50
17	3	605	CLA	CMB-C2B	-2.17	1.46	1.50
17	B	837	CLA	C1D-ND	2.17	1.40	1.37
25	F	310	HTG	C1-S1	-2.17	1.77	1.80
17	B	810	CLA	CMB-C2B	-2.17	1.46	1.50
17	A	814	CLA	MG-NB	-2.16	2.01	2.05
18	4	307	CHL	CMC-C2C	2.16	1.49	1.44
17	2	310	CLA	CMB-C2B	-2.16	1.46	1.50
17	B	825	CLA	CMB-C2B	-2.16	1.46	1.50
17	A	809	CLA	CMD-C2D	-2.16	1.46	1.50
17	1	304	CLA	CMB-C2B	-2.16	1.46	1.50
17	A	841	CLA	C3B-C4B	2.16	1.49	1.42
17	A	818	CLA	CMD-C2D	-2.16	1.46	1.50
17	4	308	CLA	MG-ND	-2.16	2.01	2.05
17	B	834	CLA	CHC-C1C	2.16	1.42	1.38
17	2	312	CLA	CMD-C2D	-2.16	1.46	1.50
17	B	805	CLA	CMB-C2B	-2.16	1.46	1.50
17	2	319	CLA	CMD-C2D	-2.15	1.46	1.50
17	B	821	CLA	CHC-C1C	2.15	1.42	1.38
17	B	833	CLA	C4B-NB	2.15	1.40	1.37
17	G	105	CLA	CMC-C2C	-2.15	1.46	1.50
17	A	818	CLA	CMB-C2B	-2.15	1.46	1.50
19	4	316	LUT	C22-C21	-2.15	1.52	1.54
18	4	301	CHL	CMA-C3A	-2.15	1.49	1.53
17	B	814	CLA	MG-NA	2.15	2.11	2.06
17	A	830	CLA	CHC-C1C	2.15	1.42	1.38
17	B	811	CLA	MG-NB	-2.15	2.01	2.05
19	1	314	LUT	C7-C6	2.15	1.52	1.45
17	A	815	CLA	CMD-C2D	-2.14	1.46	1.50
17	A	841	CLA	CMB-C2B	-2.14	1.46	1.50
17	A	827	CLA	C1D-C2D	2.14	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	826	CLA	CMD-C2D	-2.14	1.46	1.50
17	A	807	CLA	C1D-C2D	2.14	1.49	1.45
17	B	838	CLA	C1D-C2D	2.14	1.49	1.45
17	A	841	CLA	MG-NB	-2.14	2.01	2.05
18	4	301	CHL	CBD-CAD	-2.14	1.46	1.53
17	B	806	CLA	CHC-C1C	2.14	1.42	1.38
17	2	301	CLA	CMD-C2D	-2.14	1.46	1.50
22	2	317	LHG	O7-C5	-2.14	1.41	1.46
17	B	823	CLA	C3B-C4B	2.13	1.49	1.42
17	B	826	CLA	CHC-C1C	2.13	1.42	1.38
17	1	309	CLA	CMB-C2B	-2.13	1.46	1.50
17	A	838	CLA	CMB-C2B	-2.13	1.46	1.50
17	A	810	CLA	C3D-C4D	2.13	1.49	1.44
17	3	610	CLA	CHC-C1C	2.13	1.42	1.38
17	B	804	CLA	CMB-C2B	-2.12	1.46	1.50
17	4	308	CLA	CHC-C1C	2.12	1.42	1.38
17	B	813	CLA	CHC-C1C	2.12	1.42	1.38
17	B	817	CLA	CMC-C2C	-2.12	1.46	1.50
17	1	311	CLA	CMB-C2B	-2.12	1.46	1.50
21	B	849	BCR	C38-C26	-2.12	1.47	1.50
17	A	803	CLA	CMB-C2B	-2.12	1.46	1.50
21	A	847	BCR	C33-C5	-2.12	1.47	1.50
23	2	318	LMT	O2'-C2'	-2.12	1.37	1.43
17	3	602	CLA	CMB-C2B	-2.12	1.46	1.50
17	1	302	CLA	CMD-C2D	-2.12	1.46	1.50
17	B	826	CLA	CMB-C2B	-2.12	1.46	1.50
18	4	301	CHL	O2D-CGD	2.11	1.38	1.33
18	2	304	CHL	CBD-CGD	-2.11	1.49	1.52
17	1	313	CLA	CMC-C2C	-2.11	1.46	1.50
17	A	803	CLA	CMD-C2D	-2.11	1.46	1.50
17	A	812	CLA	CMB-C2B	-2.11	1.46	1.50
17	3	606	CLA	CMB-C2B	-2.11	1.46	1.50
17	B	840	CLA	C4B-NB	2.11	1.40	1.37
17	B	815	CLA	C3D-C4D	2.11	1.48	1.44
24	G	101	LMG	C4-C5	2.11	1.57	1.53
17	B	807	CLA	CMB-C2B	-2.11	1.46	1.50
17	1	310	CLA	CMD-C2D	-2.11	1.46	1.50
17	1	307	CLA	CMC-C2C	-2.11	1.46	1.50
17	B	827	CLA	CHC-C1C	2.10	1.42	1.38
17	A	825	CLA	C1D-C2D	2.10	1.49	1.45
17	A	811	CLA	C1D-C2D	2.10	1.49	1.45
17	B	841	CLA	C3C-C2C	2.10	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	818	CLA	C1D-C2D	2.10	1.49	1.45
17	A	806	CLA	CMB-C2B	-2.10	1.46	1.50
17	A	840	CLA	MG-NA	2.10	2.11	2.06
17	1	308	CLA	CMD-C2D	-2.10	1.46	1.50
17	G	103	CLA	CMB-C2B	-2.10	1.46	1.50
17	L	202	CLA	C3B-C4B	2.10	1.48	1.42
17	3	608	CLA	CMD-C2D	-2.09	1.46	1.50
17	K	201	CLA	MG-NB	-2.09	2.01	2.05
17	A	826	CLA	CHC-C1C	2.09	1.42	1.38
17	A	838	CLA	MG-NB	-2.09	2.01	2.05
17	L	202	CLA	CMD-C2D	-2.09	1.46	1.50
23	2	318	LMT	O2B-C2B	-2.09	1.37	1.43
17	A	824	CLA	CMD-C2D	-2.09	1.46	1.50
17	B	807	CLA	C4B-NB	2.09	1.40	1.37
17	1	307	CLA	CMB-C2B	-2.09	1.46	1.50
17	4	308	CLA	CMD-C2D	-2.09	1.46	1.50
17	L	203	CLA	CMD-C2D	-2.09	1.46	1.50
17	B	808	CLA	CHC-C1C	2.09	1.42	1.38
21	4	318	BCR	C30-C25	-2.09	1.51	1.53
17	A	817	CLA	CMB-C2B	-2.09	1.46	1.50
17	A	829	CLA	CMC-C2C	-2.09	1.46	1.50
17	A	841	CLA	CMC-C2C	-2.09	1.46	1.50
17	A	809	CLA	MG-NB	-2.08	2.01	2.05
17	A	833	CLA	MG-NB	-2.08	2.01	2.05
17	G	104	CLA	CHC-C1C	2.08	1.42	1.38
17	A	853	CLA	C3D-C4D	2.08	1.48	1.44
24	4	319	LMG	C7-C8	2.08	1.57	1.50
17	4	302	CLA	MG-NA	2.08	2.11	2.06
17	B	812	CLA	MG-ND	-2.08	2.01	2.05
17	1	310	CLA	CMB-C2B	-2.08	1.46	1.50
17	3	610	CLA	CMB-C2B	-2.08	1.46	1.50
17	A	822	CLA	CMD-C2D	-2.08	1.46	1.50
17	A	836	CLA	C3B-C4B	2.08	1.48	1.42
18	1	305	CHL	CMC-C2C	2.08	1.49	1.44
20	3	615	XAT	O4-C5	-2.08	1.43	1.46
26	B	850	DGD	C1E-C2E	2.07	1.58	1.52
17	B	814	CLA	O2A-CGA	2.07	1.39	1.33
20	2	315	XAT	O4-C5	-2.07	1.43	1.46
17	B	832	CLA	CHC-C1C	2.07	1.42	1.38
17	B	808	CLA	CMB-C2B	-2.07	1.46	1.50
17	B	830	CLA	CMD-C2D	-2.07	1.46	1.50
17	B	809	CLA	C1D-C2D	2.07	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	841	CLA	C3B-C4B	2.07	1.48	1.42
17	A	823	CLA	CMD-C2D	-2.07	1.46	1.50
18	4	301	CHL	O2D-CED	-2.07	1.40	1.45
21	B	847	BCR	C39-C30	-2.07	1.49	1.53
17	A	834	CLA	CMB-C2B	-2.07	1.46	1.50
17	B	831	CLA	CMB-C2B	-2.07	1.46	1.50
17	A	835	CLA	C1D-C2D	2.07	1.49	1.45
17	B	816	CLA	MG-NB	-2.07	2.01	2.05
17	1	301	CLA	MG-NA	2.07	2.11	2.06
17	2	310	CLA	MG-NB	-2.06	2.01	2.05
17	1	306	CLA	CMB-C2B	-2.06	1.46	1.50
17	B	841	CLA	CMD-C2D	-2.06	1.46	1.50
17	3	606	CLA	CMD-C2D	-2.06	1.46	1.50
17	3	604	CLA	MG-NB	-2.06	2.01	2.05
17	2	310	CLA	CMD-C2D	-2.06	1.46	1.50
17	F	306	CLA	O2A-CGA	2.06	1.37	1.30
17	B	821	CLA	C1D-C2D	2.06	1.49	1.45
17	B	824	CLA	MG-NB	-2.06	2.01	2.05
17	A	826	CLA	MG-ND	-2.06	2.01	2.05
17	A	836	CLA	MG-NB	-2.06	2.01	2.05
17	B	840	CLA	C3B-C4B	2.06	1.48	1.42
17	2	301	CLA	MG-NB	-2.06	2.01	2.05
17	3	604	CLA	CMD-C2D	-2.06	1.46	1.50
17	B	818	CLA	MG-NB	-2.06	2.01	2.05
17	1	311	CLA	MG-ND	-2.06	2.01	2.05
24	4	320	LMG	C3-C2	2.05	1.57	1.52
24	4	319	LMG	O8-C9	-2.05	1.40	1.45
17	B	831	CLA	C4B-NB	2.05	1.40	1.37
17	3	603	CLA	MG-NB	-2.05	2.01	2.05
17	4	304	CLA	MG-ND	-2.05	2.01	2.05
17	1	303	CLA	CMB-C2B	-2.05	1.46	1.50
17	1	304	CLA	CMD-C2D	-2.05	1.46	1.50
21	B	849	BCR	C33-C5	-2.05	1.47	1.50
17	K	201	CLA	CMD-C2D	-2.05	1.46	1.50
17	2	308	CLA	CMC-C2C	-2.05	1.46	1.50
17	B	812	CLA	CMB-C2B	-2.05	1.46	1.50
17	4	312	CLA	MG-ND	-2.05	2.01	2.05
20	1	315	XAT	O4-C5	-2.05	1.43	1.46
17	3	611	CLA	CMD-C2D	-2.05	1.46	1.50
17	A	820	CLA	MG-ND	-2.05	2.01	2.05
17	3	610	CLA	CMC-C2C	-2.05	1.46	1.50
17	A	834	CLA	MG-NB	-2.04	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	835	CLA	MG-NB	-2.04	2.01	2.05
17	B	806	CLA	O2A-CGA	2.04	1.37	1.30
17	B	816	CLA	O1D-CGD	2.04	1.26	1.21
17	F	307	CLA	CMB-C2B	-2.04	1.46	1.50
17	2	311	CLA	CMB-C2B	-2.04	1.46	1.50
21	A	847	BCR	C38-C26	-2.04	1.47	1.50
17	B	813	CLA	CMD-C2D	-2.04	1.46	1.50
17	1	310	CLA	MG-NB	-2.04	2.01	2.05
17	4	310	CLA	CMC-C2C	-2.04	1.46	1.50
17	3	604	CLA	CMB-C2B	-2.04	1.46	1.50
17	B	813	CLA	C1B-C2B	2.04	1.47	1.43
17	1	303	CLA	CMD-C2D	-2.04	1.46	1.50
17	B	832	CLA	C4B-NB	2.04	1.40	1.37
17	B	808	CLA	CMD-C2D	-2.04	1.46	1.50
17	B	834	CLA	CMC-C2C	-2.04	1.46	1.50
17	A	815	CLA	CMC-C2C	-2.04	1.46	1.50
17	1	306	CLA	CMD-C2D	-2.04	1.46	1.50
17	2	301	CLA	CMC-C2C	-2.04	1.46	1.50
17	2	307	CLA	CMB-C2B	-2.04	1.46	1.50
17	3	608	CLA	CMB-C2B	-2.04	1.46	1.50
17	A	821	CLA	CMB-C2B	-2.04	1.46	1.50
22	B	801	LHG	O7-C7	2.04	1.40	1.34
17	A	817	CLA	CMC-C2C	-2.03	1.46	1.50
17	A	834	CLA	CMD-C2D	-2.03	1.46	1.50
21	J	105	BCR	C33-C5	-2.03	1.47	1.50
17	B	810	CLA	CMC-C2C	-2.03	1.46	1.50
17	B	840	CLA	CHC-C1C	2.03	1.42	1.38
17	2	312	CLA	MG-NB	-2.03	2.01	2.05
24	F	309	LMG	C4-C5	2.03	1.57	1.53
17	2	307	CLA	CMD-C2D	-2.03	1.46	1.50
17	B	802	CLA	CMD-C2D	-2.03	1.46	1.50
17	4	312	CLA	O2A-CGA	2.03	1.39	1.33
17	2	303	CLA	CMD-C2D	-2.03	1.46	1.50
17	G	103	CLA	C3D-C4D	2.03	1.48	1.44
17	A	837	CLA	C1D-C2D	2.03	1.49	1.45
17	A	829	CLA	C3B-C4B	2.03	1.48	1.42
17	4	304	CLA	C4D-CHA	2.03	1.45	1.38
17	2	302	CLA	MG-NB	-2.02	2.01	2.05
17	4	311	CLA	C1D-C2D	2.02	1.49	1.45
17	B	829	CLA	O2D-CGD	2.02	1.38	1.33
17	B	828	CLA	CMB-C2B	-2.02	1.46	1.50
17	4	312	CLA	CHC-C1C	2.02	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	301	CLA	CMB-C2B	-2.02	1.46	1.50
17	A	812	CLA	CMD-C2D	-2.02	1.46	1.50
17	1	311	CLA	CMD-C2D	-2.02	1.46	1.50
17	A	831	CLA	CMB-C2B	-2.01	1.46	1.50
21	J	105	BCR	C38-C26	-2.01	1.47	1.50
17	B	836	CLA	CHC-C1C	2.01	1.42	1.38
17	A	832	CLA	CMB-C2B	-2.01	1.46	1.50
17	B	834	CLA	O2D-CGD	2.01	1.38	1.33
17	A	837	CLA	CHC-C1C	2.01	1.42	1.38
17	F	307	CLA	C1B-C2B	2.01	1.47	1.43
17	A	802	CLA	CMC-C2C	-2.01	1.46	1.50
17	2	301	CLA	MG-NA	2.01	2.11	2.06
17	4	314	CLA	C3C-C2C	2.01	1.41	1.36
17	A	816	CLA	CMC-C2C	-2.01	1.46	1.50
19	4	316	LUT	C26-C27	2.01	1.53	1.50
17	A	807	CLA	MG-ND	-2.01	2.01	2.05
17	A	803	CLA	MG-ND	-2.01	2.01	2.05
17	K	202	CLA	CMB-C2B	-2.01	1.46	1.50
17	B	807	CLA	C3C-C2C	2.01	1.41	1.36
17	A	821	CLA	CMD-C2D	-2.00	1.46	1.50
17	2	311	CLA	MG-NB	-2.00	2.01	2.05
17	2	303	CLA	CMB-C2B	-2.00	1.46	1.50
17	J	103	CLA	CMB-C2B	-2.00	1.46	1.50
17	1	310	CLA	CMC-C2C	-2.00	1.46	1.50
21	L	205	BCR	C30-C25	-2.00	1.51	1.53
17	B	833	CLA	CHC-C4B	-2.00	1.34	1.39
17	A	827	CLA	C3C-C2C	2.00	1.41	1.36
17	3	611	CLA	CMB-C2B	-2.00	1.46	1.50

All (1764) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	842	PQN	C6-C5-C10	-13.48	104.14	119.26
18	3	601	CHL	O2D-CGD-CBD	12.29	124.45	110.95
27	A	842	PQN	C9-C10-C5	-12.25	105.51	119.26
19	4	316	LUT	C31-C30-C29	-12.02	110.43	127.28
19	4	316	LUT	C11-C10-C9	-11.98	110.48	127.28
19	2	314	LUT	C35-C34-C33	-11.88	110.62	127.28
19	1	314	LUT	C31-C30-C29	-11.88	110.62	127.28
19	1	314	LUT	C15-C14-C13	-11.82	110.70	127.28
19	3	614	LUT	C15-C14-C13	-11.80	110.73	127.28
20	3	615	XAT	C35-C34-C33	-11.63	110.97	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	315	XAT	C35-C34-C33	-11.62	110.98	127.28
19	4	316	LUT	C18-C5-C6	-11.62	111.81	124.48
20	2	315	XAT	C35-C34-C33	-11.61	111.00	127.28
20	4	317	XAT	C31-C30-C29	-11.35	111.36	127.28
19	2	314	LUT	C18-C5-C6	-11.25	112.21	124.48
19	3	614	LUT	C31-C30-C29	-11.21	111.55	127.28
19	2	314	LUT	C15-C14-C13	-11.18	111.60	127.28
19	3	614	LUT	C35-C34-C33	-11.16	111.63	127.28
20	3	615	XAT	C31-C30-C29	-11.12	111.68	127.28
20	1	315	XAT	C31-C30-C29	-11.12	111.69	127.28
20	2	315	XAT	C31-C30-C29	-11.09	111.72	127.28
19	4	316	LUT	C15-C14-C13	-11.07	111.75	127.28
19	4	316	LUT	C32-C33-C34	-10.84	101.96	119.01
19	1	314	LUT	C11-C10-C9	-10.76	112.19	127.28
20	1	315	XAT	C15-C14-C13	-10.66	112.33	127.28
20	2	315	XAT	C15-C14-C13	-10.66	112.33	127.28
20	3	615	XAT	C15-C14-C13	-10.64	112.36	127.28
19	1	314	LUT	C35-C34-C33	-10.50	112.55	127.28
19	3	614	LUT	C18-C5-C6	-10.45	113.08	124.48
20	4	317	XAT	C35-C34-C33	-10.27	112.88	127.28
19	2	314	LUT	C26-C27-C28	-10.18	108.74	124.58
19	2	314	LUT	C31-C30-C29	-10.11	113.09	127.28
19	1	314	LUT	C18-C5-C6	-9.89	113.69	124.48
20	4	317	XAT	C27-C28-C29	-9.74	110.42	125.53
18	2	304	CHL	C1B-CHB-C4A	9.73	127.58	121.32
20	4	317	XAT	C15-C14-C13	-9.65	113.74	127.28
20	1	315	XAT	C8-C9-C10	-9.61	103.90	119.01
20	3	615	XAT	C8-C9-C10	-9.60	103.91	119.01
20	2	315	XAT	C8-C9-C10	-9.59	103.92	119.01
19	4	316	LUT	C35-C34-C33	-9.52	113.92	127.28
18	4	307	CHL	C1B-CHB-C4A	9.39	127.36	121.32
18	2	306	CHL	C1B-CHB-C4A	9.37	127.35	121.32
19	2	314	LUT	C11-C10-C9	-9.36	114.15	127.28
18	4	305	CHL	C1B-CHB-C4A	9.34	127.33	121.32
27	B	843	PQN	C6-C5-C10	-9.33	108.79	119.26
19	1	314	LUT	C8-C9-C10	-9.26	104.44	119.01
20	1	315	XAT	C27-C28-C29	-9.21	111.24	125.53
20	2	315	XAT	C27-C28-C29	-9.19	111.26	125.53
20	3	615	XAT	C27-C28-C29	-9.19	111.27	125.53
20	4	317	XAT	C12-C13-C14	-9.14	104.63	119.01
18	4	305	CHL	O2D-CGD-CBD	9.12	120.97	110.95
19	4	316	LUT	C8-C9-C10	-9.05	104.78	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	313	CHL	O2D-CGD-CBD	8.91	120.73	110.95
20	4	317	XAT	C11-C10-C9	-8.90	114.79	127.28
19	1	314	LUT	C26-C27-C28	-8.90	110.73	124.58
19	2	314	LUT	C28-C29-C30	-8.90	105.01	119.01
19	1	314	LUT	C7-C8-C9	-8.86	113.12	126.23
19	3	614	LUT	C11-C10-C9	-8.81	114.92	127.28
19	1	314	LUT	C32-C33-C34	-8.79	105.18	119.01
20	1	315	XAT	C12-C13-C14	-8.78	105.20	119.01
20	2	315	XAT	C12-C13-C14	-8.77	105.21	119.01
20	3	615	XAT	C12-C13-C14	-8.77	105.22	119.01
19	2	314	LUT	C7-C8-C9	-8.71	113.35	126.23
18	3	601	CHL	C1B-CHB-C4A	8.64	126.88	121.32
18	4	315	CHL	C1B-CHB-C4A	8.60	126.85	121.32
20	3	615	XAT	C11-C10-C9	-8.60	115.22	127.28
20	1	315	XAT	C11-C10-C9	-8.59	115.23	127.28
18	4	301	CHL	C1B-CHB-C4A	8.56	126.83	121.32
20	2	315	XAT	C11-C10-C9	-8.55	115.29	127.28
27	B	843	PQN	C11-C3-C4	-8.52	109.60	118.58
19	3	614	LUT	C8-C9-C10	-8.52	105.61	119.01
19	4	316	LUT	C8-C7-C6	-8.51	104.25	127.00
19	4	316	LUT	C35-C15-C14	-8.51	106.10	123.52
19	3	614	LUT	C26-C27-C28	-8.49	111.37	124.58
19	2	314	LUT	C8-C9-C10	-8.49	105.66	119.01
27	B	843	PQN	C9-C10-C5	-8.46	109.77	119.26
27	B	843	PQN	C2M-C2-C3	-8.33	110.74	124.45
18	2	313	CHL	C1B-CHB-C4A	8.33	126.68	121.32
18	2	305	CHL	C1B-CHB-C4A	8.30	126.66	121.32
18	4	306	CHL	C1B-CHB-C4A	8.25	126.63	121.32
19	4	316	LUT	C15-C35-C34	-8.19	106.77	123.52
19	2	314	LUT	C12-C13-C14	-8.11	106.25	119.01
20	2	315	XAT	C32-C33-C34	-8.06	106.33	119.01
20	1	315	XAT	C32-C33-C34	-8.06	106.34	119.01
19	2	314	LUT	C35-C15-C14	-8.04	107.06	123.52
19	3	614	LUT	C7-C8-C9	-8.04	114.34	126.23
20	3	615	XAT	C32-C33-C34	-8.03	106.38	119.01
18	3	607	CHL	C1B-CHB-C4A	8.02	126.48	121.32
20	4	317	XAT	C35-C15-C14	-8.01	107.13	123.52
27	B	843	PQN	C6-C5-C4	-7.98	108.45	120.10
18	2	304	CHL	O2D-CGD-CBD	7.96	119.69	110.95
27	B	843	PQN	C11-C12-C13	-7.94	113.14	126.83
19	1	314	LUT	C12-C13-C14	-7.92	106.55	119.01
20	1	315	XAT	C28-C29-C30	-7.89	106.60	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	615	XAT	C28-C29-C30	-7.88	106.61	119.01
20	2	315	XAT	C28-C29-C30	-7.87	106.62	119.01
20	4	317	XAT	C8-C9-C10	-7.87	106.64	119.01
18	2	305	CHL	O2D-CGD-CBD	7.81	119.53	110.95
19	3	614	LUT	C32-C33-C34	-7.80	106.75	119.01
20	4	317	XAT	C7-C8-C9	-7.75	113.51	125.53
19	4	316	LUT	C28-C29-C30	-7.72	106.86	119.01
19	4	316	LUT	C27-C28-C29	-7.69	109.78	126.32
18	3	607	CHL	O2D-CGD-CBD	7.62	119.32	110.95
20	2	315	XAT	C40-C33-C34	-7.57	110.54	122.82
17	B	821	CLA	C4A-NA-C1A	7.57	110.13	106.68
20	1	315	XAT	C40-C33-C34	-7.57	110.56	122.82
20	3	615	XAT	C40-C33-C34	-7.57	110.56	122.82
19	2	314	LUT	C32-C33-C34	-7.55	107.13	119.01
20	4	317	XAT	C39-C29-C30	-7.54	110.61	122.82
19	3	614	LUT	C27-C28-C29	-7.53	110.13	126.32
20	4	317	XAT	C20-C13-C14	-7.50	110.66	122.82
19	1	314	LUT	C8-C7-C6	-7.48	107.01	127.00
20	2	315	XAT	C6-C7-C8	-7.44	110.26	125.99
20	4	317	XAT	C26-C27-C28	-7.44	110.26	125.99
20	1	315	XAT	C6-C7-C8	-7.44	110.27	125.99
20	3	615	XAT	C6-C7-C8	-7.44	110.27	125.99
19	4	316	LUT	C12-C13-C14	-7.42	107.33	119.01
19	1	314	LUT	C27-C28-C29	-7.42	110.37	126.32
19	3	614	LUT	C15-C35-C34	-7.41	108.36	123.52
19	1	314	LUT	C1-C6-C5	-7.40	112.52	122.64
20	3	615	XAT	C15-C35-C34	-7.38	108.42	123.52
20	2	315	XAT	C15-C35-C34	-7.37	108.44	123.52
20	1	315	XAT	C15-C35-C34	-7.36	108.46	123.52
19	3	614	LUT	C1-C6-C5	-7.29	112.67	122.64
19	1	314	LUT	C28-C29-C30	-7.28	107.56	119.01
19	1	314	LUT	C39-C29-C30	-7.27	111.04	122.82
18	1	305	CHL	O2D-CGD-CBD	7.25	118.91	110.95
19	4	316	LUT	C26-C27-C28	-7.25	113.30	124.58
20	2	315	XAT	C39-C29-C30	-7.24	111.08	122.82
20	1	315	XAT	C39-C29-C30	-7.23	111.11	122.82
20	3	615	XAT	C39-C29-C30	-7.21	111.13	122.82
17	L	203	CLA	C4A-NA-C1A	7.19	109.96	106.68
20	1	315	XAT	C26-C27-C28	-7.19	110.80	125.99
20	3	615	XAT	C26-C27-C28	-7.18	110.81	125.99
20	2	315	XAT	C7-C8-C9	-7.18	114.39	125.53
17	B	840	CLA	C4A-NA-C1A	7.17	109.95	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	315	XAT	C26-C27-C28	-7.17	110.83	125.99
20	1	315	XAT	C7-C8-C9	-7.17	114.41	125.53
20	3	615	XAT	C7-C8-C9	-7.15	114.44	125.53
19	1	314	LUT	C35-C15-C14	-7.12	108.95	123.52
19	2	314	LUT	C1-C6-C5	-7.09	112.94	122.64
19	3	614	LUT	C8-C7-C6	-7.05	108.17	127.00
20	4	317	XAT	C32-C33-C34	-7.02	107.97	119.01
17	A	831	CLA	C4A-NA-C1A	7.00	109.87	106.68
19	3	614	LUT	C28-C29-C30	-6.97	108.04	119.01
17	3	610	CLA	C4A-NA-C1A	6.94	109.84	106.68
19	2	314	LUT	C15-C35-C34	-6.92	109.35	123.52
20	4	317	XAT	C28-C29-C30	-6.88	108.19	119.01
19	1	314	LUT	C15-C35-C34	-6.87	109.47	123.52
17	B	806	CLA	C4A-NA-C1A	6.87	109.81	106.68
20	4	317	XAT	O24-C25-C38	-6.85	107.39	115.05
19	4	316	LUT	C7-C8-C9	-6.82	116.14	126.23
19	3	614	LUT	C12-C13-C14	-6.81	108.30	119.01
17	B	831	CLA	C4A-NA-C1A	6.78	109.77	106.68
18	4	315	CHL	O2D-CGD-CBD	6.78	118.40	110.95
20	2	315	XAT	C20-C13-C14	-6.78	111.83	122.82
20	1	315	XAT	C20-C13-C14	-6.78	111.84	122.82
20	3	615	XAT	C20-C13-C14	-6.78	111.84	122.82
18	4	305	CHL	CBC-CAC-C3C	-6.77	103.19	112.87
19	2	314	LUT	C39-C29-C30	-6.70	111.96	122.82
17	B	808	CLA	C4A-NA-C1A	6.68	109.73	106.68
18	4	301	CHL	CHA-C1A-C2A	-6.67	117.64	133.31
17	B	822	CLA	C4A-NA-C1A	6.66	109.72	106.68
20	4	317	XAT	C15-C35-C34	-6.66	109.89	123.52
27	B	843	PQN	C9-C10-C1	-6.66	110.37	120.10
17	3	613	CLA	C4A-NA-C1A	6.66	109.72	106.68
18	2	306	CHL	O2D-CGD-CBD	6.65	118.26	110.95
20	2	315	XAT	C35-C15-C14	-6.63	109.95	123.52
20	1	315	XAT	C35-C15-C14	-6.62	109.97	123.52
19	4	316	LUT	C39-C29-C30	-6.62	112.09	122.82
20	3	615	XAT	C35-C15-C14	-6.62	109.98	123.52
19	2	314	LUT	C8-C7-C6	-6.61	109.34	127.00
27	B	843	PQN	O4-C4-C5	-6.61	111.00	121.57
19	3	614	LUT	C40-C33-C34	-6.59	112.14	122.82
19	3	614	LUT	C39-C29-C30	-6.58	112.15	122.82
17	B	811	CLA	C4A-NA-C1A	6.58	109.68	106.68
17	3	611	CLA	C4A-NA-C1A	6.57	109.68	106.68
17	A	826	CLA	C4A-NA-C1A	6.54	109.66	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	315	XAT	C19-C9-C10	-6.51	112.26	122.82
17	G	104	CLA	C4A-NA-C1A	6.51	109.65	106.68
20	1	315	XAT	C19-C9-C10	-6.50	112.28	122.82
17	K	202	CLA	C4A-NA-C1A	6.48	109.64	106.68
20	3	615	XAT	C19-C9-C10	-6.48	112.32	122.82
19	2	314	LUT	C20-C13-C14	-6.47	112.33	122.82
27	B	843	PQN	O1-C1-C2	-6.46	111.95	120.45
17	1	307	CLA	C4A-NA-C1A	6.45	109.62	106.68
17	4	304	CLA	C4A-NA-C1A	6.44	109.62	106.68
19	3	614	LUT	C35-C15-C14	-6.44	110.35	123.52
17	A	829	CLA	C4A-NA-C1A	6.41	109.60	106.68
17	3	612	CLA	C4A-NA-C1A	6.37	109.59	106.68
17	L	202	CLA	C4A-NA-C1A	6.37	109.59	106.68
19	4	316	LUT	C1-C6-C5	-6.36	113.95	122.64
27	A	842	PQN	C11-C3-C4	-6.35	111.89	118.58
17	G	103	CLA	C4A-NA-C1A	6.35	109.58	106.68
17	A	814	CLA	C4A-NA-C1A	6.35	109.58	106.68
19	2	314	LUT	C27-C28-C29	-6.34	112.69	126.32
17	A	819	CLA	C4A-NA-C1A	6.33	109.57	106.68
17	K	201	CLA	C4A-NA-C1A	6.33	109.57	106.68
17	A	822	CLA	C4A-NA-C1A	6.33	109.56	106.68
17	A	843	CLA	C4A-NA-C1A	6.33	109.56	106.68
17	A	836	CLA	C4A-NA-C1A	6.32	109.56	106.68
17	B	823	CLA	C4A-NA-C1A	6.32	109.56	106.68
18	4	305	CHL	CHA-C1A-C2A	-6.31	118.50	133.31
17	A	828	CLA	C4A-NA-C1A	6.30	109.55	106.68
17	3	603	CLA	C4A-NA-C1A	6.29	109.55	106.68
20	4	317	XAT	C19-C9-C10	-6.29	112.62	122.82
17	A	824	CLA	C4A-NA-C1A	6.28	109.55	106.68
20	3	615	XAT	C10-C11-C12	-6.26	105.07	123.20
20	1	315	XAT	C10-C11-C12	-6.25	105.09	123.20
20	2	315	XAT	C10-C11-C12	-6.23	105.14	123.20
17	A	801	CLA	O2D-CGD-CBD	6.20	122.07	111.23
17	A	853	CLA	C4A-NA-C1A	6.19	109.50	106.68
17	B	825	CLA	C4A-NA-C1A	6.18	109.50	106.68
17	2	302	CLA	C4A-NA-C1A	6.17	109.49	106.68
17	1	308	CLA	C4A-NA-C1A	6.16	109.49	106.68
19	1	314	LUT	C30-C31-C32	-6.15	105.37	123.20
18	4	306	CHL	CHA-C1A-C2A	-6.15	118.86	133.31
17	A	830	CLA	C4A-NA-C1A	6.15	109.49	106.68
19	2	314	LUT	C30-C31-C32	-6.15	105.39	123.20
18	3	601	CHL	CHA-C1A-C2A	-6.14	118.89	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	312	CLA	C4A-NA-C1A	6.13	109.48	106.68
17	3	604	CLA	C4A-NA-C1A	6.12	109.47	106.68
17	A	808	CLA	C4A-NA-C1A	6.12	109.47	106.68
17	B	803	CLA	C4A-NA-C1A	6.11	109.47	106.68
20	4	317	XAT	O24-C25-C24	-6.11	107.77	113.49
18	2	313	CHL	CHA-C1A-C2A	-6.10	118.98	133.31
17	J	103	CLA	C4A-NA-C1A	6.08	109.45	106.68
17	A	837	CLA	C4A-NA-C1A	6.05	109.44	106.68
17	G	105	CLA	C4A-NA-C1A	6.05	109.44	106.68
18	4	306	CHL	O2D-CGD-CBD	6.04	117.59	110.95
17	2	311	CLA	C4A-NA-C1A	6.03	109.43	106.68
17	A	823	CLA	C4A-NA-C1A	6.03	109.43	106.68
17	4	313	CLA	C4A-NA-C1A	6.03	109.43	106.68
17	A	853	CLA	C1-C2-C3	-6.03	116.33	126.20
19	3	614	LUT	C20-C13-C14	-6.02	113.06	122.82
19	3	614	LUT	C19-C9-C10	-6.02	113.07	122.82
19	2	314	LUT	C38-C25-C24	-6.01	109.14	123.36
19	1	314	LUT	C10-C11-C12	-6.00	105.82	123.20
27	B	843	PQN	C11-C3-C2	-5.99	114.62	124.89
19	4	316	LUT	C30-C31-C32	-5.98	105.86	123.20
17	2	309	CLA	C4A-NA-C1A	5.98	109.41	106.68
17	A	821	CLA	C4A-NA-C1A	5.98	109.41	106.68
27	A	842	PQN	C11-C12-C13	-5.97	116.54	126.83
19	1	314	LUT	C40-C33-C34	-5.97	113.15	122.82
19	2	314	LUT	C40-C33-C34	-5.96	113.15	122.82
18	4	307	CHL	CHA-C1A-C2A	-5.96	119.32	133.31
27	B	843	PQN	C7-C8-C9	-5.95	112.90	120.24
18	2	305	CHL	CHA-C1A-C2A	-5.95	119.34	133.31
17	B	841	CLA	C4A-NA-C1A	5.94	109.39	106.68
17	A	833	CLA	C4A-NA-C1A	5.93	109.39	106.68
18	2	306	CHL	CHA-C1A-C2A	-5.93	119.39	133.31
27	A	842	PQN	C7-C8-C9	-5.92	112.94	120.24
18	2	304	CHL	CHA-C1A-C2A	-5.91	119.43	133.31
17	A	801	CLA	C4A-NA-C1A	5.90	109.37	106.68
17	1	303	CLA	C4A-NA-C1A	5.89	109.37	106.68
17	A	818	CLA	C4A-NA-C1A	5.85	109.35	106.68
17	A	841	CLA	C4A-NA-C1A	5.85	109.35	106.68
17	B	837	CLA	C4A-NA-C1A	5.84	109.34	106.68
17	B	813	CLA	C4A-NA-C1A	5.83	109.34	106.68
17	A	817	CLA	C4A-NA-C1A	5.82	109.34	106.68
18	3	607	CHL	CHA-C1A-C2A	-5.81	119.66	133.31
17	B	842	CLA	C4A-NA-C1A	5.81	109.33	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	314	LUT	C19-C9-C10	-5.80	113.42	122.82
17	A	802	CLA	C4A-NA-C1A	5.78	109.32	106.68
20	4	317	XAT	C6-C7-C8	-5.77	113.78	125.99
19	3	614	LUT	C38-C25-C24	-5.77	109.71	123.36
17	L	204	CLA	C4A-NA-C1A	5.76	109.31	106.68
17	2	303	CLA	C4A-NA-C1A	5.76	109.31	106.68
17	1	304	CLA	C4A-NA-C1A	5.76	109.31	106.68
19	1	314	LUT	C20-C13-C14	-5.74	113.51	122.82
17	A	815	CLA	C4A-NA-C1A	5.74	109.30	106.68
17	B	828	CLA	C4A-NA-C1A	5.71	109.28	106.68
17	A	805	CLA	C4A-NA-C1A	5.71	109.28	106.68
19	4	316	LUT	C40-C33-C34	-5.70	113.58	122.82
17	3	609	CLA	C4A-NA-C1A	5.69	109.28	106.68
17	3	606	CLA	C4A-NA-C1A	5.67	109.27	106.68
27	A	842	PQN	O4-C4-C5	-5.67	112.51	121.57
17	A	834	CLA	C4A-NA-C1A	5.66	109.26	106.68
26	4	323	DGD	C1D-O6D-C5D	-5.65	102.68	113.72
19	3	614	LUT	C30-C31-C32	-5.65	106.84	123.20
17	F	304	CLA	C4A-NA-C1A	5.64	109.25	106.68
19	4	316	LUT	C11-C12-C13	-5.63	110.93	126.36
27	A	842	PQN	C15-C13-C12	-5.63	108.53	121.17
17	3	605	CLA	C4A-NA-C1A	5.63	109.25	106.68
17	4	311	CLA	C4A-NA-C1A	5.62	109.24	106.68
27	B	843	PQN	O1-C1-C10	-5.62	112.59	121.57
20	4	317	XAT	C10-C11-C12	-5.62	106.93	123.20
17	A	827	CLA	C4A-NA-C1A	5.61	109.24	106.68
17	B	815	CLA	C4A-NA-C1A	5.60	109.23	106.68
27	B	843	PQN	C15-C13-C12	-5.57	108.66	121.17
17	B	824	CLA	C4A-NA-C1A	5.57	109.22	106.68
17	A	825	CLA	C4A-NA-C1A	5.57	109.22	106.68
27	A	842	PQN	C7-C6-C5	-5.56	109.75	119.80
27	A	842	PQN	C11-C3-C2	-5.56	115.36	124.89
17	A	832	CLA	C4A-NA-C1A	5.55	109.21	106.68
17	A	810	CLA	C4A-NA-C1A	5.53	109.20	106.68
17	3	608	CLA	C4A-NA-C1A	5.50	109.19	106.68
19	4	316	LUT	C38-C25-C24	-5.49	110.37	123.36
19	3	614	LUT	C10-C11-C12	-5.49	107.31	123.20
17	B	814	CLA	C4A-NA-C1A	5.48	109.18	106.68
27	A	842	PQN	C2M-C2-C3	-5.48	115.44	124.45
17	A	809	CLA	C4A-NA-C1A	5.47	109.17	106.68
17	1	310	CLA	C4A-NA-C1A	5.47	109.17	106.68
17	2	308	CLA	C4A-NA-C1A	5.46	109.17	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	314	LUT	C11-C12-C13	-5.45	111.42	126.36
19	4	316	LUT	C10-C11-C12	-5.45	107.41	123.20
17	A	812	CLA	C4A-NA-C1A	5.45	109.17	106.68
25	F	305	HTG	O5-C1-C2	-5.44	102.81	110.32
17	1	313	CLA	C4A-NA-C1A	5.43	109.16	106.68
18	4	315	CHL	CHA-C1A-C2A	-5.41	120.60	133.31
19	2	314	LUT	C31-C32-C33	-5.41	111.53	126.36
19	4	316	LUT	C20-C13-C14	-5.40	114.07	122.82
17	2	310	CLA	C4A-NA-C1A	5.39	109.14	106.68
17	B	827	CLA	C4A-NA-C1A	5.38	109.13	106.68
19	2	314	LUT	C19-C9-C10	-5.34	114.16	122.82
19	3	614	LUT	C31-C32-C33	-5.33	111.75	126.36
27	B	843	PQN	C8-C7-C6	-5.33	113.66	120.24
17	A	811	CLA	C4A-NA-C1A	5.33	109.11	106.68
17	4	312	CLA	C4A-NA-C1A	5.32	109.11	106.68
17	A	816	CLA	C4A-NA-C1A	5.31	109.10	106.68
17	B	818	CLA	O2D-CGD-O1D	-5.31	113.51	123.85
20	4	317	XAT	C31-C32-C33	-5.31	111.81	126.36
27	A	842	PQN	C8-C9-C10	-5.29	110.23	119.80
19	3	614	LUT	C11-C12-C13	-5.29	111.85	126.36
17	A	835	CLA	C4A-NA-C1A	5.29	109.09	106.68
19	2	314	LUT	C10-C11-C12	-5.27	107.94	123.20
17	B	834	CLA	C4A-NA-C1A	5.26	109.08	106.68
18	4	301	CHL	O2D-CGD-CBD	5.26	116.73	110.95
17	4	308	CLA	C4A-NA-C1A	5.26	109.08	106.68
17	1	302	CLA	C4A-NA-C1A	5.25	109.08	106.68
18	1	305	CHL	CHA-C1A-C2A	-5.25	120.97	133.31
18	4	301	CHL	CBC-CAC-C3C	-5.23	105.39	112.87
17	3	602	CLA	C4A-NA-C1A	5.22	109.06	106.68
19	3	614	LUT	C4-C5-C6	-5.22	110.04	120.76
17	4	314	CLA	C4A-NA-C1A	5.21	109.06	106.68
19	2	314	LUT	C11-C12-C13	-5.21	112.09	126.36
17	1	311	CLA	C4A-NA-C1A	5.21	109.05	106.68
20	3	615	XAT	C18-C5-C4	5.17	120.05	114.24
20	1	315	XAT	C18-C5-C4	5.16	120.04	114.24
20	2	315	XAT	C18-C5-C4	5.16	120.03	114.24
20	3	615	XAT	C20-C13-C12	-5.14	110.24	118.09
20	1	315	XAT	C20-C13-C12	-5.13	110.25	118.09
20	2	315	XAT	C20-C13-C12	-5.13	110.25	118.09
19	1	314	LUT	C38-C25-C24	-5.13	111.22	123.36
17	A	806	CLA	C4A-NA-C1A	5.13	109.02	106.68
17	A	813	CLA	C4A-NA-C1A	5.12	109.02	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	843	PQN	C14-C13-C12	-5.11	110.51	123.63
17	A	820	CLA	C4A-NA-C1A	5.09	109.00	106.68
17	2	319	CLA	C4A-NA-C1A	5.07	108.99	106.68
19	2	314	LUT	C4-C5-C6	-5.03	110.43	120.76
19	1	314	LUT	C4-C5-C6	-5.02	110.45	120.76
17	J	101	CLA	O2D-CGD-O1D	-5.02	114.08	123.85
20	3	615	XAT	C30-C31-C32	-5.01	108.68	123.20
27	B	843	PQN	C5-C10-C1	-5.01	115.33	120.71
20	1	315	XAT	C30-C31-C32	-5.01	108.69	123.20
20	2	315	XAT	C30-C31-C32	-5.00	108.72	123.20
17	4	310	CLA	C4A-NA-C1A	4.99	108.96	106.68
17	B	827	CLA	O1D-CGD-CBD	4.99	134.36	124.52
17	F	306	CLA	C4A-NA-C1A	4.97	108.95	106.68
17	B	836	CLA	C4A-NA-C1A	4.96	108.94	106.68
19	3	614	LUT	C19-C9-C8	-4.96	110.52	118.09
17	4	303	CLA	C1-C2-C3	-4.95	118.09	126.20
17	B	805	CLA	C4A-NA-C1A	4.94	108.93	106.68
17	A	853	CLA	O2D-CGD-O1D	-4.93	114.25	123.85
17	1	306	CLA	C4A-NA-C1A	4.93	108.93	106.68
19	4	316	LUT	C19-C9-C10	-4.90	114.88	122.82
17	A	804	CLA	C4A-NA-C1A	4.87	108.90	106.68
19	1	314	LUT	C7-C6-C5	-4.87	110.34	121.56
17	1	309	CLA	C4A-NA-C1A	4.86	108.89	106.68
17	B	817	CLA	C4A-NA-C1A	4.85	108.89	106.68
18	4	307	CHL	O2D-CGD-CBD	4.83	116.25	110.95
26	4	323	DGD	O2G-C1B-C2B	4.82	121.91	111.48
17	F	307	CLA	C4A-NA-C1A	4.81	108.87	106.68
20	2	315	XAT	C31-C32-C33	-4.80	113.19	126.36
17	B	838	CLA	O1D-CGD-CBD	4.80	133.99	124.52
17	A	853	CLA	O2A-CGA-O1A	-4.80	111.62	123.63
20	1	315	XAT	C31-C32-C33	-4.80	113.21	126.36
19	1	314	LUT	C31-C32-C33	-4.79	113.23	126.36
20	3	615	XAT	C31-C32-C33	-4.79	113.23	126.36
17	B	838	CLA	O2D-CGD-O1D	-4.78	114.54	123.85
17	B	804	CLA	C4A-NA-C1A	4.77	108.86	106.68
18	1	305	CHL	C1B-CHB-C4A	4.77	124.39	121.32
17	1	312	CLA	C4A-NA-C1A	4.76	108.85	106.68
19	4	316	LUT	C7-C6-C5	-4.74	110.64	121.56
17	A	827	CLA	C1-C2-C3	-4.74	118.44	126.20
17	A	839	CLA	C3B-C4B-NB	-4.71	106.32	110.53
20	4	317	XAT	C40-C33-C34	-4.69	115.22	122.82
17	4	310	CLA	O2D-CGD-O1D	-4.69	114.72	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	317	XAT	C38-C25-C24	4.67	119.49	114.24
17	A	803	CLA	C4A-NA-C1A	4.65	108.80	106.68
17	B	832	CLA	C4A-NA-C1A	4.65	108.80	106.68
19	1	314	LUT	C20-C13-C12	-4.64	110.99	118.09
17	B	812	CLA	C4A-NA-C1A	4.63	108.79	106.68
17	B	837	CLA	C1-C2-C3	-4.63	118.61	126.20
17	B	839	CLA	O2D-CGD-O1D	-4.63	114.84	123.85
17	A	853	CLA	CED-O2D-CGD	-4.61	105.46	115.92
17	B	831	CLA	O2D-CGD-CBD	4.58	119.24	111.23
20	3	615	XAT	C39-C29-C28	-4.53	111.16	118.09
17	B	802	CLA	C3B-C4B-NB	-4.53	106.48	110.53
17	A	807	CLA	C4A-NA-C1A	4.53	108.75	106.68
20	1	315	XAT	C39-C29-C28	-4.53	111.17	118.09
20	4	317	XAT	C30-C31-C32	-4.51	110.14	123.20
17	B	838	CLA	C4A-NA-C1A	4.50	108.73	106.68
17	B	819	CLA	O2D-CGD-O1D	-4.50	115.08	123.85
20	2	315	XAT	C39-C29-C28	-4.50	111.21	118.09
17	B	827	CLA	O2D-CGD-O1D	-4.49	115.10	123.85
20	1	315	XAT	C19-C9-C8	-4.48	111.24	118.09
27	B	843	PQN	C2M-C2-C1	-4.48	108.43	116.68
20	3	615	XAT	C19-C9-C8	-4.48	111.25	118.09
17	B	809	CLA	C4A-NA-C1A	4.48	108.72	106.68
17	B	830	CLA	C4A-NA-C1A	4.47	108.72	106.68
20	2	315	XAT	C19-C9-C8	-4.47	111.26	118.09
17	F	304	CLA	O2A-CGA-O1A	-4.43	112.54	123.63
22	A	844	LHG	O4-P-O5	4.43	133.05	112.44
19	2	314	LUT	C19-C9-C8	-4.43	111.32	118.09
17	4	302	CLA	C4A-NA-C1A	4.43	108.70	106.68
19	2	314	LUT	C7-C6-C5	-4.42	111.37	121.56
22	2	317	LHG	O4-P-O5	4.42	133.01	112.44
17	A	838	CLA	C4A-NA-C1A	4.42	108.69	106.68
20	2	315	XAT	C38-C25-C24	4.41	119.20	114.24
20	3	615	XAT	C38-C25-C24	4.41	119.20	114.24
17	2	301	CLA	C4A-NA-C1A	4.41	108.69	106.68
17	A	840	CLA	C1-C2-C3	-4.41	118.97	126.20
20	1	315	XAT	C38-C25-C24	4.41	119.19	114.24
18	4	305	CHL	C4-C3-C5	4.40	122.87	115.23
17	B	839	CLA	O2A-CGA-O1A	-4.37	112.70	123.63
22	G	102	LHG	O4-P-O5	4.37	132.76	112.44
22	F	302	LHG	O4-P-O5	4.36	132.75	112.44
17	2	307	CLA	C4A-NA-C1A	4.36	108.67	106.68
19	3	614	LUT	C40-C33-C32	-4.35	111.45	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	838	CLA	C1-C2-C3	-4.34	119.08	126.20
20	1	315	XAT	C11-C12-C13	-4.34	114.46	126.36
20	3	615	XAT	C11-C12-C13	-4.34	114.48	126.36
20	2	315	XAT	C18-C5-C6	-4.33	115.17	122.30
20	2	315	XAT	C11-C12-C13	-4.33	114.48	126.36
18	2	304	CHL	CBC-CAC-C3C	-4.32	106.68	112.87
20	3	615	XAT	C18-C5-C6	-4.31	115.21	122.30
22	A	845	LHG	O4-P-O5	4.30	132.47	112.44
20	1	315	XAT	C18-C5-C6	-4.30	115.22	122.30
21	J	105	BCR	C2-C1-C6	4.29	116.66	110.44
19	4	316	LUT	C31-C32-C33	-4.28	114.63	126.36
24	B	852	LMG	O1-C1-C2	4.28	114.77	108.27
17	A	838	CLA	O2D-CGD-O1D	-4.27	115.53	123.85
18	1	305	CHL	CBC-CAC-C3C	-4.26	106.77	112.87
17	4	314	CLA	O2D-CGD-O1D	-4.26	115.56	123.85
17	4	309	CLA	C4A-NA-C1A	4.22	108.60	106.68
17	4	303	CLA	C4A-NA-C1A	4.21	108.60	106.68
22	1	317	LHG	O4-P-O5	4.21	132.04	112.44
22	B	801	LHG	O4-P-O5	4.19	131.93	112.44
17	B	807	CLA	C4A-NA-C1A	4.19	108.59	106.68
21	B	847	BCR	C27-C26-C25	4.19	128.36	122.70
27	B	843	PQN	C7-C6-C5	-4.18	112.24	119.80
24	4	320	LMG	O6-C5-C4	4.18	117.23	109.70
17	A	803	CLA	O2D-CGD-O1D	-4.18	115.71	123.85
19	1	314	LUT	C19-C9-C8	-4.17	111.71	118.09
17	4	308	CLA	O2D-CGD-CBD	4.16	118.51	111.23
27	B	843	PQN	O4-C4-C3	-4.16	113.99	120.67
19	3	614	LUT	C20-C13-C12	-4.16	111.74	118.09
18	4	301	CHL	O2A-CGA-CBA	4.16	124.51	111.83
17	B	816	CLA	O1D-CGD-CBD	4.15	132.70	124.52
17	A	836	CLA	O2D-CGD-O1D	-4.12	115.82	123.85
18	3	601	CHL	O2D-CGD-O1D	-4.12	115.83	123.85
17	B	839	CLA	C4A-NA-C1A	4.11	108.56	106.68
17	F	307	CLA	CAA-C2A-C3A	-4.10	101.92	113.00
25	B	851	HTG	O5-C1-C2	4.09	115.96	110.32
18	4	301	CHL	O2D-CGD-O1D	-4.09	115.89	123.85
17	B	810	CLA	C4A-NA-C1A	4.09	108.55	106.68
19	2	314	LUT	C39-C29-C28	-4.08	111.86	118.09
19	4	316	LUT	C4-C5-C6	-4.08	112.38	120.76
17	J	101	CLA	C4A-NA-C1A	4.07	108.54	106.68
26	4	323	DGD	O6D-C5D-C6D	4.06	114.75	106.69
26	B	850	DGD	O5D-C6D-C5D	-4.06	100.26	109.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	301	CHL	C1-C2-C3	-4.06	119.55	126.20
17	B	818	CLA	C3B-C4B-NB	-4.06	106.91	110.53
17	A	817	CLA	O2D-CGD-O1D	-4.05	115.95	123.85
18	4	301	CHL	CMA-C3A-C4A	-4.05	105.88	114.61
17	B	816	CLA	C4A-NA-C1A	4.05	108.53	106.68
21	3	616	BCR	C2-C1-C6	4.04	116.31	110.44
17	B	819	CLA	C4A-NA-C1A	4.04	108.52	106.68
17	B	831	CLA	O2D-CGD-O1D	-4.02	116.02	123.85
17	A	839	CLA	C4A-NA-C1A	4.02	108.51	106.68
17	J	101	CLA	O2D-CGD-CBD	4.00	118.22	111.23
19	3	614	LUT	C39-C29-C28	-3.98	112.01	118.09
17	B	832	CLA	O2D-CGD-O1D	-3.97	116.11	123.85
17	1	301	CLA	C4A-NA-C1A	3.97	108.49	106.68
17	A	839	CLA	C1-C2-C3	-3.94	119.73	126.20
20	4	317	XAT	O24-C26-C27	-3.93	105.62	116.88
27	B	843	PQN	C10-C5-C4	-3.91	116.51	120.71
17	F	304	CLA	C1-O2A-CGA	-3.89	107.23	116.65
17	B	818	CLA	O2D-CGD-CBD	3.89	118.03	111.23
17	A	829	CLA	O2D-CGD-O1D	-3.89	116.28	123.85
17	A	838	CLA	O2D-CGD-CBD	3.89	118.02	111.23
27	A	842	PQN	O1-C1-C10	-3.88	115.37	121.57
17	A	840	CLA	C3B-C4B-NB	-3.88	107.07	110.53
20	4	317	XAT	C18-C5-C4	3.87	118.58	114.24
17	A	825	CLA	O2D-CGD-O1D	-3.86	116.33	123.85
24	F	309	LMG	O1-C1-C2	-3.86	102.41	108.27
17	1	301	CLA	C3B-C4B-NB	-3.86	107.08	110.53
17	A	805	CLA	C3B-C4B-NB	-3.86	107.08	110.53
17	B	837	CLA	C3B-C4B-NB	-3.86	107.09	110.53
17	B	806	CLA	O2D-CGD-O1D	-3.86	116.34	123.85
18	2	313	CHL	O1D-CGD-CBD	-3.85	118.88	124.72
17	F	307	CLA	C3B-C4B-NB	-3.84	107.10	110.53
19	4	316	LUT	C20-C13-C12	-3.83	112.23	118.09
21	J	105	BCR	C29-C30-C25	3.82	115.99	110.44
17	B	825	CLA	CAA-C2A-C3A	-3.81	102.69	113.00
17	B	807	CLA	O2D-CGD-O1D	-3.81	116.43	123.85
17	B	835	CLA	C4A-NA-C1A	3.80	108.41	106.68
17	B	839	CLA	CAA-C2A-C1A	-3.80	99.51	111.97
17	A	804	CLA	C3B-C4B-NB	-3.80	107.14	110.53
17	A	832	CLA	O2D-CGD-O1D	-3.80	116.46	123.85
19	1	314	LUT	C40-C33-C32	-3.79	112.30	118.09
25	F	310	HTG	C3-C4-C5	3.77	117.07	110.23
21	4	318	BCR	C2-C1-C6	3.75	115.89	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	320	LMG	O6-C1-O1	-3.75	101.19	110.04
19	3	614	LUT	C7-C6-C5	-3.75	112.92	121.56
17	2	319	CLA	O2D-CGD-O1D	-3.74	116.56	123.85
27	A	842	PQN	C8-C7-C6	-3.73	115.64	120.24
19	1	314	LUT	C39-C29-C28	-3.73	112.39	118.09
17	4	310	CLA	CAA-C2A-C3A	-3.73	102.92	113.00
17	B	803	CLA	O2D-CGD-O1D	-3.73	116.60	123.85
19	4	316	LUT	C18-C5-C4	-3.72	107.58	114.42
24	F	309	LMG	O6-C1-O1	-3.72	101.26	110.04
26	B	850	DGD	O6D-C1D-O3G	-3.66	101.39	110.04
17	A	840	CLA	C4A-NA-C1A	3.65	108.34	106.68
17	B	822	CLA	O1D-CGD-CBD	3.65	131.71	124.52
17	2	319	CLA	C3B-C4B-NB	-3.64	107.28	110.53
25	B	851	HTG	C1'-S1-C1	3.64	108.32	100.45
25	B	851	HTG	C1-C2-C3	3.62	117.63	110.55
21	L	201	BCR	C15-C16-C17	-3.62	116.11	123.52
18	4	301	CHL	O2A-CGA-O1A	-3.62	114.57	123.63
17	A	808	CLA	C3B-C4B-NB	-3.61	107.30	110.53
18	2	306	CHL	C1-C2-C3	-3.61	120.92	126.76
17	F	304	CLA	C1-C2-C3	-3.61	120.28	126.20
17	B	829	CLA	C4A-NA-C1A	3.61	108.33	106.68
21	J	104	BCR	C27-C26-C25	3.61	127.58	122.70
17	4	302	CLA	O2A-CGA-O1A	-3.60	114.62	123.63
17	B	827	CLA	CED-O2D-CGD	-3.60	107.75	115.92
20	4	317	XAT	C11-C12-C13	-3.58	116.54	126.36
17	4	308	CLA	O2D-CGD-O1D	-3.57	116.89	123.85
17	A	802	CLA	O2D-CGD-O1D	-3.57	116.90	123.85
17	G	105	CLA	O2D-CGD-O1D	-3.56	116.91	123.85
17	B	835	CLA	C3B-C4B-NB	-3.55	107.36	110.53
26	4	323	DGD	C1E-O6E-C5E	3.54	120.64	113.72
17	G	103	CLA	O2D-CGD-O1D	-3.54	116.95	123.85
17	L	204	CLA	O2D-CGD-O1D	-3.54	116.97	123.85
21	A	846	BCR	C15-C14-C13	-3.54	122.32	127.28
17	2	311	CLA	O2D-CGD-O1D	-3.53	116.97	123.85
17	B	833	CLA	C4A-NA-C1A	3.53	108.29	106.68
17	4	311	CLA	O2D-CGD-O1D	-3.52	116.99	123.85
17	A	829	CLA	O2D-CGD-CBD	3.52	117.38	111.23
24	4	319	LMG	O1-C1-C2	-3.50	102.95	108.27
17	4	310	CLA	CAC-C3C-C4C	3.49	129.34	124.79
17	A	816	CLA	O2D-CGD-O1D	-3.49	117.05	123.85
17	A	853	CLA	C1-O2A-CGA	-3.49	108.20	116.65
27	A	842	PQN	C14-C13-C12	-3.49	114.67	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	843	PQN	C8-C9-C10	-3.48	113.51	119.80
17	A	838	CLA	O2A-CGA-O1A	-3.48	114.93	123.63
17	1	310	CLA	C3B-C4B-NB	-3.47	107.43	110.53
17	A	821	CLA	O2D-CGD-O1D	-3.46	117.11	123.85
21	A	850	BCR	C33-C5-C6	-3.46	120.71	124.48
17	B	842	CLA	O2A-CGA-O1A	-3.45	114.99	123.63
17	A	803	CLA	O1D-CGD-CBD	3.45	131.32	124.52
17	A	840	CLA	O2D-CGD-O1D	-3.45	117.13	123.85
18	4	307	CHL	C1-C2-C3	-3.45	121.19	126.76
20	4	317	XAT	O4-C5-C18	-3.44	111.21	115.05
17	B	834	CLA	CHB-C4A-NA	3.42	129.34	124.40
17	B	812	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
17	1	311	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
17	A	808	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
17	B	833	CLA	CMB-C2B-C1B	-3.41	120.22	125.42
24	4	319	LMG	O2-C2-C1	-3.41	101.95	110.08
17	B	826	CLA	C1-C2-C3	-3.41	120.61	126.20
17	A	827	CLA	O1D-CGD-CBD	3.41	131.24	124.52
21	B	847	BCR	C40-C30-C39	-3.40	98.91	108.63
17	B	809	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
17	A	841	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
17	B	820	CLA	C3B-C4B-NB	-3.38	107.51	110.53
18	1	305	CHL	CMA-C3A-C4A	-3.38	107.33	114.61
17	B	823	CLA	C1-C2-C3	-3.38	120.67	126.20
20	3	615	XAT	C40-C33-C32	-3.37	112.94	118.09
24	F	309	LMG	O1-C7-C8	-3.37	102.62	110.82
17	B	839	CLA	CAA-C2A-C3A	-3.37	103.89	113.00
17	A	801	CLA	C1D-ND-C4D	-3.37	103.95	106.31
17	3	602	CLA	C3B-C4B-NB	-3.37	107.52	110.53
17	4	313	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
17	A	809	CLA	C3B-C4B-NB	-3.36	107.53	110.53
17	B	825	CLA	C3B-C4B-NB	-3.36	107.53	110.53
17	B	839	CLA	CHB-C4A-NA	3.36	129.24	124.40
26	4	323	DGD	O5D-C1E-C2E	3.36	113.37	108.27
17	A	807	CLA	C3B-C4B-NB	-3.36	107.53	110.53
17	J	103	CLA	O2D-CGD-O1D	-3.35	117.32	123.85
17	B	814	CLA	O2D-CGD-CBD	3.35	117.09	111.23
20	1	315	XAT	C40-C33-C32	-3.35	112.97	118.09
20	2	315	XAT	C40-C33-C32	-3.35	112.97	118.09
17	B	817	CLA	CMB-C2B-C1B	-3.34	120.33	125.42
17	A	835	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
17	4	308	CLA	O2A-CGA-O1A	-3.33	115.30	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	304	CLA	O1D-CGD-CBD	3.33	131.08	124.52
17	A	805	CLA	O2D-CGD-O1D	-3.32	117.38	123.85
17	B	808	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
21	B	849	BCR	C27-C26-C25	3.32	127.18	122.70
17	K	202	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
17	B	814	CLA	C3B-C4B-NB	-3.31	107.57	110.53
20	3	615	XAT	C38-C25-C26	-3.31	116.85	122.30
17	B	823	CLA	CMB-C2B-C1B	-3.31	120.38	125.42
17	A	808	CLA	O2A-CGA-O1A	-3.31	115.36	123.63
18	3	601	CHL	O1D-CGD-CBD	-3.30	119.71	124.72
17	2	307	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
21	A	850	BCR	C24-C23-C22	-3.30	121.36	126.23
20	1	315	XAT	C38-C25-C26	-3.29	116.88	122.30
17	1	312	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
19	2	314	LUT	C40-C33-C32	-3.29	113.06	118.09
17	A	801	CLA	OBD-CAD-C3D	3.29	136.10	128.42
17	A	840	CLA	O2A-CGA-O1A	-3.28	115.41	123.63
17	A	836	CLA	C3B-C4B-NB	-3.28	107.60	110.53
27	A	842	PQN	C6-C5-C4	-3.28	115.31	120.10
20	2	315	XAT	C38-C25-C26	-3.28	116.91	122.30
17	A	819	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
17	A	838	CLA	C3B-C4B-NB	-3.28	107.61	110.53
17	J	101	CLA	C3B-C4B-NB	-3.28	107.61	110.53
17	B	813	CLA	O2D-CGD-O1D	-3.27	117.47	123.85
17	4	314	CLA	O2A-CGA-O1A	-3.27	115.44	123.63
17	A	817	CLA	C3B-C4B-NB	-3.27	107.61	110.53
17	4	303	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
17	B	826	CLA	O2A-CGA-O1A	-3.27	115.46	123.63
17	F	306	CLA	C3B-C4B-NB	-3.26	107.62	110.53
19	4	316	LUT	C21-C26-C27	-3.25	109.08	112.83
21	J	104	BCR	C2-C1-C6	3.25	115.16	110.44
21	A	850	BCR	C2-C1-C6	3.25	115.16	110.44
21	B	847	BCR	C15-C14-C13	-3.25	122.72	127.28
17	A	823	CLA	O2D-CGD-O1D	-3.24	117.53	123.85
17	A	810	CLA	O2D-CGD-O1D	-3.24	117.53	123.85
17	B	825	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
17	B	812	CLA	C3B-C4B-NB	-3.23	107.64	110.53
17	2	303	CLA	O2D-CGD-O1D	-3.23	117.55	123.85
17	4	309	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
18	4	305	CHL	O2D-CGD-O1D	-3.23	117.56	123.85
21	K	203	BCR	C2-C1-C6	3.23	115.13	110.44
17	B	808	CLA	C11-C12-C13	-3.23	105.24	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	306	CHL	C1C-CHC-C4B	3.22	127.61	116.07
17	B	828	CLA	CAC-C3C-C4C	3.22	128.99	124.79
17	A	816	CLA	C3B-C4B-NB	-3.22	107.65	110.53
17	2	301	CLA	C3B-C4B-NB	-3.21	107.67	110.53
17	A	834	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
17	4	302	CLA	C3B-C4B-NB	-3.20	107.67	110.53
17	B	814	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
17	B	826	CLA	C4A-NA-C1A	3.20	108.14	106.68
17	2	307	CLA	C3B-C4B-NB	-3.19	107.68	110.53
18	4	306	CHL	O2A-CGA-CBA	3.19	121.56	111.83
17	1	313	CLA	C3B-C4B-NB	-3.19	107.69	110.53
26	4	323	DGD	O6E-C5E-C4E	3.19	115.44	109.70
17	1	309	CLA	O2D-CGD-O1D	-3.18	117.65	123.85
17	B	817	CLA	C3B-C4B-NB	-3.18	107.69	110.53
17	3	605	CLA	C3B-C4B-NB	-3.18	107.69	110.53
18	4	315	CHL	CBC-CAC-C3C	-3.18	108.32	112.87
17	B	805	CLA	C3B-C4B-NB	-3.18	107.69	110.53
17	4	314	CLA	C3B-C4B-NB	-3.17	107.70	110.53
17	B	829	CLA	C3B-C4B-NB	-3.16	107.71	110.53
17	B	820	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
17	B	832	CLA	O2A-CGA-O1A	-3.16	115.73	123.63
17	B	825	CLA	CHB-C4A-NA	3.16	128.95	124.40
17	B	821	CLA	CED-O2D-CGD	3.15	123.06	115.92
17	B	816	CLA	C3B-C4B-NB	-3.15	107.72	110.53
18	4	307	CHL	C1C-CHC-C4B	3.15	127.34	116.07
17	A	833	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
17	A	827	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
17	2	312	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
17	A	835	CLA	C3B-C4B-NB	-3.14	107.73	110.53
17	A	830	CLA	C3B-C4B-NB	-3.14	107.73	110.53
18	2	305	CHL	OMC-CMC-C2C	-3.13	119.69	125.12
17	J	103	CLA	CHB-C4A-NA	3.13	128.91	124.40
17	A	801	CLA	C3B-C4B-NB	-3.12	107.74	110.53
18	2	306	CHL	O2A-CGA-CBA	3.12	121.35	111.83
17	B	839	CLA	CBA-CAA-C2A	3.12	123.07	113.79
17	A	833	CLA	C3B-C4B-NB	-3.11	107.75	110.53
17	J	103	CLA	C3B-C4B-NB	-3.11	107.75	110.53
17	B	821	CLA	CHB-C4A-NA	3.10	128.88	124.40
17	B	839	CLA	CBC-CAC-C3C	-3.10	104.01	112.42
17	A	831	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
17	1	309	CLA	C3B-C4B-NB	-3.10	107.76	110.53
17	A	838	CLA	CAC-C3C-C4C	3.09	128.81	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	819	CLA	C3B-C4B-NB	-3.09	107.77	110.53
17	B	830	CLA	C1-C2-C3	-3.09	121.14	126.20
19	4	316	LUT	C37-C21-C22	-3.09	103.65	109.41
17	4	308	CLA	C3B-C4B-NB	-3.08	107.78	110.53
17	2	301	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
18	3	607	CHL	C1C-CHC-C4B	3.08	127.09	116.07
17	B	814	CLA	CMB-C2B-C1B	-3.08	120.73	125.42
17	4	313	CLA	C3B-C4B-NB	-3.08	107.78	110.53
17	L	202	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
25	4	321	HTG	C1'-S1-C1	3.07	107.08	100.45
17	A	801	CLA	CGD-CBD-CAD	3.07	120.78	110.85
17	B	807	CLA	CAA-C2A-C1A	-3.07	101.92	111.97
17	B	810	CLA	O2A-CGA-O1A	-3.07	115.95	123.63
17	3	610	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
17	B	823	CLA	O2A-CGA-O1A	-3.07	115.96	123.63
17	2	308	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
17	L	203	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
17	G	103	CLA	C3B-C4B-NB	-3.06	107.80	110.53
17	A	809	CLA	C1-C2-C3	-3.06	121.19	126.20
21	A	846	BCR	C24-C23-C22	-3.05	121.72	126.23
17	B	820	CLA	C2D-C1D-ND	-3.05	107.10	110.13
17	F	306	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
17	B	803	CLA	C3B-C4B-NB	-3.05	107.81	110.53
21	F	308	BCR	C8-C7-C6	-3.05	118.85	127.00
17	3	602	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
17	A	853	CLA	C3B-C4B-NB	-3.04	107.81	110.53
21	4	318	BCR	C3-C4-C5	-3.04	108.63	114.06
17	B	810	CLA	O2D-CGD-CBD	3.04	116.54	111.23
17	B	830	CLA	C3B-C4B-NB	-3.04	107.82	110.53
17	B	828	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
17	B	831	CLA	C1-C2-C3	-3.04	121.22	126.20
21	1	316	BCR	C15-C16-C17	-3.03	117.31	123.52
17	B	815	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
26	4	323	DGD	O1G-C1A-C2A	3.03	121.07	111.83
21	F	308	BCR	C2-C1-C6	3.02	114.83	110.44
21	J	105	BCR	C33-C5-C6	-3.02	121.18	124.48
17	B	826	CLA	C3B-C4B-NB	-3.02	107.83	110.53
17	1	311	CLA	C3B-C4B-NB	-3.02	107.84	110.53
18	3	601	CHL	C1C-CHC-C4B	3.01	126.84	116.07
21	3	616	BCR	C15-C16-C17	-3.01	117.36	123.52
18	3	607	CHL	O1D-CGD-CBD	-3.01	120.16	124.72
24	B	852	LMG	O6-C1-C2	-3.01	104.19	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	F	303	BCR	C16-C17-C18	-3.01	123.06	127.28
17	1	303	CLA	C3B-C4B-NB	-3.01	107.85	110.53
17	B	804	CLA	C3B-C4B-NB	-3.00	107.85	110.53
17	1	312	CLA	C3B-C4B-NB	-3.00	107.85	110.53
17	A	814	CLA	C3B-C4B-NB	-3.00	107.85	110.53
22	A	845	LHG	O8-C23-C24	3.00	120.24	111.15
17	A	843	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
17	A	825	CLA	C3B-C4B-NB	-2.99	107.86	110.53
17	B	821	CLA	C3B-C4B-NB	-2.99	107.86	110.53
18	1	305	CHL	O2A-CGA-CBA	2.99	120.96	111.83
17	4	309	CLA	C3B-C4B-NB	-2.99	107.86	110.53
24	B	852	LMG	O6-C1-O1	-2.99	102.98	110.04
17	L	203	CLA	C3B-C4B-NB	-2.99	107.86	110.53
18	4	301	CHL	C1C-CHC-C4B	2.98	126.75	116.07
17	2	310	CLA	C3B-C4B-NB	-2.98	107.87	110.53
17	3	611	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
17	B	809	CLA	CHB-C4A-NA	2.98	128.71	124.40
17	B	820	CLA	CMB-C2B-C3B	2.98	133.56	126.55
17	B	842	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
18	2	305	CHL	C1C-CHC-C4B	2.98	126.73	116.07
18	2	313	CHL	C1C-CHC-C4B	2.98	126.73	116.07
17	B	820	CLA	CMB-C2B-C1B	-2.98	120.88	125.42
17	2	301	CLA	CMB-C2B-C1B	-2.98	120.89	125.42
17	1	306	CLA	C3B-C4B-NB	-2.98	107.87	110.53
17	B	830	CLA	C4-C3-C5	-2.98	110.06	115.23
17	B	830	CLA	O2A-C1-C2	2.98	119.56	108.11
21	B	844	BCR	C15-C14-C13	-2.97	123.11	127.28
18	3	601	CHL	O2A-CGA-CBA	2.97	120.90	111.83
17	2	309	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
17	A	818	CLA	CMB-C2B-C1B	-2.97	120.90	125.42
17	B	842	CLA	CAA-C2A-C3A	-2.97	104.98	113.00
17	4	311	CLA	C3B-C4B-NB	-2.97	107.88	110.53
18	3	601	CHL	C1-C2-C3	-2.97	121.34	126.20
17	A	813	CLA	C3B-C4B-NB	-2.96	107.89	110.53
17	K	201	CLA	C3B-C4B-NB	-2.96	107.89	110.53
17	B	824	CLA	C1-C2-C3	-2.96	121.35	126.20
17	A	811	CLA	C3B-C4B-NB	-2.96	107.89	110.53
17	A	840	CLA	O2D-CGD-CBD	2.95	116.39	111.23
17	B	831	CLA	O2A-CGA-O1A	-2.95	116.24	123.63
17	B	828	CLA	C1-C2-C3	-2.95	121.36	126.20
17	F	306	CLA	O2A-CGA-O1A	-2.95	115.75	123.33
17	B	810	CLA	O2D-CGD-O1D	-2.95	118.11	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	838	CLA	C3B-C4B-NB	-2.95	107.90	110.53
17	2	310	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
21	F	303	BCR	C39-C30-C25	-2.94	105.63	110.24
17	A	808	CLA	CHB-C4A-NA	2.94	128.64	124.40
17	A	830	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
17	3	606	CLA	C3B-C4B-NB	-2.93	107.91	110.53
17	4	312	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
21	2	316	BCR	C27-C26-C25	2.92	126.65	122.70
17	2	311	CLA	C3B-C4B-NB	-2.92	107.92	110.53
17	B	819	CLA	O1D-CGD-CBD	2.92	130.27	124.52
17	A	818	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
17	3	604	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
17	1	310	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
17	A	837	CLA	O2A-CGA-O1A	-2.91	116.34	123.63
17	B	829	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
17	A	821	CLA	C3B-C4B-NB	-2.91	107.94	110.53
24	4	319	LMG	O7-C10-O9	-2.91	116.91	123.70
17	B	817	CLA	CMB-C2B-C3B	2.90	133.38	126.55
17	B	822	CLA	CHB-C4A-NA	2.90	128.59	124.40
17	B	834	CLA	O2D-CGD-CBD	2.90	116.30	111.23
17	4	312	CLA	C3B-C4B-NB	-2.90	107.94	110.53
17	A	815	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
21	B	844	BCR	C7-C8-C9	-2.89	121.96	126.23
20	4	317	XAT	C39-C29-C28	-2.89	113.67	118.09
17	4	310	CLA	O2D-CGD-CBD	2.89	116.28	111.23
17	A	822	CLA	C3B-C4B-NB	-2.89	107.95	110.53
17	A	832	CLA	C3B-C4B-NB	-2.89	107.95	110.53
17	1	307	CLA	O2A-CGA-O1A	-2.89	116.41	123.63
17	A	822	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
17	B	841	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
23	2	318	LMT	C3'-C4'-C5'	-2.88	104.54	110.93
17	G	104	CLA	O2A-CGA-O1A	-2.88	116.42	123.63
17	4	303	CLA	O1D-CGD-CBD	2.88	130.20	124.52
21	2	316	BCR	C15-C14-C13	-2.88	123.24	127.28
17	A	828	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
17	A	835	CLA	C1-C2-C3	-2.88	121.48	126.20
17	B	802	CLA	C4A-NA-C1A	2.88	107.99	106.68
17	A	826	CLA	C3B-C4B-NB	-2.88	107.96	110.53
17	B	836	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
17	1	307	CLA	CHB-C4A-NA	2.88	128.55	124.40
19	2	314	LUT	C21-C26-C27	-2.88	109.52	112.83
19	2	314	LUT	C18-C5-C4	-2.88	109.13	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	846	BCR	C11-C10-C9	-2.87	123.25	127.28
24	4	319	LMG	O3-C3-C2	-2.87	103.61	110.38
21	A	847	BCR	C27-C26-C25	2.87	126.58	122.70
17	1	302	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
17	B	830	CLA	CAA-CBA-CGA	-2.86	105.08	113.21
17	B	806	CLA	O2D-CGD-CBD	2.86	116.23	111.23
21	2	316	BCR	C33-C5-C6	-2.86	121.36	124.48
17	B	825	CLA	CMB-C2B-C1B	-2.86	121.06	125.42
21	B	846	BCR	C15-C14-C13	-2.86	123.27	127.28
17	F	304	CLA	C3B-C4B-NB	-2.86	107.98	110.53
17	A	838	CLA	C1-O2A-CGA	-2.86	109.73	116.65
21	B	847	BCR	C38-C26-C27	-2.86	107.50	113.60
17	B	814	CLA	CHB-C4A-NA	2.85	128.52	124.40
19	4	316	LUT	C37-C21-C36	2.85	112.02	107.87
17	1	304	CLA	C3B-C4B-NB	-2.85	107.98	110.53
17	B	809	CLA	O2A-CGA-O1A	-2.85	116.50	123.63
17	3	606	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
17	A	823	CLA	C3B-C4B-NB	-2.85	107.99	110.53
17	A	820	CLA	C3B-C4B-NB	-2.85	107.99	110.53
17	B	820	CLA	C1-C2-C3	-2.85	121.53	126.20
17	B	834	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
17	4	302	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
17	3	613	CLA	C3B-C4B-NB	-2.85	107.99	110.53
17	B	808	CLA	C3B-C4B-NB	-2.84	107.99	110.53
17	A	836	CLA	O1D-CGD-CBD	2.84	130.12	124.52
17	4	303	CLA	C3B-C4B-NB	-2.84	107.99	110.53
17	A	834	CLA	C3B-C4B-NB	-2.84	107.99	110.53
26	B	850	DGD	CDB-CCB-CBB	-2.84	100.01	114.37
17	4	302	CLA	CED-O2D-CGD	2.84	122.36	115.92
18	4	307	CHL	O2A-CGA-CBA	2.84	120.49	111.83
17	B	826	CLA	CHA-C1A-NA	-2.84	119.96	126.39
17	A	826	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
21	L	206	BCR	C27-C26-C25	2.84	126.54	122.70
27	B	843	PQN	C17-C16-C15	-2.84	105.70	113.26
18	2	304	CHL	C1C-CHC-C4B	2.84	126.22	116.07
17	B	839	CLA	O2D-CGD-CBD	2.84	116.19	111.23
17	3	611	CLA	C3B-C4B-NB	-2.83	108.00	110.53
17	B	805	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
17	A	853	CLA	O2D-CGD-CBD	2.83	116.18	111.23
25	J	102	HTG	C1'-S1-C1	2.83	106.57	100.45
17	B	808	CLA	CHB-C4A-NA	2.83	128.49	124.40
17	B	828	CLA	O2A-CGA-O1A	-2.83	116.55	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	830	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
17	B	841	CLA	C3B-C4B-NB	-2.83	108.01	110.53
26	4	323	DGD	C6D-O5D-C1E	2.83	119.85	113.80
17	B	837	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
17	1	303	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
18	2	306	CHL	C1C-CHC-C4B	2.82	126.17	116.07
17	K	201	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
17	B	815	CLA	CHB-C4A-NA	2.82	128.47	124.40
17	B	811	CLA	CMB-C2B-C1B	-2.82	121.12	125.42
17	B	823	CLA	CMB-C2B-C3B	2.82	133.18	126.55
17	3	612	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
21	2	316	BCR	C24-C23-C22	-2.82	122.07	126.23
17	B	818	CLA	C1-O2A-CGA	2.81	123.46	116.65
21	A	851	BCR	C24-C23-C22	-2.81	122.07	126.23
21	G	106	BCR	C24-C23-C22	-2.81	122.08	126.23
21	B	845	BCR	C39-C30-C25	2.81	114.65	110.24
17	A	817	CLA	O2A-CGA-O1A	-2.81	116.60	123.63
17	A	812	CLA	C3B-C4B-NB	-2.81	108.02	110.53
17	B	819	CLA	CAA-C2A-C1A	-2.81	102.77	111.97
17	1	304	CLA	CHB-C4A-NA	2.80	128.45	124.40
18	3	607	CHL	CBC-CAC-C3C	-2.80	108.86	112.87
17	2	309	CLA	CAA-C2A-C3A	-2.80	109.81	116.23
17	B	822	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
17	A	831	CLA	O2D-CGD-CBD	2.79	116.12	111.23
17	4	310	CLA	CHB-C4A-NA	2.79	128.43	124.40
17	4	310	CLA	C3B-C4B-NB	-2.79	108.04	110.53
17	B	802	CLA	C1-C2-C3	-2.79	121.63	126.20
17	3	610	CLA	CHB-C4A-NA	2.79	128.43	124.40
26	4	323	DGD	O1G-C1A-O1A	-2.79	116.65	123.63
17	K	202	CLA	C3B-C4B-NB	-2.79	108.04	110.53
17	A	820	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
21	J	104	BCR	C15-C16-C17	-2.79	117.82	123.52
17	1	301	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
17	4	304	CLA	CHB-C4A-NA	2.78	128.42	124.40
22	A	844	LHG	O8-C23-C24	2.78	120.32	111.83
18	1	305	CHL	C1C-CHC-C4B	2.78	126.02	116.07
17	B	842	CLA	C7-C6-C5	-2.78	105.85	113.26
17	A	807	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
17	A	832	CLA	O2D-CGD-CBD	2.78	116.09	111.23
17	3	608	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
17	B	824	CLA	CHB-C4A-NA	2.78	128.41	124.40
17	A	808	CLA	CHC-C4B-NB	2.78	128.21	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	850	BCR	C27-C26-C25	2.77	126.45	122.70
18	1	305	CHL	CED-O2D-CGD	2.77	122.20	115.92
17	B	828	CLA	O1D-CGD-CBD	2.77	129.98	124.52
18	3	601	CHL	C4-C3-C5	2.77	120.03	115.23
17	B	832	CLA	C3B-C4B-NB	-2.77	108.06	110.53
22	1	317	LHG	C11-C10-C9	-2.77	100.39	114.37
17	B	806	CLA	CMB-C2B-C1B	-2.76	121.21	125.42
19	4	316	LUT	C40-C33-C32	-2.76	113.87	118.09
22	A	844	LHG	C11-C10-C9	-2.76	100.40	114.37
21	L	201	BCR	C27-C26-C25	2.76	126.44	122.70
17	B	838	CLA	CED-O2D-CGD	-2.76	109.65	115.92
17	B	834	CLA	C4-C3-C5	2.76	120.02	115.23
22	F	302	LHG	O8-C23-C24	2.76	120.24	111.83
17	B	835	CLA	C4-C3-C5	2.76	120.01	115.23
17	1	311	CLA	O2A-CGA-O1A	-2.75	116.74	123.63
17	4	312	CLA	CMB-C2B-C1B	-2.75	121.23	125.42
17	A	843	CLA	C3B-C4B-NB	-2.75	108.08	110.53
17	B	807	CLA	CMB-C2B-C1B	-2.75	121.23	125.42
21	B	848	BCR	C15-C14-C13	-2.75	123.43	127.28
18	4	301	CHL	C1C-C2C-CMC	2.75	131.75	126.80
17	B	833	CLA	CMB-C2B-C3B	2.74	133.00	126.55
17	B	816	CLA	CMB-C2B-C1B	-2.74	121.24	125.42
22	G	102	LHG	O8-C23-C24	2.74	120.19	111.83
17	B	833	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
17	3	610	CLA	C3B-C4B-NB	-2.74	108.08	110.53
17	3	608	CLA	C3B-C4B-NB	-2.74	108.09	110.53
24	G	101	LMG	C1-C2-C3	-2.74	104.25	110.01
19	2	314	LUT	C20-C13-C12	-2.74	113.91	118.09
21	B	848	BCR	C27-C26-C25	2.74	126.40	122.70
18	4	305	CHL	O2A-CGA-CBA	2.74	120.18	111.83
21	A	851	BCR	C7-C8-C9	-2.74	122.19	126.23
17	A	802	CLA	C1-C2-C3	-2.74	121.71	126.20
18	2	304	CHL	O2D-CGD-O1D	-2.73	118.53	123.85
17	4	302	CLA	O2D-CGD-CBD	2.73	116.00	111.23
17	B	807	CLA	C3B-C4B-NB	-2.73	108.09	110.53
17	F	304	CLA	CHB-C4A-NA	2.73	128.34	124.40
17	A	801	CLA	O1D-CGD-CBD	-2.73	119.14	124.52
17	A	811	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
21	L	206	BCR	C33-C5-C6	-2.72	121.51	124.48
17	2	308	CLA	C3B-C4B-NB	-2.72	108.10	110.53
17	A	803	CLA	C3B-C4B-NB	-2.72	108.10	110.53
17	1	306	CLA	O2D-CGD-O1D	-2.72	118.55	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	806	CLA	CMB-C2B-C3B	2.72	132.94	126.55
17	B	807	CLA	O1D-CGD-CBD	2.72	129.88	124.52
17	B	838	CLA	CHB-C4A-NA	2.72	128.32	124.40
18	4	315	CHL	CMA-C3A-C4A	-2.71	108.76	114.61
17	B	825	CLA	O2A-CGA-O1A	-2.71	116.84	123.63
17	A	805	CLA	O2D-CGD-CBD	2.71	115.97	111.23
17	B	823	CLA	CHB-C4A-NA	2.71	128.32	124.40
17	1	308	CLA	C3B-C4B-NB	-2.71	108.11	110.53
17	B	809	CLA	C3B-C4B-NB	-2.71	108.11	110.53
18	4	315	CHL	C1C-CHC-C4B	2.71	125.77	116.07
25	4	322	HTG	O5-C1-C2	-2.71	106.58	110.32
17	A	806	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
17	B	820	CLA	C4A-NA-C1A	2.70	107.91	106.68
21	A	846	BCR	C2-C1-C6	2.70	114.36	110.44
17	3	609	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
17	2	319	CLA	O2A-CGA-O1A	-2.70	115.14	123.20
17	A	815	CLA	C3B-C4B-NB	-2.70	108.12	110.53
21	F	303	BCR	C27-C26-C25	2.70	126.35	122.70
17	A	802	CLA	O2D-CGD-CBD	2.70	115.94	111.23
21	L	206	BCR	C11-C10-C9	-2.69	123.50	127.28
17	B	824	CLA	O2A-CGA-O1A	-2.69	116.90	123.63
21	A	846	BCR	C15-C16-C17	-2.69	118.01	123.52
21	G	106	BCR	C16-C15-C14	-2.69	118.01	123.52
17	2	303	CLA	C1-C2-C3	-2.69	121.79	126.20
18	2	304	CHL	OMC-CMC-C2C	-2.69	120.45	125.12
18	4	305	CHL	C1C-CHC-C4B	2.68	125.67	116.07
17	B	809	CLA	O2D-CGD-CBD	2.68	115.92	111.23
17	L	202	CLA	C3B-C4B-NB	-2.68	108.14	110.53
17	A	837	CLA	CMB-C2B-C1B	-2.68	121.34	125.42
17	B	830	CLA	O2A-CGA-O1A	-2.68	116.94	123.63
18	2	305	CHL	CBC-CAC-C3C	-2.68	109.04	112.87
18	3	601	CHL	CMB-C2B-C3B	2.67	130.02	124.68
17	A	832	CLA	CAC-C3C-C4C	2.67	128.27	124.79
21	B	846	BCR	C2-C1-C6	2.67	114.32	110.44
18	4	305	CHL	C4D-ND-C1D	-2.67	103.19	105.22
18	2	306	CHL	O1D-CGD-CBD	-2.67	120.67	124.72
17	B	824	CLA	C3B-C4B-NB	-2.67	108.15	110.53
17	B	820	CLA	CHD-C1D-C2D	2.67	131.04	125.49
17	B	842	CLA	CHB-C4A-NA	2.67	128.25	124.40
18	2	305	CHL	O2A-CGA-CBA	2.67	119.97	111.83
21	F	308	BCR	C27-C26-C25	2.67	126.31	122.70
17	B	824	CLA	CMB-C2B-C1B	-2.67	121.36	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	102	LHG	C11-C10-C9	-2.66	100.90	114.37
17	2	309	CLA	C3B-C4B-NB	-2.66	108.16	110.53
17	B	831	CLA	CHB-C4A-NA	2.66	128.23	124.40
17	A	802	CLA	CHB-C4A-NA	2.65	128.23	124.40
23	2	318	LMT	C3B-C4B-C5B	-2.65	105.42	110.23
17	B	819	CLA	C3B-C4B-NB	-2.65	108.16	110.53
21	K	203	BCR	C27-C26-C25	2.65	126.29	122.70
17	3	603	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
17	A	801	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
17	A	806	CLA	O2A-CGA-O1A	-2.65	117.00	123.63
25	F	310	HTG	C4-C3-C2	2.65	115.48	110.83
17	A	839	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
21	F	303	BCR	C35-C13-C14	-2.65	118.53	122.82
17	A	808	CLA	C1-O2A-CGA	-2.65	110.25	116.65
17	1	311	CLA	CHB-C4A-NA	2.64	128.22	124.40
18	4	306	CHL	CMA-C3A-C4A	-2.64	108.91	114.61
18	1	305	CHL	O1D-CGD-CBD	-2.64	120.72	124.72
17	A	829	CLA	CHB-C4A-NA	2.64	128.21	124.40
17	1	303	CLA	O2A-CGA-O1A	-2.64	117.02	123.63
21	3	616	BCR	C24-C23-C22	-2.64	122.33	126.23
17	1	309	CLA	CAA-C2A-C3A	-2.63	105.88	113.00
17	2	302	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
17	4	313	CLA	O2D-CGD-CBD	2.63	115.83	111.23
21	B	846	BCR	C24-C23-C22	-2.63	122.34	126.23
21	A	851	BCR	C2-C1-C6	2.63	114.26	110.44
17	F	304	CLA	CHD-C1D-ND	-2.63	121.11	124.80
17	B	804	CLA	CBC-CAC-C3C	-2.63	105.30	112.42
17	A	833	CLA	CHB-C4A-NA	2.63	128.19	124.40
17	A	814	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
17	B	836	CLA	CHB-C4A-NA	2.62	128.19	124.40
17	A	822	CLA	CHB-C4A-NA	2.62	128.19	124.40
17	A	815	CLA	CHB-C4A-NA	2.62	128.18	124.40
17	1	302	CLA	C3B-C4B-NB	-2.61	108.20	110.53
17	B	806	CLA	CHB-C4A-NA	2.61	128.17	124.40
17	1	304	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
17	B	840	CLA	CHB-C4A-NA	2.61	128.16	124.40
27	A	842	PQN	C2M-C2-C1	-2.61	111.87	116.68
21	B	845	BCR	C7-C8-C9	-2.61	122.38	126.23
17	G	104	CLA	CHB-C4A-NA	2.61	128.16	124.40
17	4	313	CLA	CHB-C4A-NA	2.61	128.16	124.40
17	B	836	CLA	C2A-C1A-CHA	2.60	128.39	123.87
17	A	853	CLA	C6-C5-C3	-2.60	107.13	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	J	105	BCR	C38-C26-C25	-2.60	121.64	124.48
17	2	319	CLA	CHB-C4A-NA	2.60	128.15	124.40
17	B	835	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
21	B	846	BCR	C7-C8-C9	-2.60	122.39	126.23
21	L	206	BCR	C24-C23-C22	-2.60	122.39	126.23
21	A	848	BCR	C15-C14-C13	-2.59	123.64	127.28
26	4	323	DGD	O2E-C2E-C3E	-2.59	104.26	110.38
17	B	815	CLA	CAC-C3C-C4C	2.59	128.16	124.79
17	B	832	CLA	C1D-ND-C4D	2.59	108.13	106.31
17	3	606	CLA	CHB-C4A-NA	2.59	128.14	124.40
21	A	848	BCR	C33-C5-C6	-2.59	121.66	124.48
17	L	204	CLA	C3B-C4B-NB	-2.59	108.22	110.53
17	B	806	CLA	CAC-C3C-C4C	2.59	128.16	124.79
17	A	819	CLA	CHB-C4A-NA	2.59	128.13	124.40
21	B	844	BCR	C27-C26-C25	2.58	126.20	122.70
21	B	844	BCR	C35-C13-C14	-2.58	118.63	122.82
25	J	102	HTG	O5-C5-C6	2.58	112.84	106.44
21	F	308	BCR	C33-C5-C6	-2.58	121.67	124.48
17	A	809	CLA	CHB-C4A-NA	2.58	128.12	124.40
22	2	317	LHG	O8-C23-C24	2.58	119.69	111.83
20	3	615	XAT	C37-C21-C36	2.58	111.11	107.37
17	B	802	CLA	CHB-C1B-NB	2.58	127.91	124.05
17	A	803	CLA	CHB-C4A-NA	2.57	128.12	124.40
17	F	304	CLA	C4D-CHA-C1A	2.57	124.31	121.24
21	A	849	BCR	C27-C26-C25	2.57	126.18	122.70
17	A	828	CLA	C3B-C4B-NB	-2.57	108.23	110.53
17	3	611	CLA	CHB-C4A-NA	2.57	128.11	124.40
18	4	307	CHL	C5-C3-C4	2.57	120.50	114.59
27	A	842	PQN	C9-C10-C1	-2.57	116.34	120.10
17	B	802	CLA	CAA-C2A-C1A	-2.57	103.56	111.97
17	B	833	CLA	O2A-CGA-O1A	-2.57	117.20	123.63
17	1	308	CLA	CHB-C4A-NA	2.57	128.10	124.40
21	A	847	BCR	C15-C16-C17	-2.57	118.27	123.52
21	A	847	BCR	C33-C5-C6	-2.57	121.68	124.48
17	3	609	CLA	C3B-C4B-NB	-2.57	108.24	110.53
17	B	810	CLA	C1-O2A-CGA	-2.57	110.44	116.65
17	B	811	CLA	O2D-CGD-O1D	-2.57	118.86	123.85
21	B	846	BCR	C15-C16-C17	-2.56	118.27	123.52
20	2	315	XAT	C37-C21-C36	2.56	111.10	107.37
17	A	817	CLA	O1D-CGD-CBD	2.56	129.58	124.52
17	B	816	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
17	B	823	CLA	O2D-CGD-O1D	-2.56	118.86	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	845	BCR	C33-C5-C6	-2.56	121.69	124.48
21	L	206	BCR	C7-C8-C9	-2.56	122.44	126.23
17	B	803	CLA	CHB-C4A-NA	2.56	128.09	124.40
26	B	850	DGD	O2D-C2D-C1D	-2.56	103.97	110.08
17	A	829	CLA	C3B-C4B-NB	-2.56	108.25	110.53
17	B	819	CLA	C1-C2-C3	-2.56	122.01	126.20
17	A	832	CLA	CHB-C4A-NA	2.56	128.09	124.40
17	L	203	CLA	CHB-C4A-NA	2.55	128.09	124.40
17	B	828	CLA	CHD-C1D-ND	-2.55	121.21	124.80
17	B	828	CLA	C3B-C4B-NB	-2.55	108.25	110.53
25	F	305	HTG	C1'-S1-C1	2.55	105.96	100.45
20	1	315	XAT	C37-C21-C36	2.55	111.08	107.37
17	A	840	CLA	CGD-CBD-CAD	-2.55	102.58	110.85
17	B	832	CLA	CAC-C3C-C4C	2.55	128.11	124.79
17	A	805	CLA	CAA-C2A-C3A	-2.55	106.11	113.00
21	2	316	BCR	C7-C8-C9	-2.55	122.47	126.23
17	A	836	CLA	CHB-C4A-NA	2.55	128.07	124.40
17	A	832	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
21	L	206	BCR	C15-C14-C13	-2.54	123.71	127.28
21	F	303	BCR	C29-C30-C25	2.54	114.13	110.44
17	A	853	CLA	CHA-C1A-NA	-2.54	120.64	126.39
17	B	827	CLA	CHD-C4C-NC	2.54	128.17	124.23
18	4	306	CHL	C1-O2A-CGA	2.54	122.79	116.65
17	A	825	CLA	O2D-CGD-CBD	2.54	115.67	111.23
17	A	853	CLA	O1D-CGD-CBD	2.54	129.52	124.52
18	4	305	CHL	C4C-CHD-C1D	2.54	125.14	116.07
17	A	804	CLA	CMB-C2B-C1B	-2.53	121.56	125.42
17	4	309	CLA	CHB-C4A-NA	2.53	128.06	124.40
17	J	101	CLA	CED-O2D-CGD	-2.53	110.17	115.92
18	4	307	CHL	O1D-CGD-CBD	-2.53	120.89	124.72
17	2	309	CLA	CHB-C4A-NA	2.53	128.05	124.40
22	A	845	LHG	C11-C10-C9	-2.53	101.59	114.37
17	B	834	CLA	CED-O2D-CGD	2.53	121.64	115.92
21	L	201	BCR	C33-C5-C6	-2.53	121.73	124.48
21	4	318	BCR	C7-C8-C9	-2.53	122.50	126.23
17	B	805	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
17	K	202	CLA	CHB-C4A-NA	2.52	128.04	124.40
17	A	806	CLA	CHB-C4A-NA	2.52	128.04	124.40
17	A	807	CLA	CHB-C4A-NA	2.52	128.03	124.40
17	A	827	CLA	CHB-C4A-NA	2.52	128.03	124.40
17	B	830	CLA	CHB-C4A-NA	2.52	128.03	124.40
21	B	848	BCR	C29-C30-C25	2.52	114.09	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	827	CLA	CAA-C2A-C1A	-2.52	103.73	111.97
21	B	848	BCR	C2-C1-C6	2.52	114.09	110.44
21	B	845	BCR	C27-C26-C25	2.52	126.10	122.70
17	2	311	CLA	CMB-C2B-C1B	-2.52	121.59	125.42
17	3	613	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
18	3	607	CHL	CED-O2D-CGD	2.51	121.62	115.92
22	A	844	LHG	C20-C19-C18	-2.51	101.67	114.37
17	A	831	CLA	C3B-C4B-NB	-2.51	108.29	110.53
17	L	204	CLA	O2A-CGA-O1A	-2.51	117.34	123.63
17	B	813	CLA	CAC-C3C-C4C	2.51	128.06	124.79
24	4	320	LMG	C4-C3-C2	2.51	115.24	110.83
17	A	816	CLA	O2D-CGD-CBD	2.51	115.62	111.23
17	B	820	CLA	CHB-C1B-NB	2.51	127.81	124.05
21	F	308	BCR	C11-C10-C9	-2.51	123.76	127.28
17	B	814	CLA	CMB-C2B-C3B	2.51	132.44	126.55
26	4	323	DGD	O2D-C2D-C3D	-2.51	104.47	110.38
17	A	839	CLA	CHB-C1B-NB	2.50	127.81	124.05
17	B	828	CLA	CHB-C4A-NA	2.50	128.01	124.40
25	4	322	HTG	C1'-S1-C1	2.50	105.86	100.45
17	A	821	CLA	CHB-C4A-NA	2.50	128.01	124.40
21	L	205	BCR	C29-C30-C25	2.50	114.07	110.44
21	A	848	BCR	C11-C10-C9	-2.50	123.77	127.28
21	J	105	BCR	C27-C26-C25	2.50	126.08	122.70
17	3	605	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
18	4	307	CHL	O2A-CGA-O1A	-2.50	117.39	123.63
17	1	306	CLA	CHB-C4A-NA	2.49	128.00	124.40
21	G	106	BCR	C27-C26-C25	2.49	126.07	122.70
17	B	839	CLA	C1D-ND-C4D	2.49	108.06	106.31
17	4	310	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
17	B	817	CLA	CHB-C4A-NA	2.49	127.99	124.40
17	B	831	CLA	C3A-C2A-C1A	2.49	105.06	101.34
18	2	305	CHL	O2D-CGD-O1D	-2.49	119.01	123.85
17	B	820	CLA	CHB-C4A-NA	2.48	127.98	124.40
21	A	850	BCR	C15-C14-C13	-2.48	123.80	127.28
21	A	848	BCR	C27-C26-C25	2.48	126.06	122.70
17	L	202	CLA	CHB-C4A-NA	2.48	127.98	124.40
24	B	852	LMG	C7-O1-C1	2.48	119.12	113.80
18	2	305	CHL	CMB-C2B-C3B	2.48	129.64	124.68
17	2	307	CLA	CHB-C4A-NA	2.48	127.98	124.40
18	3	607	CHL	CMB-C2B-C3B	2.48	129.64	124.68
17	2	308	CLA	CHB-C4A-NA	2.48	127.98	124.40
21	A	848	BCR	C8-C7-C6	-2.48	120.38	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	826	CLA	C4D-CHA-C1A	2.48	124.20	121.24
17	B	802	CLA	O2A-CGA-O1A	-2.48	117.43	123.63
17	A	824	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
17	B	805	CLA	O1D-CGD-CBD	2.48	129.40	124.52
17	A	809	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
20	4	317	XAT	C20-C13-C12	-2.47	114.31	118.09
17	B	822	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
17	B	825	CLA	C1-C2-C3	-2.47	122.14	126.20
17	A	831	CLA	CHB-C4A-NA	2.47	127.97	124.40
17	B	804	CLA	C1-O2A-CGA	2.47	122.63	116.65
17	B	817	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
21	F	308	BCR	C16-C15-C14	-2.47	118.47	123.52
17	F	307	CLA	CHB-C4A-NA	2.47	127.96	124.40
17	B	806	CLA	O2A-CGA-O1A	-2.47	116.99	123.33
17	B	806	CLA	C3A-C2A-C1A	2.46	105.03	101.34
18	4	305	CHL	CMA-C3A-C4A	-2.46	109.30	114.61
17	1	309	CLA	CHB-C4A-NA	2.46	127.96	124.40
17	A	818	CLA	C3B-C4B-NB	-2.46	108.33	110.53
21	A	846	BCR	C27-C26-C25	2.46	126.03	122.70
19	3	614	LUT	C18-C5-C4	-2.46	109.90	114.42
17	B	840	CLA	C3B-C4B-NB	-2.46	108.33	110.53
21	3	616	BCR	C15-C14-C13	-2.46	123.83	127.28
26	4	323	DGD	O6D-C1D-C2D	-2.46	105.33	110.37
17	4	308	CLA	CHB-C4A-NA	2.46	127.94	124.40
26	4	323	DGD	O4D-C4D-C5D	-2.45	103.28	109.32
21	L	205	BCR	C2-C1-C6	2.45	114.00	110.44
17	A	828	CLA	CHB-C4A-NA	2.44	127.93	124.40
17	B	820	CLA	CAA-CBA-CGA	-2.44	106.27	113.21
17	B	834	CLA	C3B-C4B-NB	-2.44	108.35	110.53
17	A	830	CLA	CHB-C4A-NA	2.44	127.92	124.40
17	B	818	CLA	C4A-NA-C1A	2.44	107.79	106.68
17	A	810	CLA	CAA-C2A-C3A	-2.44	106.41	113.00
17	K	201	CLA	CHB-C4A-NA	2.44	127.92	124.40
17	B	842	CLA	C4-C3-C5	2.44	119.46	115.23
22	2	317	LHG	C11-C10-C9	-2.44	102.05	114.37
17	1	310	CLA	CHB-C4A-NA	2.43	127.91	124.40
17	4	314	CLA	CAA-CBA-CGA	-2.43	106.30	113.21
17	B	827	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
17	A	804	CLA	C1-C2-C3	-2.43	122.22	126.20
21	B	846	BCR	C27-C26-C25	2.43	125.99	122.70
21	B	847	BCR	C21-C20-C19	-2.43	116.17	123.20
21	A	850	BCR	C15-C16-C17	-2.43	118.55	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	303	CLA	C3B-C4B-NB	-2.43	108.36	110.53
17	B	805	CLA	O2A-CGA-O1A	-2.43	117.56	123.63
21	I	101	BCR	C33-C5-C6	-2.42	121.84	124.48
17	A	843	CLA	CHB-C4A-NA	2.42	127.90	124.40
17	A	809	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
26	4	323	DGD	O3G-C3G-C2G	2.42	116.71	110.82
17	1	312	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
17	B	828	CLA	CMB-C2B-C1B	-2.42	121.73	125.42
17	B	808	CLA	O1D-CGD-CBD	2.42	129.29	124.52
21	B	848	BCR	C38-C26-C25	-2.42	121.85	124.48
17	A	818	CLA	C1-C2-C3	-2.42	122.24	126.20
18	4	305	CHL	CAC-C3C-C4C	2.42	130.24	124.03
21	J	105	BCR	C7-C8-C9	-2.42	122.66	126.23
17	4	312	CLA	CHB-C1B-NB	2.41	127.67	124.05
17	1	302	CLA	CAA-CBA-CGA	-2.41	106.36	113.21
17	3	612	CLA	CHB-C4A-NA	2.41	127.88	124.40
19	1	314	LUT	C21-C26-C27	-2.41	110.05	112.83
19	4	316	LUT	C19-C9-C8	-2.41	114.40	118.09
17	4	302	CLA	C4-C3-C5	2.41	119.41	115.23
17	B	840	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
17	A	827	CLA	CMB-C2B-C3B	2.41	132.22	126.55
17	A	841	CLA	O2D-CGD-CBD	2.41	115.44	111.23
17	4	304	CLA	C1D-ND-C4D	2.40	108.00	106.31
17	2	307	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
17	A	821	CLA	O2D-CGD-CBD	2.40	115.43	111.23
23	A	855	LMT	C1'-O5'-C5'	-2.40	109.03	113.72
17	G	104	CLA	C3B-C4B-NB	-2.40	108.39	110.53
21	A	847	BCR	C15-C14-C13	-2.40	123.92	127.28
21	A	849	BCR	C16-C15-C14	-2.40	118.61	123.52
21	K	203	BCR	C24-C23-C22	-2.40	122.69	126.23
17	3	612	CLA	C3B-C4B-NB	-2.40	108.39	110.53
17	B	831	CLA	CGD-CBD-CAD	2.39	118.60	110.85
17	3	613	CLA	CHB-C4A-NA	2.39	127.85	124.40
18	2	305	CHL	CAC-C3C-C4C	2.39	130.18	124.03
17	B	832	CLA	O1D-CGD-CBD	2.39	129.24	124.52
17	L	204	CLA	O2D-CGD-CBD	2.39	115.41	111.23
17	A	840	CLA	CHB-C4A-NA	2.39	127.85	124.40
17	B	839	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
17	B	806	CLA	CED-O2D-CGD	2.39	121.34	115.92
17	A	810	CLA	C3B-C4B-NB	-2.39	108.40	110.53
17	3	603	CLA	C1-C2-C3	-2.39	122.90	126.76
19	4	316	LUT	C22-C23-C24	-2.39	107.64	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	301	CLA	CMB-C2B-C3B	2.39	132.17	126.55
17	A	840	CLA	C5-C3-C2	2.39	126.53	121.17
18	4	315	CHL	C1C-C2C-CMC	2.39	131.10	126.80
17	A	804	CLA	CMC-C2C-C1C	2.39	128.76	125.03
17	A	811	CLA	CHB-C4A-NA	2.39	127.84	124.40
17	A	823	CLA	CHB-C4A-NA	2.39	127.84	124.40
17	4	314	CLA	CHB-C4A-NA	2.38	127.84	124.40
17	A	818	CLA	CMB-C2B-C3B	2.38	132.15	126.55
17	1	301	CLA	C6-C5-C3	-2.38	107.67	113.47
17	F	307	CLA	O1D-CGD-CBD	2.38	129.21	124.52
17	B	815	CLA	C3B-C4B-NB	-2.38	108.41	110.53
17	B	827	CLA	C3B-C4B-NB	-2.38	108.41	110.53
17	A	821	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
17	B	833	CLA	CAA-C2A-C3A	-2.38	106.57	113.00
17	1	312	CLA	O2D-CGD-CBD	2.38	115.39	111.23
17	A	801	CLA	CHB-C4A-NA	2.38	127.83	124.40
17	A	837	CLA	CHB-C4A-NA	2.38	127.83	124.40
21	1	316	BCR	C29-C30-C25	2.37	113.89	110.44
17	3	608	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
17	B	805	CLA	C1D-ND-C4D	2.37	107.98	106.31
21	B	845	BCR	C2-C1-C6	2.37	113.89	110.44
17	A	828	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
17	B	837	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
21	A	849	BCR	C33-C5-C6	-2.37	121.90	124.48
24	F	309	LMG	O8-C28-O10	-2.37	117.70	123.63
17	1	303	CLA	CHB-C4A-NA	2.37	127.82	124.40
17	A	808	CLA	CMB-C2B-C3B	2.37	132.12	126.55
17	1	311	CLA	O1D-CGD-CBD	2.37	129.19	124.52
17	B	824	CLA	CMB-C2B-C3B	2.37	132.12	126.55
21	F	303	BCR	C2-C1-C6	2.37	113.88	110.44
17	B	802	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
17	4	309	CLA	O2D-CGD-CBD	2.37	115.36	111.23
17	4	314	CLA	O1D-CGD-CBD	2.36	129.18	124.52
17	B	841	CLA	CAA-CBA-CGA	-2.36	106.50	113.21
18	3	601	CHL	CBC-CAC-C3C	-2.36	109.49	112.87
17	B	811	CLA	C3B-C4B-NB	-2.36	108.42	110.53
25	J	102	HTG	O4-C4-C3	-2.36	104.82	110.38
17	A	825	CLA	CHD-C1D-ND	-2.36	121.49	124.80
17	B	841	CLA	CHD-C1D-ND	-2.36	121.49	124.80
21	F	303	BCR	C15-C14-C13	-2.36	123.97	127.28
17	3	604	CLA	C3B-C4B-NB	-2.35	108.43	110.53
27	B	843	PQN	C10-C1-C2	-2.35	115.70	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	820	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
17	B	839	CLA	C2D-C1D-ND	-2.35	107.80	110.13
17	2	319	CLA	O2D-CGD-CBD	2.35	115.34	111.23
17	B	833	CLA	CBC-CAC-C3C	-2.35	106.05	112.42
17	A	838	CLA	CMA-C3A-C4A	-2.35	105.46	111.77
17	F	307	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
17	A	804	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
17	3	609	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
17	A	837	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
17	A	827	CLA	CMB-C2B-C1B	-2.34	121.85	125.42
17	G	105	CLA	C3B-C4B-NB	-2.34	108.44	110.53
21	B	847	BCR	C30-C25-C26	-2.34	119.44	122.64
21	B	845	BCR	C15-C16-C17	-2.34	118.73	123.52
17	B	842	CLA	C1-C2-C3	-2.34	122.37	126.20
17	B	816	CLA	CMB-C2B-C3B	2.33	132.04	126.55
17	A	840	CLA	CHD-C1D-ND	-2.33	121.52	124.80
17	2	311	CLA	CHB-C4A-NA	2.33	127.77	124.40
18	3	601	CHL	C4D-ND-C1D	-2.33	103.45	105.22
17	B	817	CLA	CHB-C1B-NB	2.33	127.55	124.05
17	B	819	CLA	CHB-C4A-NA	2.33	127.76	124.40
17	B	812	CLA	CHB-C4A-NA	2.33	127.76	124.40
18	4	306	CHL	CMB-C2B-C3B	2.33	129.34	124.68
17	B	810	CLA	CHB-C4A-NA	2.33	127.76	124.40
17	B	839	CLA	CMB-C2B-C3B	2.33	132.03	126.55
17	G	103	CLA	CAA-C2A-C3A	-2.33	110.89	116.23
17	B	833	CLA	CHA-C1A-NA	-2.32	121.13	126.39
21	L	205	BCR	C28-C27-C26	-2.32	109.91	114.06
17	A	818	CLA	CHB-C4A-NA	2.32	127.75	124.40
17	1	313	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
22	1	317	LHG	O8-C23-O10	-2.32	117.82	123.63
21	A	851	BCR	C28-C27-C26	-2.32	109.92	114.06
18	2	313	CHL	CED-O2D-CGD	2.32	121.18	115.92
17	1	308	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
17	B	810	CLA	C3B-C4B-NB	-2.32	108.46	110.53
17	4	304	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
17	A	813	CLA	O2D-CGD-O1D	-2.32	119.34	123.85
17	3	603	CLA	CHB-C4A-NA	2.32	127.74	124.40
25	F	310	HTG	O5-C5-C4	2.32	113.87	109.70
17	B	802	CLA	C2D-C1D-ND	-2.31	107.83	110.13
17	B	803	CLA	O2D-CGD-CBD	2.31	115.27	111.23
21	3	616	BCR	C3-C4-C5	-2.31	109.93	114.06
22	A	844	LHG	O8-C23-O10	-2.31	117.84	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	847	BCR	C2-C1-C6	2.31	113.80	110.44
25	F	310	HTG	O5-C1-C2	-2.31	107.13	110.32
21	B	844	BCR	C24-C23-C22	-2.31	122.82	126.23
18	2	305	CHL	CMA-C3A-C4A	-2.31	109.64	114.61
17	B	834	CLA	C1-C2-C3	-2.31	122.42	126.20
17	A	826	CLA	C1-C2-C3	-2.31	122.42	126.20
17	G	103	CLA	CHB-C4A-NA	2.31	127.73	124.40
17	A	824	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
17	G	104	CLA	CAA-C2A-C3A	-2.31	106.77	113.00
17	2	312	CLA	CHB-C4A-NA	2.30	127.73	124.40
17	A	834	CLA	CMB-C2B-C1B	-2.30	121.91	125.42
17	A	808	CLA	C3A-C2A-C1A	2.30	104.79	101.34
21	1	316	BCR	C33-C5-C6	-2.30	121.97	124.48
20	4	317	XAT	O23-C23-C22	-2.30	105.04	109.75
17	1	307	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
17	1	307	CLA	C3B-C4B-NB	-2.30	108.48	110.53
17	B	822	CLA	C3B-C4B-NB	-2.30	108.48	110.53
17	B	815	CLA	O2D-CGD-CBD	2.30	115.25	111.23
26	4	323	DGD	C3E-C4E-C5E	2.30	114.40	110.23
17	B	813	CLA	C1-O2A-CGA	2.30	122.21	116.65
18	4	306	CHL	C4D-ND-C1D	-2.30	103.48	105.22
17	3	605	CLA	CHB-C4A-NA	2.29	127.71	124.40
18	2	304	CHL	C4D-ND-C1D	-2.29	103.48	105.22
17	F	304	CLA	O2A-CGA-CBA	2.29	118.83	111.83
17	B	802	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
17	A	840	CLA	C7-C6-C5	-2.29	107.15	113.26
17	A	825	CLA	CAA-C2A-C1A	-2.29	104.46	111.97
21	B	846	BCR	C33-C5-C6	-2.29	121.98	124.48
17	B	825	CLA	CMC-C2C-C1C	2.29	128.62	125.03
23	2	318	LMT	O5B-C5B-C6B	2.29	112.12	106.44
27	A	842	PQN	C17-C16-C15	-2.29	107.15	113.26
21	A	848	BCR	C24-C23-C22	-2.29	122.85	126.23
17	B	816	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
21	B	847	BCR	C40-C30-C25	2.29	113.83	110.24
17	B	836	CLA	C1D-ND-C4D	2.29	107.92	106.31
17	B	822	CLA	CED-O2D-CGD	2.29	121.11	115.92
17	B	825	CLA	CMB-C2B-C3B	2.29	131.93	126.55
17	B	833	CLA	CHA-C4D-ND	2.29	137.27	132.55
18	4	306	CHL	OMC-CMC-C2C	-2.29	121.15	125.12
21	L	206	BCR	C15-C16-C17	-2.29	118.84	123.52
17	A	853	CLA	C5-C3-C2	2.29	126.30	121.17
17	B	837	CLA	CMB-C2B-C3B	2.29	131.93	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	303	CLA	CHB-C4A-NA	2.28	127.70	124.40
22	F	302	LHG	C20-C19-C18	-2.28	102.82	114.37
22	G	102	LHG	C20-C19-C18	-2.28	102.83	114.37
17	A	831	CLA	C1-C2-C3	-2.28	122.46	126.20
21	J	105	BCR	C37-C22-C21	-2.28	119.12	122.82
17	B	807	CLA	C3A-C2A-C1A	2.28	104.75	101.34
18	2	313	CHL	CMA-C3A-C4A	-2.28	109.70	114.61
24	F	309	LMG	C40-C39-C38	-2.28	102.85	114.37
17	A	814	CLA	C1-C2-C3	-2.28	123.08	126.76
17	A	805	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
17	B	819	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
17	B	810	CLA	CHA-C1A-NA	-2.28	121.24	126.39
21	L	201	BCR	C2-C1-C6	2.28	113.74	110.44
17	3	604	CLA	CHB-C4A-NA	2.27	127.68	124.40
17	A	831	CLA	CAA-CBA-CGA	-2.27	106.75	113.21
17	A	824	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
17	3	606	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
24	4	320	LMG	C7-O1-C1	2.27	118.67	113.80
21	I	101	BCR	C10-C11-C12	-2.27	116.62	123.20
17	4	314	CLA	O2D-CGD-CBD	2.27	115.20	111.23
18	2	313	CHL	C4D-ND-C1D	-2.27	103.50	105.22
21	4	318	BCR	C29-C30-C25	2.27	113.74	110.44
26	4	323	DGD	O3E-C3E-C2E	-2.27	105.02	110.38
17	4	310	CLA	O1D-CGD-CBD	2.27	129.00	124.52
25	B	851	HTG	C1-O5-C5	2.27	116.63	112.56
17	A	835	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
17	2	301	CLA	C1-C2-C3	-2.27	122.48	126.20
26	B	850	DGD	CFB-CEB-CDB	-2.27	102.91	114.37
22	F	302	LHG	C11-C10-C9	-2.27	102.91	114.37
17	A	841	CLA	C1-C2-C3	-2.27	122.48	126.20
17	2	309	CLA	CMB-C2B-C1B	-2.26	121.97	125.42
26	B	850	DGD	CBB-CAB-C9B	-2.26	102.92	114.37
21	G	106	BCR	C33-C5-C6	-2.26	122.02	124.48
17	A	804	CLA	CMB-C2B-C3B	2.26	131.87	126.55
18	4	306	CHL	C1-C2-C3	-2.26	123.10	126.76
17	B	842	CLA	C16-C15-C13	-2.26	108.45	115.97
17	A	837	CLA	C1-C2-C3	-2.26	122.50	126.20
20	4	317	XAT	C16-C1-C2	-2.26	105.00	108.97
17	G	105	CLA	O2D-CGD-CBD	2.26	115.17	111.23
21	A	849	BCR	C15-C14-C13	-2.25	124.12	127.28
21	B	849	BCR	C16-C15-C14	-2.25	118.91	123.52
17	B	839	CLA	O1D-CGD-CBD	2.25	128.96	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	816	CLA	CHB-C4A-NA	2.25	127.65	124.40
17	B	836	CLA	C3A-C2A-C1A	2.25	104.71	101.34
18	2	313	CHL	OMC-CMC-C2C	-2.25	121.21	125.12
17	B	820	CLA	CAA-C2A-C1A	-2.25	104.60	111.97
17	B	833	CLA	O2D-CGD-CBD	2.25	115.17	111.23
17	1	302	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
17	B	821	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
21	I	101	BCR	C16-C15-C14	-2.25	118.92	123.52
17	A	812	CLA	CHB-C4A-NA	2.25	127.64	124.40
17	1	306	CLA	O2A-CGA-O1A	-2.25	116.49	123.20
17	1	313	CLA	CMB-C2B-C3B	2.24	131.83	126.55
24	4	319	LMG	O6-C1-O1	-2.24	104.74	110.04
17	B	821	CLA	O2D-CGD-CBD	2.24	115.15	111.23
17	A	809	CLA	CMB-C2B-C1B	-2.24	122.00	125.42
17	A	805	CLA	CHB-C4A-NA	2.24	127.64	124.40
17	A	810	CLA	CHB-C4A-NA	2.24	127.64	124.40
26	4	323	DGD	C1D-C2D-C3D	-2.24	105.29	110.01
22	1	317	LHG	C18-C17-C16	-2.24	103.04	114.37
21	B	844	BCR	C2-C1-C6	2.24	113.69	110.44
21	4	318	BCR	C40-C30-C25	2.24	113.76	110.24
17	B	818	CLA	CMB-C2B-C3B	2.24	131.82	126.55
24	B	852	LMG	C40-C39-C38	-2.24	103.05	114.37
24	4	319	LMG	O7-C10-C11	2.24	116.32	111.48
17	B	822	CLA	C1-C2-C3	-2.24	123.14	126.76
21	A	849	BCR	C8-C7-C6	-2.24	121.02	127.00
17	A	834	CLA	CHB-C4A-NA	2.24	127.63	124.40
17	A	826	CLA	CHB-C4A-NA	2.24	127.63	124.40
24	4	319	LMG	C38-C37-C36	-2.23	103.07	114.37
17	B	836	CLA	CHA-C1A-NA	-2.23	121.34	126.39
17	4	304	CLA	CHA-C4D-ND	2.23	137.15	132.55
17	B	815	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
17	B	834	CLA	CAA-C2A-C1A	-2.23	104.67	111.97
17	B	837	CLA	CED-O2D-CGD	-2.23	110.86	115.92
17	B	820	CLA	CHB-C1B-C2B	-2.23	120.96	127.43
17	A	808	CLA	O2D-CGD-CBD	2.23	115.12	111.23
17	A	853	CLA	C2A-C1A-CHA	2.23	127.73	123.87
17	L	204	CLA	CHB-C4A-NA	2.23	127.61	124.40
21	A	849	BCR	C24-C23-C22	-2.23	122.94	126.23
17	B	832	CLA	C2D-C1D-ND	-2.23	107.92	110.13
17	A	805	CLA	O2A-CGA-CBA	2.23	118.62	111.83
17	3	609	CLA	CHB-C4A-NA	2.22	127.61	124.40
19	1	314	LUT	C18-C5-C4	-2.22	110.33	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	315	CHL	CAC-C3C-C4C	2.22	129.74	124.03
17	3	610	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
26	B	850	DGD	O2G-C1B-O1B	-2.22	118.51	123.70
17	B	831	CLA	CHB-C1B-NB	2.22	127.38	124.05
17	4	304	CLA	CAA-C2A-C3A	-2.22	107.00	113.00
24	F	309	LMG	O3-C3-C2	-2.22	105.15	110.38
17	1	310	CLA	O2A-CGA-O1A	-2.22	118.09	123.63
17	2	312	CLA	O2D-CGD-CBD	2.21	115.10	111.23
17	F	306	CLA	CHB-C4A-NA	2.21	127.59	124.40
17	3	609	CLA	C1-C2-C3	-2.21	123.19	126.76
17	2	301	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
17	B	839	CLA	CHA-C1A-NA	-2.21	121.39	126.39
17	3	604	CLA	O2A-CGA-O1A	-2.21	117.65	123.33
17	B	814	CLA	CHB-C1B-NB	2.21	127.36	124.05
17	1	301	CLA	CED-O2D-CGD	2.21	120.92	115.92
17	A	836	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
17	F	307	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
17	B	834	CLA	CMA-C3A-C4A	-2.20	105.85	111.77
17	A	807	CLA	CHB-C1B-NB	2.20	127.36	124.05
17	3	608	CLA	O2A-CGA-O1A	-2.20	118.11	123.63
17	2	307	CLA	CMB-C2B-C1B	-2.20	122.06	125.42
17	J	101	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
22	1	317	LHG	O8-C23-C24	2.20	118.55	111.83
17	B	828	CLA	CMB-C2B-C3B	2.20	131.73	126.55
17	B	831	CLA	O1A-CGA-CBA	2.20	132.38	123.78
18	2	306	CHL	C4C-CHD-C1D	2.20	123.93	116.07
17	1	302	CLA	CMB-C2B-C3B	2.20	131.72	126.55
17	A	824	CLA	CHB-C4A-NA	2.20	127.57	124.40
17	A	802	CLA	C4D-C3D-CAD	-2.19	105.72	108.11
21	1	316	BCR	C28-C27-C26	-2.19	110.14	114.06
17	2	310	CLA	CHB-C4A-NA	2.19	127.56	124.40
21	1	316	BCR	C2-C1-C6	2.19	113.62	110.44
17	A	838	CLA	CHB-C4A-NA	2.19	127.56	124.40
26	4	323	DGD	C3G-O3G-C1D	2.19	118.49	113.80
17	A	814	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
17	1	307	CLA	CAA-CBA-CGA	-2.19	107.00	113.21
18	4	305	CHL	O1D-CGD-CBD	-2.19	121.41	124.72
17	A	837	CLA	CMB-C2B-C3B	2.19	131.69	126.55
17	A	812	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
21	F	303	BCR	C38-C26-C27	-2.18	108.94	113.60
17	B	812	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
17	A	835	CLA	O2A-CGA-O1A	-2.18	118.17	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	840	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
17	A	822	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
21	A	847	BCR	C38-C26-C25	-2.18	122.10	124.48
17	A	812	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
21	J	105	BCR	C30-C25-C26	-2.18	119.66	122.64
17	3	604	CLA	O1D-CGD-CBD	2.17	128.81	124.52
21	F	303	BCR	C37-C22-C21	-2.17	119.30	122.82
17	B	804	CLA	CHB-C4A-NA	2.17	127.54	124.40
24	G	101	LMG	O6-C1-O1	-2.17	104.91	110.04
17	B	831	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
17	B	812	CLA	O2D-CGD-CBD	2.17	115.03	111.23
18	3	601	CHL	OMC-CMC-C2C	-2.17	121.35	125.12
22	2	317	LHG	C27-C26-C25	-2.17	103.42	114.37
18	2	313	CHL	OBD-CAD-C3D	-2.17	124.51	127.89
21	4	318	BCR	C16-C15-C14	-2.17	119.09	123.52
17	B	835	CLA	CHB-C4A-NA	2.16	127.52	124.40
21	F	303	BCR	C16-C15-C14	-2.16	119.09	123.52
21	K	203	BCR	C15-C16-C17	-2.16	119.09	123.52
17	B	842	CLA	O2D-CGD-CBD	2.16	115.01	111.23
17	A	810	CLA	O1D-CGD-CBD	2.16	128.79	124.52
17	B	830	CLA	CHB-C1B-NB	2.16	127.29	124.05
17	B	829	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
17	A	804	CLA	CAA-CBA-CGA	-2.16	107.07	113.21
21	2	316	BCR	C38-C26-C25	-2.16	122.13	124.48
17	B	811	CLA	CBA-CAA-C2A	-2.16	107.37	113.79
21	L	201	BCR	C7-C8-C9	-2.16	123.04	126.23
17	1	313	CLA	CHB-C4A-NA	2.16	127.52	124.40
17	B	811	CLA	C1-C2-C3	-2.16	122.66	126.20
17	A	806	CLA	CAC-C3C-C4C	2.16	127.60	124.79
17	B	840	CLA	C1-C2-C3	-2.16	122.66	126.20
17	1	302	CLA	CHB-C4A-NA	2.16	127.51	124.40
17	A	814	CLA	CHB-C4A-NA	2.16	127.51	124.40
17	A	820	CLA	CHB-C4A-NA	2.16	127.51	124.40
25	B	851	HTG	O5-C5-C6	2.16	111.78	106.44
17	L	203	CLA	O2A-CGA-O1A	-2.16	118.24	123.63
17	A	853	CLA	O2A-CGA-CBA	2.16	118.41	111.83
18	2	305	CHL	O1D-CGD-CBD	-2.15	121.45	124.72
22	G	102	LHG	C18-C17-C16	-2.15	103.48	114.37
21	A	851	BCR	C15-C16-C17	-2.15	119.11	123.52
17	B	829	CLA	CAA-C2A-C1A	2.15	119.03	111.97
24	F	309	LMG	C38-C37-C36	-2.15	103.49	114.37
17	G	104	CLA	CHD-C1D-ND	-2.15	121.77	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	616	BCR	C27-C26-C25	2.15	125.61	122.70
17	B	802	CLA	C11-C10-C8	-2.15	108.82	115.97
17	4	312	CLA	C1-C2-C3	-2.15	122.67	126.20
17	B	841	CLA	CHB-C4A-NA	2.15	127.50	124.40
17	B	829	CLA	CHA-C1A-NA	-2.15	121.52	126.39
20	1	315	XAT	O24-C25-C24	2.15	115.50	113.49
21	F	308	BCR	C30-C25-C26	-2.15	119.70	122.64
21	1	316	BCR	C15-C14-C13	-2.14	124.27	127.28
20	3	615	XAT	O24-C25-C24	2.14	115.50	113.49
17	4	314	CLA	CHD-C1D-ND	-2.14	121.79	124.80
18	4	306	CHL	CED-O2D-CGD	2.14	120.78	115.92
17	4	304	CLA	C2A-C1A-CHA	2.14	127.59	123.87
17	4	311	CLA	CHB-C4A-NA	2.14	127.49	124.40
22	F	302	LHG	C27-C26-C25	-2.14	103.54	114.37
17	4	312	CLA	CHB-C4A-NA	2.14	127.49	124.40
26	4	323	DGD	C4E-C3E-C2E	2.14	114.59	110.83
17	A	833	CLA	C1-C2-C3	-2.14	123.30	126.76
17	1	309	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
21	B	848	BCR	C15-C16-C17	-2.14	119.14	123.52
17	B	807	CLA	CHB-C1B-NB	2.14	127.26	124.05
18	2	313	CHL	C4C-CHD-C1D	2.14	123.72	116.07
24	4	320	LMG	O2-C2-C3	-2.14	105.34	110.38
17	A	801	CLA	CHA-C1A-NA	-2.14	121.55	126.39
17	A	843	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
21	A	849	BCR	C16-C17-C18	-2.14	124.28	127.28
17	A	840	CLA	CHD-C1D-C2D	2.14	129.93	125.49
17	4	304	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
17	B	818	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
17	B	836	CLA	O2A-CGA-O1A	-2.13	117.85	123.33
17	B	820	CLA	O2D-CGD-CBD	2.13	114.96	111.23
17	A	801	CLA	CMD-C2D-C3D	2.13	132.57	127.69
26	B	850	DGD	O6E-C5E-C6E	-2.13	101.16	106.44
18	2	313	CHL	CMB-C2B-C3B	2.13	128.94	124.68
17	B	805	CLA	CHA-C1A-NA	-2.13	121.57	126.39
17	A	823	CLA	O2D-CGD-CBD	2.13	114.95	111.23
17	2	302	CLA	CHB-C4A-NA	2.13	127.47	124.40
21	4	318	BCR	C11-C10-C9	-2.12	124.30	127.28
17	3	602	CLA	CHB-C4A-NA	2.12	127.46	124.40
17	B	816	CLA	CHB-C1B-NB	2.12	127.23	124.05
17	B	814	CLA	CHD-C1D-ND	-2.12	121.82	124.80
17	1	313	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
24	G	101	LMG	O3-C3-C2	-2.12	105.38	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	837	CLA	CAC-C3C-C2C	2.12	131.45	127.56
17	B	838	CLA	CMB-C2B-C3B	2.12	131.53	126.55
17	A	841	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
18	4	305	CHL	C1-C2-C3	-2.12	122.73	126.20
21	1	316	BCR	C27-C26-C25	2.12	125.56	122.70
26	B	850	DGD	CAB-C9B-C8B	-2.12	103.67	114.37
17	A	841	CLA	C3B-C4B-NB	-2.12	108.64	110.53
21	B	845	BCR	C31-C1-C6	2.12	113.56	110.24
17	A	828	CLA	CHD-C1D-ND	-2.12	121.83	124.80
17	K	202	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
17	2	309	CLA	CMA-C3A-C2A	-2.11	111.39	116.23
24	B	852	LMG	C38-C37-C36	-2.11	103.69	114.37
17	B	833	CLA	C3B-C4B-NB	-2.11	108.64	110.53
18	2	306	CHL	C5-C3-C4	2.11	119.45	114.59
21	B	844	BCR	C33-C5-C6	-2.11	122.18	124.48
17	B	805	CLA	CHB-C1B-NB	2.11	127.22	124.05
17	J	101	CLA	CBC-CAC-C3C	-2.11	106.70	112.42
21	K	203	BCR	C33-C5-C6	-2.11	122.18	124.48
18	2	304	CHL	C4C-CHD-C1D	2.11	123.61	116.07
17	1	301	CLA	O2D-CGD-CBD	2.11	114.92	111.23
17	B	818	CLA	C6-C5-C3	2.11	118.60	113.47
17	A	807	CLA	CHD-C1D-ND	-2.11	121.84	124.80
17	A	838	CLA	CHA-C1A-NA	-2.11	121.62	126.39
21	2	316	BCR	C11-C10-C9	-2.11	124.32	127.28
17	4	303	CLA	CAC-C3C-C4C	2.11	127.53	124.79
21	K	203	BCR	C3-C4-C5	-2.11	110.30	114.06
18	1	305	CHL	O2A-CGA-O1A	-2.11	118.36	123.63
17	4	308	CLA	CMB-C2B-C3B	2.11	131.50	126.55
21	J	104	BCR	C24-C23-C22	-2.10	123.12	126.23
17	1	312	CLA	CHB-C4A-NA	2.10	127.44	124.40
17	A	815	CLA	O2D-CGD-CBD	2.10	114.91	111.23
17	B	808	CLA	CHA-C4D-ND	2.10	136.89	132.55
18	4	301	CHL	C3D-C4D-ND	2.10	116.31	112.94
17	F	307	CLA	CHB-C1B-NB	2.10	127.20	124.05
20	2	315	XAT	O24-C25-C24	2.10	115.46	113.49
17	A	837	CLA	CHD-C1D-ND	-2.10	121.84	124.80
17	A	827	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
17	A	828	CLA	O1D-CGD-CBD	2.10	128.66	124.52
17	A	802	CLA	CMB-C2B-C3B	2.10	131.49	126.55
17	A	801	CLA	C4D-C3D-CAD	-2.10	105.83	108.11
18	4	307	CHL	C1C-C2C-CMC	2.10	130.59	126.80
18	4	301	CHL	C4-C3-C5	2.10	118.87	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	820	CLA	CHD-C1D-ND	-2.10	121.85	124.80
21	A	850	BCR	C20-C21-C22	-2.10	124.34	127.28
17	B	826	CLA	C2A-C1A-CHA	2.10	127.50	123.87
18	4	306	CHL	O2A-CGA-O1A	-2.10	118.39	123.63
17	A	839	CLA	CAC-C3C-C4C	2.09	127.52	124.79
20	4	317	XAT	O24-C25-C26	-2.09	57.27	58.93
18	3	601	CHL	CGD-CBD-CAD	-2.09	104.07	110.85
25	F	305	HTG	C1-C2-C3	-2.09	106.45	110.55
17	A	825	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
17	B	825	CLA	CHB-C1B-NB	2.09	127.19	124.05
27	A	842	PQN	C16-C15-C13	2.09	118.56	113.47
21	4	318	BCR	C28-C27-C26	-2.09	110.33	114.06
17	4	302	CLA	CHA-C4D-ND	2.09	136.86	132.55
17	A	835	CLA	CHB-C4A-NA	2.09	127.42	124.40
18	4	301	CHL	C4D-ND-C1D	-2.09	103.63	105.22
17	A	825	CLA	CHB-C4A-NA	2.09	127.42	124.40
17	B	830	CLA	C5-C3-C2	2.09	125.86	121.17
21	F	303	BCR	C40-C30-C25	2.09	113.52	110.24
17	B	807	CLA	CMB-C2B-C3B	2.09	131.46	126.55
17	2	311	CLA	CMB-C2B-C3B	2.09	131.46	126.55
17	A	818	CLA	CAA-C2A-C1A	-2.09	105.14	111.97
17	A	843	CLA	CBC-CAC-C3C	2.09	118.07	112.42
17	1	302	CLA	C1-C2-C3	-2.08	122.78	126.20
17	2	308	CLA	C1-C2-C3	-2.08	122.78	126.20
17	2	307	CLA	CHD-C1D-ND	-2.08	121.87	124.80
17	B	815	CLA	C12-C11-C10	-2.08	103.94	113.28
22	1	317	LHG	C20-C19-C18	-2.08	103.84	114.37
17	A	824	CLA	O2D-CGD-CBD	2.08	114.87	111.23
17	A	821	CLA	CHB-C1B-NB	2.08	127.17	124.05
27	B	843	PQN	C5-C4-C3	-2.08	114.45	118.27
21	B	845	BCR	C28-C27-C26	-2.08	110.34	114.06
17	B	820	CLA	C3C-C4C-NC	-2.08	107.76	110.43
17	K	201	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
17	4	310	CLA	C11-C10-C8	-2.08	109.05	115.97
17	A	831	CLA	CHD-C1D-ND	-2.08	121.87	124.80
18	3	607	CHL	O2A-CGA-CBA	2.08	120.00	112.14
17	A	827	CLA	C4-C3-C5	2.08	118.84	115.23
21	I	101	BCR	C15-C14-C13	-2.08	124.36	127.28
17	A	812	CLA	CED-O2D-CGD	2.08	120.63	115.92
17	A	818	CLA	CHD-C1D-ND	-2.08	121.88	124.80
17	A	825	CLA	CHD-C1D-C2D	2.08	129.81	125.49
17	A	817	CLA	CHB-C4A-NA	2.08	127.40	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	F	309	LMG	C42-C41-C40	-2.08	103.87	114.37
17	B	836	CLA	C3B-C4B-NB	-2.08	108.68	110.53
22	B	801	LHG	O8-C23-C24	2.08	121.19	112.38
17	L	202	CLA	O2D-CGD-CBD	2.08	114.86	111.23
17	A	839	CLA	C3A-C2A-C1A	2.08	104.45	101.34
18	4	301	CHL	CAC-C3C-C4C	2.07	129.36	124.03
17	B	808	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
17	B	829	CLA	CHB-C4A-NA	2.07	127.39	124.40
21	J	105	BCR	C16-C15-C14	-2.07	119.28	123.52
17	3	608	CLA	CHB-C4A-NA	2.07	127.39	124.40
17	A	808	CLA	O2A-CGA-CBA	2.07	118.16	111.83
17	A	824	CLA	C16-C15-C13	-2.07	109.08	115.97
17	B	836	CLA	CMC-C2C-C3C	2.07	131.75	126.15
17	B	826	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
21	F	303	BCR	C33-C5-C6	-2.07	122.22	124.48
17	A	830	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
21	A	847	BCR	C29-C30-C25	2.07	113.45	110.44
17	B	813	CLA	CAB-C3B-C2B	2.07	129.03	123.53
17	A	853	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
17	A	853	CLA	CHD-C1D-ND	-2.07	121.89	124.80
17	B	802	CLA	CHA-C4D-ND	2.07	136.81	132.55
17	A	801	CLA	C4D-CHA-C1A	2.07	123.71	121.24
17	A	827	CLA	CAC-C3C-C4C	2.06	127.48	124.79
17	A	825	CLA	C3A-C2A-C1A	2.06	104.43	101.34
26	B	850	DGD	O6D-C5D-C6D	-2.06	102.60	106.69
17	2	311	CLA	O1D-CGD-CBD	2.06	128.59	124.52
17	A	830	CLA	C1-C2-C3	-2.06	123.43	126.76
17	4	304	CLA	CED-O2D-CGD	2.06	120.59	115.92
17	B	802	CLA	C6-C7-C8	-2.06	109.11	115.97
17	A	809	CLA	CMB-C2B-C3B	2.06	131.40	126.55
17	G	105	CLA	CHB-C4A-NA	2.06	127.37	124.40
17	A	833	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
25	F	305	HTG	C6-C5-C4	-2.06	107.96	113.02
21	B	848	BCR	C39-C30-C25	-2.06	107.01	110.24
21	A	850	BCR	C38-C26-C25	-2.06	122.24	124.48
18	4	301	CHL	C7-C6-C5	-2.06	107.78	113.26
17	B	828	CLA	C16-C15-C13	-2.06	109.13	115.97
17	A	819	CLA	O2D-CGD-CBD	2.05	114.82	111.23
18	4	301	CHL	C4-C3-C2	-2.05	118.35	123.63
17	1	309	CLA	CHA-C1A-NA	-2.05	121.74	126.39
22	A	844	LHG	C27-C26-C25	-2.05	103.99	114.37
22	F	302	LHG	C18-C17-C16	-2.05	104.00	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	308	CLA	O2D-CGD-O1D	-2.05	119.86	123.85
17	1	312	CLA	CHD-C1D-ND	-2.05	121.92	124.80
17	G	105	CLA	C3A-C2A-C1A	2.05	104.41	101.34
21	G	106	BCR	C8-C7-C6	-2.05	121.53	127.00
17	B	837	CLA	CMA-C3A-C2A	-2.05	106.07	113.98
21	B	847	BCR	C24-C23-C22	-2.04	123.21	126.23
17	A	837	CLA	C3B-C4B-NB	-2.04	108.71	110.53
24	4	319	LMG	C3-C4-C5	-2.04	106.53	110.23
22	G	102	LHG	O8-C23-O10	-2.04	118.52	123.63
18	3	601	CHL	C4C-CHD-C1D	2.04	123.37	116.07
17	A	841	CLA	CHB-C4A-NA	2.04	127.35	124.40
17	B	826	CLA	O2D-CGD-O1D	-2.04	119.88	123.85
17	B	813	CLA	O2D-CGD-CBD	2.04	114.80	111.23
17	B	835	CLA	CHA-C1A-NA	-2.04	121.77	126.39
17	B	802	CLA	C1D-ND-C4D	2.04	107.74	106.31
17	B	828	CLA	CHA-C4D-ND	2.04	136.76	132.55
21	L	205	BCR	C33-C5-C6	-2.04	122.26	124.48
17	4	309	CLA	C2D-C1D-ND	-2.04	108.11	110.13
17	A	804	CLA	CHD-C1D-ND	-2.03	121.94	124.80
17	B	837	CLA	CMC-C2C-C3C	2.03	131.65	126.15
17	4	303	CLA	CAA-C2A-C3A	-2.03	107.51	113.00
18	2	305	CHL	C4C-CHD-C1D	2.03	123.34	116.07
17	3	603	CLA	C3B-C4B-NB	-2.03	108.72	110.53
17	B	810	CLA	C6-C5-C3	-2.03	108.52	113.47
17	B	806	CLA	C3B-C4B-NB	-2.03	108.72	110.53
17	2	307	CLA	CHB-C1B-NB	2.03	127.09	124.05
26	4	323	DGD	O3D-C3D-C4D	2.03	115.16	110.38
17	A	809	CLA	CHB-C1B-NB	2.03	127.09	124.05
18	4	305	CHL	C3D-C4D-ND	2.03	116.19	112.94
17	4	311	CLA	O1D-CGD-CBD	2.03	128.52	124.52
21	I	101	BCR	C29-C30-C25	2.03	113.39	110.44
17	A	853	CLA	CMB-C2B-C3B	2.03	131.32	126.55
17	G	104	CLA	CHD-C1D-C2D	2.03	129.71	125.49
17	A	838	CLA	CHD-C1D-ND	-2.03	121.95	124.80
17	A	830	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
17	2	319	CLA	CHB-C1B-NB	2.03	127.09	124.05
17	B	817	CLA	C3A-C2A-C1A	2.03	104.38	101.34
17	1	309	CLA	CAC-C3C-C4C	2.03	127.43	124.79
18	4	301	CHL	C4C-CHD-C1D	2.03	123.32	116.07
18	4	315	CHL	O1D-CGD-CBD	-2.03	121.65	124.72
17	4	303	CLA	CAA-CBA-CGA	-2.02	107.46	113.21
25	4	322	HTG	C3-C4-C5	2.02	113.90	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	301	CLA	CHC-C4B-NB	2.02	127.08	124.05
17	4	310	CLA	CAA-C2A-C1A	-2.02	105.35	111.97
17	B	841	CLA	CAA-C2A-C1A	-2.02	105.35	111.97
17	A	821	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
18	3	607	CHL	C4C-CHD-C1D	2.02	123.30	116.07
18	2	306	CHL	O2A-CGA-O1A	-2.02	118.57	123.63
21	L	201	BCR	C15-C14-C13	-2.02	124.44	127.28
17	4	303	CLA	CHB-C4A-NA	2.02	127.31	124.40
17	2	308	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
24	4	320	LMG	O6-C1-C2	-2.02	106.23	110.37
17	J	101	CLA	CHB-C4A-NA	2.02	127.31	124.40
17	B	841	CLA	CHD-C1D-C2D	2.02	129.68	125.49
17	B	811	CLA	CHB-C4A-NA	2.02	127.31	124.40
17	3	610	CLA	C2A-C1A-CHA	2.01	127.36	123.87
18	4	315	CHL	O2D-CGD-O1D	-2.01	119.93	123.85
17	A	827	CLA	CBC-CAC-C3C	2.01	117.87	112.42
17	2	312	CLA	C3B-C4B-NB	-2.01	108.73	110.53
17	F	304	CLA	C11-C10-C8	-2.01	109.28	115.97
18	2	304	CHL	CAC-C3C-C4C	2.01	129.20	124.03
17	1	310	CLA	O1D-CGD-CBD	2.01	128.48	124.52
17	B	820	CLA	C1D-ND-C4D	2.01	107.72	106.31
25	B	851	HTG	C3-C4-C5	-2.01	106.59	110.23
17	B	810	CLA	CHB-C1B-NB	2.01	127.06	124.05
17	B	837	CLA	CMC-C2C-C1C	-2.01	121.90	125.03
17	A	813	CLA	CHB-C4A-NA	2.00	127.29	124.40
24	B	852	LMG	O1-C7-C8	-2.00	105.94	110.82
17	1	301	CLA	CHD-C1D-C2D	2.00	129.66	125.49
26	B	850	DGD	C3G-C2G-C1G	-2.00	107.11	111.78
17	A	820	CLA	C1-C2-C3	-2.00	122.92	126.20
17	F	306	CLA	O2D-CGD-CBD	2.00	114.73	111.23
27	A	842	PQN	O1-C1-C2	-2.00	117.82	120.45
17	3	602	CLA	O2A-CGA-O1A	-2.00	118.62	123.63

All (178) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	1	301	CLA	ND
17	1	302	CLA	ND
17	1	303	CLA	ND
17	1	304	CLA	ND
17	1	306	CLA	ND
17	1	307	CLA	ND

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Mol	Chain	Res	Type	Atom
17	1	308	CLA	ND
17	1	309	CLA	ND
17	1	310	CLA	ND
17	1	311	CLA	ND
17	1	312	CLA	ND
17	1	313	CLA	ND
17	2	301	CLA	ND
17	2	302	CLA	ND
17	2	303	CLA	ND
17	2	307	CLA	ND
17	2	308	CLA	ND
17	2	309	CLA	ND
17	2	310	CLA	ND
17	2	311	CLA	ND
17	2	312	CLA	ND
17	2	319	CLA	ND
17	3	602	CLA	ND
17	3	603	CLA	ND
17	3	604	CLA	ND
17	3	605	CLA	ND
17	3	606	CLA	ND
17	3	608	CLA	ND
17	3	609	CLA	ND
17	3	610	CLA	ND
17	3	611	CLA	ND
17	3	612	CLA	ND
17	3	613	CLA	ND
17	4	302	CLA	ND
17	4	304	CLA	ND
17	4	308	CLA	ND
17	4	309	CLA	ND
17	4	310	CLA	ND
17	4	312	CLA	ND
17	4	313	CLA	ND
17	4	314	CLA	ND
17	A	801	CLA	ND
17	A	801	CLA	CBD
17	A	802	CLA	ND
17	A	803	CLA	ND
17	A	804	CLA	ND
17	A	805	CLA	ND
17	A	806	CLA	ND

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Mol	Chain	Res	Type	Atom
17	A	807	CLA	ND
17	A	808	CLA	ND
17	A	809	CLA	ND
17	A	810	CLA	ND
17	A	811	CLA	ND
17	A	812	CLA	ND
17	A	813	CLA	ND
17	A	814	CLA	ND
17	A	815	CLA	ND
17	A	816	CLA	ND
17	A	817	CLA	ND
17	A	818	CLA	ND
17	A	819	CLA	ND
17	A	820	CLA	ND
17	A	821	CLA	ND
17	A	822	CLA	ND
17	A	823	CLA	ND
17	A	824	CLA	ND
17	A	825	CLA	ND
17	A	826	CLA	ND
17	A	827	CLA	ND
17	A	828	CLA	ND
17	A	829	CLA	ND
17	A	830	CLA	ND
17	A	831	CLA	ND
17	A	832	CLA	ND
17	A	833	CLA	ND
17	A	834	CLA	ND
17	A	835	CLA	ND
17	A	836	CLA	ND
17	A	837	CLA	ND
17	A	838	CLA	ND
17	A	839	CLA	ND
17	A	840	CLA	ND
17	A	841	CLA	ND
17	A	843	CLA	ND
17	A	853	CLA	ND
17	B	802	CLA	ND
17	B	803	CLA	ND
17	B	804	CLA	ND
17	B	805	CLA	ND
17	B	806	CLA	ND

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Mol	Chain	Res	Type	Atom
17	B	807	CLA	ND
17	B	808	CLA	ND
17	B	809	CLA	ND
17	B	810	CLA	ND
17	B	811	CLA	ND
17	B	813	CLA	ND
17	B	814	CLA	ND
17	B	815	CLA	ND
17	B	816	CLA	ND
17	B	817	CLA	ND
17	B	818	CLA	ND
17	B	819	CLA	ND
17	B	820	CLA	ND
17	B	821	CLA	ND
17	B	822	CLA	ND
17	B	823	CLA	ND
17	B	824	CLA	ND
17	B	825	CLA	ND
17	B	826	CLA	ND
17	B	827	CLA	ND
17	B	828	CLA	ND
17	B	829	CLA	ND
17	B	830	CLA	ND
17	B	831	CLA	ND
17	B	832	CLA	ND
17	B	833	CLA	ND
17	B	834	CLA	ND
17	B	835	CLA	ND
17	B	836	CLA	ND
17	B	837	CLA	ND
17	B	838	CLA	ND
17	B	839	CLA	ND
17	B	840	CLA	ND
17	B	841	CLA	ND
17	B	842	CLA	ND
17	F	304	CLA	ND
17	F	306	CLA	ND
17	F	307	CLA	ND
17	G	103	CLA	ND
17	G	104	CLA	ND
17	G	105	CLA	ND
17	J	101	CLA	ND

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Mol	Chain	Res	Type	Atom
17	J	103	CLA	ND
17	L	202	CLA	ND
17	L	203	CLA	ND
17	K	201	CLA	ND
17	K	202	CLA	ND
18	1	305	CHL	NC
18	1	305	CHL	NA
18	1	305	CHL	ND
18	2	304	CHL	NC
18	2	304	CHL	NA
18	2	304	CHL	ND
18	2	305	CHL	NC
18	2	305	CHL	NA
18	2	305	CHL	ND
18	2	306	CHL	NC
18	2	306	CHL	NA
18	2	306	CHL	ND
18	2	313	CHL	NC
18	2	313	CHL	NA
18	2	313	CHL	ND
18	3	601	CHL	NC
18	3	601	CHL	NA
18	3	601	CHL	ND
18	3	607	CHL	NC
18	3	607	CHL	NA
18	3	607	CHL	ND
18	4	301	CHL	C8
18	4	301	CHL	NC
18	4	301	CHL	NA
18	4	301	CHL	ND
18	4	305	CHL	C8
18	4	305	CHL	NC
18	4	305	CHL	NA
18	4	305	CHL	ND
18	4	306	CHL	NC
18	4	306	CHL	NA
18	4	306	CHL	ND
18	4	307	CHL	NC
18	4	307	CHL	NA
18	4	307	CHL	ND
18	4	315	CHL	NC
18	4	315	CHL	NA

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Mol	Chain	Res	Type	Atom
18	4	315	CHL	ND
20	4	317	XAT	C26
20	4	317	XAT	C25
20	4	317	XAT	C6

All (1883) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	1	301	CLA	CHA-CBD-CGD-O1D
17	1	301	CLA	CHA-CBD-CGD-O2D
17	1	307	CLA	CBA-CGA-O2A-C1
17	1	307	CLA	O1A-CGA-O2A-C1
17	1	309	CLA	C1A-C2A-CAA-CBA
17	1	311	CLA	C4B-C3B-CAB-CBB
17	1	311	CLA	CBD-CGD-O2D-CED
17	1	312	CLA	C1A-C2A-CAA-CBA
17	1	313	CLA	CBA-CGA-O2A-C1
17	2	301	CLA	CHA-CBD-CGD-O1D
17	2	301	CLA	CHA-CBD-CGD-O2D
17	2	309	CLA	CBD-CGD-O2D-CED
17	2	310	CLA	CBD-CGD-O2D-CED
17	3	602	CLA	CHA-CBD-CGD-O1D
17	3	602	CLA	CHA-CBD-CGD-O2D
17	3	604	CLA	CBD-CGD-O2D-CED
17	3	606	CLA	C1A-C2A-CAA-CBA
17	3	606	CLA	C3A-C2A-CAA-CBA
17	4	304	CLA	C1A-C2A-CAA-CBA
17	4	309	CLA	CBD-CGD-O2D-CED
17	4	310	CLA	C1A-C2A-CAA-CBA
17	4	314	CLA	C2B-C3B-CAB-CBB
17	4	314	CLA	C4B-C3B-CAB-CBB
17	A	803	CLA	C1A-C2A-CAA-CBA
17	A	803	CLA	C3A-C2A-CAA-CBA
17	A	804	CLA	CAD-CBD-CGD-O1D
17	A	804	CLA	CAD-CBD-CGD-O2D
17	A	805	CLA	C1A-C2A-CAA-CBA
17	A	805	CLA	CBD-CGD-O2D-CED
17	A	807	CLA	C3A-C2A-CAA-CBA
17	A	807	CLA	CHA-CBD-CGD-O1D
17	A	807	CLA	CHA-CBD-CGD-O2D
17	A	810	CLA	C1A-C2A-CAA-CBA
17	A	814	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	A	814	CLA	C3A-C2A-CAA-CBA
17	A	814	CLA	CBA-CGA-O2A-C1
17	A	814	CLA	O1A-CGA-O2A-C1
17	A	815	CLA	CBD-CGD-O2D-CED
17	A	816	CLA	CHA-CBD-CGD-O1D
17	A	816	CLA	CHA-CBD-CGD-O2D
17	A	817	CLA	C3A-C2A-CAA-CBA
17	A	818	CLA	C1A-C2A-CAA-CBA
17	A	818	CLA	C3A-C2A-CAA-CBA
17	A	821	CLA	CHA-CBD-CGD-O1D
17	A	821	CLA	CHA-CBD-CGD-O2D
17	A	822	CLA	C2B-C3B-CAB-CBB
17	A	822	CLA	C4B-C3B-CAB-CBB
17	A	822	CLA	CBD-CGD-O2D-CED
17	A	823	CLA	C2B-C3B-CAB-CBB
17	A	823	CLA	C4B-C3B-CAB-CBB
17	A	825	CLA	C6-C7-C8-C9
17	A	829	CLA	CHA-CBD-CGD-O1D
17	A	829	CLA	CHA-CBD-CGD-O2D
17	A	831	CLA	C1A-C2A-CAA-CBA
17	A	832	CLA	CHA-CBD-CGD-O1D
17	A	832	CLA	CHA-CBD-CGD-O2D
17	A	834	CLA	C1A-C2A-CAA-CBA
17	A	834	CLA	C3A-C2A-CAA-CBA
17	A	837	CLA	C1A-C2A-CAA-CBA
17	A	840	CLA	C2B-C3B-CAB-CBB
17	A	840	CLA	C4B-C3B-CAB-CBB
17	A	843	CLA	CAD-CBD-CGD-O2D
17	B	807	CLA	C1A-C2A-CAA-CBA
17	B	807	CLA	C3A-C2A-CAA-CBA
17	B	810	CLA	CHA-CBD-CGD-O1D
17	B	810	CLA	CHA-CBD-CGD-O2D
17	B	812	CLA	CBD-CGD-O2D-CED
17	B	817	CLA	CHA-CBD-CGD-O1D
17	B	817	CLA	CHA-CBD-CGD-O2D
17	B	819	CLA	C4B-C3B-CAB-CBB
17	B	820	CLA	C3A-C2A-CAA-CBA
17	B	820	CLA	C2-C3-C5-C6
17	B	820	CLA	C6-C7-C8-C9
17	B	824	CLA	C1A-C2A-CAA-CBA
17	B	825	CLA	C1A-C2A-CAA-CBA
17	B	826	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
17	B	826	CLA	CHA-CBD-CGD-O2D
17	B	830	CLA	C1A-C2A-CAA-CBA
17	B	830	CLA	C3A-C2A-CAA-CBA
17	B	831	CLA	C1A-C2A-CAA-CBA
17	B	834	CLA	CHA-CBD-CGD-O1D
17	B	834	CLA	CHA-CBD-CGD-O2D
17	B	839	CLA	C1A-C2A-CAA-CBA
17	B	839	CLA	C3A-C2A-CAA-CBA
17	G	105	CLA	CHA-CBD-CGD-O1D
17	G	105	CLA	CHA-CBD-CGD-O2D
17	J	103	CLA	C1A-C2A-CAA-CBA
17	J	103	CLA	C3A-C2A-CAA-CBA
17	L	202	CLA	C1A-C2A-CAA-CBA
17	L	202	CLA	C3A-C2A-CAA-CBA
17	L	204	CLA	C3A-C2A-CAA-CBA
18	1	305	CHL	C1A-C2A-CAA-CBA
18	2	304	CHL	C1C-C2C-CMC-OMC
18	2	305	CHL	CHA-CBD-CGD-O1D
18	2	305	CHL	CHA-CBD-CGD-O2D
18	4	301	CHL	CBD-CGD-O2D-CED
18	4	305	CHL	CBA-CGA-O2A-C1
18	4	305	CHL	C1C-C2C-CMC-OMC
18	4	305	CHL	C3C-C2C-CMC-OMC
18	4	306	CHL	C3A-C2A-CAA-CBA
18	4	315	CHL	CBD-CGD-O2D-CED
19	1	314	LUT	C5-C6-C7-C8
19	1	314	LUT	C11-C10-C9-C19
19	1	314	LUT	C10-C11-C12-C13
19	1	314	LUT	C20-C13-C14-C15
19	1	314	LUT	C39-C29-C30-C31
19	1	314	LUT	C40-C33-C34-C35
19	2	314	LUT	C5-C6-C7-C8
19	2	314	LUT	C11-C10-C9-C8
19	2	314	LUT	C10-C11-C12-C13
19	2	314	LUT	C20-C13-C14-C15
19	2	314	LUT	C39-C29-C30-C31
19	2	314	LUT	C31-C32-C33-C40
19	2	314	LUT	C40-C33-C34-C35
19	3	614	LUT	C5-C6-C7-C8
19	3	614	LUT	C11-C10-C9-C8
19	3	614	LUT	C10-C11-C12-C13
19	3	614	LUT	C20-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
19	3	614	LUT	C39-C29-C30-C31
19	3	614	LUT	C40-C33-C34-C35
19	4	316	LUT	C5-C6-C7-C8
19	4	316	LUT	C7-C8-C9-C19
19	4	316	LUT	C11-C10-C9-C19
19	4	316	LUT	C20-C13-C14-C15
19	4	316	LUT	C39-C29-C30-C31
19	4	316	LUT	C31-C32-C33-C40
19	4	316	LUT	C40-C33-C34-C35
20	1	315	XAT	C7-C8-C9-C19
20	1	315	XAT	C11-C10-C9-C19
20	1	315	XAT	C20-C13-C14-C15
20	1	315	XAT	C39-C29-C30-C31
20	1	315	XAT	C40-C33-C34-C35
20	2	315	XAT	C7-C8-C9-C19
20	2	315	XAT	C11-C10-C9-C19
20	2	315	XAT	C20-C13-C14-C15
20	2	315	XAT	C39-C29-C30-C31
20	2	315	XAT	C40-C33-C34-C35
20	3	615	XAT	C7-C8-C9-C19
20	3	615	XAT	C11-C10-C9-C19
20	3	615	XAT	C20-C13-C14-C15
20	3	615	XAT	C39-C29-C30-C31
20	3	615	XAT	C40-C33-C34-C35
20	4	317	XAT	C11-C10-C9-C19
20	4	317	XAT	C11-C12-C13-C20
20	4	317	XAT	C20-C13-C14-C15
20	4	317	XAT	C27-C28-C29-C39
20	4	317	XAT	C39-C29-C30-C31
20	4	317	XAT	C40-C33-C34-C35
21	1	316	BCR	C11-C12-C13-C14
21	1	316	BCR	C20-C21-C22-C37
21	2	316	BCR	C10-C11-C12-C13
21	2	316	BCR	C16-C17-C18-C36
21	2	316	BCR	C21-C22-C23-C24
21	2	316	BCR	C37-C22-C23-C24
21	A	846	BCR	C21-C22-C23-C24
21	A	847	BCR	C7-C8-C9-C10
21	A	847	BCR	C7-C8-C9-C34
21	A	848	BCR	C20-C21-C22-C23
21	A	848	BCR	C20-C21-C22-C37
21	A	849	BCR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
21	A	850	BCR	C37-C22-C23-C24
21	A	850	BCR	C23-C24-C25-C26
21	B	844	BCR	C21-C22-C23-C24
21	B	844	BCR	C37-C22-C23-C24
21	B	845	BCR	C21-C22-C23-C24
21	B	845	BCR	C37-C22-C23-C24
21	B	846	BCR	C21-C22-C23-C24
21	B	848	BCR	C16-C17-C18-C36
21	B	848	BCR	C23-C24-C25-C26
21	F	303	BCR	C7-C8-C9-C34
21	F	303	BCR	C35-C13-C14-C15
21	G	106	BCR	C20-C21-C22-C37
21	G	106	BCR	C22-C23-C24-C25
21	I	101	BCR	C20-C21-C22-C37
21	J	105	BCR	C37-C22-C23-C24
21	J	105	BCR	C23-C24-C25-C26
21	L	201	BCR	C21-C22-C23-C24
21	L	205	BCR	C21-C22-C23-C24
21	L	205	BCR	C37-C22-C23-C24
21	L	205	BCR	C23-C24-C25-C26
21	L	205	BCR	C23-C24-C25-C30
21	K	203	BCR	C18-C19-C20-C21
21	K	203	BCR	C20-C21-C22-C23
21	K	203	BCR	C21-C22-C23-C24
22	1	317	LHG	C3-O3-P-O5
22	2	317	LHG	C4-O6-P-O3
22	2	317	LHG	C4-O6-P-O5
22	2	317	LHG	C24-C23-O8-C6
22	A	844	LHG	C3-O3-P-O6
22	A	845	LHG	C3-O3-P-O6
22	A	845	LHG	C4-O6-P-O3
22	B	801	LHG	C4-O6-P-O3
22	B	801	LHG	C4-O6-P-O4
22	F	302	LHG	O2-C2-C3-O3
22	F	302	LHG	C3-O3-P-O5
22	F	302	LHG	C3-O3-P-O6
22	F	302	LHG	C4-O6-P-O3
22	F	302	LHG	C4-O6-P-O4
22	F	302	LHG	C5-C4-O6-P
22	G	102	LHG	O1-C1-C2-C3
22	G	102	LHG	C4-O6-P-O3
22	G	102	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
23	2	318	LMT	C2B-C1B-O1B-C4'
23	2	318	LMT	C2'-C1'-O1'-C1
23	2	318	LMT	O5'-C1'-O1'-C1
24	4	320	LMG	O6-C1-O1-C7
24	4	320	LMG	O1-C7-C8-O7
24	4	320	LMG	O9-C10-O7-C8
24	4	320	LMG	C11-C10-O7-C8
24	B	852	LMG	C2-C1-O1-C7
24	G	101	LMG	O7-C8-C9-O8
25	4	321	HTG	C2-C1-S1-C1'
25	4	321	HTG	O5-C1-S1-C1'
25	B	851	HTG	O5-C1-S1-C1'
25	F	301	HTG	C2-C1-S1-C1'
25	F	301	HTG	O5-C1-S1-C1'
25	F	310	HTG	C2-C1-S1-C1'
25	J	102	HTG	O5-C1-S1-C1'
26	4	323	DGD	C2B-C1B-O2G-C2G
26	4	323	DGD	C2G-C3G-O3G-C1D
26	4	323	DGD	O6D-C1D-O3G-C3G
26	4	323	DGD	O6E-C1E-O5D-C6D
27	A	842	PQN	C11-C12-C13-C14
27	B	843	PQN	C12-C11-C3-C2
27	B	843	PQN	C11-C12-C13-C14
27	B	843	PQN	C14-C13-C15-C16
17	2	309	CLA	O1D-CGD-O2D-CED
17	4	304	CLA	O1D-CGD-O2D-CED
18	4	307	CHL	O1D-CGD-O2D-CED
23	2	318	LMT	O5B-C1B-O1B-C4'
17	A	815	CLA	O1D-CGD-O2D-CED
17	B	808	CLA	O1D-CGD-O2D-CED
17	1	303	CLA	CBD-CGD-O2D-CED
17	1	304	CLA	CBD-CGD-O2D-CED
17	3	602	CLA	CBD-CGD-O2D-CED
17	3	611	CLA	CBD-CGD-O2D-CED
17	4	303	CLA	CBD-CGD-O2D-CED
17	4	304	CLA	CBD-CGD-O2D-CED
17	4	311	CLA	CBD-CGD-O2D-CED
17	A	810	CLA	CBD-CGD-O2D-CED
17	A	814	CLA	CBD-CGD-O2D-CED
17	A	821	CLA	CBD-CGD-O2D-CED
17	B	808	CLA	CBD-CGD-O2D-CED
17	B	822	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	J	103	CLA	CBD-CGD-O2D-CED
17	K	201	CLA	CBD-CGD-O2D-CED
18	2	304	CHL	CBD-CGD-O2D-CED
18	4	306	CHL	CBD-CGD-O2D-CED
18	4	307	CHL	CBD-CGD-O2D-CED
17	3	608	CLA	O1A-CGA-O2A-C1
18	4	305	CHL	O1A-CGA-O2A-C1
22	2	317	LHG	O10-C23-O8-C6
17	1	313	CLA	O1A-CGA-O2A-C1
17	4	309	CLA	O1D-CGD-O2D-CED
18	4	301	CHL	O1D-CGD-O2D-CED
17	K	201	CLA	O1D-CGD-O2D-CED
17	A	831	CLA	CBD-CGD-O2D-CED
17	A	822	CLA	O1A-CGA-O2A-C1
17	A	840	CLA	O1A-CGA-O2A-C1
17	L	202	CLA	O1A-CGA-O2A-C1
17	L	204	CLA	O1A-CGA-O2A-C1
22	G	102	LHG	O10-C23-O8-C6
24	G	101	LMG	O10-C28-O8-C9
23	2	318	LMT	C4B-C5B-C6B-O6B
17	2	310	CLA	O1D-CGD-O2D-CED
17	B	822	CLA	O1D-CGD-O2D-CED
17	J	103	CLA	O1D-CGD-O2D-CED
18	4	315	CHL	O1D-CGD-O2D-CED
17	1	311	CLA	O1D-CGD-O2D-CED
17	3	604	CLA	O1D-CGD-O2D-CED
17	A	822	CLA	O1D-CGD-O2D-CED
17	B	812	CLA	O1D-CGD-O2D-CED
26	4	323	DGD	C4E-C5E-C6E-O5E
22	A	845	LHG	O9-C7-O7-C5
24	F	309	LMG	O9-C10-O7-C8
26	4	323	DGD	O1B-C1B-O2G-C2G
17	2	303	CLA	C3-C5-C6-C7
17	A	807	CLA	C3-C5-C6-C7
17	A	810	CLA	C3-C5-C6-C7
17	A	838	CLA	C3-C5-C6-C7
17	B	820	CLA	C3-C5-C6-C7
17	3	602	CLA	O1D-CGD-O2D-CED
17	3	608	CLA	CBA-CGA-O2A-C1
17	A	807	CLA	CBA-CGA-O2A-C1
17	A	840	CLA	CBA-CGA-O2A-C1
17	B	812	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	G	102	LHG	C24-C23-O8-C6
17	A	817	CLA	CBD-CGD-O2D-CED
17	A	837	CLA	CBD-CGD-O2D-CED
17	B	813	CLA	CBD-CGD-O2D-CED
17	B	826	CLA	CBD-CGD-O2D-CED
17	B	831	CLA	CBD-CGD-O2D-CED
17	G	103	CLA	CBD-CGD-O2D-CED
18	1	305	CHL	CBD-CGD-O2D-CED
18	3	607	CHL	CBD-CGD-O2D-CED
22	A	845	LHG	C8-C7-O7-C5
17	A	805	CLA	O1D-CGD-O2D-CED
17	A	821	CLA	O1D-CGD-O2D-CED
17	A	843	CLA	C2C-C3C-CAC-CBC
17	2	310	CLA	C4-C3-C5-C6
17	A	829	CLA	C4-C3-C5-C6
17	A	831	CLA	C4-C3-C5-C6
17	A	836	CLA	C4-C3-C5-C6
17	A	840	CLA	C4-C3-C5-C6
17	A	853	CLA	C4-C3-C5-C6
17	B	820	CLA	C4-C3-C5-C6
17	B	824	CLA	C4-C3-C5-C6
17	B	834	CLA	C4-C3-C5-C6
17	L	203	CLA	C4-C3-C5-C6
17	K	202	CLA	C4-C3-C5-C6
18	4	305	CHL	C4-C3-C5-C6
27	A	842	PQN	C14-C13-C15-C16
17	2	310	CLA	C2-C3-C5-C6
17	A	831	CLA	C2-C3-C5-C6
17	A	836	CLA	C2-C3-C5-C6
17	K	202	CLA	C2-C3-C5-C6
18	4	305	CHL	C2-C3-C5-C6
18	2	313	CHL	CBD-CGD-O2D-CED
17	4	311	CLA	O1D-CGD-O2D-CED
17	A	814	CLA	O1D-CGD-O2D-CED
17	A	828	CLA	C2A-CAA-CBA-CGA
18	4	306	CHL	C2A-CAA-CBA-CGA
17	2	311	CLA	C3-C5-C6-C7
17	B	808	CLA	C3-C5-C6-C7
17	B	817	CLA	C3-C5-C6-C7
17	A	822	CLA	CBA-CGA-O2A-C1
17	A	833	CLA	CBA-CGA-O2A-C1
17	B	817	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	L	202	CLA	CBA-CGA-O2A-C1
17	L	204	CLA	CBA-CGA-O2A-C1
18	4	306	CHL	CBA-CGA-O2A-C1
24	G	101	LMG	C29-C28-O8-C9
24	G	101	LMG	C4-C5-C6-O5
26	B	850	DGD	O6E-C5E-C6E-O5E
17	A	807	CLA	O1A-CGA-O2A-C1
17	A	833	CLA	O1A-CGA-O2A-C1
18	4	306	CHL	O1A-CGA-O2A-C1
17	3	611	CLA	O1D-CGD-O2D-CED
23	A	855	LMT	O5'-C5'-C6'-O6'
26	4	323	DGD	O6E-C5E-C6E-O5E
23	A	855	LMT	C4B-C5B-C6B-O6B
18	2	304	CHL	O1D-CGD-O2D-CED
17	A	816	CLA	C3-C5-C6-C7
17	A	831	CLA	C3-C5-C6-C7
17	A	832	CLA	C3-C5-C6-C7
17	B	811	CLA	C3-C5-C6-C7
17	B	823	CLA	C3-C5-C6-C7
17	1	313	CLA	CBD-CGD-O2D-CED
18	2	306	CHL	CBD-CGD-O2D-CED
17	A	843	CLA	C4C-C3C-CAC-CBC
17	1	303	CLA	O1D-CGD-O2D-CED
17	4	303	CLA	CBA-CGA-O2A-C1
17	A	818	CLA	CBA-CGA-O2A-C1
17	A	835	CLA	CBA-CGA-O2A-C1
17	B	812	CLA	O1A-CGA-O2A-C1
17	4	303	CLA	O1D-CGD-O2D-CED
26	B	850	DGD	C4E-C5E-C6E-O5E
24	F	309	LMG	C11-C10-O7-C8
25	F	301	HTG	O5-C5-C6-O6
17	A	810	CLA	O1D-CGD-O2D-CED
17	A	804	CLA	C3-C5-C6-C7
17	A	820	CLA	C3-C5-C6-C7
17	A	840	CLA	C3-C5-C6-C7
17	A	841	CLA	C3-C5-C6-C7
17	A	853	CLA	C3-C5-C6-C7
17	B	809	CLA	C3-C5-C6-C7
17	3	610	CLA	CBD-CGD-O2D-CED
17	A	816	CLA	CBD-CGD-O2D-CED
17	J	101	CLA	CBD-CGD-O2D-CED
18	4	306	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	A	841	CLA	C4-C3-C5-C6
17	B	823	CLA	C4-C3-C5-C6
17	A	841	CLA	C2-C3-C5-C6
17	A	853	CLA	C2-C3-C5-C6
17	B	823	CLA	C2-C3-C5-C6
17	B	824	CLA	C2-C3-C5-C6
17	B	834	CLA	C2-C3-C5-C6
17	L	203	CLA	C2-C3-C5-C6
17	4	303	CLA	O1A-CGA-O2A-C1
17	A	835	CLA	O1A-CGA-O2A-C1
17	B	841	CLA	CBD-CGD-O2D-CED
23	2	318	LMT	O5B-C5B-C6B-O6B
17	B	830	CLA	C2A-CAA-CBA-CGA
17	1	304	CLA	O1D-CGD-O2D-CED
17	A	818	CLA	O1A-CGA-O2A-C1
17	B	817	CLA	O1A-CGA-O2A-C1
17	B	813	CLA	C3-C5-C6-C7
24	B	852	LMG	O6-C1-O1-C7
17	A	841	CLA	CBA-CGA-O2A-C1
18	2	306	CHL	CBA-CGA-O2A-C1
17	A	827	CLA	CBD-CGD-O2D-CED
17	A	835	CLA	CBD-CGD-O2D-CED
17	A	843	CLA	CBD-CGD-O2D-CED
17	B	835	CLA	CBD-CGD-O2D-CED
17	G	104	CLA	CBD-CGD-O2D-CED
17	G	105	CLA	CBD-CGD-O2D-CED
23	A	855	LMT	O5B-C5B-C6B-O6B
24	G	101	LMG	O6-C5-C6-O5
17	A	803	CLA	C3-C5-C6-C7
17	A	805	CLA	C3-C5-C6-C7
17	B	815	CLA	C3-C5-C6-C7
17	L	202	CLA	C3-C5-C6-C7
26	4	323	DGD	C7B-C8B-C9B-CAB
17	A	831	CLA	O1D-CGD-O2D-CED
17	1	309	CLA	CBA-CGA-O2A-C1
17	3	606	CLA	CBA-CGA-O2A-C1
17	4	308	CLA	CBA-CGA-O2A-C1
17	A	830	CLA	CBA-CGA-O2A-C1
17	B	803	CLA	CBA-CGA-O2A-C1
17	G	104	CLA	CBA-CGA-O2A-C1
24	B	852	LMG	C29-C28-O8-C9
26	4	323	DGD	C2A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
17	1	302	CLA	CBD-CGD-O2D-CED
26	4	323	DGD	C3A-C4A-C5A-C6A
26	4	323	DGD	CEB-CFB-CGB-CHB
17	A	829	CLA	C2-C3-C5-C6
17	A	840	CLA	C2-C3-C5-C6
17	B	826	CLA	C3-C5-C6-C7
17	B	804	CLA	CBD-CGD-O2D-CED
17	1	302	CLA	C11-C12-C13-C14
17	2	303	CLA	C11-C10-C8-C9
17	2	308	CLA	C11-C10-C8-C9
17	4	310	CLA	C6-C7-C8-C9
17	A	804	CLA	C11-C10-C8-C9
17	A	809	CLA	C11-C10-C8-C9
17	A	812	CLA	C11-C10-C8-C9
17	A	816	CLA	C11-C12-C13-C14
17	A	836	CLA	C11-C12-C13-C14
17	A	839	CLA	C6-C7-C8-C9
17	A	839	CLA	C11-C12-C13-C14
17	A	840	CLA	C11-C10-C8-C9
17	B	803	CLA	C11-C12-C13-C14
17	B	803	CLA	C14-C13-C15-C16
17	B	805	CLA	C14-C13-C15-C16
17	B	809	CLA	C6-C7-C8-C9
17	B	809	CLA	C14-C13-C15-C16
17	B	811	CLA	C14-C13-C15-C16
17	B	815	CLA	C14-C13-C15-C16
17	B	821	CLA	C11-C12-C13-C14
17	B	829	CLA	C11-C12-C13-C14
17	B	831	CLA	C14-C13-C15-C16
17	B	835	CLA	C14-C13-C15-C16
17	B	842	CLA	C11-C12-C13-C14
18	4	301	CHL	C6-C7-C8-C9
17	B	813	CLA	O1D-CGD-O2D-CED
17	B	831	CLA	O1D-CGD-O2D-CED
17	1	309	CLA	O1A-CGA-O2A-C1
17	B	803	CLA	O1A-CGA-O2A-C1
17	3	612	CLA	CBD-CGD-O2D-CED
18	1	305	CHL	O1D-CGD-O2D-CED
19	1	314	LUT	C7-C8-C9-C19
19	1	314	LUT	C11-C12-C13-C20
19	1	314	LUT	C31-C32-C33-C40
19	2	314	LUT	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
19	2	314	LUT	C27-C28-C29-C39
19	3	614	LUT	C7-C8-C9-C19
19	3	614	LUT	C27-C28-C29-C39
19	3	614	LUT	C31-C32-C33-C40
19	4	316	LUT	C11-C12-C13-C20
20	1	315	XAT	C11-C12-C13-C20
20	1	315	XAT	C27-C28-C29-C39
20	1	315	XAT	C31-C32-C33-C40
20	2	315	XAT	C11-C12-C13-C20
20	2	315	XAT	C27-C28-C29-C39
20	2	315	XAT	C31-C32-C33-C40
20	3	615	XAT	C11-C12-C13-C20
20	3	615	XAT	C27-C28-C29-C39
20	3	615	XAT	C31-C32-C33-C40
20	4	317	XAT	C7-C8-C9-C19
20	4	317	XAT	C31-C32-C33-C40
21	1	316	BCR	C7-C8-C9-C34
21	1	316	BCR	C11-C12-C13-C35
21	2	316	BCR	C7-C8-C9-C34
21	4	318	BCR	C7-C8-C9-C34
21	A	846	BCR	C37-C22-C23-C24
21	A	848	BCR	C7-C8-C9-C34
21	A	849	BCR	C7-C8-C9-C34
21	A	851	BCR	C7-C8-C9-C34
21	B	844	BCR	C7-C8-C9-C34
21	B	844	BCR	C11-C12-C13-C35
21	B	846	BCR	C37-C22-C23-C24
21	B	849	BCR	C7-C8-C9-C34
21	J	104	BCR	C11-C12-C13-C35
21	L	201	BCR	C37-C22-C23-C24
21	K	203	BCR	C37-C22-C23-C24
21	4	318	BCR	C7-C8-C9-C10
21	A	850	BCR	C21-C22-C23-C24
21	L	205	BCR	C7-C8-C9-C10
17	3	606	CLA	C2A-CAA-CBA-CGA
17	3	606	CLA	O1A-CGA-O2A-C1
26	4	323	DGD	O1A-C1A-O1G-C1G
23	A	855	LMT	C4'-C5'-C6'-O6'
22	2	317	LHG	O9-C7-O7-C5
22	A	845	LHG	O6-C4-C5-O7
17	2	302	CLA	CBA-CGA-O2A-C1
17	A	823	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	B	810	CLA	C15-C16-C17-C18
24	4	320	LMG	C10-C11-C12-C13
22	B	801	LHG	C24-C23-O8-C6
17	B	826	CLA	O1D-CGD-O2D-CED
18	3	607	CHL	O1D-CGD-O2D-CED
25	F	301	HTG	C4-C5-C6-O6
17	A	834	CLA	CBD-CGD-O2D-CED
17	B	834	CLA	CBD-CGD-O2D-CED
22	2	317	LHG	C28-C29-C30-C31
26	4	323	DGD	CBB-CCB-CDB-CEB
17	A	810	CLA	C13-C15-C16-C17
17	A	853	CLA	C15-C16-C17-C18
17	B	803	CLA	C3-C5-C6-C7
17	2	301	CLA	C15-C16-C17-C18
17	B	829	CLA	C8-C10-C11-C12
17	A	832	CLA	CBD-CGD-O2D-CED
17	1	302	CLA	C6-C7-C8-C10
17	1	309	CLA	C11-C10-C8-C7
17	A	807	CLA	C11-C12-C13-C15
17	A	808	CLA	C6-C7-C8-C10
17	A	818	CLA	C12-C13-C15-C16
17	B	808	CLA	C11-C10-C8-C7
17	B	812	CLA	C11-C12-C13-C15
17	B	826	CLA	C12-C13-C15-C16
17	A	837	CLA	O1D-CGD-O2D-CED
17	1	308	CLA	C4-C3-C5-C6
17	A	827	CLA	C15-C16-C17-C18
17	B	820	CLA	C10-C11-C12-C13
23	A	855	LMT	O1'-C1-C2-C3
24	4	320	LMG	C11-C12-C13-C14
17	A	832	CLA	C2C-C3C-CAC-CBC
17	G	103	CLA	O1D-CGD-O2D-CED
17	2	308	CLA	C8-C10-C11-C12
22	F	302	LHG	C7-C8-C9-C10
17	4	308	CLA	O1A-CGA-O2A-C1
17	A	830	CLA	O1A-CGA-O2A-C1
17	A	841	CLA	O1A-CGA-O2A-C1
17	1	307	CLA	C15-C16-C17-C18
17	3	602	CLA	C10-C11-C12-C13
17	A	804	CLA	C15-C16-C17-C18
17	A	818	CLA	C8-C10-C11-C12
17	A	829	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
17	B	808	CLA	C10-C11-C12-C13
17	B	838	CLA	C15-C16-C17-C18
22	G	102	LHG	C5-C4-O6-P
17	B	840	CLA	C2A-CAA-CBA-CGA
17	L	203	CLA	C2A-CAA-CBA-CGA
20	4	317	XAT	C30-C31-C32-C33
17	1	302	CLA	C5-C6-C7-C8
17	1	312	CLA	C5-C6-C7-C8
17	A	827	CLA	C8-C10-C11-C12
17	A	853	CLA	C10-C11-C12-C13
17	B	816	CLA	C13-C15-C16-C17
17	B	823	CLA	C13-C15-C16-C17
17	B	833	CLA	C8-C10-C11-C12
17	B	840	CLA	C15-C16-C17-C18
27	A	842	PQN	C25-C26-C27-C28
21	K	203	BCR	C6-C7-C8-C9
17	4	310	CLA	C8-C10-C11-C12
17	A	806	CLA	C5-C6-C7-C8
17	A	812	CLA	C8-C10-C11-C12
17	A	812	CLA	C10-C11-C12-C13
17	A	817	CLA	C10-C11-C12-C13
17	B	826	CLA	C8-C10-C11-C12
17	1	310	CLA	CBD-CGD-O2D-CED
17	G	104	CLA	O1A-CGA-O2A-C1
18	2	306	CHL	O1A-CGA-O2A-C1
22	G	102	LHG	C7-C8-C9-C10
17	A	817	CLA	O1D-CGD-O2D-CED
18	2	313	CHL	O1D-CGD-O2D-CED
17	A	803	CLA	C5-C6-C7-C8
17	A	825	CLA	C15-C16-C17-C18
26	4	323	DGD	C1B-C2B-C3B-C4B
17	A	804	CLA	C10-C11-C12-C13
17	A	820	CLA	C15-C16-C17-C18
17	A	831	CLA	C15-C16-C17-C18
17	A	837	CLA	C10-C11-C12-C13
17	A	838	CLA	C5-C6-C7-C8
17	B	811	CLA	C13-C15-C16-C17
17	B	816	CLA	C15-C16-C17-C18
17	B	831	CLA	CBA-CGA-O2A-C1
17	4	310	CLA	C2C-C3C-CAC-CBC
17	2	302	CLA	O1A-CGA-O2A-C1
17	A	823	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	B	851	HTG	S1-C1'-C2'-C3'
18	2	306	CHL	O1D-CGD-O2D-CED
17	1	308	CLA	C5-C6-C7-C8
20	4	317	XAT	C29-C30-C31-C32
22	F	302	LHG	C1-C2-C3-O3
17	A	814	CLA	C2A-CAA-CBA-CGA
17	B	812	CLA	C2A-CAA-CBA-CGA
17	L	204	CLA	C2A-CAA-CBA-CGA
17	1	309	CLA	C5-C6-C7-C8
17	2	303	CLA	C5-C6-C7-C8
17	A	801	CLA	C15-C16-C17-C18
17	A	817	CLA	C8-C10-C11-C12
17	B	805	CLA	C13-C15-C16-C17
17	B	821	CLA	C13-C15-C16-C17
17	B	825	CLA	C10-C11-C12-C13
17	B	827	CLA	C10-C11-C12-C13
17	4	313	CLA	CBD-CGD-O2D-CED
17	4	314	CLA	CBD-CGD-O2D-CED
17	B	823	CLA	CBD-CGD-O2D-CED
17	4	303	CLA	C10-C11-C12-C13
17	A	804	CLA	C13-C15-C16-C17
17	A	810	CLA	C15-C16-C17-C18
17	A	805	CLA	C15-C16-C17-C18
17	A	807	CLA	C8-C10-C11-C12
17	A	836	CLA	C15-C16-C17-C18
17	B	820	CLA	C5-C6-C7-C8
17	K	202	CLA	C8-C10-C11-C12
17	1	313	CLA	O1D-CGD-O2D-CED
24	G	101	LMG	C11-C10-O7-C8
17	A	816	CLA	O1D-CGD-O2D-CED
23	A	855	LMT	C2'-C1'-O1'-C1
17	1	302	CLA	C13-C15-C16-C17
18	4	301	CHL	C11-C12-C13-C15
17	B	803	CLA	C15-C16-C17-C18
19	2	314	LUT	C11-C10-C9-C19
19	3	614	LUT	C11-C10-C9-C19
21	4	318	BCR	C20-C21-C22-C37
21	A	851	BCR	C20-C21-C22-C37
21	B	846	BCR	C16-C17-C18-C36
21	B	849	BCR	C16-C17-C18-C36
21	F	303	BCR	C16-C17-C18-C36
21	L	201	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
21	L	205	BCR	C20-C21-C22-C37
21	K	203	BCR	C20-C21-C22-C37
17	B	805	CLA	CBD-CGD-O2D-CED
18	4	301	CHL	C8-C10-C11-C12
19	1	314	LUT	C27-C28-C29-C39
19	2	314	LUT	C11-C12-C13-C20
19	3	614	LUT	C11-C12-C13-C20
19	4	316	LUT	C27-C28-C29-C39
21	A	850	BCR	C7-C8-C9-C34
21	F	303	BCR	C11-C12-C13-C35
21	L	205	BCR	C7-C8-C9-C34
25	J	102	HTG	S1-C1'-C2'-C3'
21	2	316	BCR	C7-C8-C9-C10
17	3	610	CLA	C2A-CAA-CBA-CGA
17	A	808	CLA	C2A-CAA-CBA-CGA
17	A	822	CLA	C2A-CAA-CBA-CGA
17	A	834	CLA	C2A-CAA-CBA-CGA
18	4	305	CHL	C2A-CAA-CBA-CGA
17	1	311	CLA	C5-C6-C7-C8
17	B	842	CLA	C8-C10-C11-C12
22	A	845	LHG	O1-C1-C2-C3
22	B	801	LHG	O1-C1-C2-C3
22	F	302	LHG	O1-C1-C2-C3
26	4	323	DGD	C1G-C2G-O2G-C1B
20	1	315	XAT	C29-C30-C31-C32
20	2	315	XAT	C29-C30-C31-C32
20	3	615	XAT	C29-C30-C31-C32
17	A	806	CLA	C16-C17-C18-C19
17	A	810	CLA	C16-C17-C18-C19
17	B	817	CLA	C6-C7-C8-C10
17	K	202	CLA	C3-C5-C6-C7
19	4	316	LUT	C28-C29-C30-C31
20	1	315	XAT	C12-C13-C14-C15
20	2	315	XAT	C12-C13-C14-C15
20	3	615	XAT	C12-C13-C14-C15
21	1	316	BCR	C20-C21-C22-C23
21	2	316	BCR	C12-C13-C14-C15
21	2	316	BCR	C16-C17-C18-C19
21	4	318	BCR	C20-C21-C22-C23
21	A	848	BCR	C16-C17-C18-C19
21	B	845	BCR	C11-C10-C9-C8
21	B	849	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
21	B	849	BCR	C16-C17-C18-C19
21	I	101	BCR	C20-C21-C22-C23
21	L	205	BCR	C20-C21-C22-C23
21	K	203	BCR	C16-C17-C18-C19
24	F	309	LMG	O6-C1-O1-C7
22	2	317	LHG	C8-C7-O7-C5
17	3	610	CLA	O1D-CGD-O2D-CED
17	J	101	CLA	O1D-CGD-O2D-CED
17	1	310	CLA	CBA-CGA-O2A-C1
17	B	826	CLA	C15-C16-C17-C18
22	F	302	LHG	C23-C24-C25-C26
24	B	852	LMG	C28-C29-C30-C31
17	B	835	CLA	O1D-CGD-O2D-CED
17	2	303	CLA	C2-C1-O2A-CGA
17	A	836	CLA	C16-C17-C18-C19
17	B	817	CLA	C6-C7-C8-C9
24	B	852	LMG	O10-C28-O8-C9
17	B	808	CLA	C5-C6-C7-C8
17	B	834	CLA	C5-C6-C7-C8
17	B	840	CLA	CBD-CGD-O2D-CED
21	3	616	BCR	C14-C15-C16-C17
22	2	317	LHG	C9-C10-C11-C12
22	G	102	LHG	C14-C15-C16-C17
26	B	850	DGD	CCA-CDA-CEA-CFA
22	G	102	LHG	C15-C16-C17-C18
26	4	323	DGD	C2A-C3A-C4A-C5A
26	B	850	DGD	C9A-CAA-CBA-CCA
22	A	845	LHG	O1-C1-C2-O2
24	F	309	LMG	C38-C39-C40-C41
26	4	323	DGD	C6B-C7B-C8B-C9B
17	B	815	CLA	C13-C15-C16-C17
17	1	312	CLA	C4B-C3B-CAB-CBB
17	3	611	CLA	C4B-C3B-CAB-CBB
17	4	303	CLA	C4B-C3B-CAB-CBB
17	4	310	CLA	C4B-C3B-CAB-CBB
17	A	801	CLA	C4B-C3B-CAB-CBB
17	A	805	CLA	C4B-C3B-CAB-CBB
17	A	813	CLA	C4B-C3B-CAB-CBB
17	A	833	CLA	C4B-C3B-CAB-CBB
17	G	103	CLA	C4B-C3B-CAB-CBB
17	L	204	CLA	C4B-C3B-CAB-CBB
25	J	102	HTG	C1'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
17	1	312	CLA	C6-C7-C8-C9
18	4	305	CHL	C6-C7-C8-C9
17	A	843	CLA	O1D-CGD-O2D-CED
22	A	844	LHG	C8-C7-O7-C5
26	4	323	DGD	CDB-CEB-CFB-CGB
17	4	303	CLA	C6-C7-C8-C10
17	A	827	CLA	C11-C10-C8-C7
17	B	835	CLA	C12-C13-C15-C16
24	4	319	LMG	C32-C33-C34-C35
17	4	309	CLA	C10-C11-C12-C13
22	A	844	LHG	C32-C33-C34-C35
17	1	309	CLA	C3A-C2A-CAA-CBA
17	1	310	CLA	C3A-C2A-CAA-CBA
17	1	312	CLA	C3A-C2A-CAA-CBA
17	4	303	CLA	C3A-C2A-CAA-CBA
17	4	304	CLA	C3A-C2A-CAA-CBA
17	A	810	CLA	C3A-C2A-CAA-CBA
17	A	831	CLA	C3A-C2A-CAA-CBA
17	A	835	CLA	C3A-C2A-CAA-CBA
17	B	831	CLA	C3A-C2A-CAA-CBA
17	F	307	CLA	C3A-C2A-CAA-CBA
17	J	101	CLA	C3A-C2A-CAA-CBA
18	1	305	CHL	C3A-C2A-CAA-CBA
18	4	301	CHL	C3A-C2A-CAA-CBA
17	B	841	CLA	O1D-CGD-O2D-CED
22	A	844	LHG	C17-C18-C19-C20
22	A	844	LHG	C24-C25-C26-C27
24	F	309	LMG	C34-C35-C36-C37
26	B	850	DGD	C8B-C9B-CAB-CBB
22	2	317	LHG	C11-C10-C9-C8
24	B	852	LMG	C11-C12-C13-C14
17	B	829	CLA	C13-C15-C16-C17
17	G	104	CLA	O1D-CGD-O2D-CED
17	A	832	CLA	C16-C17-C18-C19
18	4	301	CHL	C11-C12-C13-C14
17	B	831	CLA	O1A-CGA-O2A-C1
24	4	319	LMG	C36-C37-C38-C39
26	B	850	DGD	CDB-CEB-CFB-CGB
17	A	809	CLA	C5-C6-C7-C8
17	G	105	CLA	O1D-CGD-O2D-CED
17	A	816	CLA	CBA-CGA-O2A-C1
17	A	821	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	A	843	CLA	CBA-CGA-O2A-C1
24	B	852	LMG	C12-C13-C14-C15
22	1	317	LHG	C7-C8-C9-C10
22	A	844	LHG	C27-C28-C29-C30
22	G	102	LHG	C16-C17-C18-C19
22	G	102	LHG	C31-C32-C33-C34
25	A	854	HTG	C4-C5-C6-O6
22	1	317	LHG	C32-C33-C34-C35
22	2	317	LHG	C10-C11-C12-C13
24	4	320	LMG	C20-C21-C22-C23
22	A	844	LHG	C29-C30-C31-C32
24	4	320	LMG	C15-C16-C17-C18
17	B	834	CLA	O1D-CGD-O2D-CED
17	4	303	CLA	C11-C12-C13-C14
17	A	806	CLA	C16-C17-C18-C20
17	1	311	CLA	C2B-C3B-CAB-CBB
17	1	312	CLA	C2B-C3B-CAB-CBB
17	3	611	CLA	C2B-C3B-CAB-CBB
17	4	310	CLA	C2B-C3B-CAB-CBB
17	A	805	CLA	C2B-C3B-CAB-CBB
17	B	819	CLA	C2B-C3B-CAB-CBB
17	G	103	CLA	C2B-C3B-CAB-CBB
21	1	316	BCR	C23-C24-C25-C26
21	1	316	BCR	C23-C24-C25-C30
21	4	318	BCR	C23-C24-C25-C26
21	4	318	BCR	C23-C24-C25-C30
21	A	847	BCR	C1-C6-C7-C8
21	A	847	BCR	C5-C6-C7-C8
21	A	850	BCR	C23-C24-C25-C30
21	B	848	BCR	C23-C24-C25-C30
21	J	105	BCR	C23-C24-C25-C30
22	2	317	LHG	C25-C26-C27-C28
22	1	317	LHG	C8-C7-O7-C5
17	A	836	CLA	CBA-CGA-O2A-C1
17	B	824	CLA	CBA-CGA-O2A-C1
17	B	833	CLA	CBA-CGA-O2A-C1
17	2	311	CLA	C5-C6-C7-C8
17	A	831	CLA	C5-C6-C7-C8
17	B	837	CLA	C3-C5-C6-C7
22	1	317	LHG	C9-C10-C11-C12
22	1	317	LHG	C15-C16-C17-C18
26	B	850	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
22	1	317	LHG	C23-C24-C25-C26
24	F	309	LMG	C28-C29-C30-C31
26	B	850	DGD	C1B-C2B-C3B-C4B
23	A	855	LMT	C6-C7-C8-C9
17	1	310	CLA	O1A-CGA-O2A-C1
22	2	317	LHG	C27-C28-C29-C30
23	2	318	LMT	C11-C10-C9-C8
17	B	838	CLA	C4-C3-C5-C6
26	B	850	DGD	C3B-C4B-C5B-C6B
19	4	316	LUT	C10-C11-C12-C13
20	1	315	XAT	C30-C31-C32-C33
20	2	315	XAT	C30-C31-C32-C33
20	3	615	XAT	C30-C31-C32-C33
21	1	316	BCR	C10-C11-C12-C13
21	A	850	BCR	C10-C11-C12-C13
17	A	802	CLA	C10-C11-C12-C13
17	1	308	CLA	C2-C3-C5-C6
24	F	309	LMG	C29-C30-C31-C32
25	F	305	HTG	C1'-C2'-C3'-C4'
17	B	829	CLA	C3-C5-C6-C7
17	B	823	CLA	C14-C13-C15-C16
17	L	202	CLA	C14-C13-C15-C16
26	4	323	DGD	C5B-C6B-C7B-C8B
17	A	828	CLA	C15-C16-C17-C18
22	G	102	LHG	C11-C10-C9-C8
22	G	102	LHG	C17-C18-C19-C20
19	3	614	LUT	C6-C7-C8-C9
21	K	203	BCR	C22-C23-C24-C25
23	A	855	LMT	O5'-C1'-O1'-C1
24	4	320	LMG	C13-C14-C15-C16
26	4	323	DGD	C2D-C1D-O3G-C3G
17	4	303	CLA	C5-C6-C7-C8
17	A	840	CLA	C10-C11-C12-C13
17	B	835	CLA	C5-C6-C7-C8
22	1	317	LHG	C14-C15-C16-C17
23	A	855	LMT	C1-C2-C3-C4
17	B	809	CLA	C16-C17-C18-C19
17	L	202	CLA	C16-C17-C18-C19
24	G	101	LMG	C15-C16-C17-C18
25	B	851	HTG	C4-C5-C6-O6
22	G	102	LHG	C25-C26-C27-C28
26	B	850	DGD	CEB-CFB-CGB-CHB

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Mol	Chain	Res	Type	Atoms
24	G	101	LMG	O9-C10-O7-C8
24	4	319	LMG	C35-C36-C37-C38
24	F	309	LMG	C14-C15-C16-C17
26	4	323	DGD	C3B-C4B-C5B-C6B
26	B	850	DGD	C8A-C9A-CAA-CBA
17	B	809	CLA	CBD-CGD-O2D-CED
17	A	816	CLA	C13-C15-C16-C17
21	A	851	BCR	C7-C8-C9-C10
26	4	323	DGD	C5D-C6D-O5D-C1E
27	A	842	PQN	C12-C11-C3-C2
17	1	302	CLA	C15-C16-C17-C18
17	2	303	CLA	C2A-CAA-CBA-CGA
18	1	305	CHL	C2A-CAA-CBA-CGA
17	1	301	CLA	C16-C17-C18-C19
17	1	308	CLA	C11-C12-C13-C14
17	1	308	CLA	C11-C12-C13-C15
17	2	308	CLA	C11-C12-C13-C14
17	B	825	CLA	C11-C12-C13-C15
17	L	202	CLA	C16-C17-C18-C20
17	3	610	CLA	C4-C3-C5-C6
17	L	202	CLA	C4-C3-C5-C6
17	B	838	CLA	C2-C3-C5-C6
17	A	832	CLA	O1D-CGD-O2D-CED
17	A	816	CLA	O1A-CGA-O2A-C1
17	A	843	CLA	O1A-CGA-O2A-C1
17	B	838	CLA	C13-C15-C16-C17
22	A	844	LHG	C15-C16-C17-C18
24	B	852	LMG	C14-C15-C16-C17
24	B	852	LMG	C34-C35-C36-C37
24	B	852	LMG	C38-C39-C40-C41
17	A	835	CLA	O1D-CGD-O2D-CED
17	A	832	CLA	C16-C17-C18-C20
17	A	853	CLA	C16-C17-C18-C20
24	G	101	LMG	C17-C18-C19-C20
17	A	807	CLA	C5-C6-C7-C8
17	A	836	CLA	C13-C15-C16-C17
17	A	827	CLA	O1D-CGD-O2D-CED
24	4	320	LMG	O6-C5-C6-O5
17	3	608	CLA	CBD-CGD-O2D-CED
17	B	832	CLA	CBA-CGA-O2A-C1
17	A	821	CLA	O1A-CGA-O2A-C1
17	1	302	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	1	301	CLA	C16-C17-C18-C20
17	B	812	CLA	C16-C17-C18-C19
22	1	317	LHG	C11-C10-C9-C8
22	1	317	LHG	C16-C17-C18-C19
24	B	852	LMG	C16-C17-C18-C19
22	F	302	LHG	C17-C18-C19-C20
17	A	811	CLA	C3-C5-C6-C7
17	F	307	CLA	C2-C3-C5-C6
22	A	844	LHG	O9-C7-O7-C5
22	F	302	LHG	C14-C15-C16-C17
17	3	613	CLA	C2A-CAA-CBA-CGA
22	F	302	LHG	C15-C16-C17-C18
25	F	305	HTG	S1-C1'-C2'-C3'
25	B	851	HTG	C1'-C2'-C3'-C4'
17	2	303	CLA	C10-C11-C12-C13
22	A	844	LHG	C11-C10-C9-C8
24	4	319	LMG	C33-C34-C35-C36
17	2	308	CLA	C11-C12-C13-C15
18	4	305	CHL	C6-C7-C8-C10
17	B	837	CLA	C2C-C3C-CAC-CBC
24	4	319	LMG	O6-C5-C6-O5
22	F	302	LHG	O1-C1-C2-O2
22	G	102	LHG	O1-C1-C2-O2
17	A	836	CLA	O1A-CGA-O2A-C1
17	B	833	CLA	O1A-CGA-O2A-C1
17	1	306	CLA	C1A-C2A-CAA-CBA
17	1	310	CLA	C1A-C2A-CAA-CBA
17	2	303	CLA	C1A-C2A-CAA-CBA
17	2	308	CLA	C1A-C2A-CAA-CBA
17	3	609	CLA	C1A-C2A-CAA-CBA
17	4	303	CLA	C1A-C2A-CAA-CBA
17	4	313	CLA	C1A-C2A-CAA-CBA
17	A	807	CLA	C1A-C2A-CAA-CBA
17	A	808	CLA	C1A-C2A-CAA-CBA
17	A	817	CLA	C1A-C2A-CAA-CBA
17	A	835	CLA	C1A-C2A-CAA-CBA
17	B	803	CLA	C1A-C2A-CAA-CBA
17	B	806	CLA	C1A-C2A-CAA-CBA
17	B	820	CLA	C1A-C2A-CAA-CBA
17	B	822	CLA	C1A-C2A-CAA-CBA
17	B	829	CLA	C1A-C2A-CAA-CBA
17	F	304	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	F	307	CLA	C1A-C2A-CAA-CBA
17	J	101	CLA	C1A-C2A-CAA-CBA
17	L	204	CLA	C1A-C2A-CAA-CBA
17	A	824	CLA	CBD-CGD-O2D-CED
17	B	815	CLA	C2C-C3C-CAC-CBC
22	A	845	LHG	O6-C4-C5-C6
17	2	301	CLA	C3-C5-C6-C7
17	1	302	CLA	C12-C13-C15-C16
17	1	309	CLA	C11-C12-C13-C15
17	1	309	CLA	C12-C13-C15-C16
17	2	308	CLA	C11-C10-C8-C7
17	A	805	CLA	C11-C10-C8-C7
17	A	806	CLA	C6-C7-C8-C10
17	A	816	CLA	C11-C12-C13-C15
17	A	829	CLA	C11-C10-C8-C7
17	A	837	CLA	C12-C13-C15-C16
17	A	838	CLA	C11-C12-C13-C15
17	A	839	CLA	C12-C13-C15-C16
17	B	802	CLA	C11-C12-C13-C15
17	B	803	CLA	C6-C7-C8-C10
17	B	805	CLA	C11-C10-C8-C7
17	B	815	CLA	C11-C10-C8-C7
17	B	826	CLA	C11-C10-C8-C7
17	B	828	CLA	C11-C10-C8-C7
17	B	835	CLA	C11-C12-C13-C15
17	K	202	CLA	C6-C7-C8-C10
18	4	301	CHL	C11-C10-C8-C7
17	1	311	CLA	C11-C12-C13-C15
27	A	842	PQN	C26-C27-C28-C29
17	A	804	CLA	C8-C10-C11-C12
17	A	829	CLA	C5-C6-C7-C8
17	A	826	CLA	C2-C3-C5-C6
17	A	837	CLA	C2-C3-C5-C6
17	L	202	CLA	C2-C3-C5-C6
22	G	102	LHG	C9-C10-C11-C12
17	3	612	CLA	O1D-CGD-O2D-CED
25	4	321	HTG	O5-C5-C6-O6
17	K	202	CLA	C10-C11-C12-C13
17	A	802	CLA	C2A-CAA-CBA-CGA
17	A	817	CLA	C2A-CAA-CBA-CGA
17	A	853	CLA	C2A-CAA-CBA-CGA
17	1	308	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
17	1	309	CLA	C11-C10-C8-C9
17	4	302	CLA	C11-C10-C8-C9
17	A	805	CLA	C11-C12-C13-C14
17	A	807	CLA	C11-C12-C13-C14
17	A	829	CLA	C11-C10-C8-C9
17	A	832	CLA	C6-C7-C8-C9
17	A	837	CLA	C14-C13-C15-C16
17	A	838	CLA	C11-C12-C13-C14
17	A	839	CLA	C14-C13-C15-C16
17	A	840	CLA	C6-C7-C8-C9
17	B	803	CLA	C6-C7-C8-C9
17	B	805	CLA	C11-C10-C8-C9
17	B	808	CLA	C11-C10-C8-C9
17	B	815	CLA	C11-C10-C8-C9
17	B	816	CLA	C6-C7-C8-C9
17	B	820	CLA	C11-C10-C8-C9
17	B	826	CLA	C14-C13-C15-C16
17	B	837	CLA	C6-C7-C8-C9
17	B	838	CLA	C14-C13-C15-C16
26	B	850	DGD	C6B-C7B-C8B-C9B
17	B	809	CLA	C16-C17-C18-C20
17	B	830	CLA	CBA-CGA-O2A-C1
17	4	312	CLA	C5-C6-C7-C8
17	B	838	CLA	C8-C10-C11-C12
17	B	824	CLA	O1A-CGA-O2A-C1
22	1	317	LHG	C24-C25-C26-C27
22	A	845	LHG	C4-C5-C6-O8
24	4	320	LMG	O1-C7-C8-C9
24	F	309	LMG	O1-C7-C8-C9
25	B	851	HTG	O5-C5-C6-O6
17	A	836	CLA	C10-C11-C12-C13
17	1	302	CLA	C16-C17-C18-C20
17	1	309	CLA	C16-C17-C18-C20
17	B	812	CLA	C16-C17-C18-C20
22	F	302	LHG	C25-C26-C27-C28
22	1	317	LHG	C17-C18-C19-C20
18	4	315	CHL	CHA-CBD-CGD-O1D
21	K	203	BCR	C16-C17-C18-C36
17	B	837	CLA	C5-C6-C7-C8
23	2	318	LMT	O5'-C5'-C6'-O6'
19	1	314	LUT	C14-C15-C35-C34
17	B	830	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	A	837	CLA	C4-C3-C5-C6
17	F	307	CLA	C4-C3-C5-C6
17	A	828	CLA	C2-C3-C5-C6
17	B	840	CLA	C2-C3-C5-C6
17	1	307	CLA	C8-C10-C11-C12
17	2	311	CLA	C13-C15-C16-C17
17	A	839	CLA	C5-C6-C7-C8
17	A	834	CLA	O1D-CGD-O2D-CED
24	4	320	LMG	C28-C29-C30-C31
17	A	828	CLA	C13-C15-C16-C17
17	K	202	CLA	C5-C6-C7-C8
17	1	309	CLA	C2A-CAA-CBA-CGA
17	1	310	CLA	C3-C5-C6-C7
24	B	852	LMG	O6-C5-C6-O5
17	2	311	CLA	C8-C10-C11-C12
24	4	319	LMG	C30-C31-C32-C33
24	F	309	LMG	C31-C32-C33-C34
19	4	316	LUT	C30-C31-C32-C33
21	3	616	BCR	C18-C19-C20-C21
21	B	847	BCR	C10-C11-C12-C13
17	A	816	CLA	C10-C11-C12-C13
17	B	809	CLA	C5-C6-C7-C8
24	4	320	LMG	C14-C15-C16-C17
18	2	304	CHL	C3C-C2C-CMC-OMC
21	K	203	BCR	C15-C16-C17-C18
17	A	853	CLA	C16-C17-C18-C19
17	2	303	CLA	CBA-CGA-O2A-C1
17	B	818	CLA	CBA-CGA-O2A-C1
17	B	840	CLA	C4-C3-C5-C6
26	B	850	DGD	C4B-C5B-C6B-C7B
22	A	844	LHG	O7-C5-C6-O8
17	A	824	CLA	CBA-CGA-O2A-C1
17	K	201	CLA	C2C-C3C-CAC-CBC
24	4	320	LMG	C18-C19-C20-C21
17	A	811	CLA	C6-C7-C8-C9
17	A	836	CLA	C16-C17-C18-C20
24	4	319	LMG	C31-C32-C33-C34
17	B	832	CLA	O1A-CGA-O2A-C1
17	A	816	CLA	C15-C16-C17-C18
17	A	826	CLA	CBA-CGA-O2A-C1
24	B	852	LMG	C39-C40-C41-C42
26	B	850	DGD	CFB-CGB-CHB-CIB

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Mol	Chain	Res	Type	Atoms
17	A	829	CLA	CBD-CGD-O2D-CED
24	4	320	LMG	C21-C22-C23-C24
25	A	854	HTG	O5-C5-C6-O6
17	B	829	CLA	C15-C16-C17-C18
17	1	310	CLA	O1D-CGD-O2D-CED
17	A	810	CLA	C8-C10-C11-C12
17	B	827	CLA	C16-C17-C18-C20
17	A	828	CLA	C4-C3-C5-C6
17	A	803	CLA	C2-C3-C5-C6
17	1	302	CLA	CBA-CGA-O2A-C1
17	2	303	CLA	C8-C10-C11-C12
17	B	811	CLA	C15-C16-C17-C18
22	A	844	LHG	C26-C27-C28-C29
22	B	801	LHG	O1-C1-C2-O2
23	A	855	LMT	C2-C1-O1'-C1'
17	1	302	CLA	C14-C13-C15-C16
17	1	307	CLA	C14-C13-C15-C16
17	1	309	CLA	C11-C12-C13-C14
17	1	309	CLA	C14-C13-C15-C16
17	A	805	CLA	C11-C10-C8-C9
17	A	805	CLA	C14-C13-C15-C16
17	A	806	CLA	C6-C7-C8-C9
17	A	808	CLA	C6-C7-C8-C9
17	A	812	CLA	C11-C12-C13-C14
17	A	818	CLA	C14-C13-C15-C16
17	A	831	CLA	C14-C13-C15-C16
17	B	826	CLA	C11-C10-C8-C9
17	B	827	CLA	C14-C13-C15-C16
17	B	828	CLA	C11-C12-C13-C14
17	B	834	CLA	C11-C10-C8-C9
17	B	835	CLA	C6-C7-C8-C9
17	B	835	CLA	C11-C12-C13-C14
17	F	304	CLA	C14-C13-C15-C16
17	K	202	CLA	C6-C7-C8-C9
18	4	301	CHL	C11-C10-C8-C9
17	4	309	CLA	C5-C6-C7-C8
17	B	841	CLA	C15-C16-C17-C18
17	3	606	CLA	C4B-C3B-CAB-CBB
17	A	819	CLA	C4B-C3B-CAB-CBB
17	A	820	CLA	C4B-C3B-CAB-CBB
17	B	825	CLA	C4B-C3B-CAB-CBB
17	B	834	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	B	840	CLA	O1D-CGD-O2D-CED
17	B	837	CLA	C4C-C3C-CAC-CBC
22	1	317	LHG	C28-C29-C30-C31
26	4	323	DGD	C2E-C1E-O5D-C6D
22	G	102	LHG	O6-C4-C5-C6
23	2	318	LMT	C4-C5-C6-C7
24	G	101	LMG	C14-C15-C16-C17
22	F	302	LHG	C26-C27-C28-C29
17	A	805	CLA	CAA-CBA-CGA-O2A
17	4	302	CLA	C11-C10-C8-C7
17	A	805	CLA	C11-C12-C13-C15
17	A	805	CLA	C12-C13-C15-C16
17	A	812	CLA	C11-C12-C13-C15
17	A	828	CLA	C12-C13-C15-C16
17	A	832	CLA	C6-C7-C8-C10
17	A	839	CLA	C6-C7-C8-C10
17	A	839	CLA	C11-C12-C13-C15
17	A	840	CLA	C6-C7-C8-C10
17	B	816	CLA	C6-C7-C8-C10
17	B	820	CLA	C6-C7-C8-C10
17	B	828	CLA	C11-C12-C13-C15
17	B	834	CLA	C6-C7-C8-C10
17	B	834	CLA	C11-C10-C8-C7
17	B	835	CLA	C6-C7-C8-C10
17	B	837	CLA	C6-C7-C8-C10
17	B	840	CLA	C12-C13-C15-C16
17	F	304	CLA	C12-C13-C15-C16
17	L	202	CLA	C11-C12-C13-C15
17	B	807	CLA	C13-C15-C16-C17
24	F	309	LMG	C18-C19-C20-C21
17	4	310	CLA	C4-C3-C5-C6
17	A	805	CLA	C3A-C2A-CAA-CBA
17	A	837	CLA	C3A-C2A-CAA-CBA
17	B	814	CLA	C4-C3-C5-C6
17	1	309	CLA	C15-C16-C17-C18
17	1	307	CLA	C2-C3-C5-C6
17	4	310	CLA	C2-C3-C5-C6
17	B	813	CLA	C2-C3-C5-C6
22	B	801	LHG	C7-C8-C9-C10
18	3	601	CHL	CBA-CGA-O2A-C1
21	1	316	BCR	C19-C20-C21-C22
21	2	316	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
17	B	804	CLA	C15-C16-C17-C18
17	1	302	CLA	O1A-CGA-O2A-C1
24	F	309	LMG	C40-C41-C42-C43
22	G	102	LHG	C27-C28-C29-C30
26	B	850	DGD	C2B-C3B-C4B-C5B
24	G	101	LMG	C7-C8-C9-O8
26	B	850	DGD	O1G-C1G-C2G-C3G
17	A	832	CLA	C4C-C3C-CAC-CBC
22	2	317	LHG	C23-C24-C25-C26
17	B	813	CLA	C6-C7-C8-C10
18	4	301	CHL	C1A-C2A-CAA-CBA
18	4	306	CHL	C1A-C2A-CAA-CBA
17	B	812	CLA	C5-C6-C7-C8
17	1	307	CLA	C4-C3-C5-C6
17	A	803	CLA	C4-C3-C5-C6
17	A	826	CLA	C4-C3-C5-C6
17	B	813	CLA	C4-C3-C5-C6
17	B	814	CLA	C2-C3-C5-C6
17	1	307	CLA	C3-C5-C6-C7
17	4	310	CLA	C10-C11-C12-C13
17	B	804	CLA	O1D-CGD-O2D-CED
17	B	809	CLA	O1D-CGD-O2D-CED
26	B	850	DGD	C5A-C6A-C7A-C8A
17	A	810	CLA	C16-C17-C18-C20
17	B	813	CLA	C6-C7-C8-C9
17	B	826	CLA	C16-C17-C18-C20
17	B	837	CLA	C11-C12-C13-C15
17	A	819	CLA	C2B-C3B-CAB-CBB
21	2	316	BCR	C1-C6-C7-C8
21	3	616	BCR	C23-C24-C25-C30
21	A	849	BCR	C1-C6-C7-C8
21	B	847	BCR	C23-C24-C25-C30
21	B	849	BCR	C1-C6-C7-C8
21	G	106	BCR	C23-C24-C25-C30
21	J	105	BCR	C1-C6-C7-C8
21	L	201	BCR	C23-C24-C25-C30
21	L	206	BCR	C23-C24-C25-C30
17	1	312	CLA	CAA-CBA-CGA-O2A
17	B	808	CLA	C8-C10-C11-C12
22	F	302	LHG	C11-C10-C9-C8
17	A	809	CLA	C8-C10-C11-C12
17	B	809	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
17	B	818	CLA	C5-C6-C7-C8
22	A	844	LHG	C19-C20-C21-C22
17	1	302	CLA	C16-C17-C18-C19
17	B	823	CLA	O1D-CGD-O2D-CED
24	F	309	LMG	O7-C8-C9-O8
25	F	310	HTG	O5-C1-S1-C1'
17	B	805	CLA	O1D-CGD-O2D-CED
22	1	317	LHG	C19-C20-C21-C22
17	B	818	CLA	O1A-CGA-O2A-C1
24	4	319	LMG	C17-C18-C19-C20
17	1	312	CLA	C6-C7-C8-C10
17	B	826	CLA	C16-C17-C18-C19
27	A	842	PQN	C26-C27-C28-C30
24	4	320	LMG	C29-C30-C31-C32
24	B	852	LMG	C15-C16-C17-C18
26	B	850	DGD	C9B-CAB-CBB-CCB
24	4	319	LMG	C18-C19-C20-C21
17	A	825	CLA	C11-C12-C13-C14
17	A	832	CLA	C11-C12-C13-C14
17	B	840	CLA	C14-C13-C15-C16
17	B	841	CLA	C6-C7-C8-C9
24	B	852	LMG	C29-C30-C31-C32
26	4	323	DGD	C6A-C7A-C8A-C9A
17	2	303	CLA	O1A-CGA-O2A-C1
24	G	101	LMG	C16-C17-C18-C19
17	4	303	CLA	C11-C12-C13-C15
22	F	302	LHG	C18-C19-C20-C21
24	4	320	LMG	C2-C1-O1-C7
22	A	844	LHG	C10-C11-C12-C13
17	L	203	CLA	C3-C5-C6-C7
17	A	831	CLA	CBA-CGA-O2A-C1
26	4	323	DGD	O1G-C1A-C2A-C3A
17	1	311	CLA	C11-C12-C13-C14
17	B	827	CLA	C16-C17-C18-C19
22	A	844	LHG	C1-C2-C3-O3
21	3	616	BCR	C11-C10-C9-C34
21	4	318	BCR	C16-C17-C18-C36
17	A	824	CLA	O1A-CGA-O2A-C1
17	A	811	CLA	CBA-CGA-O2A-C1
17	B	825	CLA	C11-C12-C13-C14
17	3	611	CLA	C5-C6-C7-C8
24	F	309	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
17	1	302	CLA	C11-C12-C13-C15
17	2	303	CLA	C6-C7-C8-C10
17	A	807	CLA	C12-C13-C15-C16
17	A	812	CLA	C11-C10-C8-C7
17	A	818	CLA	C11-C12-C13-C15
17	A	825	CLA	C11-C12-C13-C15
17	A	831	CLA	C12-C13-C15-C16
17	A	832	CLA	C11-C12-C13-C15
17	A	841	CLA	C11-C12-C13-C15
17	B	805	CLA	C12-C13-C15-C16
17	B	809	CLA	C6-C7-C8-C10
17	B	811	CLA	C6-C7-C8-C10
17	B	826	CLA	C11-C12-C13-C15
17	B	831	CLA	C11-C12-C13-C15
17	B	838	CLA	C12-C13-C15-C16
17	B	841	CLA	C6-C7-C8-C10
17	B	842	CLA	C11-C12-C13-C15
17	L	202	CLA	C6-C7-C8-C10
21	3	616	BCR	C21-C22-C23-C24
21	B	845	BCR	C7-C8-C9-C10
17	3	608	CLA	O1D-CGD-O2D-CED
17	B	819	CLA	C2A-CAA-CBA-CGA
17	A	816	CLA	C16-C17-C18-C19
17	4	313	CLA	O1D-CGD-O2D-CED
24	B	852	LMG	O9-C10-O7-C8
17	A	810	CLA	C4-C3-C5-C6
17	J	101	CLA	C10-C11-C12-C13
17	B	814	CLA	O2A-C1-C2-C3
17	A	826	CLA	O1A-CGA-O2A-C1
17	A	838	CLA	C15-C16-C17-C18
17	A	829	CLA	O1D-CGD-O2D-CED
17	1	309	CLA	C16-C17-C18-C19
17	A	819	CLA	C2C-C3C-CAC-CBC
18	3	601	CHL	O1A-CGA-O2A-C1
17	A	805	CLA	C8-C10-C11-C12
21	2	316	BCR	C20-C21-C22-C23
22	B	801	LHG	O6-C4-C5-O7
17	A	839	CLA	O1D-CGD-O2D-CED
24	F	309	LMG	C7-C8-C9-O8
17	B	807	CLA	C10-C11-C12-C13
17	B	826	CLA	C13-C15-C16-C17
17	B	829	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
17	B	810	CLA	C16-C17-C18-C19
17	B	820	CLA	C11-C12-C13-C15
17	A	808	CLA	C3-C5-C6-C7
22	G	102	LHG	C10-C11-C12-C13
17	A	838	CLA	C4-C3-C5-C6
17	3	610	CLA	C2-C3-C5-C6
17	A	838	CLA	C2-C3-C5-C6
25	B	851	HTG	C2-C1-S1-C1'
25	J	102	HTG	C2-C1-S1-C1'
17	B	812	CLA	C13-C15-C16-C17
17	A	836	CLA	C3-C5-C6-C7
17	B	810	CLA	C3-C5-C6-C7
22	A	845	LHG	O7-C5-C6-O8
17	2	301	CLA	C6-C7-C8-C9
17	2	303	CLA	C6-C7-C8-C9
17	A	807	CLA	C14-C13-C15-C16
17	A	817	CLA	C14-C13-C15-C16
17	A	818	CLA	C11-C10-C8-C9
17	A	827	CLA	C11-C10-C8-C9
17	B	827	CLA	C11-C10-C8-C9
24	F	309	LMG	C39-C40-C41-C42
17	A	811	CLA	O1A-CGA-O2A-C1
17	A	824	CLA	C10-C11-C12-C13
17	A	839	CLA	C8-C10-C11-C12
24	4	319	LMG	C22-C23-C24-C25
17	A	809	CLA	C10-C11-C12-C13
17	B	835	CLA	C2-C1-O2A-CGA
17	2	311	CLA	CBA-CGA-O2A-C1
17	4	309	CLA	C11-C12-C13-C14
17	4	302	CLA	C10-C11-C12-C13
17	A	810	CLA	C5-C6-C7-C8
17	B	823	CLA	C5-C6-C7-C8
22	A	844	LHG	O2-C2-C3-O3
22	F	302	LHG	C10-C11-C12-C13
17	3	611	CLA	C6-C7-C8-C9
21	L	201	BCR	C14-C15-C16-C17
26	4	323	DGD	C4B-C5B-C6B-C7B
22	B	801	LHG	O10-C23-O8-C6
17	A	838	CLA	C8-C10-C11-C12
21	B	849	BCR	C10-C11-C12-C13
17	B	828	CLA	C2C-C3C-CAC-CBC
17	1	303	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	3	605	CLA	C4B-C3B-CAB-CBB
17	3	610	CLA	C4B-C3B-CAB-CBB
17	4	312	CLA	C4B-C3B-CAB-CBB
17	4	313	CLA	C4B-C3B-CAB-CBB
17	A	823	CLA	C1A-C2A-CAA-CBA
17	B	812	CLA	C4B-C3B-CAB-CBB
17	B	815	CLA	C1A-C2A-CAA-CBA
17	B	821	CLA	C4B-C3B-CAB-CBB
17	B	833	CLA	C1A-C2A-CAA-CBA
17	B	841	CLA	C4B-C3B-CAB-CBB
17	K	202	CLA	C1A-C2A-CAA-CBA
17	A	824	CLA	O1D-CGD-O2D-CED
17	3	609	CLA	CBA-CGA-O2A-C1
20	4	317	XAT	C7-C8-C9-C10
21	J	105	BCR	C21-C22-C23-C24
23	2	318	LMT	O1'-C1-C2-C3
17	A	831	CLA	O1A-CGA-O2A-C1
17	4	304	CLA	C2A-CAA-CBA-CGA
24	4	319	LMG	C29-C30-C31-C32
26	B	850	DGD	CDA-CEA-CFA-CGA
22	B	801	LHG	O6-C4-C5-C6
17	1	303	CLA	C2-C3-C5-C6
17	A	822	CLA	C2-C3-C5-C6
17	A	820	CLA	C13-C15-C16-C17
17	1	301	CLA	C11-C12-C13-C15
17	2	303	CLA	C11-C10-C8-C7
17	2	311	CLA	C6-C7-C8-C10
17	2	311	CLA	C11-C10-C8-C7
17	A	807	CLA	C11-C10-C8-C7
17	A	824	CLA	C11-C12-C13-C15
17	B	803	CLA	C11-C12-C13-C15
17	B	815	CLA	C11-C12-C13-C15
17	B	815	CLA	C12-C13-C15-C16
17	B	816	CLA	C11-C12-C13-C15
17	B	829	CLA	C11-C12-C13-C15
17	B	841	CLA	C12-C13-C15-C16
17	L	203	CLA	C12-C13-C15-C16
17	K	202	CLA	C11-C10-C8-C7
24	F	309	LMG	C37-C38-C39-C40
17	B	837	CLA	C11-C12-C13-C14
17	B	807	CLA	CBA-CGA-O2A-C1
22	F	302	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	A	855	LMT	C5-C6-C7-C8
17	4	310	CLA	C3A-C2A-CAA-CBA
17	B	805	CLA	C16-C17-C18-C19
17	A	853	CLA	C8-C10-C11-C12
18	4	301	CHL	C10-C11-C12-C13
22	A	844	LHG	C13-C14-C15-C16
17	2	311	CLA	O1A-CGA-O2A-C1
17	B	816	CLA	CBA-CGA-O2A-C1
22	A	844	LHG	O6-C4-C5-O7
22	G	102	LHG	O6-C4-C5-O7
17	A	819	CLA	C4C-C3C-CAC-CBC
17	A	818	CLA	C11-C12-C13-C14
17	A	828	CLA	C14-C13-C15-C16
17	A	838	CLA	C11-C10-C8-C9
17	A	841	CLA	C11-C12-C13-C14
17	A	853	CLA	C11-C12-C13-C14
17	B	811	CLA	C6-C7-C8-C9
17	B	826	CLA	C11-C12-C13-C14
17	B	831	CLA	C11-C12-C13-C14
17	B	816	CLA	O1A-CGA-O2A-C1
19	1	314	LUT	C13-C14-C15-C35
21	L	201	BCR	C13-C14-C15-C16
21	K	203	BCR	C19-C20-C21-C22
22	G	102	LHG	C33-C34-C35-C36
17	A	821	CLA	C1-C2-C3-C4
22	F	302	LHG	C13-C14-C15-C16
17	B	841	CLA	C3-C5-C6-C7
17	3	609	CLA	O1A-CGA-O2A-C1
22	1	317	LHG	O9-C7-O7-C5
22	F	302	LHG	O9-C7-O7-C5
24	F	309	LMG	O1-C7-C8-O7
25	F	305	HTG	C2'-C3'-C4'-C5'
22	1	317	LHG	C24-C23-O8-C6
17	A	816	CLA	C16-C17-C18-C20
17	B	828	CLA	C10-C11-C12-C13
24	B	852	LMG	C33-C34-C35-C36
17	B	807	CLA	CAD-CBD-CGD-O2D
17	J	103	CLA	CAD-CBD-CGD-O2D
17	B	807	CLA	O1A-CGA-O2A-C1
17	B	840	CLA	C13-C15-C16-C17
17	B	823	CLA	O1A-CGA-O2A-C1
17	3	612	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
17	4	302	CLA	CHA-CBD-CGD-O1D
17	4	302	CLA	CHA-CBD-CGD-O2D
17	A	824	CLA	CHA-CBD-CGD-O1D
17	A	824	CLA	CHA-CBD-CGD-O2D
17	A	830	CLA	CHA-CBD-CGD-O1D
17	A	830	CLA	CHA-CBD-CGD-O2D
17	A	843	CLA	CAD-CBD-CGD-O1D
17	B	807	CLA	CAD-CBD-CGD-O1D
17	J	103	CLA	CAD-CBD-CGD-O1D
18	3	601	CHL	CHA-CBD-CGD-O2D
18	4	315	CHL	CHA-CBD-CGD-O2D
22	2	317	LHG	C3-O3-P-O5
22	2	317	LHG	C4-O6-P-O4
22	A	844	LHG	C3-O3-P-O5
22	A	845	LHG	C3-O3-P-O5
22	A	845	LHG	C4-O6-P-O5
22	G	102	LHG	C4-O6-P-O5
17	A	839	CLA	CBD-CGD-O2D-CED
17	A	824	CLA	C15-C16-C17-C18
17	4	314	CLA	O1D-CGD-O2D-CED
17	3	606	CLA	C2B-C3B-CAB-CBB
17	3	610	CLA	C2B-C3B-CAB-CBB
17	4	312	CLA	C2B-C3B-CAB-CBB
17	A	813	CLA	C2B-C3B-CAB-CBB
17	A	820	CLA	C2B-C3B-CAB-CBB
17	A	833	CLA	C2B-C3B-CAB-CBB
17	B	821	CLA	C2B-C3B-CAB-CBB
21	2	316	BCR	C5-C6-C7-C8
21	A	847	BCR	C23-C24-C25-C30
22	G	102	LHG	C2-C3-O3-P
17	A	828	CLA	C3-C5-C6-C7
17	A	837	CLA	C3-C5-C6-C7
17	3	611	CLA	C6-C7-C8-C10
17	A	827	CLA	C16-C17-C18-C19
17	B	814	CLA	C6-C7-C8-C10
25	J	102	HTG	C4'-C5'-C6'-C7'
17	B	823	CLA	CBA-CGA-O2A-C1
17	A	835	CLA	C2A-CAA-CBA-CGA
17	B	813	CLA	O1A-CGA-O2A-C1
17	F	304	CLA	C13-C15-C16-C17
22	F	302	LHG	C4-C5-O7-C7
17	4	310	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
17	B	828	CLA	C8-C10-C11-C12
23	2	318	LMT	C5-C6-C7-C8
17	A	805	CLA	CBA-CGA-O2A-C1
17	1	307	CLA	C11-C12-C13-C14
17	2	311	CLA	C14-C13-C15-C16
17	A	802	CLA	C11-C10-C8-C9
17	A	838	CLA	C14-C13-C15-C16
17	B	819	CLA	C11-C10-C8-C9
17	B	828	CLA	C11-C10-C8-C9
17	B	834	CLA	C6-C7-C8-C9
17	B	838	CLA	C11-C12-C13-C14
17	L	202	CLA	C6-C7-C8-C9
17	L	202	CLA	C11-C12-C13-C14
17	A	802	CLA	C11-C10-C8-C7
17	A	809	CLA	C11-C10-C8-C7
17	A	809	CLA	C12-C13-C15-C16
17	A	818	CLA	C11-C10-C8-C7
17	B	820	CLA	C11-C10-C8-C7
17	B	817	CLA	C5-C6-C7-C8
21	A	851	BCR	C16-C17-C18-C19
17	A	807	CLA	C2A-CAA-CBA-CGA
17	A	801	CLA	C3-C5-C6-C7
22	F	302	LHG	C19-C20-C21-C22
22	1	317	LHG	C27-C28-C29-C30
17	B	803	CLA	C4-C3-C5-C6
17	A	810	CLA	C2-C3-C5-C6
17	A	826	CLA	C16-C17-C18-C20
17	A	839	CLA	C16-C17-C18-C19
17	B	810	CLA	C16-C17-C18-C20
24	B	852	LMG	C36-C37-C38-C39
17	B	807	CLA	C15-C16-C17-C18
17	B	842	CLA	CAA-CBA-CGA-O2A
24	4	320	LMG	C36-C37-C38-C39
17	B	815	CLA	C4C-C3C-CAC-CBC
17	1	303	CLA	O1A-CGA-O2A-C1
17	1	303	CLA	CBA-CGA-O2A-C1
17	B	829	CLA	CBA-CGA-O2A-C1
21	2	316	BCR	C9-C10-C11-C12
17	B	841	CLA	C16-C17-C18-C20
26	B	850	DGD	CBB-CCB-CDB-CEB
17	1	308	CLA	CBA-CGA-O2A-C1
17	1	308	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	4	304	CLA	C2-C1-O2A-CGA
22	A	844	LHG	C16-C17-C18-C19
17	A	841	CLA	C10-C11-C12-C13
17	B	819	CLA	CAA-CBA-CGA-O2A
17	4	309	CLA	C11-C12-C13-C15
25	J	102	HTG	C2'-C1'-S1-C1
17	A	853	CLA	CBD-CGD-O2D-CED
24	4	319	LMG	C37-C38-C39-C40
22	A	845	LHG	O10-C23-C24-C25
17	2	311	CLA	C2A-CAA-CBA-CGA
17	4	313	CLA	C2A-CAA-CBA-CGA
22	F	302	LHG	C12-C13-C14-C15
22	A	845	LHG	O8-C23-C24-C25
17	1	301	CLA	C11-C12-C13-C14
17	2	311	CLA	C11-C10-C8-C9
17	A	824	CLA	C11-C12-C13-C14
17	B	808	CLA	C11-C12-C13-C14
17	B	815	CLA	C11-C12-C13-C14
17	K	202	CLA	C11-C10-C8-C9
17	B	813	CLA	CBA-CGA-O2A-C1
17	4	312	CLA	O1A-CGA-O2A-C1
17	A	817	CLA	C4B-C3B-CAB-CBB
17	A	826	CLA	C4B-C3B-CAB-CBB
17	B	803	CLA	C4B-C3B-CAB-CBB
17	A	839	CLA	C13-C15-C16-C17
17	4	312	CLA	CBA-CGA-O2A-C1
17	A	809	CLA	CBA-CGA-O2A-C1
22	F	302	LHG	C24-C23-O8-C6
17	B	829	CLA	O1A-CGA-O2A-C1
17	B	836	CLA	C2C-C3C-CAC-CBC
19	4	316	LUT	C13-C14-C15-C35
17	B	805	CLA	C16-C17-C18-C20
24	4	319	LMG	C12-C13-C14-C15
17	2	308	CLA	C6-C7-C8-C10
17	A	806	CLA	C11-C12-C13-C15
17	A	853	CLA	C12-C13-C15-C16
17	B	808	CLA	C11-C12-C13-C15
17	B	810	CLA	C6-C7-C8-C10
17	B	811	CLA	C12-C13-C15-C16
17	4	302	CLA	C8-C10-C11-C12
22	G	102	LHG	C11-C12-C13-C14
24	4	319	LMG	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
25	F	310	HTG	C1'-C2'-C3'-C4'
17	1	304	CLA	C2C-C3C-CAC-CBC
17	1	301	CLA	C15-C16-C17-C18
26	B	850	DGD	O1G-C1G-C2G-O2G
17	A	822	CLA	C3A-C2A-CAA-CBA
17	A	839	CLA	C4-C3-C5-C6
17	B	815	CLA	C3A-C2A-CAA-CBA
17	B	818	CLA	C4-C3-C5-C6
17	L	203	CLA	C3A-C2A-CAA-CBA
23	A	855	LMT	C2B-C1B-O1B-C4'
24	F	309	LMG	C20-C21-C22-C23
21	A	851	BCR	C11-C10-C9-C34
21	A	851	BCR	C16-C17-C18-C36
21	B	845	BCR	C11-C10-C9-C34
21	B	846	BCR	C11-C10-C9-C34
21	B	846	BCR	C20-C21-C22-C37
21	J	105	BCR	C35-C13-C14-C15
21	L	201	BCR	C11-C10-C9-C34
22	1	317	LHG	C29-C30-C31-C32
22	2	317	LHG	C29-C30-C31-C32
24	B	852	LMG	C18-C19-C20-C21
17	A	853	CLA	C2-C1-O2A-CGA
21	I	101	BCR	C19-C20-C21-C22
17	B	827	CLA	C13-C15-C16-C17
17	B	838	CLA	C5-C6-C7-C8
17	1	303	CLA	C4-C3-C5-C6
17	A	822	CLA	C4-C3-C5-C6
17	A	818	CLA	C4-C3-C5-C6
17	A	805	CLA	CAA-CBA-CGA-O1A
21	B	849	BCR	C14-C15-C16-C17
17	2	311	CLA	C6-C7-C8-C9
17	4	312	CLA	C6-C7-C8-C9
17	A	806	CLA	C11-C12-C13-C14
17	A	816	CLA	C6-C7-C8-C9
17	A	820	CLA	C11-C10-C8-C9
17	A	820	CLA	C14-C13-C15-C16
17	A	836	CLA	C6-C7-C8-C9
17	B	807	CLA	C11-C10-C8-C9
17	B	829	CLA	C14-C13-C15-C16
17	J	101	CLA	C11-C10-C8-C9
17	A	820	CLA	C16-C17-C18-C19
17	4	310	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
24	G	101	LMG	C21-C22-C23-C24
18	2	306	CHL	C1A-C2A-CAA-CBA
18	3	607	CHL	C1A-C2A-CAA-CBA
17	A	805	CLA	C2-C3-C5-C6
17	3	611	CLA	C2A-CAA-CBA-CGA
17	3	610	CLA	C1A-C2A-CAA-CBA
17	A	802	CLA	C1A-C2A-CAA-CBA
17	A	809	CLA	C1A-C2A-CAA-CBA
17	A	822	CLA	C1A-C2A-CAA-CBA
21	A	851	BCR	C11-C10-C9-C8
21	B	846	BCR	C20-C21-C22-C23
21	G	106	BCR	C20-C21-C22-C23
21	L	201	BCR	C11-C10-C9-C8
17	1	303	CLA	C2B-C3B-CAB-CBB
17	3	605	CLA	C2B-C3B-CAB-CBB
17	4	303	CLA	C2B-C3B-CAB-CBB
17	4	313	CLA	C2B-C3B-CAB-CBB
17	A	801	CLA	C2B-C3B-CAB-CBB
17	A	817	CLA	C2B-C3B-CAB-CBB
17	A	826	CLA	C2B-C3B-CAB-CBB
17	B	803	CLA	C2B-C3B-CAB-CBB
17	B	812	CLA	C2B-C3B-CAB-CBB
17	B	841	CLA	C2B-C3B-CAB-CBB
17	L	204	CLA	C2B-C3B-CAB-CBB
21	2	316	BCR	C23-C24-C25-C30
21	3	616	BCR	C23-C24-C25-C26
21	A	847	BCR	C23-C24-C25-C26
21	A	848	BCR	C1-C6-C7-C8
21	A	850	BCR	C1-C6-C7-C8
21	B	847	BCR	C23-C24-C25-C26
21	B	849	BCR	C5-C6-C7-C8
21	G	106	BCR	C23-C24-C25-C26
21	J	105	BCR	C5-C6-C7-C8
21	L	201	BCR	C1-C6-C7-C8
21	L	201	BCR	C23-C24-C25-C26
21	L	206	BCR	C1-C6-C7-C8
21	L	206	BCR	C23-C24-C25-C26
17	A	805	CLA	C4-C3-C5-C6
17	A	839	CLA	C2-C3-C5-C6
17	1	301	CLA	C6-C7-C8-C10
17	1	309	CLA	C6-C7-C8-C10
17	2	311	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
17	A	801	CLA	C12-C13-C15-C16
17	A	804	CLA	C11-C10-C8-C7
17	A	825	CLA	C6-C7-C8-C10
17	A	836	CLA	C11-C12-C13-C15
17	A	837	CLA	C6-C7-C8-C10
17	A	838	CLA	C11-C10-C8-C7
17	A	840	CLA	C11-C10-C8-C7
17	B	807	CLA	C11-C10-C8-C7
17	B	809	CLA	C12-C13-C15-C16
17	B	827	CLA	C11-C12-C13-C15
17	J	101	CLA	C11-C10-C8-C7
18	4	301	CHL	C6-C7-C8-C10
17	A	840	CLA	C2A-CAA-CBA-CGA
17	A	839	CLA	C15-C16-C17-C18
25	B	851	HTG	C4'-C5'-C6'-C7'
24	4	320	LMG	C33-C34-C35-C36
17	A	827	CLA	C10-C11-C12-C13
17	A	826	CLA	C16-C17-C18-C19
17	B	841	CLA	C16-C17-C18-C19
24	4	319	LMG	O9-C10-O7-C8
22	G	102	LHG	C28-C29-C30-C31
17	4	313	CLA	CAA-CBA-CGA-O1A
17	A	807	CLA	C4-C3-C5-C6
17	A	843	CLA	C4-C3-C5-C6
25	4	322	HTG	C4-C5-C6-O6
17	F	307	CLA	C5-C6-C7-C8
17	A	818	CLA	C2-C3-C5-C6
24	G	101	LMG	C19-C20-C21-C22
17	A	809	CLA	O1A-CGA-O2A-C1
17	4	308	CLA	C2-C1-O2A-CGA
17	2	319	CLA	C2A-CAA-CBA-CGA
17	4	313	CLA	CAA-CBA-CGA-O2A
17	A	809	CLA	C11-C12-C13-C14
17	B	837	CLA	C11-C10-C8-C9
17	A	818	CLA	C5-C6-C7-C8
17	A	801	CLA	C13-C15-C16-C17
17	A	804	CLA	C4-C3-C5-C6
17	A	805	CLA	O1A-CGA-O2A-C1
17	F	304	CLA	C10-C11-C12-C13
17	F	304	CLA	C15-C16-C17-C18
17	4	303	CLA	C8-C10-C11-C12
22	2	317	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
17	A	819	CLA	CAA-CBA-CGA-O2A
17	B	819	CLA	C11-C12-C13-C14
17	A	839	CLA	C16-C17-C18-C20
17	B	814	CLA	O1A-CGA-O2A-C1
17	A	807	CLA	C2-C3-C5-C6
17	4	310	CLA	C11-C12-C13-C15
24	F	309	LMG	C16-C17-C18-C19
17	3	603	CLA	C4B-C3B-CAB-CBB
17	A	814	CLA	C4B-C3B-CAB-CBB
17	B	840	CLA	C4B-C3B-CAB-CBB
17	A	815	CLA	CAA-CBA-CGA-O2A
17	A	803	CLA	C6-C7-C8-C9
17	B	824	CLA	C6-C7-C8-C9
18	2	304	CHL	CHA-CBD-CGD-O1D
18	3	601	CHL	CHA-CBD-CGD-O1D
18	4	301	CHL	CHA-CBD-CGD-O1D
18	4	301	CHL	CHA-CBD-CGD-O2D
18	4	306	CHL	CHA-CBD-CGD-O1D
18	4	306	CHL	CHA-CBD-CGD-O2D
21	2	316	BCR	C11-C10-C9-C34
21	F	308	BCR	C35-C13-C14-C15
21	J	104	BCR	C20-C21-C22-C37
22	F	302	LHG	O7-C5-C6-O8
17	3	612	CLA	CAA-CBA-CGA-O2A
17	A	817	CLA	CAA-CBA-CGA-O2A
17	A	836	CLA	C6-C7-C8-C10
17	B	829	CLA	C12-C13-C15-C16
21	2	316	BCR	C19-C20-C21-C22
21	F	308	BCR	C9-C10-C11-C12
22	A	844	LHG	C30-C31-C32-C33
17	1	302	CLA	C6-C7-C8-C9
17	A	801	CLA	C14-C13-C15-C16
17	A	806	CLA	C14-C13-C15-C16
17	A	807	CLA	C11-C10-C8-C9
17	A	829	CLA	C6-C7-C8-C9
17	A	829	CLA	C14-C13-C15-C16
17	B	809	CLA	C11-C10-C8-C9
17	B	840	CLA	C6-C7-C8-C9
24	4	320	LMG	C8-C7-O1-C1
24	G	101	LMG	C8-C7-O1-C1
26	B	850	DGD	CAA-CBA-CCA-CDA
17	1	312	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
17	A	811	CLA	C2A-CAA-CBA-CGA
17	A	823	CLA	C2A-CAA-CBA-CGA
17	A	841	CLA	C2A-CAA-CBA-CGA
17	B	805	CLA	C2A-CAA-CBA-CGA
17	A	837	CLA	C2-C1-O2A-CGA
17	B	823	CLA	C2-C1-O2A-CGA
17	1	307	CLA	C3A-C2A-CAA-CBA
17	A	802	CLA	C3A-C2A-CAA-CBA
17	A	808	CLA	C3A-C2A-CAA-CBA
17	B	835	CLA	C3A-C2A-CAA-CBA
17	B	818	CLA	C2-C3-C5-C6
17	4	309	CLA	C8-C10-C11-C12
17	2	319	CLA	CAA-CBA-CGA-O2A
22	F	302	LHG	C6-C5-O7-C7
21	1	316	BCR	C18-C19-C20-C21
26	B	850	DGD	CAB-CBB-CCB-CDB
17	B	810	CLA	C10-C11-C12-C13
21	1	316	BCR	C14-C15-C16-C17
17	A	815	CLA	CAA-CBA-CGA-O1A
17	A	819	CLA	CAA-CBA-CGA-O1A
17	A	831	CLA	C2A-CAA-CBA-CGA
23	A	855	LMT	O5B-C1B-O1B-C4'
17	A	843	CLA	C2-C3-C5-C6
18	4	301	CHL	C2-C3-C5-C6
20	1	315	XAT	O4-C6-C7-C8
20	1	315	XAT	C11-C10-C9-C8
20	2	315	XAT	O4-C6-C7-C8
20	2	315	XAT	C11-C10-C9-C8
20	3	615	XAT	O4-C6-C7-C8
20	3	615	XAT	C11-C10-C9-C8
21	B	846	BCR	C11-C10-C9-C8
21	F	308	BCR	C12-C13-C14-C15
22	B	801	LHG	C2-C3-O3-P
22	A	844	LHG	C4-C5-C6-O8
22	F	302	LHG	C4-C5-C6-O8
17	2	308	CLA	O1A-CGA-O2A-C1
22	1	317	LHG	C31-C32-C33-C34
24	4	320	LMG	C17-C18-C19-C20
17	B	822	CLA	C2A-CAA-CBA-CGA
22	A	844	LHG	C34-C35-C36-C37
22	G	102	LHG	C23-C24-C25-C26
17	A	809	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
17	A	841	CLA	C5-C6-C7-C8
26	4	323	DGD	O1A-C1A-C2A-C3A
17	A	827	CLA	C11-C12-C13-C14
17	B	841	CLA	C14-C13-C15-C16
17	L	203	CLA	C14-C13-C15-C16
17	B	824	CLA	C6-C7-C8-C10
17	4	311	CLA	CAA-CBA-CGA-O2A
17	B	829	CLA	C5-C6-C7-C8
18	4	301	CHL	C4-C3-C5-C6
17	3	612	CLA	CAA-CBA-CGA-O1A
17	1	311	CLA	C2A-CAA-CBA-CGA
17	2	308	CLA	C2A-CAA-CBA-CGA
17	3	612	CLA	C2A-CAA-CBA-CGA
17	A	830	CLA	C2A-CAA-CBA-CGA
17	1	308	CLA	C11-C10-C8-C7
17	A	809	CLA	C11-C12-C13-C15
17	A	838	CLA	C6-C7-C8-C10
17	A	841	CLA	C6-C7-C8-C10
17	B	803	CLA	C12-C13-C15-C16
17	B	809	CLA	C11-C10-C8-C7
17	B	821	CLA	C11-C12-C13-C15
17	B	823	CLA	C12-C13-C15-C16
17	B	837	CLA	C11-C10-C8-C7
17	B	840	CLA	C6-C7-C8-C10
17	J	101	CLA	C6-C7-C8-C10
17	A	814	CLA	C2B-C3B-CAB-CBB
17	B	825	CLA	C2B-C3B-CAB-CBB
17	B	833	CLA	C2B-C3B-CAB-CBB
17	B	834	CLA	C2B-C3B-CAB-CBB
21	2	316	BCR	C23-C24-C25-C26
21	3	616	BCR	C1-C6-C7-C8
21	A	848	BCR	C5-C6-C7-C8
21	A	849	BCR	C5-C6-C7-C8
21	A	849	BCR	C23-C24-C25-C26
21	A	849	BCR	C23-C24-C25-C30
21	A	850	BCR	C5-C6-C7-C8
21	B	844	BCR	C23-C24-C25-C26
21	B	844	BCR	C23-C24-C25-C30
21	I	101	BCR	C1-C6-C7-C8
21	L	201	BCR	C5-C6-C7-C8
21	L	205	BCR	C1-C6-C7-C8
21	L	205	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	L	206	BCR	C5-C6-C7-C8
21	K	203	BCR	C1-C6-C7-C8
24	B	852	LMG	C11-C10-O7-C8
23	A	855	LMT	C4-C5-C6-C7
17	B	808	CLA	C2-C1-O2A-CGA
17	B	829	CLA	C2-C1-O2A-CGA
18	3	601	CHL	C2-C1-O2A-CGA
17	A	821	CLA	O2A-C1-C2-C3
17	B	824	CLA	CAA-CBA-CGA-O2A
17	B	836	CLA	CBD-CGD-O2D-CED
17	B	840	CLA	CBA-CGA-O2A-C1
17	B	812	CLA	C4-C3-C5-C6
22	A	844	LHG	O7-C7-C8-C9
17	B	812	CLA	C2-C3-C5-C6
17	B	836	CLA	CAA-CBA-CGA-O2A
17	B	841	CLA	C13-C15-C16-C17
24	G	101	LMG	C22-C23-C24-C25
17	2	308	CLA	CBA-CGA-O2A-C1
17	K	202	CLA	CAA-CBA-CGA-O2A
17	L	203	CLA	C5-C6-C7-C8
17	1	302	CLA	CAA-CBA-CGA-O2A
17	1	304	CLA	C4C-C3C-CAC-CBC
17	B	803	CLA	C2-C3-C5-C6
17	G	105	CLA	CBA-CGA-O2A-C1
17	B	840	CLA	O1A-CGA-O2A-C1
17	2	310	CLA	CAA-CBA-CGA-O2A
17	1	301	CLA	C6-C7-C8-C9
17	B	815	CLA	O1D-CGD-O2D-CED
17	3	610	CLA	CAA-CBA-CGA-O2A
17	A	808	CLA	CAA-CBA-CGA-O2A
17	A	812	CLA	O1A-CGA-O2A-C1
17	1	307	CLA	C1A-C2A-CAA-CBA
17	1	310	CLA	C4B-C3B-CAB-CBB
17	A	816	CLA	C4B-C3B-CAB-CBB
17	A	831	CLA	C4B-C3B-CAB-CBB
17	A	834	CLA	C4B-C3B-CAB-CBB
17	A	840	CLA	C1A-C2A-CAA-CBA
17	A	843	CLA	C4B-C3B-CAB-CBB
17	B	817	CLA	C1A-C2A-CAA-CBA
17	B	842	CLA	C1A-C2A-CAA-CBA
17	A	812	CLA	CBA-CGA-O2A-C1
19	2	314	LUT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
17	B	812	CLA	CAA-CBA-CGA-O2A
17	F	307	CLA	CAA-CBA-CGA-O2A
21	A	849	BCR	C7-C8-C9-C10
21	F	303	BCR	C7-C8-C9-C10
19	2	314	LUT	C13-C14-C15-C35
17	L	203	CLA	C16-C17-C18-C19
17	A	803	CLA	CAA-CBA-CGA-O2A
17	B	811	CLA	CAA-CBA-CGA-O2A
24	B	852	LMG	C23-C24-C25-C26
18	2	305	CHL	C2-C1-O2A-CGA
17	1	302	CLA	C10-C11-C12-C13
22	A	844	LHG	O8-C23-C24-C25
17	B	815	CLA	C15-C16-C17-C18
17	A	840	CLA	C2-C1-O2A-CGA
17	B	807	CLA	C2-C1-O2A-CGA
17	B	817	CLA	C2-C1-O2A-CGA
17	K	202	CLA	C2-C1-O2A-CGA
17	4	310	CLA	C6-C7-C8-C10
17	4	310	CLA	C11-C10-C8-C7
17	A	817	CLA	C11-C12-C13-C15
17	A	829	CLA	C12-C13-C15-C16
17	A	831	CLA	C6-C7-C8-C10
17	B	825	CLA	C6-C7-C8-C10
17	B	827	CLA	C6-C7-C8-C10
17	B	831	CLA	C12-C13-C15-C16
17	B	814	CLA	CBA-CGA-O2A-C1
17	4	312	CLA	C2A-CAA-CBA-CGA
17	A	835	CLA	CAA-CBA-CGA-O2A
17	2	311	CLA	C10-C11-C12-C13
18	3	607	CHL	CBA-CGA-O2A-C1
17	2	303	CLA	C3A-C2A-CAA-CBA
17	B	824	CLA	C3A-C2A-CAA-CBA
17	F	304	CLA	C3A-C2A-CAA-CBA
17	B	820	CLA	C11-C12-C13-C14
22	1	317	LHG	O8-C23-C24-C25
17	B	824	CLA	CAA-CBA-CGA-O1A
17	B	802	CLA	C15-C16-C17-C18
17	B	836	CLA	CAA-CBA-CGA-O1A
17	4	303	CLA	C6-C7-C8-C9
17	A	809	CLA	C14-C13-C15-C16
17	A	831	CLA	C6-C7-C8-C9
17	A	841	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
17	B	816	CLA	C11-C12-C13-C14
17	B	825	CLA	C6-C7-C8-C9
17	B	812	CLA	CAA-CBA-CGA-O1A
22	A	844	LHG	O9-C7-C8-C9
17	1	302	CLA	CAA-CBA-CGA-O1A
22	F	302	LHG	C24-C25-C26-C27
17	4	311	CLA	CAA-CBA-CGA-O1A
26	B	850	DGD	C4A-C5A-C6A-C7A
17	B	820	CLA	O1A-CGA-O2A-C1
17	A	803	CLA	C6-C7-C8-C10
17	1	307	CLA	C10-C11-C12-C13
17	A	809	CLA	CAA-CBA-CGA-O1A
17	2	307	CLA	O1A-CGA-O2A-C1
22	2	317	LHG	O7-C5-C6-O8
17	2	310	CLA	CAA-CBA-CGA-O1A
17	3	610	CLA	CAA-CBA-CGA-O1A
17	B	808	CLA	CAA-CBA-CGA-O2A
17	A	812	CLA	C2A-CAA-CBA-CGA
17	A	808	CLA	CAA-CBA-CGA-O1A
22	2	317	LHG	C11-C12-C13-C14
17	G	105	CLA	O1A-CGA-O2A-C1
17	F	307	CLA	CAA-CBA-CGA-O1A
17	K	202	CLA	CAA-CBA-CGA-O1A
17	4	309	CLA	CAD-CBD-CGD-O2D
17	A	840	CLA	CAD-CBD-CGD-O2D
17	B	812	CLA	CAD-CBD-CGD-O2D
22	A	844	LHG	O6-C4-C5-C6
17	1	307	CLA	C2-C1-O2A-CGA
17	F	307	CLA	C2-C1-O2A-CGA
17	3	603	CLA	CAA-CBA-CGA-O2A
17	B	804	CLA	C16-C17-C18-C20
17	A	818	CLA	C13-C15-C16-C17
17	A	823	CLA	C5-C6-C7-C8
17	2	303	CLA	CAA-CBA-CGA-O2A
17	3	613	CLA	CAA-CBA-CGA-O2A
17	F	304	CLA	CAA-CBA-CGA-O2A
17	1	310	CLA	CAA-CBA-CGA-O2A
17	3	606	CLA	CAA-CBA-CGA-O2A
17	A	801	CLA	CAA-CBA-CGA-O2A
17	3	611	CLA	CBA-CGA-O2A-C1
17	3	611	CLA	O1A-CGA-O2A-C1
17	A	835	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
17	B	811	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

190 monomers are involved in 543 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	3	602	CLA	6	0
17	A	824	CLA	1	0
17	A	823	CLA	4	0
17	F	304	CLA	2	0
20	2	315	XAT	9	0
21	A	851	BCR	5	0
17	3	605	CLA	1	0
17	B	837	CLA	7	0
21	3	616	BCR	4	0
17	A	826	CLA	1	0
18	2	306	CHL	6	0
25	4	322	HTG	2	0
17	1	303	CLA	2	0
17	A	841	CLA	4	0
17	F	307	CLA	2	0
17	A	814	CLA	4	0
17	L	204	CLA	2	0
17	B	836	CLA	2	0
20	3	615	XAT	12	0
17	2	311	CLA	4	0
17	2	312	CLA	1	0
17	A	839	CLA	3	0
17	A	806	CLA	1	0
17	A	811	CLA	3	0
17	1	312	CLA	2	0
25	F	305	HTG	1	0
17	1	307	CLA	3	0
17	3	610	CLA	1	0
21	A	848	BCR	3	0
17	A	809	CLA	3	0
17	2	307	CLA	1	0
18	2	304	CHL	2	0
17	B	841	CLA	1	0
17	1	302	CLA	2	0
17	A	843	CLA	6	0
17	2	310	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	3	608	CLA	3	0
17	B	825	CLA	3	0
17	1	301	CLA	1	0
17	1	311	CLA	6	0
18	4	307	CHL	4	0
19	1	314	LUT	7	0
21	J	105	BCR	5	0
17	1	310	CLA	3	0
18	1	305	CHL	4	0
17	B	818	CLA	2	0
25	J	102	HTG	3	0
21	A	846	BCR	10	0
17	A	832	CLA	2	0
21	L	206	BCR	4	0
17	B	828	CLA	2	0
17	F	306	CLA	4	0
17	A	834	CLA	2	0
25	B	851	HTG	1	0
17	B	833	CLA	1	0
24	4	320	LMG	7	0
17	B	838	CLA	4	0
21	A	850	BCR	3	0
17	A	810	CLA	7	0
17	A	827	CLA	1	0
17	A	836	CLA	3	0
17	B	803	CLA	6	0
21	A	847	BCR	1	0
18	4	315	CHL	4	0
17	G	105	CLA	1	0
21	I	101	BCR	4	0
17	B	829	CLA	6	0
17	K	201	CLA	3	0
17	K	202	CLA	2	0
22	A	845	LHG	1	0
24	F	309	LMG	1	0
17	4	310	CLA	1	0
17	A	812	CLA	2	0
17	A	815	CLA	1	0
17	A	820	CLA	6	0
17	B	815	CLA	2	0
17	B	816	CLA	3	0
17	B	824	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	839	CLA	2	0
23	A	855	LMT	2	0
17	B	804	CLA	2	0
17	A	805	CLA	3	0
17	3	603	CLA	2	0
17	A	819	CLA	4	0
17	B	834	CLA	2	0
18	2	313	CHL	5	0
18	3	601	CHL	18	0
21	L	205	BCR	4	0
24	B	852	LMG	4	0
17	B	810	CLA	6	0
25	4	321	HTG	2	0
18	3	607	CHL	2	0
17	B	811	CLA	5	0
27	B	843	PQN	3	0
21	A	849	BCR	3	0
17	A	807	CLA	2	0
17	4	304	CLA	5	0
17	A	840	CLA	4	0
17	B	812	CLA	3	0
17	A	801	CLA	1	0
17	2	308	CLA	5	0
17	A	853	CLA	7	0
17	1	304	CLA	4	0
17	G	103	CLA	1	0
17	A	825	CLA	4	0
17	B	802	CLA	3	0
20	4	317	XAT	9	0
21	B	844	BCR	4	0
21	B	848	BCR	4	0
17	A	817	CLA	5	0
23	2	318	LMT	3	0
21	B	847	BCR	8	0
18	4	301	CHL	11	0
17	B	826	CLA	7	0
17	B	806	CLA	2	0
17	A	835	CLA	3	0
17	1	309	CLA	5	0
17	J	101	CLA	5	0
17	3	609	CLA	2	0
17	G	104	CLA	3	0

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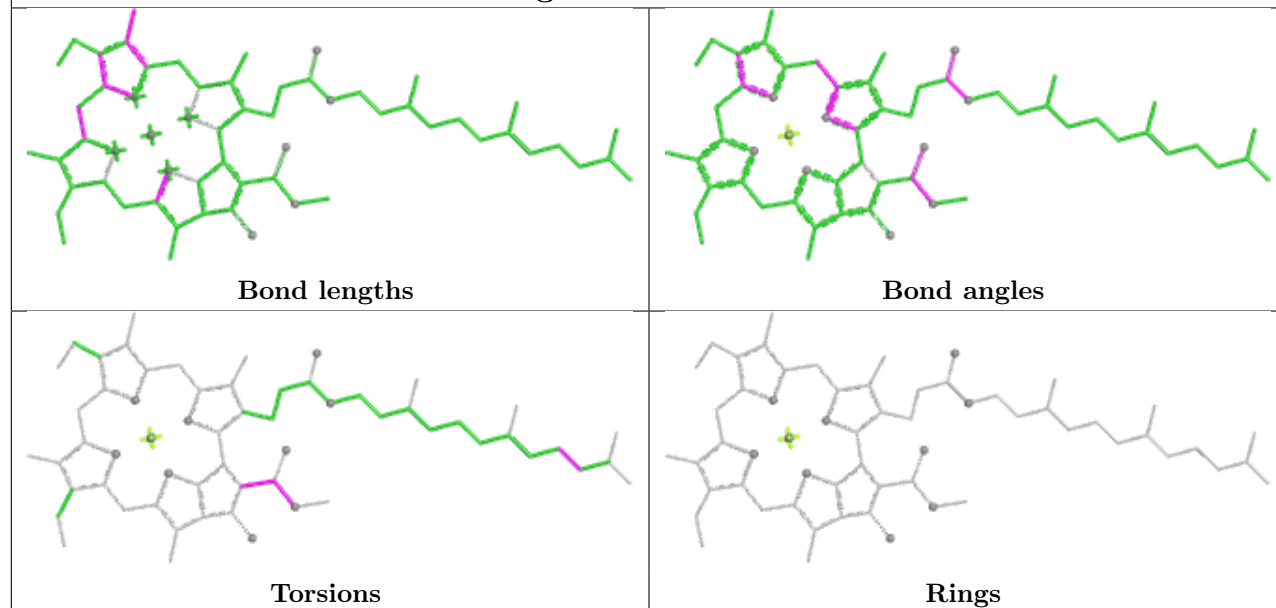
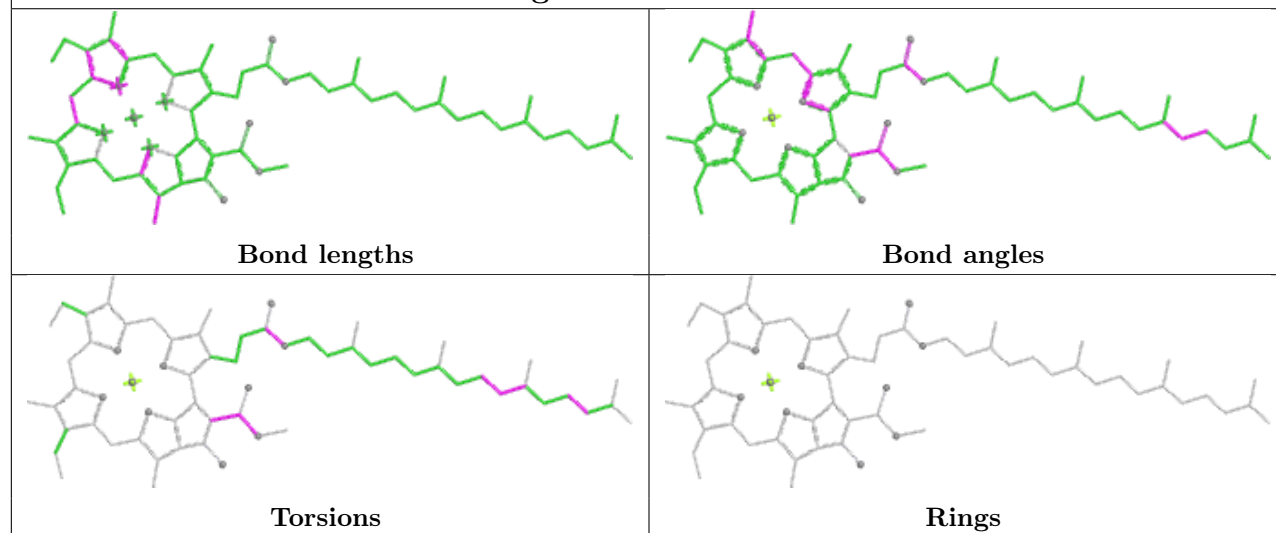
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	821	CLA	1	0
17	B	820	CLA	2	0
17	B	835	CLA	3	0
17	4	309	CLA	1	0
17	2	309	CLA	1	0
17	1	308	CLA	6	0
21	2	316	BCR	9	0
17	B	831	CLA	2	0
17	A	818	CLA	3	0
21	L	201	BCR	2	0
17	B	805	CLA	3	0
17	4	303	CLA	4	0
17	L	202	CLA	5	0
27	A	842	PQN	6	0
17	B	809	CLA	6	0
18	2	305	CHL	2	0
17	A	822	CLA	1	0
17	A	828	CLA	3	0
17	B	821	CLA	2	0
17	4	311	CLA	2	0
17	B	832	CLA	3	0
20	1	315	XAT	3	0
18	4	305	CHL	5	0
21	B	849	BCR	3	0
21	G	106	BCR	2	0
26	B	850	DGD	7	0
17	L	203	CLA	5	0
17	B	842	CLA	3	0
17	A	803	CLA	7	0
17	B	808	CLA	1	0
17	B	807	CLA	3	0
21	J	104	BCR	2	0
24	G	101	LMG	3	0
17	B	823	CLA	4	0
17	B	830	CLA	2	0
17	A	829	CLA	2	0
19	3	614	LUT	4	0
17	B	822	CLA	2	0
21	B	846	BCR	3	0
17	2	301	CLA	4	0
17	A	816	CLA	4	0
22	B	801	LHG	1	0

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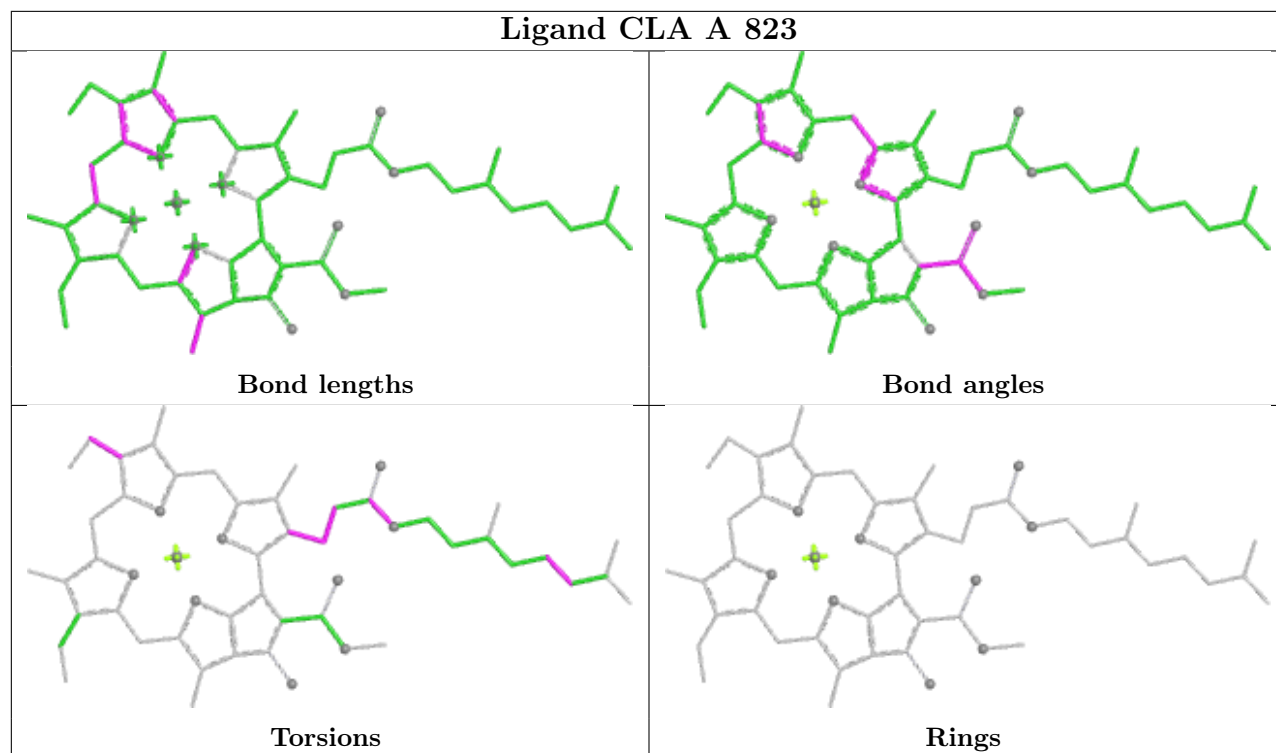
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	804	CLA	6	0
25	F	310	HTG	1	0
26	4	323	DGD	29	0
22	1	317	LHG	6	0
17	2	303	CLA	1	0
21	B	845	BCR	4	0
17	3	613	CLA	2	0
17	B	817	CLA	1	0
17	B	827	CLA	9	0
22	2	317	LHG	6	0
17	4	314	CLA	2	0
19	4	316	LUT	3	0
17	A	831	CLA	2	0
17	A	808	CLA	5	0
21	F	308	BCR	3	0
17	A	813	CLA	1	0
22	A	844	LHG	2	0
18	4	306	CHL	7	0
17	4	308	CLA	1	0
21	K	203	BCR	5	0
17	A	838	CLA	4	0
22	F	302	LHG	2	0
22	G	102	LHG	2	0
17	A	837	CLA	6	0
17	B	819	CLA	6	0
21	4	318	BCR	14	0
19	2	314	LUT	4	0
17	4	302	CLA	6	0

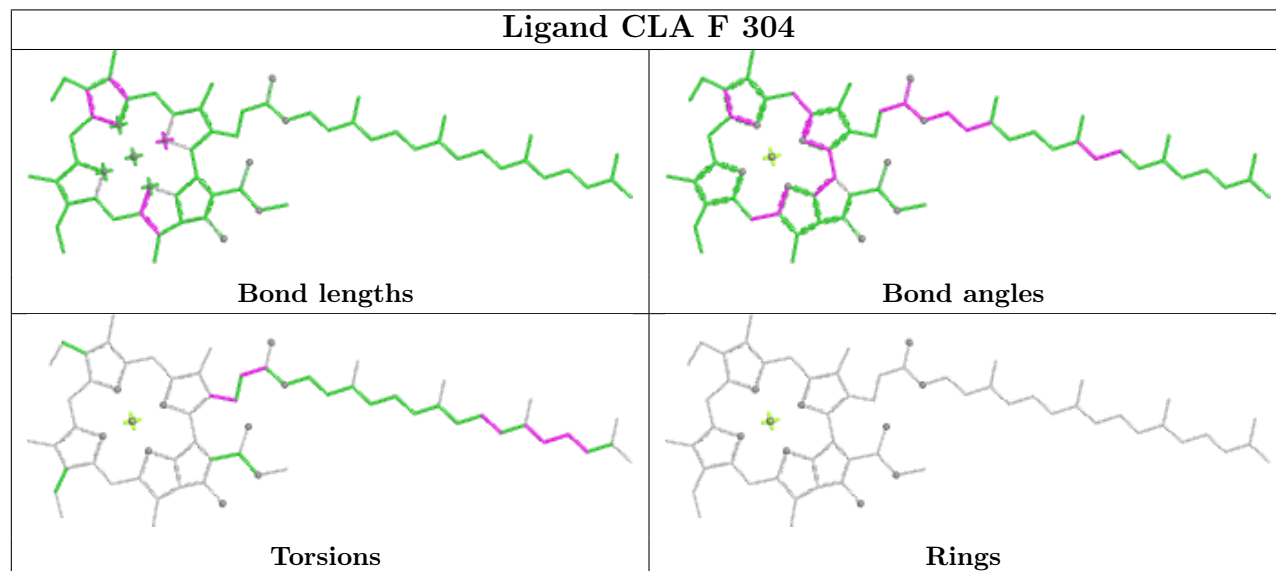
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 3 602**Ligand CLA A 824**

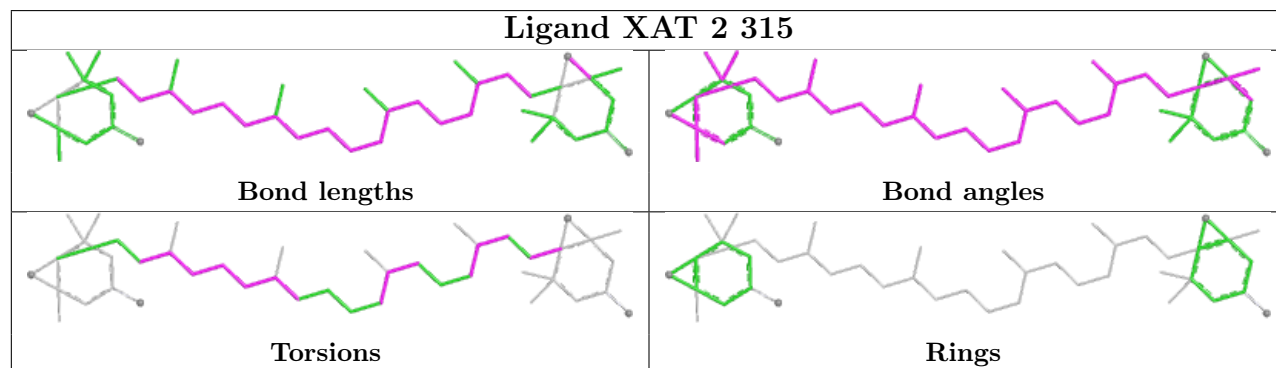
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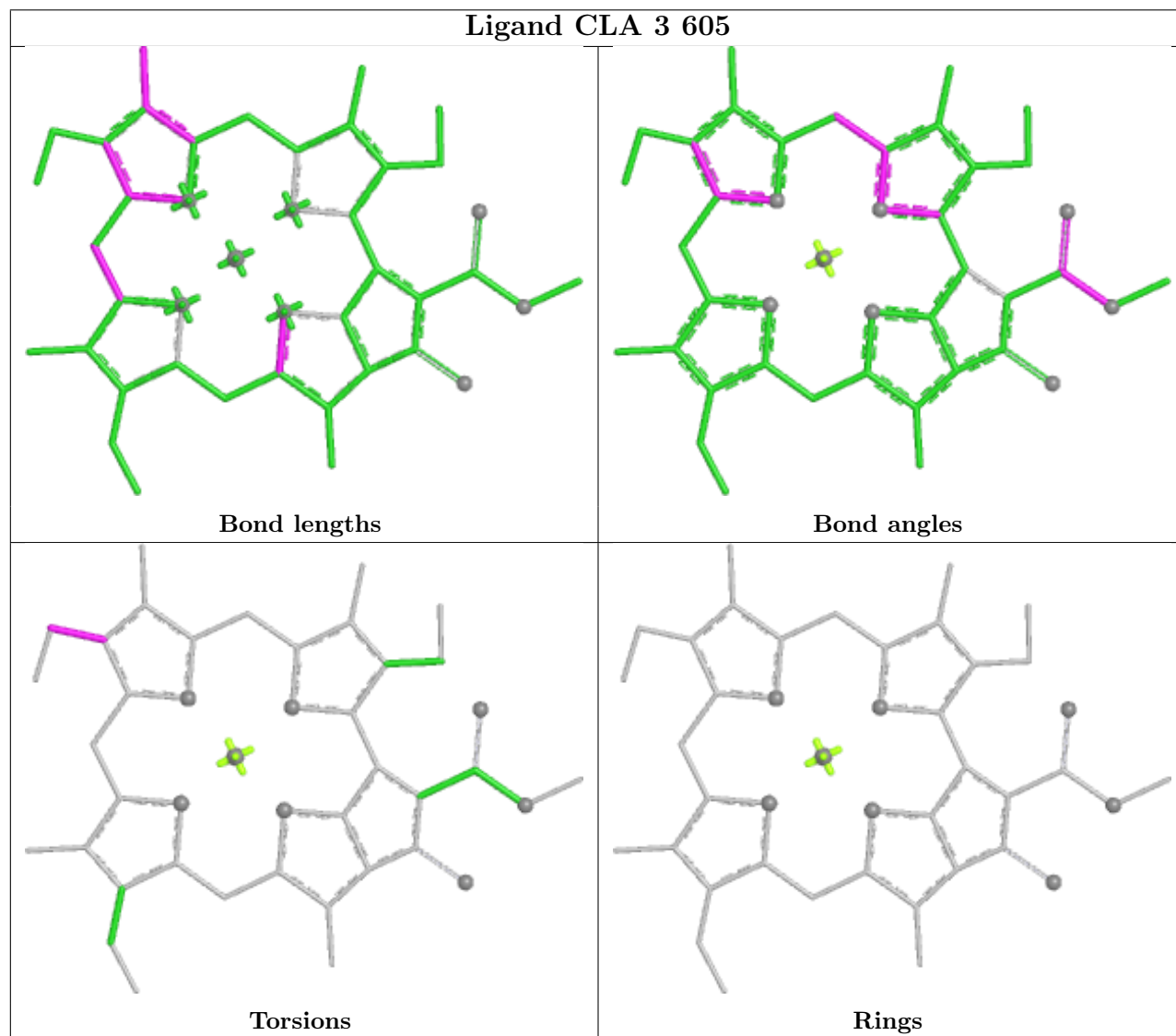
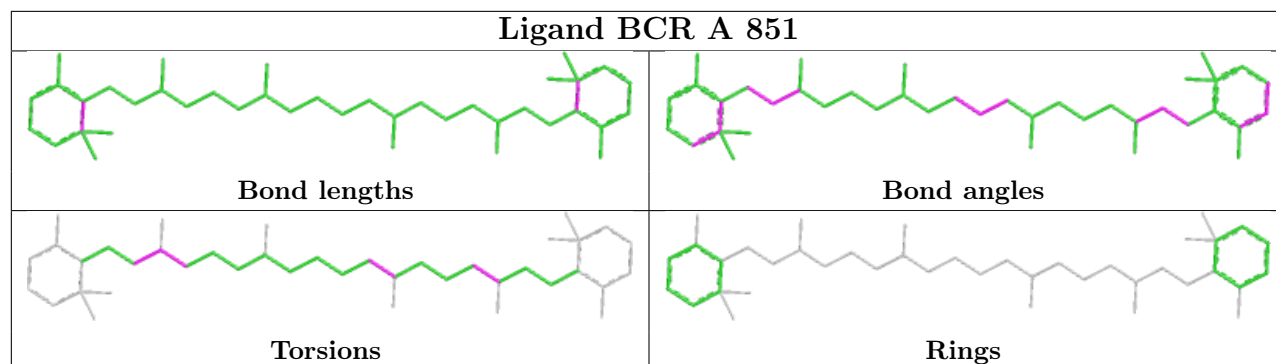


Ligand CLA F 304

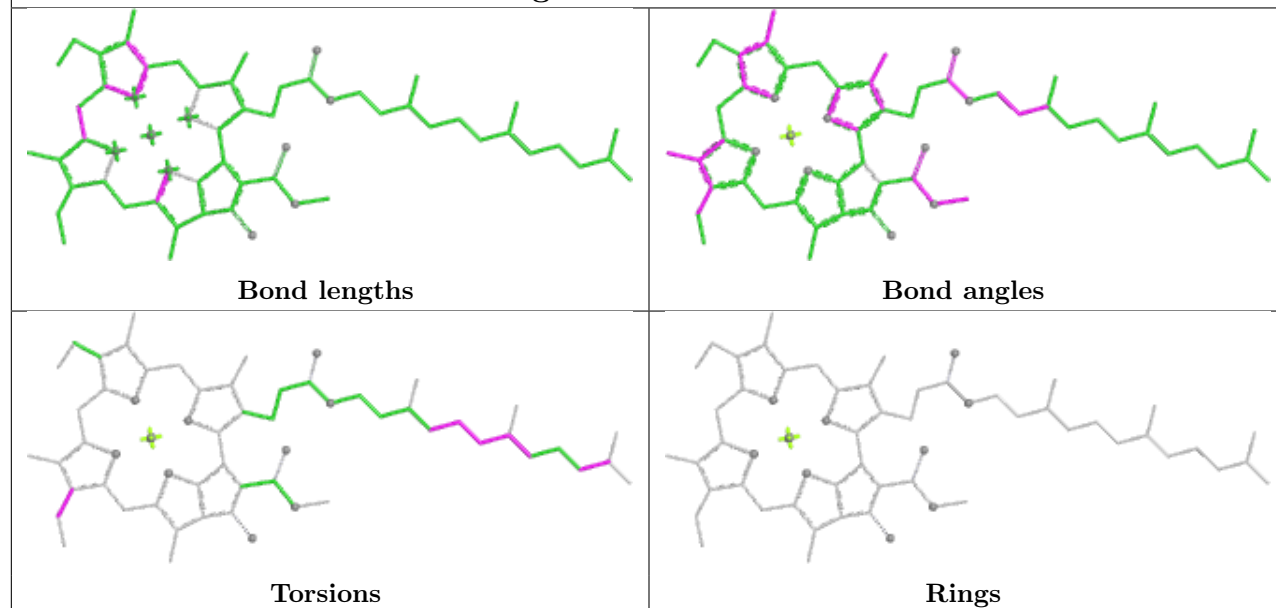


Ligand XAT 2 315

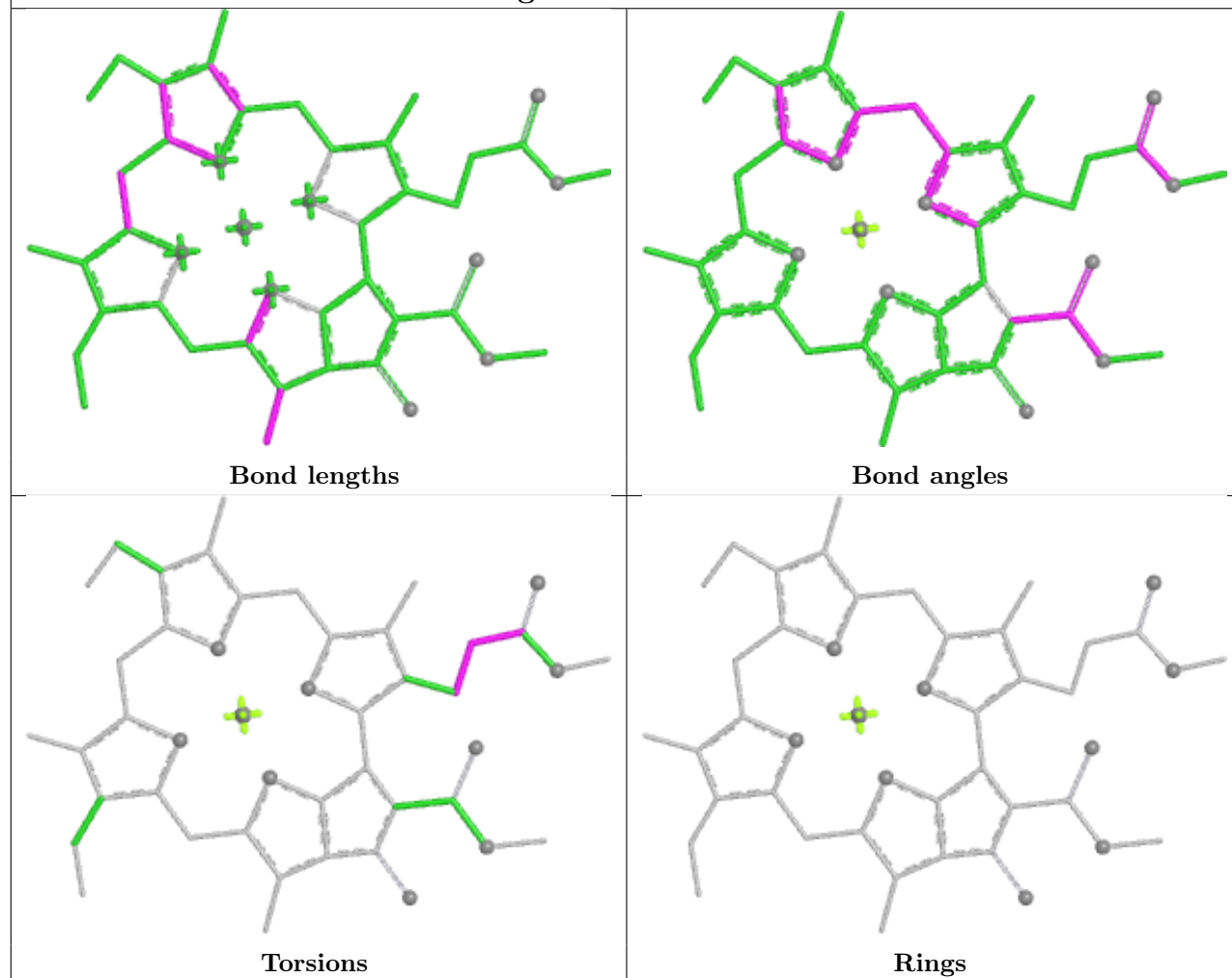




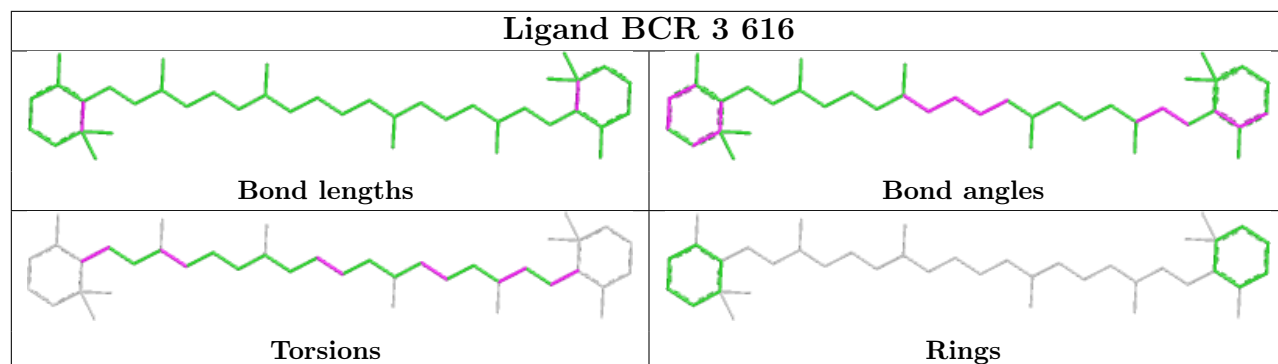
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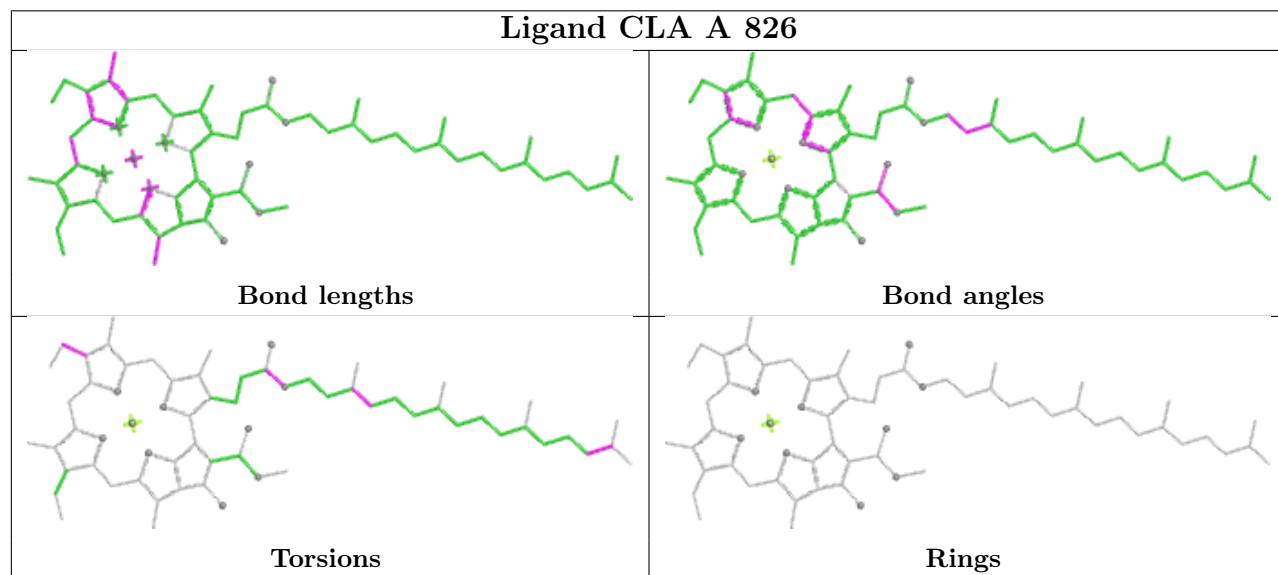
Ligand CLA 2 319



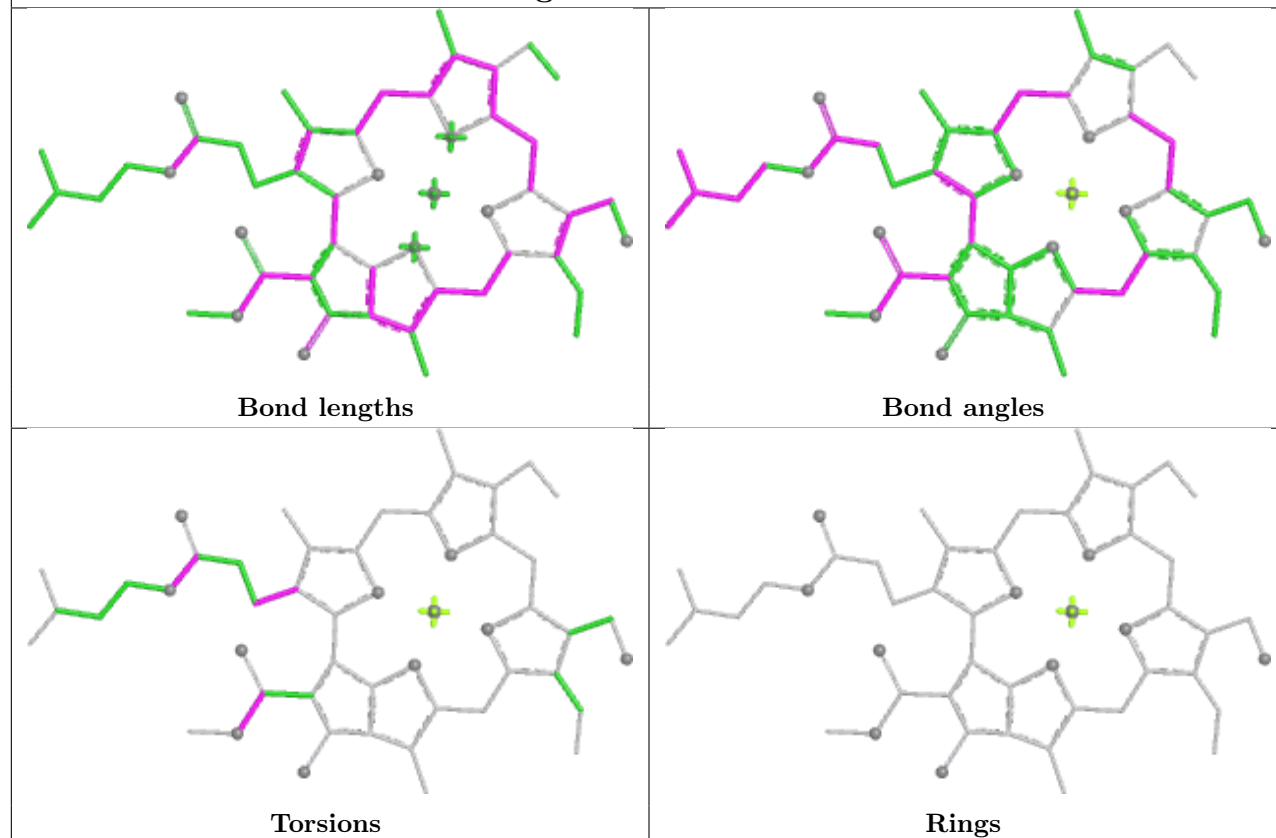
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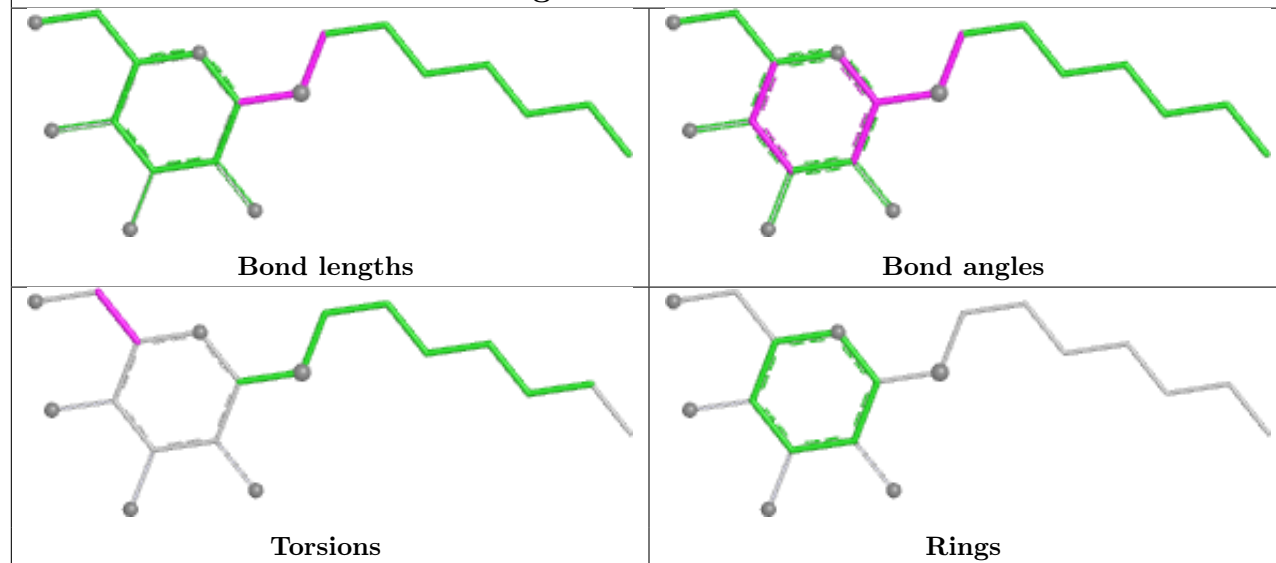
Ligand CLA A 826



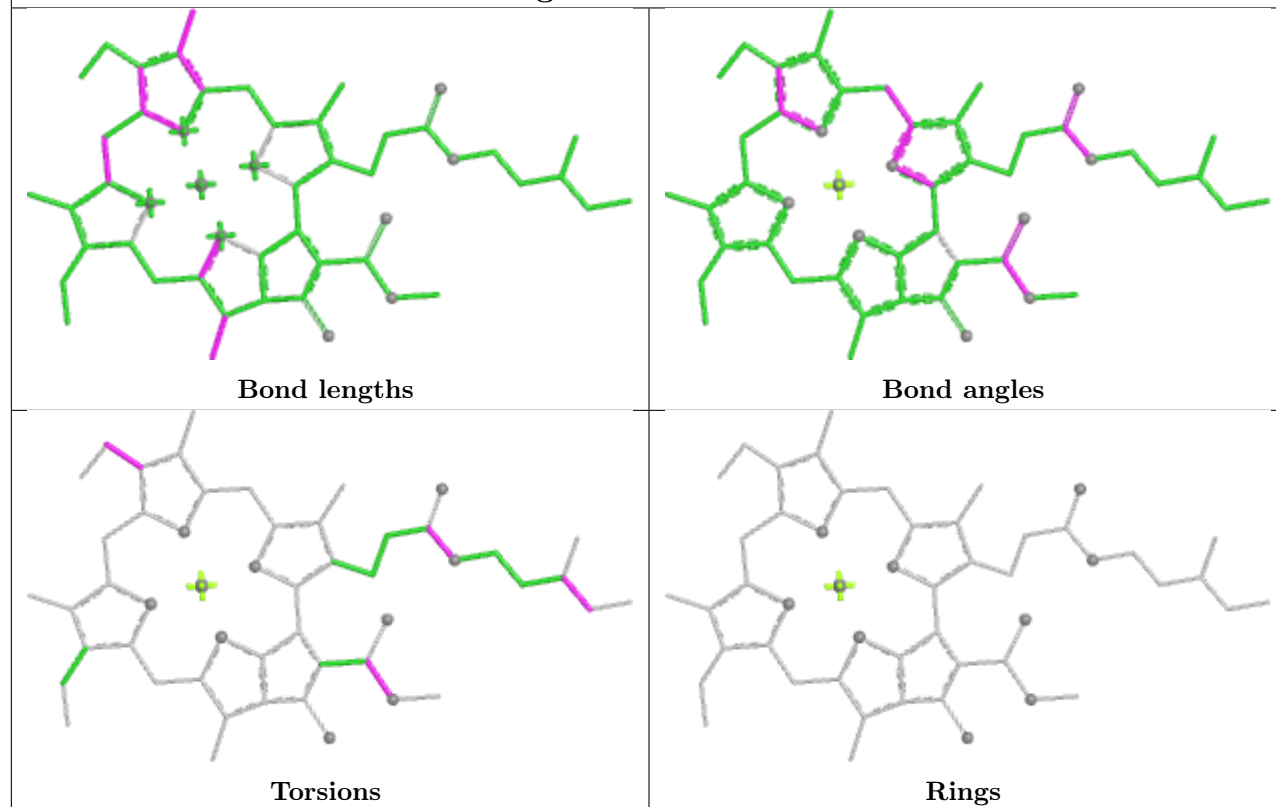
Ligand CHL 2 306



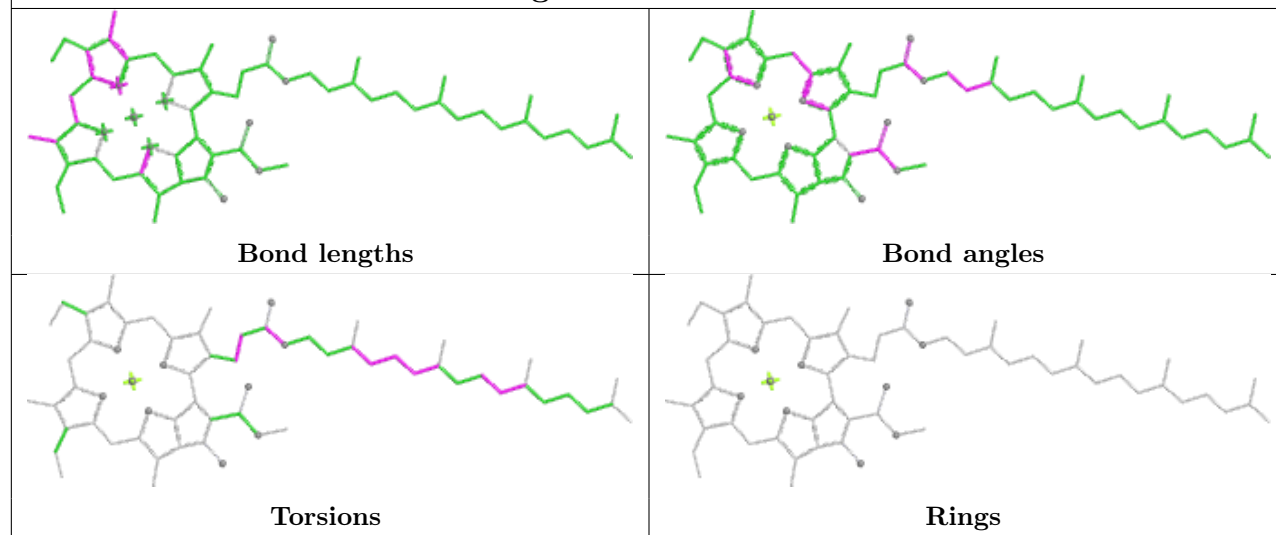
Ligand HTG 4 322



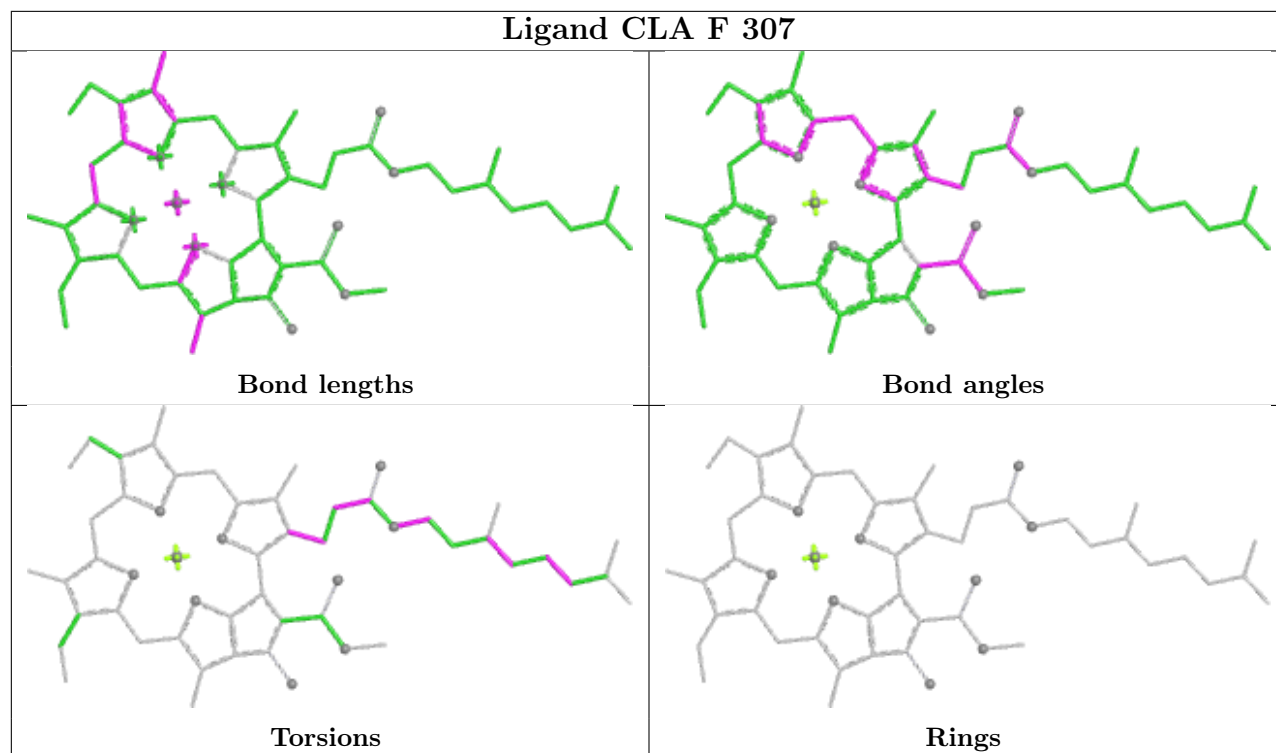
Ligand CLA 1 303



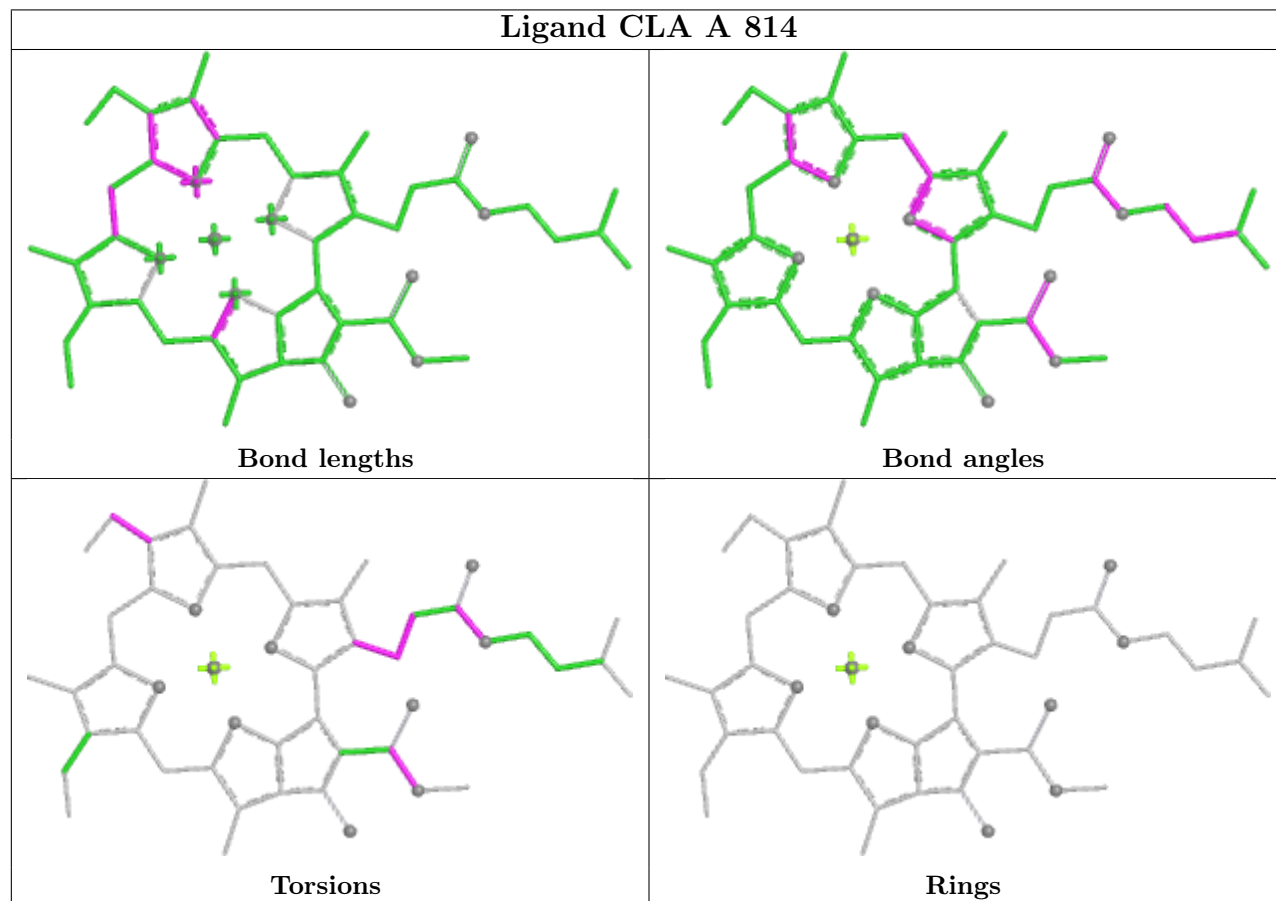
Ligand CLA A 841



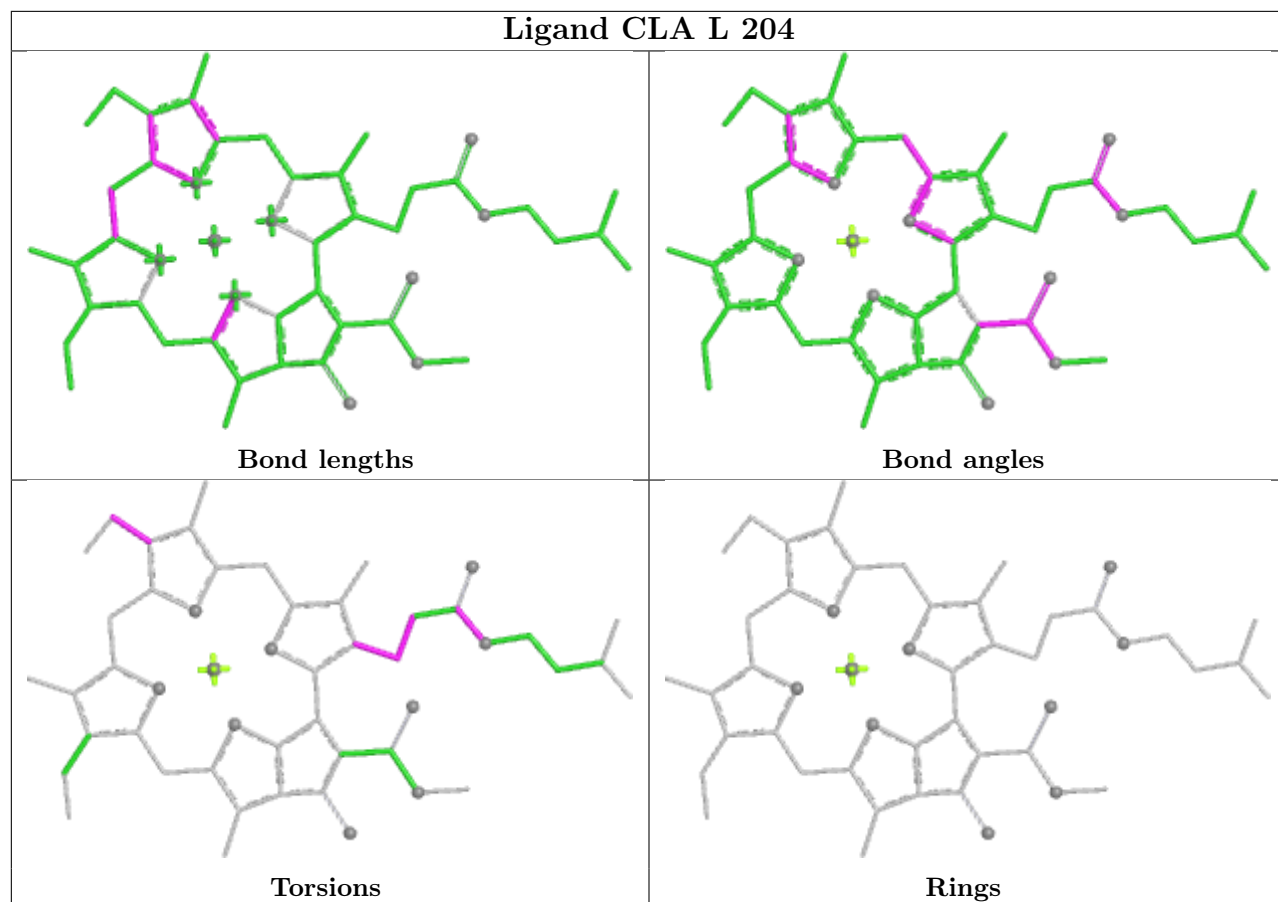
Ligand CLA F 307



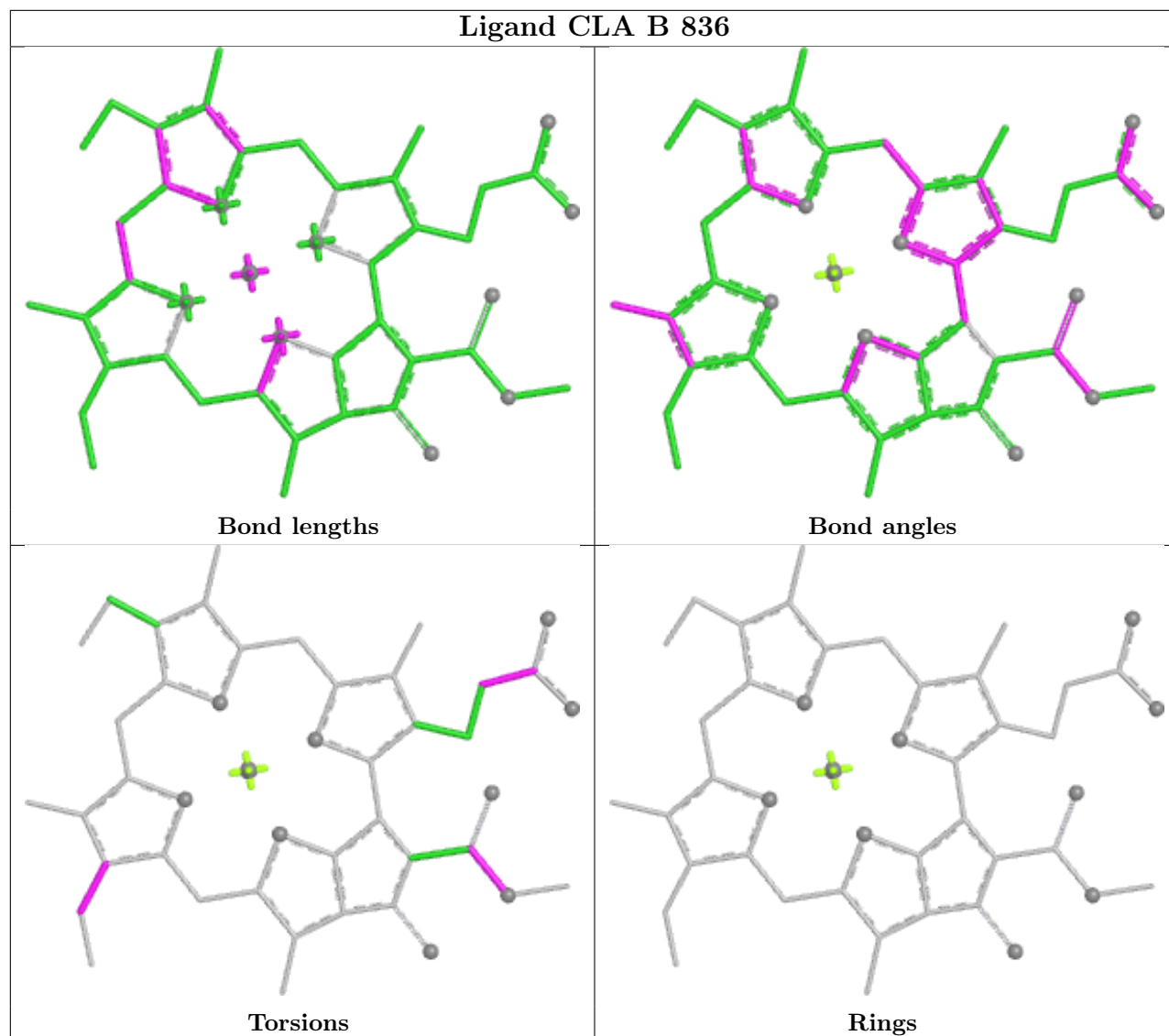
Ligand CLA A 814



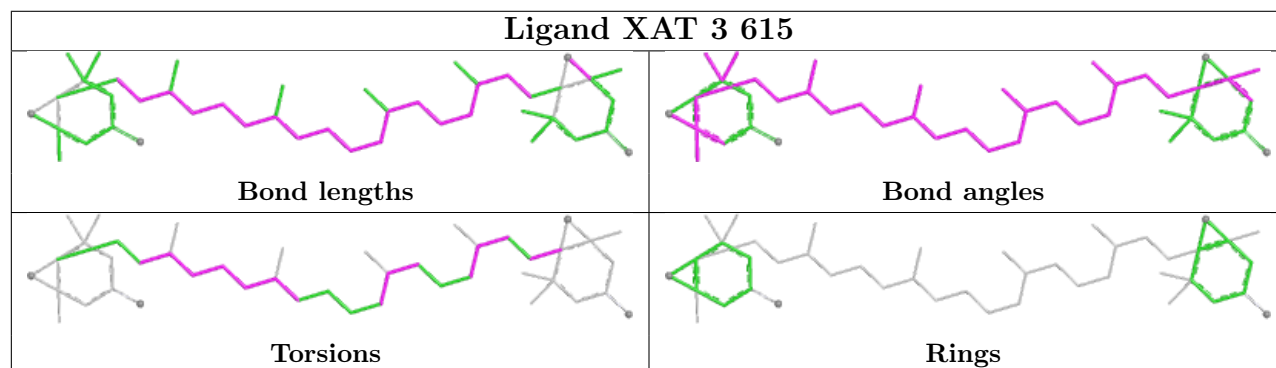
Ligand CLA L 204



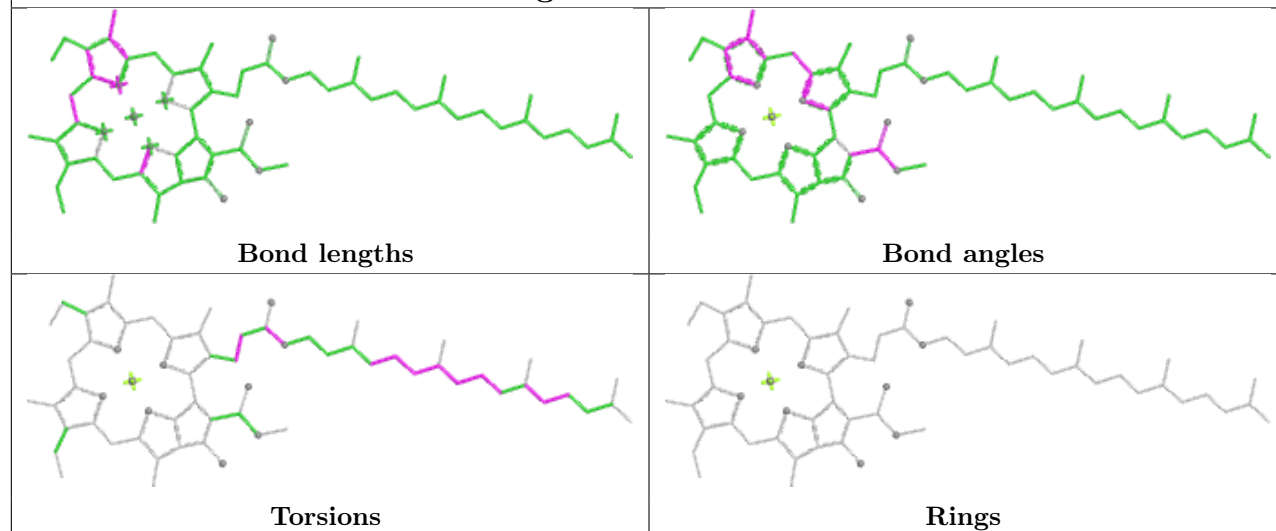
Ligand CLA B 836



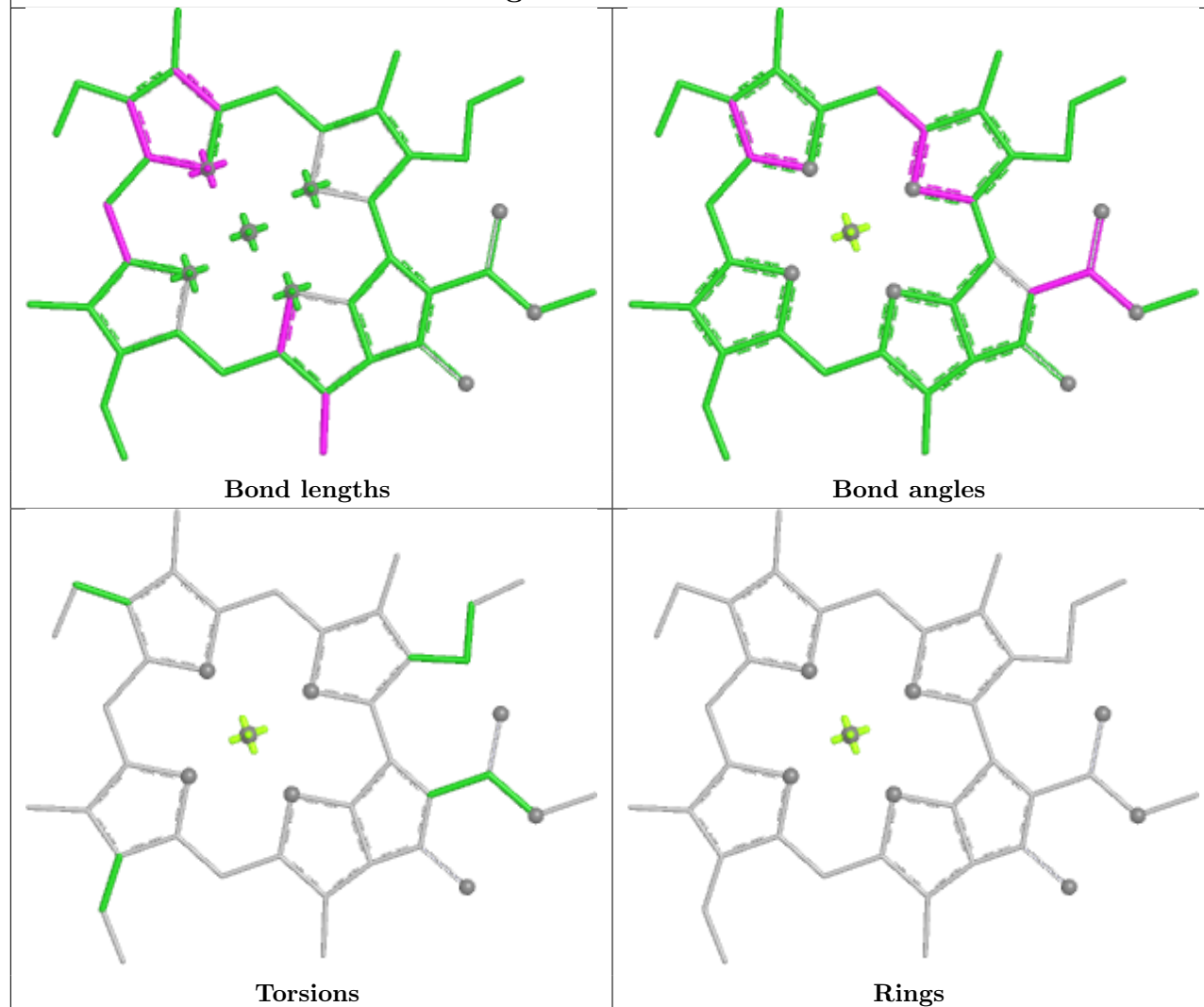
Ligand XAT 3 615

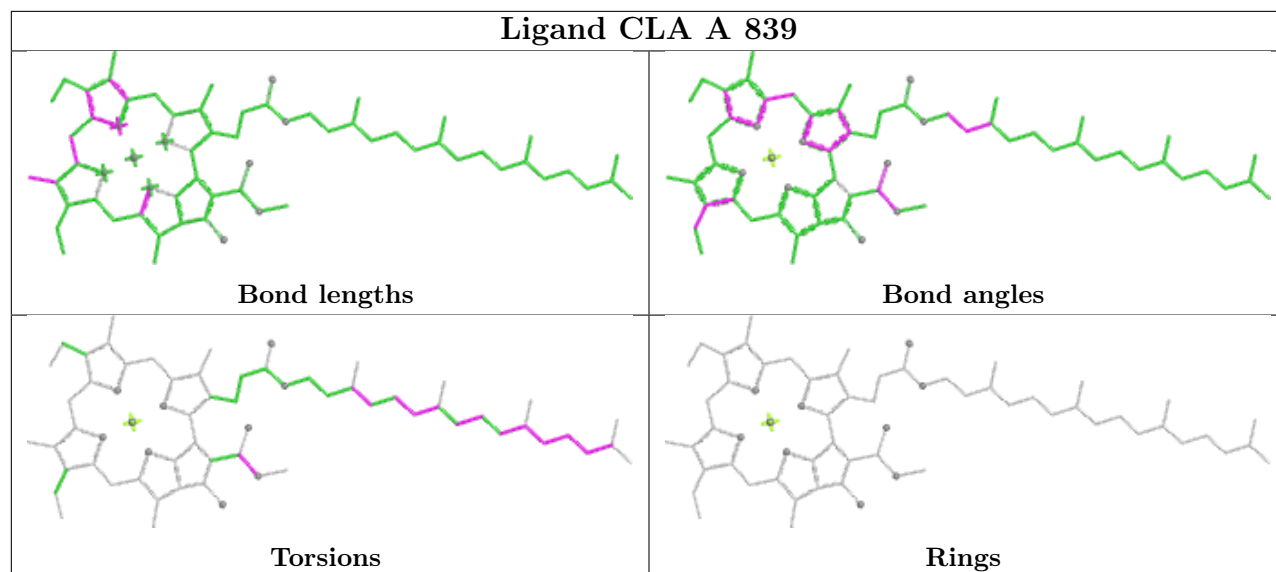
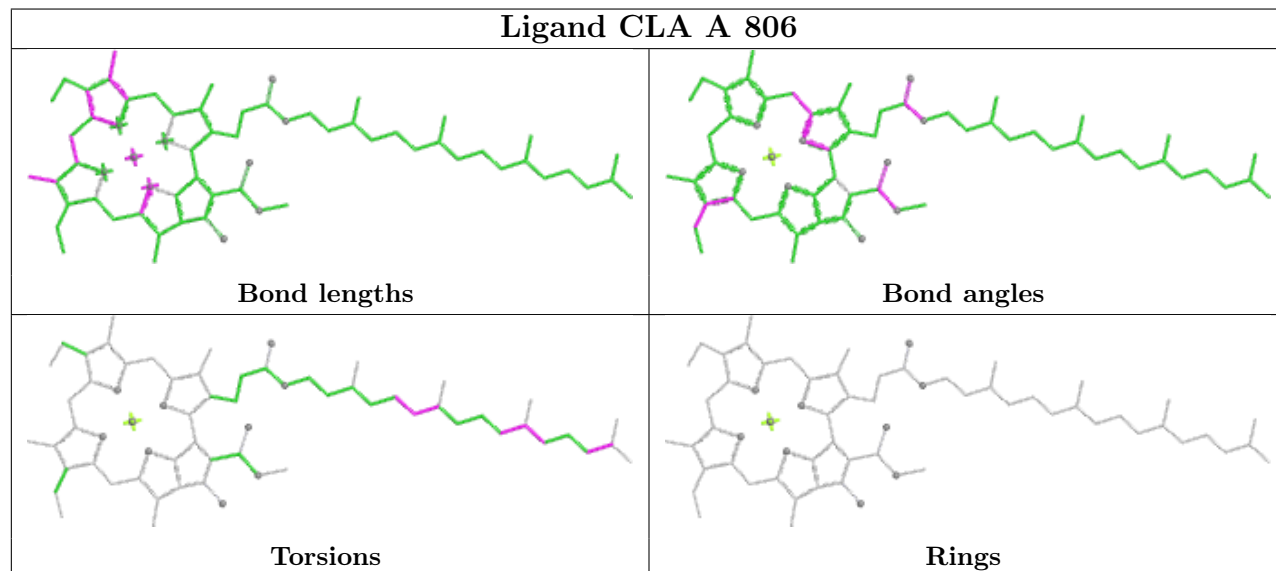


Ligand CLA 2 311

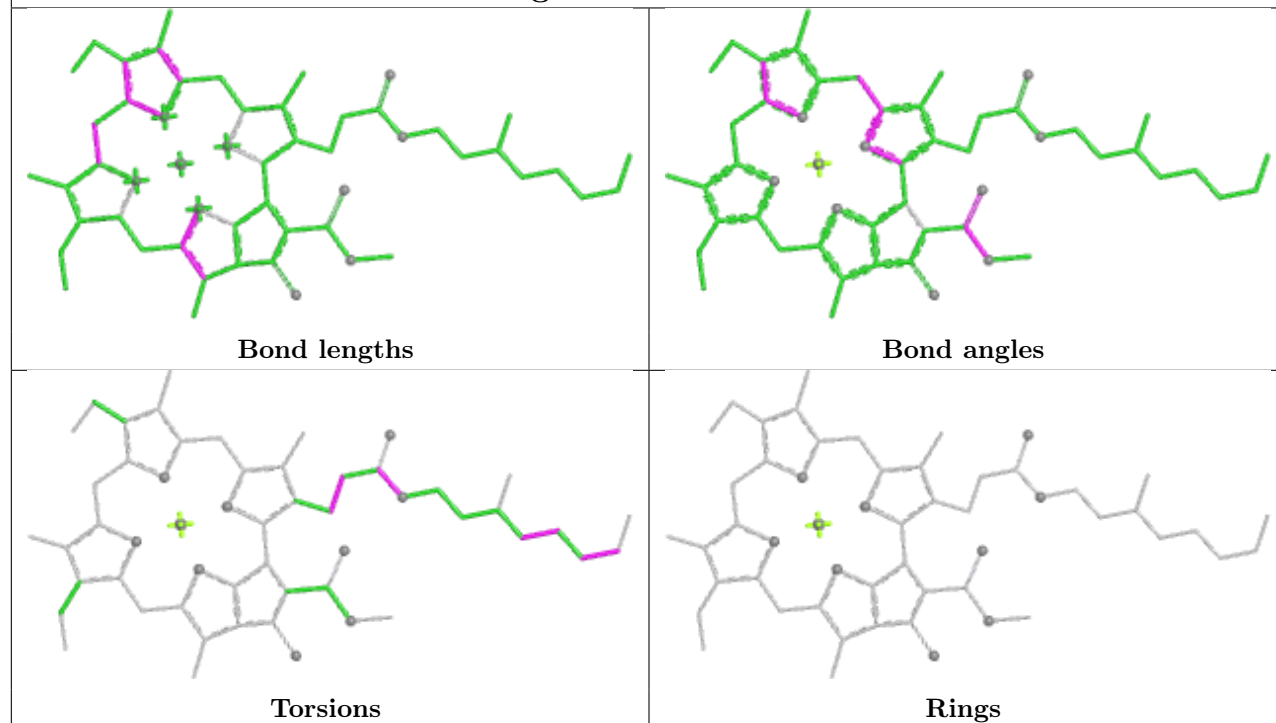


Ligand CLA 2 312

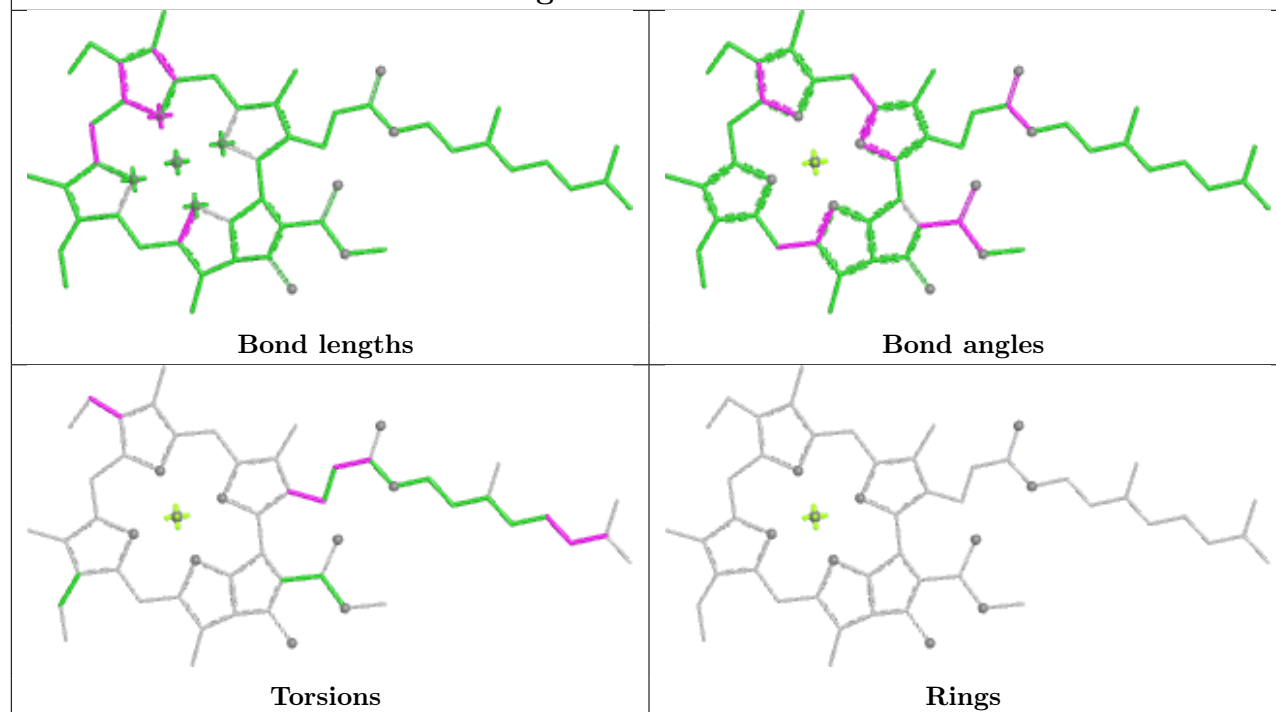


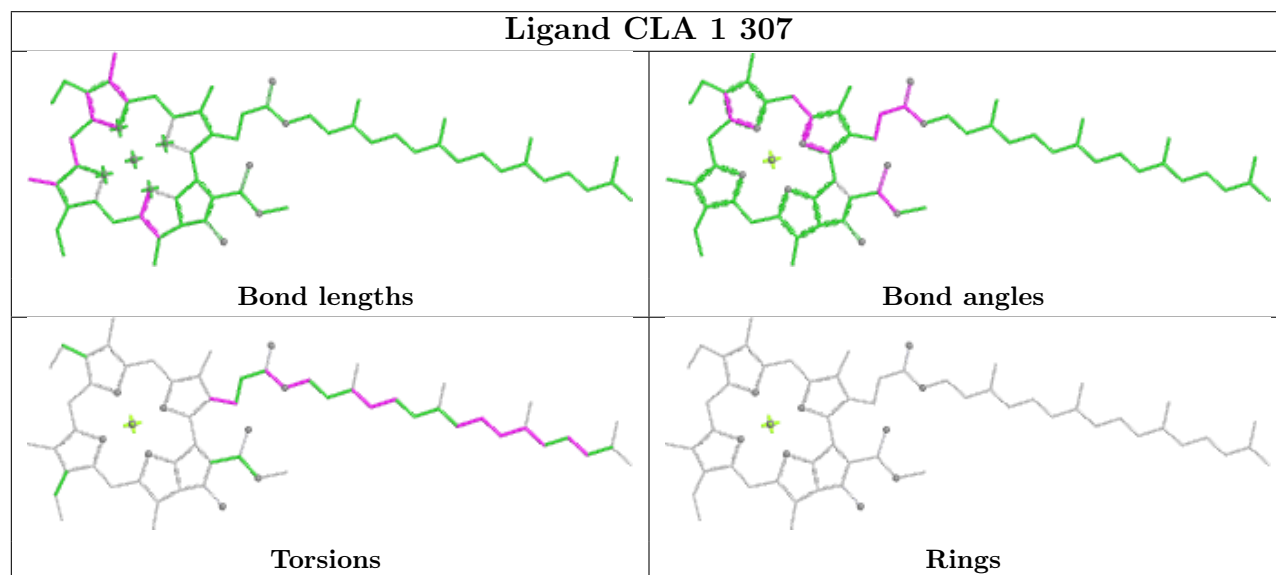
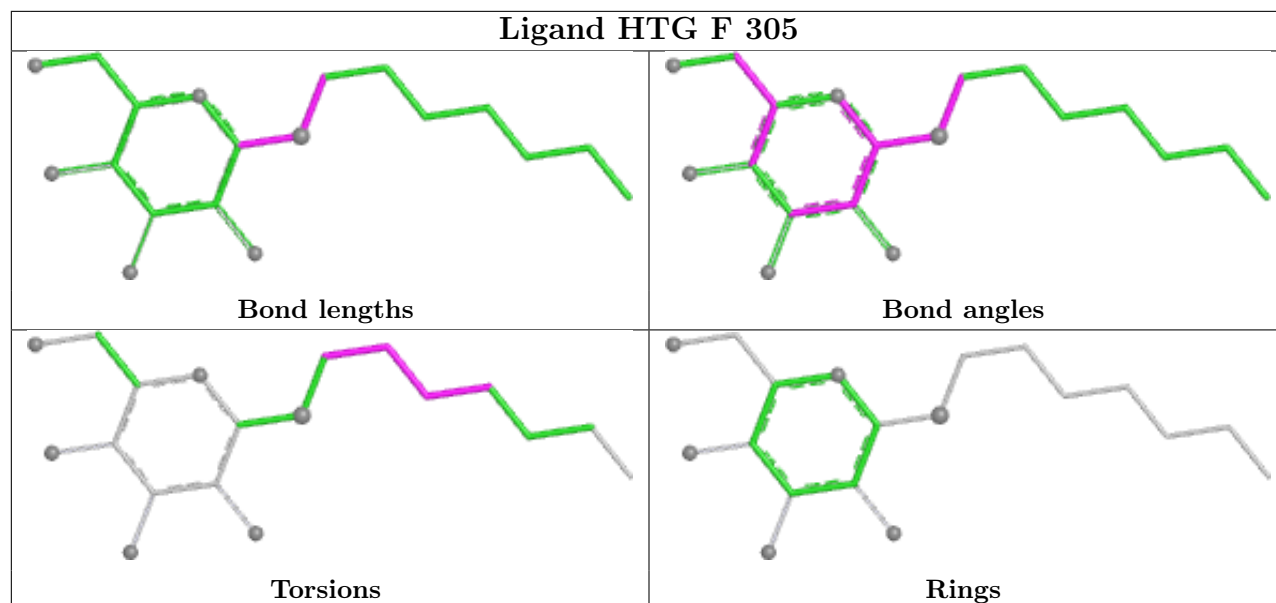
Ligand CLA A 839**Ligand CLA A 806**

Ligand CLA A 811

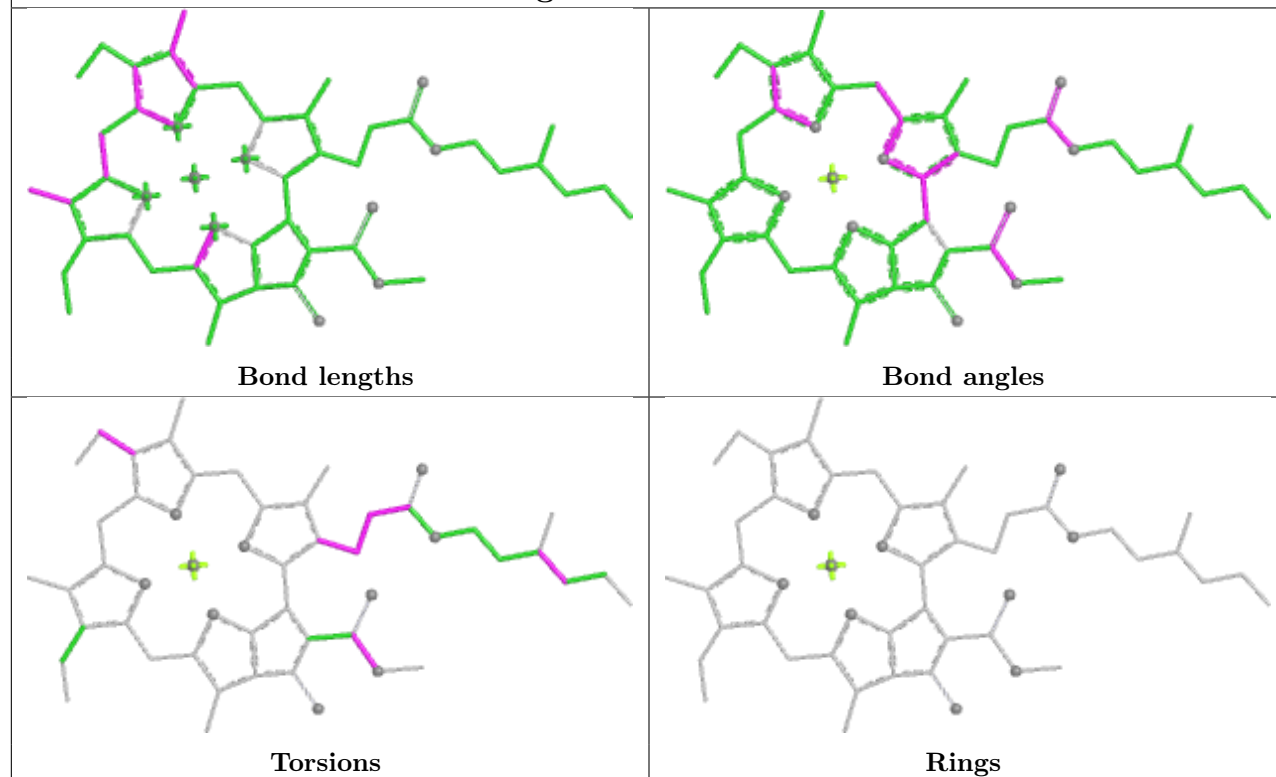


Ligand CLA 1 312

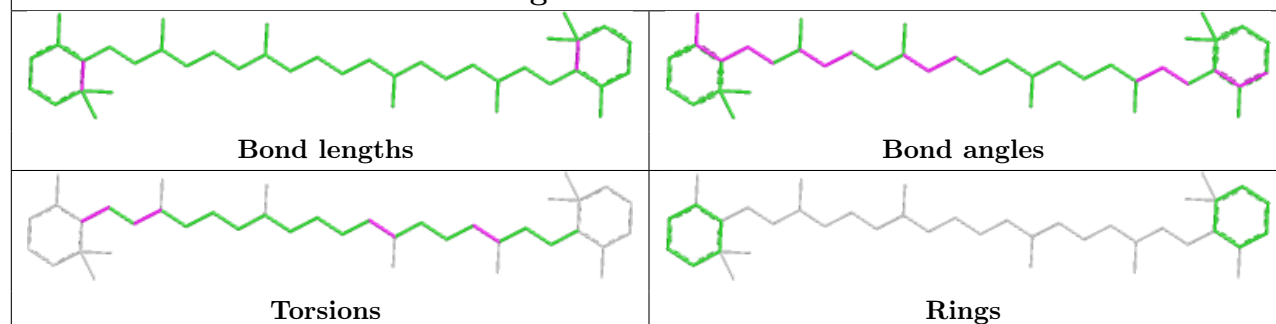




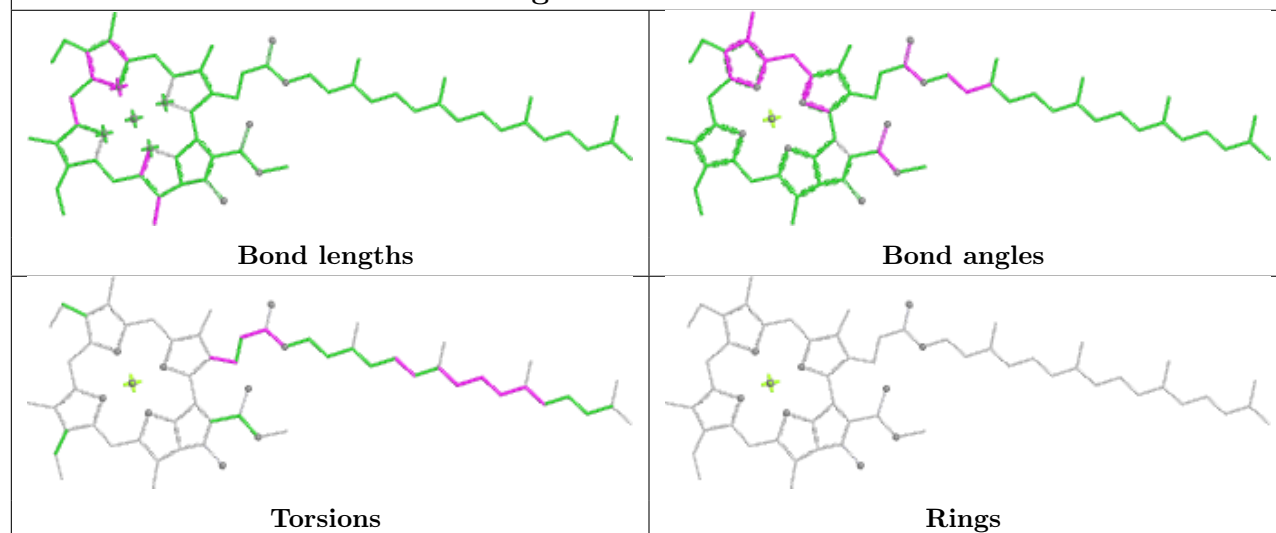
Ligand CLA 3 610



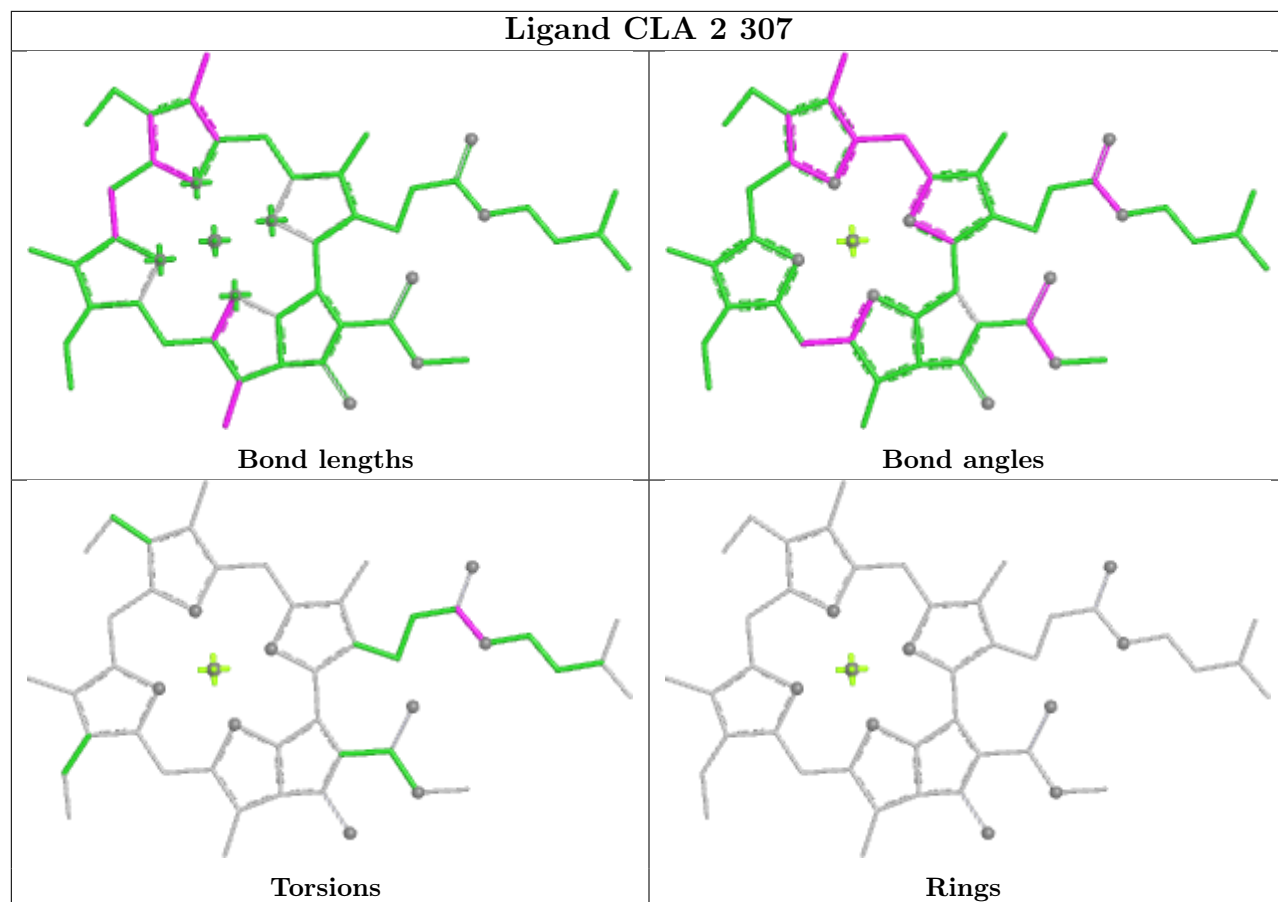
Ligand BCR A 848



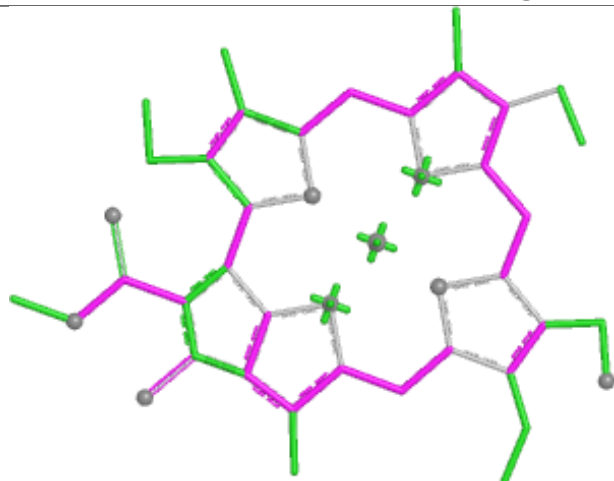
Ligand CLA A 809



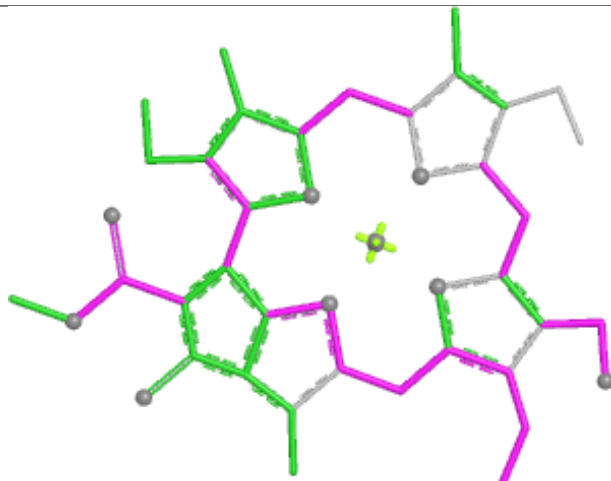
Ligand CLA 2 307



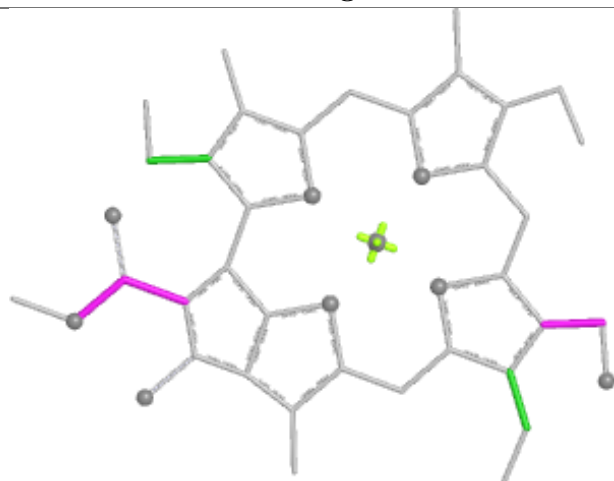
Ligand CHL 2 304



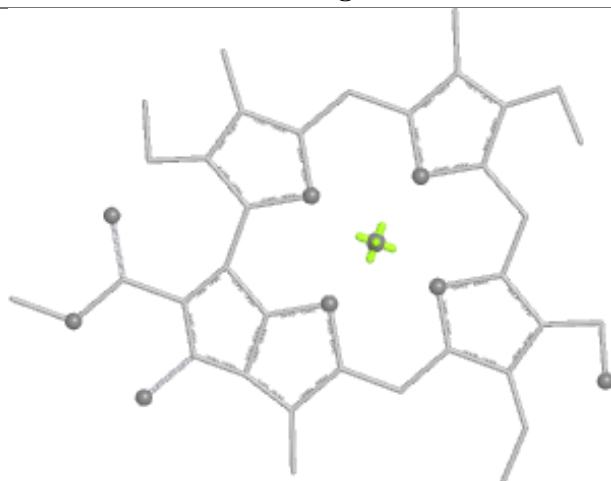
Bond lengths



Bond angles

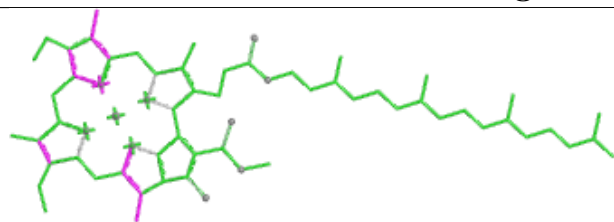


Torsions

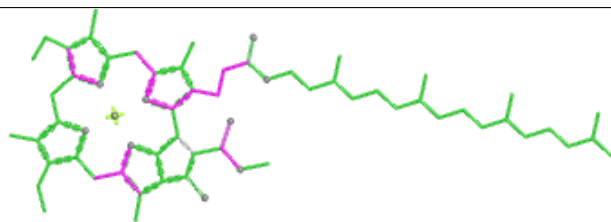


Rings

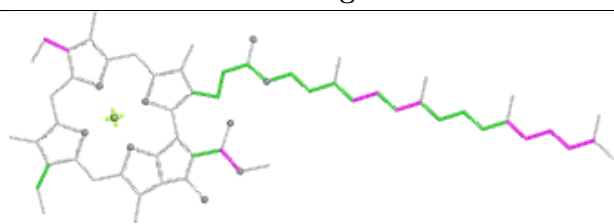
Ligand CLA B 841



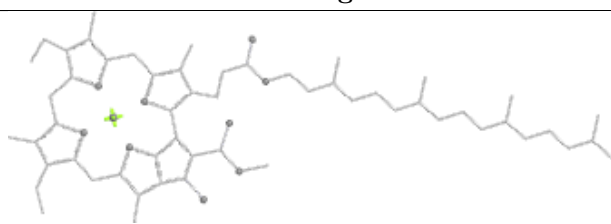
Bond lengths



Bond angles

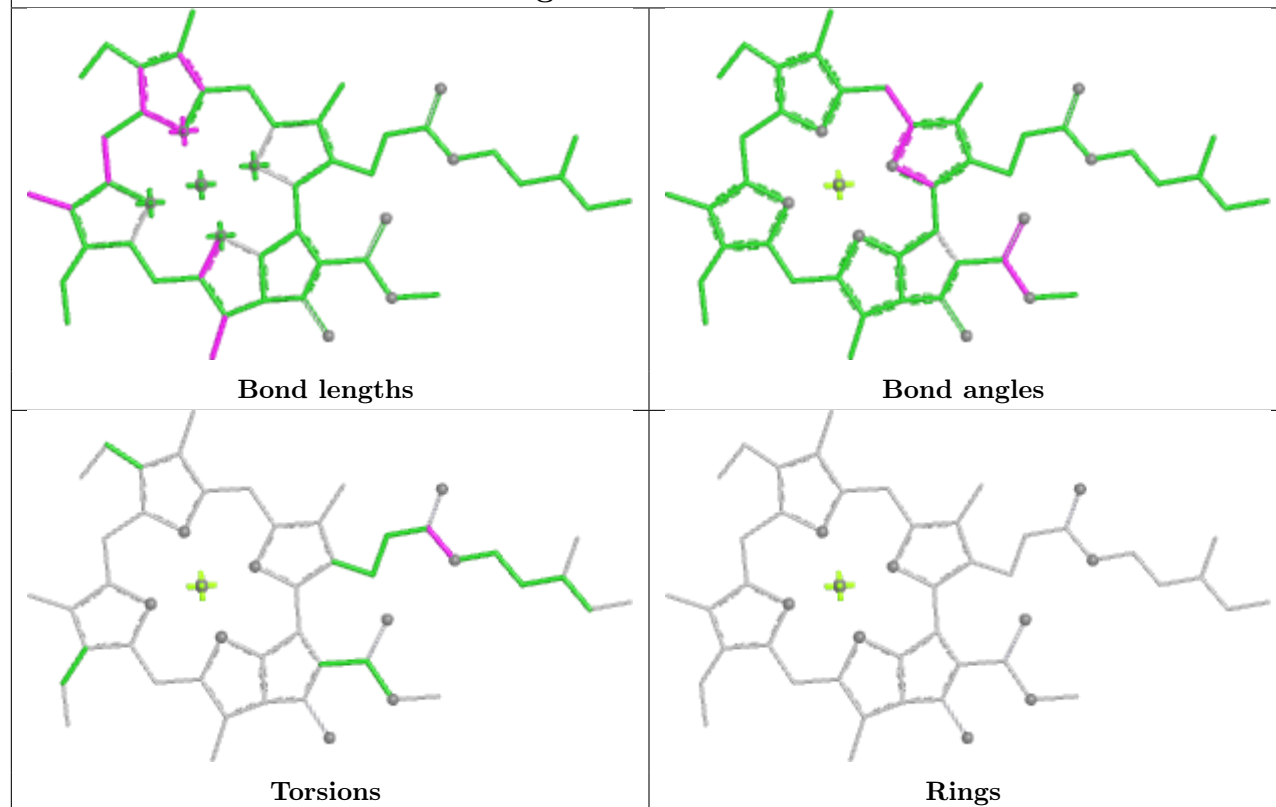


Torsions

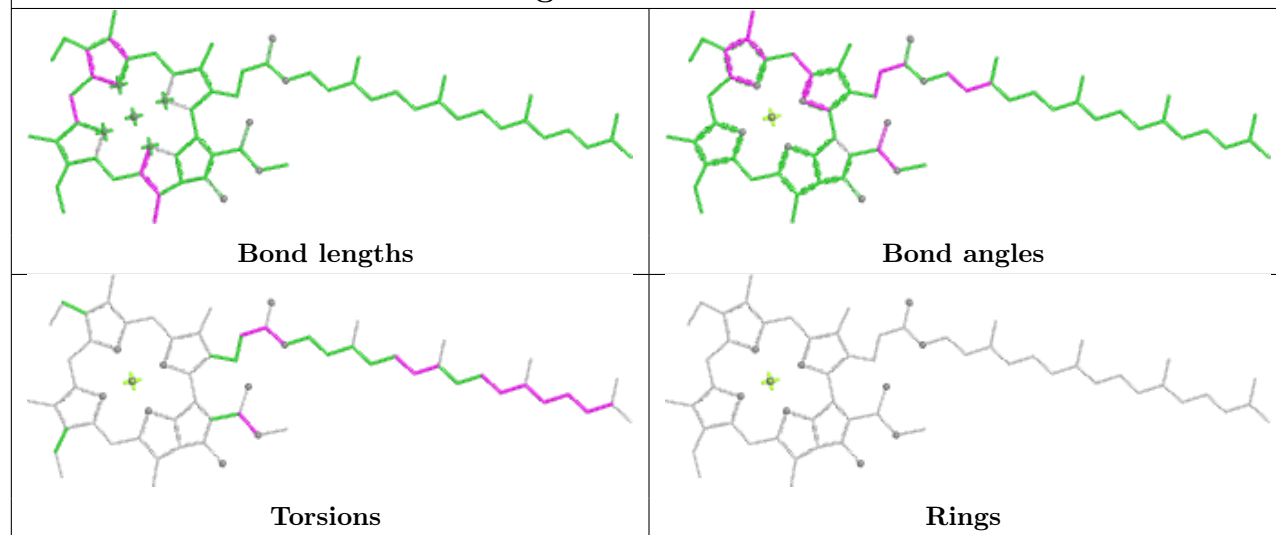


Rings

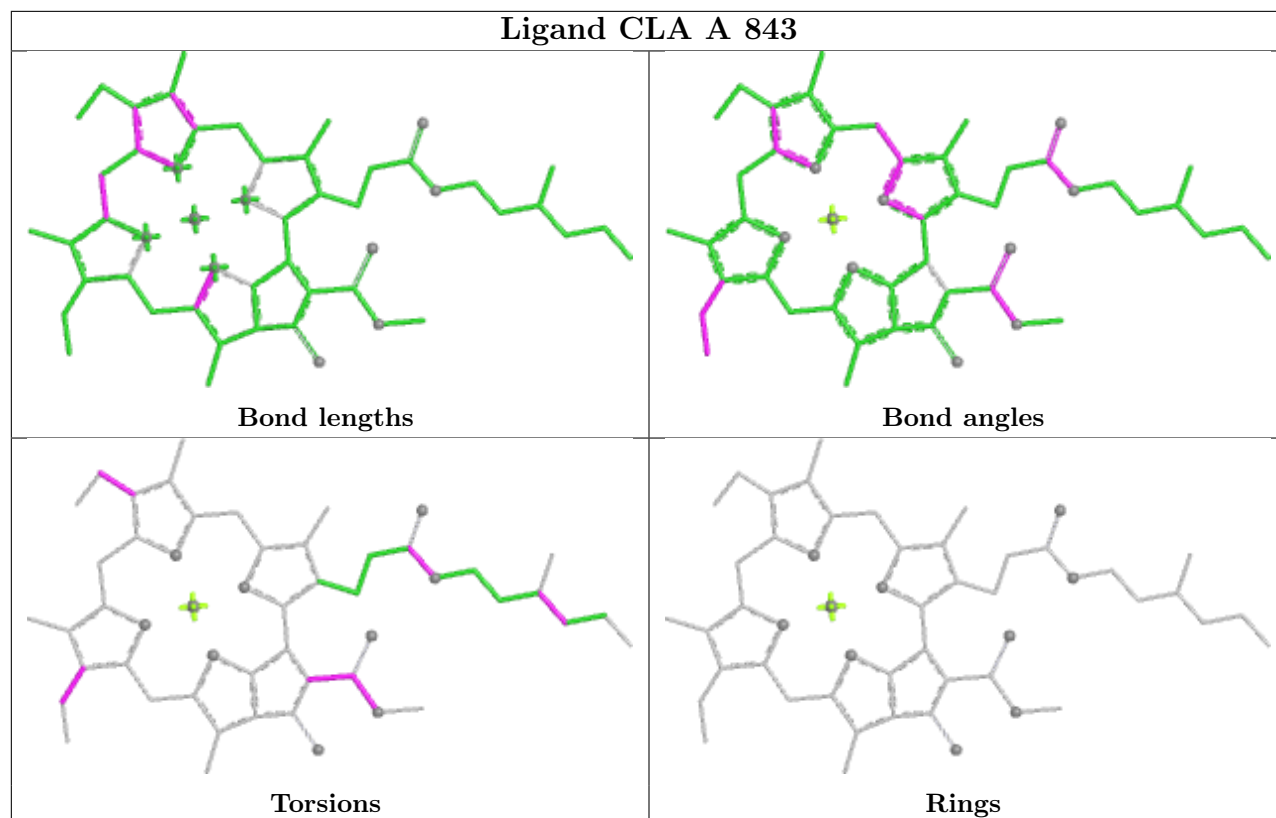
Ligand CLA 2 302



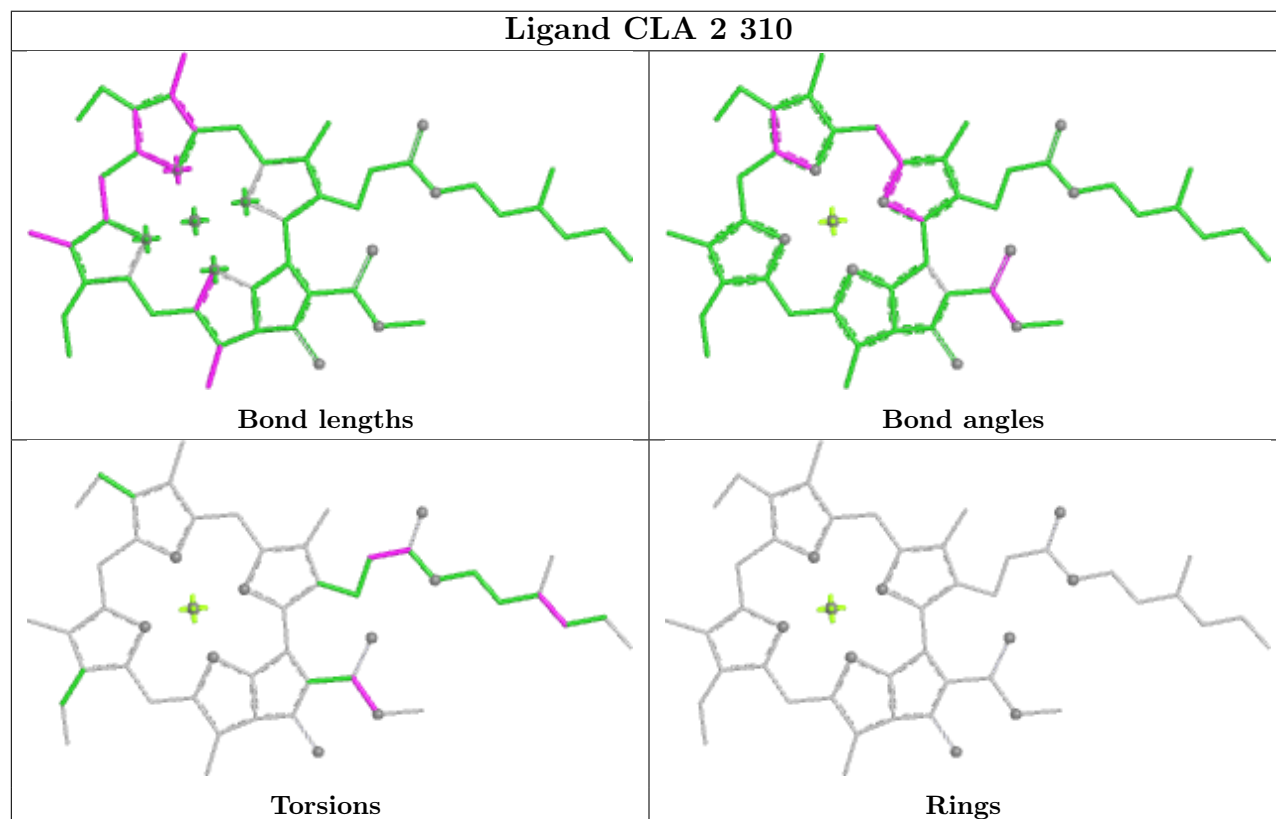
Ligand CLA 1 302



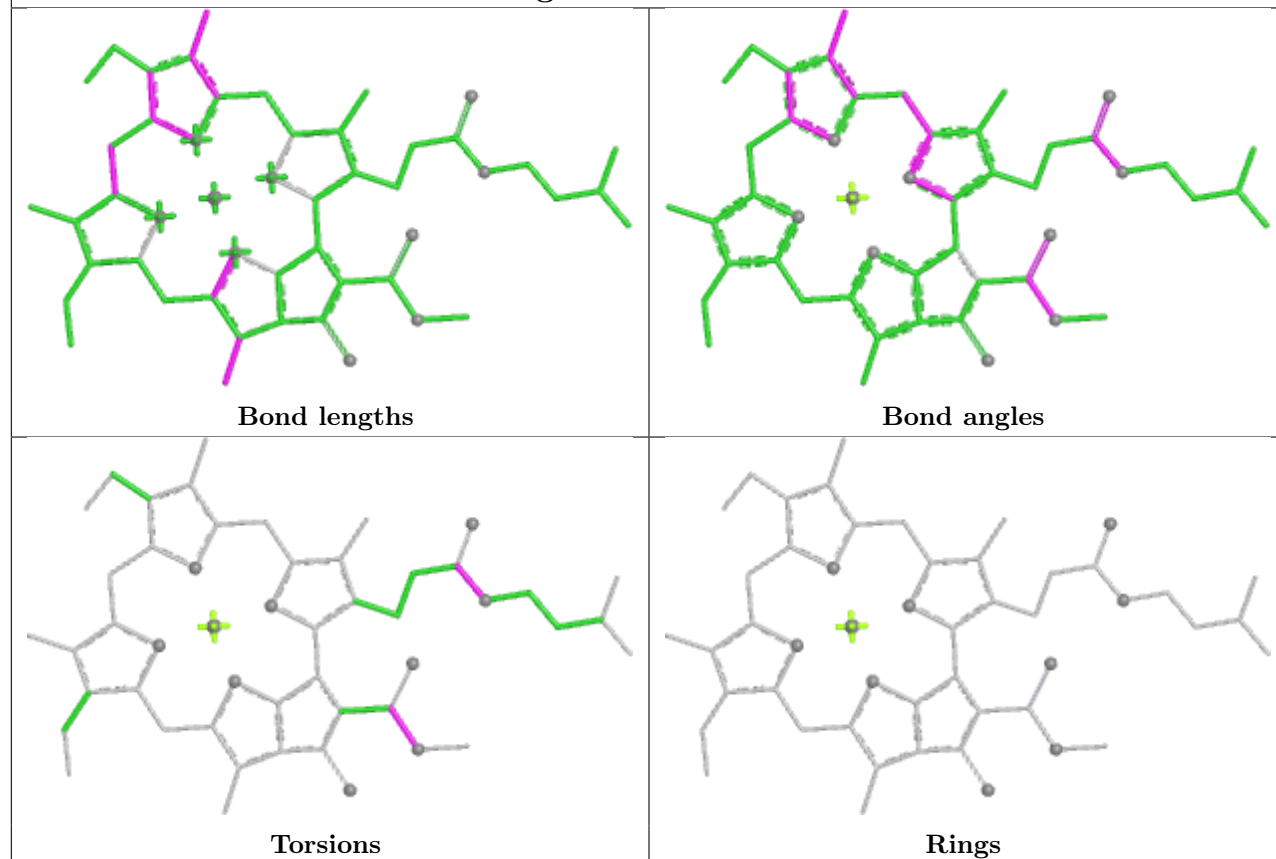
Ligand CLA A 843



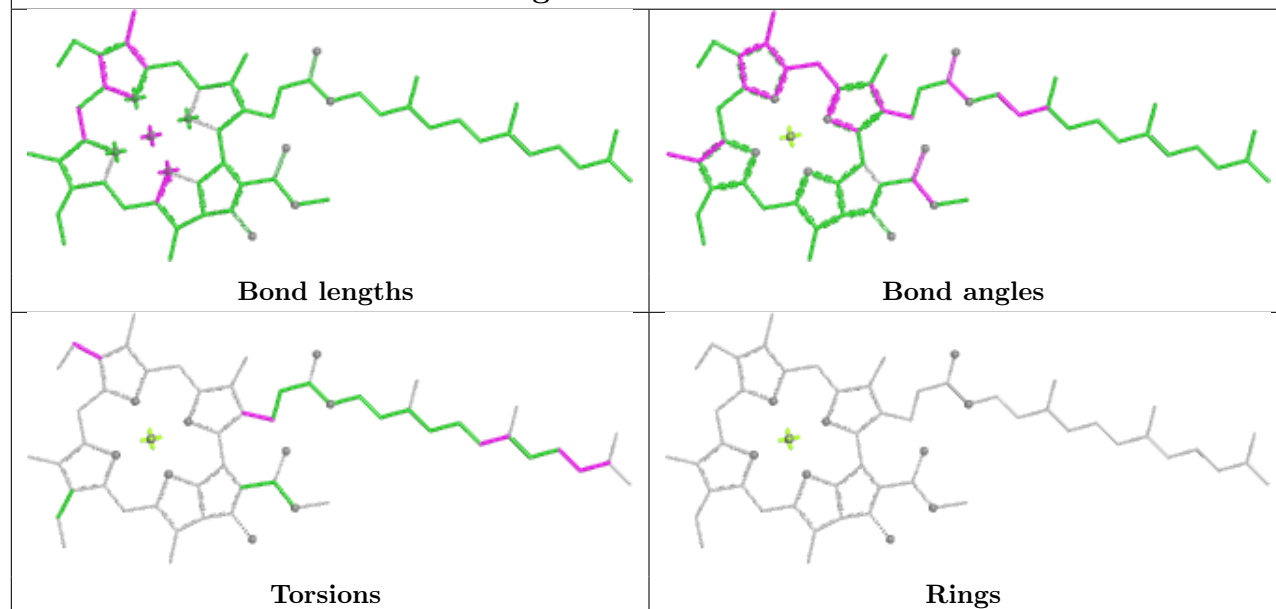
Ligand CLA 2 310

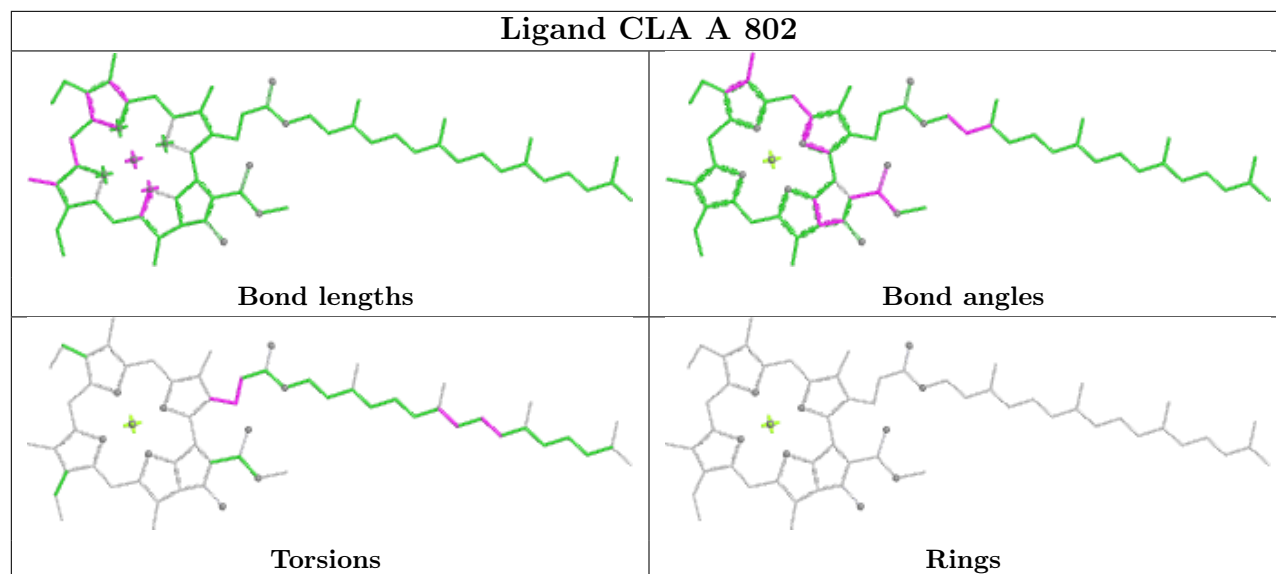
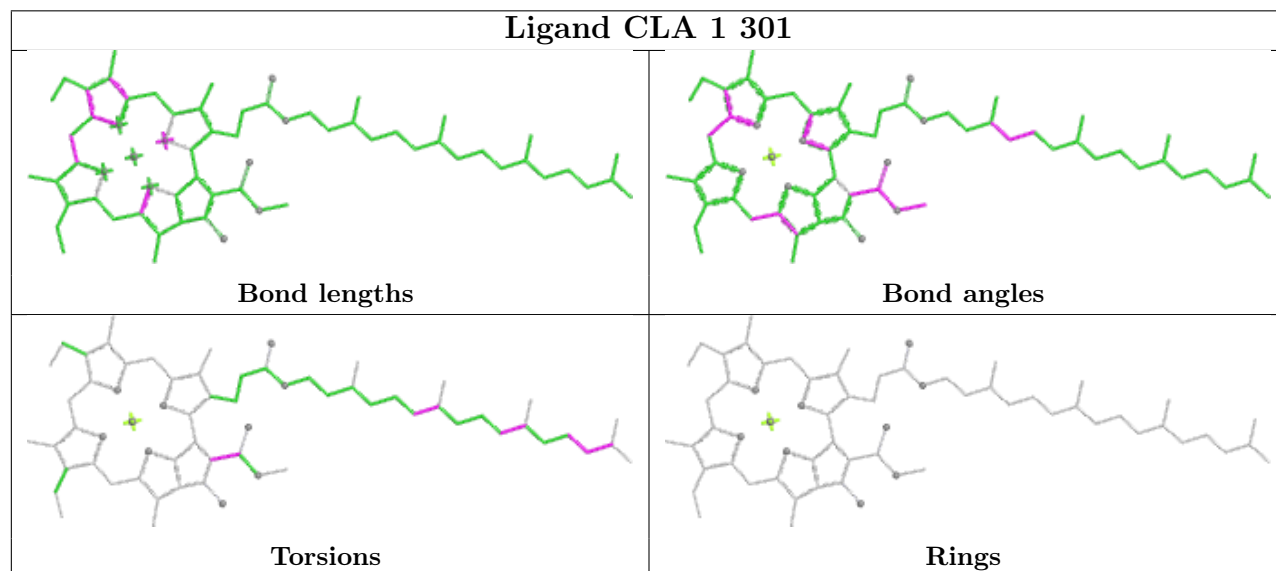


Ligand CLA 3 608

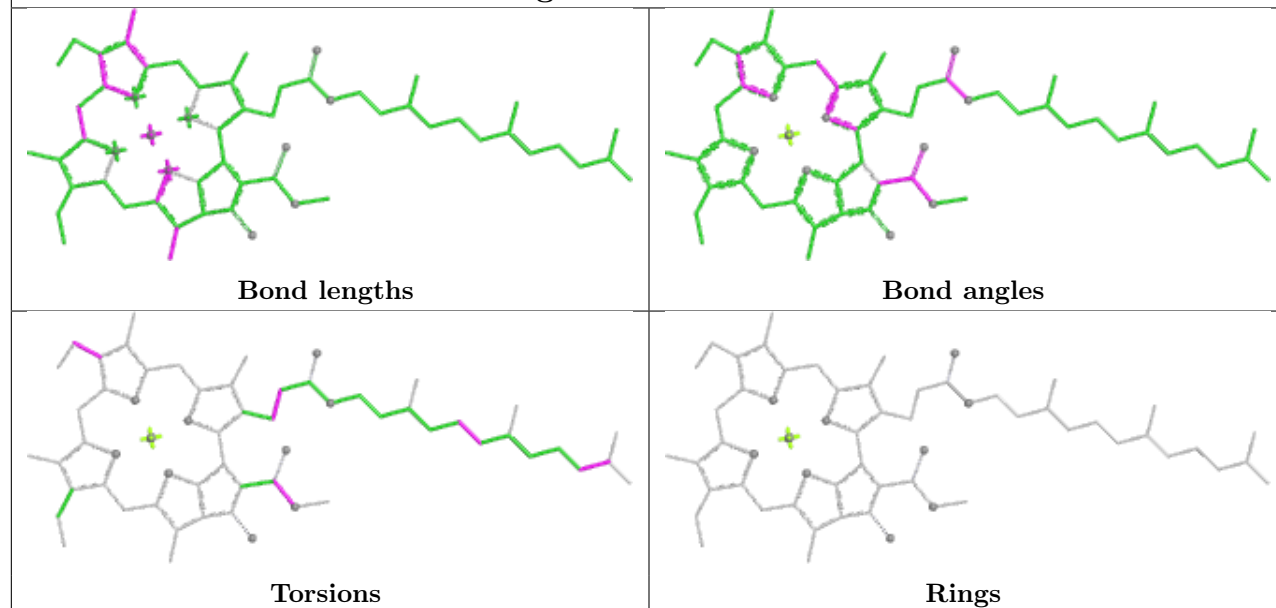


Ligand CLA B 825

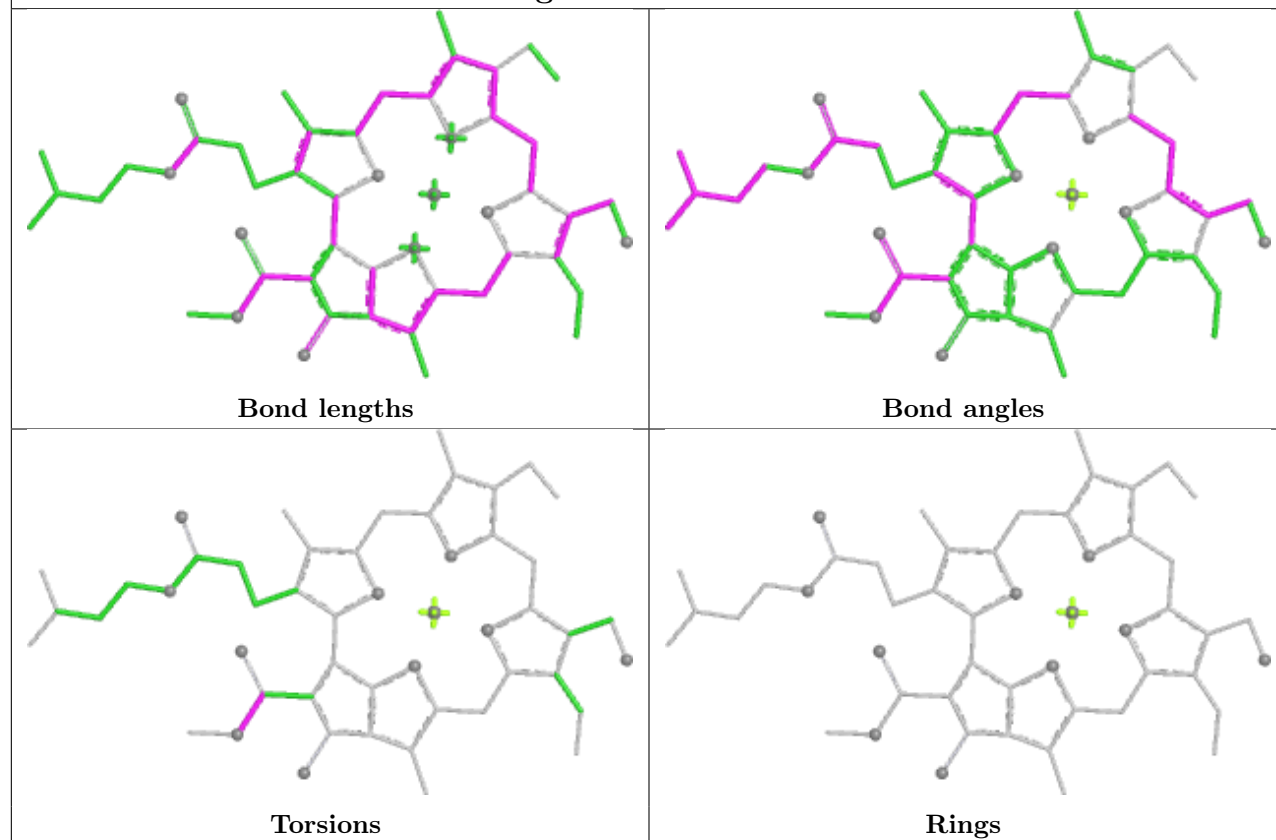


Ligand CLA A 802**Ligand CLA 1 301**

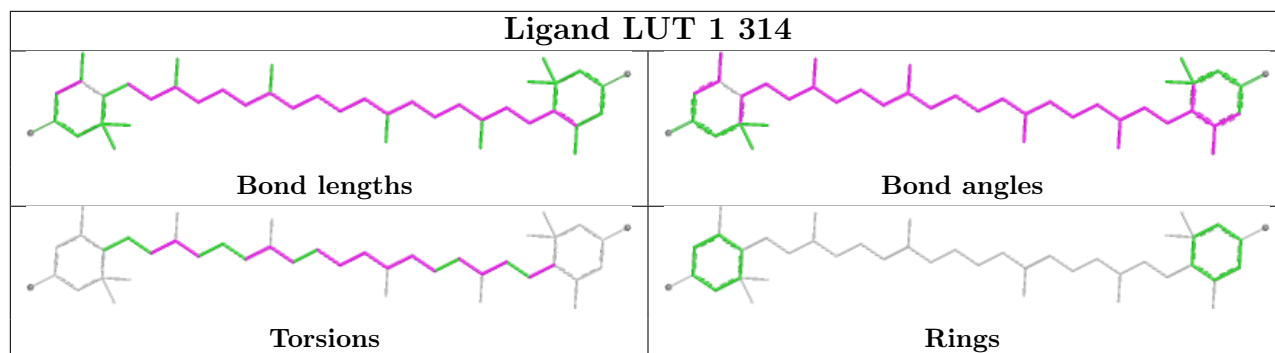
Ligand CLA 1 311



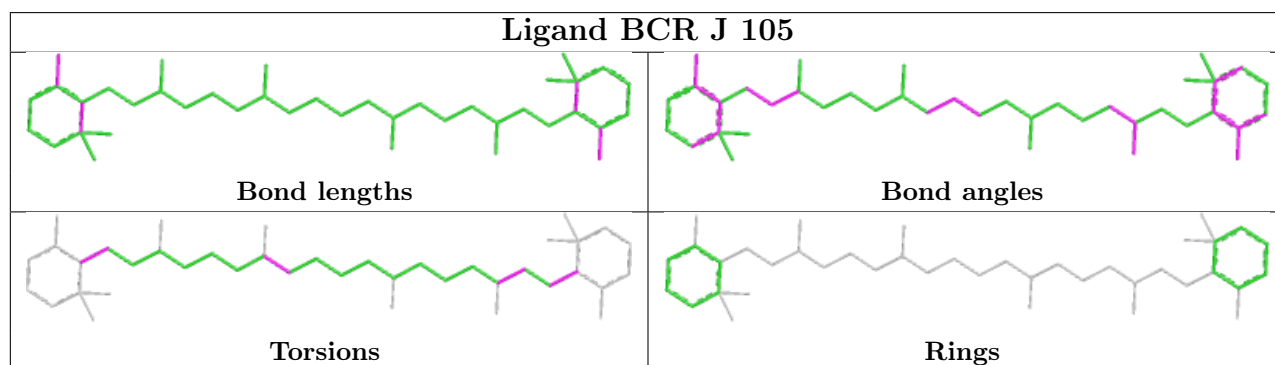
Ligand CHL 4 307



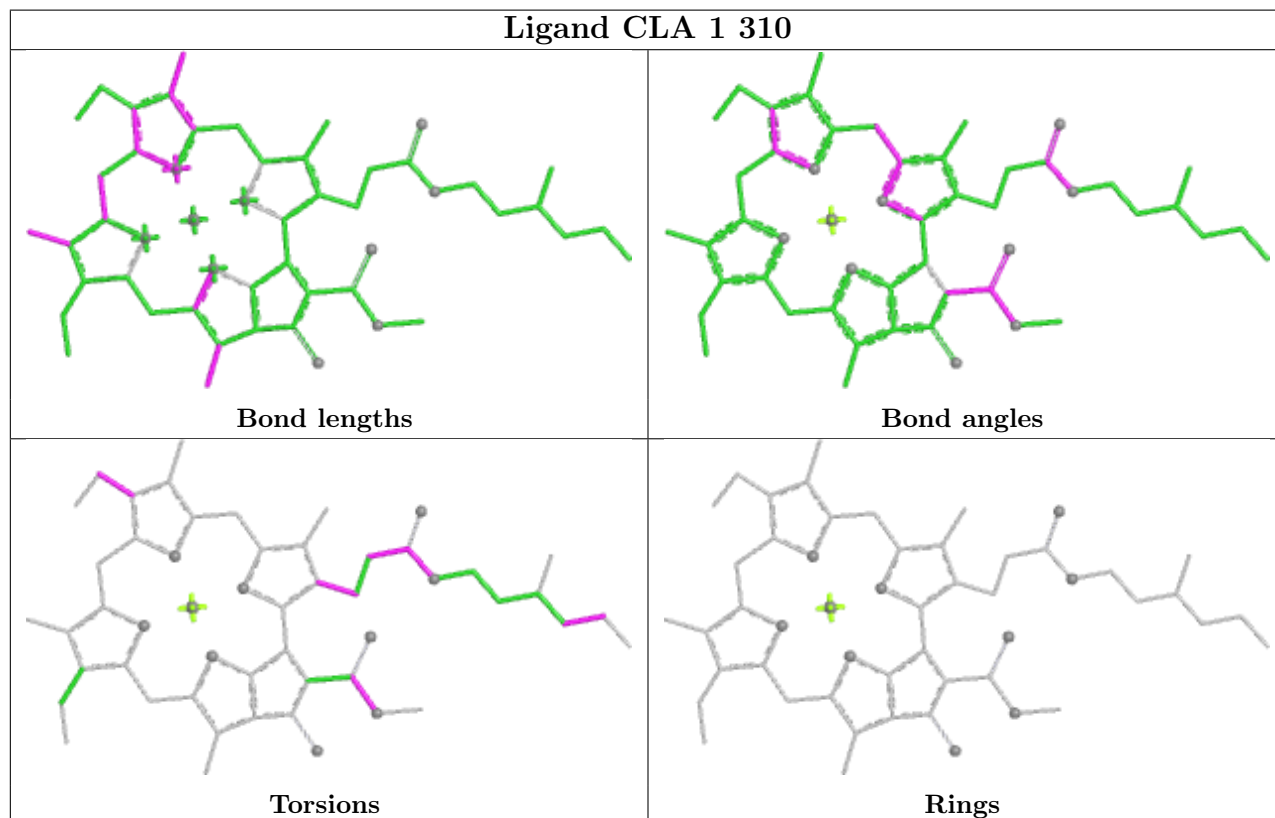
Ligand LUT 1 314



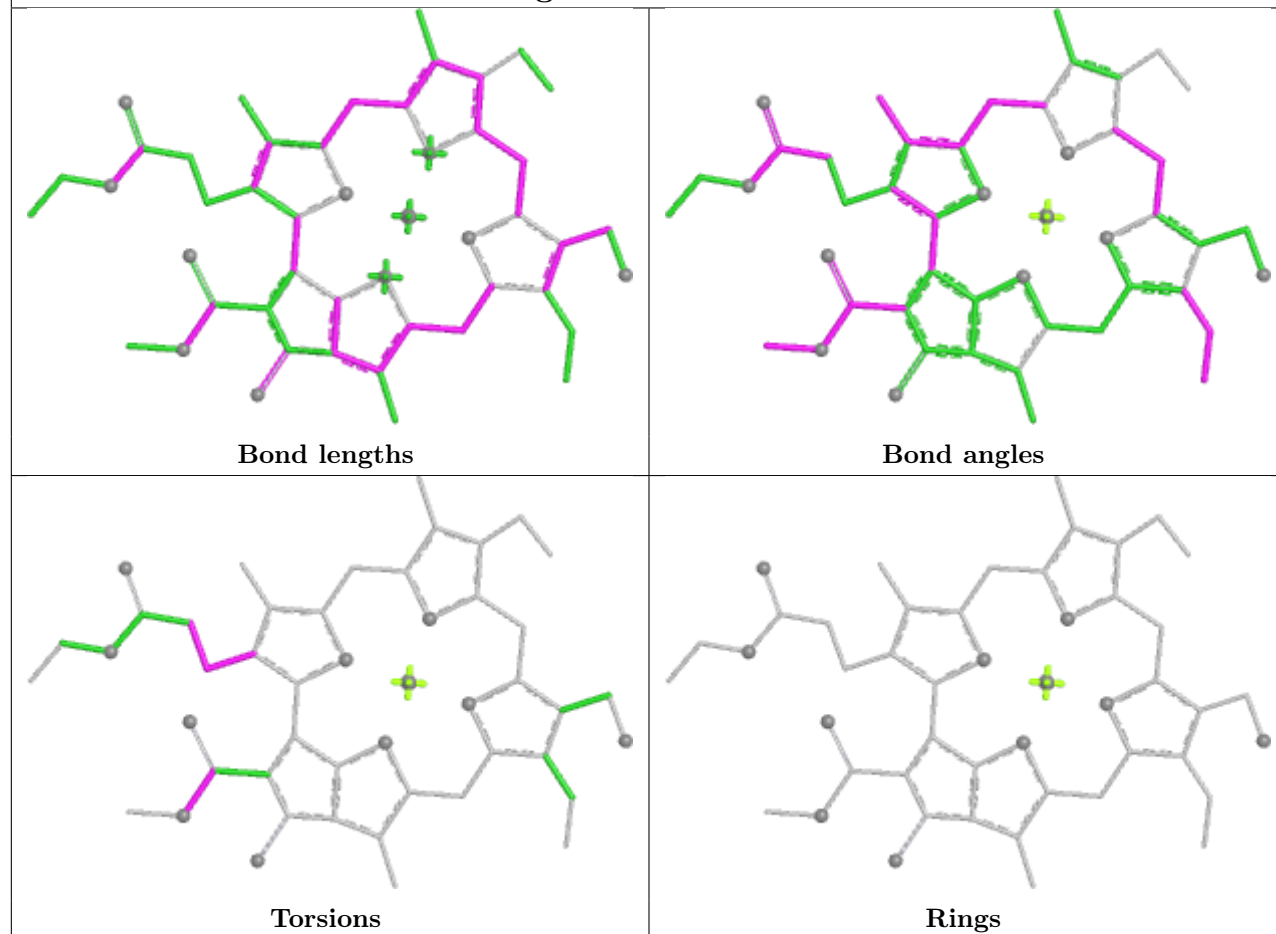
Ligand BCR J 105



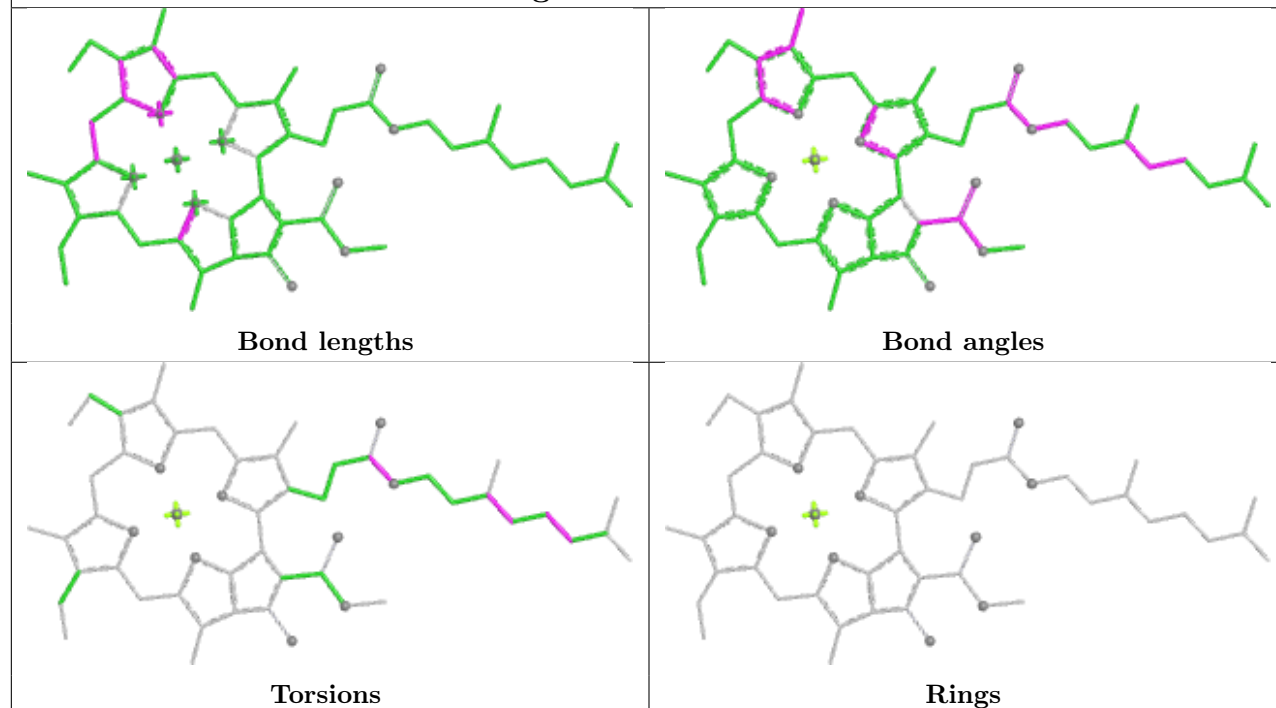
Ligand CLA 1 310



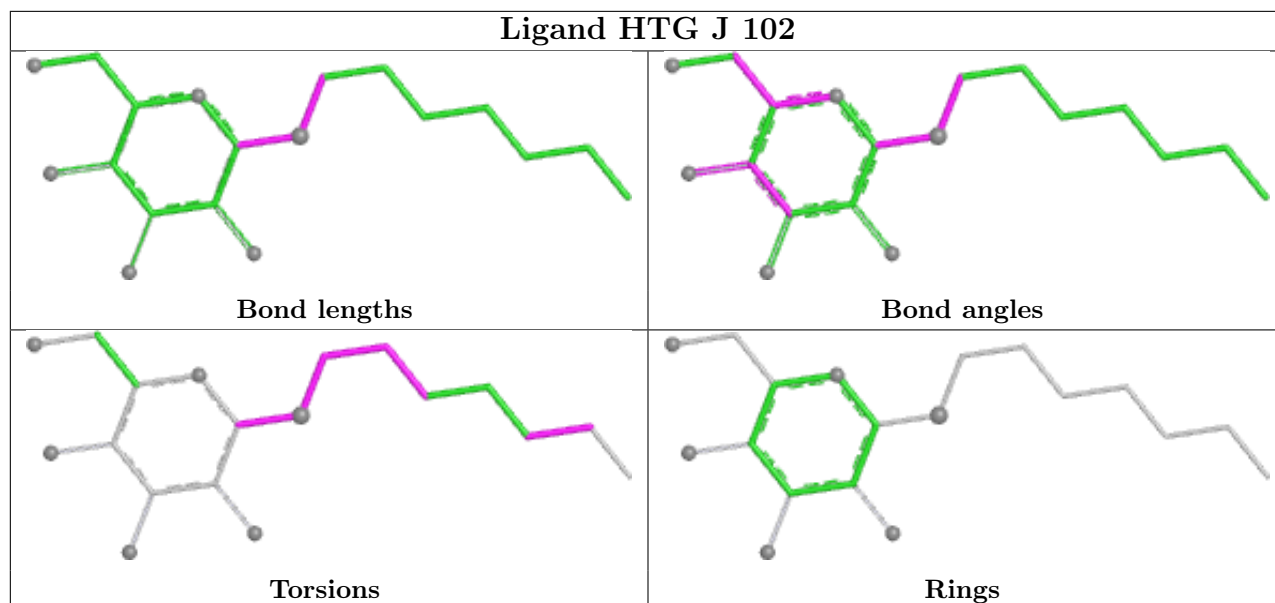
Ligand CHL 1 305



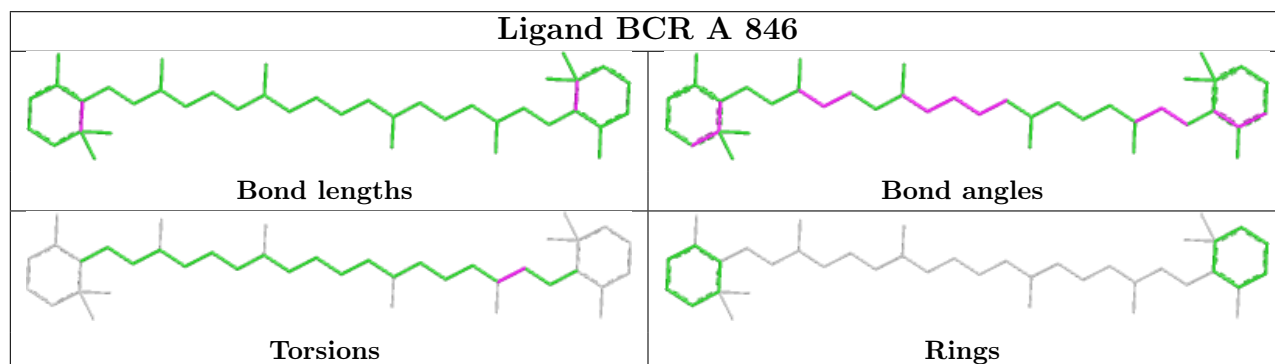
Ligand CLA B 818



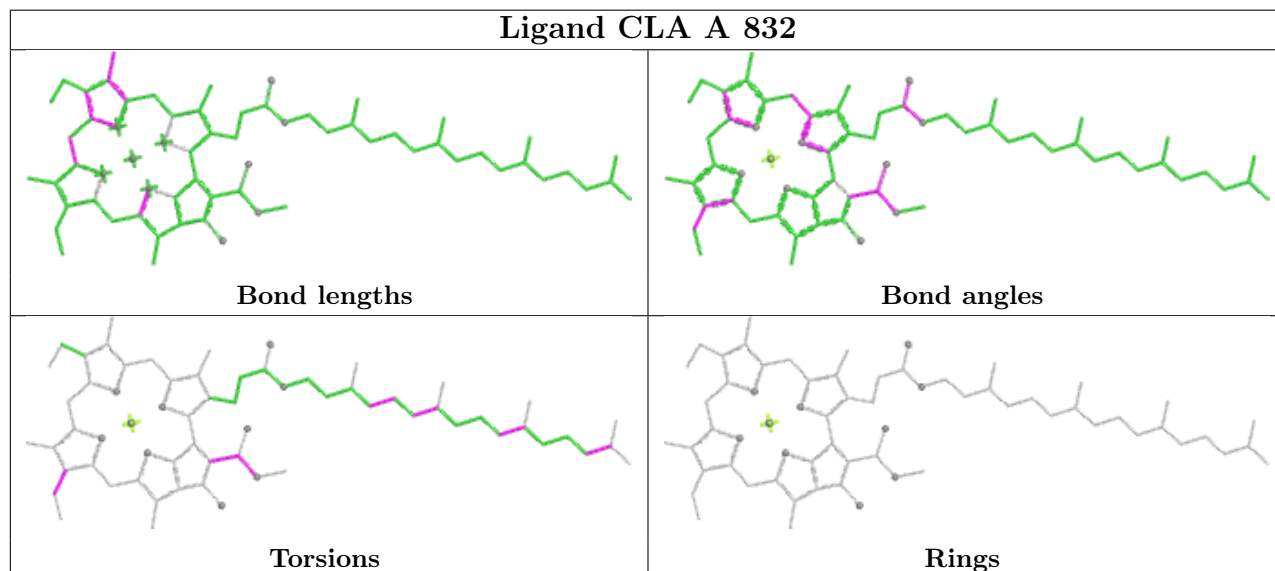
Ligand HTG J 102



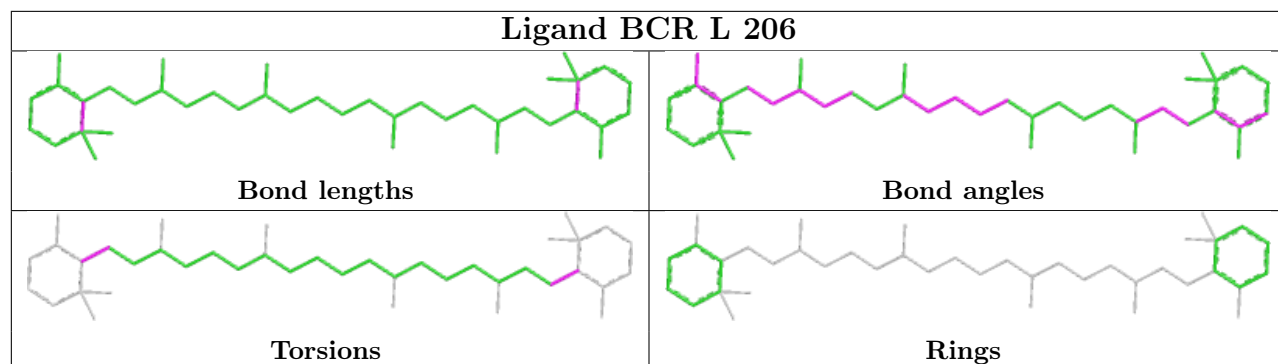
Ligand BCR A 846



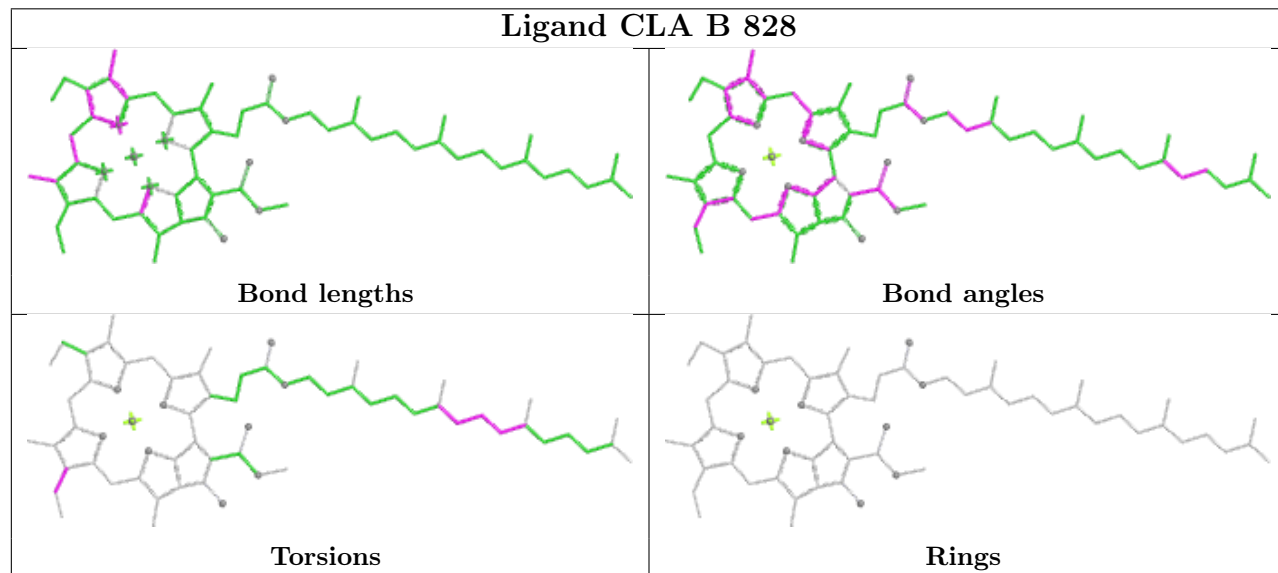
Ligand CLA A 832



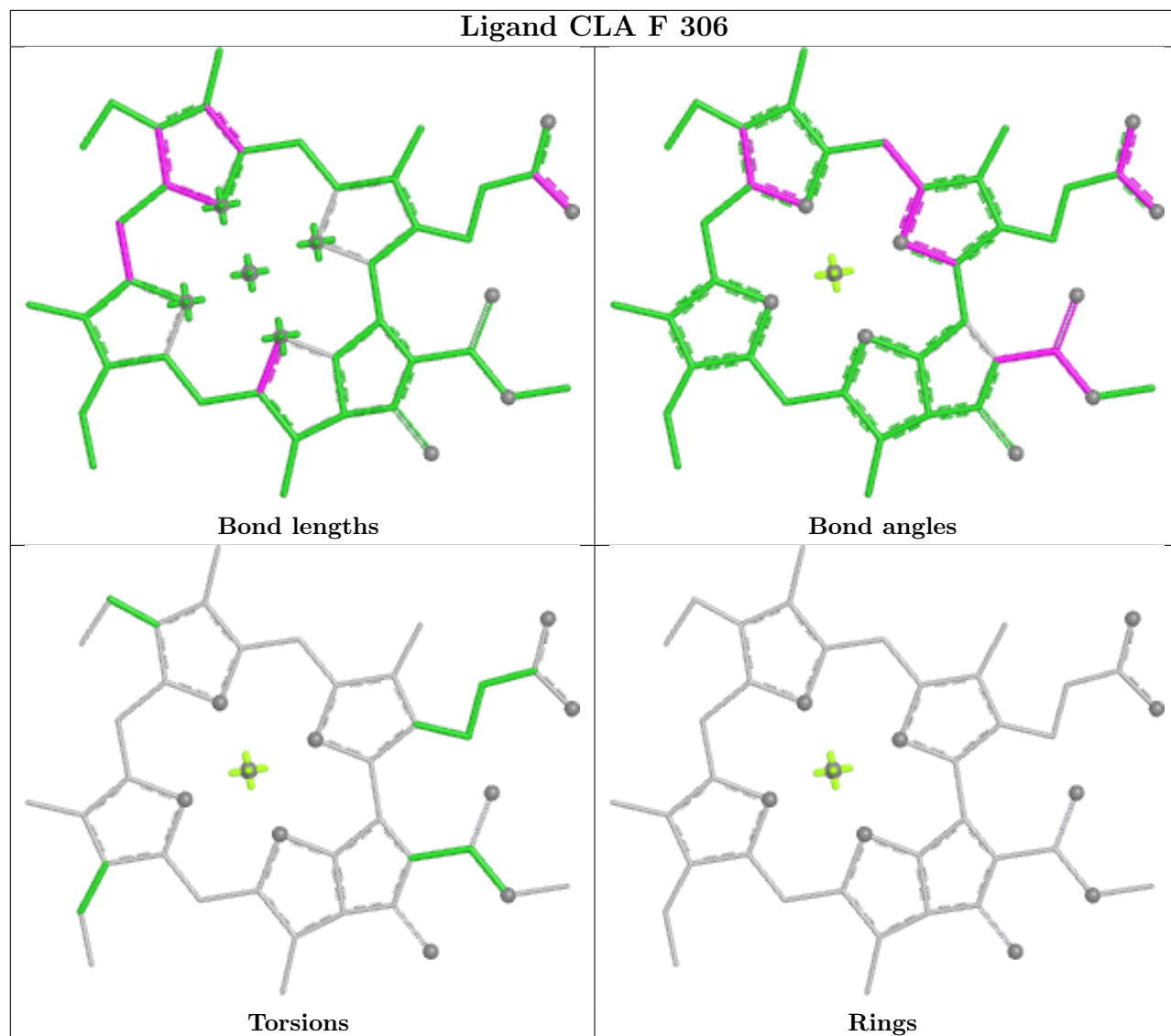
Ligand BCR L 206



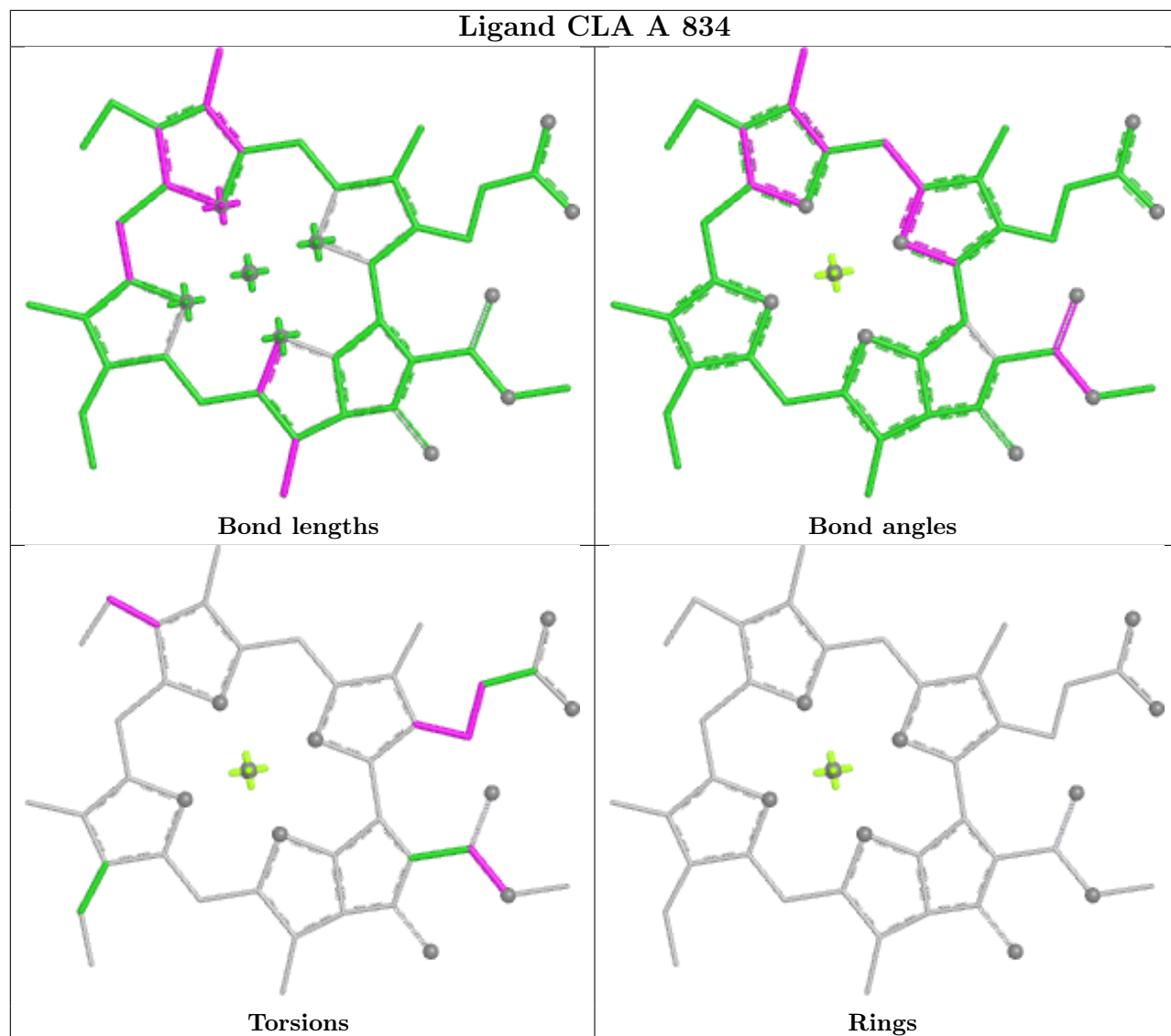
Ligand CLA B 828



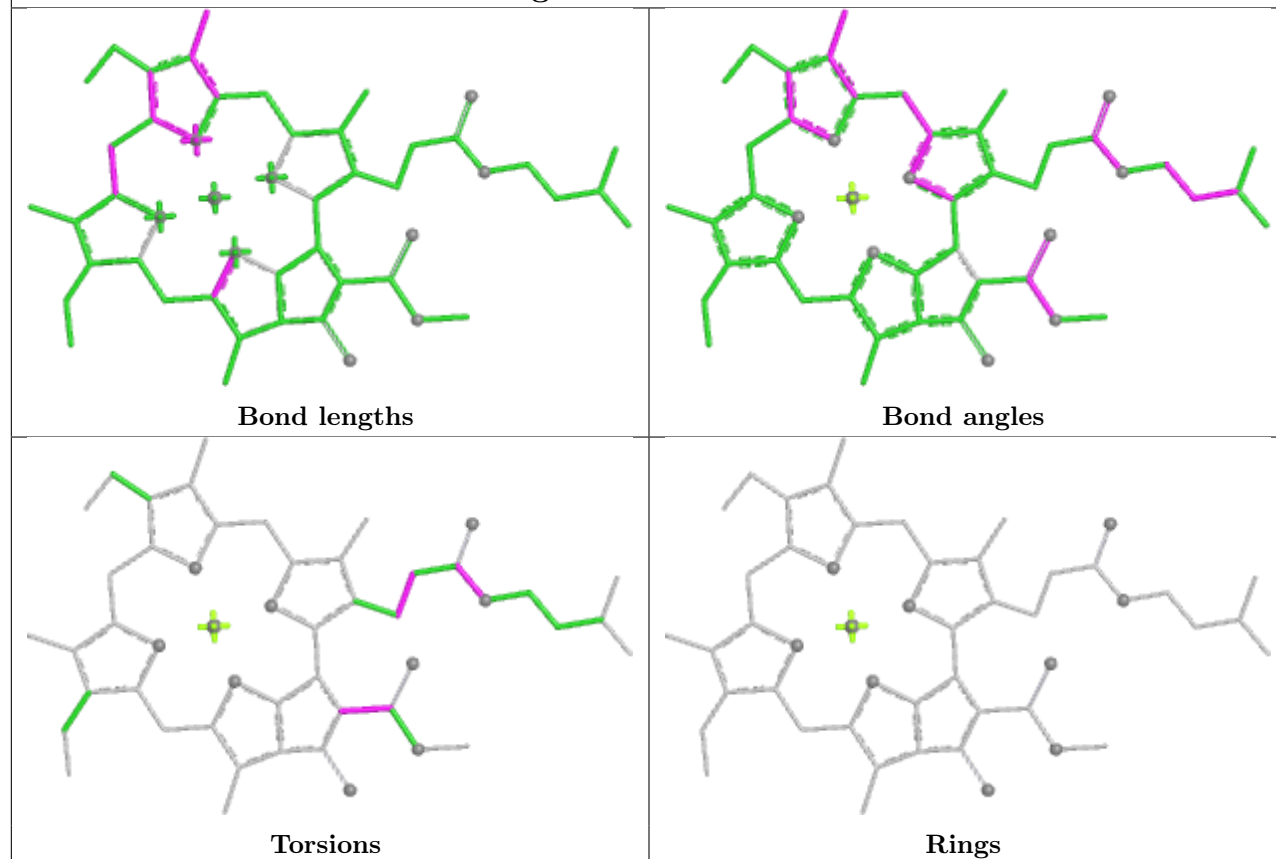
Ligand CLA F 306



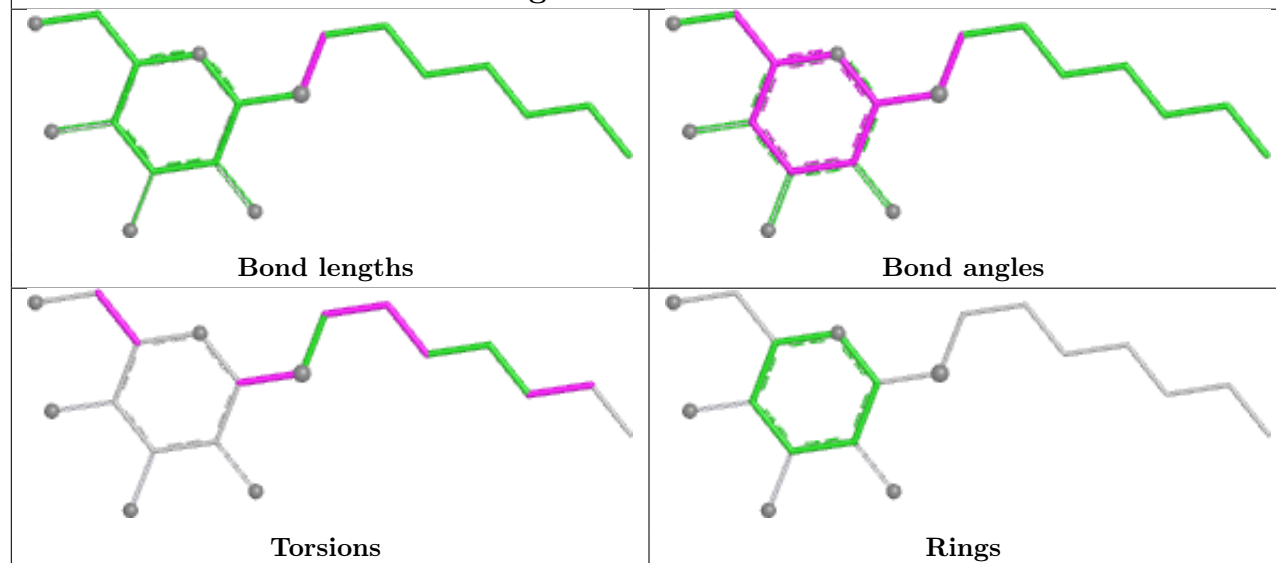
Ligand CLA A 834



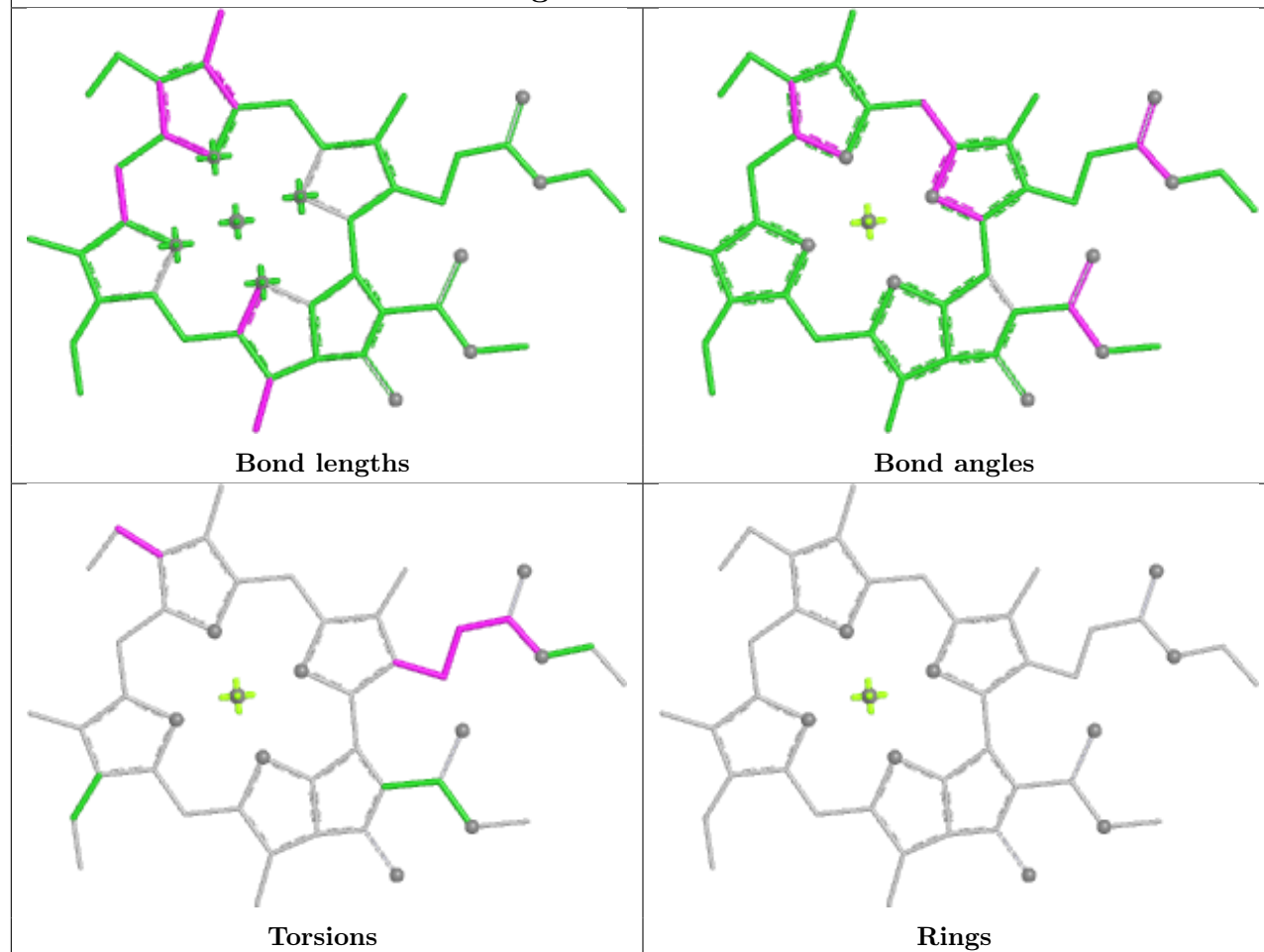
Ligand CLA A 830



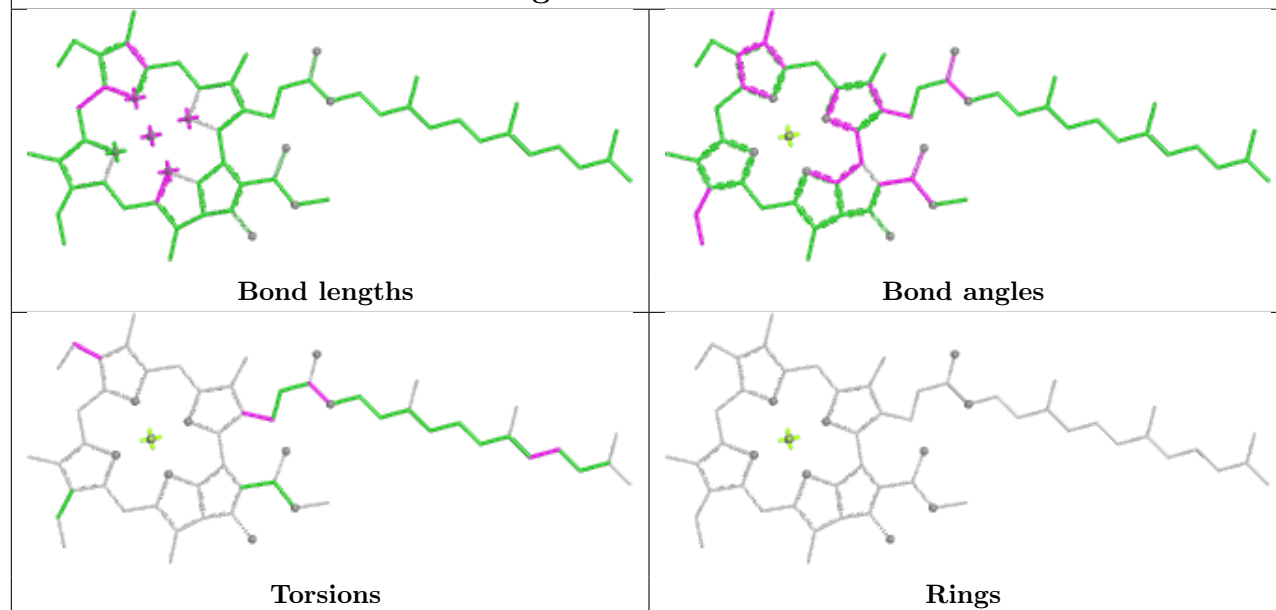
Ligand HTG B 851

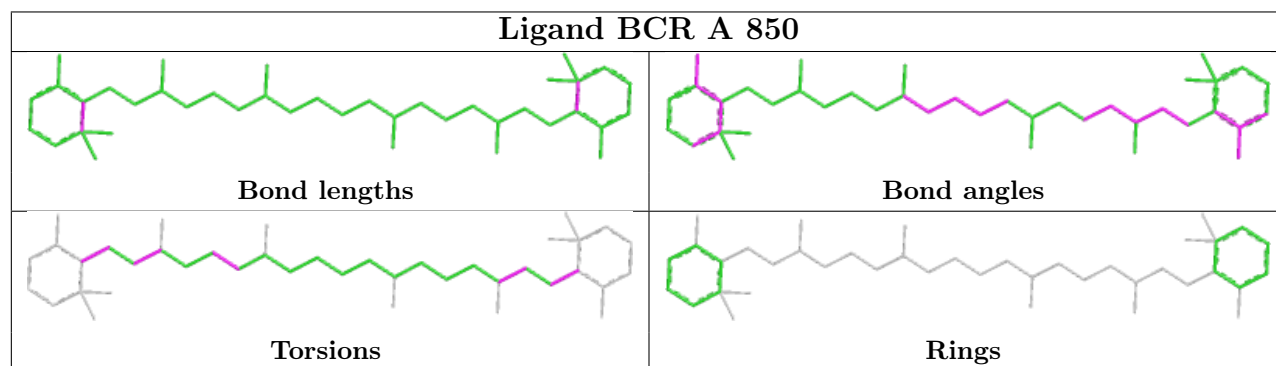
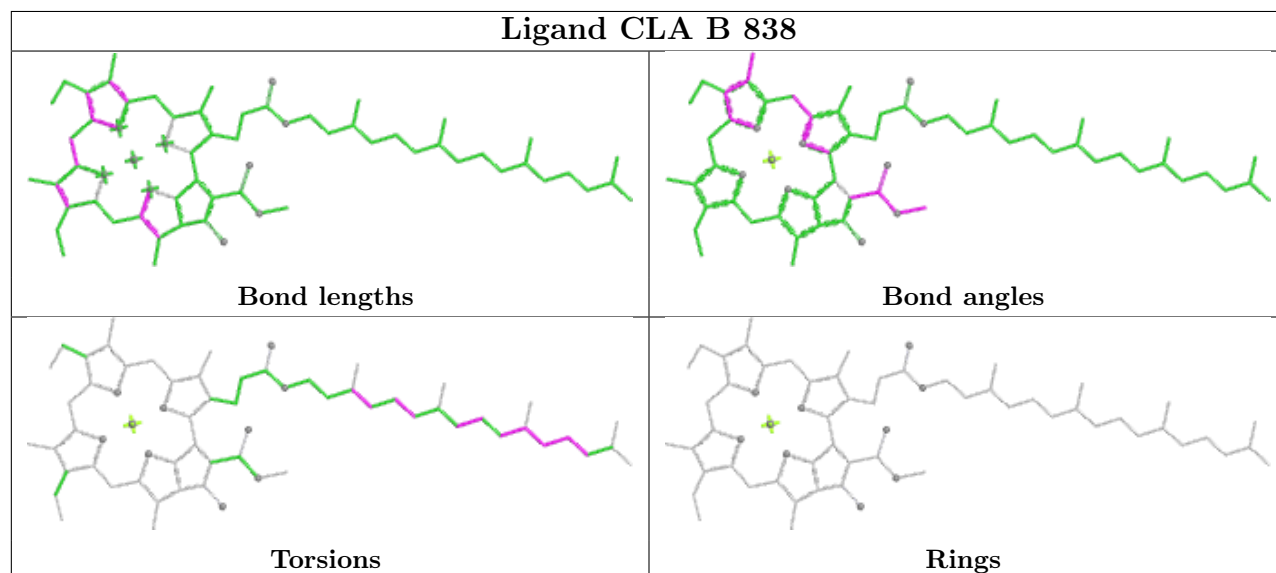
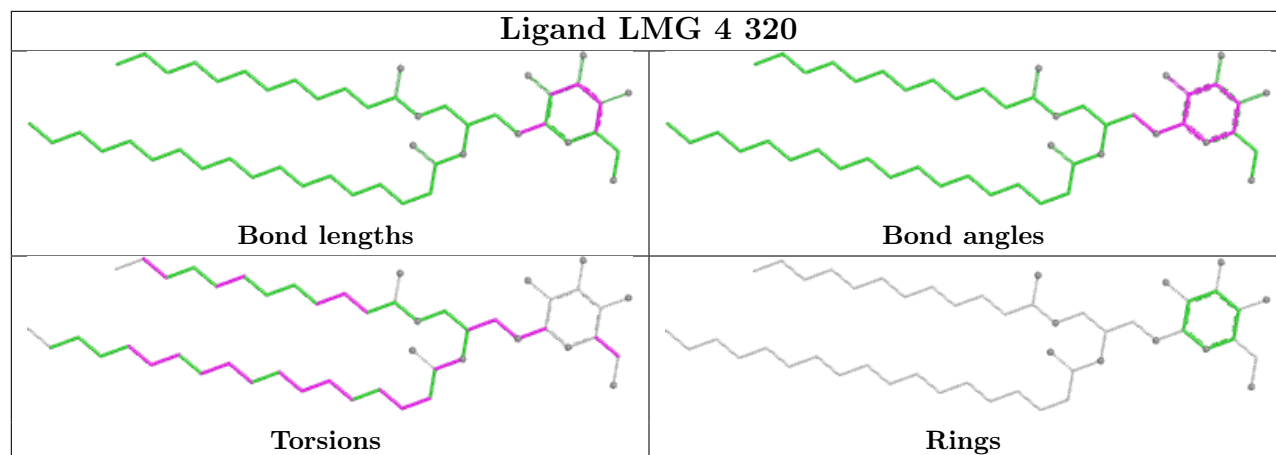


Ligand CLA 3 606

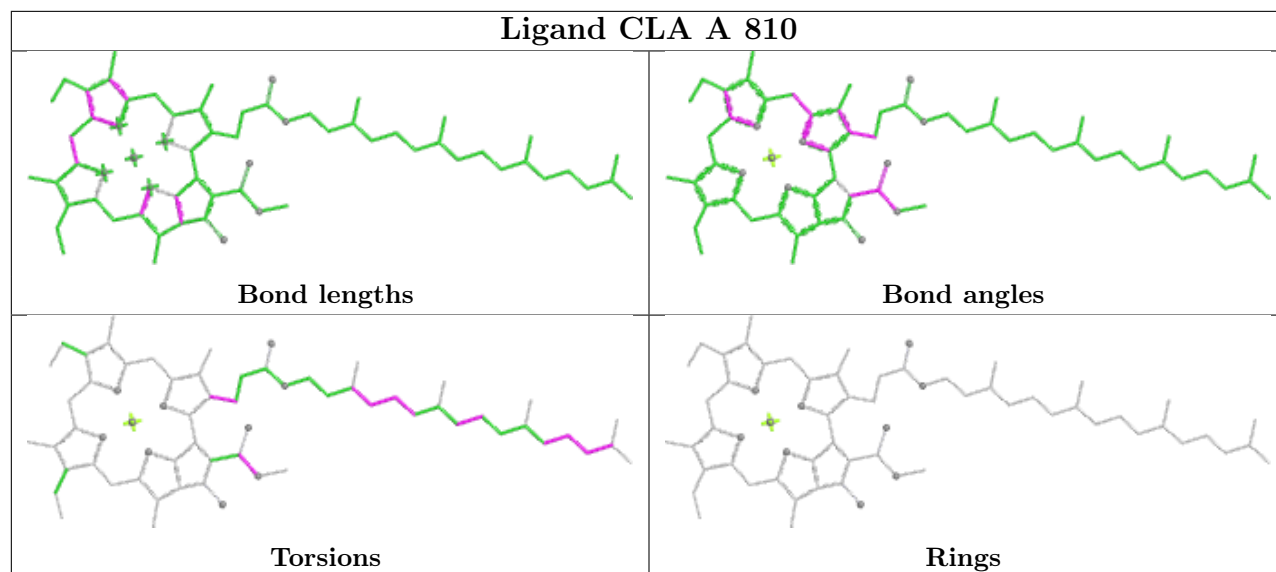


Ligand CLA B 833

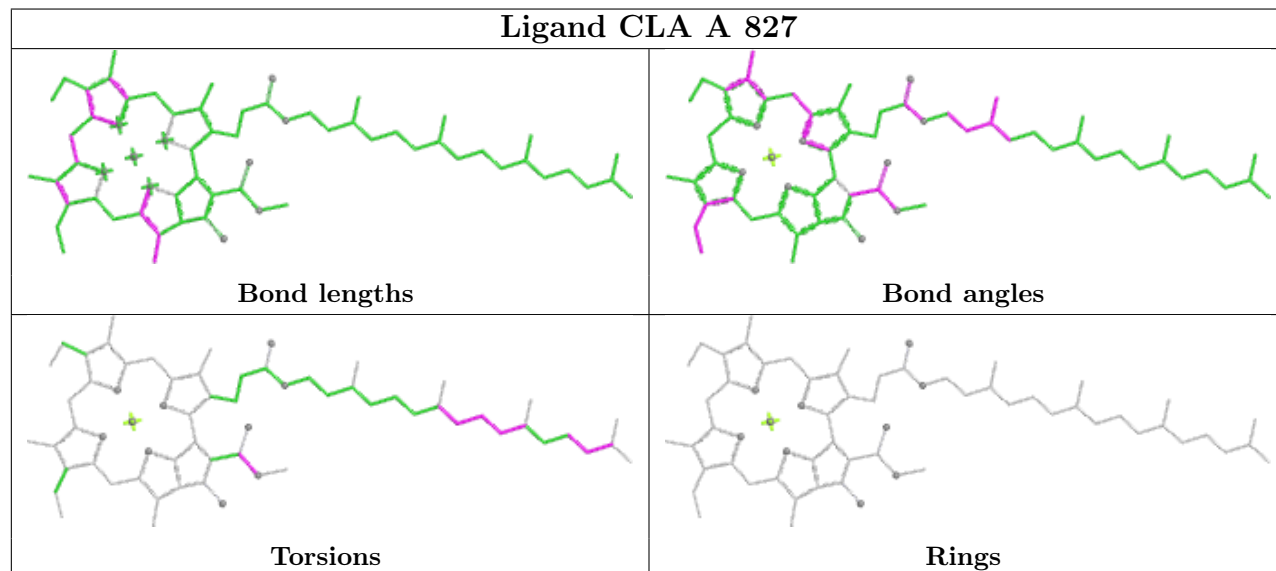




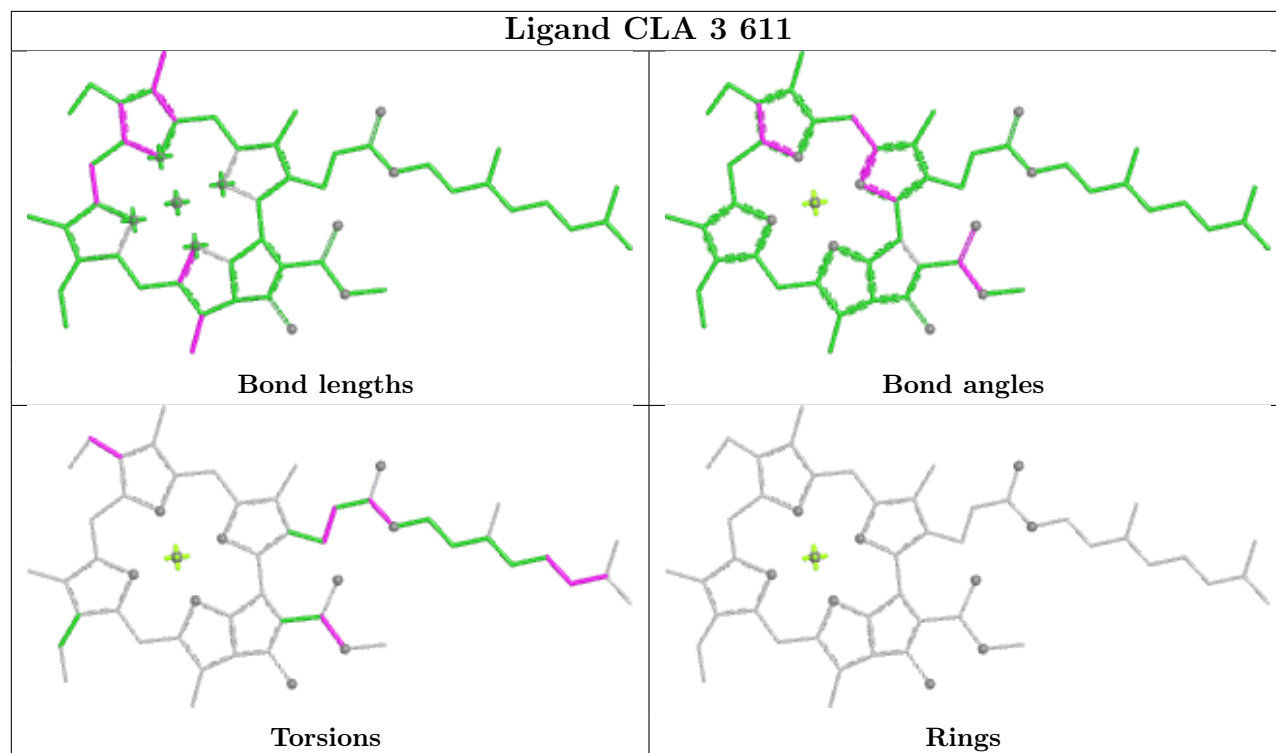
Ligand CLA A 810



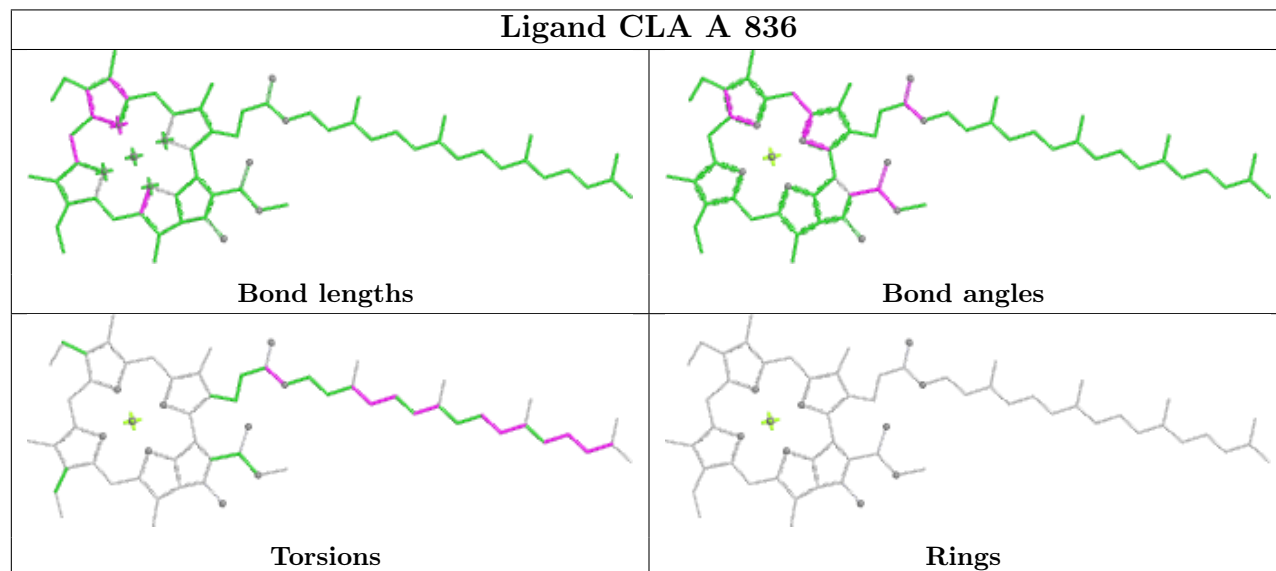
Ligand CLA A 827

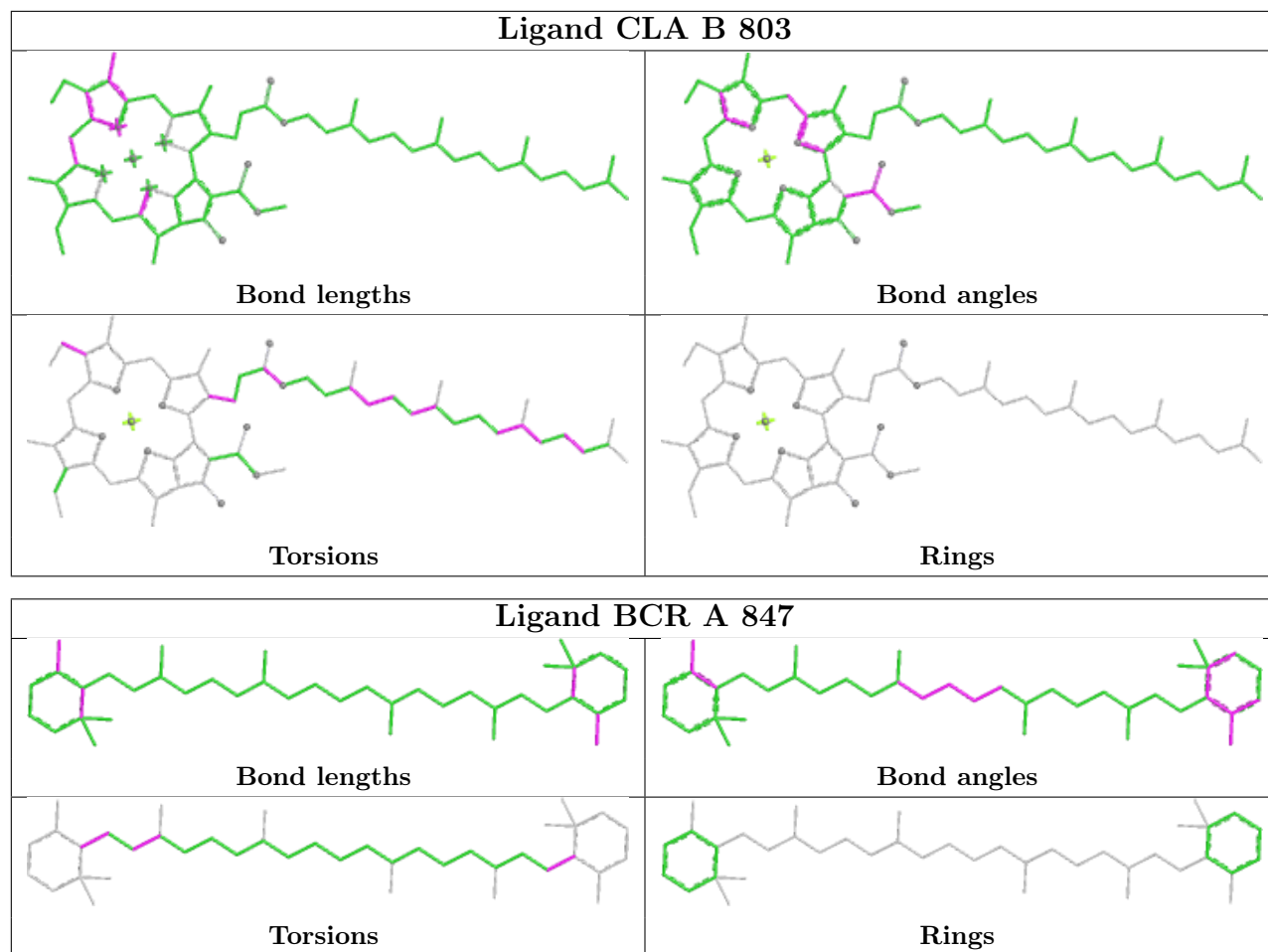


Ligand CLA 3 611

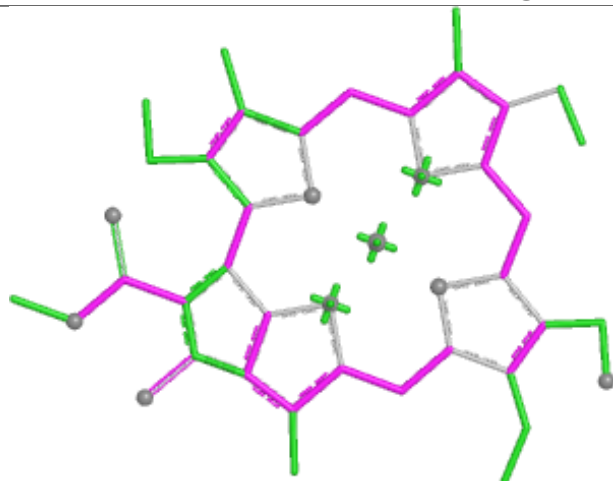


Ligand CLA A 836

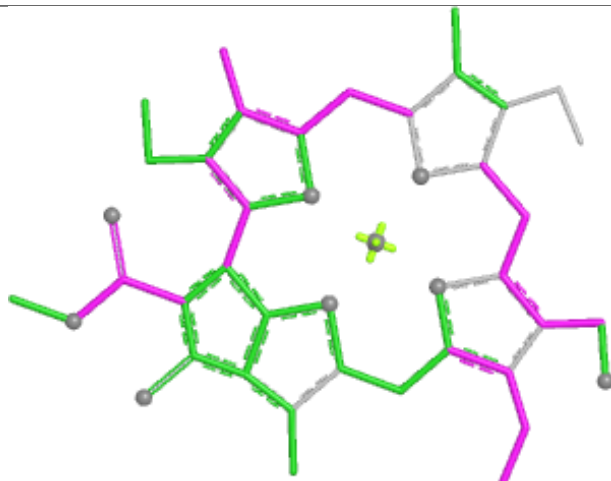




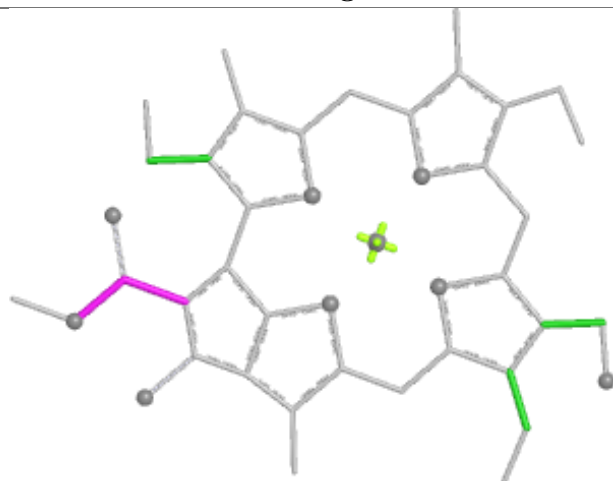
Ligand CHL 4 315



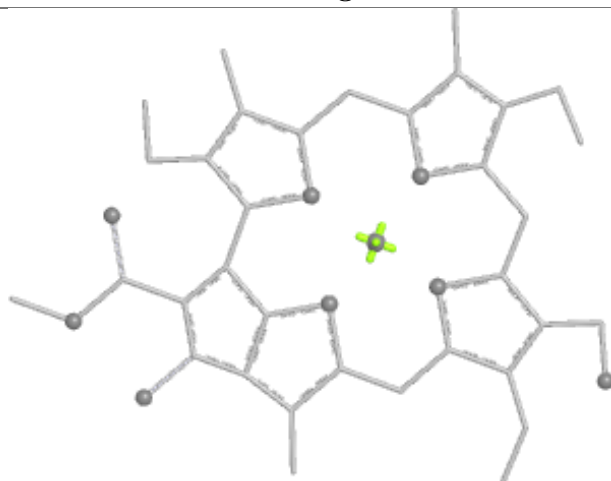
Bond lengths



Bond angles

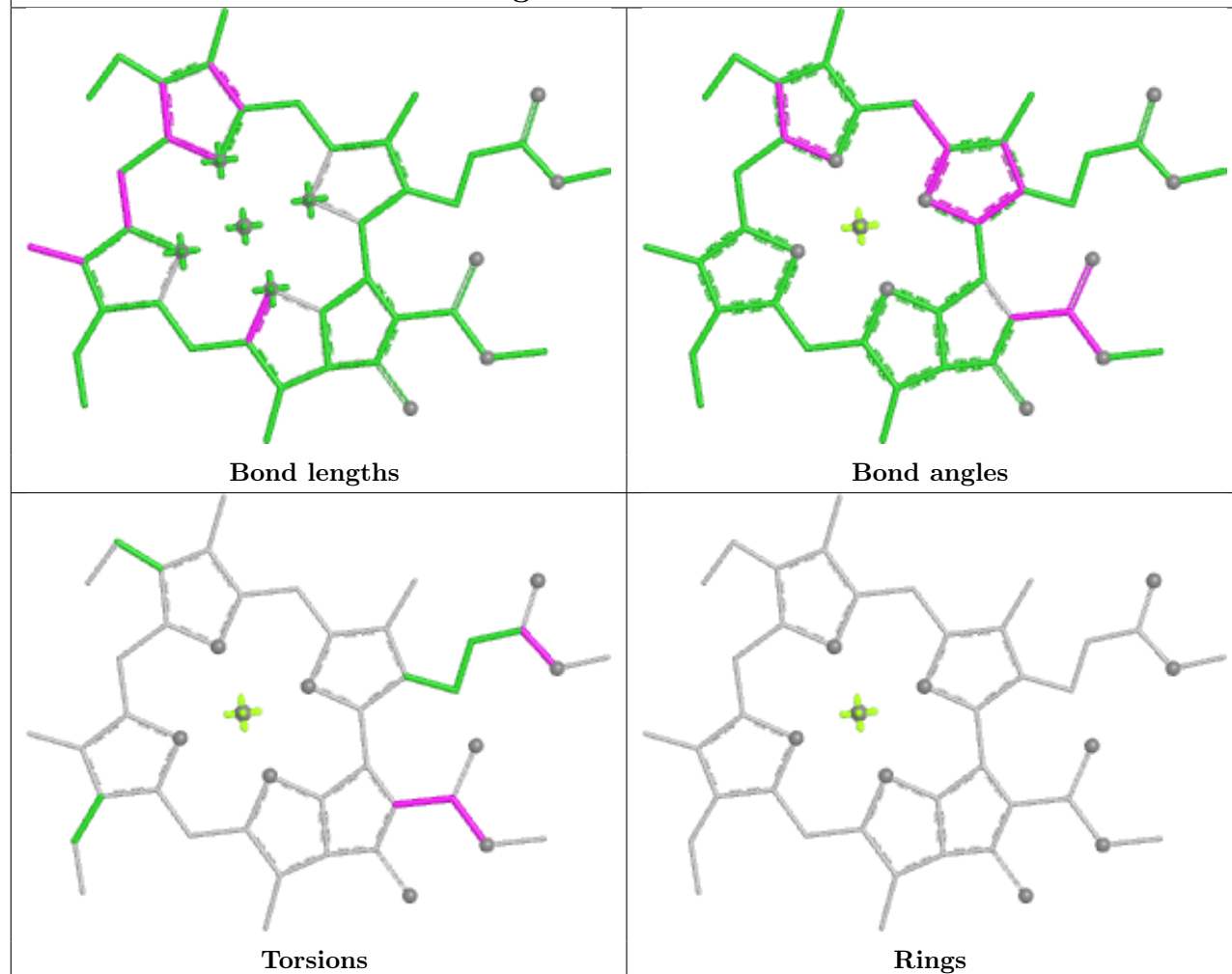


Torsions

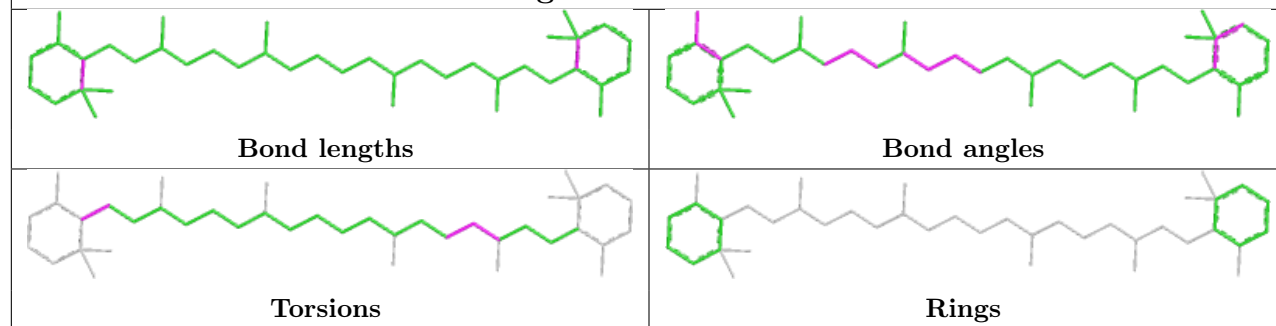


Rings

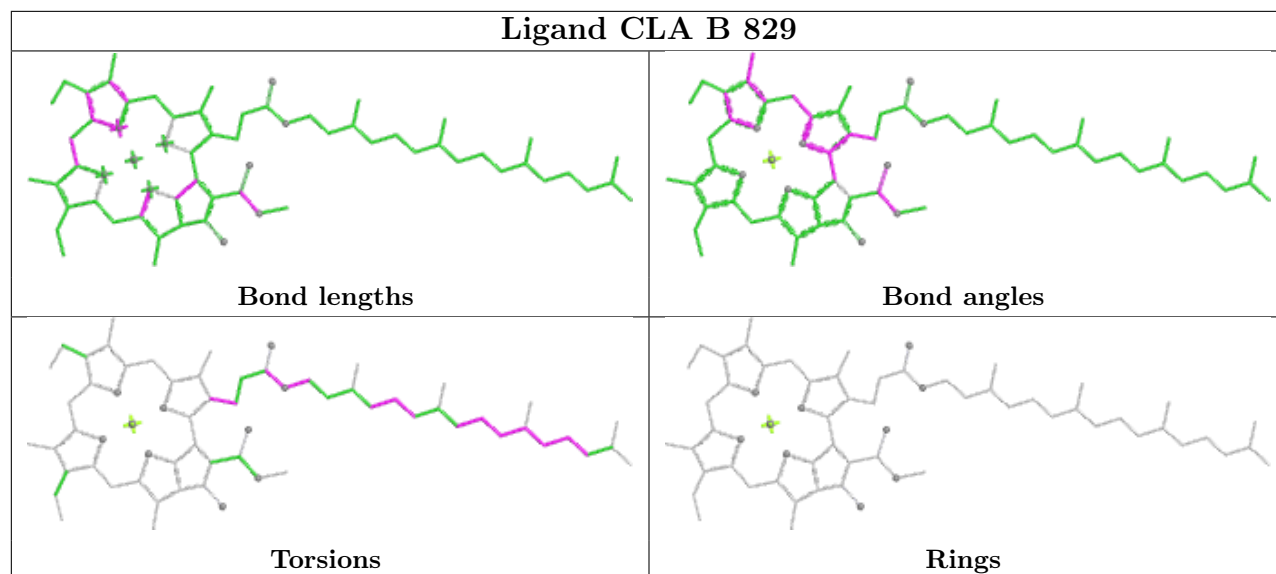
Ligand CLA G 105



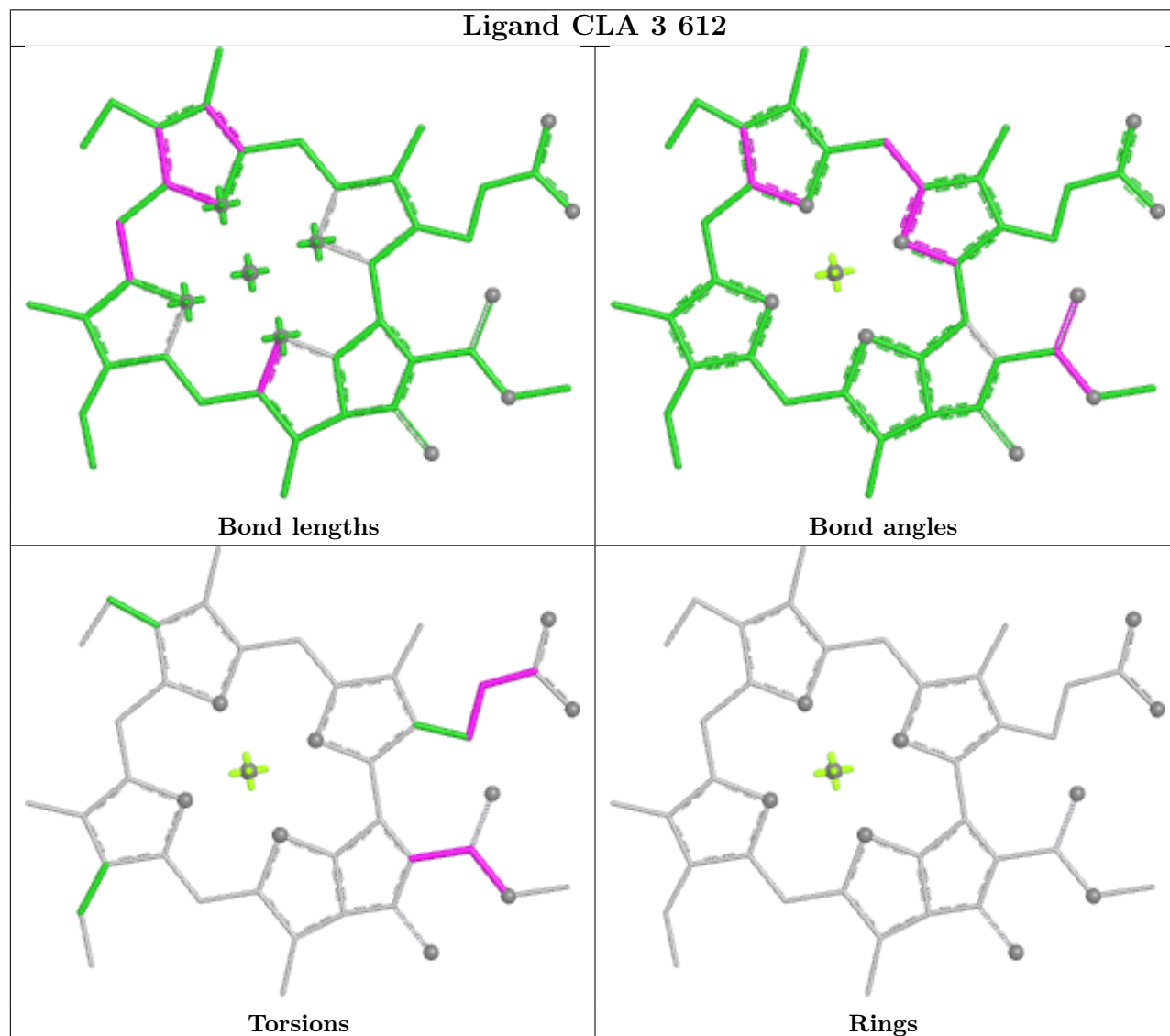
Ligand BCR I 101



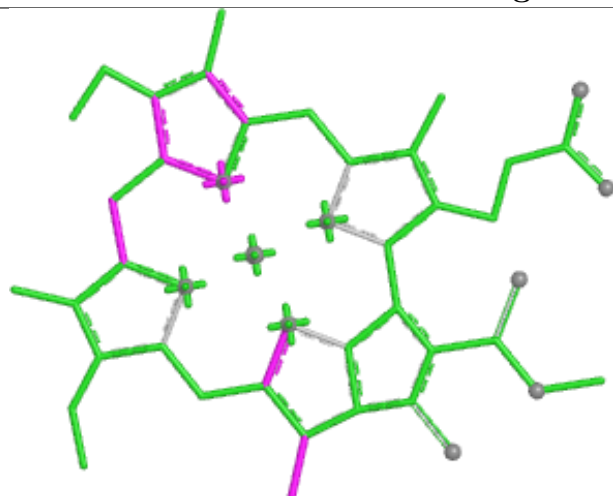
Ligand CLA B 829



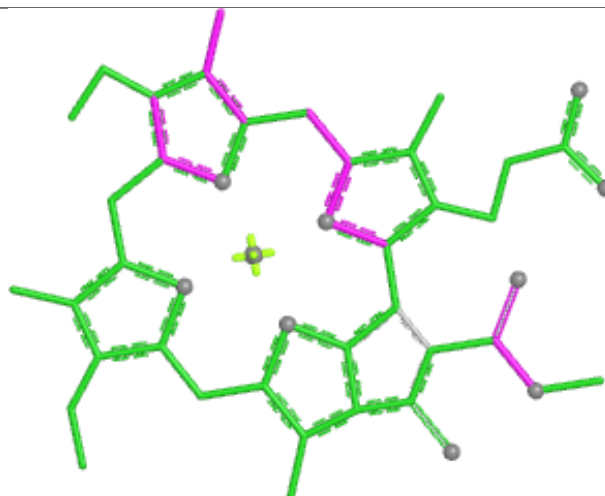
Ligand CLA 3 612



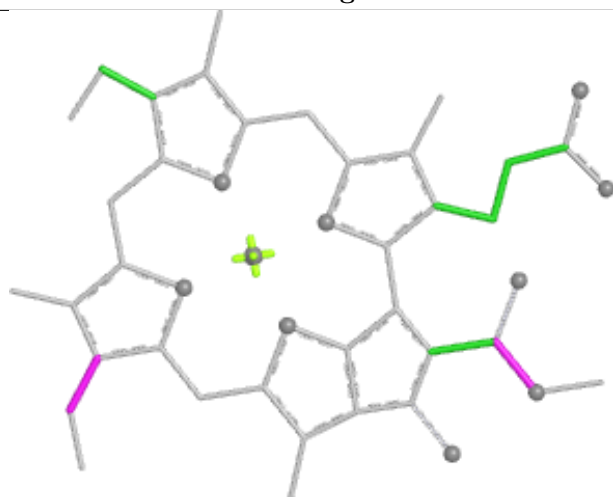
Ligand CLA K 201



Bond lengths



Bond angles

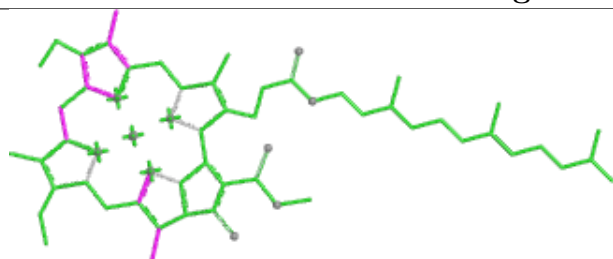


Torsions

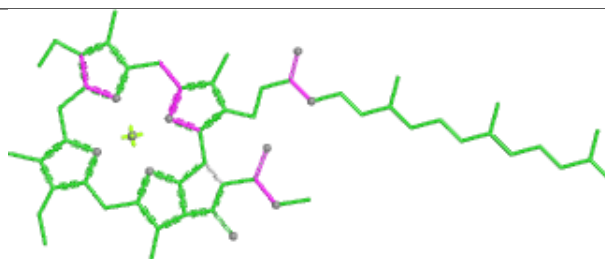


Rings

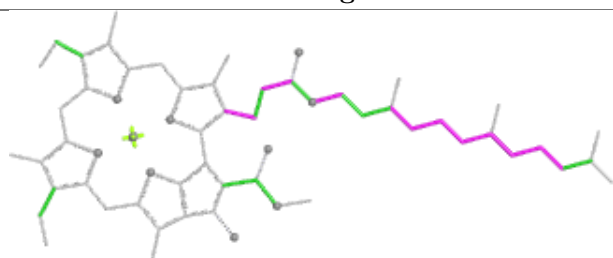
Ligand CLA K 202



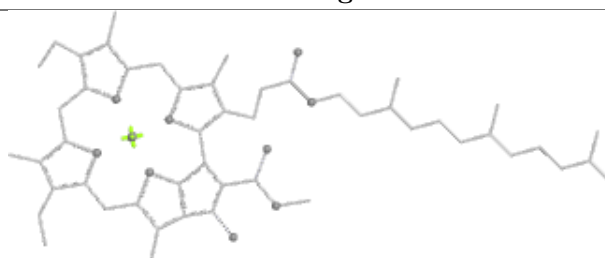
Bond lengths



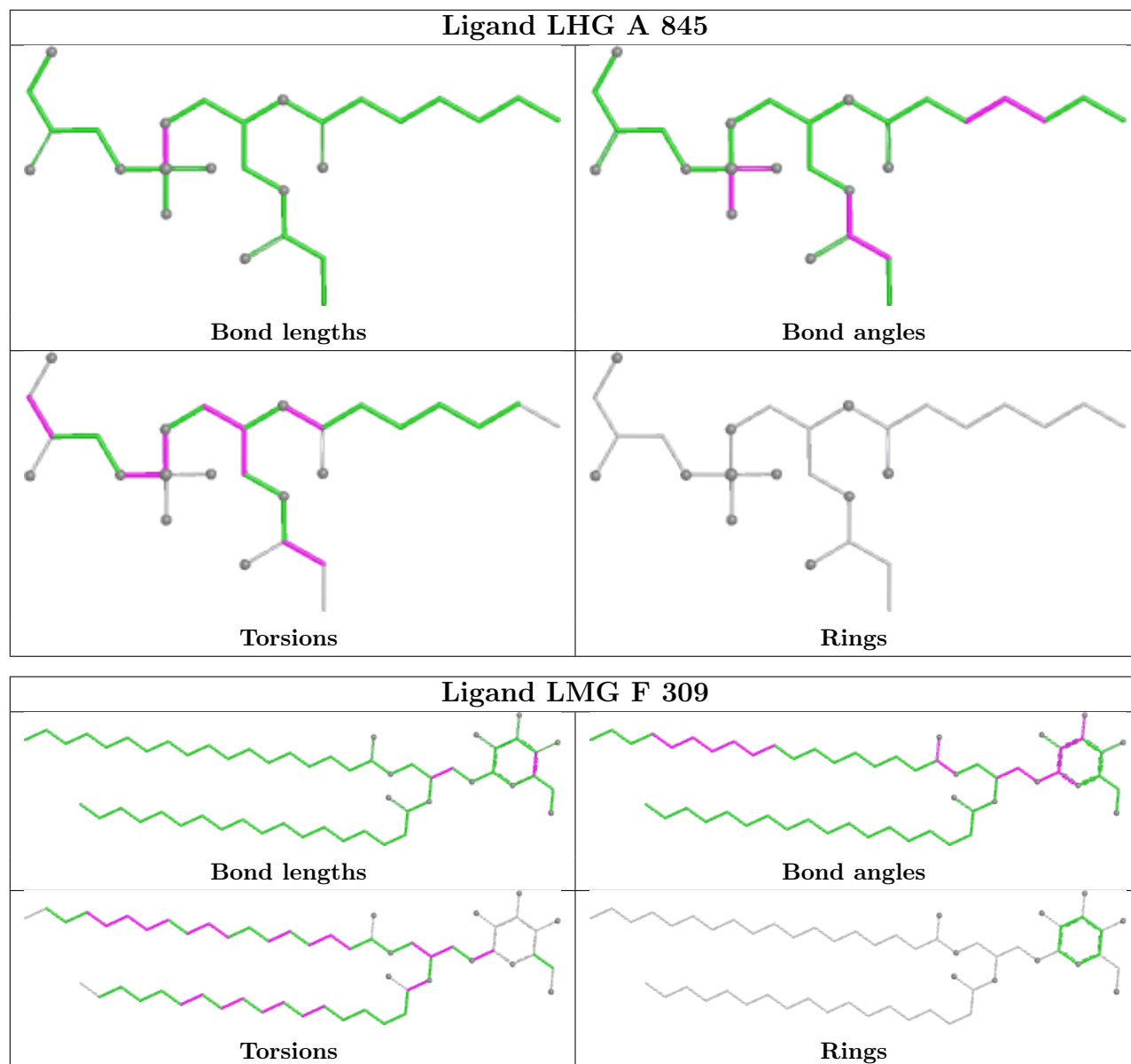
Bond angles



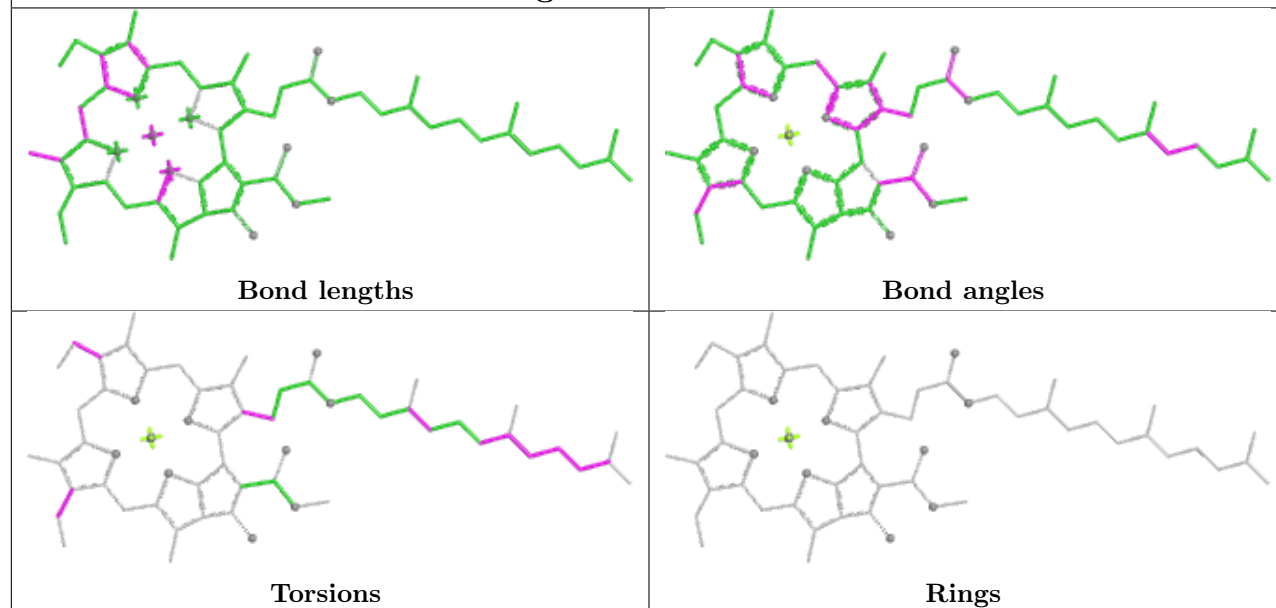
Torsions



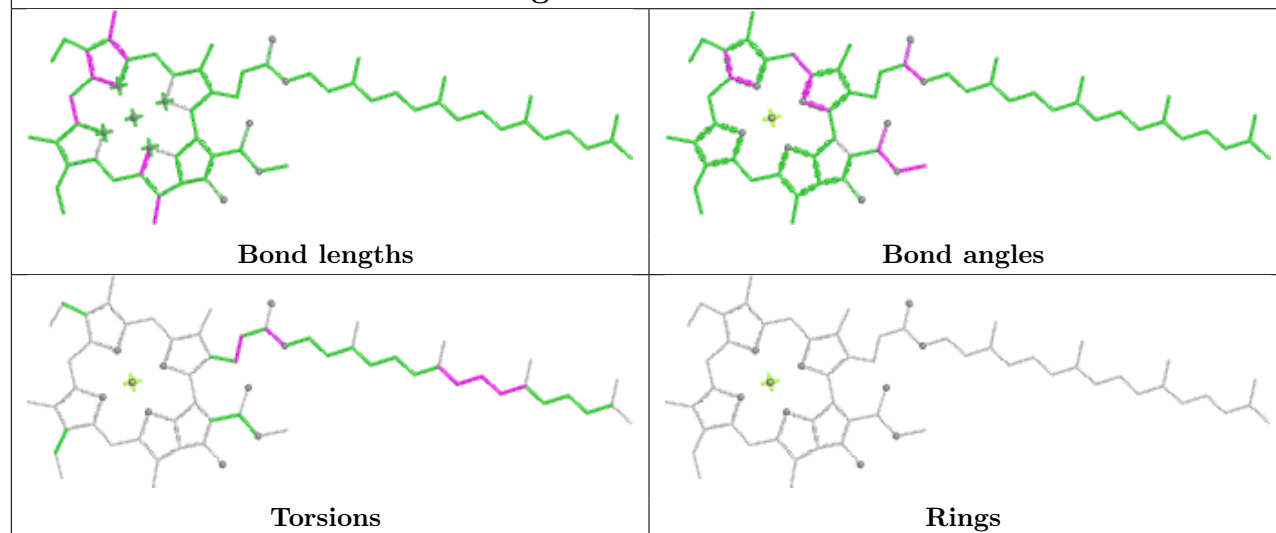
Rings



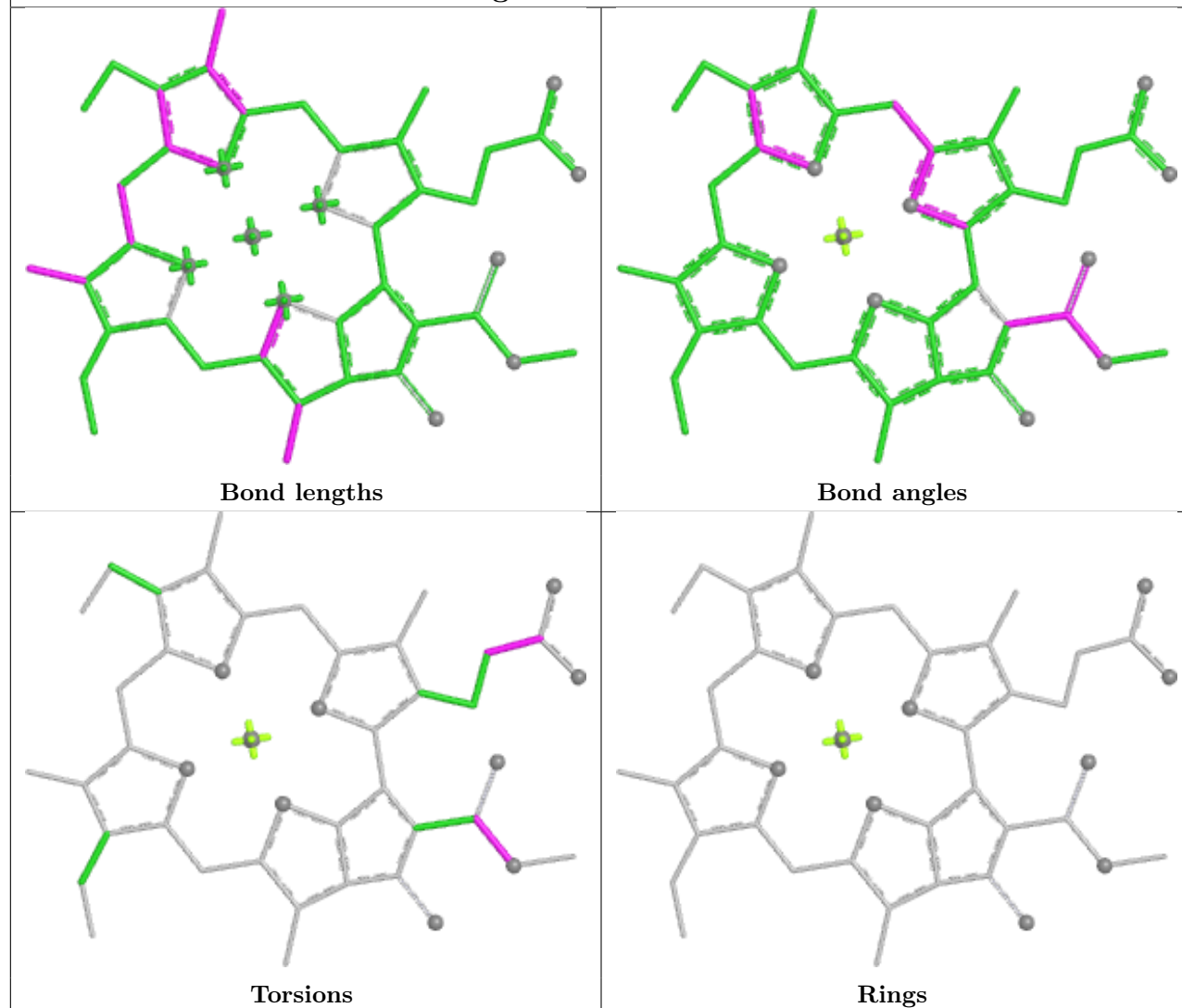
Ligand CLA 4 310



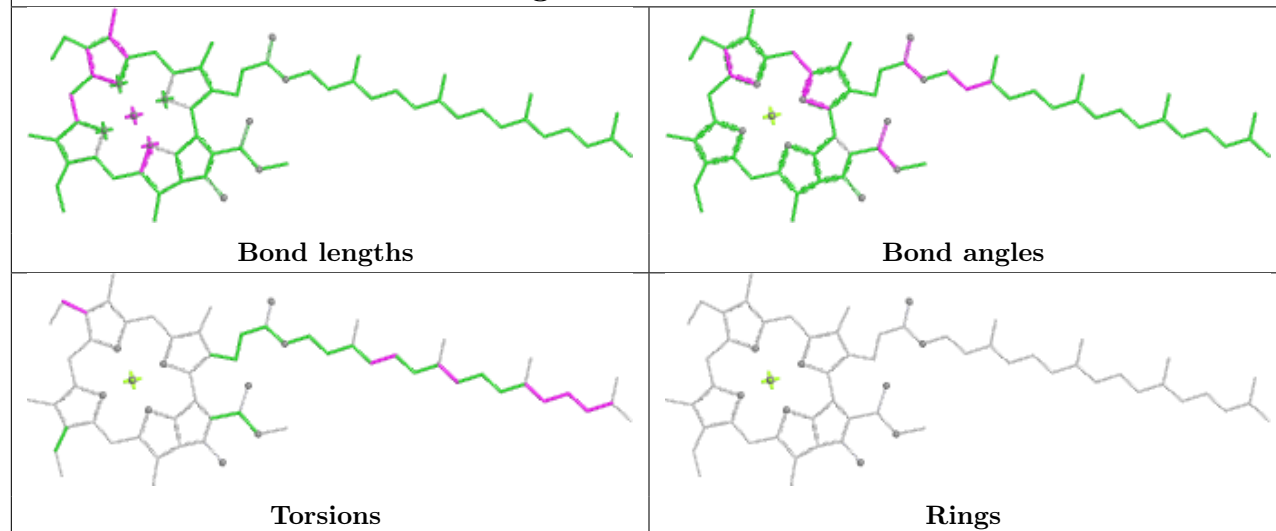
Ligand CLA A 812



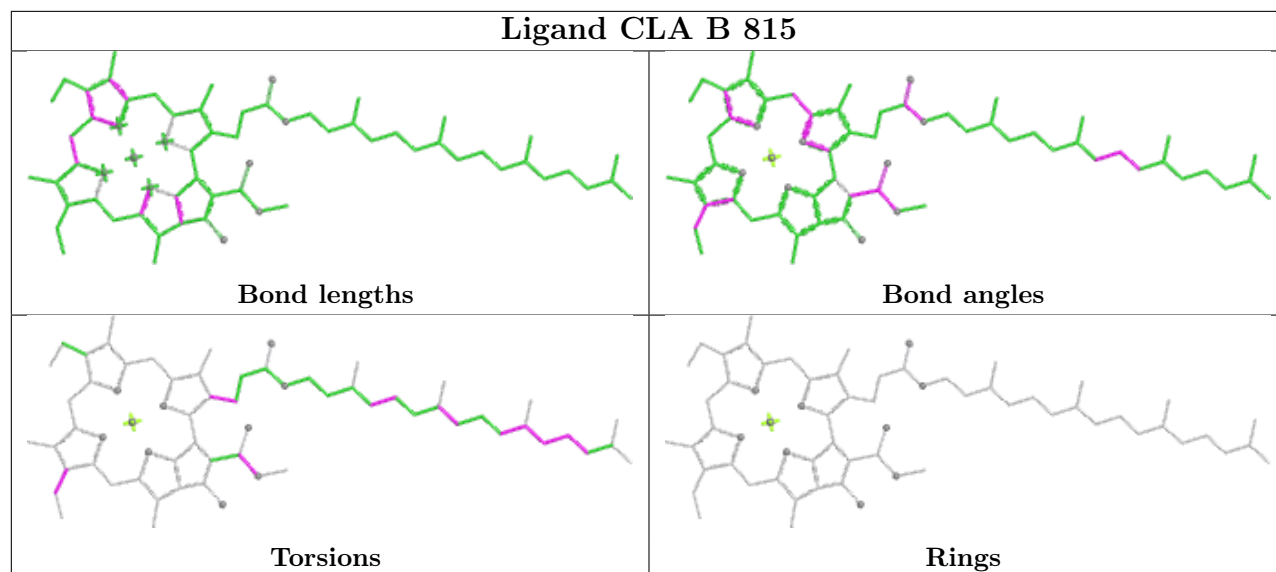
Ligand CLA A 815



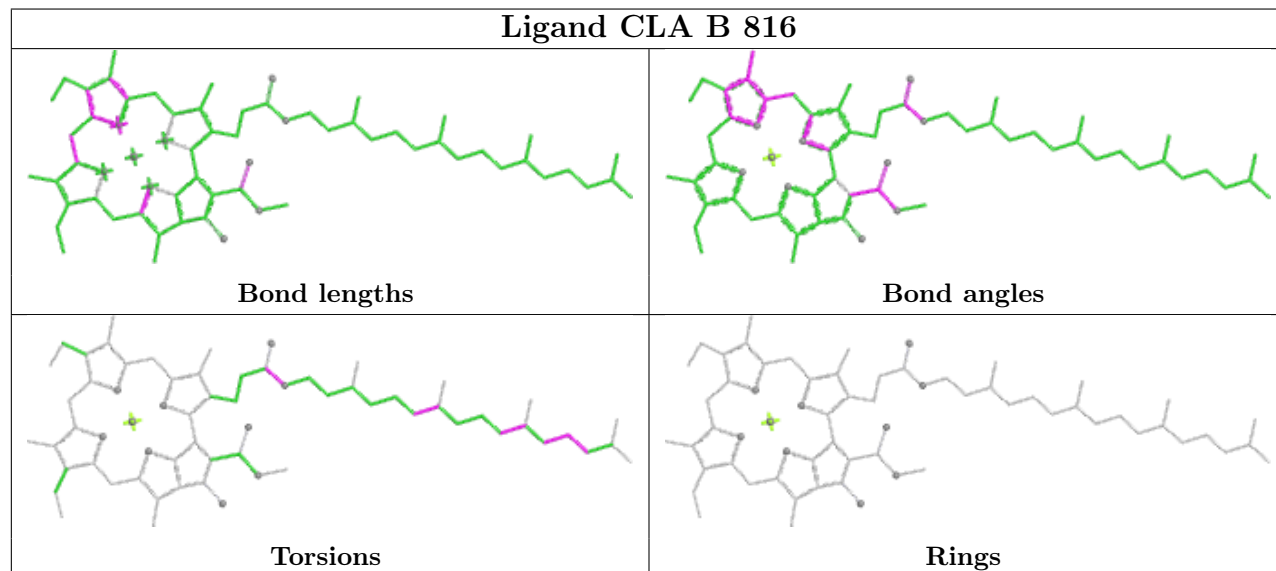
Ligand CLA A 820



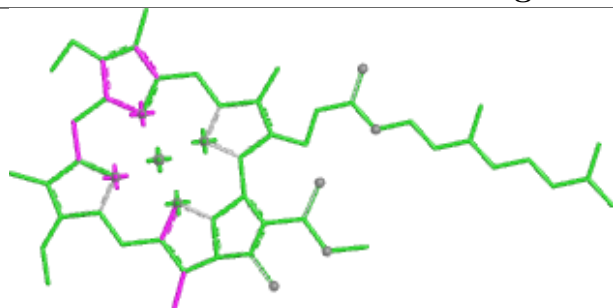
Ligand CLA B 815



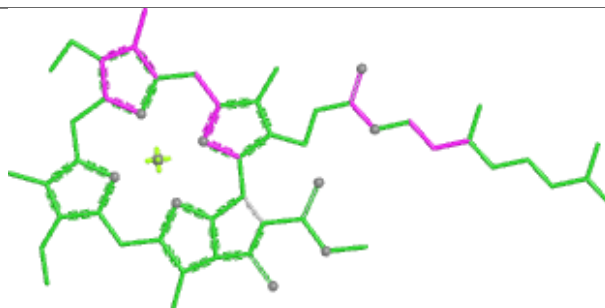
Ligand CLA B 816



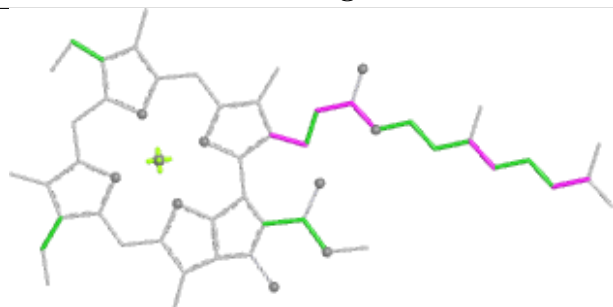
Ligand CLA B 824



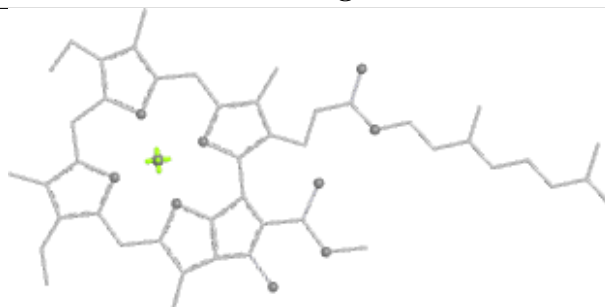
Bond lengths



Bond angles

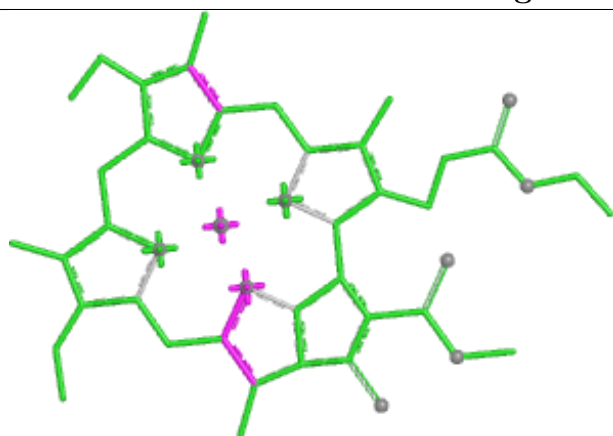


Torsions

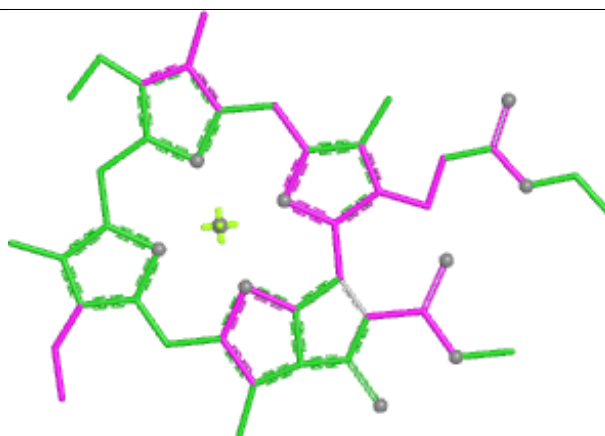


Rings

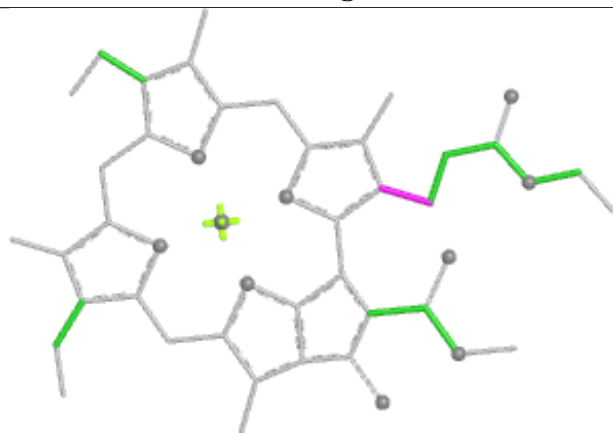
Ligand CLA B 839



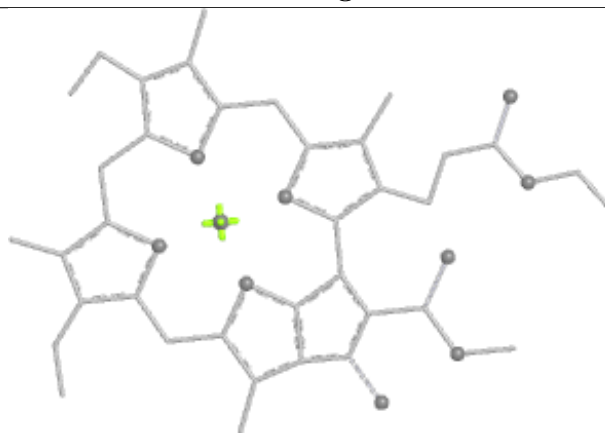
Bond lengths



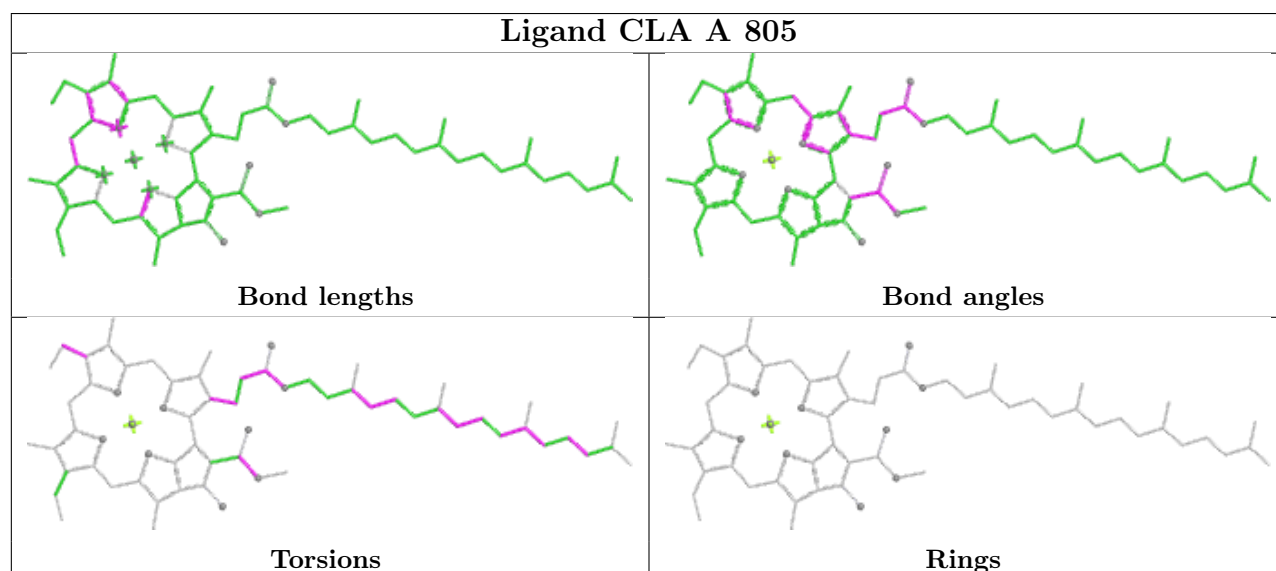
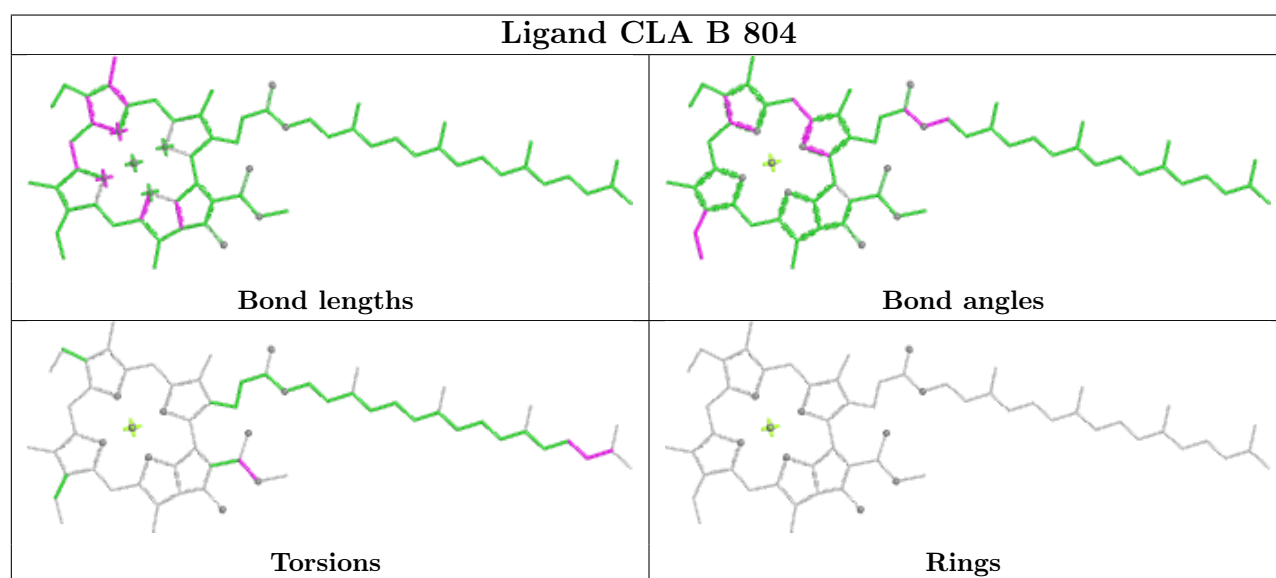
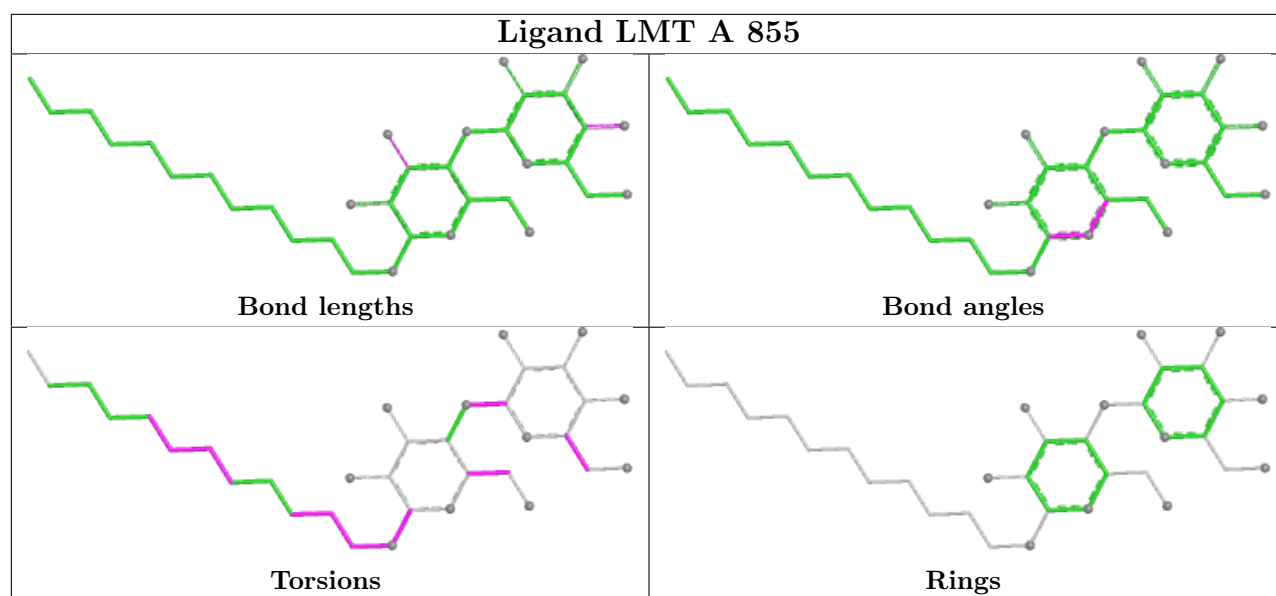
Bond angles



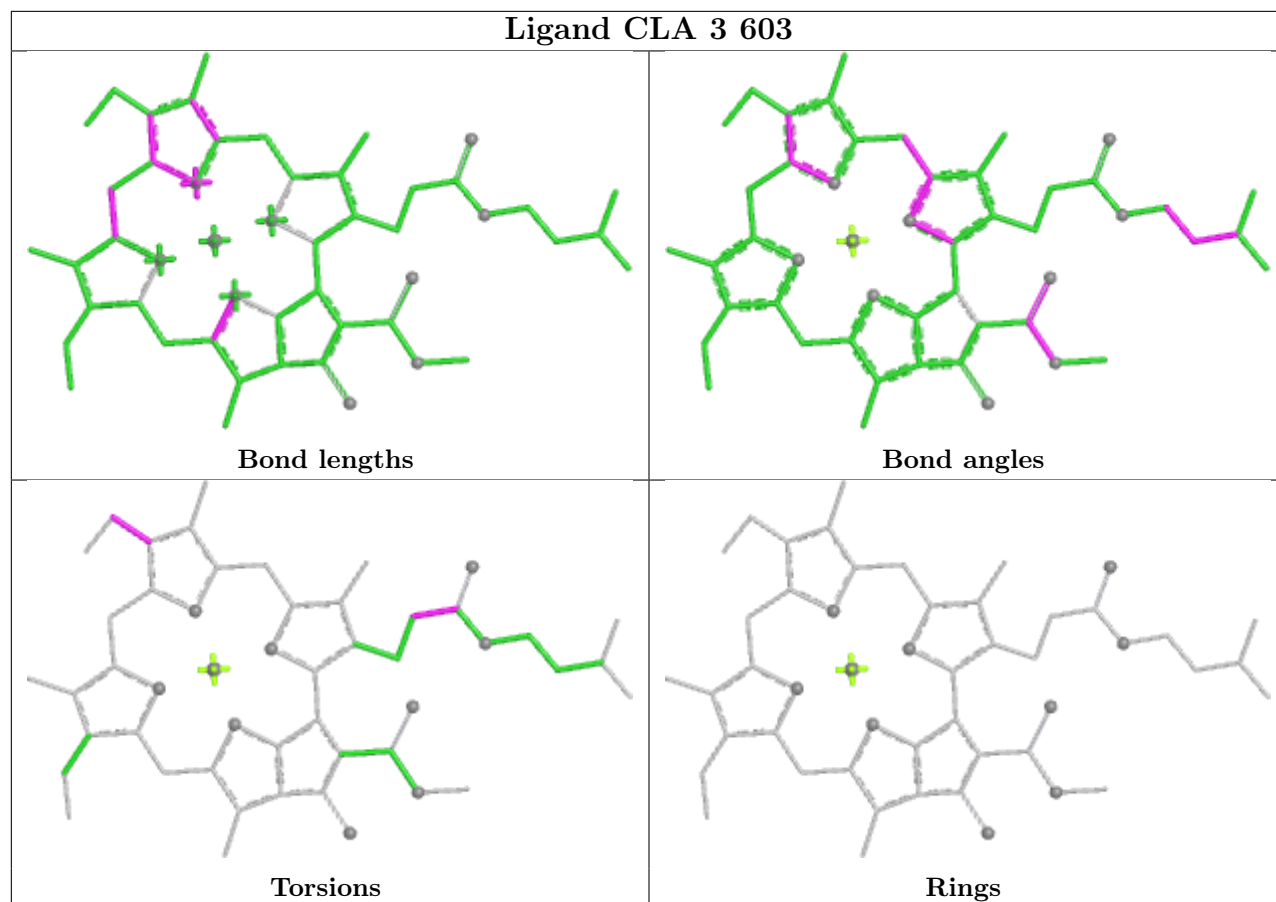
Torsions



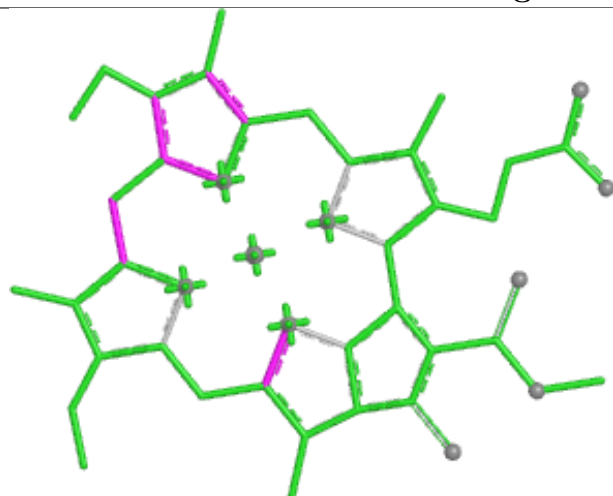
Rings



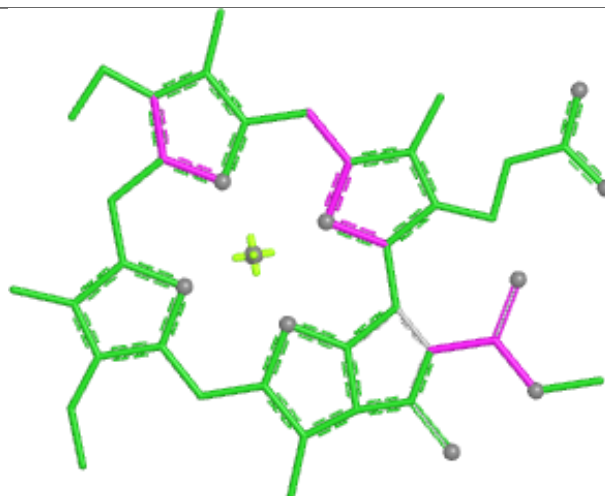
Ligand CLA 3 603



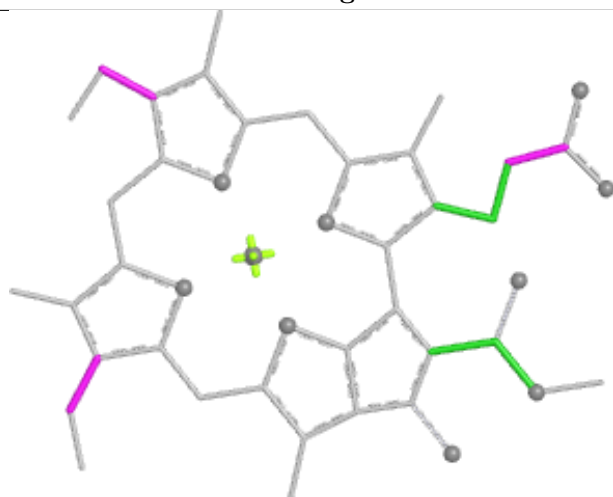
Ligand CLA A 819



Bond lengths



Bond angles

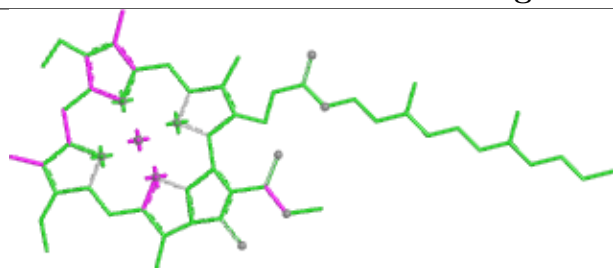


Torsions

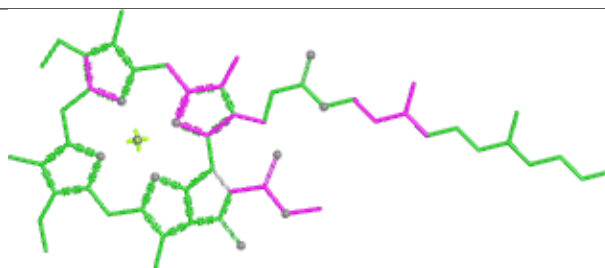


Rings

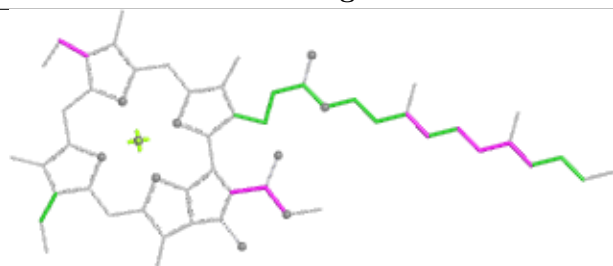
Ligand CLA B 834



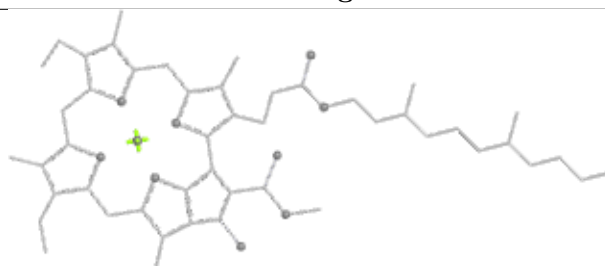
Bond lengths



Bond angles

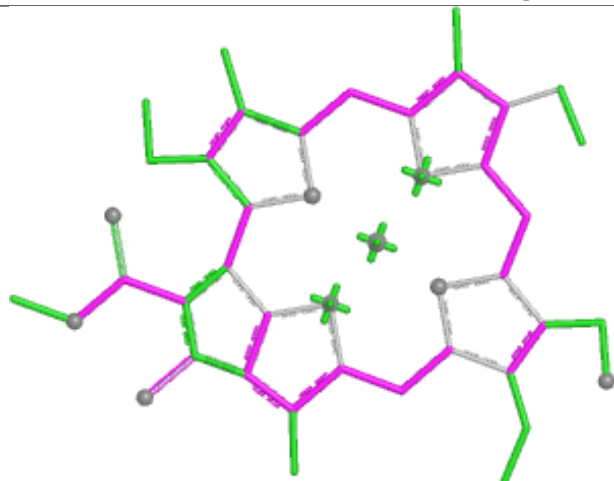


Torsions

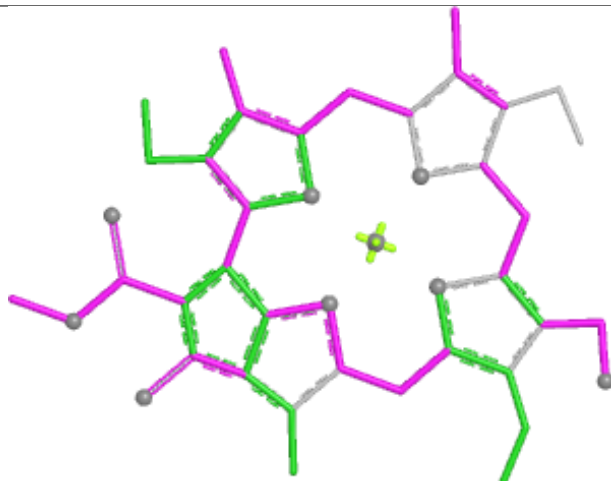


Rings

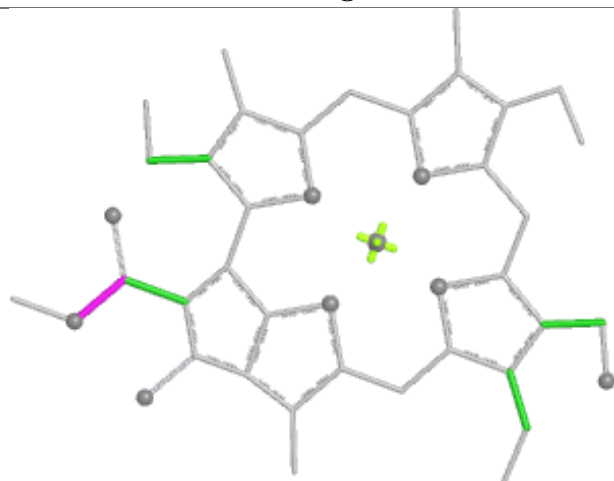
Ligand CHL 2 313



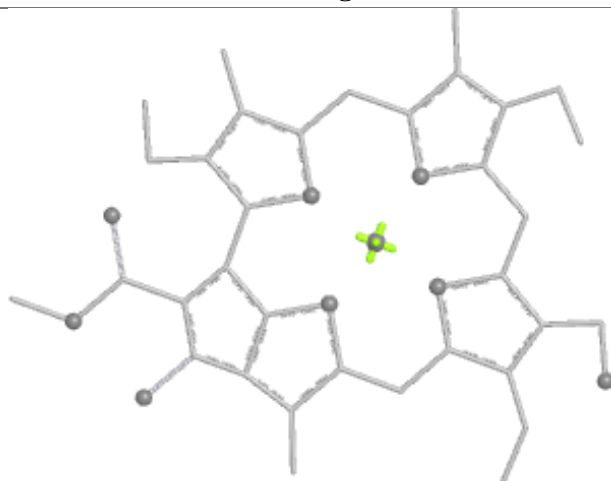
Bond lengths



Bond angles

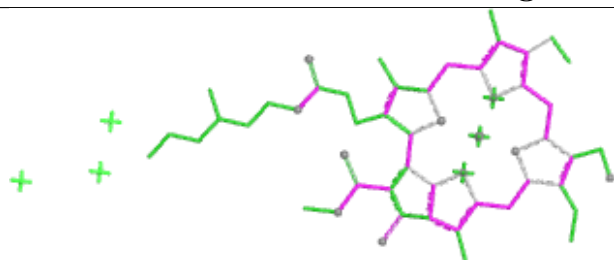


Torsions

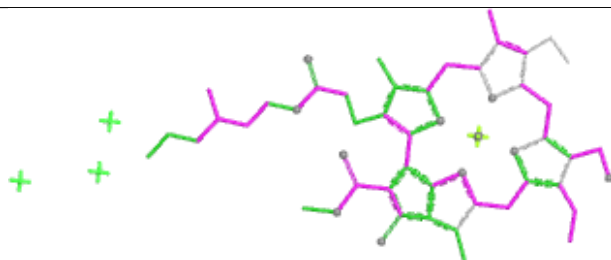


Rings

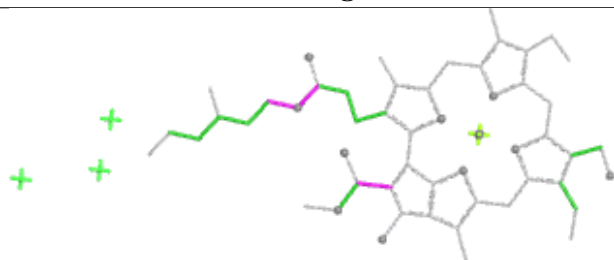
Ligand CHL 3 601



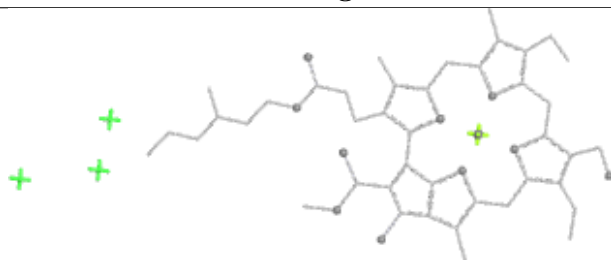
Bond lengths



Bond angles

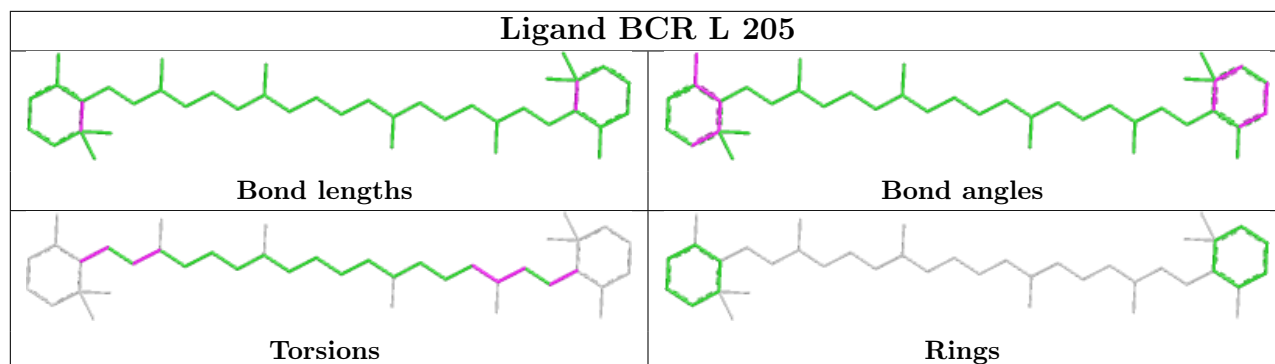


Torsions

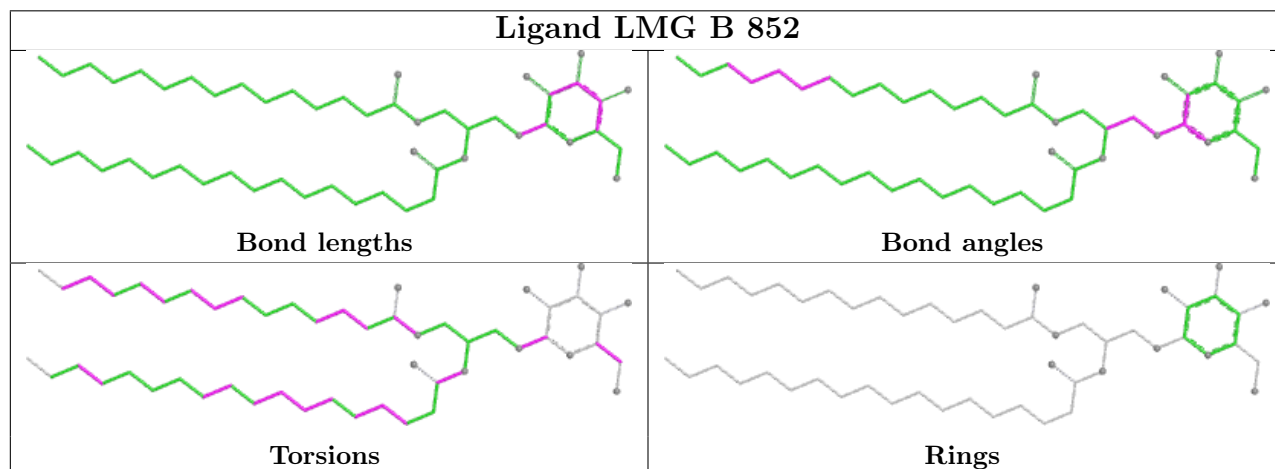


Rings

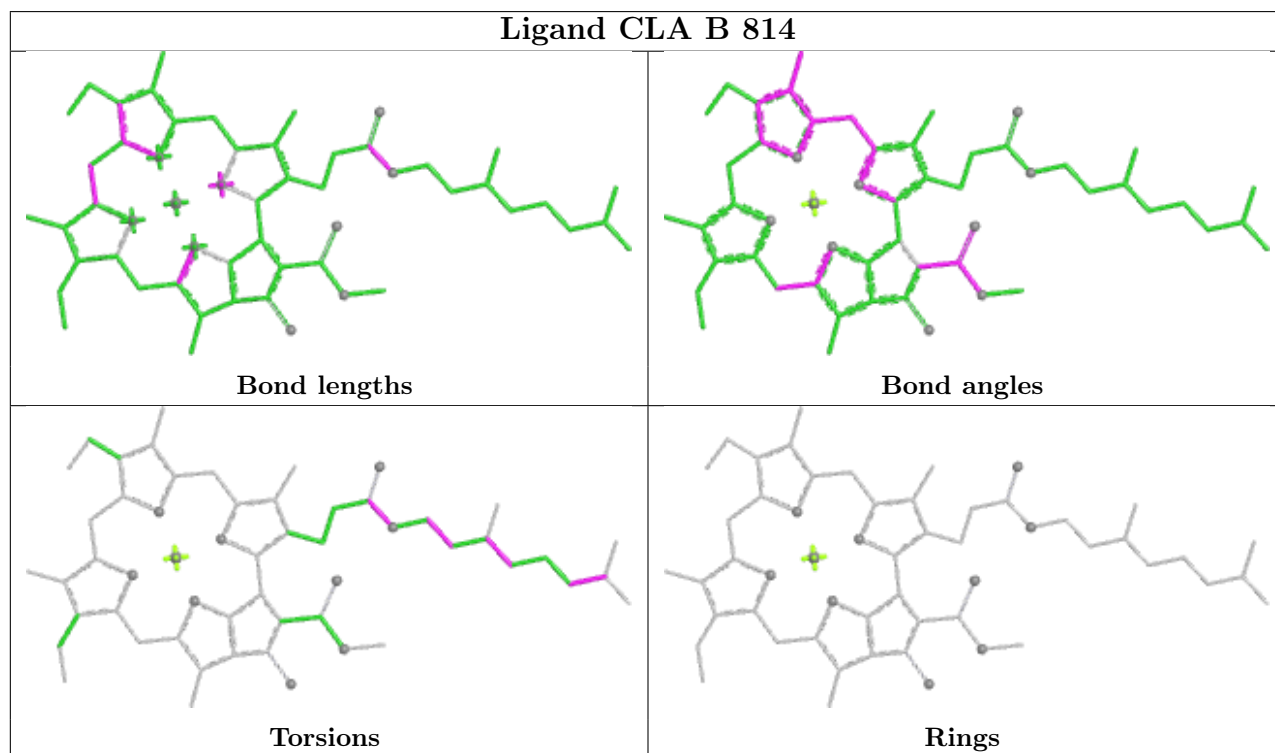
Ligand BCR L 205



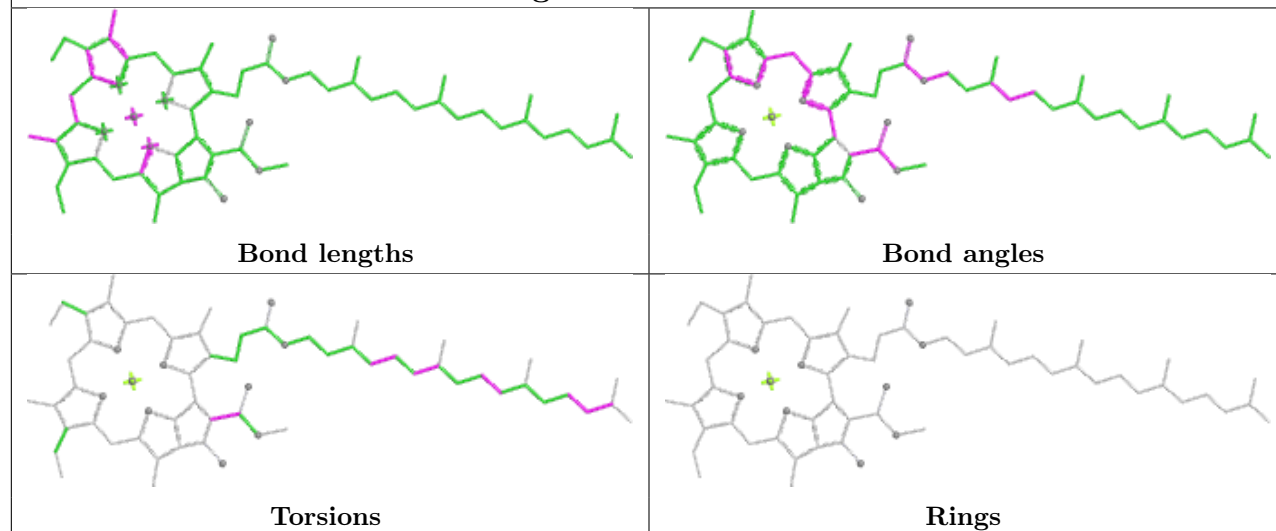
Ligand LMG B 852



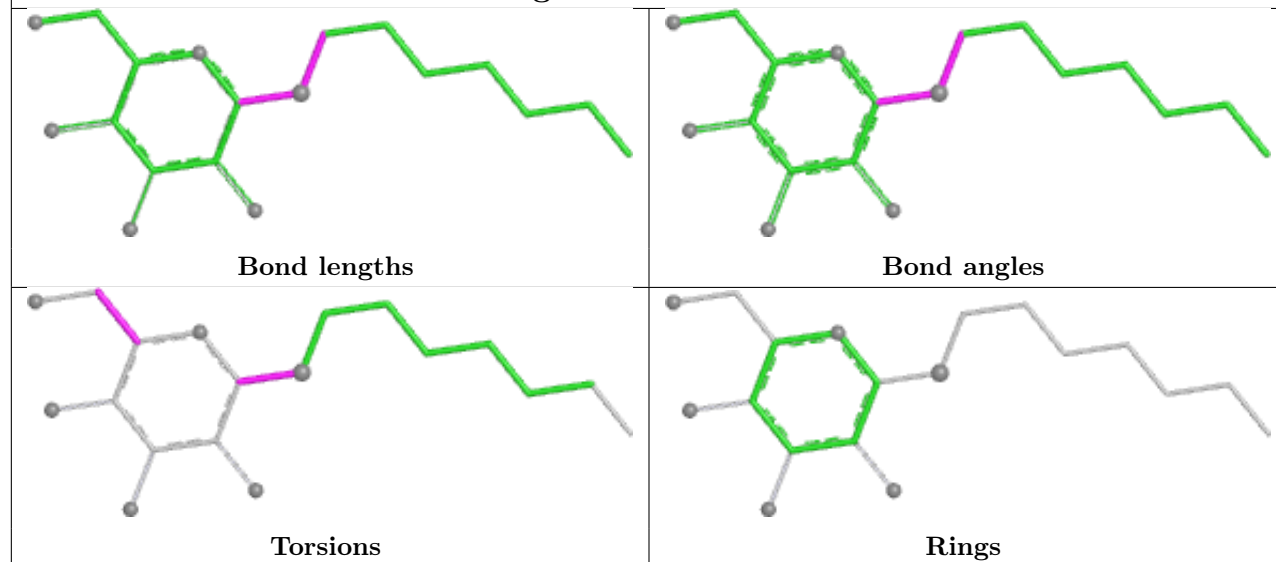
Ligand CLA B 814



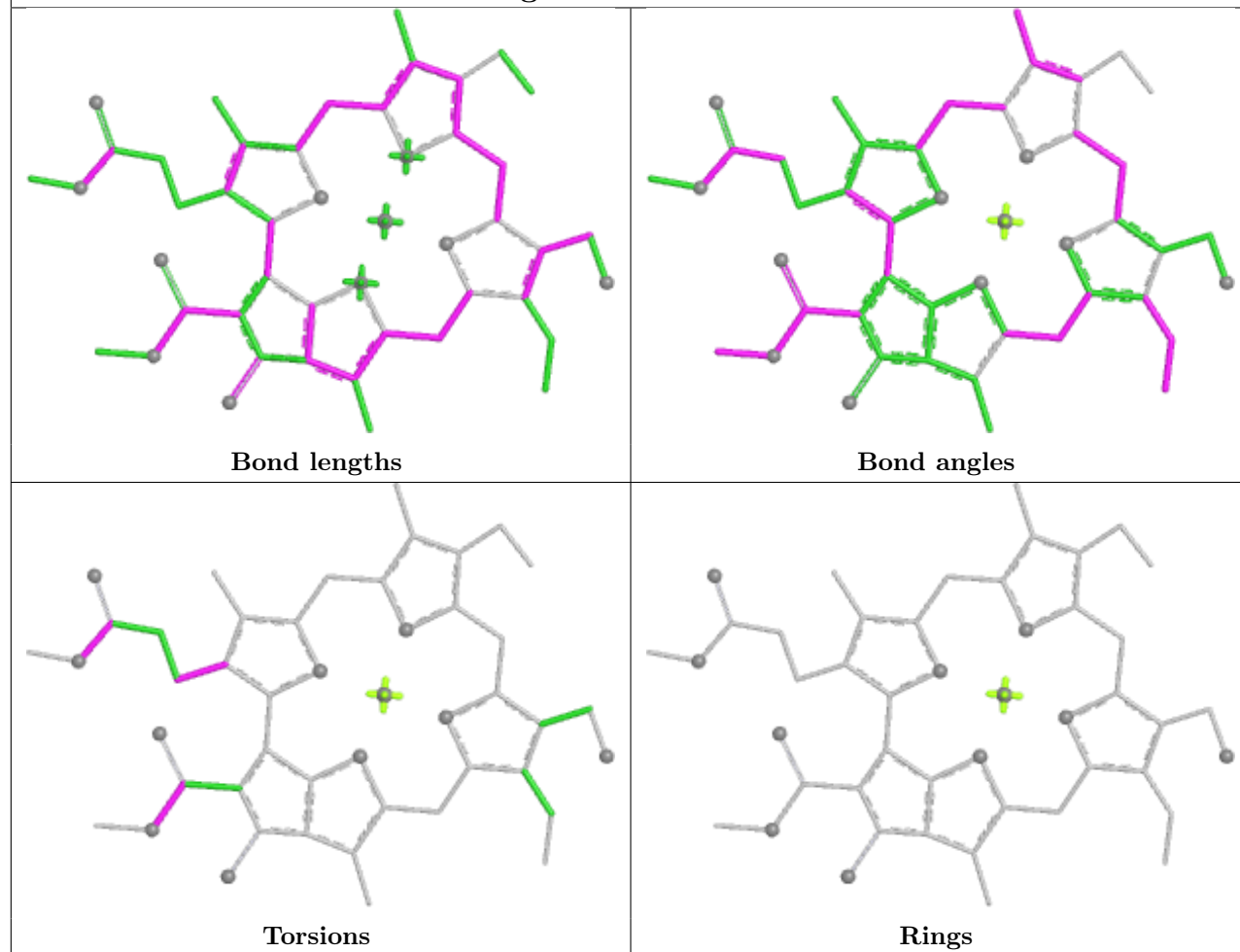
Ligand CLA B 810



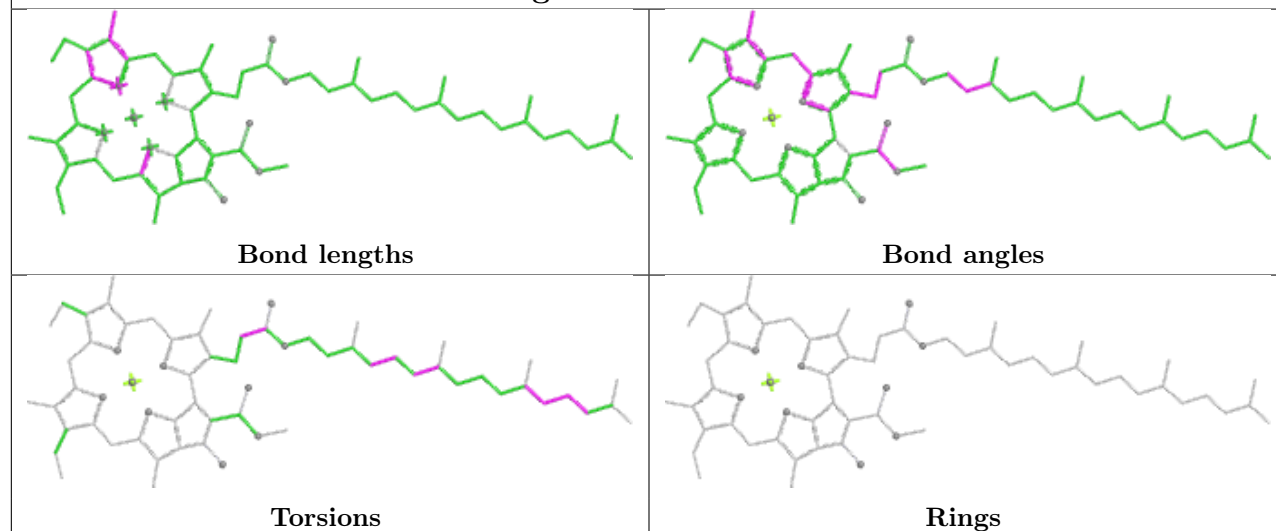
Ligand HTG 4 321

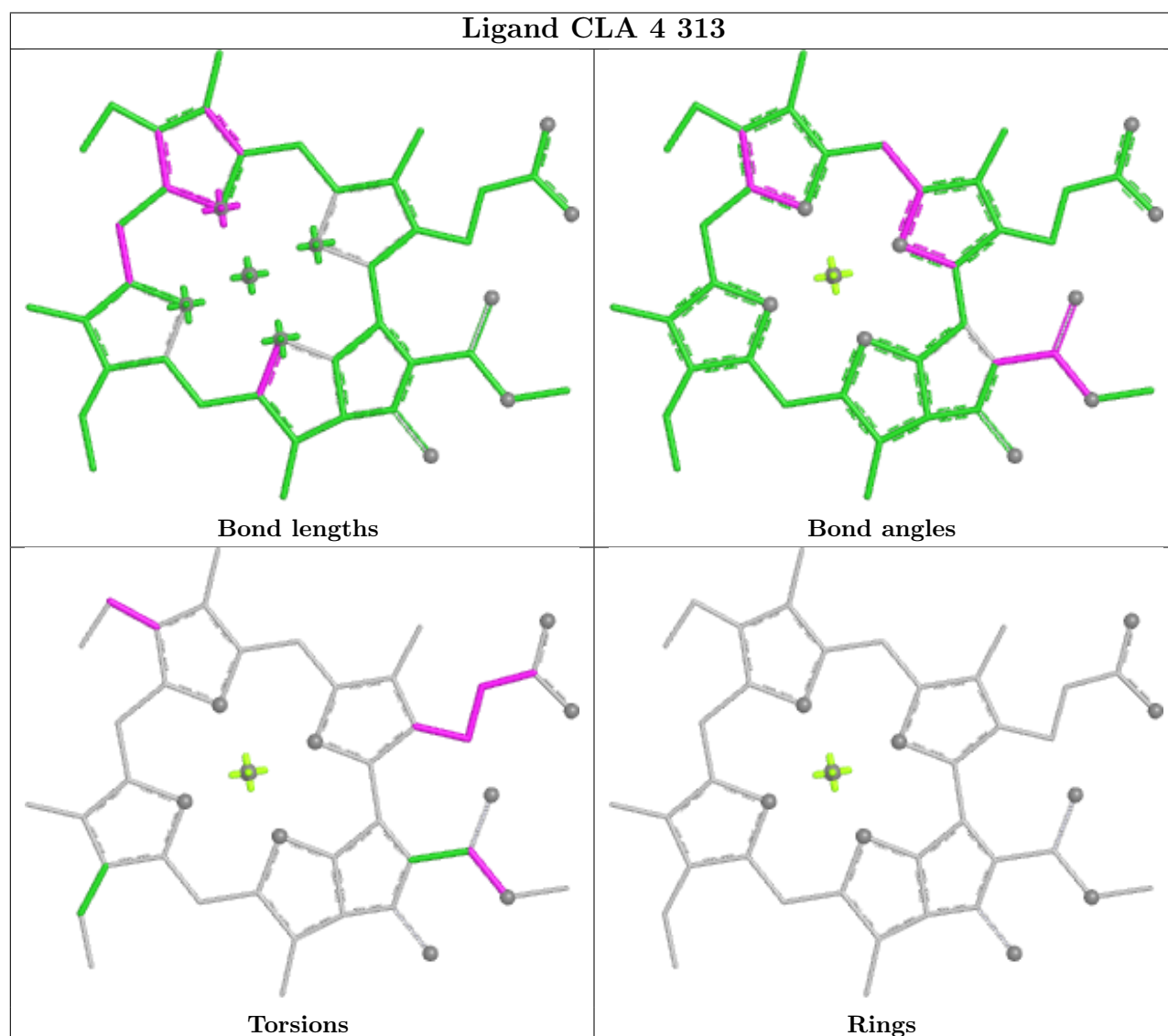
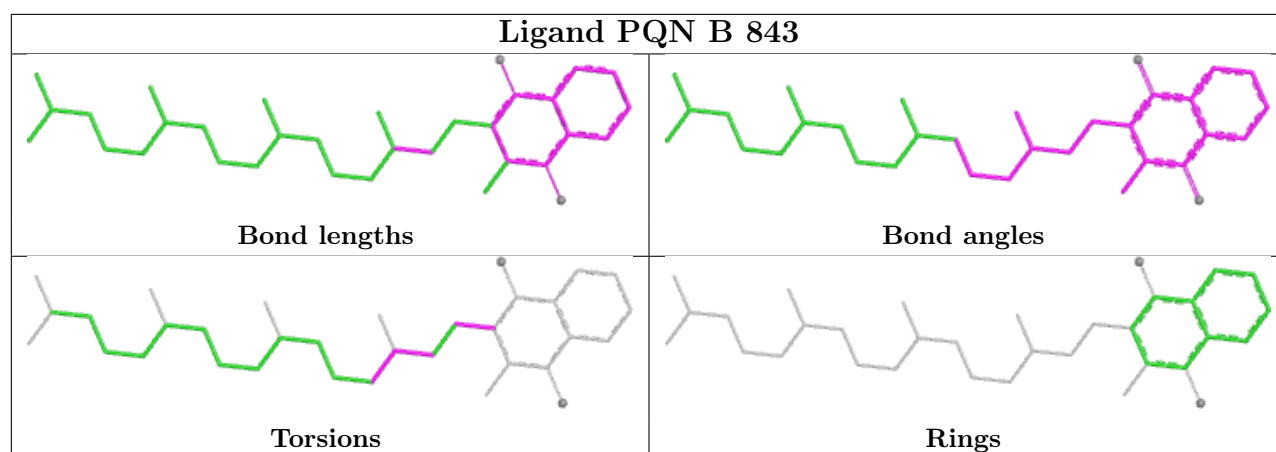


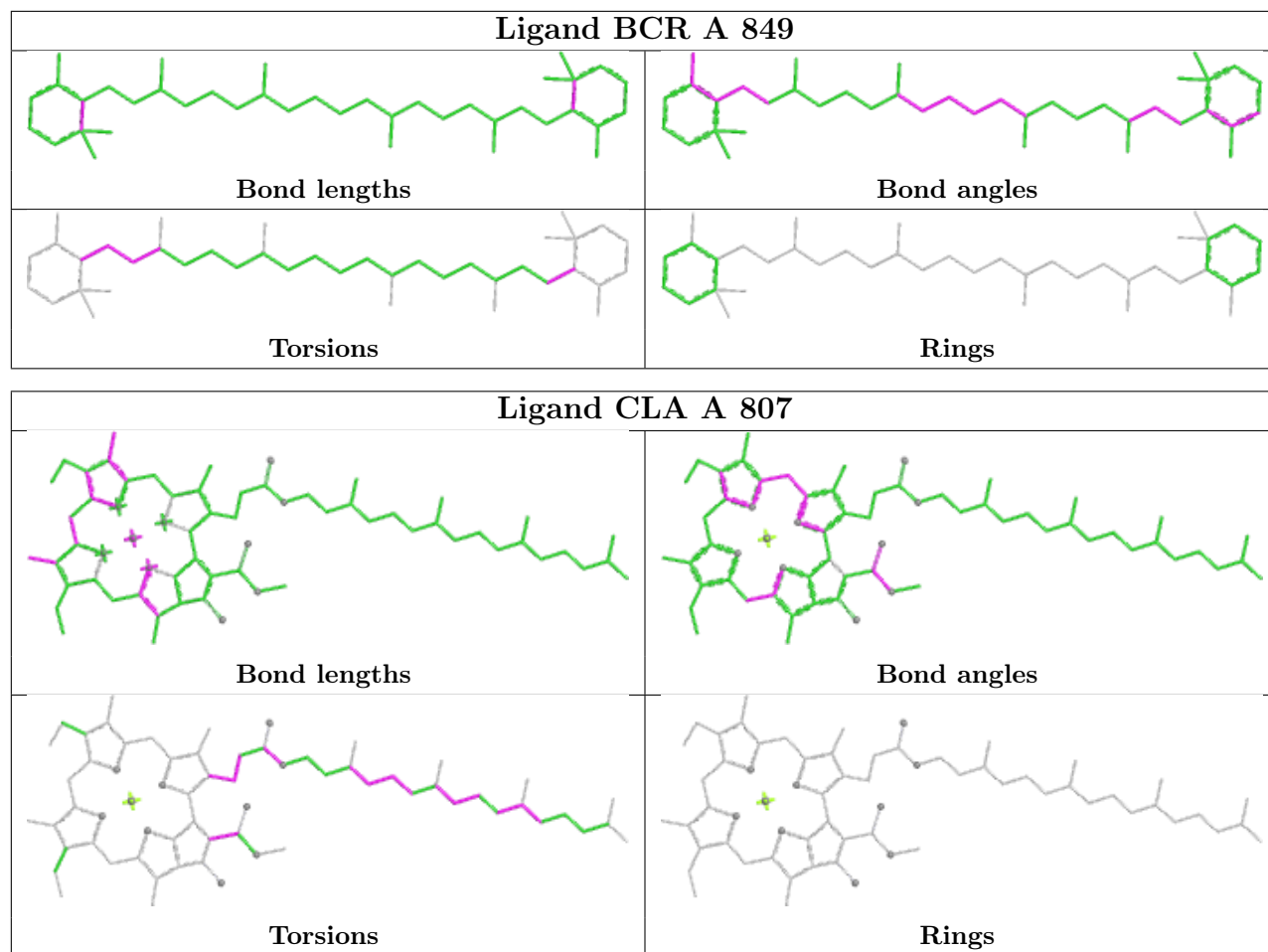
Ligand CHL 3 607



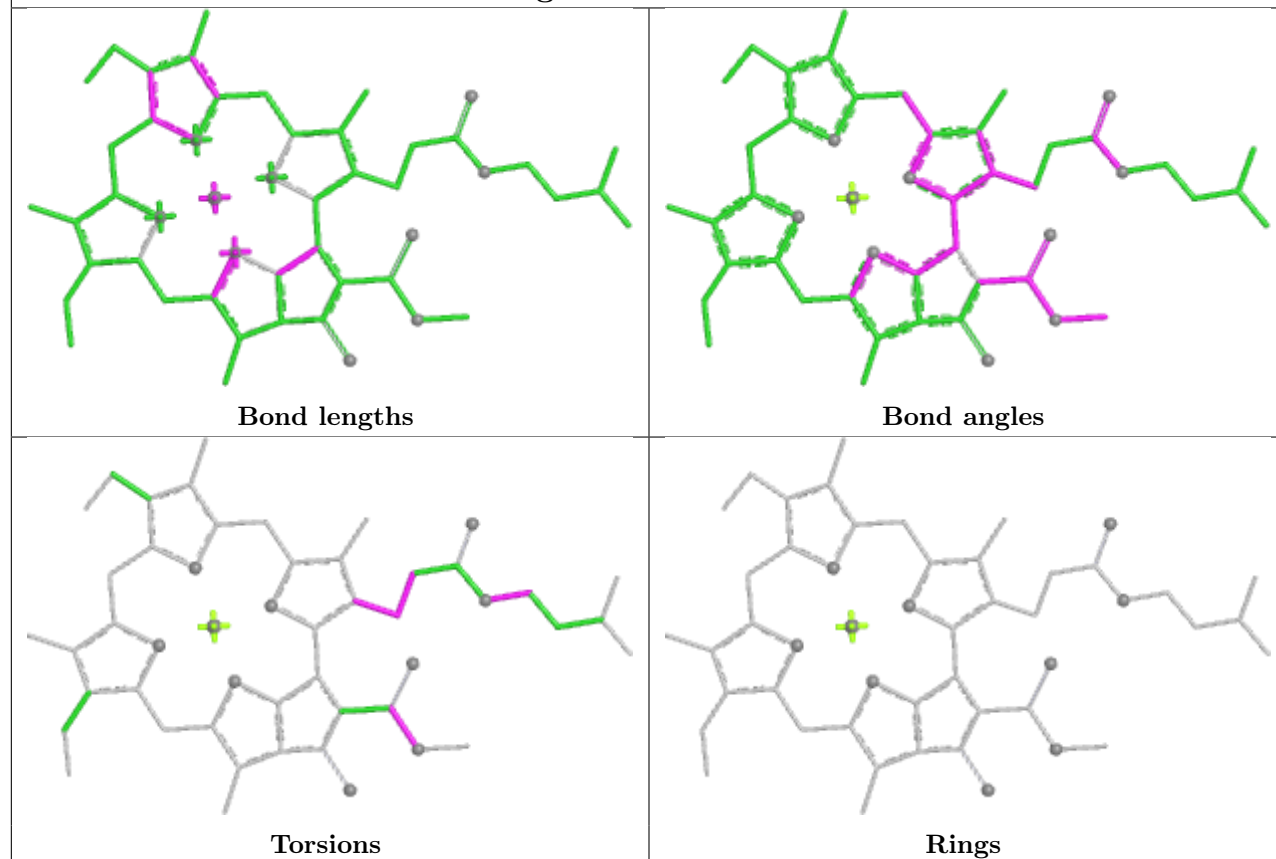
Ligand CLA B 811



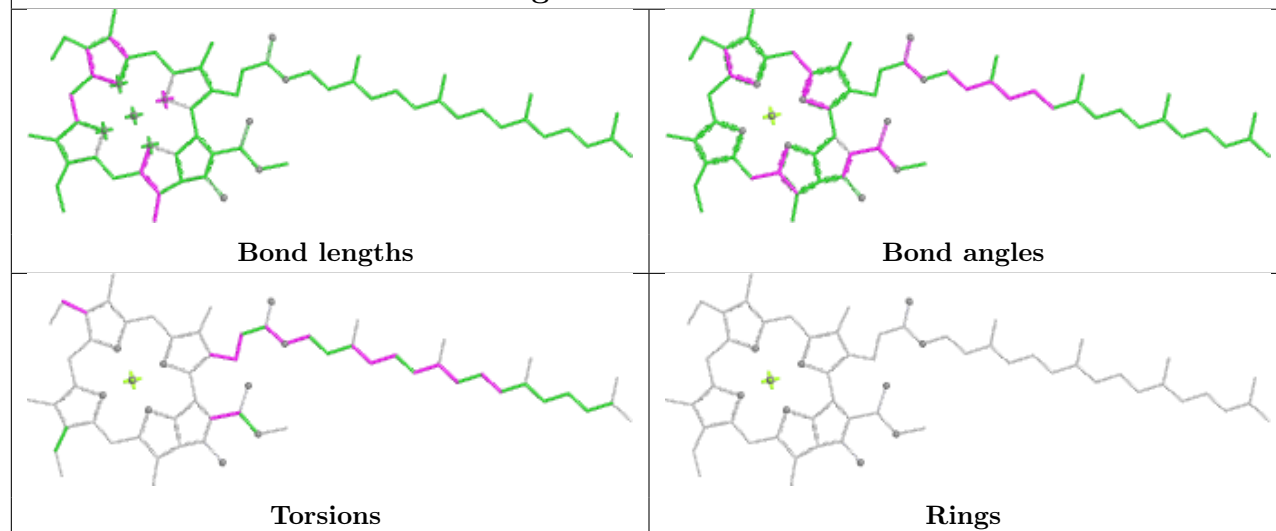




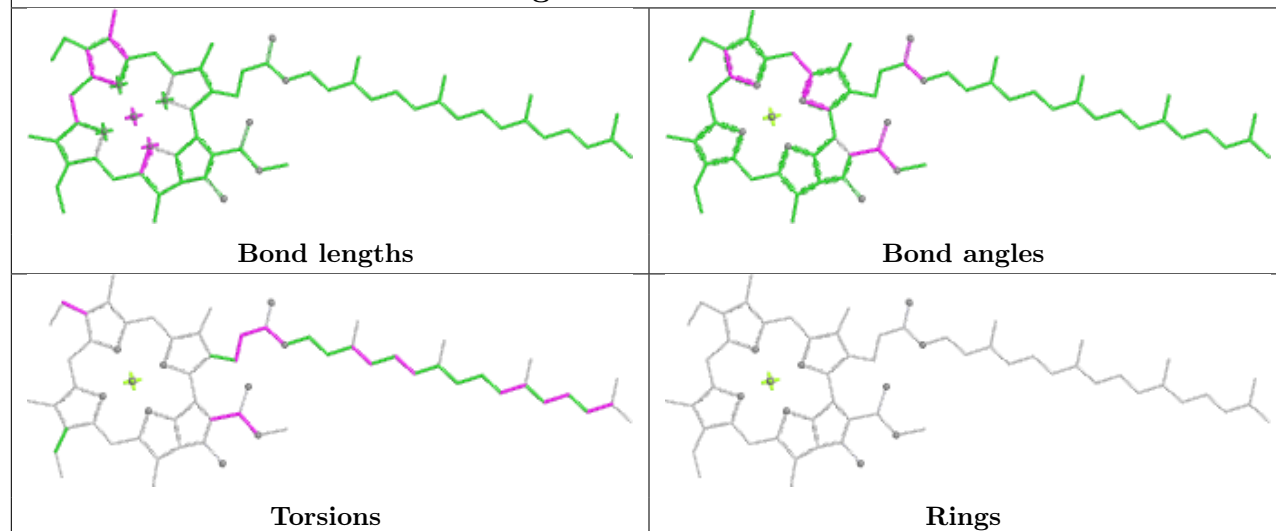
Ligand CLA 4 304



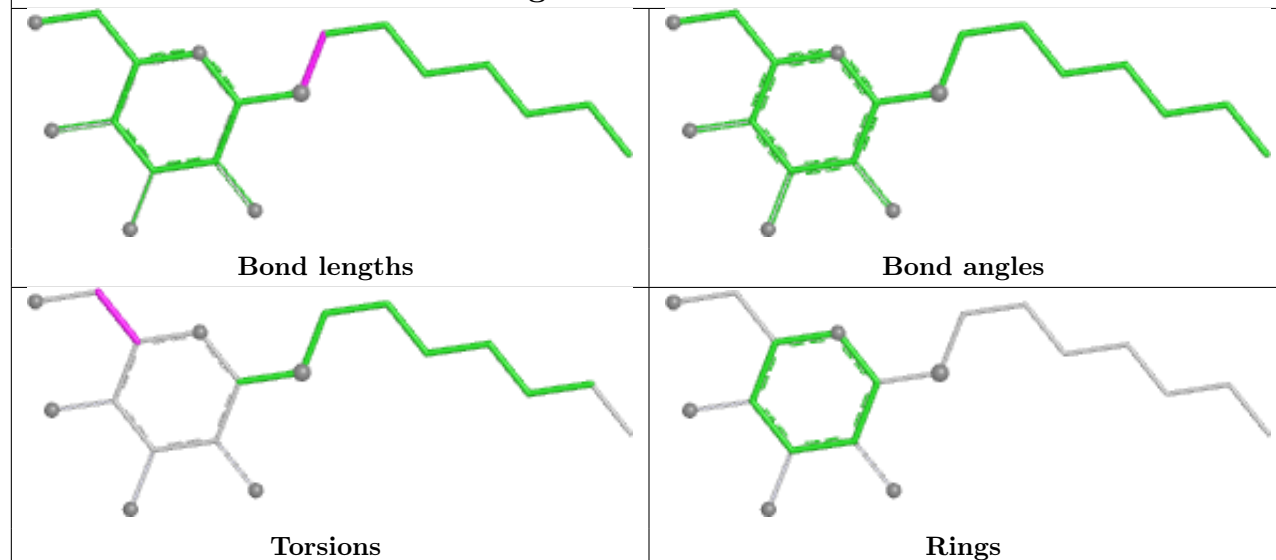
Ligand CLA A 840



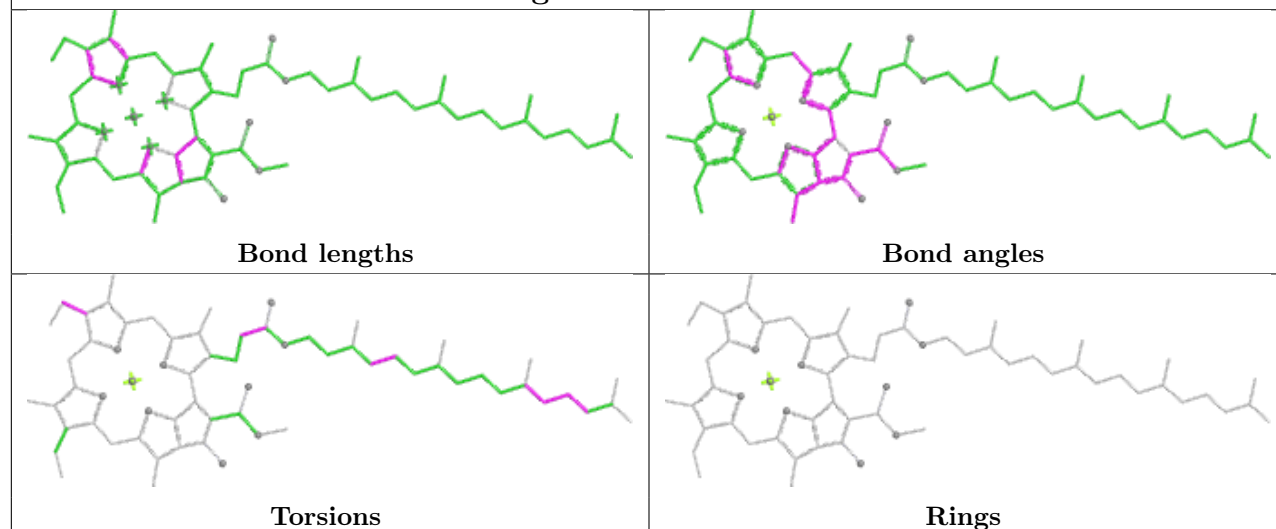
Ligand CLA B 812



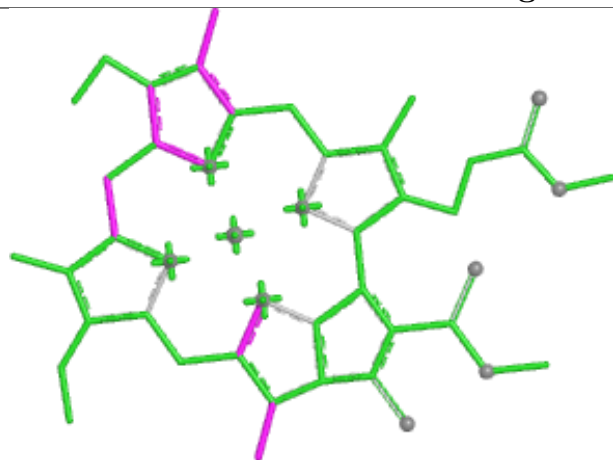
Ligand HTG A 854



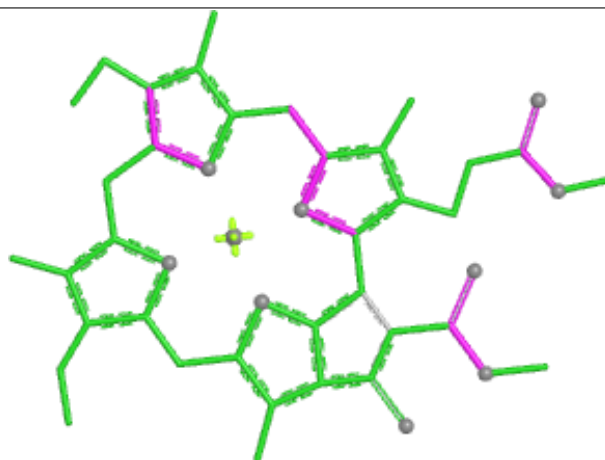
Ligand CLA A 801



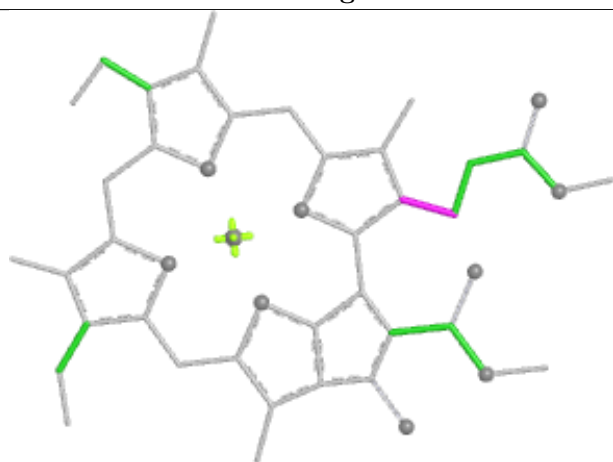
Ligand CLA 1 306



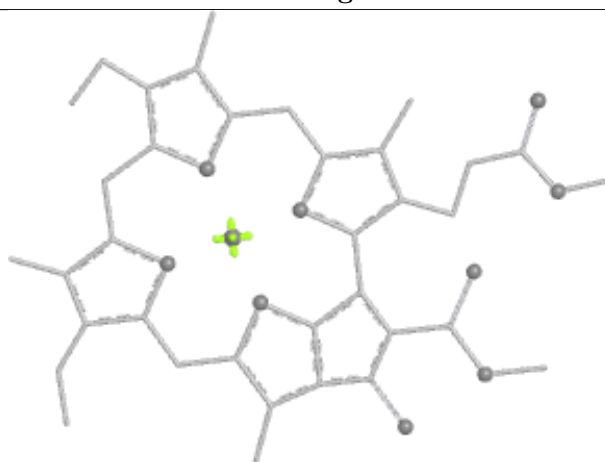
Bond lengths



Bond angles

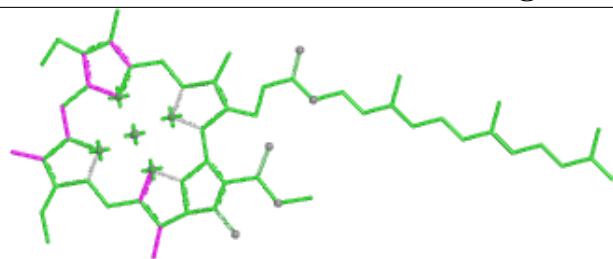


Torsions

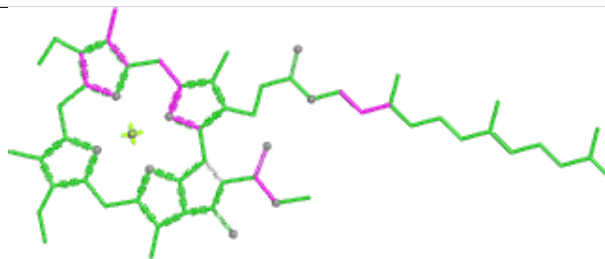


Rings

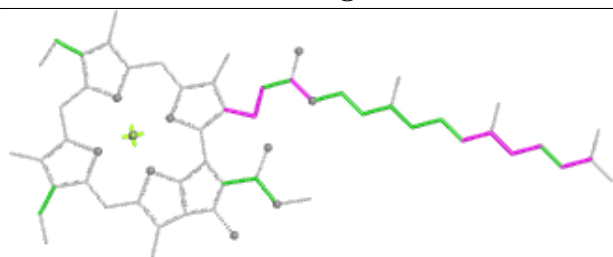
Ligand CLA 2 308



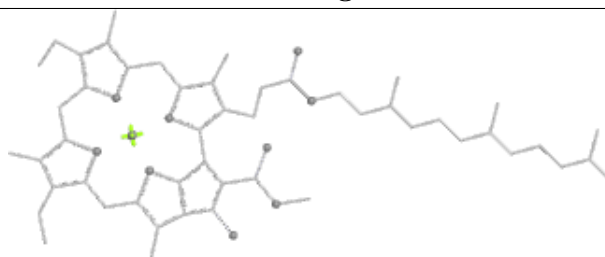
Bond lengths



Bond angles

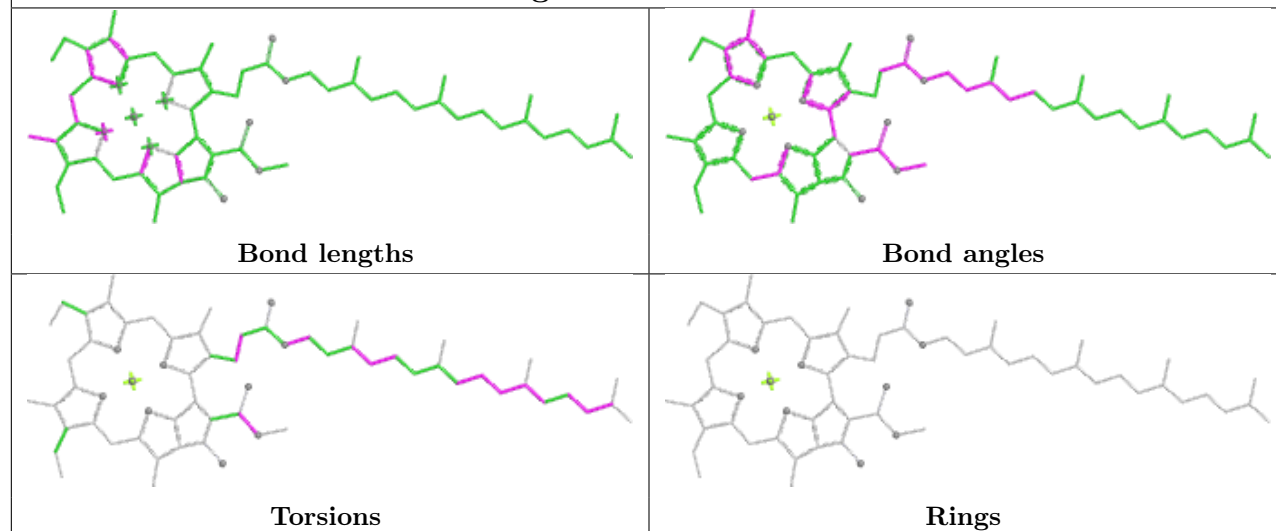


Torsions

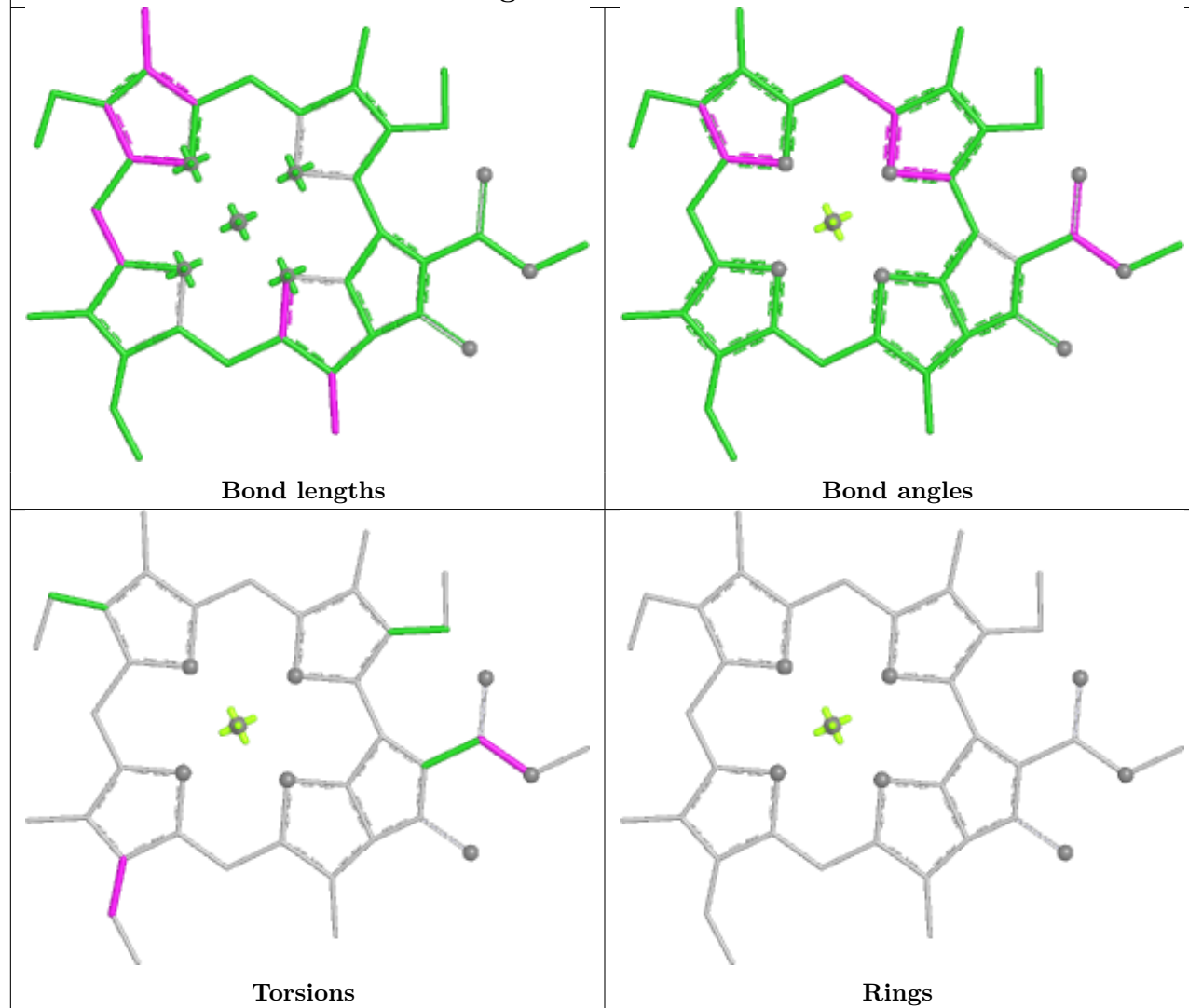


Rings

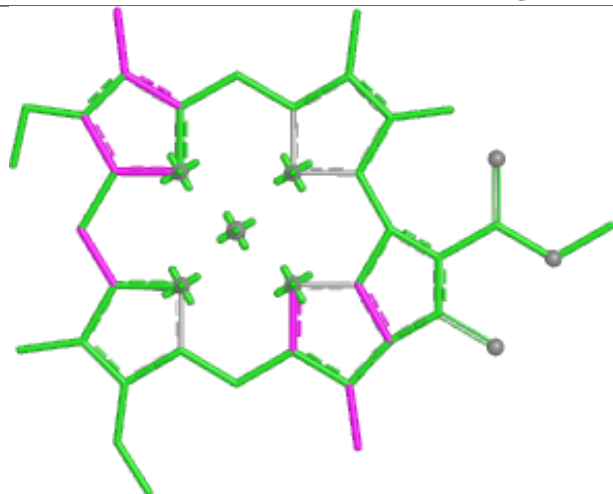
Ligand CLA A 853



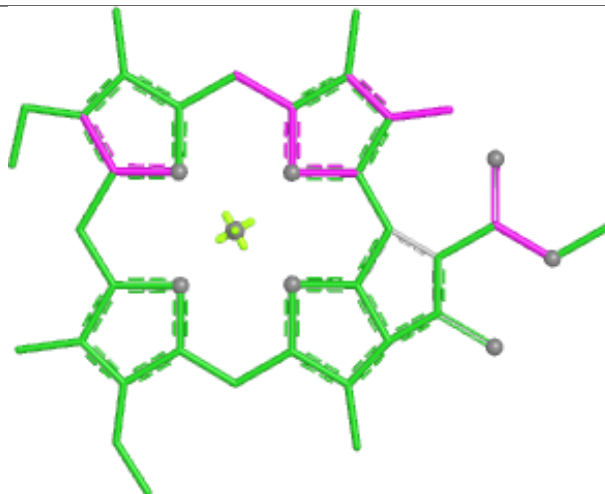
Ligand CLA 1 304



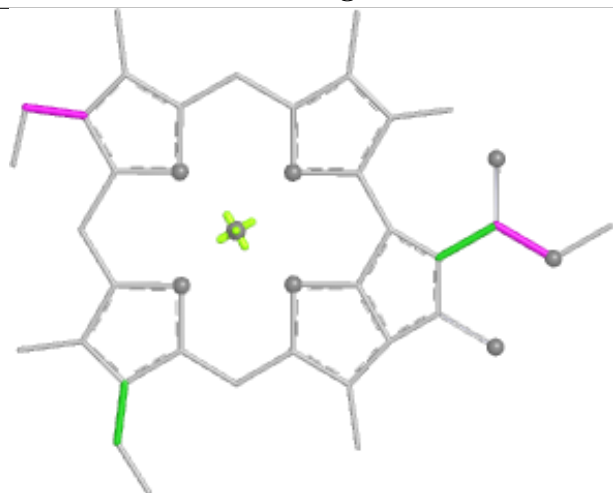
Ligand CLA G 103



Bond lengths



Bond angles

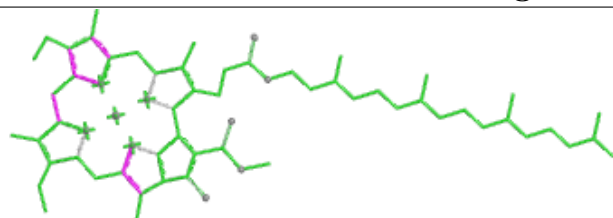


Torsions

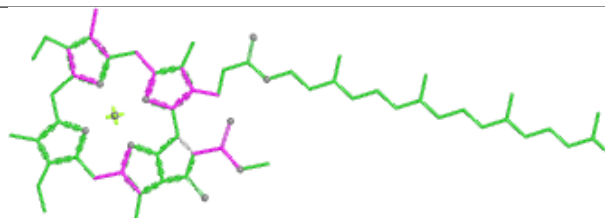


Rings

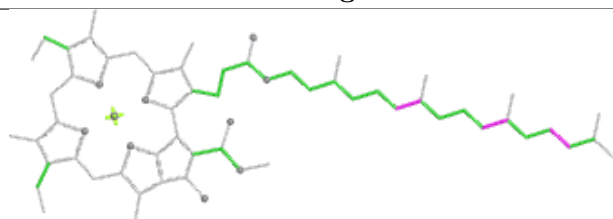
Ligand CLA A 825



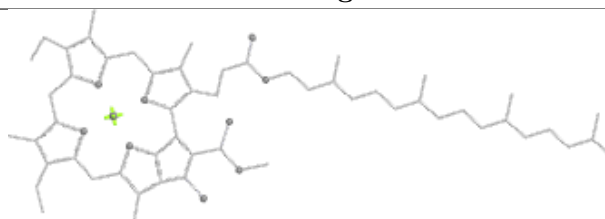
Bond lengths



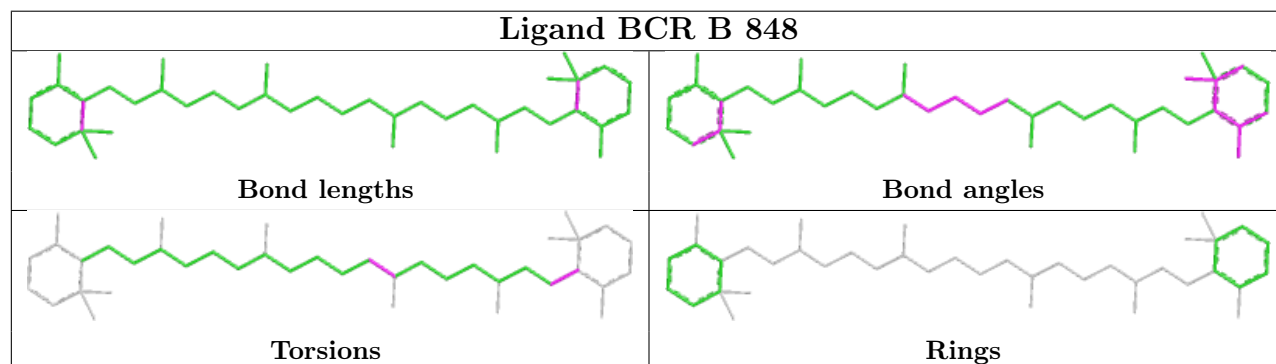
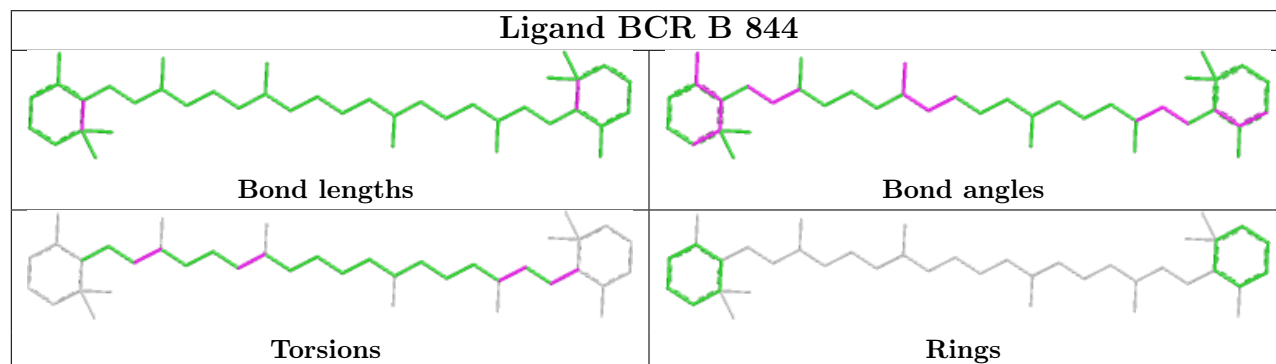
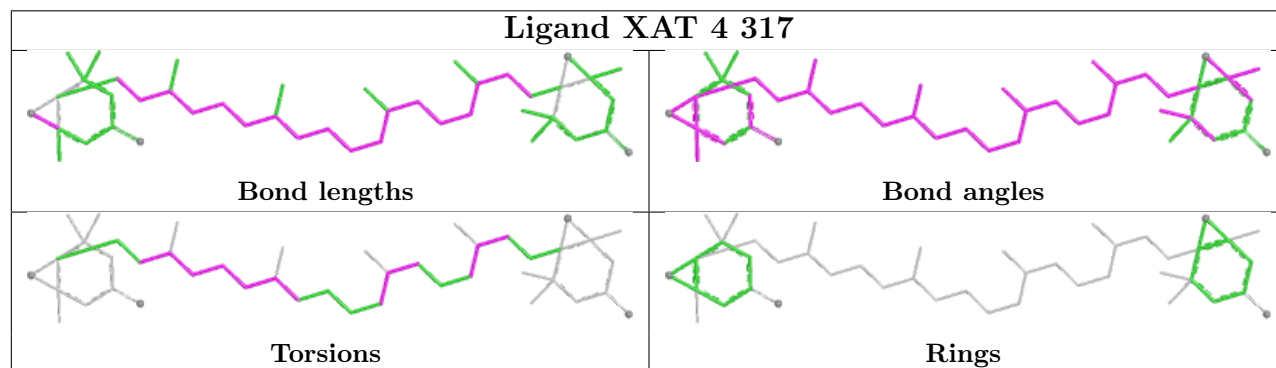
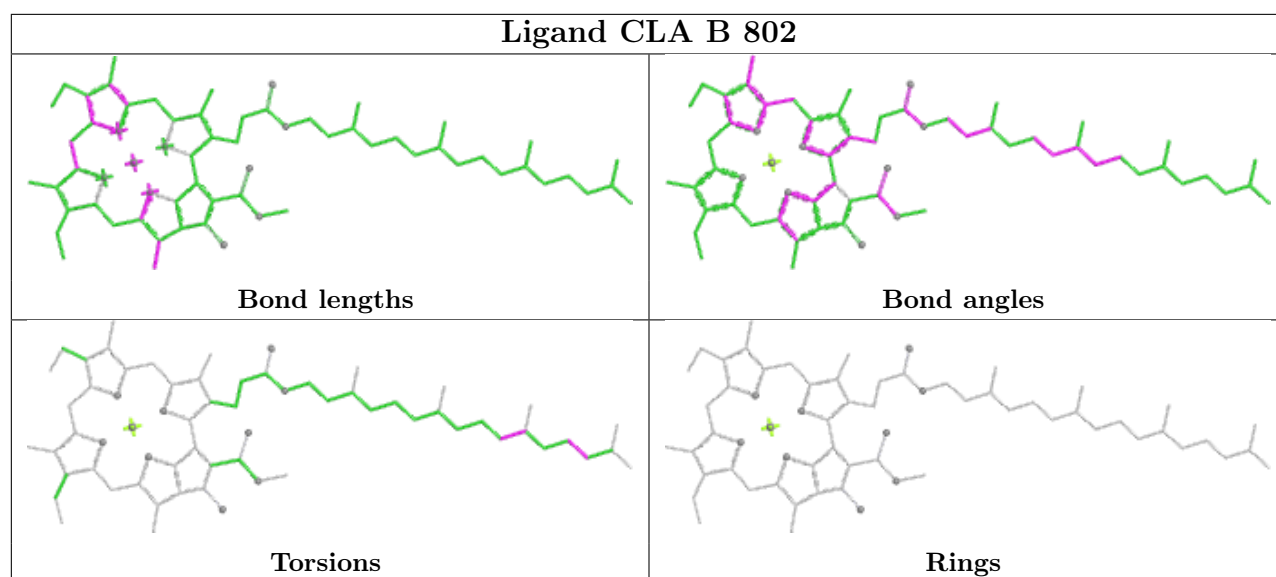
Bond angles

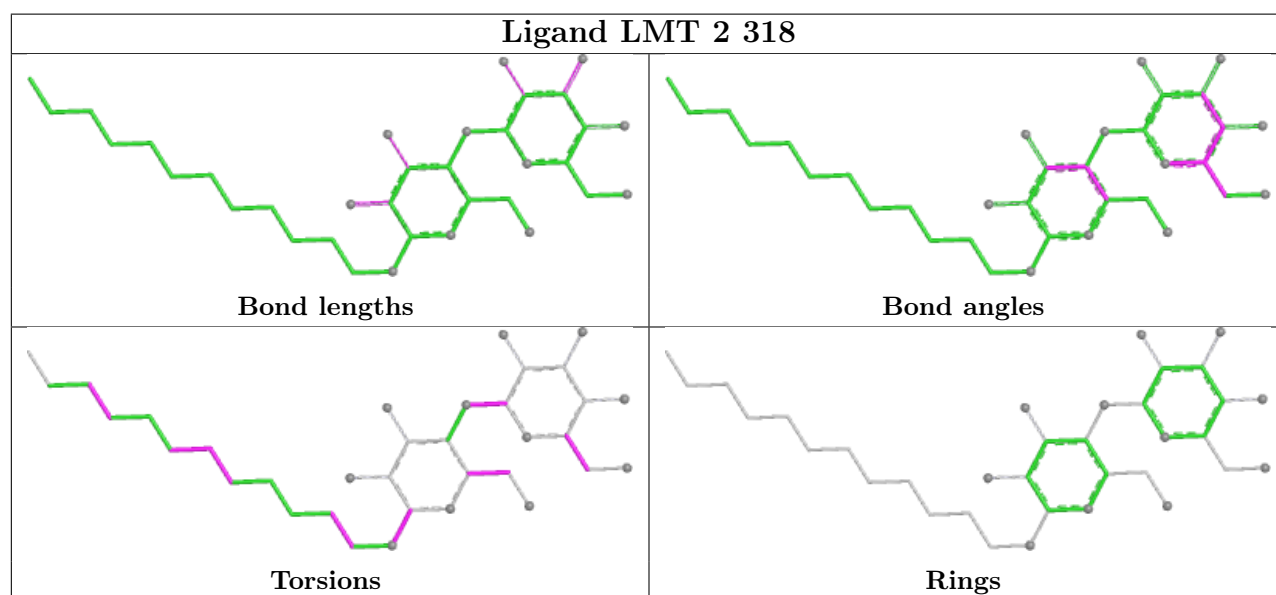
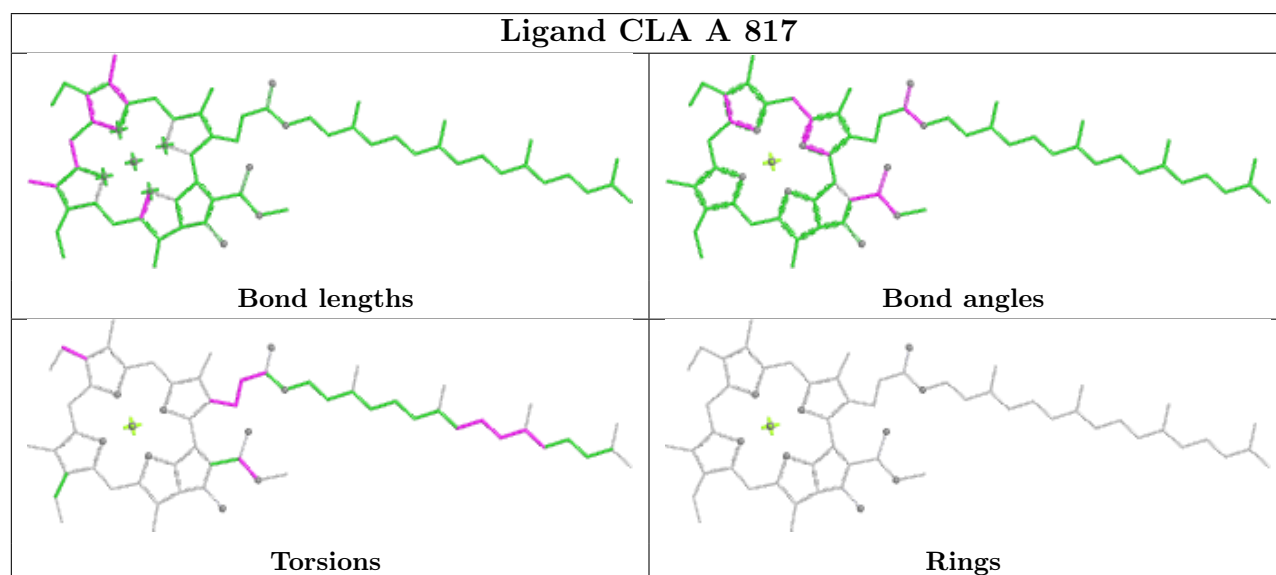
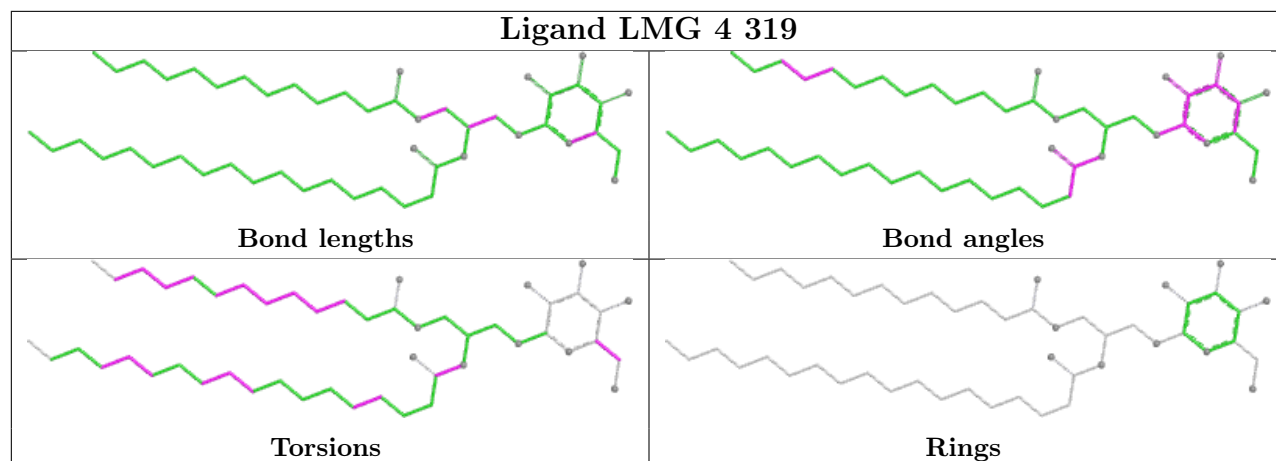


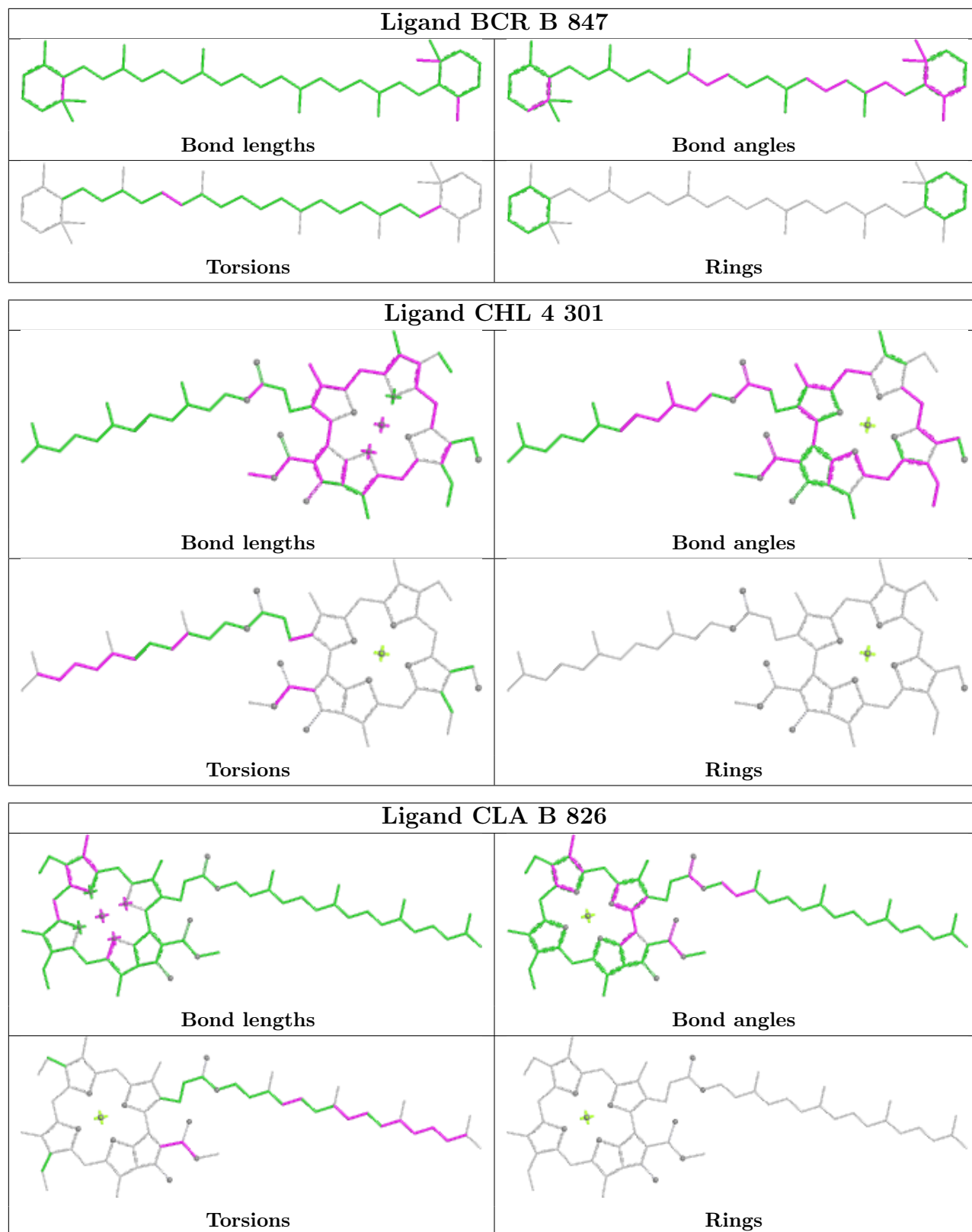
Torsions



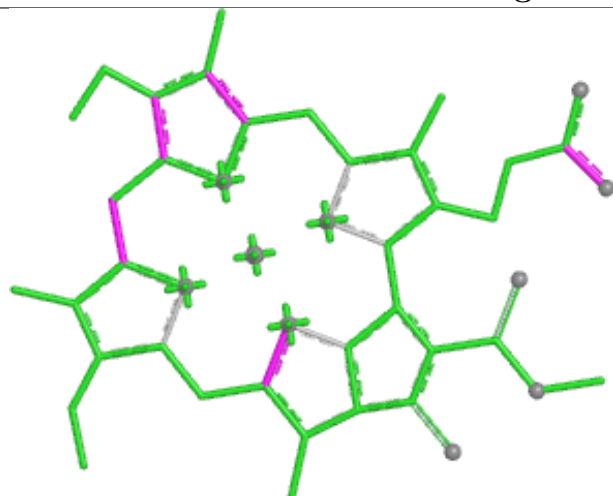
Rings



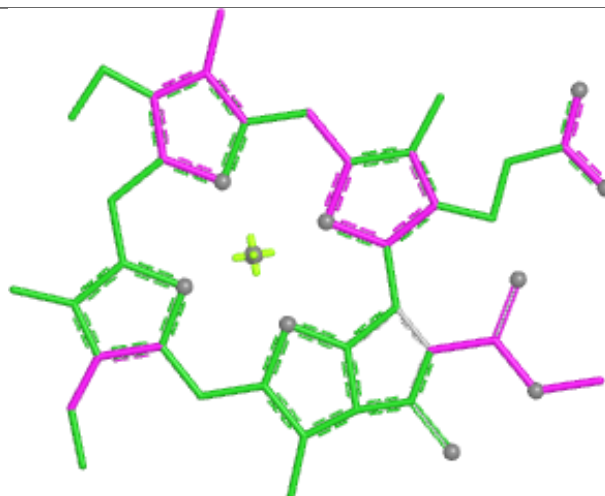




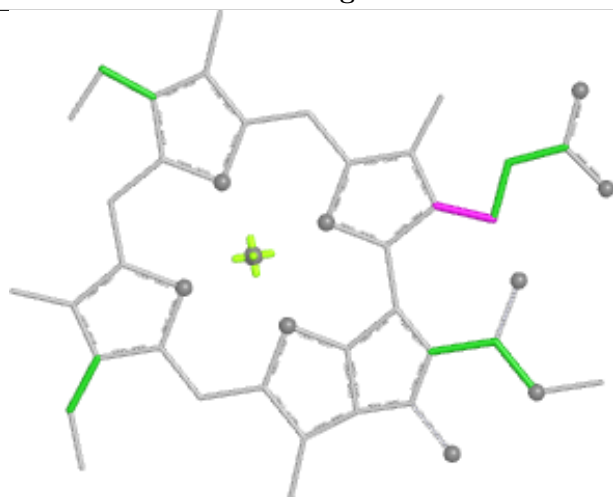
Ligand CLA B 806



Bond lengths



Bond angles

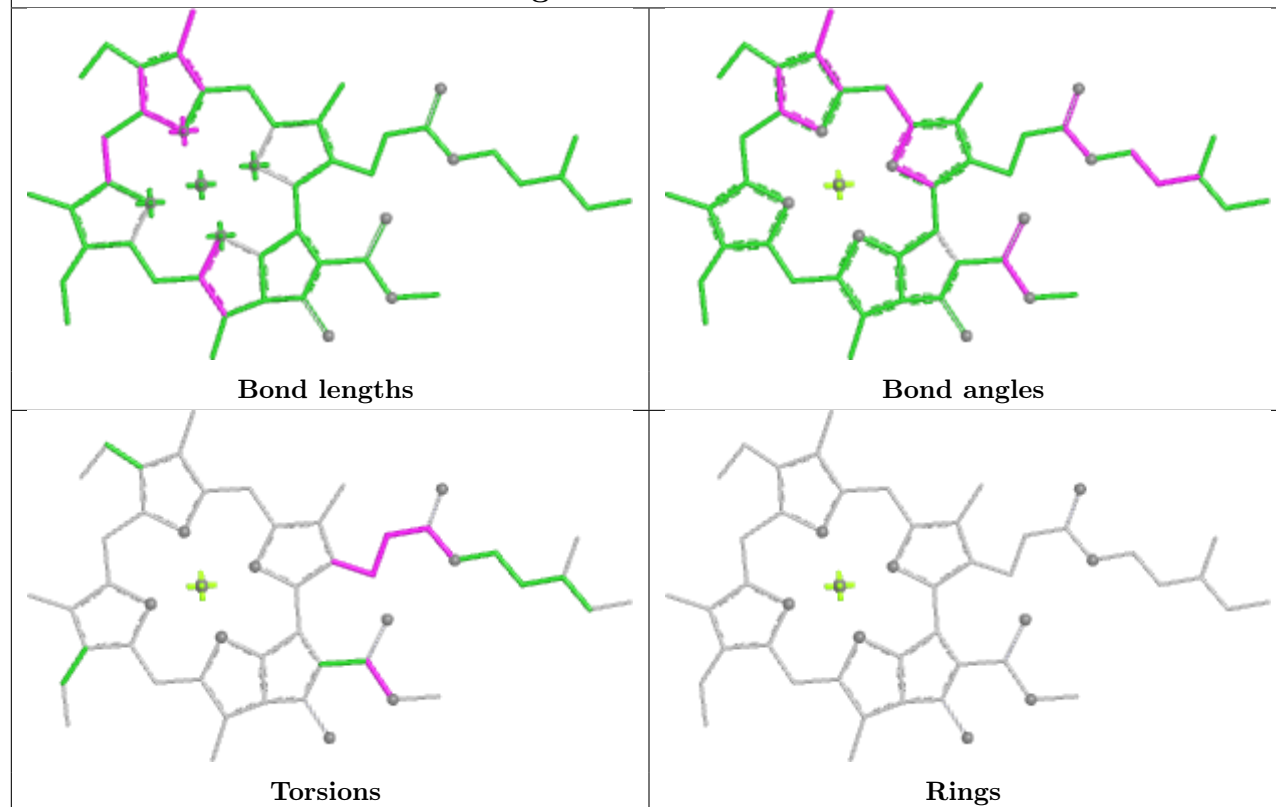


Torsions

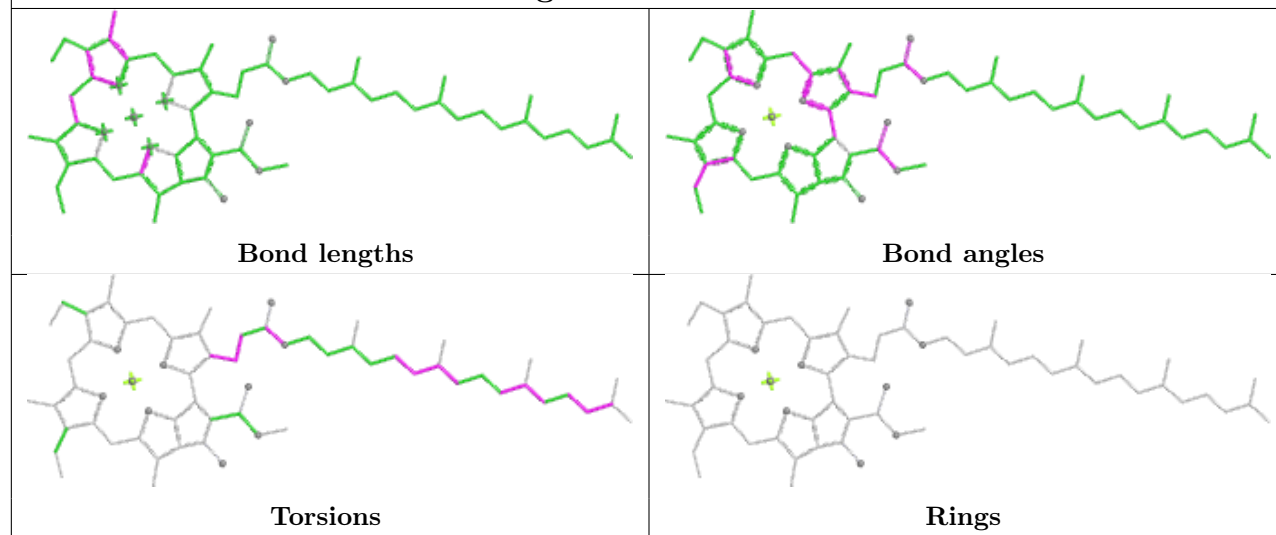


Rings

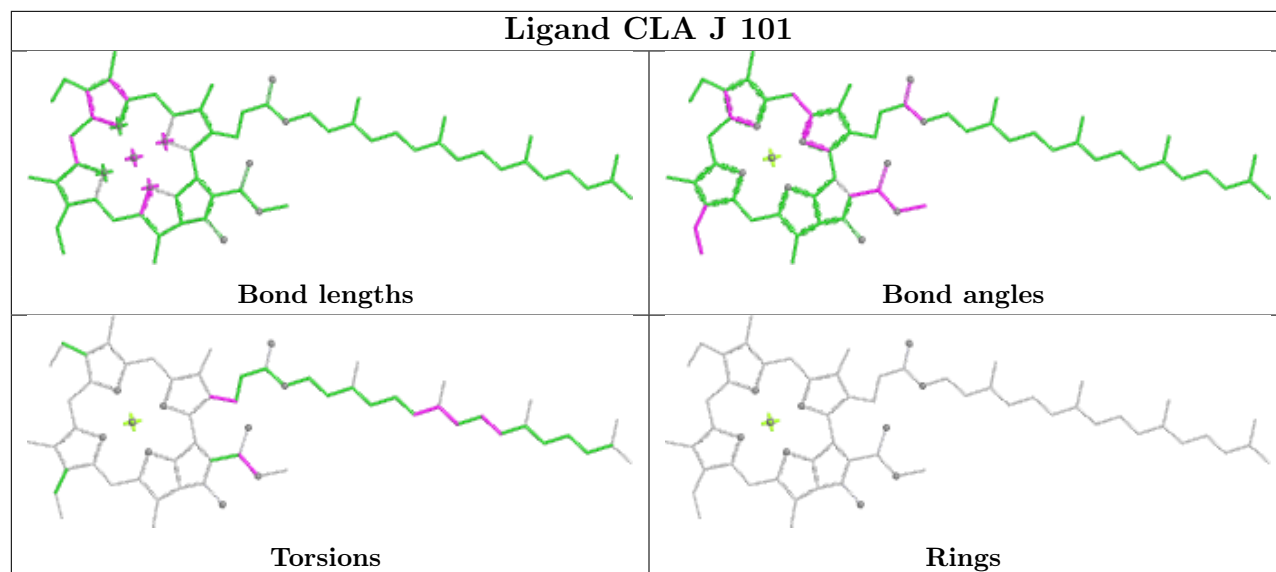
Ligand CLA A 835



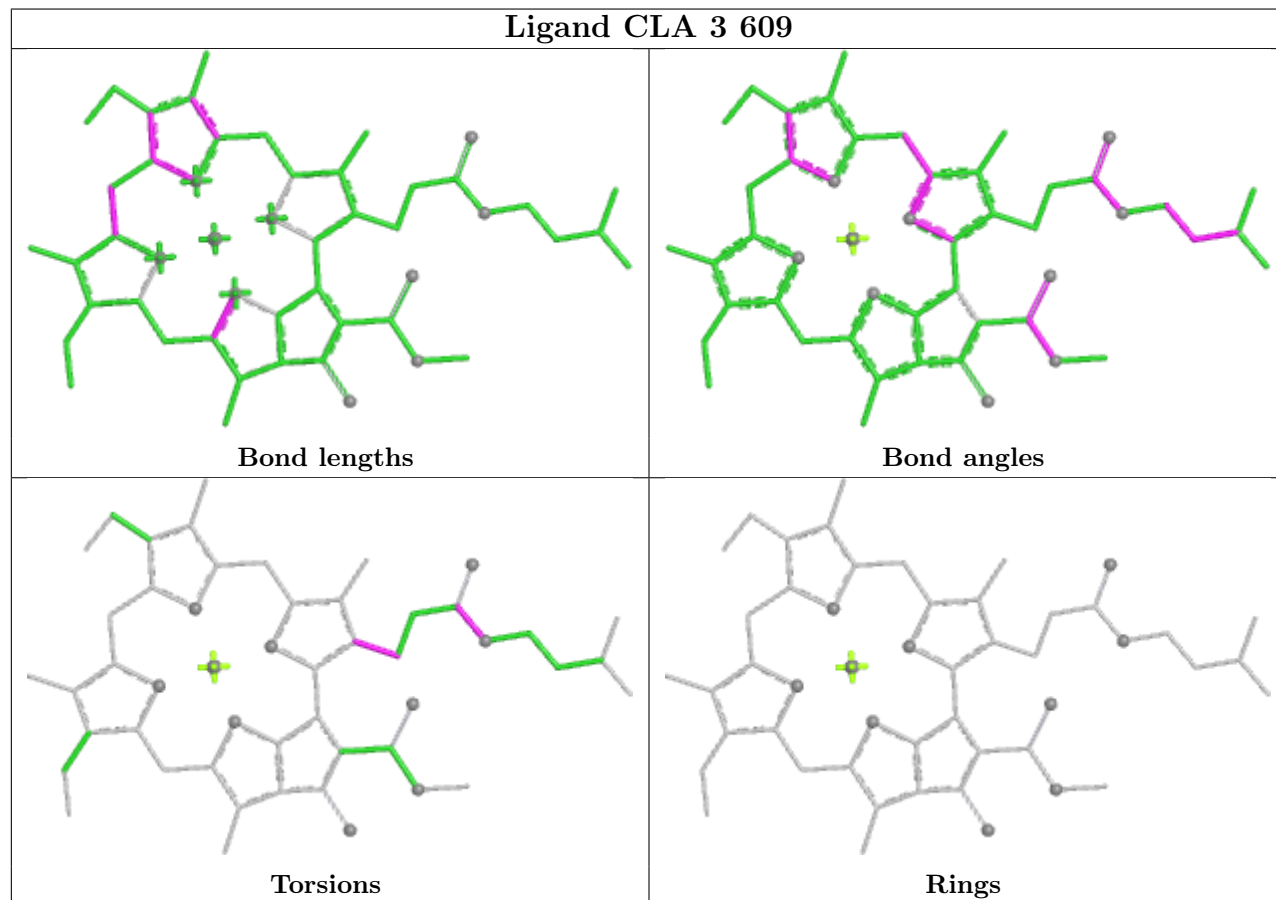
Ligand CLA 1 309

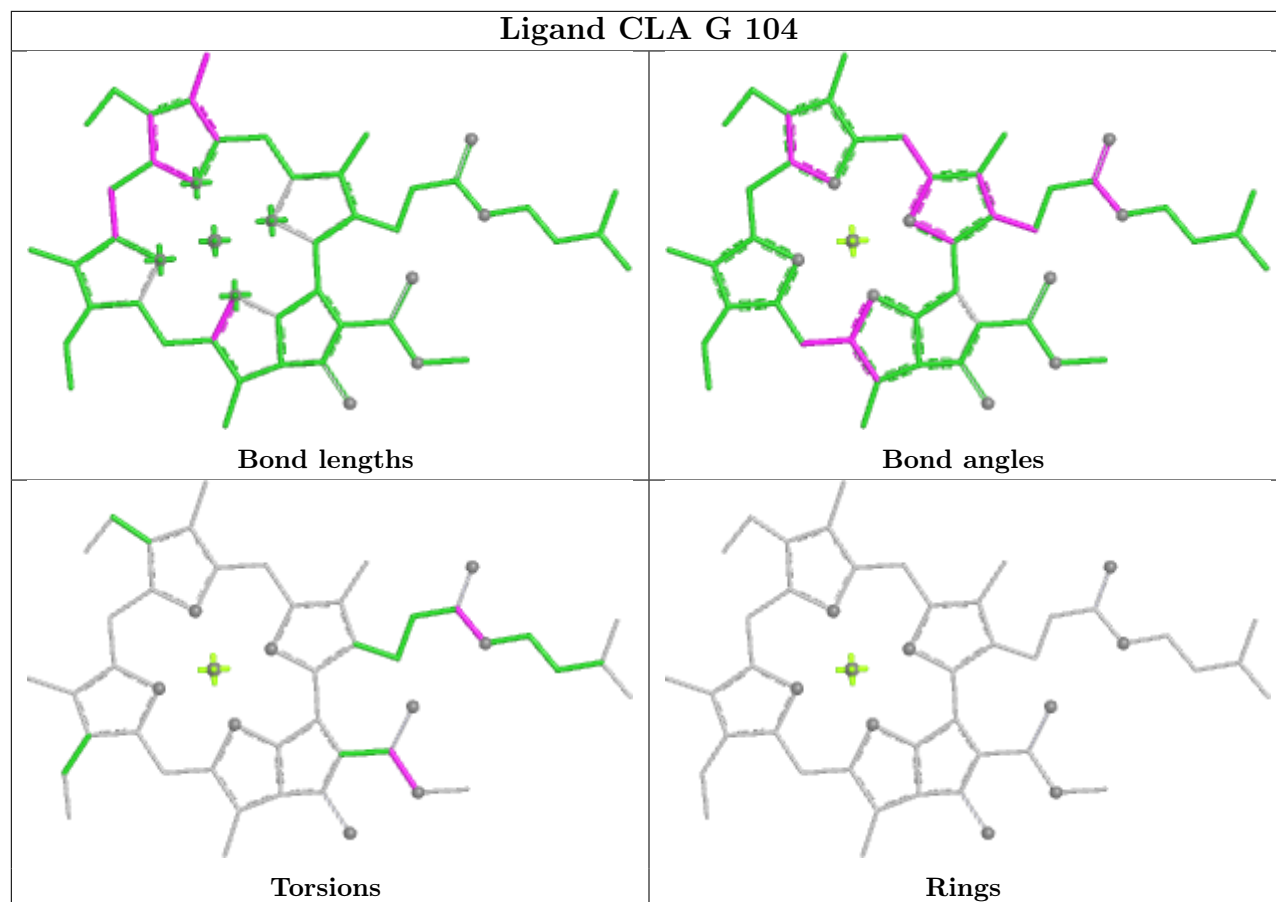


Ligand CLA J 101

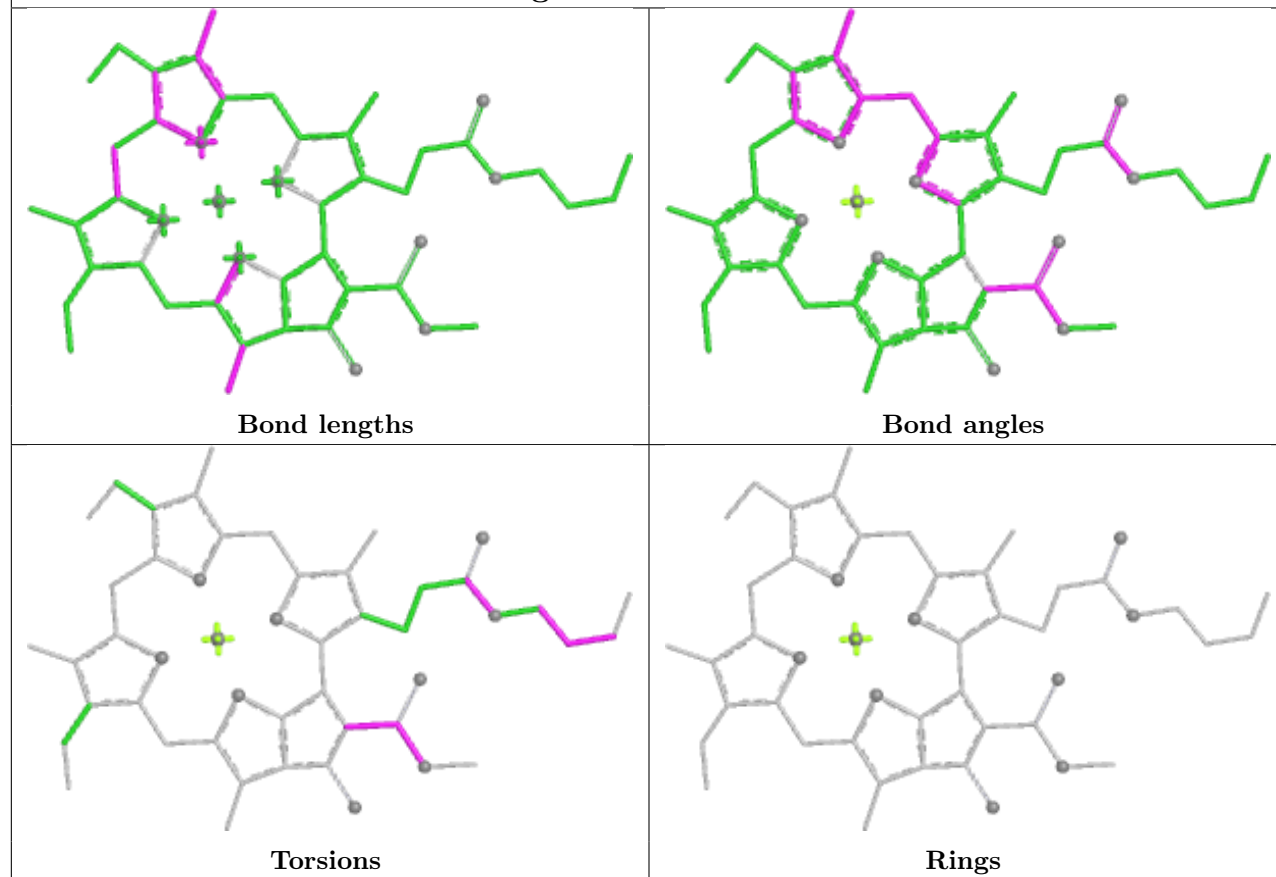


Ligand CLA 3 609

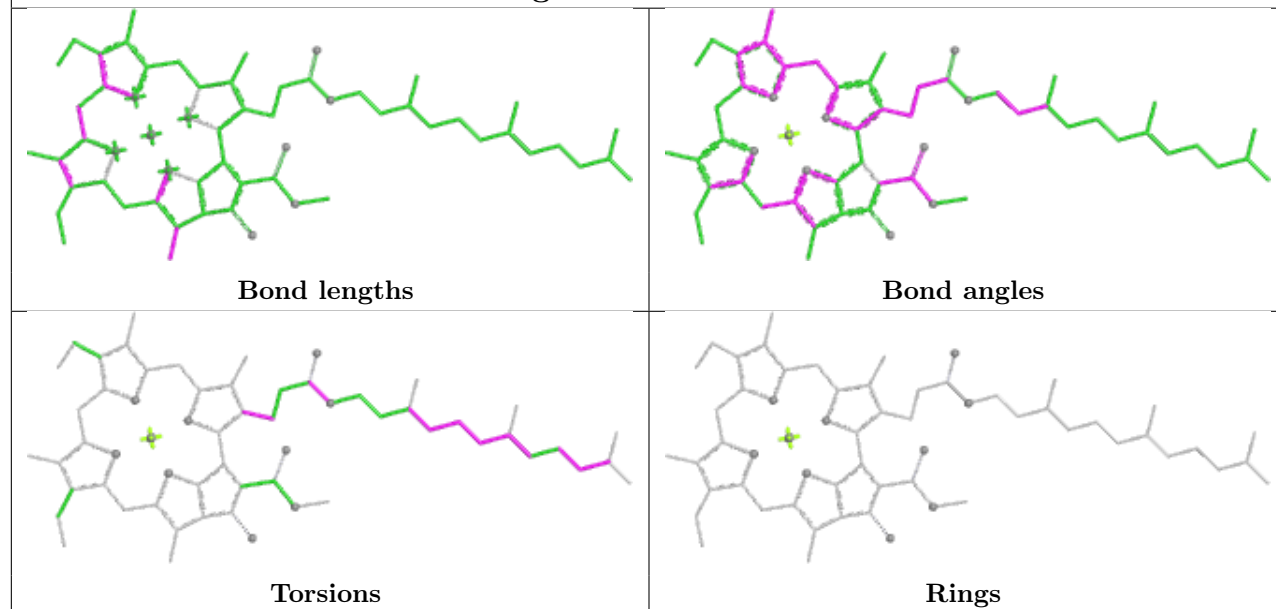




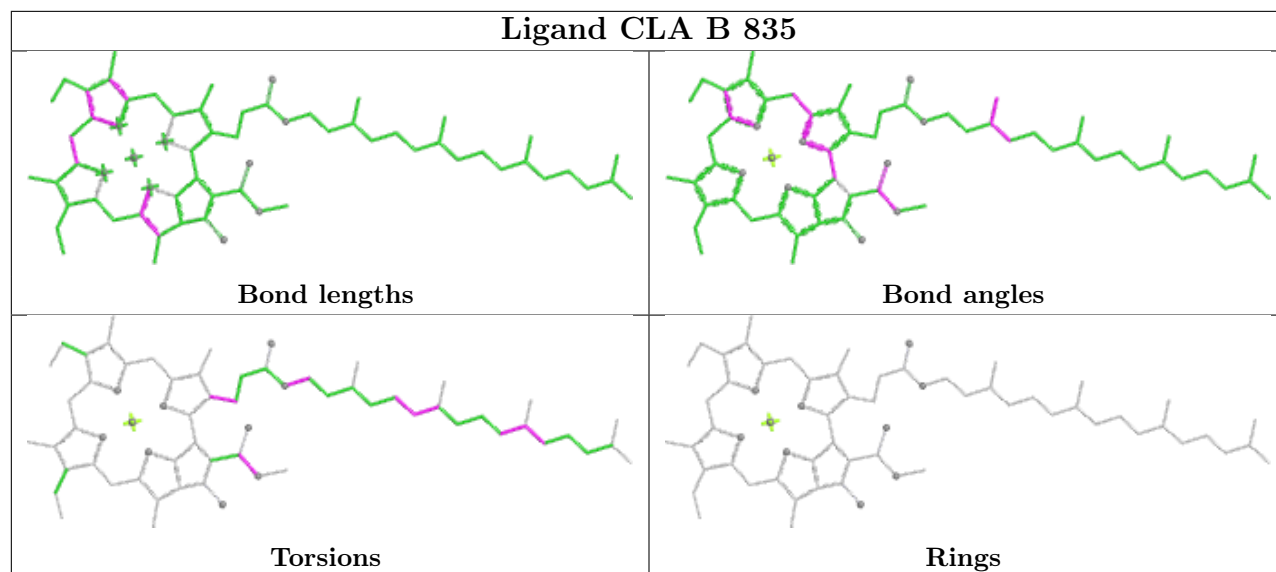
Ligand CLA A 821



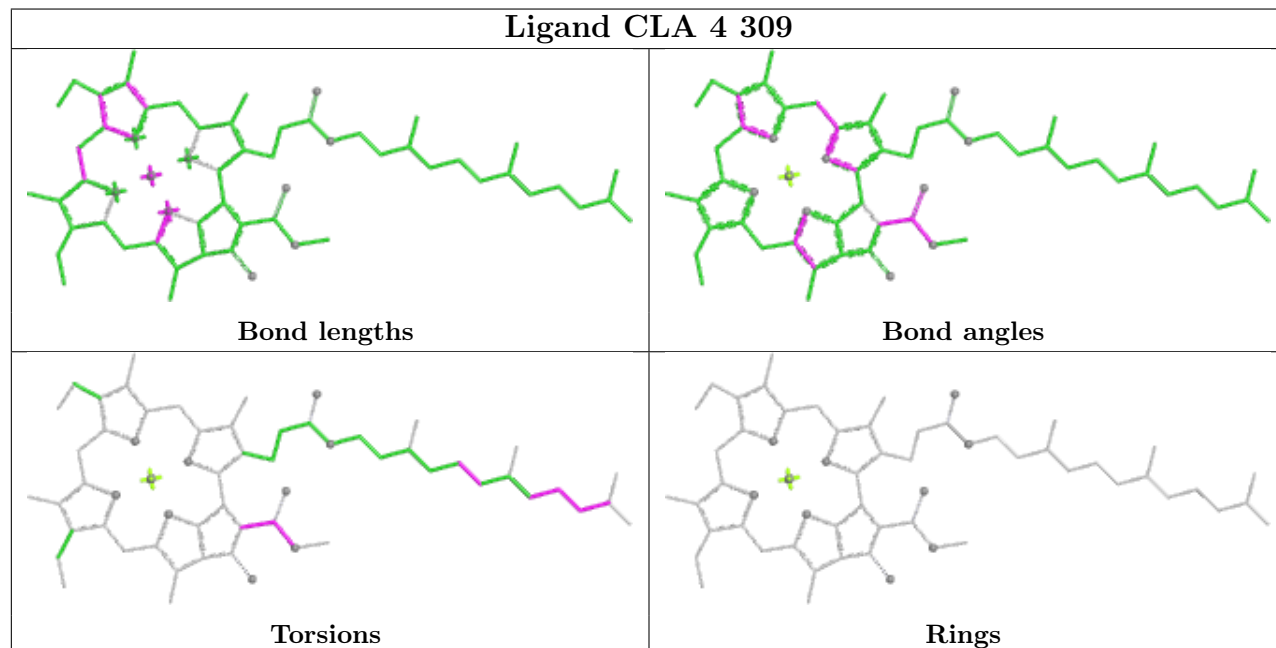
Ligand CLA B 820



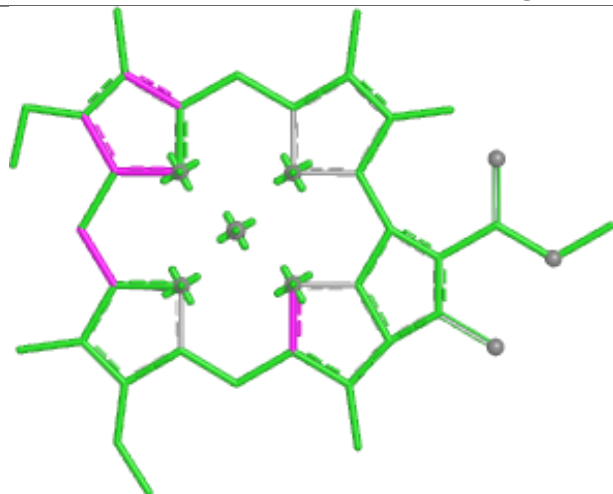
Ligand CLA B 835



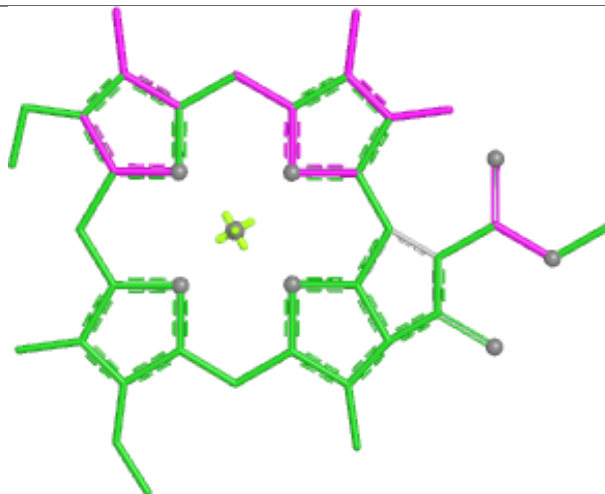
Ligand CLA 4 309



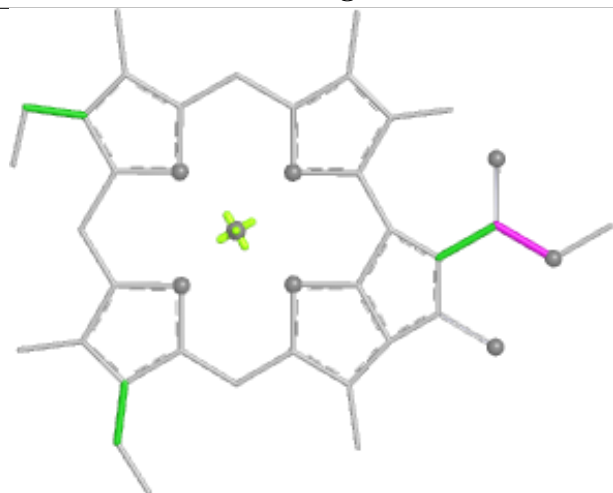
Ligand CLA 2 309



Bond lengths



Bond angles

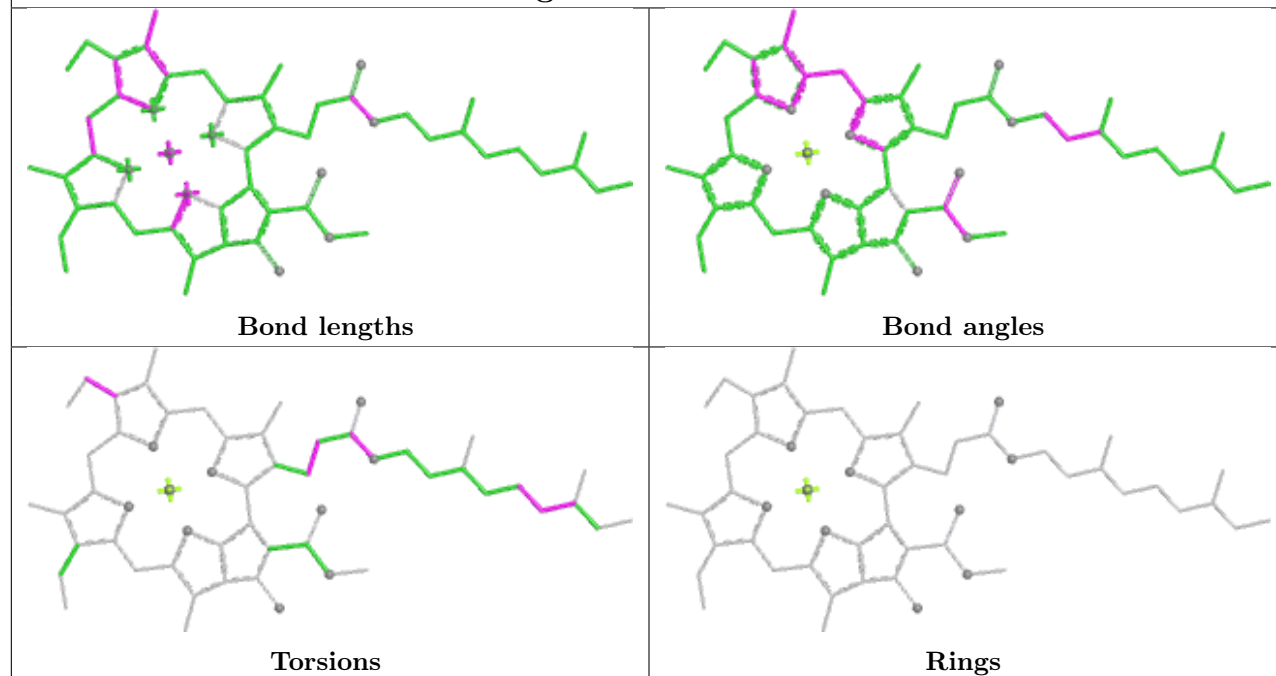


Torsions

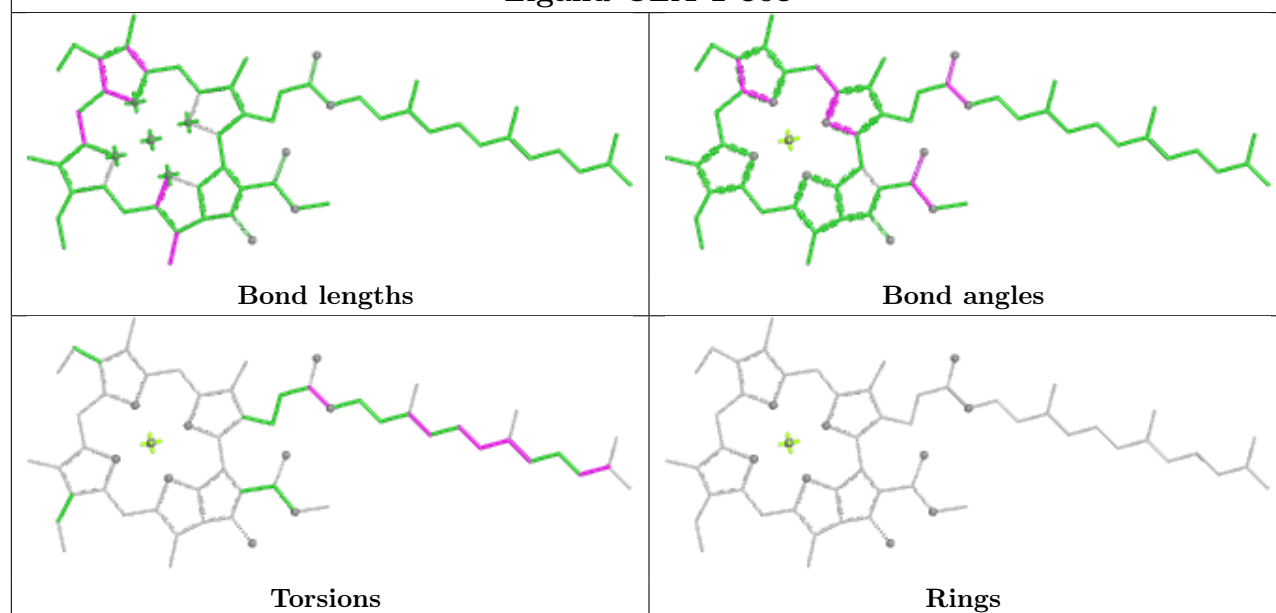


Rings

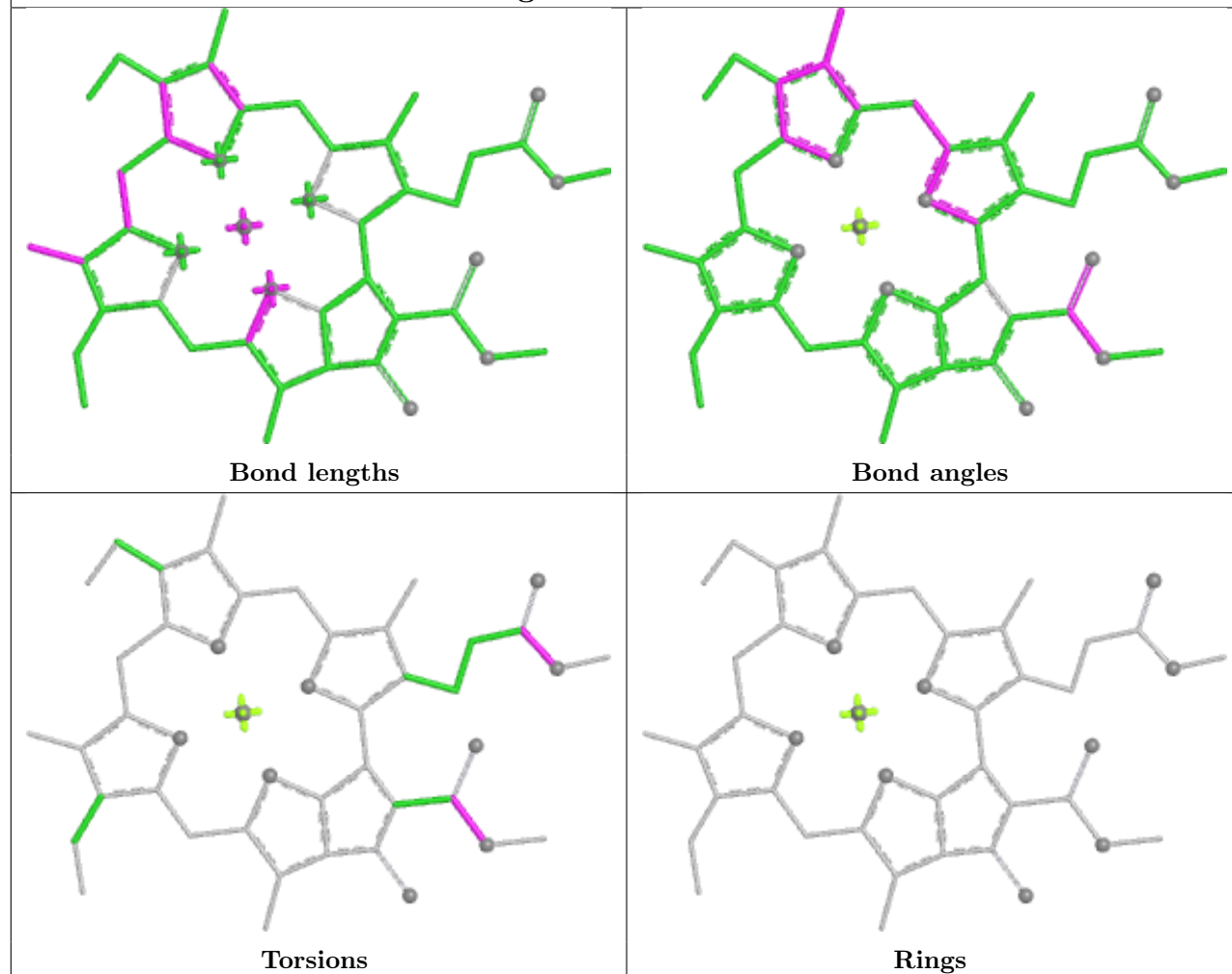
Ligand CLA 4 312



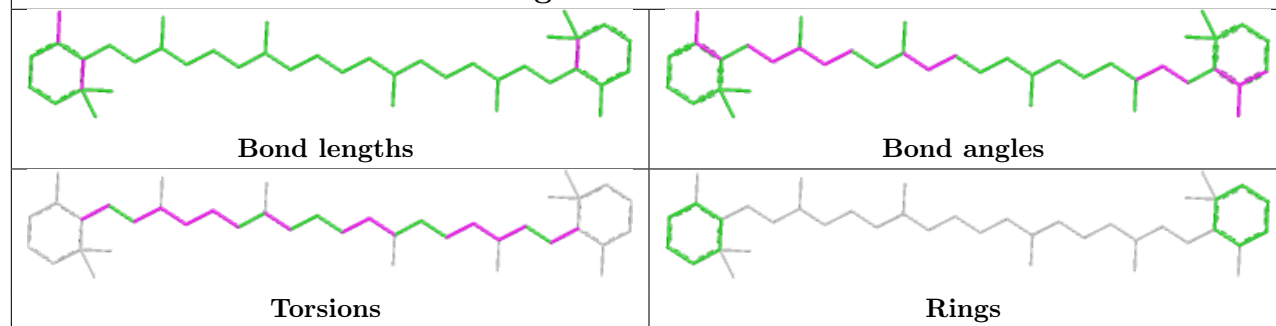
Ligand CLA 1 308

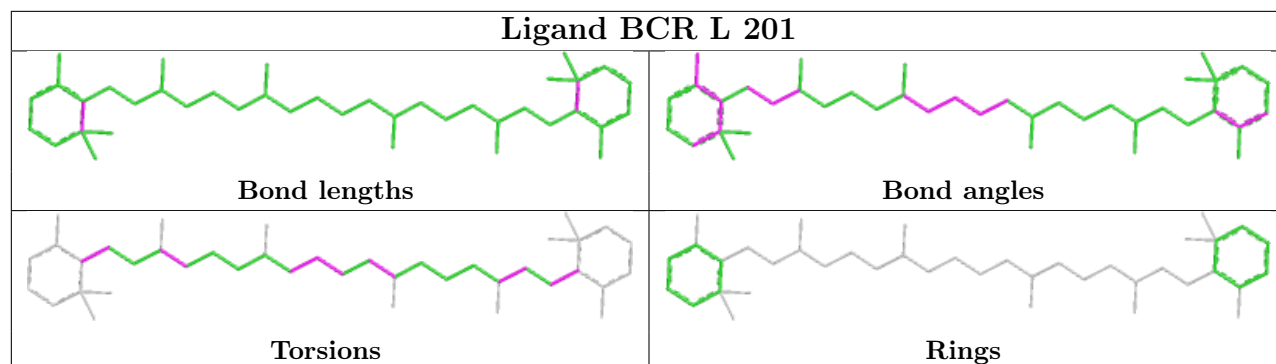
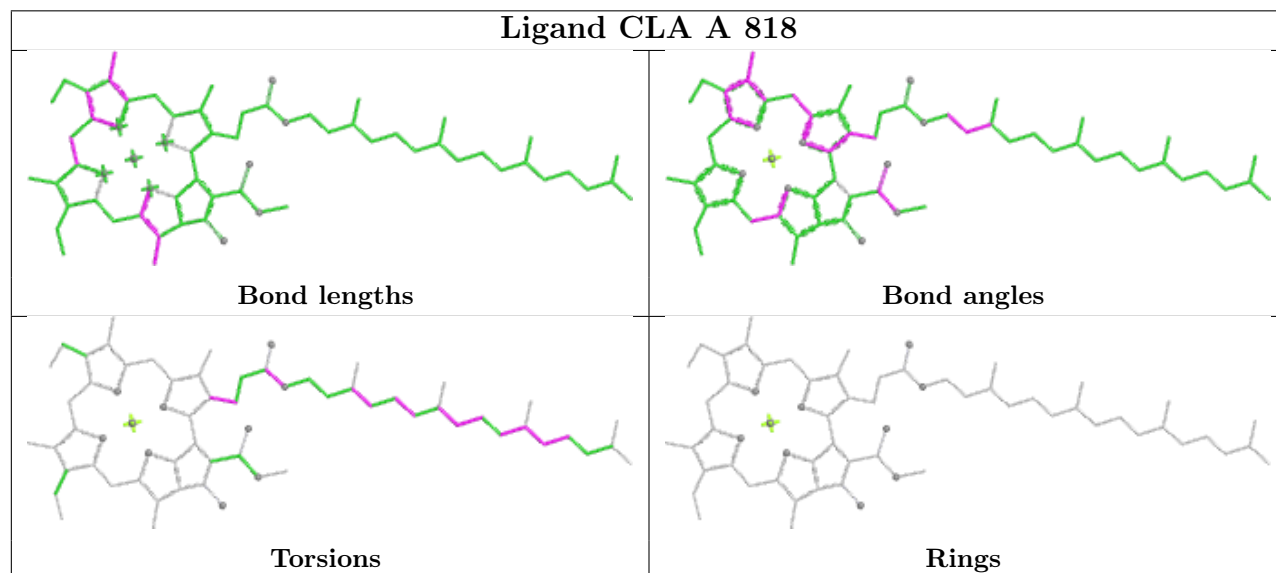
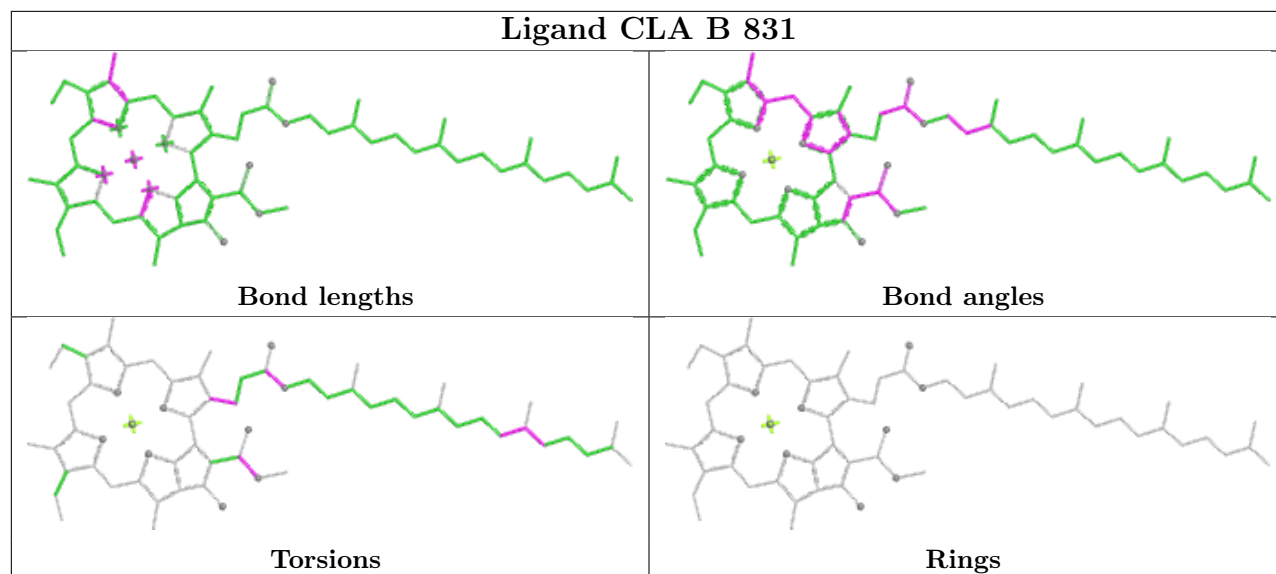


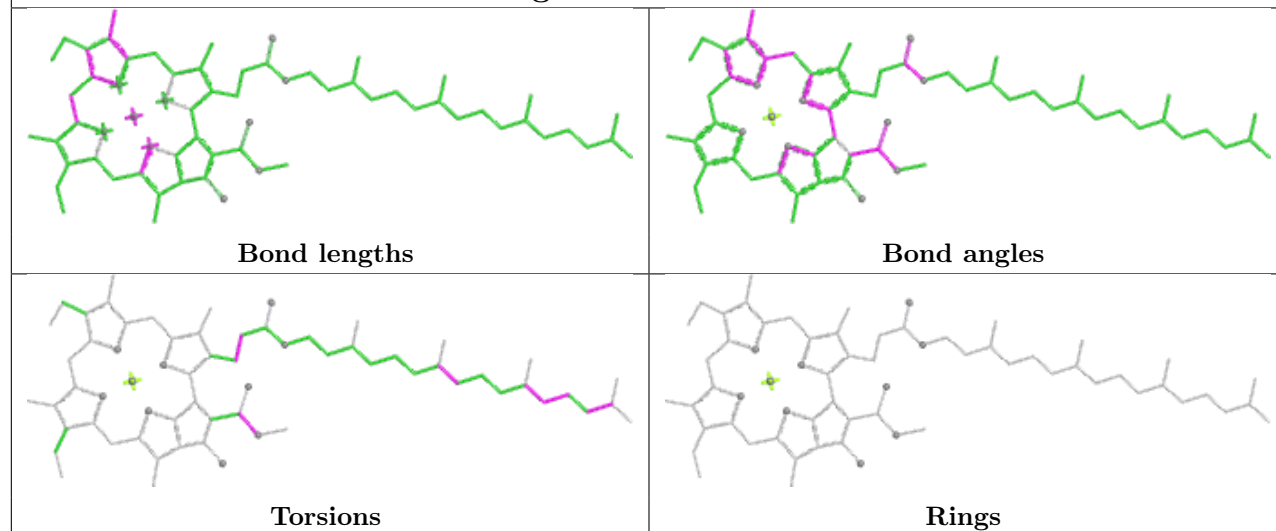
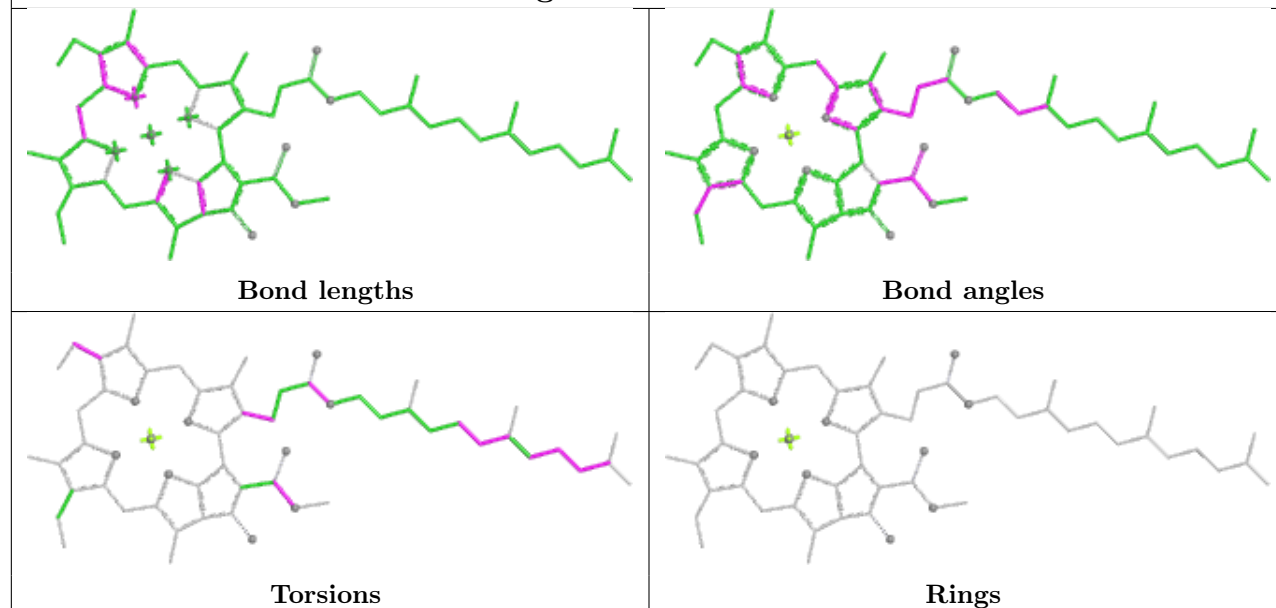
Ligand CLA 1 313



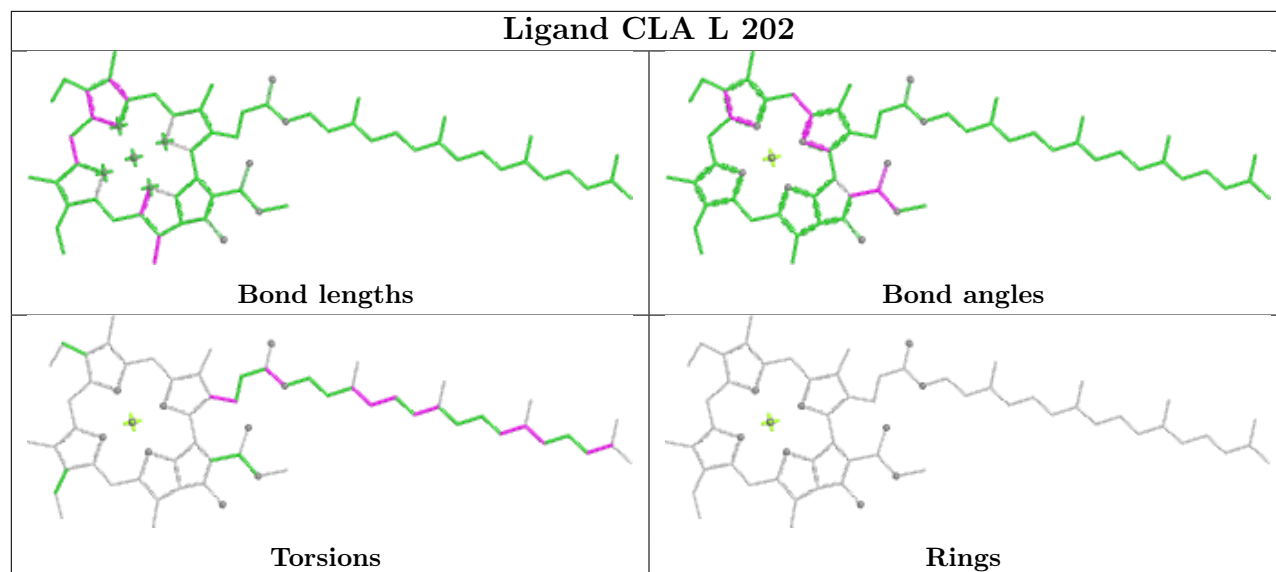
Ligand BCR 2 316



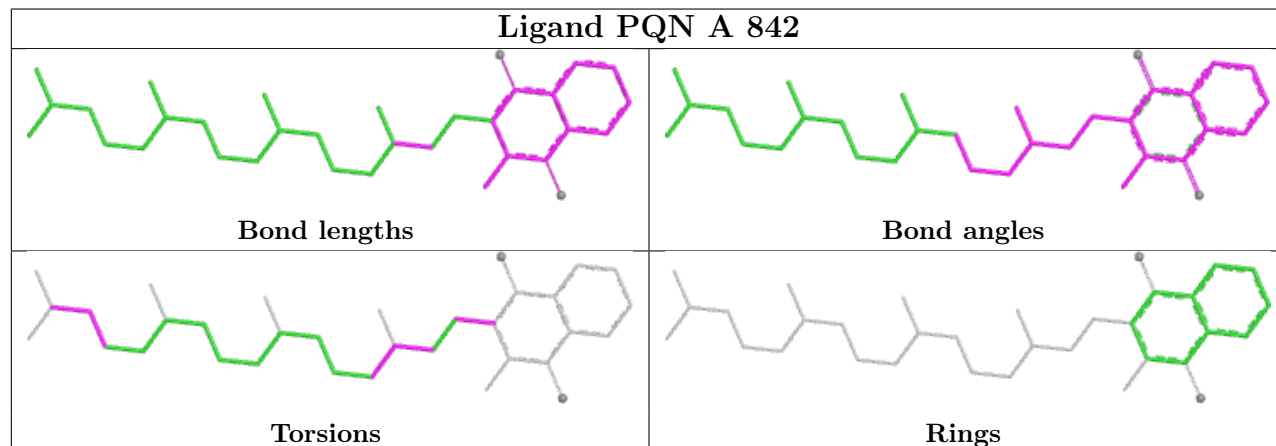


Ligand CLA B 805**Ligand CLA 4 303**

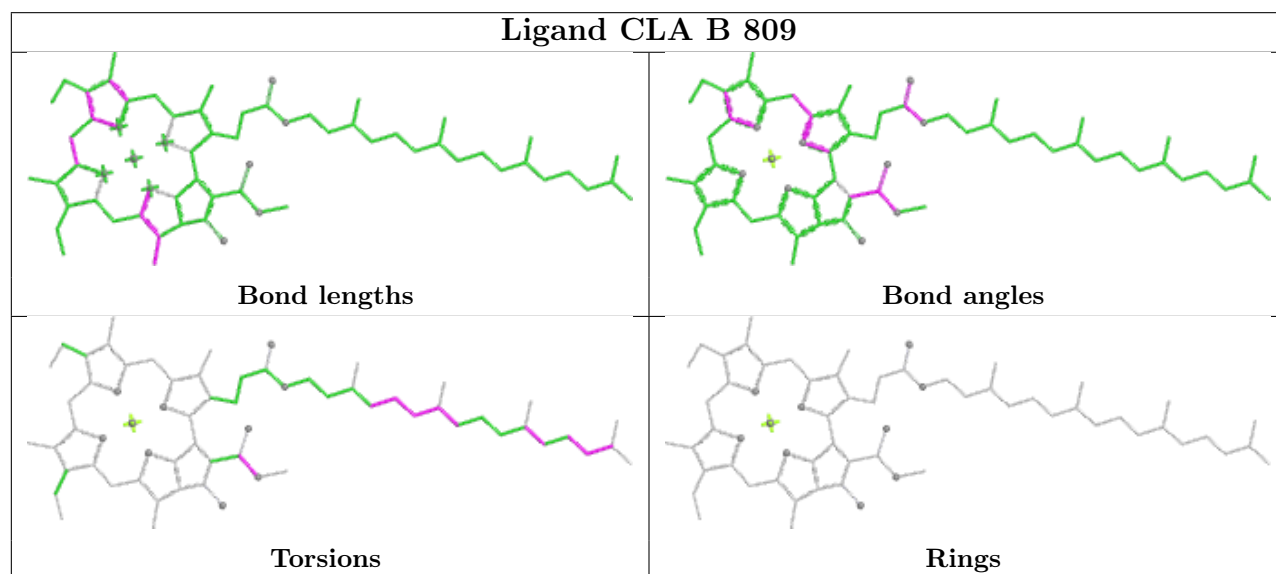
Ligand CLA L 202



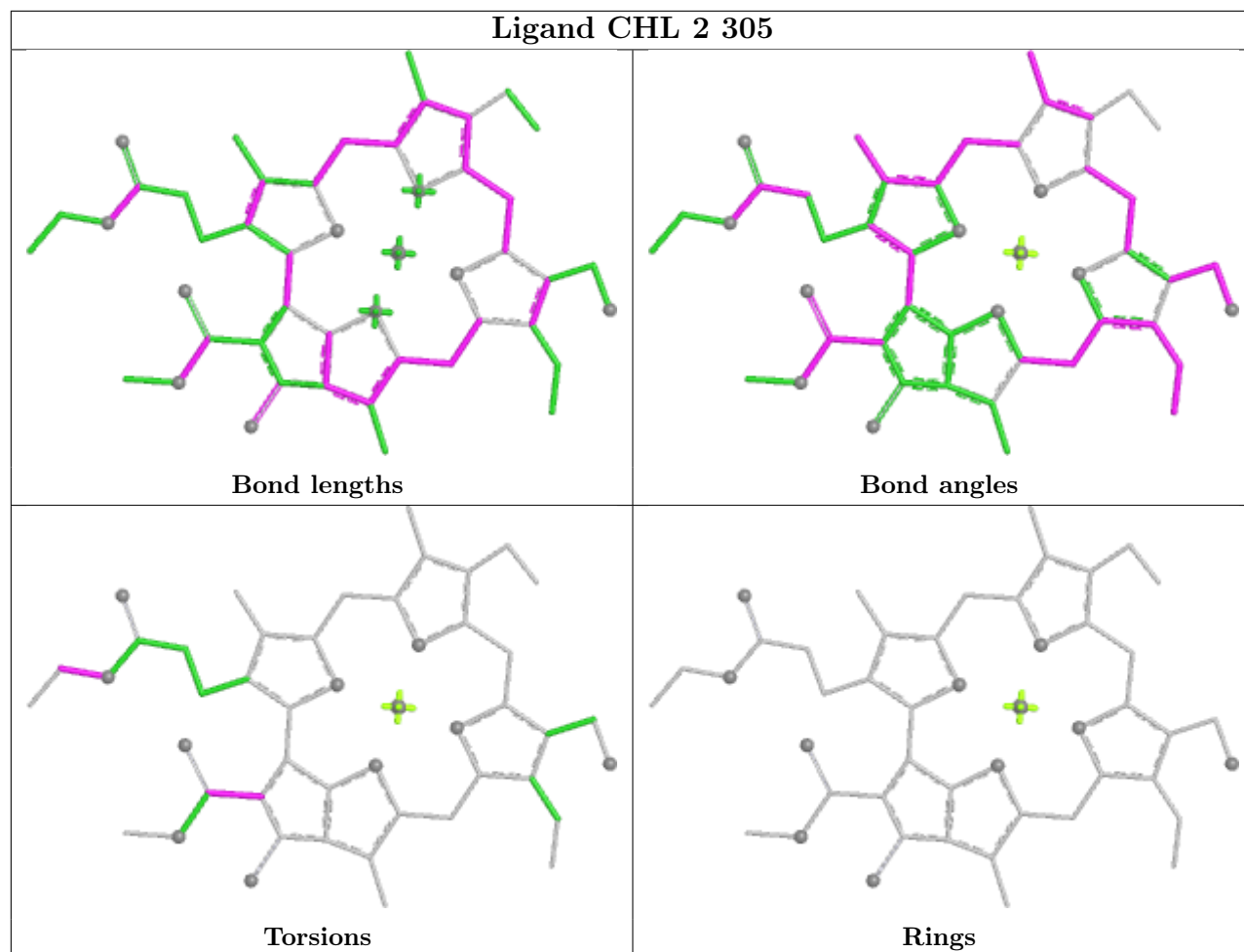
Ligand PQN A 842



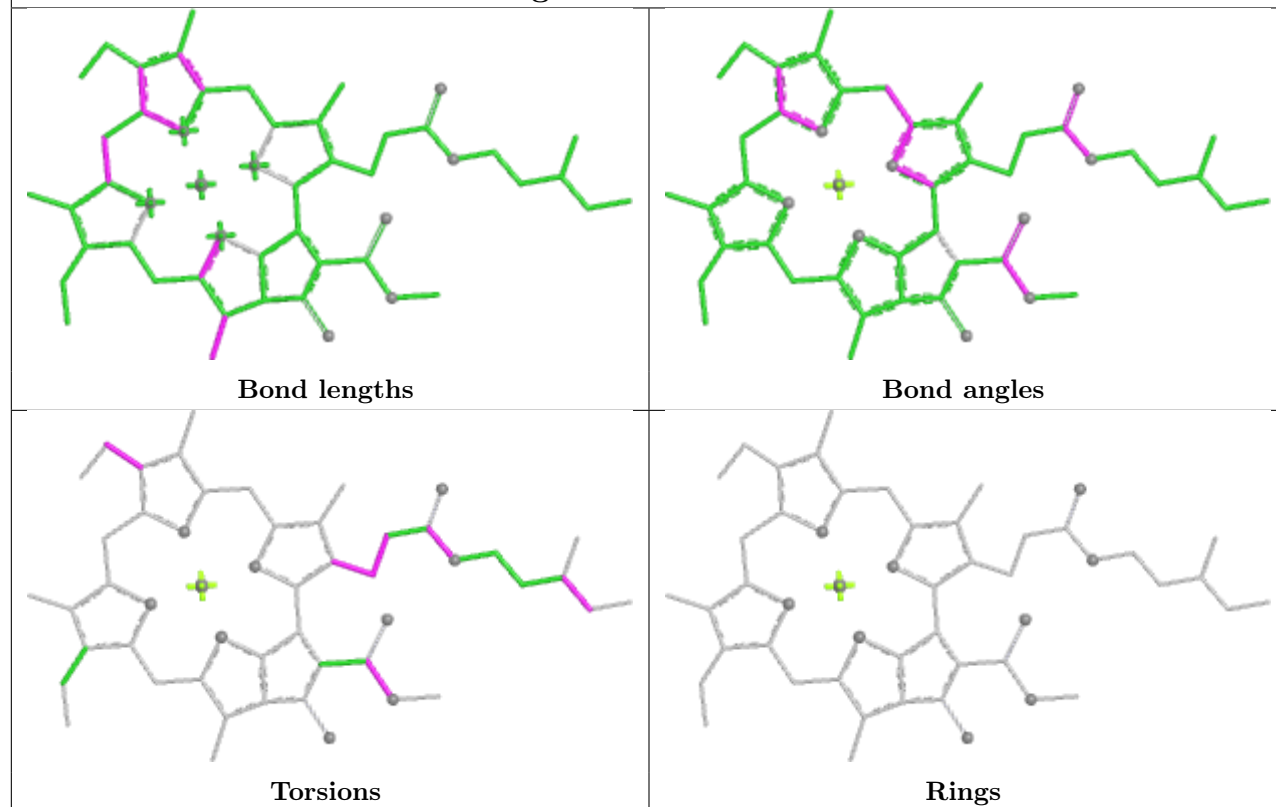
Ligand CLA B 809



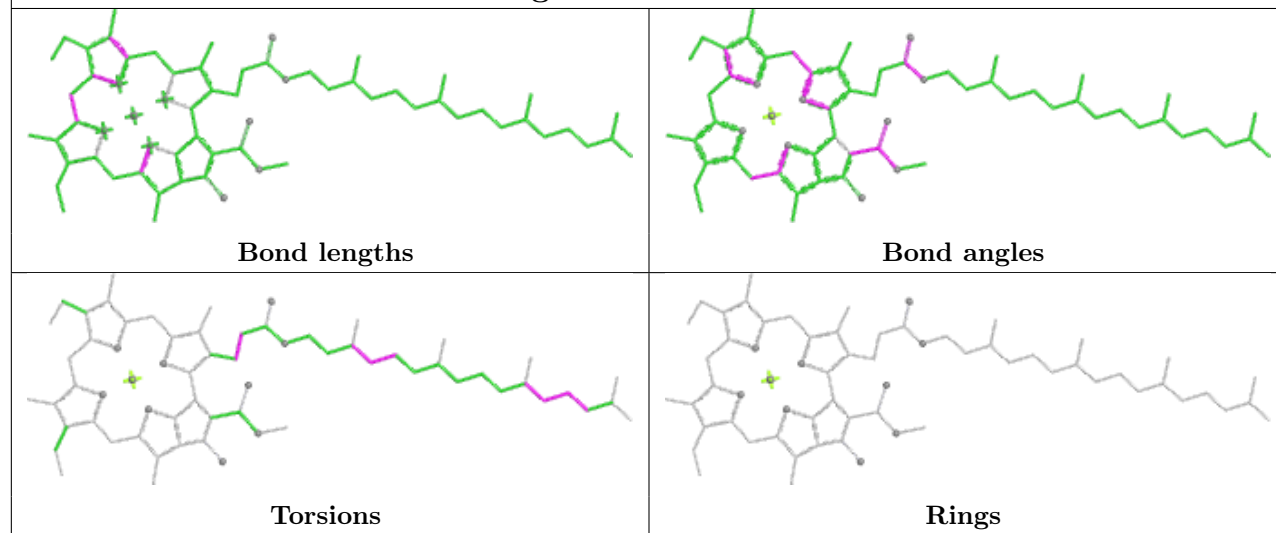
Ligand CHL 2 305



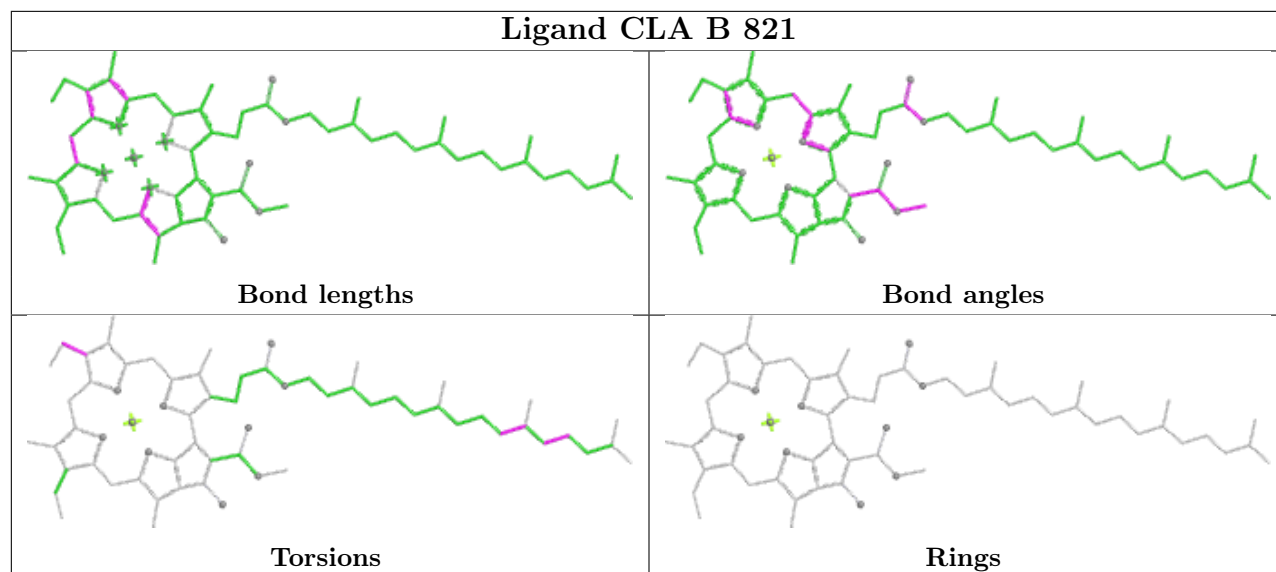
Ligand CLA A 822



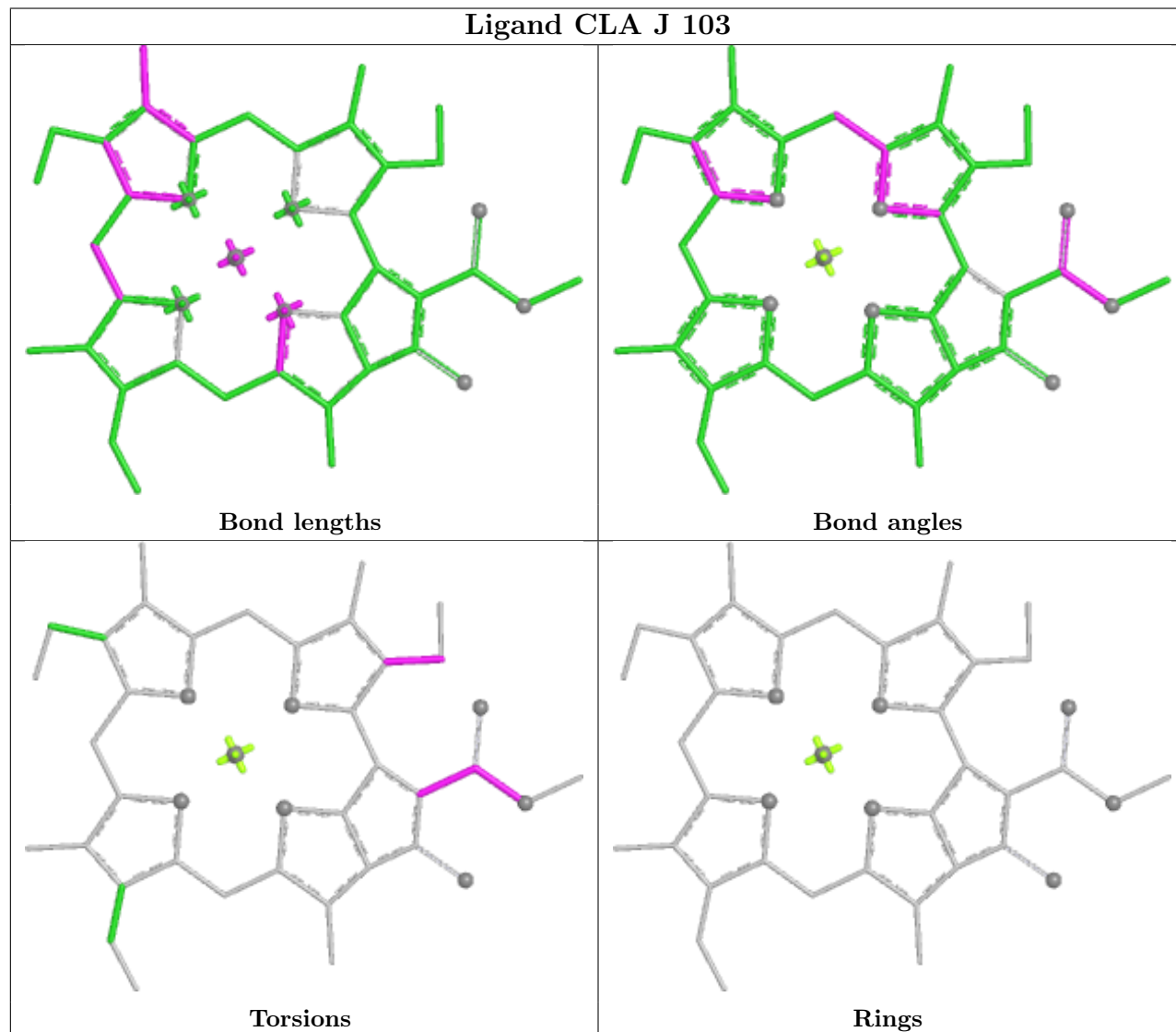
Ligand CLA A 828



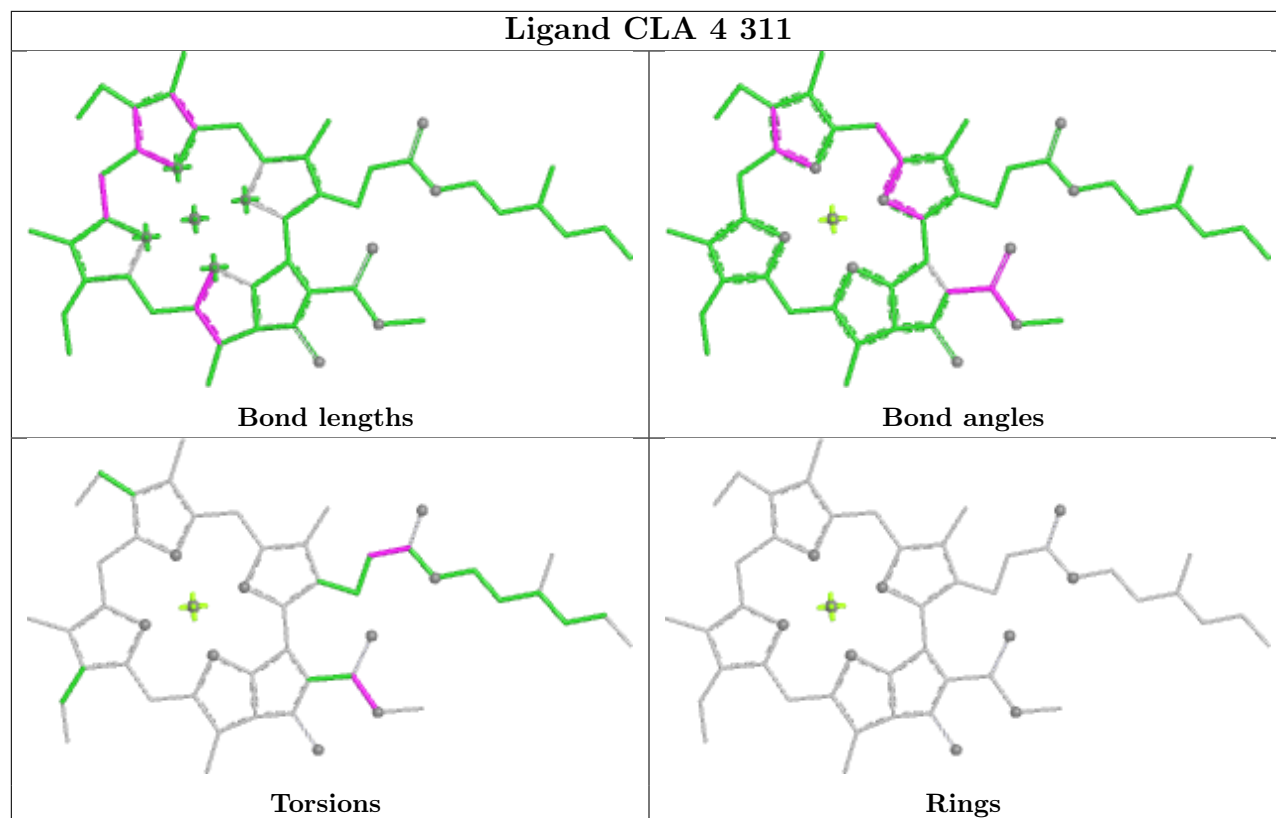
Ligand CLA B 821



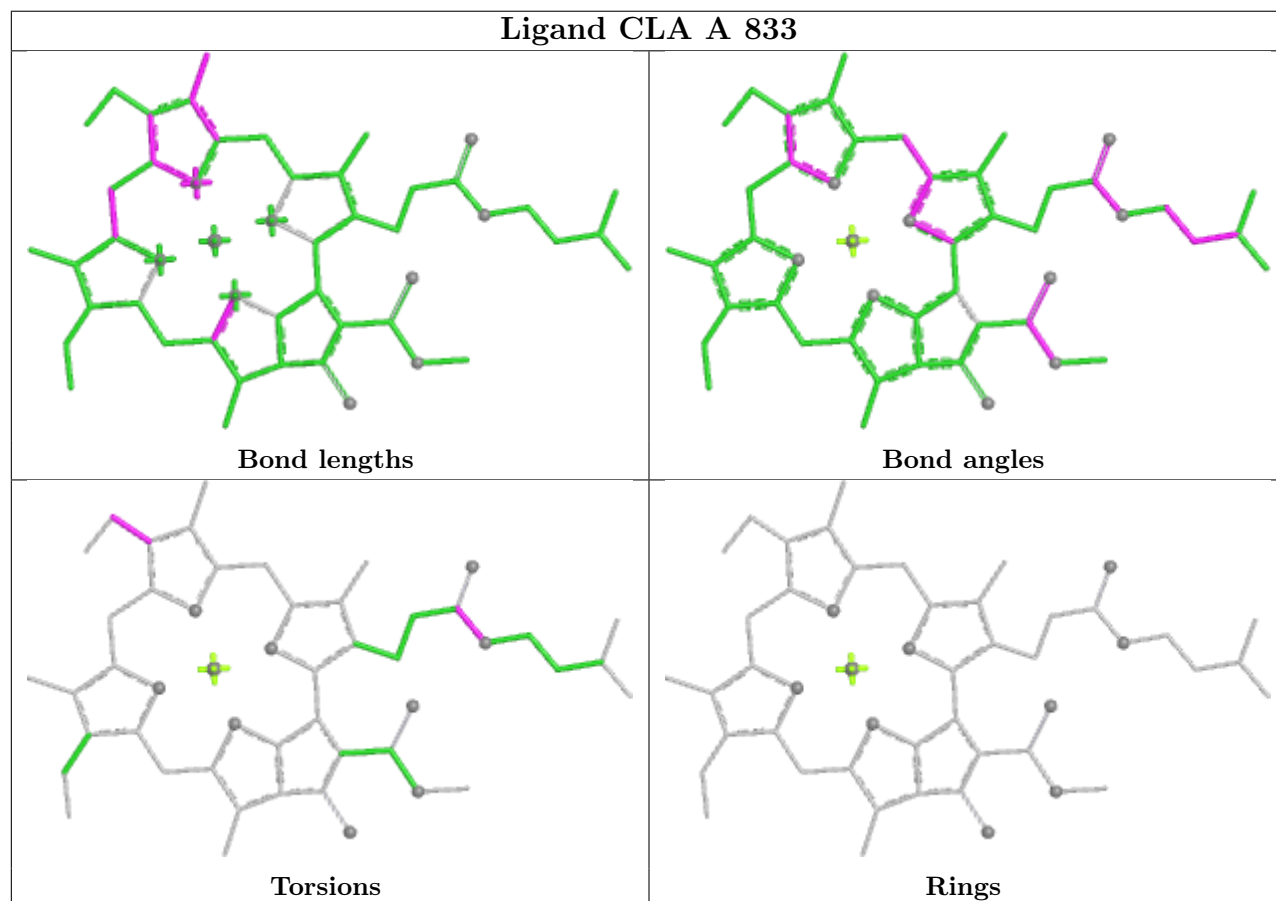
Ligand CLA J 103



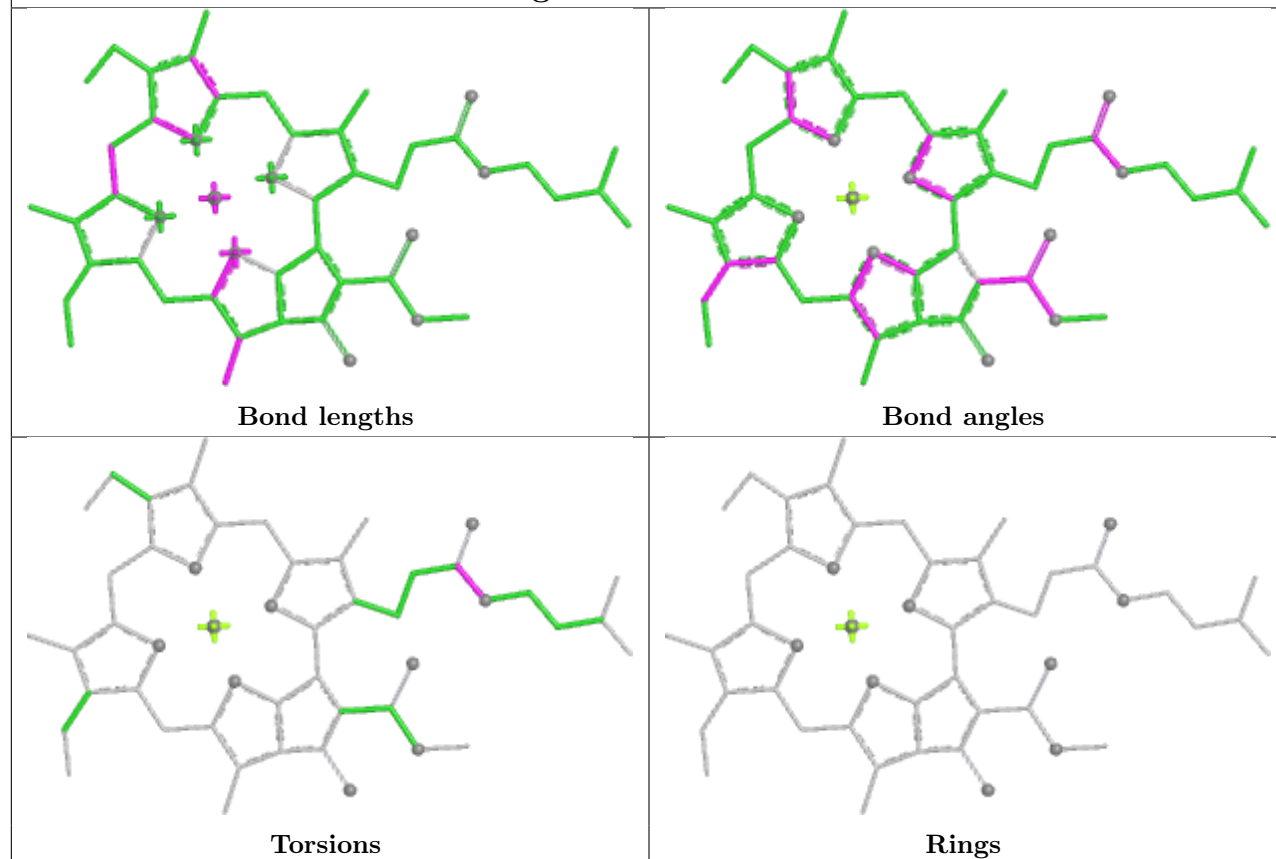
Ligand CLA 4 311



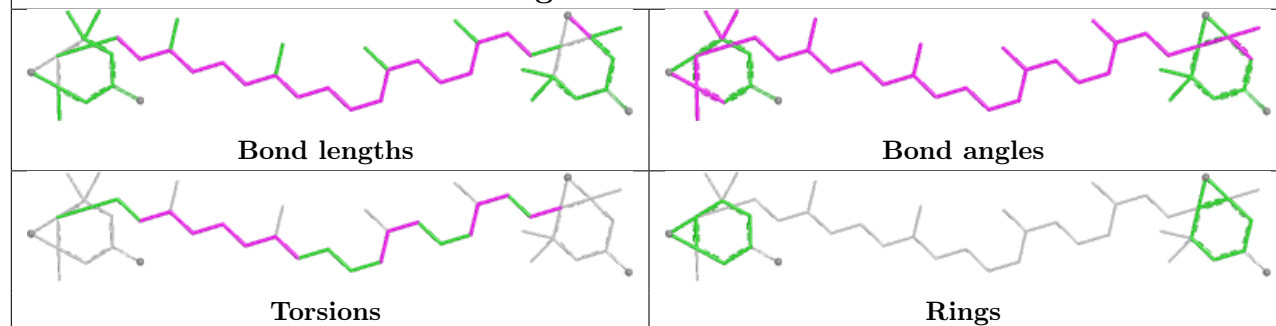
Ligand CLA A 833

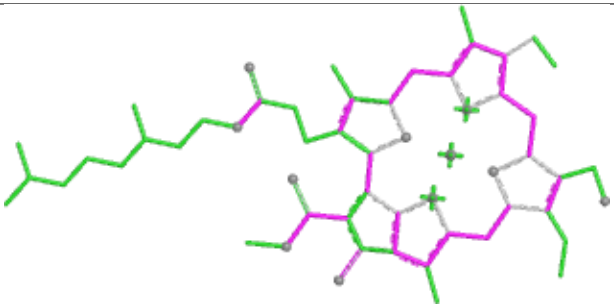
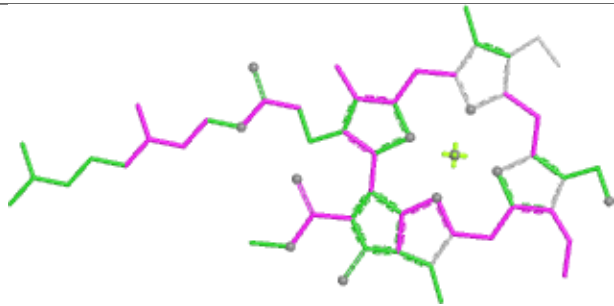
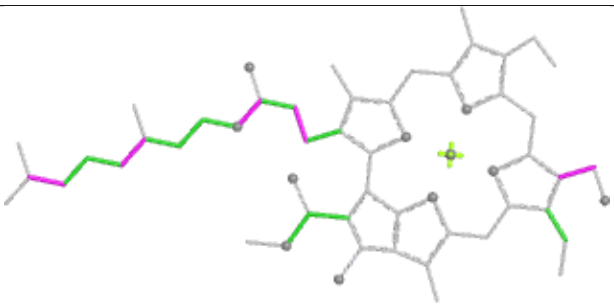
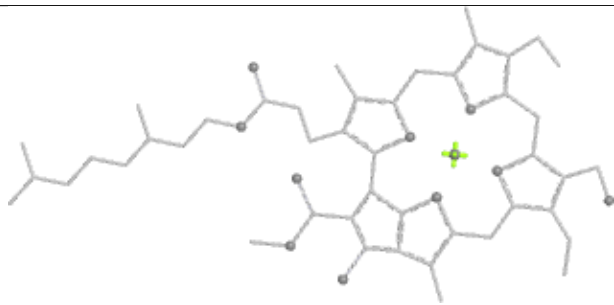


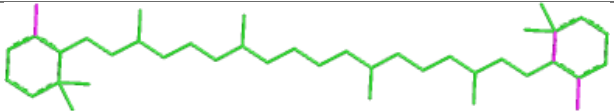
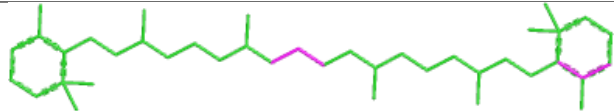
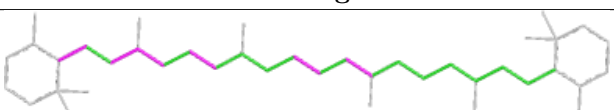
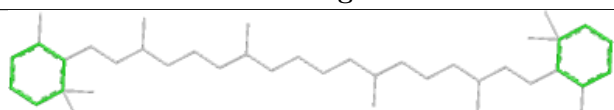
Ligand CLA B 832

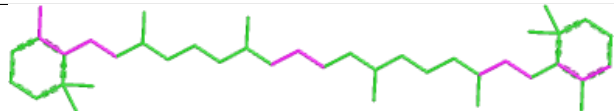
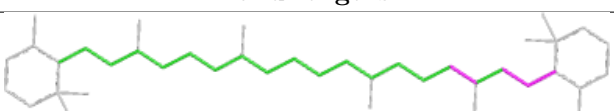
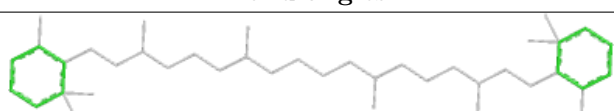


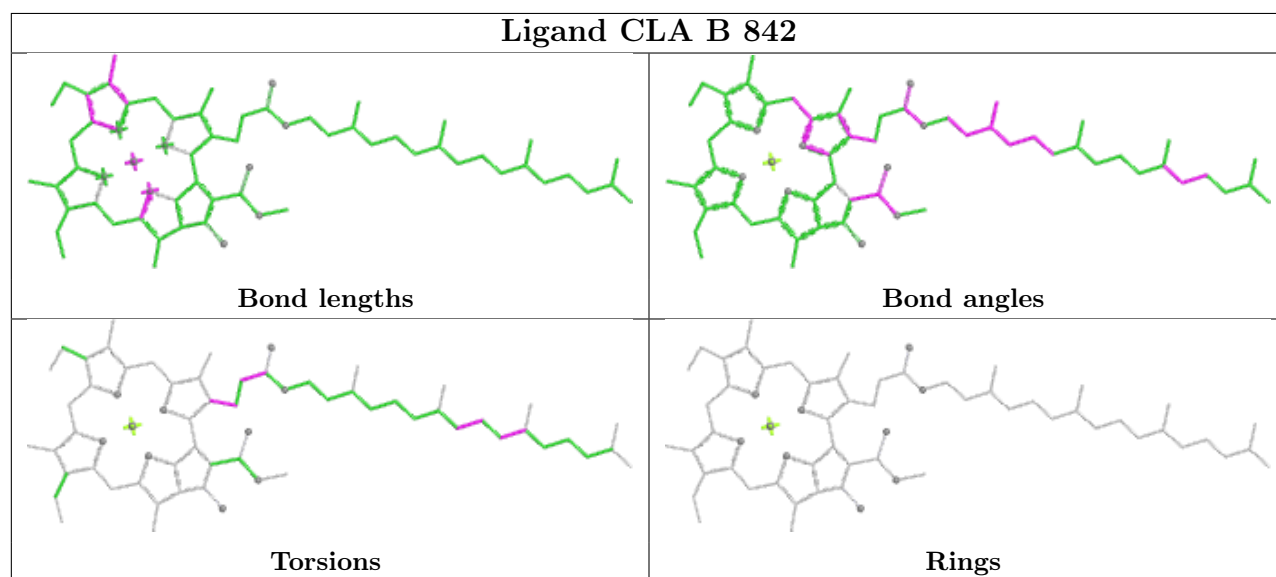
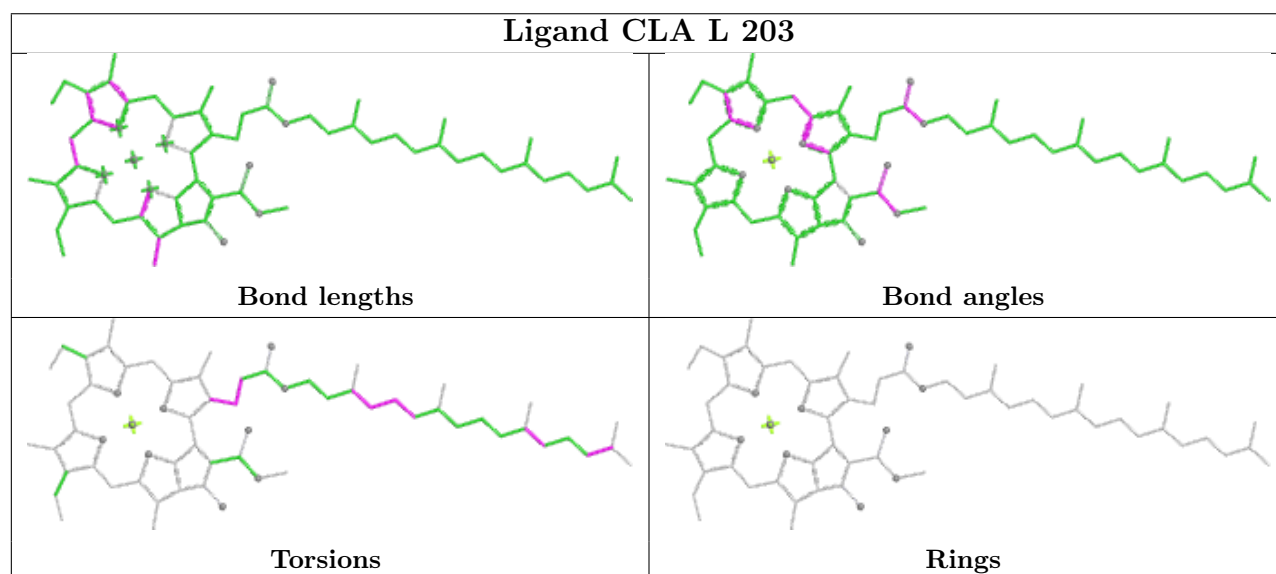
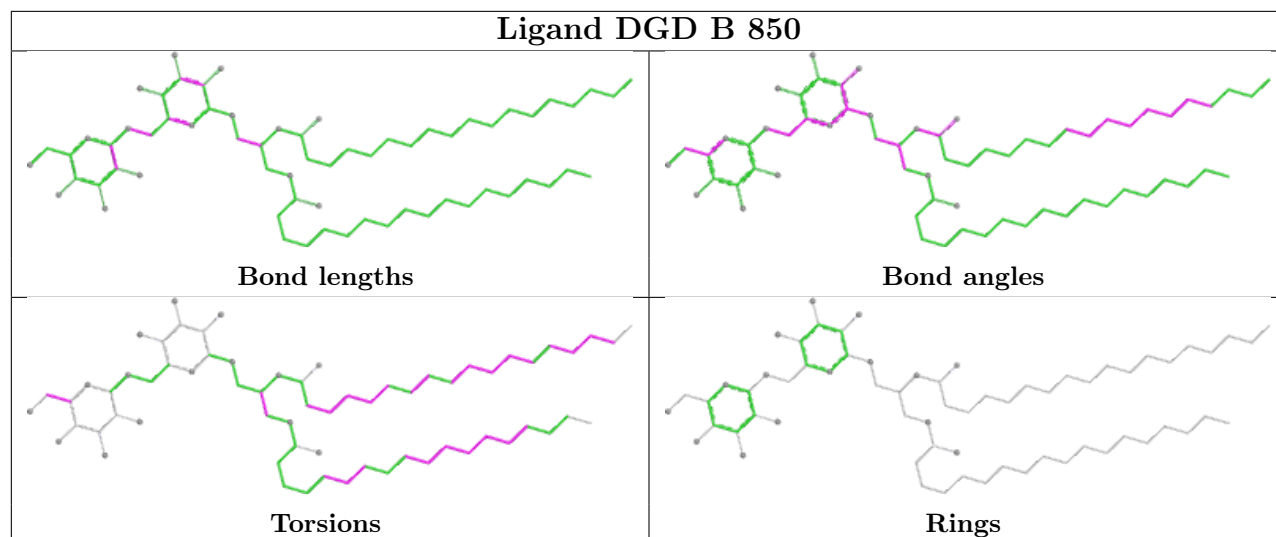
Ligand XAT 1 315



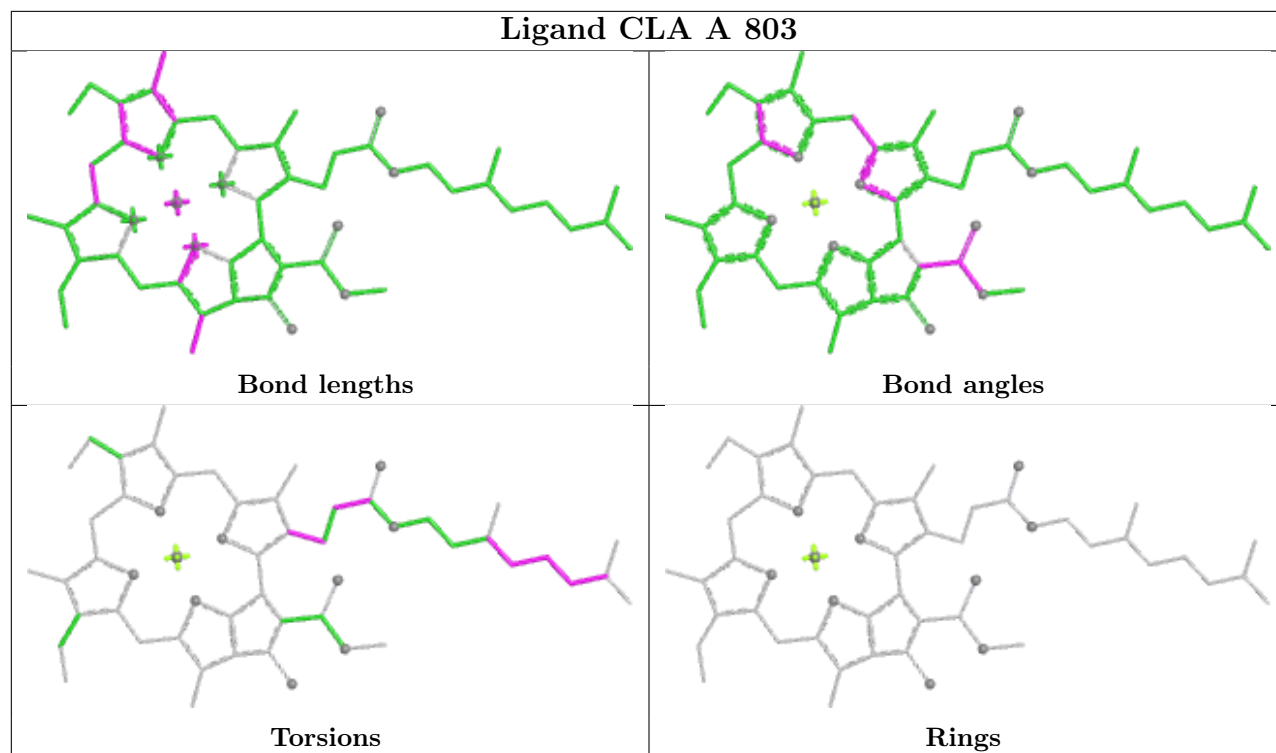
Ligand CHL 4 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 849	
	
Bond lengths	Bond angles
	
Torsions	Rings

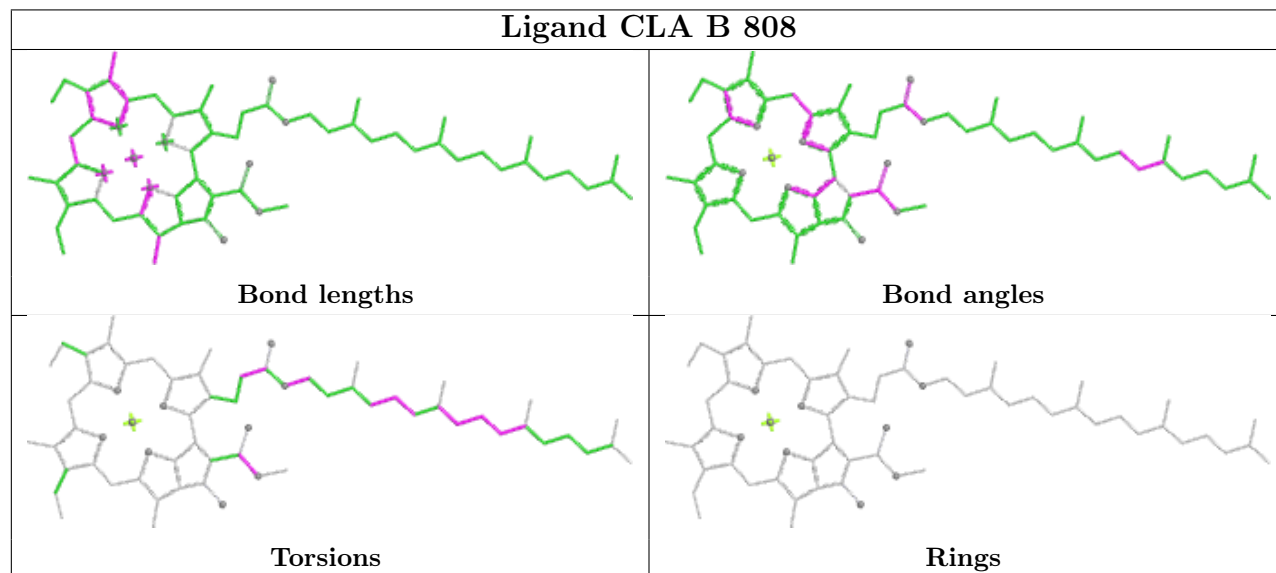
Ligand BCR G 106	
	
Bond lengths	Bond angles
	
Torsions	Rings

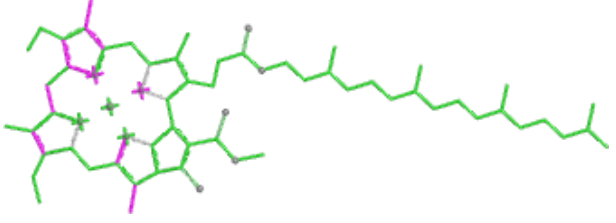
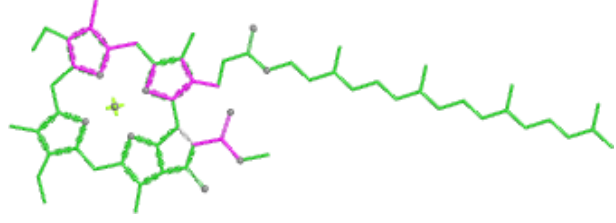
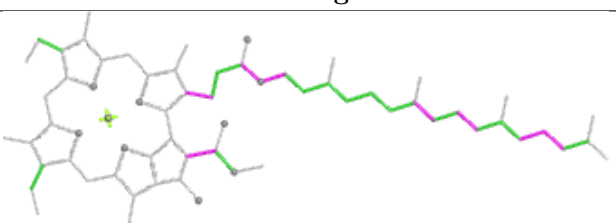
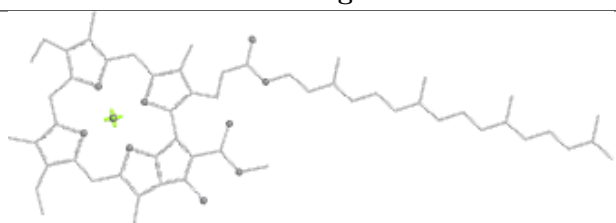
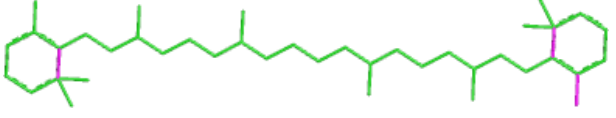
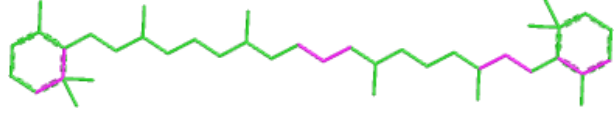
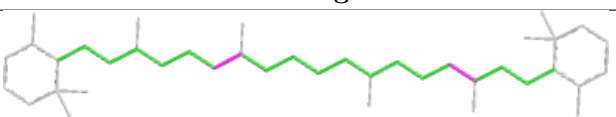
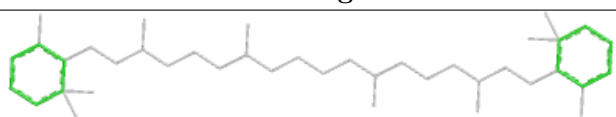
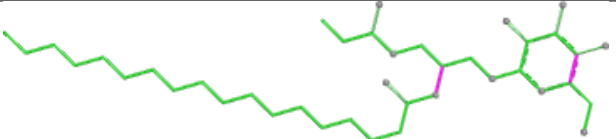
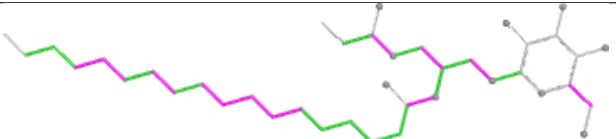


Ligand CLA A 803

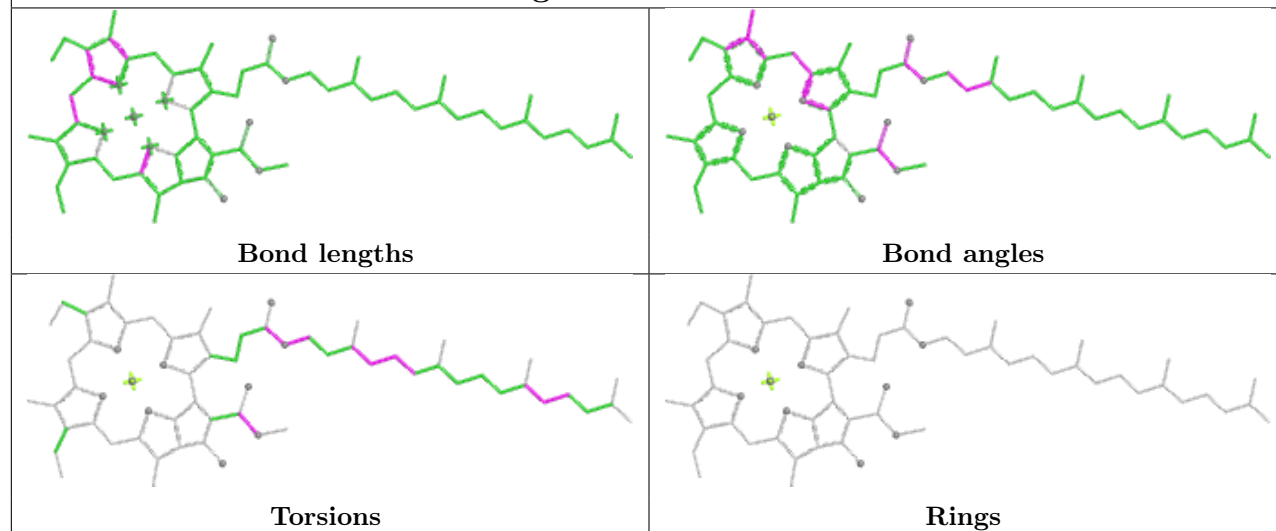


Ligand CLA B 808

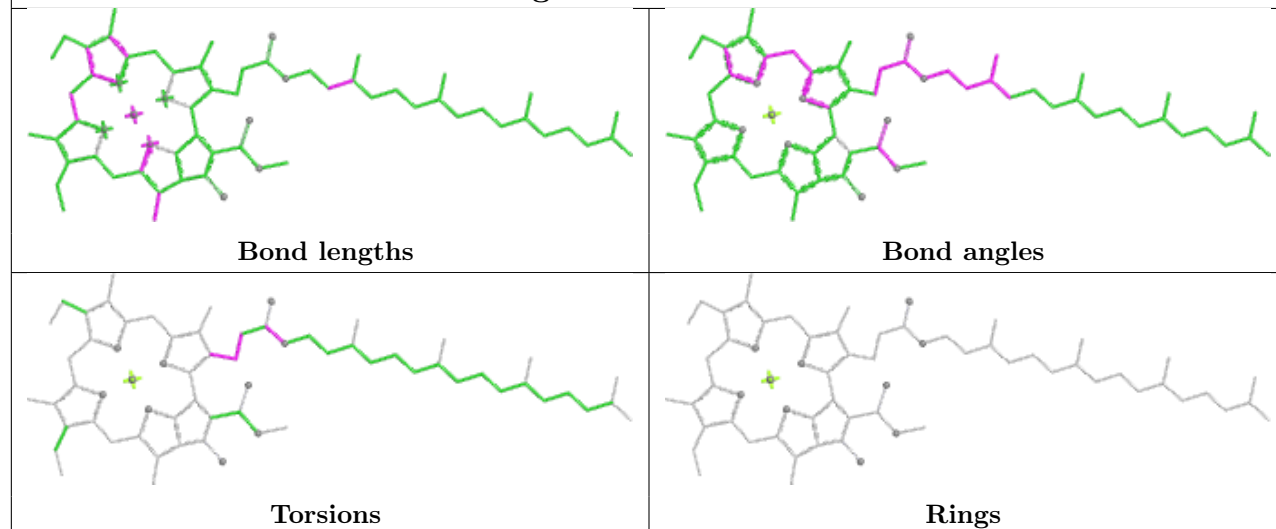


Ligand CLA B 807	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR J 104	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG G 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

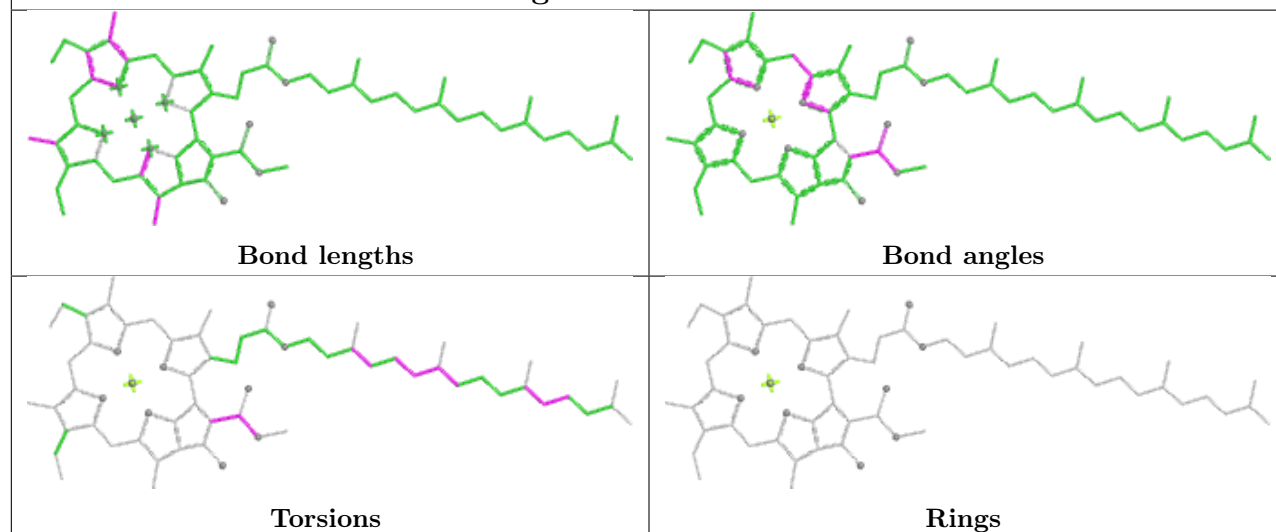
Ligand CLA B 823



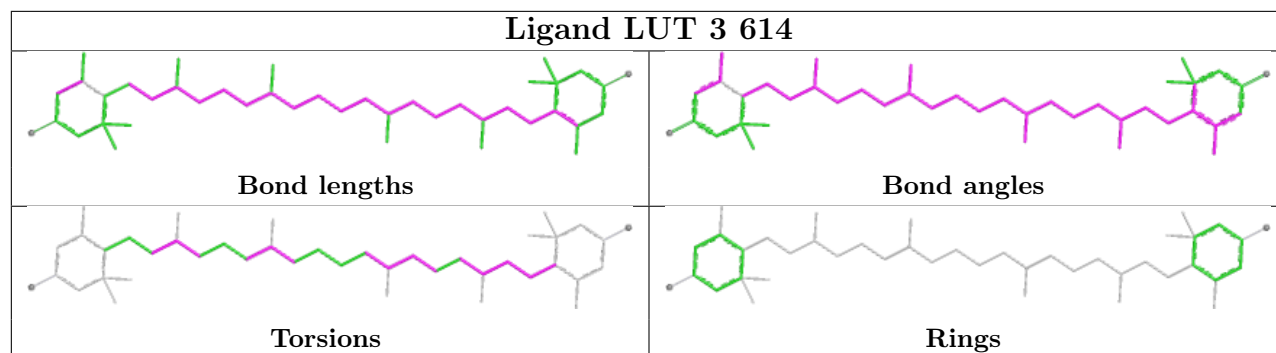
Ligand CLA B 830



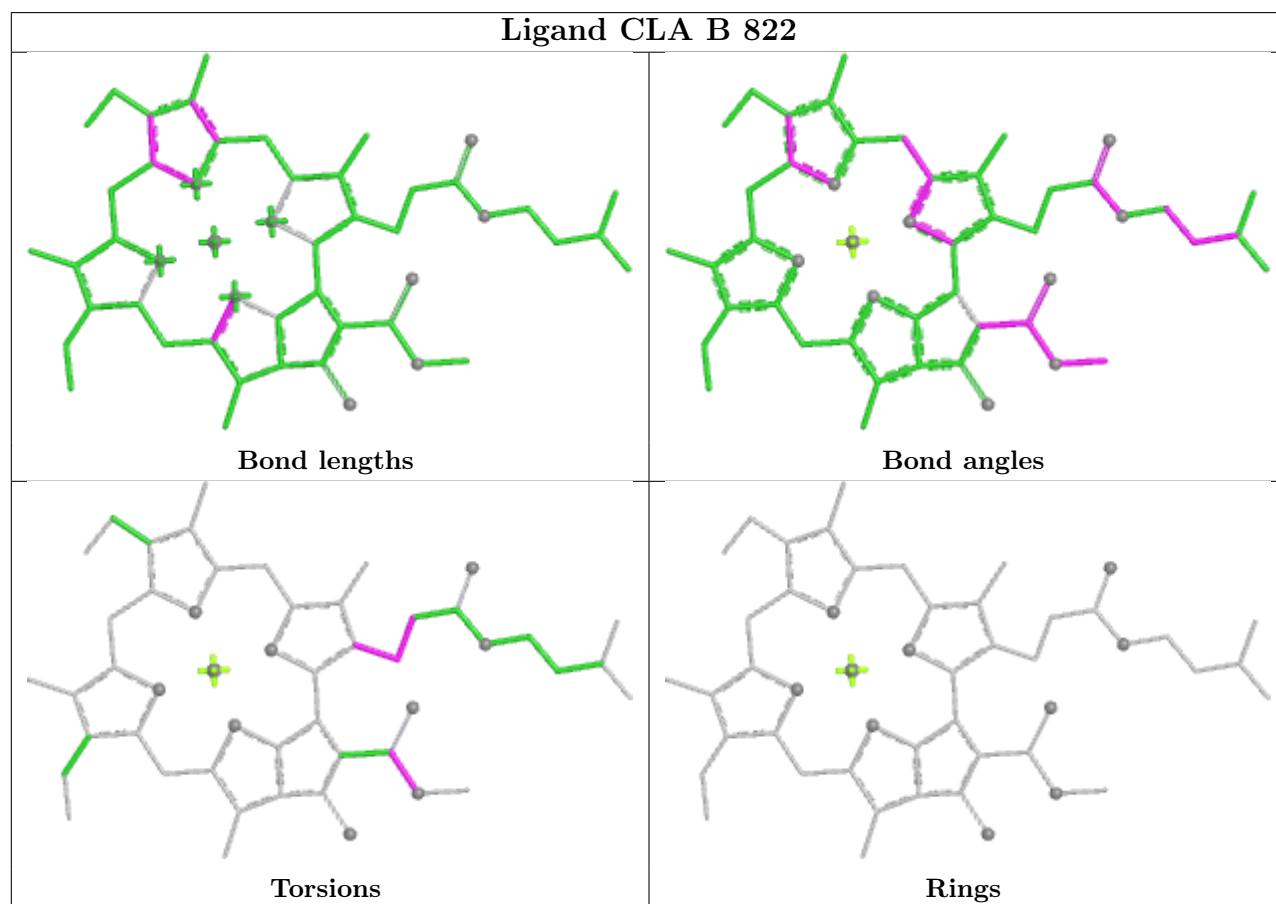
Ligand CLA A 829



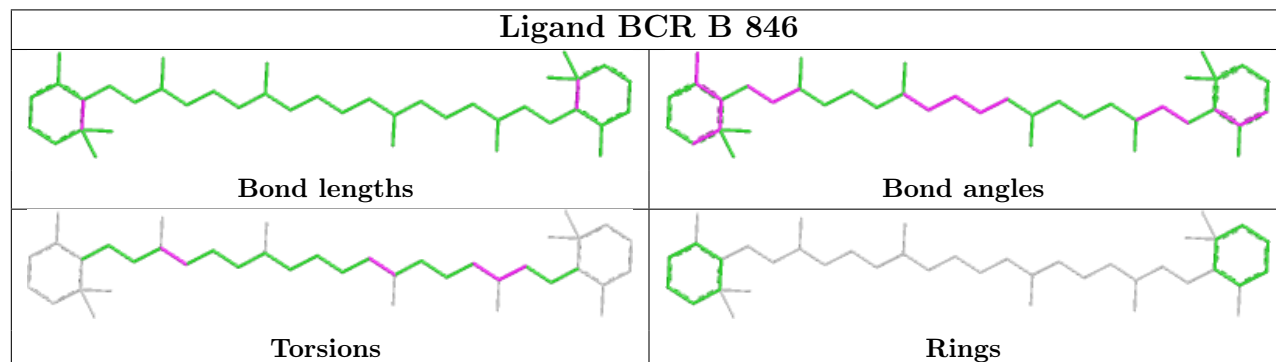
Ligand LUT 3 614



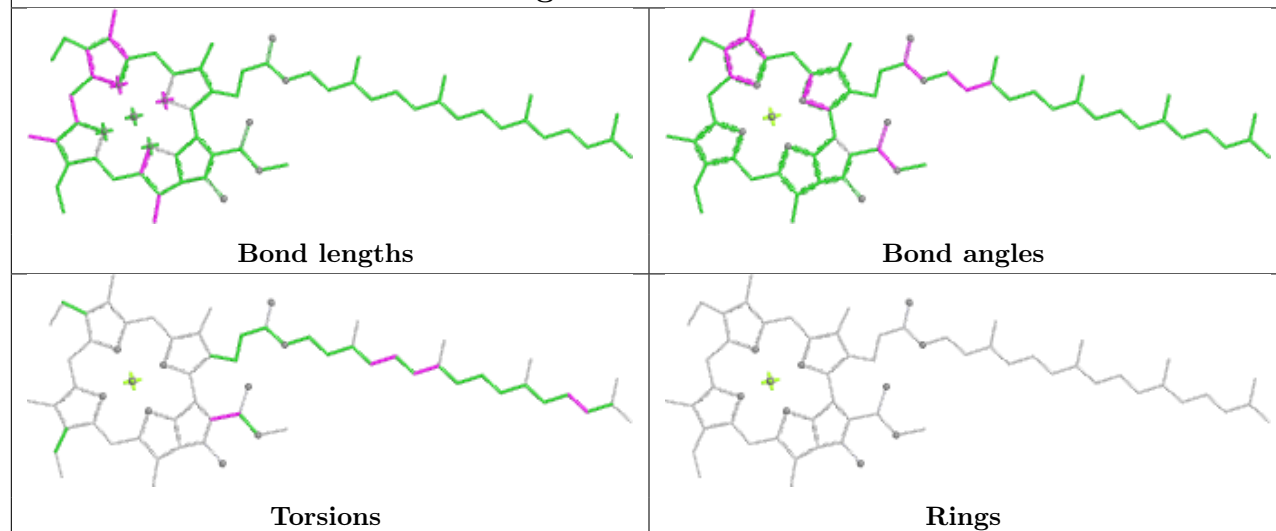
Ligand CLA B 822



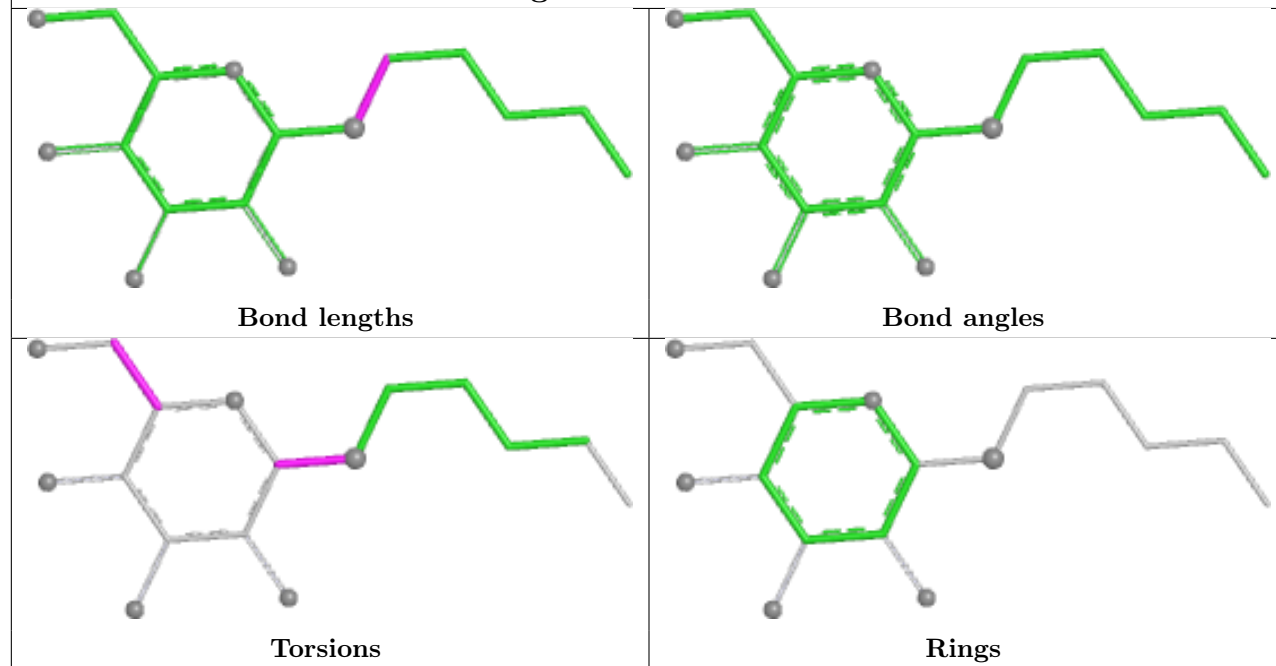
Ligand BCR B 846



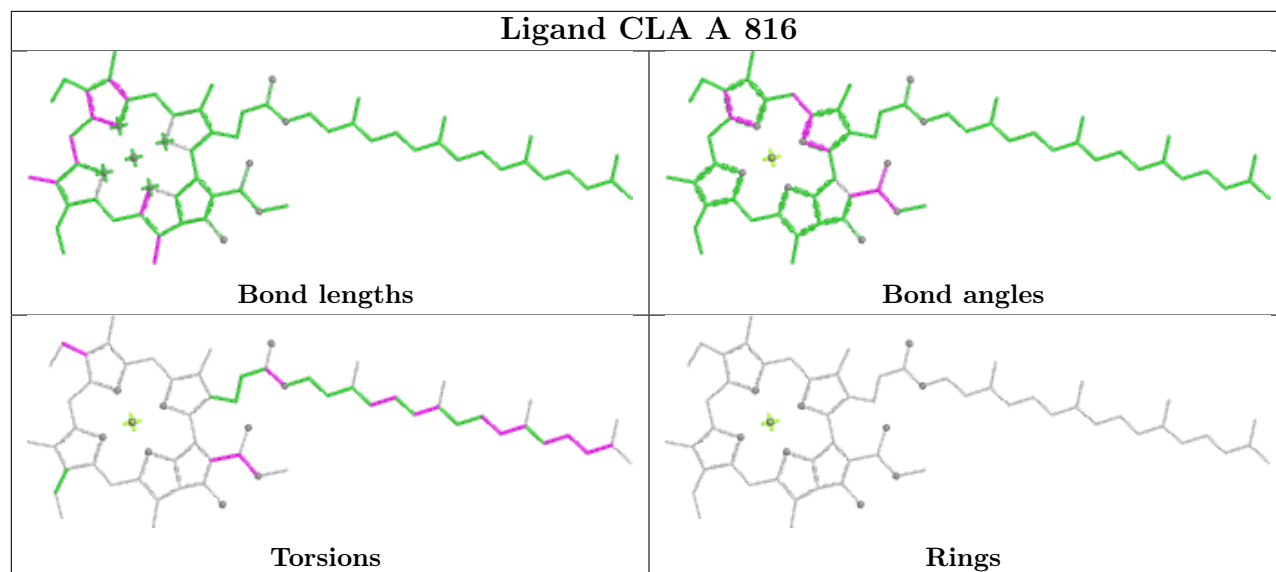
Ligand CLA 2 301



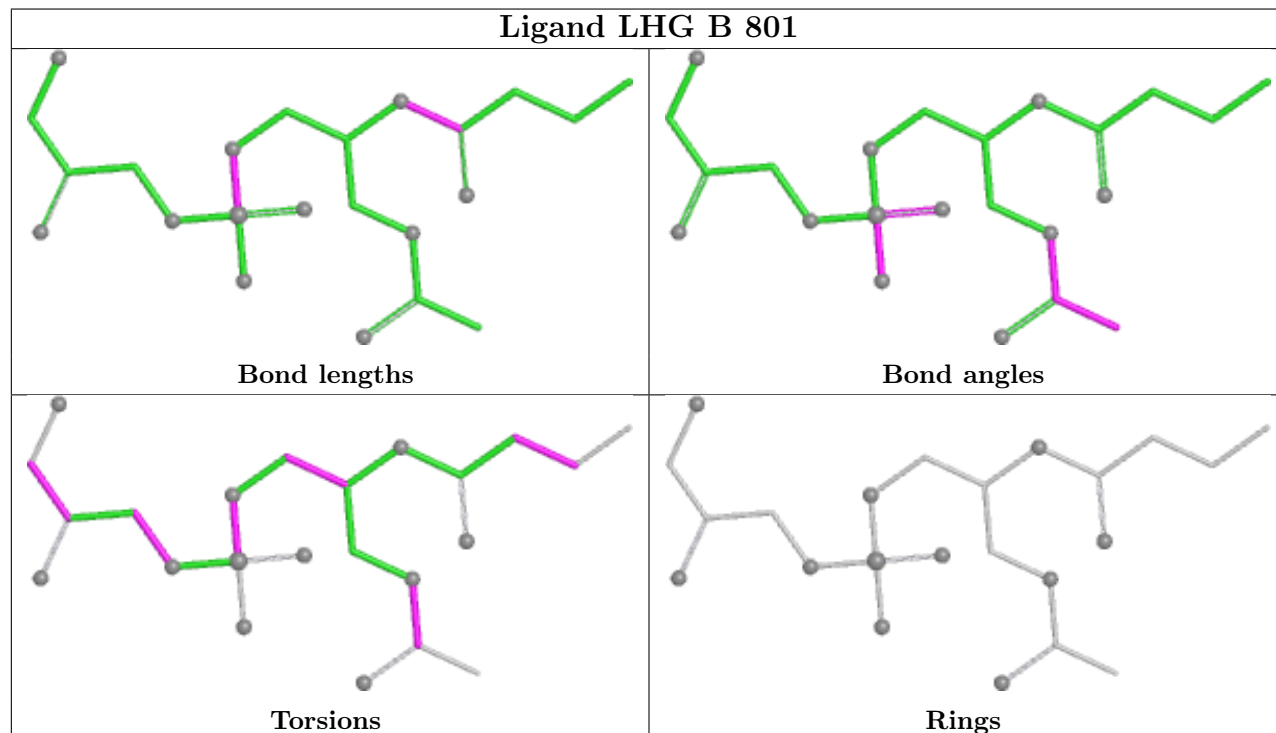
Ligand HTG F 301



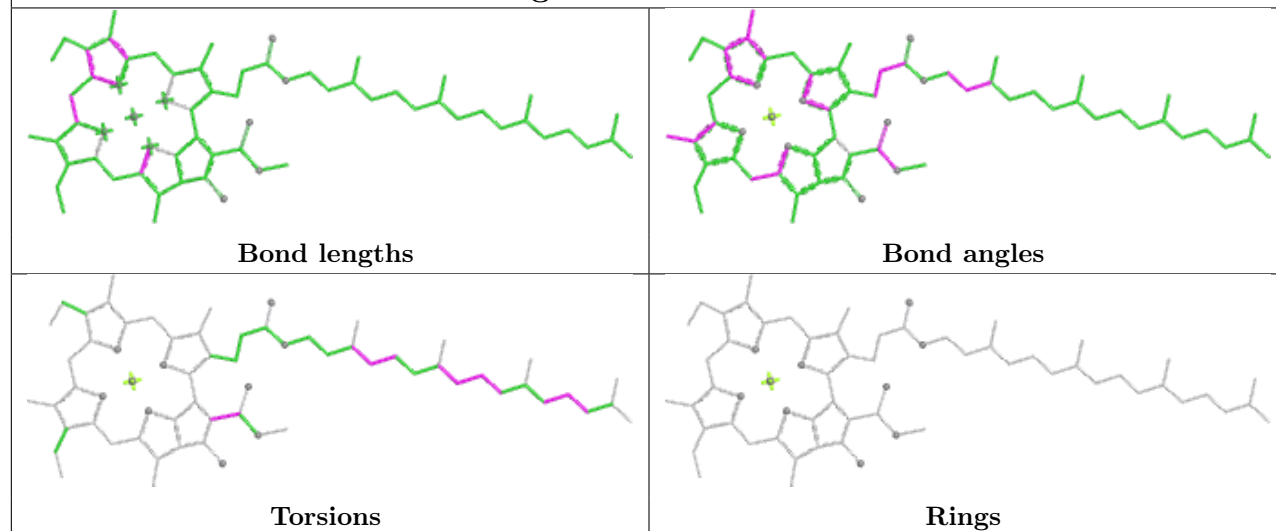
Ligand CLA A 816



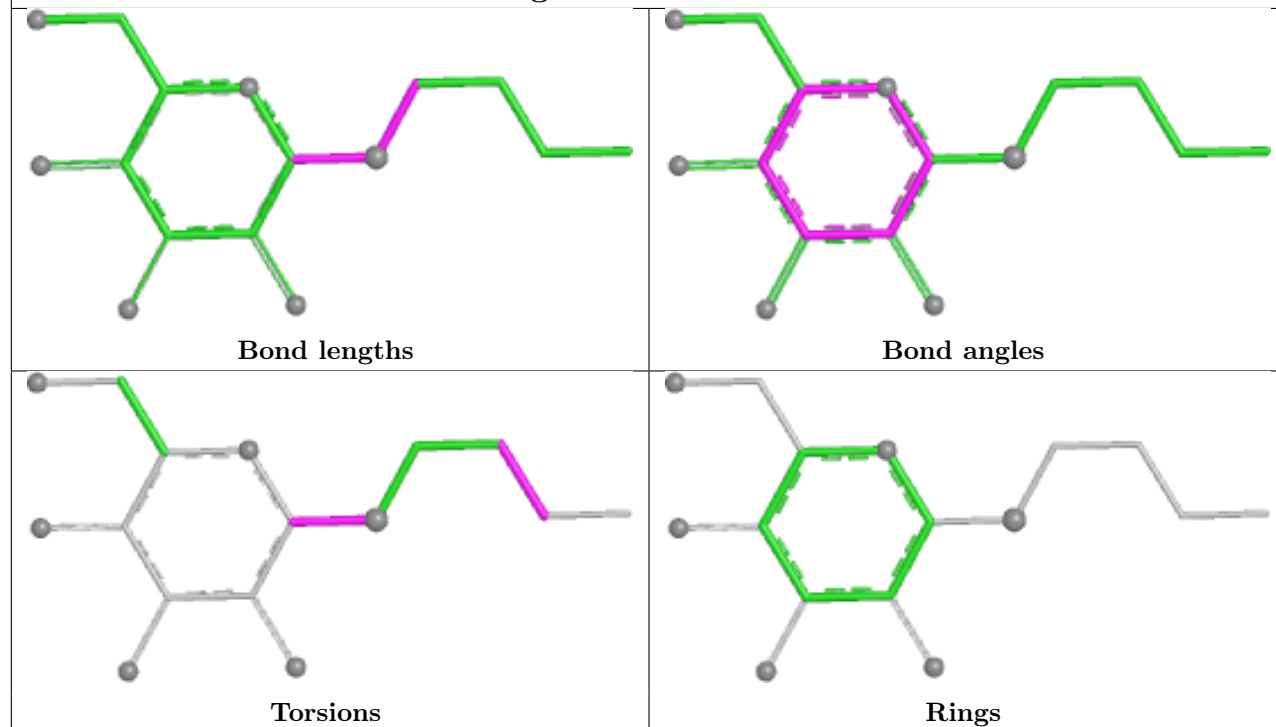
Ligand LHG B 801



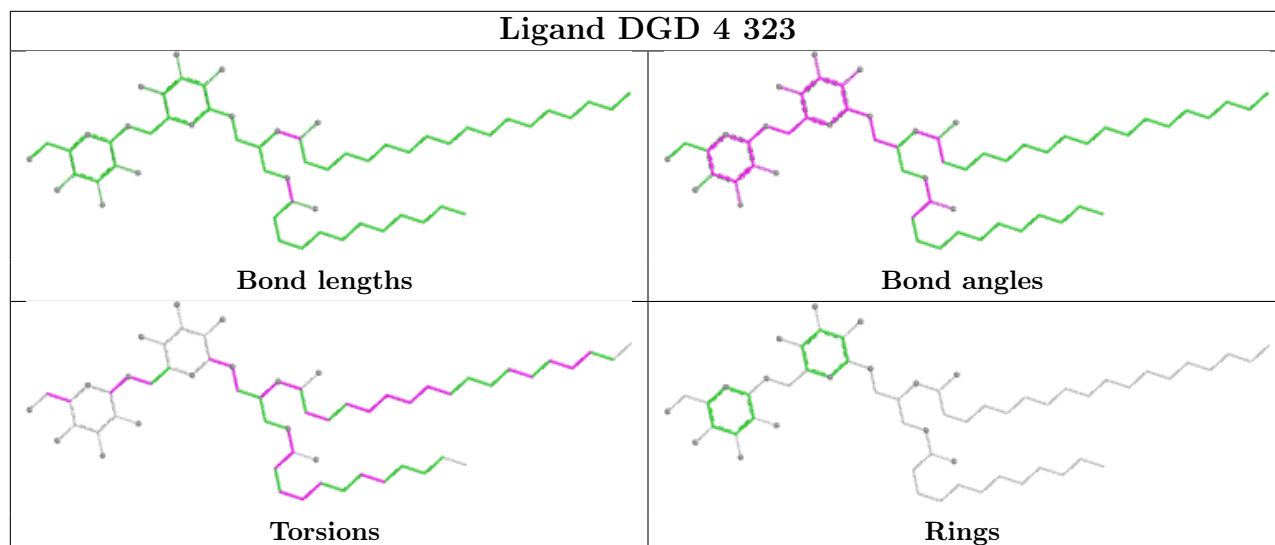
Ligand CLA A 804



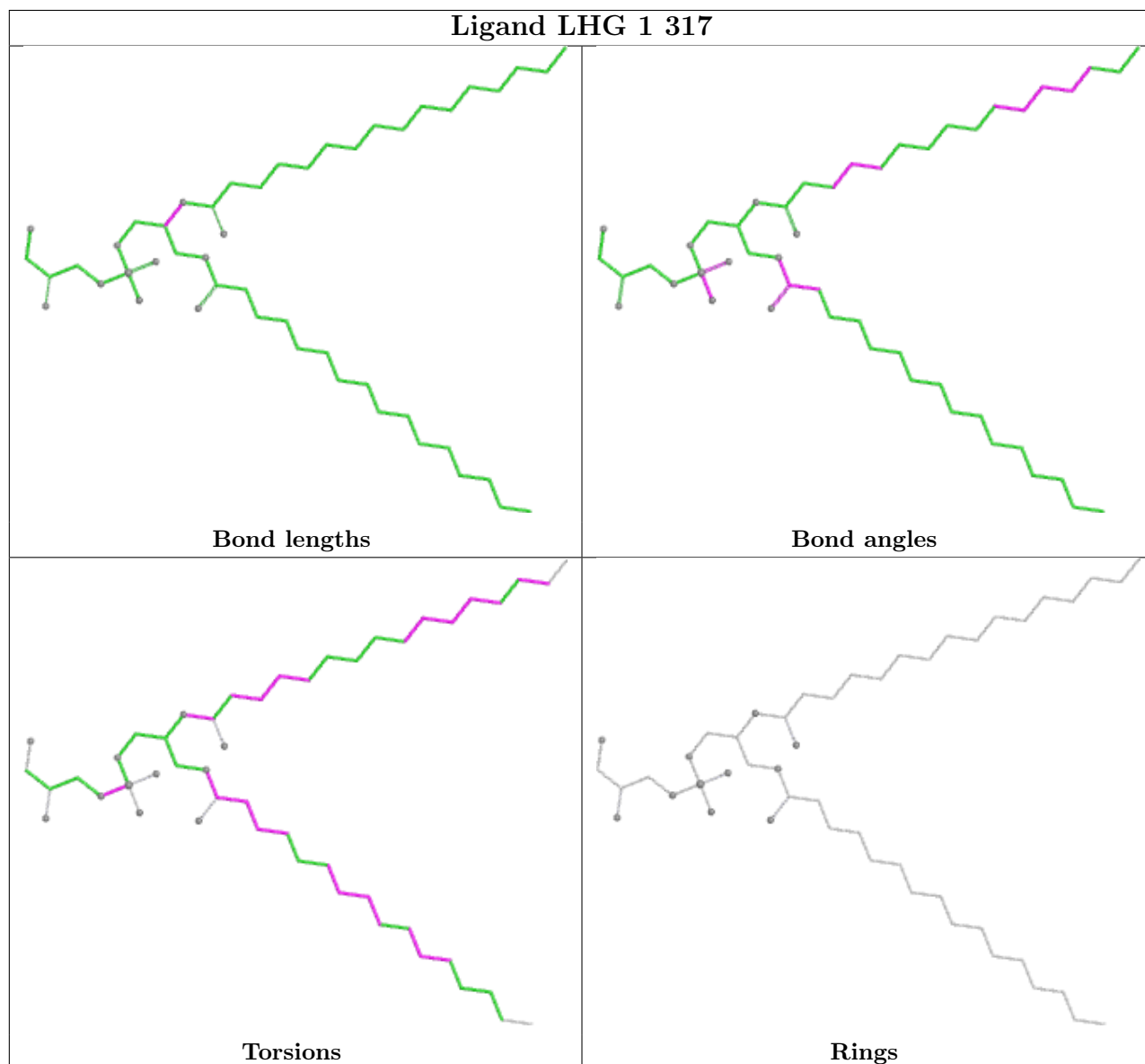
Ligand HTG F 310



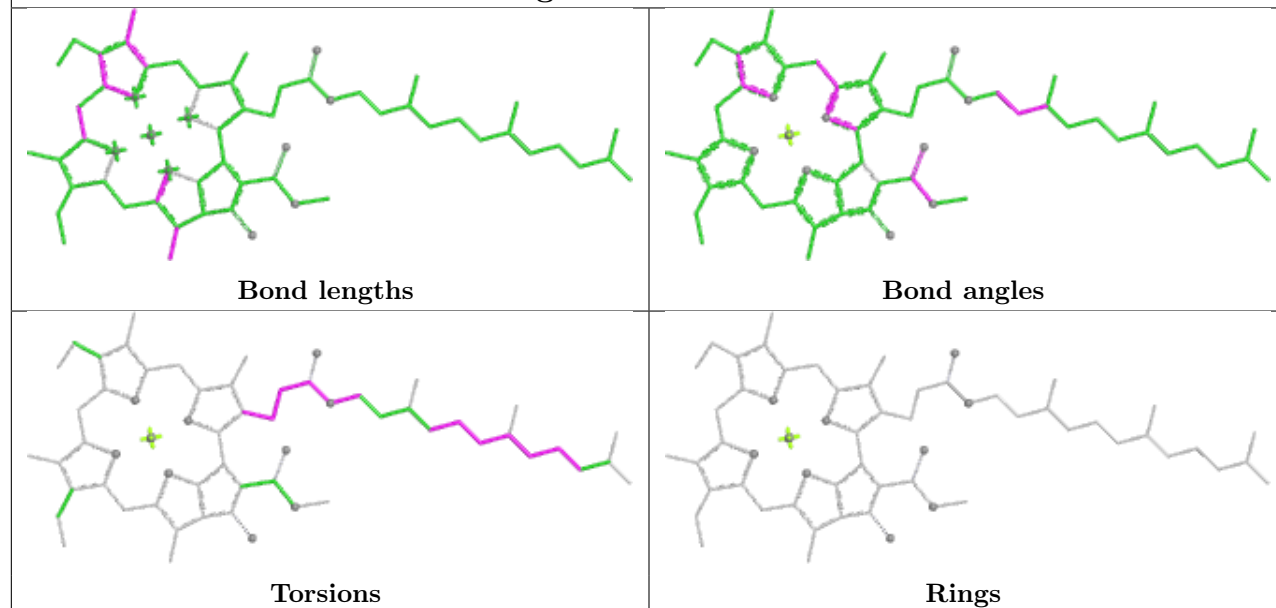
Ligand DGD 4 323



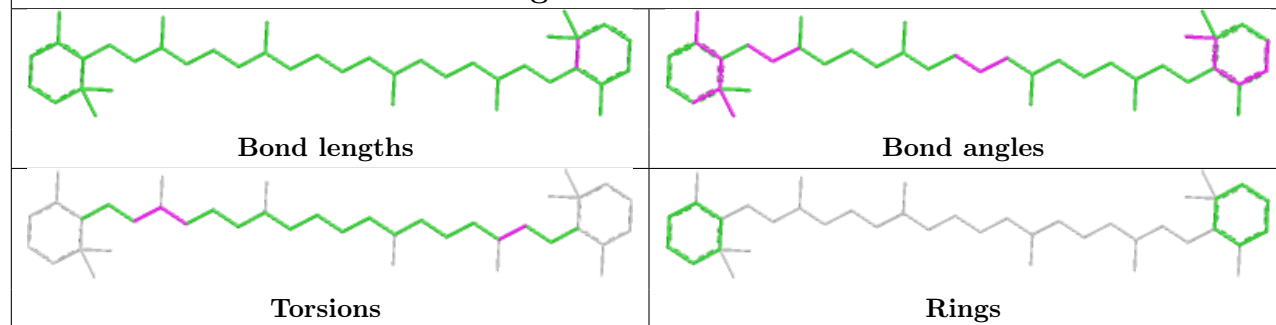
Ligand LHG 1 317



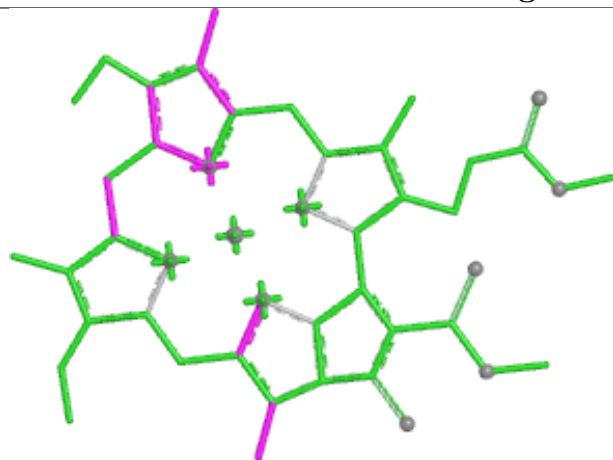
Ligand CLA 2 303



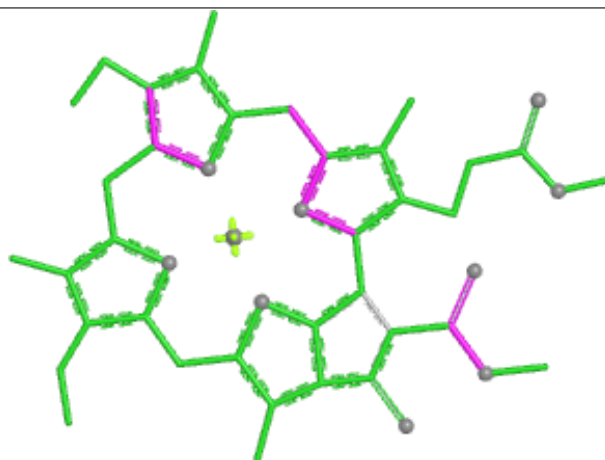
Ligand BCR B 845



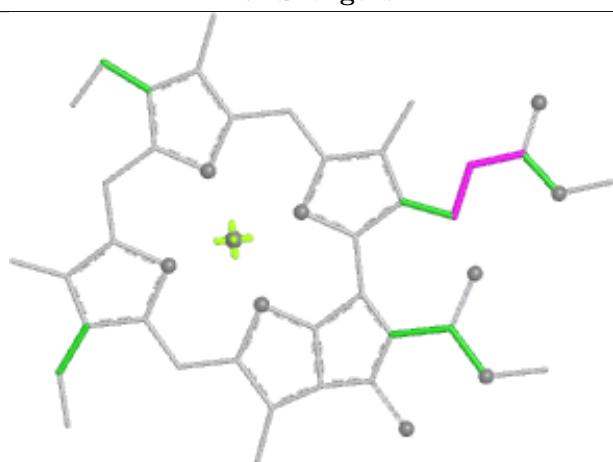
Ligand CLA 3 613



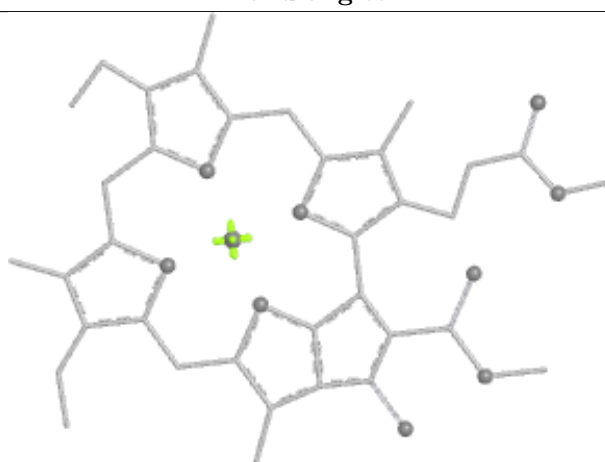
Bond lengths



Bond angles

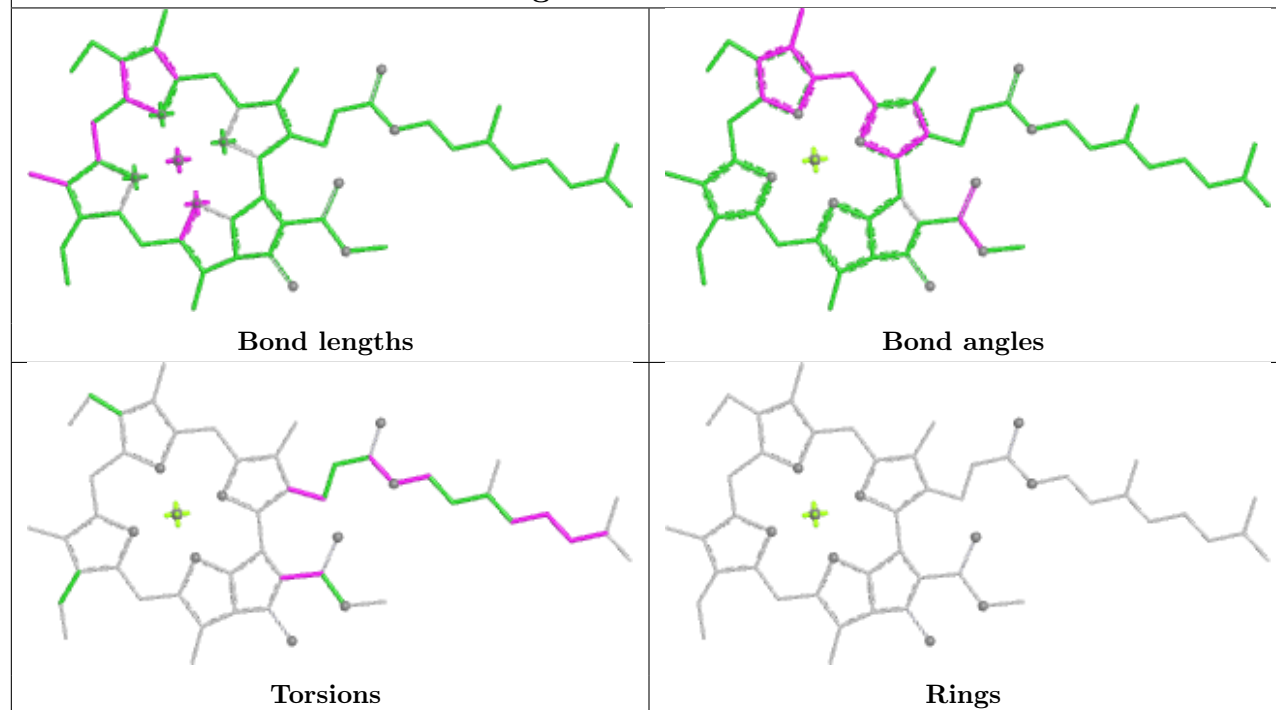


Torsions

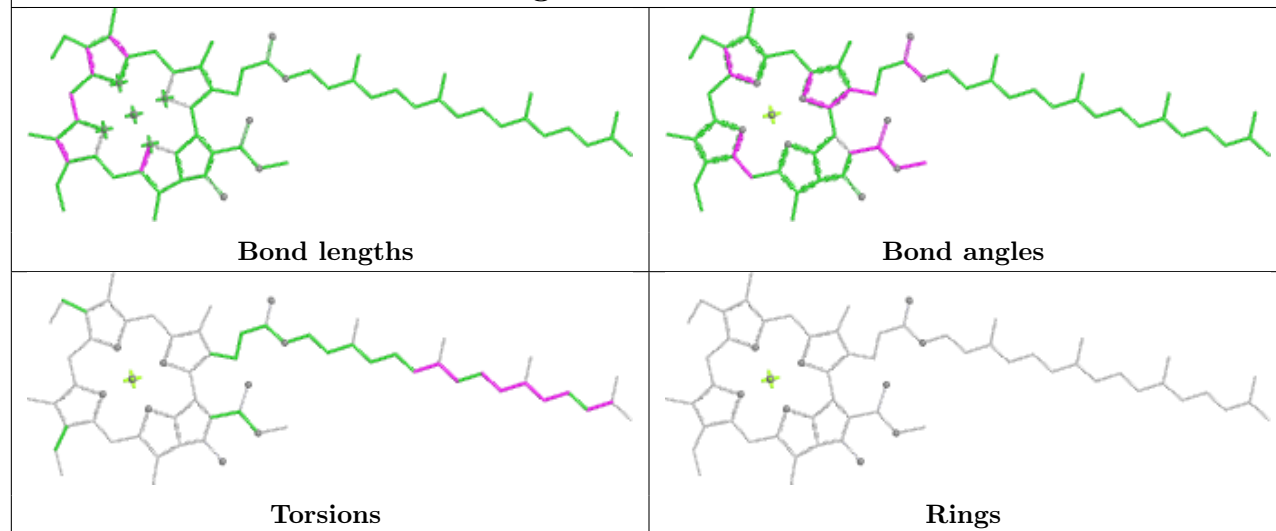


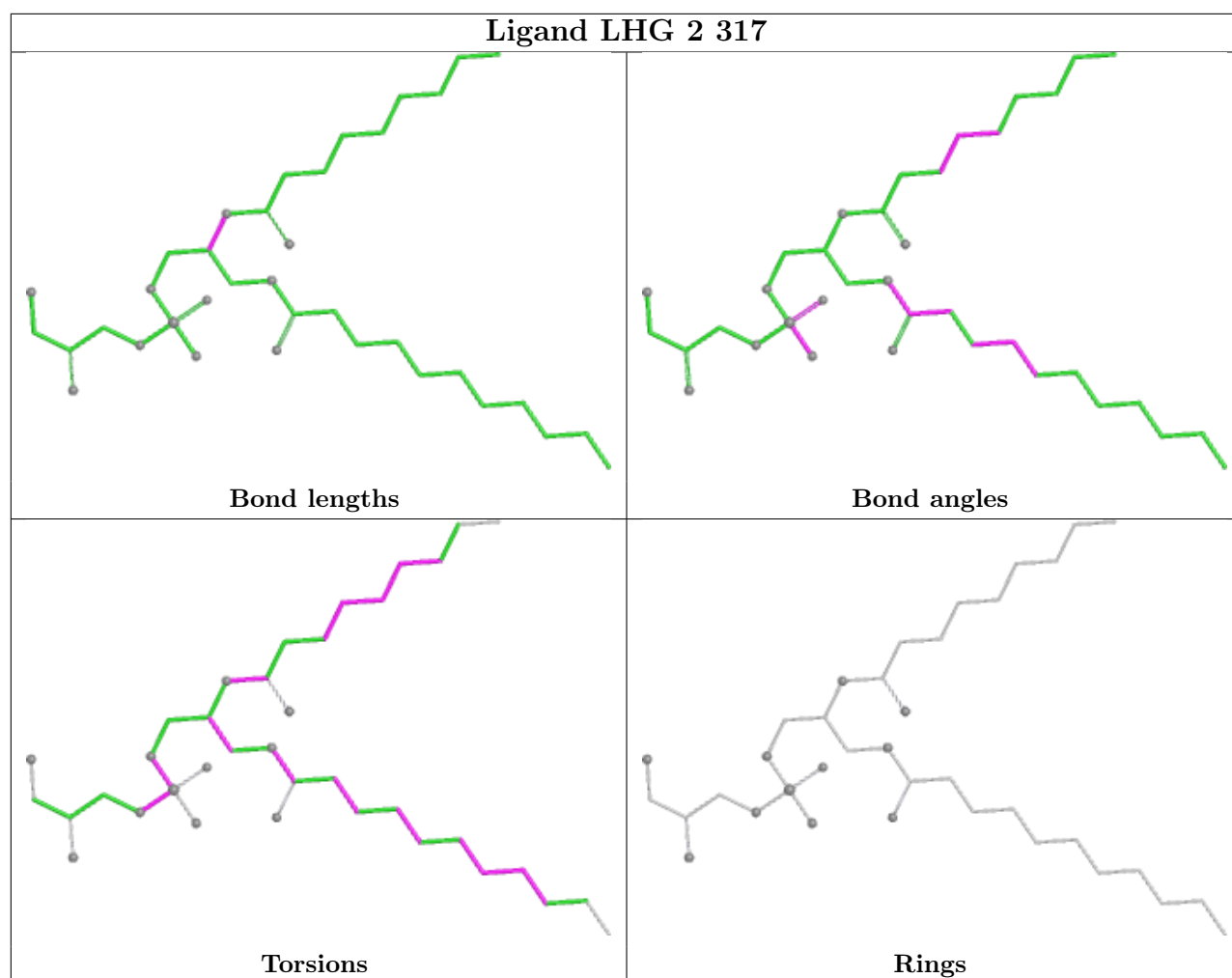
Rings

Ligand CLA B 817

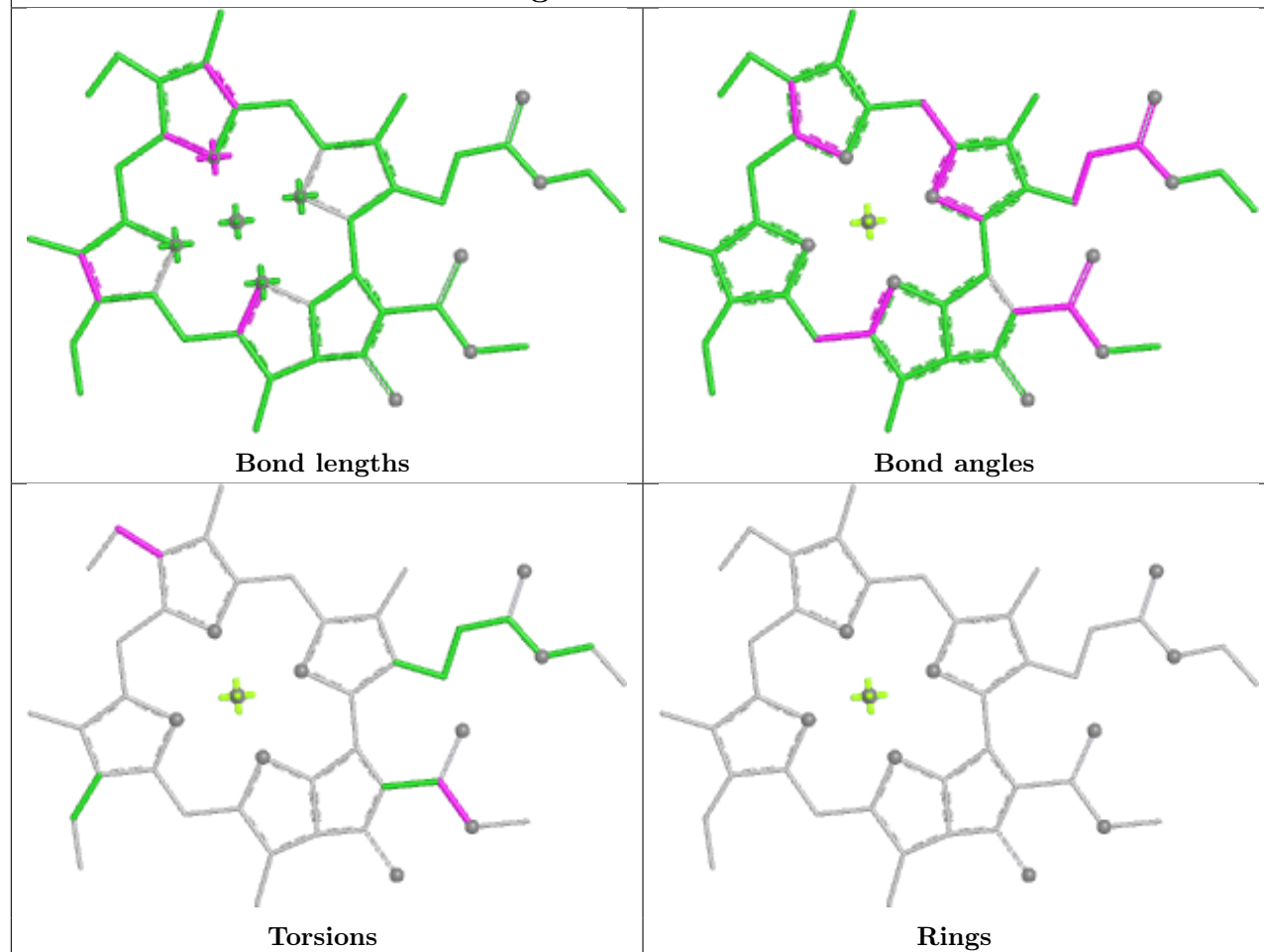


Ligand CLA B 827

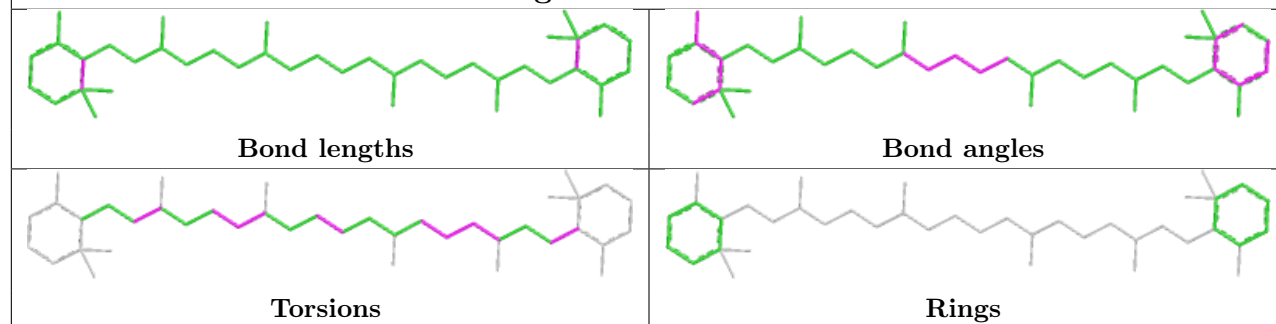




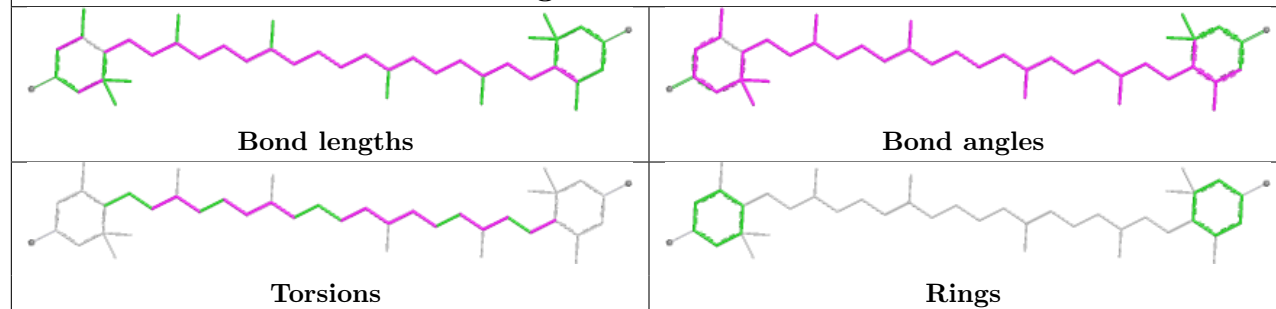
Ligand CLA 4 314



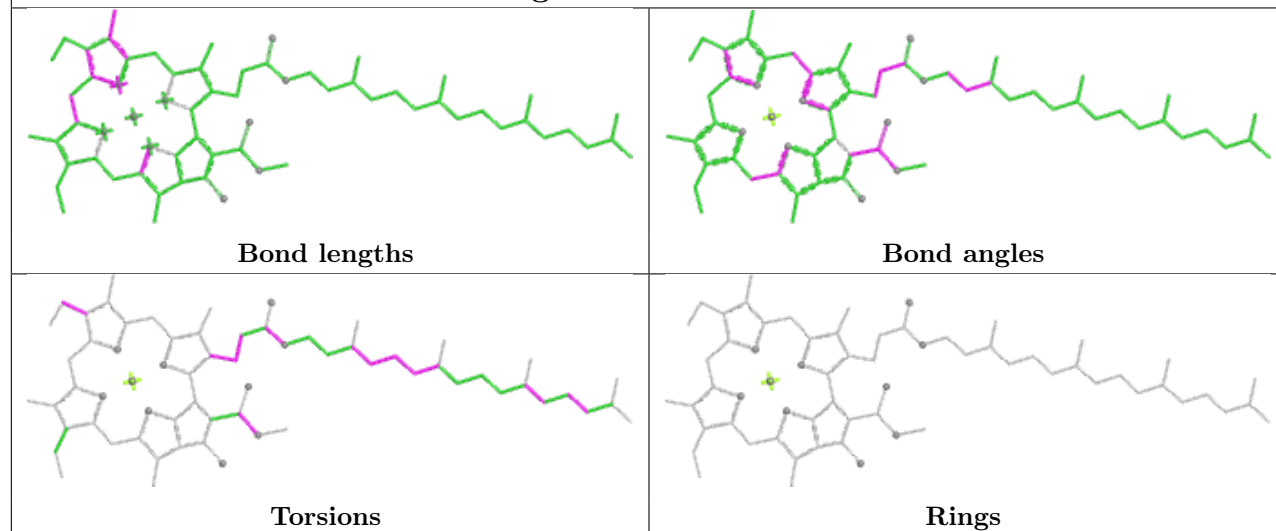
Ligand BCR 1 316



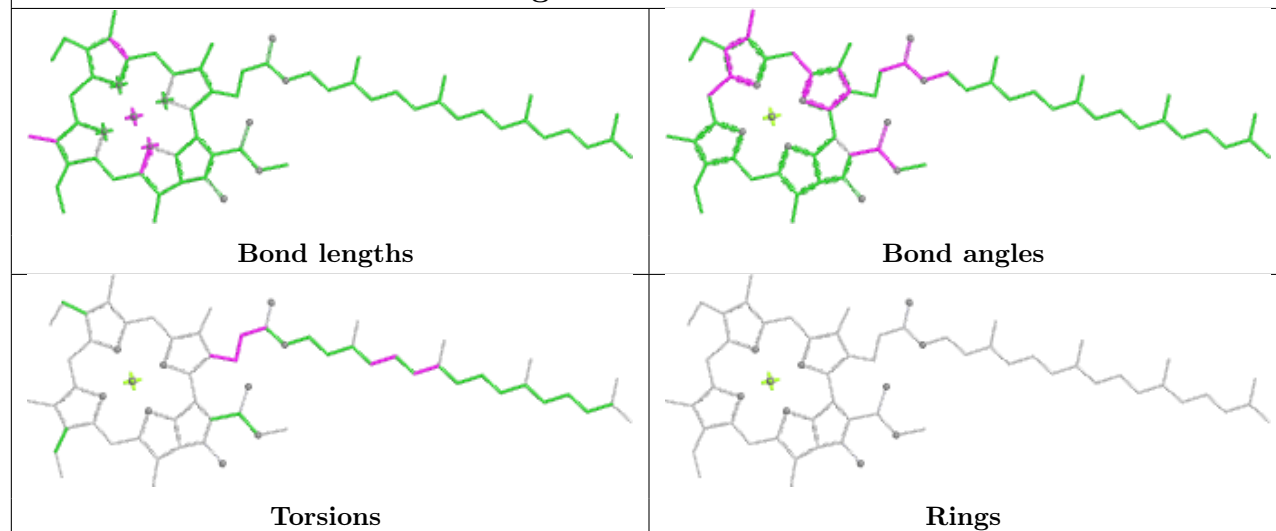
Ligand LUT 4 316



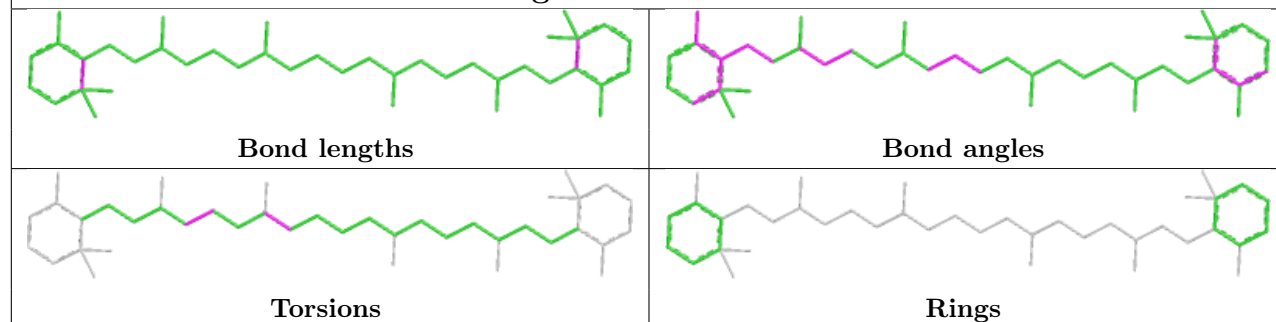
Ligand CLA A 831



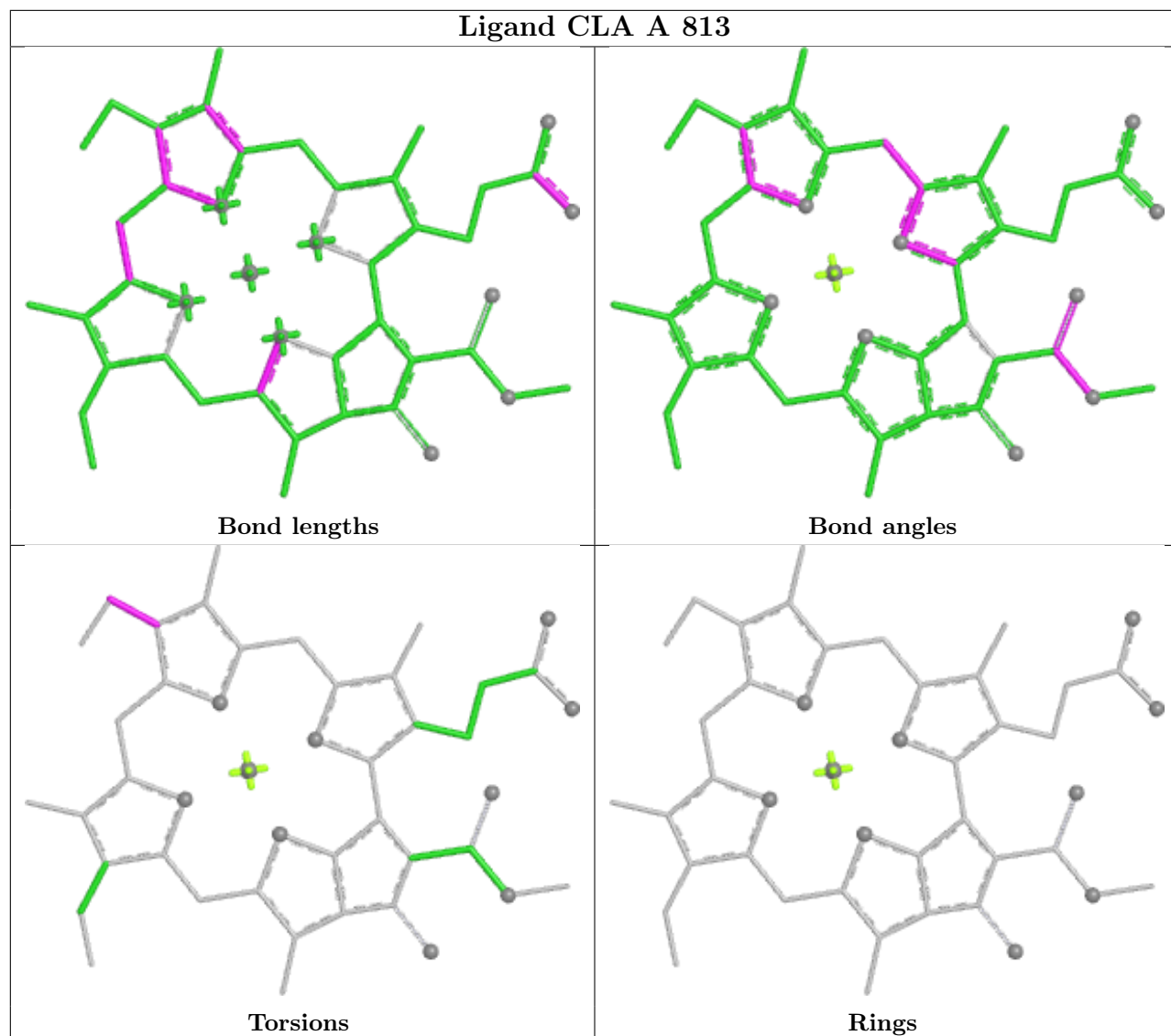
Ligand CLA A 808

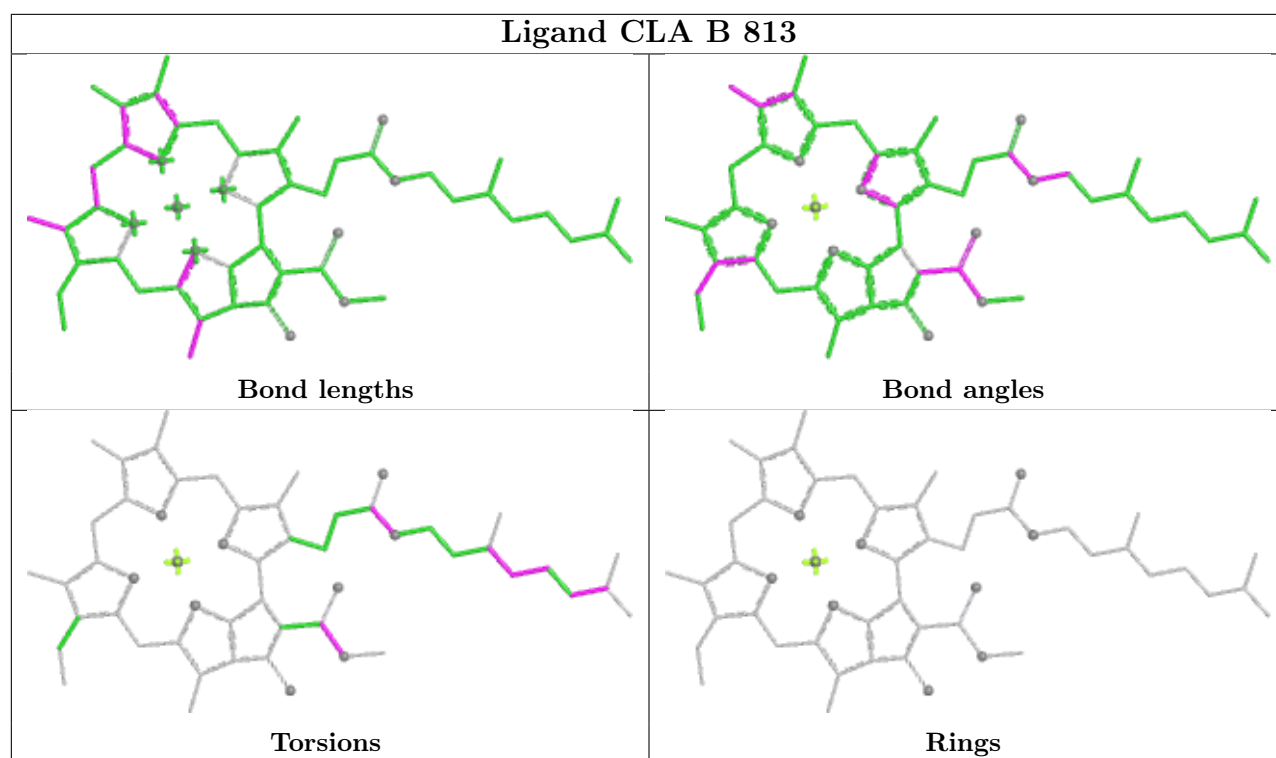


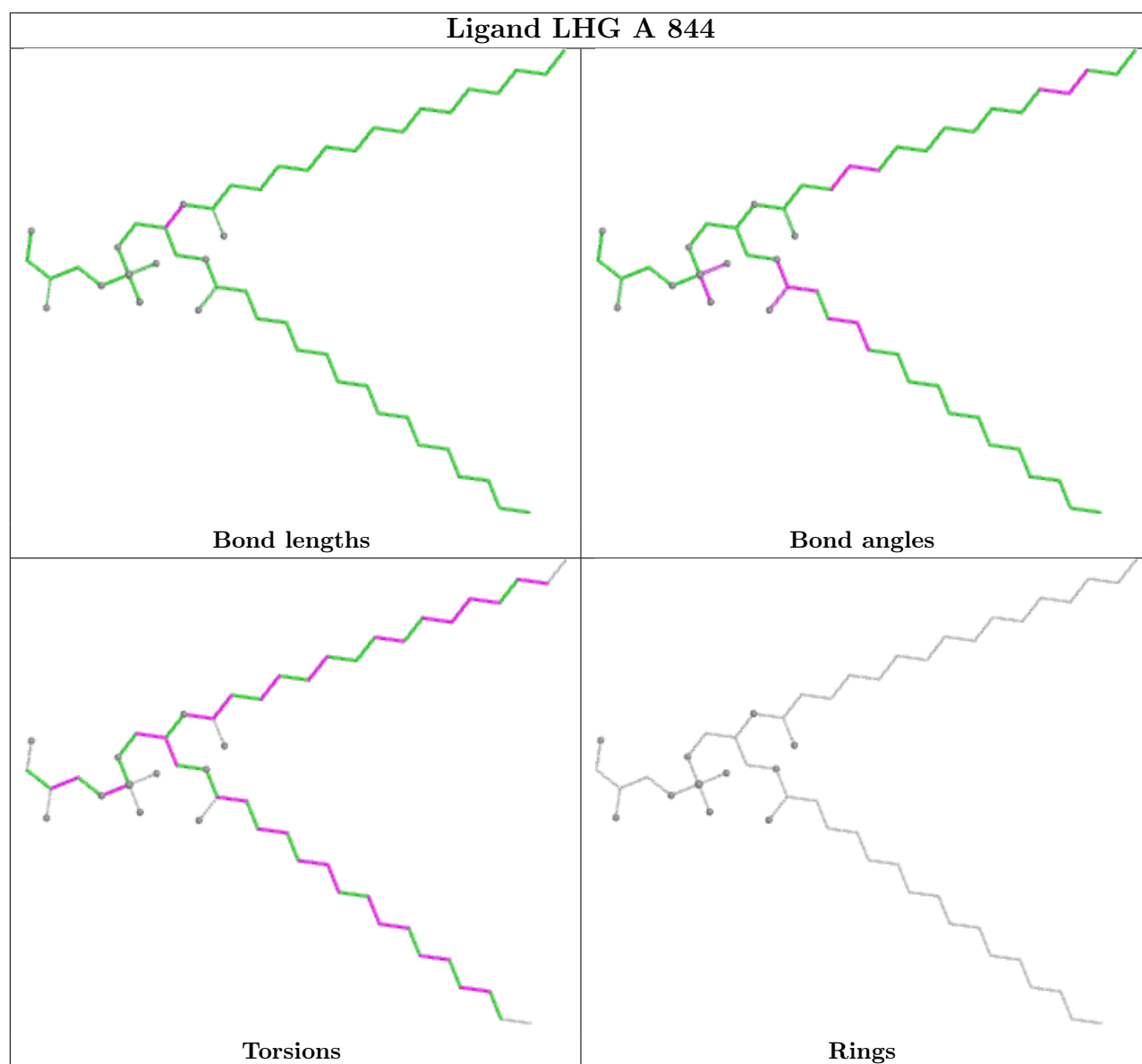
Ligand BCR F 308



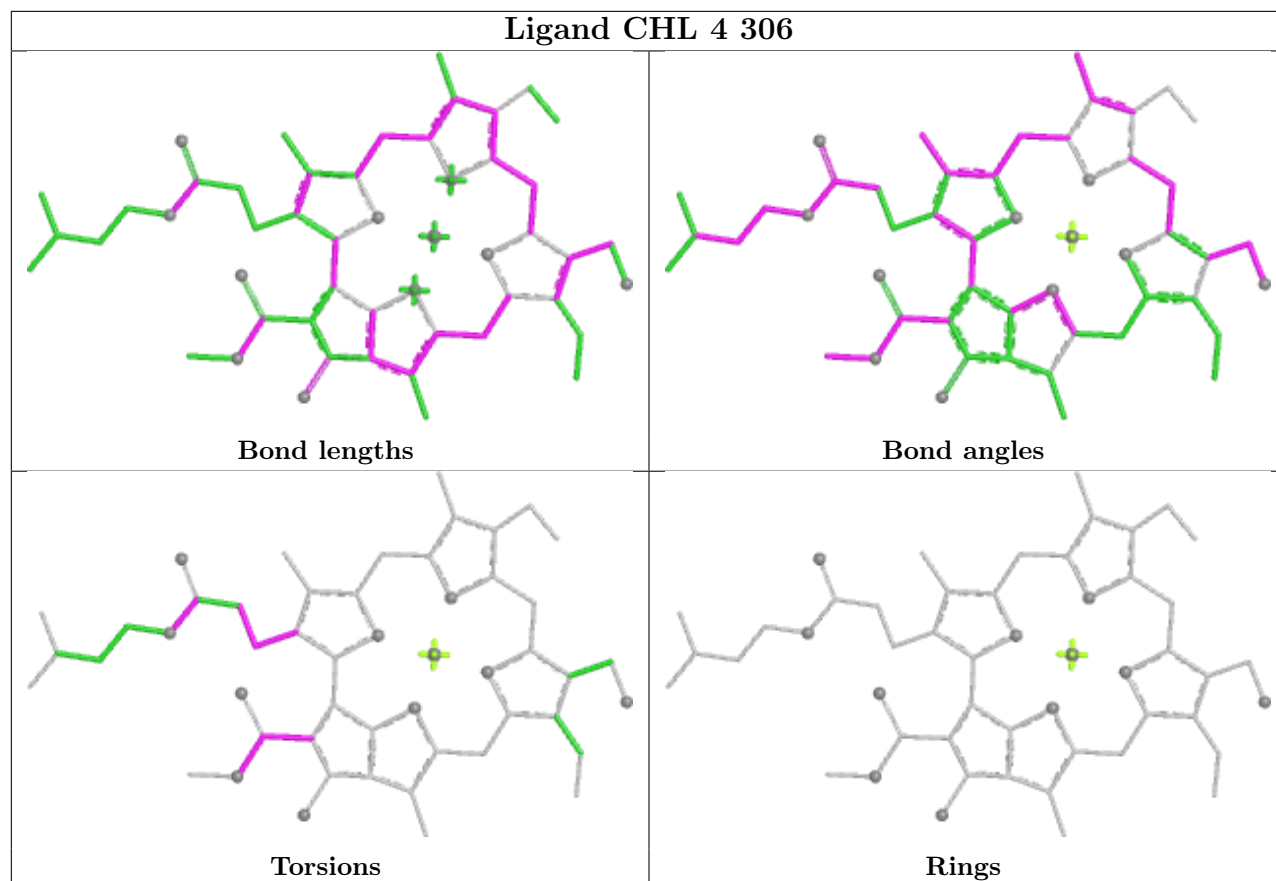
Ligand CLA A 813



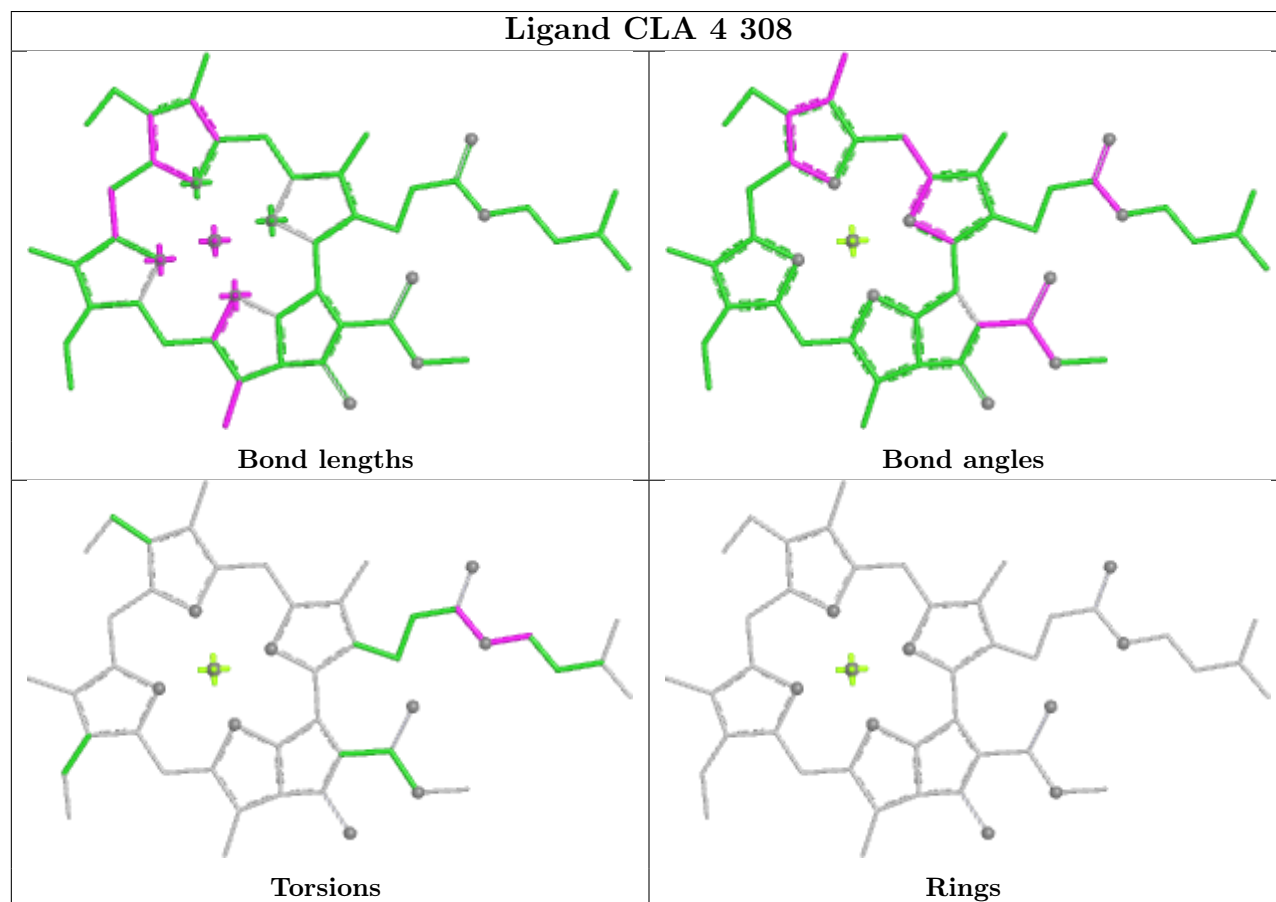


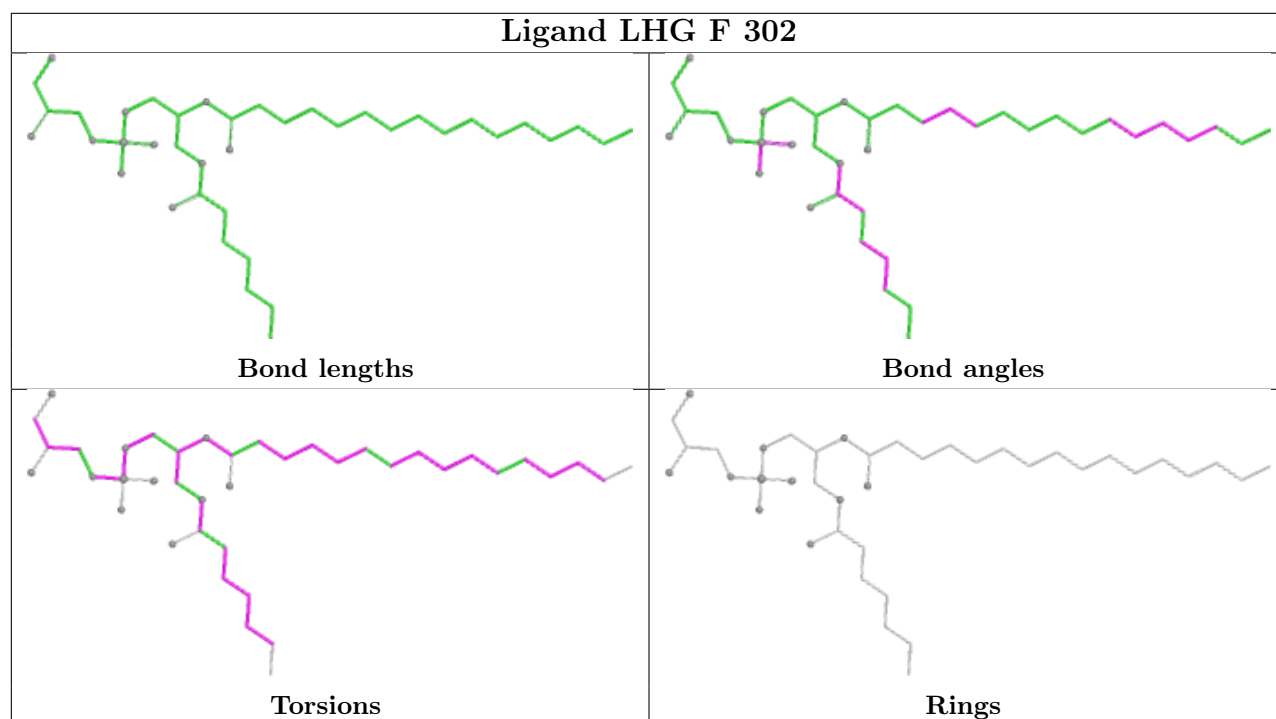
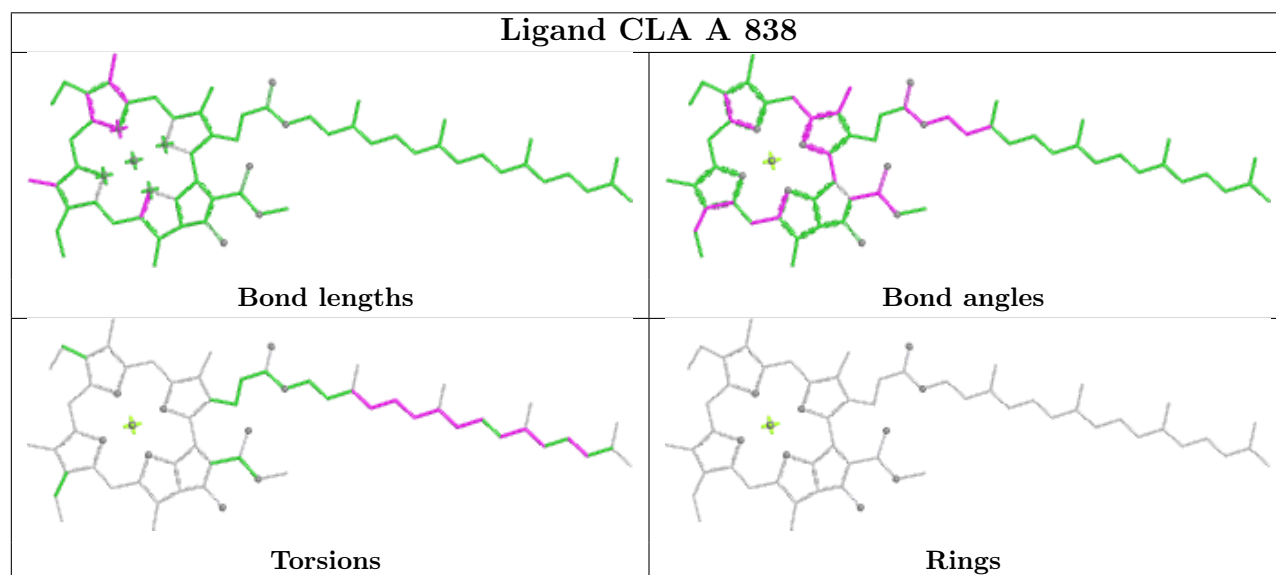
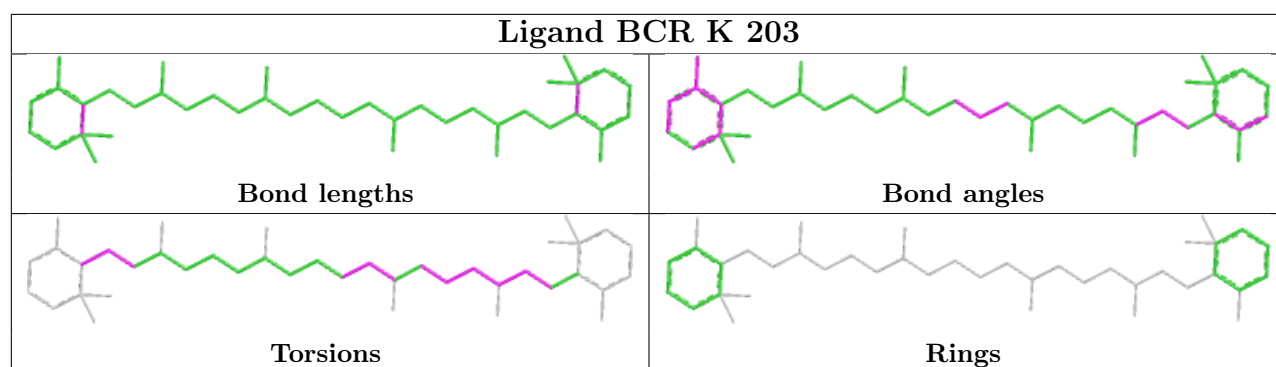


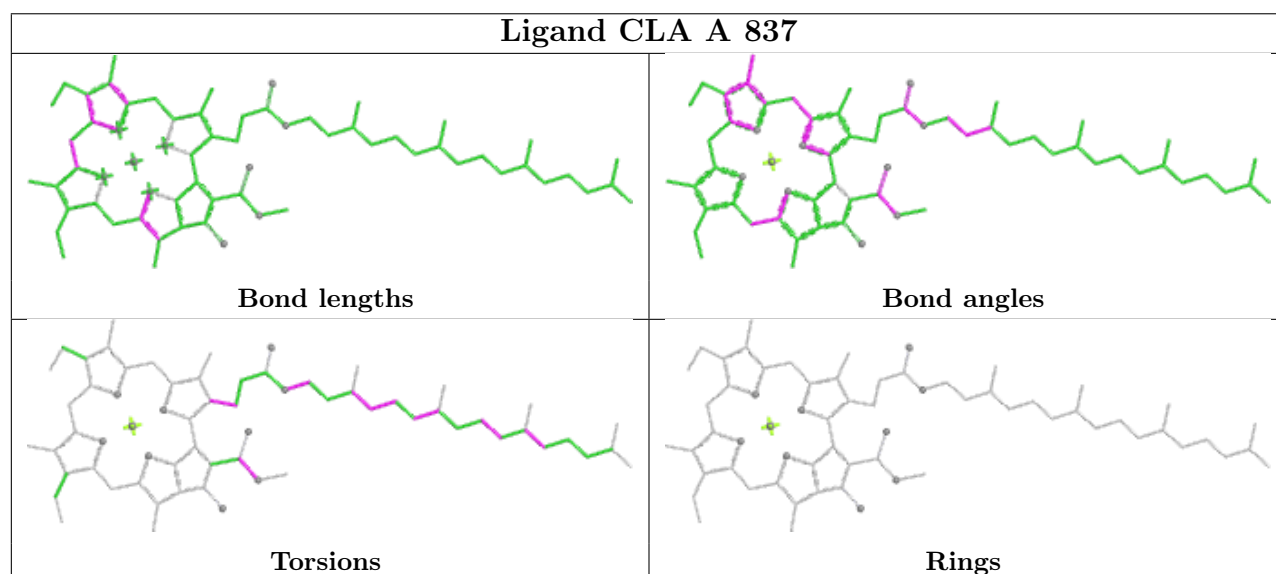
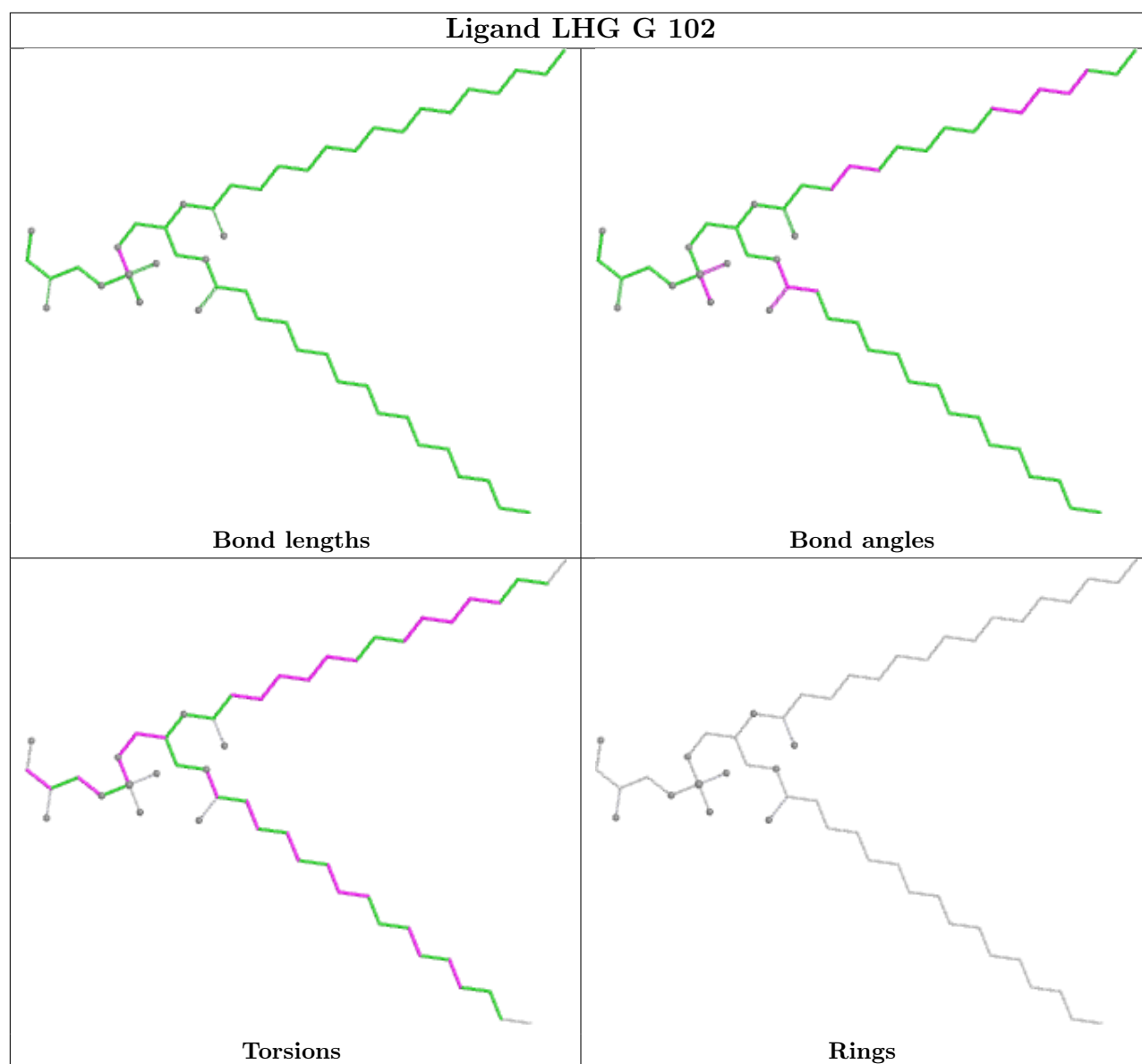
Ligand CHL 4 306



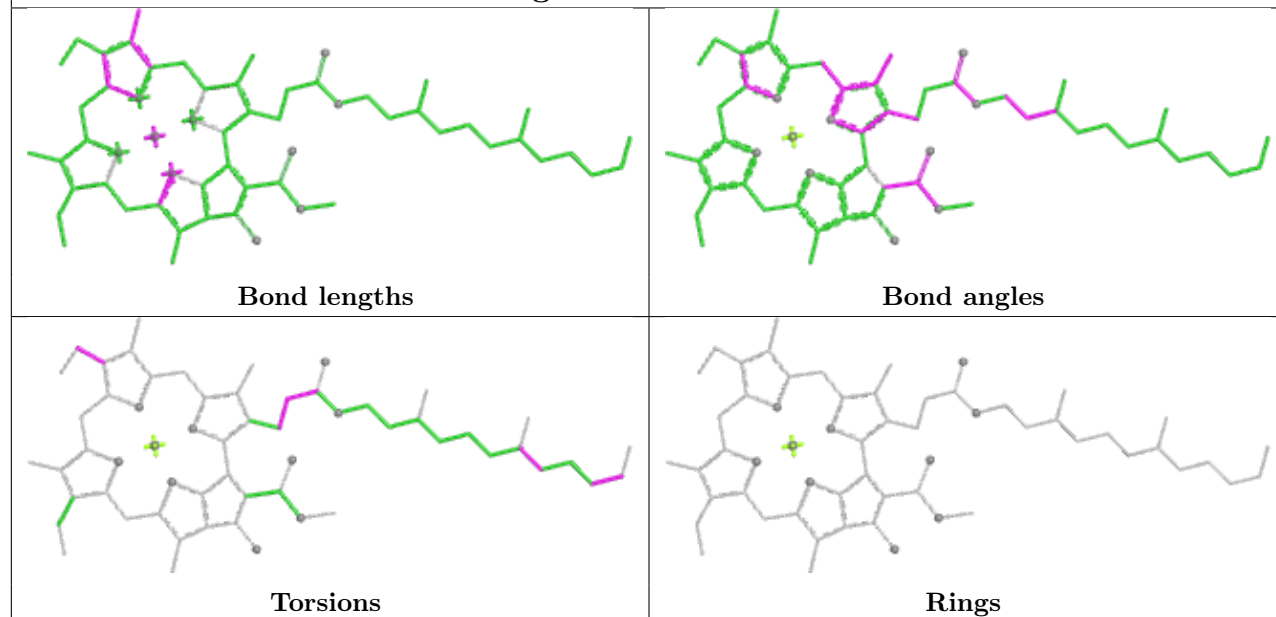
Ligand CLA 4 308



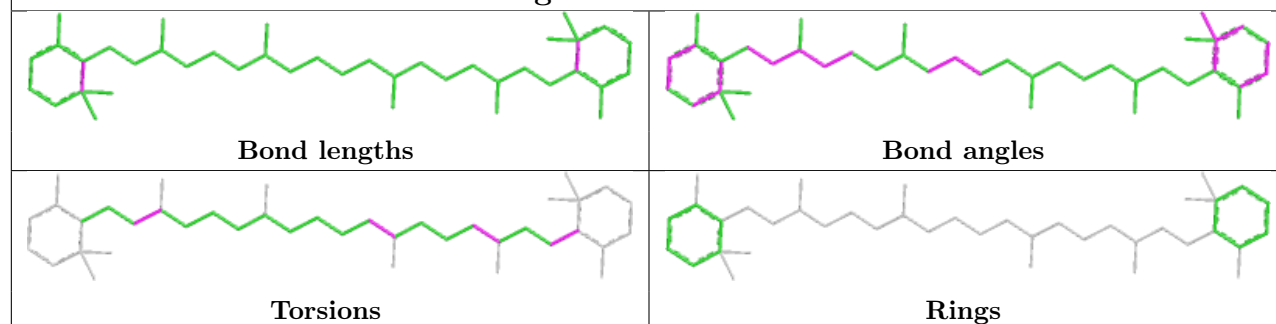




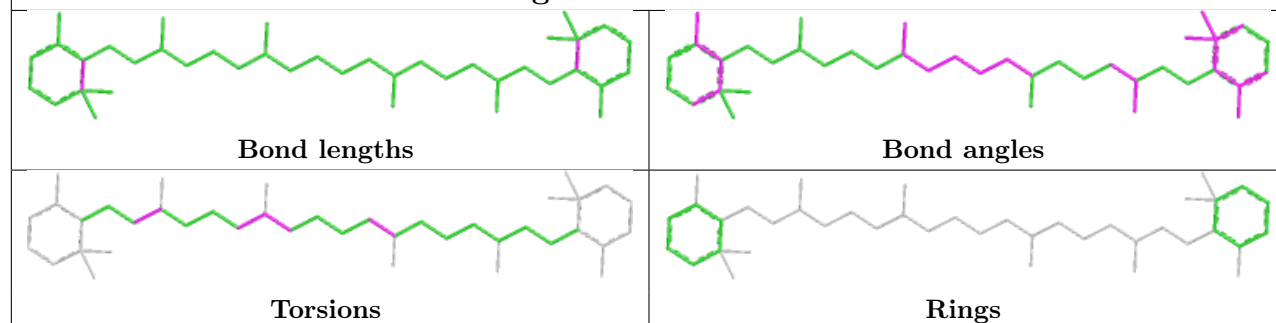
Ligand CLA B 819



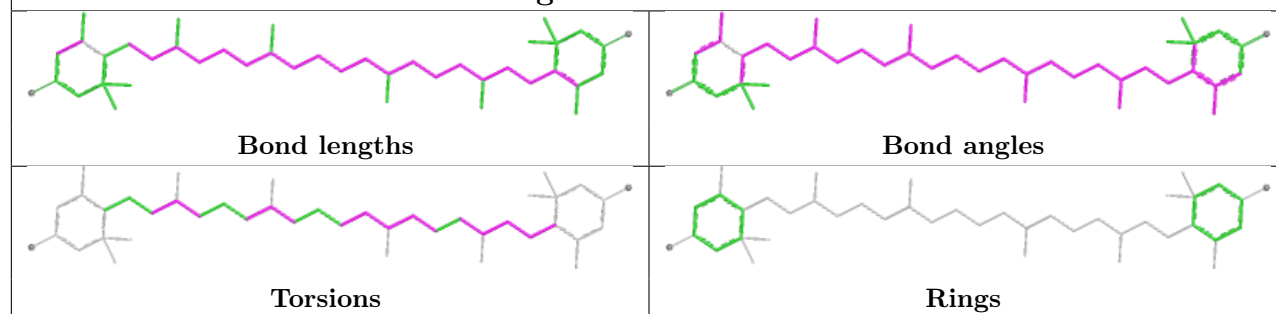
Ligand BCR 4 318



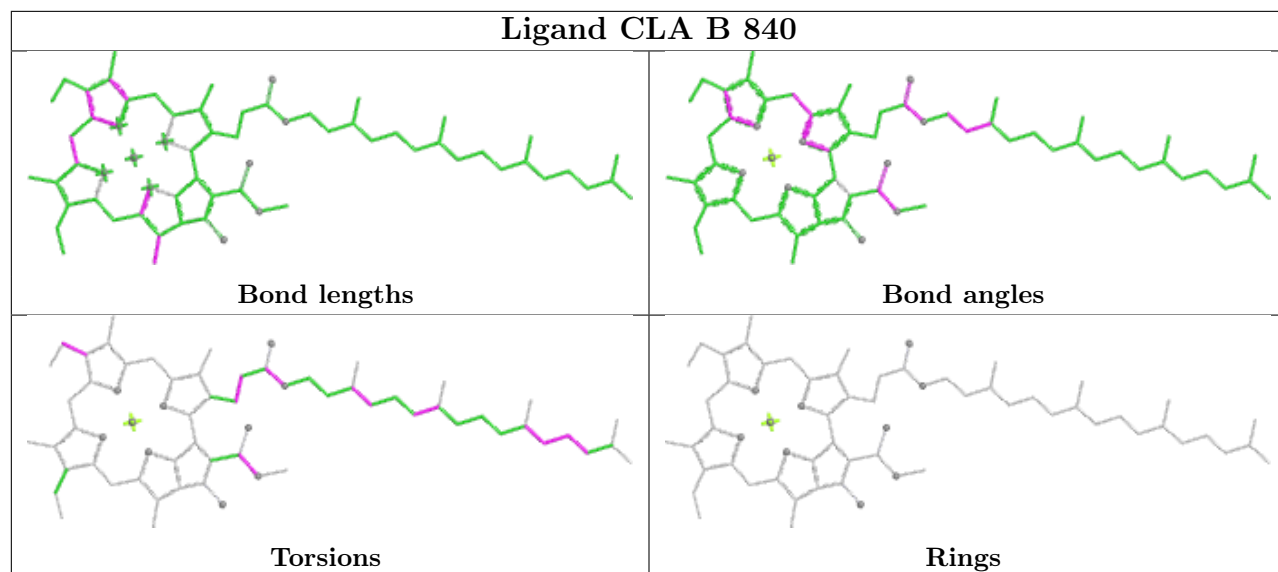
Ligand BCR F 303



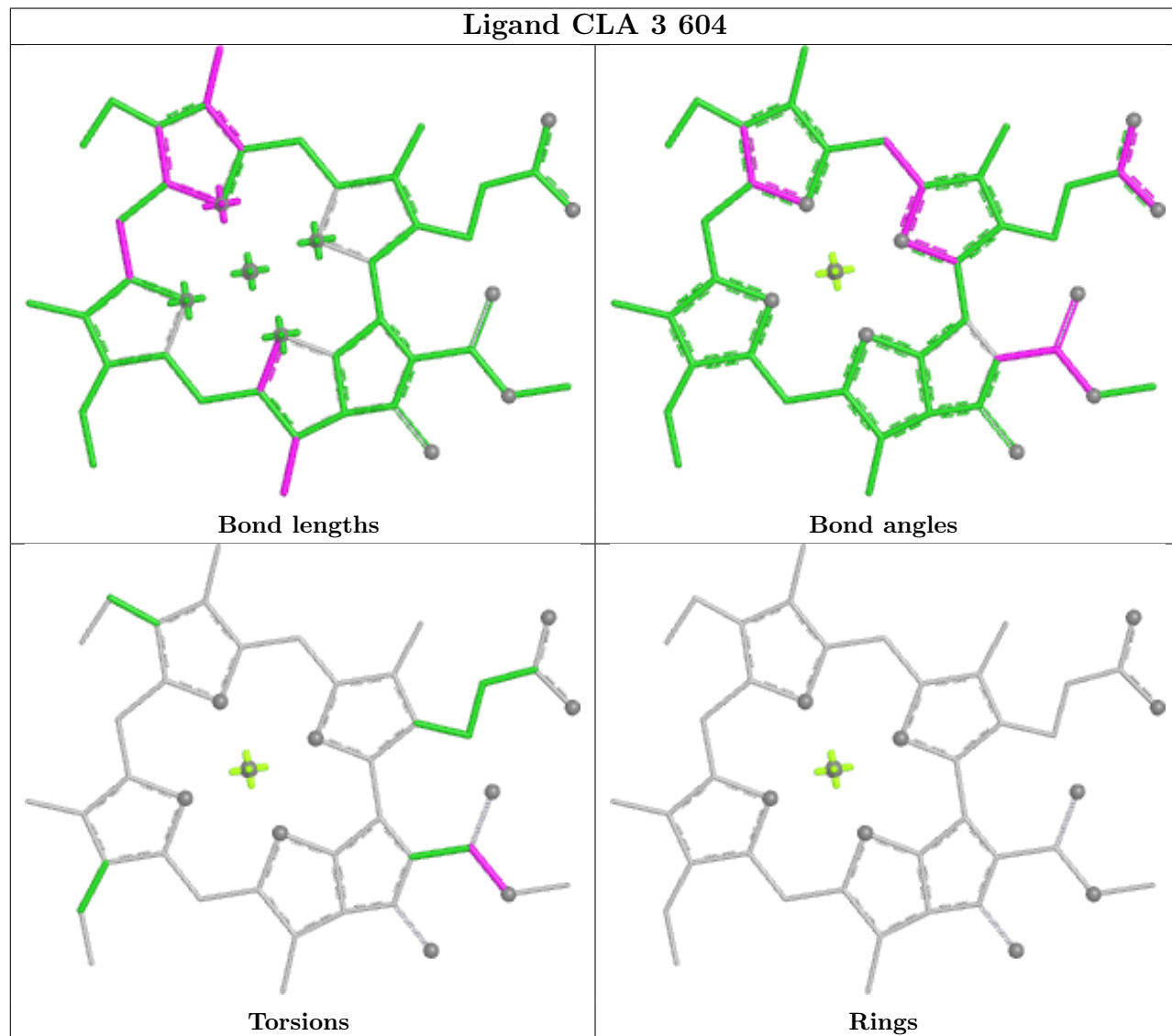
Ligand LUT 2 314

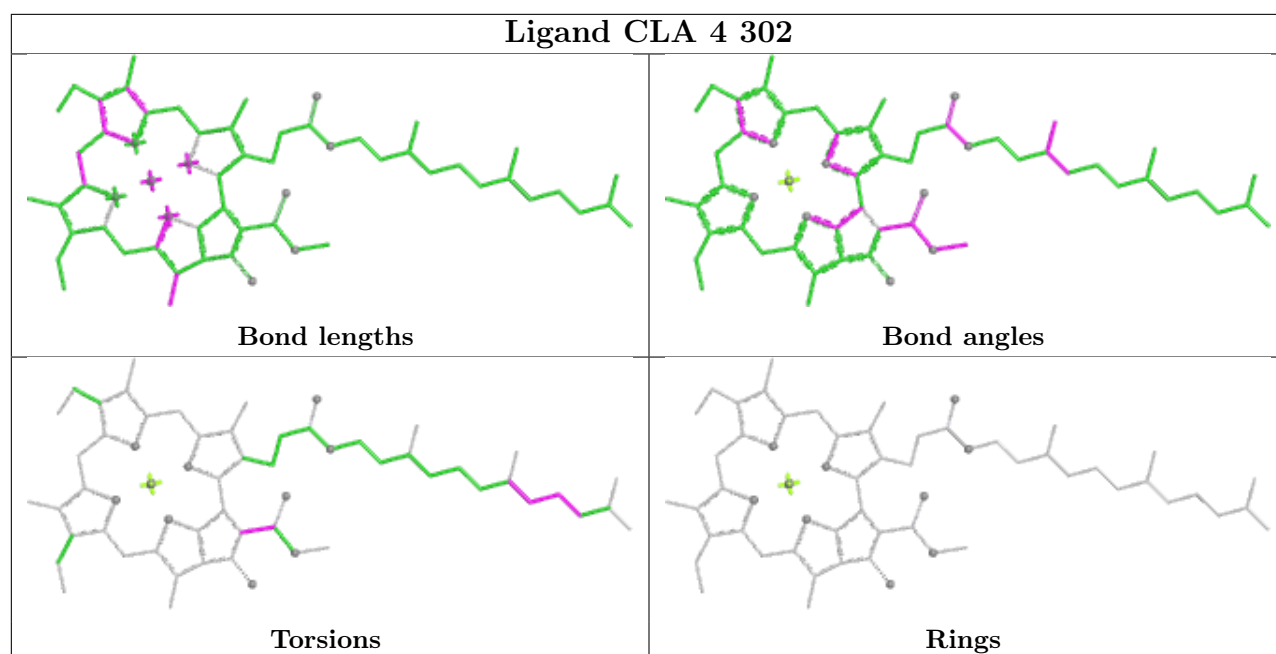


Ligand CLA B 840



Ligand CLA 3 604





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	1	195/195 (100%)	0.58	15 (7%) 19 16	66, 95, 152, 193	0
2	2	204/269 (75%)	0.68	17 (8%) 17 14	87, 121, 159, 212	0
3	3	216/275 (78%)	0.76	23 (10%) 11 8	114, 161, 229, 257	0
4	4	195/198 (98%)	0.12	4 (2%) 63 59	60, 74, 111, 143	0
5	A	742/758 (97%)	0.30	26 (3%) 47 43	52, 94, 150, 233	0
6	B	733/734 (99%)	0.03	18 (2%) 58 54	30, 69, 98, 132	0
7	C	80/81 (98%)	0.33	4 (5%) 34 30	30, 78, 94, 120	0
8	D	140/143 (97%)	0.32	6 (4%) 40 36	66, 101, 137, 158	0
9	E	63/66 (95%)	-0.03	1 (1%) 70 66	65, 84, 111, 129	0
10	F	152/154 (98%)	0.11	6 (3%) 43 39	30, 70, 96, 138	0
11	G	95/97 (97%)	0.41	8 (8%) 17 14	30, 91, 125, 156	0
12	H	88/88 (100%)	0.76	10 (11%) 10 7	96, 132, 182, 259	0
13	I	30/40 (75%)	0.60	2 (6%) 24 20	92, 108, 146, 208	0
14	J	39/42 (92%)	0.23	4 (10%) 12 9	60, 73, 101, 112	0
15	L	151/157 (96%)	0.41	4 (2%) 57 53	102, 137, 165, 192	0
16	K	77/80 (96%)	1.33	18 (23%) 2 1	137, 198, 248, 302	0
All	All	3200/3377 (94%)	0.33	166 (5%) 33 29	30, 91, 178, 302	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
16	K	90	LEU	6.2
3	3	128	LEU	5.9
12	H	142	LEU	5.7
1	1	109	ALA	5.5
16	K	72	PRO	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	B	734	GLY	5.1
5	A	159	THR	5.1
6	B	5	PHE	5.0
2	2	231	TYR	4.7
16	K	80	ALA	4.5
1	1	229	ALA	4.4
5	A	227	LEU	4.2
1	1	128	PRO	4.1
5	A	436	LEU	4.0
2	2	128	TYR	4.0
4	4	246	VAL	3.8
13	I	2	ILE	3.8
16	K	51	THR	3.8
3	3	116	LEU	3.8
5	A	323	ILE	3.8
2	2	67	LEU	3.7
14	J	39	PHE	3.7
5	A	111	ASN	3.6
16	K	71	ALA	3.6
4	4	247	GLN	3.6
6	B	667	TRP	3.6
3	3	91	TRP	3.6
16	K	74	ALA	3.6
1	1	51	ALA	3.5
5	A	263	ALA	3.5
16	K	112	ILE	3.5
2	2	97	LEU	3.5
16	K	73	SER	3.5
16	K	97	GLY	3.5
10	F	228	LYS	3.4
3	3	170	TRP	3.4
3	3	129	ALA	3.4
3	3	121	LEU	3.4
2	2	129	THR	3.4
2	2	60	GLY	3.4
4	4	245	ILE	3.3
7	C	63	LEU	3.3
5	A	517	GLY	3.3
1	1	212	THR	3.3
12	H	56	VAL	3.3
2	2	52	PRO	3.2
10	F	207	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
16	K	125	GLY	3.2
5	A	34	TRP	3.2
1	1	35	ALA	3.2
2	2	254	ALA	3.1
1	1	98	LEU	3.1
1	1	227	ILE	3.1
3	3	52	TRP	3.1
16	K	47	ILE	3.0
3	3	265	SER	3.0
6	B	94	PRO	3.0
1	1	121	PRO	3.0
10	F	203	THR	2.9
11	G	50	THR	2.9
2	2	158	TRP	2.9
2	2	76	GLY	2.9
14	J	37	LEU	2.9
2	2	132	GLU	2.9
11	G	89	THR	2.9
2	2	131	GLY	2.9
6	B	6	PRO	2.9
11	G	96	PRO	2.9
1	1	110	LEU	2.8
2	2	68	ASP	2.8
6	B	458	ILE	2.8
7	C	61	ASP	2.7
12	H	140	PRO	2.7
1	1	127	LEU	2.7
6	B	42	LEU	2.7
11	G	23	PHE	2.7
5	A	70	ASP	2.7
1	1	218	TRP	2.7
11	G	35	GLY	2.6
5	A	334	HIS	2.6
11	G	36	LEU	2.6
8	D	132	ALA	2.6
6	B	733	PHE	2.6
3	3	115	TYR	2.6
5	A	529	LEU	2.6
6	B	690	LEU	2.6
15	L	116	LEU	2.6
5	A	377	TYR	2.6
8	D	111	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
13	I	31	ARG	2.6
6	B	92	TRP	2.6
3	3	122	ILE	2.5
11	G	94	TYR	2.5
5	A	184	PHE	2.5
12	H	126	LEU	2.5
5	A	251	ASN	2.5
12	H	143	GLY	2.5
11	G	34	GLN	2.5
1	1	161	PHE	2.5
12	H	141	ARG	2.5
16	K	115	VAL	2.5
5	A	657	LEU	2.5
2	2	255	ALA	2.5
5	A	266	ALA	2.5
8	D	154	PHE	2.4
2	2	111	PHE	2.4
2	2	56	LEU	2.4
3	3	62	LEU	2.4
3	3	149	TYR	2.4
5	A	254	LEU	2.4
12	H	85	GLN	2.4
8	D	76	PRO	2.4
6	B	298	GLY	2.4
12	H	128	ILE	2.4
3	3	127	ALA	2.3
14	J	32	PHE	2.3
5	A	368	LEU	2.3
6	B	213	LEU	2.3
10	F	131	ASN	2.3
15	L	60	LEU	2.3
3	3	86	PHE	2.3
8	D	210	LEU	2.3
5	A	340	GLY	2.3
3	3	167	PHE	2.2
6	B	241	ASN	2.2
6	B	569	ASP	2.2
5	A	480	THR	2.2
12	H	72	LEU	2.2
3	3	123	PRO	2.2
6	B	2	ALA	2.2
1	1	107	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
6	B	476	VAL	2.2
5	A	518	GLY	2.2
3	3	112	ALA	2.2
5	A	511	THR	2.2
16	K	79	THR	2.2
6	B	687	LEU	2.2
16	K	50	PRO	2.2
7	C	2	SER	2.2
14	J	38	THR	2.2
16	K	70	LEU	2.1
3	3	209	LYS	2.1
5	A	501	GLY	2.1
9	E	27	ALA	2.1
3	3	94	TYR	2.1
12	H	134	LEU	2.1
16	K	121	LEU	2.1
16	K	98	PHE	2.1
3	3	195	ALA	2.1
15	L	18	SER	2.1
2	2	237	ILE	2.1
3	3	240	LEU	2.1
15	L	75	ILE	2.1
3	3	241	VAL	2.1
7	C	45	THR	2.1
5	A	108	ALA	2.1
5	A	481	ALA	2.1
10	F	135	GLN	2.1
16	K	113	ILE	2.1
8	D	117	GLY	2.1
5	A	333	ALA	2.0
10	F	79	ALA	2.0
3	3	74	PRO	2.0
4	4	135	PHE	2.0
1	1	219	HIS	2.0
6	B	14	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	CLA	A	843	52/65	0.66	0.14	173,188,196,199	0
25	HTG	4	322	19/19	0.71	0.16	107,129,140,145	0
25	HTG	F	310	16/19	0.71	0.14	114,141,144,146	0
26	DGD	4	323	60/66	0.72	0.17	90,115,130,138	0
22	LHG	G	102	49/49	0.74	0.20	92,119,171,174	0
25	HTG	F	301	17/19	0.75	0.16	124,149,155,159	0
25	HTG	B	851	19/19	0.77	0.16	107,134,142,143	0
22	LHG	F	302	40/49	0.77	0.21	111,140,164,167	0
17	CLA	3	610	52/65	0.77	0.14	177,188,210,215	0
21	BCR	K	203	40/40	0.77	0.18	142,185,227,229	0
24	LMG	B	852	52/55	0.78	0.17	100,127,143,148	0
21	BCR	2	316	40/40	0.78	0.19	148,157,172,173	0
20	XAT	3	615	44/44	0.79	0.15	62,89,98,100	0
24	LMG	4	320	49/55	0.80	0.16	96,119,174,176	0
24	LMG	F	309	55/55	0.81	0.14	91,108,120,124	0
17	CLA	L	204	50/65	0.82	0.12	122,147,157,163	0
17	CLA	J	103	42/65	0.82	0.12	83,101,120,125	0
24	LMG	G	101	40/55	0.83	0.15	110,157,180,181	0
23	LMT	2	318	35/35	0.83	0.15	120,133,143,146	0
22	LHG	A	845	27/49	0.83	0.12	128,174,191,196	0
17	CLA	A	821	49/65	0.84	0.12	130,142,169,175	0
21	BCR	3	616	40/40	0.85	0.14	156,164,187,189	0
17	CLA	L	202	65/65	0.85	0.12	142,154,170,175	0
17	CLA	3	612	45/65	0.85	0.11	197,212,229,235	0
22	LHG	B	801	23/49	0.85	0.15	67,88,119,120	0
23	LMT	A	855	35/35	0.86	0.13	97,154,171,172	0
17	CLA	A	822	51/65	0.86	0.11	137,148,164,169	0
18	CHL	3	601	56/66	0.86	0.13	108,134,146,147	0
20	XAT	2	315	44/44	0.86	0.14	62,89,98,100	0
17	CLA	2	303	60/65	0.86	0.11	120,132,139,142	0
17	CLA	L	203	65/65	0.87	0.13	119,143,157,167	0
17	CLA	K	201	45/65	0.87	0.11	172,184,191,193	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	CHL	2	305	48/66	0.87	0.13	105,129,162,162	0
24	LMG	4	319	50/55	0.87	0.15	68,89,131,132	0
25	HTG	4	321	19/19	0.87	0.16	125,139,147,147	0
17	CLA	4	304	50/65	0.88	0.11	55,78,112,117	0
21	BCR	L	206	40/40	0.88	0.12	156,168,177,178	0
17	CLA	3	609	50/65	0.88	0.10	147,163,173,175	0
22	LHG	2	317	37/49	0.88	0.19	155,163,179,187	0
17	CLA	1	304	42/65	0.88	0.12	80,107,125,133	0
17	CLA	A	837	65/65	0.88	0.13	92,103,174,177	0
17	CLA	3	604	45/65	0.88	0.11	137,162,170,173	0
17	CLA	3	605	42/65	0.89	0.11	125,135,143,147	0
17	CLA	G	103	41/65	0.89	0.14	105,122,131,136	0
17	CLA	1	307	65/65	0.89	0.12	74,93,123,129	0
18	CHL	4	301	61/66	0.89	0.12	66,78,116,118	0
26	DGD	B	850	66/66	0.89	0.14	80,94,119,120	0
17	CLA	3	602	60/65	0.90	0.12	132,157,174,178	0
17	CLA	A	817	65/65	0.90	0.13	103,129,169,173	0
17	CLA	2	310	52/65	0.90	0.09	106,113,156,164	0
19	LUT	3	614	42/42	0.90	0.11	127,146,163,166	0
22	LHG	1	317	49/49	0.90	0.16	85,100,127,130	0
17	CLA	2	312	43/65	0.90	0.10	122,142,146,147	0
17	CLA	K	202	60/65	0.90	0.09	146,176,193,196	0
21	BCR	1	316	40/40	0.90	0.12	98,125,149,151	0
17	CLA	2	309	41/65	0.91	0.10	126,134,143,146	0
17	CLA	A	819	45/65	0.91	0.11	126,138,151,155	0
17	CLA	1	303	51/65	0.91	0.12	112,124,138,143	0
17	CLA	1	312	55/65	0.91	0.11	74,88,119,123	0
17	CLA	A	825	65/65	0.91	0.11	76,98,163,165	0
18	CHL	1	305	48/66	0.91	0.13	102,114,132,134	0
17	CLA	A	833	50/65	0.91	0.11	120,135,146,157	0
17	CLA	A	834	45/65	0.91	0.09	156,170,177,185	0
17	CLA	A	835	51/65	0.91	0.11	78,102,129,135	0
17	CLA	2	302	51/65	0.91	0.10	89,102,120,127	0
17	CLA	1	306	46/65	0.91	0.11	91,101,117,120	0
17	CLA	B	803	65/65	0.91	0.11	106,119,153,161	0
17	CLA	B	814	55/65	0.91	0.11	61,75,121,123	0
17	CLA	B	817	55/65	0.91	0.11	72,86,123,134	0
17	CLA	4	310	60/65	0.91	0.10	68,89,116,121	0
21	BCR	4	318	40/40	0.91	0.12	61,90,99,104	0
21	BCR	A	846	40/40	0.91	0.12	116,137,151,153	0
21	BCR	J	105	40/40	0.91	0.14	73,85,100,101	0
17	CLA	G	105	46/65	0.91	0.10	92,122,136,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	CLA	A	814	50/65	0.91	0.14	119,141,161,164	0
17	CLA	4	311	52/65	0.92	0.10	72,83,118,119	0
17	CLA	B	824	55/65	0.92	0.12	63,74,104,112	0
21	BCR	A	849	40/40	0.92	0.14	100,137,196,199	0
21	BCR	B	845	40/40	0.92	0.11	62,73,118,122	0
21	BCR	B	847	40/40	0.92	0.12	49,65,85,92	0
18	CHL	2	313	43/66	0.92	0.08	99,119,137,139	0
17	CLA	A	830	50/65	0.92	0.12	102,117,152,156	0
17	CLA	A	809	65/65	0.92	0.13	100,120,149,151	0
17	CLA	3	613	46/65	0.92	0.09	106,121,156,159	0
17	CLA	A	816	65/65	0.92	0.12	116,134,152,155	0
17	CLA	4	303	60/65	0.92	0.10	52,67,108,113	0
17	CLA	2	301	65/65	0.92	0.12	86,105,122,135	0
25	HTG	J	102	19/19	0.92	0.10	75,82,115,120	0
17	CLA	4	309	60/65	0.92	0.11	61,72,98,100	0
17	CLA	1	309	65/65	0.92	0.10	84,105,142,147	0
21	BCR	J	104	40/40	0.93	0.11	63,73,87,91	0
17	CLA	B	812	65/65	0.93	0.13	76,107,137,144	0
21	BCR	L	201	40/40	0.93	0.10	95,107,120,123	0
18	CHL	2	304	43/66	0.93	0.11	101,117,129,137	0
17	CLA	B	813	54/65	0.93	0.09	61,90,114,117	0
17	CLA	3	606	47/65	0.93	0.09	113,124,135,138	0
17	CLA	1	302	65/65	0.93	0.10	70,87,125,128	0
17	CLA	B	818	55/65	0.93	0.11	63,73,95,102	0
18	CHL	4	305	56/66	0.93	0.10	68,77,116,118	0
18	CHL	4	306	51/66	0.93	0.09	66,79,130,133	0
18	CHL	4	315	43/66	0.93	0.09	67,88,102,117	0
19	LUT	1	314	42/42	0.93	0.10	67,95,116,120	0
19	LUT	2	314	42/42	0.93	0.10	97,114,124,130	0
17	CLA	B	820	60/65	0.93	0.10	46,66,85,87	0
19	LUT	4	316	42/42	0.93	0.10	63,72,86,91	0
17	CLA	1	313	46/65	0.93	0.08	73,84,105,117	0
17	CLA	3	611	55/65	0.93	0.10	143,177,193,195	0
17	CLA	G	104	50/65	0.93	0.09	76,95,125,133	0
17	CLA	A	811	54/65	0.93	0.11	107,127,140,140	0
17	CLA	2	307	50/65	0.93	0.10	90,95,110,113	0
25	HTG	A	854	19/19	0.93	0.07	63,78,85,96	0
17	CLA	A	815	45/65	0.93	0.09	114,125,135,140	0
17	CLA	A	836	65/65	0.93	0.11	86,106,146,154	0
25	HTG	F	305	19/19	0.93	0.14	62,83,100,104	0
17	CLA	3	603	50/65	0.93	0.10	116,128,132,135	0
17	CLA	2	308	60/65	0.93	0.12	111,122,145,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	CLA	1	310	52/65	0.93	0.10	88,103,145,147	0
21	BCR	F	303	40/40	0.93	0.12	48,60,65,66	0
17	CLA	2	311	65/65	0.94	0.09	109,127,142,147	0
17	CLA	A	826	65/65	0.94	0.10	90,119,149,154	0
17	CLA	B	816	65/65	0.94	0.12	65,78,97,99	0
17	CLA	4	308	50/65	0.94	0.09	52,64,103,109	0
17	CLA	1	301	65/65	0.94	0.10	60,72,107,115	0
17	CLA	1	308	60/65	0.94	0.11	89,100,129,133	0
18	CHL	2	306	51/66	0.94	0.12	84,101,141,144	0
17	CLA	B	822	50/65	0.94	0.10	70,80,109,113	0
21	BCR	A	847	40/40	0.94	0.12	87,120,171,173	0
21	BCR	A	848	40/40	0.94	0.12	92,116,163,164	0
17	CLA	3	608	50/65	0.94	0.09	120,130,136,139	0
18	CHL	3	607	47/66	0.94	0.10	124,135,160,166	0
21	BCR	B	846	40/40	0.94	0.10	62,77,125,126	0
17	CLA	B	834	58/65	0.94	0.10	46,59,102,105	0
17	CLA	4	312	56/65	0.94	0.09	70,84,109,112	0
21	BCR	G	106	40/40	0.94	0.10	71,90,129,130	0
21	BCR	I	101	40/40	0.94	0.10	92,99,112,114	0
17	CLA	A	820	65/65	0.94	0.11	103,126,143,144	0
17	CLA	4	314	47/65	0.94	0.08	57,70,104,106	0
17	CLA	1	311	60/65	0.94	0.10	64,75,111,113	0
21	BCR	L	205	40/40	0.94	0.13	101,116,137,137	0
17	CLA	B	809	65/65	0.94	0.11	71,88,138,144	0
17	CLA	A	824	65/65	0.94	0.11	90,102,108,111	0
17	CLA	B	833	60/65	0.95	0.08	44,58,104,110	0
17	CLA	A	803	55/65	0.95	0.10	64,82,119,124	0
17	CLA	B	835	65/65	0.95	0.09	53,67,106,116	0
17	CLA	B	836	45/65	0.95	0.07	62,71,94,97	0
17	CLA	B	839	47/65	0.95	0.08	52,58,84,93	0
17	CLA	F	304	65/65	0.95	0.10	44,58,76,84	0
21	BCR	A	850	40/40	0.95	0.11	72,108,147,148	0
21	BCR	A	851	40/40	0.95	0.09	45,63,77,79	0
17	CLA	F	307	55/65	0.95	0.07	49,67,123,125	0
17	CLA	A	804	65/65	0.95	0.10	77,91,115,117	0
17	CLA	A	827	65/65	0.95	0.10	64,76,89,94	0
17	CLA	A	829	65/65	0.95	0.09	68,82,94,98	0
21	BCR	F	308	40/40	0.95	0.09	53,62,72,78	0
17	CLA	J	101	65/65	0.95	0.11	62,76,93,101	0
17	CLA	A	853	65/65	0.95	0.11	48,61,88,96	0
17	CLA	A	806	65/65	0.95	0.10	72,81,131,134	0
17	CLA	2	319	46/65	0.95	0.09	68,80,109,111	0

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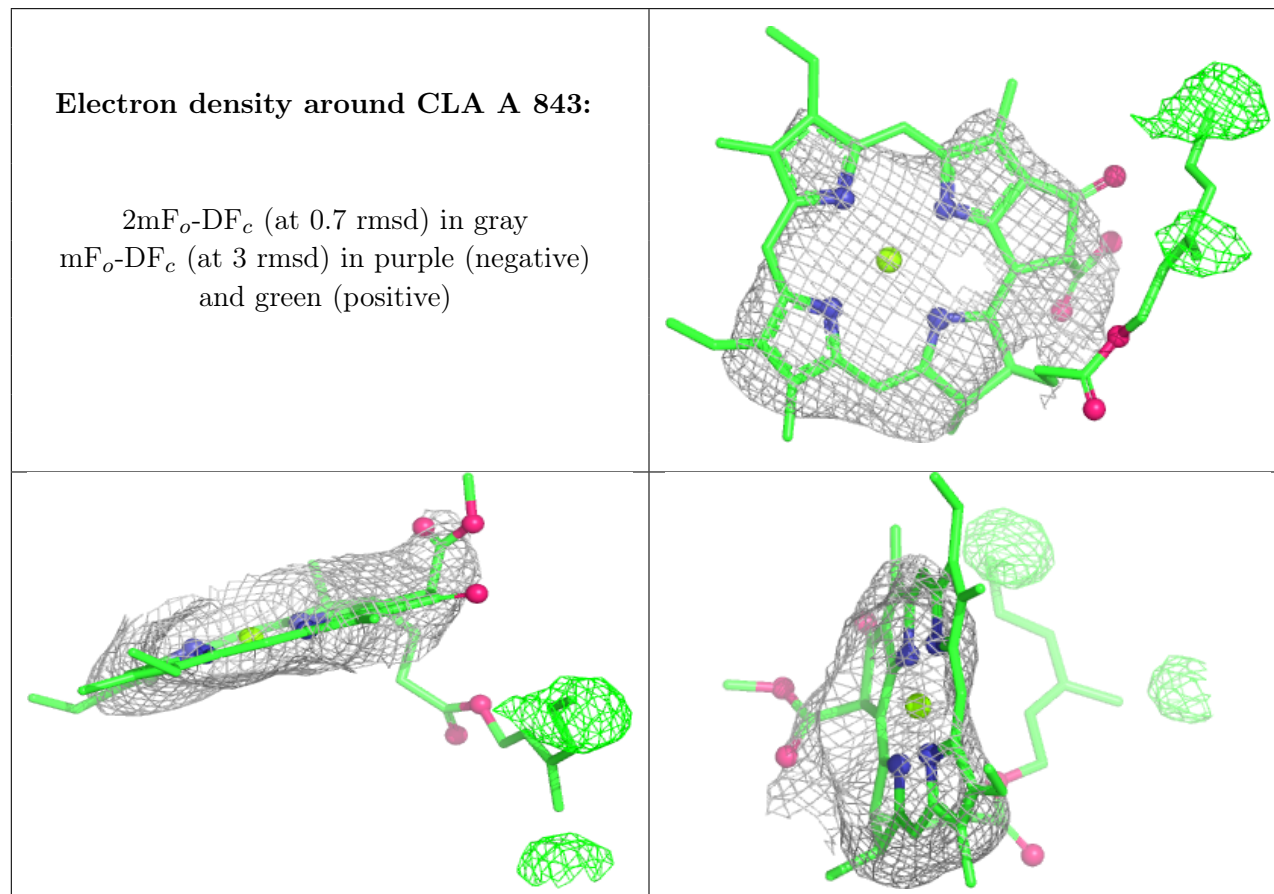
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	CLA	B	823	65/65	0.95	0.10	62,75,131,140	0
17	CLA	A	810	65/65	0.95	0.10	80,88,102,113	0
20	XAT	4	317	44/44	0.95	0.09	58,67,81,88	0
17	CLA	B	825	60/65	0.95	0.09	51,60,107,115	0
17	CLA	B	826	65/65	0.95	0.09	50,67,87,92	0
17	CLA	A	812	65/65	0.96	0.09	88,112,121,122	0
21	BCR	B	848	40/40	0.96	0.07	48,58,74,79	0
21	BCR	B	849	40/40	0.96	0.07	60,75,82,83	0
17	CLA	A	823	55/65	0.96	0.09	105,121,137,143	0
17	CLA	A	805	65/65	0.96	0.10	69,82,91,93	0
17	CLA	B	821	65/65	0.96	0.07	56,67,98,103	0
17	CLA	A	801	65/65	0.96	0.10	52,67,83,87	0
17	CLA	A	838	65/65	0.96	0.09	45,55,71,78	0
17	CLA	A	839	65/65	0.96	0.09	47,59,97,101	0
17	CLA	A	840	65/65	0.96	0.08	52,63,76,90	0
17	CLA	A	841	65/65	0.96	0.10	82,100,138,149	0
17	CLA	B	827	65/65	0.96	0.08	43,58,106,109	0
17	CLA	B	829	65/65	0.96	0.10	54,65,124,133	0
17	CLA	B	830	65/65	0.96	0.09	48,68,83,97	0
17	CLA	B	831	65/65	0.96	0.10	48,63,105,107	0
17	CLA	B	832	50/65	0.96	0.08	53,62,96,105	0
17	CLA	A	807	65/65	0.96	0.09	59,73,104,120	0
17	CLA	A	808	65/65	0.96	0.08	54,69,114,118	0
17	CLA	A	828	65/65	0.96	0.09	73,89,106,107	0
17	CLA	B	804	65/65	0.96	0.10	50,60,68,74	0
17	CLA	B	837	60/65	0.96	0.09	46,57,105,106	0
17	CLA	B	838	65/65	0.96	0.08	43,58,72,81	0
17	CLA	B	805	65/65	0.96	0.09	62,78,101,112	0
17	CLA	B	840	65/65	0.96	0.08	70,91,118,124	0
17	CLA	B	841	65/65	0.96	0.09	57,72,127,136	0
17	CLA	B	842	65/65	0.96	0.09	57,69,84,94	0
17	CLA	B	806	45/65	0.96	0.07	62,71,90,114	0
17	CLA	B	808	65/65	0.96	0.08	49,70,88,92	0
17	CLA	A	802	65/65	0.96	0.09	59,73,82,90	0
17	CLA	B	811	65/65	0.96	0.09	70,83,118,125	0
17	CLA	4	313	45/65	0.96	0.07	73,98,120,127	0
17	CLA	A	831	65/65	0.96	0.08	84,103,108,110	0
17	CLA	A	832	65/65	0.96	0.10	89,101,142,149	0
21	BCR	B	844	40/40	0.96	0.11	69,83,97,102	0
17	CLA	B	815	65/65	0.96	0.08	57,67,75,77	0
17	CLA	4	302	60/65	0.96	0.08	50,62,94,97	0
27	PQN	A	842	33/33	0.96	0.10	49,61,85,91	0

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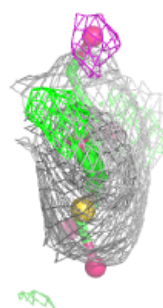
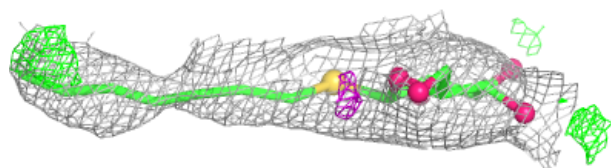
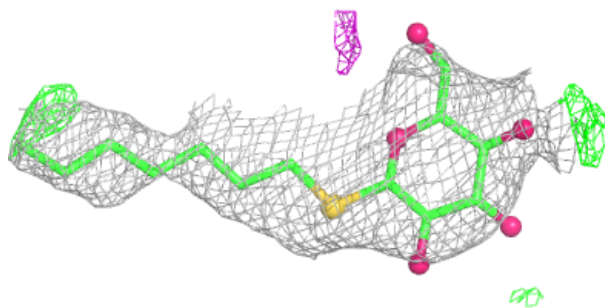
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	PQN	B	843	33/33	0.96	0.10	65,84,91,97	0
17	CLA	B	810	65/65	0.97	0.09	63,73,95,101	0
18	CHL	4	307	51/66	0.97	0.07	60,73,90,101	0
17	CLA	B	828	65/65	0.97	0.07	45,58,72,78	0
17	CLA	A	818	65/65	0.97	0.10	91,103,125,130	0
17	CLA	F	306	45/65	0.97	0.06	55,66,75,85	0
17	CLA	B	807	65/65	0.97	0.10	57,69,79,82	0
17	CLA	A	813	45/65	0.97	0.08	89,111,120,126	0
20	XAT	1	315	44/44	0.97	0.09	62,89,98,100	0
17	CLA	B	819	59/65	0.97	0.09	55,66,81,85	0
22	LHG	A	844	49/49	0.97	0.09	69,83,92,96	0
17	CLA	B	802	65/65	0.97	0.07	48,60,81,93	0
28	SF4	A	852	8/8	0.99	0.04	55,67,73,74	0
28	SF4	C	101	8/8	0.99	0.03	69,76,84,85	0
28	SF4	C	102	8/8	0.99	0.03	75,76,85,89	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.

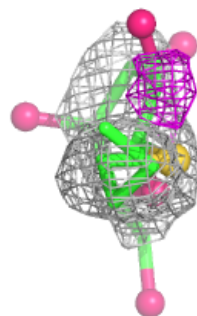
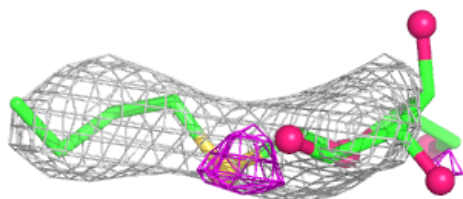
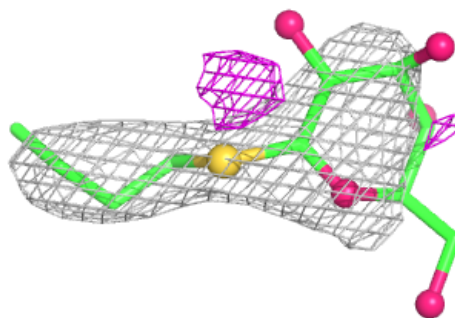


Electron density around HTG 4 322:

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

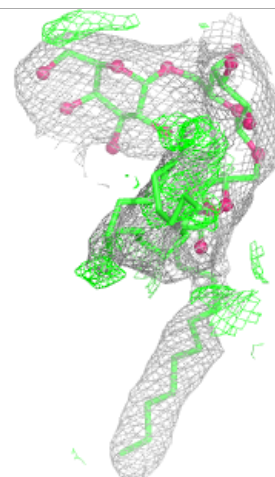
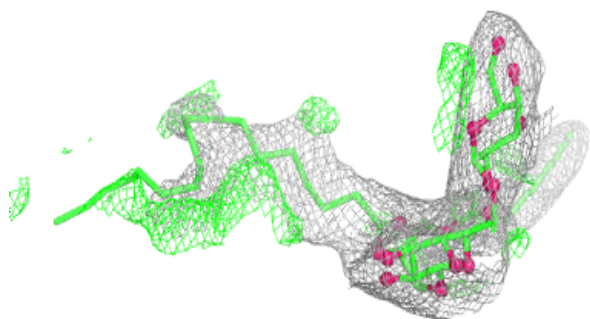
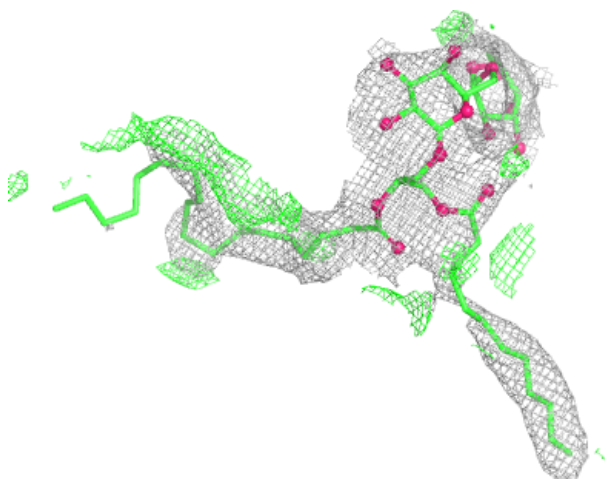
**Electron density around HTG F 310:**

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



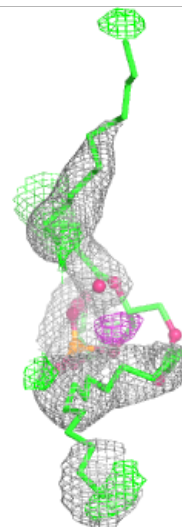
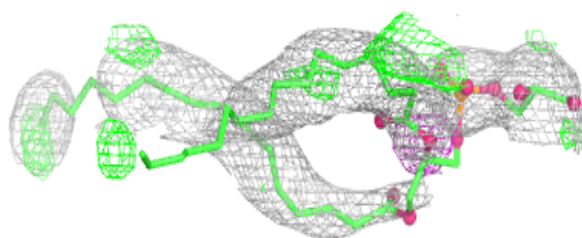
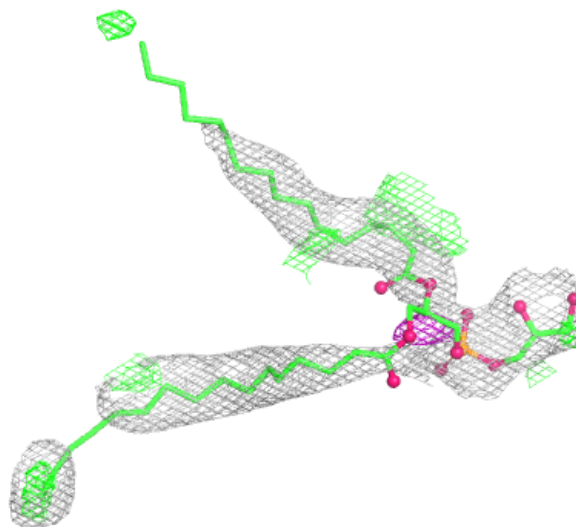
Electron density around DGD 4 323:

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



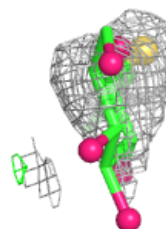
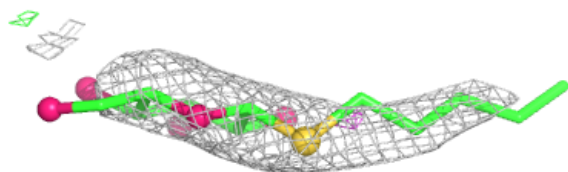
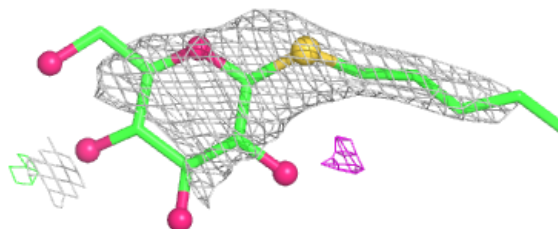
Electron density around LHG G 102:

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

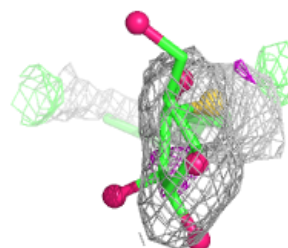
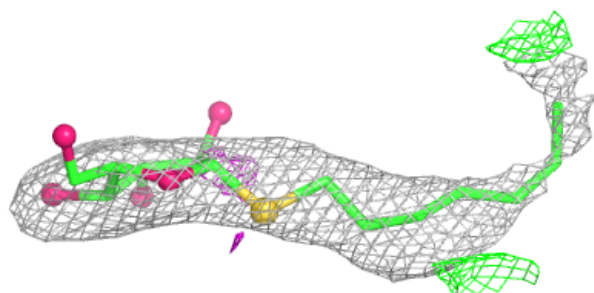
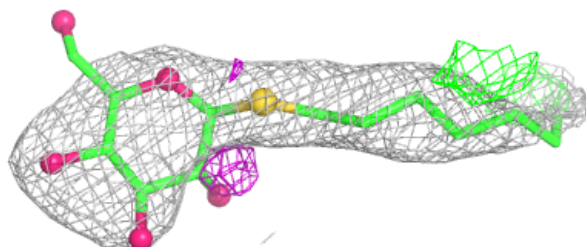


Electron density around HTG F 301:

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

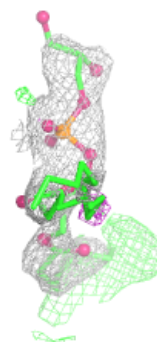
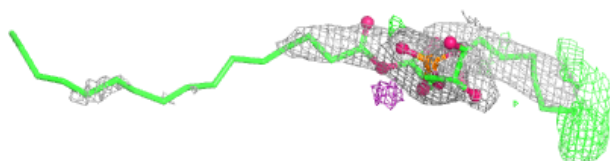
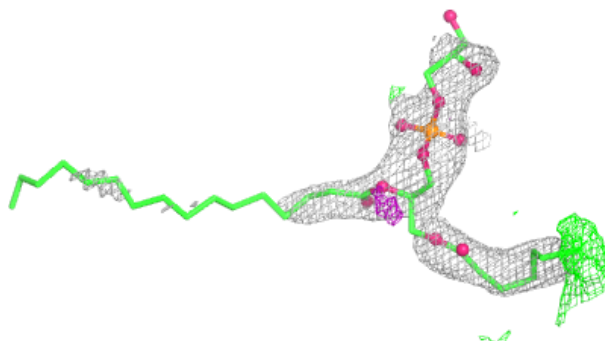
**Electron density around HTG B 851:**

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

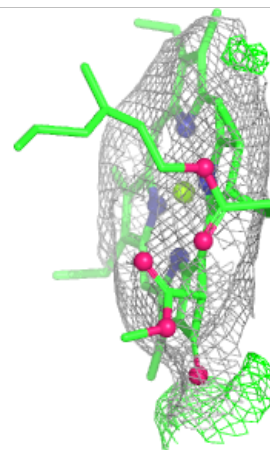
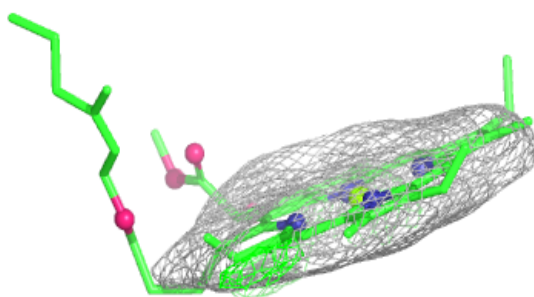
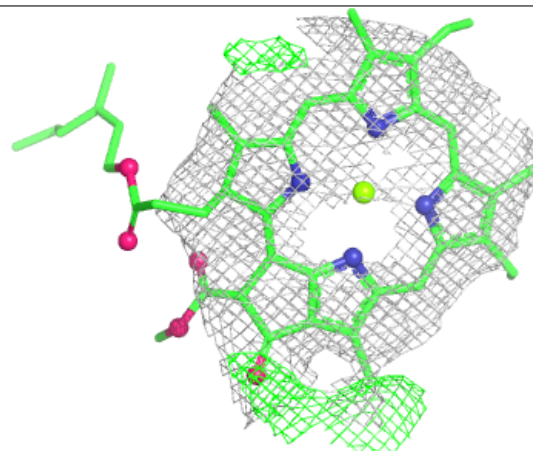


Electron density around LHG F 302:

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

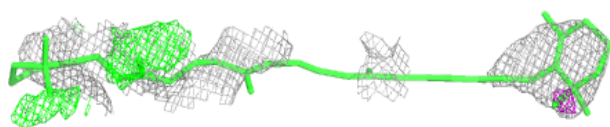
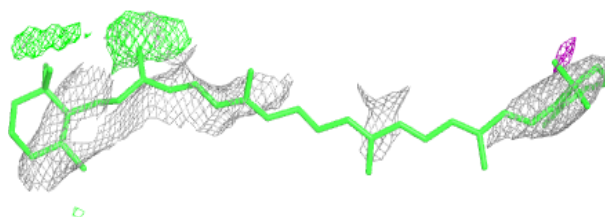
**Electron density around CLA 3 610:**

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

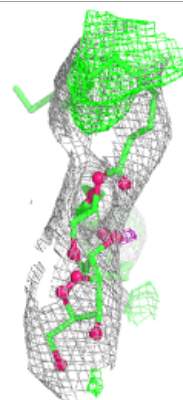
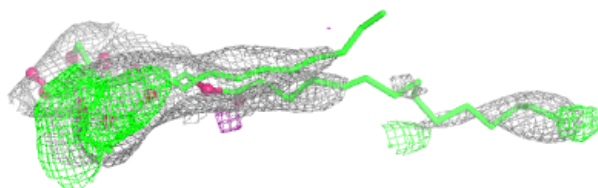
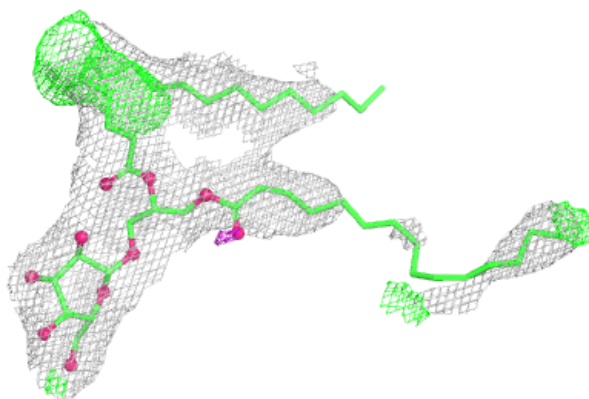


Electron density around BCR K 203:

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

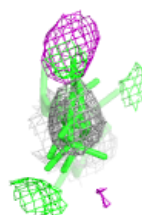
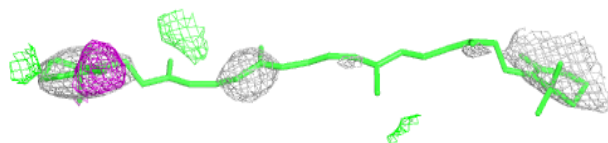
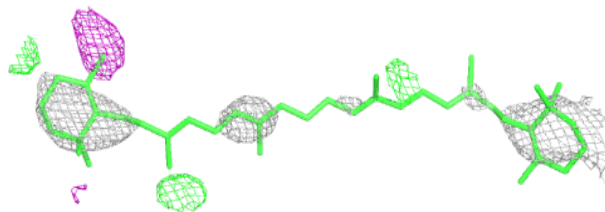
**Electron density around LMG B 852:**

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

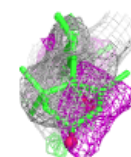
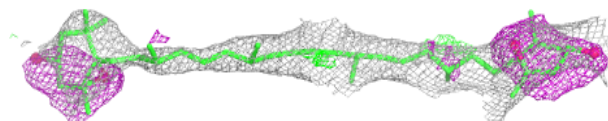
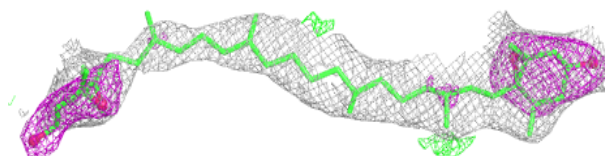


Electron density around BCR 2 316:

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

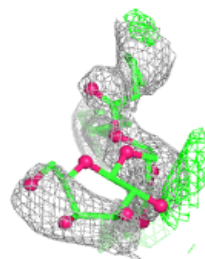
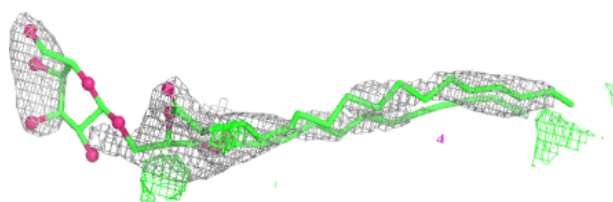
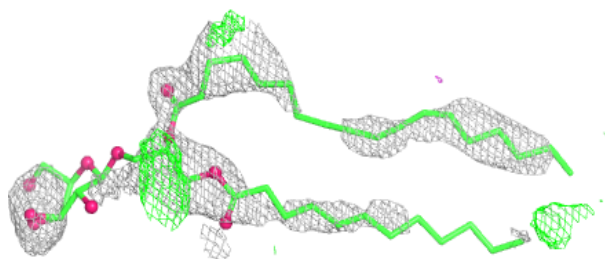
**Electron density around XAT 3 615:**

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



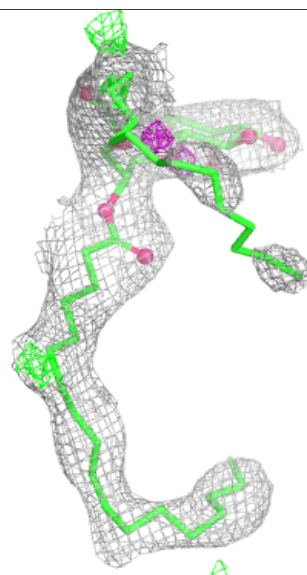
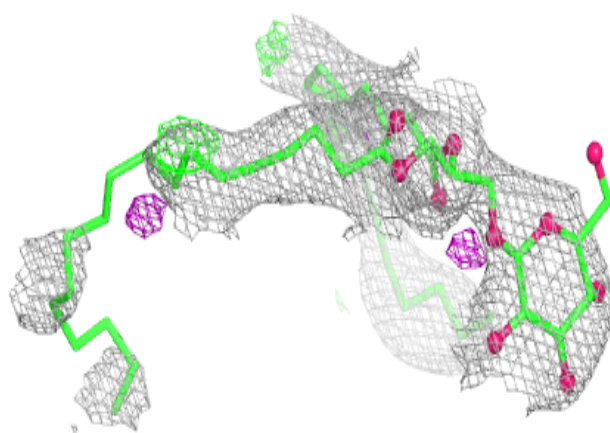
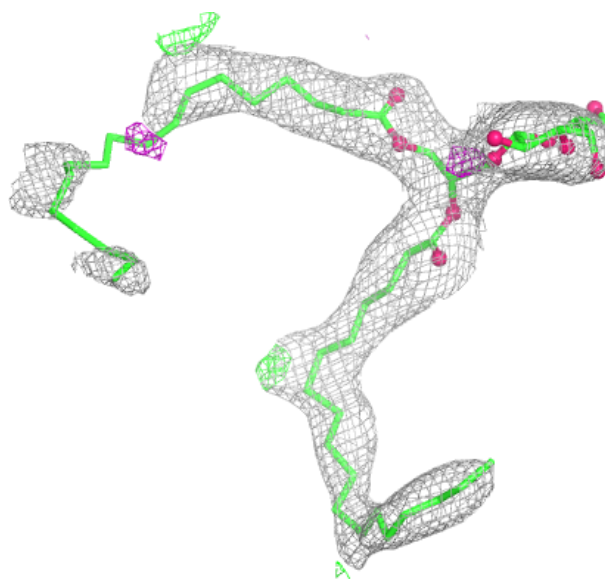
Electron density around LMG 4 320:

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



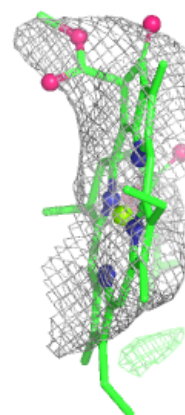
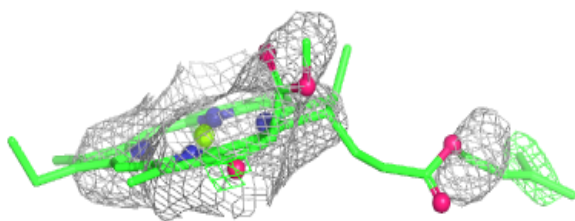
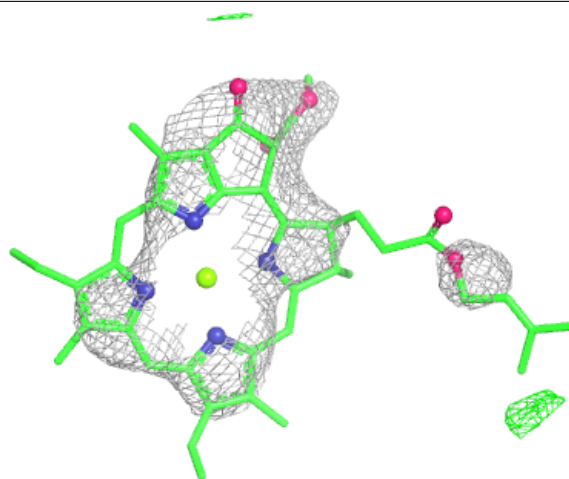
Electron density around LMG F 309:

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



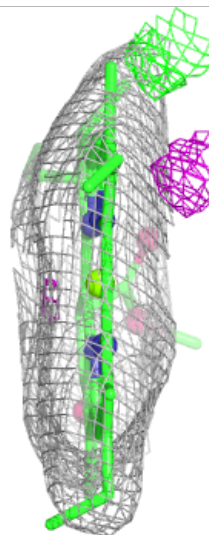
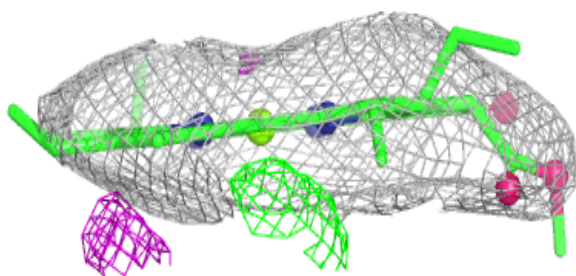
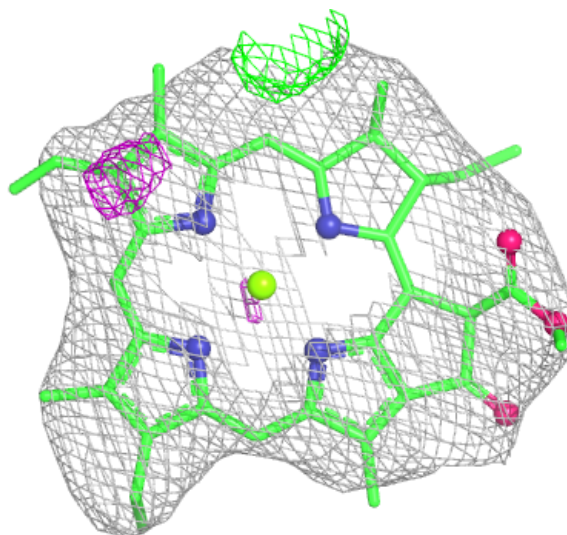
Electron density around CLA L 204:

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



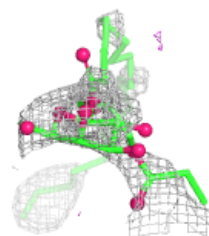
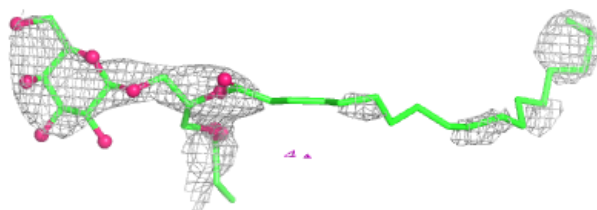
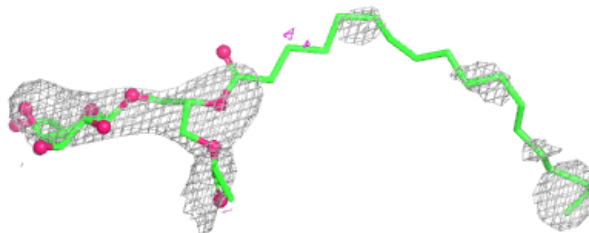
Electron density around CLA J 103:

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

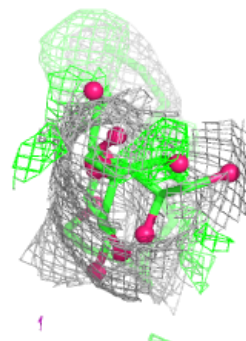
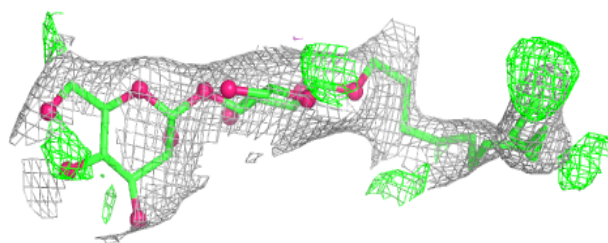
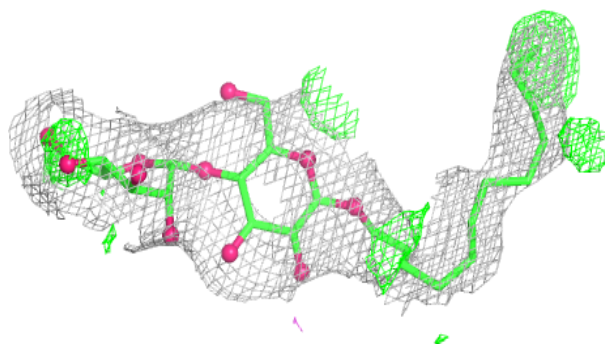


Electron density around LMG G 101:

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

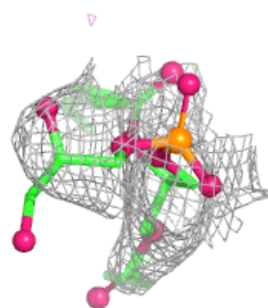
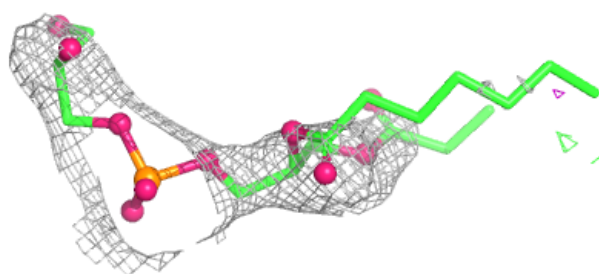
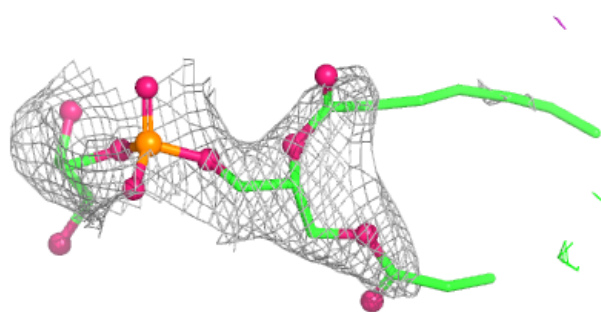
**Electron density around LMT 2 318:**

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

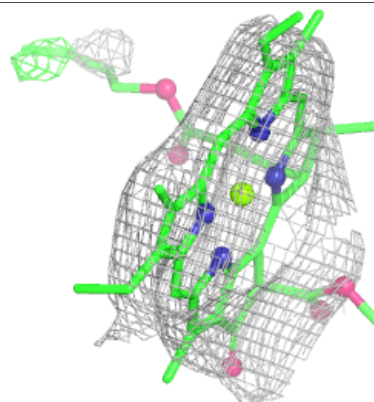
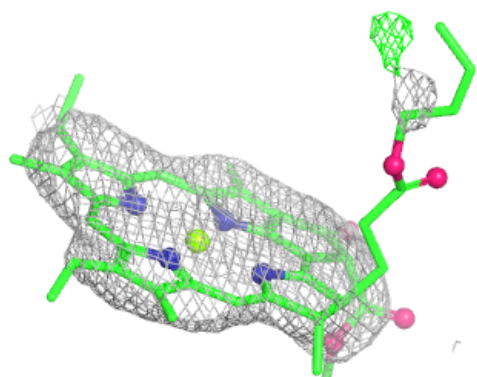
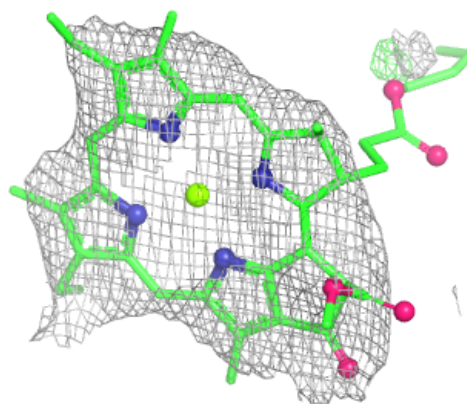


Electron density around LHG A 845:

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and green (positive)

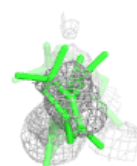
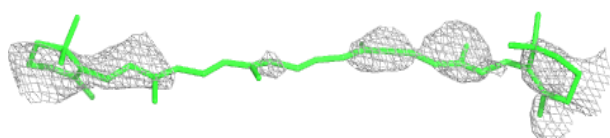
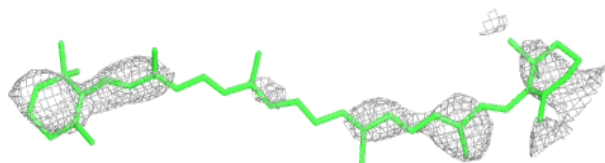
**Electron density around CLA A 821:**

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and green (positive)

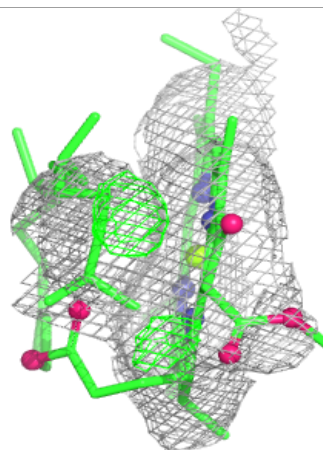
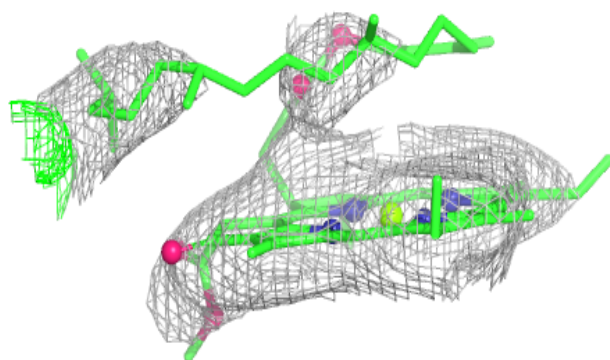
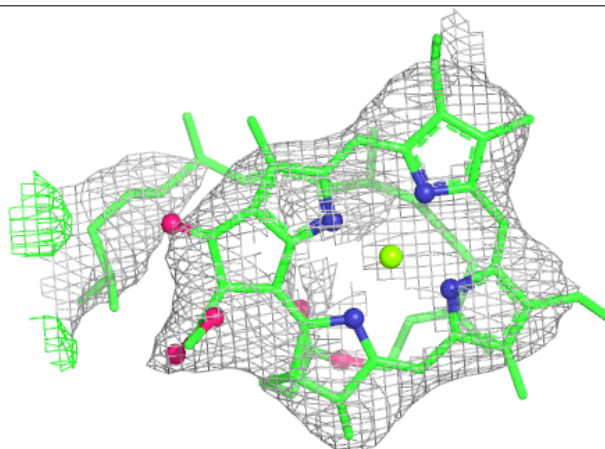


Electron density around BCR 3 616:

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and green (positive)

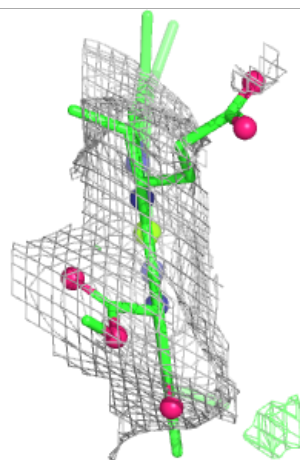
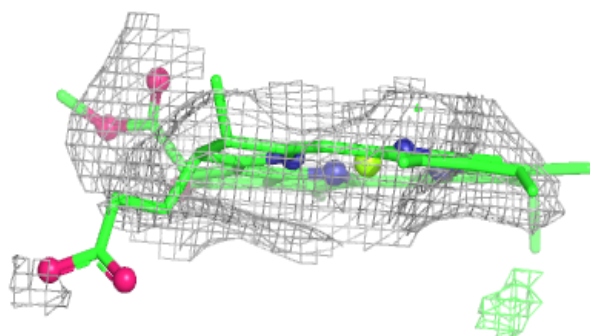
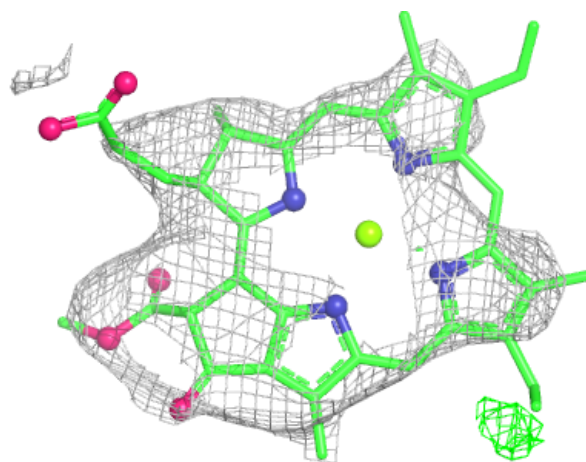
**Electron density around CLA L 202:**

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



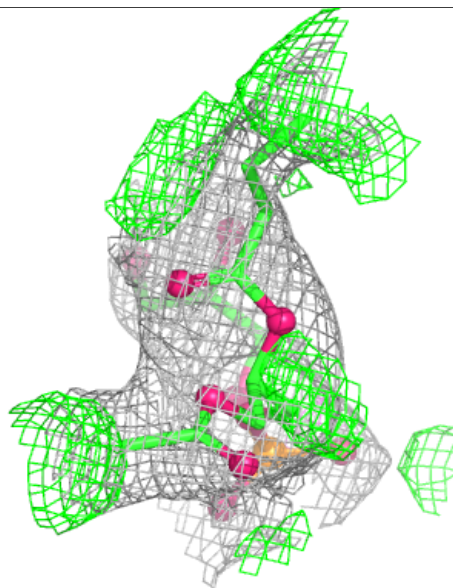
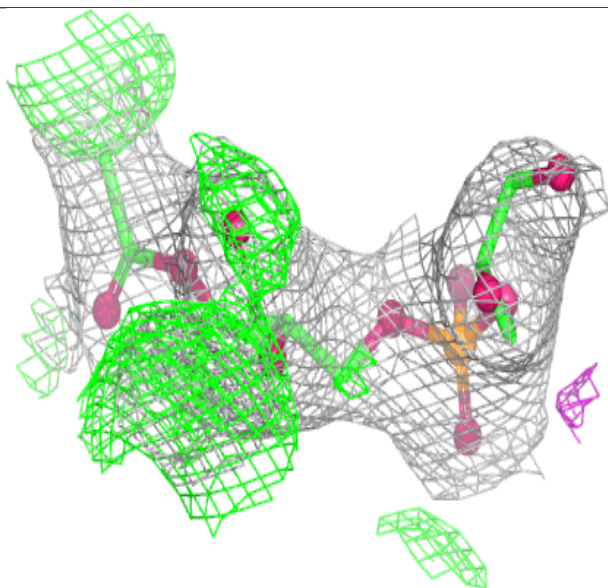
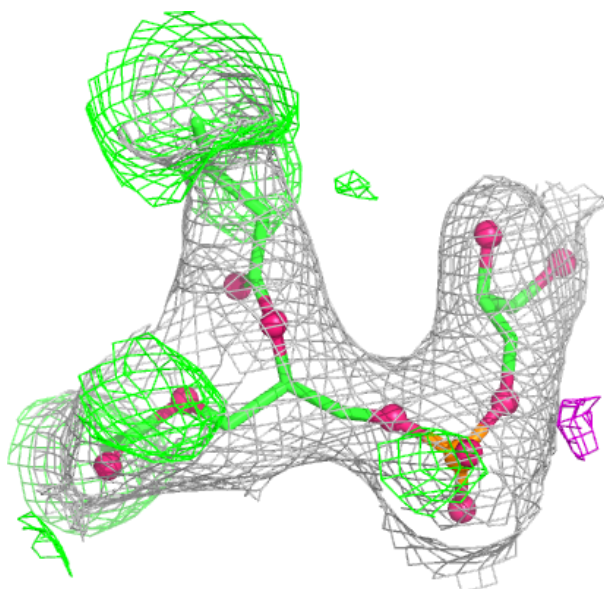
Electron density around CLA 3 612:

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



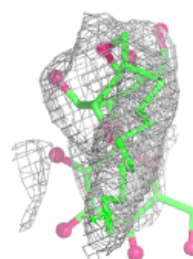
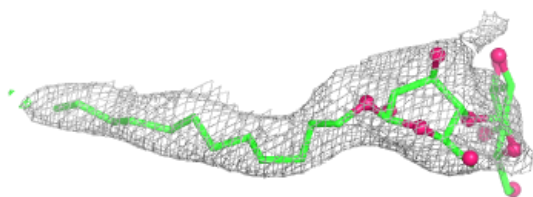
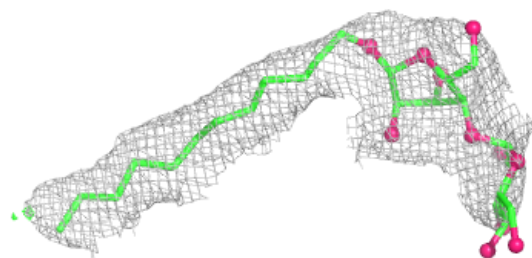
Electron density around LHG B 801:

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



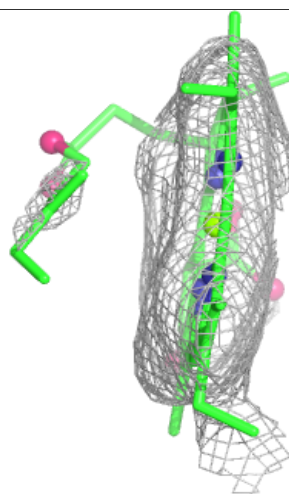
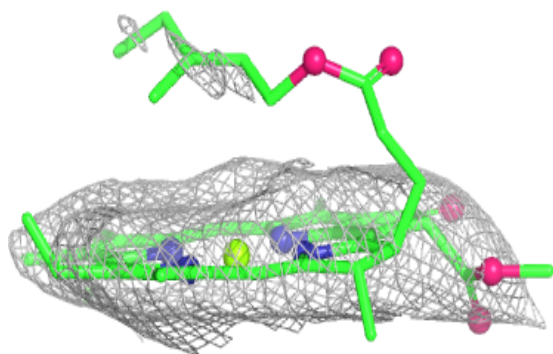
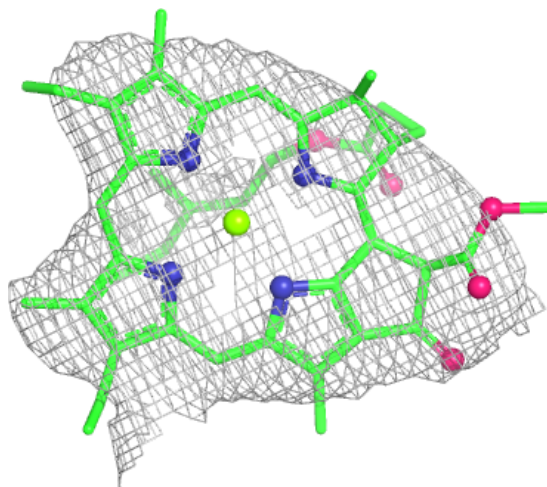
Electron density around LMT A 855:

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



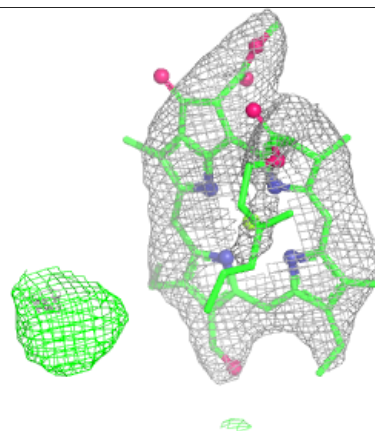
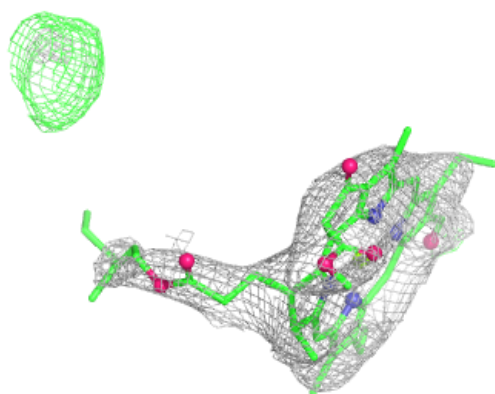
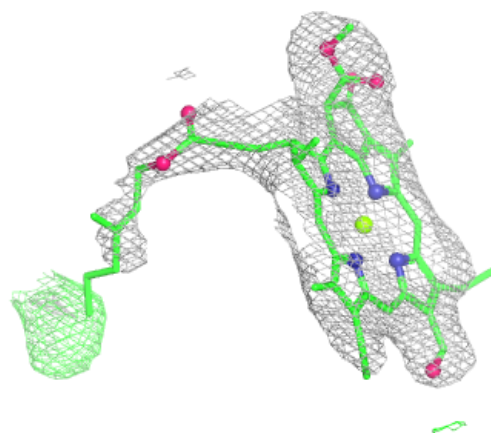
Electron density around CLA A 822:

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

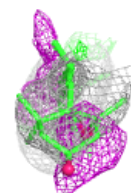
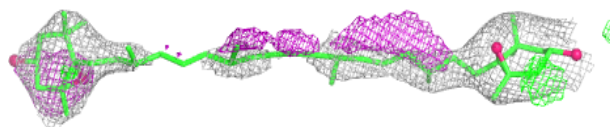
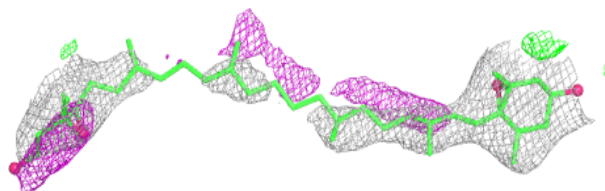


Electron density around CHL 3 601:

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

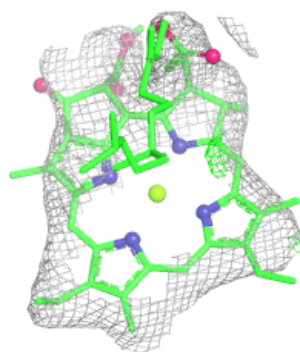
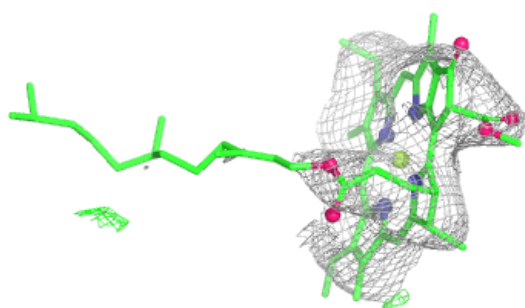
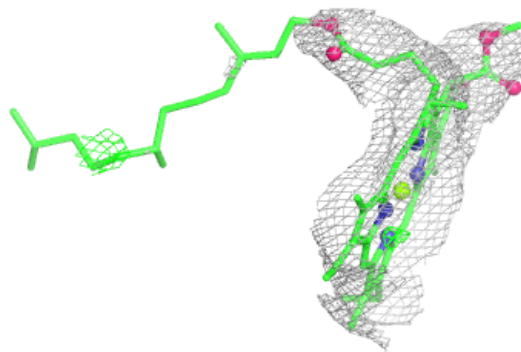
**Electron density around XAT 2 315:**

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

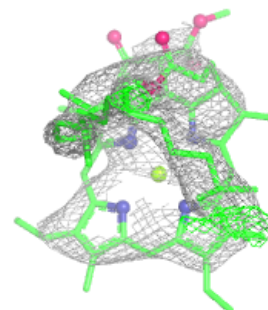
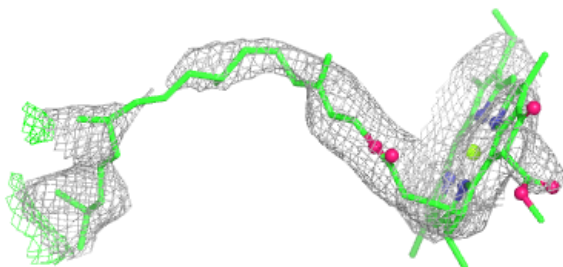
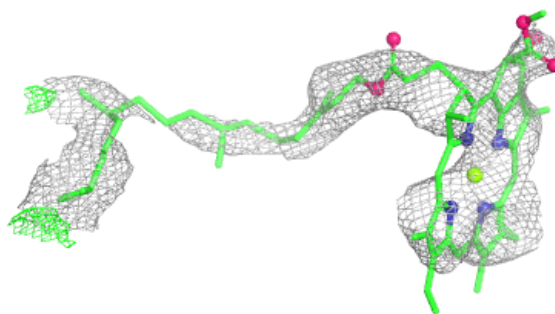


Electron density around CLA 2 303:

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

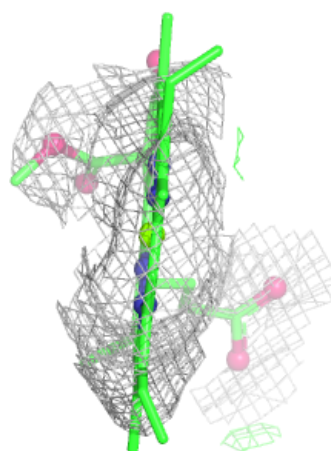
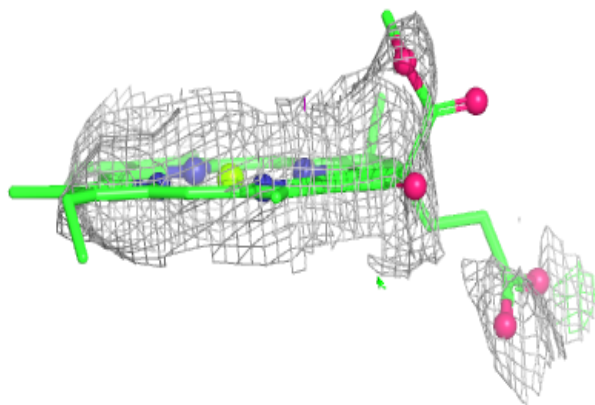
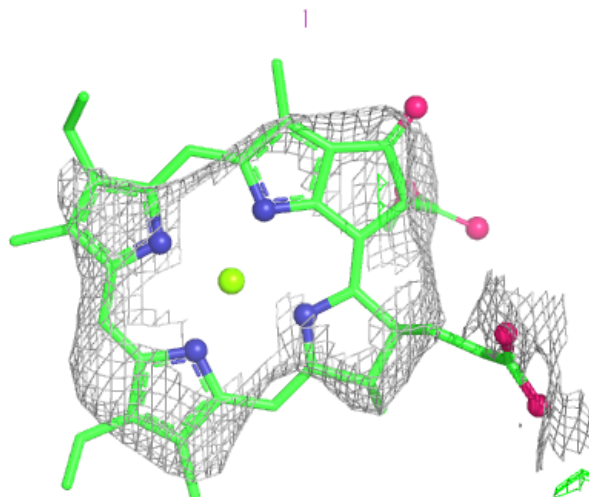
**Electron density around CLA L 203:**

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



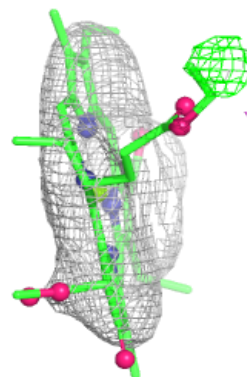
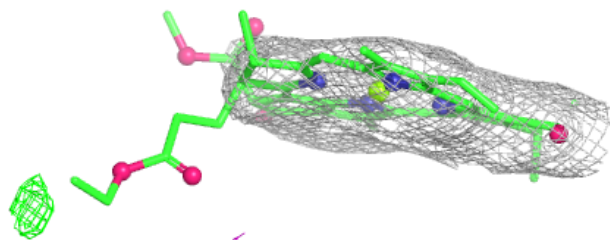
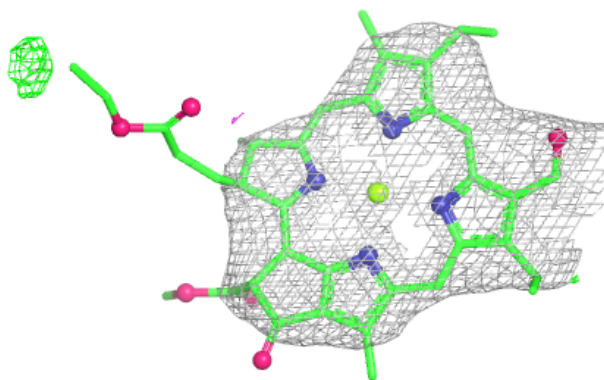
Electron density around CLA K 201:

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

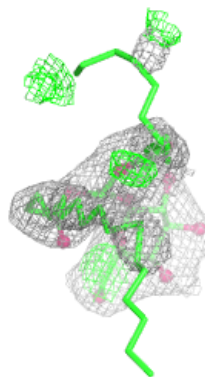
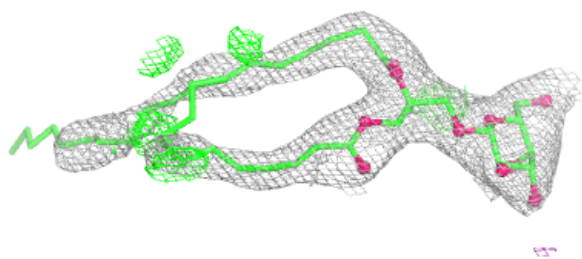
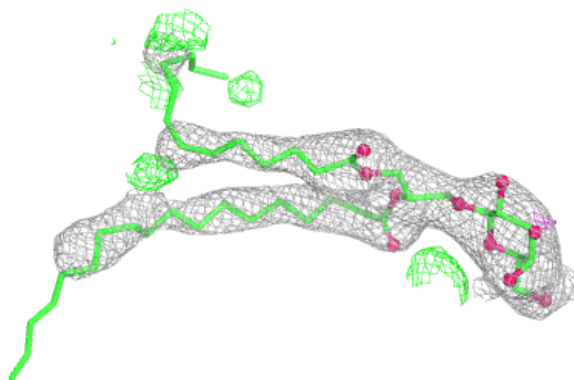


Electron density around CHL 2 305:

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

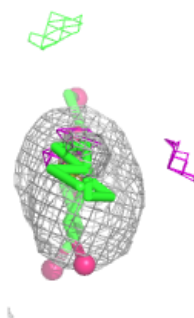
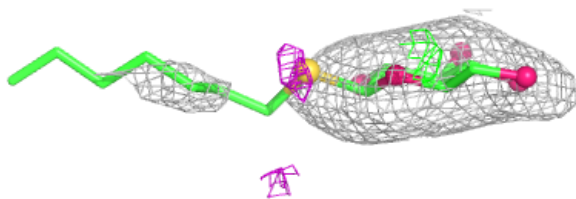
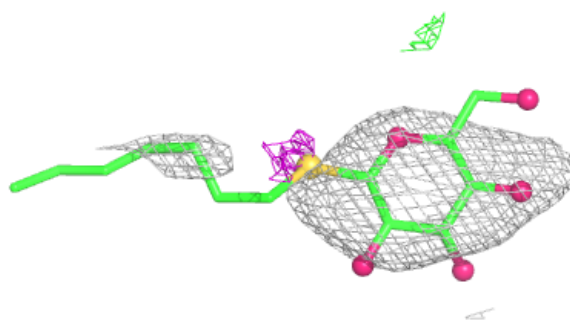
**Electron density around LMG 4 319:**

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



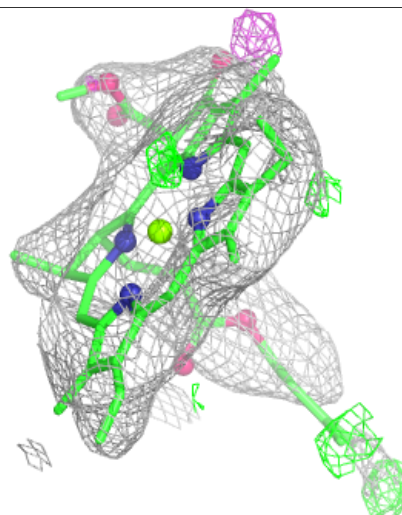
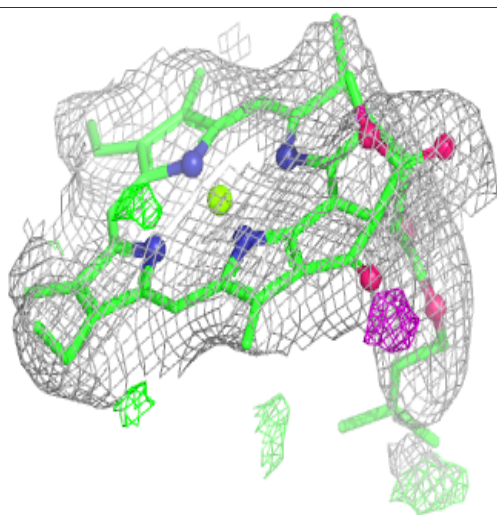
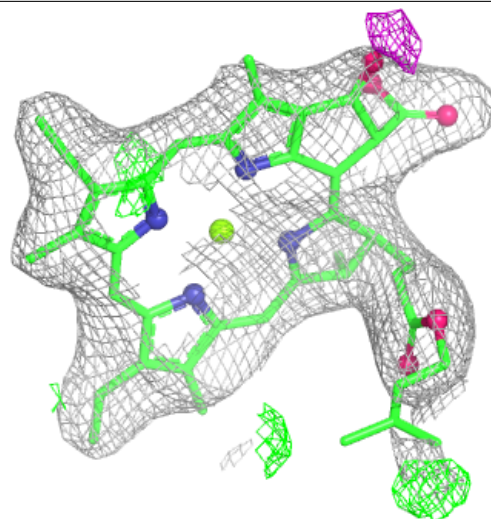
Electron density around HTG 4 321:

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



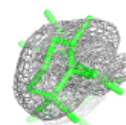
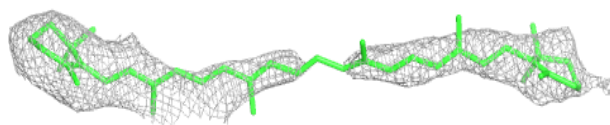
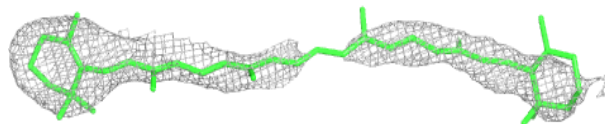
Electron density around CLA 4 304:

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



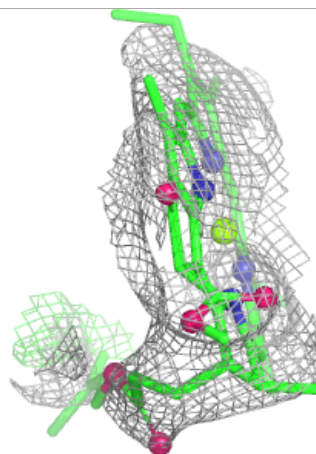
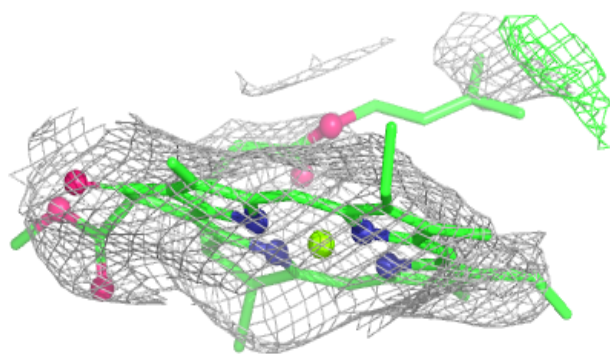
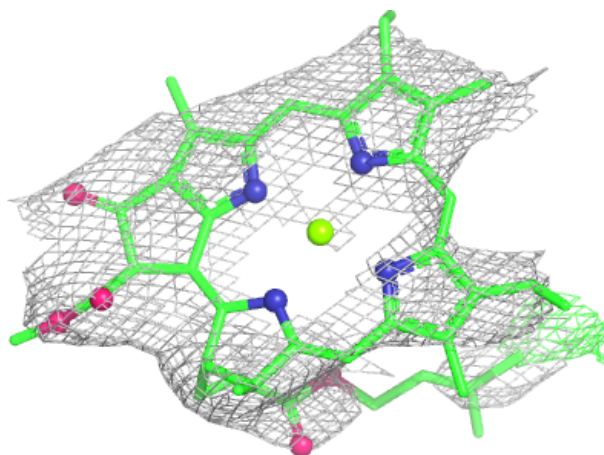
Electron density around BCR L 206:

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



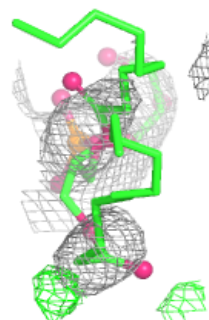
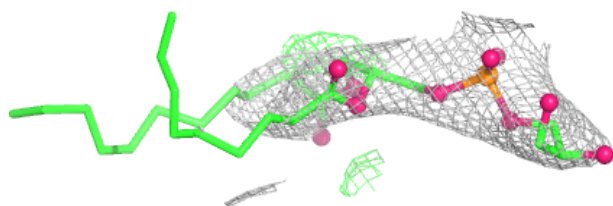
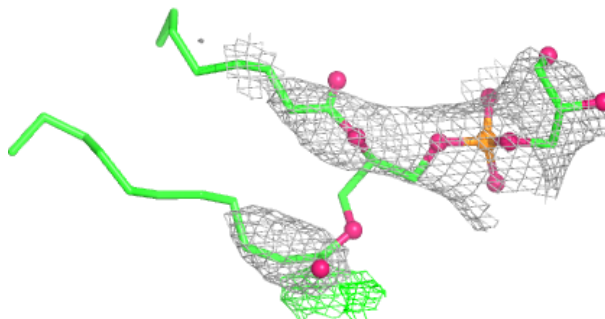
Electron density around CLA 3 609:

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



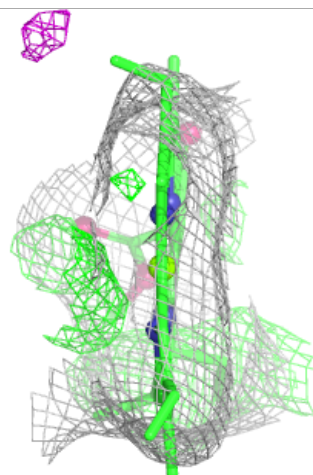
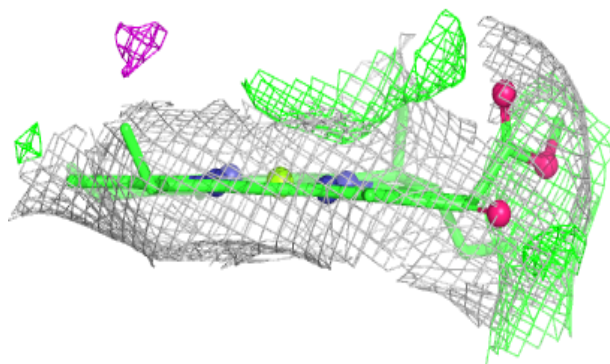
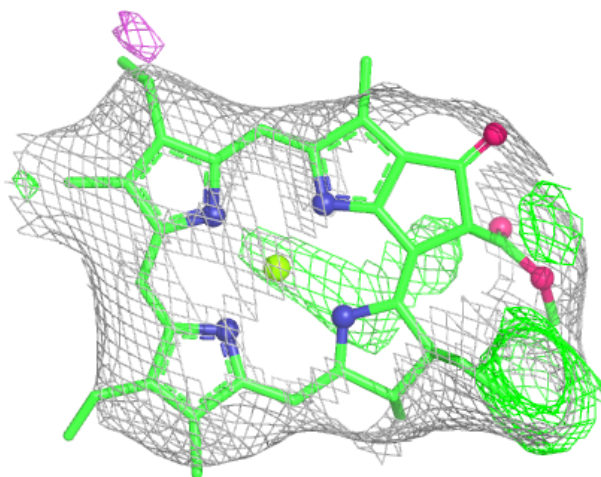
Electron density around LHG 2 317:

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



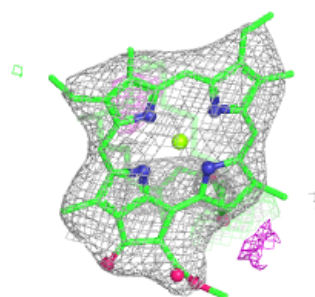
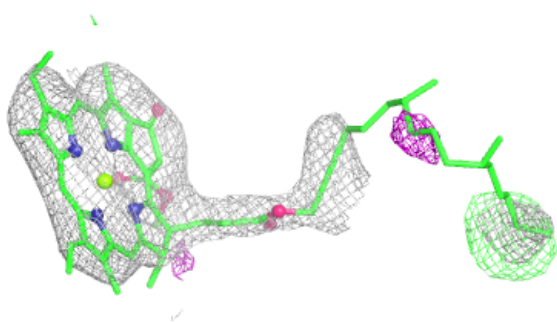
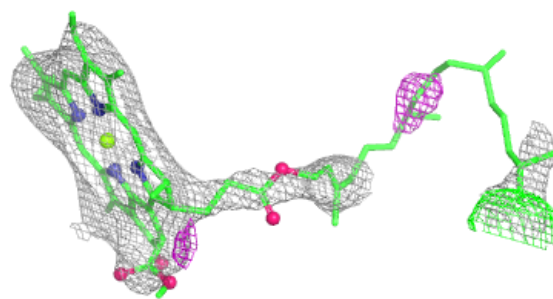
Electron density around CLA 1 304:

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



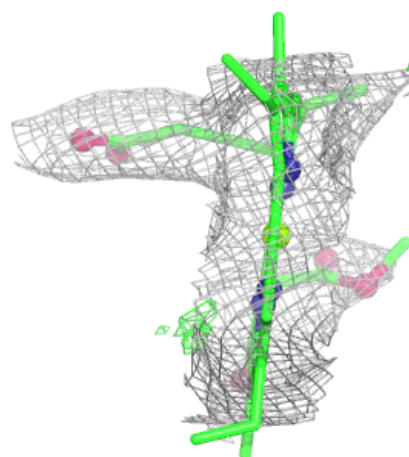
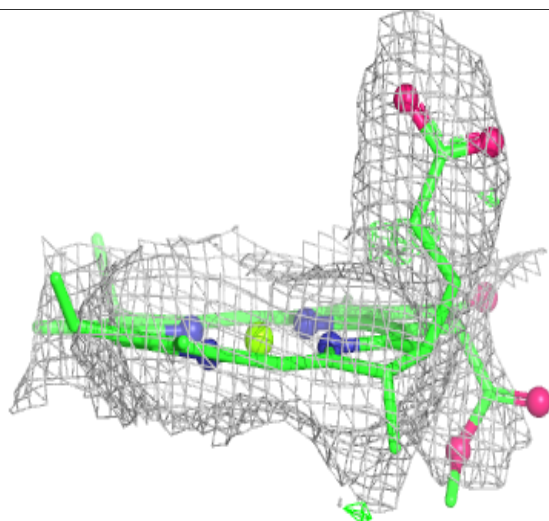
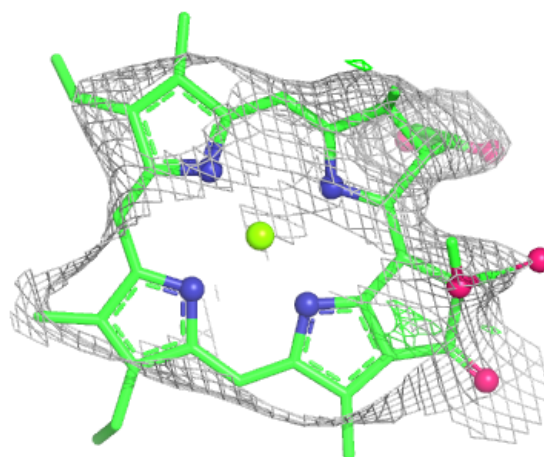
Electron density around CLA A 837:

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



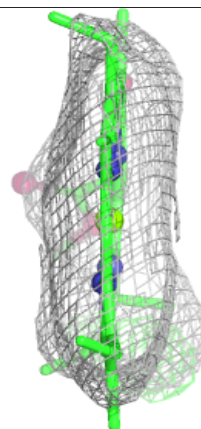
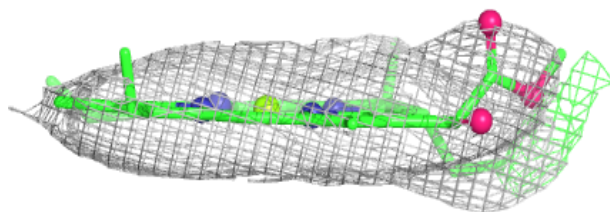
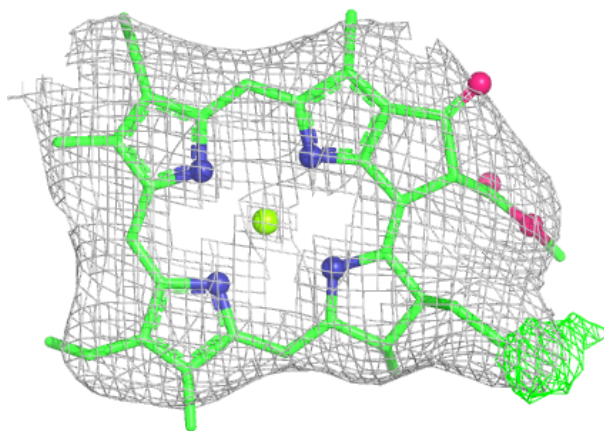
Electron density around CLA 3 604:

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



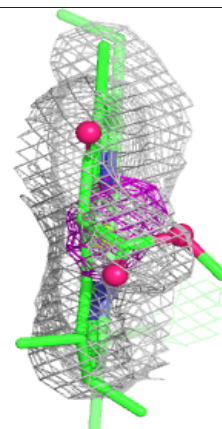
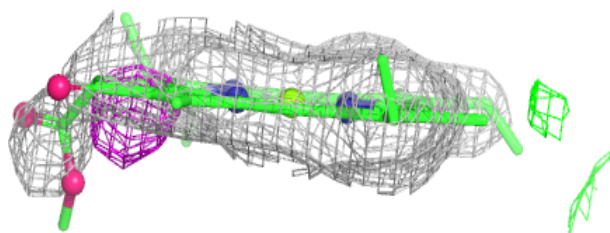
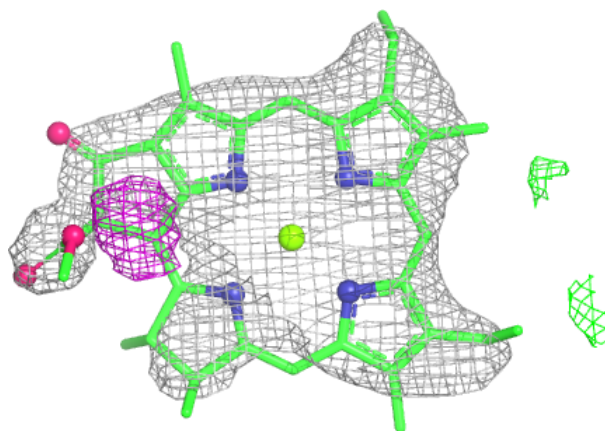
Electron density around CLA 3 605:

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

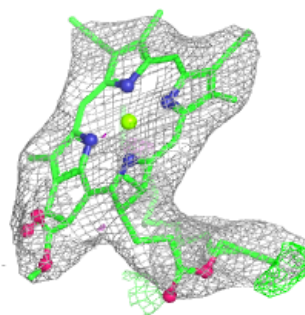
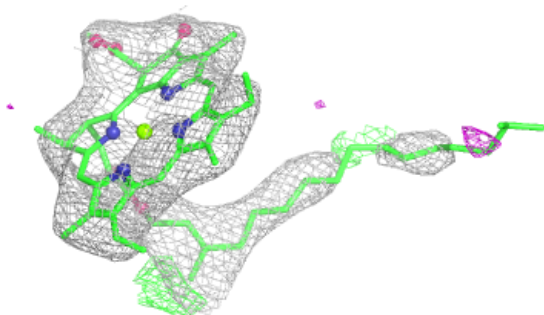
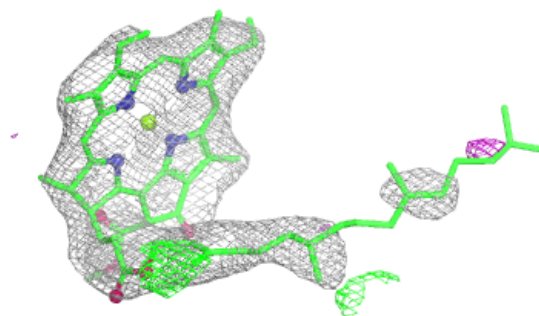


Electron density around CLA G 103:

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

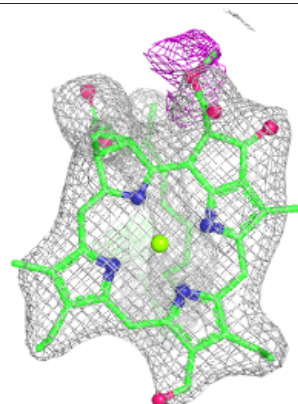
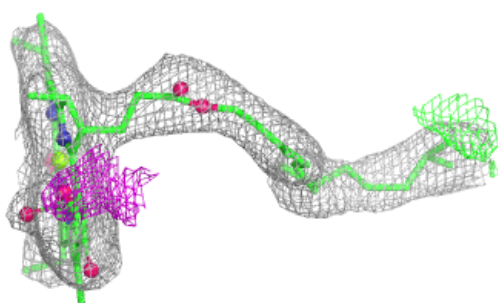
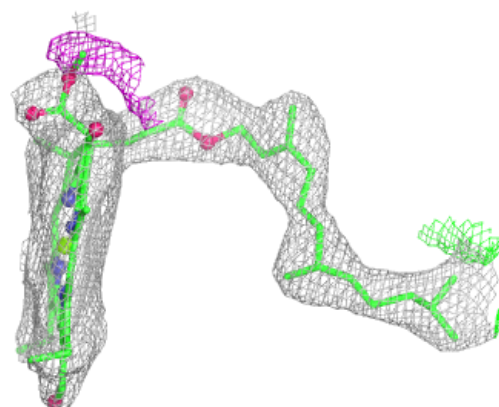
**Electron density around CLA 1 307:**

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

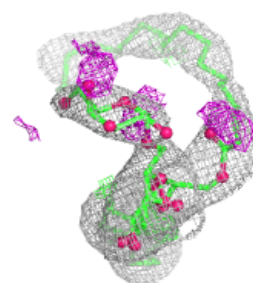
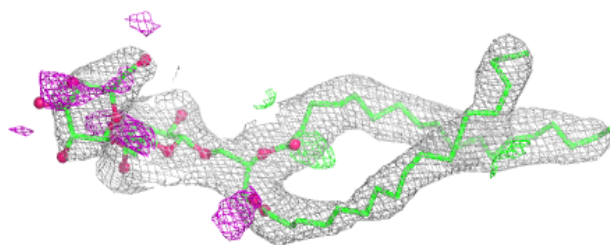
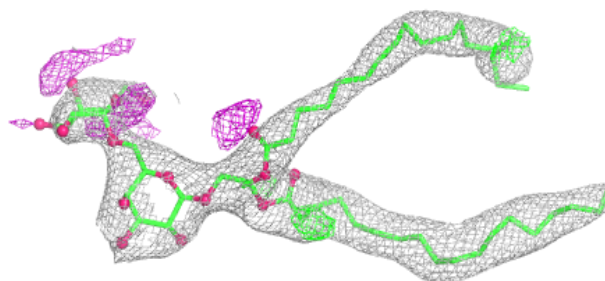


Electron density around CHL 4 301:

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

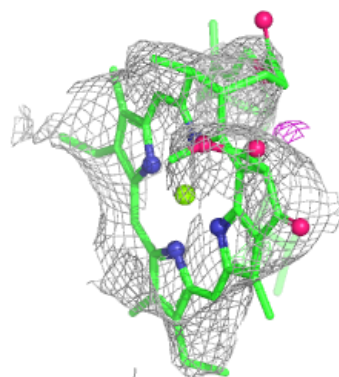
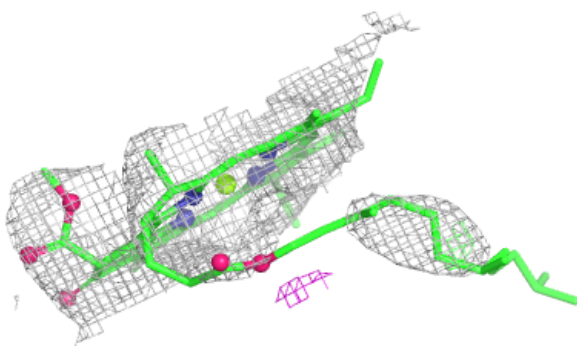
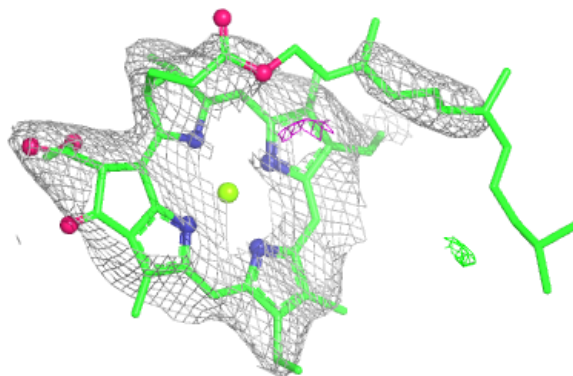
**Electron density around DGD B 850:**

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

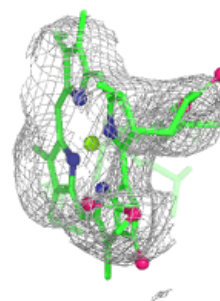
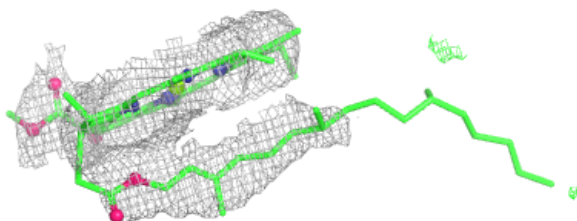
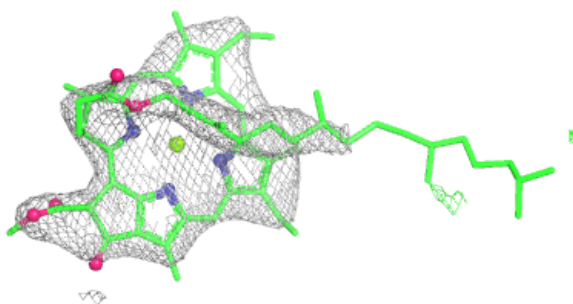


Electron density around CLA 3 602:

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

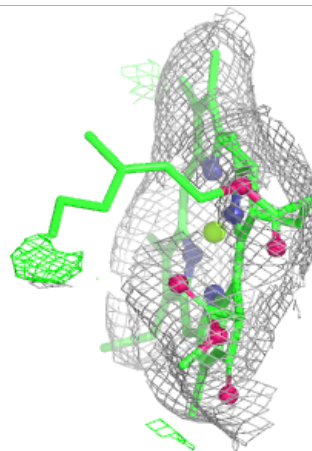
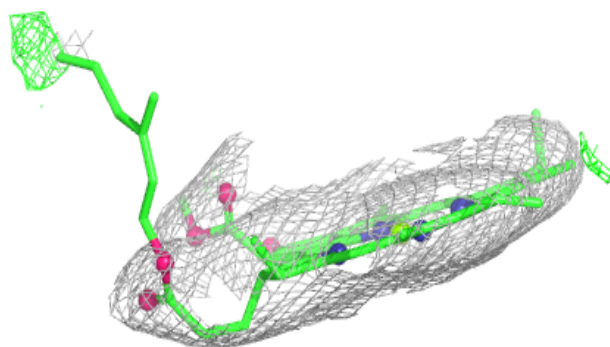
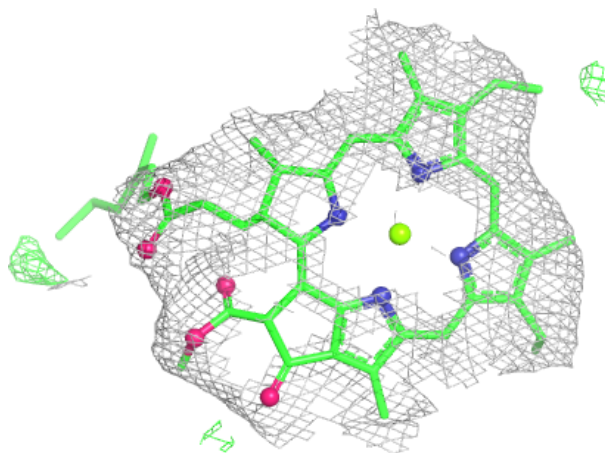
**Electron density around CLA A 817:**

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



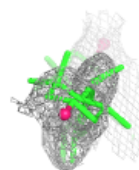
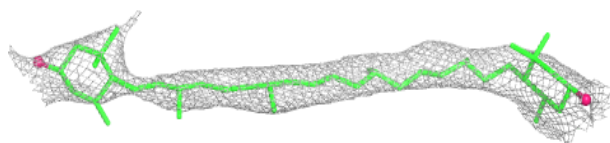
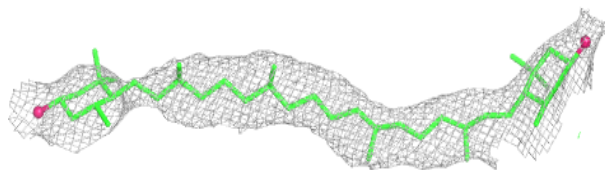
Electron density around CLA 2 310:

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

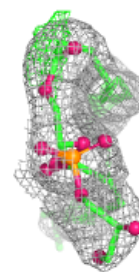
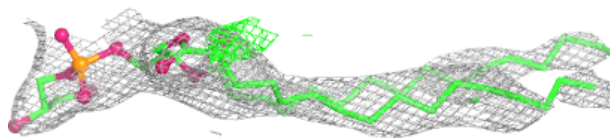
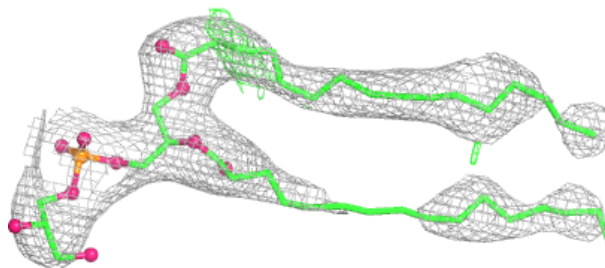


Electron density around LUT 3 614:

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

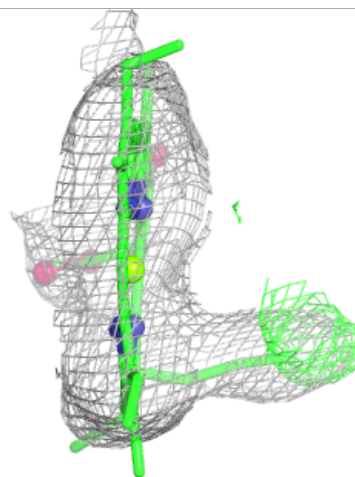
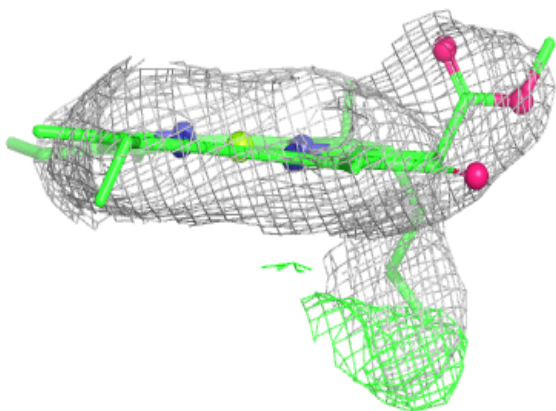
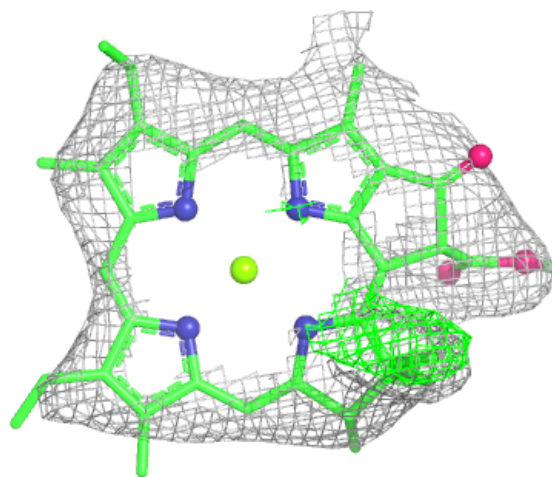
**Electron density around LHG 1 317:**

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



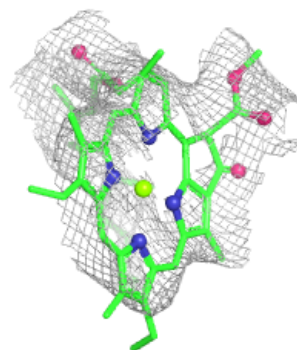
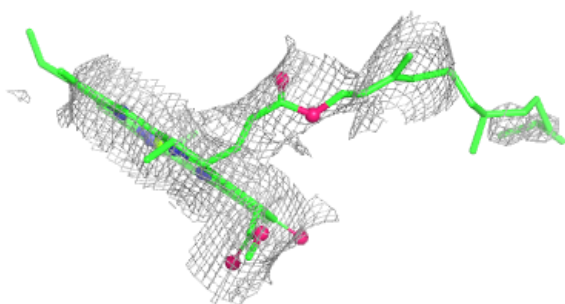
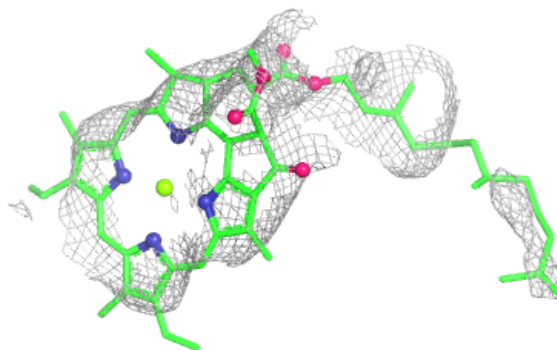
Electron density around CLA 2 312:

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

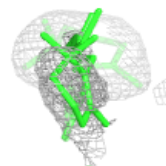
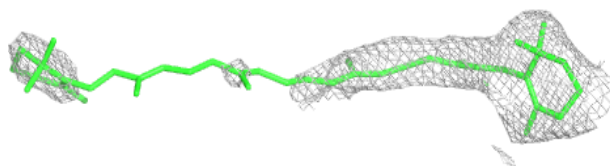
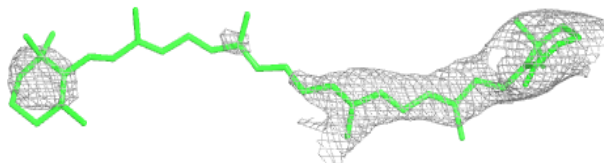


Electron density around CLA K 202:

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

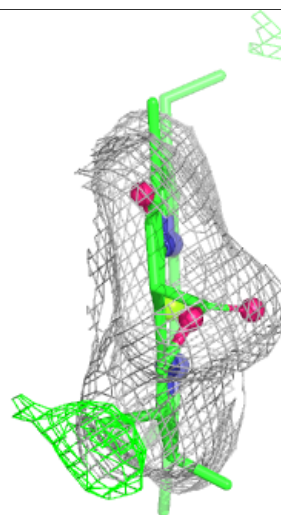
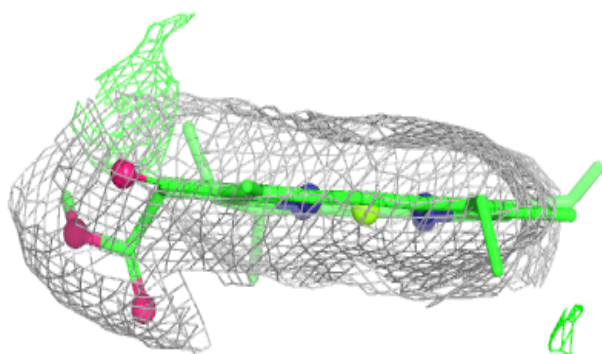
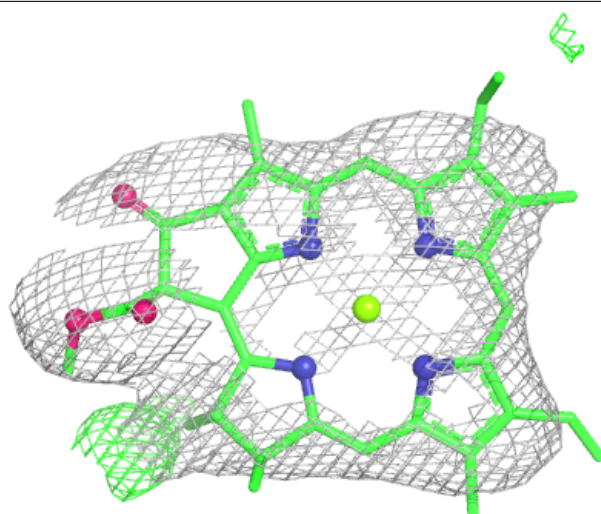
**Electron density around BCR 1 316:**

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



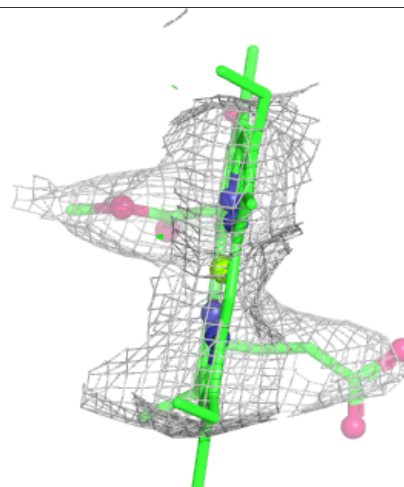
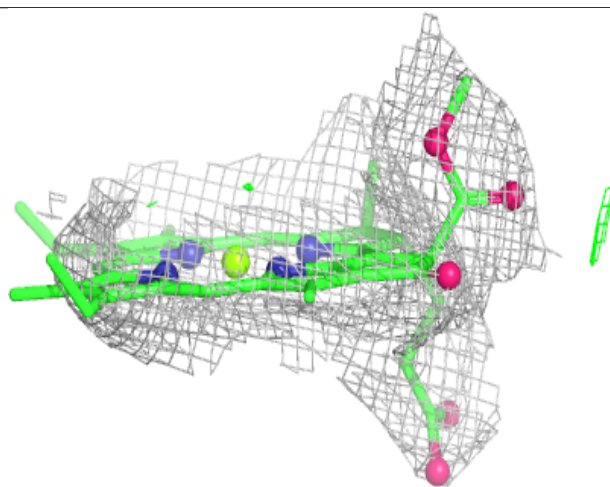
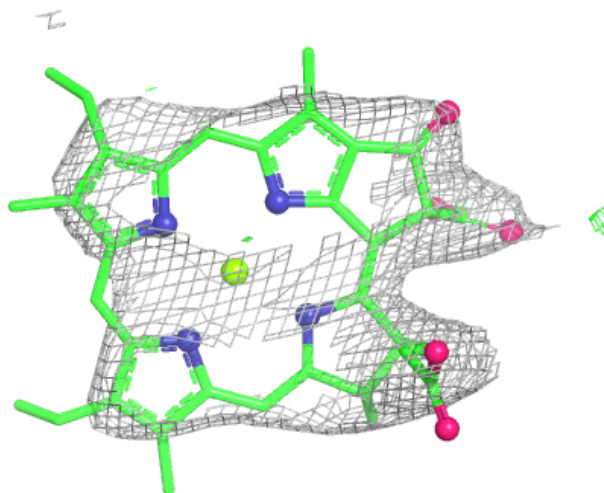
Electron density around CLA 2 309:

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



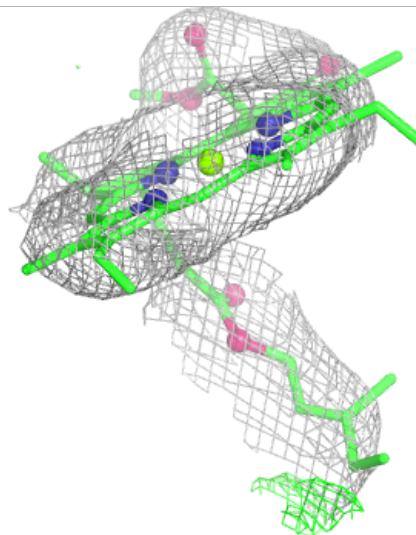
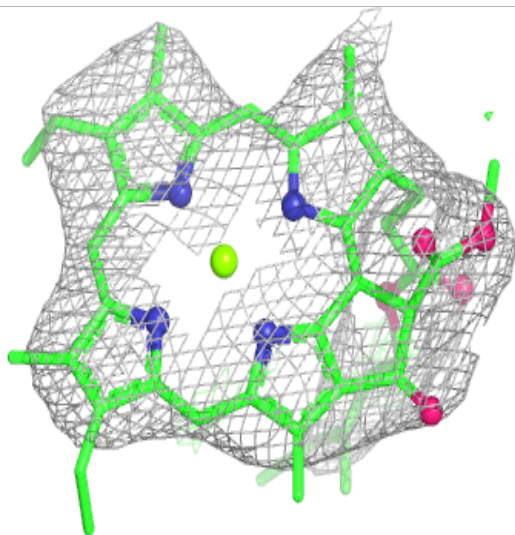
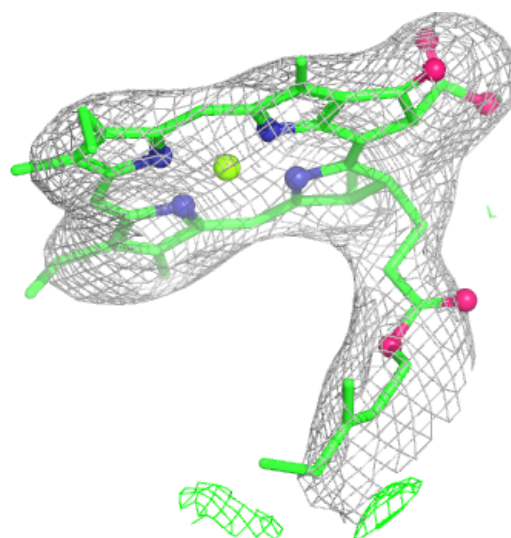
Electron density around CLA A 819:

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



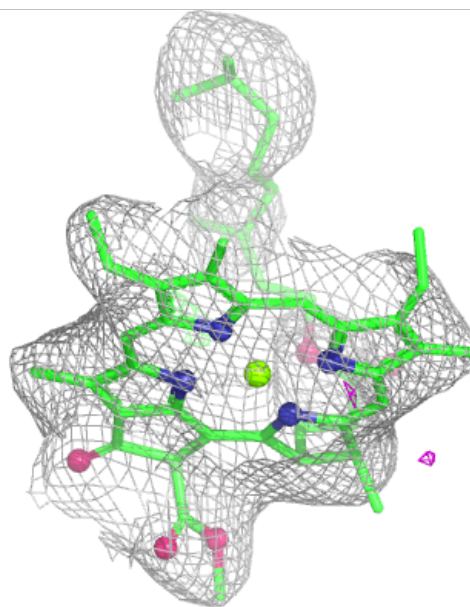
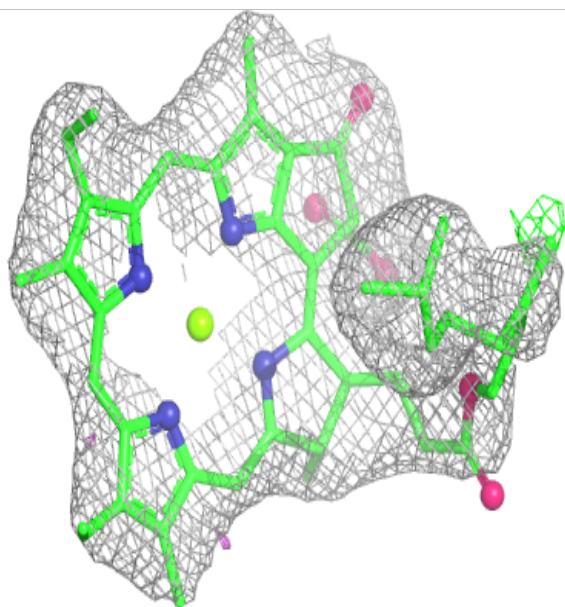
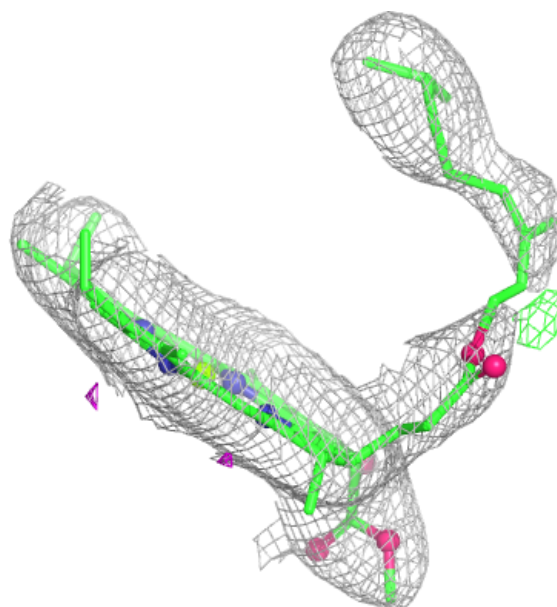
Electron density around CLA 1 303:

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



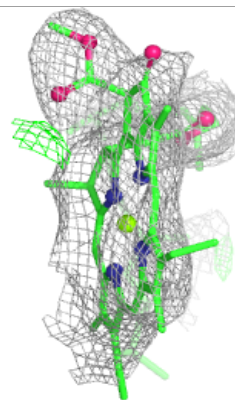
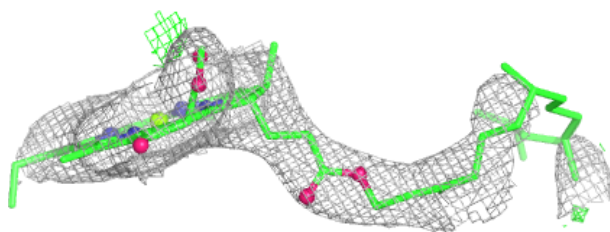
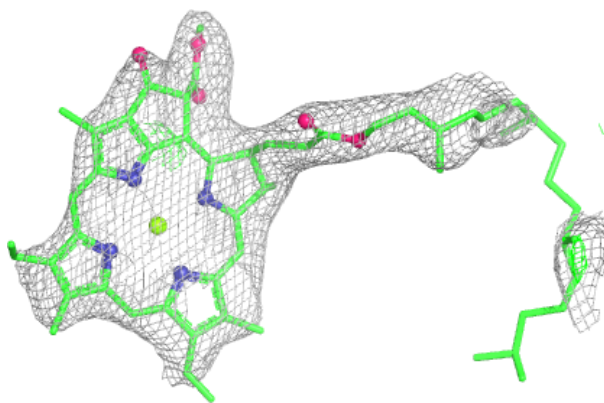
Electron density around CLA 1 312:

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

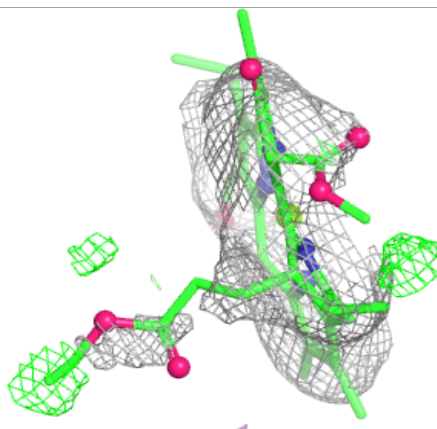
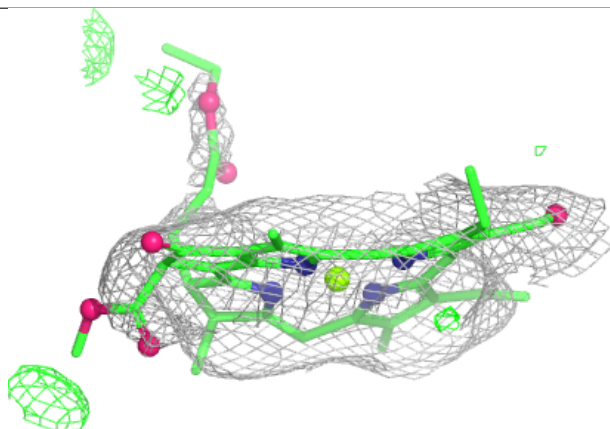
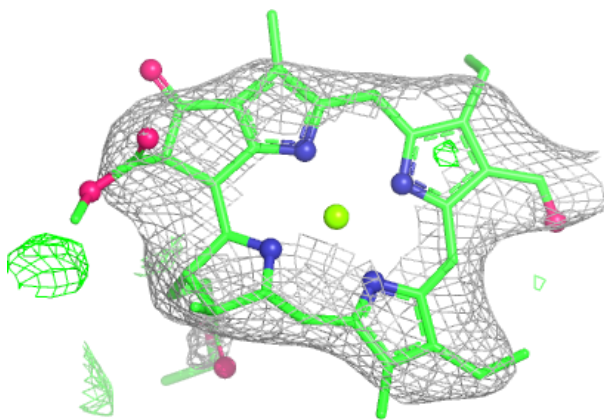


Electron density around CLA A 825:

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

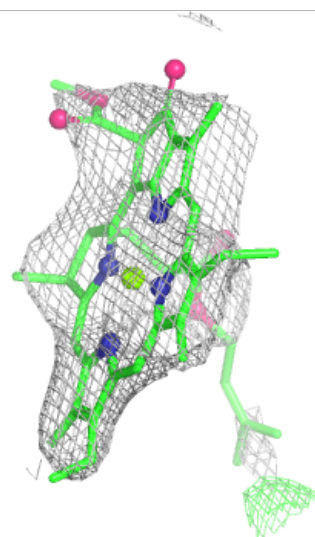
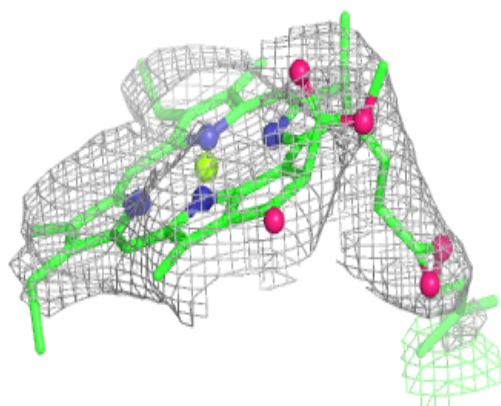
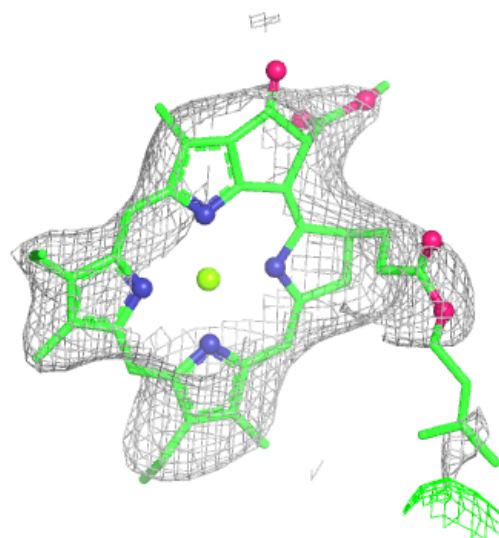
**Electron density around CHL 1 305:**

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



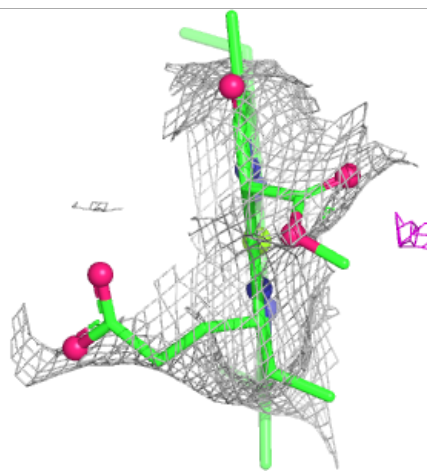
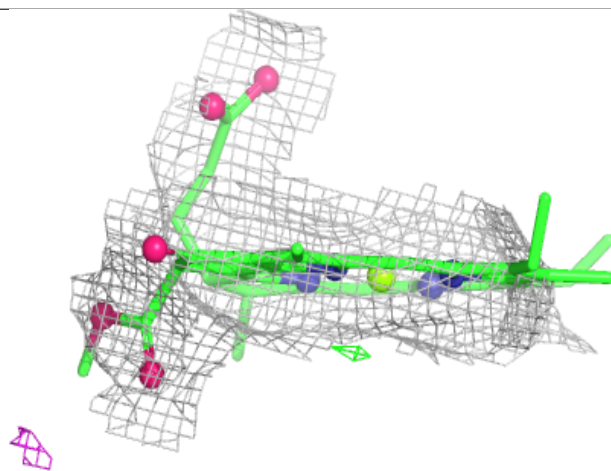
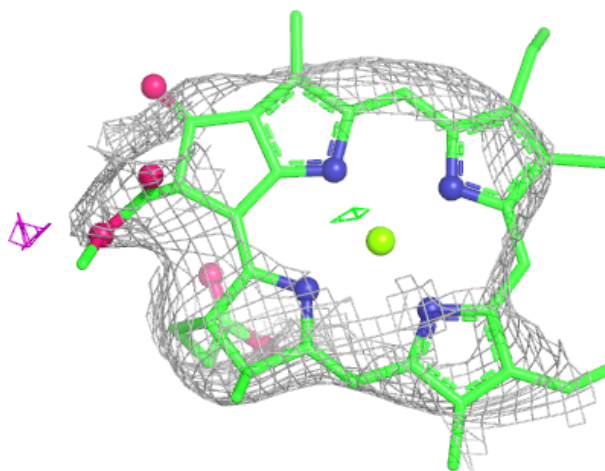
Electron density around CLA A 833:

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



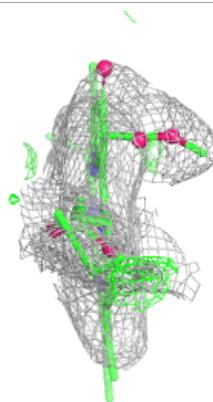
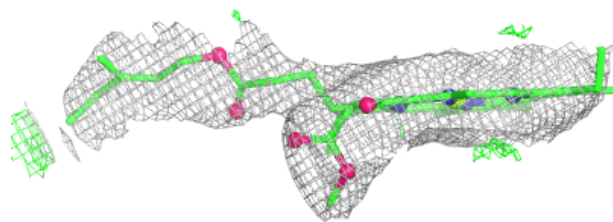
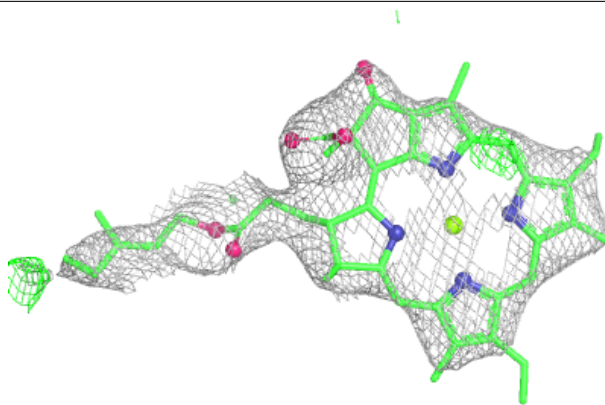
Electron density around CLA A 834:

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



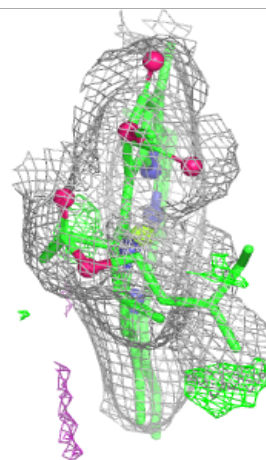
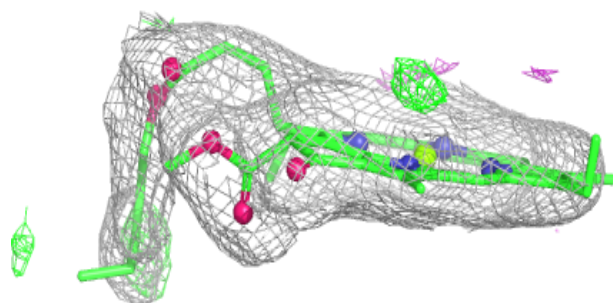
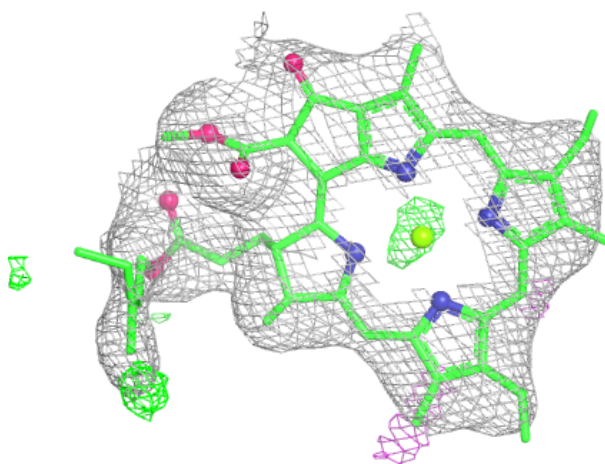
Electron density around CLA A 835:

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



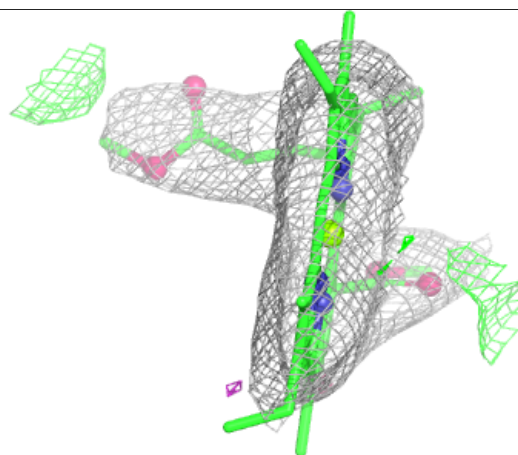
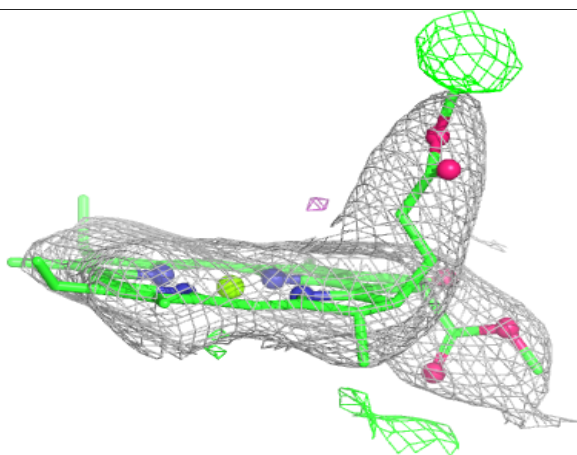
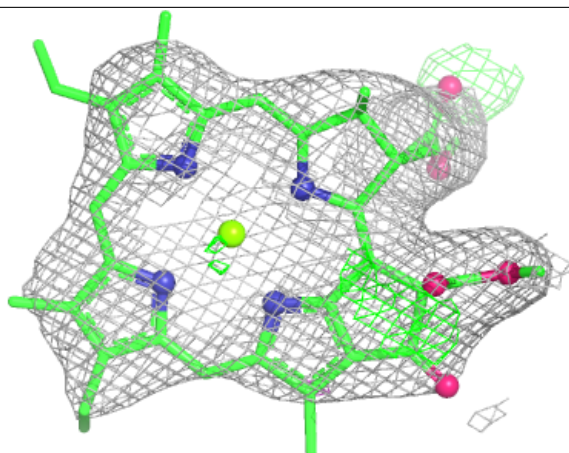
Electron density around CLA 2 302:

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



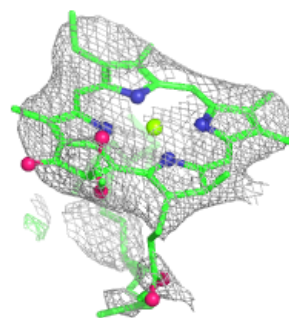
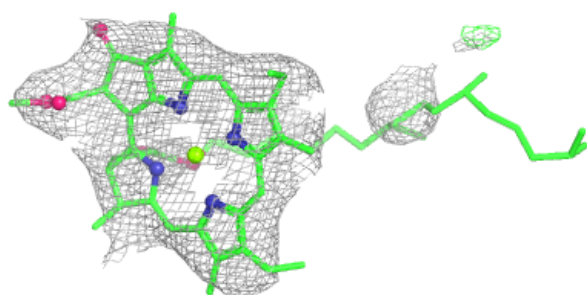
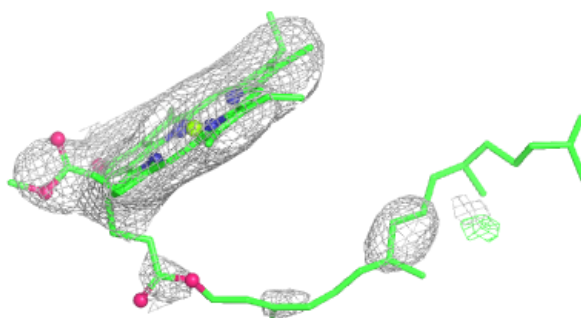
Electron density around CLA 1 306:

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

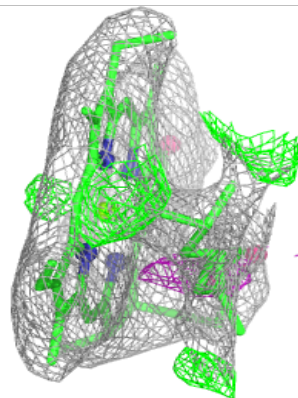
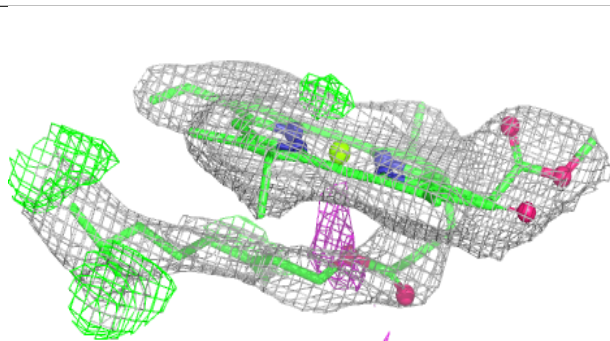
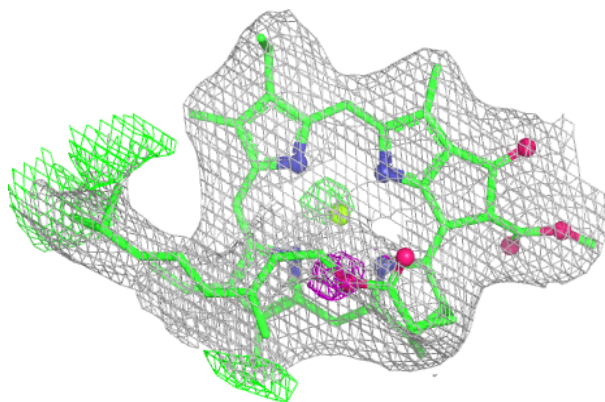


Electron density around CLA B 803:

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

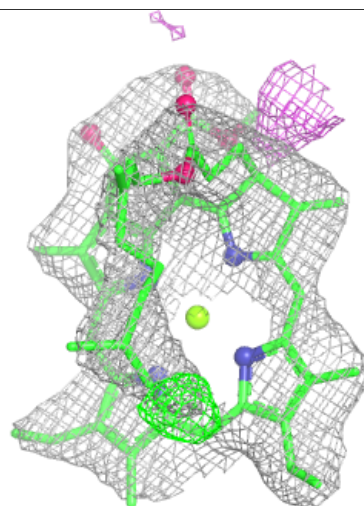
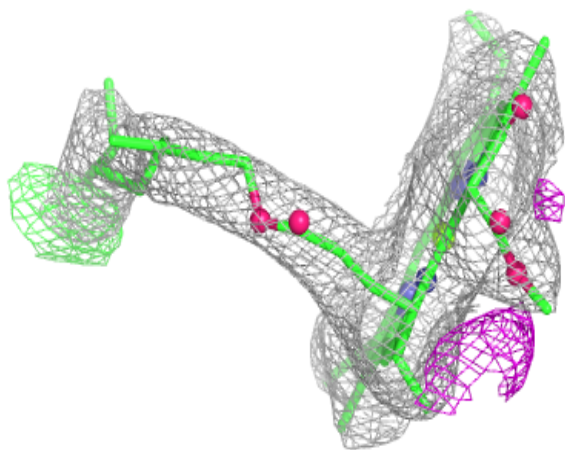
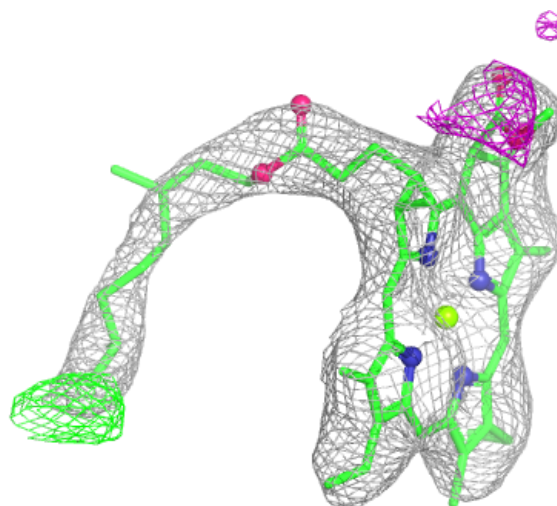
**Electron density around CLA B 814:**

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



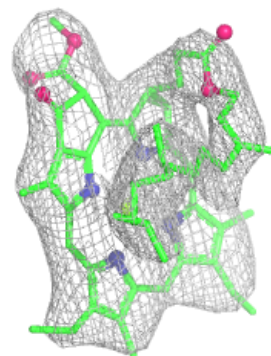
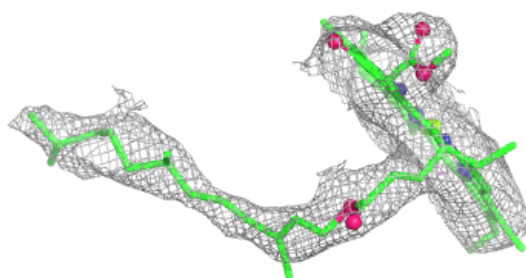
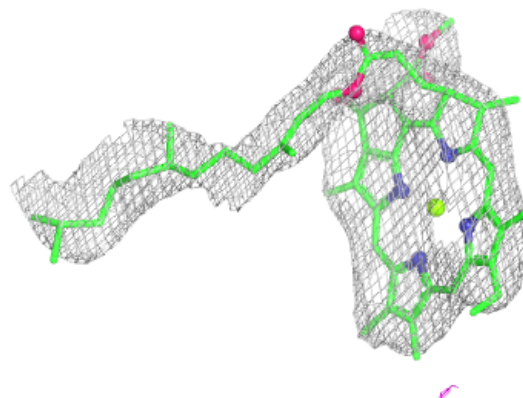
Electron density around CLA B 817:

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

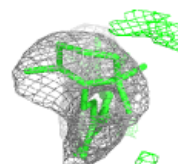
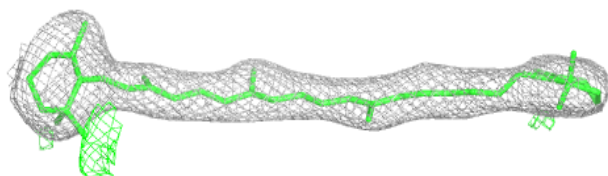
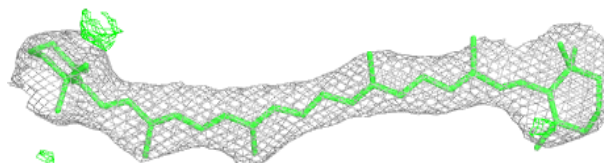


Electron density around CLA 4 310:

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

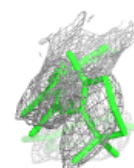
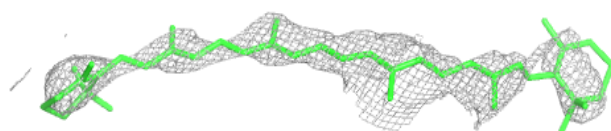
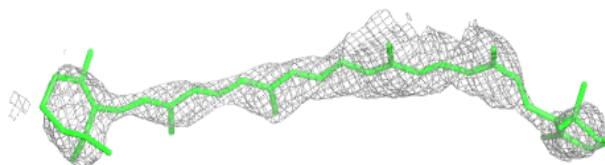
**Electron density around BCR 4 318:**

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

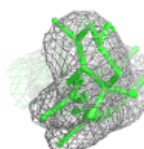
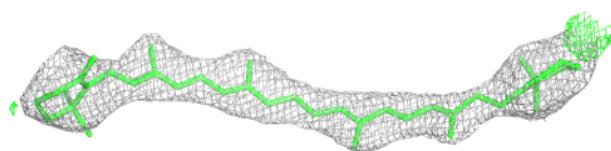
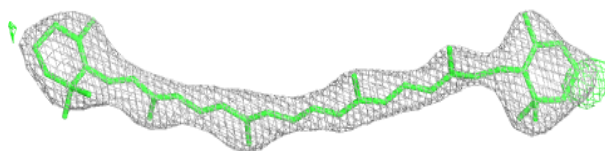


Electron density around BCR A 846:

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

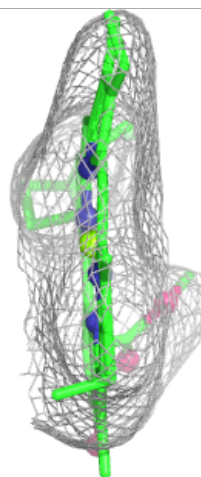
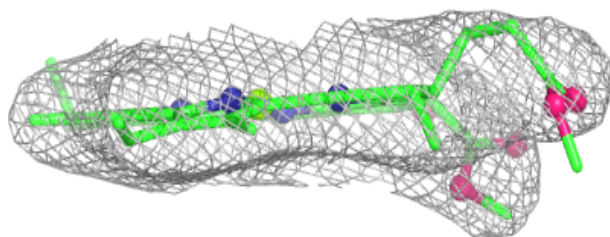
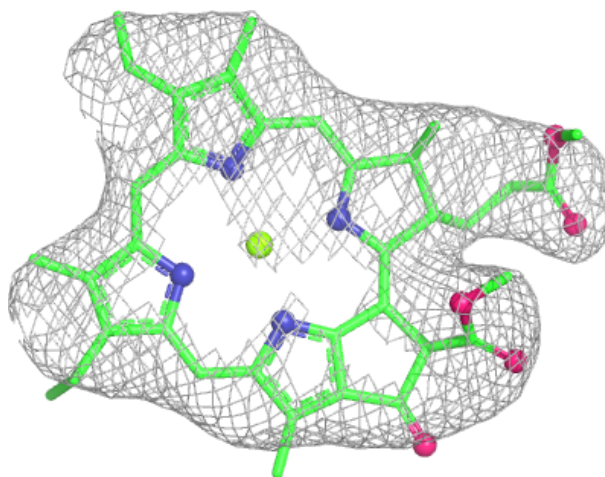
**Electron density around BCR J 105:**

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



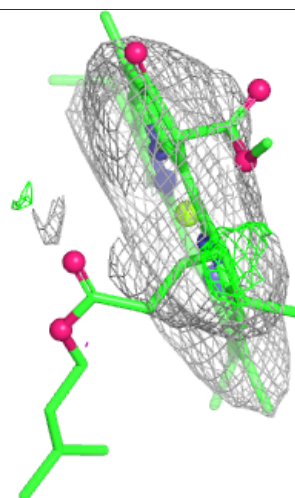
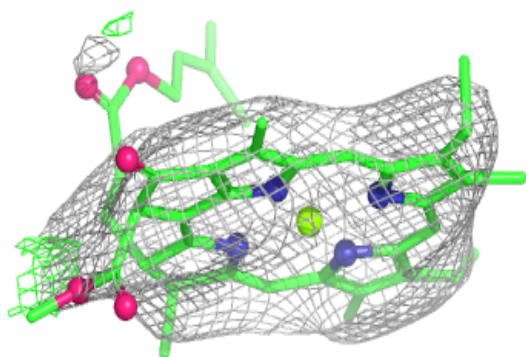
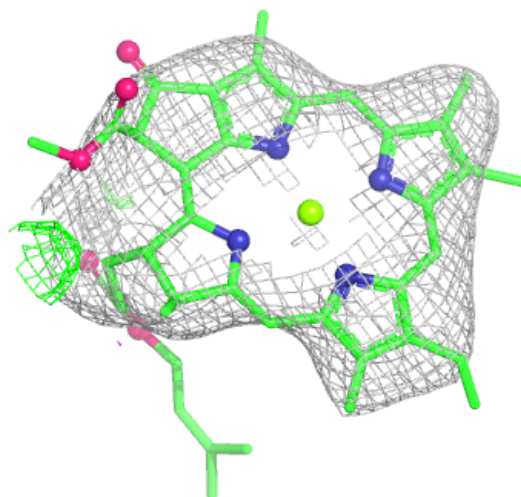
Electron density around CLA G 105:

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



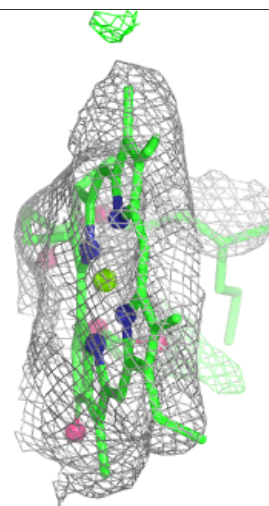
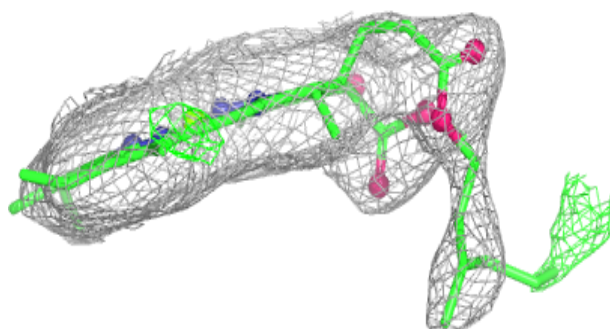
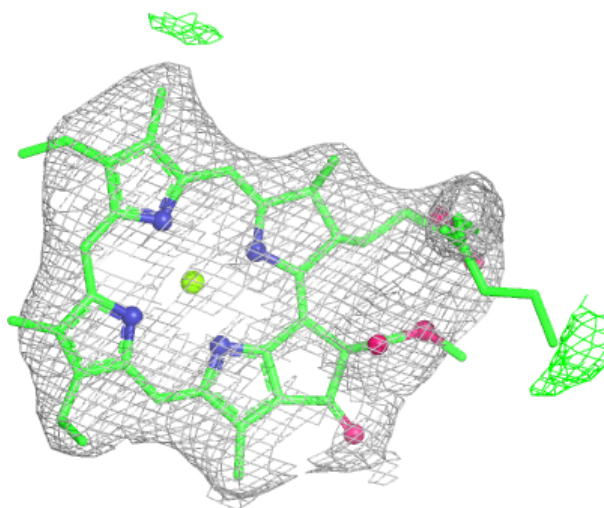
Electron density around CLA A 814:

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



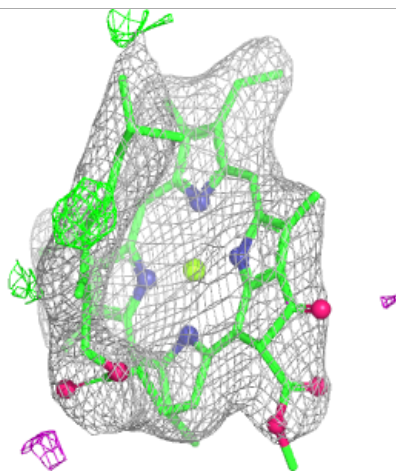
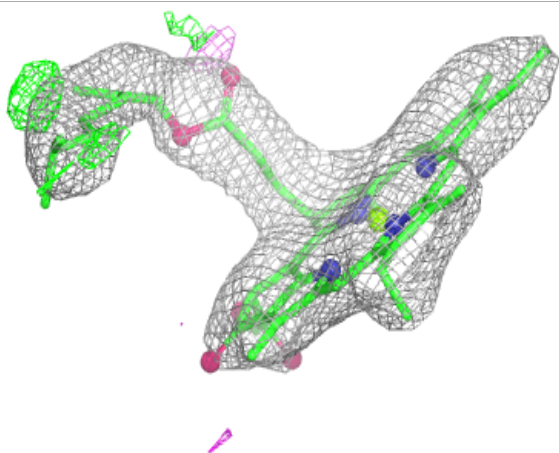
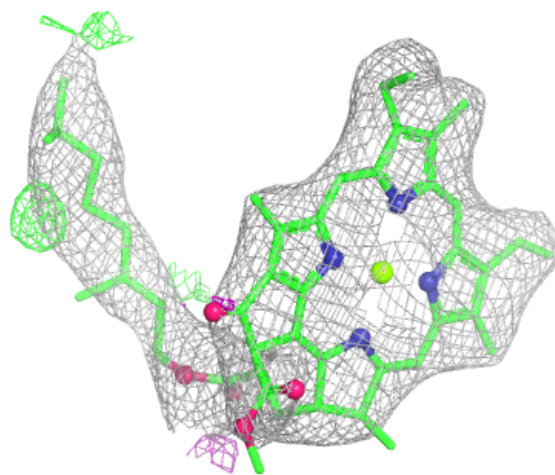
Electron density around CLA 4 311:

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



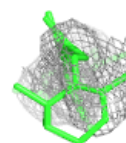
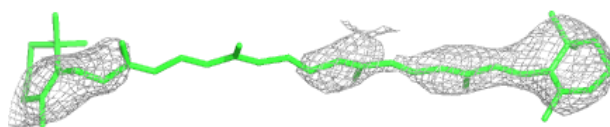
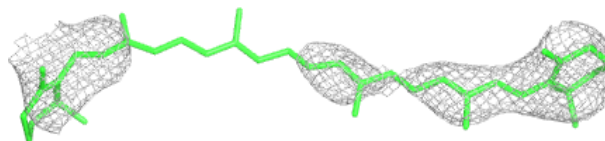
Electron density around CLA B 824:

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

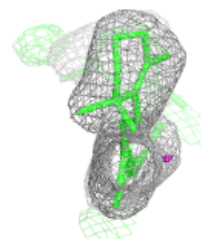
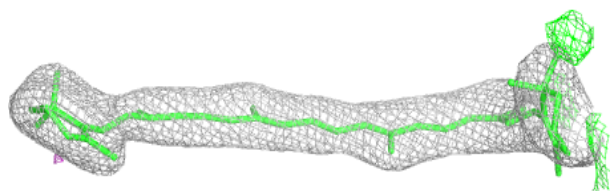
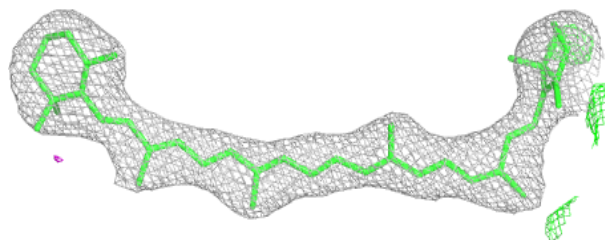


Electron density around BCR A 849:

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

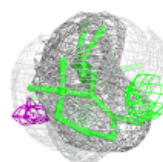
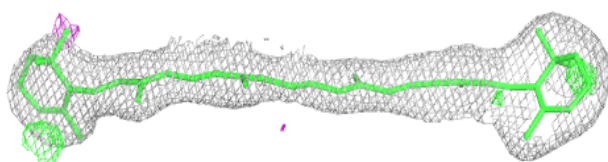
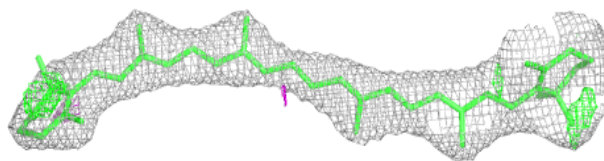
**Electron density around BCR B 845:**

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



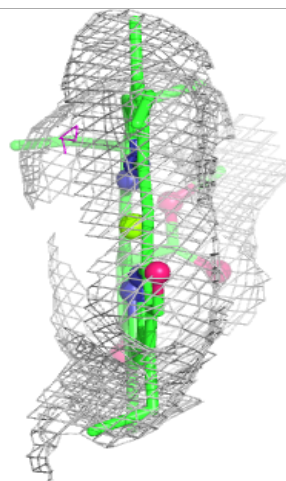
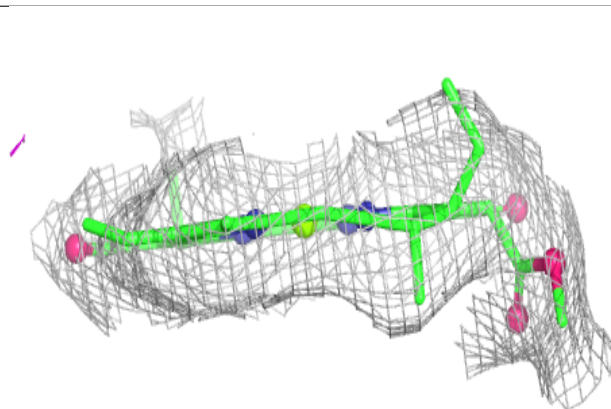
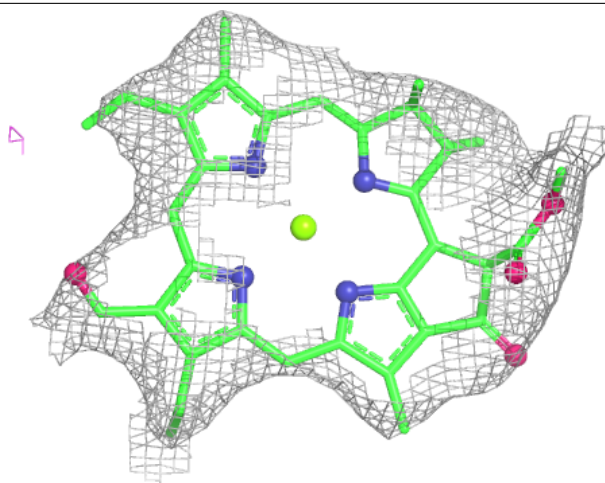
Electron density around BCR B 847:

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



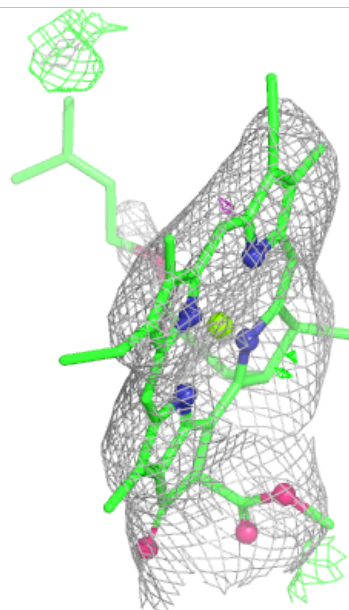
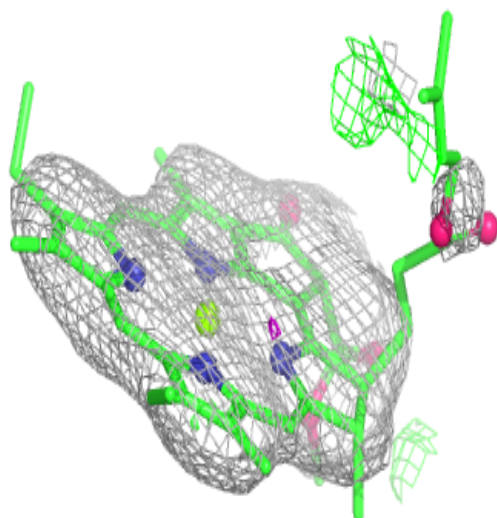
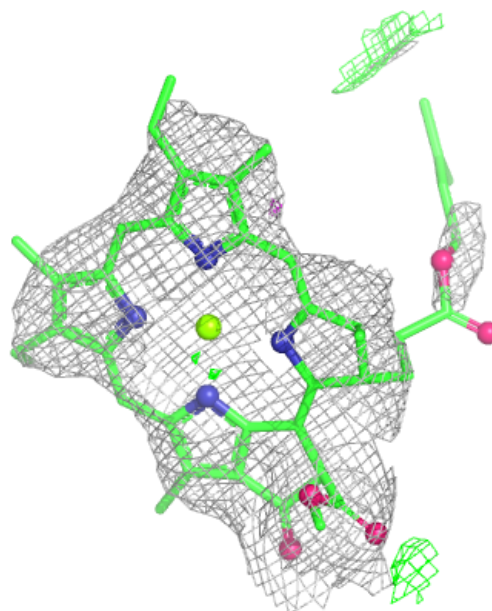
Electron density around CHL 2 313:

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



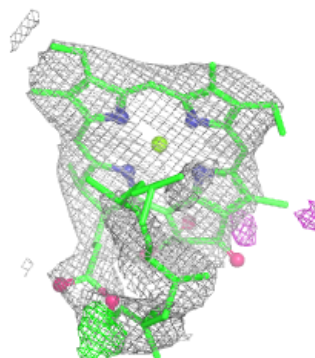
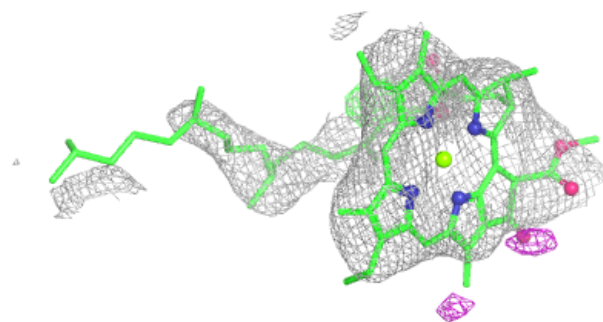
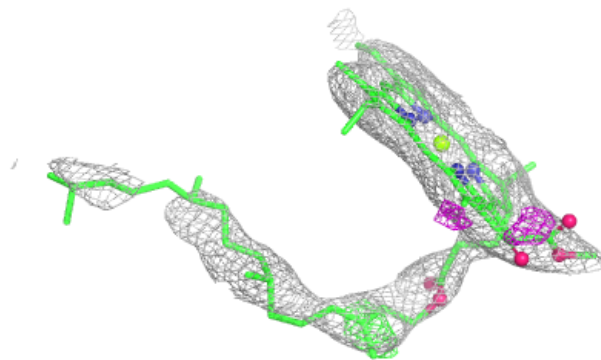
Electron density around CLA A 830:

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

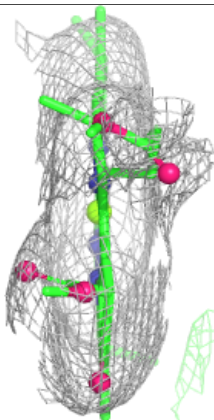
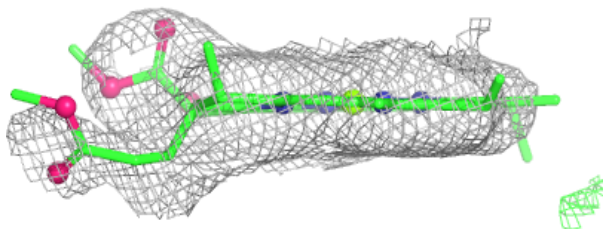
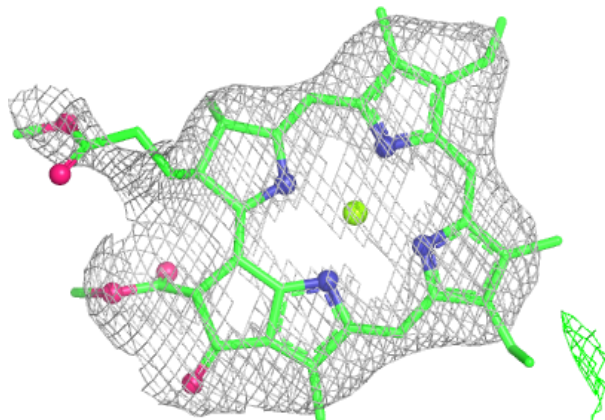


Electron density around CLA A 809:

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

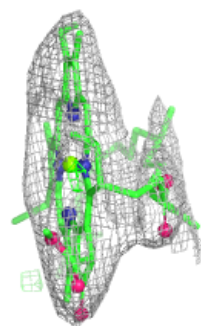
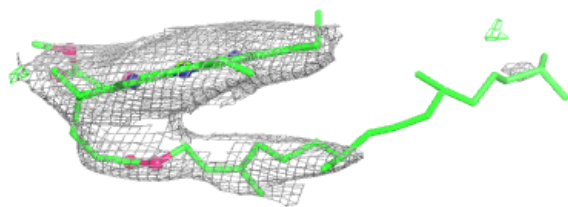
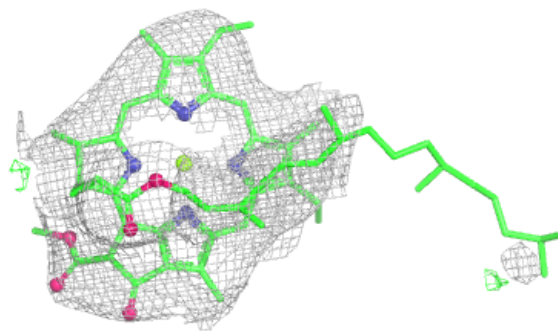
**Electron density around CLA 3 613:**

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



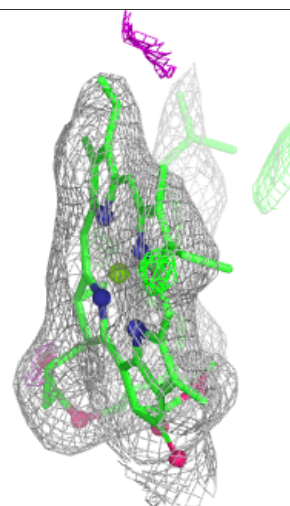
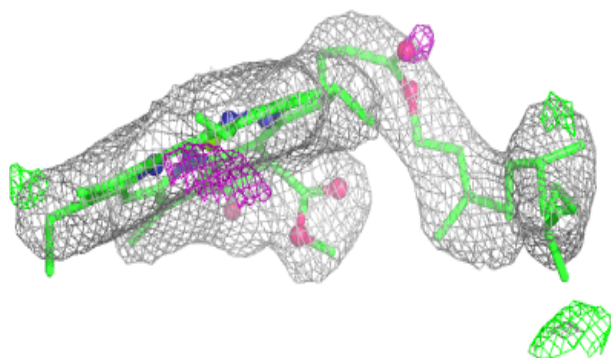
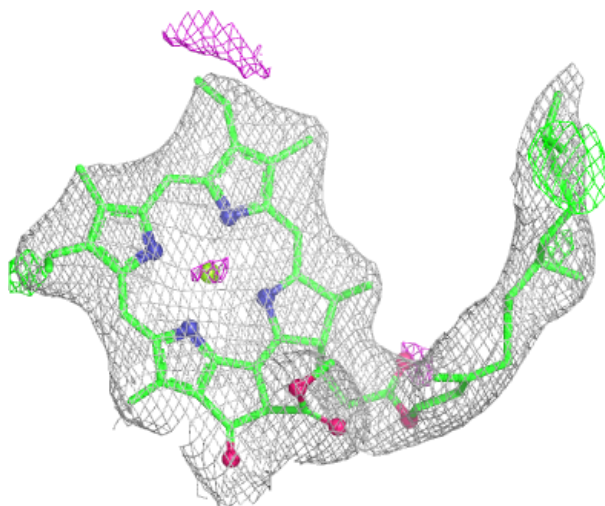
Electron density around CLA A 816:

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



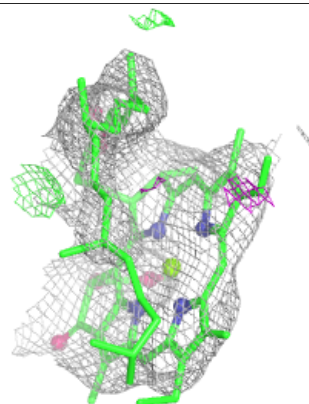
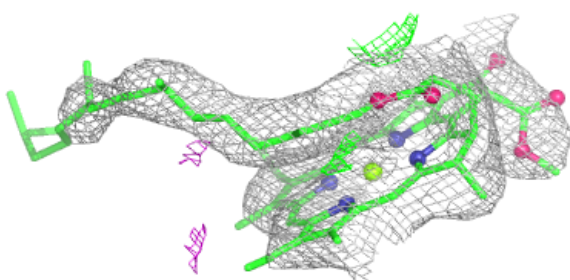
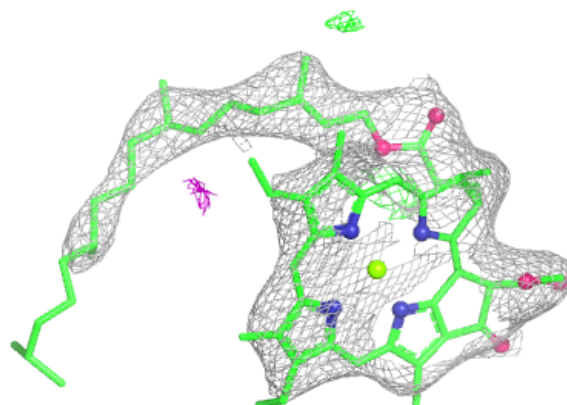
Electron density around CLA 4 303:

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

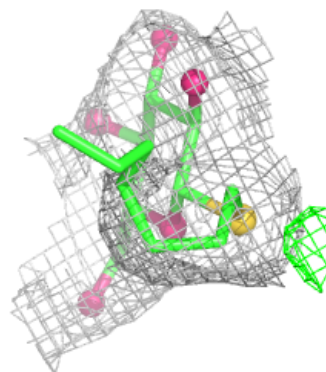
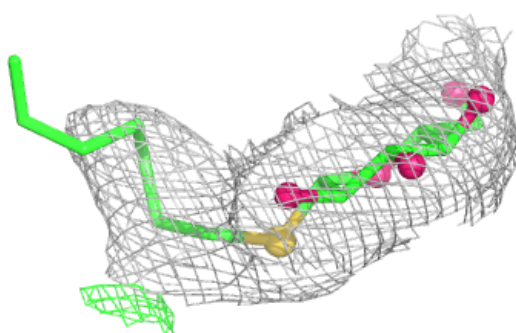
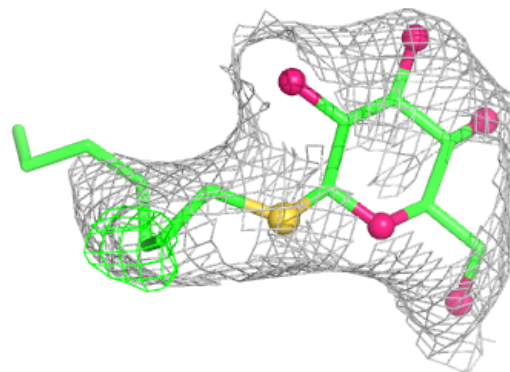


Electron density around CLA 2 301:

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

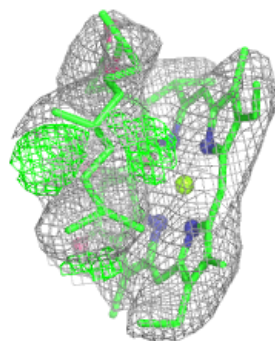
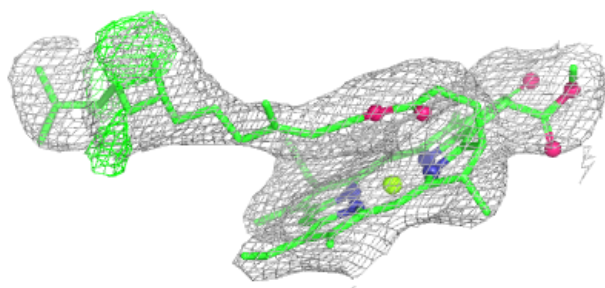
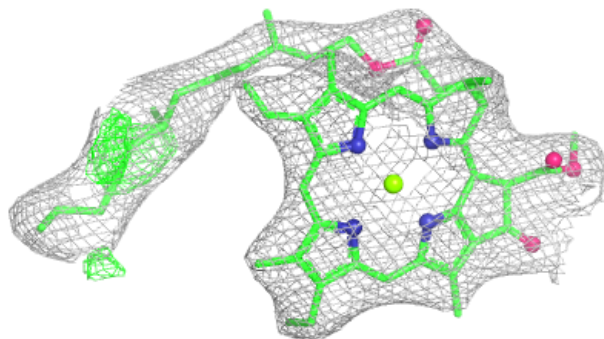
**Electron density around HTG J 102:**

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

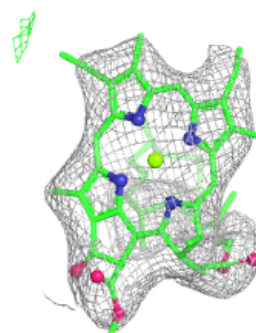
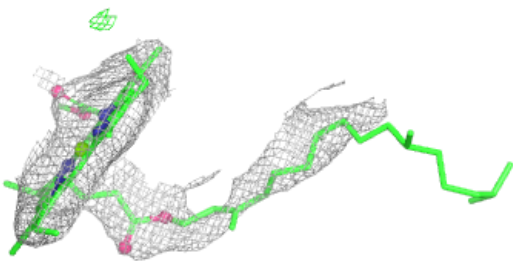
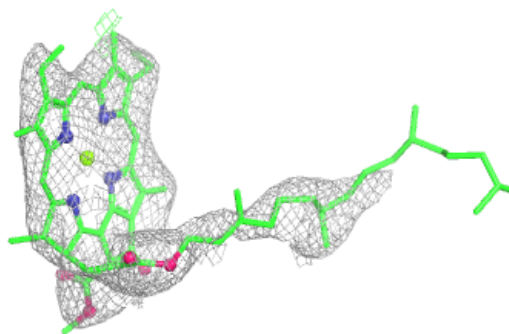


Electron density around CLA 4 309:

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

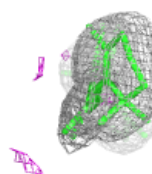
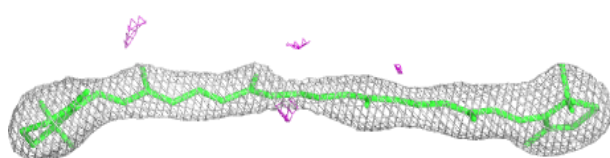
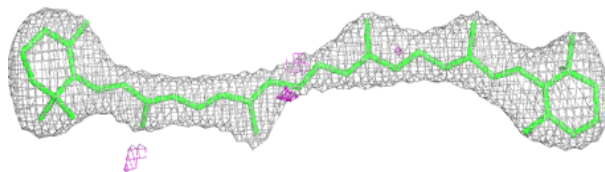
**Electron density around CLA 1 309:**

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



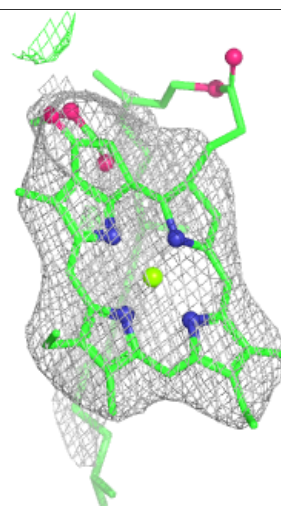
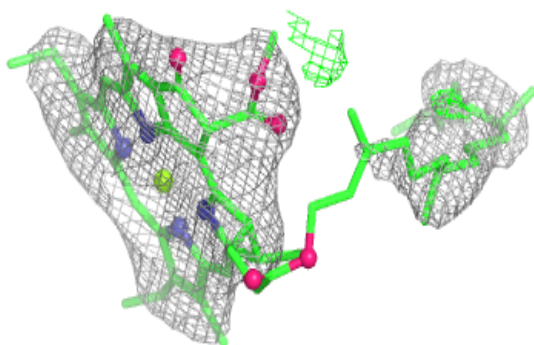
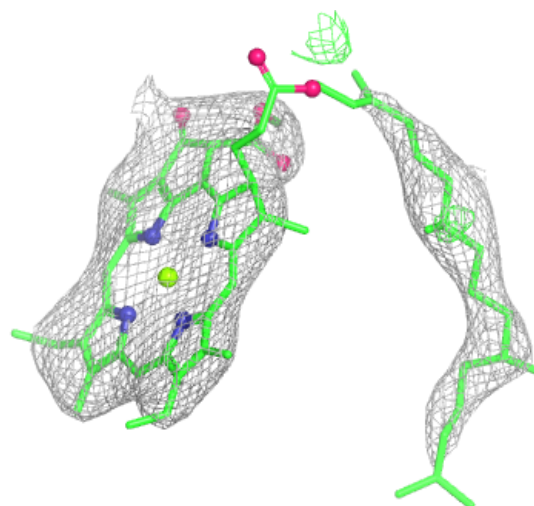
Electron density around BCR J 104:

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



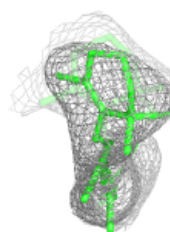
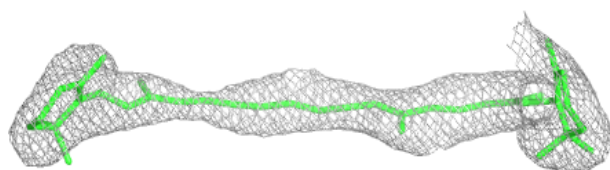
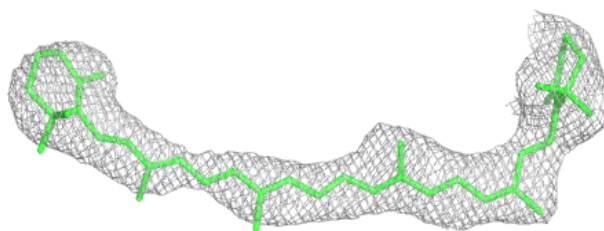
Electron density around CLA B 812:

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

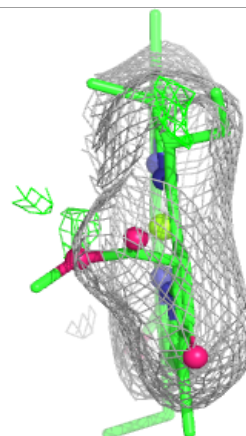
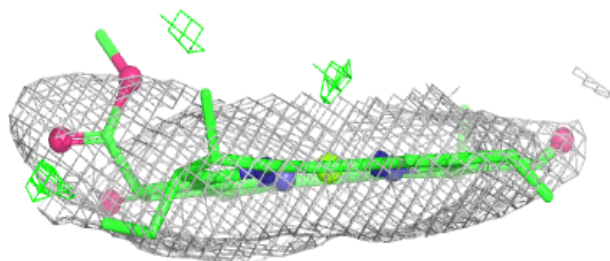
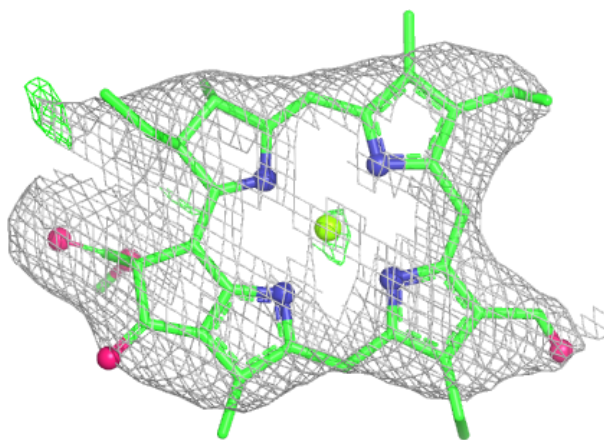


Electron density around BCR L 201:

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

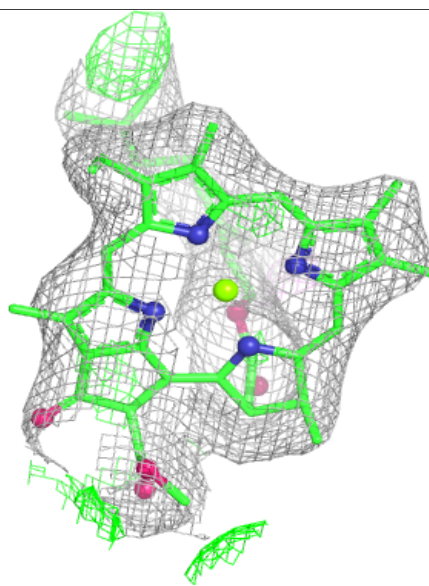
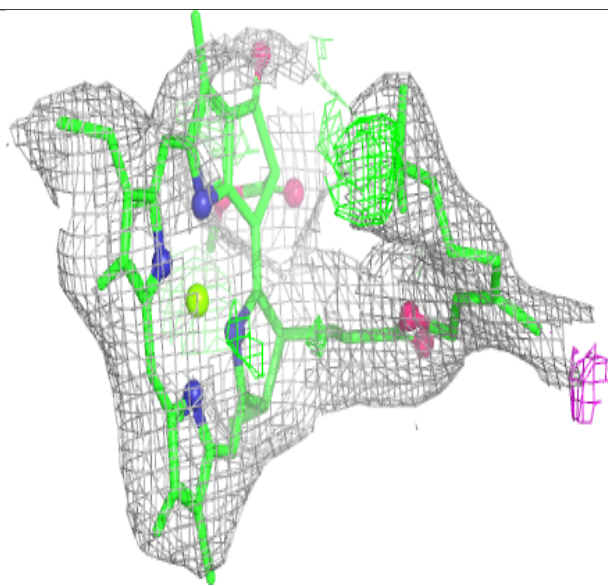
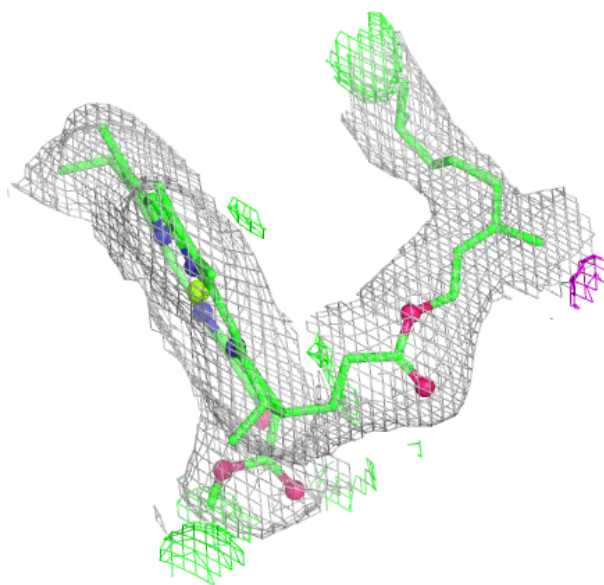
**Electron density around CHL 2 304:**

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



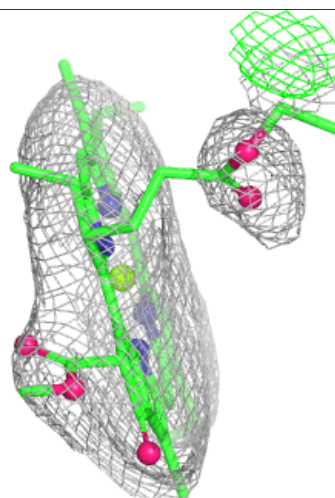
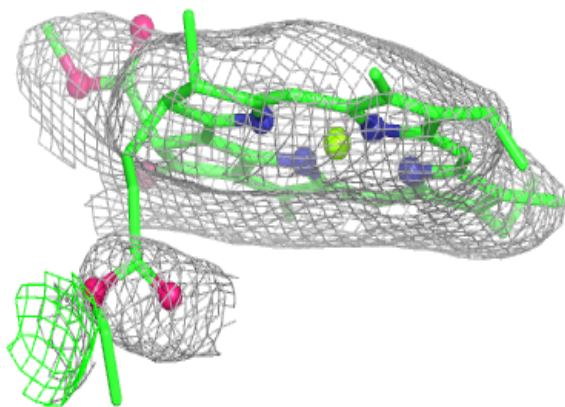
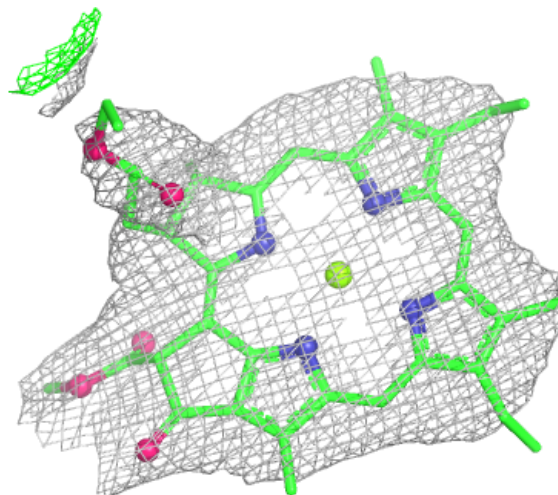
Electron density around CLA B 813:

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



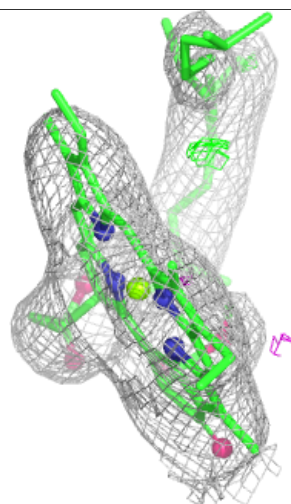
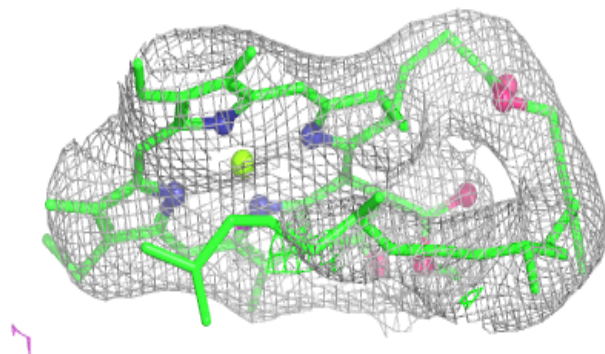
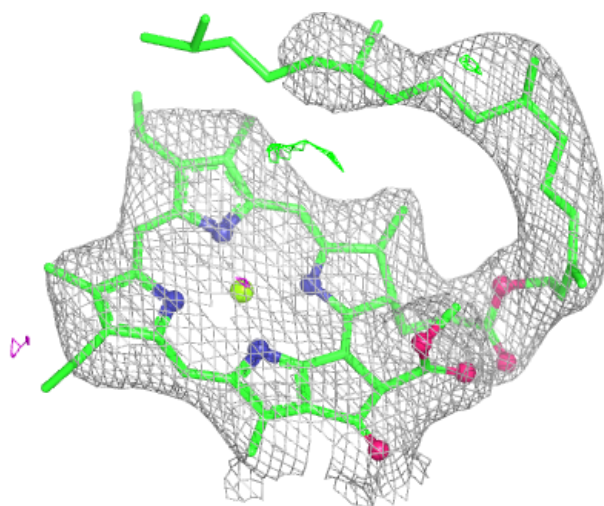
Electron density around CLA 3 606:

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



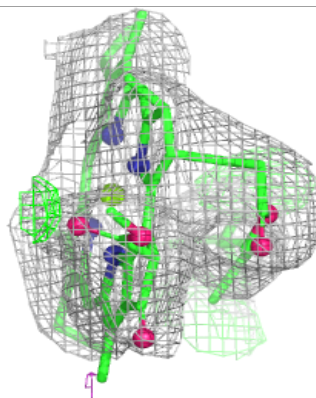
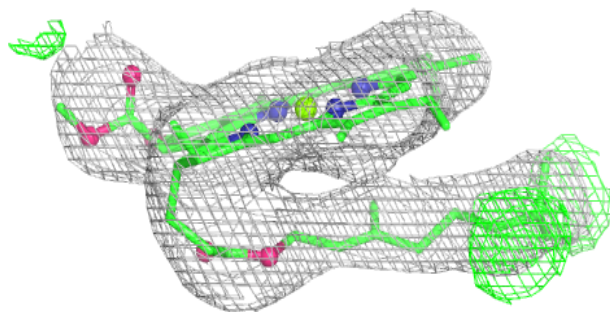
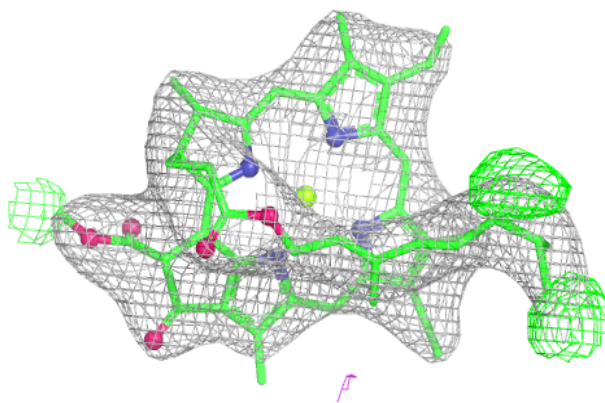
Electron density around CLA 1 302:

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

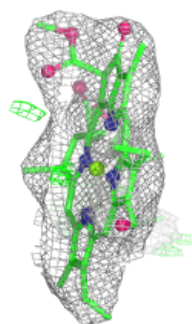
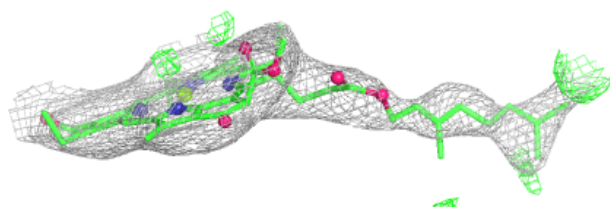
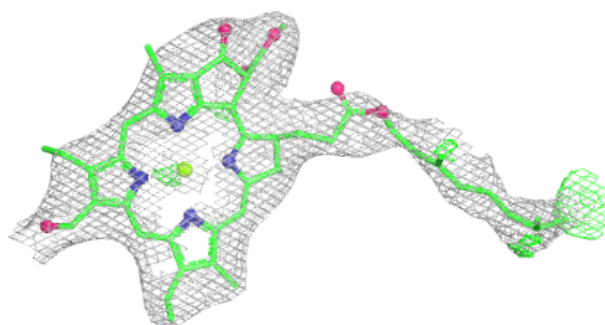


Electron density around CLA B 818:

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

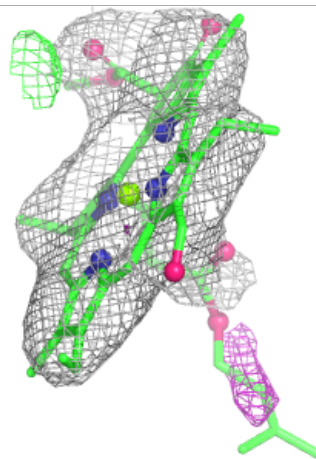
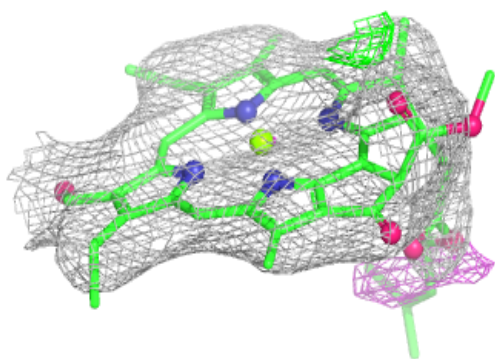
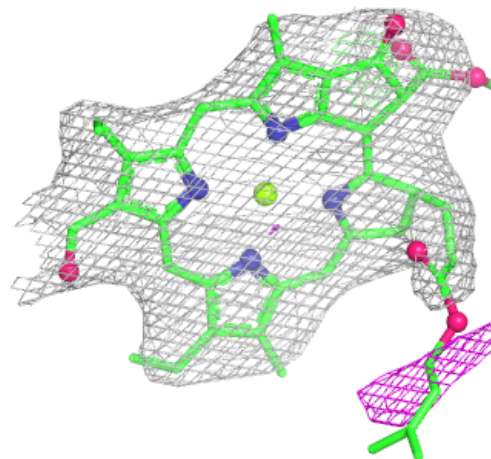
**Electron density around CHL 4 305:**

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



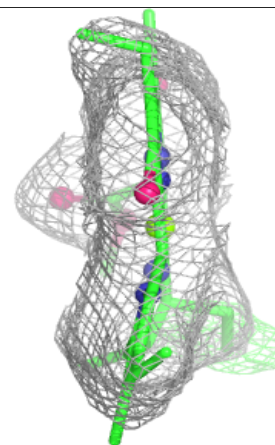
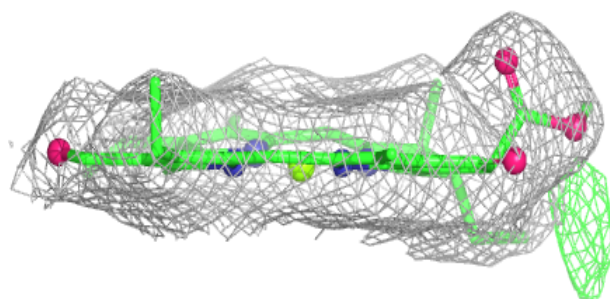
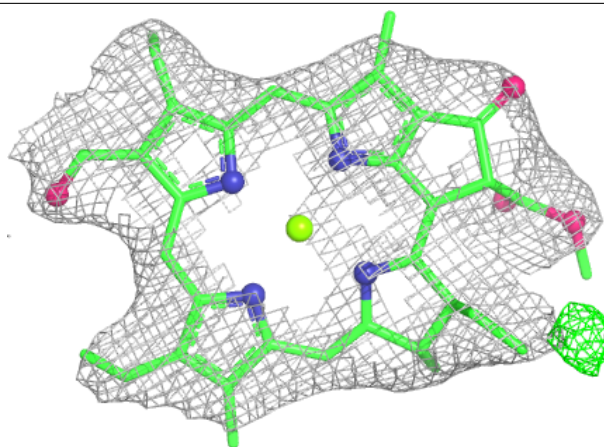
Electron density around CHL 4 306:

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

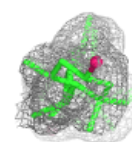
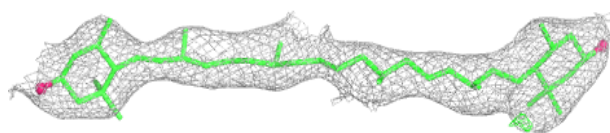
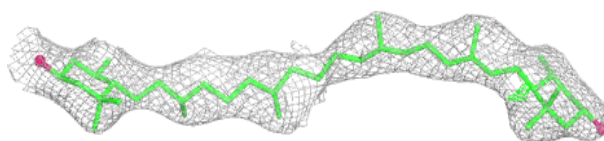


Electron density around CHL 4 315:

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

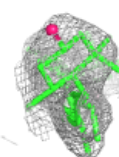
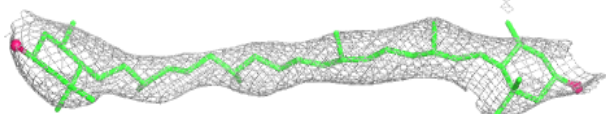
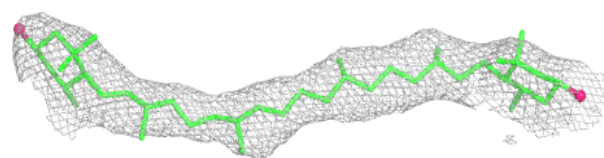
**Electron density around LUT 1 314:**

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

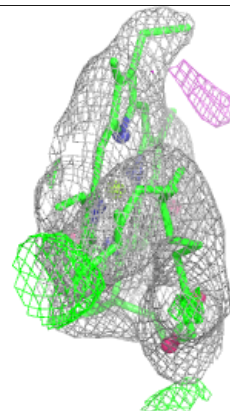
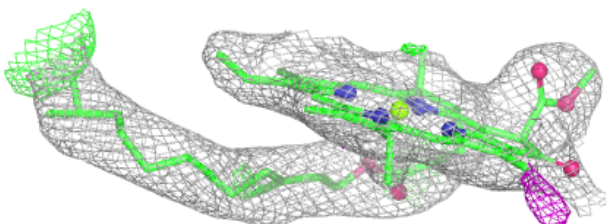
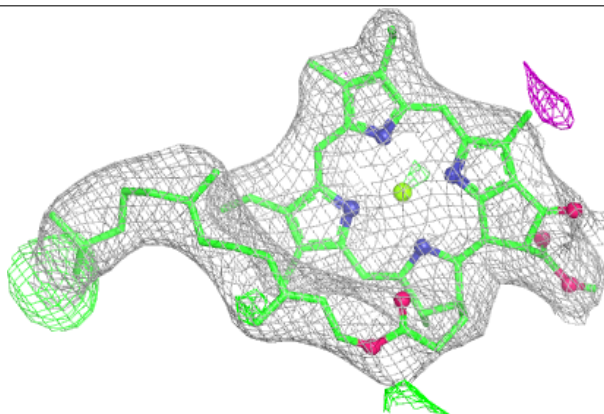


Electron density around LUT 2 314:

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

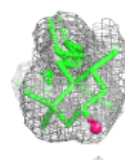
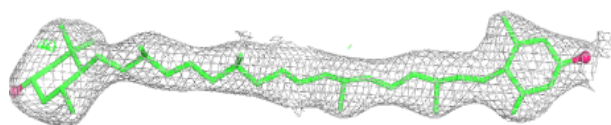
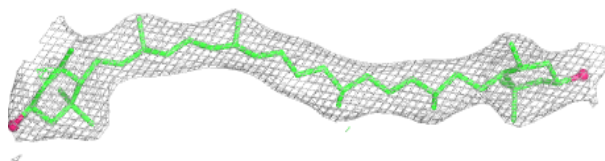
**Electron density around CLA B 820:**

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

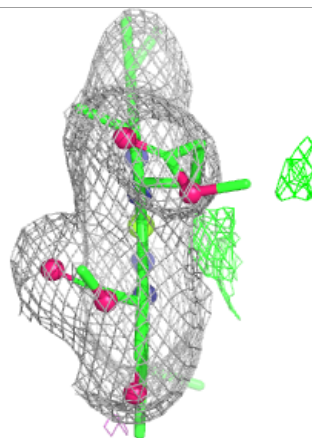
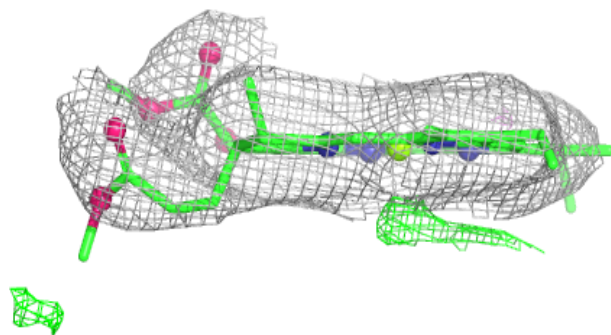
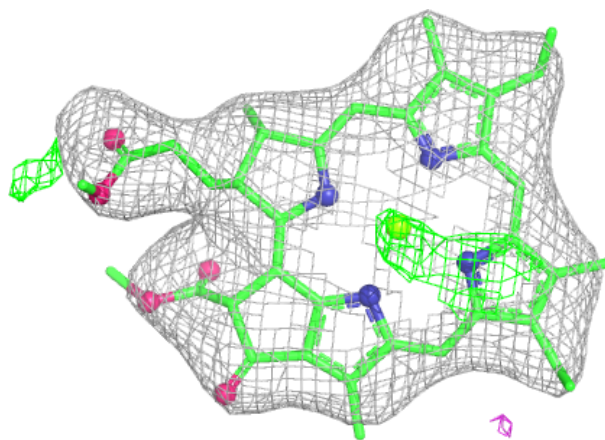


Electron density around LUT 4 316:

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

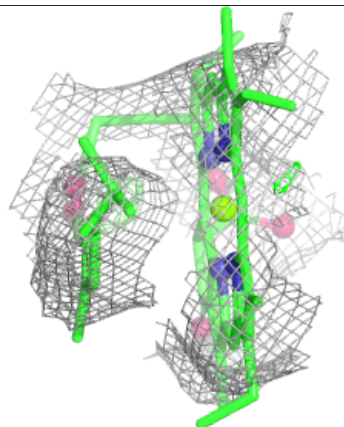
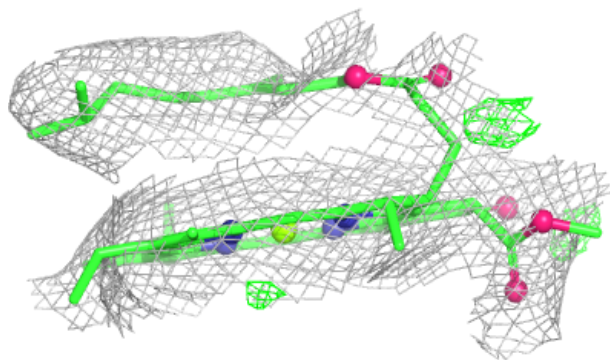
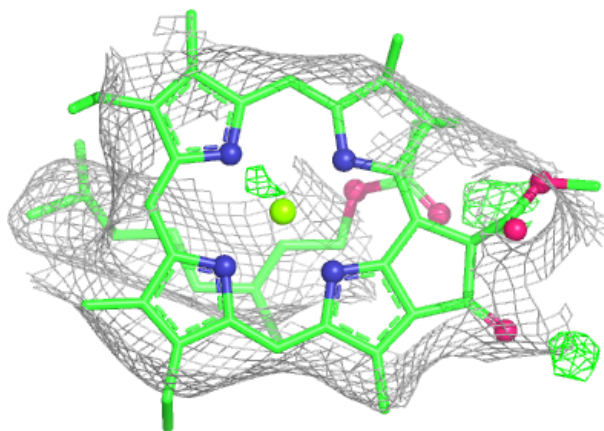
**Electron density around CLA 1 313:**

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

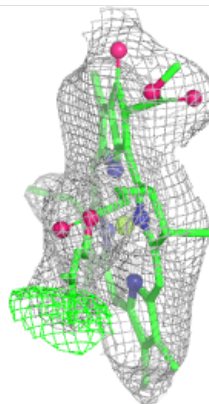
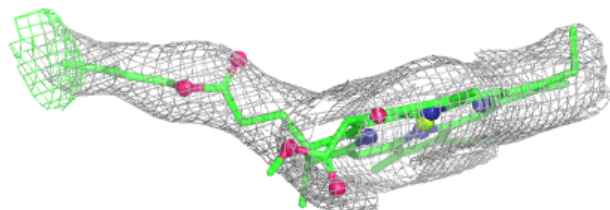
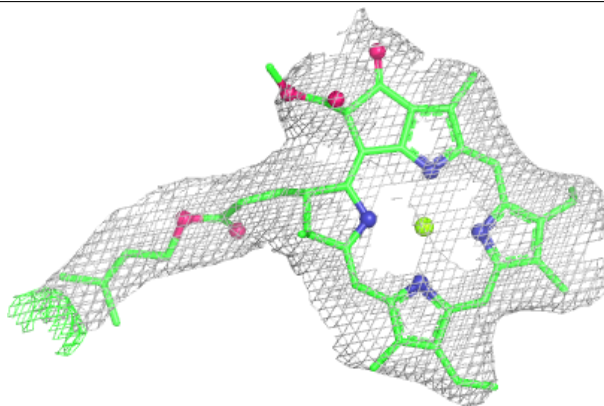


Electron density around CLA 3 611:

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

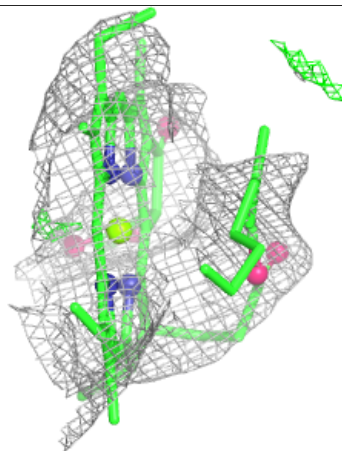
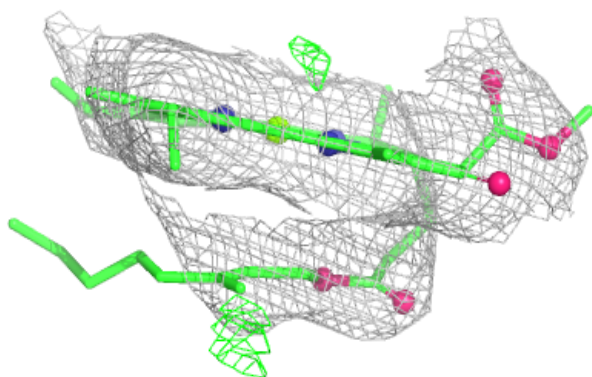
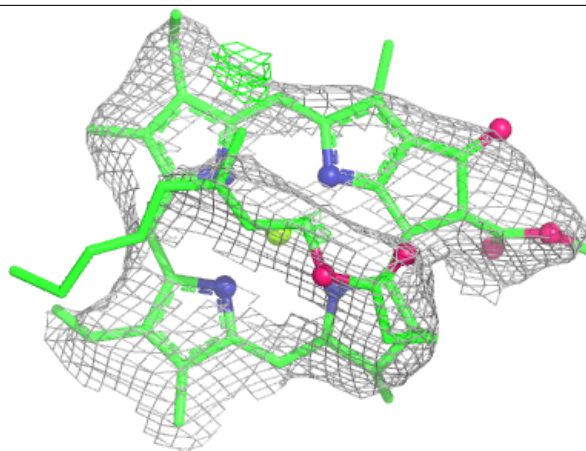
**Electron density around CLA G 104:**

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



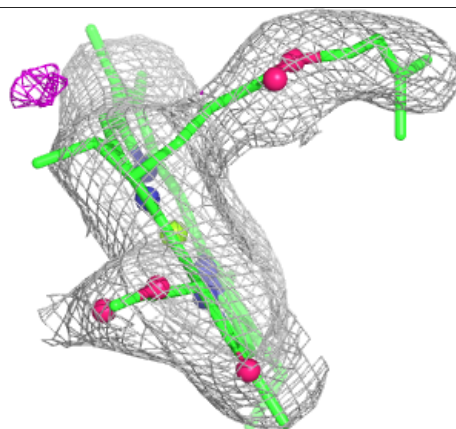
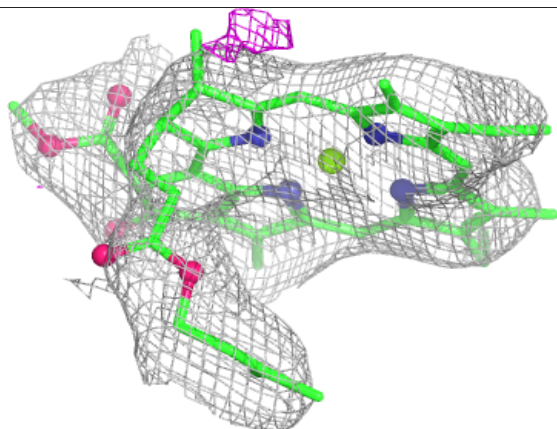
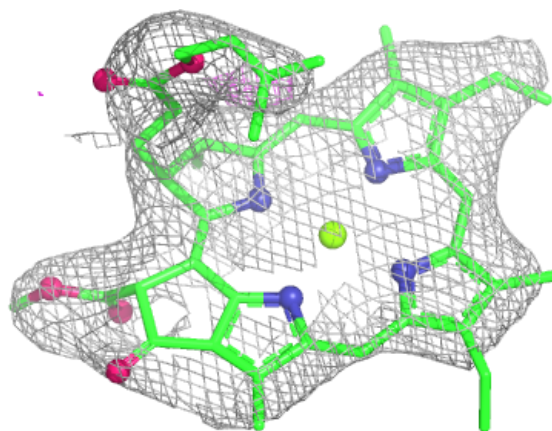
Electron density around CLA A 811:

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

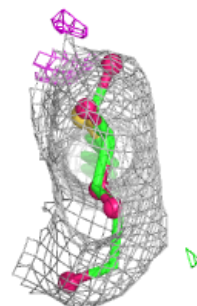
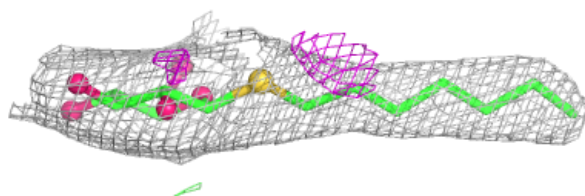
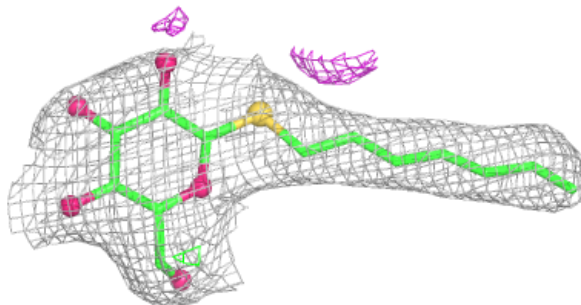


Electron density around CLA 2 307:

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

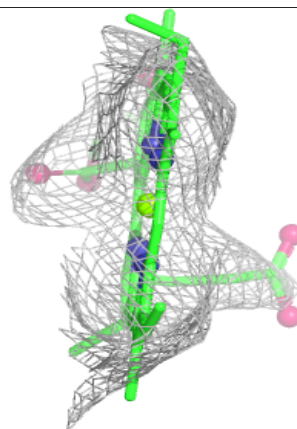
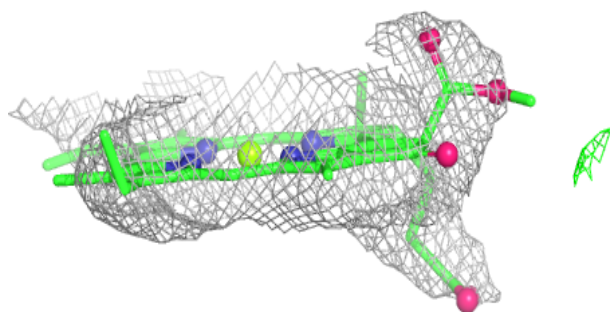
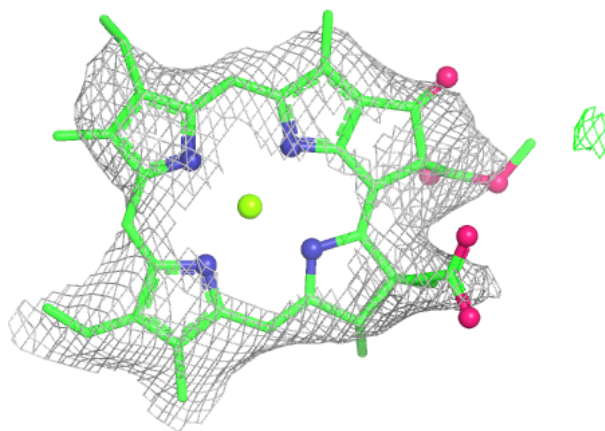
**Electron density around HTG A 854:**

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

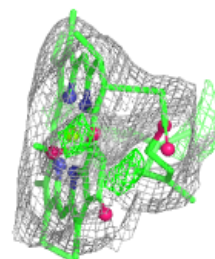
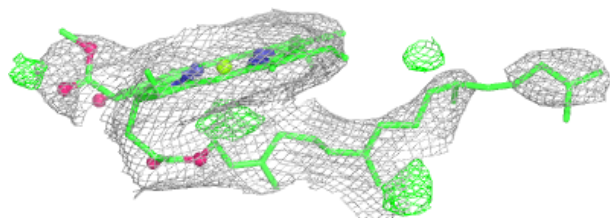
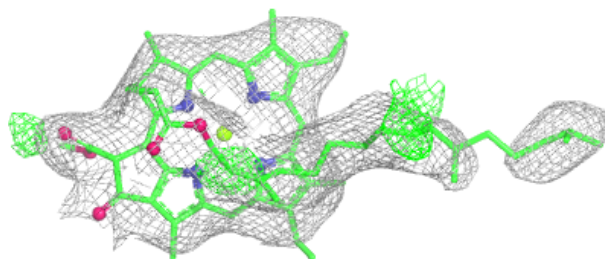


Electron density around CLA A 815:

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

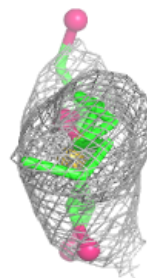
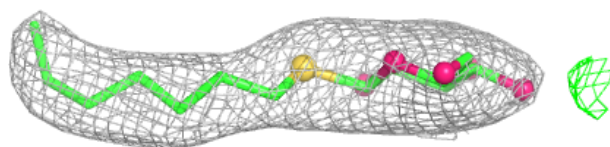
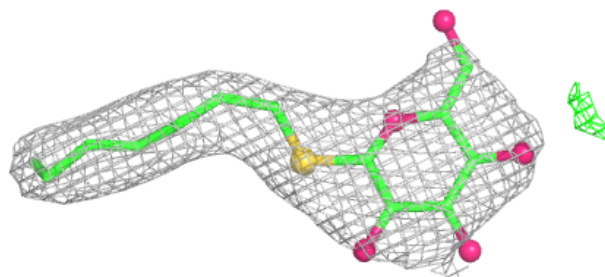
**Electron density around CLA A 836:**

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



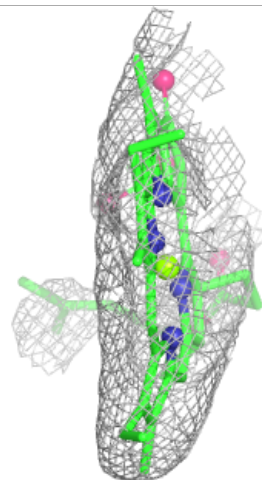
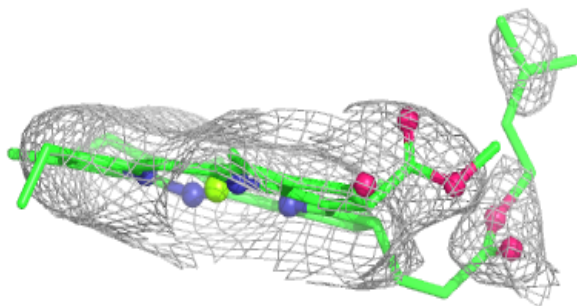
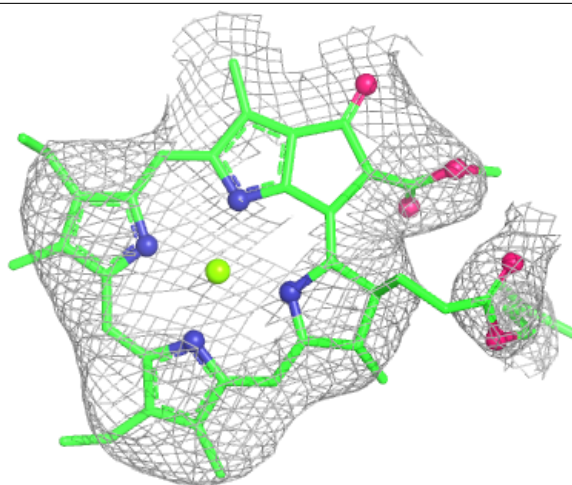
Electron density around HTG F 305:

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



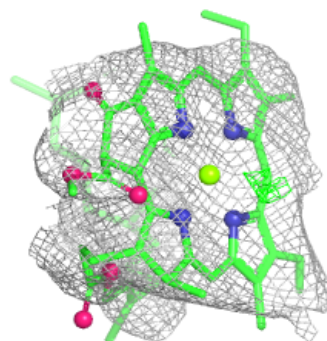
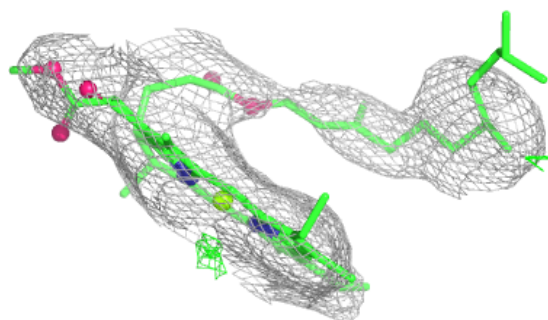
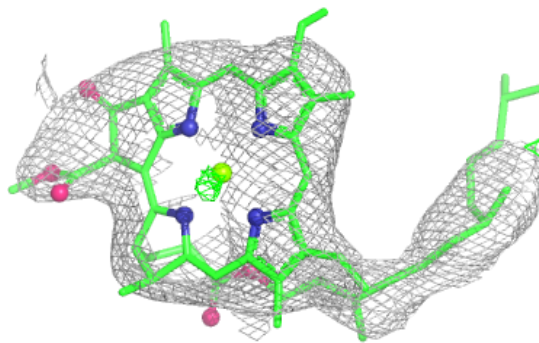
Electron density around CLA 3 603:

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



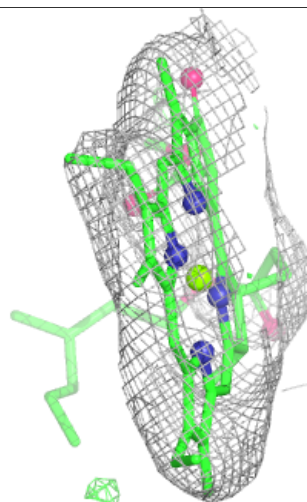
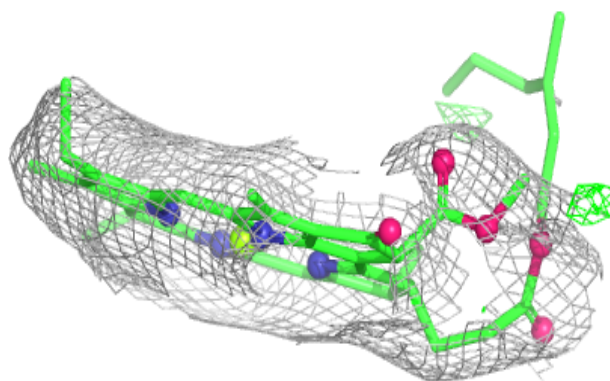
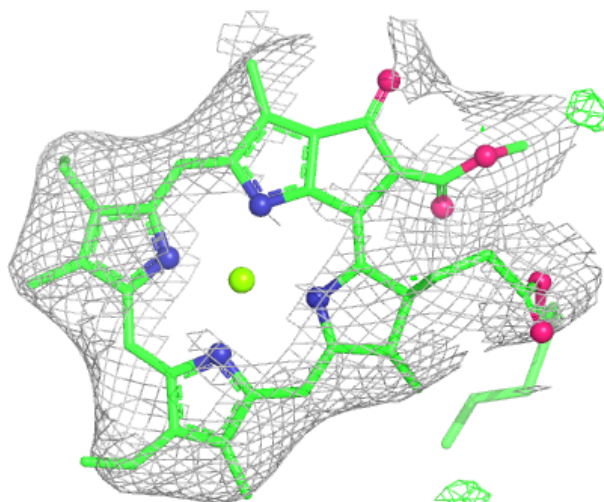
Electron density around CLA 2 308:

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



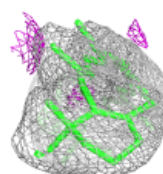
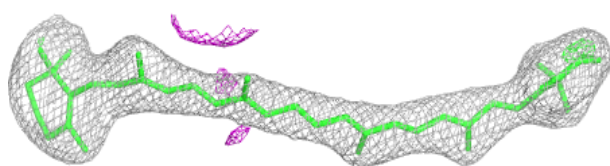
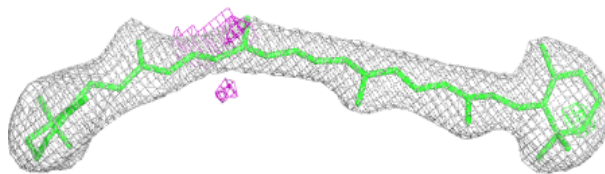
Electron density around CLA 1 310:

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

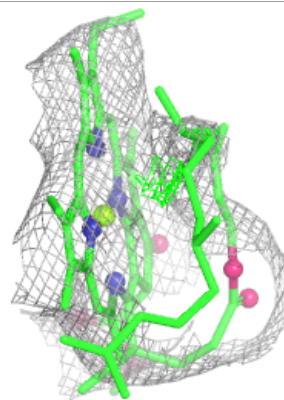
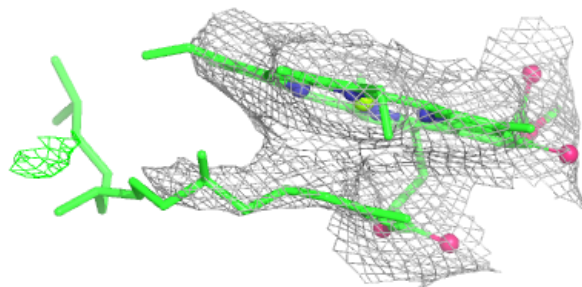
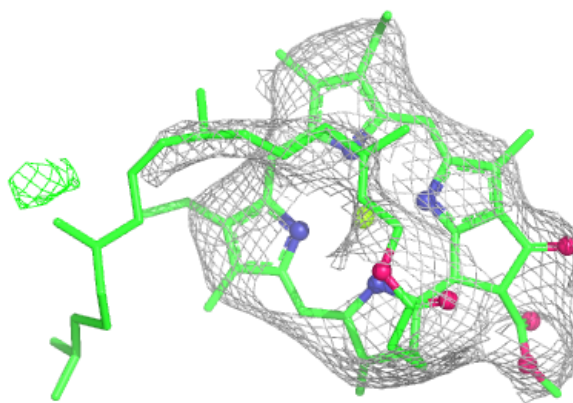


Electron density around BCR F 303:

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

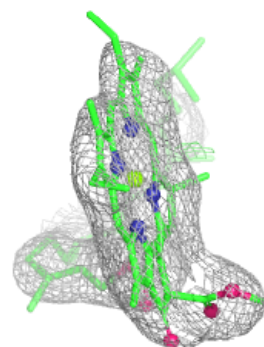
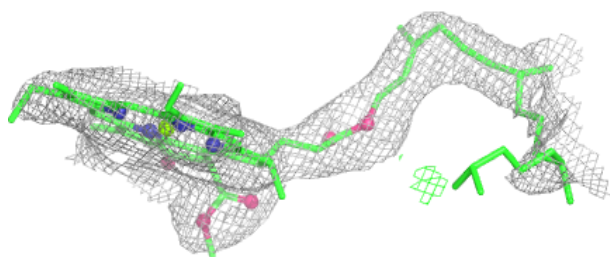
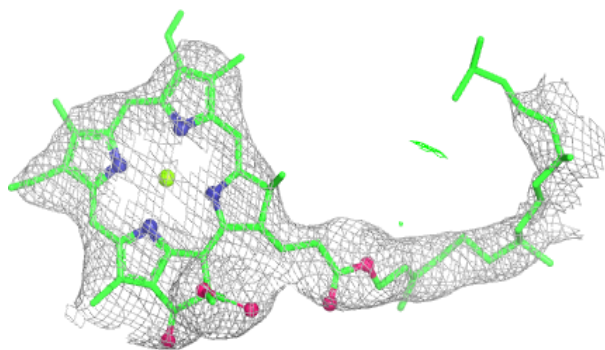
**Electron density around CLA 2 311:**

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

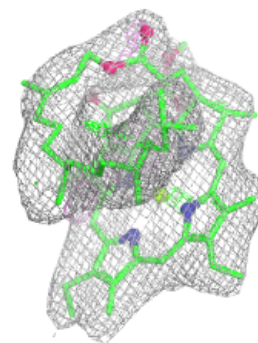
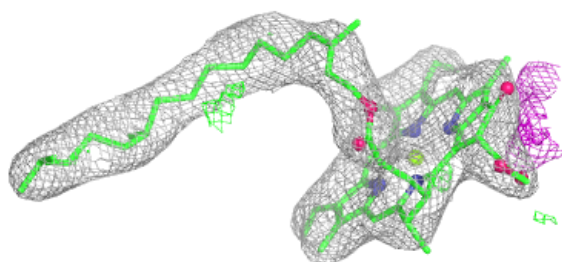
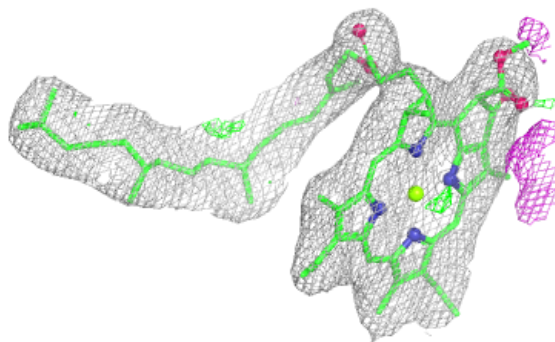


Electron density around CLA A 826:

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

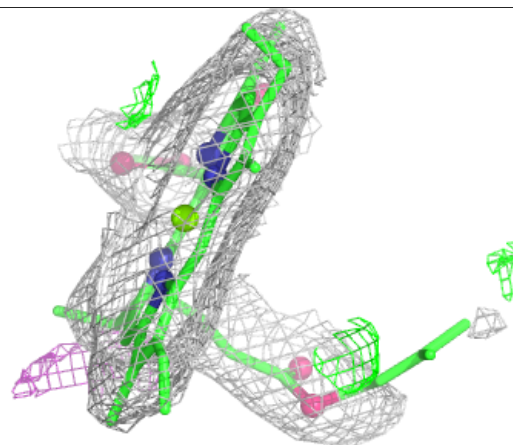
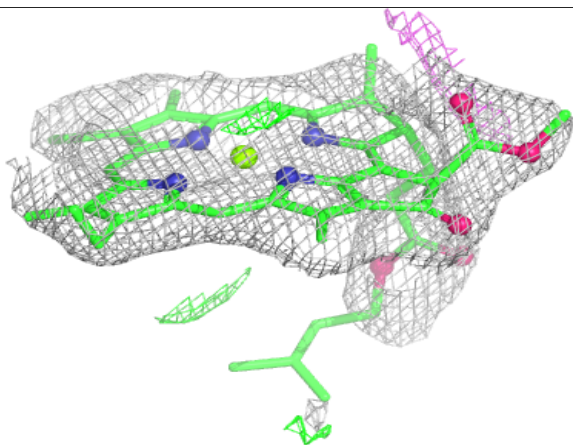
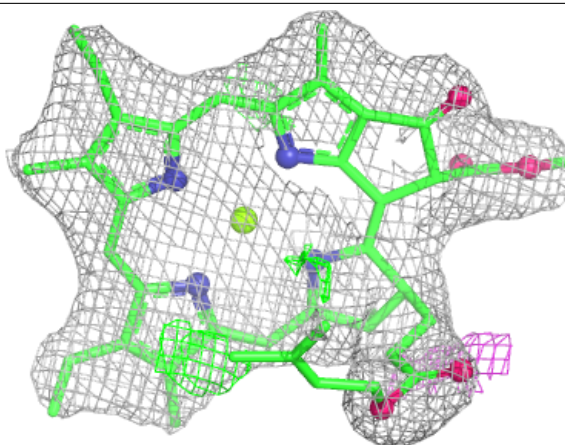
**Electron density around CLA B 816:**

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

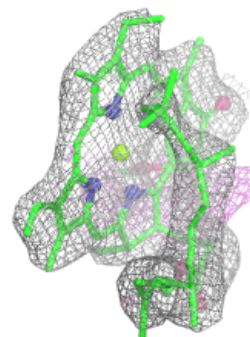
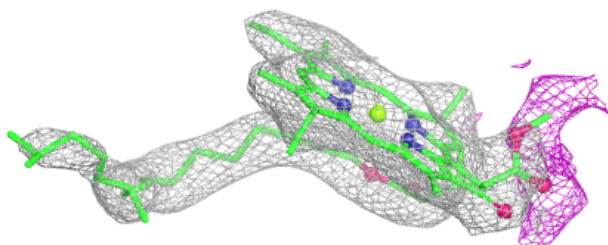
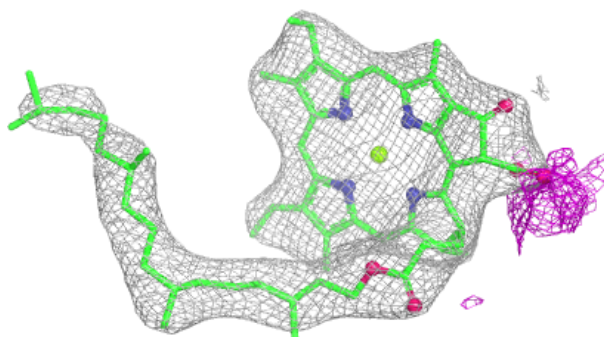


Electron density around CLA 4 308:

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

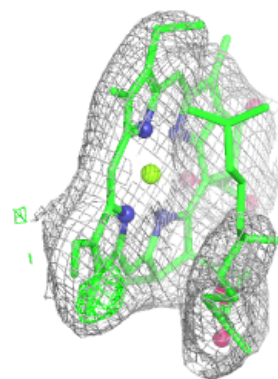
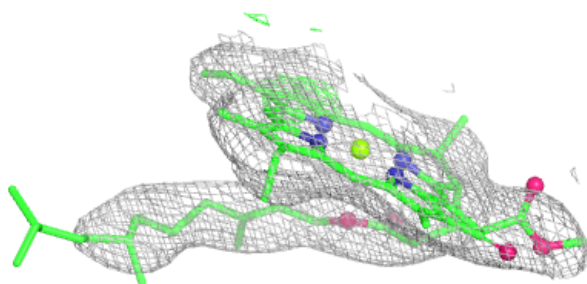
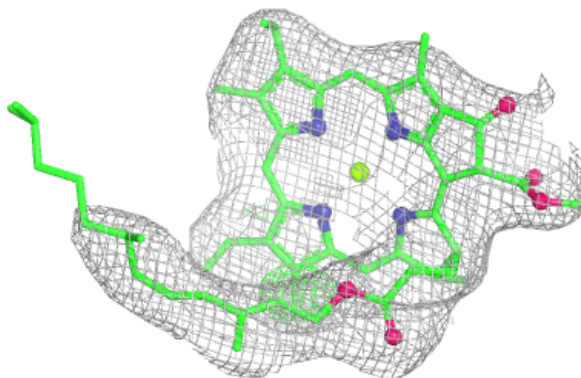
**Electron density around CLA 1 301:**

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

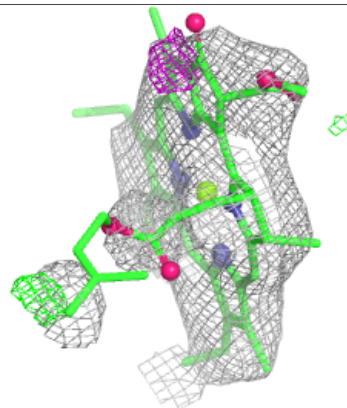
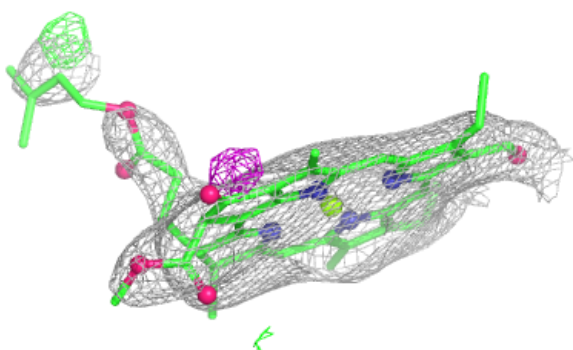
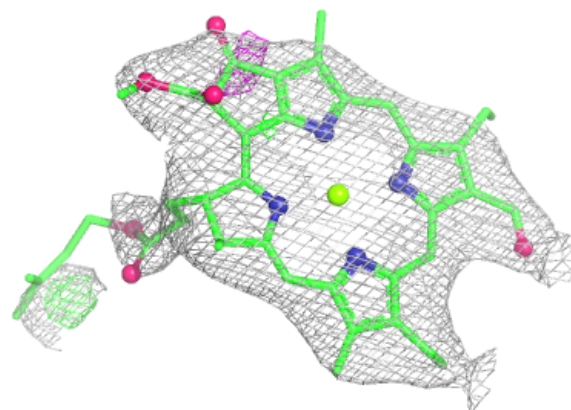


Electron density around CLA 1 308:

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

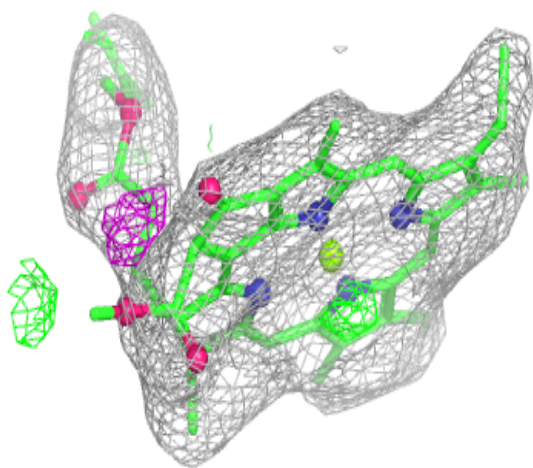
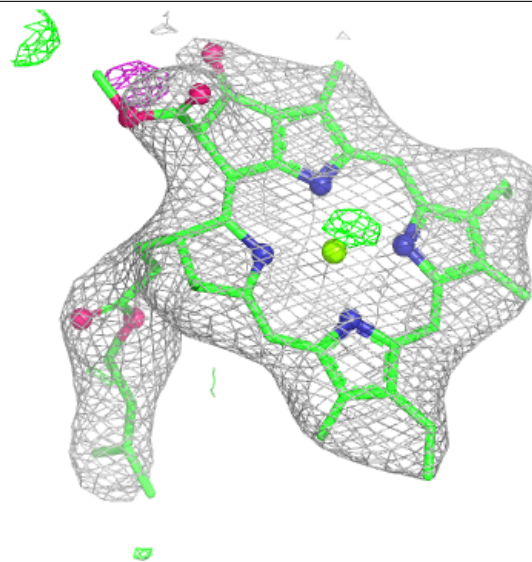
**Electron density around CHL 2 306:**

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



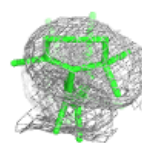
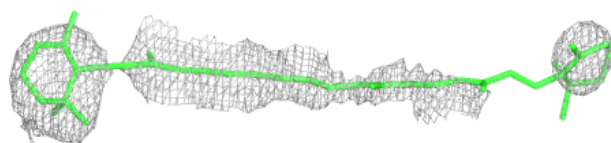
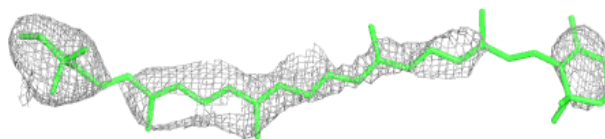
Electron density around CLA B 822:

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

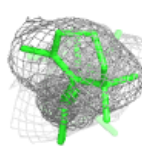
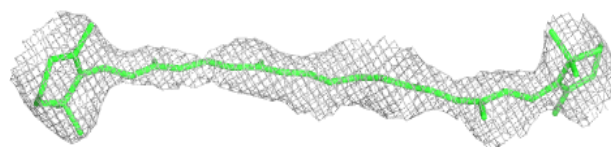
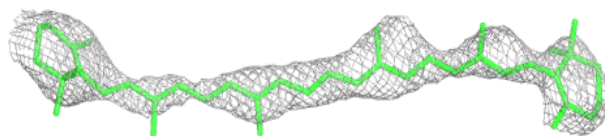


Electron density around BCR A 847:

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

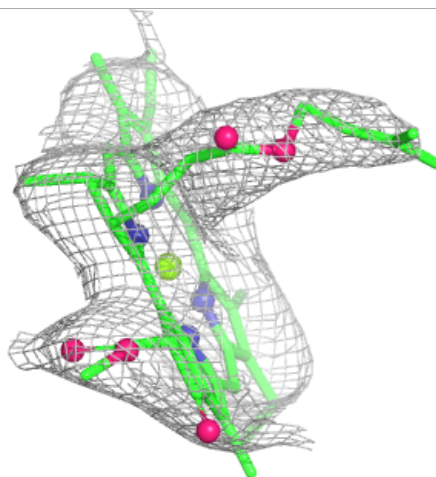
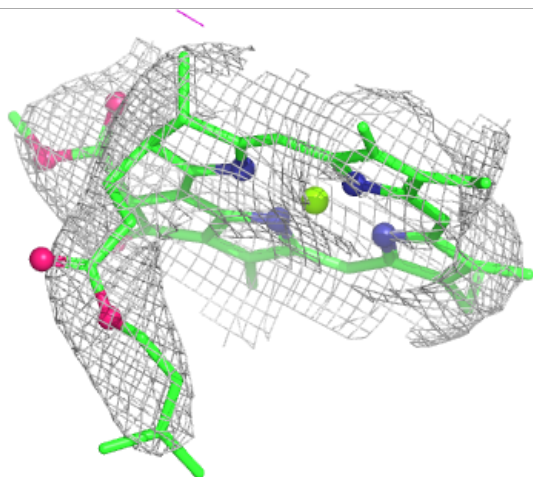
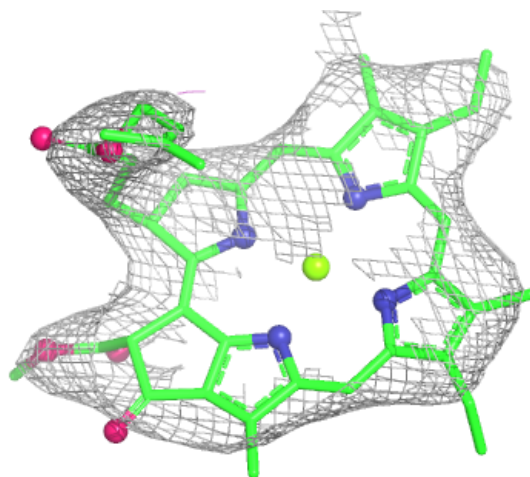
**Electron density around BCR A 848:**

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



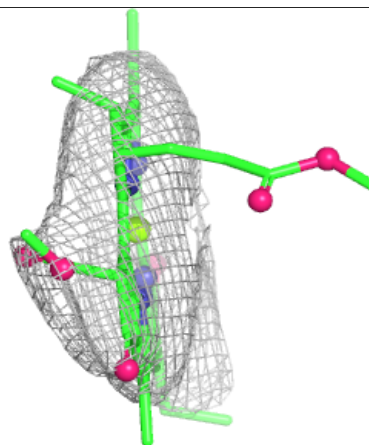
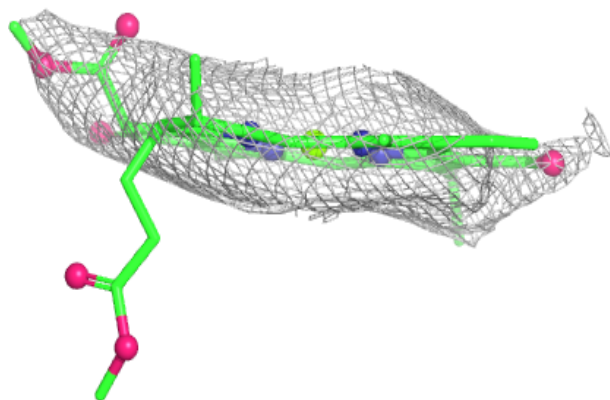
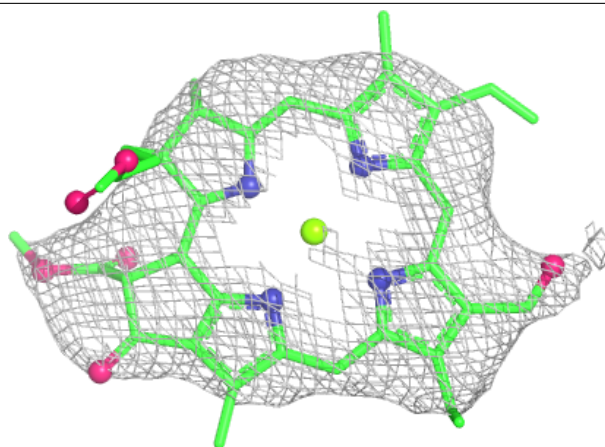
Electron density around CLA 3 608:

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

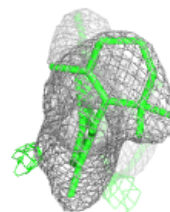
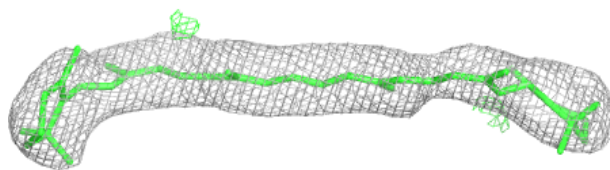
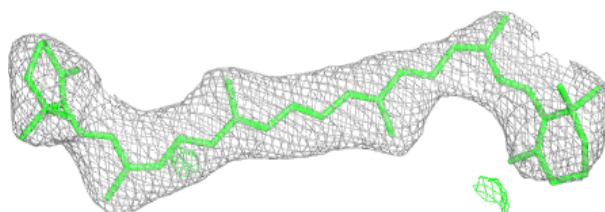


Electron density around CHL 3 607:

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

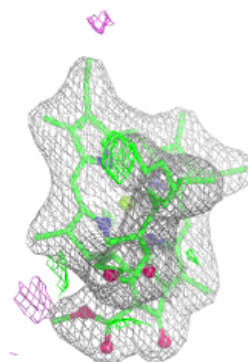
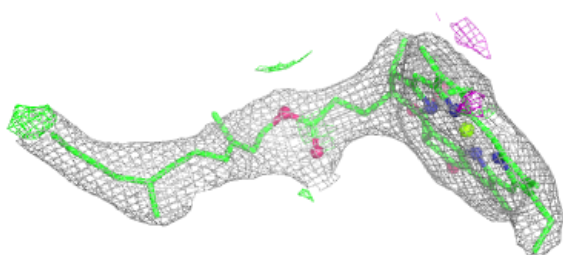
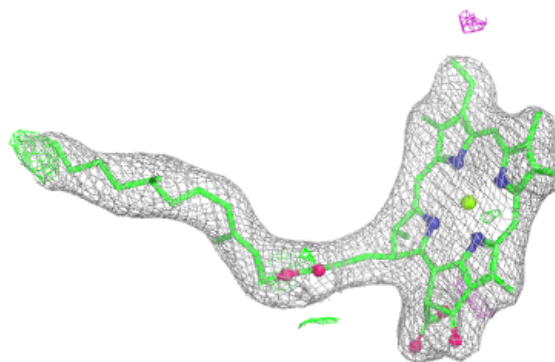
**Electron density around BCR B 846:**

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



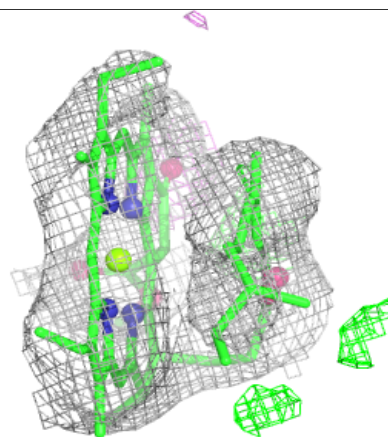
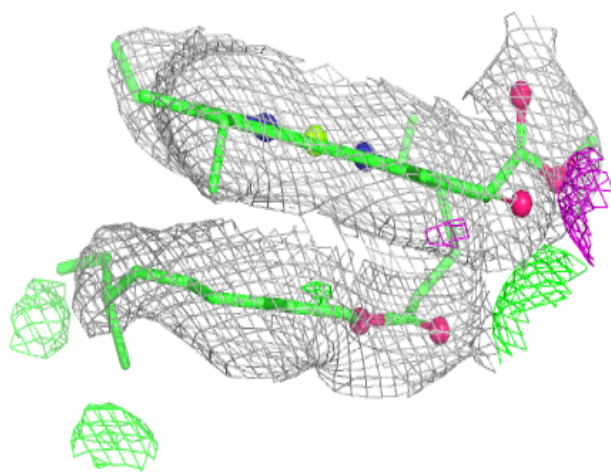
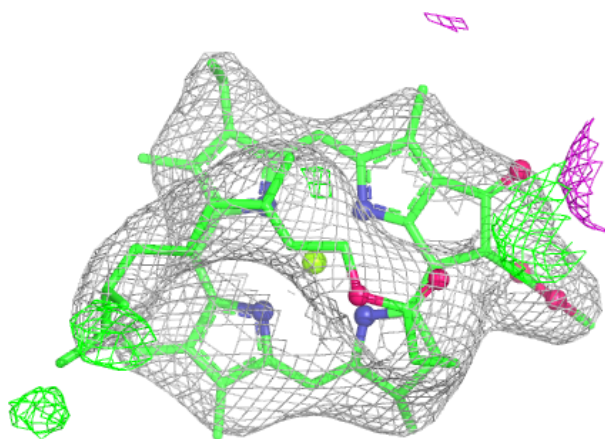
Electron density around CLA B 834:

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



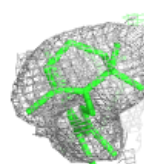
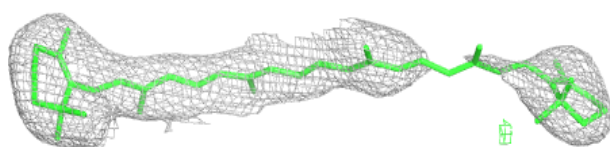
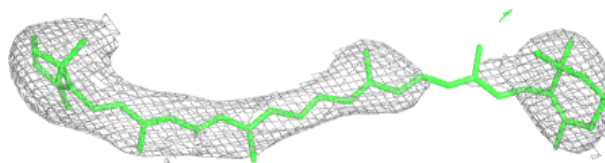
Electron density around CLA 4 312:

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

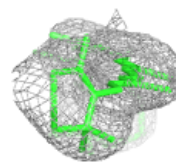
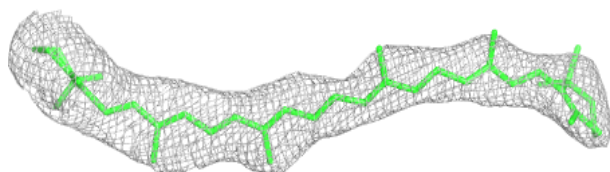
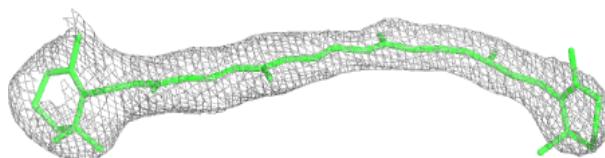


Electron density around BCR G 106:

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

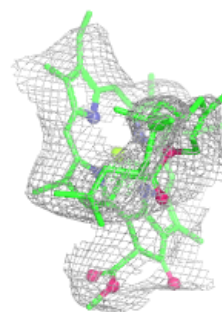
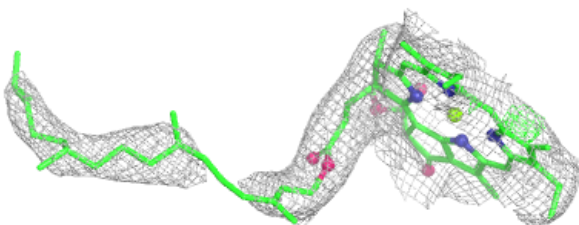
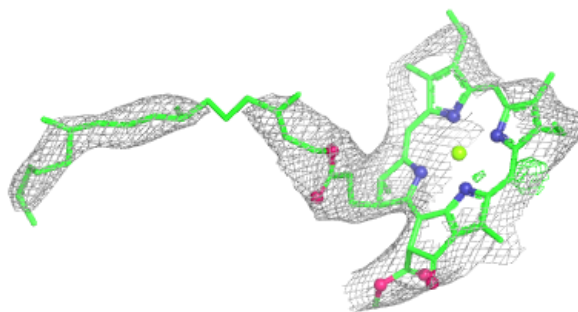
**Electron density around BCR I 101:**

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



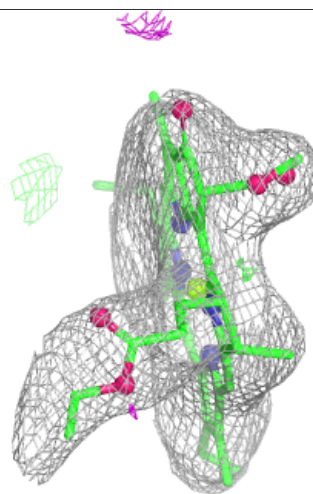
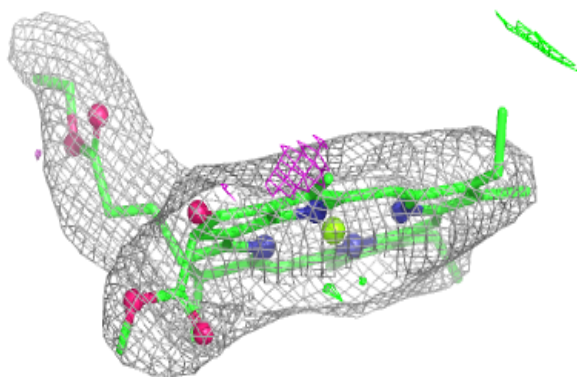
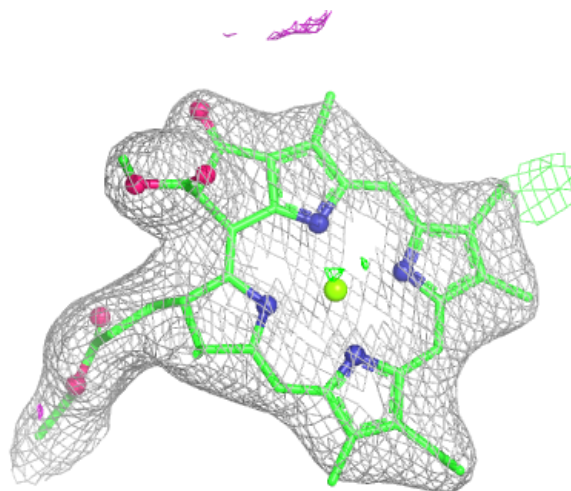
Electron density around CLA A 820:

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



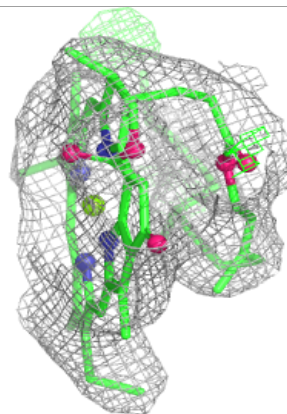
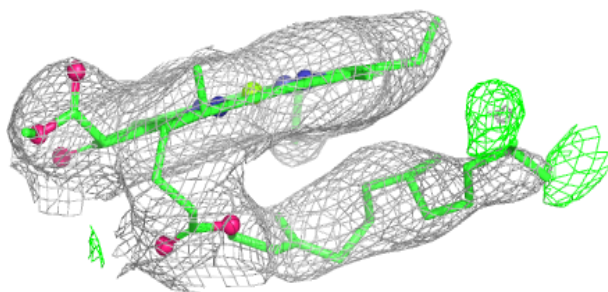
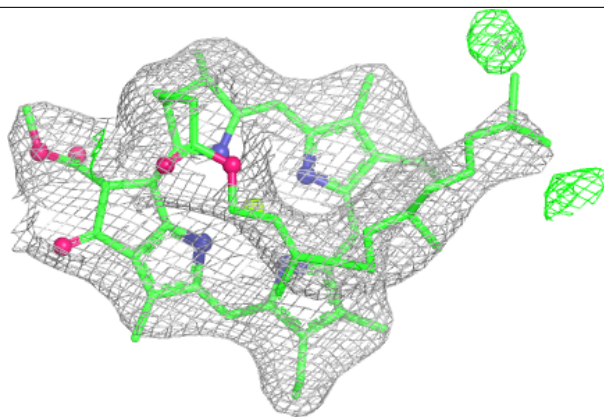
Electron density around CLA 4 314:

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

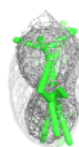
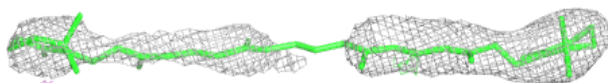
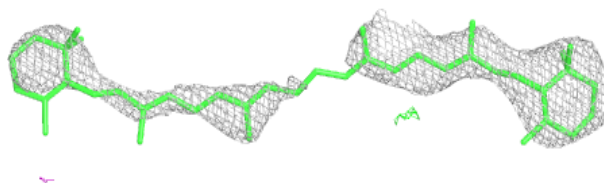


Electron density around CLA 1 311:

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

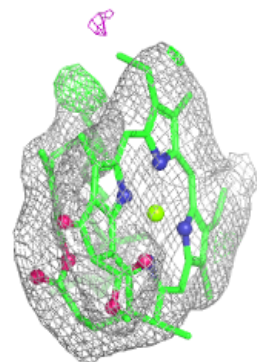
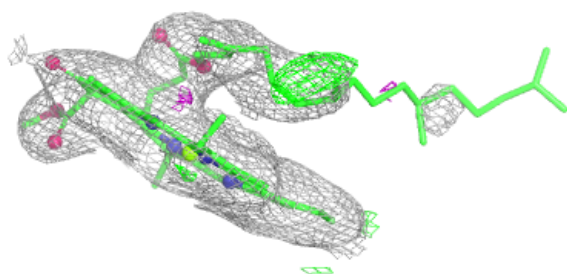
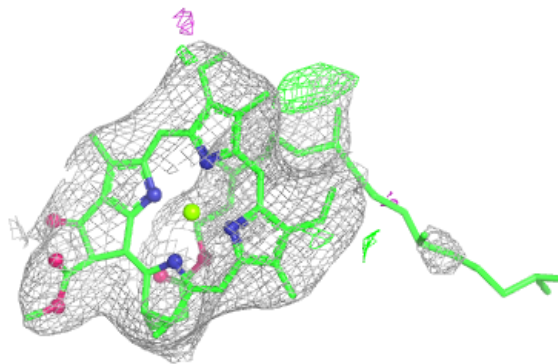
**Electron density around BCR L 205:**

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



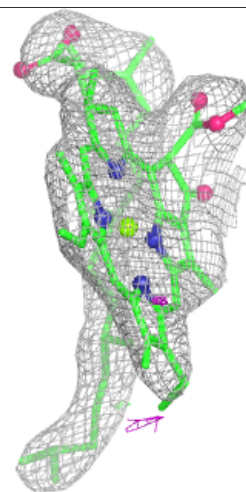
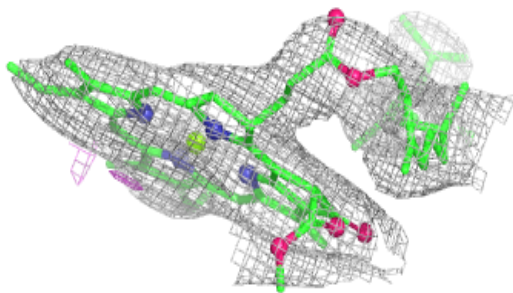
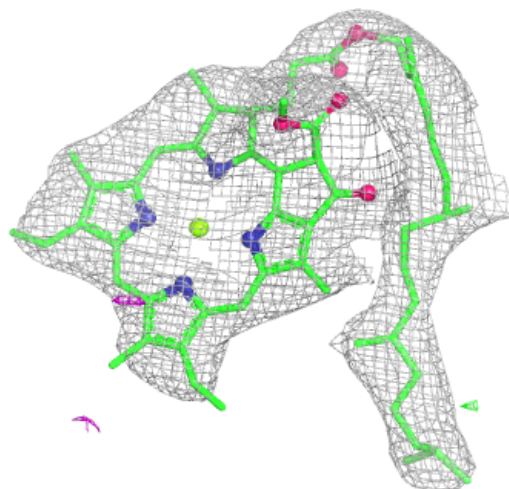
Electron density around CLA B 809:

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



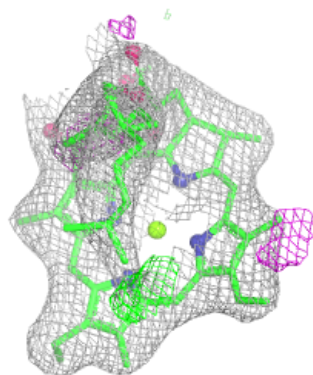
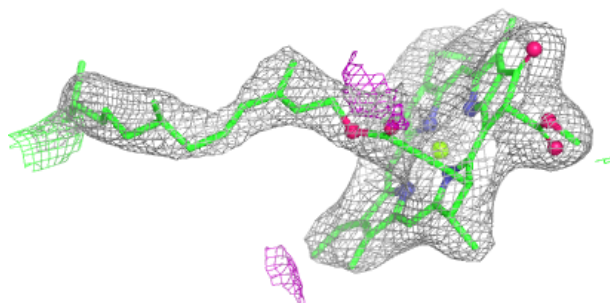
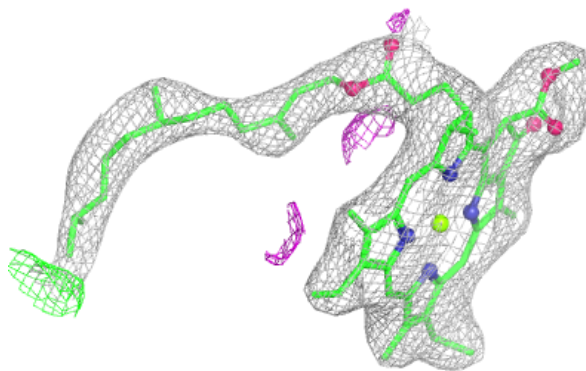
Electron density around CLA A 824:

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



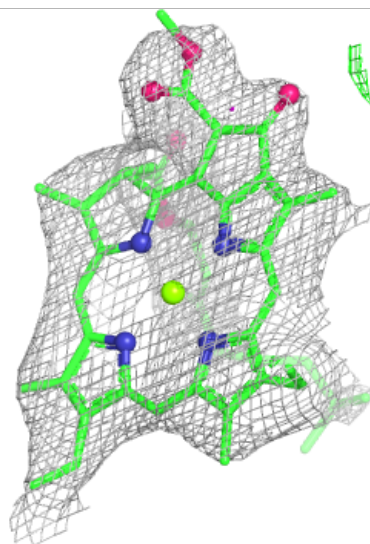
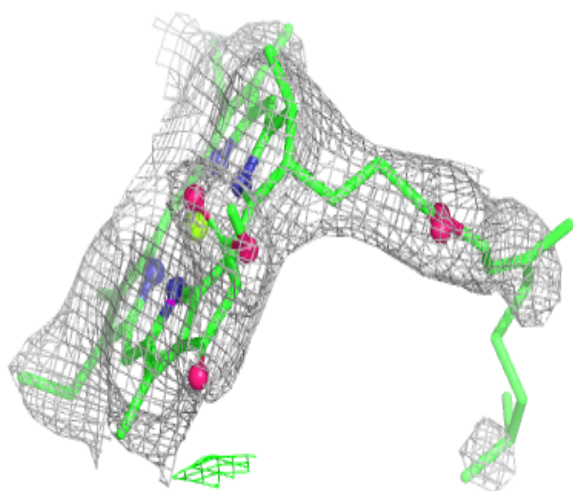
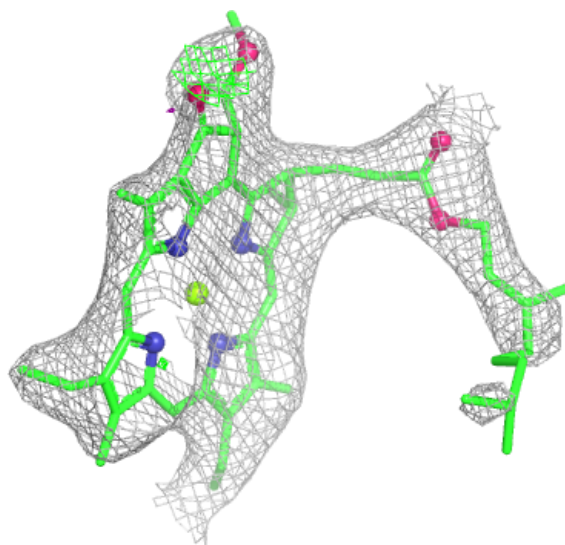
Electron density around CLA B 833:

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



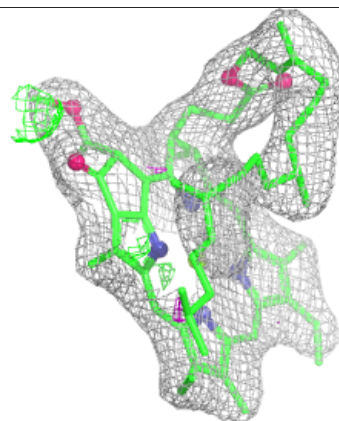
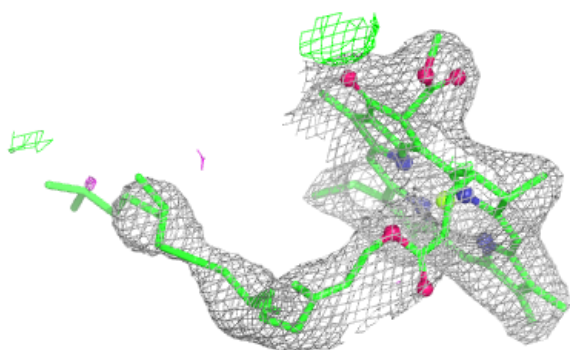
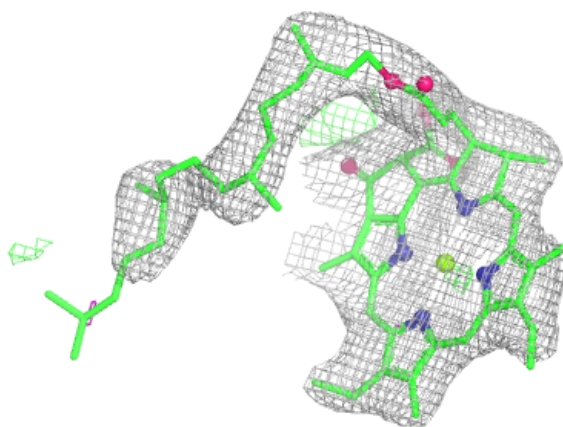
Electron density around CLA A 803:

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



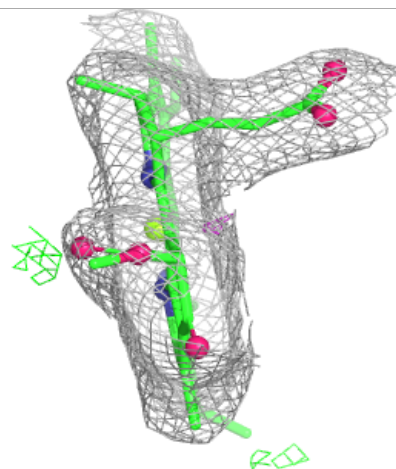
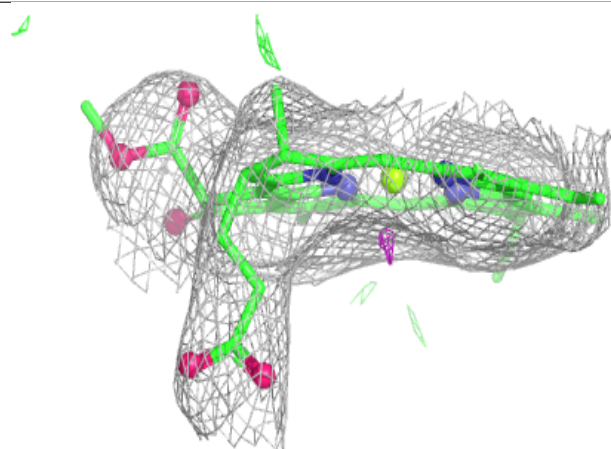
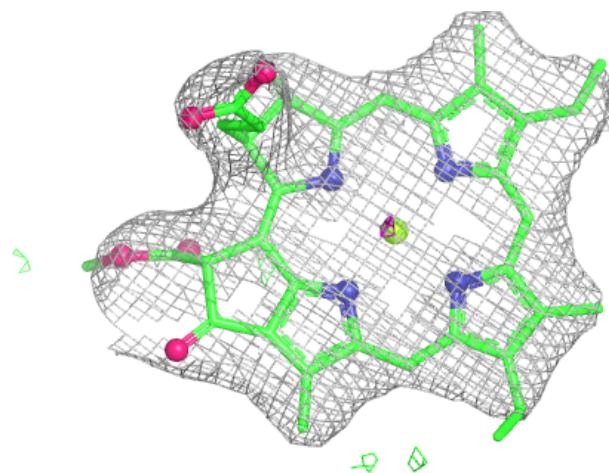
Electron density around CLA B 835:

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



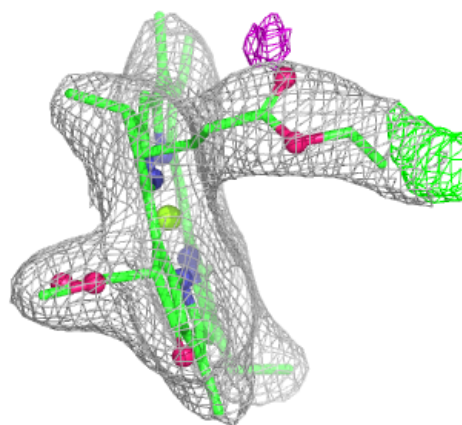
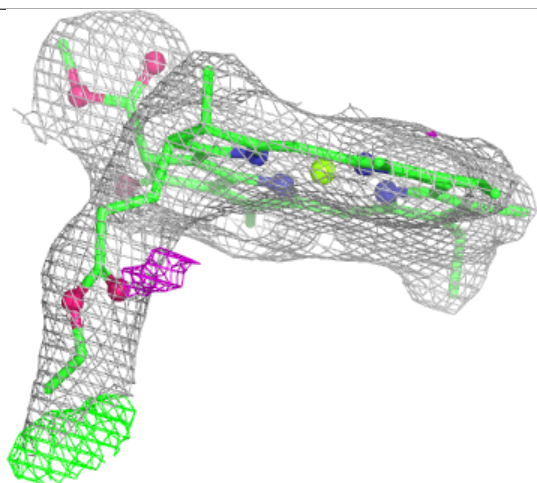
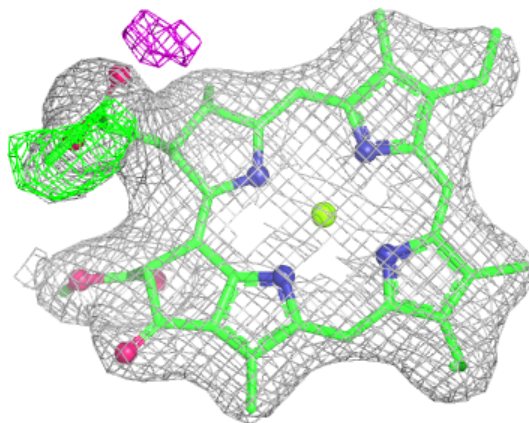
Electron density around CLA B 836:

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



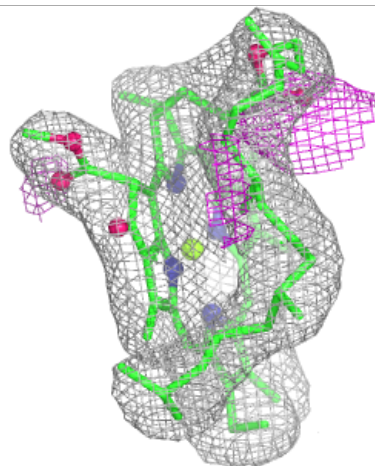
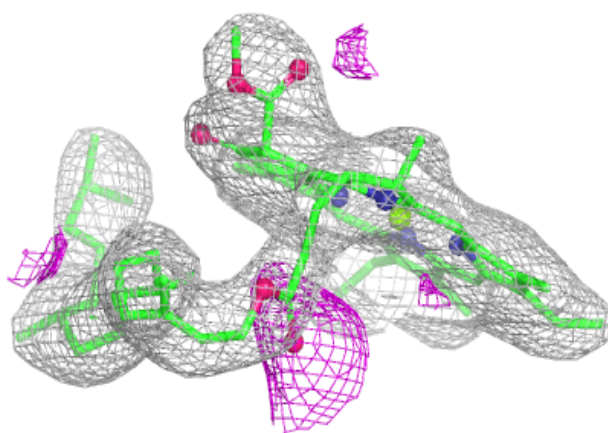
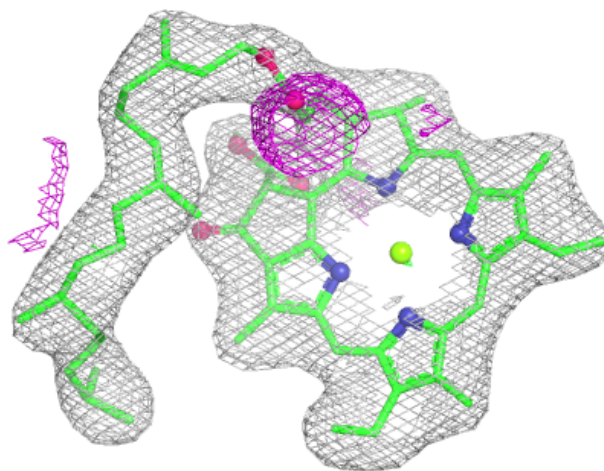
Electron density around CLA B 839:

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



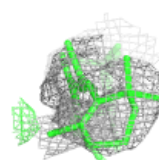
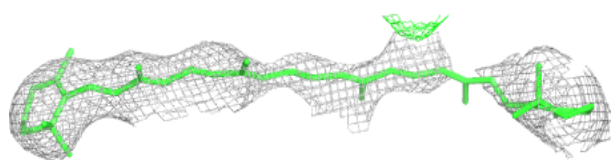
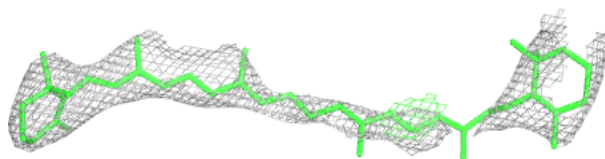
Electron density around CLA F 304:

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

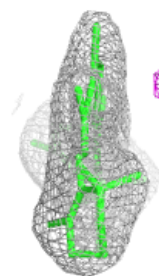
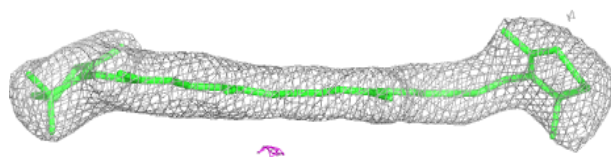
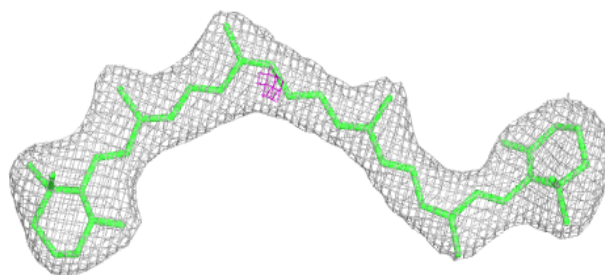


Electron density around BCR A 850:

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

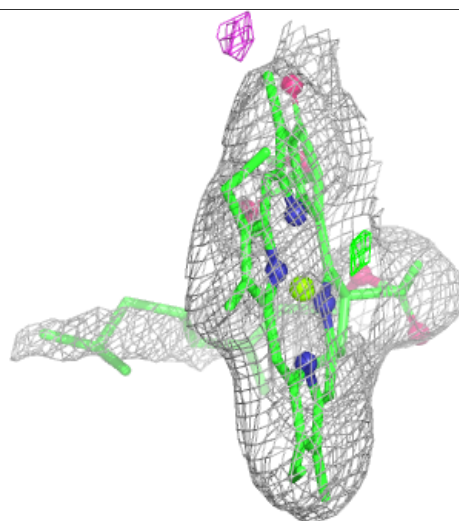
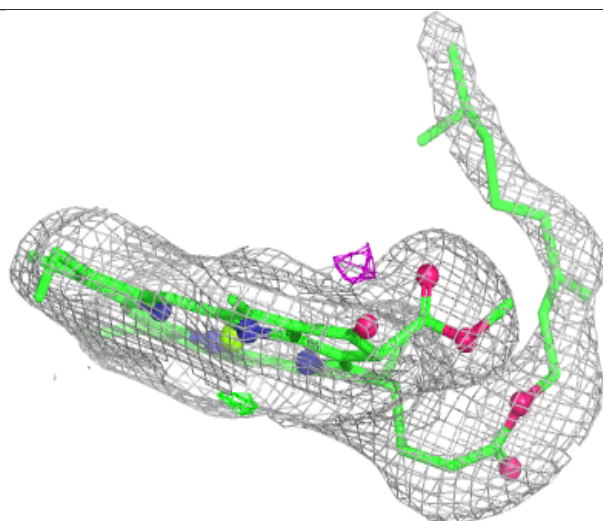
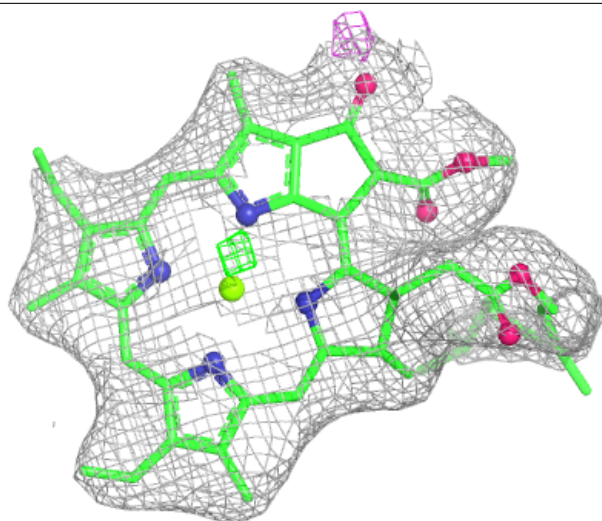
**Electron density around BCR A 851:**

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



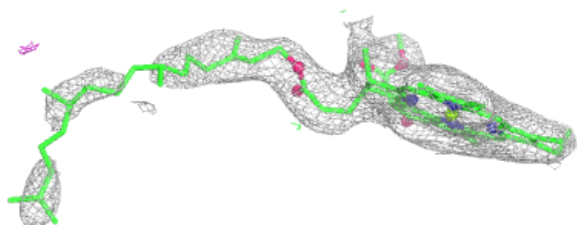
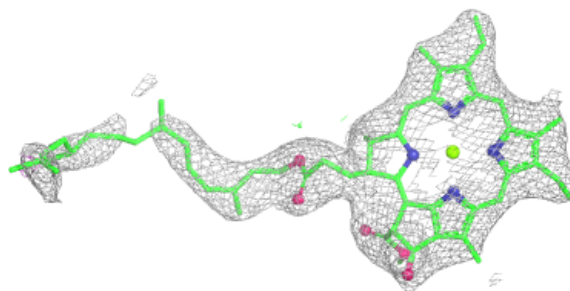
Electron density around CLA F 307:

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

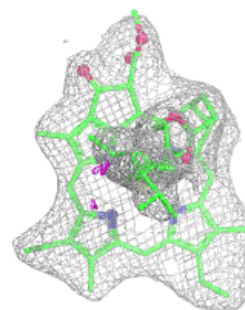
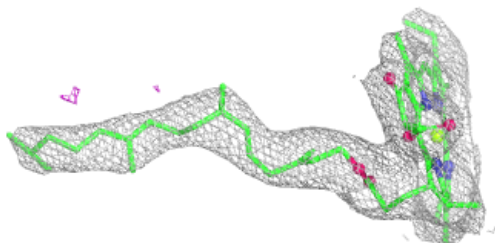
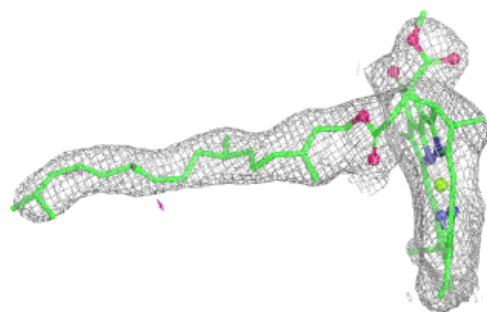


Electron density around CLA A 804:

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

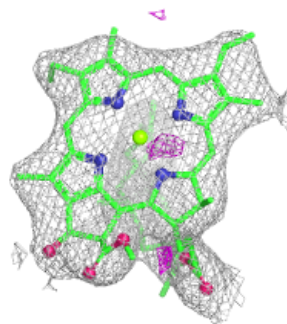
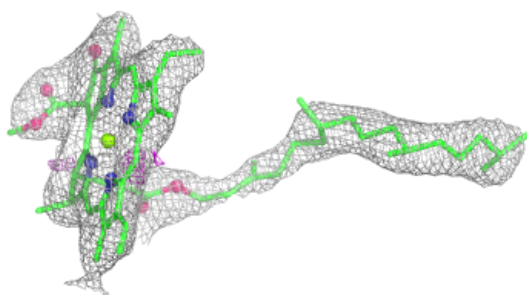
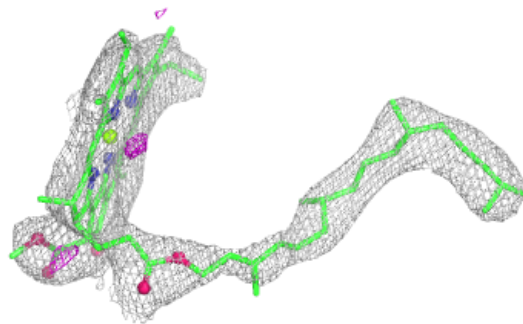
**Electron density around CLA A 827:**

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

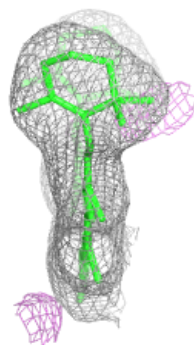
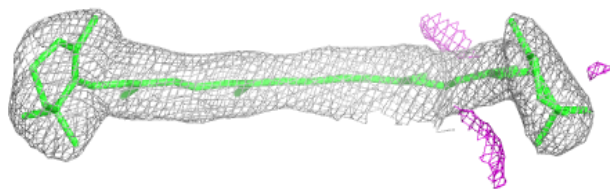
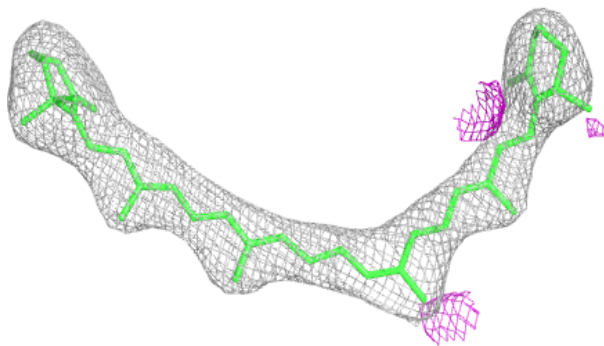


Electron density around CLA A 829:

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

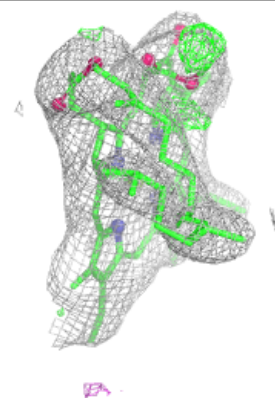
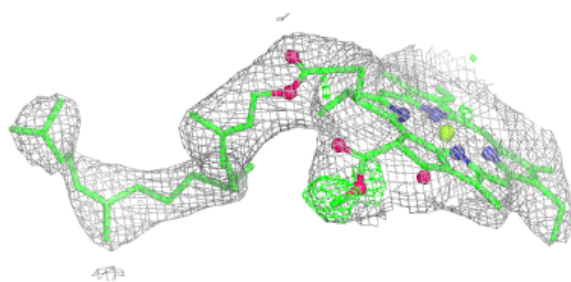
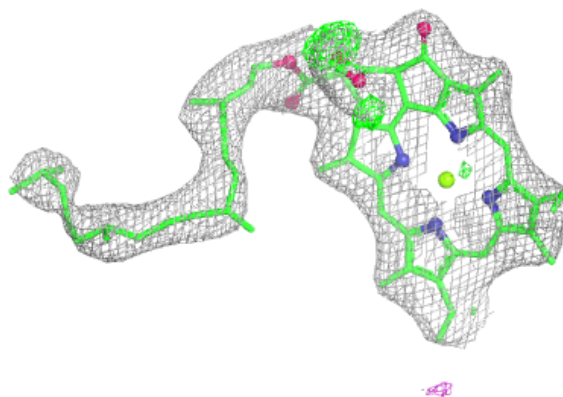
**Electron density around BCR F 308:**

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

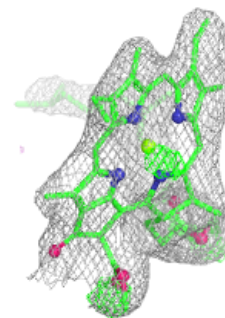
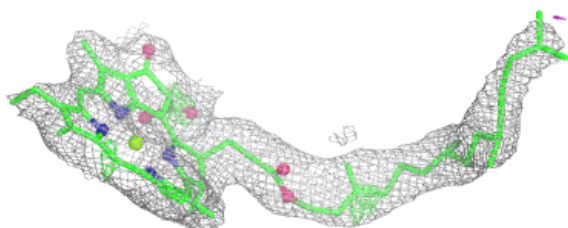
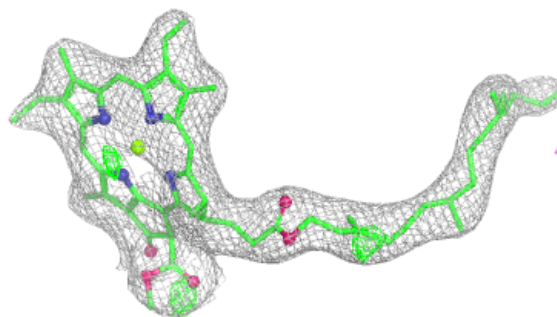


Electron density around CLA J 101:

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

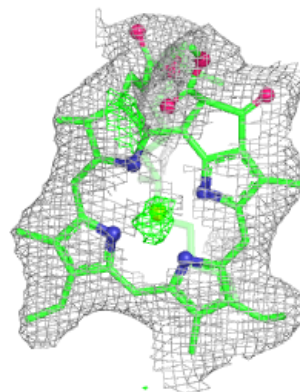
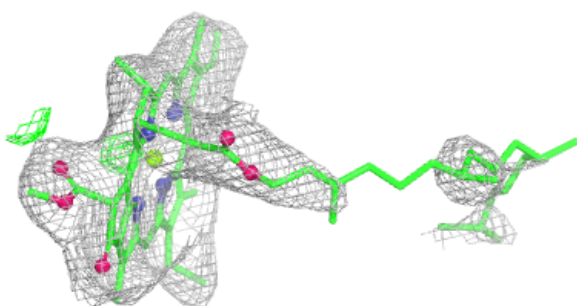
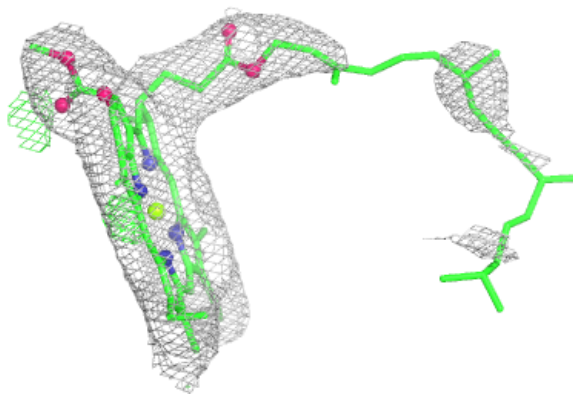
**Electron density around CLA A 853:**

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



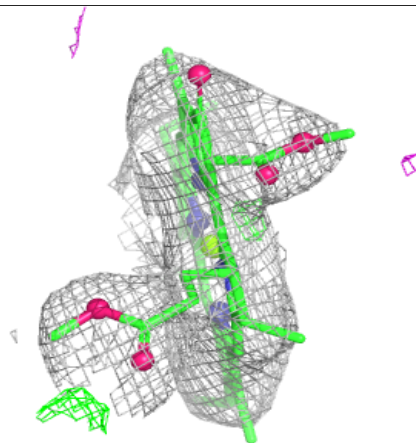
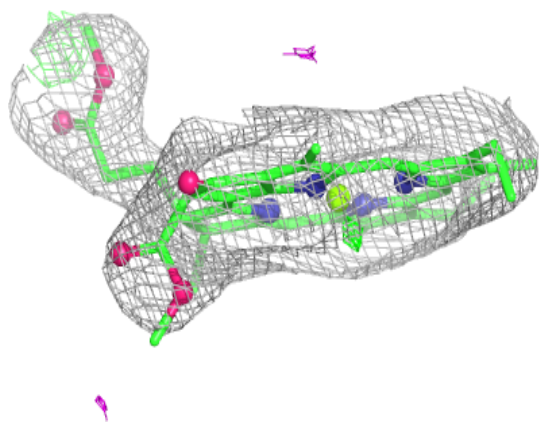
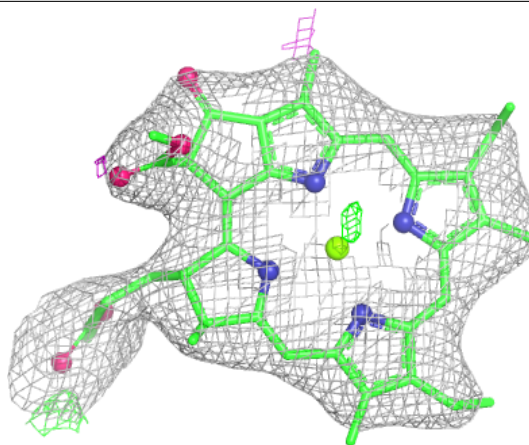
Electron density around CLA A 806:

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



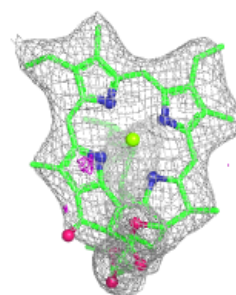
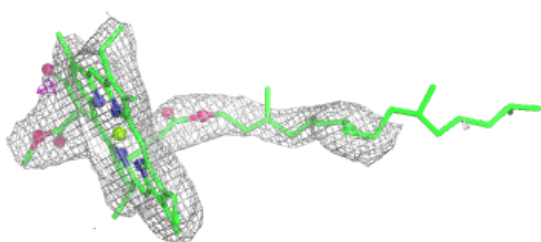
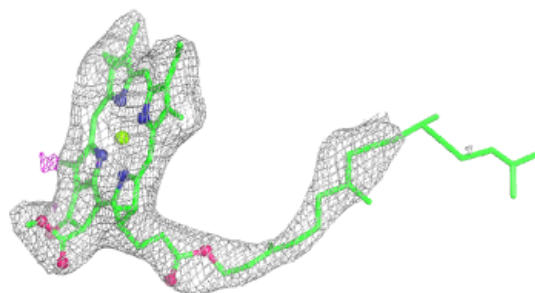
Electron density around CLA 2 319:

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

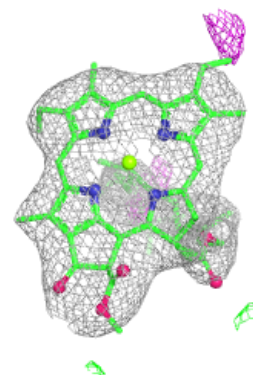
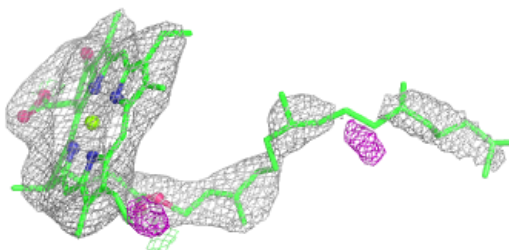
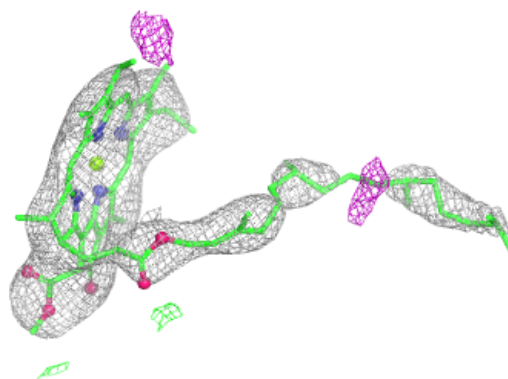


Electron density around CLA B 823:

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

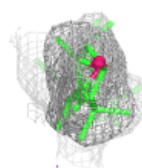
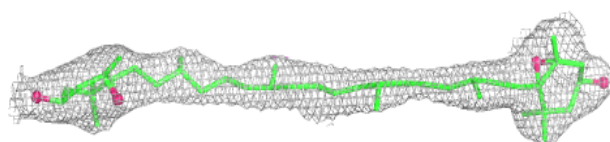
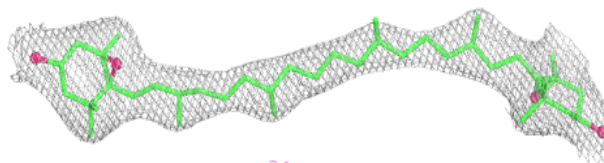
**Electron density around CLA A 810:**

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

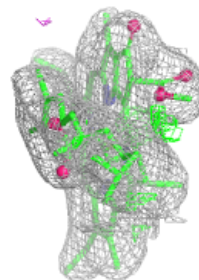
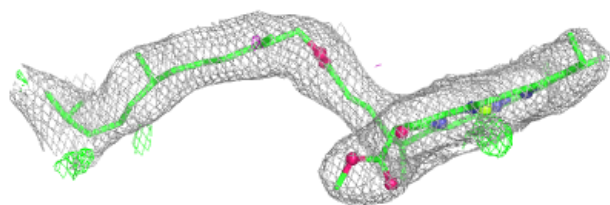
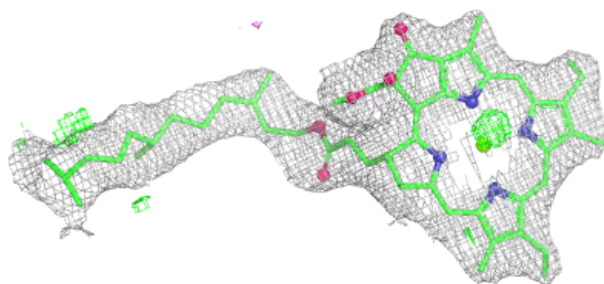


Electron density around XAT 4 317:

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

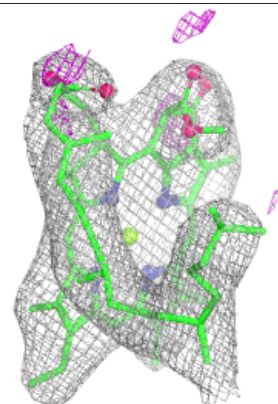
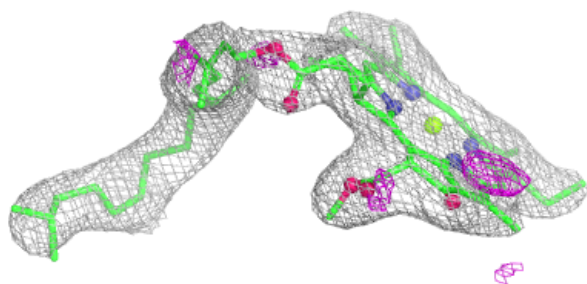
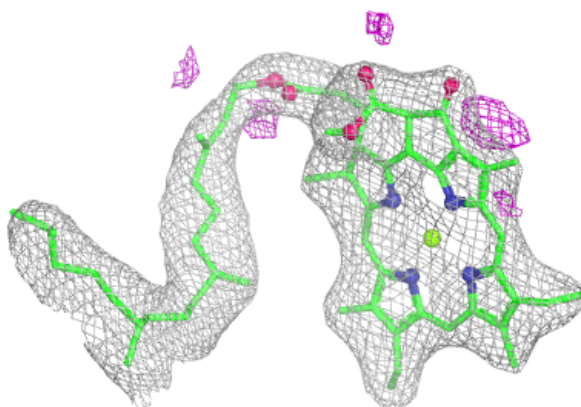
**Electron density around CLA B 825:**

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



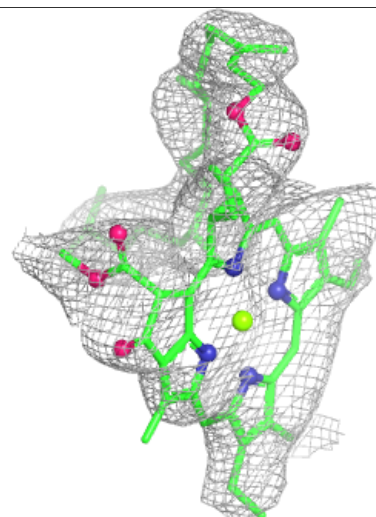
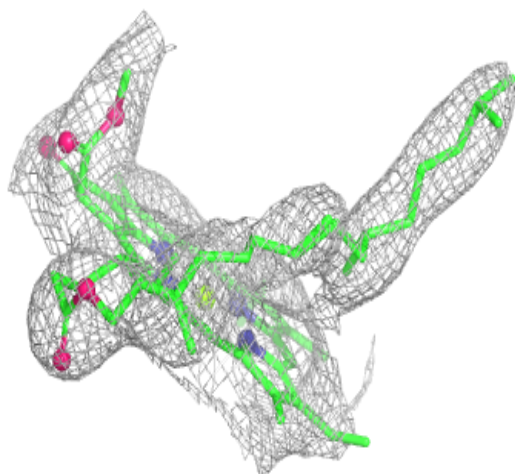
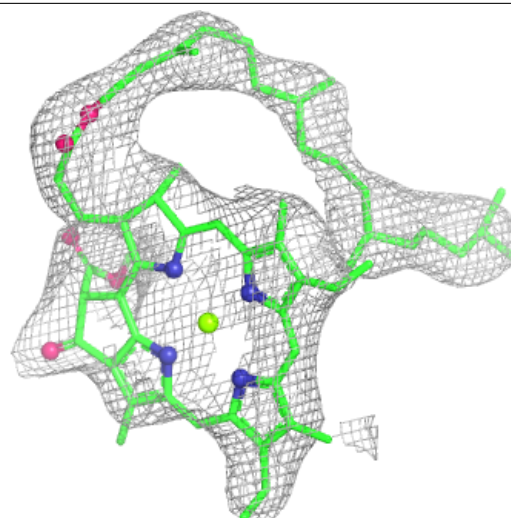
Electron density around CLA B 826:

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



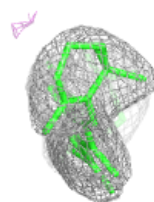
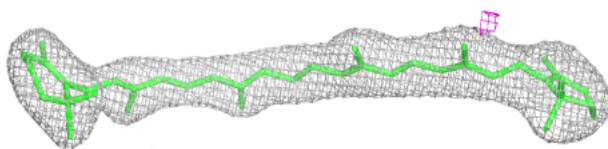
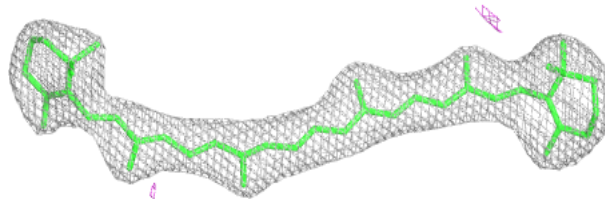
Electron density around CLA A 812:

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

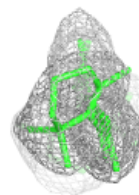
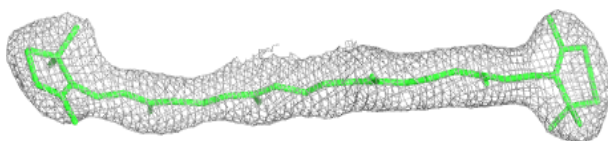
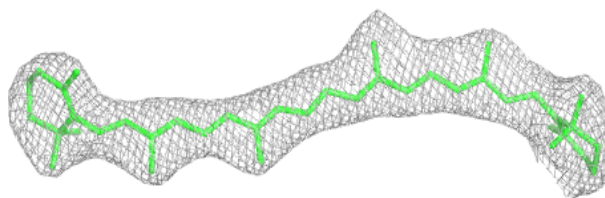


Electron density around BCR B 848:

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

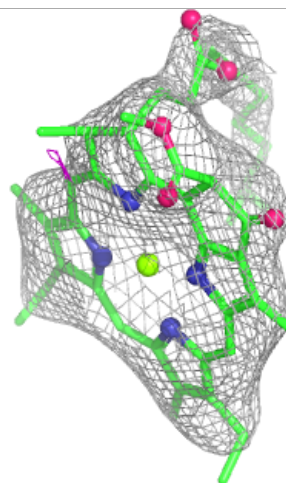
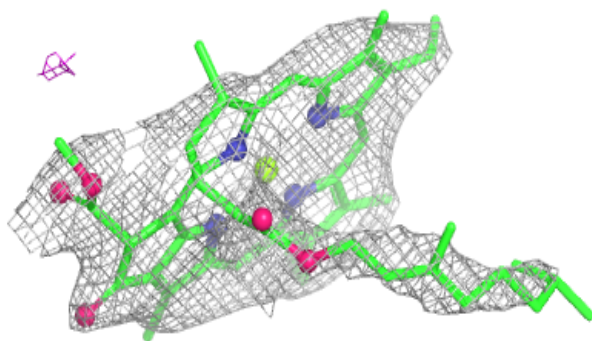
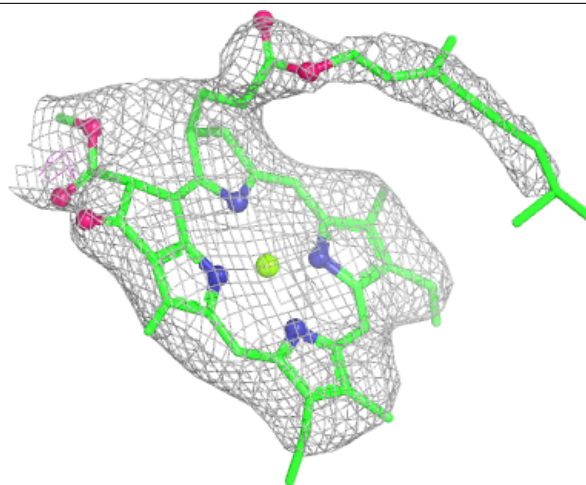
**Electron density around BCR B 849:**

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



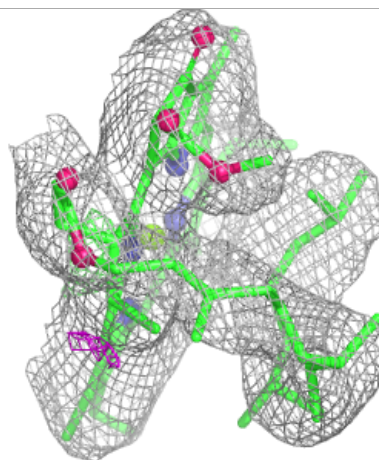
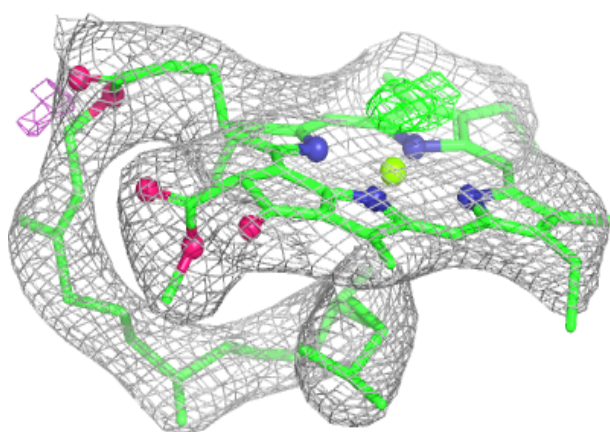
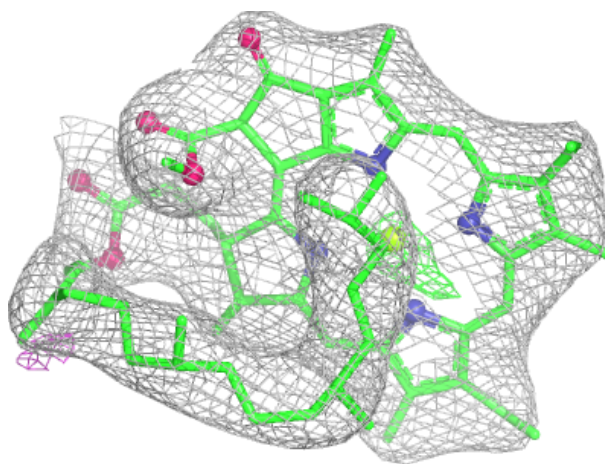
Electron density around CLA A 823:

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



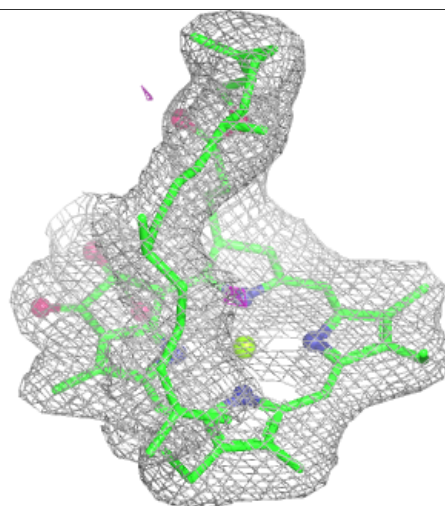
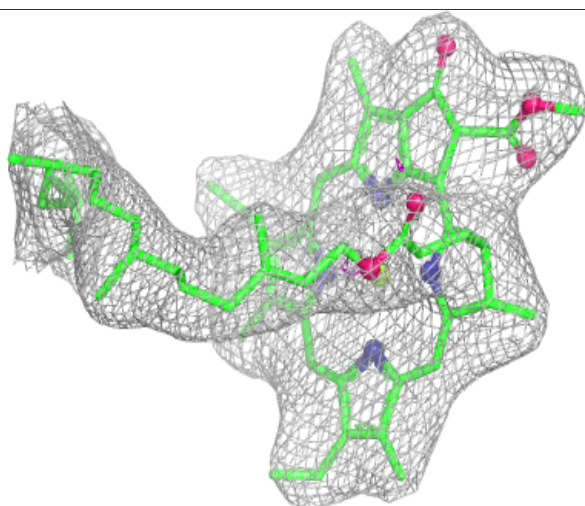
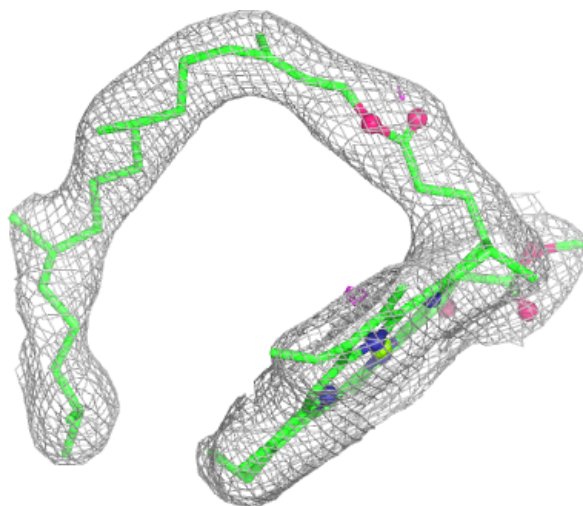
Electron density around CLA A 805:

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



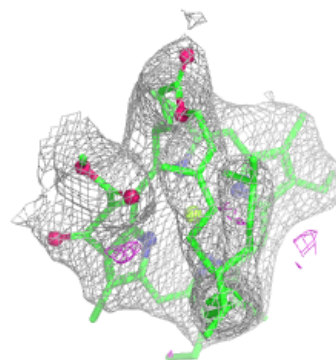
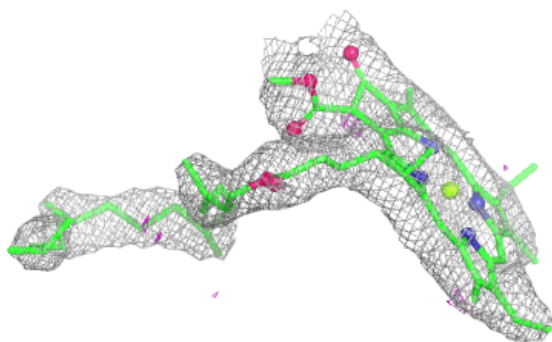
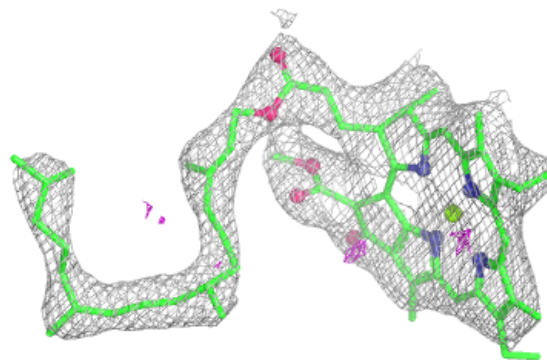
Electron density around CLA B 821:

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

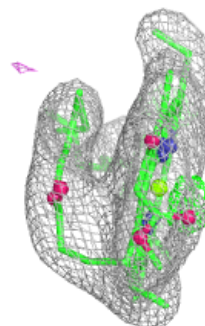
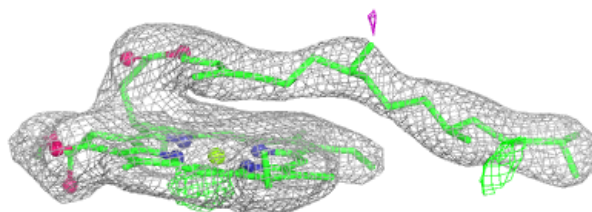
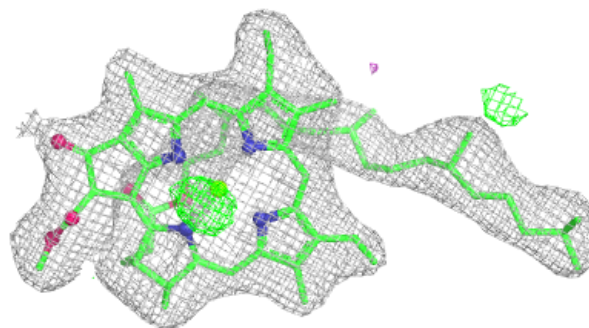


Electron density around CLA A 801:

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

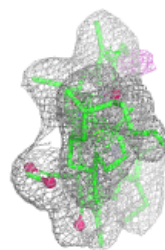
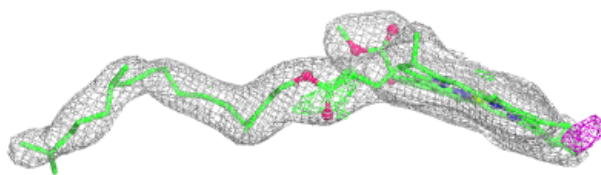
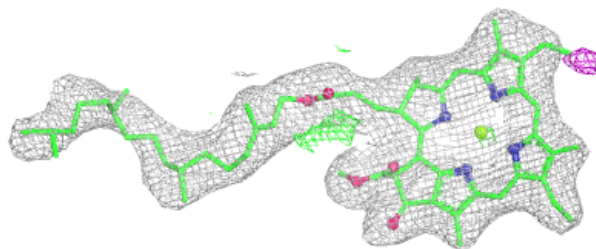
**Electron density around CLA A 838:**

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

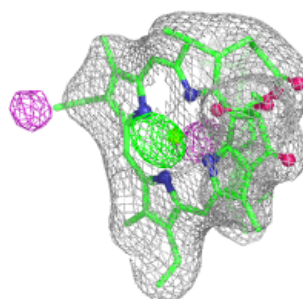
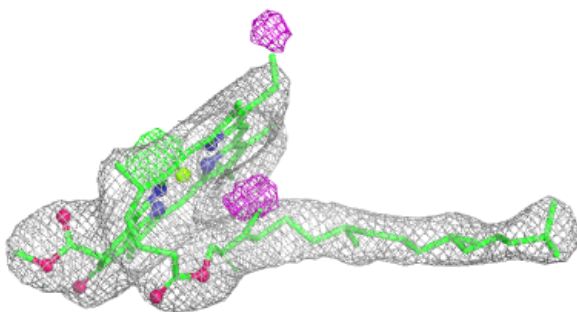
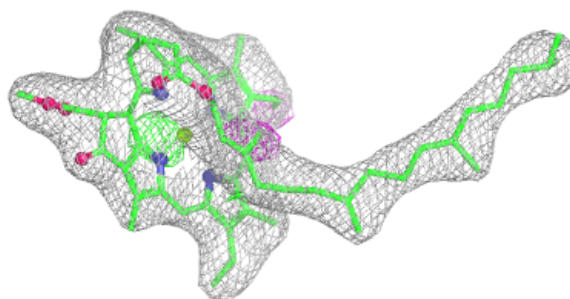


Electron density around CLA A 839:

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

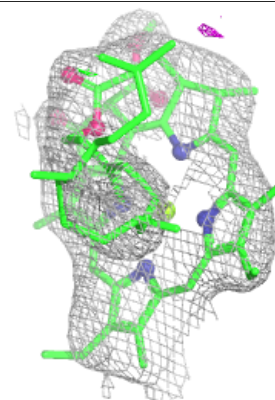
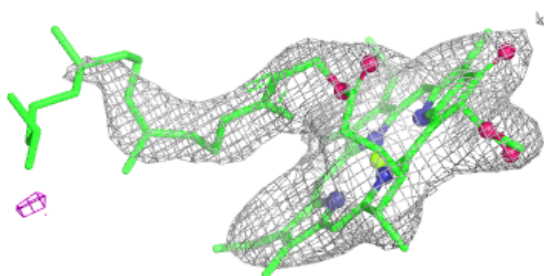
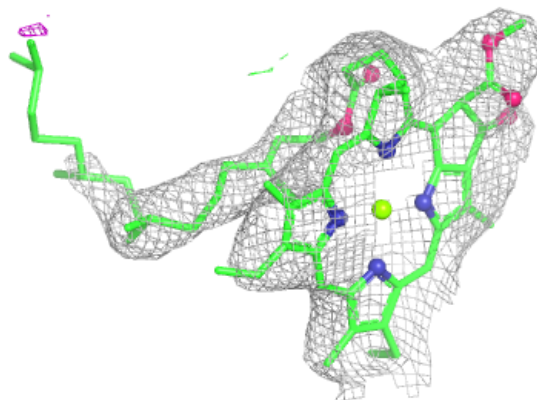
**Electron density around CLA A 840:**

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

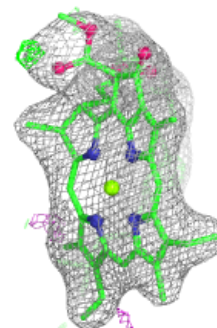
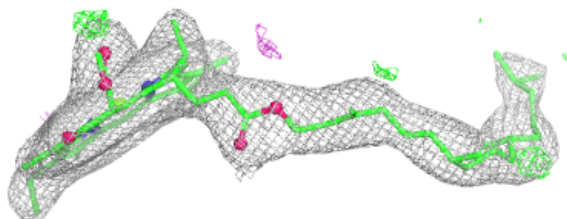
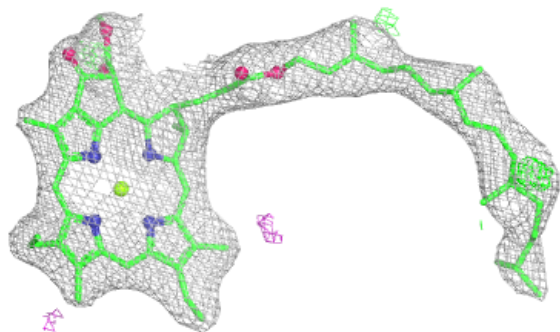


Electron density around CLA A 841:

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

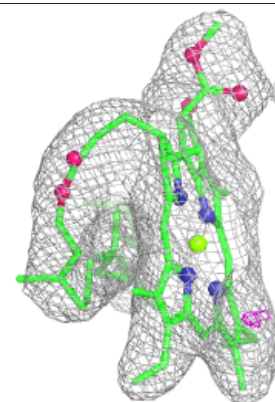
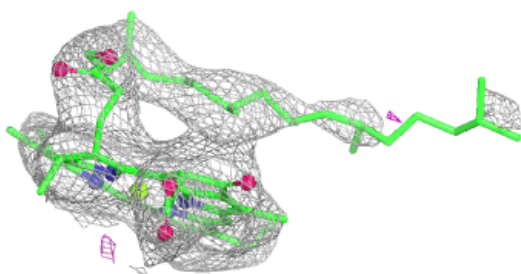
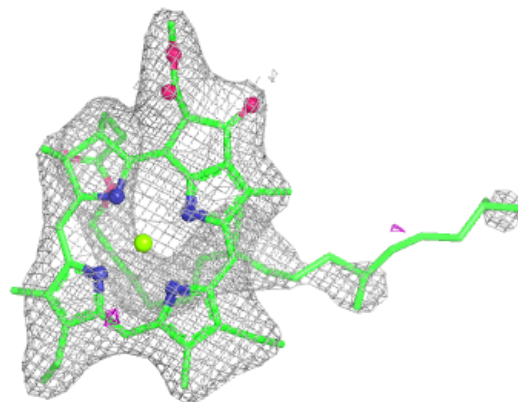
**Electron density around CLA B 827:**

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

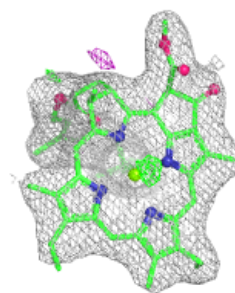
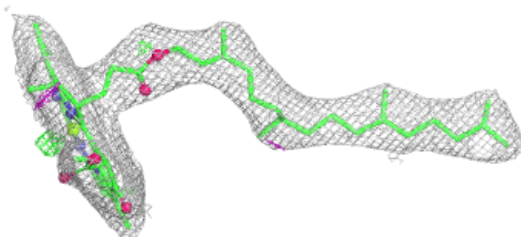
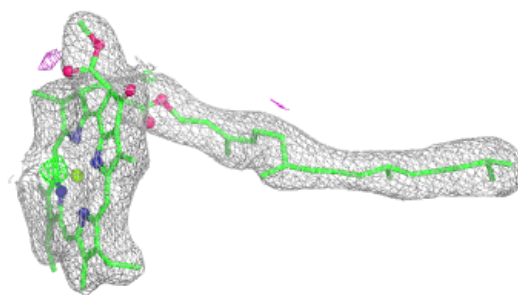


Electron density around CLA B 829:

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

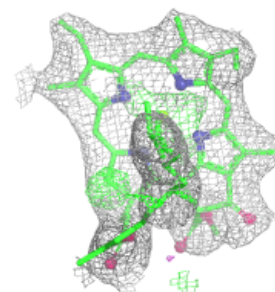
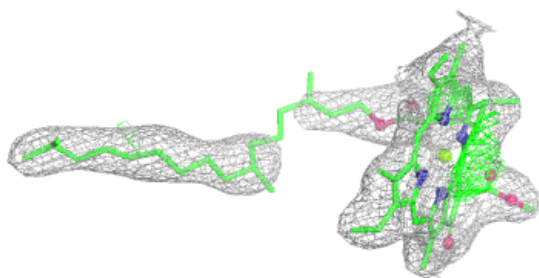
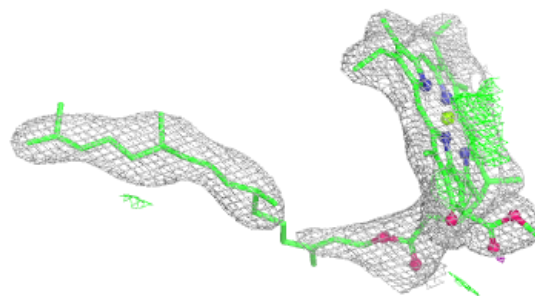
**Electron density around CLA B 830:**

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



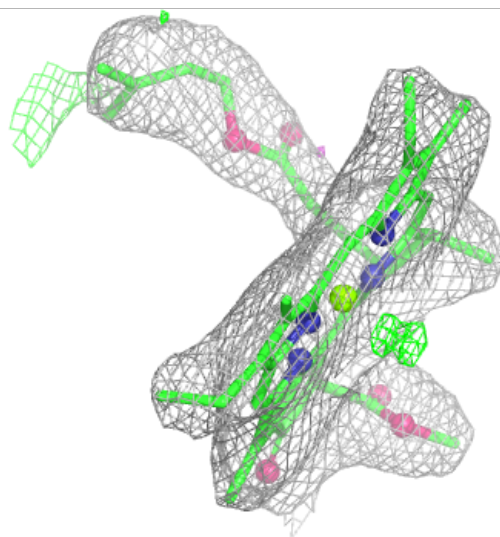
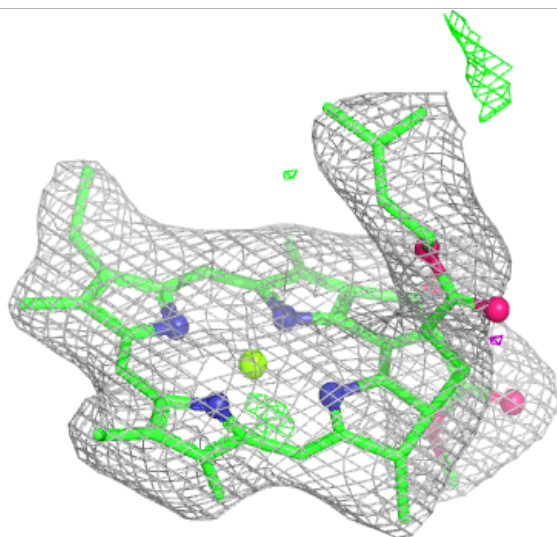
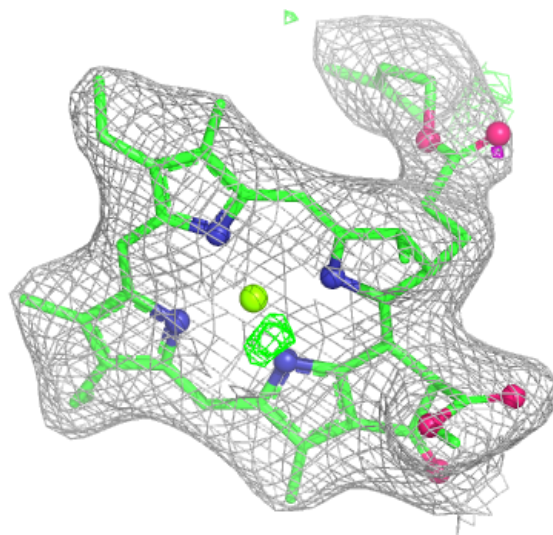
Electron density around CLA B 831:

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



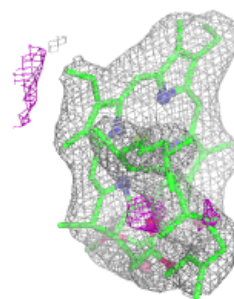
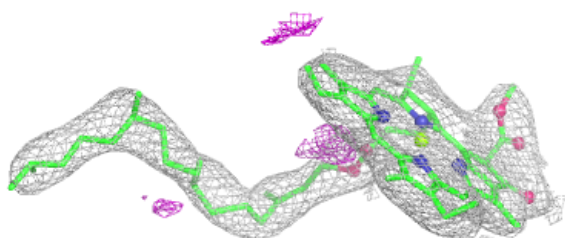
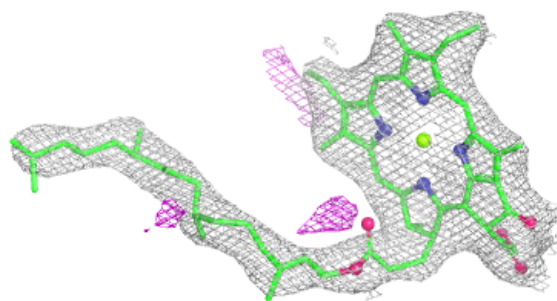
Electron density around CLA B 832:

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

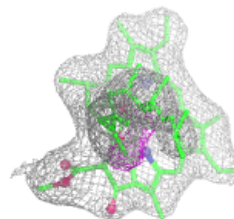
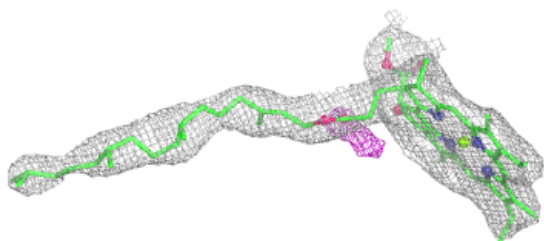
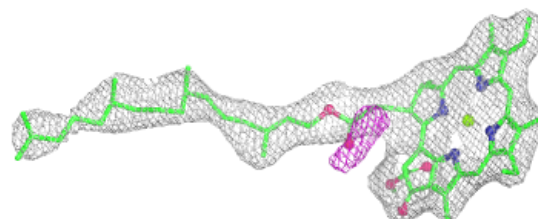


Electron density around CLA A 807:

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

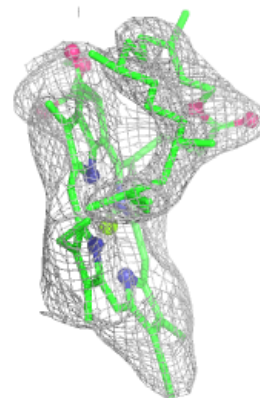
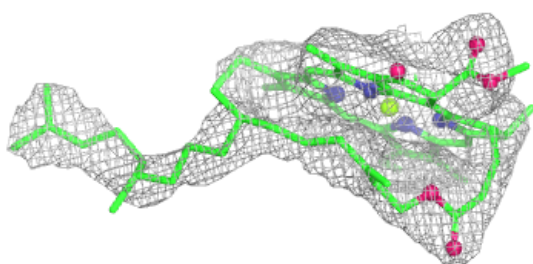
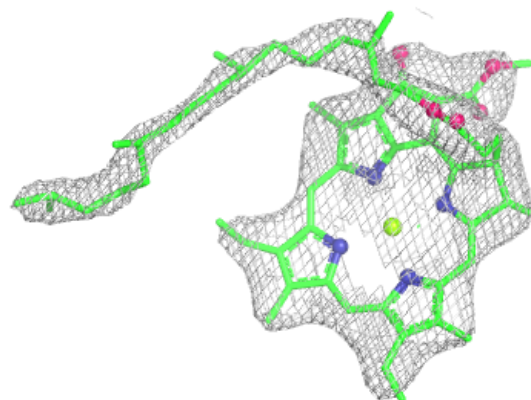
**Electron density around CLA A 808:**

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

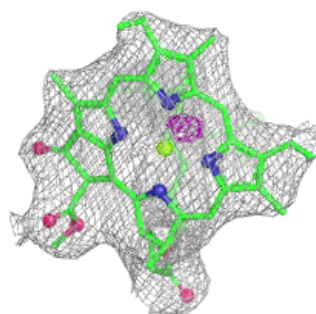
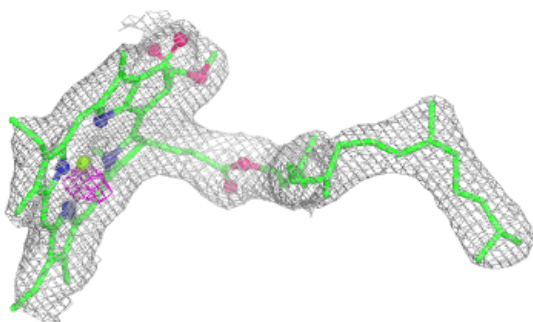
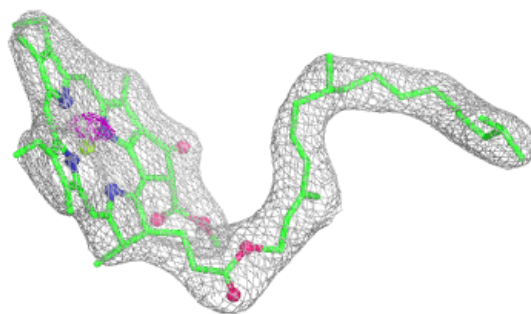


Electron density around CLA A 828:

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

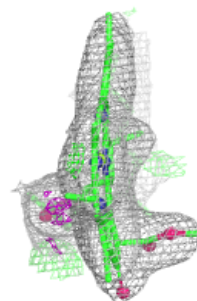
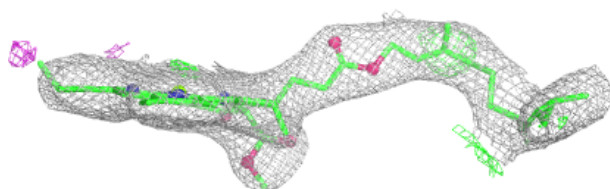
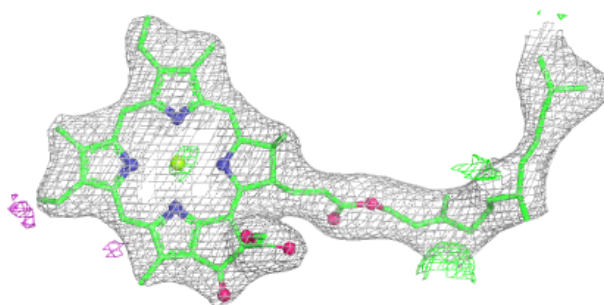
**Electron density around CLA B 804:**

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

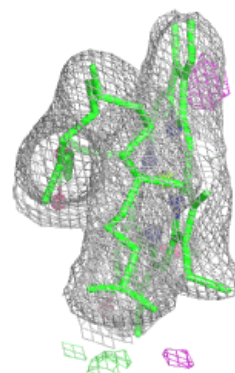
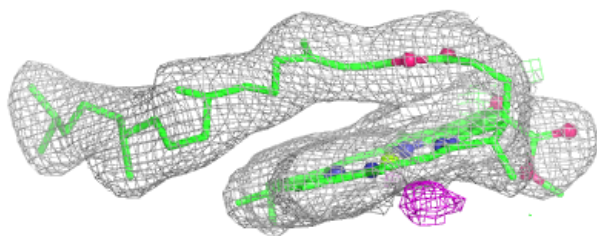
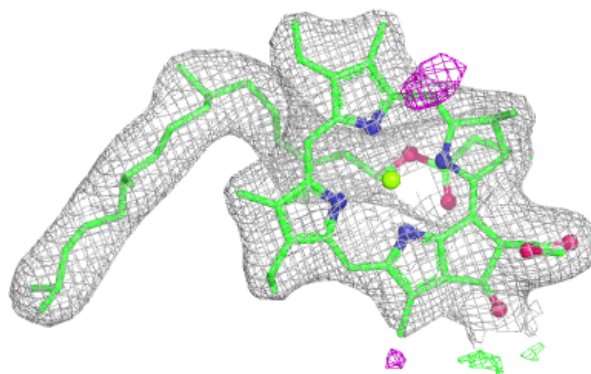


Electron density around CLA B 837:

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

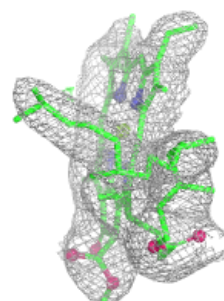
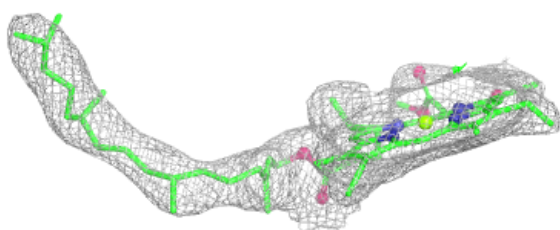
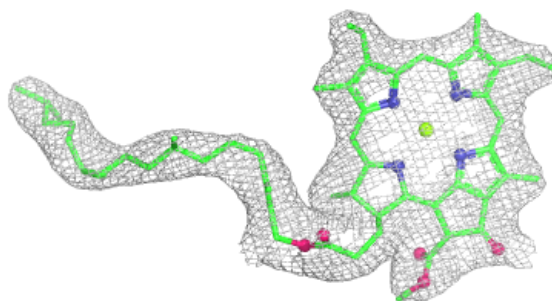
**Electron density around CLA B 838:**

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

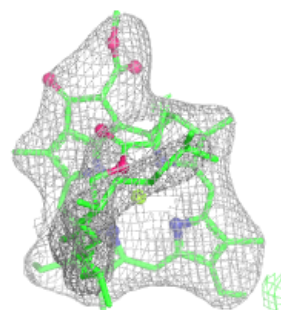
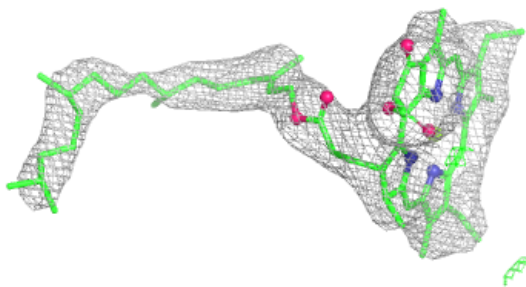
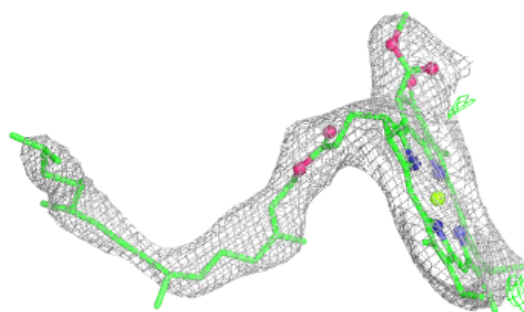


Electron density around CLA B 805:

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

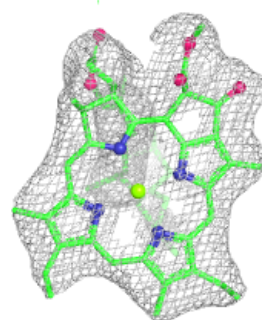
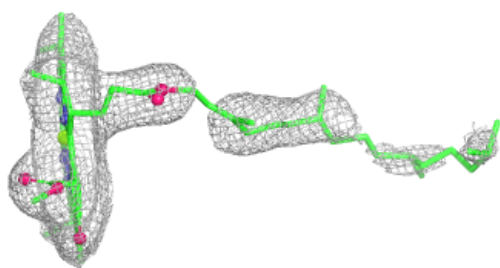
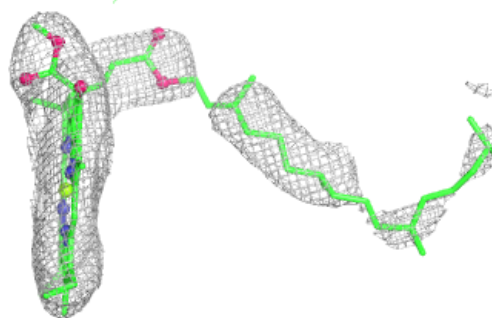
**Electron density around CLA B 840:**

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

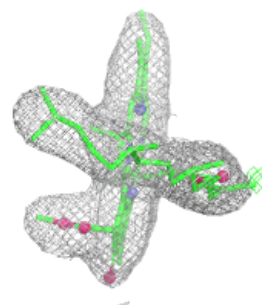
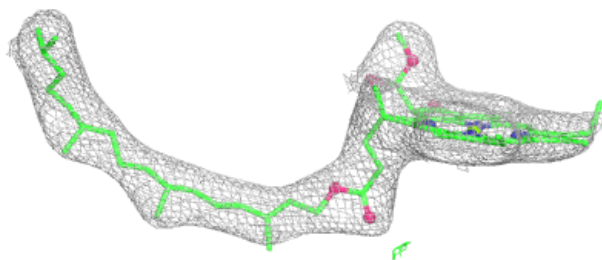
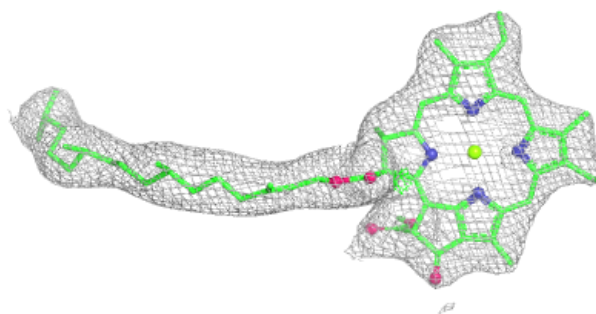


Electron density around CLA B 841:

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

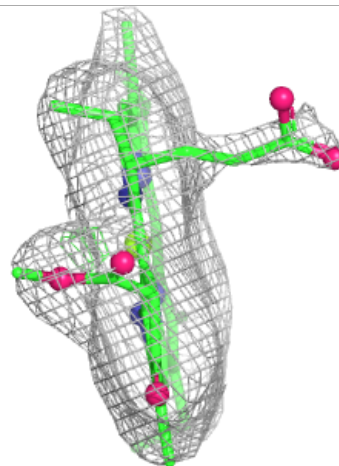
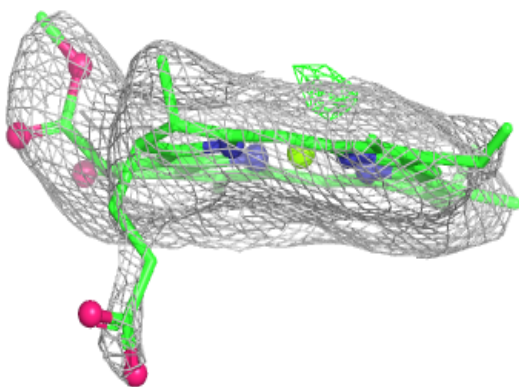
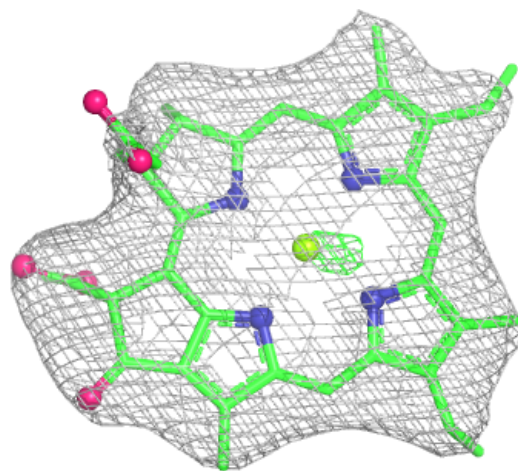
**Electron density around CLA B 842:**

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



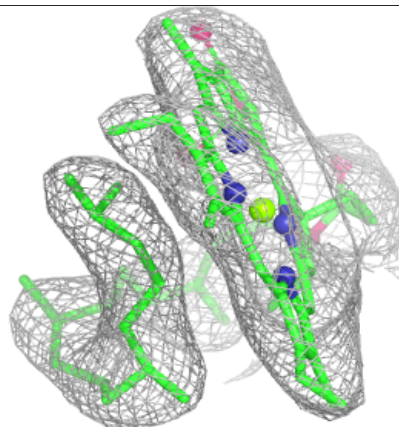
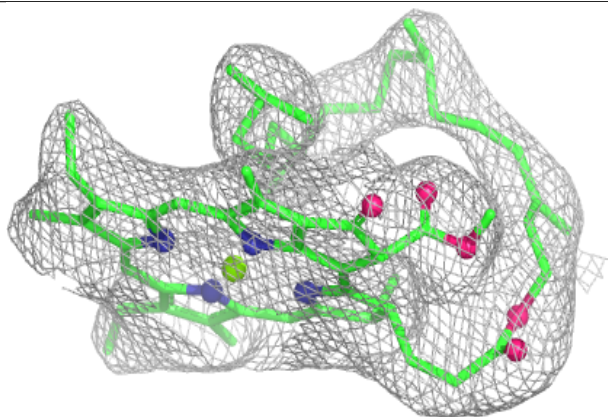
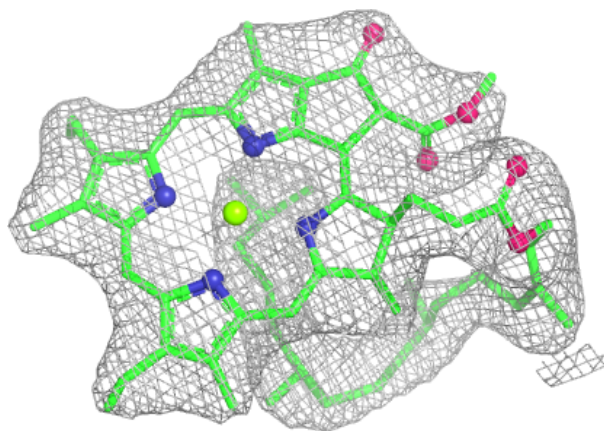
Electron density around CLA B 806:

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

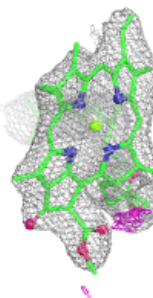
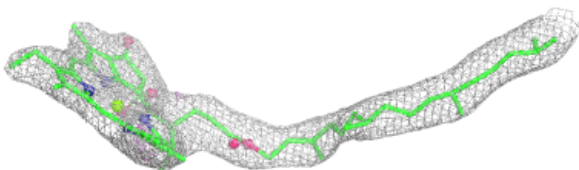
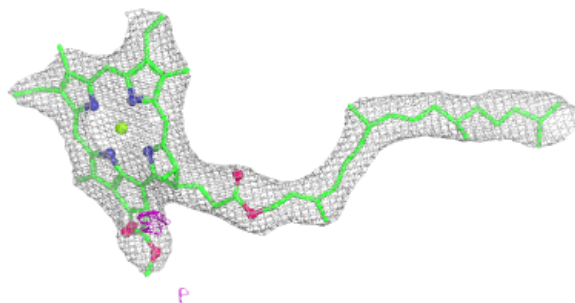


Electron density around CLA B 808:

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

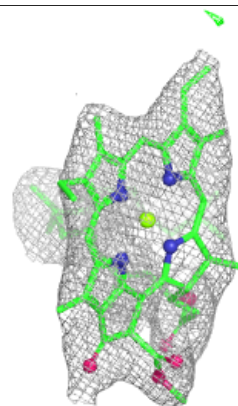
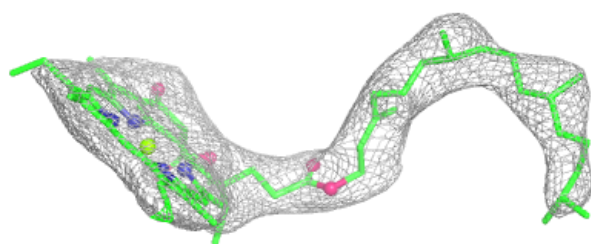
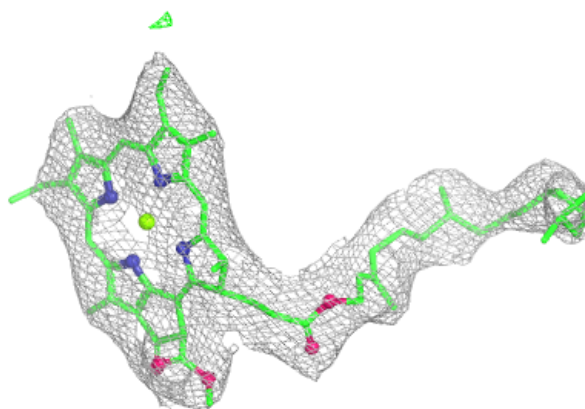
**Electron density around CLA A 802:**

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



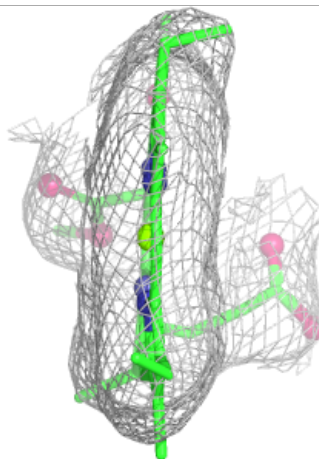
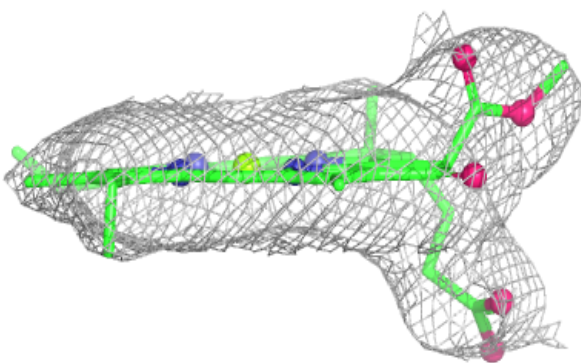
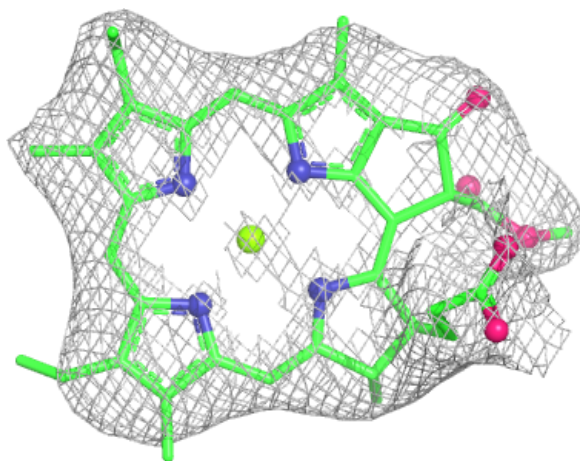
Electron density around CLA B 811:

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



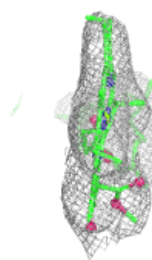
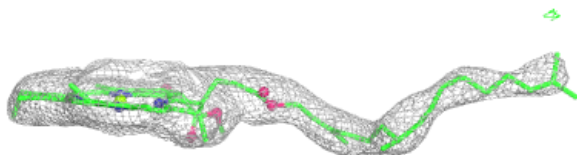
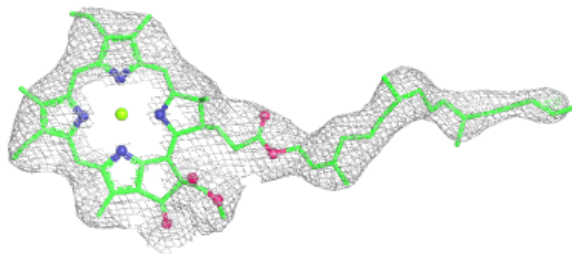
Electron density around CLA 4 313:

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

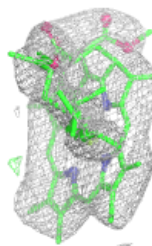
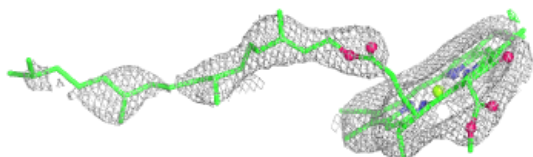
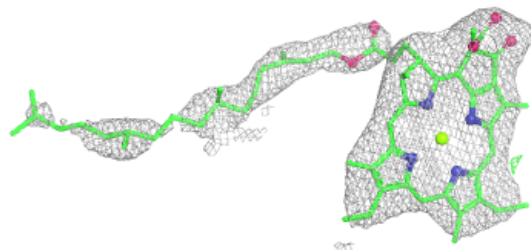


Electron density around CLA A 831:

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

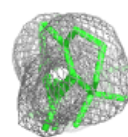
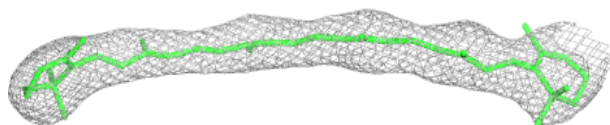
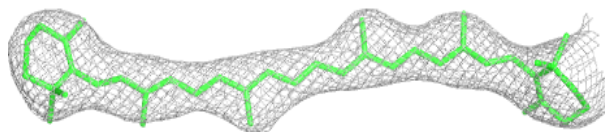
**Electron density around CLA A 832:**

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

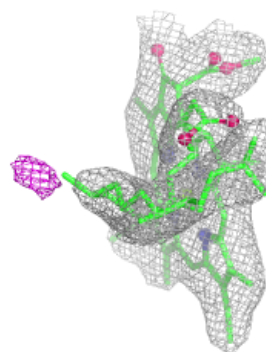
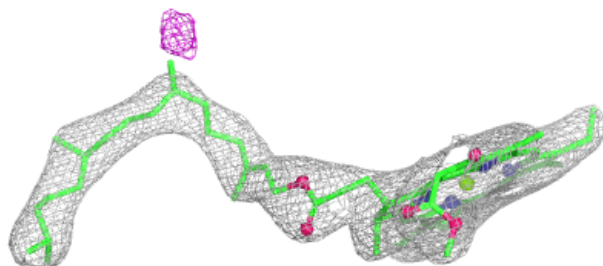
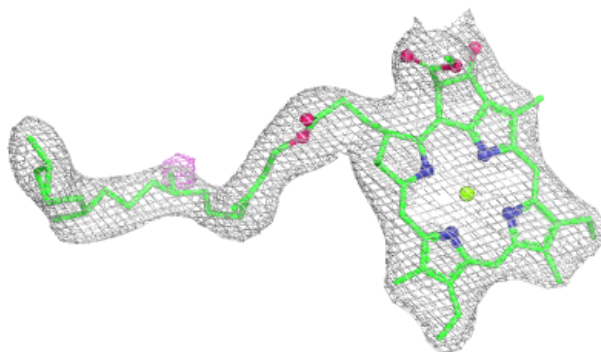


Electron density around BCR B 844:

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

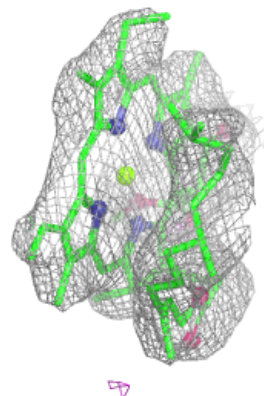
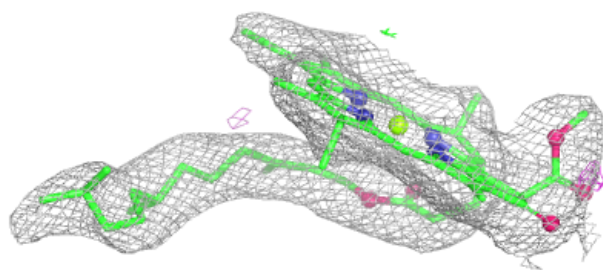
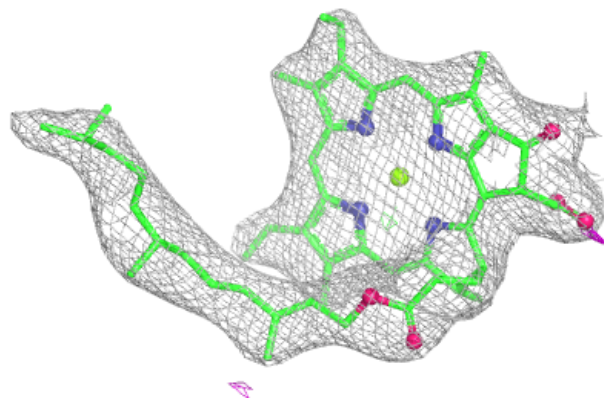
**Electron density around CLA B 815:**

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

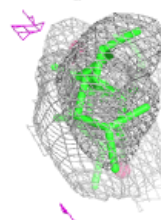
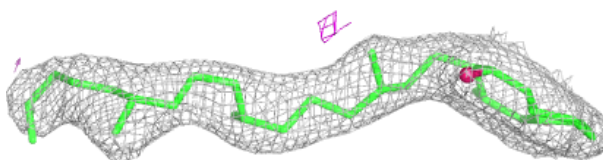
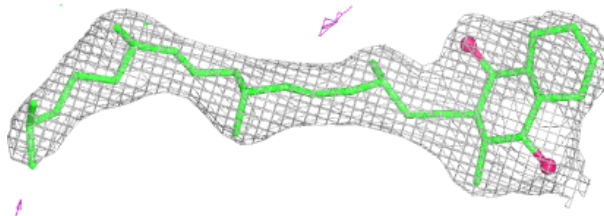


Electron density around CLA 4 302:

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

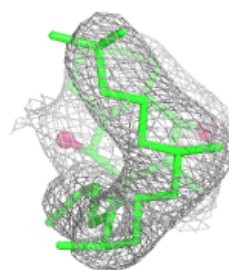
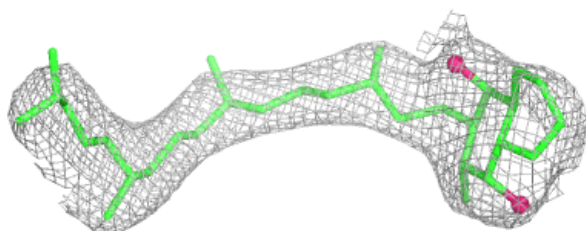
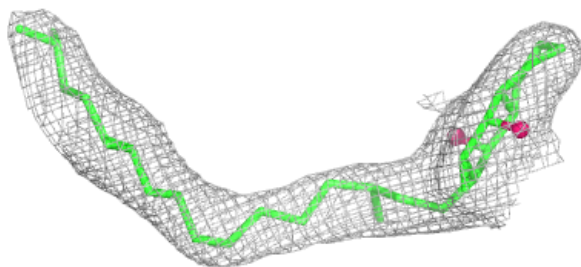
**Electron density around PQN A 842:**

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



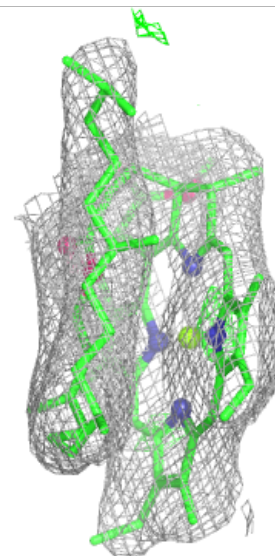
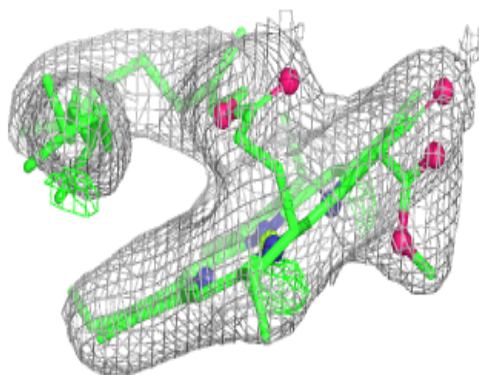
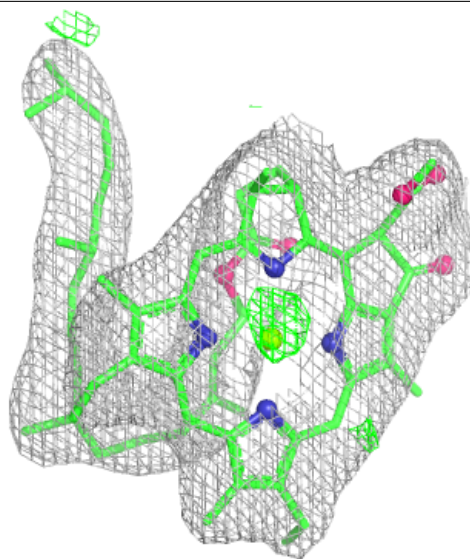
Electron density around PQN B 843:

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



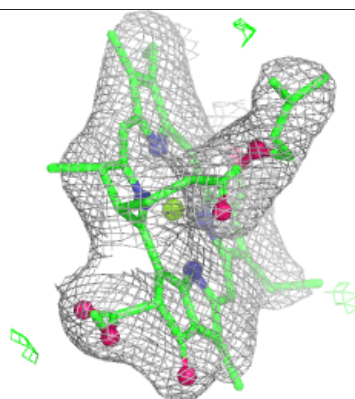
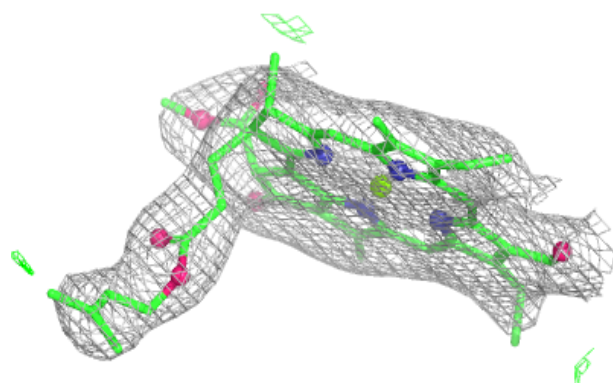
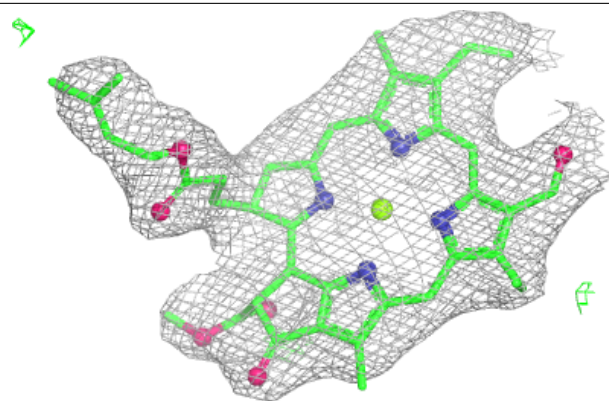
Electron density around CLA B 810:

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

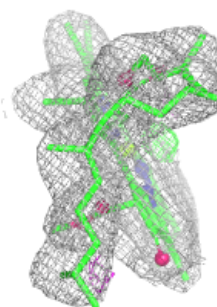
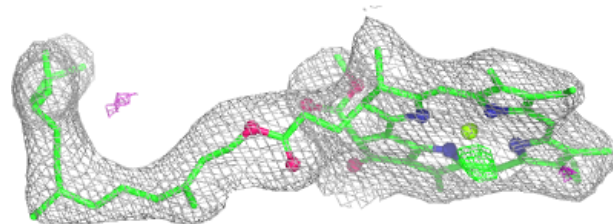
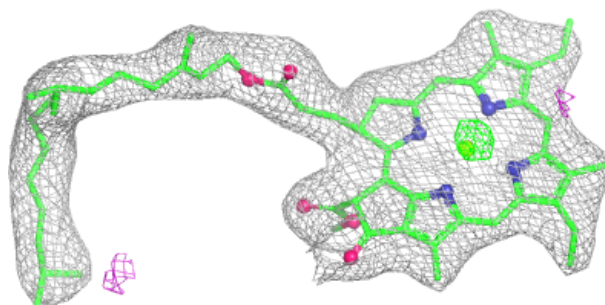


Electron density around CHL 4 307:

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

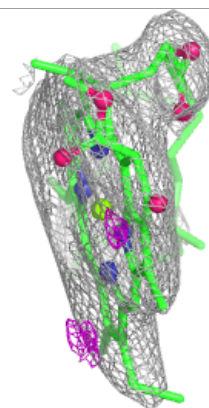
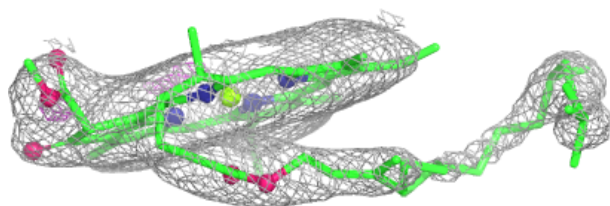
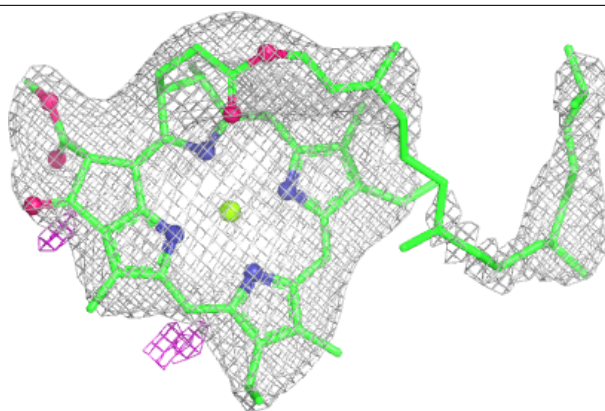
**Electron density around CLA B 828:**

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

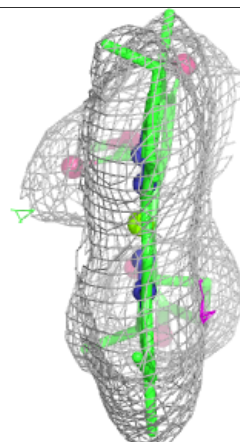
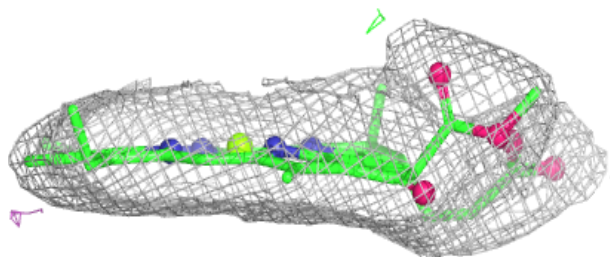
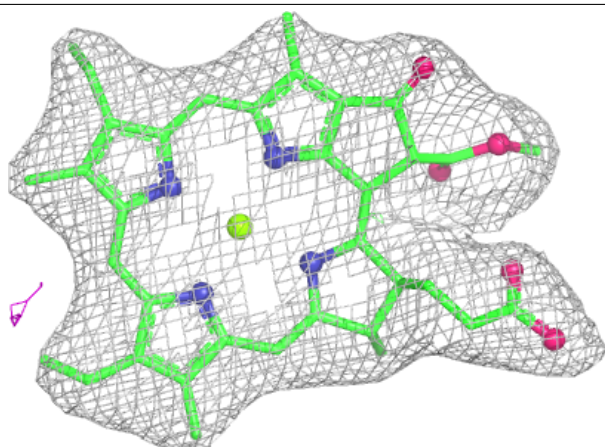


Electron density around CLA A 818:

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

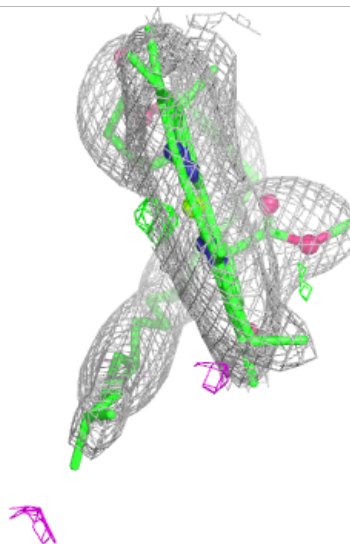
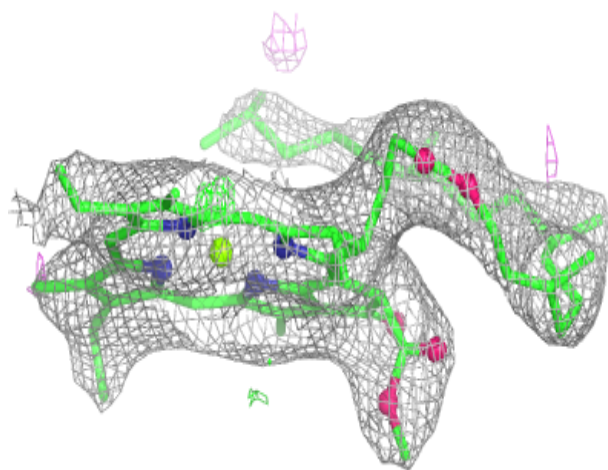
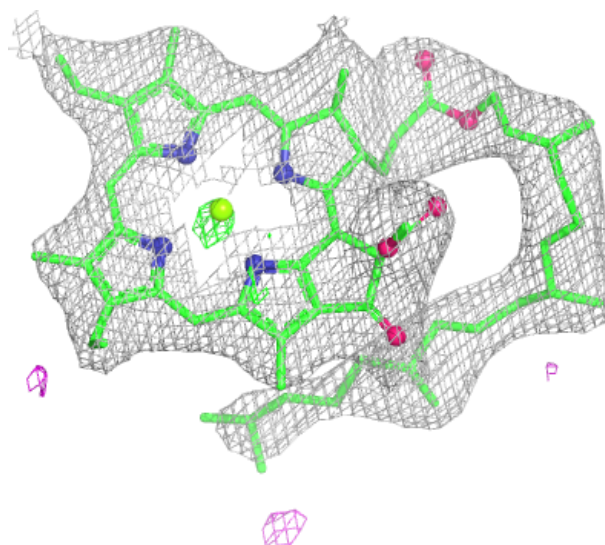
**Electron density around CLA F 306:**

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



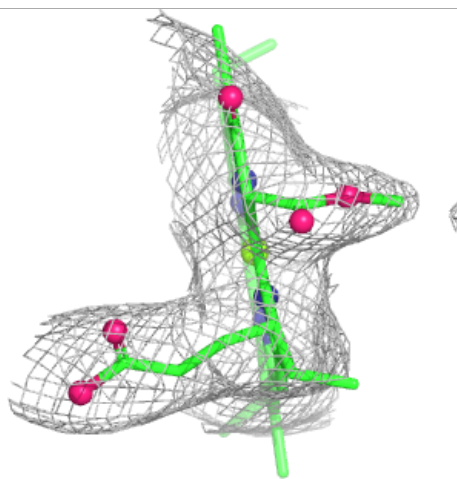
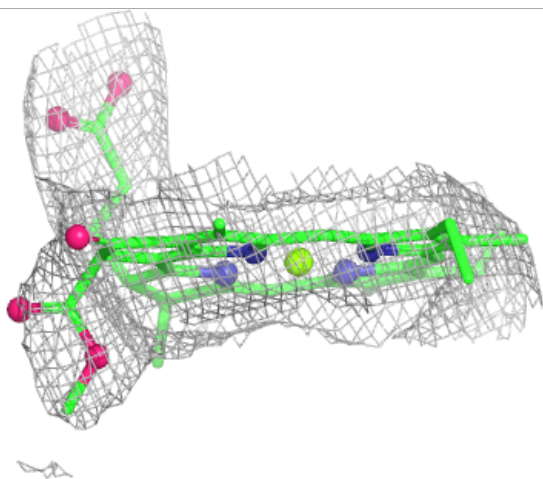
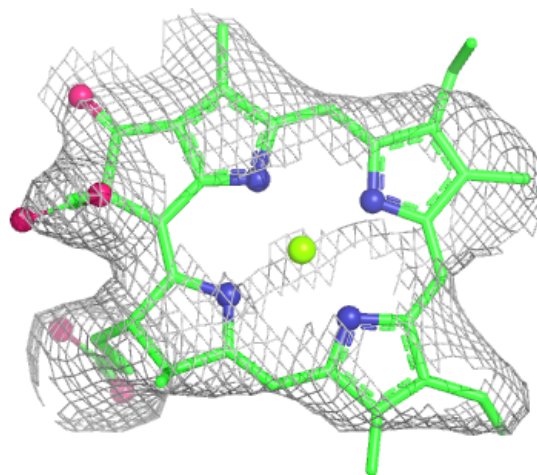
Electron density around CLA B 807:

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



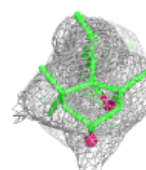
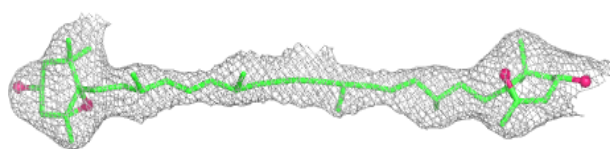
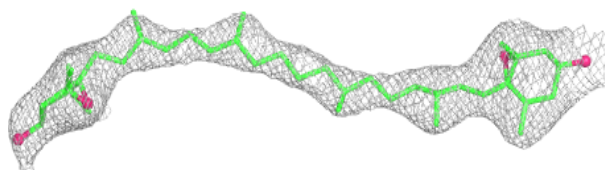
Electron density around CLA A 813:

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

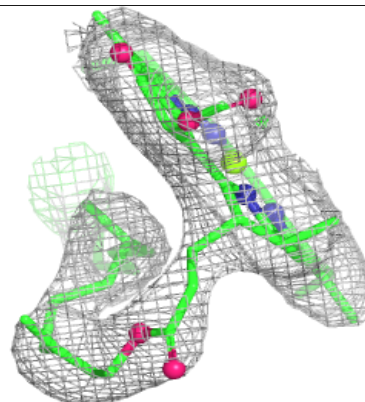
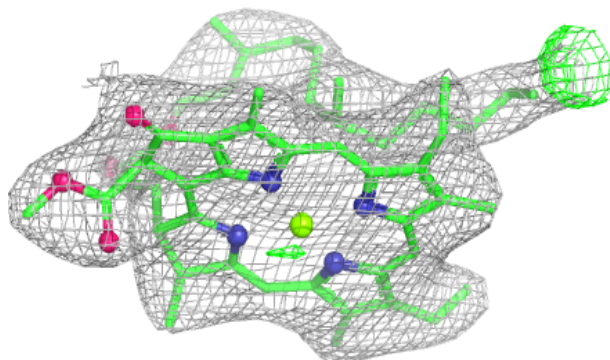
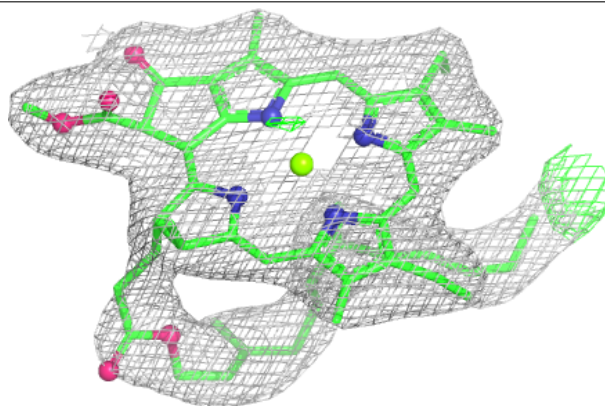


Electron density around XAT 1 315:

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

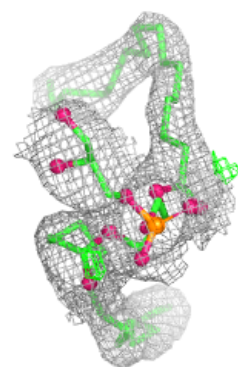
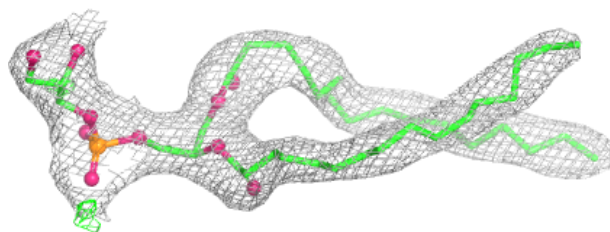
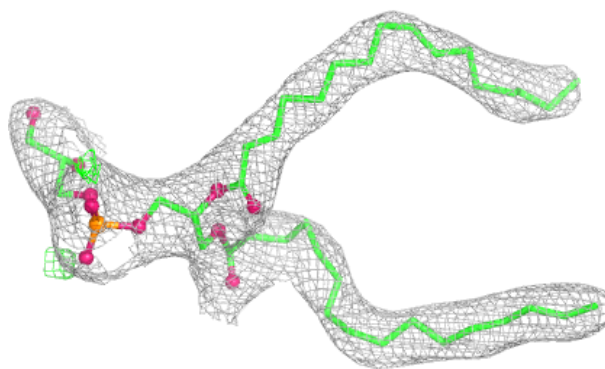
**Electron density around CLA B 819:**

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

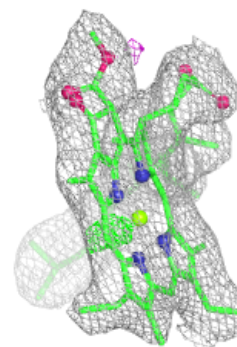
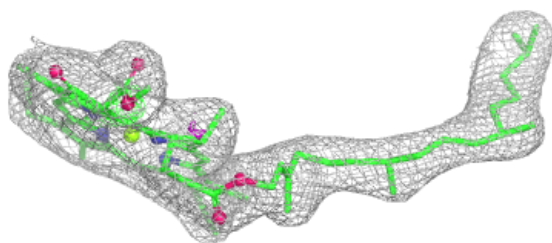
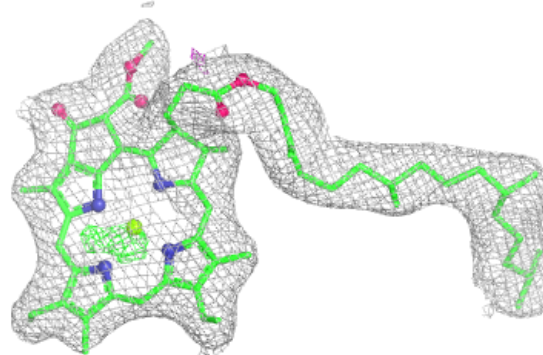


Electron density around LHG A 844:

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

**Electron density around CLA B 802:**

$2mF_o-DF_c$ (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.