



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:38 AM UTC

PDB ID : 6ZXS / pdb\_00006zxs  
Title : Cold grown Pea Photosystem I  
Authors : Caspy, I.; Borovikova-Sheinker, A.; Subramanyam, R.; Nelson, N.  
Deposited on : 2020-07-30  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

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

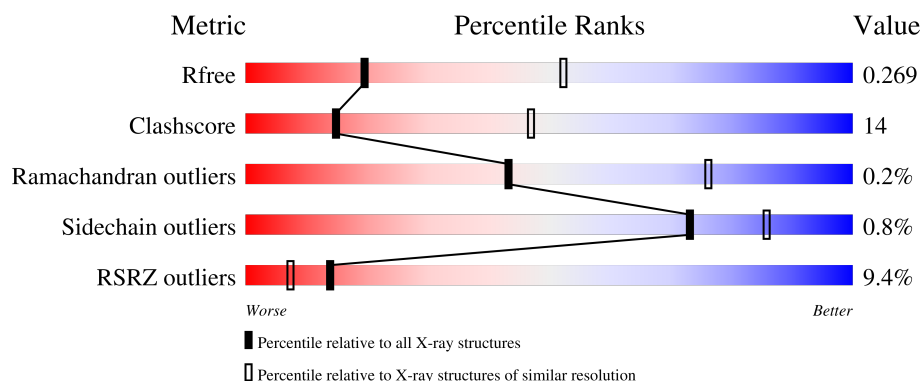
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	743	<div> <div>6%</div> <div>78%</div> <div>22%</div> </div>
2	B	733	<div> <div>9%</div> <div>76%</div> <div>23%</div> </div>
3	C	80	<div> <div>9%</div> <div>81%</div> <div>19%</div> </div>
4	D	143	<div> <div>12%</div> <div>77%</div> <div>23%</div> </div>
5	E	66	<div> <div>11%</div> <div>91%</div> <div>9%</div> </div>

*Continued on next page...*



Continued from previous page...

Mol	Chain	Length	Quality of chain
6	F	154	
7	G	97	
8	H	88	
9	I	30	
10	J	42	
11	K	80	
12	L	157	
13	1	193	
14	2	208	
15	3	221	
16	4	198	

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	CL0	A	801	X	-	-	-
18	CLA	1	5006	X	-	-	-
18	CLA	1	5007	X	-	-	-
18	CLA	1	5008	X	-	-	-
18	CLA	1	5009	X	-	-	-
18	CLA	1	5010	X	-	-	-
18	CLA	1	5011	X	-	-	-
18	CLA	1	5012	X	-	-	-
18	CLA	1	5013	X	-	-	-
18	CLA	1	5015	X	-	-	-
18	CLA	1	5017	X	-	-	-
18	CLA	1	5018	X	-	-	-
18	CLA	2	306	X	-	-	-
18	CLA	2	307	X	-	-	-
18	CLA	2	308	X	-	-	-
18	CLA	2	309	X	-	-	-
18	CLA	2	310	X	-	-	-
18	CLA	2	311	X	-	-	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	2	312	X	-	-	-
18	CLA	2	313	X	-	-	-
18	CLA	2	317	X	-	-	-
18	CLA	2	326	X	-	-	-
18	CLA	3	301	X	-	-	-
18	CLA	3	307	X	-	-	-
18	CLA	3	308	X	-	-	-
18	CLA	3	309	X	-	-	-
18	CLA	3	311	X	-	-	-
18	CLA	3	314	X	-	-	-
18	CLA	3	315	X	-	-	-
18	CLA	3	317	X	-	-	-
18	CLA	3	318	X	-	-	-
18	CLA	3	319	X	-	-	-
18	CLA	4	305	X	-	-	-
18	CLA	4	306	X	-	-	-
18	CLA	4	307	X	-	-	-
18	CLA	4	308	X	-	-	-
18	CLA	4	309	X	-	-	-
18	CLA	4	310	X	-	-	-
18	CLA	4	311	X	-	-	-
18	CLA	4	312	X	-	-	-
18	CLA	4	315	X	-	-	-
18	CLA	A	802	X	-	-	-
18	CLA	A	803	X	-	-	-
18	CLA	A	804	X	-	-	-
18	CLA	A	805	X	-	-	-
18	CLA	A	806	X	-	-	-
18	CLA	A	807	X	-	-	-
18	CLA	A	808	X	-	-	-
18	CLA	A	809	X	-	-	-
18	CLA	A	810	X	-	-	-
18	CLA	A	811	X	-	-	-
18	CLA	A	812	X	-	-	-
18	CLA	A	813	X	-	-	-
18	CLA	A	814	X	-	-	-
18	CLA	A	815	X	-	-	-
18	CLA	A	816	X	-	-	-
18	CLA	A	817	X	-	-	-
18	CLA	A	818	X	-	-	-
18	CLA	A	819	X	-	-	-
18	CLA	A	820	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	A	821	X	-	-	-
18	CLA	A	822	X	-	-	-
18	CLA	A	823	X	-	-	-
18	CLA	A	824	X	-	-	-
18	CLA	A	825	X	-	-	-
18	CLA	A	826	X	-	-	-
18	CLA	A	827	X	-	-	-
18	CLA	A	828	X	-	-	-
18	CLA	A	829	X	-	-	-
18	CLA	A	830	X	-	-	-
18	CLA	A	831	X	-	-	-
18	CLA	A	832	X	-	-	-
18	CLA	A	833	X	-	-	-
18	CLA	A	834	X	-	-	-
18	CLA	A	835	X	-	-	-
18	CLA	A	836	X	-	-	-
18	CLA	A	837	X	-	-	-
18	CLA	A	838	X	-	-	-
18	CLA	A	839	X	-	-	-
18	CLA	A	840	X	-	-	-
18	CLA	A	852	X	-	-	-
18	CLA	A	853	X	-	-	-
18	CLA	B	801	X	-	-	-
18	CLA	B	803	X	-	-	-
18	CLA	B	804	X	-	-	-
18	CLA	B	805	X	-	-	-
18	CLA	B	806	X	-	-	-
18	CLA	B	807	X	-	-	-
18	CLA	B	808	X	-	-	-
18	CLA	B	809	X	-	-	-
18	CLA	B	810	X	-	-	-
18	CLA	B	811	X	-	-	-
18	CLA	B	812	X	-	-	-
18	CLA	B	813	X	-	-	-
18	CLA	B	814	X	-	-	-
18	CLA	B	815	X	-	-	-
18	CLA	B	816	X	-	-	-
18	CLA	B	817	X	-	-	-
18	CLA	B	818	X	-	-	-
18	CLA	B	819	X	-	-	-
18	CLA	B	820	X	-	-	-
18	CLA	B	821	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	822	X	-	-	-
18	CLA	B	823	X	-	-	-
18	CLA	B	824	X	-	-	-
18	CLA	B	825	X	-	-	-
18	CLA	B	826	X	-	-	-
18	CLA	B	827	X	-	-	-
18	CLA	B	828	X	-	-	-
18	CLA	B	829	X	-	-	-
18	CLA	B	830	X	-	-	-
18	CLA	B	831	X	-	-	-
18	CLA	B	832	X	-	-	-
18	CLA	B	833	X	-	-	-
18	CLA	B	834	X	-	-	-
18	CLA	B	835	X	-	-	-
18	CLA	B	836	X	-	-	-
18	CLA	B	837	X	-	-	-
18	CLA	B	838	X	-	-	-
18	CLA	B	839	X	-	-	-
18	CLA	B	840	X	-	-	-
18	CLA	B	841	X	-	-	-
18	CLA	F	301	X	-	-	-
18	CLA	F	302	X	-	-	-
18	CLA	F	303	X	-	-	-
18	CLA	G	1601	X	-	-	-
18	CLA	G	1602	X	-	-	-
18	CLA	G	1603	X	-	-	-
18	CLA	H	1701	X	-	-	-
18	CLA	J	1101	X	-	-	-
18	CLA	J	1103	X	-	-	-
18	CLA	K	1401	X	-	-	-
18	CLA	K	1402	X	-	-	-
18	CLA	K	1403	X	-	-	-
18	CLA	K	1404	X	-	-	-
18	CLA	L	301	X	-	-	-
18	CLA	L	304	X	-	-	-
18	CLA	L	305	X	-	-	-
18	CLA	L	306	X	-	-	-
29	LUT	1	5004	X	-	-	-
29	LUT	2	303	X	-	-	-
29	LUT	3	304	X	-	-	-
29	LUT	J	1105	X	-	-	-
30	CHL	1	5014	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CHL	1	5016	X	-	-	-
30	CHL	2	314	X	-	-	-
30	CHL	2	315	X	-	-	-
30	CHL	2	316	X	-	-	-
30	CHL	2	318	X	-	-	-
30	CHL	2	319	X	-	-	-
30	CHL	3	310	X	-	-	-
30	CHL	3	312	X	-	-	-
30	CHL	3	313	X	-	-	-
30	CHL	3	316	X	-	-	-
30	CHL	4	302	X	-	-	-
30	CHL	4	313	X	-	-	-
30	CHL	4	314	X	-	-	-
30	CHL	4	316	X	-	-	-
30	CHL	4	317	X	-	-	-
30	CHL	4	318	X	-	-	-
31	XAT	2	304	X	-	-	-
31	XAT	4	304	X	-	-	-

## 2 Entry composition [i](#)

There are 31 unique types of molecules in this entry. The entry contains 37423 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	743	Total	C	N	O	S	0	0	0
			5858	3839	998	1003	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	733	Total	C	N	O	S	0	0	0
			5857	3848	998	997	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			612	379	107	115	11			

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	143	Total	C	N	O	S	0	0	0
			1132	731	194	204	3			

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	66	Total	C	N	O	0	0	0
			528	336	93	99			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	154	Total	C	N	O	S	0	0	0
			1206	782	207	215	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	80	ALA	SER	conflict	UNP A0A0M3KL12
F	87	ASP	GLU	conflict	UNP A0A0M3KL12
F	108	LEU	ILE	conflict	UNP A0A0M3KL12
F	111	PRO	ALA	conflict	UNP A0A0M3KL12
F	134	GLY	ALA	conflict	UNP A0A0M3KL12
F	188	ASP	GLU	conflict	UNP A0A0M3KL12
F	204	THR	SER	conflict	UNP A0A0M3KL12
F	205	GLY	ARG	conflict	UNP A0A0M3KL12

- Molecule 7 is a protein called PsaG.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	97	Total	C	N	O	0	0	0
			757	492	125	140			

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

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	60	LEU	ILE	conflict	UNP A0A0M3KL10
H	79	ASN	SER	conflict	UNP A0A0M3KL10
H	80	SER	PRO	conflict	UNP A0A0M3KL10
H	116	ALA	THR	conflict	UNP A0A0M3KL10
H	126	LYS	VAL	conflict	UNP A0A0M3KL10
H	134	GLN	LYS	conflict	UNP A0A0M3KL10
H	139	LEU	-	insertion	UNP A0A0M3KL10
H	?	-	LYS	deletion	UNP A0A0M3KL10

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	30	Total	C	N	O	S	0	0	0
			232	159	37	35	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	42	Total	C	N	O	S	0	0	0
			338	231	51	55	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 11 is a protein called Photosystem I reaction center subunit X psaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	80	Total	C	N	O	S	0	0	0
			558	353	98	104	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	86	ALA	VAL	conflict	UNP E1C9L3

- Molecule 12 is a protein called PsaL domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	157	Total	C	N	O	S	0	0	0
			1174	772	189	212	1			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	57	VAL	ILE	conflict	UNP E1C9L1
L	79	VAL	ILE	conflict	UNP E1C9L1
L	88	GLY	ALA	conflict	UNP E1C9L1
L	94	ASN	SER	conflict	UNP E1C9L1
L	108	PHE	TYR	conflict	UNP E1C9L1
L	143	ILE	LEU	conflict	UNP E1C9L1
L	157	ASP	ALA	conflict	UNP E1C9L1
L	172	GLN	GLU	conflict	UNP E1C9L1
L	201	PHE	TYR	conflict	UNP E1C9L1

- Molecule 13 is a protein called Lhca1.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1	193	Total	C	N	O	S	0	0	0
			1508	982	252	269	5			

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	2	208	Total	C	N	O	S	0	0	0
			1620	1059	265	292	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	3	221	Total	C	N	O	S	0	0	0
			1706	1118	278	305	5			

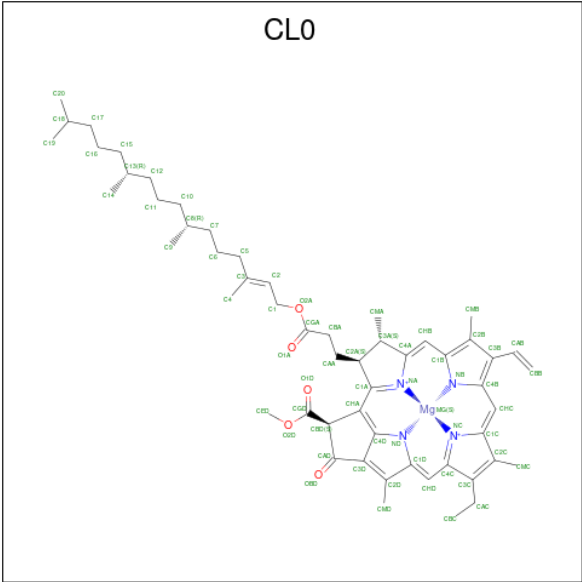
- Molecule 16 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	4	198	Total	C	N	O	S	0	0	0
			1559	1022	253	281	3			

There are 3 discrepancies between the modelled and reference sequences:

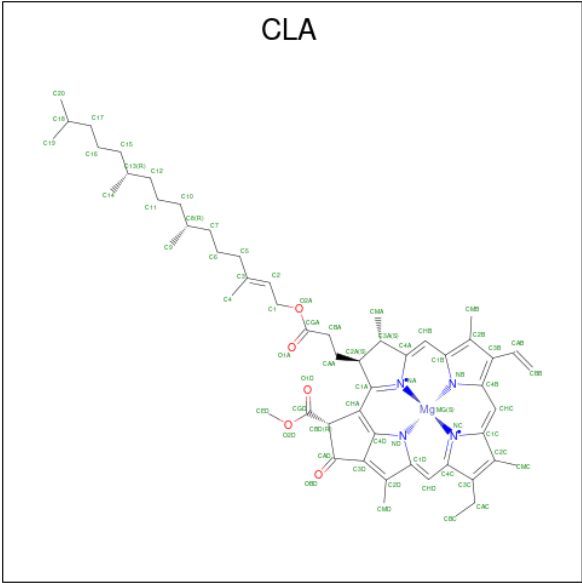
Chain	Residue	Modelled	Actual	Comment	Reference
4	89	LYS	ARG	conflict	UNP Q9SQL2
4	128	ASP	ALA	conflict	UNP Q9SQL2
4	149	PHE	SER	conflict	UNP Q9SQL2

- Molecule 17 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
18	A	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
18	B	1	Total 58	C 48	Mg 1	N 4	O 5	0	0
18	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
18	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
18	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	F	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	F	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	F	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	G	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
18	G	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
18	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	H	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	J	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	J	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
18	K	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	K	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
18	K	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		

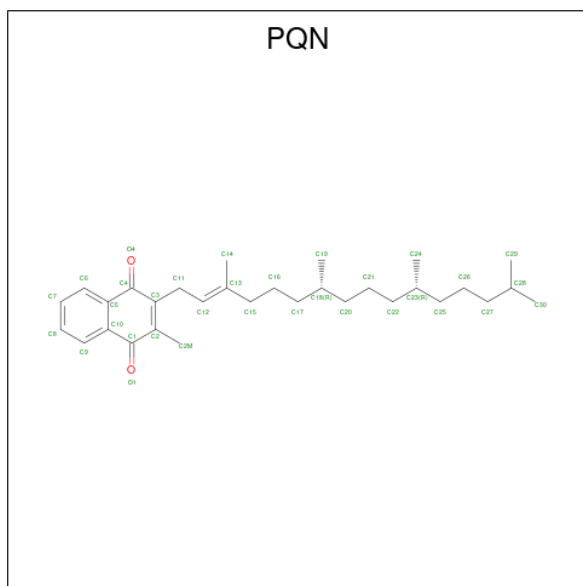
*Continued on next page...*



Continued from previous page...

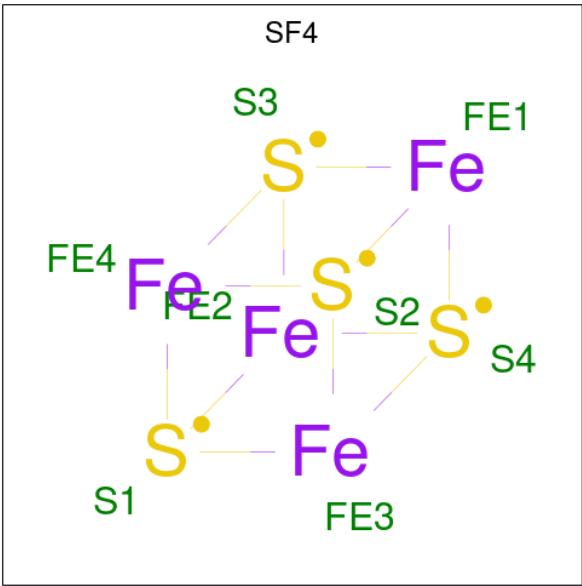
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 19 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ).



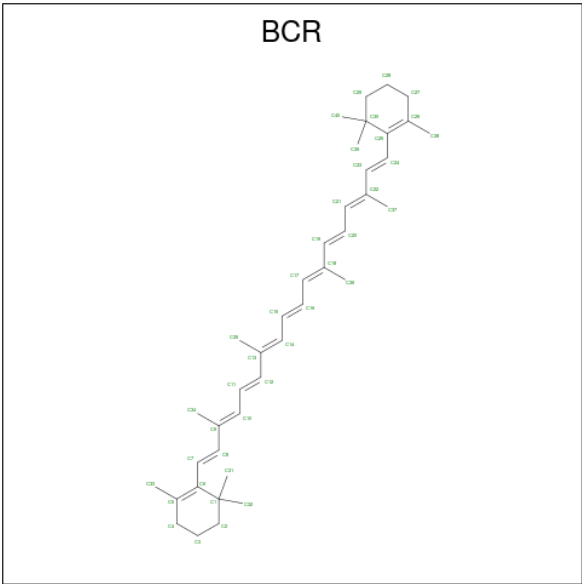
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	O			0	0
			33	31	2				
19	B	1	Total	C	O			0	0
			33	31	2				

- Molecule 20 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



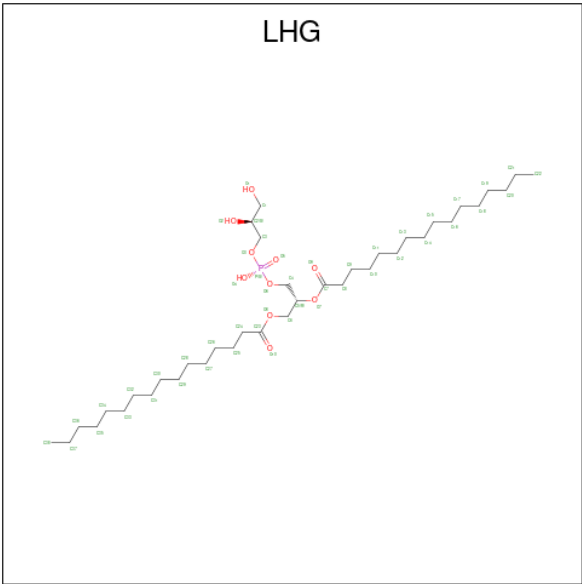
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total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

Continued on next page...

Continued from previous page...

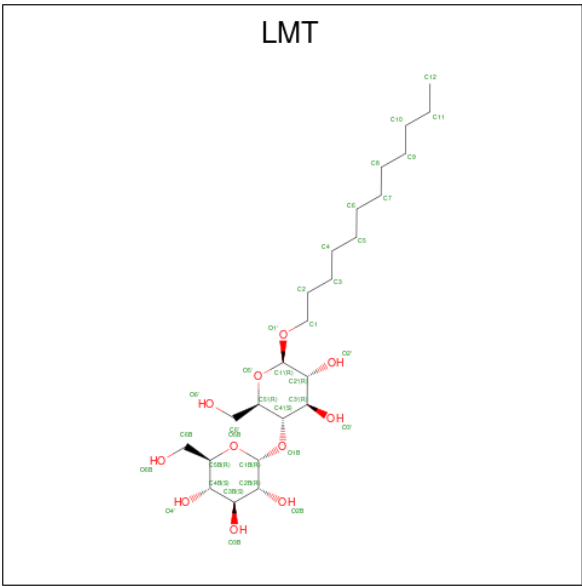
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	1	1	Total C 40 40	0	0
21	2	1	Total C 40 40	0	0
21	3	1	Total C 40 40	0	0
21	3	1	Total C 40 40	0	0
21	4	1	Total C 40 40	0	0

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



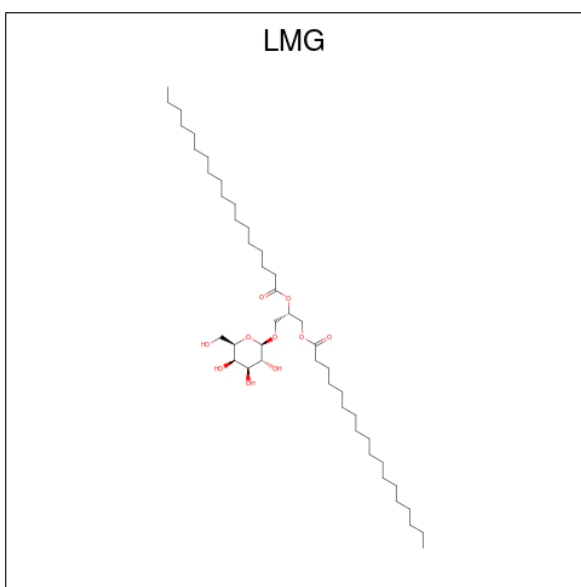
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C O P 49 38 10 1	0	0
22	A	1	Total C O P 40 29 10 1	0	0
22	B	1	Total C O P 21 10 10 1	0	0
22	B	1	Total C O P 49 38 10 1	0	0
22	1	1	Total C O P 49 38 10 1	0	0
22	2	1	Total C O P 35 24 10 1	0	0

- Molecule 23 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			35	24	11		
23	B	1	Total	C	O	0	0
			35	24	11		
23	B	1	Total	C	O	0	0
			32	21	11		
23	B	1	Total	C	O	0	0
			31	20	11		
23	G	1	Total	C	O	0	0
			35	24	11		
23	G	1	Total	C	O	0	0
			31	20	11		
23	J	1	Total	C	O	0	0
			25	14	11		
23	2	1	Total	C	O	0	0
			35	24	11		
23	4	1	Total	C	O	0	0
			35	24	11		

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



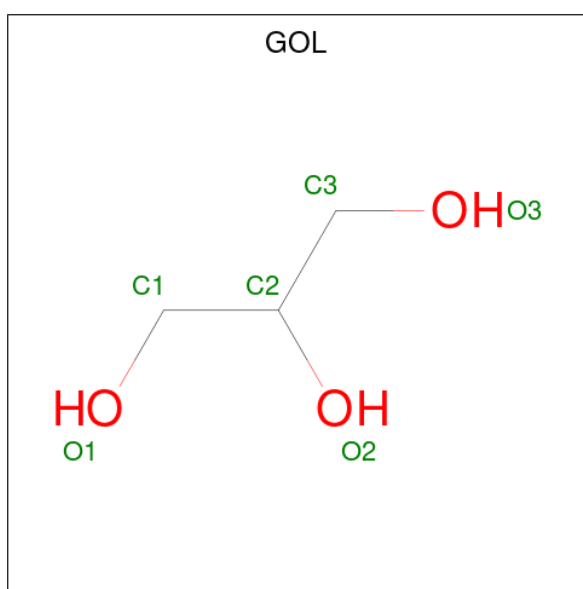
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	A	1	Total	C	O	0	0
			50	40	10		
24	B	1	Total	C	O	0	0
			35	25	10		
24	B	1	Total	C	O	0	0
			33	23	10		
24	B	1	Total	C	O	0	0
			13	7	6		
24	F	1	Total	C	O	0	0
			47	37	10		
24	F	1	Total	C	O	0	0
			36	26	10		
24	F	1	Total	C	O	0	0
			34	24	10		
24	G	1	Total	C	O	0	0
			25	15	10		
24	J	1	Total	C	O	0	0
			30	20	10		
24	1	1	Total	C	O	0	0
			49	39	10		
24	1	1	Total	C	O	0	0
			46	36	10		
24	2	1	Total	C	O	0	0
			13	7	6		
24	2	1	Total	C	O	0	0
			13	7	6		
24	2	1	Total	C	O	0	0
			25	15	10		

*Continued on next page...*

Continued from previous page...

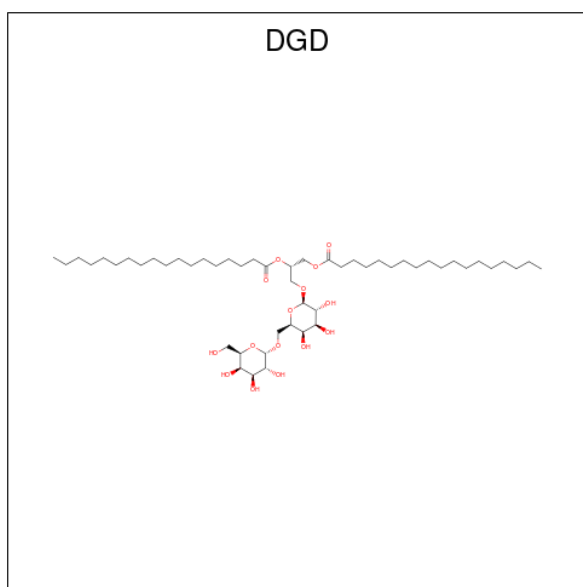
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	2	1	Total	C	O	0	0
			36	26	10		
24	2	1	Total	C	O	0	0
			13	7	6		
24	2	1	Total	C	O	0	0
			13	7	6		
24	4	1	Total	C	O	0	0
			13	7	6		

- Molecule 25 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	O	0	0
			6	3	3		
25	4	1	Total	C	O	0	0
			6	3	3		

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



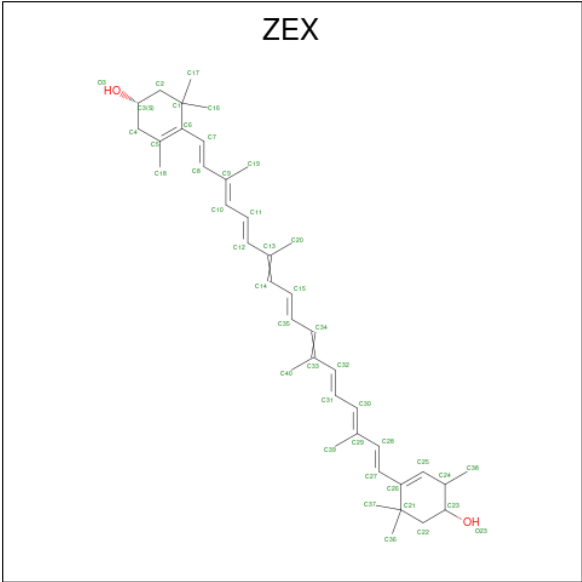
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	B	1	Total	C	O	0	0
			61	46	15		
26	F	1	Total	C	O	0	0
			57	42	15		
26	J	1	Total	C	O	0	0
			58	43	15		
26	1	1	Total	C	O	0	0
			35	26	9		
26	2	1	Total	C	O	0	0
			51	36	15		

- Molecule 27 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	B	1	Total	Ca	0	0
			1	1		
27	3	1	Total	Ca	0	0
			1	1		

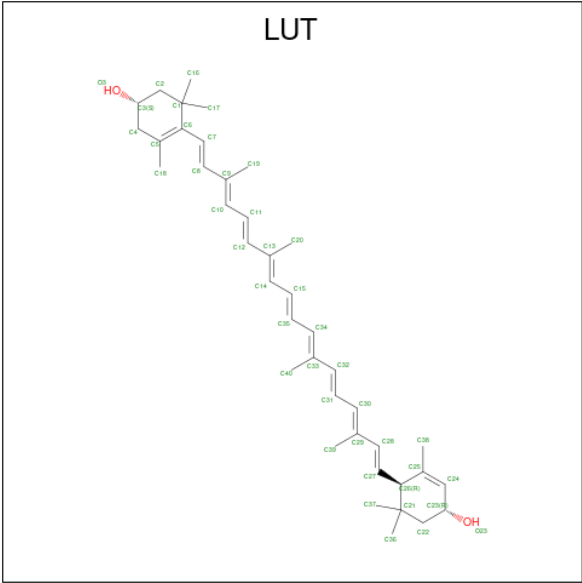
- Molecule 28 is (1R,2S)-4-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl]-2,5,5-trimethylcyclohex-3-en-1-ol (CCD ID: ZEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).





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

- Molecule 29 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



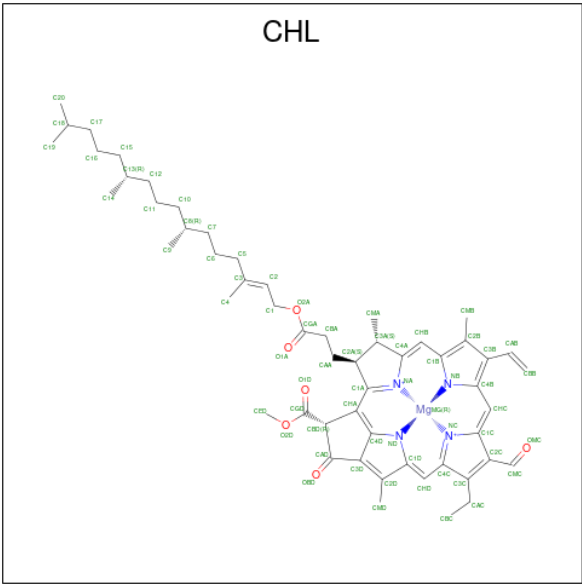
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	J	1	Total	C	O	0	0
			42	40	2		
29	1	1	Total	C	O	0	0
			42	40	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	1	1	Total	C	O	0	0
			42	40	2		
29	2	1	Total	C	O	0	0
			42	40	2		
29	3	1	Total	C	O	0	0
			42	40	2		
29	3	1	Total	C	O	0	0
			42	40	2		
29	4	1	Total	C	O	0	0
			42	40	2		

- Molecule 30 is CHLOROPHYLL B (CCD ID: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>).



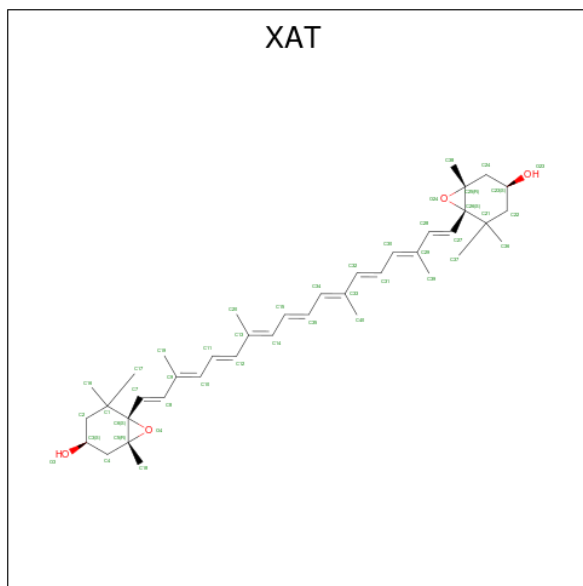
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	1	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
30	1	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
30	2	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
30	2	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
30	2	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
30	2	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	2	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
30	3	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
30	3	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
30	3	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
30	3	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
30	4	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
30	4	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
30	4	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
30	4	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
30	4	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
30	4	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		

- Molecule 31 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: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	2	1	Total 44	C 40	O 4	0	0
31	4	1	Total 44	C 40	O 4	0	0

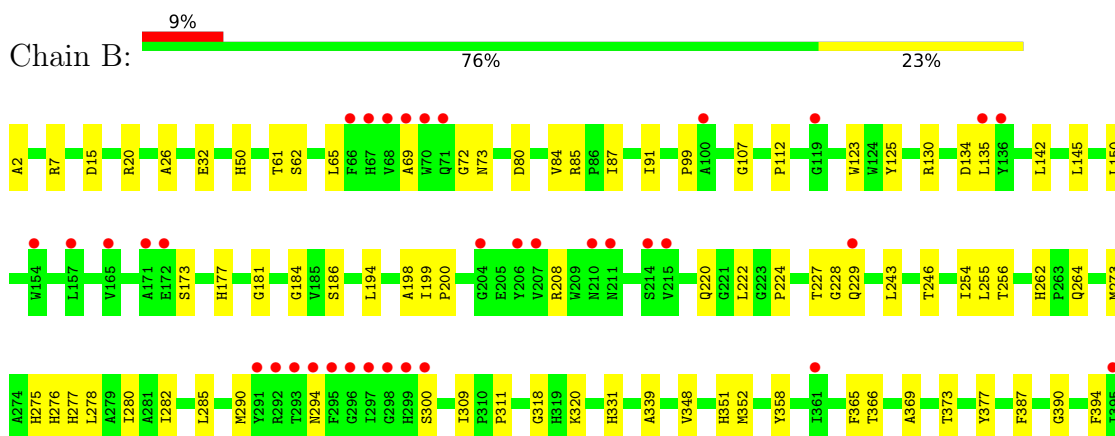
### 3 Residue-property plots

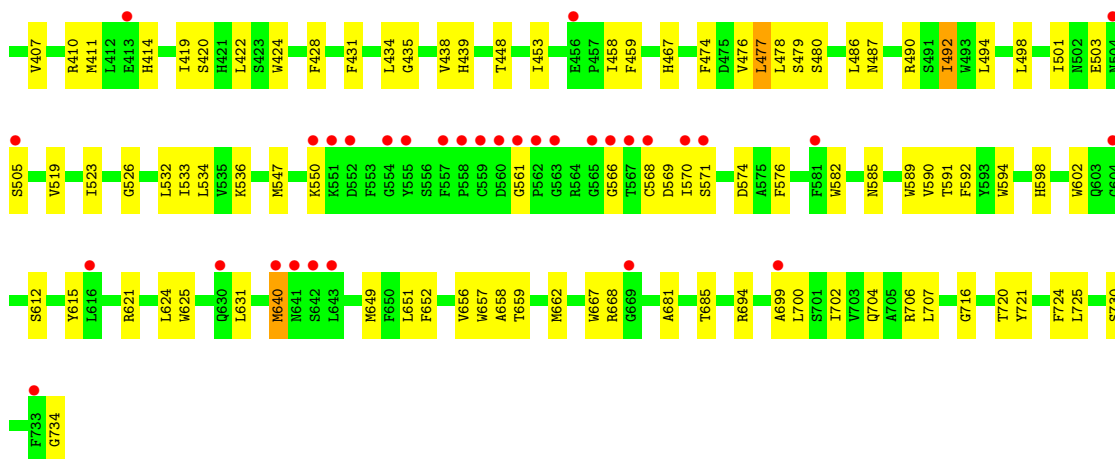
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

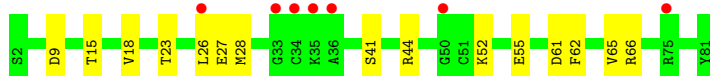
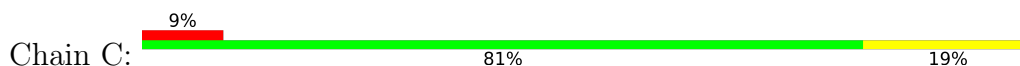


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

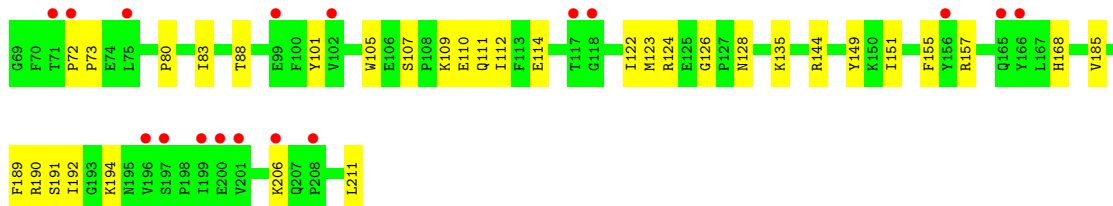
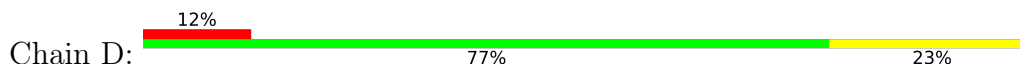




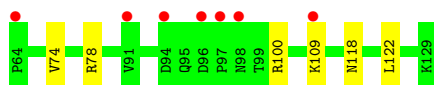
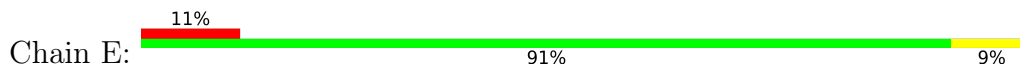
• Molecule 3: Photosystem I iron-sulfur center



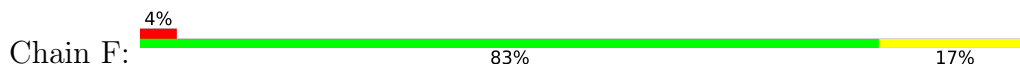
• Molecule 4: Psad



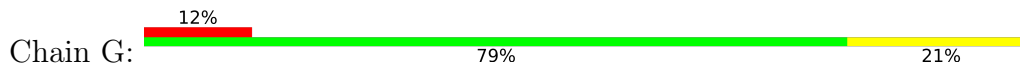
• Molecule 5: Psae

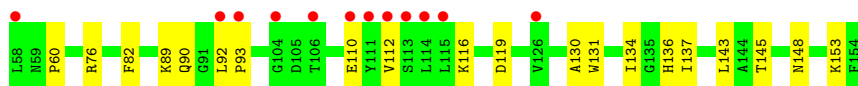


• Molecule 6: Photosystem I reaction center subunit III

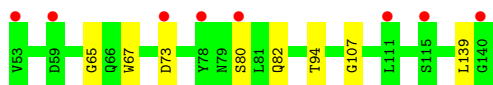
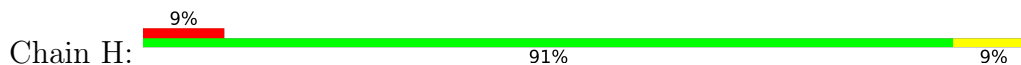


• Molecule 7: Psag

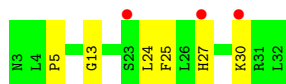
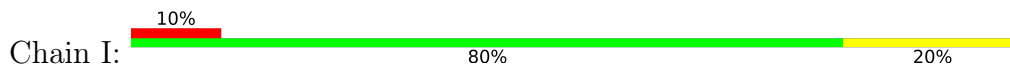




- Molecule 8: Photosystem I reaction center subunit VI



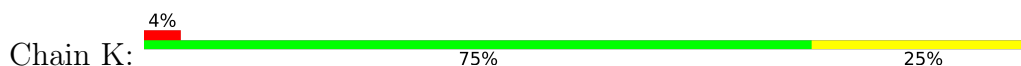
- Molecule 9: Photosystem I reaction center subunit VIII



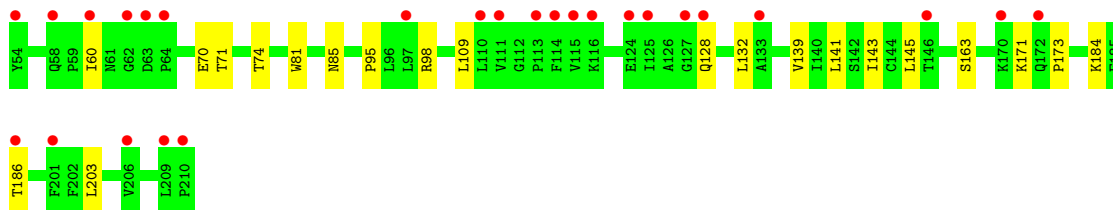
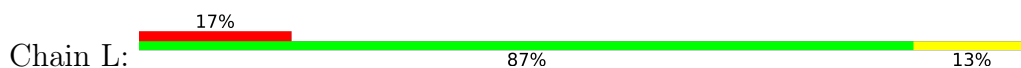
- Molecule 10: Photosystem I reaction center subunit IX



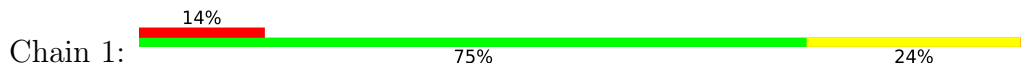
- Molecule 11: Photosystem I reaction center subunit X psaK

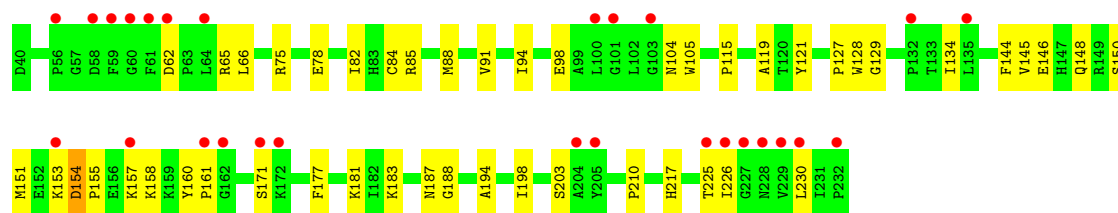


- Molecule 12: PsaL domain-containing protein

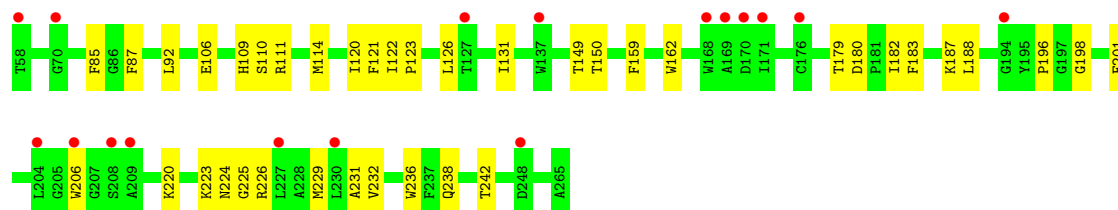
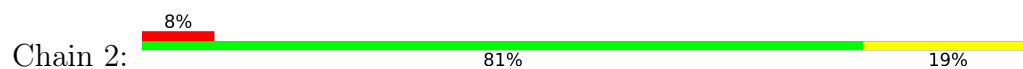


- Molecule 13: Lhca1

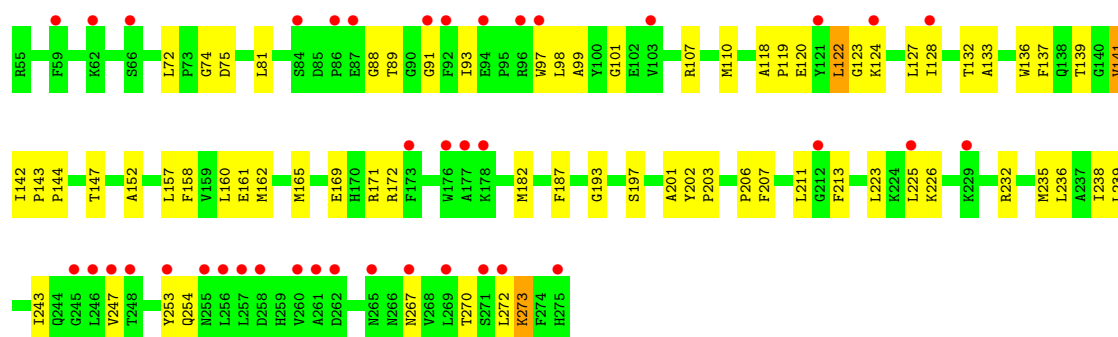




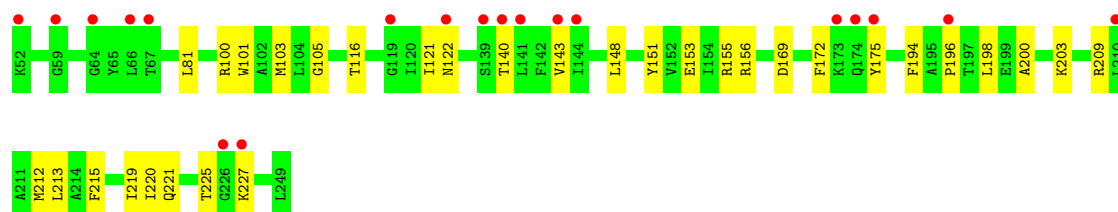
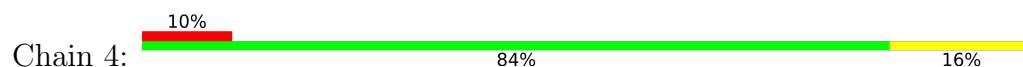
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



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



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	190.20Å 201.79Å 213.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 3.00 49.63 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.7 (49.63-3.00) 91.6 (49.63-3.00)	Depositor EDS
$R_{merge}$	0.33	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.04 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.239 , 0.270 0.239 , 0.269	Depositor DCC
$R_{free}$ test set	3337 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	96.1	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 41.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	37423	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, CHL, DGD, BCR, LHG, CA, CL0, PQN, GOL, CLA, ZEX, XAT, SF4, LMT, LUT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.12	0/6057	0.29	0/8264
2	B	0.10	0/6069	0.27	0/8286
3	C	0.11	0/625	0.32	0/846
4	D	0.10	0/1163	0.31	0/1572
5	E	0.10	0/540	0.32	0/734
6	F	0.10	0/1234	0.27	0/1670
7	G	0.08	0/776	0.23	0/1054
8	H	0.09	0/693	0.26	0/942
9	I	0.10	0/238	0.26	0/324
10	J	0.10	0/349	0.27	0/476
11	K	0.09	0/564	0.29	0/763
12	L	0.09	0/1207	0.26	0/1651
13	1	0.10	0/1558	0.27	0/2125
14	2	0.10	0/1679	0.26	0/2302
15	3	0.10	0/1760	0.29	0/2390
16	4	0.09	0/1608	0.25	0/2191
All	All	0.10	0/26120	0.28	0/35590

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5858	0	5717	143	0
2	B	5857	0	5653	141	0
3	C	612	0	591	13	0
4	D	1132	0	1141	19	0
5	E	528	0	528	6	0
6	F	1206	0	1231	20	0
7	G	757	0	743	16	0
8	H	673	0	667	7	0
9	I	232	0	253	5	0
10	J	338	0	345	13	0
11	K	558	0	587	18	0
12	L	1174	0	1183	17	0
13	1	1508	0	1489	43	0
14	2	1620	0	1554	33	0
15	3	1706	0	1659	62	0
16	4	1559	0	1524	28	0
17	A	65	0	72	7	0
18	1	608	0	562	37	0
18	2	572	0	538	34	0
18	3	531	0	456	29	0
18	4	516	0	488	19	0
18	A	2543	0	2661	203	0
18	B	2480	0	2602	191	0
18	F	195	0	215	12	0
18	G	166	0	152	5	0
18	H	60	0	59	6	0
18	J	115	0	110	8	0
18	K	199	0	158	16	0
18	L	215	0	183	7	0
19	A	33	0	46	5	0
19	B	33	0	46	2	0
20	A	8	0	0	0	0
20	C	16	0	0	1	0
21	1	40	0	53	3	0
21	2	40	0	53	10	0
21	3	80	0	106	6	0
21	4	40	0	52	7	0
21	A	240	0	317	33	0
21	B	240	0	317	27	0
21	F	80	0	105	11	0
21	G	40	0	53	4	0
21	I	80	0	105	4	0
21	J	40	0	53	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	K	40	0	53	2	0
21	L	120	0	159	7	0
22	1	49	0	74	3	0
22	2	35	0	40	1	0
22	A	89	0	127	16	0
22	B	70	0	86	8	0
23	2	35	0	46	1	0
23	4	35	0	46	0	0
23	A	35	0	45	0	0
23	B	98	0	118	3	0
23	G	66	0	80	3	0
23	J	25	0	22	0	0
24	1	95	0	136	9	0
24	2	113	0	106	5	0
24	4	13	0	11	0	0
24	A	50	0	73	6	0
24	B	81	0	87	2	0
24	F	117	0	147	5	0
24	G	25	0	20	1	0
24	J	30	0	30	0	0
25	4	6	0	8	0	0
25	A	6	0	8	1	0
26	1	35	0	39	0	0
26	2	51	0	60	5	0
26	B	61	0	83	8	0
26	F	57	0	75	0	0
26	J	58	0	77	4	0
27	3	1	0	0	0	0
27	B	1	0	0	0	0
28	F	42	0	56	3	0
29	1	84	0	110	14	0
29	2	42	0	55	5	0
29	3	84	0	110	12	0
29	4	42	0	55	2	0
29	J	42	0	55	9	0
30	1	108	0	87	10	0
30	2	272	0	224	19	0
30	3	215	0	172	23	0
30	4	314	0	243	20	0
31	2	44	0	56	7	0
31	4	44	0	56	6	0
All	All	37423	0	37562	1032	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 14.

All (1032) 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)
11:K:61:LEU:HB3	18:K:1403:CLA:HAB	1.45	0.97
31:2:304:XAT:H8	18:2:311:CLA:HBB1	1.50	0.94
1:A:401:TRP:CD1	18:A:826:CLA:HAB	2.10	0.87
18:B:807:CLA:H152	18:B:829:CLA:HBB2	1.58	0.85
24:1:5001:LMG:H122	30:1:5016:CHL:HBA1	1.61	0.83
18:A:853:CLA:H141	21:L:303:BCR:H17C	1.62	0.82
2:B:582:TRP:CH2	18:B:801:CLA:HAB	2.17	0.79
29:3:304:LUT:H32	30:3:310:CHL:HAB	1.64	0.79
14:2:159:PHE:HB3	21:2:305:BCR:H16C	1.65	0.78
1:A:401:TRP:HD1	18:A:826:CLA:HAB	1.48	0.77
24:2:301:LMG:HC2	24:2:302:LMG:HC5	1.68	0.76
14:2:232:VAL:HG11	31:2:304:XAT:H12	1.68	0.76
12:L:145:LEU:HB3	12:L:186:THR:HG22	1.68	0.76
29:J:1105:LUT:H181	29:J:1105:LUT:H8	1.68	0.75
18:B:805:CLA:HBC1	26:B:855:DGD:HA92	1.69	0.75
4:D:83:ILE:HB	4:D:122:ILE:HB	1.68	0.75
21:B:843:BCR:HC31	21:B:845:BCR:H333	1.68	0.74
13:1:85:ARG:HB3	18:1:5006:CLA:HBC2	1.69	0.74
2:B:311:PRO:HG2	22:B:848:LHG:HC32	1.69	0.73
18:F:303:CLA:HAB	24:F:306:LMG:H382	1.71	0.73
1:A:310:PHE:HE1	18:A:819:CLA:HAB	1.53	0.73
18:A:804:CLA:H61	21:A:844:BCR:H24C	1.68	0.73
18:B:812:CLA:HHC	18:B:812:CLA:HBB1	1.72	0.72
18:B:801:CLA:HED2	18:B:803:CLA:H71	1.71	0.72
18:A:803:CLA:HBB1	18:A:810:CLA:H122	1.69	0.72
1:A:204:ASN:HB3	18:A:818:CLA:HMD2	1.71	0.72
15:3:239:LEU:HD13	18:3:311:CLA:HBB2	1.70	0.72
1:A:270:PHE:HA	18:K:1401:CLA:HAC2	1.72	0.72
3:C:18:VAL:HG22	3:C:26:LEU:HB3	1.71	0.72
29:2:303:LUT:H362	18:2:313:CLA:HBC1	1.70	0.71
15:3:110:MET:SD	18:3:307:CLA:HAB	2.31	0.71
18:B:823:CLA:HHC	18:B:823:CLA:HBB1	1.71	0.70
2:B:656:VAL:HG22	18:B:840:CLA:HMB2	1.72	0.70
30:1:5014:CHL:HHC	30:1:5014:CHL:HBB1	1.73	0.70
18:A:814:CLA:HHC	18:A:814:CLA:HBB1	1.72	0.70
10:J:34:PRO:O	26:J:1106:DGD:O2D	2.10	0.69
18:A:822:CLA:HMA1	18:A:840:CLA:HAB	1.72	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:25:PHE:HB2	21:I:102:BCR:H14C	1.74	0.69
18:B:830:CLA:H143	26:B:855:DGD:HAW1	1.74	0.69
18:A:802:CLA:H111	21:A:847:BCR:H23C	1.74	0.69
18:A:822:CLA:HHC	18:A:822:CLA:HBB1	1.73	0.69
14:2:120:ILE:HG13	31:2:304:XAT:H163	1.72	0.69
29:3:303:LUT:H31	21:3:306:BCR:H363	1.75	0.69
29:1:5003:LUT:H30	18:1:5006:CLA:H52	1.74	0.68
18:A:852:CLA:H122	21:B:802:BCR:H352	1.75	0.68
2:B:2:ALA:HB1	2:B:7:ARG:HE	1.57	0.68
2:B:255:LEU:HD11	18:B:816:CLA:HBC1	1.74	0.68
2:B:615:TYR:OH	2:B:621:ARG:NH2	2.26	0.68
18:2:313:CLA:HBA1	15:3:160:LEU:HD13	1.76	0.68
18:B:834:CLA:H143	18:B:835:CLA:H71	1.75	0.68
13:1:88:MET:SD	18:1:5006:CLA:HAB	2.34	0.68
2:B:373:THR:HG23	2:B:591:THR:HG21	1.75	0.68
18:A:805:CLA:HED1	18:A:828:CLA:H2	1.75	0.67
18:A:813:CLA:C2B	21:A:843:BCR:H10C	2.24	0.67
16:4:151:TYR:HB2	30:4:302:CHL:H11	1.75	0.67
21:A:845:BCR:H24C	24:A:851:LMG:H362	1.75	0.67
21:A:847:BCR:H16C	18:B:801:CLA:H122	1.76	0.67
6:F:196:ILE:HD12	6:F:197:ILE:HG13	1.76	0.66
15:3:139:THR:HG23	30:3:312:CHL:HED2	1.76	0.66
18:2:308:CLA:HMA1	18:2:313:CLA:HBC3	1.76	0.66
18:4:310:CLA:HMA1	30:4:316:CHL:HBC3	1.78	0.66
18:A:810:CLA:H202	22:A:848:LHG:H211	1.78	0.66
18:A:820:CLA:H62	18:A:821:CLA:H12	1.76	0.66
18:4:306:CLA:H12	18:4:306:CLA:HMA1	1.77	0.66
1:A:492:ILE:HD13	18:A:832:CLA:HBB1	1.77	0.65
2:B:99:PRO:HB2	2:B:640:MET:HE2	1.78	0.65
21:4:301:BCR:H403	21:4:301:BCR:H23C	1.77	0.65
18:K:1404:CLA:HHC	18:K:1404:CLA:HBB1	1.77	0.65
14:2:110:SER:HB3	14:2:225:GLY:HA3	1.79	0.65
24:F:307:LMG:H131	24:F:307:LMG:HC91	1.78	0.65
22:1:5019:LHG:H171	30:4:318:CHL:HED1	1.78	0.65
15:3:160:LEU:HD21	18:3:318:CLA:HED3	1.77	0.65
7:G:131:TRP:HA	7:G:134:ILE:HD12	1.78	0.64
1:A:453:LEU:HB3	1:A:547:PHE:HB2	1.78	0.64
18:A:806:CLA:HMB2	21:J:1104:BCR:H23C	1.80	0.64
18:B:826:CLA:H191	18:B:841:CLA:H122	1.78	0.64
21:A:846:BCR:HC7	18:K:1402:CLA:H122	1.79	0.64
18:B:832:CLA:HBC2	18:B:838:CLA:HMC2	1.78	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:305:BCR:H333	18:4:311:CLA:HMC2	1.79	0.64
30:2:318:CHL:HHC	30:2:318:CHL:HBB1	1.80	0.64
18:A:820:CLA:H2	24:A:851:LMG:H162	1.79	0.64
18:B:826:CLA:H51	18:B:837:CLA:HBA1	1.79	0.64
18:B:841:CLA:HBA1	22:B:848:LHG:HC42	1.78	0.64
1:A:37:PRO:HA	18:J:1101:CLA:HBC1	1.80	0.64
18:1:5010:CLA:HBC1	30:1:5014:CHL:HBB2	1.78	0.64
18:B:811:CLA:H92	12:L:132:LEU:HB3	1.80	0.64
1:A:602:LEU:HD21	18:A:828:CLA:HBC1	1.79	0.63
1:A:462:ILE:HG22	18:A:831:CLA:HBC2	1.80	0.63
13:1:154:ASP:H	13:1:155:PRO:HA	1.64	0.63
1:A:330:ILE:O	1:A:334:HIS:ND1	2.32	0.63
21:3:306:BCR:H10C	30:3:316:CHL:O1A	1.99	0.63
15:3:247:VAL:HA	15:3:273:LYS:HG3	1.81	0.63
30:3:313:CHL:HHC	30:3:313:CHL:HBB1	1.81	0.63
18:A:806:CLA:HAB	21:J:1104:BCR:H271	1.80	0.62
18:B:836:CLA:HMB1	18:B:838:CLA:HED1	1.80	0.62
1:A:434:ARG:HH11	18:A:829:CLA:HED2	1.63	0.62
2:B:721:TYR:HB2	18:B:803:CLA:HED3	1.81	0.62
1:A:173:VAL:HG21	18:A:813:CLA:H91	1.80	0.62
18:B:832:CLA:H2	21:F:305:BCR:H372	1.82	0.62
1:A:76:ARG:HD2	1:A:190:ALA:HB1	1.82	0.62
2:B:576:PHE:HE1	18:B:830:CLA:HAC2	1.65	0.62
13:1:75:ARG:NH1	18:1:5010:CLA:O1A	2.33	0.62
1:A:126:ILE:HG13	1:A:127:VAL:HG13	1.81	0.61
22:A:848:LHG:H161	18:J:1101:CLA:HMB1	1.81	0.61
14:2:114:MET:SD	18:2:306:CLA:HAB	2.40	0.61
21:4:301:BCR:H10C	30:4:317:CHL:HBB2	1.82	0.61
2:B:65:LEU:HD11	21:B:845:BCR:H291	1.82	0.61
18:B:806:CLA:H93	18:B:814:CLA:H2	1.83	0.61
18:B:831:CLA:HAB	18:B:838:CLA:CBB	2.29	0.61
30:1:5016:CHL:HHC	30:1:5016:CHL:HBB1	1.81	0.61
2:B:309:ILE:HG22	2:B:318:GLY:HA3	1.83	0.61
30:2:315:CHL:HAB	30:2:318:CHL:HBB2	1.83	0.61
30:4:318:CHL:HHC	30:4:318:CHL:HBB1	1.81	0.61
1:A:687:ALA:HB3	18:A:802:CLA:HBB2	1.83	0.61
18:B:807:CLA:H43	26:B:855:DGD:HB61	1.83	0.61
14:2:121:PHE:HE2	14:2:231:ALA:HB1	1.66	0.61
26:2:327:DGD:HA31	16:4:213:LEU:HD12	1.82	0.61
15:3:202:TYR:HB3	18:3:307:CLA:HED3	1.82	0.61
15:3:236:LEU:HG	30:3:310:CHL:HMC	1.82	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:ALA:HB2	2:B:135:LEU:HB2	1.83	0.60
14:2:162:TRP:HH2	21:2:305:BCR:H321	1.65	0.60
2:B:410:ARG:HH22	24:B:850:LMG:HC61	1.66	0.60
18:1:5013:CLA:HED1	16:4:140:THR:HG23	1.82	0.60
18:2:326:CLA:HBC3	26:2:327:DGD:HG32	1.83	0.60
1:A:375:HIS:ND1	18:A:816:CLA:OBD	2.34	0.60
1:A:226:SER:O	1:A:230:ASN:HB2	2.01	0.60
18:A:819:CLA:H111	21:A:845:BCR:H10C	1.82	0.60
18:B:818:CLA:H142	18:B:818:CLA:HBB1	1.81	0.60
30:4:302:CHL:HHC	30:4:302:CHL:HBB1	1.84	0.60
18:B:818:CLA:HBA2	18:B:827:CLA:HBB2	1.83	0.60
12:L:85:ASN:HB3	18:L:304:CLA:HAC1	1.83	0.60
18:2:310:CLA:H12	24:2:321:LMG:HC72	1.82	0.60
1:A:593:SER:OG	1:A:596:ASP:OD1	2.18	0.60
18:A:824:CLA:HAB	21:A:846:BCR:C23	2.32	0.60
2:B:228:GLY:HA3	7:G:143:LEU:HB3	1.83	0.60
1:A:321:TRP:HD1	11:K:91:LEU:HD22	1.66	0.60
18:B:812:CLA:HBD	23:G:1605:LMT:H1'	1.84	0.60
30:2:316:CHL:HHC	30:2:316:CHL:HBB1	1.82	0.60
2:B:582:TRP:HH2	18:B:801:CLA:HAB	1.67	0.60
21:B:843:BCR:H332	21:B:844:BCR:HC31	1.83	0.60
18:B:837:CLA:H52	21:F:305:BCR:H343	1.84	0.59
30:2:319:CHL:HHC	30:2:319:CHL:HBB1	1.84	0.59
18:H:1701:CLA:H121	12:L:81:TRP:HE1	1.66	0.59
18:2:326:CLA:HHC	18:2:326:CLA:HBB1	1.84	0.59
2:B:458:ILE:HG21	6:F:151:SER:HB3	1.83	0.59
2:B:707:LEU:HD22	26:B:855:DGD:HB21	1.85	0.59
18:B:819:CLA:H3A	18:B:819:CLA:CGA	2.32	0.59
4:D:114:GLU:O	4:D:144:ARG:NH2	2.36	0.59
16:4:203:LYS:HD2	18:4:306:CLA:HAA2	1.85	0.59
18:B:815:CLA:H2	21:B:845:BCR:H362	1.84	0.59
13:1:154:ASP:HB3	13:1:157:LYS:H	1.66	0.59
15:3:152:ALA:HB3	15:3:157:LEU:HG	1.85	0.59
2:B:181:GLY:HA3	18:B:814:CLA:HBB1	1.85	0.59
1:A:308:ILE:HD11	21:A:855:BCR:H341	1.83	0.58
18:A:837:CLA:HBB1	18:A:837:CLA:HMB1	1.85	0.58
18:B:826:CLA:HED2	18:B:827:CLA:HBD	1.85	0.58
29:4:303:LUT:H373	18:4:305:CLA:H51	1.85	0.58
18:H:1701:CLA:HAB	21:L:307:BCR:H321	1.84	0.58
18:A:839:CLA:HAC1	19:A:841:PQN:H171	1.85	0.58
21:B:802:BCR:H362	18:B:804:CLA:H122	1.84	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:317:CHL:HHC	30:4:317:CHL:HBB1	1.85	0.58
1:A:360:ILE:HD11	21:A:845:BCR:HC7	1.86	0.58
12:L:71:THR:H	12:L:74:THR:HG1	1.49	0.58
13:1:91:VAL:HG11	29:1:5003:LUT:H10	1.83	0.58
1:A:245:PRO:HG3	18:A:813:CLA:HED2	1.84	0.58
18:A:822:CLA:H161	22:A:849:LHG:H161	1.84	0.58
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.86	0.58
2:B:150:LEU:HD21	22:B:849:LHG:H371	1.86	0.58
18:F:303:CLA:H3A	21:F:305:BCR:H333	1.85	0.58
18:3:317:CLA:H12	18:3:319:CLA:CBB	2.33	0.58
2:B:73:ASN:ND2	2:B:107:GLY:O	2.30	0.58
18:B:810:CLA:H112	18:B:828:CLA:H192	1.85	0.58
1:A:684:PHE:CG	21:A:847:BCR:H363	2.39	0.58
18:A:829:CLA:HMA2	12:L:71:THR:HG21	1.84	0.58
4:D:80:PRO:HB3	4:D:124:ARG:HH21	1.68	0.58
12:L:81:TRP:O	12:L:85:ASN:ND2	2.28	0.58
2:B:387:PHE:CZ	18:B:826:CLA:HAB	2.39	0.57
1:A:21:LEU:HA	15:3:88:GLY:HA3	1.87	0.57
18:B:834:CLA:HMB1	18:B:834:CLA:HBB1	1.86	0.57
12:L:95:PRO:HA	12:L:98:ARG:HD3	1.86	0.57
1:A:141:ARG:HE	25:A:854:GOL:H11	1.70	0.57
1:A:567:ARG:NH2	4:D:88:THR:O	2.37	0.57
2:B:32:GLU:OE2	2:B:331:HIS:NE2	2.37	0.57
2:B:438:VAL:HG22	18:B:801:CLA:H42	1.86	0.57
2:B:657:TRP:CD2	18:B:803:CLA:HMA2	2.40	0.57
18:2:310:CLA:H192	30:2:315:CHL:H8	1.86	0.57
2:B:254:ILE:HG13	2:B:255:LEU:HG	1.85	0.57
2:B:668:ARG:NH1	2:B:699:ALA:O	2.38	0.57
15:3:193:GLY:HA2	15:3:206:PRO:HD2	1.86	0.57
18:A:813:CLA:C1B	21:A:843:BCR:H10C	2.35	0.57
18:B:819:CLA:H193	18:B:820:CLA:H143	1.85	0.57
14:2:126:LEU:HD23	14:2:131:ILE:HG21	1.86	0.57
1:A:372:VAL:HG22	18:A:817:CLA:H42	1.87	0.57
18:B:839:CLA:H161	21:I:101:BCR:H353	1.86	0.57
12:L:163:SER:HB3	12:L:173:PRO:HG3	1.87	0.57
13:1:128:TRP:HD1	13:1:134:ILE:HD11	1.70	0.57
1:A:604:TRP:CH2	18:A:852:CLA:HAB	2.40	0.56
2:B:486:LEU:HD12	2:B:494:LEU:HD13	1.86	0.56
6:F:78:ASP:N	6:F:82:LEU:O	2.38	0.56
2:B:428:PHE:CE1	18:B:837:CLA:HAB	2.40	0.56
13:1:98:GLU:HG2	13:1:104:ASN:HA	1.86	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:315:CHL:CAB	30:2:318:CHL:HBB2	2.35	0.56
30:4:314:CHL:HHC	30:4:314:CHL:HBB1	1.87	0.56
18:B:826:CLA:HAA2	18:B:827:CLA:OBD	2.05	0.56
2:B:276:HIS:HB2	18:B:818:CLA:C1B	2.36	0.56
22:B:848:LHG:O3	22:B:848:LHG:O1	2.24	0.56
2:B:681:ALA:O	2:B:685:THR:OG1	2.20	0.56
30:4:316:CHL:HHC	30:4:316:CHL:HBB1	1.88	0.56
1:A:653:LEU:HD22	2:B:651:LEU:HD21	1.88	0.56
18:B:824:CLA:CMD	18:B:825:CLA:HAB	2.35	0.56
10:J:1:MET:HE3	10:J:5:LYS:HE3	1.86	0.56
18:A:802:CLA:H92	2:B:431:PHE:HE1	1.69	0.56
18:A:816:CLA:HAC1	18:A:832:CLA:H42	1.86	0.56
2:B:576:PHE:CE1	18:B:830:CLA:HAC2	2.41	0.56
2:B:351:HIS:HB3	18:B:818:CLA:HED2	1.87	0.55
18:B:821:CLA:HAB	21:B:843:BCR:H351	1.88	0.55
1:A:201:SER:O	1:A:205:HIS:ND1	2.21	0.55
2:B:434:LEU:O	2:B:438:VAL:HG23	2.06	0.55
17:A:801:CL0:H12	18:B:801:CLA:CAD	2.36	0.55
18:A:838:CLA:H161	10:J:18:TRP:HE3	1.72	0.55
18:B:805:CLA:HAB	18:B:807:CLA:CAD	2.37	0.55
18:B:824:CLA:HBA2	21:B:846:BCR:H16C	1.86	0.55
1:A:80:SER:OG	1:A:186:TYR:HB2	2.07	0.55
2:B:387:PHE:HZ	18:B:826:CLA:HAB	1.71	0.55
18:A:811:CLA:H8	18:A:811:CLA:HBB1	1.88	0.55
3:C:62:PHE:HD1	4:D:192:ILE:HD13	1.71	0.55
18:B:841:CLA:HBB2	13:1:66:LEU:HD13	1.88	0.55
2:B:273:MET:O	2:B:277:HIS:ND1	2.31	0.55
18:A:828:CLA:H91	22:A:848:LHG:H331	1.89	0.55
18:A:837:CLA:H92	21:F:304:BCR:H16C	1.88	0.55
18:A:853:CLA:H111	18:B:839:CLA:H102	1.87	0.55
30:2:314:CHL:HHC	30:2:314:CHL:HBB1	1.88	0.55
1:A:512:SER:H	1:A:515:TRP:HD1	1.53	0.55
14:2:226:ARG:HA	14:2:229:MET:HE3	1.88	0.55
18:3:319:CLA:H2A	18:3:319:CLA:HED2	1.88	0.55
1:A:205:HIS:CG	18:A:812:CLA:HMC1	2.42	0.54
18:A:837:CLA:HED3	2:B:420:SER:HB2	1.88	0.54
14:2:121:PHE:CE2	14:2:231:ALA:HB1	2.42	0.54
18:A:804:CLA:H203	18:A:812:CLA:H62	1.89	0.54
16:4:212:MET:SD	18:4:308:CLA:HAB	2.47	0.54
1:A:72:GLU:O	1:A:76:ARG:HG3	2.08	0.54
18:A:833:CLA:H2	18:K:1402:CLA:HBA2	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:839:CLA:H111	18:B:840:CLA:H13	1.90	0.54
12:L:60:ILE:HA	12:L:70:GLU:HG3	1.89	0.54
24:2:322:LMG:HC71	24:2:322:LMG:H122	1.89	0.54
18:A:822:CLA:H18	21:A:845:BCR:H363	1.89	0.54
18:A:853:CLA:H71	18:B:839:CLA:H43	1.90	0.54
18:3:317:CLA:H12	18:3:319:CLA:HBB2	1.90	0.54
10:J:16:THR:HG22	18:J:1101:CLA:H8	1.90	0.54
18:B:803:CLA:HMB1	18:B:803:CLA:HBB1	1.90	0.54
18:B:809:CLA:O1A	18:B:828:CLA:HBD	2.08	0.54
18:B:824:CLA:HMD3	18:B:825:CLA:HAB	1.89	0.54
11:K:79:THR:OG1	11:K:80:ALA:N	2.39	0.54
22:B:849:LHG:H201	22:B:849:LHG:H361	1.89	0.54
24:1:5020:LMG:H151	30:4:318:CHL:HMD2	1.89	0.54
18:A:806:CLA:HBA1	18:A:808:CLA:H12	1.90	0.54
18:B:822:CLA:C1D	21:B:843:BCR:H402	2.38	0.54
15:3:122:LEU:HD12	15:3:128:ILE:HB	1.90	0.54
15:3:165:MET:HG3	18:3:317:CLA:HMC2	1.90	0.54
1:A:302:HIS:HB2	18:A:816:CLA:C1B	2.38	0.53
2:B:352:MET:HE3	18:B:819:CLA:HBA1	1.90	0.53
18:B:828:CLA:CGA	18:B:828:CLA:H3A	2.38	0.53
30:2:315:CHL:HMB1	30:2:315:CHL:HBB1	1.90	0.53
15:3:211:LEU:HD12	29:3:303:LUT:H222	1.91	0.53
18:B:831:CLA:H191	24:F:306:LMG:H451	1.91	0.53
14:2:149:THR:HG21	30:2:315:CHL:HMD3	1.90	0.53
14:2:182:ILE:HD11	21:2:305:BCR:H312	1.89	0.53
18:B:801:CLA:HMB3	18:B:803:CLA:H201	1.89	0.53
18:B:815:CLA:HMB1	18:B:815:CLA:HBB1	1.91	0.53
1:A:310:PHE:CE1	18:A:819:CLA:HAB	2.39	0.53
1:A:512:SER:H	1:A:515:TRP:CD1	2.26	0.53
1:A:261:SER:HB2	1:A:280:PHE:HE2	1.72	0.53
18:A:823:CLA:HBA1	18:A:827:CLA:H191	1.91	0.53
18:B:840:CLA:HED2	26:B:855:DGD:HA52	1.90	0.53
14:2:111:ARG:NH1	30:2:316:CHL:OBD	2.40	0.53
1:A:199:VAL:HG11	18:A:823:CLA:HAC2	1.90	0.53
1:A:356:ALA:HB1	21:A:845:BCR:H312	1.91	0.53
21:A:847:BCR:H24C	18:B:833:CLA:HMC2	1.91	0.53
2:B:487:ASN:O	7:G:153:LYS:NZ	2.42	0.53
18:B:829:CLA:H142	21:B:845:BCR:H372	1.91	0.53
15:3:187:PHE:HE2	30:3:316:CHL:HBB2	1.74	0.53
18:B:811:CLA:HAB	9:I:13:GLY:HA3	1.89	0.53
18:2:312:CLA:HBB2	21:3:305:BCR:HC7	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ALA:HB2	1:A:314:GLY:HA3	1.91	0.53
18:A:802:CLA:HMD3	2:B:533:ILE:HG12	1.91	0.53
18:A:822:CLA:H12	21:A:845:BCR:H15C	1.91	0.53
18:A:852:CLA:H172	21:B:802:BCR:H343	1.91	0.53
2:B:276:HIS:CE1	2:B:280:ILE:HD13	2.44	0.53
13:1:226:ILE:HG12	13:1:230:LEU:HG	1.91	0.53
30:4:313:CHL:HHC	30:4:313:CHL:HBB1	1.91	0.53
8:H:80:SER:O	8:H:82:GLN:N	2.41	0.52
15:3:107:ARG:HB3	18:3:307:CLA:HBC3	1.89	0.52
18:A:808:CLA:HBB1	18:A:808:CLA:HMB3	1.92	0.52
2:B:125:TYR:O	2:B:130:ARG:NH1	2.38	0.52
18:2:310:CLA:H111	18:2:317:CLA:H91	1.90	0.52
30:3:316:CHL:HHC	30:3:316:CHL:HBB1	1.91	0.52
16:4:155:ARG:NH1	30:4:302:CHL:OBD	2.42	0.52
18:B:815:CLA:CHB	21:B:845:BCR:H21C	2.40	0.52
14:2:179:THR:HG22	14:2:187:LYS:HG2	1.91	0.52
1:A:124:TRP:HB3	29:J:1105:LUT:H183	1.90	0.52
1:A:195:TRP:CE2	18:A:812:CLA:HBC3	2.44	0.52
18:A:822:CLA:H8	18:A:822:CLA:H202	1.92	0.52
18:A:837:CLA:H52	21:F:304:BCR:H14C	1.92	0.52
2:B:435:GLY:HA3	18:B:833:CLA:HAB	1.92	0.52
1:A:368:LEU:HD11	18:A:817:CLA:H62	1.92	0.52
1:A:727:ILE:HD11	2:B:566:GLY:HA3	1.92	0.52
18:A:803:CLA:HAA1	18:A:810:CLA:H51	1.91	0.52
18:B:833:CLA:H122	18:F:302:CLA:H43	1.91	0.52
9:I:24:LEU:HD13	21:I:102:BCR:HC8	1.92	0.52
18:1:5009:CLA:HHD	30:4:302:CHL:HBB2	1.90	0.52
18:1:5012:CLA:HBB1	21:4:301:BCR:HC42	1.91	0.52
14:2:196:PRO:HB3	30:2:316:CHL:HBC2	1.91	0.52
13:1:153:LYS:HE3	13:1:158:LYS:HE3	1.91	0.52
30:1:5014:CHL:OMC	18:1:5017:CLA:HAB	2.10	0.52
18:2:309:CLA:HHD	30:2:314:CHL:HBB2	1.92	0.52
1:A:354:TRP:HB3	18:A:804:CLA:HAC1	1.92	0.52
1:A:435:VAL:HA	1:A:438:HIS:CE1	2.45	0.52
13:1:146:GLU:HG2	30:1:5016:CHL:NB	2.25	0.52
18:A:839:CLA:H91	19:A:841:PQN:H292	1.92	0.52
4:D:126:GLY:O	4:D:128:ASN:ND2	2.42	0.52
13:1:128:TRP:NE1	18:1:5017:CLA:OBD	2.40	0.52
16:4:100:ARG:HA	16:4:103:MET:HE3	1.92	0.52
15:3:141:VAL:HG21	29:3:304:LUT:H22	1.92	0.52
21:A:855:BCR:H353	21:K:1405:BCR:H323	1.91	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:GLN:NE2	18:A:808:CLA:OBD	2.43	0.51
1:A:400:MET:HE2	1:A:612:VAL:HG11	1.91	0.51
18:A:825:CLA:CAB	18:A:832:CLA:HMA2	2.39	0.51
2:B:585:ASN:HB2	18:B:801:CLA:HBC2	1.93	0.51
10:J:16:THR:HG21	29:J:1105:LUT:H371	1.92	0.51
2:B:477:LEU:HD13	18:B:834:CLA:HMD2	1.93	0.51
2:B:631:LEU:HD22	2:B:724:PHE:HA	1.92	0.51
18:B:828:CLA:HBC3	26:B:855:DGD:HBG3	1.92	0.51
1:A:541:VAL:HG11	1:A:615:HIS:CG	2.45	0.51
22:1:5019:LHG:H192	24:1:5020:LMG:H251	1.92	0.51
18:A:828:CLA:H13	22:A:848:LHG:H202	1.92	0.51
18:K:1401:CLA:HMB1	18:K:1401:CLA:HBB1	1.93	0.51
13:1:183:LYS:HG2	18:1:5007:CLA:HBD	1.93	0.51
18:A:837:CLA:H72	21:F:304:BCR:H14C	1.93	0.51
13:1:183:LYS:O	13:1:187:ASN:ND2	2.28	0.51
1:A:90:PHE:HE2	21:A:843:BCR:HC21	1.76	0.51
18:A:830:CLA:HAB	18:A:831:CLA:HHB	1.93	0.51
16:4:225:THR:HG23	16:4:227:LYS:H	1.76	0.51
18:B:824:CLA:H71	24:1:5001:LMG:H421	1.91	0.51
18:B:835:CLA:O1A	18:G:1603:CLA:HHB	2.10	0.51
4:D:155:PHE:CZ	4:D:168:HIS:HB3	2.45	0.51
18:A:803:CLA:H201	18:A:808:CLA:H8	1.93	0.51
18:A:803:CLA:HBD	18:A:810:CLA:H12	1.93	0.50
2:B:459:PHE:HB3	18:B:836:CLA:H42	1.93	0.50
3:C:27:GLU:HG3	3:C:44:ARG:HH22	1.76	0.50
1:A:302:HIS:HB2	18:A:816:CLA:CHB	2.40	0.50
1:A:364:MET:HE3	18:A:819:CLA:H93	1.92	0.50
1:A:687:ALA:O	18:A:802:CLA:HAB	2.11	0.50
18:A:819:CLA:H193	18:A:822:CLA:HAC2	1.94	0.50
2:B:658:ALA:HB3	18:B:804:CLA:HBB2	1.91	0.50
1:A:580:PRO:HB3	1:A:727:ILE:HB	1.92	0.50
2:B:275:HIS:HB3	18:B:818:CLA:HMB2	1.94	0.50
18:B:831:CLA:HAB	18:B:838:CLA:HBB2	1.94	0.50
1:A:57:LEU:HD21	18:J:1101:CLA:HBC2	1.93	0.50
1:A:98:PHE:CG	18:A:806:CLA:HBC3	2.47	0.50
13:1:66:LEU:HD12	29:1:5004:LUT:H41	1.92	0.50
13:1:145:VAL:HG21	21:1:5005:BCR:H16C	1.92	0.50
15:3:232:ARG:NH1	30:3:310:CHL:O1D	2.45	0.50
2:B:26:ALA:HB1	26:B:855:DGD:HB22	1.94	0.50
2:B:422:LEU:HD13	2:B:532:LEU:HA	1.93	0.50
18:B:805:CLA:H92	18:B:808:CLA:H172	1.94	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:84:CYS:HB3	13:1:188:GLY:HA3	1.93	0.50
14:2:150:THR:HG23	24:2:322:LMG:HC61	1.93	0.50
18:G:1601:CLA:HMB1	18:G:1601:CLA:HBB1	1.93	0.50
15:3:267:ASN:HB3	18:3:309:CLA:OBD	2.11	0.50
18:A:819:CLA:HBC3	18:A:825:CLA:H18	1.93	0.50
13:1:62:ASP:O	13:1:65:ARG:NH1	2.43	0.50
13:1:145:VAL:CG2	21:1:5005:BCR:H16C	2.41	0.50
14:2:85:PHE:HZ	14:2:223:LYS:HE2	1.76	0.50
29:J:1105:LUT:H28	29:J:1105:LUT:H361	1.93	0.49
29:1:5003:LUT:H32	18:1:5006:CLA:CAB	2.42	0.49
15:3:187:PHE:CE2	30:3:316:CHL:HBB2	2.47	0.49
21:4:301:BCR:H342	30:4:302:CHL:H51	1.94	0.49
1:A:18:VAL:N	1:A:320:ASN:OD1	2.40	0.49
1:A:24:ARG:HH21	15:3:89:THR:HB	1.76	0.49
18:B:823:CLA:HBB2	21:B:846:BCR:H343	1.93	0.49
18:B:841:CLA:HED1	21:B:846:BCR:H353	1.94	0.49
4:D:112:ILE:O	4:D:149:TYR:OH	2.30	0.49
13:1:105:TRP:HE3	29:1:5004:LUT:H221	1.77	0.49
2:B:194:LEU:HA	2:B:198:ALA:HB3	1.94	0.49
2:B:474:PHE:HD1	23:B:853:LMT:H6E	1.77	0.49
1:A:397:THR:HG23	1:A:613:ILE:HG21	1.95	0.49
18:2:312:CLA:HBB1	18:2:312:CLA:HMB3	1.94	0.49
15:3:124:LYS:NZ	15:3:254:GLN:OE1	2.45	0.49
1:A:686:TRP:CE3	17:A:801:CL0:H6	2.48	0.49
2:B:65:LEU:HD21	21:B:845:BCR:H291	1.94	0.49
14:2:220:LYS:O	14:2:224:ASN:ND2	2.43	0.49
18:A:811:CLA:C4C	18:A:811:CLA:H42	2.43	0.49
2:B:222:LEU:HD12	23:B:856:LMT:H3B	1.93	0.49
15:3:74:GLY:H	15:3:225:LEU:HD12	1.78	0.49
15:3:162:MET:HE1	18:3:317:CLA:HMC1	1.94	0.49
18:A:819:CLA:H101	21:A:846:BCR:H21C	1.94	0.49
21:A:855:BCR:H362	11:K:109:VAL:HG21	1.93	0.49
3:C:65:VAL:HG23	20:C:102:SF4:S1	2.53	0.49
10:J:10:VAL:HG13	10:J:12:PRO:HD2	1.94	0.49
18:A:815:CLA:H121	18:K:1402:CLA:HMD1	1.95	0.49
29:1:5003:LUT:H373	18:1:5006:CLA:H42	1.94	0.49
1:A:305:ALA:CB	18:A:816:CLA:HAB	2.43	0.49
1:A:604:TRP:HE1	18:B:804:CLA:C1D	2.25	0.49
18:A:836:CLA:HMC2	18:L:301:CLA:HBC2	1.93	0.49
2:B:526:GLY:HA2	2:B:582:TRP:CZ3	2.48	0.49
18:A:824:CLA:HBA1	18:A:825:CLA:HED2	1.94	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:TRP:CH2	21:B:845:BCR:H272	2.48	0.48
18:B:836:CLA:H61	18:B:836:CLA:H2	1.63	0.48
3:C:15:THR:HG22	3:C:28:MET:HE2	1.94	0.48
14:2:122:ILE:HB	14:2:123:PRO:HD3	1.94	0.48
1:A:387:THR:HG21	1:A:523:VAL:HB	1.95	0.48
1:A:596:ASP:HA	1:A:599:PHE:HB3	1.94	0.48
2:B:243:LEU:HB2	2:B:246:THR:OG1	2.13	0.48
2:B:369:ALA:HB1	2:B:725:LEU:HD11	1.96	0.48
2:B:571:SER:OG	2:B:574:ASP:OD1	2.24	0.48
13:1:144:PHE:O	13:1:148:GLN:HG2	2.12	0.48
14:2:159:PHE:HB3	21:2:305:BCR:H363	1.95	0.48
15:3:98:LEU:HD22	30:3:310:CHL:H11	1.95	0.48
16:4:105:GLY:HA2	31:4:304:XAT:H181	1.94	0.48
18:B:834:CLA:H61	18:B:835:CLA:H12	1.96	0.48
4:D:189:PHE:HB3	5:E:100:ARG:HH12	1.78	0.48
6:F:163:PRO:HG3	10:J:39:PHE:HB2	1.96	0.48
18:2:310:CLA:HBB1	18:2:310:CLA:HMB3	1.95	0.48
15:3:107:ARG:NH2	15:3:201:ALA:O	2.45	0.48
18:A:806:CLA:H12	18:A:808:CLA:H2	1.95	0.48
19:A:841:PQN:H241	18:J:1101:CLA:HED1	1.94	0.48
2:B:309:ILE:HD13	2:B:320:LYS:HE3	1.95	0.48
18:A:811:CLA:H52	15:3:81:LEU:HD13	1.96	0.48
22:A:849:LHG:H202	22:A:849:LHG:H172	1.68	0.48
2:B:547:MET:HE3	2:B:550:LYS:HG3	1.95	0.48
18:B:825:CLA:H72	18:B:827:CLA:H42	1.94	0.48
14:2:162:TRP:CH2	21:2:305:BCR:H321	2.48	0.48
18:A:821:CLA:CBB	24:A:851:LMG:H192	2.44	0.48
2:B:224:PRO:HB3	2:B:229:GLN:HG3	1.95	0.48
18:B:816:CLA:HBB1	21:B:844:BCR:HC42	1.96	0.48
4:D:109:LYS:HG3	4:D:111:GLN:HG3	1.96	0.48
11:K:57:THR:O	11:K:61:LEU:HB2	2.14	0.48
18:A:822:CLA:H43	21:A:846:BCR:H351	1.95	0.48
18:A:840:CLA:CHB	22:A:849:LHG:HC62	2.43	0.48
18:B:811:CLA:H91	18:B:811:CLA:H112	1.70	0.48
14:2:201:PHE:HA	30:2:316:CHL:H11	1.96	0.48
18:A:802:CLA:H143	18:A:802:CLA:H162	1.72	0.48
18:A:810:CLA:H141	18:A:810:CLA:H161	1.73	0.48
2:B:612:SER:HA	2:B:615:TYR:HE1	1.78	0.48
18:B:830:CLA:C2D	26:B:855:DGD:HB62	2.43	0.48
18:2:306:CLA:H41	18:2:307:CLA:HMA2	1.95	0.48
21:4:301:BCR:H373	30:4:316:CHL:HMB1	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:823:CLA:HBB1	18:A:823:CLA:HMB1	1.96	0.48
18:B:808:CLA:H203	18:B:808:CLA:H161	1.70	0.48
18:B:827:CLA:C4B	18:B:834:CLA:HMA3	2.43	0.48
18:B:841:CLA:C4B	18:1:5010:CLA:H52	2.44	0.48
18:1:5010:CLA:H62	18:1:5010:CLA:H41	1.43	0.48
18:1:5012:CLA:HBB1	18:1:5012:CLA:HHC	1.96	0.48
1:A:261:SER:HB2	1:A:280:PHE:CE2	2.48	0.48
18:B:826:CLA:HBA2	18:B:838:CLA:HAA1	1.96	0.48
1:A:259:TYR:CD1	1:A:280:PHE:HB3	2.49	0.47
1:A:338:PHE:CD2	22:A:849:LHG:HC42	2.48	0.47
1:A:397:THR:HB	18:A:826:CLA:HMB2	1.94	0.47
18:B:837:CLA:HMA3	18:B:838:CLA:HED2	1.96	0.47
7:G:136:HIS:CE1	21:G:1604:BCR:H16C	2.48	0.47
24:2:321:LMG:H112	24:2:321:LMG:HC8	1.51	0.47
31:4:304:XAT:H183	18:4:310:CLA:C3B	2.44	0.47
1:A:696:GLY:HA3	2:B:568:CYS:HB2	1.95	0.47
2:B:142:LEU:HG	21:B:845:BCR:H402	1.96	0.47
18:B:823:CLA:HMC2	24:1:5001:LMG:H412	1.96	0.47
7:G:92:LEU:HD12	7:G:93:PRO:HD2	1.96	0.47
11:K:61:LEU:HB3	18:K:1403:CLA:CAB	2.32	0.47
13:1:217:HIS:CG	18:1:5008:CLA:HAA2	2.49	0.47
1:A:195:TRP:CZ2	18:A:812:CLA:HBC3	2.49	0.47
18:A:826:CLA:H8	21:A:847:BCR:H343	1.95	0.47
18:A:832:CLA:H72	21:A:846:BCR:H10C	1.95	0.47
18:B:831:CLA:H61	18:B:831:CLA:H102	1.60	0.47
21:2:305:BCR:HC41	26:2:327:DGD:HB21	1.96	0.47
18:A:829:CLA:H102	18:A:829:CLA:H61	1.49	0.47
2:B:352:MET:HG2	18:B:819:CLA:O1A	2.14	0.47
18:B:806:CLA:HED2	18:B:830:CLA:HBB2	1.96	0.47
18:H:1701:CLA:H41	18:H:1701:CLA:H61	1.55	0.47
10:J:31:ARG:HD2	29:J:1105:LUT:H41	1.96	0.47
1:A:614:PHE:HB3	1:A:652:TRP:HZ3	1.79	0.47
2:B:476:VAL:O	2:B:480:SER:N	2.48	0.47
18:A:824:CLA:HAA2	18:A:825:CLA:OBD	2.14	0.47
18:A:826:CLA:H71	18:A:826:CLA:H112	1.58	0.47
18:B:810:CLA:H91	18:B:810:CLA:H111	1.75	0.47
18:B:812:CLA:HBA2	23:G:1605:LMT:H11	1.96	0.47
18:A:817:CLA:H203	18:A:825:CLA:H11	1.95	0.47
2:B:547:MET:HE2	2:B:570:ILE:HD13	1.97	0.47
6:F:113:SER:OG	6:F:115:PRO:HD2	2.14	0.47
28:F:310:ZEX:O3	18:1:5018:CLA:H2	2.14	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:119:ALA:H	13:1:129:GLY:HA3	1.79	0.47
18:2:312:CLA:H8	18:2:312:CLA:H122	1.52	0.47
30:3:310:CHL:HBB1	30:3:310:CHL:HMB1	1.96	0.47
1:A:91:LEU:HD23	21:J:1104:BCR:H282	1.96	0.47
1:A:370:ILE:HG22	18:A:824:CLA:HED2	1.97	0.47
1:A:467:MET:HB2	1:A:476:MET:HG2	1.96	0.47
1:A:547:PHE:HZ	18:A:852:CLA:HBB2	1.80	0.47
18:A:809:CLA:H42	18:3:311:CLA:H2	1.97	0.47
15:3:197:SER:OG	15:3:202:TYR:O	2.33	0.47
18:A:810:CLA:H61	18:A:810:CLA:H41	1.57	0.47
18:A:853:CLA:H171	12:L:141:LEU:HD11	1.95	0.47
18:B:806:CLA:H122	18:B:806:CLA:HBD	1.96	0.47
4:D:206:LYS:HD3	4:D:211:LEU:HD21	1.96	0.47
13:1:121:TYR:CD1	18:1:5011:CLA:H2	2.50	0.47
18:1:5006:CLA:H41	18:1:5006:CLA:H61	1.48	0.47
15:3:72:LEU:HD21	15:3:99:ALA:HB2	1.97	0.47
30:4:316:CHL:HBA1	30:4:316:CHL:H3A	1.61	0.47
4:D:110:GLU:HA	4:D:123:MET:O	2.14	0.46
15:3:142:ILE:HG22	15:3:144:PRO:HG2	1.97	0.46
1:A:402:ILE:HD12	18:A:805:CLA:H143	1.96	0.46
1:A:446:LEU:HB3	1:A:554:LEU:HD13	1.97	0.46
18:A:803:CLA:H91	18:A:803:CLA:H111	1.65	0.46
18:B:826:CLA:HBA1	18:B:826:CLA:H3A	1.51	0.46
6:F:156:HIS:HB3	6:F:159:GLU:CD	2.40	0.46
15:3:141:VAL:HG22	18:3:318:CLA:HMC2	1.98	0.46
18:A:803:CLA:H11	18:A:810:CLA:H62	1.97	0.46
2:B:50:HIS:HE1	18:B:806:CLA:H161	1.80	0.46
2:B:184:GLY:HA3	2:B:285:LEU:HD12	1.97	0.46
18:B:815:CLA:H3A	21:B:845:BCR:H392	1.96	0.46
18:F:302:CLA:H3A	18:F:302:CLA:HBA1	1.64	0.46
21:G:1604:BCR:H351	21:G:1604:BCR:H15C	1.60	0.46
15:3:98:LEU:HB3	30:3:310:CHL:H11	1.97	0.46
18:A:805:CLA:H162	18:A:805:CLA:H122	1.65	0.46
2:B:300:SER:H	7:G:90:GLN:HE21	1.62	0.46
6:F:154:GLN:NE2	24:F:306:LMG:O9	2.48	0.46
6:F:188:ASP:OD1	6:F:189:LYS:N	2.46	0.46
1:A:155:ALA:HB2	1:A:383:PRO:HD2	1.98	0.46
18:A:835:CLA:H13	18:A:835:CLA:H102	1.58	0.46
21:L:303:BCR:H351	21:L:303:BCR:H15C	1.76	0.46
29:1:5004:LUT:H12	18:1:5009:CLA:CBB	2.46	0.46
18:2:312:CLA:H61	18:2:312:CLA:H41	1.44	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:314:CHL:H62	30:2:314:CHL:H41	1.56	0.46
15:3:213:PHE:HB2	18:3:307:CLA:HBA1	1.97	0.46
18:4:315:CLA:H162	18:4:315:CLA:H203	1.69	0.46
18:A:811:CLA:H11	15:3:81:LEU:HD13	1.98	0.46
18:B:814:CLA:H151	18:B:814:CLA:H111	1.70	0.46
18:F:303:CLA:H112	18:F:303:CLA:H143	1.73	0.46
28:F:310:ZEX:H191	30:4:318:CHL:H2	1.97	0.46
18:K:1403:CLA:O1D	18:K:1403:CLA:H2	2.15	0.46
31:4:304:XAT:H31	31:4:304:XAT:H391	1.70	0.46
1:A:93:LEU:O	1:A:97:TYR:HD2	1.99	0.46
18:B:824:CLA:HMD3	18:B:825:CLA:HHC	1.98	0.46
15:3:182:MET:HA	15:3:182:MET:HE2	1.97	0.46
15:3:203:PRO:HG3	30:3:316:CHL:HMD2	1.98	0.46
30:3:312:CHL:HMB1	30:3:312:CHL:HBB1	1.97	0.46
1:A:206:HIS:HB3	18:A:823:CLA:HED3	1.98	0.46
1:A:283:PHE:HZ	18:A:816:CLA:H51	1.81	0.46
1:A:321:TRP:CD1	11:K:91:LEU:HD22	2.49	0.46
1:A:389:TYR:HB3	1:A:754:ILE:HD11	1.98	0.46
18:A:802:CLA:H203	18:A:839:CLA:H2	1.97	0.46
18:A:820:CLA:H111	18:A:820:CLA:H93	1.74	0.46
18:A:822:CLA:H41	18:A:822:CLA:H61	1.56	0.46
2:B:142:LEU:HD23	2:B:145:LEU:HD12	1.97	0.46
2:B:428:PHE:CD1	18:B:837:CLA:HAB	2.51	0.46
18:1:5006:CLA:H92	18:1:5006:CLA:H62	1.67	0.46
29:2:303:LUT:H15	29:2:303:LUT:H201	1.74	0.46
18:B:830:CLA:HMB1	18:B:830:CLA:HBB1	1.97	0.46
6:F:167:PHE:HB2	21:F:304:BCR:H403	1.98	0.46
18:1:5006:CLA:HAC1	18:1:5015:CLA:O1A	2.15	0.46
15:3:161:GLU:HG3	15:3:162:MET:HE2	1.98	0.46
1:A:521:VAL:HG12	1:A:528:ALA:HB3	1.98	0.46
1:A:611:VAL:HG21	17:A:801:CL0:H64	1.98	0.46
1:A:711:HIS:NE2	18:A:838:CLA:HAC1	2.31	0.46
18:A:819:CLA:H72	18:A:822:CLA:H42	1.98	0.46
18:A:840:CLA:HMA2	24:A:851:LMG:H392	1.97	0.46
18:B:820:CLA:HED2	18:B:824:CLA:HED2	1.98	0.46
18:1:5006:CLA:H192	18:1:5015:CLA:H201	1.98	0.46
16:4:203:LYS:HG3	18:4:311:CLA:HED2	1.98	0.46
1:A:218:TRP:NE1	18:A:817:CLA:O1D	2.38	0.45
18:B:806:CLA:H3A	18:B:806:CLA:HBA1	1.46	0.45
18:B:820:CLA:H203	18:B:820:CLA:H161	1.75	0.45
1:A:321:TRP:O	1:A:323:ILE:N	2.47	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:822:CLA:H141	22:A:849:LHG:H202	1.99	0.45
2:B:519:VAL:O	2:B:523:ILE:HG12	2.17	0.45
29:1:5004:LUT:H28	29:1:5004:LUT:H361	1.98	0.45
18:1:5018:CLA:H2A	18:1:5018:CLA:HED2	1.98	0.45
1:A:417:PHE:CD1	1:A:421:ASP:HB2	2.51	0.45
18:B:805:CLA:H61	22:B:849:LHG:H191	1.97	0.45
3:C:61:ASP:O	5:E:118:ASN:ND2	2.46	0.45
26:2:327:DGD:HG11	18:4:311:CLA:CHD	2.47	0.45
16:4:175:TYR:HB3	30:4:317:CHL:C3D	2.47	0.45
1:A:461:TYR:CE2	1:A:540:LEU:HB3	2.52	0.45
1:A:471:GLY:HA3	2:B:99:PRO:HG2	1.97	0.45
18:A:834:CLA:H11	18:A:835:CLA:O1A	2.16	0.45
2:B:477:LEU:C	2:B:479:SER:H	2.24	0.45
2:B:612:SER:HA	2:B:615:TYR:CE1	2.52	0.45
21:B:802:BCR:H363	18:B:804:CLA:H72	1.97	0.45
18:B:808:CLA:HED2	9:I:5:PRO:HB3	1.99	0.45
18:B:813:CLA:HMB1	18:B:813:CLA:HBB1	1.98	0.45
18:H:1701:CLA:H121	12:L:81:TRP:NE1	2.32	0.45
29:3:304:LUT:H24	30:3:310:CHL:O1A	2.16	0.45
18:A:819:CLA:H2	18:A:823:CLA:HBB1	1.99	0.45
2:B:448:THR:O	2:B:448:THR:OG1	2.35	0.45
18:B:806:CLA:H161	18:B:806:CLA:H202	1.73	0.45
18:B:835:CLA:H62	18:B:835:CLA:H41	1.60	0.45
18:K:1402:CLA:H61	18:K:1402:CLA:H41	1.52	0.45
18:3:311:CLA:HED2	18:3:317:CLA:H2	1.98	0.45
1:A:453:LEU:HD21	18:A:835:CLA:HAB	1.98	0.45
18:A:819:CLA:HBA1	18:A:823:CLA:C3B	2.46	0.45
18:A:835:CLA:H111	18:A:835:CLA:H72	1.82	0.45
18:A:835:CLA:H161	18:A:835:CLA:H122	1.68	0.45
18:A:835:CLA:HMA3	18:A:836:CLA:HED2	1.98	0.45
18:A:835:CLA:HBB2	18:A:836:CLA:HBC3	1.99	0.45
18:A:853:CLA:H102	18:B:839:CLA:H61	1.99	0.45
2:B:498:LEU:HA	2:B:501:ILE:HG22	1.98	0.45
6:F:213:TRP:CG	6:F:214:PRO:HD3	2.52	0.45
18:F:302:CLA:HMB1	10:J:26:LEU:HD11	1.98	0.45
13:1:177:PHE:CE2	13:1:181:LYS:HE3	2.52	0.45
29:3:303:LUT:H401	29:3:303:LUT:H35	1.80	0.45
1:A:411:ALA:HB2	21:A:846:BCR:H402	1.99	0.45
18:A:806:CLA:CAB	21:J:1104:BCR:H271	2.44	0.45
18:A:811:CLA:H62	18:A:811:CLA:H92	1.83	0.45
16:4:215:PHE:CD2	31:4:304:XAT:H12	2.51	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:ILE:HD13	18:A:837:CLA:HMD1	1.98	0.45
18:A:813:CLA:H62	18:A:813:CLA:H102	1.64	0.45
18:A:828:CLA:H162	18:A:828:CLA:H122	1.52	0.45
2:B:173:SER:O	2:B:177:HIS:ND1	2.33	0.45
24:G:1607:LMG:HC71	24:G:1607:LMG:HC2	1.42	0.45
13:1:225:THR:HG22	13:1:226:ILE:H	1.82	0.45
29:3:304:LUT:H32	30:3:310:CHL:CAB	2.42	0.45
18:A:840:CLA:H93	18:A:840:CLA:H111	1.70	0.45
18:B:813:CLA:HMC1	21:B:844:BCR:H10C	1.98	0.45
3:C:9:ASP:OD2	5:E:100:ARG:NH1	2.48	0.45
18:F:303:CLA:H3A	18:F:303:CLA:HBA1	1.76	0.45
18:G:1603:CLA:H111	18:G:1603:CLA:H142	1.69	0.45
18:J:1101:CLA:HBB1	29:J:1105:LUT:H383	1.98	0.45
1:A:55:TRP:HE3	22:A:848:LHG:H111	1.81	0.45
18:A:816:CLA:H62	18:A:816:CLA:H41	1.55	0.45
2:B:486:LEU:O	2:B:490:ARG:HG3	2.17	0.45
18:B:803:CLA:H3A	18:B:803:CLA:HBA2	1.75	0.45
23:B:856:LMT:H51	23:G:1606:LMT:H52	1.99	0.45
13:1:85:ARG:HB3	18:1:5006:CLA:CBC	2.43	0.45
17:A:801:CL0:H21	2:B:625:TRP:HD1	1.82	0.44
18:A:802:CLA:H91	18:A:802:CLA:H112	1.56	0.44
18:A:825:CLA:H91	18:A:825:CLA:H111	1.69	0.44
18:A:853:CLA:HAA2	18:L:301:CLA:HMB1	1.99	0.44
2:B:199:ILE:HB	2:B:200:PRO:HD3	1.99	0.44
2:B:348:VAL:O	2:B:352:MET:HG3	2.17	0.44
2:B:351:HIS:ND1	18:B:818:CLA:OBD	2.48	0.44
2:B:365:PHE:HD2	2:B:734:GLY:HA2	1.82	0.44
18:B:807:CLA:H161	18:B:807:CLA:H122	1.75	0.44
18:B:819:CLA:H41	18:B:819:CLA:H61	1.46	0.44
26:J:1106:DGD:HAS1	26:J:1106:DGD:HAH2	1.68	0.44
18:2:307:CLA:OBD	18:2:312:CLA:H2	2.17	0.44
15:3:223:LEU:HA	15:3:226:LYS:HD2	1.98	0.44
15:3:238:ILE:HG21	29:3:304:LUT:H14	1.99	0.44
18:A:815:CLA:H41	18:A:815:CLA:H62	1.47	0.44
18:A:831:CLA:H141	18:A:831:CLA:H161	1.80	0.44
2:B:662:MET:HB2	18:B:804:CLA:C1C	2.47	0.44
18:B:809:CLA:CGA	18:B:809:CLA:C1A	2.95	0.44
15:3:132:THR:O	30:3:312:CHL:HED3	2.16	0.44
29:3:304:LUT:H35	29:3:304:LUT:H401	1.72	0.44
2:B:526:GLY:HA2	2:B:582:TRP:HZ3	1.81	0.44
13:1:121:TYR:CE1	18:1:5011:CLA:H2	2.52	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3:315:CLA:H161	18:3:315:CLA:H122	1.45	0.44
18:A:804:CLA:H121	21:A:843:BCR:HC41	2.00	0.44
18:B:806:CLA:H151	18:B:814:CLA:CAD	2.48	0.44
18:B:816:CLA:CAB	21:B:843:BCR:H333	2.48	0.44
1:A:23:ASP:HB2	1:A:76:ARG:HH12	1.83	0.44
1:A:682:ALA:HA	1:A:685:VAL:HG22	1.99	0.44
2:B:80:ASP:HB2	2:B:84:VAL:HG23	2.00	0.44
2:B:366:THR:HG21	2:B:730:SER:HB3	1.98	0.44
18:B:829:CLA:HBB1	18:B:829:CLA:HMB3	1.99	0.44
18:B:840:CLA:H3A	18:B:840:CLA:HBA2	1.52	0.44
18:1:5009:CLA:H202	18:1:5009:CLA:H162	1.74	0.44
18:3:314:CLA:CHA	18:3:314:CLA:HBA1	2.48	0.44
16:4:116:THR:HA	16:4:121:ILE:O	2.17	0.44
21:4:301:BCR:H271	18:4:310:CLA:NB	2.32	0.44
1:A:227:LEU:HB3	1:A:259:TYR:CE2	2.53	0.44
1:A:378:ALA:CB	18:A:825:CLA:HAC2	2.48	0.44
1:A:466:THR:HG21	18:B:810:CLA:HAB	1.99	0.44
2:B:365:PHE:CD2	2:B:734:GLY:HA2	2.53	0.44
18:B:809:CLA:H8	18:B:809:CLA:H51	1.58	0.44
6:F:172:GLY:HA3	6:F:213:TRP:CE2	2.53	0.44
6:F:203:ALA:O	6:F:207:VAL:HG13	2.17	0.44
8:H:65:GLY:HA2	8:H:67:TRP:CE2	2.53	0.44
21:2:305:BCR:H402	30:2:318:CHL:HAA2	1.99	0.44
16:4:209:ARG:HA	16:4:212:MET:HE3	2.00	0.44
18:A:808:CLA:H62	18:A:808:CLA:H41	1.87	0.44
18:A:828:CLA:HMB3	18:A:828:CLA:HBB1	1.99	0.44
2:B:294:ASN:HB3	7:G:110:GLU:HA	1.99	0.44
2:B:658:ALA:C	18:B:804:CLA:HAB	2.42	0.44
13:1:150:SER:HB2	30:1:5016:CHL:HMA1	1.99	0.44
30:3:310:CHL:H61	18:3:311:CLA:HMA2	2.00	0.44
16:4:148:LEU:HB3	21:4:301:BCR:C16	2.47	0.44
18:B:808:CLA:H62	18:B:808:CLA:H101	1.65	0.44
13:1:94:ILE:HG21	13:1:198:ILE:HD13	1.99	0.44
18:4:315:CLA:H3A	18:4:315:CLA:HBA1	1.57	0.44
1:A:751:LEU:HD23	1:A:751:LEU:HA	1.81	0.44
2:B:91:ILE:HB	2:B:112:PRO:HB2	1.99	0.44
2:B:594:TRP:HB2	18:B:836:CLA:HMC1	1.99	0.44
6:F:213:TRP:CD1	6:F:214:PRO:HD3	2.53	0.44
29:1:5003:LUT:H35	29:1:5003:LUT:H401	1.75	0.44
18:1:5006:CLA:H51	18:1:5007:CLA:HMA2	2.00	0.44
15:3:136:TRP:CE2	15:3:137:PHE:HD1	2.35	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:813:CLA:C3B	21:A:843:BCR:H10C	2.47	0.43
18:B:823:CLA:H41	18:B:823:CLA:H61	1.43	0.43
3:C:66:ARG:HD3	3:C:66:ARG:HA	1.76	0.43
10:J:12:PRO:HB2	29:J:1105:LUT:H372	1.99	0.43
1:A:195:TRP:CD1	18:A:811:CLA:HED2	2.52	0.43
1:A:355:HIS:CE1	1:A:416:ILE:HG21	2.53	0.43
1:A:396:PHE:O	1:A:400:MET:HG2	2.18	0.43
1:A:684:PHE:CD2	21:A:847:BCR:H363	2.53	0.43
18:A:832:CLA:C2D	18:A:833:CLA:HAB	2.48	0.43
2:B:377:TYR:CD2	18:B:828:CLA:HAB	2.53	0.43
2:B:640:MET:HE3	2:B:640:MET:O	2.18	0.43
13:1:65:ARG:HH21	24:1:5020:LMG:HC3	1.83	0.43
18:2:309:CLA:H3A	18:2:309:CLA:HBA2	1.62	0.43
18:2:317:CLA:H3A	18:2:317:CLA:HBA1	1.61	0.43
21:3:306:BCR:H392	21:3:306:BCR:H23C	2.00	0.43
1:A:66:SER:HB3	1:A:420:ARG:HH22	1.82	0.43
1:A:544:ILE:HG21	17:A:801:CL0:H60	2.01	0.43
2:B:72:GLY:HA2	2:B:87:ILE:HB	1.99	0.43
18:B:823:CLA:H203	7:G:134:ILE:HA	1.99	0.43
18:2:306:CLA:H3A	18:2:306:CLA:HBA2	1.44	0.43
16:4:215:PHE:CE2	31:4:304:XAT:H10	2.53	0.43
29:4:303:LUT:H11	29:4:303:LUT:H191	1.92	0.43
1:A:53:TRP:HE3	1:A:54:ILE:HG13	1.84	0.43
18:A:803:CLA:H11	18:A:803:CLA:H52	1.63	0.43
2:B:62:SER:HA	2:B:65:LEU:HD12	2.00	0.43
21:B:843:BCR:H382	7:G:130:ALA:HB1	2.00	0.43
18:2:307:CLA:H41	18:2:307:CLA:H61	1.57	0.43
1:A:225:VAL:HG13	1:A:245:PRO:HB3	2.00	0.43
17:A:801:CL0:H58	17:A:801:CL0:H50	1.78	0.43
2:B:373:THR:HB	18:B:828:CLA:HMB1	2.01	0.43
2:B:390:GLY:HA2	21:B:847:BCR:H393	1.99	0.43
7:G:137:ILE:HG12	21:G:1604:BCR:H392	2.00	0.43
18:K:1403:CLA:H2A	18:K:1403:CLA:HED2	2.00	0.43
13:1:127:PRO:HG2	13:1:128:TRP:CE3	2.53	0.43
1:A:64:PHE:CD1	18:A:804:CLA:HMC2	2.54	0.43
1:A:604:TRP:HH2	18:A:852:CLA:HAB	1.83	0.43
18:A:840:CLA:H62	24:A:851:LMG:H332	1.99	0.43
18:B:811:CLA:H51	18:B:811:CLA:H11	1.79	0.43
18:B:841:CLA:H62	18:B:841:CLA:H41	1.60	0.43
18:B:841:CLA:HBC1	24:1:5001:LMG:HC62	1.99	0.43
18:3:317:CLA:HMB2	18:3:319:CLA:C4B	2.49	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:HIS:HB2	22:A:848:LHG:H112	2.01	0.43
1:A:499:ALA:N	1:A:500:PRO:HD2	2.34	0.43
1:A:680:LEU:HD13	18:B:801:CLA:H2	2.01	0.43
1:A:699:TYR:OH	18:A:802:CLA:OBD	2.27	0.43
18:A:807:CLA:CHC	18:A:808:CLA:HMD2	2.49	0.43
18:A:816:CLA:HBA2	18:A:816:CLA:H3A	1.44	0.43
18:A:822:CLA:HHB	18:A:840:CLA:CAB	2.49	0.43
2:B:262:HIS:CE1	2:B:264:GLN:HB3	2.53	0.43
18:B:806:CLA:HHC	18:B:806:CLA:HBB1	2.00	0.43
4:D:191:SER:HB2	4:D:194:LYS:HG3	2.01	0.43
13:1:198:ILE:HG23	13:1:210:PRO:HG3	2.00	0.43
18:1:5009:CLA:HED2	18:1:5009:CLA:H2A	2.01	0.43
15:3:75:ASP:HA	30:3:310:CHL:HED2	2.01	0.43
16:4:220:ILE:HD12	18:4:307:CLA:HAC2	2.01	0.43
18:4:307:CLA:H61	18:4:307:CLA:H41	1.83	0.43
1:A:272:LEU:HD21	11:K:116:VAL:HG22	1.99	0.43
18:A:836:CLA:H111	18:A:836:CLA:H142	1.68	0.43
19:A:841:PQN:H161	19:A:841:PQN:H141	1.57	0.43
18:B:811:CLA:H141	8:H:107:GLY:HA2	2.01	0.43
4:D:72:PRO:HA	4:D:73:PRO:HD3	1.93	0.43
24:1:5001:LMG:H162	30:1:5016:CHL:C2B	2.48	0.43
14:2:206:TRP:C	18:2:306:CLA:HBA1	2.44	0.43
18:2:311:CLA:HMA3	30:2:318:CHL:C3C	2.49	0.43
15:3:158:PHE:HA	15:3:161:GLU:HG2	2.01	0.43
30:4:318:CHL:H61	30:4:318:CHL:H41	1.67	0.43
18:A:803:CLA:H3A	18:A:803:CLA:HBA2	1.40	0.43
18:A:808:CLA:CBB	21:J:1104:BCR:HC8	2.49	0.43
18:A:811:CLA:HBD	18:A:811:CLA:HBA1	1.99	0.43
2:B:467:HIS:HA	2:B:478:LEU:HD12	2.01	0.43
18:B:809:CLA:HBB1	18:B:809:CLA:H91	2.00	0.43
18:B:826:CLA:H71	18:B:837:CLA:H12	2.01	0.43
3:C:61:ASP:O	5:E:78:ARG:NH1	2.50	0.43
18:F:303:CLA:H11	18:F:303:CLA:H52	1.82	0.43
8:H:73:ASP:HB2	12:L:171:LYS:HE2	2.01	0.43
1:A:55:TRP:CE3	22:A:848:LHG:H111	2.53	0.43
18:A:803:CLA:HBB2	18:A:805:CLA:HMD3	2.01	0.43
18:A:805:CLA:H41	18:A:805:CLA:H61	1.40	0.43
18:A:823:CLA:H62	18:A:823:CLA:H102	1.56	0.43
18:A:839:CLA:H192	10:J:22:LEU:HD23	2.01	0.43
21:A:845:BCR:H15C	21:A:845:BCR:H351	1.69	0.43
18:B:818:CLA:H143	18:B:818:CLA:H111	1.68	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:215:ILE:HG12	18:4:309:CLA:H2	2.00	0.43
11:K:67:ARG:HD2	11:K:99:PHE:HB2	2.01	0.43
13:1:171:SER:HA	13:1:177:PHE:HB2	2.00	0.43
18:2:313:CLA:CAD	30:2:314:CHL:H102	2.48	0.43
18:A:833:CLA:C2	18:K:1402:CLA:H2	2.49	0.42
2:B:61:THR:HB	2:B:142:LEU:HD13	2.00	0.42
3:C:41:SER:HB2	4:D:185:VAL:H	1.84	0.42
15:3:202:TYR:HA	18:3:307:CLA:O1D	2.19	0.42
18:A:840:CLA:HBA1	24:A:851:LMG:H321	2.01	0.42
18:A:852:CLA:H18	18:B:811:CLA:HMC1	2.00	0.42
2:B:186:SER:O	18:B:815:CLA:HBB2	2.20	0.42
18:B:801:CLA:H161	18:B:801:CLA:H202	1.74	0.42
18:B:828:CLA:H193	18:B:828:CLA:H162	1.71	0.42
5:E:122:LEU:HD23	5:E:122:LEU:HA	1.86	0.42
23:2:325:LMT:H11	23:2:325:LMT:H41	1.87	0.42
15:3:123:GLY:HA3	15:3:133:ALA:HB1	2.01	0.42
16:4:103:MET:SD	18:4:305:CLA:HAB	2.59	0.42
2:B:659:THR:HA	18:B:804:CLA:HAB	2.00	0.42
2:B:667:TRP:HA	19:B:842:PQN:H8	2.01	0.42
22:B:848:LHG:HC12	13:1:66:LEU:HA	2.01	0.42
7:G:82:PHE:HB2	13:1:151:MET:SD	2.59	0.42
29:J:1105:LUT:H181	29:J:1105:LUT:C8	2.45	0.42
18:1:5010:CLA:H43	18:1:5010:CLA:HED3	2.01	0.42
21:2:305:BCR:H392	21:2:305:BCR:H282	1.33	0.42
15:3:101:GLY:HA2	18:3:317:CLA:HED2	2.01	0.42
15:3:169:GLU:OE1	15:3:172:ARG:NH2	2.41	0.42
16:4:153:GLU:OE2	16:4:156:ARG:NH2	2.49	0.42
1:A:516:GLY:O	1:A:531:PRO:HG3	2.19	0.42
18:A:834:CLA:HMB3	18:A:834:CLA:HBB1	2.00	0.42
2:B:339:ALA:HB2	21:B:847:BCR:H372	2.02	0.42
2:B:407:VAL:O	2:B:411:MET:HG2	2.20	0.42
2:B:410:ARG:O	2:B:414:HIS:ND1	2.49	0.42
2:B:700:LEU:HD22	2:B:704:GLN:NE2	2.34	0.42
18:B:818:CLA:H193	18:B:818:CLA:H162	1.84	0.42
18:B:823:CLA:HBC2	18:B:824:CLA:HAA2	2.01	0.42
7:G:145:THR:HA	7:G:148:ASN:ND2	2.34	0.42
14:2:180:ASP:HB3	14:2:183:PHE:O	2.20	0.42
14:2:236:TRP:CZ3	30:2:315:CHL:HHB	2.54	0.42
15:3:193:GLY:HA3	15:3:207:PHE:CD2	2.54	0.42
1:A:339:THR:HG1	22:A:849:LHG:H02	1.66	0.42
18:A:812:CLA:H41	18:A:812:CLA:H61	1.70	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:817:CLA:H71	18:A:817:CLA:C3B	2.50	0.42
18:A:828:CLA:H61	18:A:828:CLA:H92	1.67	0.42
18:A:837:CLA:HED2	2:B:424:TRP:HB2	2.02	0.42
21:K:1405:BCR:H351	21:K:1405:BCR:H15C	1.81	0.42
12:L:203:LEU:HD11	21:L:302:BCR:H381	2.02	0.42
14:2:92:LEU:HD13	18:2:309:CLA:H42	2.01	0.42
2:B:278:LEU:O	2:B:282:ILE:HG22	2.19	0.42
7:G:76:ARG:NH1	7:G:119:ASP:OD2	2.53	0.42
14:2:109:HIS:HB3	14:2:229:MET:SD	2.60	0.42
29:2:303:LUT:H11	29:2:303:LUT:H191	1.88	0.42
15:3:273:LYS:HG2	18:3:301:CLA:CGA	2.49	0.42
29:3:304:LUT:H31	29:3:304:LUT:H391	1.85	0.42
18:3:309:CLA:H12	18:3:314:CLA:CAD	2.50	0.42
18:3:319:CLA:H41	18:3:319:CLA:H61	1.45	0.42
16:4:169:ASP:HB3	16:4:172:PHE:O	2.19	0.42
1:A:85:GLN:HG2	18:A:804:CLA:CMA	2.50	0.42
18:A:807:CLA:H192	18:A:807:CLA:H162	1.74	0.42
18:A:809:CLA:H11	18:A:811:CLA:H43	2.01	0.42
21:A:844:BCR:H351	21:A:844:BCR:H15C	1.92	0.42
2:B:589:TRP:CE2	18:B:803:CLA:H161	2.54	0.42
18:B:823:CLA:HED1	7:G:89:LYS:HE3	2.01	0.42
18:B:833:CLA:HBA2	18:B:833:CLA:H3A	1.77	0.42
18:B:837:CLA:H91	18:B:837:CLA:H111	1.78	0.42
6:F:138:LEU:HD13	6:F:146:PRO:HB3	2.02	0.42
30:4:316:CHL:H62	30:4:316:CHL:H101	1.87	0.42
18:A:802:CLA:H201	18:A:807:CLA:H202	2.02	0.42
18:A:825:CLA:C3B	18:A:832:CLA:HMA2	2.49	0.42
2:B:478:LEU:HA	2:B:486:LEU:HD13	2.02	0.42
4:D:105:TRP:CD1	4:D:151:ILE:HG21	2.54	0.42
18:F:301:CLA:HMB2	21:F:304:BCR:H21C	2.00	0.42
18:F:302:CLA:H61	18:F:302:CLA:H41	1.70	0.42
11:K:55:MET:HG3	18:K:1401:CLA:HMD3	2.01	0.42
11:K:67:ARG:HH12	11:K:97:ALA:HB3	1.85	0.42
29:1:5004:LUT:H12	18:1:5009:CLA:CAB	2.49	0.42
15:3:232:ARG:HA	15:3:235:MET:HE3	2.02	0.42
15:3:270:THR:HG22	15:3:272:LEU:H	1.85	0.42
18:A:811:CLA:HBB1	18:A:811:CLA:HHC	2.02	0.42
18:B:811:CLA:H3A	18:B:811:CLA:HBA1	1.67	0.42
7:G:112:VAL:O	7:G:116:LYS:HG3	2.19	0.42
18:G:1603:CLA:H92	18:G:1603:CLA:H62	1.70	0.42
29:1:5003:LUT:H11	29:1:5003:LUT:H191	1.86	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1:5015:CLA:H203	18:1:5015:CLA:H161	1.71	0.42
14:2:106:GLU:HB2	18:2:309:CLA:CHB	2.50	0.42
15:3:107:ARG:HB3	18:3:307:CLA:CBC	2.50	0.42
1:A:22:VAL:HA	1:A:191:PRO:HA	2.02	0.42
1:A:584:PRO:HD3	2:B:561:GLY:HA2	2.02	0.42
18:A:819:CLA:C2	18:A:823:CLA:HBB1	2.50	0.42
18:A:838:CLA:H93	6:F:203:ALA:HB1	2.02	0.42
2:B:282:ILE:HD11	21:G:1604:BCR:H393	2.01	0.42
18:B:824:CLA:HBA1	18:B:824:CLA:H3A	1.80	0.42
11:K:87:ARG:HG2	11:K:88:ASP:N	2.35	0.42
21:L:303:BCR:C19	18:L:305:CLA:HAB	2.50	0.42
13:1:78:GLU:O	13:1:82:ILE:HG12	2.20	0.42
14:2:220:LYS:HG3	18:2:312:CLA:HED2	2.01	0.42
31:2:304:XAT:H391	31:2:304:XAT:H31	1.67	0.42
15:3:171:ARG:HD3	30:3:316:CHL:CBB	2.50	0.42
1:A:100:GLY:O	1:A:104:SER:OG	2.29	0.41
18:A:837:CLA:HAA2	18:B:832:CLA:HMB1	2.02	0.41
18:B:807:CLA:H91	18:B:828:CLA:HBC1	2.01	0.41
3:C:23:THR:O	4:D:135:LYS:NZ	2.53	0.41
21:2:305:BCR:HC32	26:2:327:DGD:O2E	2.20	0.41
15:3:143:PRO:N	15:3:144:PRO:HD2	2.35	0.41
15:3:158:PHE:CD1	18:3:315:CLA:HBD	2.55	0.41
1:A:343:HIS:HA	1:A:346:LEU:HD12	2.01	0.41
1:A:701:GLN:O	1:A:705:GLU:HG3	2.21	0.41
18:A:811:CLA:H52	18:A:811:CLA:H11	1.83	0.41
18:B:829:CLA:H62	18:B:829:CLA:H41	1.95	0.41
6:F:162:THR:HB	6:F:163:PRO:HD3	2.00	0.41
6:F:173:TRP:CD1	6:F:210:GLY:HA3	2.55	0.41
18:J:1101:CLA:H71	18:J:1101:CLA:H112	1.86	0.41
16:4:198:LEU:O	16:4:200:ALA:N	2.51	0.41
19:A:841:PQN:H111	19:A:841:PQN:H2M1	1.89	0.41
2:B:503:GLU:HG3	2:B:505:SER:H	1.85	0.41
18:B:829:CLA:H8	21:B:844:BCR:H21C	2.02	0.41
18:F:303:CLA:ND	24:F:306:LMG:H302	2.35	0.41
18:H:1701:CLA:HBB2	21:L:307:BCR:H311	2.02	0.41
18:L:306:CLA:CHA	18:L:306:CLA:HBA1	2.48	0.41
14:2:188:LEU:HD23	14:2:198:GLY:HA3	2.02	0.41
18:2:326:CLA:H3A	18:2:326:CLA:HBA2	1.58	0.41
16:4:221:GLN:O	16:4:225:THR:HG22	2.20	0.41
18:A:822:CLA:H161	22:A:849:LHG:H142	2.03	0.41
2:B:590:VAL:HG22	18:B:836:CLA:HAB	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:812:CLA:H41	18:B:812:CLA:H62	1.78	0.41
18:B:822:CLA:H111	18:B:822:CLA:H91	1.84	0.41
18:B:833:CLA:H61	18:B:833:CLA:H41	1.75	0.41
18:B:841:CLA:H143	18:B:841:CLA:H161	1.84	0.41
8:H:94:THR:HG22	12:L:184:LYS:HA	2.02	0.41
10:J:29:ILE:HG23	26:J:1106:DGD:HB22	2.03	0.41
29:J:1105:LUT:H35	29:J:1105:LUT:H401	1.73	0.41
29:1:5004:LUT:H11	29:1:5004:LUT:H191	1.79	0.41
29:2:303:LUT:H173	18:2:306:CLA:H12	2.03	0.41
30:2:314:CHL:H71	30:2:314:CHL:H112	1.55	0.41
18:A:823:CLA:H142	18:A:823:CLA:H111	1.83	0.41
18:A:830:CLA:H143	19:B:842:PQN:H191	2.02	0.41
18:A:837:CLA:H62	18:A:837:CLA:H102	1.89	0.41
18:A:839:CLA:H18	18:J:1101:CLA:H193	2.02	0.41
21:A:855:BCR:H351	21:A:855:BCR:H15C	1.68	0.41
6:F:129:ARG:HB2	10:J:35:ASP:OD2	2.20	0.41
11:K:47:ILE:HD12	11:K:47:ILE:HA	1.92	0.41
15:3:97:TRP:CZ2	18:3:317:CLA:HAA2	2.55	0.41
1:A:195:TRP:NE1	18:A:809:CLA:HMA3	2.36	0.41
18:A:807:CLA:H3A	18:A:807:CLA:HBA2	1.40	0.41
18:A:815:CLA:H3A	18:A:815:CLA:HBA2	1.87	0.41
2:B:222:LEU:HD11	18:B:816:CLA:HBA2	2.01	0.41
18:B:805:CLA:HMB1	18:B:805:CLA:HBB1	2.01	0.41
18:B:819:CLA:HBB2	18:B:825:CLA:H191	2.03	0.41
4:D:101:TYR:CE1	4:D:157:ARG:HD3	2.56	0.41
11:K:73:SER:OG	11:K:74:ALA:N	2.54	0.41
18:A:819:CLA:H41	18:A:819:CLA:H62	1.56	0.41
18:A:832:CLA:C7	21:A:846:BCR:H10C	2.51	0.41
18:A:836:CLA:HHC	18:A:836:CLA:HBB1	2.02	0.41
18:B:805:CLA:HMA2	22:B:849:LHG:H282	2.02	0.41
18:B:818:CLA:H162	18:B:818:CLA:H141	1.83	0.41
21:F:304:BCR:H351	21:F:304:BCR:H15C	1.74	0.41
13:1:194:ALA:HB1	29:1:5003:LUT:H171	2.01	0.41
29:1:5003:LUT:H15	29:1:5003:LUT:H201	1.86	0.41
14:2:110:SER:CB	14:2:225:GLY:HA3	2.49	0.41
18:2:312:CLA:HBC3	22:2:320:LHG:H252	2.02	0.41
15:3:123:GLY:HA3	15:3:133:ALA:CB	2.51	0.41
16:4:81:LEU:HD13	18:4:308:CLA:H42	2.03	0.41
1:A:729:GLN:HB2	22:A:848:LHG:HC41	2.02	0.41
18:A:838:CLA:H62	18:A:838:CLA:H41	1.39	0.41
2:B:134:ASP:OD2	2:B:208:ARG:NH2	2.50	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:MET:HE1	18:B:820:CLA:CAD	2.51	0.41
2:B:358:TYR:CE2	18:B:829:CLA:HED2	2.55	0.41
2:B:439:HIS:CD2	2:B:453:ILE:HG13	2.55	0.41
2:B:694:ARG:HG3	18:B:839:CLA:HED3	2.03	0.41
18:B:806:CLA:H102	18:B:806:CLA:H61	1.90	0.41
18:B:821:CLA:HAB	21:B:843:BCR:H14C	2.02	0.41
18:B:831:CLA:H122	18:B:831:CLA:H202	2.03	0.41
11:K:125:ILE:HD11	18:K:1402:CLA:HMA1	2.03	0.41
16:4:121:ILE:HG22	16:4:122:ASN:H	1.86	0.41
1:A:207:LEU:O	1:A:310:PHE:HB3	2.20	0.41
1:A:213:LEU:HD22	21:A:843:BCR:H361	2.03	0.41
1:A:721:GLN:NE2	5:E:109:LYS:HB2	2.36	0.41
17:A:801:CL0:H10	17:A:801:CL0:H72	1.65	0.41
18:A:807:CLA:CAD	18:A:826:CLA:HAA2	2.50	0.41
21:A:855:BCR:H291	11:K:72:PRO:HB2	2.02	0.41
2:B:419:ILE:HG21	2:B:536:LYS:HG3	2.03	0.41
2:B:716:GLY:O	2:B:720:THR:OG1	2.29	0.41
18:B:825:CLA:H61	18:B:825:CLA:H41	1.96	0.41
3:C:52:LYS:HD3	3:C:55:GLU:OE2	2.20	0.41
3:C:61:ASP:HA	3:C:62:PHE:HA	1.71	0.41
4:D:190:ARG:HH12	4:D:211:LEU:C	2.28	0.41
18:F:301:CLA:H61	21:F:305:BCR:H393	2.01	0.41
28:F:310:ZEX:H27	28:F:310:ZEX:H391	1.88	0.41
8:H:65:GLY:HA2	8:H:67:TRP:CZ2	2.56	0.41
11:K:94:GLY:C	18:K:1404:CLA:HAA1	2.46	0.41
12:L:139:VAL:O	12:L:143:ILE:HG13	2.20	0.41
18:L:304:CLA:HAA2	21:L:307:BCR:H352	2.02	0.41
13:1:150:SER:HB2	30:1:5016:CHL:CMA	2.51	0.41
13:1:154:ASP:N	13:1:155:PRO:HA	2.33	0.41
13:1:203:SER:OG	18:1:5018:CLA:H71	2.21	0.41
14:2:238:GLN:HE21	18:2:308:CLA:C1A	2.34	0.41
15:3:272:LEU:C	15:3:273:LYS:HD3	2.46	0.41
16:4:101:TRP:HD1	18:4:315:CLA:HMD3	1.84	0.41
1:A:296:LEU:HD23	1:A:296:LEU:HA	1.90	0.41
1:A:364:MET:HG3	18:A:823:CLA:HHB	2.03	0.41
18:A:853:CLA:H61	18:A:853:CLA:H41	1.49	0.41
2:B:453:ILE:HD13	26:J:1106:DGD:HA82	2.03	0.41
2:B:592:PHE:CE2	2:B:624:LEU:HD21	2.56	0.41
18:B:826:CLA:CAD	18:B:836:CLA:HBB1	2.51	0.41
18:G:1602:CLA:HMB1	18:G:1602:CLA:HBB1	2.02	0.41
14:2:87:PHE:HZ	31:2:304:XAT:H362	1.85	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:3:91:GLY:C	15:3:93:ILE:H	2.29	0.41
21:3:305:BCR:H402	30:3:312:CHL:C1B	2.51	0.41
18:4:305:CLA:H61	18:4:305:CLA:H41	1.95	0.41
1:A:325:HIS:CG	1:A:330:ILE:HD11	2.56	0.40
1:A:545:HIS:CE1	1:A:612:VAL:HA	2.56	0.40
2:B:649:MET:HA	2:B:652:PHE:HB3	2.03	0.40
18:B:832:CLA:HMC1	18:B:838:CLA:HAC1	2.03	0.40
11:K:104:THR:CG2	18:K:1404:CLA:HAB	2.51	0.40
13:1:160:TYR:HB3	18:1:5006:CLA:HED3	2.02	0.40
31:2:304:XAT:H15	31:2:304:XAT:H201	1.72	0.40
31:2:304:XAT:H28	18:2:309:CLA:H61	2.03	0.40
15:3:118:ALA:HB3	15:3:119:PRO:HD3	2.04	0.40
29:3:304:LUT:H15	29:3:304:LUT:H201	1.97	0.40
31:4:304:XAT:H201	31:4:304:XAT:H15	1.77	0.40
1:A:445:HIS:O	1:A:449:VAL:HG23	2.20	0.40
1:A:556:LEU:HD21	1:A:601:GLY:HA3	2.02	0.40
18:A:830:CLA:H143	18:A:830:CLA:H111	1.85	0.40
2:B:387:PHE:HB2	2:B:534:LEU:HD13	2.03	0.40
18:B:814:CLA:H193	18:B:814:CLA:H161	1.85	0.40
6:F:213:TRP:CZ3	21:F:305:BCR:H381	2.56	0.40
18:H:1701:CLA:HHB	18:L:304:CLA:HBA2	2.03	0.40
9:I:27:HIS:HA	9:I:30:LYS:HE3	2.03	0.40
21:1:5005:BCR:H351	21:1:5005:BCR:H15C	1.79	0.40
15:3:120:GLU:HG2	15:3:253:TYR:HB3	2.02	0.40
15:3:243:ILE:HG13	18:3:309:CLA:HAC2	2.04	0.40
1:A:529:LEU:HD23	1:A:529:LEU:HA	1.95	0.40
1:A:694:PHE:HB2	18:A:802:CLA:HBC2	2.03	0.40
2:B:227:THR:HG23	7:G:60:PRO:HG3	2.03	0.40
18:B:810:CLA:H193	21:I:101:BCR:H372	2.02	0.40
18:B:837:CLA:H3A	18:B:837:CLA:HBA2	1.80	0.40
12:L:128:GLN:H	12:L:128:GLN:HG2	1.63	0.40
18:1:5012:CLA:NC	22:1:5019:LHG:HC42	2.35	0.40
18:1:5013:CLA:HED3	16:4:143:VAL:HB	2.03	0.40
21:3:305:BCR:H383	30:3:312:CHL:CAB	2.50	0.40
1:A:455:PHE:HB3	18:A:831:CLA:HBB2	2.04	0.40
18:A:836:CLA:H102	22:A:849:LHG:H281	2.02	0.40
2:B:410:ARG:HH22	24:B:850:LMG:C6	2.33	0.40
2:B:569:ASP:OD1	2:B:706:ARG:NE	2.54	0.40
18:B:805:CLA:H162	18:B:805:CLA:H141	1.70	0.40
18:B:808:CLA:H112	18:B:808:CLA:H93	1.77	0.40
18:B:822:CLA:H92	24:1:5001:LMG:H161	2.03	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3:307:CLA:H3A	18:3:307:CLA:HBA2	1.41	0.40
16:4:215:PHE:O	16:4:219:ILE:HG12	2.21	0.40
1:A:382:TYR:CE1	18:A:827:CLA:HED2	2.57	0.40
1:A:416:ILE:HG23	1:A:420:ARG:HD3	2.03	0.40
2:B:85:ARG:HG3	8:H:139:LEU:HB2	2.03	0.40
2:B:598:HIS:HB3	2:B:602:TRP:CZ2	2.57	0.40
18:B:805:CLA:H3A	18:B:805:CLA:HBA2	1.55	0.40
30:1:5014:CHL:HHC	30:1:5014:CHL:CBB	2.48	0.40
29:2:303:LUT:H381	18:2:308:CLA:HBB1	2.04	0.40
29:3:304:LUT:H183	30:3:312:CHL:C3B	2.51	0.40
16:4:194:PHE:O	16:4:196:PRO:HD3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	741/743 (100%)	700 (94%)	40 (5%)	1 (0%)	48	80
2	B	731/733 (100%)	707 (97%)	23 (3%)	1 (0%)	48	80
3	C	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
4	D	141/143 (99%)	131 (93%)	9 (6%)	1 (1%)	18	53
5	E	64/66 (97%)	59 (92%)	5 (8%)	0	100	100
6	F	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
7	G	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
8	H	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
9	I	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
10	J	40/42 (95%)	38 (95%)	2 (5%)	0	100	100
11	K	78/80 (98%)	70 (90%)	8 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	155/157 (99%)	147 (95%)	8 (5%)	0	100	100
13	1	191/193 (99%)	181 (95%)	7 (4%)	3 (2%)	7	34
14	2	206/208 (99%)	189 (92%)	17 (8%)	0	100	100
15	3	219/221 (99%)	201 (92%)	18 (8%)	0	100	100
16	4	196/198 (99%)	188 (96%)	8 (4%)	0	100	100
All	All	3201/3233 (99%)	3034 (95%)	161 (5%)	6 (0%)	43	76

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	1	161	PRO
1	A	720	THR
2	B	492	ILE
13	1	115	PRO
13	1	154	ASP
4	D	107	SER

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	604/604 (100%)	599 (99%)	5 (1%)	73	86
2	B	598/598 (100%)	591 (99%)	7 (1%)	63	82
3	C	69/69 (100%)	69 (100%)	0	100	100
4	D	122/122 (100%)	122 (100%)	0	100	100
5	E	58/58 (100%)	57 (98%)	1 (2%)	53	78
6	F	125/126 (99%)	125 (100%)	0	100	100
7	G	82/82 (100%)	82 (100%)	0	100	100
8	H	71/71 (100%)	71 (100%)	0	100	100
9	I	26/26 (100%)	26 (100%)	0	100	100
10	J	35/35 (100%)	35 (100%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	58/58 (100%)	58 (100%)	0	100	100
12	L	124/124 (100%)	123 (99%)	1 (1%)	73	86
13	1	158/158 (100%)	158 (100%)	0	100	100
14	2	167/167 (100%)	166 (99%)	1 (1%)	78	88
15	3	171/172 (99%)	166 (97%)	5 (3%)	37	70
16	4	164/164 (100%)	164 (100%)	0	100	100
All	All	2632/2634 (100%)	2612 (99%)	20 (1%)	73	86

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	217	SER
1	A	230	ASN
1	A	267	THR
1	A	282	THR
1	A	377	TYR
2	B	220	GLN
2	B	256	THR
2	B	394	PHE
2	B	477	LEU
2	B	492	ILE
2	B	640	MET
2	B	702	ILE
5	E	74	VAL
12	L	109	LEU
14	2	242	THR
15	3	122	LEU
15	3	127	LEU
15	3	141	VAL
15	3	147	THR
15	3	273	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	HIS
1	A	485	GLN
1	A	712	ASN
2	B	98	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	B	241	ASN
2	B	482	ASN
2	B	603	GLN
2	B	608	GLN
7	G	90	GLN
8	H	130	GLN
13	1	217	HIS
13	1	228	ASN
14	2	186	ASN
15	3	244	GLN
16	4	222	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 240 ligands modelled in this entry, 2 are monoatomic - leaving 238 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	2	312	22	64,68,73	1.41	8 (12%)	76,107,113	1.91	16 (21%)
18	CLA	2	326	16	54,58,73	1.53	8 (14%)	64,95,113	2.04	16 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	3	309	-	59,63,73	1.47	8 (13%)	70,101,113	2.07	22 (31%)
23	LMT	J	1107	-	26,26,36	1.29	4 (15%)	37,37,47	1.07	2 (5%)
18	CLA	B	829	-	69,73,73	1.36	8 (11%)	82,113,113	1.81	17 (20%)
18	CLA	A	806	-	64,68,73	1.42	7 (10%)	76,107,113	1.90	17 (22%)
18	CLA	A	839	-	69,73,73	1.36	8 (11%)	82,113,113	1.80	16 (19%)
24	LMG	1	5020	-	46,46,55	1.04	3 (6%)	54,54,63	1.08	4 (7%)
24	LMG	2	324	-	13,13,55	0.58	0	18,18,63	0.68	0
22	LHG	A	848	-	48,48,48	0.38	0	51,54,54	1.05	3 (5%)
18	CLA	A	840	22	64,68,73	1.41	7 (10%)	76,107,113	1.93	17 (22%)
18	CLA	B	817	-	64,68,73	1.40	7 (10%)	76,107,113	1.90	19 (25%)
18	CLA	A	814	-	50,54,73	1.59	7 (14%)	59,90,113	2.03	15 (25%)
19	PQN	B	842	-	34,34,34	0.42	0	43,45,45	1.10	3 (6%)
30	CHL	2	316	-	42,56,74	1.56	9 (21%)	36,92,114	2.01	12 (33%)
18	CLA	J	1101	-	69,73,73	1.35	6 (8%)	82,113,113	1.91	19 (23%)
18	CLA	K	1401	-	49,53,73	1.61	8 (16%)	58,89,113	2.03	15 (25%)
18	CLA	1	5012	-	50,54,73	1.58	7 (14%)	59,90,113	2.03	15 (25%)
21	BCR	B	846	-	41,41,41	1.60	4 (9%)	56,56,56	4.40	13 (23%)
18	CLA	2	317	-	59,63,73	1.46	7 (11%)	70,101,113	1.96	16 (22%)
21	BCR	A	846	-	41,41,41	1.60	4 (9%)	56,56,56	4.41	14 (25%)
18	CLA	4	315	-	69,73,73	1.35	7 (10%)	82,113,113	1.88	17 (20%)
18	CLA	G	1603	-	69,73,73	1.36	8 (11%)	82,113,113	1.86	19 (23%)
18	CLA	A	812	-	69,73,73	1.34	7 (10%)	82,113,113	1.89	20 (24%)
18	CLA	B	809	-	69,73,73	1.35	6 (8%)	82,113,113	1.84	15 (18%)
18	CLA	1	5011	-	54,58,73	1.53	7 (12%)	64,95,113	2.05	17 (26%)
18	CLA	B	805	-	69,73,73	1.35	7 (10%)	82,113,113	1.83	17 (20%)
18	CLA	4	307	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	19 (23%)
20	SF4	C	101	3	0,12,12	-	-	-	-	-
18	CLA	A	810	-	69,73,73	1.35	7 (10%)	82,113,113	1.83	15 (18%)
21	BCR	I	101	-	41,41,41	1.64	4 (9%)	56,56,56	4.46	18 (32%)
24	LMG	2	301	-	13,13,55	0.57	0	18,18,63	0.59	0
23	LMT	2	325	-	36,36,36	1.13	4 (11%)	47,47,47	1.10	3 (6%)
18	CLA	1	5007	13	50,54,73	1.58	7 (14%)	59,90,113	2.02	17 (28%)
30	CHL	3	312	-	45,59,74	1.46	7 (15%)	40,96,114	1.97	11 (27%)
21	BCR	B	802	-	41,41,41	1.60	4 (9%)	56,56,56	4.86	18 (32%)
21	BCR	A	843	-	41,41,41	1.59	4 (9%)	56,56,56	4.48	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	B	807	2	69,73,73	1.35	7 (10%)	82,113,113	1.83	16 (19%)
18	CLA	1	5018	13	64,68,73	1.42	8 (12%)	76,107,113	1.89	20 (26%)
18	CLA	4	311	-	64,68,73	1.40	7 (10%)	76,107,113	1.92	19 (25%)
21	BCR	3	306	-	41,41,41	1.62	4 (9%)	56,56,56	4.21	19 (33%)
18	CLA	1	5008	-	59,63,73	1.46	7 (11%)	70,101,113	2.02	17 (24%)
24	LMG	F	306	-	47,47,55	1.09	4 (8%)	55,55,63	1.12	4 (7%)
18	CLA	A	853	-	69,73,73	1.35	5 (7%)	82,113,113	1.91	16 (19%)
24	LMG	B	850	-	35,35,55	0.79	1 (2%)	43,43,63	1.15	5 (11%)
18	CLA	1	5010	-	69,73,73	1.36	6 (8%)	82,113,113	1.90	19 (23%)
21	BCR	L	302	-	41,41,41	1.59	4 (9%)	56,56,56	4.61	20 (35%)
18	CLA	B	835	-	59,63,73	1.47	7 (11%)	70,101,113	1.99	20 (28%)
18	CLA	A	804	-	69,73,73	1.35	7 (10%)	82,113,113	1.90	18 (21%)
22	LHG	1	5019	-	48,48,48	0.40	0	51,54,54	1.06	3 (5%)
21	BCR	L	307	-	41,41,41	1.60	4 (9%)	56,56,56	4.50	15 (26%)
24	LMG	A	851	-	50,50,55	1.18	5 (10%)	58,58,63	1.07	3 (5%)
18	CLA	B	801	-	69,73,73	1.36	8 (11%)	82,113,113	1.90	18 (21%)
24	LMG	F	308	-	34,34,55	0.51	0	42,42,63	1.10	2 (4%)
25	GOL	4	321	-	5,5,5	0.56	0	5,5,5	0.29	0
17	CL0	A	801	-	58,73,73	3.28	17 (29%)	60,113,113	2.79	16 (26%)
18	CLA	A	852	-	69,73,73	1.36	8 (11%)	82,113,113	1.85	18 (21%)
18	CLA	B	838	-	54,58,73	1.53	7 (12%)	64,95,113	2.07	20 (31%)
29	LUT	3	303	-	42,43,43	2.47	1 (2%)	51,60,60	1.82	15 (29%)
18	CLA	L	305	-	64,68,73	1.40	7 (10%)	76,107,113	1.95	19 (25%)
18	CLA	4	312	-	50,54,73	1.58	7 (14%)	59,90,113	2.06	15 (25%)
18	CLA	2	307	14	56,60,73	1.51	8 (14%)	65,97,113	2.04	19 (29%)
18	CLA	A	828	-	69,73,73	1.36	7 (10%)	82,113,113	1.90	16 (19%)
21	BCR	B	847	-	41,41,41	1.60	4 (9%)	56,56,56	4.54	14 (25%)
24	LMG	B	854	-	13,13,55	0.56	0	18,18,63	0.73	0
26	DGD	F	309	-	58,58,67	1.12	4 (6%)	72,72,81	1.07	2 (2%)
30	CHL	2	319	-	50,64,74	1.36	8 (16%)	46,102,114	1.86	12 (26%)
18	CLA	B	834	-	64,68,73	1.41	8 (12%)	76,107,113	1.88	14 (18%)
29	LUT	4	303	-	42,43,43	2.48	1 (2%)	51,60,60	1.81	13 (25%)
24	LMG	F	307	-	36,36,55	0.79	1 (2%)	44,44,63	1.05	2 (4%)
18	CLA	B	841	22	69,73,73	1.36	7 (10%)	82,113,113	1.82	20 (24%)
18	CLA	A	813	-	69,73,73	1.35	6 (8%)	82,113,113	1.91	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	B	804	-	69,73,73	1.35	6 (8%)	82,113,113	1.82	19 (23%)
28	ZEX	F	310	-	43,43,43	0.74	1 (2%)	51,60,60	2.01	13 (25%)
21	BCR	B	844	-	41,41,41	1.59	4 (9%)	56,56,56	4.51	17 (30%)
18	CLA	1	5015	-	69,73,73	1.35	7 (10%)	82,113,113	1.85	16 (19%)
18	CLA	1	5009	-	69,73,73	1.36	6 (8%)	82,113,113	1.89	18 (21%)
18	CLA	2	308	-	69,73,73	1.35	7 (10%)	82,113,113	1.96	18 (21%)
18	CLA	A	816	-	60,64,73	1.45	7 (11%)	71,102,113	1.96	19 (26%)
30	CHL	4	317	-	37,51,74	1.58	9 (24%)	30,86,114	2.27	10 (33%)
18	CLA	B	831	-	69,73,73	1.36	7 (10%)	82,113,113	1.89	19 (23%)
18	CLA	A	837	-	69,73,73	1.36	7 (10%)	82,113,113	1.84	15 (18%)
18	CLA	H	1701	-	64,68,73	1.41	6 (9%)	76,107,113	1.93	18 (23%)
18	CLA	F	302	-	69,73,73	1.36	8 (11%)	82,113,113	1.82	18 (21%)
18	CLA	B	839	-	69,73,73	1.36	7 (10%)	82,113,113	1.86	17 (20%)
18	CLA	B	819	-	69,73,73	1.34	7 (10%)	82,113,113	1.92	19 (23%)
18	CLA	2	313	-	54,58,73	1.53	7 (12%)	64,95,113	2.12	19 (29%)
24	LMG	2	322	-	36,36,55	0.69	1 (2%)	44,44,63	1.07	2 (4%)
18	CLA	B	830	-	69,73,73	1.38	8 (11%)	82,113,113	1.91	16 (19%)
18	CLA	G	1601	-	59,63,73	1.47	7 (11%)	70,101,113	1.98	17 (24%)
20	SF4	C	102	3	0,12,12	-	-	-	-	-
21	BCR	F	304	-	41,41,41	1.60	4 (9%)	56,56,56	4.50	16 (28%)
18	CLA	1	5017	-	49,53,73	1.61	7 (14%)	58,89,113	2.03	14 (24%)
21	BCR	A	855	-	41,41,41	1.60	4 (9%)	56,56,56	4.56	17 (30%)
18	CLA	3	308	-	56,60,73	1.50	7 (12%)	65,97,113	2.04	18 (27%)
18	CLA	4	309	-	64,68,73	1.41	7 (10%)	76,107,113	1.94	20 (26%)
22	LHG	2	320	18	34,34,48	0.45	0	37,40,54	1.16	3 (8%)
18	CLA	A	805	-	69,73,73	1.36	7 (10%)	82,113,113	1.82	18 (21%)
18	CLA	B	816	-	59,63,73	1.46	7 (11%)	70,101,113	2.05	21 (30%)
18	CLA	B	820	-	69,73,73	1.34	7 (10%)	82,113,113	1.81	17 (20%)
18	CLA	A	823	-	69,73,73	1.36	8 (11%)	82,113,113	1.94	19 (23%)
26	DGD	2	327	-	52,52,67	0.98	3 (5%)	66,66,81	1.10	5 (7%)
30	CHL	2	318	-	40,54,74	1.52	9 (22%)	34,90,114	2.11	10 (29%)
21	BCR	K	1405	-	41,41,41	1.61	4 (9%)	56,56,56	4.45	18 (32%)
30	CHL	2	314	14	60,74,74	1.34	8 (13%)	58,114,114	1.70	12 (20%)
24	LMG	G	1607	-	25,25,55	0.69	1 (4%)	33,33,63	1.29	5 (15%)
18	CLA	A	807	1	69,73,73	1.35	7 (10%)	82,113,113	1.89	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	BCR	1	5005	-	41,41,41	1.59	4 (9%)	56,56,56	4.51	15 (26%)
25	GOL	A	854	-	5,5,5	0.56	0	5,5,5	0.30	0
30	CHL	4	316	-	55,69,74	1.35	10 (18%)	52,108,114	1.76	12 (23%)
18	CLA	B	822	-	69,73,73	1.36	7 (10%)	82,113,113	1.89	18 (21%)
24	LMG	1	5001	-	49,49,55	1.14	5 (10%)	57,57,63	1.13	4 (7%)
18	CLA	3	315	15	69,73,73	1.35	7 (10%)	82,113,113	1.81	17 (20%)
18	CLA	2	311	-	54,58,73	1.51	7 (12%)	64,95,113	2.09	18 (28%)
18	CLA	3	307	-	59,63,73	1.48	7 (11%)	70,101,113	1.97	20 (28%)
18	CLA	A	824	-	59,63,73	1.48	8 (13%)	70,101,113	1.95	16 (22%)
30	CHL	3	313	-	45,59,74	1.42	7 (15%)	40,96,114	2.02	11 (27%)
18	CLA	B	811	-	69,73,73	1.36	8 (11%)	82,113,113	1.83	18 (21%)
18	CLA	A	831	-	69,73,73	1.35	7 (10%)	82,113,113	1.88	21 (25%)
24	LMG	2	323	-	13,13,55	0.63	0	18,18,63	0.93	1 (5%)
31	XAT	2	304	-	41,47,47	0.71	1 (2%)	54,74,74	1.82	10 (18%)
18	CLA	B	810	2	69,73,73	1.36	7 (10%)	82,113,113	1.81	17 (20%)
18	CLA	K	1403	-	52,56,73	1.56	6 (11%)	61,92,113	2.19	17 (27%)
30	CHL	4	318	-	50,64,74	1.35	7 (14%)	46,102,114	1.86	12 (26%)
18	CLA	4	308	-	64,68,73	1.41	7 (10%)	76,107,113	1.97	18 (23%)
20	SF4	A	842	2,1	0,12,12	-	-	-	-	-
18	CLA	A	836	-	69,73,73	1.35	7 (10%)	82,113,113	1.85	20 (24%)
18	CLA	B	803	-	69,73,73	1.37	6 (8%)	82,113,113	1.78	13 (15%)
18	CLA	B	837	-	69,73,73	1.34	7 (10%)	82,113,113	1.90	18 (21%)
18	CLA	A	803	-	69,73,73	1.34	7 (10%)	82,113,113	1.90	21 (25%)
18	CLA	2	306	-	64,68,73	1.40	7 (10%)	76,107,113	1.93	19 (25%)
18	CLA	1	5013	-	50,54,73	1.58	6 (12%)	59,90,113	2.10	13 (22%)
22	LHG	B	849	-	48,48,48	0.40	0	51,54,54	1.03	2 (3%)
30	CHL	1	5014	-	41,55,74	1.43	7 (17%)	35,91,114	2.10	11 (31%)
18	CLA	B	821	-	50,54,73	1.59	7 (14%)	59,90,113	2.04	14 (23%)
23	LMT	B	852	-	36,36,36	1.12	4 (11%)	47,47,47	1.08	2 (4%)
18	CLA	A	829	-	69,73,73	1.35	8 (11%)	82,113,113	1.91	18 (21%)
18	CLA	3	318	-	50,54,73	1.59	6 (12%)	59,90,113	1.99	14 (23%)
18	CLA	3	314	-	52,56,73	1.56	8 (15%)	61,92,113	2.09	18 (29%)
18	CLA	B	828	-	69,73,73	1.36	6 (8%)	82,113,113	1.88	16 (19%)
18	CLA	A	815	-	69,73,73	1.35	7 (10%)	82,113,113	1.84	18 (21%)
18	CLA	4	305	-	64,68,73	1.41	7 (10%)	76,107,113	1.90	21 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	B	827	-	69,73,73	1.37	7 (10%)	82,113,113	1.92	19 (23%)
19	PQN	A	841	-	34,34,34	0.43	0	43,45,45	1.15	4 (9%)
30	CHL	4	313	-	41,55,74	1.51	8 (19%)	35,91,114	2.14	11 (31%)
18	CLA	4	310	-	54,58,73	1.52	7 (12%)	64,95,113	2.03	15 (23%)
18	CLA	3	317	-	54,58,73	1.51	7 (12%)	64,95,113	2.14	19 (29%)
21	BCR	4	301	-	41,41,41	1.62	4 (9%)	56,56,56	4.45	17 (30%)
30	CHL	1	5016	-	55,69,74	1.39	8 (14%)	52,108,114	1.72	11 (21%)
18	CLA	B	815	-	69,73,73	1.35	7 (10%)	82,113,113	1.90	16 (19%)
18	CLA	B	833	-	62,66,73	1.43	6 (9%)	73,104,113	2.03	19 (26%)
18	CLA	J	1103	-	54,58,73	1.54	8 (14%)	64,95,113	2.08	19 (29%)
21	BCR	F	305	-	41,41,41	1.60	4 (9%)	56,56,56	4.61	19 (33%)
24	LMG	2	321	-	25,25,55	0.56	0	33,33,63	1.07	3 (9%)
24	LMG	4	320	-	13,13,55	0.56	0	18,18,63	0.68	0
18	CLA	A	802	-	69,73,73	1.35	7 (10%)	82,113,113	1.75	16 (19%)
18	CLA	A	827	-	69,73,73	1.36	7 (10%)	82,113,113	1.83	15 (18%)
18	CLA	A	809	-	54,58,73	1.52	7 (12%)	64,95,113	2.04	18 (28%)
21	BCR	A	847	-	41,41,41	1.60	4 (9%)	56,56,56	4.48	19 (33%)
29	LUT	2	303	-	42,43,43	2.43	1 (2%)	51,60,60	1.94	13 (25%)
30	CHL	4	314	-	45,59,74	1.59	8 (17%)	40,96,114	2.05	12 (30%)
18	CLA	3	301	-	49,53,73	1.60	7 (14%)	58,89,113	1.97	14 (24%)
18	CLA	L	306	-	54,58,73	1.53	7 (12%)	64,95,113	2.05	18 (28%)
18	CLA	B	812	-	64,68,73	1.41	6 (9%)	76,107,113	1.86	18 (23%)
18	CLA	L	304	12	54,58,73	1.52	6 (11%)	64,95,113	2.09	17 (26%)
18	CLA	B	826	-	69,73,73	1.35	7 (10%)	82,113,113	1.93	17 (20%)
18	CLA	L	301	-	59,63,73	1.47	7 (11%)	70,101,113	1.94	19 (27%)
18	CLA	B	836	-	59,63,73	1.48	8 (13%)	70,101,113	1.98	18 (25%)
18	CLA	1	5006	13	69,73,73	1.37	7 (10%)	82,113,113	1.85	19 (23%)
21	BCR	B	843	-	41,41,41	1.61	4 (9%)	56,56,56	4.79	19 (33%)
18	CLA	B	825	-	69,73,73	1.36	7 (10%)	82,113,113	1.92	16 (19%)
18	CLA	B	813	-	50,54,73	1.59	6 (12%)	59,90,113	2.03	12 (20%)
21	BCR	L	303	-	41,41,41	1.61	4 (9%)	56,56,56	4.52	14 (25%)
18	CLA	A	825	-	69,73,73	1.37	8 (11%)	82,113,113	1.91	20 (24%)
23	LMT	4	319	-	36,36,36	1.12	4 (11%)	47,47,47	0.98	2 (4%)
18	CLA	A	835	-	69,73,73	1.35	7 (10%)	82,113,113	1.87	17 (20%)
18	CLA	G	1602	7	50,54,73	1.60	8 (16%)	59,90,113	2.02	12 (20%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	4	306	-	54,58,73	1.53	8 (14%)	64,95,113	2.12	20 (31%)
21	BCR	3	305	-	41,41,41	1.59	4 (9%)	56,56,56	4.51	14 (25%)
26	DGD	1	5002	-	35,35,67	0.98	2 (5%)	43,43,81	1.11	3 (6%)
18	CLA	K	1404	-	50,54,73	1.60	8 (16%)	59,90,113	2.03	13 (22%)
30	CHL	2	315	-	50,64,74	1.31	8 (16%)	46,102,114	1.85	12 (26%)
22	LHG	B	848	18	20,20,48	0.59	0	23,26,54	1.56	2 (8%)
18	CLA	A	817	-	69,73,73	1.36	7 (10%)	82,113,113	1.82	18 (21%)
18	CLA	A	834	-	55,59,73	1.52	7 (12%)	64,96,113	2.06	17 (26%)
18	CLA	B	840	-	69,73,73	1.35	6 (8%)	82,113,113	1.88	19 (23%)
18	CLA	A	821	-	64,68,73	1.41	7 (10%)	76,107,113	1.93	17 (22%)
21	BCR	B	845	-	41,41,41	1.59	4 (9%)	56,56,56	4.23	19 (33%)
21	BCR	J	1104	-	41,41,41	1.60	4 (9%)	56,56,56	4.45	14 (25%)
23	LMT	A	850	-	36,36,36	1.09	3 (8%)	47,47,47	1.17	1 (2%)
29	LUT	J	1105	-	42,43,43	2.45	1 (2%)	51,60,60	2.17	11 (21%)
18	CLA	A	838	-	69,73,73	1.37	8 (11%)	82,113,113	1.83	15 (18%)
18	CLA	A	830	-	69,73,73	1.35	7 (10%)	82,113,113	1.83	17 (20%)
26	DGD	B	855	-	62,62,67	1.21	6 (9%)	76,76,81	0.99	3 (3%)
30	CHL	4	302	13	50,64,74	1.34	8 (16%)	46,102,114	1.94	12 (26%)
30	CHL	3	316	-	41,55,74	1.58	9 (21%)	35,91,114	2.09	9 (25%)
18	CLA	B	814	-	69,73,73	1.36	6 (8%)	82,113,113	1.92	18 (21%)
18	CLA	B	832	-	64,68,73	1.41	6 (9%)	76,107,113	1.90	18 (23%)
18	CLA	B	818	-	69,73,73	1.35	6 (8%)	82,113,113	1.83	18 (21%)
18	CLA	2	309	14	69,73,73	1.36	7 (10%)	82,113,113	1.90	17 (20%)
18	CLA	A	818	-	54,58,73	1.54	7 (12%)	64,95,113	2.06	17 (26%)
18	CLA	F	303	6	69,73,73	1.36	7 (10%)	82,113,113	1.84	19 (23%)
18	CLA	A	808	1	69,73,73	1.37	7 (10%)	82,113,113	1.85	18 (21%)
18	CLA	3	319	-	64,68,73	1.40	7 (10%)	76,107,113	1.92	17 (22%)
30	CHL	3	310	-	60,74,74	1.26	7 (11%)	58,114,114	1.80	11 (18%)
24	LMG	2	302	-	13,13,55	0.57	0	18,18,63	0.62	0
21	BCR	A	845	-	41,41,41	1.63	4 (9%)	56,56,56	4.49	18 (32%)
18	CLA	B	806	-	69,73,73	1.33	7 (10%)	82,113,113	1.91	18 (21%)
18	CLA	A	822	-	69,73,73	1.36	7 (10%)	82,113,113	1.83	18 (21%)
23	LMT	G	1606	-	32,32,36	1.18	4 (12%)	43,43,47	1.01	1 (2%)
23	LMT	B	853	-	33,33,36	1.19	5 (15%)	44,44,47	1.13	2 (4%)
18	CLA	F	301	-	69,73,73	1.36	7 (10%)	82,113,113	1.84	20 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	XAT	4	304	-	41,47,47	0.69	1 (2%)	54,74,74	1.93	12 (22%)
18	CLA	3	311	-	59,63,73	1.48	8 (13%)	70,101,113	1.96	19 (27%)
18	CLA	A	833	1	59,63,73	1.47	8 (13%)	70,101,113	1.98	17 (24%)
21	BCR	G	1604	-	41,41,41	1.60	4 (9%)	56,56,56	4.52	14 (25%)
18	CLA	B	808	-	69,73,73	1.36	7 (10%)	82,113,113	1.82	17 (20%)
29	LUT	1	5004	-	42,43,43	2.48	1 (2%)	51,60,60	1.97	12 (23%)
18	CLA	A	811	-	59,63,73	1.46	6 (10%)	70,101,113	1.99	19 (27%)
23	LMT	B	856	-	32,32,36	1.19	5 (15%)	43,43,47	1.04	3 (6%)
21	BCR	A	844	-	41,41,41	1.59	4 (9%)	56,56,56	4.46	16 (28%)
18	CLA	2	310	-	69,73,73	1.34	7 (10%)	82,113,113	2.04	20 (24%)
18	CLA	A	820	-	64,68,73	1.41	7 (10%)	76,107,113	1.91	16 (21%)
26	DGD	J	1106	-	59,59,67	1.16	6 (10%)	73,73,81	1.21	5 (6%)
29	LUT	1	5003	-	42,43,43	2.50	1 (2%)	51,60,60	1.87	13 (25%)
21	BCR	I	102	-	41,41,41	1.59	4 (9%)	56,56,56	4.42	14 (25%)
21	BCR	2	305	-	41,41,41	1.63	4 (9%)	56,56,56	5.13	27 (48%)
18	CLA	K	1402	-	64,68,73	1.42	8 (12%)	76,107,113	1.90	17 (22%)
18	CLA	B	824	-	59,63,73	1.47	7 (11%)	70,101,113	1.92	17 (24%)
29	LUT	3	304	-	42,43,43	2.45	1 (2%)	51,60,60	1.92	10 (19%)
22	LHG	A	849	18	39,39,48	0.42	0	42,45,54	1.26	5 (11%)
23	LMT	G	1605	-	36,36,36	1.12	4 (11%)	47,47,47	1.01	1 (2%)
18	CLA	A	826	-	69,73,73	1.35	6 (8%)	82,113,113	1.86	17 (20%)
18	CLA	A	819	-	69,73,73	1.35	7 (10%)	82,113,113	1.74	16 (19%)
24	LMG	J	1102	-	30,30,55	0.55	0	38,38,63	1.11	3 (7%)
18	CLA	A	832	-	69,73,73	1.35	7 (10%)	82,113,113	1.81	21 (25%)
24	LMG	B	851	-	33,33,55	0.58	1 (3%)	41,41,63	1.45	7 (17%)
18	CLA	B	823	-	69,73,73	1.35	7 (10%)	82,113,113	1.85	18 (21%)

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
18	CLA	2	312	22	1/1/14/20	17/33/109/115	-
18	CLA	2	326	16	1/1/12/20	9/21/97/115	-
18	CLA	3	309	-	1/1/13/20	11/27/103/115	-

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LMT	J	1107	-	-	5/11/51/61	0/2/2/2
18	CLA	B	829	-	1/1/15/20	18/39/115/115	-
18	CLA	A	806	-	1/1/14/20	16/33/109/115	-
18	CLA	A	839	-	1/1/15/20	5/39/115/115	-
24	LMG	1	5020	-	-	10/41/61/70	0/1/1/1
24	LMG	2	324	-	-	4/4/24/70	0/1/1/1
22	LHG	A	848	-	-	31/53/53/53	-
18	CLA	A	840	22	1/1/14/20	10/33/109/115	-
18	CLA	B	817	-	1/1/14/20	9/33/109/115	-
18	CLA	A	814	-	1/1/11/20	8/17/93/115	-
30	CHL	2	316	-	3/3/16/26	2/18/116/137	-
19	PQN	B	842	-	-	8/23/43/43	0/2/2/2
18	CLA	J	1101	-	1/1/15/20	14/39/115/115	-
18	CLA	K	1401	-	1/1/11/20	5/15/91/115	-
18	CLA	1	5012	-	1/1/11/20	5/17/93/115	-
21	BCR	B	846	-	-	8/29/63/63	0/2/2/2
18	CLA	2	317	-	1/1/13/20	8/27/103/115	-
21	BCR	A	846	-	-	14/29/63/63	0/2/2/2
18	CLA	4	315	-	1/1/15/20	19/39/115/115	-
18	CLA	G	1603	-	1/1/15/20	18/39/115/115	-
18	CLA	A	812	-	1/1/15/20	17/39/115/115	-
18	CLA	B	809	-	1/1/15/20	8/39/115/115	-
18	CLA	1	5011	-	1/1/12/20	5/21/97/115	-
18	CLA	B	805	-	1/1/15/20	20/39/115/115	-
18	CLA	4	307	-	1/1/15/20	15/39/115/115	-
21	BCR	I	101	-	-	15/29/63/63	0/2/2/2
18	CLA	A	810	-	1/1/15/20	19/39/115/115	-
24	LMG	2	301	-	-	3/4/24/70	0/1/1/1
20	SF4	C	101	3	-	-	0/6/5/5
23	LMT	2	325	-	-	9/21/61/61	0/2/2/2
18	CLA	1	5007	13	1/1/11/20	7/17/93/115	-
30	CHL	3	312	-	3/3/17/26	2/21/119/137	-
21	BCR	B	802	-	-	7/29/63/63	0/2/2/2
21	BCR	A	843	-	-	14/29/63/63	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	807	2	1/1/15/20	13/39/115/115	-
18	CLA	1	5018	13	1/1/14/20	18/33/109/115	-
18	CLA	4	311	-	1/1/14/20	12/33/109/115	-
21	BCR	3	306	-	-	14/29/63/63	0/2/2/2
18	CLA	1	5008	-	1/1/13/20	7/27/103/115	-
24	LMG	F	306	-	-	7/42/62/70	0/1/1/1
18	CLA	A	853	-	1/1/15/20	17/39/115/115	-
24	LMG	B	850	-	-	9/30/50/70	0/1/1/1
18	CLA	1	5010	-	1/1/15/20	12/39/115/115	-
21	BCR	L	302	-	-	12/29/63/63	0/2/2/2
18	CLA	B	835	-	1/1/13/20	9/27/103/115	-
18	CLA	A	804	-	1/1/15/20	23/39/115/115	-
22	LHG	1	5019	-	-	22/53/53/53	-
21	BCR	L	307	-	-	14/29/63/63	0/2/2/2
24	LMG	A	851	-	-	18/45/65/70	0/1/1/1
18	CLA	B	801	-	1/1/15/20	15/39/115/115	-
24	LMG	F	308	-	-	12/29/49/70	0/1/1/1
25	GOL	4	321	-	-	0/4/4/4	-
17	CL0	A	801	-	3/3/20/25	7/37/135/135	-
18	CLA	A	852	-	1/1/15/20	16/39/115/115	-
18	CLA	B	838	-	1/1/12/20	5/21/97/115	-
29	LUT	3	303	-	-	3/29/67/67	0/2/2/2
18	CLA	L	305	-	1/1/14/20	17/33/109/115	-
18	CLA	4	312	-	1/1/11/20	7/17/93/115	-
18	CLA	2	307	14	1/1/12/20	8/24/100/115	-
18	CLA	A	828	-	1/1/15/20	15/39/115/115	-
21	BCR	B	847	-	-	14/29/63/63	0/2/2/2
30	CHL	2	319	-	4/4/18/26	7/27/125/137	-
24	LMG	B	851	-	-	10/28/48/70	0/1/1/1
24	LMG	B	854	-	-	1/4/24/70	0/1/1/1
26	DGD	F	309	-	-	17/46/86/95	0/2/2/2
18	CLA	B	834	-	1/1/14/20	12/33/109/115	-
29	LUT	4	303	-	-	4/29/67/67	0/2/2/2
24	LMG	F	307	-	-	9/31/51/70	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	841	22	1/1/15/20	15/39/115/115	-
18	CLA	A	813	-	1/1/15/20	15/39/115/115	-
18	CLA	B	804	-	1/1/15/20	14/39/115/115	-
28	ZEX	F	310	-	-	3/29/67/67	0/2/2/2
21	BCR	B	844	-	-	10/29/63/63	0/2/2/2
18	CLA	1	5015	-	1/1/15/20	18/39/115/115	-
18	CLA	1	5009	-	1/1/15/20	15/39/115/115	-
18	CLA	2	308	-	1/1/15/20	17/39/115/115	-
18	CLA	A	816	-	1/1/13/20	16/29/105/115	-
18	CLA	B	831	-	1/1/15/20	15/39/115/115	-
18	CLA	A	837	-	1/1/15/20	7/39/115/115	-
18	CLA	H	1701	-	1/1/14/20	11/33/109/115	-
18	CLA	F	302	-	1/1/15/20	19/39/115/115	-
18	CLA	B	839	-	1/1/15/20	18/39/115/115	-
18	CLA	B	819	-	1/1/15/20	18/39/115/115	-
18	CLA	2	313	-	1/1/12/20	12/21/97/115	-
24	LMG	2	322	-	-	17/31/51/70	0/1/1/1
18	CLA	B	830	-	1/1/15/20	14/39/115/115	-
18	CLA	G	1601	-	1/1/13/20	9/27/103/115	-
20	SF4	C	102	3	-	-	0/6/5/5
21	BCR	F	304	-	-	8/29/63/63	0/2/2/2
18	CLA	1	5017	-	1/1/11/20	6/15/91/115	-
21	BCR	A	855	-	-	9/29/63/63	0/2/2/2
18	CLA	3	308	-	1/1/12/20	9/24/100/115	-
18	CLA	4	309	-	1/1/14/20	14/33/109/115	-
22	LHG	2	320	18	-	17/39/39/53	-
18	CLA	A	805	-	1/1/15/20	17/39/115/115	-
18	CLA	B	816	-	1/1/13/20	5/27/103/115	-
18	CLA	B	820	-	1/1/15/20	13/39/115/115	-
18	CLA	A	823	-	1/1/15/20	18/39/115/115	-
30	CHL	2	318	-	3/3/16/26	4/15/113/137	-
26	DGD	2	327	-	-	15/40/80/95	0/2/2/2
21	BCR	K	1405	-	-	13/29/63/63	0/2/2/2
30	CHL	2	314	14	4/4/20/26	9/39/137/137	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LMG	G	1607	-	-	8/20/40/70	0/1/1/1
18	CLA	A	807	1	1/1/15/20	15/39/115/115	-
21	BCR	1	5005	-	-	9/29/63/63	0/2/2/2
25	GOL	A	854	-	-	1/4/4/4	-
30	CHL	4	316	-	4/4/19/26	7/33/131/137	-
18	CLA	B	822	-	1/1/15/20	14/39/115/115	-
24	LMG	1	5001	-	-	15/44/64/70	0/1/1/1
18	CLA	3	315	15	1/1/15/20	23/39/115/115	-
18	CLA	2	311	-	1/1/12/20	9/21/97/115	-
18	CLA	3	307	-	1/1/13/20	9/27/103/115	-
18	CLA	A	824	-	1/1/13/20	15/27/103/115	-
30	CHL	3	313	-	3/3/17/26	3/21/119/137	-
18	CLA	B	811	-	1/1/15/20	16/39/115/115	-
18	CLA	A	831	-	1/1/15/20	23/39/115/115	-
31	XAT	2	304	-	1/1/12/26	4/31/93/93	0/4/4/4
24	LMG	2	323	-	-	0/4/24/70	0/1/1/1
18	CLA	B	810	2	1/1/15/20	14/39/115/115	-
18	CLA	K	1403	-	1/1/11/20	10/19/95/115	-
30	CHL	4	318	-	4/4/18/26	6/27/125/137	-
18	CLA	4	308	-	1/1/14/20	19/33/109/115	-
20	SF4	A	842	2,1	-	-	0/6/5/5
18	CLA	A	836	-	1/1/15/20	15/39/115/115	-
18	CLA	B	803	-	1/1/15/20	11/39/115/115	-
18	CLA	B	837	-	1/1/15/20	20/39/115/115	-
18	CLA	A	803	-	1/1/15/20	21/39/115/115	-
18	CLA	2	306	-	1/1/14/20	9/33/109/115	-
18	CLA	1	5013	-	1/1/11/20	8/17/93/115	-
22	LHG	B	849	-	-	34/53/53/53	-
30	CHL	1	5014	-	3/3/16/26	3/17/115/137	-
18	CLA	B	821	-	1/1/11/20	7/17/93/115	-
23	LMT	B	852	-	-	13/21/61/61	0/2/2/2
18	CLA	A	829	-	1/1/15/20	15/39/115/115	-
18	CLA	3	318	-	1/1/11/20	6/17/93/115	-
18	CLA	3	314	-	1/1/11/20	7/19/95/115	-
18	CLA	B	828	-	1/1/15/20	22/39/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	815	-	1/1/15/20	11/39/115/115	-
18	CLA	4	305	-	1/1/14/20	9/33/109/115	-
18	CLA	B	827	-	1/1/15/20	9/39/115/115	-
30	CHL	4	313	-	3/3/16/26	1/17/115/137	-
19	PQN	A	841	-	-	6/23/43/43	0/2/2/2
18	CLA	4	310	-	1/1/12/20	8/21/97/115	-
18	CLA	3	317	-	1/1/12/20	7/21/97/115	-
21	BCR	4	301	-	-	13/29/63/63	0/2/2/2
30	CHL	1	5016	-	4/4/19/26	7/33/131/137	-
18	CLA	B	815	-	1/1/15/20	16/39/115/115	-
18	CLA	B	833	-	1/1/13/20	14/31/107/115	-
18	CLA	J	1103	-	1/1/12/20	7/21/97/115	-
21	BCR	F	305	-	-	14/29/63/63	0/2/2/2
24	LMG	2	321	-	-	5/20/40/70	0/1/1/1
24	LMG	4	320	-	-	0/4/24/70	0/1/1/1
18	CLA	A	802	-	1/1/15/20	20/39/115/115	-
18	CLA	A	827	-	1/1/15/20	15/39/115/115	-
18	CLA	A	809	-	1/1/12/20	8/21/97/115	-
21	BCR	A	847	-	-	13/29/63/63	0/2/2/2
29	LUT	2	303	-	1/1/12/27	3/29/67/67	0/2/2/2
30	CHL	4	314	-	3/3/17/26	2/21/119/137	-
18	CLA	3	301	-	1/1/11/20	4/15/91/115	-
18	CLA	L	306	-	1/1/12/20	8/21/97/115	-
18	CLA	B	812	-	1/1/14/20	9/33/109/115	-
18	CLA	L	304	12	1/1/12/20	7/21/97/115	-
18	CLA	B	826	-	1/1/15/20	18/39/115/115	-
18	CLA	L	301	-	1/1/13/20	10/27/103/115	-
18	CLA	B	836	-	1/1/13/20	9/27/103/115	-
18	CLA	1	5006	13	1/1/15/20	15/39/115/115	-
21	BCR	B	843	-	-	10/29/63/63	0/2/2/2
18	CLA	B	825	-	1/1/15/20	13/39/115/115	-
18	CLA	B	813	-	1/1/11/20	4/17/93/115	-
21	BCR	L	303	-	-	12/29/63/63	0/2/2/2
18	CLA	A	825	-	1/1/15/20	16/39/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LMT	4	319	-	-	4/21/61/61	0/2/2/2
18	CLA	A	835	-	1/1/15/20	11/39/115/115	-
18	CLA	G	1602	7	1/1/11/20	6/17/93/115	-
18	CLA	4	306	-	1/1/12/20	9/21/97/115	-
21	BCR	3	305	-	-	12/29/63/63	0/2/2/2
26	DGD	1	5002	-	-	11/29/49/95	0/1/1/2
18	CLA	K	1404	-	1/1/11/20	8/17/93/115	-
30	CHL	2	315	-	4/4/18/26	7/27/125/137	-
22	LHG	B	848	18	-	9/23/23/53	-
18	CLA	A	817	-	1/1/15/20	16/39/115/115	-
18	CLA	A	834	-	1/1/12/20	9/23/99/115	-
18	CLA	B	840	-	1/1/15/20	18/39/115/115	-
18	CLA	A	821	-	1/1/14/20	9/33/109/115	-
29	LUT	J	1105	-	1/1/12/27	4/29/67/67	0/2/2/2
21	BCR	B	845	-	-	14/29/63/63	0/2/2/2
21	BCR	J	1104	-	-	15/29/63/63	0/2/2/2
23	LMT	A	850	-	-	11/21/61/61	0/2/2/2
18	CLA	A	838	-	1/1/15/20	15/39/115/115	-
18	CLA	A	830	-	1/1/15/20	12/39/115/115	-
30	CHL	4	302	13	4/4/18/26	4/27/125/137	-
26	DGD	B	855	-	-	19/50/90/95	0/2/2/2
30	CHL	3	316	-	3/3/16/26	4/17/115/137	-
18	CLA	B	814	-	1/1/15/20	13/39/115/115	-
18	CLA	B	832	-	1/1/14/20	18/33/109/115	-
18	CLA	B	818	-	1/1/15/20	15/39/115/115	-
18	CLA	2	309	14	1/1/15/20	19/39/115/115	-
18	CLA	A	818	-	1/1/12/20	7/21/97/115	-
18	CLA	F	303	6	1/1/15/20	18/39/115/115	-
18	CLA	A	808	1	1/1/15/20	19/39/115/115	-
18	CLA	3	319	-	1/1/14/20	20/33/109/115	-
30	CHL	3	310	-	4/4/20/26	12/39/137/137	-
24	LMG	2	302	-	-	0/4/24/70	0/1/1/1
21	BCR	A	845	-	-	11/29/63/63	0/2/2/2
18	CLA	B	806	-	1/1/15/20	16/39/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	822	-	1/1/15/20	15/39/115/115	-
23	LMT	G	1606	-	-	13/17/57/61	0/2/2/2
23	LMT	B	853	-	-	9/18/58/61	0/2/2/2
18	CLA	F	301	-	1/1/15/20	18/39/115/115	-
31	XAT	4	304	-	1/1/12/26	0/31/93/93	0/4/4/4
18	CLA	3	311	-	1/1/13/20	7/27/103/115	-
18	CLA	A	833	1	1/1/13/20	9/27/103/115	-
29	LUT	1	5004	-	1/1/12/27	4/29/67/67	0/2/2/2
18	CLA	B	808	-	1/1/15/20	13/39/115/115	-
21	BCR	G	1604	-	-	8/29/63/63	0/2/2/2
18	CLA	A	811	-	1/1/13/20	7/27/103/115	-
23	LMT	B	856	-	-	3/17/57/61	0/2/2/2
21	BCR	A	844	-	-	10/29/63/63	0/2/2/2
18	CLA	2	310	-	1/1/15/20	12/39/115/115	-
18	CLA	A	820	-	1/1/14/20	14/33/109/115	-
26	DGD	J	1106	-	-	14/47/87/95	0/2/2/2
29	LUT	1	5003	-	-	5/29/67/67	0/2/2/2
21	BCR	I	102	-	-	16/29/63/63	0/2/2/2
21	BCR	2	305	-	-	10/29/63/63	0/2/2/2
18	CLA	K	1402	-	1/1/14/20	18/33/109/115	-
18	CLA	B	824	-	1/1/13/20	13/27/103/115	-
29	LUT	3	304	-	1/1/12/27	7/29/67/67	0/2/2/2
22	LHG	A	849	18	-	22/44/44/53	-
23	LMT	G	1605	-	-	10/21/61/61	0/2/2/2
18	CLA	A	826	-	1/1/15/20	21/39/115/115	-
18	CLA	A	819	-	1/1/15/20	18/39/115/115	-
24	LMG	J	1102	-	-	6/25/45/70	0/1/1/1
18	CLA	A	832	-	1/1/15/20	19/39/115/115	-
30	CHL	4	317	-	3/3/15/26	0/12/110/137	-
18	CLA	B	823	-	1/1/15/20	14/39/115/115	-

All (1323) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	1	5003	LUT	C24-C25	15.43	1.51	1.33
29	4	303	LUT	C24-C25	15.33	1.51	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	3	303	LUT	C24-C25	15.29	1.51	1.33
29	1	5004	LUT	C24-C25	15.27	1.51	1.33
29	J	1105	LUT	C24-C25	15.12	1.51	1.33
29	3	304	LUT	C24-C25	15.11	1.51	1.33
29	2	303	LUT	C24-C25	15.00	1.51	1.33
17	A	801	CL0	C1A-CHA	9.65	1.51	1.40
17	A	801	CL0	C1B-C2B	9.32	1.50	1.39
17	A	801	CL0	C1D-C2D	9.28	1.50	1.39
17	A	801	CL0	C3B-C4B	7.40	1.48	1.41
18	K	1402	CLA	MG-NA	6.53	2.21	2.06
18	J	1103	CLA	MG-NA	6.48	2.21	2.06
18	1	5018	CLA	MG-NA	6.48	2.21	2.06
18	K	1404	CLA	MG-NA	6.48	2.21	2.06
18	B	836	CLA	MG-NA	6.47	2.21	2.06
18	K	1403	CLA	MG-NA	6.46	2.21	2.06
18	A	838	CLA	MG-NA	6.46	2.21	2.06
18	1	5012	CLA	MG-NA	6.46	2.21	2.06
18	G	1603	CLA	MG-NA	6.46	2.21	2.06
18	2	307	CLA	MG-NA	6.45	2.21	2.06
18	3	314	CLA	MG-NA	6.44	2.21	2.06
18	B	822	CLA	MG-NA	6.44	2.21	2.06
18	2	326	CLA	MG-NA	6.44	2.21	2.06
18	A	808	CLA	MG-NA	6.44	2.21	2.06
18	3	311	CLA	MG-NA	6.43	2.21	2.06
18	F	302	CLA	MG-NA	6.42	2.21	2.06
18	4	306	CLA	MG-NA	6.42	2.21	2.06
18	F	303	CLA	MG-NA	6.42	2.21	2.06
18	3	308	CLA	MG-NA	6.42	2.21	2.06
18	B	824	CLA	MG-NA	6.42	2.21	2.06
18	A	833	CLA	MG-NA	6.41	2.21	2.06
18	A	834	CLA	MG-NA	6.41	2.21	2.06
18	3	309	CLA	MG-NA	6.41	2.21	2.06
18	B	811	CLA	MG-NA	6.41	2.21	2.06
18	A	823	CLA	MG-NA	6.40	2.21	2.06
18	G	1601	CLA	MG-NA	6.40	2.21	2.06
18	A	820	CLA	MG-NA	6.40	2.21	2.06
18	A	822	CLA	MG-NA	6.40	2.21	2.06
18	B	810	CLA	MG-NA	6.40	2.21	2.06
18	A	814	CLA	MG-NA	6.40	2.21	2.06
18	G	1602	CLA	MG-NA	6.40	2.21	2.06
18	L	306	CLA	MG-NA	6.39	2.21	2.06
18	A	840	CLA	MG-NA	6.39	2.21	2.06

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	312	CLA	MG-NA	6.39	2.21	2.06
18	B	813	CLA	MG-NA	6.39	2.21	2.06
18	3	301	CLA	MG-NA	6.39	2.21	2.06
18	K	1401	CLA	MG-NA	6.39	2.21	2.06
18	H	1701	CLA	MG-NA	6.38	2.21	2.06
18	1	5010	CLA	MG-NA	6.38	2.21	2.06
18	B	823	CLA	MG-NA	6.38	2.21	2.06
18	3	315	CLA	MG-NA	6.38	2.21	2.06
18	B	827	CLA	MG-NA	6.38	2.21	2.06
18	B	801	CLA	MG-NA	6.37	2.21	2.06
18	1	5017	CLA	MG-NA	6.37	2.21	2.06
18	A	825	CLA	MG-NA	6.37	2.21	2.06
18	4	309	CLA	MG-NA	6.37	2.21	2.06
18	4	307	CLA	MG-NA	6.37	2.21	2.06
18	4	311	CLA	MG-NA	6.37	2.21	2.06
18	A	839	CLA	MG-NA	6.37	2.21	2.06
18	2	308	CLA	MG-NA	6.37	2.21	2.06
18	2	313	CLA	MG-NA	6.37	2.21	2.06
18	A	813	CLA	MG-NA	6.36	2.21	2.06
18	1	5007	CLA	MG-NA	6.36	2.21	2.06
18	A	816	CLA	MG-NA	6.36	2.21	2.06
18	A	852	CLA	MG-NA	6.36	2.21	2.06
18	A	836	CLA	MG-NA	6.36	2.21	2.06
18	A	806	CLA	MG-NA	6.36	2.21	2.06
18	L	301	CLA	MG-NA	6.35	2.21	2.06
18	B	841	CLA	MG-NA	6.35	2.21	2.06
18	1	5008	CLA	MG-NA	6.35	2.21	2.06
18	B	821	CLA	MG-NA	6.35	2.21	2.06
18	B	812	CLA	MG-NA	6.35	2.21	2.06
18	B	832	CLA	MG-NA	6.35	2.21	2.06
18	B	817	CLA	MG-NA	6.34	2.21	2.06
18	B	830	CLA	MG-NA	6.34	2.21	2.06
18	B	840	CLA	MG-NA	6.34	2.21	2.06
18	A	824	CLA	MG-NA	6.34	2.21	2.06
18	F	301	CLA	MG-NA	6.34	2.21	2.06
18	B	831	CLA	MG-NA	6.34	2.21	2.06
18	3	318	CLA	MG-NA	6.34	2.21	2.06
18	4	305	CLA	MG-NA	6.34	2.21	2.06
18	A	811	CLA	MG-NA	6.34	2.21	2.06
18	A	832	CLA	MG-NA	6.34	2.21	2.06
18	B	829	CLA	MG-NA	6.34	2.21	2.06
18	J	1101	CLA	MG-NA	6.34	2.21	2.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	5015	CLA	MG-NA	6.34	2.21	2.06
18	B	839	CLA	MG-NA	6.33	2.21	2.06
18	3	307	CLA	MG-NA	6.33	2.21	2.06
18	A	827	CLA	MG-NA	6.33	2.21	2.06
18	A	829	CLA	MG-NA	6.33	2.21	2.06
18	B	818	CLA	MG-NA	6.33	2.21	2.06
18	A	817	CLA	MG-NA	6.32	2.21	2.06
18	B	835	CLA	MG-NA	6.32	2.21	2.06
18	1	5009	CLA	MG-NA	6.32	2.21	2.06
18	L	304	CLA	MG-NA	6.32	2.21	2.06
18	A	818	CLA	MG-NA	6.32	2.21	2.06
18	B	828	CLA	MG-NA	6.32	2.21	2.06
18	A	821	CLA	MG-NA	6.32	2.21	2.06
18	A	803	CLA	MG-NA	6.31	2.21	2.06
18	B	833	CLA	MG-NA	6.31	2.21	2.06
18	A	810	CLA	MG-NA	6.31	2.21	2.06
18	B	805	CLA	MG-NA	6.31	2.21	2.06
18	1	5006	CLA	MG-NA	6.31	2.21	2.06
18	B	808	CLA	MG-NA	6.31	2.21	2.06
18	1	5011	CLA	MG-NA	6.30	2.21	2.06
18	3	319	CLA	MG-NA	6.30	2.21	2.06
18	B	816	CLA	MG-NA	6.29	2.21	2.06
18	2	309	CLA	MG-NA	6.29	2.21	2.06
18	A	837	CLA	MG-NA	6.29	2.21	2.06
18	B	814	CLA	MG-NA	6.29	2.21	2.06
18	A	815	CLA	MG-NA	6.29	2.21	2.06
18	4	308	CLA	MG-NA	6.28	2.21	2.06
18	A	805	CLA	MG-NA	6.28	2.21	2.06
18	B	825	CLA	MG-NA	6.28	2.21	2.06
18	4	312	CLA	MG-NA	6.28	2.21	2.06
18	A	830	CLA	MG-NA	6.27	2.21	2.06
18	B	834	CLA	MG-NA	6.26	2.21	2.06
18	A	804	CLA	MG-NA	6.26	2.21	2.06
18	B	838	CLA	MG-NA	6.26	2.21	2.06
18	4	315	CLA	MG-NA	6.26	2.21	2.06
18	A	802	CLA	MG-NA	6.26	2.21	2.06
18	1	5013	CLA	MG-NA	6.26	2.21	2.06
18	B	809	CLA	MG-NA	6.25	2.21	2.06
18	A	831	CLA	MG-NA	6.25	2.21	2.06
18	L	305	CLA	MG-NA	6.24	2.21	2.06
18	4	310	CLA	MG-NA	6.24	2.21	2.06
18	B	807	CLA	MG-NA	6.24	2.21	2.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	804	CLA	MG-NA	6.24	2.21	2.06
18	A	835	CLA	MG-NA	6.23	2.21	2.06
18	2	310	CLA	MG-NA	6.22	2.21	2.06
18	A	853	CLA	MG-NA	6.22	2.21	2.06
18	A	809	CLA	MG-NA	6.22	2.21	2.06
18	B	815	CLA	MG-NA	6.21	2.21	2.06
18	2	306	CLA	MG-NA	6.20	2.21	2.06
18	A	807	CLA	MG-NA	6.20	2.21	2.06
18	B	826	CLA	MG-NA	6.19	2.21	2.06
18	B	819	CLA	MG-NA	6.19	2.21	2.06
18	B	820	CLA	MG-NA	6.18	2.21	2.06
18	B	806	CLA	MG-NA	6.18	2.20	2.06
18	2	317	CLA	MG-NA	6.17	2.20	2.06
18	B	803	CLA	MG-NA	6.17	2.20	2.06
18	2	311	CLA	MG-NA	6.17	2.20	2.06
18	A	819	CLA	MG-NA	6.17	2.20	2.06
18	A	828	CLA	MG-NA	6.17	2.20	2.06
18	3	317	CLA	MG-NA	6.16	2.20	2.06
18	A	826	CLA	MG-NA	6.15	2.20	2.06
18	A	812	CLA	MG-NA	6.15	2.20	2.06
18	B	837	CLA	MG-NA	6.13	2.20	2.06
21	2	305	BCR	C24-C23	5.98	1.50	1.33
21	L	303	BCR	C24-C23	5.95	1.50	1.33
21	B	843	BCR	C24-C23	5.93	1.50	1.33
21	B	802	BCR	C24-C23	5.91	1.50	1.33
21	3	306	BCR	C24-C23	5.90	1.50	1.33
21	L	302	BCR	C24-C23	5.90	1.50	1.33
21	I	102	BCR	C24-C23	5.89	1.50	1.33
21	K	1405	BCR	C24-C23	5.85	1.50	1.33
21	4	301	BCR	C24-C23	5.82	1.50	1.33
21	A	845	BCR	C24-C23	5.81	1.50	1.33
21	I	101	BCR	C24-C23	5.81	1.50	1.33
21	L	307	BCR	C24-C23	5.80	1.50	1.33
21	A	855	BCR	C24-C23	5.78	1.50	1.33
21	F	304	BCR	C24-C23	5.78	1.50	1.33
21	G	1604	BCR	C24-C23	5.78	1.50	1.33
21	F	305	BCR	C24-C23	5.77	1.50	1.33
21	A	843	BCR	C24-C23	5.76	1.50	1.33
21	1	5005	BCR	C24-C23	5.74	1.50	1.33
21	A	844	BCR	C24-C23	5.72	1.50	1.33
21	A	846	BCR	C24-C23	5.71	1.50	1.33
21	B	847	BCR	C24-C23	5.71	1.50	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	J	1104	BCR	C24-C23	5.70	1.50	1.33
21	3	305	BCR	C24-C23	5.68	1.50	1.33
21	B	844	BCR	C24-C23	5.67	1.50	1.33
21	A	847	BCR	C24-C23	5.66	1.50	1.33
21	B	846	BCR	C24-C23	5.62	1.49	1.33
30	4	314	CHL	C3B-C4B	5.52	1.46	1.41
30	1	5016	CHL	C3A-C2A	-5.50	1.50	1.54
21	B	845	BCR	C24-C23	5.47	1.49	1.33
30	3	316	CHL	C3B-C4B	5.42	1.46	1.41
21	A	845	BCR	C11-C12	-5.41	1.20	1.34
30	4	317	CHL	C3B-C4B	5.38	1.46	1.41
17	A	801	CL0	O2A-C1	5.38	1.60	1.46
30	4	313	CHL	C3B-C4B	5.35	1.46	1.41
21	I	101	BCR	C11-C12	-5.35	1.20	1.34
17	A	801	CL0	CHC-C4B	5.31	1.48	1.39
17	A	801	CL0	CHB-C1B	5.28	1.48	1.39
30	2	319	CHL	C3B-C4B	5.24	1.46	1.41
30	2	314	CHL	C3B-C4B	5.21	1.46	1.41
21	J	1104	BCR	C11-C12	-5.21	1.21	1.34
21	B	845	BCR	C11-C12	-5.20	1.21	1.34
21	4	301	BCR	C11-C12	-5.20	1.21	1.34
21	A	844	BCR	C11-C12	-5.16	1.21	1.34
21	A	847	BCR	C11-C12	-5.16	1.21	1.34
21	A	855	BCR	C11-C12	-5.15	1.21	1.34
30	4	316	CHL	C3B-C4B	5.14	1.46	1.41
17	A	801	CL0	OBD-CAD	5.14	1.29	1.22
17	A	801	CL0	O2D-CGD	5.14	1.45	1.33
21	F	305	BCR	C11-C12	-5.13	1.21	1.34
21	F	304	BCR	C11-C12	-5.12	1.21	1.34
21	3	305	BCR	C11-C12	-5.11	1.21	1.34
21	G	1604	BCR	C11-C12	-5.10	1.21	1.34
21	L	307	BCR	C11-C12	-5.10	1.21	1.34
30	3	310	CHL	C3B-C4B	5.10	1.46	1.41
21	A	843	BCR	C11-C12	-5.09	1.21	1.34
21	A	846	BCR	C11-C12	-5.09	1.21	1.34
21	B	847	BCR	C11-C12	-5.09	1.21	1.34
21	B	846	BCR	C11-C12	-5.07	1.21	1.34
21	K	1405	BCR	C11-C12	-5.06	1.21	1.34
17	A	801	CL0	CHD-C1D	5.06	1.47	1.39
21	1	5005	BCR	C11-C12	-5.06	1.21	1.34
21	B	844	BCR	C11-C12	-5.05	1.21	1.34
30	4	314	CHL	C3A-C2A	-5.00	1.50	1.54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	L	303	BCR	C11-C12	-4.99	1.21	1.34
21	2	305	BCR	C11-C12	-4.98	1.21	1.34
30	4	318	CHL	C3B-C4B	4.98	1.46	1.41
21	I	102	BCR	C11-C12	-4.95	1.21	1.34
30	3	313	CHL	C3B-C4B	4.90	1.46	1.41
17	A	801	CL0	C3B-C2B	4.90	1.47	1.40
30	4	302	CHL	C3B-C4B	4.89	1.46	1.41
17	A	801	CL0	CHD-C4C	4.87	1.48	1.39
30	2	314	CHL	C3A-C2A	-4.87	1.50	1.54
21	3	306	BCR	C11-C12	-4.87	1.22	1.34
21	L	302	BCR	C11-C12	-4.85	1.22	1.34
21	B	802	BCR	C11-C12	-4.81	1.22	1.34
21	B	843	BCR	C11-C12	-4.80	1.22	1.34
30	2	318	CHL	C3B-C4B	4.75	1.46	1.41
30	3	312	CHL	C3B-C4B	4.68	1.45	1.41
17	A	801	CL0	CHC-C1C	4.59	1.48	1.39
17	A	801	CL0	C3D-C2D	4.57	1.47	1.39
30	1	5014	CHL	C3B-C4B	4.55	1.45	1.41
17	A	801	CL0	C3D-C4D	-4.50	1.34	1.41
30	2	316	CHL	C3B-C4B	4.49	1.45	1.41
21	B	843	BCR	C10-C9	4.46	1.46	1.35
30	1	5016	CHL	C3B-C4B	4.46	1.45	1.41
18	B	811	CLA	CBB-CAB	4.43	1.51	1.30
18	J	1103	CLA	CBB-CAB	4.43	1.51	1.30
18	B	826	CLA	CBB-CAB	4.43	1.51	1.30
18	A	828	CLA	CBB-CAB	4.43	1.51	1.30
18	B	801	CLA	CBB-CAB	4.43	1.51	1.30
18	A	837	CLA	CBB-CAB	4.43	1.51	1.30
18	B	832	CLA	CBB-CAB	4.43	1.51	1.30
18	A	805	CLA	CBB-CAB	4.43	1.51	1.30
18	A	817	CLA	CBB-CAB	4.43	1.51	1.30
18	K	1402	CLA	CBB-CAB	4.43	1.51	1.30
18	K	1403	CLA	CBB-CAB	4.42	1.51	1.30
18	B	830	CLA	CBB-CAB	4.42	1.51	1.30
18	G	1602	CLA	CBB-CAB	4.42	1.51	1.30
18	2	306	CLA	CBB-CAB	4.42	1.51	1.30
18	4	308	CLA	CBB-CAB	4.42	1.51	1.30
18	4	310	CLA	CBB-CAB	4.42	1.51	1.30
18	K	1404	CLA	CBB-CAB	4.42	1.51	1.30
18	3	317	CLA	CBB-CAB	4.42	1.51	1.30
18	B	833	CLA	CBB-CAB	4.42	1.51	1.30
18	1	5009	CLA	CBB-CAB	4.42	1.51	1.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	838	CLA	CBB-CAB	4.42	1.51	1.30
18	F	301	CLA	CBB-CAB	4.42	1.51	1.30
30	3	312	CHL	C3A-C2A	-4.42	1.50	1.54
18	A	819	CLA	CBB-CAB	4.42	1.51	1.30
18	A	802	CLA	CBB-CAB	4.42	1.51	1.30
18	B	816	CLA	CBB-CAB	4.42	1.51	1.30
18	3	315	CLA	CBB-CAB	4.42	1.51	1.30
18	B	812	CLA	CBB-CAB	4.42	1.51	1.30
18	1	5017	CLA	CBB-CAB	4.42	1.51	1.30
18	A	834	CLA	CBB-CAB	4.42	1.51	1.30
18	2	310	CLA	CBB-CAB	4.42	1.51	1.30
18	K	1401	CLA	CBB-CAB	4.42	1.51	1.30
18	A	814	CLA	CBB-CAB	4.42	1.51	1.30
18	A	839	CLA	CBB-CAB	4.42	1.51	1.30
18	1	5008	CLA	CBB-CAB	4.42	1.51	1.30
18	3	307	CLA	CBB-CAB	4.42	1.51	1.30
18	A	807	CLA	CBB-CAB	4.42	1.51	1.30
18	B	805	CLA	CBB-CAB	4.42	1.51	1.30
18	B	840	CLA	CBB-CAB	4.42	1.51	1.30
18	B	807	CLA	CBB-CAB	4.42	1.51	1.30
18	B	813	CLA	CBB-CAB	4.42	1.51	1.30
18	L	304	CLA	CBB-CAB	4.42	1.51	1.30
18	1	5010	CLA	CBB-CAB	4.41	1.51	1.30
21	B	802	BCR	C10-C9	4.41	1.46	1.35
18	L	306	CLA	CBB-CAB	4.41	1.51	1.30
18	1	5018	CLA	CBB-CAB	4.41	1.51	1.30
18	B	819	CLA	CBB-CAB	4.41	1.51	1.30
18	1	5007	CLA	CBB-CAB	4.41	1.51	1.30
18	1	5011	CLA	CBB-CAB	4.41	1.51	1.30
18	A	811	CLA	CBB-CAB	4.41	1.51	1.30
18	G	1601	CLA	CBB-CAB	4.41	1.51	1.30
18	2	317	CLA	CBB-CAB	4.41	1.51	1.30
18	B	822	CLA	CBB-CAB	4.41	1.51	1.30
18	B	825	CLA	CBB-CAB	4.41	1.51	1.30
18	L	301	CLA	CBB-CAB	4.41	1.51	1.30
18	A	812	CLA	CBB-CAB	4.41	1.51	1.30
18	4	311	CLA	CBB-CAB	4.41	1.51	1.30
18	L	305	CLA	CBB-CAB	4.41	1.51	1.30
18	3	309	CLA	CBB-CAB	4.41	1.51	1.30
18	2	326	CLA	CBB-CAB	4.41	1.51	1.30
18	3	311	CLA	CBB-CAB	4.41	1.51	1.30
18	B	827	CLA	CBB-CAB	4.41	1.51	1.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	810	CLA	CBB-CAB	4.41	1.51	1.30
18	B	821	CLA	CBB-CAB	4.41	1.51	1.30
18	2	307	CLA	CBB-CAB	4.41	1.51	1.30
18	1	5015	CLA	CBB-CAB	4.41	1.51	1.30
18	A	827	CLA	CBB-CAB	4.41	1.51	1.30
18	B	804	CLA	CBB-CAB	4.41	1.51	1.30
18	3	308	CLA	CBB-CAB	4.41	1.51	1.30
18	B	835	CLA	CBB-CAB	4.41	1.51	1.30
18	F	302	CLA	CBB-CAB	4.41	1.51	1.30
18	J	1101	CLA	CBB-CAB	4.41	1.51	1.30
18	3	318	CLA	CBB-CAB	4.40	1.51	1.30
18	A	831	CLA	CBB-CAB	4.40	1.51	1.30
18	B	834	CLA	CBB-CAB	4.40	1.51	1.30
18	A	816	CLA	CBB-CAB	4.40	1.51	1.30
18	A	825	CLA	CBB-CAB	4.40	1.51	1.30
18	A	853	CLA	CBB-CAB	4.40	1.51	1.30
18	B	837	CLA	CBB-CAB	4.40	1.51	1.30
18	G	1603	CLA	CBB-CAB	4.40	1.51	1.30
18	A	804	CLA	CBB-CAB	4.40	1.51	1.30
18	A	838	CLA	CBB-CAB	4.40	1.51	1.30
18	A	826	CLA	CBB-CAB	4.40	1.51	1.30
18	A	818	CLA	CBB-CAB	4.40	1.51	1.30
18	B	803	CLA	CBB-CAB	4.40	1.51	1.30
18	A	810	CLA	CBB-CAB	4.40	1.51	1.30
18	A	836	CLA	CBB-CAB	4.40	1.51	1.30
18	2	309	CLA	CBB-CAB	4.40	1.51	1.30
18	A	806	CLA	CBB-CAB	4.40	1.51	1.30
18	B	828	CLA	CBB-CAB	4.40	1.51	1.30
18	3	301	CLA	CBB-CAB	4.40	1.51	1.30
18	1	5006	CLA	CBB-CAB	4.40	1.51	1.30
18	4	307	CLA	CBB-CAB	4.40	1.51	1.30
18	A	823	CLA	CBB-CAB	4.40	1.51	1.30
18	B	831	CLA	CBB-CAB	4.40	1.51	1.30
18	4	306	CLA	CBB-CAB	4.40	1.51	1.30
18	B	836	CLA	CBB-CAB	4.40	1.51	1.30
18	B	814	CLA	CBB-CAB	4.40	1.51	1.30
18	A	840	CLA	CBB-CAB	4.40	1.51	1.30
18	4	305	CLA	CBB-CAB	4.40	1.51	1.30
18	B	841	CLA	CBB-CAB	4.39	1.51	1.30
18	2	313	CLA	CBB-CAB	4.39	1.51	1.30
18	A	813	CLA	CBB-CAB	4.39	1.51	1.30
18	B	808	CLA	CBB-CAB	4.39	1.51	1.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	312	CLA	CBB-CAB	4.39	1.51	1.30
18	A	808	CLA	CBB-CAB	4.39	1.51	1.30
18	B	817	CLA	CBB-CAB	4.39	1.51	1.30
18	4	315	CLA	CBB-CAB	4.39	1.51	1.30
18	B	815	CLA	CBB-CAB	4.39	1.51	1.30
18	4	309	CLA	CBB-CAB	4.39	1.51	1.30
18	B	809	CLA	CBB-CAB	4.39	1.51	1.30
18	3	314	CLA	CBB-CAB	4.39	1.51	1.30
18	B	818	CLA	CBB-CAB	4.39	1.51	1.30
18	A	824	CLA	CBB-CAB	4.39	1.51	1.30
18	1	5013	CLA	CBB-CAB	4.39	1.51	1.30
18	A	833	CLA	CBB-CAB	4.38	1.51	1.30
18	A	852	CLA	CBB-CAB	4.38	1.51	1.30
18	A	830	CLA	CBB-CAB	4.38	1.51	1.30
18	F	303	CLA	CBB-CAB	4.38	1.51	1.30
21	L	302	BCR	C10-C9	4.38	1.45	1.35
18	A	809	CLA	CBB-CAB	4.38	1.51	1.30
18	B	824	CLA	CBB-CAB	4.38	1.51	1.30
18	B	839	CLA	CBB-CAB	4.38	1.51	1.30
18	A	835	CLA	CBB-CAB	4.38	1.51	1.30
18	B	806	CLA	CBB-CAB	4.37	1.51	1.30
18	2	312	CLA	CBB-CAB	4.37	1.51	1.30
18	B	829	CLA	CBB-CAB	4.37	1.51	1.30
18	B	823	CLA	CBB-CAB	4.37	1.51	1.30
18	A	821	CLA	CBB-CAB	4.37	1.51	1.30
18	B	820	CLA	CBB-CAB	4.37	1.51	1.30
18	A	815	CLA	CBB-CAB	4.36	1.51	1.30
21	3	306	BCR	C10-C9	4.36	1.45	1.35
18	2	308	CLA	CBB-CAB	4.36	1.51	1.30
18	1	5012	CLA	CBB-CAB	4.36	1.51	1.30
30	2	315	CHL	C3A-C2A	-4.35	1.51	1.54
21	B	846	BCR	C16-C17	-4.35	1.29	1.43
18	H	1701	CLA	CBB-CAB	4.35	1.51	1.30
18	A	832	CLA	CBB-CAB	4.35	1.51	1.30
18	A	829	CLA	CBB-CAB	4.35	1.51	1.30
18	A	820	CLA	CBB-CAB	4.34	1.51	1.30
18	2	311	CLA	CBB-CAB	4.34	1.51	1.30
21	4	301	BCR	C16-C17	-4.33	1.29	1.43
26	B	855	DGD	O1G-C1A	4.33	1.46	1.33
18	A	822	CLA	CBB-CAB	4.32	1.51	1.30
18	A	803	CLA	CBB-CAB	4.29	1.51	1.30
26	1	5002	DGD	O1G-C1A	4.29	1.45	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	F	309	DGD	O1G-C1A	4.29	1.45	1.33
21	J	1104	BCR	C16-C17	-4.28	1.29	1.43
21	B	847	BCR	C16-C17	-4.27	1.29	1.43
21	B	845	BCR	C16-C17	-4.25	1.30	1.43
21	3	306	BCR	C16-C17	-4.23	1.30	1.43
21	F	304	BCR	C16-C17	-4.23	1.30	1.43
18	3	319	CLA	CBB-CAB	4.22	1.50	1.30
21	A	845	BCR	C16-C17	-4.22	1.30	1.43
21	A	847	BCR	C16-C17	-4.22	1.30	1.43
21	I	102	BCR	C10-C9	4.21	1.45	1.35
21	1	5005	BCR	C16-C17	-4.21	1.30	1.43
21	L	303	BCR	C10-C9	4.20	1.45	1.35
21	1	5005	BCR	C10-C9	4.20	1.45	1.35
26	J	1106	DGD	O1G-C1A	4.20	1.45	1.33
21	B	844	BCR	C10-C9	4.20	1.45	1.35
21	3	305	BCR	C16-C17	-4.20	1.30	1.43
21	A	844	BCR	C16-C17	-4.19	1.30	1.43
21	K	1405	BCR	C10-C9	4.19	1.45	1.35
21	A	843	BCR	C16-C17	-4.18	1.30	1.43
21	G	1604	BCR	C16-C17	-4.18	1.30	1.43
21	2	305	BCR	C10-C9	4.18	1.45	1.35
21	A	846	BCR	C16-C17	-4.17	1.30	1.43
21	A	846	BCR	C10-C9	4.17	1.45	1.35
21	A	855	BCR	C16-C17	-4.17	1.30	1.43
26	2	327	DGD	O1G-C1A	4.16	1.45	1.33
21	B	847	BCR	C10-C9	4.15	1.45	1.35
21	B	846	BCR	C10-C9	4.15	1.45	1.35
21	L	307	BCR	C16-C17	-4.15	1.30	1.43
21	B	844	BCR	C16-C17	-4.14	1.30	1.43
21	K	1405	BCR	C16-C17	-4.13	1.30	1.43
21	F	304	BCR	C10-C9	4.12	1.45	1.35
21	G	1604	BCR	C10-C9	4.12	1.45	1.35
21	L	307	BCR	C10-C9	4.11	1.45	1.35
21	3	305	BCR	C10-C9	4.11	1.45	1.35
21	A	843	BCR	C10-C9	4.11	1.45	1.35
21	2	305	BCR	C16-C17	-4.10	1.30	1.43
21	F	305	BCR	C16-C17	-4.10	1.30	1.43
21	A	855	BCR	C10-C9	4.10	1.45	1.35
21	F	305	BCR	C10-C9	4.09	1.45	1.35
21	L	303	BCR	C16-C17	-4.08	1.30	1.43
21	B	802	BCR	C16-C17	-4.08	1.30	1.43
21	I	101	BCR	C16-C17	-4.08	1.30	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	I	102	BCR	C16-C17	-4.04	1.30	1.43
18	B	830	CLA	MG-ND	-4.02	1.97	2.05
21	I	101	BCR	C10-C9	4.02	1.45	1.35
21	4	301	BCR	C10-C9	4.02	1.45	1.35
21	A	844	BCR	C10-C9	4.01	1.45	1.35
21	B	845	BCR	C10-C9	4.00	1.45	1.35
21	L	302	BCR	C16-C17	-4.00	1.30	1.43
21	A	847	BCR	C10-C9	4.00	1.45	1.35
21	B	843	BCR	C16-C17	-3.98	1.30	1.43
21	J	1104	BCR	C10-C9	3.98	1.45	1.35
18	B	803	CLA	MG-ND	-3.96	1.97	2.05
18	A	824	CLA	MG-ND	-3.92	1.98	2.05
18	B	828	CLA	MG-ND	-3.92	1.98	2.05
18	B	827	CLA	MG-ND	-3.90	1.98	2.05
18	A	828	CLA	MG-ND	-3.90	1.98	2.05
18	A	827	CLA	MG-ND	-3.89	1.98	2.05
18	B	801	CLA	MG-ND	-3.89	1.98	2.05
18	A	818	CLA	MG-ND	-3.87	1.98	2.05
18	L	301	CLA	MG-ND	-3.86	1.98	2.05
18	B	825	CLA	MG-ND	-3.85	1.98	2.05
18	B	804	CLA	MG-ND	-3.84	1.98	2.05
18	A	852	CLA	MG-ND	-3.84	1.98	2.05
18	A	802	CLA	MG-ND	-3.83	1.98	2.05
18	B	809	CLA	MG-ND	-3.83	1.98	2.05
18	3	311	CLA	MG-ND	-3.81	1.98	2.05
18	4	309	CLA	MG-ND	-3.81	1.98	2.05
18	B	838	CLA	MG-ND	-3.81	1.98	2.05
18	1	5017	CLA	MG-ND	-3.81	1.98	2.05
18	B	814	CLA	MG-ND	-3.80	1.98	2.05
18	B	821	CLA	MG-ND	-3.80	1.98	2.05
18	A	825	CLA	MG-ND	-3.80	1.98	2.05
18	2	312	CLA	MG-ND	-3.80	1.98	2.05
18	A	826	CLA	MG-ND	-3.80	1.98	2.05
18	B	810	CLA	MG-ND	-3.80	1.98	2.05
21	A	845	BCR	C10-C9	3.79	1.44	1.35
18	A	808	CLA	MG-ND	-3.79	1.98	2.05
18	3	318	CLA	MG-ND	-3.79	1.98	2.05
18	B	831	CLA	MG-ND	-3.79	1.98	2.05
18	B	835	CLA	MG-ND	-3.78	1.98	2.05
18	A	820	CLA	MG-ND	-3.78	1.98	2.05
18	A	831	CLA	MG-ND	-3.77	1.98	2.05
18	A	840	CLA	MG-ND	-3.77	1.98	2.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	819	CLA	MG-ND	-3.77	1.98	2.05
30	2	316	CHL	C3A-C2A	-3.76	1.51	1.54
26	J	1106	DGD	CDA-CCA	-3.76	1.33	1.51
18	B	811	CLA	MG-ND	-3.76	1.98	2.05
18	L	305	CLA	MG-ND	-3.76	1.98	2.05
18	A	816	CLA	MG-ND	-3.76	1.98	2.05
18	A	823	CLA	MG-ND	-3.76	1.98	2.05
18	3	307	CLA	MG-ND	-3.76	1.98	2.05
18	A	838	CLA	MG-ND	-3.76	1.98	2.05
18	A	803	CLA	MG-ND	-3.76	1.98	2.05
30	3	310	CHL	C1A-CHA	-3.75	1.35	1.40
18	A	830	CLA	MG-ND	-3.75	1.98	2.05
18	B	815	CLA	MG-ND	-3.75	1.98	2.05
18	K	1404	CLA	MG-ND	-3.75	1.98	2.05
26	J	1106	DGD	CAA-C9A	-3.75	1.33	1.51
18	H	1701	CLA	MG-ND	-3.74	1.98	2.05
18	A	817	CLA	MG-ND	-3.74	1.98	2.05
18	3	319	CLA	MG-ND	-3.74	1.98	2.05
18	B	836	CLA	MG-ND	-3.74	1.98	2.05
18	4	315	CLA	MG-ND	-3.74	1.98	2.05
18	4	305	CLA	MG-ND	-3.74	1.98	2.05
18	B	826	CLA	MG-ND	-3.74	1.98	2.05
18	3	301	CLA	MG-ND	-3.74	1.98	2.05
18	4	306	CLA	MG-ND	-3.74	1.98	2.05
18	2	317	CLA	MG-ND	-3.74	1.98	2.05
18	A	837	CLA	MG-ND	-3.74	1.98	2.05
18	1	5006	CLA	MG-ND	-3.74	1.98	2.05
30	3	316	CHL	C3A-C2A	-3.74	1.51	1.54
18	1	5013	CLA	MG-ND	-3.73	1.98	2.05
18	A	806	CLA	MG-ND	-3.73	1.98	2.05
18	B	820	CLA	MG-ND	-3.73	1.98	2.05
18	B	818	CLA	MG-ND	-3.73	1.98	2.05
18	A	811	CLA	MG-ND	-3.73	1.98	2.05
18	B	819	CLA	MG-ND	-3.73	1.98	2.05
18	3	309	CLA	MG-ND	-3.73	1.98	2.05
18	K	1401	CLA	MG-ND	-3.73	1.98	2.05
18	2	307	CLA	MG-ND	-3.73	1.98	2.05
18	A	821	CLA	MG-ND	-3.73	1.98	2.05
18	B	805	CLA	MG-ND	-3.73	1.98	2.05
18	A	839	CLA	MG-ND	-3.72	1.98	2.05
18	B	841	CLA	MG-ND	-3.72	1.98	2.05
18	B	822	CLA	MG-ND	-3.72	1.98	2.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	F	306	LMG	C40-C39	-3.72	1.33	1.51
24	F	306	LMG	C43-C42	-3.72	1.33	1.51
18	A	836	CLA	MG-ND	-3.72	1.98	2.05
18	4	312	CLA	MG-ND	-3.72	1.98	2.05
18	B	823	CLA	MG-ND	-3.72	1.98	2.05
18	1	5015	CLA	MG-ND	-3.72	1.98	2.05
18	A	814	CLA	MG-ND	-3.72	1.98	2.05
18	B	834	CLA	MG-ND	-3.72	1.98	2.05
18	B	813	CLA	MG-ND	-3.71	1.98	2.05
18	1	5010	CLA	MG-ND	-3.71	1.98	2.05
18	3	314	CLA	MG-ND	-3.71	1.98	2.05
18	G	1602	CLA	MG-ND	-3.71	1.98	2.05
18	G	1603	CLA	MG-ND	-3.71	1.98	2.05
18	A	829	CLA	MG-ND	-3.71	1.98	2.05
18	1	5007	CLA	MG-ND	-3.71	1.98	2.05
18	4	311	CLA	MG-ND	-3.71	1.98	2.05
18	B	824	CLA	MG-ND	-3.71	1.98	2.05
18	B	816	CLA	MG-ND	-3.71	1.98	2.05
18	2	326	CLA	MG-ND	-3.71	1.98	2.05
18	B	832	CLA	MG-ND	-3.70	1.98	2.05
18	4	308	CLA	MG-ND	-3.70	1.98	2.05
18	A	807	CLA	MG-ND	-3.70	1.98	2.05
26	B	855	DGD	CAB-C9B	-3.70	1.33	1.51
18	A	815	CLA	MG-ND	-3.70	1.98	2.05
18	A	805	CLA	MG-ND	-3.70	1.98	2.05
18	B	808	CLA	MG-ND	-3.70	1.98	2.05
18	A	853	CLA	MG-ND	-3.70	1.98	2.05
18	B	807	CLA	MG-ND	-3.70	1.98	2.05
18	2	311	CLA	MG-ND	-3.70	1.98	2.05
24	1	5020	LMG	C19-C18	-3.70	1.33	1.51
18	A	834	CLA	MG-ND	-3.70	1.98	2.05
18	L	304	CLA	MG-ND	-3.70	1.98	2.05
18	2	309	CLA	MG-ND	-3.70	1.98	2.05
18	B	839	CLA	MG-ND	-3.70	1.98	2.05
18	A	813	CLA	MG-ND	-3.69	1.98	2.05
18	4	310	CLA	MG-ND	-3.69	1.98	2.05
30	2	315	CHL	C3B-C4B	3.69	1.45	1.41
18	1	5008	CLA	MG-ND	-3.69	1.98	2.05
18	2	308	CLA	MG-ND	-3.69	1.98	2.05
18	3	315	CLA	MG-ND	-3.69	1.98	2.05
18	G	1601	CLA	MG-ND	-3.69	1.98	2.05
18	1	5018	CLA	MG-ND	-3.69	1.98	2.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	310	CLA	MG-ND	-3.69	1.98	2.05
24	F	306	LMG	C37-C36	-3.69	1.33	1.51
18	F	302	CLA	MG-ND	-3.69	1.98	2.05
18	J	1103	CLA	MG-ND	-3.69	1.98	2.05
18	B	833	CLA	MG-ND	-3.69	1.98	2.05
24	A	851	LMG	C22-C21	-3.69	1.33	1.51
18	K	1403	CLA	MG-ND	-3.69	1.98	2.05
18	3	308	CLA	MG-ND	-3.69	1.98	2.05
18	A	833	CLA	MG-ND	-3.69	1.98	2.05
26	F	309	DGD	CGA-CFA	-3.68	1.33	1.51
18	A	804	CLA	MG-ND	-3.68	1.98	2.05
26	B	855	DGD	CGB-CFB	-3.68	1.33	1.51
18	A	812	CLA	MG-ND	-3.68	1.98	2.05
18	F	301	CLA	MG-ND	-3.68	1.98	2.05
18	2	313	CLA	MG-ND	-3.68	1.98	2.05
24	A	851	LMG	C25-C24	-3.68	1.33	1.51
24	1	5001	LMG	C19-C18	-3.68	1.33	1.51
18	1	5011	CLA	MG-ND	-3.68	1.98	2.05
24	1	5020	LMG	C25-C24	-3.68	1.33	1.51
26	J	1106	DGD	CGA-CFA	-3.68	1.33	1.51
18	K	1402	CLA	MG-ND	-3.68	1.98	2.05
26	2	327	DGD	CAA-C9A	-3.68	1.33	1.51
18	L	306	CLA	MG-ND	-3.68	1.98	2.05
26	B	855	DGD	CDB-CCB	-3.68	1.33	1.51
18	4	307	CLA	MG-ND	-3.67	1.98	2.05
18	B	840	CLA	MG-ND	-3.67	1.98	2.05
18	B	829	CLA	MG-ND	-3.67	1.98	2.05
18	1	5012	CLA	MG-ND	-3.67	1.98	2.05
24	A	851	LMG	C37-C36	-3.67	1.33	1.51
24	F	307	LMG	C37-C36	-3.67	1.33	1.51
24	1	5020	LMG	C22-C21	-3.67	1.33	1.51
18	B	837	CLA	MG-ND	-3.66	1.98	2.05
26	F	309	DGD	CAA-C9A	-3.66	1.33	1.51
24	1	5001	LMG	C43-C42	-3.66	1.33	1.51
26	F	309	DGD	CDA-CCA	-3.66	1.33	1.51
18	2	306	CLA	MG-ND	-3.66	1.98	2.05
24	A	851	LMG	C19-C18	-3.66	1.33	1.51
18	A	809	CLA	MG-ND	-3.66	1.98	2.05
18	1	5009	CLA	MG-ND	-3.66	1.98	2.05
18	A	832	CLA	MG-ND	-3.65	1.98	2.05
18	A	835	CLA	MG-ND	-3.65	1.98	2.05
18	3	317	CLA	MG-ND	-3.65	1.98	2.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	5001	LMG	C37-C36	-3.65	1.33	1.51
18	B	817	CLA	MG-ND	-3.65	1.98	2.05
24	B	850	LMG	C19-C18	-3.65	1.33	1.51
18	F	303	CLA	MG-ND	-3.64	1.98	2.05
18	B	812	CLA	MG-ND	-3.64	1.98	2.05
26	B	855	DGD	CAA-C9A	-3.64	1.33	1.51
24	1	5001	LMG	C40-C39	-3.64	1.33	1.51
18	J	1101	CLA	MG-ND	-3.64	1.98	2.05
18	A	822	CLA	MG-ND	-3.63	1.98	2.05
18	B	806	CLA	MG-ND	-3.63	1.98	2.05
18	A	810	CLA	MG-ND	-3.60	1.98	2.05
30	3	312	CHL	CBB-CAB	3.60	1.51	1.29
30	3	310	CHL	CBB-CAB	3.59	1.51	1.29
30	4	318	CHL	CBB-CAB	3.57	1.51	1.29
30	3	313	CHL	CBB-CAB	3.56	1.51	1.29
30	1	5016	CHL	CBB-CAB	3.56	1.51	1.29
30	2	319	CHL	CBB-CAB	3.54	1.51	1.29
30	4	313	CHL	CBB-CAB	3.51	1.51	1.29
30	1	5014	CHL	CBB-CAB	3.50	1.51	1.29
30	4	302	CHL	CBB-CAB	3.49	1.51	1.29
30	2	314	CHL	CBB-CAB	3.48	1.51	1.29
30	4	317	CHL	CBB-CAB	3.48	1.51	1.29
30	2	318	CHL	CBB-CAB	3.46	1.51	1.29
30	4	318	CHL	C3A-C2A	-3.40	1.51	1.54
30	3	316	CHL	CBB-CAB	3.35	1.50	1.29
30	2	315	CHL	CBB-CAB	3.35	1.50	1.29
30	2	316	CHL	CBB-CAB	3.33	1.50	1.29
30	4	316	CHL	CBB-CAB	3.33	1.50	1.29
18	A	828	CLA	C1C-NC	-3.32	1.32	1.37
30	4	314	CHL	CBB-CAB	3.28	1.49	1.29
18	B	814	CLA	C1C-NC	-3.27	1.32	1.37
30	4	302	CHL	C3A-C2A	-3.27	1.51	1.54
18	K	1404	CLA	C1C-NC	-3.23	1.32	1.37
30	2	316	CHL	C3B-C2B	-3.23	1.36	1.40
30	4	316	CHL	C3B-C2B	-3.20	1.36	1.40
18	A	811	CLA	C1C-NC	-3.20	1.32	1.37
18	4	311	CLA	C1C-NC	-3.19	1.32	1.37
18	B	827	CLA	C1C-NC	-3.19	1.32	1.37
18	B	812	CLA	C1C-NC	-3.18	1.32	1.37
18	B	840	CLA	C1C-NC	-3.17	1.32	1.37
18	A	853	CLA	C1C-NC	-3.17	1.32	1.37
18	A	822	CLA	C1C-NC	-3.17	1.32	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	839	CLA	C1C-NC	-3.16	1.32	1.37
18	A	812	CLA	C1C-NC	-3.16	1.32	1.37
18	A	836	CLA	C1C-NC	-3.16	1.32	1.37
18	B	823	CLA	C1C-NC	-3.14	1.32	1.37
18	1	5006	CLA	C1C-NC	-3.14	1.32	1.37
18	3	318	CLA	C1C-NC	-3.14	1.32	1.37
18	B	830	CLA	C1C-NC	-3.14	1.32	1.37
18	A	806	CLA	C1C-NC	-3.14	1.32	1.37
18	A	824	CLA	C1C-NC	-3.13	1.32	1.37
18	1	5007	CLA	C1C-NC	-3.13	1.33	1.37
18	1	5008	CLA	C1C-NC	-3.13	1.33	1.37
18	A	825	CLA	C1C-NC	-3.13	1.33	1.37
18	A	813	CLA	C1C-NC	-3.13	1.33	1.37
18	A	814	CLA	C1C-NC	-3.12	1.33	1.37
18	4	309	CLA	C1C-NC	-3.12	1.33	1.37
18	A	807	CLA	C1C-NC	-3.12	1.33	1.37
18	B	833	CLA	C1C-NC	-3.11	1.33	1.37
18	B	809	CLA	C1C-NC	-3.11	1.33	1.37
18	J	1103	CLA	C1C-NC	-3.11	1.33	1.37
18	2	311	CLA	C1C-NC	-3.11	1.33	1.37
18	B	832	CLA	C1C-NC	-3.11	1.33	1.37
18	B	811	CLA	C1C-NC	-3.10	1.33	1.37
18	4	315	CLA	C1C-NC	-3.10	1.33	1.37
18	B	806	CLA	C1C-NC	-3.10	1.33	1.37
18	3	317	CLA	C1C-NC	-3.10	1.33	1.37
18	B	813	CLA	C1C-NC	-3.10	1.33	1.37
18	L	301	CLA	C1C-NC	-3.10	1.33	1.37
18	B	803	CLA	C1C-NC	-3.09	1.33	1.37
18	B	804	CLA	C1C-NC	-3.09	1.33	1.37
18	A	831	CLA	C1C-NC	-3.09	1.33	1.37
18	H	1701	CLA	C1C-NC	-3.09	1.33	1.37
18	4	305	CLA	C1C-NC	-3.09	1.33	1.37
18	B	815	CLA	C1C-NC	-3.09	1.33	1.37
18	B	835	CLA	C1C-NC	-3.09	1.33	1.37
18	B	819	CLA	C1C-NC	-3.09	1.33	1.37
18	L	305	CLA	C1C-NC	-3.08	1.33	1.37
18	B	826	CLA	C1C-NC	-3.08	1.33	1.37
18	B	839	CLA	C1C-NC	-3.08	1.33	1.37
18	2	317	CLA	C1C-NC	-3.08	1.33	1.37
18	2	306	CLA	C1C-NC	-3.08	1.33	1.37
30	1	5014	CHL	C3A-C2A	-3.08	1.52	1.54
18	G	1601	CLA	C1C-NC	-3.08	1.33	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	309	CLA	C1C-NC	-3.08	1.33	1.37
18	B	818	CLA	C1C-NC	-3.08	1.33	1.37
18	B	822	CLA	C1C-NC	-3.07	1.33	1.37
18	F	301	CLA	C1C-NC	-3.07	1.33	1.37
18	B	841	CLA	C1C-NC	-3.07	1.33	1.37
18	3	307	CLA	C1C-NC	-3.07	1.33	1.37
18	A	835	CLA	C1C-NC	-3.07	1.33	1.37
18	A	827	CLA	C1C-NC	-3.07	1.33	1.37
18	A	821	CLA	C1C-NC	-3.07	1.33	1.37
18	1	5009	CLA	C1C-NC	-3.07	1.33	1.37
18	K	1403	CLA	C1C-NC	-3.06	1.33	1.37
18	A	804	CLA	C1C-NC	-3.06	1.33	1.37
18	B	807	CLA	C1C-NC	-3.06	1.33	1.37
18	F	303	CLA	C1C-NC	-3.06	1.33	1.37
18	A	808	CLA	C1C-NC	-3.06	1.33	1.37
18	A	826	CLA	C1C-NC	-3.06	1.33	1.37
18	L	304	CLA	C1C-NC	-3.06	1.33	1.37
18	A	810	CLA	C1C-NC	-3.06	1.33	1.37
18	A	815	CLA	C1C-NC	-3.06	1.33	1.37
18	A	820	CLA	C1C-NC	-3.06	1.33	1.37
18	A	809	CLA	C1C-NC	-3.05	1.33	1.37
18	K	1402	CLA	C1C-NC	-3.05	1.33	1.37
18	J	1101	CLA	C1C-NC	-3.05	1.33	1.37
18	A	805	CLA	C1C-NC	-3.05	1.33	1.37
18	B	808	CLA	C1C-NC	-3.05	1.33	1.37
18	B	810	CLA	C1C-NC	-3.05	1.33	1.37
18	K	1401	CLA	C1C-NC	-3.05	1.33	1.37
18	L	306	CLA	C1C-NC	-3.05	1.33	1.37
18	2	310	CLA	C1C-NC	-3.05	1.33	1.37
18	B	816	CLA	C1C-NC	-3.05	1.33	1.37
18	1	5010	CLA	C1C-NC	-3.05	1.33	1.37
18	F	302	CLA	C1C-NC	-3.04	1.33	1.37
18	2	308	CLA	C1C-NC	-3.04	1.33	1.37
18	4	308	CLA	C1C-NC	-3.04	1.33	1.37
18	2	326	CLA	C1C-NC	-3.04	1.33	1.37
18	B	829	CLA	C1C-NC	-3.04	1.33	1.37
18	3	301	CLA	C1C-NC	-3.04	1.33	1.37
18	3	308	CLA	C1C-NC	-3.04	1.33	1.37
18	1	5012	CLA	C1C-NC	-3.04	1.33	1.37
18	4	312	CLA	C1C-NC	-3.04	1.33	1.37
18	A	819	CLA	C1C-NC	-3.03	1.33	1.37
18	B	837	CLA	C1C-NC	-3.03	1.33	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	307	CLA	C1C-NC	-3.03	1.33	1.37
18	A	840	CLA	C1C-NC	-3.03	1.33	1.37
18	A	837	CLA	C1C-NC	-3.03	1.33	1.37
18	2	312	CLA	C1C-NC	-3.03	1.33	1.37
18	B	821	CLA	C1C-NC	-3.03	1.33	1.37
30	4	313	CHL	C3A-C2A	-3.02	1.52	1.54
18	1	5015	CLA	C1C-NC	-3.02	1.33	1.37
18	B	824	CLA	C1C-NC	-3.02	1.33	1.37
18	4	310	CLA	C1C-NC	-3.02	1.33	1.37
18	B	828	CLA	C1C-NC	-3.02	1.33	1.37
18	1	5013	CLA	C1C-NC	-3.02	1.33	1.37
18	3	311	CLA	C1C-NC	-3.02	1.33	1.37
18	3	315	CLA	C1C-NC	-3.02	1.33	1.37
18	3	319	CLA	C1C-NC	-3.02	1.33	1.37
18	A	852	CLA	C1C-NC	-3.02	1.33	1.37
18	A	838	CLA	C1C-NC	-3.01	1.33	1.37
18	2	309	CLA	C1C-NC	-3.01	1.33	1.37
18	A	818	CLA	C1C-NC	-3.01	1.33	1.37
18	2	313	CLA	C1C-NC	-3.01	1.33	1.37
18	B	831	CLA	C1C-NC	-3.01	1.33	1.37
30	4	317	CHL	C3A-C2A	-3.01	1.52	1.54
18	A	832	CLA	C1C-NC	-3.01	1.33	1.37
18	4	306	CLA	C1C-NC	-3.01	1.33	1.37
18	B	838	CLA	C1C-NC	-3.01	1.33	1.37
18	A	816	CLA	C1C-NC	-3.00	1.33	1.37
18	B	834	CLA	C1C-NC	-3.00	1.33	1.37
18	A	829	CLA	C1C-NC	-3.00	1.33	1.37
18	B	836	CLA	C1C-NC	-3.00	1.33	1.37
18	A	830	CLA	C1C-NC	-3.00	1.33	1.37
18	G	1602	CLA	C1C-NC	-3.00	1.33	1.37
18	B	820	CLA	C1C-NC	-2.98	1.33	1.37
18	3	314	CLA	C1C-NC	-2.98	1.33	1.37
18	A	817	CLA	C1C-NC	-2.98	1.33	1.37
18	B	805	CLA	C1C-NC	-2.98	1.33	1.37
18	1	5011	CLA	C1C-NC	-2.98	1.33	1.37
18	1	5018	CLA	C1C-NC	-2.98	1.33	1.37
30	3	313	CHL	C3A-C2A	-2.98	1.52	1.54
18	G	1603	CLA	C1C-NC	-2.98	1.33	1.37
18	A	802	CLA	C1C-NC	-2.98	1.33	1.37
18	A	803	CLA	C1C-NC	-2.98	1.33	1.37
18	B	817	CLA	C1C-NC	-2.98	1.33	1.37
18	A	833	CLA	C1C-NC	-2.98	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	5017	CLA	C1C-NC	-2.97	1.33	1.37
18	4	307	CLA	C1C-NC	-2.97	1.33	1.37
18	A	834	CLA	C1C-NC	-2.96	1.33	1.37
24	2	322	LMG	C19-C18	-2.94	1.33	1.51
30	2	319	CHL	C3A-C2A	-2.94	1.52	1.54
17	A	801	CL0	CHB-C4A	-2.92	1.35	1.38
30	3	316	CHL	C3B-C2B	-2.91	1.36	1.40
18	B	801	CLA	C1C-NC	-2.90	1.33	1.37
18	B	825	CLA	C1C-NC	-2.89	1.33	1.37
30	4	314	CHL	C3B-C2B	-2.86	1.36	1.40
17	A	801	CL0	C3A-C2A	-2.85	1.52	1.54
18	A	823	CLA	C1C-NC	-2.84	1.33	1.37
18	2	317	CLA	C4B-NB	-2.80	1.34	1.37
30	3	312	CHL	C1D-C2D	2.79	1.42	1.39
30	2	318	CHL	C3A-C2A	-2.79	1.52	1.54
30	2	315	CHL	C1D-C2D	2.79	1.42	1.39
30	3	310	CHL	C1B-C2B	2.78	1.42	1.39
30	3	310	CHL	C1D-C2D	2.78	1.42	1.39
30	3	316	CHL	C1D-C2D	2.78	1.42	1.39
18	B	814	CLA	C4B-NB	-2.77	1.34	1.37
30	1	5016	CHL	C1D-C2D	2.77	1.42	1.39
30	1	5016	CHL	C1B-C2B	2.77	1.42	1.39
30	2	314	CHL	C1D-C2D	2.77	1.42	1.39
30	4	317	CHL	C1D-C2D	2.76	1.42	1.39
30	3	316	CHL	CHB-C4A	-2.76	1.35	1.38
30	2	316	CHL	C1D-C2D	2.76	1.42	1.39
30	2	316	CHL	C2C-C3C	2.75	1.39	1.36
30	2	319	CHL	C1D-C2D	2.75	1.42	1.39
18	A	807	CLA	C4B-NB	-2.75	1.34	1.37
18	A	826	CLA	C4B-NB	-2.74	1.34	1.37
30	4	318	CHL	C1B-C2B	2.74	1.42	1.39
30	2	318	CHL	C1D-C2D	2.74	1.42	1.39
18	B	815	CLA	C4B-NB	-2.74	1.34	1.37
30	1	5014	CHL	C1B-C2B	2.74	1.42	1.39
30	2	319	CHL	C1B-C2B	2.74	1.42	1.39
30	3	313	CHL	C1B-C2B	2.73	1.42	1.39
18	4	315	CLA	C4B-NB	-2.73	1.34	1.37
30	4	313	CHL	C1D-C2D	2.73	1.42	1.39
30	1	5014	CHL	C1D-C2D	2.73	1.42	1.39
30	4	302	CHL	C1B-C2B	2.73	1.42	1.39
30	2	318	CHL	C1B-C2B	2.72	1.42	1.39
30	4	316	CHL	C1D-C2D	2.72	1.42	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	3	312	CHL	CHB-C4A	-2.72	1.35	1.38
18	B	834	CLA	C4B-NB	-2.72	1.34	1.37
30	4	314	CHL	C1D-C2D	2.72	1.42	1.39
18	B	827	CLA	C4B-NB	-2.72	1.34	1.37
30	3	312	CHL	C1B-C2B	2.72	1.42	1.39
18	2	312	CLA	C4B-NB	-2.72	1.34	1.37
18	A	808	CLA	C4B-NB	-2.72	1.34	1.37
18	B	803	CLA	C4B-NB	-2.72	1.34	1.37
18	G	1601	CLA	C4B-NB	-2.71	1.34	1.37
30	2	315	CHL	C1B-C2B	2.71	1.42	1.39
30	4	314	CHL	CHB-C4A	-2.71	1.35	1.38
18	F	301	CLA	C4B-NB	-2.70	1.34	1.37
30	4	313	CHL	C1B-C2B	2.70	1.42	1.39
30	4	316	CHL	C1B-C2B	2.70	1.42	1.39
18	A	813	CLA	C4B-NB	-2.70	1.34	1.37
30	2	316	CHL	CHB-C4A	-2.70	1.35	1.38
30	2	314	CHL	C1B-C2B	2.69	1.42	1.39
30	4	317	CHL	C1B-C2B	2.69	1.42	1.39
30	3	313	CHL	C1D-C2D	2.69	1.42	1.39
30	4	302	CHL	C1D-C2D	2.69	1.42	1.39
18	A	821	CLA	C4B-NB	-2.69	1.34	1.37
18	A	825	CLA	C4B-NB	-2.69	1.34	1.37
18	1	5010	CLA	C4B-NB	-2.69	1.34	1.37
30	3	310	CHL	C3A-C2A	-2.69	1.52	1.54
18	3	301	CLA	C4B-NB	-2.69	1.34	1.37
30	2	318	CHL	C2C-C3C	2.68	1.39	1.36
30	4	318	CHL	C1D-C2D	2.68	1.42	1.39
18	1	5006	CLA	C4B-NB	-2.68	1.34	1.37
30	2	315	CHL	CHB-C4A	-2.68	1.35	1.38
18	B	829	CLA	C4B-NB	-2.68	1.34	1.37
18	2	311	CLA	C4B-NB	-2.67	1.34	1.37
18	B	813	CLA	C4B-NB	-2.66	1.34	1.37
18	B	830	CLA	C4B-NB	-2.66	1.34	1.37
18	A	812	CLA	C4B-NB	-2.66	1.34	1.37
18	A	828	CLA	C4B-NB	-2.66	1.34	1.37
18	J	1101	CLA	C4B-NB	-2.66	1.34	1.37
18	B	825	CLA	C4B-NB	-2.66	1.34	1.37
18	A	805	CLA	C4B-NB	-2.66	1.34	1.37
18	B	828	CLA	C4B-NB	-2.66	1.34	1.37
18	B	841	CLA	C4B-NB	-2.65	1.34	1.37
18	A	819	CLA	C4B-NB	-2.65	1.34	1.37
18	L	301	CLA	C4B-NB	-2.65	1.34	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	310	CLA	C4B-NB	-2.65	1.34	1.37
18	K	1401	CLA	C4B-NB	-2.65	1.34	1.37
18	4	309	CLA	C4B-NB	-2.64	1.34	1.37
18	A	829	CLA	C4B-NB	-2.64	1.34	1.37
18	A	815	CLA	C4B-NB	-2.64	1.34	1.37
18	A	840	CLA	C4B-NB	-2.64	1.34	1.37
18	B	819	CLA	C4B-NB	-2.63	1.34	1.37
18	A	838	CLA	C4B-NB	-2.63	1.34	1.37
30	4	314	CHL	C1B-C2B	2.63	1.42	1.39
18	4	305	CLA	C4B-NB	-2.63	1.34	1.37
18	B	826	CLA	C4B-NB	-2.63	1.34	1.37
18	4	310	CLA	C4B-NB	-2.63	1.34	1.37
18	A	820	CLA	C4B-NB	-2.63	1.34	1.37
30	2	316	CHL	C1B-C2B	2.63	1.42	1.39
18	A	852	CLA	C4B-NB	-2.62	1.34	1.37
18	3	311	CLA	C4B-NB	-2.62	1.34	1.37
18	B	816	CLA	C4B-NB	-2.62	1.34	1.37
30	4	317	CHL	CHB-C4A	-2.62	1.35	1.38
18	A	823	CLA	C4B-NB	-2.62	1.34	1.37
18	4	308	CLA	C4B-NB	-2.62	1.34	1.37
18	B	807	CLA	C4B-NB	-2.62	1.34	1.37
30	2	314	CHL	CHB-C4A	-2.61	1.35	1.38
18	A	834	CLA	C4B-NB	-2.61	1.34	1.37
18	A	818	CLA	C4B-NB	-2.61	1.34	1.37
18	L	305	CLA	C4B-NB	-2.61	1.34	1.37
30	4	313	CHL	CHB-C4A	-2.61	1.35	1.38
18	B	820	CLA	C4B-NB	-2.61	1.34	1.37
18	B	805	CLA	C4B-NB	-2.61	1.34	1.37
18	B	804	CLA	C4B-NB	-2.61	1.34	1.37
18	A	817	CLA	C4B-NB	-2.61	1.34	1.37
18	A	824	CLA	C4B-NB	-2.61	1.34	1.37
18	F	302	CLA	C4B-NB	-2.61	1.34	1.37
18	B	838	CLA	C4B-NB	-2.61	1.34	1.37
18	H	1701	CLA	C4B-NB	-2.60	1.34	1.37
30	3	310	CHL	CHB-C4A	-2.60	1.35	1.38
18	2	306	CLA	C4B-NB	-2.60	1.34	1.37
18	B	809	CLA	C4B-NB	-2.60	1.34	1.37
18	A	802	CLA	C4B-NB	-2.60	1.34	1.37
18	3	318	CLA	C4B-NB	-2.60	1.34	1.37
30	3	316	CHL	C1B-C2B	2.60	1.42	1.39
18	B	836	CLA	C4B-NB	-2.60	1.34	1.37
18	1	5011	CLA	C4B-NB	-2.60	1.34	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	317	CLA	C4B-NB	-2.60	1.34	1.37
18	A	804	CLA	C4B-NB	-2.59	1.34	1.37
18	2	309	CLA	C4B-NB	-2.59	1.34	1.37
18	A	837	CLA	C4B-NB	-2.59	1.34	1.37
18	A	806	CLA	C4B-NB	-2.59	1.34	1.37
18	A	827	CLA	C4B-NB	-2.59	1.34	1.37
18	3	315	CLA	C4B-NB	-2.59	1.34	1.37
30	4	316	CHL	C3A-C2A	-2.59	1.52	1.54
30	3	313	CHL	CHB-C4A	-2.59	1.35	1.38
18	B	832	CLA	C4B-NB	-2.59	1.34	1.37
18	B	833	CLA	C4B-NB	-2.58	1.34	1.37
18	B	808	CLA	C4B-NB	-2.58	1.34	1.37
30	2	318	CHL	CHB-C4A	-2.58	1.35	1.38
18	3	307	CLA	C4B-NB	-2.58	1.34	1.37
18	G	1602	CLA	C4B-NB	-2.57	1.34	1.37
18	1	5013	CLA	C4B-NB	-2.57	1.34	1.37
18	B	810	CLA	C4B-NB	-2.57	1.34	1.37
18	1	5009	CLA	C4B-NB	-2.56	1.34	1.37
18	L	306	CLA	C4B-NB	-2.56	1.34	1.37
18	1	5015	CLA	C4B-NB	-2.56	1.34	1.37
30	4	316	CHL	CHB-C4A	-2.56	1.35	1.38
18	A	853	CLA	C4B-NB	-2.56	1.34	1.37
18	B	839	CLA	C4B-NB	-2.56	1.34	1.37
18	B	831	CLA	C4B-NB	-2.56	1.34	1.37
18	A	831	CLA	C4B-NB	-2.56	1.34	1.37
30	1	5014	CHL	CHB-C4A	-2.55	1.35	1.38
30	4	302	CHL	CHB-C4A	-2.55	1.35	1.38
30	2	319	CHL	CHB-C4A	-2.55	1.35	1.38
18	L	304	CLA	C4B-NB	-2.55	1.34	1.37
18	2	313	CLA	C4B-NB	-2.55	1.34	1.37
18	B	821	CLA	C4B-NB	-2.55	1.34	1.37
30	4	318	CHL	CHB-C4A	-2.54	1.35	1.38
18	A	809	CLA	C4B-NB	-2.54	1.34	1.37
18	2	308	CLA	C4B-NB	-2.54	1.34	1.37
18	3	319	CLA	C4B-NB	-2.54	1.34	1.37
18	K	1403	CLA	C4B-NB	-2.54	1.34	1.37
18	A	803	CLA	C4B-NB	-2.54	1.34	1.37
18	4	312	CLA	C4B-NB	-2.54	1.34	1.37
18	B	837	CLA	C4B-NB	-2.53	1.34	1.37
18	G	1603	CLA	C4B-NB	-2.53	1.34	1.37
18	A	816	CLA	C4B-NB	-2.53	1.34	1.37
30	1	5016	CHL	CHB-C4A	-2.52	1.35	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	G	1605	LMT	O3'-C3'	-2.52	1.36	1.43
18	B	801	CLA	C4B-NB	-2.52	1.34	1.37
18	1	5018	CLA	C4B-NB	-2.51	1.34	1.37
18	A	833	CLA	C4B-NB	-2.50	1.34	1.37
18	4	306	CLA	C4B-NB	-2.50	1.34	1.37
18	A	830	CLA	C4B-NB	-2.50	1.34	1.37
31	2	304	XAT	O24-C25	-2.50	1.43	1.46
24	G	1607	LMG	O1-C1	2.50	1.44	1.40
23	A	850	LMT	O3'-C3'	-2.48	1.36	1.43
18	1	5017	CLA	C4B-NB	-2.48	1.34	1.37
18	B	817	CLA	C4B-NB	-2.48	1.34	1.37
23	J	1107	LMT	O3'-C3'	-2.48	1.36	1.43
18	B	818	CLA	C4B-NB	-2.47	1.34	1.37
23	4	319	LMT	O3'-C3'	-2.47	1.36	1.43
23	B	856	LMT	O3'-C3'	-2.47	1.36	1.43
30	4	316	CHL	C2C-C3C	2.45	1.38	1.36
18	B	824	CLA	C4B-NB	-2.45	1.34	1.37
30	2	319	CHL	C1A-CHA	-2.45	1.37	1.40
18	3	314	CLA	C4B-NB	-2.44	1.34	1.37
18	F	303	CLA	C4B-NB	-2.44	1.34	1.37
18	2	307	CLA	C4B-NB	-2.44	1.34	1.37
23	B	852	LMT	O3'-C3'	-2.42	1.37	1.43
18	K	1404	CLA	C4B-NB	-2.42	1.34	1.37
18	A	835	CLA	C4B-NB	-2.42	1.34	1.37
18	B	835	CLA	C4B-NB	-2.42	1.34	1.37
18	3	308	CLA	C4B-NB	-2.41	1.34	1.37
23	G	1606	LMT	O3'-C3'	-2.40	1.37	1.43
31	4	304	XAT	O24-C25	-2.40	1.43	1.46
23	B	853	LMT	O3'-C3'	-2.40	1.37	1.43
18	B	822	CLA	C4B-NB	-2.39	1.34	1.37
18	4	307	CLA	C4B-NB	-2.37	1.34	1.37
26	1	5002	DGD	CAB-C9B	-2.37	1.33	1.50
26	2	327	DGD	CDA-CCA	-2.37	1.33	1.50
24	A	851	LMG	C40-C39	-2.37	1.33	1.50
18	1	5008	CLA	C4B-NB	-2.37	1.34	1.37
26	B	855	DGD	CDA-CCA	-2.37	1.33	1.50
18	B	840	CLA	C4B-NB	-2.37	1.34	1.37
24	F	306	LMG	C19-C18	-2.36	1.33	1.50
26	J	1106	DGD	CAB-C9B	-2.36	1.33	1.50
23	2	325	LMT	O3'-C3'	-2.36	1.37	1.43
18	3	309	CLA	C4B-NB	-2.35	1.34	1.37
18	A	836	CLA	C4B-NB	-2.34	1.34	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	810	CLA	C4B-NB	-2.33	1.34	1.37
18	1	5007	CLA	C4B-NB	-2.33	1.34	1.37
18	A	839	CLA	C4B-NB	-2.32	1.34	1.37
18	A	832	CLA	C4B-NB	-2.32	1.34	1.37
18	B	811	CLA	C4B-NB	-2.32	1.34	1.37
30	3	313	CHL	C1A-CHA	-2.32	1.37	1.40
18	4	311	CLA	C4B-NB	-2.32	1.34	1.37
18	J	1103	CLA	C4B-NB	-2.31	1.34	1.37
18	A	811	CLA	C4B-NB	-2.31	1.34	1.37
18	A	824	CLA	C1C-C2C	2.30	1.49	1.44
18	K	1402	CLA	C4B-NB	-2.28	1.34	1.37
18	1	5012	CLA	C4B-NB	-2.26	1.34	1.37
18	A	822	CLA	C4B-NB	-2.25	1.34	1.37
18	B	806	CLA	C4B-NB	-2.25	1.34	1.37
30	1	5016	CHL	CHA-CBD	2.25	1.54	1.51
30	1	5014	CHL	CHA-CBD	2.24	1.54	1.51
18	A	823	CLA	MG-NC	2.23	2.11	2.06
18	A	816	CLA	C1C-C2C	2.23	1.49	1.44
18	2	326	CLA	C4B-NB	-2.23	1.34	1.37
18	A	814	CLA	C4B-NB	-2.22	1.34	1.37
18	1	5018	CLA	C1C-C2C	2.22	1.49	1.44
18	3	307	CLA	C1C-C2C	2.21	1.49	1.44
18	F	301	CLA	C1C-C2C	2.21	1.49	1.44
18	2	326	CLA	C1A-CHA	2.21	1.52	1.43
18	J	1103	CLA	C1A-CHA	2.21	1.52	1.43
30	4	314	CHL	CHA-CBD	2.21	1.54	1.51
23	B	856	LMT	O2'-C2'	-2.21	1.37	1.43
30	2	316	CHL	CHA-CBD	2.21	1.54	1.51
18	B	823	CLA	C4B-NB	-2.20	1.35	1.37
18	B	830	CLA	CHD-C1D	2.20	1.42	1.38
30	4	313	CHL	CHA-CBD	2.20	1.54	1.51
18	B	801	CLA	C1C-C2C	2.20	1.49	1.44
23	B	856	LMT	O3B-C3B	-2.19	1.37	1.43
30	2	315	CHL	CHA-CBD	2.19	1.54	1.51
30	4	313	CHL	C3B-C2B	-2.19	1.37	1.40
18	B	810	CLA	C1A-CHA	2.19	1.52	1.43
18	1	5017	CLA	C1C-C2C	2.19	1.49	1.44
30	2	318	CHL	CHA-CBD	2.19	1.54	1.51
23	B	852	LMT	O3B-C3B	-2.19	1.37	1.43
18	B	817	CLA	C1C-C2C	2.19	1.49	1.44
23	B	856	LMT	O2B-C2B	-2.19	1.37	1.43
18	4	311	CLA	C1C-C2C	2.18	1.49	1.44

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	301	CLA	C1A-CHA	2.18	1.52	1.43
18	2	312	CLA	C1A-CHA	2.18	1.52	1.43
23	G	1605	LMT	O2B-C2B	-2.18	1.37	1.43
18	A	825	CLA	C1C-C2C	2.18	1.48	1.44
23	4	319	LMT	O2B-C2B	-2.18	1.37	1.43
18	A	823	CLA	C1A-CHA	2.18	1.52	1.43
23	J	1107	LMT	O2B-C2B	-2.18	1.37	1.43
23	G	1605	LMT	O3B-C3B	-2.18	1.37	1.43
18	B	812	CLA	C1C-C2C	2.17	1.48	1.44
23	G	1606	LMT	O3B-C3B	-2.17	1.37	1.43
18	3	314	CLA	C1A-CHA	2.17	1.52	1.43
23	2	325	LMT	O2B-C2B	-2.17	1.37	1.43
23	B	852	LMT	O2B-C2B	-2.17	1.37	1.43
30	2	319	CHL	CHA-CBD	2.17	1.54	1.51
18	B	825	CLA	C1A-CHA	2.17	1.52	1.43
18	B	816	CLA	C1A-CHA	2.17	1.52	1.43
18	A	836	CLA	C1C-C2C	2.17	1.48	1.44
18	4	306	CLA	C1A-CHA	2.17	1.52	1.43
18	3	309	CLA	C1A-CHA	2.16	1.52	1.43
23	4	319	LMT	O3B-C3B	-2.16	1.37	1.43
30	4	317	CHL	CHA-CBD	2.16	1.54	1.51
18	A	822	CLA	C1C-C2C	2.16	1.48	1.44
18	1	5010	CLA	C1A-CHA	2.16	1.52	1.43
18	B	812	CLA	C4B-NB	-2.16	1.35	1.37
23	B	853	LMT	O3B-C3B	-2.16	1.37	1.43
18	B	828	CLA	C1A-CHA	2.16	1.52	1.43
18	4	305	CLA	C1A-CHA	2.16	1.52	1.43
30	1	5016	CHL	C1A-CHA	-2.16	1.37	1.40
18	A	821	CLA	C1A-CHA	2.16	1.52	1.43
18	A	832	CLA	C1C-C2C	2.16	1.48	1.44
18	L	301	CLA	C1C-C2C	2.16	1.48	1.44
18	L	306	CLA	C1A-CHA	2.15	1.52	1.43
18	B	841	CLA	C1C-C2C	2.15	1.48	1.44
18	B	813	CLA	C1A-CHA	2.15	1.52	1.43
18	3	308	CLA	C1A-CHA	2.15	1.52	1.43
30	2	318	CHL	C3B-C2B	-2.15	1.37	1.40
18	B	805	CLA	C1C-C2C	2.15	1.48	1.44
18	A	838	CLA	C1C-C2C	2.15	1.48	1.44
30	4	302	CHL	CHA-CBD	2.15	1.54	1.51
23	J	1107	LMT	O2'-C2'	-2.15	1.37	1.43
23	4	319	LMT	O2'-C2'	-2.15	1.37	1.43
18	A	835	CLA	C1C-C2C	2.15	1.48	1.44

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	804	CLA	C1A-CHA	2.15	1.51	1.43
18	B	833	CLA	C1A-CHA	2.14	1.51	1.43
18	4	310	CLA	C1A-CHA	2.14	1.51	1.43
18	1	5017	CLA	C1A-CHA	2.14	1.51	1.43
18	A	810	CLA	C1A-CHA	2.14	1.51	1.43
18	G	1601	CLA	C1A-CHA	2.14	1.51	1.43
18	2	306	CLA	C1A-CHA	2.14	1.51	1.43
18	3	319	CLA	C1C-C2C	2.14	1.48	1.44
30	4	318	CHL	CHA-CBD	2.14	1.54	1.51
23	B	856	LMT	O1'-C1'	-2.14	1.36	1.40
18	A	840	CLA	C1A-CHA	2.14	1.51	1.43
30	3	316	CHL	CHA-CBD	2.14	1.54	1.51
18	F	303	CLA	C1C-C2C	2.14	1.48	1.44
23	B	853	LMT	O2B-C2B	-2.14	1.37	1.43
18	A	834	CLA	C1C-C2C	2.14	1.48	1.44
18	J	1103	CLA	C1C-C2C	2.13	1.48	1.44
18	B	822	CLA	C1A-CHA	2.13	1.51	1.43
18	A	803	CLA	C1A-CHA	2.13	1.51	1.43
30	2	314	CHL	CHA-CBD	2.13	1.54	1.51
30	3	312	CHL	CHA-CBD	2.13	1.54	1.51
23	A	850	LMT	O3B-C3B	-2.13	1.37	1.43
18	B	821	CLA	C1A-CHA	2.13	1.51	1.43
18	2	308	CLA	C1A-CHA	2.13	1.51	1.43
18	2	311	CLA	C1A-CHA	2.13	1.51	1.43
18	B	835	CLA	C1C-C2C	2.13	1.48	1.44
18	B	839	CLA	C1C-C2C	2.13	1.48	1.44
18	2	308	CLA	C1C-C2C	2.13	1.48	1.44
18	A	807	CLA	C1C-C2C	2.13	1.48	1.44
18	A	837	CLA	C1A-CHA	2.13	1.51	1.43
23	G	1606	LMT	O2'-C2'	-2.13	1.37	1.43
18	A	838	CLA	C1A-CHA	2.13	1.51	1.43
18	K	1404	CLA	C1A-CHA	2.13	1.51	1.43
18	3	308	CLA	C1C-C2C	2.13	1.48	1.44
18	1	5012	CLA	C1A-CHA	2.13	1.51	1.43
18	A	803	CLA	C1C-C2C	2.13	1.48	1.44
18	A	802	CLA	C1C-C2C	2.13	1.48	1.44
18	4	311	CLA	C1A-CHA	2.13	1.51	1.43
18	B	823	CLA	C1C-C2C	2.13	1.48	1.44
18	B	826	CLA	C1C-C2C	2.13	1.48	1.44
18	G	1602	CLA	C1A-CHA	2.13	1.51	1.43
18	A	837	CLA	C1C-C2C	2.13	1.48	1.44
18	3	315	CLA	C1C-C2C	2.13	1.48	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	5009	CLA	C1C-C2C	2.12	1.48	1.44
18	L	304	CLA	C1A-CHA	2.12	1.51	1.43
18	B	840	CLA	C1A-CHA	2.12	1.51	1.43
18	K	1403	CLA	C1A-CHA	2.12	1.51	1.43
18	B	826	CLA	C1A-CHA	2.12	1.51	1.43
18	3	309	CLA	C1C-C2C	2.12	1.48	1.44
30	4	302	CHL	C3B-C2B	-2.12	1.37	1.40
30	2	314	CHL	C3B-C2B	-2.12	1.37	1.40
18	1	5006	CLA	C1C-C2C	2.12	1.48	1.44
18	A	830	CLA	C1C-C2C	2.12	1.48	1.44
18	1	5013	CLA	C1A-CHA	2.12	1.51	1.43
23	J	1107	LMT	O3B-C3B	-2.12	1.37	1.43
18	B	838	CLA	C1C-C2C	2.12	1.48	1.44
18	L	305	CLA	C1C-C2C	2.12	1.48	1.44
30	4	316	CHL	CHA-CBD	2.12	1.54	1.51
18	1	5007	CLA	C1C-C2C	2.12	1.48	1.44
18	A	833	CLA	C1A-CHA	2.12	1.51	1.43
18	B	835	CLA	C1A-CHA	2.12	1.51	1.43
18	H	1701	CLA	C1A-CHA	2.12	1.51	1.43
18	A	806	CLA	C1C-C2C	2.12	1.48	1.44
28	F	310	ZEX	C21-C26	-2.12	1.51	1.53
18	A	802	CLA	C1A-CHA	2.12	1.51	1.43
18	A	816	CLA	C1A-CHA	2.12	1.51	1.43
18	F	302	CLA	C1A-CHA	2.12	1.51	1.43
23	2	325	LMT	O3B-C3B	-2.11	1.37	1.43
18	1	5018	CLA	C1A-CHA	2.11	1.51	1.43
18	B	801	CLA	C1A-CHA	2.11	1.51	1.43
30	4	316	CHL	C1A-CHA	-2.11	1.37	1.40
18	2	307	CLA	C1A-CHA	2.11	1.51	1.43
23	G	1605	LMT	O2'-C2'	-2.11	1.37	1.43
18	B	832	CLA	C1A-CHA	2.11	1.51	1.43
18	2	309	CLA	C1C-C2C	2.11	1.48	1.44
18	A	807	CLA	C1A-CHA	2.11	1.51	1.43
23	B	852	LMT	O2'-C2'	-2.11	1.37	1.43
18	A	805	CLA	C1C-C2C	2.11	1.48	1.44
26	J	1106	DGD	O5D-C1E	2.11	1.43	1.40
18	A	813	CLA	C1A-CHA	2.11	1.51	1.43
18	A	829	CLA	C1C-C2C	2.11	1.48	1.44
18	K	1402	CLA	C1C-C2C	2.11	1.48	1.44
18	A	852	CLA	C1C-C2C	2.11	1.48	1.44
18	B	815	CLA	C1A-CHA	2.11	1.51	1.43
18	4	315	CLA	C1A-CHA	2.11	1.51	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	809	CLA	C1A-CHA	2.11	1.51	1.43
18	2	310	CLA	C1A-CHA	2.11	1.51	1.43
18	2	312	CLA	C1C-C2C	2.11	1.48	1.44
18	4	307	CLA	C1A-CHA	2.11	1.51	1.43
18	A	825	CLA	C1A-CHA	2.11	1.51	1.43
18	3	315	CLA	C1A-CHA	2.10	1.51	1.43
18	1	5015	CLA	C1A-CHA	2.10	1.51	1.43
18	4	305	CLA	C1C-C2C	2.10	1.48	1.44
18	B	827	CLA	C1A-CHA	2.10	1.51	1.43
18	A	817	CLA	C1C-C2C	2.10	1.48	1.44
18	1	5015	CLA	C1C-C2C	2.10	1.48	1.44
18	A	831	CLA	C1A-CHA	2.10	1.51	1.43
18	2	307	CLA	C1C-C2C	2.10	1.48	1.44
18	B	838	CLA	C1A-CHA	2.10	1.51	1.43
18	1	5008	CLA	C1A-CHA	2.10	1.51	1.43
18	G	1603	CLA	C1C-C2C	2.10	1.48	1.44
18	K	1401	CLA	C1A-CHA	2.10	1.51	1.43
18	1	5007	CLA	C1A-CHA	2.09	1.51	1.43
18	G	1602	CLA	C1C-C2C	2.09	1.48	1.44
18	A	809	CLA	C1C-C2C	2.09	1.48	1.44
18	A	833	CLA	C1C-C2C	2.09	1.48	1.44
18	3	314	CLA	C1C-C2C	2.09	1.48	1.44
18	2	317	CLA	CHD-C1D	2.09	1.42	1.38
18	B	823	CLA	C1A-CHA	2.09	1.51	1.43
18	B	830	CLA	C1A-CHA	2.09	1.51	1.43
18	A	820	CLA	C1A-CHA	2.09	1.51	1.43
18	2	313	CLA	C1A-CHA	2.09	1.51	1.43
18	4	308	CLA	C1C-C2C	2.09	1.48	1.44
18	A	817	CLA	C1A-CHA	2.09	1.51	1.43
18	B	837	CLA	C1C-C2C	2.09	1.48	1.44
18	B	816	CLA	C1C-C2C	2.09	1.48	1.44
18	3	307	CLA	C1A-CHA	2.09	1.51	1.43
18	B	831	CLA	C1A-CHA	2.09	1.51	1.43
18	3	317	CLA	C1A-CHA	2.09	1.51	1.43
18	2	326	CLA	MG-NC	2.08	2.11	2.06
18	A	818	CLA	C1A-CHA	2.08	1.51	1.43
18	A	810	CLA	C1C-C2C	2.08	1.48	1.44
18	1	5012	CLA	C1C-C2C	2.08	1.48	1.44
18	B	829	CLA	C1A-CHA	2.08	1.51	1.43
18	A	822	CLA	C1A-CHA	2.08	1.51	1.43
18	A	811	CLA	C1A-CHA	2.08	1.51	1.43
30	4	317	CHL	C3B-C2B	-2.08	1.37	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	840	CLA	C1C-C2C	2.08	1.48	1.44
18	B	824	CLA	C1C-C2C	2.08	1.48	1.44
18	B	805	CLA	C1A-CHA	2.08	1.51	1.43
23	2	325	LMT	O2'-C2'	-2.08	1.37	1.43
23	B	853	LMT	O2'-C2'	-2.08	1.37	1.43
18	A	839	CLA	C1A-CHA	2.08	1.51	1.43
18	A	814	CLA	C1A-CHA	2.08	1.51	1.43
18	2	313	CLA	C1C-C2C	2.08	1.48	1.44
18	4	307	CLA	C1C-C2C	2.08	1.48	1.44
18	B	818	CLA	C1A-CHA	2.08	1.51	1.43
18	K	1404	CLA	C1C-C2C	2.08	1.48	1.44
18	2	326	CLA	C1C-C2C	2.08	1.48	1.44
18	L	306	CLA	C1C-C2C	2.07	1.48	1.44
18	J	1103	CLA	MG-NC	2.07	2.11	2.06
18	A	808	CLA	C1A-CHA	2.07	1.51	1.43
18	B	827	CLA	C3D-C4D	-2.07	1.39	1.44
23	G	1606	LMT	O2B-C2B	-2.07	1.37	1.43
18	B	806	CLA	C1A-CHA	2.07	1.51	1.43
18	A	808	CLA	C1C-C2C	2.07	1.48	1.44
18	F	303	CLA	C1A-CHA	2.07	1.51	1.43
18	B	822	CLA	C1C-C2C	2.07	1.48	1.44
18	B	824	CLA	C1A-CHA	2.07	1.51	1.43
18	K	1401	CLA	C1C-C2C	2.07	1.48	1.44
18	A	824	CLA	C1A-CHA	2.07	1.51	1.43
18	2	310	CLA	C1C-C2C	2.07	1.48	1.44
18	B	808	CLA	C1C-C2C	2.07	1.48	1.44
18	A	819	CLA	C1C-C2C	2.07	1.48	1.44
18	F	302	CLA	C1C-C2C	2.06	1.48	1.44
18	A	826	CLA	C1C-C2C	2.06	1.48	1.44
18	B	815	CLA	C1C-C2C	2.06	1.48	1.44
18	A	828	CLA	CHD-C1D	2.06	1.42	1.38
18	A	827	CLA	C1C-C2C	2.06	1.48	1.44
18	1	5011	CLA	C1C-C2C	2.06	1.48	1.44
18	3	311	CLA	C1C-C2C	2.06	1.48	1.44
18	A	834	CLA	C1A-CHA	2.06	1.51	1.43
18	A	818	CLA	C1C-C2C	2.06	1.48	1.44
18	1	5008	CLA	C1C-C2C	2.06	1.48	1.44
18	B	836	CLA	MG-NC	2.06	2.11	2.06
18	4	306	CLA	C1C-C2C	2.06	1.48	1.44
18	1	5011	CLA	C1A-CHA	2.06	1.51	1.43
18	A	831	CLA	C1C-C2C	2.06	1.48	1.44
18	4	312	CLA	C1C-C2C	2.06	1.48	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	5006	CLA	C1A-CHA	2.06	1.51	1.43
18	4	312	CLA	C1A-CHA	2.06	1.51	1.43
18	4	310	CLA	C1C-C2C	2.06	1.48	1.44
18	B	830	CLA	C3D-C4D	-2.06	1.39	1.44
18	3	319	CLA	C1A-CHA	2.06	1.51	1.43
24	1	5001	LMG	O1-C1	2.06	1.43	1.40
18	B	831	CLA	C1C-C2C	2.06	1.48	1.44
18	L	301	CLA	C1A-CHA	2.06	1.51	1.43
18	2	306	CLA	C1C-C2C	2.06	1.48	1.44
18	3	318	CLA	C1A-CHA	2.06	1.51	1.43
18	A	838	CLA	MG-NC	2.06	2.11	2.06
18	B	811	CLA	C1C-C2C	2.05	1.48	1.44
18	B	820	CLA	C1C-C2C	2.05	1.48	1.44
18	B	825	CLA	C1C-C2C	2.05	1.48	1.44
18	B	837	CLA	C1A-CHA	2.05	1.51	1.43
18	4	309	CLA	C1A-CHA	2.05	1.51	1.43
18	A	821	CLA	C1C-C2C	2.05	1.48	1.44
18	3	301	CLA	C1C-C2C	2.05	1.48	1.44
30	3	316	CHL	C1A-CHA	-2.05	1.37	1.40
18	K	1402	CLA	C1A-CHA	2.05	1.51	1.43
18	G	1603	CLA	C1A-CHA	2.05	1.51	1.43
18	4	308	CLA	C1A-CHA	2.05	1.51	1.43
18	B	819	CLA	C1A-CHA	2.05	1.51	1.43
18	K	1404	CLA	MG-NC	2.05	2.11	2.06
18	G	1601	CLA	C1C-C2C	2.05	1.48	1.44
18	B	836	CLA	C1C-C2C	2.04	1.48	1.44
18	F	301	CLA	C1A-CHA	2.04	1.51	1.43
18	B	834	CLA	CHD-C1D	2.04	1.42	1.38
18	K	1402	CLA	MG-NC	2.04	2.11	2.06
18	B	820	CLA	C1A-CHA	2.04	1.51	1.43
18	B	829	CLA	C1C-C2C	2.04	1.48	1.44
18	A	804	CLA	C1A-CHA	2.04	1.51	1.43
18	B	803	CLA	C1C-C2C	2.04	1.48	1.44
18	B	834	CLA	C1C-C2C	2.04	1.48	1.44
18	2	317	CLA	C1A-CHA	2.04	1.51	1.43
18	A	806	CLA	C1A-CHA	2.04	1.51	1.43
23	A	850	LMT	O2'-C2'	-2.04	1.37	1.43
18	3	317	CLA	C1C-C2C	2.04	1.48	1.44
18	B	836	CLA	C1A-CHA	2.04	1.51	1.43
30	2	315	CHL	C1A-CHA	-2.04	1.37	1.40
18	B	841	CLA	C1A-CHA	2.04	1.51	1.43
18	B	806	CLA	C1C-C2C	2.04	1.48	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	811	CLA	C1A-CHA	2.03	1.51	1.43
18	A	839	CLA	C1C-C2C	2.03	1.48	1.44
18	A	815	CLA	C1A-CHA	2.03	1.51	1.43
18	3	311	CLA	C1A-CHA	2.03	1.51	1.43
18	A	833	CLA	MG-NC	2.03	2.11	2.06
18	B	834	CLA	C1A-CHA	2.03	1.51	1.43
18	B	801	CLA	MG-NC	2.03	2.11	2.06
18	A	812	CLA	C1A-CHA	2.03	1.51	1.43
18	3	311	CLA	C3D-C4D	-2.03	1.39	1.44
18	A	835	CLA	C1A-CHA	2.03	1.51	1.43
18	A	823	CLA	C1C-C2C	2.03	1.48	1.44
23	B	853	LMT	O5'-C5'	-2.03	1.39	1.44
18	A	827	CLA	C1A-CHA	2.03	1.51	1.43
18	B	817	CLA	C1A-CHA	2.03	1.51	1.43
24	B	851	LMG	O1-C1	2.03	1.43	1.40
18	A	814	CLA	C1C-C2C	2.03	1.48	1.44
18	A	820	CLA	C1C-C2C	2.03	1.48	1.44
18	A	836	CLA	C1A-CHA	2.03	1.51	1.43
18	J	1101	CLA	C1A-CHA	2.03	1.51	1.43
18	A	812	CLA	C1C-C2C	2.03	1.48	1.44
18	3	314	CLA	MG-NC	2.02	2.11	2.06
18	B	839	CLA	C1A-CHA	2.02	1.51	1.43
18	B	810	CLA	C1C-C2C	2.02	1.48	1.44
18	2	307	CLA	MG-NC	2.02	2.11	2.06
18	B	814	CLA	C1A-CHA	2.02	1.51	1.43
18	B	821	CLA	C1C-C2C	2.02	1.48	1.44
18	A	852	CLA	MG-NC	2.02	2.11	2.06
18	4	315	CLA	CHD-C1D	2.02	1.42	1.38
18	B	808	CLA	C1A-CHA	2.02	1.51	1.43
18	4	309	CLA	C3D-C4D	-2.02	1.39	1.44
18	2	309	CLA	C3D-C4D	-2.02	1.39	1.44
18	B	807	CLA	C1C-C2C	2.02	1.48	1.44
18	A	828	CLA	C1A-CHA	2.02	1.51	1.43
18	F	302	CLA	MG-NC	2.02	2.11	2.06
18	A	819	CLA	C3D-C4D	-2.02	1.39	1.44
18	B	807	CLA	C3D-C4D	-2.02	1.39	1.44
18	G	1602	CLA	MG-NC	2.02	2.11	2.06
18	K	1401	CLA	MG-NC	2.02	2.11	2.06
18	A	815	CLA	C1C-C2C	2.01	1.48	1.44
18	2	311	CLA	C1C-C2C	2.01	1.48	1.44
18	2	312	CLA	MG-NC	2.01	2.11	2.06
18	A	824	CLA	MG-NC	2.01	2.11	2.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	852	CLA	C3D-C4D	-2.01	1.39	1.44
18	G	1603	CLA	MG-NC	2.01	2.11	2.06
18	B	819	CLA	C1C-C2C	2.01	1.48	1.44
18	A	829	CLA	C3D-C4D	-2.01	1.39	1.44
18	1	5018	CLA	MG-NC	2.01	2.11	2.06
18	A	829	CLA	C1A-CHA	2.01	1.51	1.43
18	A	804	CLA	C1C-C2C	2.01	1.48	1.44
18	A	839	CLA	CHD-C1D	2.01	1.42	1.38
18	4	306	CLA	MG-NC	2.01	2.11	2.06
18	A	825	CLA	C3D-C4D	-2.00	1.39	1.44
18	A	832	CLA	C1A-CHA	2.00	1.51	1.43
18	L	305	CLA	C1A-CHA	2.00	1.51	1.43
18	A	805	CLA	C3D-C4D	-2.00	1.39	1.44
18	A	809	CLA	C3D-C4D	-2.00	1.39	1.44
18	A	830	CLA	C1A-CHA	2.00	1.51	1.43
30	4	317	CHL	C1A-CHA	-2.00	1.37	1.40
18	B	811	CLA	C3D-C4D	-2.00	1.39	1.44
18	B	829	CLA	MG-NC	2.00	2.11	2.06
18	3	309	CLA	MG-NC	2.00	2.11	2.06

All (3306) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	I	101	BCR	C10-C11-C12	19.60	180.00	123.20
21	G	1604	BCR	C10-C11-C12	19.21	178.87	123.20
21	K	1405	BCR	C10-C11-C12	19.06	178.43	123.20
21	F	304	BCR	C10-C11-C12	18.93	178.06	123.20
21	A	855	BCR	C10-C11-C12	18.90	177.97	123.20
21	A	845	BCR	C10-C11-C12	18.86	177.84	123.20
21	F	305	BCR	C10-C11-C12	18.73	177.46	123.20
21	B	845	BCR	C10-C11-C12	18.65	177.25	123.20
21	B	843	BCR	C10-C11-C12	18.60	177.09	123.20
21	A	846	BCR	C10-C11-C12	18.53	176.90	123.20
21	I	102	BCR	C10-C11-C12	18.52	176.85	123.20
21	3	305	BCR	C10-C11-C12	18.46	176.70	123.20
21	B	802	BCR	C10-C11-C12	18.46	176.68	123.20
21	B	846	BCR	C10-C11-C12	18.43	176.61	123.20
21	2	305	BCR	C10-C11-C12	18.42	176.56	123.20
21	1	5005	BCR	C10-C11-C12	18.36	176.41	123.20
21	B	847	BCR	C10-C11-C12	18.36	176.39	123.20
21	3	306	BCR	C10-C11-C12	18.33	176.32	123.20
21	L	303	BCR	C10-C11-C12	18.23	176.03	123.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	843	BCR	C10-C11-C12	18.15	175.78	123.20
21	L	302	BCR	C10-C11-C12	18.12	175.71	123.20
21	L	307	BCR	C10-C11-C12	18.08	175.60	123.20
21	A	844	BCR	C10-C11-C12	18.08	175.59	123.20
21	4	301	BCR	C10-C11-C12	18.07	175.55	123.20
21	J	1104	BCR	C10-C11-C12	17.82	174.84	123.20
21	B	844	BCR	C10-C11-C12	17.64	174.32	123.20
21	A	847	BCR	C10-C11-C12	17.45	173.78	123.20
21	B	802	BCR	C16-C15-C14	16.94	158.19	123.52
21	B	843	BCR	C11-C10-C9	15.87	149.53	127.28
21	B	843	BCR	C21-C20-C19	15.50	168.12	123.20
21	2	305	BCR	C29-C30-C25	-15.06	88.57	110.44
21	B	844	BCR	C11-C10-C9	14.73	147.93	127.28
21	A	855	BCR	C21-C20-C19	14.51	165.24	123.20
21	L	307	BCR	C11-C10-C9	14.45	147.54	127.28
21	F	305	BCR	C16-C15-C14	14.37	152.93	123.52
21	L	302	BCR	C11-C10-C9	14.16	147.13	127.28
21	A	846	BCR	C11-C10-C9	14.14	147.11	127.28
21	1	5005	BCR	C11-C10-C9	14.09	147.03	127.28
21	L	303	BCR	C11-C10-C9	13.96	146.86	127.28
17	A	801	CL0	C1B-CHB-C4A	13.96	130.30	121.32
21	J	1104	BCR	C11-C10-C9	13.92	146.79	127.28
21	4	301	BCR	C11-C10-C9	13.90	146.77	127.28
21	A	844	BCR	C21-C20-C19	13.86	163.36	123.20
21	3	306	BCR	C21-C20-C19	13.66	162.77	123.20
21	A	847	BCR	C11-C10-C9	13.64	146.41	127.28
21	A	843	BCR	C11-C10-C9	13.62	146.39	127.28
21	B	847	BCR	C11-C10-C9	13.51	146.22	127.28
21	B	802	BCR	C21-C20-C19	13.46	162.20	123.20
21	B	802	BCR	C11-C10-C9	13.44	146.13	127.28
21	A	843	BCR	C21-C20-C19	13.41	162.07	123.20
21	G	1604	BCR	C16-C15-C14	13.37	150.88	123.52
21	A	845	BCR	C21-C20-C19	13.34	161.85	123.20
21	B	847	BCR	C16-C15-C14	13.32	150.78	123.52
21	3	305	BCR	C11-C10-C9	13.19	145.78	127.28
21	F	305	BCR	C11-C10-C9	13.17	145.75	127.28
21	I	101	BCR	C16-C15-C14	13.12	150.37	123.52
21	A	844	BCR	C11-C10-C9	13.10	145.65	127.28
21	3	305	BCR	C16-C15-C14	13.10	150.32	123.52
21	J	1104	BCR	C21-C20-C19	13.08	161.10	123.20
21	G	1604	BCR	C21-C20-C19	13.08	161.09	123.20
21	A	847	BCR	C11-C12-C13	12.94	161.84	126.36

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	846	BCR	C11-C10-C9	12.93	145.41	127.28
21	L	303	BCR	C21-C20-C19	12.90	160.58	123.20
21	F	304	BCR	C16-C15-C14	12.86	149.84	123.52
21	I	102	BCR	C11-C10-C9	12.77	145.19	127.28
21	2	305	BCR	C11-C10-C9	12.74	145.14	127.28
21	L	302	BCR	C21-C20-C19	12.70	159.99	123.20
21	A	855	BCR	C11-C10-C9	12.68	145.06	127.28
21	1	5005	BCR	C16-C15-C14	12.67	149.44	123.52
21	A	855	BCR	C16-C15-C14	12.65	149.40	123.52
21	I	102	BCR	C16-C15-C14	12.62	149.34	123.52
21	L	307	BCR	C16-C15-C14	12.53	149.15	123.52
21	F	304	BCR	C11-C10-C9	12.50	144.81	127.28
21	L	307	BCR	C21-C20-C19	12.46	159.29	123.20
21	K	1405	BCR	C11-C10-C9	12.32	144.55	127.28
21	I	102	BCR	C21-C20-C19	12.31	158.88	123.20
21	B	844	BCR	C11-C12-C13	12.25	159.96	126.36
21	A	845	BCR	C11-C10-C9	12.23	144.43	127.28
21	A	845	BCR	C16-C15-C14	12.22	148.52	123.52
21	B	847	BCR	C21-C20-C19	12.21	158.57	123.20
21	A	846	BCR	C21-C20-C19	12.19	158.52	123.20
21	K	1405	BCR	C21-C20-C19	12.14	158.36	123.20
21	K	1405	BCR	C16-C15-C14	12.13	148.33	123.52
21	L	303	BCR	C16-C15-C14	12.10	148.29	123.52
21	A	844	BCR	C11-C12-C13	12.04	159.38	126.36
21	L	302	BCR	C16-C15-C14	12.00	148.07	123.52
21	F	305	BCR	C21-C20-C19	12.00	157.96	123.20
21	B	845	BCR	C11-C10-C9	11.95	144.04	127.28
21	3	305	BCR	C21-C20-C19	11.86	157.56	123.20
21	1	5005	BCR	C21-C20-C19	11.83	157.48	123.20
21	L	302	BCR	C11-C12-C13	11.80	158.73	126.36
21	A	843	BCR	C16-C15-C14	11.76	147.59	123.52
21	B	844	BCR	C21-C20-C19	11.76	157.27	123.20
21	B	846	BCR	C11-C12-C13	11.75	158.59	126.36
21	I	101	BCR	C21-C20-C19	11.68	157.03	123.20
21	G	1604	BCR	C11-C10-C9	11.68	143.65	127.28
21	F	304	BCR	C21-C20-C19	11.63	156.91	123.20
21	2	305	BCR	C11-C12-C13	11.63	158.26	126.36
21	2	305	BCR	C21-C20-C19	11.62	156.87	123.20
21	B	844	BCR	C16-C15-C14	11.60	147.25	123.52
21	3	306	BCR	C16-C15-C14	11.60	147.25	123.52
21	4	301	BCR	C11-C12-C13	11.42	157.68	126.36
21	B	847	BCR	C11-C12-C13	11.41	157.66	126.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	846	BCR	C16-C15-C14	11.38	146.81	123.52
21	J	1104	BCR	C16-C15-C14	11.36	146.77	123.52
21	L	303	BCR	C11-C12-C13	11.34	157.46	126.36
21	B	846	BCR	C21-C20-C19	11.32	155.99	123.20
21	3	305	BCR	C11-C12-C13	11.22	157.14	126.36
21	I	102	BCR	C11-C12-C13	11.21	157.09	126.36
21	1	5005	BCR	C11-C12-C13	11.20	157.06	126.36
21	K	1405	BCR	C11-C12-C13	11.18	157.02	126.36
21	A	847	BCR	C16-C15-C14	11.14	146.31	123.52
21	A	847	BCR	C21-C20-C19	11.08	155.30	123.20
21	4	301	BCR	C16-C15-C14	11.07	146.16	123.52
21	J	1104	BCR	C11-C12-C13	11.02	156.57	126.36
21	A	846	BCR	C16-C15-C14	11.01	146.04	123.52
21	I	101	BCR	C11-C10-C9	10.99	142.70	127.28
21	B	845	BCR	C11-C12-C13	10.98	156.48	126.36
21	F	304	BCR	C11-C12-C13	10.95	156.39	126.36
21	A	843	BCR	C11-C12-C13	10.93	156.33	126.36
21	B	845	BCR	C16-C15-C14	10.91	145.84	123.52
21	A	855	BCR	C11-C12-C13	10.90	156.25	126.36
21	L	307	BCR	C11-C12-C13	10.81	156.01	126.36
21	A	845	BCR	C11-C12-C13	10.75	155.84	126.36
21	G	1604	BCR	C11-C12-C13	10.64	155.54	126.36
21	F	305	BCR	C11-C12-C13	10.60	155.44	126.36
21	B	802	BCR	C11-C12-C13	10.54	155.26	126.36
21	4	301	BCR	C21-C20-C19	10.43	153.43	123.20
21	A	844	BCR	C16-C15-C14	10.35	144.70	123.52
21	2	305	BCR	C16-C15-C14	10.32	144.64	123.52
21	A	846	BCR	C11-C12-C13	10.25	154.47	126.36
21	4	301	BCR	C20-C19-C18	9.89	153.48	126.36
21	A	847	BCR	C20-C19-C18	9.75	153.11	126.36
21	I	101	BCR	C20-C19-C18	9.57	152.61	126.36
21	F	305	BCR	C20-C19-C18	9.46	152.30	126.36
18	A	823	CLA	C4A-NA-C1A	9.16	110.86	106.68
18	2	311	CLA	C4A-NA-C1A	9.10	110.83	106.68
18	K	1403	CLA	C4A-NA-C1A	9.10	110.83	106.68
18	B	837	CLA	C4A-NA-C1A	9.04	110.80	106.68
18	B	806	CLA	C4A-NA-C1A	9.02	110.79	106.68
18	1	5008	CLA	C4A-NA-C1A	9.02	110.79	106.68
18	3	317	CLA	C4A-NA-C1A	9.01	110.79	106.68
18	B	809	CLA	C4A-NA-C1A	9.00	110.79	106.68
18	B	833	CLA	C4A-NA-C1A	8.96	110.77	106.68
18	L	304	CLA	C4A-NA-C1A	8.96	110.77	106.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	F	304	BCR	C20-C19-C18	8.95	150.91	126.36
18	J	1103	CLA	C4A-NA-C1A	8.95	110.76	106.68
18	2	308	CLA	C4A-NA-C1A	8.95	110.76	106.68
21	B	846	BCR	C20-C19-C18	8.94	150.86	126.36
18	A	812	CLA	C4A-NA-C1A	8.93	110.75	106.68
18	L	306	CLA	C4A-NA-C1A	8.91	110.75	106.68
18	B	816	CLA	C4A-NA-C1A	8.88	110.73	106.68
18	A	813	CLA	C4A-NA-C1A	8.85	110.72	106.68
18	2	310	CLA	C4A-NA-C1A	8.85	110.72	106.68
18	A	825	CLA	C4A-NA-C1A	8.85	110.72	106.68
18	A	807	CLA	C4A-NA-C1A	8.85	110.72	106.68
21	B	844	BCR	C20-C19-C18	8.85	150.62	126.36
18	4	315	CLA	C4A-NA-C1A	8.84	110.71	106.68
18	1	5015	CLA	C4A-NA-C1A	8.83	110.71	106.68
18	B	825	CLA	C4A-NA-C1A	8.82	110.70	106.68
18	3	308	CLA	C4A-NA-C1A	8.82	110.70	106.68
18	2	312	CLA	C4A-NA-C1A	8.80	110.69	106.68
18	1	5013	CLA	C4A-NA-C1A	8.79	110.69	106.68
18	3	309	CLA	C4A-NA-C1A	8.79	110.69	106.68
18	3	314	CLA	C4A-NA-C1A	8.79	110.69	106.68
18	B	826	CLA	C4A-NA-C1A	8.78	110.69	106.68
18	B	810	CLA	C4A-NA-C1A	8.76	110.68	106.68
21	L	307	BCR	C20-C19-C18	8.76	150.38	126.36
18	B	813	CLA	C4A-NA-C1A	8.75	110.67	106.68
18	B	840	CLA	C4A-NA-C1A	8.74	110.67	106.68
21	I	101	BCR	C11-C12-C13	8.74	150.33	126.36
18	4	306	CLA	C4A-NA-C1A	8.74	110.67	106.68
18	H	1701	CLA	C4A-NA-C1A	8.70	110.65	106.68
21	1	5005	BCR	C20-C19-C18	8.68	150.18	126.36
18	2	306	CLA	C4A-NA-C1A	8.68	110.64	106.68
18	A	853	CLA	C4A-NA-C1A	8.68	110.64	106.68
18	A	821	CLA	C4A-NA-C1A	8.67	110.64	106.68
18	B	815	CLA	C4A-NA-C1A	8.67	110.64	106.68
18	A	810	CLA	C4A-NA-C1A	8.67	110.64	106.68
18	4	310	CLA	C4A-NA-C1A	8.67	110.63	106.68
18	A	815	CLA	C4A-NA-C1A	8.66	110.63	106.68
18	A	804	CLA	C4A-NA-C1A	8.65	110.62	106.68
18	A	837	CLA	C4A-NA-C1A	8.65	110.62	106.68
18	A	820	CLA	C4A-NA-C1A	8.64	110.62	106.68
18	4	311	CLA	C4A-NA-C1A	8.64	110.62	106.68
18	4	307	CLA	C4A-NA-C1A	8.63	110.62	106.68
18	K	1401	CLA	C4A-NA-C1A	8.63	110.61	106.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	804	CLA	C4A-NA-C1A	8.63	110.61	106.68
18	1	5010	CLA	C4A-NA-C1A	8.62	110.61	106.68
18	B	821	CLA	C4A-NA-C1A	8.62	110.61	106.68
18	4	305	CLA	C4A-NA-C1A	8.62	110.61	106.68
18	B	819	CLA	C4A-NA-C1A	8.62	110.61	106.68
18	B	822	CLA	C4A-NA-C1A	8.61	110.61	106.68
18	2	313	CLA	C4A-NA-C1A	8.61	110.61	106.68
18	2	317	CLA	C4A-NA-C1A	8.60	110.60	106.68
18	B	808	CLA	C4A-NA-C1A	8.60	110.60	106.68
18	G	1602	CLA	C4A-NA-C1A	8.59	110.60	106.68
18	B	829	CLA	C4A-NA-C1A	8.59	110.60	106.68
18	A	808	CLA	C4A-NA-C1A	8.59	110.60	106.68
18	A	818	CLA	C4A-NA-C1A	8.58	110.59	106.68
18	B	838	CLA	C4A-NA-C1A	8.58	110.59	106.68
18	A	840	CLA	C4A-NA-C1A	8.58	110.59	106.68
21	B	847	BCR	C20-C19-C18	8.57	149.88	126.36
18	A	811	CLA	C4A-NA-C1A	8.57	110.59	106.68
18	A	835	CLA	C4A-NA-C1A	8.57	110.59	106.68
18	A	833	CLA	C4A-NA-C1A	8.56	110.58	106.68
18	B	827	CLA	C4A-NA-C1A	8.56	110.58	106.68
18	3	301	CLA	C4A-NA-C1A	8.53	110.57	106.68
21	B	843	BCR	C16-C15-C14	8.53	140.96	123.52
18	A	828	CLA	C4A-NA-C1A	8.52	110.57	106.68
18	J	1101	CLA	C4A-NA-C1A	8.52	110.57	106.68
21	3	305	BCR	C20-C19-C18	8.52	149.74	126.36
18	A	831	CLA	C4A-NA-C1A	8.52	110.56	106.68
18	K	1404	CLA	C4A-NA-C1A	8.51	110.56	106.68
18	A	816	CLA	C4A-NA-C1A	8.49	110.55	106.68
18	B	831	CLA	C4A-NA-C1A	8.48	110.55	106.68
18	B	832	CLA	C4A-NA-C1A	8.48	110.55	106.68
18	A	806	CLA	C4A-NA-C1A	8.48	110.55	106.68
18	1	5017	CLA	C4A-NA-C1A	8.47	110.54	106.68
18	1	5007	CLA	C4A-NA-C1A	8.46	110.54	106.68
18	B	805	CLA	C4A-NA-C1A	8.46	110.54	106.68
18	4	312	CLA	C4A-NA-C1A	8.45	110.53	106.68
21	I	102	BCR	C20-C19-C18	8.44	149.51	126.36
18	G	1603	CLA	C4A-NA-C1A	8.44	110.53	106.68
18	A	803	CLA	C4A-NA-C1A	8.42	110.52	106.68
18	F	302	CLA	C4A-NA-C1A	8.41	110.52	106.68
18	4	308	CLA	C4A-NA-C1A	8.41	110.51	106.68
18	G	1601	CLA	C4A-NA-C1A	8.40	110.51	106.68
18	B	834	CLA	C4A-NA-C1A	8.40	110.51	106.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	5012	CLA	C4A-NA-C1A	8.39	110.51	106.68
18	A	824	CLA	C4A-NA-C1A	8.39	110.50	106.68
18	A	814	CLA	C4A-NA-C1A	8.37	110.50	106.68
18	3	318	CLA	C4A-NA-C1A	8.36	110.49	106.68
18	4	309	CLA	C4A-NA-C1A	8.36	110.49	106.68
18	A	838	CLA	C4A-NA-C1A	8.35	110.49	106.68
18	B	817	CLA	C4A-NA-C1A	8.35	110.49	106.68
18	1	5011	CLA	C4A-NA-C1A	8.35	110.49	106.68
18	3	315	CLA	C4A-NA-C1A	8.35	110.49	106.68
18	2	326	CLA	C4A-NA-C1A	8.34	110.48	106.68
18	B	814	CLA	C4A-NA-C1A	8.33	110.48	106.68
18	B	835	CLA	C4A-NA-C1A	8.32	110.48	106.68
17	A	801	CL0	O2D-CGD-CBD	8.32	120.09	110.95
18	A	834	CLA	C4A-NA-C1A	8.32	110.47	106.68
18	B	803	CLA	C4A-NA-C1A	8.31	110.47	106.68
18	B	818	CLA	C4A-NA-C1A	8.31	110.47	106.68
18	3	319	CLA	C4A-NA-C1A	8.31	110.47	106.68
18	A	827	CLA	C4A-NA-C1A	8.31	110.47	106.68
18	2	307	CLA	C4A-NA-C1A	8.31	110.47	106.68
21	B	843	BCR	C11-C12-C13	8.31	149.14	126.36
18	B	828	CLA	C4A-NA-C1A	8.30	110.47	106.68
18	A	839	CLA	C4A-NA-C1A	8.30	110.47	106.68
21	A	846	BCR	C20-C19-C18	8.28	149.08	126.36
18	A	826	CLA	C4A-NA-C1A	8.27	110.45	106.68
18	B	823	CLA	C4A-NA-C1A	8.27	110.45	106.68
18	1	5018	CLA	C4A-NA-C1A	8.25	110.44	106.68
18	F	301	CLA	C4A-NA-C1A	8.24	110.44	106.68
18	L	305	CLA	C4A-NA-C1A	8.24	110.44	106.68
21	B	845	BCR	C21-C20-C19	8.22	147.03	123.20
18	3	307	CLA	C4A-NA-C1A	8.22	110.43	106.68
18	B	839	CLA	C4A-NA-C1A	8.20	110.42	106.68
18	B	824	CLA	C4A-NA-C1A	8.20	110.42	106.68
29	J	1105	LUT	C21-C26-C27	8.18	122.23	112.83
18	2	309	CLA	C4A-NA-C1A	8.18	110.41	106.68
18	B	841	CLA	C4A-NA-C1A	8.18	110.41	106.68
18	B	836	CLA	C4A-NA-C1A	8.17	110.41	106.68
18	A	829	CLA	C4A-NA-C1A	8.17	110.41	106.68
18	A	836	CLA	C4A-NA-C1A	8.16	110.40	106.68
18	A	809	CLA	C4A-NA-C1A	8.15	110.40	106.68
18	A	819	CLA	C4A-NA-C1A	8.13	110.39	106.68
18	B	801	CLA	C4A-NA-C1A	8.11	110.38	106.68
18	1	5009	CLA	C4A-NA-C1A	8.11	110.38	106.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	1402	CLA	C4A-NA-C1A	8.11	110.38	106.68
18	L	301	CLA	C4A-NA-C1A	8.11	110.38	106.68
21	3	306	BCR	C11-C10-C9	8.11	138.65	127.28
18	F	303	CLA	C4A-NA-C1A	8.09	110.37	106.68
18	B	807	CLA	C4A-NA-C1A	8.07	110.36	106.68
21	J	1104	BCR	C20-C19-C18	8.06	148.45	126.36
18	A	817	CLA	C4A-NA-C1A	8.06	110.35	106.68
18	A	802	CLA	C4A-NA-C1A	8.05	110.35	106.68
18	A	830	CLA	C4A-NA-C1A	8.05	110.35	106.68
18	B	830	CLA	C4A-NA-C1A	8.05	110.35	106.68
18	B	820	CLA	C4A-NA-C1A	8.02	110.34	106.68
18	A	852	CLA	C4A-NA-C1A	8.02	110.34	106.68
18	1	5006	CLA	C4A-NA-C1A	8.00	110.33	106.68
21	L	302	BCR	C20-C19-C18	7.98	148.24	126.36
18	B	811	CLA	C4A-NA-C1A	7.83	110.25	106.68
18	A	805	CLA	C4A-NA-C1A	7.82	110.25	106.68
18	3	311	CLA	C4A-NA-C1A	7.79	110.23	106.68
18	A	832	CLA	C4A-NA-C1A	7.77	110.22	106.68
21	A	845	BCR	C20-C19-C18	7.76	147.63	126.36
18	A	822	CLA	C4A-NA-C1A	7.72	110.20	106.68
21	2	305	BCR	C40-C30-C29	-7.72	79.32	108.95
21	3	306	BCR	C20-C19-C18	7.65	147.34	126.36
18	B	812	CLA	C4A-NA-C1A	7.65	110.17	106.68
21	G	1604	BCR	C20-C19-C18	7.61	147.24	126.36
21	K	1405	BCR	C20-C19-C18	7.60	147.20	126.36
21	L	303	BCR	C20-C19-C18	7.56	147.09	126.36
21	A	843	BCR	C20-C19-C18	7.47	146.83	126.36
21	B	843	BCR	C19-C18-C17	7.44	130.72	119.01
30	2	314	CHL	C1B-CHB-C4A	7.14	125.91	121.32
30	4	302	CHL	C1B-CHB-C4A	7.05	125.86	121.32
30	4	317	CHL	C1B-CHB-C4A	6.96	125.80	121.32
30	4	313	CHL	C1B-CHB-C4A	6.88	125.75	121.32
21	B	802	BCR	C15-C14-C13	-6.86	117.66	127.28
30	2	318	CHL	C1B-CHB-C4A	6.81	125.70	121.32
21	B	802	BCR	C20-C19-C18	6.77	144.93	126.36
21	2	305	BCR	C20-C19-C18	6.74	144.84	126.36
21	A	844	BCR	C20-C19-C18	6.71	144.78	126.36
30	4	314	CHL	C1B-CHB-C4A	6.65	125.60	121.32
30	3	316	CHL	C1B-CHB-C4A	6.46	125.48	121.32
21	2	305	BCR	C40-C30-C25	6.44	120.35	110.24
21	A	855	BCR	C20-C19-C18	6.42	143.96	126.36
30	1	5014	CHL	C1B-CHB-C4A	6.36	125.42	121.32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	814	CLA	O2D-CGD-CBD	6.33	122.29	111.23
21	3	306	BCR	C11-C12-C13	6.28	143.59	126.36
21	3	306	BCR	C12-C13-C14	6.26	128.85	119.01
18	K	1403	CLA	CMD-C2D-C1D	6.18	135.61	124.73
18	B	833	CLA	O2D-CGD-CBD	6.16	122.00	111.23
21	B	843	BCR	C12-C13-C14	6.13	128.65	119.01
18	B	834	CLA	CMD-C2D-C1D	6.11	135.49	124.73
30	4	318	CHL	C1B-CHB-C4A	6.07	125.23	121.32
18	B	830	CLA	CMD-C2D-C1D	6.02	135.32	124.73
29	1	5004	LUT	C21-C26-C27	6.00	119.72	112.83
29	J	1105	LUT	C31-C30-C29	-5.99	118.88	127.28
18	A	820	CLA	CMD-C2D-C1D	5.98	135.26	124.73
18	A	829	CLA	CMD-C2D-C1D	5.97	135.25	124.73
18	A	828	CLA	O2D-CGD-CBD	5.94	121.61	111.23
31	2	304	XAT	C31-C30-C29	-5.92	118.97	127.28
18	A	823	CLA	O2D-CGD-CBD	5.91	121.56	111.23
30	2	319	CHL	C1B-CHB-C4A	5.90	125.12	121.32
18	1	5013	CLA	O2D-CGD-CBD	5.88	121.50	111.23
18	2	309	CLA	CMD-C2D-C1D	5.86	135.05	124.73
18	4	308	CLA	O2D-CGD-CBD	5.83	121.42	111.23
18	1	5009	CLA	CMD-C2D-C1D	5.83	135.00	124.73
18	A	807	CLA	O2D-CGD-CBD	5.81	121.38	111.23
18	B	828	CLA	CMD-C2D-C1D	5.81	134.95	124.73
30	3	312	CHL	C1B-CHB-C4A	5.80	125.05	121.32
18	A	813	CLA	O2D-CGD-CBD	5.79	121.35	111.23
30	3	310	CHL	C1B-CHB-C4A	5.79	125.05	121.32
18	3	307	CLA	CMD-C2D-C1D	5.76	134.87	124.73
29	3	304	LUT	C21-C26-C27	5.75	119.44	112.83
30	2	315	CHL	C1B-CHB-C4A	5.75	125.02	121.32
18	A	805	CLA	CMD-C2D-C1D	5.75	134.85	124.73
28	F	310	ZEX	C15-C14-C13	-5.75	119.22	127.28
18	B	830	CLA	O2D-CGD-CBD	5.75	121.28	111.23
18	B	801	CLA	O2D-CGD-CBD	5.74	121.26	111.23
18	1	5006	CLA	CMD-C2D-C1D	5.74	134.83	124.73
30	3	313	CHL	C1B-CHB-C4A	5.73	125.01	121.32
30	4	316	CHL	C1B-CHB-C4A	5.73	125.01	121.32
18	A	831	CLA	O2D-CGD-CBD	5.72	121.23	111.23
18	B	831	CLA	O2D-CGD-CBD	5.71	121.22	111.23
18	1	5009	CLA	O2D-CGD-CBD	5.71	121.21	111.23
18	B	815	CLA	O2D-CGD-CBD	5.69	121.18	111.23
18	A	822	CLA	CMD-C2D-C1D	5.69	134.74	124.73
18	A	829	CLA	O2D-CGD-CBD	5.67	121.14	111.23

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	312	CLA	CMD-C2D-C1D	5.66	134.70	124.73
18	B	826	CLA	CMD-C2D-C1D	5.65	134.69	124.73
18	J	1101	CLA	CMD-C2D-C1D	5.65	134.67	124.73
18	A	809	CLA	CMD-C2D-C1D	5.64	134.66	124.73
18	B	837	CLA	CMD-C2D-C1D	5.64	134.66	124.73
18	2	313	CLA	CMD-C2D-C1D	5.64	134.66	124.73
18	G	1601	CLA	CMD-C2D-C1D	5.63	134.65	124.73
18	A	825	CLA	CMD-C2D-C1D	5.62	134.62	124.73
18	1	5017	CLA	CMD-C2D-C1D	5.62	134.62	124.73
18	J	1101	CLA	O2D-CGD-CBD	5.62	121.05	111.23
30	2	316	CHL	C1B-CHB-C4A	5.61	124.93	121.32
18	2	326	CLA	O2D-CGD-CBD	5.60	121.02	111.23
18	4	309	CLA	CMD-C2D-C1D	5.60	134.59	124.73
18	B	811	CLA	CMD-C2D-C1D	5.59	134.58	124.73
18	H	1701	CLA	CMD-C2D-C1D	5.59	134.58	124.73
18	B	825	CLA	CMD-C2D-C1D	5.59	134.57	124.73
18	B	840	CLA	CMD-C2D-C1D	5.59	134.57	124.73
18	A	812	CLA	O2D-CGD-CBD	5.59	121.00	111.23
18	B	826	CLA	O2D-CGD-CBD	5.59	121.00	111.23
18	A	823	CLA	CMD-C2D-C1D	5.58	134.56	124.73
18	B	827	CLA	CMD-C2D-C1D	5.58	134.56	124.73
18	4	305	CLA	CMD-C2D-C1D	5.58	134.55	124.73
18	3	309	CLA	CMD-C2D-C1D	5.58	134.55	124.73
18	B	821	CLA	O2D-CGD-CBD	5.58	120.98	111.23
18	A	810	CLA	CMD-C2D-C1D	5.58	134.55	124.73
18	3	311	CLA	CMD-C2D-C1D	5.57	134.54	124.73
18	4	308	CLA	CMD-C2D-C1D	5.57	134.54	124.73
18	A	803	CLA	O2D-CGD-CBD	5.56	120.96	111.23
18	B	807	CLA	CMD-C2D-C1D	5.56	134.52	124.73
18	1	5015	CLA	CMD-C2D-C1D	5.55	134.51	124.73
18	4	307	CLA	CMD-C2D-C1D	5.55	134.51	124.73
18	L	304	CLA	O2D-CGD-CBD	5.55	120.93	111.23
18	1	5017	CLA	O2D-CGD-CBD	5.54	120.92	111.23
18	3	308	CLA	CMD-C2D-C1D	5.54	134.49	124.73
18	1	5013	CLA	CMD-C2D-C1D	5.54	134.48	124.73
21	B	843	BCR	C15-C14-C13	5.54	135.04	127.28
18	B	827	CLA	O2D-CGD-CBD	5.54	120.91	111.23
18	2	308	CLA	CMD-C2D-C1D	5.53	134.47	124.73
18	F	302	CLA	CMD-C2D-C1D	5.53	134.46	124.73
18	B	831	CLA	CMD-C2D-C1D	5.53	134.46	124.73
18	B	819	CLA	O2D-CGD-CBD	5.52	120.88	111.23
18	A	814	CLA	CMD-C2D-C1D	5.52	134.45	124.73

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	1402	CLA	CMD-C2D-C1D	5.51	134.44	124.73
18	2	310	CLA	CMD-C2D-C1D	5.51	134.44	124.73
18	L	306	CLA	CMD-C2D-C1D	5.51	134.44	124.73
18	A	835	CLA	CMD-C2D-C1D	5.51	134.44	124.73
18	A	832	CLA	CMD-C2D-C1D	5.51	134.44	124.73
18	B	814	CLA	CMD-C2D-C1D	5.51	134.43	124.73
18	L	305	CLA	CMD-C2D-C1D	5.51	134.42	124.73
18	3	318	CLA	CMD-C2D-C1D	5.50	134.42	124.73
18	2	311	CLA	CMD-C2D-C1D	5.50	134.42	124.73
18	A	813	CLA	CMD-C2D-C1D	5.50	134.42	124.73
18	L	304	CLA	CMD-C2D-C1D	5.50	134.42	124.73
18	B	839	CLA	CMD-C2D-C1D	5.50	134.41	124.73
18	2	313	CLA	O2D-CGD-CBD	5.50	120.84	111.23
18	A	834	CLA	CMD-C2D-C1D	5.50	134.41	124.73
18	B	819	CLA	CMD-C2D-C1D	5.50	134.41	124.73
18	A	812	CLA	CMD-C2D-C1D	5.50	134.41	124.73
18	A	840	CLA	CMD-C2D-C1D	5.49	134.40	124.73
18	B	817	CLA	CMD-C2D-C1D	5.49	134.40	124.73
18	G	1603	CLA	CMD-C2D-C1D	5.49	134.39	124.73
18	G	1602	CLA	CMD-C2D-C1D	5.49	134.39	124.73
18	K	1401	CLA	CMD-C2D-C1D	5.48	134.38	124.73
18	A	807	CLA	CMD-C2D-C1D	5.48	134.38	124.73
18	B	822	CLA	CMD-C2D-C1D	5.48	134.38	124.73
18	A	819	CLA	CMD-C2D-C1D	5.48	134.38	124.73
18	K	1404	CLA	CMD-C2D-C1D	5.48	134.37	124.73
18	A	826	CLA	CMD-C2D-C1D	5.47	134.37	124.73
18	A	833	CLA	CMD-C2D-C1D	5.47	134.37	124.73
18	4	306	CLA	O2D-CGD-CBD	5.47	120.79	111.23
18	B	805	CLA	CMD-C2D-C1D	5.47	134.36	124.73
18	A	806	CLA	CMD-C2D-C1D	5.47	134.36	124.73
18	F	303	CLA	CMD-C2D-C1D	5.47	134.35	124.73
18	2	307	CLA	CMD-C2D-C1D	5.47	134.35	124.73
18	3	319	CLA	CMD-C2D-C1D	5.46	134.35	124.73
18	1	5011	CLA	CMD-C2D-C1D	5.46	134.35	124.73
18	4	312	CLA	O2D-CGD-CBD	5.46	120.78	111.23
18	B	818	CLA	CMD-C2D-C1D	5.46	134.34	124.73
18	B	823	CLA	CMD-C2D-C1D	5.46	134.34	124.73
18	A	804	CLA	CMD-C2D-C1D	5.46	134.34	124.73
18	B	806	CLA	CMD-C2D-C1D	5.46	134.34	124.73
18	A	817	CLA	CMD-C2D-C1D	5.46	134.34	124.73
18	A	831	CLA	CMD-C2D-C1D	5.46	134.34	124.73
18	4	306	CLA	CMD-C2D-C1D	5.46	134.34	124.73

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	813	CLA	CMD-C2D-C1D	5.46	134.34	124.73
18	1	5010	CLA	CMD-C2D-C1D	5.46	134.34	124.73
18	1	5018	CLA	CMD-C2D-C1D	5.45	134.33	124.73
18	A	838	CLA	CMD-C2D-C1D	5.45	134.33	124.73
18	B	812	CLA	CMD-C2D-C1D	5.45	134.33	124.73
18	1	5012	CLA	CMD-C2D-C1D	5.45	134.32	124.73
18	3	315	CLA	CMD-C2D-C1D	5.45	134.32	124.73
18	B	833	CLA	CMD-C2D-C1D	5.45	134.32	124.73
18	A	830	CLA	CMD-C2D-C1D	5.44	134.31	124.73
18	B	824	CLA	CMD-C2D-C1D	5.44	134.31	124.73
18	B	808	CLA	CMD-C2D-C1D	5.44	134.30	124.73
18	2	306	CLA	CMD-C2D-C1D	5.44	134.30	124.73
18	B	816	CLA	O2D-CGD-CBD	5.44	120.73	111.23
18	4	310	CLA	CMD-C2D-C1D	5.43	134.29	124.73
18	G	1603	CLA	O2D-CGD-CBD	5.43	120.72	111.23
18	A	815	CLA	CMD-C2D-C1D	5.42	134.28	124.73
30	1	5016	CHL	C1B-CHB-C4A	5.41	124.81	121.32
18	A	836	CLA	CMD-C2D-C1D	5.41	134.26	124.73
18	A	837	CLA	CMD-C2D-C1D	5.41	134.26	124.73
18	A	808	CLA	O2D-CGD-CBD	5.41	120.69	111.23
18	3	301	CLA	CMD-C2D-C1D	5.41	134.26	124.73
31	4	304	XAT	C31-C30-C29	-5.41	119.69	127.28
18	3	318	CLA	O2D-CGD-CBD	5.41	120.68	111.23
18	B	820	CLA	CMD-C2D-C1D	5.40	134.24	124.73
18	A	853	CLA	CMD-C2D-C1D	5.40	134.24	124.73
18	J	1103	CLA	CMD-C2D-C1D	5.40	134.23	124.73
18	B	828	CLA	O2D-CGD-CBD	5.40	120.67	111.23
18	B	837	CLA	O2D-CGD-CBD	5.40	120.67	111.23
18	B	825	CLA	O2D-CGD-CBD	5.39	120.66	111.23
18	B	806	CLA	O2D-CGD-CBD	5.39	120.65	111.23
18	A	816	CLA	CMD-C2D-C1D	5.39	134.21	124.73
18	A	803	CLA	CMD-C2D-C1D	5.38	134.21	124.73
18	A	830	CLA	O2D-CGD-CBD	5.38	120.64	111.23
18	A	818	CLA	O2D-CGD-CBD	5.38	120.63	111.23
18	B	832	CLA	CMD-C2D-C1D	5.37	134.19	124.73
18	2	326	CLA	CMD-C2D-C1D	5.37	134.19	124.73
18	B	815	CLA	CMD-C2D-C1D	5.37	134.19	124.73
18	A	811	CLA	CMD-C2D-C1D	5.36	134.17	124.73
18	3	314	CLA	CMD-C2D-C1D	5.36	134.17	124.73
18	A	852	CLA	CMD-C2D-C1D	5.36	134.17	124.73
21	2	305	BCR	C39-C30-C25	5.35	118.64	110.24
18	B	821	CLA	CMD-C2D-C1D	5.35	134.16	124.73

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	311	CLA	O2D-CGD-CBD	5.35	120.58	111.23
18	B	835	CLA	CMD-C2D-C1D	5.34	134.13	124.73
18	3	317	CLA	CMD-C2D-C1D	5.34	134.13	124.73
18	B	829	CLA	CMD-C2D-C1D	5.34	134.13	124.73
18	B	817	CLA	O2D-CGD-CBD	5.33	120.56	111.23
18	A	821	CLA	CMD-C2D-C1D	5.33	134.12	124.73
18	B	816	CLA	CMD-C2D-C1D	5.32	134.10	124.73
18	A	808	CLA	CMD-C2D-C1D	5.32	134.10	124.73
18	B	836	CLA	CMD-C2D-C1D	5.32	134.10	124.73
18	F	301	CLA	CMD-C2D-C1D	5.32	134.10	124.73
18	A	804	CLA	O2D-CGD-CBD	5.32	120.53	111.23
18	B	841	CLA	CMD-C2D-C1D	5.32	134.09	124.73
18	1	5010	CLA	O2D-CGD-CBD	5.32	120.52	111.23
18	B	810	CLA	CMD-C2D-C1D	5.31	134.07	124.73
18	B	838	CLA	CMD-C2D-C1D	5.30	134.06	124.73
18	L	305	CLA	O2D-CGD-CBD	5.30	120.49	111.23
18	1	5008	CLA	CMD-C2D-C1D	5.29	134.05	124.73
18	4	311	CLA	CMD-C2D-C1D	5.29	134.05	124.73
18	2	309	CLA	O2D-CGD-CBD	5.28	120.47	111.23
31	4	304	XAT	O4-C5-C18	-5.28	109.14	115.05
18	A	824	CLA	O2D-CGD-CBD	5.28	120.46	111.23
18	3	315	CLA	O2D-CGD-CBD	5.28	120.45	111.23
18	2	307	CLA	O2D-CGD-CBD	5.28	120.45	111.23
18	B	811	CLA	O2D-CGD-CBD	5.27	120.44	111.23
18	B	822	CLA	O2D-CGD-CBD	5.27	120.44	111.23
18	2	317	CLA	CMD-C2D-C1D	5.27	134.00	124.73
18	2	312	CLA	O2D-CGD-CBD	5.27	120.44	111.23
18	B	805	CLA	O2D-CGD-CBD	5.26	120.43	111.23
18	1	5007	CLA	CMD-C2D-C1D	5.25	133.98	124.73
18	A	825	CLA	O2D-CGD-CBD	5.25	120.41	111.23
18	A	834	CLA	O2D-CGD-CBD	5.25	120.40	111.23
18	4	315	CLA	CMD-C2D-C1D	5.24	133.95	124.73
18	1	5007	CLA	O2D-CGD-CBD	5.24	120.39	111.23
18	A	835	CLA	O2D-CGD-CBD	5.23	120.38	111.23
18	B	809	CLA	CMD-C2D-C1D	5.23	133.94	124.73
29	2	303	LUT	C26-C27-C28	-5.23	116.45	124.58
18	B	840	CLA	O2D-CGD-CBD	5.23	120.36	111.23
18	A	839	CLA	CMD-C2D-C1D	5.22	133.93	124.73
18	B	801	CLA	CMD-C2D-C1D	5.22	133.93	124.73
18	B	836	CLA	O2D-CGD-CBD	5.22	120.36	111.23
18	L	301	CLA	CMD-C2D-C1D	5.22	133.91	124.73
18	A	816	CLA	O2D-CGD-CBD	5.21	120.35	111.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	H	1701	CLA	O2D-CGD-CBD	5.21	120.34	111.23
18	1	5018	CLA	O2D-CGD-CBD	5.21	120.33	111.23
22	B	848	LHG	O7-C7-C8	5.21	120.37	111.09
18	2	310	CLA	C1-C2-C3	-5.19	117.69	126.20
18	B	818	CLA	O2D-CGD-CBD	5.19	120.30	111.23
17	A	801	CL0	O2A-CGA-O1A	-5.19	110.65	123.63
18	A	853	CLA	O2D-CGD-CBD	5.19	120.30	111.23
18	1	5011	CLA	O2D-CGD-CBD	5.18	120.28	111.23
18	F	301	CLA	O2D-CGD-CBD	5.18	120.28	111.23
18	3	309	CLA	O2D-CGD-CBD	5.17	120.27	111.23
18	B	804	CLA	CMD-C2D-C1D	5.17	133.83	124.73
18	2	312	CLA	CMD-C2D-C1D	5.17	133.82	124.73
18	A	827	CLA	O2D-CGD-CBD	5.16	120.25	111.23
18	B	839	CLA	O2D-CGD-CBD	5.16	120.25	111.23
18	F	303	CLA	O2D-CGD-CBD	5.16	120.25	111.23
18	A	839	CLA	O2D-CGD-CBD	5.15	120.24	111.23
18	A	836	CLA	O2D-CGD-CBD	5.14	120.22	111.23
18	A	833	CLA	O2D-CGD-CBD	5.14	120.22	111.23
18	A	832	CLA	O2D-CGD-CBD	5.14	120.22	111.23
18	3	314	CLA	O2D-CGD-CBD	5.14	120.21	111.23
18	1	5015	CLA	O2D-CGD-CBD	5.14	120.21	111.23
18	A	818	CLA	CMD-C2D-C1D	5.12	133.75	124.73
18	2	308	CLA	O2D-CGD-CBD	5.12	120.18	111.23
18	B	813	CLA	O2D-CGD-CBD	5.12	120.18	111.23
29	J	1105	LUT	C35-C34-C33	-5.12	120.10	127.28
18	A	828	CLA	CMD-C2D-C1D	5.11	133.72	124.73
18	2	306	CLA	O2D-CGD-CBD	5.10	120.15	111.23
28	F	310	ZEX	C28-C27-C26	-5.09	118.74	126.94
18	4	309	CLA	O2D-CGD-CBD	5.09	120.12	111.23
18	B	838	CLA	O2D-CGD-CBD	5.08	120.10	111.23
29	3	304	LUT	C35-C34-C33	-5.07	120.17	127.28
18	A	809	CLA	O2D-CGD-CBD	5.06	120.08	111.23
18	A	806	CLA	O2D-CGD-CBD	5.06	120.08	111.23
18	A	837	CLA	O2D-CGD-CBD	5.06	120.08	111.23
18	A	840	CLA	O2D-CGD-CBD	5.06	120.08	111.23
18	3	307	CLA	O2D-CGD-CBD	5.06	120.08	111.23
18	4	311	CLA	O2D-CGD-CBD	5.06	120.07	111.23
18	3	319	CLA	O2D-CGD-CBD	5.04	120.05	111.23
18	G	1602	CLA	O2D-CGD-CBD	5.04	120.04	111.23
18	B	812	CLA	O2D-CGD-CBD	5.04	120.03	111.23
18	4	315	CLA	O2D-CGD-CBD	5.02	120.01	111.23
18	1	5012	CLA	O2D-CGD-CBD	5.02	120.00	111.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	1401	CLA	O2D-CGD-CBD	5.01	119.99	111.23
18	B	808	CLA	O2D-CGD-CBD	5.00	119.97	111.23
18	B	829	CLA	O2D-CGD-CBD	5.00	119.97	111.23
18	2	317	CLA	O2D-CGD-CBD	4.98	119.94	111.23
31	2	304	XAT	C15-C14-C13	-4.98	120.30	127.28
18	A	815	CLA	O2D-CGD-CBD	4.98	119.93	111.23
18	2	310	CLA	O2D-CGD-CBD	4.98	119.93	111.23
18	1	5006	CLA	O2D-CGD-CBD	4.97	119.92	111.23
18	G	1601	CLA	O2D-CGD-CBD	4.97	119.91	111.23
18	2	311	CLA	O2D-CGD-CBD	4.96	119.90	111.23
18	A	820	CLA	O2D-CGD-CBD	4.95	119.88	111.23
18	B	807	CLA	O2D-CGD-CBD	4.94	119.86	111.23
18	K	1403	CLA	O2D-CGD-CBD	4.94	119.86	111.23
24	B	851	LMG	O7-C10-C11	4.93	122.14	111.48
18	A	817	CLA	O2D-CGD-CBD	4.93	119.84	111.23
18	A	821	CLA	O2D-CGD-CBD	4.92	119.84	111.23
18	4	307	CLA	O2D-CGD-CBD	4.92	119.83	111.23
18	3	317	CLA	O2D-CGD-CBD	4.91	119.82	111.23
29	3	304	LUT	C31-C30-C29	-4.91	120.39	127.28
18	K	1402	CLA	O2D-CGD-CBD	4.91	119.81	111.23
18	K	1404	CLA	O2D-CGD-CBD	4.91	119.81	111.23
29	4	303	LUT	C21-C26-C27	4.91	118.47	112.83
29	1	5003	LUT	C35-C34-C33	-4.90	120.40	127.28
18	A	814	CLA	O2D-CGD-CBD	4.90	119.80	111.23
18	B	809	CLA	O2D-CGD-CBD	4.90	119.79	111.23
18	L	301	CLA	O2D-CGD-CBD	4.90	119.79	111.23
18	A	819	CLA	O2D-CGD-CBD	4.88	119.77	111.23
18	B	841	CLA	O2D-CGD-CBD	4.87	119.75	111.23
18	B	820	CLA	O2D-CGD-CBD	4.87	119.74	111.23
18	A	852	CLA	O2D-CGD-CBD	4.87	119.74	111.23
18	1	5008	CLA	O2D-CGD-CBD	4.84	119.69	111.23
18	A	824	CLA	CMD-C2D-C1D	4.84	133.25	124.73
18	A	826	CLA	O2D-CGD-CBD	4.84	119.69	111.23
30	3	313	CHL	C1C-CHC-C4B	4.83	133.36	116.07
21	B	845	BCR	C29-C30-C25	-4.83	103.42	110.44
29	2	303	LUT	C15-C14-C13	-4.83	120.51	127.28
18	F	302	CLA	O2D-CGD-CBD	4.82	119.66	111.23
18	A	827	CLA	CMD-C2D-C1D	4.82	133.21	124.73
18	J	1103	CLA	O2D-CGD-CBD	4.82	119.65	111.23
30	3	310	CHL	C1C-CHC-C4B	4.80	133.25	116.07
30	4	316	CHL	C1C-CHC-C4B	4.80	133.23	116.07
18	4	305	CLA	O2D-CGD-CBD	4.79	119.61	111.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	318	CHL	C1C-CHC-C4B	4.79	133.20	116.07
29	3	303	LUT	C21-C26-C27	4.79	118.33	112.83
18	B	823	CLA	O2D-CGD-CBD	4.78	119.59	111.23
18	A	805	CLA	O2D-CGD-CBD	4.78	119.59	111.23
31	2	304	XAT	C38-C25-C24	4.77	119.60	114.24
18	B	804	CLA	O2D-CGD-CBD	4.77	119.58	111.23
18	L	306	CLA	O2D-CGD-CBD	4.77	119.57	111.23
18	A	811	CLA	O2D-CGD-CBD	4.76	119.55	111.23
30	2	319	CHL	C1C-CHC-C4B	4.76	133.09	116.07
18	4	310	CLA	O2D-CGD-CBD	4.76	119.55	111.23
30	1	5014	CHL	C1C-CHC-C4B	4.74	133.02	116.07
30	1	5016	CHL	C1C-CHC-C4B	4.74	133.02	116.07
21	2	305	BCR	C28-C27-C26	-4.73	105.61	114.06
30	3	312	CHL	C1C-CHC-C4B	4.71	132.92	116.07
30	2	316	CHL	C1C-CHC-C4B	4.71	132.91	116.07
18	B	832	CLA	O2D-CGD-CBD	4.68	119.41	111.23
18	3	308	CLA	O2D-CGD-CBD	4.68	119.41	111.23
18	B	803	CLA	O2D-CGD-CBD	4.67	119.40	111.23
30	2	318	CHL	C1C-CHC-C4B	4.66	132.74	116.07
21	2	305	BCR	C39-C30-C29	-4.66	91.08	108.95
21	B	843	BCR	C8-C9-C10	4.65	126.33	119.01
30	2	315	CHL	C1C-CHC-C4B	4.65	132.71	116.07
18	A	802	CLA	CMD-C2D-C1D	4.64	132.89	124.73
29	1	5004	LUT	C15-C14-C13	-4.63	120.78	127.28
31	4	304	XAT	C38-C25-C24	4.62	119.43	114.24
18	A	822	CLA	O2D-CGD-CBD	4.62	119.30	111.23
18	B	835	CLA	O2D-CGD-CBD	4.61	119.29	111.23
29	4	303	LUT	C35-C34-C33	-4.60	120.83	127.28
18	A	802	CLA	O2D-CGD-CBD	4.60	119.27	111.23
18	B	810	CLA	O2D-CGD-CBD	4.60	119.27	111.23
30	4	302	CHL	C1C-CHC-C4B	4.59	132.50	116.07
30	4	313	CHL	C1C-CHC-C4B	4.59	132.49	116.07
30	3	316	CHL	C1C-CHC-C4B	4.57	132.42	116.07
21	A	855	BCR	C33-C5-C6	-4.56	119.51	124.48
21	B	845	BCR	C19-C18-C17	4.55	126.17	119.01
30	4	317	CHL	C1C-CHC-C4B	4.54	132.32	116.07
30	2	314	CHL	C1C-CHC-C4B	4.54	132.32	116.07
18	B	803	CLA	CMD-C2D-C1D	4.54	132.72	124.73
30	4	314	CHL	C1C-CHC-C4B	4.52	132.24	116.07
18	A	810	CLA	O2D-CGD-CBD	4.51	119.11	111.23
22	A	849	LHG	O7-C7-C8	4.51	121.23	111.48
18	A	838	CLA	O2D-CGD-CBD	4.49	119.09	111.23

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	1	5004	LUT	C35-C34-C33	-4.48	121.00	127.28
21	B	843	BCR	C36-C18-C17	-4.47	115.57	122.82
18	B	834	CLA	O2D-CGD-CBD	4.46	119.03	111.23
29	2	303	LUT	C21-C26-C27	4.45	117.94	112.83
30	3	310	CHL	C1-C2-C3	-4.44	118.93	126.20
21	4	301	BCR	C33-C5-C6	-4.42	119.66	124.48
18	3	317	CLA	C1-C2-C3	-4.40	119.65	126.76
18	B	806	CLA	C1-C2-C3	-4.39	119.01	126.20
18	B	826	CLA	C1-C2-C3	-4.38	119.03	126.20
24	1	5020	LMG	O7-C10-C11	4.37	120.93	111.48
24	F	308	LMG	O7-C10-C11	4.34	120.86	111.48
17	A	801	CL0	O2A-CGA-CBA	4.33	125.03	111.83
17	A	801	CL0	CHA-C1A-C2A	-4.32	123.15	133.31
29	1	5003	LUT	C21-C26-C27	4.32	117.79	112.83
21	3	306	BCR	C35-C13-C14	-4.31	115.83	122.82
21	B	843	BCR	C35-C13-C14	-4.30	115.85	122.82
18	A	803	CLA	C1-C2-C3	-4.30	119.16	126.20
18	A	853	CLA	C1-C2-C3	-4.30	119.16	126.20
18	B	838	CLA	C1-C2-C3	-4.29	119.82	126.76
18	A	828	CLA	C1-C2-C3	-4.28	119.18	126.20
21	B	843	BCR	C20-C19-C18	4.26	138.05	126.36
30	1	5016	CHL	C3D-C4D-CHA	4.26	115.01	108.54
18	2	310	CLA	O2A-C1-C2	4.25	124.44	108.11
18	A	827	CLA	C1-C2-C3	-4.24	119.24	126.20
18	B	807	CLA	C1-C2-C3	-4.24	119.25	126.20
18	B	815	CLA	C1-C2-C3	-4.22	119.28	126.20
21	B	845	BCR	C33-C5-C6	-4.22	119.88	124.48
18	A	826	CLA	C1-C2-C3	-4.21	119.30	126.20
30	4	314	CHL	C3D-C4D-CHA	4.21	114.94	108.54
30	2	316	CHL	C3D-C4D-CHA	4.21	114.93	108.54
31	4	304	XAT	C15-C14-C13	-4.20	121.38	127.28
29	3	303	LUT	C35-C34-C33	-4.19	121.40	127.28
26	2	327	DGD	O2G-C1B-C2B	4.18	120.53	111.48
30	2	315	CHL	C3D-C4D-CHA	4.16	114.87	108.54
21	2	305	BCR	C33-C5-C6	-4.16	119.94	124.48
18	B	825	CLA	O2A-C1-C2	4.15	124.10	108.11
24	F	306	LMG	O7-C10-C11	4.15	120.45	111.48
18	3	317	CLA	O2A-C1-C2	4.14	124.05	108.11
31	4	304	XAT	C18-C5-C4	4.14	118.89	114.24
30	1	5014	CHL	C3D-C4D-CHA	4.13	114.82	108.54
30	2	318	CHL	C3D-C4D-CHA	4.13	114.82	108.54
26	1	5002	DGD	O2G-C1B-C2B	4.13	120.42	111.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	313	CHL	C3D-C4D-CHA	4.12	114.80	108.54
29	3	303	LUT	C15-C14-C13	-4.12	121.50	127.28
18	4	307	CLA	C1-C2-C3	-4.11	119.47	126.20
21	3	305	BCR	C23-C24-C25	-4.11	116.02	127.00
18	B	816	CLA	C1-C2-C3	-4.11	119.47	126.20
18	A	805	CLA	C1-C2-C3	-4.10	119.48	126.20
24	2	322	LMG	O7-C10-C11	4.10	120.34	111.48
30	4	302	CHL	C3D-C4D-CHA	4.10	114.77	108.54
30	3	310	CHL	CHA-C1A-C2A	-4.09	123.71	133.31
21	L	303	BCR	C33-C5-C6	-4.07	120.04	124.48
30	2	314	CHL	C3D-C4D-CHA	4.06	114.72	108.54
29	J	1105	LUT	C27-C28-C29	-4.06	117.59	126.32
18	B	824	CLA	C1-C2-C3	-4.06	119.55	126.20
30	3	312	CHL	C3D-C4D-CHA	4.05	114.70	108.54
22	1	5019	LHG	O7-C7-C8	4.05	120.24	111.48
30	4	317	CHL	C3D-C4D-CHA	4.05	114.69	108.54
30	3	316	CHL	C3D-C4D-CHA	4.04	114.68	108.54
28	F	310	ZEX	C35-C34-C33	-4.04	121.62	127.28
18	B	819	CLA	O2A-C1-C2	4.03	123.64	108.11
18	B	824	CLA	O2D-CGD-CBD	4.03	118.28	111.23
18	3	301	CLA	O2D-CGD-CBD	4.03	118.27	111.23
18	B	835	CLA	O2A-C1-C2	4.02	123.59	108.11
22	B	849	LHG	O7-C7-C8	4.02	120.18	111.48
18	J	1101	CLA	O2A-C1-C2	4.02	123.58	108.11
18	4	306	CLA	C1-C2-C3	-4.01	120.27	126.76
24	B	850	LMG	O7-C10-C11	4.01	120.16	111.48
30	4	318	CHL	C3D-C4D-CHA	4.01	114.63	108.54
30	2	319	CHL	C3D-C4D-CHA	3.99	114.61	108.54
21	B	847	BCR	C33-C5-C6	-3.99	120.13	124.48
18	B	803	CLA	C1-C2-C3	-3.99	119.66	126.20
21	3	305	BCR	C33-C5-C6	-3.99	120.13	124.48
18	2	308	CLA	C1-C2-C3	-3.99	119.67	126.20
22	2	320	LHG	O7-C7-C8	3.98	120.10	111.48
22	A	848	LHG	O7-C7-C8	3.98	120.09	111.48
24	J	1102	LMG	O7-C10-C11	3.96	120.06	111.48
21	B	802	BCR	C19-C18-C17	3.96	125.23	119.01
21	B	844	BCR	C33-C5-C6	-3.96	120.17	124.48
18	B	816	CLA	O2A-C1-C2	3.95	123.31	108.11
18	1	5010	CLA	C1-C2-C3	-3.95	119.73	126.20
17	A	801	CL0	C1C-CHC-C4B	3.94	130.17	116.07
18	G	1601	CLA	C1-C2-C3	-3.93	119.76	126.20
18	A	834	CLA	O2A-C1-C2	3.92	123.20	108.11

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	2	304	XAT	C18-C5-C4	3.92	118.65	114.24
30	4	316	CHL	C3D-C4D-CHA	3.92	114.50	108.54
21	B	845	BCR	C20-C19-C18	3.92	137.11	126.36
29	1	5004	LUT	C11-C10-C9	-3.92	121.78	127.28
18	F	302	CLA	O2A-C1-C2	3.90	123.12	108.11
26	F	309	DGD	O2G-C1B-C2B	3.90	119.92	111.48
23	A	850	LMT	C3'-C4'-C5'	-3.90	102.29	110.93
30	3	313	CHL	C3D-C4D-CHA	3.90	114.46	108.54
29	4	303	LUT	C18-C5-C6	-3.89	120.24	124.48
18	B	839	CLA	O2A-C1-C2	3.89	123.08	108.11
18	1	5006	CLA	C1-C2-C3	-3.89	119.82	126.20
21	3	306	BCR	C33-C5-C6	-3.89	120.24	124.48
21	2	305	BCR	C40-C30-C39	3.89	119.76	108.63
18	2	309	CLA	O2A-C1-C2	3.88	123.04	108.11
21	J	1104	BCR	C33-C5-C6	-3.88	120.25	124.48
24	1	5001	LMG	O7-C10-C11	3.88	119.87	111.48
18	B	823	CLA	O2A-C1-C2	3.88	123.03	108.11
30	2	319	CHL	CHA-C1A-C2A	-3.87	124.22	133.31
30	3	313	CHL	C1A-CHA-C4D	3.87	125.43	118.98
18	A	825	CLA	C1-C2-C3	-3.86	119.87	126.20
21	A	844	BCR	C33-C5-C6	-3.86	120.27	124.48
21	A	847	BCR	C23-C24-C25	-3.86	116.70	127.00
18	3	311	CLA	O2A-C1-C2	3.85	122.94	108.11
18	1	5010	CLA	O2A-C1-C2	3.85	122.94	108.11
24	F	307	LMG	O7-C10-C11	3.85	119.81	111.48
18	B	815	CLA	O2A-C1-C2	3.85	122.93	108.11
29	1	5003	LUT	C18-C5-C6	-3.84	120.29	124.48
18	4	310	CLA	C1-C2-C3	-3.84	120.54	126.76
18	2	313	CLA	C1-C2-C3	-3.84	120.55	126.76
21	A	846	BCR	C23-C24-C25	-3.83	116.77	127.00
18	2	311	CLA	C1-C2-C3	-3.81	120.59	126.76
18	A	806	CLA	O2A-C1-C2	3.81	122.76	108.11
29	3	304	LUT	C18-C5-C6	-3.81	120.33	124.48
21	2	305	BCR	C19-C18-C17	3.80	124.99	119.01
18	B	817	CLA	O2A-C1-C2	3.80	122.72	108.11
18	2	313	CLA	O2A-C1-C2	3.80	122.71	108.11
21	B	845	BCR	C39-C30-C25	3.79	116.19	110.24
18	A	829	CLA	C1-C2-C3	-3.79	119.98	126.20
29	J	1105	LUT	C15-C14-C13	-3.79	121.97	127.28
18	A	818	CLA	C1-C2-C3	-3.79	120.64	126.76
26	B	855	DGD	O2G-C1B-C2B	3.78	119.65	111.48
21	1	5005	BCR	C33-C5-C6	-3.78	120.36	124.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	305	CLA	O2A-C1-C2	3.78	122.64	108.11
30	3	310	CHL	C3D-C4D-CHA	3.78	114.28	108.54
28	F	310	ZEX	C21-C26-C25	-3.77	119.92	122.84
18	1	5008	CLA	O2A-C1-C2	3.77	122.63	108.11
18	B	820	CLA	C1-C2-C3	-3.77	120.02	126.20
18	B	819	CLA	C1-C2-C3	-3.77	120.02	126.20
18	B	836	CLA	O2A-C1-C2	3.77	122.60	108.11
24	A	851	LMG	O7-C10-C11	3.76	119.62	111.48
17	A	801	CL0	C1-C2-C3	-3.76	120.03	126.20
18	A	803	CLA	O2A-C1-C2	3.76	122.59	108.11
18	L	305	CLA	C1-C2-C3	-3.76	120.04	126.20
18	A	804	CLA	O2A-C1-C2	3.76	122.57	108.11
18	A	825	CLA	O2A-C1-C2	3.76	122.56	108.11
18	B	807	CLA	O2A-C1-C2	3.76	122.56	108.11
18	1	5009	CLA	C1-C2-C3	-3.75	120.05	126.20
30	3	310	CHL	C1A-CHA-C4D	3.75	125.24	118.98
18	A	809	CLA	C1-C2-C3	-3.75	120.69	126.76
18	A	832	CLA	O2A-C1-C2	3.75	122.55	108.11
18	2	310	CLA	CAA-C2A-C3A	-3.75	102.87	113.00
18	A	816	CLA	O2A-C1-C2	3.74	122.52	108.11
18	3	309	CLA	O2A-C1-C2	3.74	122.51	108.11
18	A	853	CLA	O2A-C1-C2	3.74	122.50	108.11
18	A	805	CLA	O2A-C1-C2	3.74	122.49	108.11
18	L	301	CLA	C1-C2-C3	-3.74	120.07	126.20
18	B	832	CLA	C1-C2-C3	-3.74	120.08	126.20
18	J	1103	CLA	C1-C2-C3	-3.74	120.72	126.76
18	A	836	CLA	C1-C2-C3	-3.74	120.08	126.20
21	B	846	BCR	C23-C24-C25	-3.73	117.04	127.00
18	A	811	CLA	C1-C2-C3	-3.72	120.10	126.20
18	B	831	CLA	O2A-C1-C2	3.72	122.42	108.11
18	B	833	CLA	C1-C2-C3	-3.71	120.11	126.20
18	A	815	CLA	O2A-C1-C2	3.71	122.39	108.11
26	J	1106	DGD	O5D-C1E-C2E	3.71	113.91	108.27
30	4	318	CHL	CHA-C1A-C2A	-3.71	124.59	133.31
18	4	306	CLA	O2A-C1-C2	3.71	122.37	108.11
30	4	316	CHL	C1-O2A-CGA	3.71	125.62	116.65
18	A	840	CLA	O2A-C1-C2	3.70	122.35	108.11
18	3	314	CLA	O2A-C1-C2	3.70	121.83	109.44
18	B	804	CLA	O2A-C1-C2	3.70	122.34	108.11
30	4	316	CHL	CHA-C1A-C2A	-3.69	124.64	133.31
18	3	311	CLA	C1-C2-C3	-3.69	120.15	126.20
18	A	822	CLA	C1-C2-C3	-3.68	120.16	126.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	5011	CLA	O2A-C1-C2	3.68	122.27	108.11
18	2	308	CLA	CMA-C3A-C4A	3.68	121.67	111.77
21	B	845	BCR	C23-C22-C21	-3.68	113.22	119.01
18	A	829	CLA	O2A-C1-C2	3.68	122.25	108.11
21	G	1604	BCR	C15-C14-C13	-3.67	122.13	127.28
18	1	5006	CLA	O2A-C1-C2	3.67	122.23	108.11
31	4	304	XAT	C7-C8-C9	-3.67	119.84	125.53
18	3	319	CLA	O2A-C1-C2	3.67	122.21	108.11
18	B	808	CLA	O2A-C1-C2	3.66	122.19	108.11
18	4	309	CLA	C1-C2-C3	-3.66	120.20	126.20
18	2	317	CLA	O2A-C1-C2	3.66	122.18	108.11
21	B	843	BCR	C33-C5-C6	-3.66	120.49	124.48
30	3	313	CHL	CHA-C1A-C2A	-3.65	124.72	133.31
18	4	309	CLA	O2A-C1-C2	3.65	122.16	108.11
18	A	827	CLA	O2A-C1-C2	3.65	122.16	108.11
21	B	844	BCR	C23-C24-C25	-3.65	117.25	127.00
18	B	832	CLA	O2A-C1-C2	3.65	122.15	108.11
18	K	1403	CLA	O2A-C1-C2	3.65	121.65	109.44
21	B	843	BCR	C34-C9-C10	-3.65	116.91	122.82
18	B	824	CLA	O2A-C1-C2	3.64	122.12	108.11
21	G	1604	BCR	C33-C5-C6	-3.64	120.51	124.48
18	B	836	CLA	C1-C2-C3	-3.63	120.25	126.20
18	A	836	CLA	O2A-C1-C2	3.63	122.08	108.11
18	B	801	CLA	O2A-C1-C2	3.63	122.07	108.11
18	L	301	CLA	O2A-C1-C2	3.63	122.07	108.11
21	B	802	BCR	C33-C5-C6	-3.62	120.53	124.48
18	A	823	CLA	C1-C2-C3	-3.62	120.26	126.20
18	3	309	CLA	C1-C2-C3	-3.62	120.26	126.20
30	2	315	CHL	CHA-C1A-C2A	-3.62	124.81	133.31
18	A	822	CLA	O2A-C1-C2	3.62	122.03	108.11
18	B	840	CLA	O2A-C1-C2	3.62	122.02	108.11
18	A	828	CLA	O2A-C1-C2	3.61	122.02	108.11
18	1	5018	CLA	O2A-C1-C2	3.61	122.01	108.11
21	A	844	BCR	C19-C18-C17	3.61	124.69	119.01
18	A	834	CLA	C1-C2-C3	-3.61	120.29	126.20
18	4	308	CLA	O2A-C1-C2	3.60	121.97	108.11
29	2	303	LUT	C7-C8-C9	-3.60	120.91	126.23
30	1	5014	CHL	CHA-C1A-C2A	-3.60	124.85	133.31
18	A	808	CLA	O2A-C1-C2	3.60	121.95	108.11
18	B	814	CLA	O2A-C1-C2	3.60	121.95	108.11
18	B	829	CLA	O2A-C1-C2	3.60	121.94	108.11
18	B	801	CLA	C1-C2-C3	-3.59	120.31	126.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	311	CLA	O2A-C1-C2	3.59	121.94	108.11
18	A	831	CLA	O2A-C1-C2	3.59	121.91	108.11
18	4	315	CLA	O2A-C1-C2	3.59	121.91	108.11
21	L	302	BCR	C19-C18-C17	3.59	124.65	119.01
18	A	811	CLA	O2A-C1-C2	3.59	121.91	108.11
18	A	821	CLA	O2A-C1-C2	3.58	121.90	108.11
18	1	5009	CLA	O2A-C1-C2	3.58	121.90	108.11
18	2	311	CLA	O2A-C1-C2	3.58	121.89	108.11
30	4	317	CHL	CHA-C1A-C2A	-3.58	124.90	133.31
30	4	316	CHL	C1A-CHA-C4D	3.58	124.95	118.98
18	B	811	CLA	O2A-C1-C2	3.58	121.87	108.11
18	4	305	CLA	O2A-C1-C2	3.58	121.87	108.11
18	B	830	CLA	C1-C2-C3	-3.58	120.34	126.20
18	A	807	CLA	O2A-C1-C2	3.57	121.85	108.11
17	A	801	CL0	O2A-C1-C2	3.57	121.85	108.11
18	4	310	CLA	O2A-C1-C2	3.56	121.82	108.11
18	2	326	CLA	C1-C2-C3	-3.56	121.00	126.76
30	1	5016	CHL	CHA-C1A-C2A	-3.56	124.96	133.31
30	4	313	CHL	CHA-C1A-C2A	-3.56	124.96	133.31
18	B	805	CLA	O2A-C1-C2	3.55	121.77	108.11
18	B	826	CLA	O2A-C1-C2	3.55	121.77	108.11
18	4	308	CLA	C1-C2-C3	-3.54	120.40	126.20
21	A	843	BCR	C33-C5-C6	-3.54	120.62	124.48
18	B	812	CLA	O2A-C1-C2	3.54	121.72	108.11
18	4	307	CLA	O2A-C1-C2	3.54	121.72	108.11
18	1	5011	CLA	C1-C2-C3	-3.53	121.05	126.76
18	A	824	CLA	O2A-C1-C2	3.53	121.68	108.11
21	L	303	BCR	C19-C18-C17	3.53	124.56	119.01
21	I	101	BCR	C33-C5-C6	-3.52	120.64	124.48
18	H	1701	CLA	O2A-C1-C2	3.52	121.66	108.11
18	1	5008	CLA	C1-C2-C3	-3.52	120.43	126.20
18	J	1103	CLA	CMA-C3A-C4A	3.52	121.24	111.77
18	B	835	CLA	C1-C2-C3	-3.52	120.43	126.20
18	4	311	CLA	C1-C2-C3	-3.52	120.43	126.20
30	4	302	CHL	CHA-C1A-C2A	-3.52	125.05	133.31
21	B	846	BCR	C33-C5-C6	-3.52	120.65	124.48
18	A	816	CLA	C1-C2-C3	-3.51	120.44	126.20
21	B	847	BCR	C23-C24-C25	-3.51	117.62	127.00
18	L	306	CLA	C1-C2-C3	-3.51	121.09	126.76
29	3	303	LUT	C18-C5-C6	-3.51	120.66	124.48
30	3	316	CHL	CHA-C1A-C2A	-3.51	125.08	133.31
18	A	833	CLA	O2A-C1-C2	3.50	121.59	108.11

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	314	CHL	CHA-C1A-C2A	-3.50	125.08	133.31
29	1	5003	LUT	C15-C14-C13	-3.50	122.37	127.28
18	A	852	CLA	O2A-C1-C2	3.50	121.57	108.11
24	G	1607	LMG	O1-C1-C2	3.50	113.58	108.27
18	3	307	CLA	O2A-C1-C2	3.50	121.56	108.11
18	H	1701	CLA	C1-C2-C3	-3.50	120.47	126.20
18	G	1601	CLA	O2A-C1-C2	3.50	121.56	108.11
18	K	1402	CLA	O2A-C1-C2	3.50	121.56	108.11
21	L	303	BCR	C36-C18-C17	-3.49	117.16	122.82
18	B	827	CLA	O2A-C1-C2	3.49	121.53	108.11
18	B	837	CLA	O2A-C1-C2	3.49	121.52	108.11
21	B	845	BCR	C36-C18-C17	-3.48	117.17	122.82
18	2	306	CLA	O2A-C1-C2	3.48	121.51	108.11
30	2	316	CHL	CHA-C1A-C2A	-3.48	125.13	133.31
18	B	827	CLA	C1-C2-C3	-3.48	120.50	126.20
18	A	837	CLA	C1-C2-C3	-3.48	120.50	126.20
21	3	306	BCR	C15-C14-C13	3.48	132.15	127.28
18	B	841	CLA	O2A-C1-C2	3.47	121.47	108.11
18	A	840	CLA	C1-C2-C3	-3.47	120.51	126.20
18	B	828	CLA	C1-C2-C3	-3.47	120.52	126.20
18	2	307	CLA	O2A-C1-C2	3.47	121.44	108.11
30	3	312	CHL	CHA-C1A-C2A	-3.47	125.17	133.31
18	B	830	CLA	O2A-C1-C2	3.46	121.44	108.11
28	F	310	ZEX	C11-C10-C9	-3.46	122.43	127.28
23	2	325	LMT	C1'-O5'-C5'	-3.46	106.97	113.72
28	F	310	ZEX	C31-C30-C29	-3.46	122.43	127.28
18	A	813	CLA	C1-C2-C3	-3.45	120.54	126.20
18	B	812	CLA	C1-C2-C3	-3.45	120.54	126.20
18	B	825	CLA	C1-O2A-CGA	3.45	125.01	116.65
18	A	807	CLA	C1-C2-C3	-3.45	120.54	126.20
18	2	309	CLA	C1-C2-C3	-3.45	120.55	126.20
21	A	846	BCR	C33-C5-C6	-3.44	120.73	124.48
28	F	310	ZEX	C18-C5-C6	-3.44	120.73	124.48
30	3	312	CHL	C1-C2-C3	-3.44	121.20	126.76
30	3	310	CHL	C1-O2A-CGA	3.44	124.97	116.65
18	A	830	CLA	O2A-C1-C2	3.43	121.32	108.11
18	2	308	CLA	O2A-C1-C2	3.43	121.30	108.11
18	A	830	CLA	C1-C2-C3	-3.43	120.58	126.20
30	2	316	CHL	C1A-CHA-C4D	3.43	124.70	118.98
21	L	302	BCR	C33-C5-C6	-3.42	120.75	124.48
29	2	303	LUT	C18-C5-C6	-3.42	120.75	124.48
21	L	307	BCR	C33-C5-C6	-3.42	120.75	124.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	806	CLA	O2A-C1-C2	3.42	121.25	108.11
18	L	304	CLA	C1-C2-C3	-3.42	121.24	126.76
18	B	838	CLA	O2A-C1-C2	3.41	121.24	108.11
18	A	810	CLA	O2A-C1-C2	3.41	121.23	108.11
18	A	815	CLA	C1-C2-C3	-3.41	120.62	126.20
21	F	304	BCR	C2-C1-C6	3.39	115.37	110.44
30	2	314	CHL	CHA-C1A-C2A	-3.38	125.36	133.31
21	A	845	BCR	C33-C5-C6	-3.38	120.80	124.48
21	I	101	BCR	C12-C13-C14	3.38	124.32	119.01
18	A	823	CLA	O2A-C1-C2	3.38	121.11	108.11
30	1	5016	CHL	C3C-C4C-NC	-3.37	106.40	114.65
29	1	5003	LUT	C26-C27-C28	-3.36	119.34	124.58
18	F	303	CLA	C1-C2-C3	-3.36	120.69	126.20
18	A	804	CLA	C1-C2-C3	-3.36	120.69	126.20
30	4	318	CHL	C1A-CHA-C4D	3.36	124.59	118.98
18	3	308	CLA	C1-C2-C3	-3.36	120.69	126.20
18	3	308	CLA	O2A-C1-C2	3.36	121.02	108.11
18	G	1603	CLA	CMA-C3A-C4A	3.36	120.79	111.77
18	A	818	CLA	O2A-C1-C2	3.35	121.00	108.11
18	B	834	CLA	O2A-C1-C2	3.34	120.98	108.11
18	B	837	CLA	C1-C2-C3	-3.34	120.72	126.20
18	A	838	CLA	C1-C2-C3	-3.34	120.72	126.20
18	A	812	CLA	C1-C2-C3	-3.34	120.73	126.20
18	B	808	CLA	C1-C2-C3	-3.34	120.73	126.20
18	L	306	CLA	O2A-C1-C2	3.33	120.94	108.11
18	B	814	CLA	C1-C2-C3	-3.33	120.74	126.20
22	A	849	LHG	C5-O7-C7	-3.33	109.83	117.80
30	3	316	CHL	C1A-CHA-C4D	3.33	124.53	118.98
18	A	835	CLA	O2A-C1-C2	3.32	120.89	108.11
29	4	303	LUT	C7-C8-C9	-3.32	121.33	126.23
18	A	820	CLA	O2A-C1-C2	3.31	120.86	108.11
21	F	305	BCR	C33-C5-C6	-3.31	120.87	124.48
18	B	820	CLA	O2A-C1-C2	3.31	120.84	108.11
18	B	828	CLA	O2A-C1-C2	3.31	120.83	108.11
18	A	838	CLA	O2A-C1-C2	3.30	120.80	108.11
18	2	312	CLA	O2A-C1-C2	3.30	120.80	108.11
18	4	315	CLA	C1-C2-C3	-3.29	120.80	126.20
18	F	303	CLA	O2A-C1-C2	3.28	120.72	108.11
18	A	813	CLA	O2A-C1-C2	3.27	120.70	108.11
21	B	845	BCR	C37-C22-C23	3.27	123.08	118.09
18	A	812	CLA	O2A-C1-C2	3.27	120.69	108.11
23	B	853	LMT	C1'-O5'-C5'	-3.27	107.34	113.72

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	833	CLA	O2A-C1-C2	3.26	120.66	108.11
18	A	821	CLA	C1-C2-C3	-3.26	120.85	126.20
21	A	847	BCR	C12-C13-C14	-3.26	113.88	119.01
18	2	307	CLA	C1-C2-C3	-3.26	120.86	126.20
18	3	307	CLA	C1-C2-C3	-3.25	120.86	126.20
30	2	319	CHL	C1A-CHA-C4D	3.25	124.41	118.98
18	A	837	CLA	O2A-C1-C2	3.25	120.63	108.11
21	A	845	BCR	C27-C26-C25	-3.25	118.31	122.70
21	A	847	BCR	C35-C13-C12	3.24	123.04	118.09
30	3	316	CHL	C3C-C4C-NC	-3.24	106.74	114.65
21	L	302	BCR	C3-C4-C5	-3.24	108.29	114.06
30	3	312	CHL	C3C-C4C-NC	-3.23	106.75	114.65
18	2	310	CLA	C1C-C2C-C3C	-3.23	103.58	106.98
18	A	809	CLA	O2A-C1-C2	3.23	120.55	108.11
18	A	823	CLA	C2C-C1C-NC	3.23	113.38	109.98
18	K	1403	CLA	C2C-C1C-NC	3.23	113.37	109.98
18	A	817	CLA	O2A-C1-C2	3.22	120.49	108.11
18	B	803	CLA	O2A-C1-C2	3.22	120.48	108.11
21	F	304	BCR	C28-C27-C26	-3.22	108.32	114.06
21	L	302	BCR	C2-C1-C6	3.21	115.11	110.44
21	I	102	BCR	C33-C5-C6	-3.21	120.98	124.48
30	2	318	CHL	CHA-C1A-C2A	-3.21	125.77	133.31
18	K	1404	CLA	C2C-C1C-NC	3.21	113.35	109.98
21	L	302	BCR	C33-C5-C4	3.21	120.44	113.60
18	2	326	CLA	O2A-C1-C2	3.21	120.45	108.11
21	I	101	BCR	C31-C1-C6	-3.21	105.21	110.24
18	J	1103	CLA	O2A-C1-C2	3.20	120.43	108.11
30	3	312	CHL	C1A-CHA-C4D	3.20	124.33	118.98
21	F	305	BCR	C23-C24-C25	-3.20	118.46	127.00
18	3	319	CLA	C1-C2-C3	-3.19	120.97	126.20
26	J	1106	DGD	O2G-C1B-C2B	3.19	118.38	111.48
18	G	1603	CLA	O2A-C1-C2	3.19	120.37	108.11
30	2	315	CHL	C1A-CHA-C4D	3.18	124.29	118.98
18	3	319	CLA	C3B-C4B-NB	-3.18	107.69	110.53
21	2	305	BCR	C33-C5-C4	3.18	120.37	113.60
18	3	315	CLA	O2A-C1-C2	3.17	120.32	108.11
21	F	304	BCR	C23-C24-C25	-3.17	118.53	127.00
19	A	841	PQN	C14-C13-C15	3.16	120.72	115.23
21	A	855	BCR	C15-C14-C13	-3.16	122.84	127.28
30	4	314	CHL	C1-C2-C3	-3.16	121.64	126.76
18	B	809	CLA	O2A-C1-C2	3.16	120.28	108.11
30	2	318	CHL	C1A-CHA-C4D	3.16	124.26	118.98

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	309	CLA	CMA-C3A-C4A	3.16	120.27	111.77
19	B	842	PQN	C11-C12-C13	-3.16	121.39	126.83
18	A	853	CLA	CMA-C3A-C4A	3.15	120.25	111.77
18	B	819	CLA	O2A-CGA-CBA	3.15	121.44	111.83
18	K	1402	CLA	CMA-C3A-C4A	3.15	120.24	111.77
18	A	838	CLA	CMA-C3A-C4A	3.15	120.23	111.77
18	B	831	CLA	C1-C2-C3	-3.15	121.04	126.20
30	4	313	CHL	C1A-CHA-C4D	3.14	124.23	118.98
18	A	817	CLA	CMA-C3A-C4A	3.14	120.22	111.77
30	1	5014	CHL	C1A-CHA-C4D	3.14	124.22	118.98
30	4	317	CHL	C3C-C4C-NC	-3.14	106.98	114.65
18	B	810	CLA	O2A-C1-C2	3.14	120.17	108.11
29	2	303	LUT	C11-C10-C9	-3.13	122.89	127.28
18	3	315	CLA	C1-C2-C3	-3.13	121.07	126.20
18	B	822	CLA	O2A-C1-C2	3.13	120.13	108.11
18	A	822	CLA	C3B-C4B-NB	-3.12	107.74	110.53
18	A	810	CLA	CMA-C3A-C4A	3.12	120.16	111.77
26	J	1106	DGD	O1G-C1A-C2A	3.12	121.34	111.83
29	4	303	LUT	C15-C14-C13	-3.12	122.91	127.28
30	2	315	CHL	C3C-C4C-NC	-3.12	107.03	114.65
18	F	301	CLA	O2A-C1-C2	3.12	120.10	108.11
18	4	308	CLA	CMA-C3A-C4A	3.12	120.15	111.77
18	L	304	CLA	O2A-C1-C2	3.11	120.09	108.11
30	4	317	CHL	C1A-CHA-C4D	3.11	124.18	118.98
18	B	801	CLA	C3B-C4B-NB	-3.11	107.75	110.53
29	3	304	LUT	C35-C15-C14	-3.11	117.16	123.52
18	B	839	CLA	C1-C2-C3	-3.11	121.11	126.20
18	1	5013	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
22	A	849	LHG	O8-C23-C24	3.10	121.30	111.83
21	I	101	BCR	C33-C5-C4	3.10	120.21	113.60
21	J	1104	BCR	C35-C13-C12	3.10	122.82	118.09
21	J	1104	BCR	C12-C13-C14	-3.09	114.14	119.01
30	4	314	CHL	C1A-CHA-C4D	3.09	124.14	118.98
21	A	844	BCR	C36-C18-C17	-3.09	117.81	122.82
18	A	833	CLA	C1-C2-C3	-3.09	121.13	126.20
18	2	306	CLA	C1-C2-C3	-3.09	121.13	126.20
18	B	840	CLA	C2C-C1C-NC	3.09	113.23	109.98
30	4	302	CHL	C1A-CHA-C4D	3.09	124.14	118.98
18	1	5008	CLA	O2A-CGA-CBA	3.08	121.24	111.83
30	2	319	CHL	C3C-C4C-NC	-3.08	107.11	114.65
18	B	805	CLA	C1-C2-C3	-3.08	121.14	126.20
18	G	1603	CLA	C1-C2-C3	-3.08	121.14	126.20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	2	314	CHL	C3C-C4C-NC	-3.08	107.12	114.65
18	B	834	CLA	C1-C2-C3	-3.08	121.15	126.20
22	B	848	LHG	C5-O7-C7	-3.08	112.41	117.85
29	1	5003	LUT	C11-C10-C9	-3.08	122.96	127.28
30	4	314	CHL	C3C-C4C-NC	-3.08	107.12	114.65
30	3	310	CHL	C3C-C4C-NC	-3.08	107.13	114.65
18	K	1404	CLA	CMA-C3A-C4A	3.08	120.04	111.77
21	2	305	BCR	C27-C26-C25	-3.07	118.55	122.70
18	2	317	CLA	C2C-C1C-NC	3.07	113.21	109.98
18	B	801	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
21	A	844	BCR	C27-C26-C25	-3.07	118.56	122.70
30	4	318	CHL	C3C-C4C-NC	-3.07	107.15	114.65
18	B	817	CLA	O2A-CGA-CBA	3.06	121.17	111.83
18	4	311	CLA	CMA-C3A-C4A	3.06	120.00	111.77
30	2	319	CHL	C1-O2A-CGA	3.06	124.06	116.65
18	A	831	CLA	C1-C2-C3	-3.06	121.19	126.20
18	1	5008	CLA	CMA-C3A-C4A	3.06	119.99	111.77
18	F	301	CLA	CMA-C3A-C4A	3.06	119.99	111.77
21	L	302	BCR	C23-C24-C25	-3.06	118.83	127.00
18	4	307	CLA	CMA-C3A-C4A	3.06	119.99	111.77
18	A	822	CLA	CMA-C3A-C4A	3.06	119.99	111.77
30	3	313	CHL	C1-C2-C3	-3.06	121.82	126.76
30	4	313	CHL	C3C-C4C-NC	-3.05	107.19	114.65
24	B	850	LMG	O8-C28-C29	3.05	121.14	111.83
18	B	830	CLA	C2C-C1C-NC	3.05	113.19	109.98
18	A	806	CLA	C1-C2-C3	-3.05	121.20	126.20
29	1	5003	LUT	C35-C15-C14	-3.05	117.28	123.52
18	2	312	CLA	CMA-C3A-C4A	3.05	119.96	111.77
18	A	817	CLA	C1-C2-C3	-3.05	121.20	126.20
29	1	5004	LUT	C7-C8-C9	-3.05	121.73	126.23
18	K	1403	CLA	CMA-C3A-C4A	3.05	119.96	111.77
21	A	847	BCR	C4-C5-C6	-3.04	118.60	122.70
18	3	309	CLA	CMA-C3A-C4A	3.04	119.94	111.77
18	A	826	CLA	O2A-C1-C2	3.04	119.80	108.11
18	1	5015	CLA	CMA-C3A-C4A	3.04	119.94	111.77
18	A	814	CLA	CMA-C3A-C4A	3.04	119.93	111.77
21	4	301	BCR	C35-C13-C12	3.03	122.72	118.09
18	B	822	CLA	C1-C2-C3	-3.03	121.22	126.20
18	J	1101	CLA	C1-C2-C3	-3.03	121.22	126.20
18	4	305	CLA	C1-C2-C3	-3.03	121.23	126.20
18	1	5015	CLA	O2A-C1-C2	3.03	119.78	108.11
29	3	304	LUT	C27-C28-C29	-3.03	119.81	126.32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	L	302	BCR	C36-C18-C17	-3.03	117.91	122.82
18	B	822	CLA	CMA-C3A-C4A	3.03	119.91	111.77
18	B	841	CLA	C1-C2-C3	-3.03	121.23	126.20
18	J	1103	CLA	C2C-C1C-NC	3.02	113.16	109.98
30	3	313	CHL	C3C-C4C-NC	-3.02	107.27	114.65
18	1	5012	CLA	CMA-C3A-C4A	3.02	119.89	111.77
18	2	326	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
21	B	845	BCR	C23-C24-C25	-3.02	118.94	127.00
30	2	314	CHL	C1A-CHA-C4D	3.02	124.02	118.98
18	A	835	CLA	C1-C2-C3	-3.01	121.26	126.20
24	1	5001	LMG	O8-C28-C29	3.01	121.02	111.83
21	B	844	BCR	C27-C26-C25	-3.01	118.64	122.70
30	1	5016	CHL	C1A-CHA-C4D	3.01	124.00	118.98
30	4	302	CHL	C3C-C4C-NC	-3.01	107.30	114.65
21	A	845	BCR	C23-C24-C25	-3.00	118.97	127.00
18	2	310	CLA	CMA-C3A-C4A	3.00	119.85	111.77
18	A	819	CLA	O2A-C1-C2	3.00	119.67	108.11
18	A	813	CLA	CMA-C3A-C4A	3.00	119.84	111.77
24	2	321	LMG	O7-C10-C11	3.00	121.95	110.93
18	B	830	CLA	CMD-C2D-C3D	-3.00	120.81	127.69
21	A	855	BCR	C27-C26-C25	-3.00	118.66	122.70
18	B	819	CLA	CMA-C3A-C4A	3.00	119.82	111.77
18	2	313	CLA	CMA-C3A-C4A	2.99	119.82	111.77
18	A	813	CLA	C2C-C1C-NC	2.99	113.12	109.98
18	A	827	CLA	CMA-C3A-C4A	2.99	119.81	111.77
29	3	304	LUT	C10-C11-C12	-2.99	114.53	123.20
18	2	326	CLA	C2C-C1C-NC	2.99	113.12	109.98
18	4	315	CLA	C2C-C1C-NC	2.99	113.12	109.98
18	L	301	CLA	CMA-C3A-C4A	2.99	119.81	111.77
29	2	303	LUT	C15-C35-C34	-2.99	117.41	123.52
18	B	810	CLA	C2C-C1C-NC	2.98	113.11	109.98
18	A	820	CLA	CMA-C3A-C4A	2.98	119.79	111.77
23	J	1107	LMT	C1'-O5'-C5'	-2.98	107.90	113.72
18	A	823	CLA	CMA-C3A-C4A	2.98	119.78	111.77
18	1	5018	CLA	CMA-C3A-C4A	2.98	119.78	111.77
30	1	5014	CHL	C3C-C4C-NC	-2.98	107.38	114.65
18	3	317	CLA	O2A-CGA-CBA	2.98	120.91	111.83
21	B	802	BCR	C34-C9-C10	-2.98	118.00	122.82
18	B	839	CLA	CMA-C3A-C4A	2.97	119.77	111.77
21	4	301	BCR	C24-C25-C26	-2.97	114.71	121.56
18	B	823	CLA	C1-C2-C3	-2.97	121.33	126.20
18	B	830	CLA	O2D-CGD-O1D	-2.97	118.06	123.85

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	852	LMT	C1'-O5'-C5'	-2.97	107.92	113.72
18	B	816	CLA	CMA-C3A-C4A	2.97	119.76	111.77
21	1	5005	BCR	C38-C26-C25	-2.97	121.25	124.48
18	B	809	CLA	C2C-C1C-NC	2.97	113.10	109.98
18	B	818	CLA	C2C-C1C-NC	2.97	113.10	109.98
24	2	321	LMG	O8-C28-C29	2.97	120.15	111.15
18	H	1701	CLA	C2C-C1C-NC	2.97	113.10	109.98
18	A	808	CLA	CMA-C3A-C4A	2.97	119.74	111.77
18	4	315	CLA	CMA-C3A-C4A	2.96	119.74	111.77
18	A	839	CLA	O2A-C1-C2	2.96	119.52	108.11
21	4	301	BCR	C38-C26-C25	-2.96	121.25	124.48
18	2	308	CLA	O2A-CGA-CBA	2.96	120.86	111.83
18	B	840	CLA	C1C-C2C-C3C	-2.96	103.87	106.98
18	B	826	CLA	CMA-C3A-C4A	2.96	119.72	111.77
18	B	811	CLA	C1-C2-C3	-2.96	121.35	126.20
29	1	5004	LUT	C18-C5-C6	-2.96	121.26	124.48
18	A	821	CLA	CMA-C3A-C4A	2.96	119.72	111.77
18	1	5010	CLA	C1C-C2C-C3C	-2.96	103.87	106.98
18	B	812	CLA	CMA-C3A-C4A	2.96	119.72	111.77
26	J	1106	DGD	O6D-C5D-C6D	2.96	112.56	106.69
18	B	813	CLA	CMA-C3A-C4A	2.96	119.72	111.77
18	A	833	CLA	CMA-C3A-C4A	2.95	119.71	111.77
31	4	304	XAT	C38-C25-C26	-2.95	117.44	122.30
21	A	855	BCR	C19-C18-C17	2.95	123.65	119.01
18	3	315	CLA	CMA-C3A-C4A	2.95	119.69	111.77
18	A	814	CLA	C2C-C1C-NC	2.94	113.07	109.98
18	K	1403	CLA	C1C-C2C-C3C	-2.94	103.88	106.98
21	A	844	BCR	C35-C13-C12	2.94	122.58	118.09
18	A	835	CLA	CMA-C3A-C4A	2.94	119.68	111.77
18	A	825	CLA	CMA-C3A-C4A	2.94	119.67	111.77
30	4	302	CHL	C1-O2A-CGA	2.94	123.76	116.65
18	B	836	CLA	C2C-C1C-NC	2.94	113.07	109.98
18	B	832	CLA	CMA-C3A-C4A	2.94	119.66	111.77
21	B	802	BCR	C8-C9-C10	2.93	123.62	119.01
18	B	827	CLA	OBD-CAD-C3D	-2.93	121.56	128.42
18	B	833	CLA	CAA-CBA-CGA	-2.93	104.88	113.21
18	G	1602	CLA	CMA-C3A-C4A	2.93	119.65	111.77
21	2	305	BCR	C36-C18-C17	-2.93	118.07	122.82
18	3	314	CLA	CMA-C3A-C4A	2.93	119.64	111.77
18	A	803	CLA	C3B-C4B-NB	-2.93	107.92	110.53
18	A	802	CLA	O2A-C1-C2	2.93	119.36	108.11
18	A	824	CLA	C3B-C4B-NB	-2.92	107.92	110.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	852	CLA	C3B-C4B-NB	-2.92	107.92	110.53
30	2	316	CHL	C3C-C4C-NC	-2.92	107.51	114.65
18	2	317	CLA	C1-C2-C3	-2.92	121.42	126.20
18	2	310	CLA	CBC-CAC-C3C	-2.92	104.51	112.42
26	2	327	DGD	C2G-O2G-C1B	-2.92	110.81	117.80
18	G	1601	CLA	C2C-C1C-NC	2.92	113.05	109.98
18	L	305	CLA	CMA-C3A-C4A	2.92	119.61	111.77
18	A	828	CLA	C2C-C1C-NC	2.91	113.04	109.98
18	1	5010	CLA	C2C-C1C-NC	2.91	113.04	109.98
18	A	840	CLA	CMA-C3A-C4A	2.91	119.60	111.77
18	J	1101	CLA	C2C-C1C-NC	2.91	113.04	109.98
18	B	841	CLA	CMA-C3A-C4A	2.91	119.59	111.77
29	1	5004	LUT	C27-C28-C29	-2.90	120.08	126.32
18	K	1402	CLA	C2C-C1C-NC	2.90	113.03	109.98
18	B	836	CLA	CMA-C3A-C4A	2.90	119.58	111.77
24	F	306	LMG	O8-C28-C29	2.90	120.68	111.83
21	A	845	BCR	C15-C14-C13	-2.90	123.21	127.28
23	G	1605	LMT	C3'-C4'-C5'	-2.90	104.50	110.93
24	G	1607	LMG	O8-C28-C29	2.90	119.95	111.15
18	B	835	CLA	C3B-C4B-NB	-2.90	107.94	110.53
21	F	304	BCR	C4-C5-C6	-2.90	118.79	122.70
21	G	1604	BCR	C23-C24-C25	-2.90	119.26	127.00
18	A	824	CLA	CMA-C3A-C4A	2.90	119.55	111.77
18	A	852	CLA	CMA-C3A-C4A	2.89	119.55	111.77
18	A	823	CLA	C1C-C2C-C3C	-2.89	103.94	106.98
21	4	301	BCR	C12-C13-C14	-2.89	114.46	119.01
18	1	5009	CLA	CMA-C3A-C4A	2.89	119.53	111.77
18	B	829	CLA	CMA-C3A-C4A	2.89	119.53	111.77
21	I	101	BCR	C1-C6-C5	-2.88	118.70	122.64
21	L	302	BCR	C4-C5-C6	-2.88	118.81	122.70
18	B	821	CLA	C2C-C1C-NC	2.88	113.01	109.98
30	4	316	CHL	C3C-C4C-NC	-2.88	107.61	114.65
18	A	811	CLA	CMA-C3A-C4A	2.88	119.51	111.77
21	B	843	BCR	C36-C18-C19	-2.88	113.69	118.09
18	2	307	CLA	CMA-C3A-C4A	2.88	119.51	111.77
26	B	855	DGD	O1G-C1A-C2A	2.88	120.61	111.83
18	B	830	CLA	C1C-C2C-C3C	-2.88	103.95	106.98
18	B	835	CLA	CMA-C3A-C4A	2.87	119.50	111.77
18	F	302	CLA	C2C-C1C-NC	2.87	113.00	109.98
18	A	832	CLA	C3B-C4B-NB	-2.87	107.97	110.53
21	A	843	BCR	C35-C13-C12	2.87	122.47	118.09
18	3	308	CLA	CMA-C3A-C4A	2.87	119.49	111.77

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	2	318	CHL	C4D-CHA-CBD	-2.87	106.07	108.97
18	A	838	CLA	C2C-C1C-NC	2.87	113.00	109.98
28	F	310	ZEX	C27-C28-C29	-2.87	121.99	126.23
18	1	5008	CLA	C2C-C1C-NC	2.87	112.99	109.98
18	1	5012	CLA	C2C-C1C-NC	2.87	112.99	109.98
24	A	851	LMG	O8-C28-C29	2.87	120.58	111.83
18	B	829	CLA	C2C-C1C-NC	2.87	112.99	109.98
18	K	1404	CLA	C4B-CHC-C1C	2.87	132.99	126.25
21	A	843	BCR	C23-C24-C25	-2.86	119.35	127.00
18	A	833	CLA	C2C-C1C-NC	2.86	112.99	109.98
18	A	831	CLA	C3B-C4B-NB	-2.86	107.98	110.53
24	J	1102	LMG	O8-C28-C29	2.86	119.83	111.15
18	K	1401	CLA	CMA-C3A-C4A	2.86	119.46	111.77
21	G	1604	BCR	C33-C5-C4	2.86	119.69	113.60
18	A	839	CLA	CMA-C3A-C4A	2.86	119.46	111.77
18	A	808	CLA	C2C-C1C-NC	2.86	112.98	109.98
18	B	801	CLA	OBD-CAD-C3D	-2.86	121.73	128.42
18	2	312	CLA	C2C-C1C-NC	2.86	112.98	109.98
18	A	809	CLA	CMA-C3A-C4A	2.86	119.45	111.77
18	A	852	CLA	C2C-C1C-NC	2.86	112.98	109.98
18	B	808	CLA	C2C-C1C-NC	2.86	112.98	109.98
18	B	823	CLA	C3B-C4B-NB	-2.86	107.98	110.53
29	4	303	LUT	C31-C30-C29	-2.85	123.28	127.28
24	F	307	LMG	O8-C28-C29	2.85	120.53	111.83
18	A	832	CLA	C1-C2-C3	-2.85	121.52	126.20
18	1	5013	CLA	C2C-C1C-NC	2.85	112.98	109.98
18	L	305	CLA	C3B-C4B-NB	-2.85	107.99	110.53
23	G	1606	LMT	C1'-O5'-C5'	-2.85	108.16	113.72
18	A	820	CLA	C2C-C1C-NC	2.85	112.97	109.98
21	B	802	BCR	C36-C18-C17	-2.85	118.20	122.82
18	A	806	CLA	CMA-C3A-C4A	2.85	119.42	111.77
18	L	304	CLA	C2C-C1C-NC	2.84	112.97	109.98
18	A	839	CLA	C2C-C1C-NC	2.84	112.97	109.98
18	B	810	CLA	C1C-C2C-C3C	-2.84	103.99	106.98
18	2	311	CLA	C1C-C2C-C3C	-2.84	103.99	106.98
18	A	818	CLA	C2C-C1C-NC	2.84	112.97	109.98
18	B	834	CLA	CMD-C2D-C3D	-2.84	121.17	127.69
18	J	1101	CLA	C1C-C2C-C3C	-2.84	103.99	106.98
18	A	836	CLA	C3B-C4B-NB	-2.84	108.00	110.53
18	3	314	CLA	C2C-C1C-NC	2.84	112.96	109.98
21	K	1405	BCR	C33-C5-C4	2.84	119.65	113.60
18	A	826	CLA	C3B-C4B-NB	-2.84	108.00	110.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	842	PQN	C14-C13-C15	2.84	120.15	115.23
18	A	822	CLA	C4B-CHC-C1C	2.83	132.91	126.25
18	B	827	CLA	C2C-C1C-NC	2.83	112.96	109.98
26	1	5002	DGD	O1G-C1A-C2A	2.83	120.48	111.83
18	A	838	CLA	C1C-C2C-C3C	-2.83	104.00	106.98
18	B	809	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
18	A	852	CLA	OBD-CAD-C3D	-2.83	121.80	128.42
18	B	819	CLA	C1C-C2C-C3C	-2.83	104.00	106.98
18	B	840	CLA	C1-C2-C3	-2.83	121.56	126.20
18	1	5018	CLA	C1-C2-C3	-2.83	121.56	126.20
18	B	822	CLA	C2C-C1C-NC	2.83	112.95	109.98
18	B	828	CLA	C2C-C1C-NC	2.83	112.95	109.98
18	L	304	CLA	CMA-C3A-C4A	2.83	119.37	111.77
18	G	1603	CLA	C2C-C1C-NC	2.83	112.95	109.98
18	K	1403	CLA	CMD-C2D-C3D	-2.82	121.21	127.69
18	G	1601	CLA	C1C-C2C-C3C	-2.82	104.01	106.98
18	G	1602	CLA	C2C-C1C-NC	2.82	112.95	109.98
18	B	831	CLA	CMA-C3A-C4A	2.82	119.35	111.77
18	B	814	CLA	C2C-C1C-NC	2.82	112.94	109.98
29	3	303	LUT	C26-C27-C28	-2.82	120.19	124.58
21	F	305	BCR	C15-C14-C13	-2.82	123.32	127.28
18	B	836	CLA	O2A-CGA-CBA	2.82	120.43	111.83
18	F	301	CLA	O2A-CGA-CBA	2.82	120.43	111.83
18	3	308	CLA	C2C-C1C-NC	2.82	112.94	109.98
18	B	818	CLA	O2A-C1-C2	2.82	118.95	108.11
30	2	315	CHL	C1-O2A-CGA	2.82	123.47	116.65
30	3	310	CHL	CMA-C3A-C4A	2.81	120.67	114.61
18	A	804	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
18	A	806	CLA	C2C-C1C-NC	2.81	112.94	109.98
18	B	813	CLA	C2C-C1C-NC	2.81	112.94	109.98
18	B	818	CLA	C1C-C2C-C3C	-2.81	104.02	106.98
18	3	307	CLA	CMA-C3A-C4A	2.81	119.33	111.77
18	B	812	CLA	C4B-CHC-C1C	2.81	132.86	126.25
18	B	814	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
18	1	5007	CLA	CMA-C3A-C4A	2.81	119.33	111.77
21	B	845	BCR	C35-C13-C12	2.81	122.38	118.09
18	K	1404	CLA	C1C-C2C-C3C	-2.81	104.03	106.98
18	K	1401	CLA	C2C-C1C-NC	2.81	112.93	109.98
18	A	835	CLA	C3B-C4B-NB	-2.81	108.02	110.53
18	2	307	CLA	C2C-C1C-NC	2.81	112.93	109.98
18	A	831	CLA	CMA-C3A-C4A	2.80	119.31	111.77
18	4	306	CLA	C2C-C1C-NC	2.80	112.93	109.98

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	827	CLA	CMA-C3A-C4A	2.80	119.31	111.77
18	L	306	CLA	CMA-C3A-C4A	2.80	119.31	111.77
21	K	1405	BCR	C33-C5-C6	-2.80	121.43	124.48
30	2	318	CHL	C3C-C4C-NC	-2.80	107.81	114.65
18	A	827	CLA	C2C-C1C-NC	2.80	112.92	109.98
18	4	315	CLA	C1C-C2C-C3C	-2.80	104.04	106.98
18	4	308	CLA	O2A-CGA-CBA	2.80	120.36	111.83
18	B	812	CLA	C3B-C4B-NB	-2.80	108.03	110.53
18	2	313	CLA	C2C-C1C-NC	2.80	112.92	109.98
21	K	1405	BCR	C4-C5-C6	-2.80	118.93	122.70
21	B	802	BCR	C23-C24-C25	-2.80	119.53	127.00
21	A	847	BCR	C3-C4-C5	-2.80	109.07	114.06
18	A	839	CLA	C1-C2-C3	-2.79	121.62	126.20
18	A	835	CLA	O2A-CGA-CBA	2.79	120.35	111.83
18	2	312	CLA	C1-C2-C3	-2.79	121.62	126.20
18	A	821	CLA	C2C-C1C-NC	2.79	112.91	109.98
18	A	852	CLA	C1-C2-C3	-2.79	121.63	126.20
18	3	301	CLA	C2C-C1C-NC	2.79	112.91	109.98
18	2	307	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
29	1	5003	LUT	C8-C7-C6	-2.79	119.56	127.00
18	A	837	CLA	CMA-C3A-C4A	2.78	119.26	111.77
18	1	5012	CLA	C3B-C4B-NB	-2.78	108.05	110.53
18	A	804	CLA	CMA-C3A-C4A	2.78	119.25	111.77
18	2	311	CLA	C2C-C1C-NC	2.78	112.90	109.98
18	2	313	CLA	C1C-C2C-C3C	-2.78	104.05	106.98
18	2	317	CLA	C1C-C2C-C3C	-2.78	104.06	106.98
18	2	308	CLA	C2C-C1C-NC	2.78	112.90	109.98
18	B	825	CLA	C2C-C1C-NC	2.78	112.90	109.98
18	L	304	CLA	C1C-C2C-C3C	-2.78	104.06	106.98
30	2	316	CHL	C4D-CHA-CBD	-2.78	106.17	108.97
18	3	319	CLA	CMA-C3A-C4A	2.78	119.23	111.77
18	B	837	CLA	O2A-CGA-CBA	2.78	120.30	111.83
18	4	311	CLA	C3B-C4B-NB	-2.77	108.05	110.53
18	3	309	CLA	C2C-C1C-NC	2.77	112.89	109.98
18	B	804	CLA	C1-C2-C3	-2.77	121.65	126.20
18	F	303	CLA	C3B-C4B-NB	-2.77	108.06	110.53
18	2	310	CLA	C1-O2A-CGA	2.77	123.36	116.65
18	A	823	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
18	3	318	CLA	C2C-C1C-NC	2.77	112.89	109.98
18	B	823	CLA	C1-O2A-CGA	2.77	123.35	116.65
18	A	840	CLA	C2C-C1C-NC	2.77	112.89	109.98
21	B	846	BCR	C35-C13-C12	2.77	122.32	118.09

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	829	CLA	C3B-C4B-NB	-2.77	108.06	110.53
18	3	301	CLA	CMA-C3A-C4A	2.77	119.21	111.77
18	B	828	CLA	O2A-CGA-CBA	2.76	120.26	111.83
17	A	801	CL0	CBC-CAC-C3C	-2.76	108.92	112.87
18	4	307	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
18	B	823	CLA	C4B-CHC-C1C	2.76	132.74	126.25
18	B	821	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
18	4	311	CLA	C4B-CHC-C1C	2.76	132.73	126.25
21	A	847	BCR	C33-C5-C4	2.76	119.47	113.60
18	A	813	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
18	L	304	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
18	2	308	CLA	C1C-C2C-C3C	-2.75	104.08	106.98
18	A	853	CLA	C2C-C1C-NC	2.75	112.88	109.98
21	B	846	BCR	C38-C26-C25	-2.75	121.48	124.48
21	K	1405	BCR	C27-C26-C25	-2.75	118.98	122.70
18	A	832	CLA	C1-O2A-CGA	2.75	123.31	116.65
18	B	840	CLA	CMA-C3A-C4A	2.75	119.17	111.77
18	B	819	CLA	C2C-C1C-NC	2.75	112.87	109.98
18	B	823	CLA	C2C-C1C-NC	2.75	112.87	109.98
21	A	844	BCR	C28-C27-C26	-2.75	109.15	114.06
18	K	1402	CLA	O2A-CGA-CBA	2.75	120.22	111.83
18	1	5017	CLA	C3B-C4B-NB	-2.75	108.08	110.53
24	B	850	LMG	C8-O7-C10	-2.75	111.22	117.80
18	A	834	CLA	C2C-C1C-NC	2.75	112.87	109.98
18	B	811	CLA	C3B-C4B-NB	-2.75	108.08	110.53
18	B	808	CLA	C1C-C2C-C3C	-2.74	104.09	106.98
18	4	307	CLA	C2C-C1C-NC	2.74	112.86	109.98
18	A	808	CLA	C1-C2-C3	-2.74	121.70	126.20
18	A	829	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
18	B	814	CLA	O2A-CGA-CBA	2.74	120.20	111.83
30	1	5014	CHL	CMA-C3A-C4A	2.74	120.52	114.61
22	1	5019	LHG	C5-O7-C7	-2.74	111.23	117.80
18	B	806	CLA	C2C-C1C-NC	2.74	112.86	109.98
22	B	849	LHG	O8-C23-C24	2.74	120.19	111.83
18	J	1103	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
18	B	839	CLA	C2C-C1C-NC	2.74	112.86	109.98
18	B	831	CLA	C2C-C1C-NC	2.74	112.86	109.98
18	1	5007	CLA	C2C-C1C-NC	2.74	112.86	109.98
24	1	5020	LMG	O8-C28-C29	2.73	120.17	111.83
18	1	5008	CLA	C1C-C2C-C3C	-2.73	104.10	106.98
18	A	814	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
18	A	834	CLA	C1C-C2C-C3C	-2.73	104.11	106.98

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	818	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
18	1	5015	CLA	C2C-C1C-NC	2.73	112.85	109.98
18	B	803	CLA	C2C-C1C-NC	2.73	112.85	109.98
18	B	813	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
18	B	823	CLA	CMA-C3A-C4A	2.73	119.11	111.77
18	A	807	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
18	A	840	CLA	O2A-CGA-CBA	2.73	120.15	111.83
21	A	844	BCR	C12-C13-C14	-2.73	114.72	119.01
18	A	815	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
18	1	5007	CLA	C4B-CHC-C1C	2.73	132.66	126.25
18	A	836	CLA	C4B-CHC-C1C	2.73	132.66	126.25
18	B	818	CLA	CMA-C3A-C4A	2.72	119.10	111.77
23	4	319	LMT	C1'-O5'-C5'	-2.72	108.40	113.72
30	4	316	CHL	C4D-CHA-CBD	-2.72	106.22	108.97
18	A	814	CLA	C4B-CHC-C1C	2.72	132.65	126.25
18	K	1404	CLA	C3B-C4B-NB	-2.72	108.10	110.53
30	1	5016	CHL	C1-O2A-CGA	2.72	123.24	116.65
29	2	303	LUT	C30-C31-C32	-2.72	115.32	123.20
18	4	308	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
29	J	1105	LUT	C1-C6-C5	-2.72	118.92	122.64
18	B	835	CLA	C2C-C1C-NC	2.72	112.84	109.98
24	2	322	LMG	O8-C28-C29	2.72	120.12	111.83
18	A	816	CLA	CMA-C3A-C4A	2.72	119.07	111.77
30	4	314	CHL	CMA-C3A-C4A	2.72	120.46	114.61
18	B	820	CLA	C3B-C4B-NB	-2.72	108.11	110.53
18	B	830	CLA	O2A-CGA-CBA	2.71	120.11	111.83
18	1	5007	CLA	C3B-C4B-NB	-2.71	108.11	110.53
26	2	327	DGD	O1G-C1A-C2A	2.71	120.10	111.83
18	A	812	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
18	B	822	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
18	B	824	CLA	CMA-C3A-C4A	2.71	119.06	111.77
18	B	816	CLA	C2C-C1C-NC	2.71	112.83	109.98
18	B	809	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
30	4	318	CHL	C4D-CHA-CBD	-2.71	106.24	108.97
18	A	826	CLA	CMA-C3A-C4A	2.71	119.05	111.77
18	4	305	CLA	CMA-C3A-C4A	2.71	119.05	111.77
18	1	5011	CLA	C2C-C1C-NC	2.71	112.83	109.98
30	1	5016	CHL	C4D-CHA-CBD	-2.71	106.24	108.97
18	B	809	CLA	C1-C2-C3	-2.71	121.77	126.20
18	1	5017	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
18	J	1101	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
18	B	830	CLA	CMA-C3A-C4A	2.70	119.03	111.77

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	834	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
18	F	302	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
30	4	313	CHL	CMA-C3A-C4A	2.70	120.43	114.61
18	F	303	CLA	C2C-C1C-NC	2.70	112.82	109.98
18	B	825	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
24	B	851	LMG	C1-C2-C3	2.70	115.69	110.01
18	3	308	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
29	4	303	LUT	C26-C27-C28	-2.70	120.38	124.58
18	L	306	CLA	C2C-C1C-NC	2.70	112.82	109.98
18	B	811	CLA	C4B-CHC-C1C	2.70	132.59	126.25
30	1	5016	CHL	C1-C2-C3	-2.70	121.78	126.20
18	4	308	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
18	A	818	CLA	CMA-C3A-C4A	2.70	119.02	111.77
18	A	829	CLA	CMD-C2D-C3D	-2.70	121.51	127.69
18	4	312	CLA	C2C-C1C-NC	2.69	112.81	109.98
18	1	5015	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
18	B	815	CLA	C2C-C1C-NC	2.69	112.81	109.98
29	3	303	LUT	C31-C30-C29	-2.69	123.50	127.28
18	K	1402	CLA	C4B-CHC-C1C	2.69	132.58	126.25
18	A	825	CLA	C2C-C1C-NC	2.69	112.81	109.98
18	G	1603	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
18	B	834	CLA	C2C-C1C-NC	2.69	112.81	109.98
18	A	852	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
18	B	838	CLA	C2C-C1C-NC	2.69	112.80	109.98
18	3	307	CLA	C3B-C4B-NB	-2.69	108.13	110.53
18	B	803	CLA	C1C-C2C-C3C	-2.69	104.16	106.98
18	B	835	CLA	C1C-C2C-C3C	-2.69	104.16	106.98
18	B	839	CLA	C1C-C2C-C3C	-2.69	104.16	106.98
30	2	314	CHL	C1-O2A-CGA	2.69	123.15	116.65
18	1	5013	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
18	A	811	CLA	C2C-C1C-NC	2.68	112.80	109.98
18	A	826	CLA	CHD-C1D-ND	-2.68	121.02	124.80
30	4	302	CHL	CMA-C3A-C4A	2.68	120.40	114.61
18	A	815	CLA	CMA-C3A-C4A	2.68	118.99	111.77
18	1	5012	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
21	L	302	BCR	C32-C1-C6	-2.68	106.03	110.24
18	B	831	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
30	1	5014	CHL	C4D-CHA-CBD	-2.68	106.26	108.97
28	F	310	ZEX	C15-C35-C34	-2.68	118.03	123.52
30	4	302	CHL	C4D-CHA-CBD	-2.68	106.26	108.97
18	B	838	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
18	A	833	CLA	C1C-C2C-C3C	-2.68	104.16	106.98

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	5009	CLA	O2A-CGA-CBA	2.68	120.01	111.83
29	1	5003	LUT	C31-C30-C29	-2.68	123.52	127.28
18	B	809	CLA	CMA-C3A-C4A	2.68	118.97	111.77
18	A	810	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
18	2	312	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
21	I	101	BCR	C23-C24-C25	-2.68	119.84	127.00
22	2	320	LHG	O8-C23-C24	2.68	120.00	111.83
18	1	5018	CLA	O2A-CGA-CBA	2.68	120.00	111.83
21	J	1104	BCR	C27-C26-C25	-2.68	119.09	122.70
18	G	1602	CLA	C1C-C2C-C3C	-2.68	104.17	106.98
18	4	310	CLA	C1C-C2C-C3C	-2.68	104.17	106.98
18	A	830	CLA	C2C-C1C-NC	2.68	112.79	109.98
18	2	307	CLA	C3B-C4B-NB	-2.67	108.14	110.53
18	A	808	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
18	1	5012	CLA	C4B-CHC-C1C	2.67	132.53	126.25
18	4	312	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
18	A	804	CLA	C2C-C1C-NC	2.67	112.79	109.98
23	B	856	LMT	C1'-O5'-C5'	-2.67	108.50	113.72
18	A	809	CLA	C3B-C4B-NB	-2.67	108.14	110.53
18	2	326	CLA	C4B-CHC-C1C	2.67	132.53	126.25
18	A	853	CLA	O2A-CGA-CBA	2.67	119.98	111.83
18	A	830	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
18	4	309	CLA	CMA-C3A-C4A	2.67	118.94	111.77
18	1	5011	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
18	B	833	CLA	C2C-C1C-NC	2.67	112.78	109.98
18	A	806	CLA	O2A-CGA-CBA	2.67	119.97	111.83
30	4	314	CHL	C4D-CHA-CBD	-2.67	106.28	108.97
18	K	1402	CLA	C1C-C2C-C3C	-2.67	104.18	106.98
18	F	302	CLA	O2A-CGA-CBA	2.67	119.96	111.83
18	A	817	CLA	C1C-C2C-C3C	-2.67	104.18	106.98
18	4	310	CLA	C2C-C1C-NC	2.66	112.78	109.98
18	3	314	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
18	A	836	CLA	CMA-C3A-C4A	2.66	118.93	111.77
18	2	326	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
21	B	846	BCR	C33-C5-C4	2.66	119.27	113.60
18	1	5010	CLA	CMA-C3A-C4A	2.66	118.92	111.77
18	3	309	CLA	C3B-C4B-NB	-2.66	108.16	110.53
18	4	312	CLA	C3B-C4B-NB	-2.66	108.16	110.53
18	A	819	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
18	A	840	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
18	A	827	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
24	A	851	LMG	C8-O7-C10	-2.66	111.43	117.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	830	CLA	CHA-C4D-ND	2.66	138.03	132.55
18	A	802	CLA	C1C-C2C-C3C	-2.66	104.19	106.98
18	B	806	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
18	2	309	CLA	C1C-C2C-C3C	-2.66	104.19	106.98
30	3	313	CHL	C4D-CHA-CBD	-2.66	106.29	108.97
18	J	1103	CLA	C4B-CHC-C1C	2.66	132.49	126.25
18	B	833	CLA	O1D-CGD-CBD	-2.66	119.28	124.52
18	A	807	CLA	C2C-C1C-NC	2.66	112.77	109.98
18	A	830	CLA	C3B-C4B-NB	-2.65	108.16	110.53
18	B	815	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
18	1	5007	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
18	4	306	CLA	O2A-CGA-CBA	2.65	119.93	111.83
18	A	828	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
18	B	803	CLA	O2A-CGA-CBA	2.65	119.92	111.83
18	B	810	CLA	O2A-CGA-CBA	2.65	119.92	111.83
18	B	828	CLA	O1D-CGD-CBD	-2.65	119.29	124.52
18	3	315	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
21	I	101	BCR	C4-C5-C6	-2.65	119.12	122.70
18	1	5013	CLA	CMA-C3A-C4A	2.65	118.89	111.77
18	B	827	CLA	O2A-CGA-CBA	2.65	119.91	111.83
18	A	803	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
21	A	855	BCR	C36-C18-C17	-2.65	118.53	122.82
21	A	846	BCR	C27-C26-C25	-2.65	119.13	122.70
18	H	1701	CLA	C1C-C2C-C3C	-2.65	104.20	106.98
18	B	835	CLA	O2A-CGA-CBA	2.65	119.91	111.83
18	B	821	CLA	CMA-C3A-C4A	2.65	118.89	111.77
18	B	811	CLA	C2C-C1C-NC	2.65	112.76	109.98
18	4	312	CLA	CMA-C3A-C4A	2.65	118.88	111.77
18	A	820	CLA	CMD-C2D-C3D	-2.64	121.63	127.69
18	B	824	CLA	C3B-C4B-NB	-2.64	108.17	110.53
29	1	5004	LUT	C31-C30-C29	-2.64	123.57	127.28
22	1	5019	LHG	O8-C23-C24	2.64	119.89	111.83
18	B	806	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
18	1	5017	CLA	CHA-C4D-ND	2.64	138.00	132.55
18	2	306	CLA	CMA-C3A-C4A	2.64	118.87	111.77
18	B	816	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
18	3	301	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
18	3	315	CLA	C2C-C1C-NC	2.64	112.75	109.98
21	A	844	BCR	C33-C5-C4	2.64	119.22	113.60
18	B	829	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
21	G	1604	BCR	C28-C27-C26	-2.64	109.35	114.06
18	3	311	CLA	C2C-C1C-NC	2.64	112.75	109.98

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	827	CLA	CHA-C4D-ND	2.64	137.99	132.55
18	A	815	CLA	C2C-C1C-NC	2.64	112.75	109.98
18	A	821	CLA	C1C-C2C-C3C	-2.64	104.21	106.98
18	A	839	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
18	2	309	CLA	C2C-C1C-NC	2.63	112.75	109.98
18	A	805	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
18	1	5006	CLA	CAA-C2A-C3A	-2.63	105.89	113.00
18	B	810	CLA	C1-C2-C3	-2.63	121.88	126.20
18	B	833	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
18	3	317	CLA	CMA-C3A-C4A	2.63	118.85	111.77
18	1	5011	CLA	O2A-CGA-CBA	2.63	119.86	111.83
18	A	853	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
18	A	814	CLA	C3B-C4B-NB	-2.63	108.18	110.53
18	L	305	CLA	CHD-C1D-ND	-2.63	121.10	124.80
18	B	833	CLA	CMA-C3A-C4A	2.63	118.84	111.77
18	B	828	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
18	B	814	CLA	O1D-CGD-CBD	-2.63	119.33	124.52
18	B	809	CLA	O2A-CGA-CBA	2.63	119.85	111.83
18	2	326	CLA	C3B-C4B-NB	-2.63	108.18	110.53
18	3	319	CLA	C1C-C2C-C3C	-2.63	104.22	106.98
21	B	847	BCR	C37-C22-C23	2.63	122.10	118.09
18	B	827	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
18	B	812	CLA	C1C-C2C-C3C	-2.63	104.22	106.98
18	B	837	CLA	C1C-C2C-C3C	-2.63	104.22	106.98
30	2	314	CHL	C4D-CHA-CBD	-2.63	106.32	108.97
18	B	832	CLA	C2C-C1C-NC	2.63	112.74	109.98
18	4	309	CLA	C2C-C1C-NC	2.62	112.74	109.98
18	1	5006	CLA	CMA-C3A-C4A	2.62	118.83	111.77
18	A	811	CLA	C4B-CHC-C1C	2.62	132.42	126.25
18	B	804	CLA	O2A-CGA-CBA	2.62	119.83	111.83
18	K	1402	CLA	C3B-C4B-NB	-2.62	108.19	110.53
18	B	801	CLA	C2C-C1C-NC	2.62	112.74	109.98
18	B	824	CLA	C2C-C1C-NC	2.62	112.74	109.98
30	2	319	CHL	CMA-C3A-C4A	2.62	120.26	114.61
18	3	309	CLA	O2A-CGA-CBA	2.62	119.83	111.83
18	4	311	CLA	C2C-C1C-NC	2.62	112.73	109.98
18	2	309	CLA	CMD-C2D-C3D	-2.62	121.68	127.69
18	B	834	CLA	CHD-C1D-ND	-2.62	121.12	124.80
18	B	812	CLA	C2C-C1C-NC	2.62	112.73	109.98
18	G	1603	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
21	3	306	BCR	C30-C25-C24	2.62	122.75	115.65
18	B	813	CLA	C1C-C2C-C3C	-2.62	104.23	106.98

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	836	CLA	C1C-C2C-C3C	-2.62	104.23	106.98
18	B	825	CLA	CHA-C4D-ND	2.62	137.95	132.55
18	A	824	CLA	C1-C2-C3	-2.62	121.91	126.20
18	3	319	CLA	C2C-C1C-NC	2.61	112.73	109.98
18	K	1402	CLA	C1-C2-C3	-2.61	121.91	126.20
18	B	821	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
18	A	806	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
18	A	820	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
18	B	819	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
18	F	303	CLA	CMA-C3A-C4A	2.61	118.80	111.77
18	3	315	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
29	J	1105	LUT	C11-C10-C9	-2.61	123.61	127.28
18	A	828	CLA	CMA-C3A-C4A	2.61	118.79	111.77
22	A	848	LHG	O8-C23-C24	2.61	119.79	111.83
18	3	309	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
21	1	5005	BCR	C34-C9-C10	-2.61	118.59	122.82
18	G	1601	CLA	CMA-C3A-C4A	2.61	118.78	111.77
24	B	851	LMG	O8-C28-C29	2.61	119.79	111.83
18	A	835	CLA	C1C-C2C-C3C	-2.61	104.24	106.98
18	4	306	CLA	CMA-C3A-C4A	2.61	118.78	111.77
18	B	820	CLA	C1C-C2C-C3C	-2.61	104.24	106.98
21	3	305	BCR	C33-C5-C4	2.61	119.15	113.60
18	2	310	CLA	C2C-C1C-NC	2.61	112.72	109.98
18	1	5006	CLA	C4B-CHC-C1C	2.60	132.37	126.25
21	L	303	BCR	C38-C26-C25	-2.60	121.64	124.48
18	B	815	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
18	A	824	CLA	C2C-C1C-NC	2.60	112.72	109.98
18	1	5009	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
18	A	804	CLA	C6-C5-C3	-2.60	107.13	113.47
18	4	306	CLA	C3B-C4B-NB	-2.60	108.21	110.53
18	B	817	CLA	CMA-C3A-C4A	2.60	118.76	111.77
18	A	829	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
18	B	805	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
18	3	311	CLA	CMA-C3A-C4A	2.60	118.76	111.77
18	3	308	CLA	C3B-C4B-NB	-2.60	108.21	110.53
21	2	305	BCR	C32-C1-C6	-2.60	106.17	110.24
29	4	303	LUT	C35-C15-C14	-2.60	118.20	123.52
18	B	807	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
30	2	314	CHL	C1-C2-C3	-2.60	121.94	126.20
18	4	308	CLA	C2C-C1C-NC	2.60	112.71	109.98
18	A	822	CLA	C2C-C1C-NC	2.60	112.71	109.98
18	1	5018	CLA	C2C-C1C-NC	2.60	112.71	109.98

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	3	313	CHL	C1-O2A-CGA	2.60	122.94	116.65
21	4	301	BCR	C33-C5-C4	2.60	119.13	113.60
18	1	5009	CLA	CMD-C2D-C3D	-2.60	121.74	127.69
19	A	841	PQN	C11-C12-C13	-2.59	122.36	126.83
18	B	831	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
18	A	825	CLA	C1C-C2C-C3C	-2.59	104.25	106.98
18	A	809	CLA	CHD-C1D-ND	-2.59	121.15	124.80
18	A	820	CLA	CHD-C1D-ND	-2.59	121.15	124.80
18	B	823	CLA	C1C-C2C-C3C	-2.59	104.25	106.98
18	B	814	CLA	C4B-CHC-C1C	2.59	132.34	126.25
18	3	309	CLA	OBD-CAD-C3D	-2.59	122.36	128.42
21	K	1405	BCR	C23-C24-C25	-2.59	120.08	127.00
18	A	828	CLA	C1C-C2C-C3C	-2.59	104.25	106.98
18	B	812	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
18	B	837	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
18	A	817	CLA	C2C-C1C-NC	2.59	112.70	109.98
18	A	804	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
18	B	806	CLA	C3B-C4B-NB	-2.59	108.22	110.53
18	F	303	CLA	C4B-CHC-C1C	2.59	132.33	126.25
18	F	303	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
18	3	311	CLA	CHA-C4D-ND	2.59	137.89	132.55
30	4	317	CHL	CMA-C3A-C4A	2.59	120.18	114.61
18	B	822	CLA	C3B-C4B-NB	-2.59	108.22	110.53
18	4	307	CLA	C3B-C4B-NB	-2.59	108.22	110.53
18	A	807	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
21	B	802	BCR	C35-C13-C14	-2.58	118.63	122.82
18	3	309	CLA	C4B-CHC-C1C	2.58	132.32	126.25
31	2	304	XAT	C38-C25-C26	-2.58	118.05	122.30
18	A	803	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
18	A	834	CLA	O2A-CGA-CBA	2.58	119.71	111.83
18	A	810	CLA	C2C-C1C-NC	2.58	112.69	109.98
18	A	829	CLA	C2C-C1C-NC	2.58	112.69	109.98
30	4	313	CHL	C4D-CHA-CBD	-2.58	106.36	108.97
18	A	839	CLA	C4B-CHC-C1C	2.58	132.31	126.25
18	3	307	CLA	CMD-C2D-C3D	-2.58	121.77	127.69
18	3	317	CLA	C1-O2A-CGA	2.58	122.89	116.65
18	2	312	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
18	B	840	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
21	F	304	BCR	C31-C1-C6	-2.58	106.20	110.24
18	4	306	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
18	A	819	CLA	C2C-C1C-NC	2.58	112.69	109.98
18	B	828	CLA	CMD-C2D-C3D	-2.57	121.78	127.69

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	317	CHL	C4D-CHA-CBD	-2.57	106.37	108.97
18	A	822	CLA	C1C-C2C-C3C	-2.57	104.27	106.98
18	B	811	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
18	B	801	CLA	C1C-C2C-C3C	-2.57	104.27	106.98
18	B	824	CLA	C1C-C2C-C3C	-2.57	104.28	106.98
18	3	311	CLA	C1C-C2C-C3C	-2.57	104.28	106.98
18	2	317	CLA	O2A-CGA-CBA	2.57	119.67	111.83
18	A	826	CLA	C2C-C1C-NC	2.57	112.68	109.98
18	A	831	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
18	2	307	CLA	C1C-C2C-C3C	-2.57	104.28	106.98
18	B	839	CLA	C3B-C4B-NB	-2.57	108.24	110.53
21	B	802	BCR	C27-C26-C25	-2.57	119.23	122.70
18	2	309	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
18	A	829	CLA	CHD-C1D-ND	-2.57	121.19	124.80
18	B	826	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
18	1	5008	CLA	C4B-CHC-C1C	2.57	132.28	126.25
18	A	802	CLA	C3B-C4B-NB	-2.57	108.24	110.53
18	A	839	CLA	C1C-C2C-C3C	-2.57	104.28	106.98
18	A	809	CLA	C1D-ND-C4D	-2.56	104.51	106.31
21	A	846	BCR	C36-C18-C17	-2.56	118.66	122.82
18	1	5018	CLA	C1C-C2C-C3C	-2.56	104.28	106.98
18	B	828	CLA	CMA-C3A-C4A	2.56	118.66	111.77
18	3	314	CLA	C3B-C4B-NB	-2.56	108.24	110.53
17	A	801	CL0	C4-C3-C5	2.56	119.68	115.23
18	A	802	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
18	A	835	CLA	C4B-CHC-C1C	2.56	132.27	126.25
18	B	804	CLA	C3B-C4B-NB	-2.56	108.25	110.53
18	A	813	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
21	2	305	BCR	C35-C13-C12	2.56	122.00	118.09
30	3	316	CHL	CMA-C3A-C4A	2.56	120.12	114.61
24	F	306	LMG	C8-O7-C10	-2.56	111.67	117.80
18	A	818	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
18	A	812	CLA	C2C-C1C-NC	2.56	112.67	109.98
18	A	835	CLA	C2C-C1C-NC	2.56	112.67	109.98
21	4	301	BCR	C28-C27-C26	-2.56	109.50	114.06
18	A	816	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
18	1	5015	CLA	C1-C2-C3	-2.55	122.01	126.20
18	L	305	CLA	C1C-C2C-C3C	-2.55	104.29	106.98
18	B	806	CLA	C4B-CHC-C1C	2.55	132.25	126.25
18	2	310	CLA	C1D-ND-C4D	-2.55	104.52	106.31
18	B	801	CLA	O2A-CGA-CBA	2.55	119.62	111.83
18	A	811	CLA	C1C-C2C-C3C	-2.55	104.30	106.98

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	834	CLA	CHA-C4D-ND	2.55	137.81	132.55
18	A	808	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
18	A	812	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
18	B	835	CLA	CAA-C2A-C3A	-2.55	106.11	113.00
18	B	829	CLA	C1-C2-C3	-2.55	122.02	126.20
18	A	831	CLA	O2A-CGA-CBA	2.55	119.61	111.83
18	A	832	CLA	CHD-C1D-ND	-2.55	121.21	124.80
21	J	1104	BCR	C23-C24-C25	-2.55	120.19	127.00
17	A	801	CL0	CMC-C2C-C1C	2.55	129.32	124.73
18	B	817	CLA	C3B-C4B-NB	-2.55	108.25	110.53
18	B	840	CLA	C4B-CHC-C1C	2.55	132.24	126.25
18	A	810	CLA	CHD-C1D-ND	-2.55	121.22	124.80
18	B	837	CLA	CHD-C1D-ND	-2.55	121.22	124.80
18	A	810	CLA	C3B-C4B-NB	-2.55	108.26	110.53
18	A	812	CLA	CHD-C1D-ND	-2.55	121.22	124.80
18	K	1401	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
18	4	309	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
21	A	845	BCR	C38-C26-C27	2.55	119.02	113.60
21	F	304	BCR	C3-C4-C5	-2.55	109.52	114.06
18	A	803	CLA	C2C-C1C-NC	2.54	112.66	109.98
18	1	5017	CLA	C2C-C1C-NC	2.54	112.66	109.98
18	A	825	CLA	CHA-C4D-ND	2.54	137.80	132.55
21	3	306	BCR	C33-C5-C4	2.54	119.02	113.60
18	B	836	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
18	A	833	CLA	C3B-C4B-NB	-2.54	108.26	110.53
18	A	832	CLA	C1C-C2C-C3C	-2.54	104.31	106.98
30	3	312	CHL	C1-O2A-CGA	2.54	122.80	116.65
18	A	830	CLA	CHD-C1D-ND	-2.54	121.23	124.80
18	A	837	CLA	C2C-C1C-NC	2.54	112.65	109.98
18	B	835	CLA	C4B-CHC-C1C	2.54	132.22	126.25
18	A	802	CLA	CAA-C2A-C3A	-2.54	106.14	113.00
30	4	318	CHL	C1-C2-C3	-2.54	122.04	126.20
18	A	832	CLA	C4B-CHC-C1C	2.54	132.22	126.25
18	2	307	CLA	C4B-CHC-C1C	2.54	132.22	126.25
18	4	311	CLA	C1C-C2C-C3C	-2.54	104.31	106.98
18	K	1403	CLA	CHA-C4D-ND	2.54	137.78	132.55
18	A	811	CLA	C3B-C4B-NB	-2.54	108.27	110.53
21	4	301	BCR	C37-C22-C23	2.54	121.96	118.09
18	4	305	CLA	C2C-C1C-NC	2.54	112.65	109.98
29	3	303	LUT	C10-C11-C12	-2.54	115.85	123.20
18	A	830	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
18	B	805	CLA	C2C-C1C-NC	2.54	112.64	109.98

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	805	CLA	CAA-C2A-C3A	-2.53	106.15	113.00
17	A	801	CL0	O1D-CGD-CBD	-2.53	120.88	124.72
18	2	326	CLA	CHA-C4D-ND	2.53	137.78	132.55
18	A	835	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
18	A	836	CLA	C2C-C1C-NC	2.53	112.64	109.98
18	B	837	CLA	C2C-C1C-NC	2.53	112.64	109.98
18	2	307	CLA	O2A-CGA-CBA	2.53	119.56	111.83
18	A	805	CLA	C2C-C1C-NC	2.53	112.64	109.98
18	A	805	CLA	CMD-C2D-C3D	-2.53	121.88	127.69
18	B	819	CLA	CHD-C1D-ND	-2.53	121.24	124.80
18	B	822	CLA	C4B-CHC-C1C	2.53	132.20	126.25
18	B	807	CLA	C2C-C1C-NC	2.53	112.64	109.98
18	A	824	CLA	C4B-CHC-C1C	2.53	132.19	126.25
18	1	5018	CLA	C3B-C4B-NB	-2.53	108.27	110.53
30	3	312	CHL	C4D-CHA-CBD	-2.53	106.42	108.97
18	L	306	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
18	4	309	CLA	CHA-C4D-ND	2.53	137.76	132.55
18	A	816	CLA	C3B-C4B-NB	-2.53	108.28	110.53
18	A	826	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
18	2	310	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
18	A	809	CLA	C1C-C2C-C3C	-2.52	104.33	106.98
18	4	306	CLA	CHA-C4D-ND	2.52	137.75	132.55
18	B	829	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
21	A	843	BCR	C36-C18-C17	-2.52	118.73	122.82
18	A	821	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
18	A	829	CLA	CHA-C4D-ND	2.52	137.75	132.55
18	A	837	CLA	C1C-C2C-C3C	-2.52	104.33	106.98
18	1	5015	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
18	B	818	CLA	C1-C2-C3	-2.52	122.07	126.20
18	B	828	CLA	CHA-C4D-ND	2.52	137.75	132.55
18	3	307	CLA	C4B-CHC-C1C	2.52	132.17	126.25
18	A	807	CLA	C4B-CHC-C1C	2.52	132.17	126.25
21	L	307	BCR	C8-C7-C6	-2.52	120.27	127.00
18	J	1101	CLA	O2A-CGA-CBA	2.52	119.51	111.83
18	B	820	CLA	C2C-C1C-NC	2.52	112.63	109.98
18	B	838	CLA	C3B-C4B-NB	-2.52	108.28	110.53
18	3	309	CLA	CHA-C4D-ND	2.52	137.74	132.55
18	A	824	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
21	B	844	BCR	C34-C9-C10	-2.51	118.74	122.82
18	1	5006	CLA	CHD-C1D-ND	-2.51	121.26	124.80
18	A	805	CLA	C4B-CHC-C1C	2.51	132.16	126.25
18	4	305	CLA	C1C-C2C-C3C	-2.51	104.34	106.98

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	5006	CLA	C2C-C1C-NC	2.51	112.62	109.98
29	2	303	LUT	C35-C34-C33	-2.51	123.75	127.28
18	2	313	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
30	4	318	CHL	CMA-C3A-C4A	2.51	120.02	114.61
21	F	305	BCR	C27-C26-C25	-2.51	119.31	122.70
18	B	811	CLA	CHA-C4D-ND	2.51	137.73	132.55
18	B	808	CLA	CMA-C3A-C4A	2.51	118.52	111.77
18	A	836	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
18	B	811	CLA	CMD-C2D-C3D	-2.51	121.93	127.69
18	3	317	CLA	CHD-C1D-ND	-2.51	121.27	124.80
18	2	307	CLA	CHA-C4D-ND	2.51	137.72	132.55
18	B	822	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
29	3	303	LUT	C7-C8-C9	-2.51	122.53	126.23
18	3	308	CLA	C4B-CHC-C1C	2.51	132.14	126.25
18	1	5017	CLA	CMD-C2D-C3D	-2.51	121.94	127.69
18	B	838	CLA	CMA-C3A-C4A	2.51	118.51	111.77
18	3	311	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
18	J	1103	CLA	C3B-C4B-NB	-2.51	108.29	110.53
18	L	305	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
18	2	309	CLA	CHD-C1D-ND	-2.51	121.28	124.80
18	A	834	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
18	A	820	CLA	CHA-C4D-ND	2.50	137.72	132.55
18	4	312	CLA	CHD-C1D-ND	-2.50	121.28	124.80
18	B	811	CLA	C1C-C2C-C3C	-2.50	104.35	106.98
18	1	5006	CLA	CMD-C2D-C3D	-2.50	121.95	127.69
18	3	307	CLA	C1C-C2C-C3C	-2.50	104.35	106.98
18	B	821	CLA	CHA-C4D-ND	2.50	137.71	132.55
18	B	805	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
18	A	835	CLA	C1D-ND-C4D	-2.50	104.56	106.31
18	B	803	CLA	CHA-C4D-ND	2.50	137.71	132.55
18	A	810	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
21	3	305	BCR	C35-C13-C12	2.50	121.91	118.09
21	B	847	BCR	C35-C13-C12	2.50	121.91	118.09
18	B	811	CLA	CMA-C3A-C4A	2.50	118.49	111.77
18	B	837	CLA	CMA-C3A-C4A	2.50	118.49	111.77
18	B	816	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
18	A	817	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
18	3	318	CLA	C1C-C2C-C3C	-2.50	104.35	106.98
18	A	853	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
18	B	839	CLA	O2D-CGD-O1D	-2.49	118.99	123.85
18	F	301	CLA	C4B-CHC-C1C	2.49	132.11	126.25
18	A	823	CLA	CHA-C4D-ND	2.49	137.69	132.55

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	841	CLA	C4B-CHC-C1C	2.49	132.11	126.25
19	A	841	PQN	C2M-C2-C3	-2.49	120.35	124.45
18	B	801	CLA	CHA-C4D-ND	2.49	137.69	132.55
30	2	318	CHL	CMA-C3A-C4A	2.49	119.98	114.61
21	A	847	BCR	C8-C7-C6	-2.49	120.34	127.00
18	1	5008	CLA	C3B-C4B-NB	-2.49	108.31	110.53
18	1	5009	CLA	C4B-CHC-C1C	2.49	132.10	126.25
18	A	831	CLA	CHD-C1D-ND	-2.49	121.30	124.80
18	F	301	CLA	C2C-C1C-NC	2.49	112.60	109.98
21	3	306	BCR	C8-C9-C10	2.49	122.93	119.01
18	A	830	CLA	O2A-CGA-CBA	2.49	119.42	111.83
31	2	304	XAT	C18-C5-C6	-2.49	118.21	122.30
18	1	5011	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
18	B	815	CLA	O2A-CGA-CBA	2.49	119.42	111.83
18	B	831	CLA	CHA-C4D-ND	2.49	137.68	132.55
29	1	5004	LUT	C31-C32-C33	-2.49	119.54	126.36
24	G	1607	LMG	O7-C10-C11	2.49	120.06	110.93
18	F	301	CLA	C1D-ND-C4D	-2.49	104.57	106.31
18	B	818	CLA	C4B-CHC-C1C	2.49	132.09	126.25
18	A	824	CLA	C1C-C2C-C3C	-2.49	104.37	106.98
18	A	817	CLA	CHD-C1D-ND	-2.49	121.31	124.80
18	B	838	CLA	CHD-C1D-ND	-2.49	121.31	124.80
18	A	825	CLA	C4B-CHC-C1C	2.48	132.09	126.25
23	2	325	LMT	C2'-C3'-C4'	2.48	115.32	109.68
18	A	819	CLA	CHA-C4D-ND	2.48	137.67	132.55
18	A	809	CLA	C2C-C1C-NC	2.48	112.59	109.98
18	A	852	CLA	CHA-C4D-ND	2.48	137.67	132.55
30	2	315	CHL	CMA-C3A-C4A	2.48	119.96	114.61
18	B	803	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
18	2	313	CLA	CHD-C1D-ND	-2.48	121.31	124.80
18	3	308	CLA	CHA-C4D-ND	2.48	137.67	132.55
18	1	5009	CLA	C1C-C2C-C3C	-2.48	104.37	106.98
18	F	303	CLA	C1D-ND-C4D	-2.48	104.57	106.31
18	3	307	CLA	C1-O2A-CGA	2.48	122.66	116.65
21	A	843	BCR	C12-C13-C14	-2.48	115.11	119.01
18	A	802	CLA	C2C-C1C-NC	2.48	112.59	109.98
17	A	801	CL0	O2D-CGD-O1D	-2.48	119.02	123.85
18	F	302	CLA	CMA-C3A-C4A	2.48	118.44	111.77
18	B	818	CLA	C3B-C4B-NB	-2.48	108.32	110.53
18	1	5009	CLA	CHD-C1D-ND	-2.48	121.32	124.80
24	1	5001	LMG	C8-O7-C10	-2.48	111.87	117.80
18	B	826	CLA	CHA-C4D-ND	2.48	137.66	132.55

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	306	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
18	1	5009	CLA	C2C-C1C-NC	2.48	112.58	109.98
18	A	837	CLA	CHD-C1D-ND	-2.48	121.32	124.80
18	3	319	CLA	CHD-C1D-ND	-2.48	121.32	124.80
21	4	301	BCR	C36-C18-C17	-2.48	118.81	122.82
18	1	5012	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
18	3	317	CLA	C2C-C1C-NC	2.48	112.58	109.98
18	A	834	CLA	CMA-C3A-C4A	2.48	118.43	111.77
18	L	305	CLA	O2A-CGA-CBA	2.47	119.38	111.83
18	G	1602	CLA	CHA-C4D-ND	2.47	137.66	132.55
26	F	309	DGD	O1G-C1A-C2A	2.47	119.38	111.83
21	1	5005	BCR	C33-C5-C4	2.47	118.87	113.60
18	B	822	CLA	CHD-C1D-ND	-2.47	121.32	124.80
18	2	306	CLA	C1-O2A-CGA	2.47	122.64	116.65
18	2	313	CLA	C3B-C4B-NB	-2.47	108.32	110.53
18	1	5011	CLA	CHA-C4D-ND	2.47	137.65	132.55
18	G	1601	CLA	C4B-CHC-C1C	2.47	132.06	126.25
18	4	315	CLA	CHD-C1D-ND	-2.47	121.32	124.80
21	L	303	BCR	C23-C22-C21	2.47	122.90	119.01
18	A	812	CLA	C1D-ND-C4D	-2.47	104.58	106.31
18	A	815	CLA	CHD-C1D-ND	-2.47	121.32	124.80
18	1	5017	CLA	C1C-C2C-C3C	-2.47	104.38	106.98
21	K	1405	BCR	C34-C9-C10	-2.47	118.81	122.82
18	A	837	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
18	B	820	CLA	CHD-C1D-ND	-2.47	121.33	124.80
18	J	1103	CLA	CHA-C4D-ND	2.47	137.65	132.55
18	3	319	CLA	C4B-CHC-C1C	2.47	132.06	126.25
18	3	317	CLA	C1C-C2C-C3C	-2.47	104.38	106.98
18	2	309	CLA	CHA-C4D-ND	2.47	137.65	132.55
18	A	825	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
18	1	5009	CLA	CHA-C4D-ND	2.47	137.64	132.55
18	B	817	CLA	CHD-C1D-ND	-2.47	121.33	124.80
18	K	1401	CLA	CHD-C1D-ND	-2.47	121.33	124.80
18	A	827	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
23	4	319	LMT	C3'-C4'-C5'	-2.47	105.46	110.93
18	B	815	CLA	CHA-C4D-ND	2.47	137.64	132.55
18	1	5012	CLA	CHA-C4D-ND	2.47	137.64	132.55
18	B	820	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
18	L	301	CLA	C1C-C2C-C3C	-2.47	104.39	106.98
18	A	834	CLA	CHA-C4D-ND	2.47	137.64	132.55
18	A	807	CLA	CMA-C3A-C4A	2.47	118.40	111.77
18	4	308	CLA	C4B-CHC-C1C	2.46	132.04	126.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	2	319	CHL	C4D-CHA-CBD	-2.46	106.48	108.97
18	B	834	CLA	C4B-CHC-C1C	2.46	132.04	126.25
18	3	307	CLA	C2C-C1C-NC	2.46	112.57	109.98
18	A	852	CLA	CHD-C1D-ND	-2.46	121.33	124.80
18	B	807	CLA	CHA-C4D-ND	2.46	137.63	132.55
30	4	302	CHL	C1-C2-C3	-2.46	122.16	126.20
18	A	813	CLA	O2A-CGA-CBA	2.46	119.34	111.83
30	4	314	CHL	C1-O2A-CGA	2.46	122.61	116.65
18	A	822	CLA	CMD-C2D-C3D	-2.46	122.05	127.69
18	A	819	CLA	CHD-C1D-ND	-2.46	121.34	124.80
21	L	303	BCR	C37-C22-C21	-2.46	118.83	122.82
18	2	306	CLA	C4B-CHC-C1C	2.46	132.03	126.25
18	B	807	CLA	CHD-C1D-ND	-2.46	121.34	124.80
18	A	818	CLA	CHA-C4D-ND	2.46	137.62	132.55
18	1	5013	CLA	CHA-C4D-ND	2.46	137.62	132.55
18	1	5007	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
18	B	836	CLA	CHA-C4D-ND	2.46	137.62	132.55
18	3	318	CLA	CHA-C4D-ND	2.46	137.62	132.55
18	2	309	CLA	C3B-C4B-NB	-2.46	108.34	110.53
18	B	827	CLA	C4B-CHC-C1C	2.46	132.03	126.25
18	3	307	CLA	CHA-C4D-ND	2.46	137.62	132.55
18	2	312	CLA	CHA-C4D-ND	2.46	137.62	132.55
18	B	841	CLA	C3B-C4B-NB	-2.46	108.34	110.53
18	2	313	CLA	O2A-CGA-CBA	2.46	119.33	111.83
18	H	1701	CLA	CHA-C4D-ND	2.46	137.62	132.55
18	B	804	CLA	CHA-C4D-ND	2.46	137.62	132.55
18	1	5010	CLA	CHA-C4D-ND	2.46	137.62	132.55
18	A	813	CLA	CHD-C1D-ND	-2.45	121.35	124.80
30	2	316	CHL	CMA-C3A-C4A	2.45	119.90	114.61
18	A	828	CLA	O2A-CGA-CBA	2.45	119.32	111.83
18	4	305	CLA	C4B-CHC-C1C	2.45	132.02	126.25
18	B	804	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
18	2	310	CLA	CHD-C1D-ND	-2.45	121.35	124.80
18	A	805	CLA	CHA-C4D-ND	2.45	137.61	132.55
18	B	826	CLA	C1C-C2C-C3C	-2.45	104.40	106.98
18	4	312	CLA	CMD-C2D-C3D	-2.45	122.07	127.69
18	4	309	CLA	C1C-C2C-C3C	-2.45	104.40	106.98
18	K	1403	CLA	CHD-C1D-ND	-2.45	121.35	124.80
18	2	306	CLA	C1D-ND-C4D	-2.45	104.59	106.31
18	1	5018	CLA	CHA-C4D-ND	2.45	137.60	132.55
18	A	820	CLA	O2A-CGA-CBA	2.45	119.30	111.83
18	B	817	CLA	C1D-ND-C4D	-2.45	104.59	106.31

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	314	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
18	2	311	CLA	CHD-C1D-ND	-2.45	121.36	124.80
18	B	833	CLA	C1C-C2C-C3C	-2.45	104.41	106.98
18	B	801	CLA	CMA-C3A-C4A	2.45	118.35	111.77
18	4	310	CLA	CHA-C4D-ND	2.45	137.60	132.55
18	A	816	CLA	O2A-CGA-CBA	2.45	119.30	111.83
18	B	826	CLA	C3B-C4B-NB	-2.45	108.35	110.53
18	L	301	CLA	O2A-CGA-CBA	2.45	119.29	111.83
18	B	809	CLA	CHA-C4D-ND	2.45	137.59	132.55
18	2	309	CLA	C4B-CHC-C1C	2.45	132.00	126.25
18	G	1601	CLA	CHA-C4D-ND	2.44	137.59	132.55
18	4	307	CLA	CHA-C4D-ND	2.44	137.59	132.55
21	1	5005	BCR	C37-C22-C23	2.44	121.82	118.09
18	2	308	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
21	B	845	BCR	C33-C5-C4	2.44	118.81	113.60
18	1	5007	CLA	CHA-C4D-ND	2.44	137.59	132.55
18	A	810	CLA	C4B-CHC-C1C	2.44	131.99	126.25
18	B	833	CLA	CHA-C4D-ND	2.44	137.59	132.55
18	A	833	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
18	A	840	CLA	CHA-C4D-ND	2.44	137.59	132.55
21	A	843	BCR	C27-C26-C25	-2.44	119.41	122.70
18	B	828	CLA	CHD-C1D-ND	-2.44	121.37	124.80
18	B	833	CLA	O2A-CGA-CBA	2.44	119.28	111.83
18	B	817	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
18	L	301	CLA	C2C-C1C-NC	2.44	112.55	109.98
18	2	317	CLA	CHA-C4D-ND	2.44	137.58	132.55
18	A	806	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
18	B	808	CLA	CHD-C1D-ND	-2.44	121.37	124.80
18	3	307	CLA	CHD-C1D-ND	-2.44	121.37	124.80
18	K	1404	CLA	CHA-C4D-ND	2.44	137.58	132.55
18	3	319	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
28	F	310	ZEX	C8-C7-C6	-2.44	120.48	127.00
18	A	828	CLA	O1D-CGD-CBD	-2.44	119.71	124.52
18	B	813	CLA	CHA-C4D-ND	2.44	137.58	132.55
18	1	5006	CLA	CHA-C4D-ND	2.44	137.58	132.55
18	A	853	CLA	CHD-C1D-ND	-2.44	121.37	124.80
18	B	837	CLA	C3B-C4B-NB	-2.44	108.36	110.53
30	2	315	CHL	C4D-CHA-CBD	-2.44	106.51	108.97
23	B	852	LMT	O5B-C5B-C4B	2.44	114.09	109.70
18	A	835	CLA	CHD-C1D-ND	-2.44	121.38	124.80
18	F	302	CLA	C4B-CHC-C1C	2.44	131.97	126.25
18	A	837	CLA	CHA-C4D-ND	2.43	137.57	132.55

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	822	CLA	CHD-C1D-ND	-2.43	121.38	124.80
21	2	305	BCR	C1-C6-C7	2.43	122.25	115.65
18	2	306	CLA	CHD-C1D-ND	-2.43	121.38	124.80
18	A	806	CLA	C4B-CHC-C1C	2.43	131.97	126.25
18	L	305	CLA	C4B-CHC-C1C	2.43	131.97	126.25
29	2	303	LUT	C39-C29-C28	2.43	121.81	118.09
18	3	301	CLA	C4B-CHC-C1C	2.43	131.97	126.25
18	J	1101	CLA	CHD-C1D-ND	-2.43	121.38	124.80
18	B	826	CLA	C4B-CHC-C1C	2.43	131.97	126.25
18	F	302	CLA	CHA-C4D-ND	2.43	137.57	132.55
18	4	305	CLA	CHA-C4D-ND	2.43	137.57	132.55
18	B	810	CLA	CHA-C4D-ND	2.43	137.56	132.55
18	B	815	CLA	C4B-CHC-C1C	2.43	131.96	126.25
18	J	1101	CLA	CHA-C4D-ND	2.43	137.56	132.55
18	B	814	CLA	C1C-C2C-C3C	-2.43	104.42	106.98
21	4	301	BCR	C30-C25-C24	2.43	122.24	115.65
29	3	303	LUT	C35-C15-C14	-2.43	118.55	123.52
18	A	822	CLA	CHA-C4D-ND	2.43	137.56	132.55
18	F	301	CLA	C3B-C4B-NB	-2.43	108.36	110.53
18	A	823	CLA	CHD-C1D-ND	-2.43	121.39	124.80
18	A	827	CLA	O2A-CGA-CBA	2.43	119.24	111.83
18	F	301	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
18	A	808	CLA	CHA-C4D-ND	2.43	137.56	132.55
18	3	308	CLA	O2A-CGA-CBA	2.43	119.24	111.83
18	A	839	CLA	C3B-C4B-NB	-2.43	108.36	110.53
18	B	816	CLA	C4B-CHC-C1C	2.43	131.95	126.25
29	4	303	LUT	C11-C10-C9	-2.43	123.88	127.28
18	A	821	CLA	CAA-C2A-C3A	-2.43	106.44	113.00
18	4	308	CLA	CHD-C1D-ND	-2.43	121.39	124.80
18	L	301	CLA	C3B-C4B-NB	-2.43	108.36	110.53
21	A	846	BCR	C19-C18-C17	2.42	122.82	119.01
18	B	841	CLA	C1D-ND-C4D	-2.42	104.61	106.31
18	4	312	CLA	C4B-CHC-C1C	2.42	131.95	126.25
18	4	308	CLA	CHA-C4D-ND	2.42	137.55	132.55
21	A	845	BCR	C31-C1-C6	-2.42	106.44	110.24
18	A	803	CLA	CHA-C4D-ND	2.42	137.55	132.55
18	B	831	CLA	C3B-C4B-NB	-2.42	108.37	110.53
18	B	824	CLA	CHA-C4D-ND	2.42	137.55	132.55
21	G	1604	BCR	C19-C18-C17	2.42	122.82	119.01
18	B	826	CLA	CHD-C1D-ND	-2.42	121.39	124.80
18	A	828	CLA	CHD-C1D-ND	-2.42	121.39	124.80
18	1	5006	CLA	C3B-C4B-NB	-2.42	108.37	110.53

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	315	CLA	C4B-CHC-C1C	2.42	131.94	126.25
18	A	820	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
18	B	818	CLA	O2A-CGA-CBA	2.42	119.22	111.83
18	4	312	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
21	2	305	BCR	C38-C26-C27	2.42	118.76	113.60
18	B	823	CLA	CHA-C4D-ND	2.42	137.54	132.55
18	B	812	CLA	CHD-C1D-ND	-2.42	121.40	124.80
18	2	317	CLA	CHD-C1D-ND	-2.42	121.40	124.80
21	B	845	BCR	C29-C28-C27	2.42	116.60	111.28
18	B	822	CLA	CHA-C4D-ND	2.42	137.54	132.55
18	1	5010	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
18	B	828	CLA	C3B-C4B-NB	-2.42	108.37	110.53
18	A	816	CLA	CHA-C4D-ND	2.42	137.54	132.55
18	F	302	CLA	C1-C2-C3	-2.42	122.23	126.20
18	H	1701	CLA	CMA-C3A-C4A	2.42	118.28	111.77
18	K	1402	CLA	CHA-C4D-ND	2.42	137.54	132.55
28	F	310	ZEX	C7-C8-C9	-2.42	122.66	126.23
18	B	820	CLA	CHA-C4D-ND	2.42	137.54	132.55
18	J	1103	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
18	A	805	CLA	CHD-C1D-ND	-2.42	121.40	124.80
26	B	855	DGD	C2G-O2G-C1B	-2.42	112.01	117.80
18	A	814	CLA	CHA-C4D-ND	2.42	137.53	132.55
18	B	832	CLA	O2A-CGA-CBA	2.42	119.20	111.83
18	A	833	CLA	CHA-C4D-ND	2.41	137.53	132.55
18	G	1602	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
21	B	802	BCR	C33-C5-C4	2.41	118.74	113.60
21	A	845	BCR	C33-C5-C4	2.41	118.74	113.60
18	B	808	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
18	B	839	CLA	CHA-C4D-ND	2.41	137.53	132.55
18	1	5015	CLA	CHA-C4D-ND	2.41	137.53	132.55
18	B	832	CLA	C1C-C2C-C3C	-2.41	104.44	106.98
18	2	306	CLA	C1C-C2C-C3C	-2.41	104.44	106.98
18	F	301	CLA	CHD-C1D-ND	-2.41	121.41	124.80
18	J	1101	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
21	L	303	BCR	C33-C5-C4	2.41	118.74	113.60
18	B	837	CLA	C1D-ND-C4D	-2.41	104.62	106.31
18	A	840	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
18	A	807	CLA	CHA-C4D-ND	2.41	137.52	132.55
18	3	317	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
18	A	804	CLA	CHA-C4D-ND	2.41	137.52	132.55
18	B	805	CLA	CHA-C4D-ND	2.41	137.52	132.55
21	J	1104	BCR	C33-C5-C4	2.41	118.73	113.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	806	CLA	CHD-C1D-ND	-2.41	121.41	124.80
18	B	818	CLA	CHA-C4D-ND	2.41	137.52	132.55
18	B	825	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
18	1	5013	CLA	CHD-C1D-ND	-2.41	121.41	124.80
18	B	826	CLA	CMD-C2D-C3D	-2.41	122.17	127.69
18	K	1401	CLA	C4B-CHC-C1C	2.41	131.91	126.25
18	L	306	CLA	C4B-CHC-C1C	2.41	131.91	126.25
17	A	801	CL0	C4C-CHD-C1D	2.41	124.68	116.07
18	B	837	CLA	CMD-C2D-C3D	-2.41	122.17	127.69
18	B	804	CLA	CMA-C3A-C4A	2.41	118.24	111.77
18	4	315	CLA	CAA-C2A-C3A	-2.41	106.50	113.00
18	A	821	CLA	C4B-CHC-C1C	2.41	131.91	126.25
18	A	821	CLA	CHA-C4D-ND	2.41	137.51	132.55
18	G	1603	CLA	CHA-C4D-ND	2.41	137.51	132.55
18	L	305	CLA	C2C-C1C-NC	2.41	112.51	109.98
18	K	1401	CLA	CHA-C4D-ND	2.41	137.51	132.55
18	A	809	CLA	C4B-CHC-C1C	2.40	131.90	126.25
18	A	834	CLA	C4B-CHC-C1C	2.40	131.90	126.25
18	A	838	CLA	CHA-C4D-ND	2.40	137.51	132.55
18	B	814	CLA	CHA-C4D-ND	2.40	137.51	132.55
18	B	832	CLA	CHD-C1D-ND	-2.40	121.42	124.80
18	B	818	CLA	CHD-C1D-ND	-2.40	121.42	124.80
18	3	311	CLA	CMD-C2D-C3D	-2.40	122.18	127.69
18	B	832	CLA	C4B-CHC-C1C	2.40	131.90	126.25
21	2	305	BCR	C1-C6-C5	-2.40	119.35	122.64
18	A	819	CLA	C4B-CHC-C1C	2.40	131.90	126.25
21	B	845	BCR	C8-C7-C6	-2.40	120.58	127.00
21	B	843	BCR	C30-C25-C26	-2.40	119.35	122.64
18	2	317	CLA	C4B-CHC-C1C	2.40	131.90	126.25
18	2	310	CLA	CHA-C4D-ND	2.40	137.50	132.55
18	A	806	CLA	CHD-C1D-ND	-2.40	121.42	124.80
22	2	320	LHG	C5-O7-C7	-2.40	112.05	117.80
18	G	1603	CLA	CHD-C1D-ND	-2.40	121.42	124.80
18	B	817	CLA	C1C-C2C-C3C	-2.40	104.46	106.98
18	1	5018	CLA	C4B-CHC-C1C	2.40	131.89	126.25
18	B	817	CLA	C4B-CHC-C1C	2.40	131.89	126.25
18	3	314	CLA	CHA-C4D-ND	2.40	137.50	132.55
18	2	311	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
18	2	308	CLA	C3B-C4B-NB	-2.40	108.39	110.53
18	A	852	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
21	B	847	BCR	C23-C22-C21	-2.40	115.24	119.01
18	B	819	CLA	C4B-CHC-C1C	2.40	131.89	126.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	839	CLA	C4B-CHC-C1C	2.40	131.89	126.25
18	K	1403	CLA	C4B-CHC-C1C	2.40	131.89	126.25
18	H	1701	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
18	4	312	CLA	CHA-C4D-ND	2.40	137.49	132.55
18	K	1401	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
18	B	805	CLA	CHD-C1D-ND	-2.40	121.43	124.80
18	A	828	CLA	CHA-C4D-ND	2.40	137.49	132.55
21	4	301	BCR	C8-C7-C6	-2.40	120.60	127.00
18	B	812	CLA	C1D-ND-C4D	-2.40	104.63	106.31
18	A	836	CLA	CHD-C1D-ND	-2.40	121.43	124.80
18	A	831	CLA	CHA-C4D-ND	2.40	137.49	132.55
18	1	5010	CLA	C4B-CHC-C1C	2.40	131.88	126.25
18	3	319	CLA	CHA-C4D-ND	2.39	137.49	132.55
18	L	304	CLA	CHD-C1D-ND	-2.39	121.43	124.80
18	B	805	CLA	C4B-CHC-C1C	2.39	131.88	126.25
18	4	307	CLA	C4B-CHC-C1C	2.39	131.88	126.25
18	1	5018	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
18	2	317	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
29	3	304	LUT	C20-C13-C12	2.39	121.75	118.09
18	2	313	CLA	CHA-C4D-ND	2.39	137.49	132.55
23	B	856	LMT	O1'-C1'-C2'	2.39	111.91	108.27
18	K	1401	CLA	C1D-ND-C4D	-2.39	104.63	106.31
30	3	313	CHL	CMA-C3A-C4A	2.39	119.77	114.61
18	1	5011	CLA	C4B-CHC-C1C	2.39	131.87	126.25
18	A	833	CLA	CHD-C1D-ND	-2.39	121.44	124.80
18	A	817	CLA	C3B-C4B-NB	-2.39	108.39	110.53
18	B	834	CLA	O2A-CGA-CBA	2.39	119.13	111.83
18	A	824	CLA	O2A-CGA-CBA	2.39	119.13	111.83
18	A	834	CLA	CHD-C1D-ND	-2.39	121.44	124.80
18	A	812	CLA	C4B-CHC-C1C	2.39	131.87	126.25
29	3	303	LUT	C11-C10-C9	-2.39	123.92	127.28
18	A	807	CLA	O1D-CGD-CBD	-2.39	119.80	124.52
18	A	839	CLA	CHA-C4D-ND	2.39	137.48	132.55
18	A	814	CLA	CHD-C1D-ND	-2.39	121.44	124.80
18	B	806	CLA	CMA-C3A-C4A	2.39	118.20	111.77
18	B	829	CLA	CHA-C4D-ND	2.39	137.48	132.55
18	A	810	CLA	CMD-C2D-C3D	-2.39	122.21	127.69
18	1	5013	CLA	C3B-C4B-NB	-2.39	108.40	110.53
18	4	307	CLA	CHD-C1D-ND	-2.39	121.44	124.80
18	F	301	CLA	C1C-C2C-C3C	-2.39	104.47	106.98
30	3	316	CHL	C4D-CHA-CBD	-2.39	106.56	108.97
21	L	302	BCR	C35-C13-C12	2.39	121.74	118.09

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	5006	CLA	C1C-C2C-C3C	-2.39	104.47	106.98
21	F	305	BCR	C38-C26-C27	2.39	118.69	113.60
18	L	301	CLA	C4B-CHC-C1C	2.39	131.86	126.25
18	A	832	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
18	B	823	CLA	O2A-CGA-CBA	2.39	119.11	111.83
18	4	305	CLA	CHD-C1D-ND	-2.39	121.44	124.80
18	B	827	CLA	C1C-C2C-C3C	-2.39	104.47	106.98
18	K	1403	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
18	1	5007	CLA	C1D-ND-C4D	-2.39	104.64	106.31
18	A	837	CLA	C4B-CHC-C1C	2.39	131.86	126.25
18	A	809	CLA	CMD-C2D-C3D	-2.39	122.22	127.69
18	G	1601	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
18	F	303	CLA	CHA-C4D-ND	2.39	137.47	132.55
18	3	301	CLA	CHA-C4D-ND	2.39	137.47	132.55
18	1	5015	CLA	C4B-CHC-C1C	2.38	131.85	126.25
18	A	832	CLA	CHA-C4D-ND	2.38	137.47	132.55
18	B	835	CLA	CHA-C4D-ND	2.38	137.47	132.55
18	B	807	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
18	B	840	CLA	CHA-C4D-ND	2.38	137.47	132.55
21	3	306	BCR	C34-C9-C10	-2.38	118.95	122.82
18	2	326	CLA	CMA-C3A-C4A	2.38	118.18	111.77
18	2	312	CLA	O2A-CGA-CBA	2.38	119.10	111.83
18	L	305	CLA	C1D-ND-C4D	-2.38	104.64	106.31
18	3	315	CLA	CHD-C1D-ND	-2.38	121.45	124.80
18	A	817	CLA	C4B-CHC-C1C	2.38	131.85	126.25
18	B	812	CLA	CAA-C2A-C3A	-2.38	106.56	113.00
18	B	808	CLA	C4B-CHC-C1C	2.38	131.85	126.25
18	L	301	CLA	CHA-C4D-ND	2.38	137.46	132.55
18	L	304	CLA	CHA-C4D-ND	2.38	137.46	132.55
18	3	311	CLA	C4B-CHC-C1C	2.38	131.85	126.25
18	A	806	CLA	CHA-C4D-ND	2.38	137.46	132.55
18	1	5009	CLA	C3B-C4B-NB	-2.38	108.40	110.53
18	A	829	CLA	CMA-C3A-C4A	2.38	118.17	111.77
18	A	811	CLA	CHA-C4D-ND	2.38	137.46	132.55
18	B	841	CLA	C1C-C2C-C3C	-2.38	104.48	106.98
18	B	824	CLA	C4B-CHC-C1C	2.38	131.84	126.25
18	A	816	CLA	C4B-CHC-C1C	2.38	131.84	126.25
18	B	824	CLA	CMD-C2D-C3D	-2.38	122.23	127.69
18	4	310	CLA	C4B-CHC-C1C	2.38	131.84	126.25
21	G	1604	BCR	C36-C18-C17	-2.38	118.96	122.82
18	B	839	CLA	CHD-C1D-ND	-2.38	121.46	124.80
18	B	808	CLA	CHA-C4D-ND	2.38	137.46	132.55

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	310	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
18	4	306	CLA	C4B-CHC-C1C	2.38	131.84	126.25
18	B	807	CLA	C4B-CHC-C1C	2.38	131.84	126.25
18	4	307	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
18	B	819	CLA	CHA-C4D-ND	2.38	137.45	132.55
18	B	833	CLA	C4B-CHC-C1C	2.38	131.84	126.25
18	K	1402	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
18	A	817	CLA	CHA-C4D-ND	2.38	137.45	132.55
18	B	837	CLA	CHA-C4D-ND	2.38	137.45	132.55
18	A	838	CLA	C4B-CHC-C1C	2.38	131.83	126.25
18	A	802	CLA	CHD-C1D-ND	-2.38	121.46	124.80
18	B	801	CLA	CHD-C1D-ND	-2.38	121.46	124.80
18	1	5011	CLA	CHD-C1D-ND	-2.37	121.46	124.80
18	3	317	CLA	C4B-CHC-C1C	2.37	131.83	126.25
18	A	819	CLA	C1-C2-C3	-2.37	122.31	126.20
18	A	813	CLA	CHA-C4D-ND	2.37	137.45	132.55
18	4	315	CLA	CHA-C4D-ND	2.37	137.44	132.55
18	4	311	CLA	C1D-ND-C4D	-2.37	104.65	106.31
18	A	836	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
18	A	824	CLA	CHA-C4D-ND	2.37	137.44	132.55
18	B	830	CLA	CHD-C1D-ND	-2.37	121.47	124.80
18	4	311	CLA	CHA-C4D-ND	2.37	137.44	132.55
18	B	807	CLA	C3B-C4B-NB	-2.37	108.41	110.53
18	A	815	CLA	C1-O2A-CGA	2.37	122.39	116.65
18	A	803	CLA	CHD-C1D-ND	-2.37	121.47	124.80
18	A	804	CLA	C4B-CHC-C1C	2.37	131.82	126.25
18	2	310	CLA	C2D-C1D-ND	2.37	112.47	110.13
18	3	318	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
18	J	1101	CLA	C4B-CHC-C1C	2.37	131.81	126.25
18	A	808	CLA	C4B-CHC-C1C	2.37	131.81	126.25
18	2	313	CLA	CMD-C2D-C3D	-2.37	122.26	127.69
21	F	305	BCR	C36-C18-C19	2.37	121.70	118.09
18	F	301	CLA	C1-C2-C3	-2.37	122.32	126.20
18	G	1601	CLA	CMD-C2D-C3D	-2.37	122.26	127.69
21	A	845	BCR	C3-C4-C5	-2.37	109.83	114.06
18	A	815	CLA	CHA-C4D-ND	2.37	137.43	132.55
18	B	806	CLA	CHA-C4D-ND	2.37	137.43	132.55
18	A	853	CLA	C4B-CHC-C1C	2.37	131.81	126.25
21	B	844	BCR	C35-C13-C12	2.37	121.70	118.09
18	B	816	CLA	CHA-C4D-ND	2.37	137.43	132.55
18	B	806	CLA	C1D-ND-C4D	-2.37	104.65	106.31
18	A	840	CLA	CHD-C1D-ND	-2.37	121.47	124.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	829	CLA	O2A-CGA-CBA	2.37	119.05	111.83
18	B	837	CLA	C4B-CHC-C1C	2.37	131.81	126.25
21	3	306	BCR	C30-C25-C26	-2.36	119.40	122.64
18	B	832	CLA	CHA-C4D-ND	2.36	137.43	132.55
18	B	840	CLA	C3B-C4B-NB	-2.36	108.42	110.53
18	2	311	CLA	C1D-ND-C4D	-2.36	104.65	106.31
18	B	831	CLA	CMD-C2D-C3D	-2.36	122.27	127.69
18	L	304	CLA	CMD-C2D-C3D	-2.36	122.27	127.69
18	B	805	CLA	CMA-C3A-C4A	2.36	118.13	111.77
18	2	311	CLA	CHA-C4D-ND	2.36	137.43	132.55
21	3	305	BCR	C37-C22-C23	2.36	121.70	118.09
18	A	803	CLA	CMA-C3A-C4A	2.36	118.12	111.77
18	A	835	CLA	CHA-C4D-ND	2.36	137.42	132.55
18	A	831	CLA	C2C-C1C-NC	2.36	112.46	109.98
18	2	308	CLA	CHA-C4D-ND	2.36	137.42	132.55
29	4	303	LUT	C10-C11-C12	-2.36	116.36	123.20
18	1	5015	CLA	C3B-C4B-NB	-2.36	108.42	110.53
18	A	819	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
18	B	818	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
18	B	803	CLA	C4B-CHC-C1C	2.36	131.80	126.25
18	2	312	CLA	C4B-CHC-C1C	2.36	131.80	126.25
18	B	838	CLA	C4B-CHC-C1C	2.36	131.79	126.25
18	4	309	CLA	C3B-C4B-NB	-2.36	108.42	110.53
18	1	5011	CLA	CMD-C2D-C3D	-2.36	122.28	127.69
18	A	802	CLA	O2A-CGA-CBA	2.36	119.03	111.83
18	H	1701	CLA	CMD-C2D-C3D	-2.36	122.28	127.69
18	B	814	CLA	CHD-C1D-ND	-2.36	121.48	124.80
18	4	315	CLA	C4B-CHC-C1C	2.36	131.79	126.25
18	A	827	CLA	CHA-C4D-ND	2.36	137.41	132.55
18	A	832	CLA	C2C-C1C-NC	2.36	112.46	109.98
24	F	308	LMG	O8-C28-C29	2.36	119.02	111.83
21	A	855	BCR	C33-C5-C4	2.36	118.62	113.60
18	A	836	CLA	CHA-C4D-ND	2.36	137.41	132.55
18	L	306	CLA	CHA-C4D-ND	2.36	137.41	132.55
18	B	840	CLA	CHD-C1D-ND	-2.36	121.49	124.80
18	1	5015	CLA	CHD-C1D-ND	-2.36	121.49	124.80
18	4	305	CLA	CAA-C2A-C3A	-2.36	106.63	113.00
18	A	830	CLA	CHA-C4D-ND	2.36	137.41	132.55
30	2	315	CHL	C1-C2-C3	-2.36	122.34	126.20
31	2	304	XAT	C6-C7-C8	-2.36	121.01	125.99
18	F	302	CLA	O2D-CGD-O1D	-2.36	119.26	123.85
18	B	825	CLA	CMD-C2D-C3D	-2.35	122.29	127.69

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	839	CLA	CMD-C2D-C3D	-2.35	122.29	127.69
18	A	833	CLA	C4B-CHC-C1C	2.35	131.78	126.25
18	B	815	CLA	CMD-C2D-C3D	-2.35	122.29	127.69
18	A	826	CLA	C4B-CHC-C1C	2.35	131.78	126.25
23	2	325	LMT	O5B-C5B-C4B	2.35	113.94	109.70
18	B	822	CLA	O2A-CGA-CBA	2.35	119.01	111.83
18	B	841	CLA	C2C-C1C-NC	2.35	112.45	109.98
18	A	829	CLA	C4B-CHC-C1C	2.35	131.78	126.25
18	3	301	CLA	CHD-C1D-ND	-2.35	121.49	124.80
30	2	314	CHL	C4C-CHD-C1D	2.35	124.48	116.07
18	B	813	CLA	C4B-CHC-C1C	2.35	131.78	126.25
18	1	5008	CLA	C1D-ND-C4D	-2.35	104.66	106.31
21	A	843	BCR	C19-C18-C17	2.35	122.71	119.01
31	4	304	XAT	C6-C7-C8	-2.35	121.02	125.99
18	B	840	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
18	4	310	CLA	CHD-C1D-ND	-2.35	121.49	124.80
29	3	303	LUT	C22-C23-C24	-2.35	107.69	111.18
18	2	308	CLA	C4B-CHC-C1C	2.35	131.77	126.25
18	A	836	CLA	C1D-ND-C4D	-2.35	104.66	106.31
26	2	327	DGD	C3G-O3G-C1D	-2.35	108.76	113.80
18	B	836	CLA	C4B-CHC-C1C	2.35	131.77	126.25
18	3	314	CLA	C4B-CHC-C1C	2.35	131.77	126.25
21	I	102	BCR	C36-C18-C17	-2.35	119.01	122.82
21	A	847	BCR	C2-C1-C6	2.35	113.85	110.44
18	F	301	CLA	C2D-C1D-ND	2.35	112.45	110.13
18	B	838	CLA	CHA-C4D-ND	2.35	137.39	132.55
21	1	5005	BCR	C8-C9-C10	2.35	122.70	119.01
18	B	841	CLA	CHD-C1D-ND	-2.35	121.50	124.80
18	B	829	CLA	C4B-CHC-C1C	2.35	131.77	126.25
18	4	311	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
18	A	833	CLA	O2A-CGA-CBA	2.35	118.99	111.83
18	L	306	CLA	CHD-C1D-ND	-2.35	121.50	124.80
18	4	308	CLA	CMD-C2D-C3D	-2.35	122.31	127.69
18	A	810	CLA	CHA-C4D-ND	2.35	137.39	132.55
18	2	308	CLA	CHD-C1D-ND	-2.35	121.50	124.80
18	A	814	CLA	O2D-CGD-O1D	-2.34	119.28	123.85
18	K	1404	CLA	O2D-CGD-O1D	-2.34	119.28	123.85
18	B	835	CLA	C1-O2A-CGA	2.34	122.33	116.65
18	3	315	CLA	CHA-C4D-ND	2.34	137.38	132.55
18	A	807	CLA	CHD-C1D-ND	-2.34	121.51	124.80
18	3	317	CLA	CHA-C4D-ND	2.34	137.38	132.55
18	A	804	CLA	CHD-C1D-ND	-2.34	121.51	124.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	830	CLA	C4B-CHC-C1C	2.34	131.75	126.25
18	B	812	CLA	CHA-C4D-ND	2.34	137.38	132.55
18	A	822	CLA	C1D-ND-C4D	-2.34	104.67	106.31
18	G	1603	CLA	C4B-CHC-C1C	2.34	131.75	126.25
18	L	306	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
18	A	810	CLA	O2A-CGA-CBA	2.34	118.97	111.83
21	A	847	BCR	C33-C5-C6	-2.34	121.93	124.48
18	A	809	CLA	CHA-C4D-ND	2.34	137.38	132.55
31	4	304	XAT	C26-C27-C28	-2.34	121.05	125.99
18	A	820	CLA	C3B-C4B-NB	-2.34	108.44	110.53
18	B	831	CLA	C4B-CHC-C1C	2.34	131.75	126.25
18	A	815	CLA	C4B-CHC-C1C	2.34	131.75	126.25
18	B	820	CLA	C4B-CHC-C1C	2.34	131.75	126.25
18	A	812	CLA	CHA-C4D-ND	2.34	137.37	132.55
18	1	5015	CLA	CMD-C2D-C3D	-2.34	122.33	127.69
18	2	313	CLA	C4B-CHC-C1C	2.34	131.74	126.25
18	B	817	CLA	CHA-C4D-ND	2.34	137.37	132.55
21	K	1405	BCR	C1-C6-C5	-2.34	119.44	122.64
18	B	816	CLA	CAA-C2A-C3A	-2.34	106.68	113.00
18	1	5008	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
18	F	302	CLA	CHD-C1D-ND	-2.34	121.52	124.80
18	3	318	CLA	CMD-C2D-C3D	-2.34	122.33	127.69
18	B	825	CLA	CHD-C1D-ND	-2.34	121.52	124.80
18	G	1602	CLA	C4B-CHC-C1C	2.34	131.74	126.25
18	A	818	CLA	C3B-C4B-NB	-2.33	108.45	110.53
18	G	1601	CLA	CHD-C1D-ND	-2.33	121.52	124.80
18	A	837	CLA	O2A-CGA-CBA	2.33	118.95	111.83
18	2	310	CLA	C4B-CHC-C1C	2.33	131.73	126.25
18	K	1402	CLA	CHD-C1D-ND	-2.33	121.52	124.80
18	3	309	CLA	CHD-C1D-ND	-2.33	121.52	124.80
18	B	807	CLA	CMD-C2D-C3D	-2.33	122.34	127.69
18	B	820	CLA	CAA-C2A-C3A	-2.33	106.70	113.00
18	1	5017	CLA	C4B-CHC-C1C	2.33	131.72	126.25
18	2	306	CLA	CHA-C4D-ND	2.33	137.35	132.55
18	A	823	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
18	4	309	CLA	C4B-CHC-C1C	2.33	131.72	126.25
18	B	817	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
18	A	831	CLA	O1D-CGD-CBD	-2.33	119.93	124.52
18	A	819	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
18	A	827	CLA	C3B-C4B-NB	-2.33	108.45	110.53
18	4	307	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
18	B	832	CLA	O2D-CGD-O1D	-2.33	119.32	123.85

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	838	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
18	A	829	CLA	O2A-CGA-CBA	2.33	118.93	111.83
18	K	1401	CLA	C2D-C1D-ND	2.33	112.43	110.13
18	K	1402	CLA	CMD-C2D-C3D	-2.33	122.36	127.69
18	B	825	CLA	O2A-CGA-CBA	2.32	118.92	111.83
18	A	838	CLA	CHD-C1D-ND	-2.32	121.53	124.80
18	B	823	CLA	CHD-C1D-ND	-2.32	121.53	124.80
21	B	843	BCR	C33-C5-C4	2.32	118.55	113.60
18	H	1701	CLA	CHD-C1D-ND	-2.32	121.53	124.80
18	3	314	CLA	CHD-C1D-ND	-2.32	121.53	124.80
18	G	1603	CLA	C3B-C4B-NB	-2.32	108.46	110.53
18	2	306	CLA	C3B-C4B-NB	-2.32	108.46	110.53
18	F	302	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
18	B	824	CLA	CHD-C1D-ND	-2.32	121.54	124.80
18	F	303	CLA	CHD-C1D-ND	-2.32	121.54	124.80
18	B	825	CLA	CHA-C1A-NA	-2.32	121.14	126.39
18	B	806	CLA	O2A-CGA-CBA	2.32	118.91	111.83
18	2	311	CLA	C4B-CHC-C1C	2.32	131.71	126.25
21	B	802	BCR	C30-C25-C26	-2.32	119.46	122.64
21	B	846	BCR	C37-C22-C23	2.32	121.63	118.09
18	L	306	CLA	C1D-ND-C4D	-2.32	104.68	106.31
23	B	853	LMT	C2'-C3'-C4'	2.32	114.95	109.68
21	F	304	BCR	C33-C5-C4	2.32	118.54	113.60
18	4	310	CLA	O2A-CGA-CBA	2.32	118.91	111.83
18	1	5013	CLA	CMD-C2D-C3D	-2.32	122.37	127.69
18	H	1701	CLA	C4B-CHC-C1C	2.32	131.70	126.25
18	2	306	CLA	C2C-C1C-NC	2.32	112.42	109.98
18	1	5008	CLA	CHA-C4D-ND	2.32	137.33	132.55
18	A	838	CLA	CMD-C2D-C3D	-2.32	122.37	127.69
18	A	852	CLA	C4B-CHC-C1C	2.32	131.70	126.25
18	J	1101	CLA	CMA-C3A-C4A	2.32	118.00	111.77
18	A	827	CLA	C4B-CHC-C1C	2.32	131.70	126.25
18	A	835	CLA	CMD-C2D-C3D	-2.32	122.37	127.69
18	A	840	CLA	C4B-CHC-C1C	2.32	131.70	126.25
18	3	318	CLA	CHD-C1D-ND	-2.32	121.54	124.80
29	3	304	LUT	C7-C8-C9	-2.32	122.81	126.23
18	B	829	CLA	CHD-C1D-ND	-2.32	121.54	124.80
18	A	816	CLA	C2C-C1C-NC	2.32	112.42	109.98
18	2	311	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
18	1	5009	CLA	C1D-ND-C4D	-2.32	104.69	106.31
21	L	302	BCR	C30-C25-C26	-2.32	119.47	122.64
18	A	809	CLA	CAA-C2A-C3A	-2.32	106.74	113.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	304	CLA	C4B-CHC-C1C	2.32	131.69	126.25
18	F	301	CLA	CHA-C4D-ND	2.31	137.32	132.55
18	A	811	CLA	CHD-C1D-ND	-2.31	121.55	124.80
18	G	1602	CLA	CHD-C1D-ND	-2.31	121.55	124.80
18	1	5010	CLA	CMD-C2D-C3D	-2.31	122.38	127.69
18	4	315	CLA	O2D-CGD-O1D	-2.31	119.34	123.85
18	3	311	CLA	C3B-C4B-NB	-2.31	108.46	110.53
18	A	815	CLA	O2D-CGD-O1D	-2.31	119.34	123.85
18	B	826	CLA	C2C-C1C-NC	2.31	112.41	109.98
18	1	5008	CLA	CHD-C1D-ND	-2.31	121.55	124.80
18	G	1602	CLA	CMD-C2D-C3D	-2.31	122.38	127.69
18	A	832	CLA	C1D-ND-C4D	-2.31	104.69	106.31
21	K	1405	BCR	C30-C25-C26	-2.31	119.48	122.64
24	B	851	LMG	O6-C5-C6	2.31	112.17	106.44
18	1	5013	CLA	C4B-CHC-C1C	2.31	131.68	126.25
24	J	1102	LMG	C8-O7-C10	-2.31	112.27	117.80
18	A	839	CLA	CHD-C1D-ND	-2.31	121.55	124.80
18	A	853	CLA	CHA-C4D-ND	2.31	137.31	132.55
21	F	304	BCR	C37-C22-C23	2.31	121.62	118.09
18	A	816	CLA	CHD-C1D-ND	-2.31	121.55	124.80
18	A	826	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
18	3	301	CLA	C3B-C4B-NB	-2.31	108.47	110.53
18	A	817	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
18	3	318	CLA	C4B-CHC-C1C	2.31	131.68	126.25
18	B	841	CLA	CHA-C4D-ND	2.31	137.31	132.55
18	A	823	CLA	O1D-CGD-CBD	-2.31	119.97	124.52
18	B	813	CLA	CMD-C2D-C3D	-2.31	122.40	127.69
18	H	1701	CLA	C3B-C4B-NB	-2.31	108.47	110.53
18	A	853	CLA	CMD-C2D-C3D	-2.30	122.40	127.69
21	B	847	BCR	C8-C7-C6	-2.30	120.84	127.00
24	2	321	LMG	O7-C10-O9	-2.30	118.32	123.70
18	B	808	CLA	CMD-C2D-C3D	-2.30	122.40	127.69
18	A	813	CLA	C4B-CHC-C1C	2.30	131.67	126.25
18	A	818	CLA	C4B-CHC-C1C	2.30	131.67	126.25
31	2	304	XAT	O4-C5-C18	-2.30	112.47	115.05
18	3	308	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
18	L	301	CLA	CHD-C1D-ND	-2.30	121.56	124.80
30	2	314	CHL	CMA-C3A-C4A	2.30	119.58	114.61
18	4	310	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
18	A	812	CLA	CMA-C3A-C4A	2.30	117.96	111.77
21	A	846	BCR	C38-C26-C27	2.30	118.51	113.60
18	B	831	CLA	CHD-C1D-ND	-2.30	121.56	124.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	804	CLA	C2C-C1C-NC	2.30	112.40	109.98
18	B	819	CLA	C3B-C4B-NB	-2.30	108.47	110.53
18	B	808	CLA	C1D-ND-C4D	-2.30	104.70	106.31
18	A	836	CLA	O2A-CGA-CBA	2.30	118.85	111.83
18	B	821	CLA	C3B-C4B-NB	-2.30	108.48	110.53
18	A	802	CLA	C4B-CHC-C1C	2.30	131.66	126.25
18	2	308	CLA	C1D-ND-C4D	-2.30	104.70	106.31
18	A	802	CLA	CHA-C1A-NA	-2.30	121.18	126.39
18	B	805	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
18	4	309	CLA	CHA-C1A-NA	-2.30	121.18	126.39
18	A	830	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
18	4	305	CLA	C3B-C4B-NB	-2.30	108.48	110.53
29	3	303	LUT	C27-C28-C29	-2.30	121.38	126.32
18	A	808	CLA	O2A-CGA-CBA	2.30	118.84	111.83
18	B	831	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
22	A	848	LHG	C5-O7-C7	-2.30	112.30	117.80
18	1	5018	CLA	CHD-C1D-ND	-2.30	121.57	124.80
18	B	810	CLA	C4B-CHC-C1C	2.30	131.65	126.25
18	2	308	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
18	B	819	CLA	CAA-C2A-C1A	-2.30	104.45	111.97
18	B	823	CLA	O2D-CGD-O1D	-2.30	119.38	123.85
18	B	814	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
18	A	821	CLA	CHD-C1D-ND	-2.30	121.57	124.80
30	4	314	CHL	C4C-CHD-C1D	2.30	124.29	116.07
18	2	310	CLA	CAA-C2A-C1A	-2.30	104.45	111.97
18	A	805	CLA	C1D-ND-C4D	-2.30	104.70	106.31
18	A	814	CLA	C1D-ND-C4D	-2.30	104.70	106.31
18	B	807	CLA	C1D-ND-C4D	-2.30	104.70	106.31
18	B	819	CLA	C1D-ND-C4D	-2.30	104.70	106.31
18	B	801	CLA	CHA-C1A-NA	-2.30	121.19	126.39
17	A	801	CL0	CMB-C2B-C3B	2.30	129.27	124.68
21	A	845	BCR	C36-C18-C17	-2.29	119.10	122.82
18	L	301	CLA	O2D-CGD-O1D	-2.29	119.38	123.85
18	A	853	CLA	C1D-ND-C4D	-2.29	104.70	106.31
18	B	839	CLA	O2A-CGA-CBA	2.29	118.83	111.83
18	A	814	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
18	3	315	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
18	A	802	CLA	CHA-C4D-ND	2.29	137.28	132.55
18	B	813	CLA	CHD-C1D-ND	-2.29	121.58	124.80
21	K	1405	BCR	C19-C18-C17	2.29	122.62	119.01
18	K	1404	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
18	3	307	CLA	O1D-CGD-CBD	-2.29	120.00	124.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	825	CLA	C4B-CHC-C1C	2.29	131.64	126.25
18	A	804	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
18	3	308	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
18	A	838	CLA	O2A-CGA-CBA	2.29	118.82	111.83
18	A	825	CLA	C2D-C1D-ND	2.29	112.39	110.13
18	B	840	CLA	O2A-CGA-CBA	2.29	118.82	111.83
18	2	306	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
18	A	840	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
18	B	819	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
18	B	838	CLA	O2A-CGA-CBA	2.29	118.82	111.83
18	J	1101	CLA	C1D-ND-C4D	-2.29	104.70	106.31
18	B	812	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
18	B	828	CLA	C4B-CHC-C1C	2.29	131.63	126.25
18	1	5009	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
29	1	5004	LUT	C39-C29-C28	2.29	121.58	118.09
18	B	814	CLA	CHA-C1A-NA	-2.29	121.21	126.39
18	A	803	CLA	C4B-CHC-C1C	2.29	131.63	126.25
18	1	5015	CLA	O2A-CGA-CBA	2.29	118.81	111.83
18	1	5012	CLA	CHD-C1D-ND	-2.29	121.59	124.80
18	4	308	CLA	CAA-C2A-C3A	-2.28	106.83	113.00
29	3	304	LUT	C19-C9-C8	2.28	121.58	118.09
18	A	806	CLA	CMD-C2D-C3D	-2.28	122.45	127.69
18	B	821	CLA	C4B-CHC-C1C	2.28	131.62	126.25
18	A	803	CLA	C1-O2A-CGA	2.28	122.18	116.65
18	B	838	CLA	C1D-ND-C4D	-2.28	104.71	106.31
18	A	831	CLA	C4B-CHC-C1C	2.28	131.62	126.25
18	2	311	CLA	O2A-CGA-CBA	2.28	118.80	111.83
18	A	811	CLA	CMD-C2D-C3D	-2.28	122.45	127.69
18	B	815	CLA	CHD-C1D-ND	-2.28	121.59	124.80
18	L	306	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
18	1	5010	CLA	C1-O2A-CGA	2.28	122.17	116.65
18	B	823	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
18	B	820	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
18	2	309	CLA	C1-O2A-CGA	2.28	122.17	116.65
18	A	826	CLA	CHA-C4D-ND	2.28	137.25	132.55
18	4	308	CLA	O1D-CGD-CBD	-2.28	120.02	124.52
18	A	834	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
21	F	305	BCR	C38-C26-C25	-2.28	122.00	124.48
21	3	306	BCR	C38-C26-C25	-2.28	122.00	124.48
18	A	825	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
18	A	831	CLA	C1C-C2C-C3C	-2.28	104.58	106.98
18	B	809	CLA	CMD-C2D-C3D	-2.28	122.47	127.69

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	1402	CLA	CHA-C1A-NA	-2.28	121.23	126.39
18	K	1403	CLA	C3B-C4B-NB	-2.28	108.50	110.53
24	B	851	LMG	O7-C10-O9	-2.28	118.38	123.70
18	L	305	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
18	L	306	CLA	O2A-CGA-CBA	2.28	118.78	111.83
21	K	1405	BCR	C36-C18-C17	-2.28	119.13	122.82
18	A	833	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
18	A	804	CLA	C1-O2A-CGA	2.28	122.16	116.65
31	4	304	XAT	O4-C6-C7	-2.28	110.36	116.88
18	B	816	CLA	CHD-C1D-ND	-2.28	121.60	124.80
18	A	823	CLA	C4B-CHC-C1C	2.28	131.60	126.25
18	3	309	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
21	A	843	BCR	C31-C1-C6	-2.28	106.67	110.24
18	4	310	CLA	C3B-C4B-NB	-2.28	108.50	110.53
18	A	821	CLA	O2A-CGA-CBA	2.27	118.77	111.83
18	3	317	CLA	C1D-ND-C4D	-2.27	104.72	106.31
18	B	804	CLA	CAC-C3C-C4C	2.27	127.75	124.79
18	F	303	CLA	O2A-CGA-CBA	2.27	118.77	111.83
18	B	815	CLA	O1D-CGD-CBD	-2.27	120.03	124.52
21	A	847	BCR	C32-C1-C6	-2.27	106.68	110.24
18	A	832	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
18	2	309	CLA	O2A-CGA-CBA	2.27	118.76	111.83
18	4	315	CLA	C3B-C4B-NB	-2.27	108.50	110.53
18	B	821	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
18	A	826	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
21	B	843	BCR	C30-C25-C24	2.27	121.81	115.65
18	B	809	CLA	C4B-CHC-C1C	2.27	131.58	126.25
18	F	303	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
18	G	1603	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
18	B	835	CLA	CHD-C1D-ND	-2.27	121.61	124.80
18	A	818	CLA	O2A-CGA-CBA	2.27	118.75	111.83
18	B	804	CLA	C4B-CHC-C1C	2.27	131.58	126.25
18	4	305	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
18	L	305	CLA	CHA-C4D-ND	2.27	137.22	132.55
18	3	311	CLA	O2A-CGA-CBA	2.27	118.75	111.83
18	A	806	CLA	C3B-C4B-NB	-2.27	108.51	110.53
18	A	820	CLA	C4B-CHC-C1C	2.27	131.57	126.25
18	A	813	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
18	3	319	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
18	A	826	CLA	O2A-CGA-CBA	2.26	118.74	111.83
18	K	1403	CLA	C1D-ND-C4D	-2.26	104.72	106.31
18	4	309	CLA	CHD-C1D-ND	-2.26	121.62	124.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	J	1101	CLA	C1-O2A-CGA	2.26	122.13	116.65
21	I	101	BCR	C3-C4-C5	-2.26	110.02	114.06
30	4	318	CHL	C1-O2A-CGA	2.26	122.12	116.65
18	B	801	CLA	C4B-CHC-C1C	2.26	131.56	126.25
18	B	817	CLA	C2C-C1C-NC	2.26	112.36	109.98
24	B	851	LMG	O1-C1-C2	2.26	111.71	108.27
18	4	311	CLA	C2D-C1D-ND	2.26	112.36	110.13
18	A	809	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
18	B	818	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
21	L	307	BCR	C33-C5-C4	2.26	118.41	113.60
18	A	825	CLA	C1D-ND-C4D	-2.26	104.73	106.31
18	A	811	CLA	CAA-C2A-C3A	-2.26	106.90	113.00
18	G	1601	CLA	O2A-CGA-CBA	2.26	118.72	111.83
18	A	811	CLA	C1D-ND-C4D	-2.26	104.73	106.31
18	B	836	CLA	C3B-C4B-NB	-2.26	108.52	110.53
18	B	822	CLA	CMD-C2D-C3D	-2.26	122.52	127.69
18	B	810	CLA	CHD-C1D-ND	-2.25	121.63	124.80
18	G	1603	CLA	C1D-ND-C4D	-2.25	104.73	106.31
18	2	326	CLA	O2A-CGA-CBA	2.25	118.70	111.83
18	4	309	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
18	A	817	CLA	O2A-CGA-CBA	2.25	118.70	111.83
18	A	816	CLA	C1C-C2C-C3C	-2.25	104.61	106.98
18	B	809	CLA	C3B-C4B-NB	-2.25	108.52	110.53
18	3	318	CLA	CMA-C3A-C4A	2.25	117.82	111.77
30	4	302	CHL	C4C-CHD-C1D	2.25	124.12	116.07
18	1	5011	CLA	C3B-C4B-NB	-2.25	108.52	110.53
21	3	305	BCR	C27-C26-C25	-2.25	119.67	122.70
18	2	326	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
18	4	312	CLA	O1D-CGD-CBD	-2.25	120.09	124.52
18	3	318	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
18	B	833	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
18	A	837	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
18	4	306	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
18	2	317	CLA	CMD-C2D-C3D	-2.24	122.54	127.69
19	B	842	PQN	C2M-C2-C3	-2.24	120.76	124.45
18	L	304	CLA	O2A-CGA-CBA	2.24	118.68	111.83
18	B	817	CLA	C1-C2-C3	-2.24	122.52	126.20
18	3	311	CLA	CHA-C1A-NA	-2.24	121.31	126.39
26	J	1106	DGD	C3E-C4E-C5E	2.24	114.30	110.23
18	3	308	CLA	C1D-ND-C4D	-2.24	104.74	106.31
30	2	319	CHL	C1-C2-C3	-2.24	122.52	126.20
30	3	310	CHL	C4D-CHA-CBD	-2.24	106.71	108.97

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	5012	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
18	B	810	CLA	CMA-C3A-C4A	2.24	117.80	111.77
18	B	808	CLA	C3B-C4B-NB	-2.24	108.53	110.53
18	B	832	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
18	A	826	CLA	C6-C5-C3	-2.24	108.01	113.47
21	I	101	BCR	C35-C13-C14	-2.24	119.19	122.82
30	2	315	CHL	C4C-CHD-C1D	2.24	124.08	116.07
21	L	307	BCR	C23-C24-C25	-2.24	121.02	127.00
18	B	820	CLA	O2A-CGA-CBA	2.24	118.66	111.83
18	2	309	CLA	C1D-ND-C4D	-2.24	104.74	106.31
21	A	843	BCR	C33-C5-C4	2.24	118.37	113.60
29	2	303	LUT	C18-C5-C4	2.24	118.53	114.42
18	A	811	CLA	O2A-CGA-CBA	2.24	118.65	111.83
21	A	855	BCR	C37-C22-C21	-2.24	119.19	122.82
18	1	5018	CLA	C1D-ND-C4D	-2.24	104.74	106.31
18	A	808	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
18	3	317	CLA	C3B-C4B-NB	-2.24	108.53	110.53
18	A	812	CLA	O2A-CGA-CBA	2.24	118.65	111.83
21	L	307	BCR	C35-C13-C12	2.23	121.50	118.09
31	2	304	XAT	O4-C6-C7	-2.23	110.48	116.88
21	2	305	BCR	C4-C5-C6	-2.23	119.69	122.70
29	2	303	LUT	C10-C11-C12	-2.23	116.73	123.20
18	3	301	CLA	CHA-C1A-NA	-2.23	121.33	126.39
18	2	306	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
18	A	812	CLA	O1D-CGD-CBD	-2.23	120.11	124.52
18	A	834	CLA	CHA-C1A-NA	-2.23	121.33	126.39
18	K	1403	CLA	O2A-CGA-CBA	2.23	118.64	111.83
21	B	845	BCR	C12-C13-C14	-2.23	115.50	119.01
30	2	316	CHL	C1-O2A-CGA	2.23	123.01	116.67
18	L	306	CLA	CHA-C1A-NA	-2.23	121.34	126.39
18	A	815	CLA	C3B-C4B-NB	-2.23	108.54	110.53
18	2	311	CLA	C3B-C4B-NB	-2.23	108.54	110.53
24	G	1607	LMG	C1-O6-C5	2.23	118.07	113.72
21	F	305	BCR	C30-C25-C24	2.23	121.69	115.65
21	K	1405	BCR	C38-C26-C27	2.23	118.34	113.60
18	B	806	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
19	A	841	PQN	C11-C3-C2	-2.22	121.08	124.89
21	B	847	BCR	C28-C27-C26	-2.22	110.09	114.06
18	A	812	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
18	2	312	CLA	CHD-C1D-ND	-2.22	121.67	124.80
18	A	831	CLA	CAA-C2A-C3A	-2.22	106.99	113.00
18	2	311	CLA	CAA-C2A-C3A	-2.22	106.99	113.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	307	CLA	C1D-ND-C4D	-2.22	104.75	106.31
18	B	804	CLA	CHD-C1D-ND	-2.22	121.67	124.80
18	A	822	CLA	O2A-CGA-CBA	2.22	118.61	111.83
18	3	309	CLA	C1D-ND-C4D	-2.22	104.75	106.31
21	A	843	BCR	C38-C26-C27	2.22	118.33	113.60
18	A	805	CLA	C3B-C4B-NB	-2.22	108.55	110.53
18	A	831	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
18	B	827	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
18	A	825	CLA	CHD-C1D-ND	-2.22	121.68	124.80
18	A	829	CLA	C1D-ND-C4D	-2.22	104.75	106.31
18	B	810	CLA	CHA-C1A-NA	-2.22	121.37	126.39
18	A	805	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
18	A	839	CLA	O2A-CGA-CBA	2.22	118.60	111.83
21	A	846	BCR	C37-C22-C23	2.22	121.48	118.09
30	2	318	CHL	C4C-CHD-C1D	2.22	124.00	116.07
18	4	311	CLA	CHD-C1D-ND	-2.22	121.68	124.80
18	1	5006	CLA	O2A-CGA-CBA	2.22	118.59	111.83
18	A	852	CLA	CMD-C2D-C3D	-2.22	122.61	127.69
18	B	814	CLA	CMA-C3A-C4A	2.22	117.73	111.77
18	A	807	CLA	CMD-C2D-C3D	-2.22	122.61	127.69
18	B	829	CLA	CMD-C2D-C3D	-2.22	122.61	127.69
18	1	5018	CLA	CMD-C2D-C3D	-2.22	122.61	127.69
18	B	836	CLA	CHA-C1A-NA	-2.22	121.38	126.39
18	B	805	CLA	O2A-CGA-CBA	2.21	118.59	111.83
18	B	826	CLA	O1D-CGD-CBD	-2.21	120.15	124.52
18	2	307	CLA	CMD-C2D-C3D	-2.21	122.61	127.69
21	A	855	BCR	C23-C24-C25	-2.21	121.09	127.00
23	J	1107	LMT	C3'-C4'-C5'	-2.21	106.03	110.93
18	1	5007	CLA	C2D-C1D-ND	2.21	112.32	110.13
18	3	314	CLA	CHA-C1A-NA	-2.21	121.38	126.39
18	A	815	CLA	C1D-ND-C4D	-2.21	104.76	106.31
18	A	824	CLA	C1D-ND-C4D	-2.21	104.76	106.31
18	B	840	CLA	C1D-ND-C4D	-2.21	104.76	106.31
21	B	844	BCR	C38-C26-C27	2.21	118.31	113.60
18	A	819	CLA	O2A-CGA-CBA	2.21	118.58	111.83
18	F	303	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
18	3	309	CLA	O2D-CGD-O1D	-2.21	119.54	123.85
18	A	813	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
18	A	811	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
18	A	804	CLA	C1D-ND-C4D	-2.21	104.76	106.31
18	1	5010	CLA	CHD-C1D-ND	-2.21	121.69	124.80
18	B	826	CLA	C1D-ND-C4D	-2.21	104.76	106.31

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	804	CLA	CHA-C1A-NA	-2.21	121.39	126.39
30	4	313	CHL	C1-O2A-CGA	2.21	123.14	116.07
18	B	832	CLA	C3B-C4B-NB	-2.21	108.56	110.53
18	4	306	CLA	CHD-C1D-ND	-2.21	121.70	124.80
21	2	305	BCR	C12-C13-C14	-2.21	115.54	119.01
18	B	825	CLA	O1D-CGD-CBD	-2.21	120.17	124.52
18	A	813	CLA	CHA-C1A-NA	-2.21	121.39	126.39
18	3	308	CLA	CHD-C1D-ND	-2.21	121.70	124.80
18	B	821	CLA	CHD-C1D-ND	-2.20	121.70	124.80
18	B	836	CLA	CHD-C1D-ND	-2.20	121.70	124.80
18	2	307	CLA	CHD-C1D-ND	-2.20	121.70	124.80
18	B	803	CLA	CHA-C1A-NA	-2.20	121.40	126.39
18	B	810	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
18	B	841	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
18	4	305	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
18	B	824	CLA	C1D-ND-C4D	-2.20	104.77	106.31
18	3	318	CLA	CHA-C1A-NA	-2.20	121.40	126.39
21	I	102	BCR	C38-C26-C25	-2.20	122.08	124.48
18	A	815	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
18	A	823	CLA	O2A-CGA-CBA	2.20	118.55	111.83
18	B	811	CLA	C1D-ND-C4D	-2.20	104.77	106.31
18	4	306	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
18	B	833	CLA	CHD-C1D-ND	-2.20	121.70	124.80
18	3	315	CLA	C3B-C4B-NB	-2.20	108.56	110.53
18	2	307	CLA	CHA-C1A-NA	-2.20	121.41	126.39
18	B	827	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
21	F	304	BCR	C34-C9-C10	-2.20	119.25	122.82
18	B	816	CLA	C1-O2A-CGA	2.20	121.97	116.65
18	K	1403	CLA	CHA-C1A-NA	-2.20	121.41	126.39
30	4	313	CHL	C4C-CHD-C1D	2.20	123.93	116.07
30	4	317	CHL	C4C-CHD-C1D	2.20	123.93	116.07
21	L	302	BCR	C34-C9-C10	-2.20	119.25	122.82
18	A	853	CLA	C3B-C4B-NB	-2.20	108.57	110.53
18	B	838	CLA	C2D-C1D-ND	2.20	112.30	110.13
18	G	1603	CLA	O2A-CGA-CBA	2.20	118.53	111.83
30	1	5014	CHL	C4C-CHD-C1D	2.20	123.93	116.07
18	A	825	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
18	A	825	CLA	C3B-C4B-NB	-2.20	108.57	110.53
29	1	5003	LUT	C7-C8-C9	-2.20	122.99	126.23
18	B	840	CLA	C1-O2A-CGA	2.20	121.97	116.65
18	A	808	CLA	CHD-C1D-ND	-2.20	121.71	124.80
18	A	824	CLA	C1-O2A-CGA	2.20	121.96	116.65

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	305	BCR	C34-C9-C10	-2.19	119.26	122.82
24	2	323	LMG	C1-O6-C5	2.19	118.00	113.72
18	3	309	CLA	O1D-CGD-CBD	-2.19	120.19	124.52
18	A	802	CLA	C2D-C1D-ND	2.19	112.30	110.13
18	B	807	CLA	O2A-CGA-CBA	2.19	118.52	111.83
18	4	305	CLA	C1D-ND-C4D	-2.19	104.77	106.31
21	A	845	BCR	C30-C25-C26	-2.19	119.64	122.64
29	1	5003	LUT	C18-C5-C4	2.19	118.45	114.42
18	3	311	CLA	CHD-C1D-ND	-2.19	121.72	124.80
18	3	301	CLA	CMD-C2D-C3D	-2.19	122.66	127.69
18	A	822	CLA	O2D-CGD-O1D	-2.19	119.58	123.85
18	2	313	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
18	J	1103	CLA	CHD-C1D-ND	-2.19	121.72	124.80
18	3	317	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
24	1	5001	LMG	O8-C28-O10	-2.19	118.15	123.63
18	B	827	CLA	CHA-C1A-NA	-2.19	121.43	126.39
18	A	816	CLA	C2D-C1D-ND	2.19	112.29	110.13
18	B	829	CLA	C1D-ND-C4D	-2.19	104.78	106.31
18	B	809	CLA	CHD-C1D-ND	-2.19	121.72	124.80
18	A	812	CLA	C2D-C1D-ND	2.19	112.29	110.13
18	L	306	CLA	C3B-C4B-NB	-2.19	108.58	110.53
18	1	5006	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
18	B	839	CLA	C1D-ND-C4D	-2.19	104.78	106.31
18	A	818	CLA	CHD-C1D-ND	-2.19	121.73	124.80
18	F	303	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
29	1	5004	LUT	C18-C5-C4	2.19	118.44	114.42
18	J	1103	CLA	CMD-C2D-C3D	-2.18	122.68	127.69
18	2	310	CLA	CMD-C2D-C3D	-2.18	122.68	127.69
18	B	827	CLA	C3B-C4B-NB	-2.18	108.58	110.53
18	4	307	CLA	C1D-ND-C4D	-2.18	104.78	106.31
18	2	307	CLA	C1D-ND-C4D	-2.18	104.78	106.31
18	A	852	CLA	O2A-CGA-CBA	2.18	118.48	111.83
18	A	839	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
18	A	810	CLA	C1D-ND-C4D	-2.18	104.78	106.31
21	I	101	BCR	C27-C26-C25	-2.18	119.76	122.70
18	A	803	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
18	J	1103	CLA	O2A-CGA-CBA	2.18	118.48	111.83
18	L	304	CLA	C1D-ND-C4D	-2.18	104.78	106.31
30	1	5016	CHL	C4C-CHD-C1D	2.18	123.86	116.07
18	A	836	CLA	CMD-C2D-C3D	-2.18	122.70	127.69
18	A	821	CLA	CMD-C2D-C3D	-2.18	122.70	127.69
18	4	305	CLA	C1-O2A-CGA	2.18	121.92	116.65

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	828	CLA	CHA-C1A-NA	-2.18	121.47	126.39
21	F	305	BCR	C37-C22-C23	2.18	121.41	118.09
18	3	315	CLA	C1D-ND-C4D	-2.17	104.79	106.31
18	F	302	CLA	CHA-C1A-NA	-2.17	121.47	126.39
18	A	828	CLA	C4B-CHC-C1C	2.17	131.36	126.25
18	4	315	CLA	CMD-C2D-C3D	-2.17	122.70	127.69
18	4	305	CLA	CHA-C1A-NA	-2.17	121.47	126.39
18	4	308	CLA	C1D-ND-C4D	-2.17	104.79	106.31
18	B	816	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
21	K	1405	BCR	C35-C13-C12	2.17	121.41	118.09
18	J	1103	CLA	CHA-C1A-NA	-2.17	121.47	126.39
18	B	834	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
21	A	847	BCR	C34-C9-C10	-2.17	119.30	122.82
18	3	314	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
18	A	807	CLA	O2A-CGA-CBA	2.17	118.45	111.83
18	A	838	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
18	B	841	CLA	CHA-C1A-NA	-2.17	121.48	126.39
18	B	835	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
21	F	305	BCR	C35-C13-C12	2.17	121.40	118.09
18	L	301	CLA	C1D-ND-C4D	-2.17	104.79	106.31
24	B	851	LMG	C1-O6-C5	2.17	117.95	113.72
30	3	316	CHL	C4C-CHD-C1D	2.17	123.82	116.07
18	K	1401	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
18	B	816	CLA	C1D-ND-C4D	-2.16	104.79	106.31
18	B	823	CLA	C1D-ND-C4D	-2.16	104.79	106.31
18	1	5015	CLA	C1D-ND-C4D	-2.16	104.79	106.31
21	I	102	BCR	C28-C27-C26	-2.16	110.19	114.06
18	K	1404	CLA	CHD-C1D-ND	-2.16	121.76	124.80
18	A	803	CLA	CMD-C2D-C3D	-2.16	122.72	127.69
18	2	306	CLA	C2D-C1D-ND	2.16	112.27	110.13
30	4	316	CHL	CMA-C3A-C4A	2.16	119.27	114.61
18	A	825	CLA	O2A-CGA-CBA	2.16	118.43	111.83
18	2	310	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
18	4	306	CLA	CHA-C1A-NA	-2.16	121.49	126.39
21	A	855	BCR	C29-C28-C27	2.16	116.03	111.28
18	B	811	CLA	CHD-C1D-ND	-2.16	121.76	124.80
21	L	302	BCR	C30-C25-C24	2.16	121.51	115.65
18	1	5017	CLA	CMA-C3A-C4A	2.16	117.58	111.77
18	4	309	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
29	2	303	LUT	C40-C33-C32	2.16	121.39	118.09
18	B	821	CLA	O1D-CGD-CBD	-2.16	120.26	124.52
18	B	803	CLA	C6-C5-C3	-2.16	108.20	113.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	3	312	CHL	C4C-CHD-C1D	2.16	123.80	116.07
18	A	804	CLA	C3B-C4B-NB	-2.16	108.60	110.53
18	1	5008	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
18	3	319	CLA	C1D-ND-C4D	-2.16	104.80	106.31
18	1	5018	CLA	CHA-C1A-NA	-2.16	121.50	126.39
24	1	5020	LMG	C8-O7-C10	-2.16	112.63	117.80
18	A	832	CLA	CMA-C3A-C4A	2.16	117.58	111.77
18	A	806	CLA	C1D-ND-C4D	-2.16	104.80	106.31
18	A	816	CLA	C1D-ND-C4D	-2.16	104.80	106.31
29	4	303	LUT	C31-C32-C33	-2.16	120.45	126.36
18	A	838	CLA	CHA-C1A-NA	-2.16	121.51	126.39
18	B	839	CLA	C1-O2A-CGA	2.16	121.87	116.65
21	L	307	BCR	C38-C26-C25	-2.16	122.13	124.48
18	K	1403	CLA	CBC-CAC-C3C	-2.16	106.58	112.42
21	G	1604	BCR	C4-C5-C6	-2.15	119.79	122.70
21	L	302	BCR	C27-C26-C25	-2.15	119.79	122.70
18	A	803	CLA	CHA-C1A-NA	-2.15	121.51	126.39
18	B	841	CLA	C2D-C1D-ND	2.15	112.26	110.13
18	B	830	CLA	C4B-CHC-C1C	2.15	131.31	126.25
18	K	1402	CLA	C1D-ND-C4D	-2.15	104.80	106.31
18	3	318	CLA	C3B-C4B-NB	-2.15	108.61	110.53
18	B	806	CLA	C2D-C1D-ND	2.15	112.25	110.13
18	L	304	CLA	C3B-C4B-NB	-2.15	108.61	110.53
18	K	1401	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
18	B	833	CLA	C1D-ND-C4D	-2.15	104.80	106.31
18	B	835	CLA	O2D-CGD-O1D	-2.15	119.67	123.85
18	B	816	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
18	B	822	CLA	CHA-C1A-NA	-2.15	121.53	126.39
18	H	1701	CLA	CHA-C1A-NA	-2.15	121.53	126.39
30	2	316	CHL	C4C-CHD-C1D	2.15	123.75	116.07
18	4	312	CLA	C1D-ND-C4D	-2.15	104.81	106.31
18	A	837	CLA	C3B-C4B-NB	-2.15	108.61	110.53
21	I	102	BCR	C34-C9-C10	-2.15	119.34	122.82
18	J	1103	CLA	CMA-C3A-C2A	2.15	122.28	113.98
18	A	819	CLA	C3B-C4B-NB	-2.15	108.61	110.53
18	B	825	CLA	C3B-C4B-NB	-2.15	108.61	110.53
18	B	812	CLA	C1-O2A-CGA	2.15	121.84	116.65
18	A	818	CLA	CMD-C2D-C3D	-2.14	122.77	127.69
30	4	318	CHL	CMD-C2D-C3D	2.14	128.97	124.68
21	B	802	BCR	C38-C26-C27	2.14	118.17	113.60
21	A	847	BCR	C27-C26-C25	-2.14	119.81	122.70
18	A	813	CLA	C1D-ND-C4D	-2.14	104.81	106.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	305	BCR	C36-C18-C17	-2.14	119.34	122.82
18	B	811	CLA	O2A-CGA-CBA	2.14	118.37	111.83
18	1	5012	CLA	C1D-ND-C4D	-2.14	104.81	106.31
18	4	315	CLA	O2A-CGA-CBA	2.14	118.37	111.83
18	A	805	CLA	O2A-CGA-CBA	2.14	118.36	111.83
18	B	810	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
18	B	836	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
21	1	5005	BCR	C35-C13-C12	2.14	121.36	118.09
21	1	5005	BCR	C15-C14-C13	-2.14	124.28	127.28
18	1	5011	CLA	C1-O2A-CGA	2.14	121.83	116.65
18	A	808	CLA	CHA-C1A-NA	-2.14	121.55	126.39
18	A	834	CLA	C1D-ND-C4D	-2.14	104.81	106.31
29	1	5003	LUT	C22-C23-C24	-2.14	108.01	111.18
18	G	1603	CLA	CHA-C1A-NA	-2.14	121.55	126.39
30	4	316	CHL	C1-C2-C3	-2.14	122.69	126.20
18	F	303	CLA	C2D-C1D-ND	2.14	112.24	110.13
18	L	301	CLA	CMD-C2D-C3D	-2.14	122.79	127.69
18	1	5012	CLA	CHA-C1A-NA	-2.14	121.55	126.39
18	A	836	CLA	C2D-C1D-ND	2.14	112.24	110.13
18	4	310	CLA	CHA-C1A-NA	-2.14	121.56	126.39
24	G	1607	LMG	O6-C5-C6	2.14	111.73	106.44
18	4	308	CLA	C3B-C4B-NB	-2.14	108.62	110.53
31	4	304	XAT	O24-C25-C24	2.14	115.49	113.49
18	1	5010	CLA	C1D-ND-C4D	-2.13	104.81	106.31
21	A	843	BCR	C3-C4-C5	-2.13	110.25	114.06
18	4	305	CLA	C2D-C1D-ND	2.13	112.24	110.13
18	L	304	CLA	CHA-C1A-NA	-2.13	121.56	126.39
18	3	309	CLA	C2D-C1D-ND	2.13	112.24	110.13
18	1	5017	CLA	CHD-C1D-ND	-2.13	121.80	124.80
18	G	1601	CLA	C1D-ND-C4D	-2.13	104.82	106.31
18	F	302	CLA	C1-O2A-CGA	2.13	121.81	116.65
18	A	827	CLA	CHD-C1D-ND	-2.13	121.80	124.80
18	2	317	CLA	CHA-C1A-NA	-2.13	121.57	126.39
18	4	309	CLA	C1D-ND-C4D	-2.13	104.82	106.31
18	A	836	CLA	CHA-C1A-NA	-2.13	121.57	126.39
18	B	822	CLA	C1D-ND-C4D	-2.13	104.82	106.31
18	A	812	CLA	C3B-C4B-NB	-2.13	108.63	110.53
18	2	326	CLA	CHD-C1D-ND	-2.13	121.81	124.80
18	1	5006	CLA	C1D-ND-C4D	-2.13	104.82	106.31
18	B	841	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
18	A	852	CLA	CHA-C1A-NA	-2.13	121.58	126.39
21	A	847	BCR	C37-C22-C23	2.13	121.33	118.09

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	828	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
29	J	1105	LUT	C31-C32-C33	-2.13	120.54	126.36
18	A	819	CLA	C1D-ND-C4D	-2.13	104.82	106.31
30	3	313	CHL	CMD-C2D-C3D	2.12	128.93	124.68
18	A	832	CLA	CHA-C1A-NA	-2.12	121.58	126.39
18	G	1601	CLA	CHA-C1A-NA	-2.12	121.58	126.39
18	A	816	CLA	CMD-C2D-C3D	-2.12	122.82	127.69
17	A	801	CL0	C4C-C3C-C2C	-2.12	104.98	113.37
18	2	312	CLA	CHA-C1A-NA	-2.12	121.58	126.39
21	I	102	BCR	C19-C18-C17	2.12	122.35	119.01
18	B	823	CLA	CHA-C1A-NA	-2.12	121.59	126.39
18	B	830	CLA	CAC-C3C-C4C	2.12	127.55	124.79
18	B	818	CLA	CHA-C1A-NA	-2.12	121.59	126.39
18	3	309	CLA	CHA-C1A-NA	-2.12	121.59	126.39
18	B	831	CLA	O2A-CGA-CBA	2.12	118.30	111.83
18	A	808	CLA	C1-O2A-CGA	2.12	121.78	116.65
18	1	5010	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
18	2	313	CLA	C1D-ND-C4D	-2.12	104.83	106.31
18	3	314	CLA	C1D-ND-C4D	-2.12	104.83	106.31
18	1	5018	CLA	C2D-C1D-ND	2.12	112.22	110.13
21	3	306	BCR	C37-C22-C21	-2.12	119.39	122.82
18	B	817	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
18	2	326	CLA	CHA-C1A-NA	-2.12	121.60	126.39
29	4	303	LUT	C27-C28-C29	-2.11	121.78	126.32
18	A	825	CLA	CHA-C1A-NA	-2.11	121.60	126.39
18	B	805	CLA	C3B-C4B-NB	-2.11	108.64	110.53
21	J	1104	BCR	C38-C26-C27	2.11	118.10	113.60
18	B	824	CLA	O2D-CGD-O1D	-2.11	119.73	123.85
29	1	5003	LUT	C31-C32-C33	-2.11	120.57	126.36
18	3	308	CLA	C2D-C1D-ND	2.11	112.22	110.13
18	A	802	CLA	C1D-ND-C4D	-2.11	104.83	106.31
18	A	829	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
18	B	819	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
18	F	301	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
18	B	827	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
18	A	821	CLA	C3B-C4B-NB	-2.11	108.65	110.53
21	F	305	BCR	C33-C5-C4	2.11	118.09	113.60
30	4	316	CHL	CMD-C2D-C3D	2.11	128.90	124.68
18	2	307	CLA	C2D-C1D-ND	2.11	112.21	110.13
18	A	807	CLA	C1D-ND-C4D	-2.11	104.83	106.31
18	B	836	CLA	C1D-ND-C4D	-2.11	104.83	106.31
21	B	844	BCR	C33-C5-C4	2.11	118.09	113.60

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	5007	CLA	CHD-C1D-ND	-2.11	121.84	124.80
18	A	811	CLA	C6-C5-C3	-2.11	108.34	113.47
18	4	305	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
18	A	824	CLA	C2D-C1D-ND	2.11	112.21	110.13
18	A	817	CLA	C1D-ND-C4D	-2.11	104.83	106.31
18	B	834	CLA	CHA-C1A-NA	-2.10	121.62	126.39
29	3	303	LUT	C19-C9-C8	2.10	121.30	118.09
18	J	1101	CLA	O1D-CGD-CBD	-2.10	120.37	124.52
21	B	844	BCR	C8-C9-C10	2.10	122.32	119.01
18	K	1404	CLA	CHA-C1A-NA	-2.10	121.63	126.39
18	L	306	CLA	C2D-C1D-ND	2.10	112.21	110.13
18	A	826	CLA	C1D-ND-C4D	-2.10	104.84	106.31
18	1	5011	CLA	C1D-ND-C4D	-2.10	104.84	106.31
18	4	305	CLA	O2A-CGA-CBA	2.10	118.25	111.83
18	A	805	CLA	CHA-C1A-NA	-2.10	121.63	126.39
18	A	803	CLA	C2D-C1D-ND	2.10	112.21	110.13
18	B	833	CLA	C3B-C4B-NB	-2.10	108.65	110.53
21	A	844	BCR	C38-C26-C27	2.10	118.08	113.60
21	B	844	BCR	C12-C13-C14	-2.10	115.70	119.01
18	B	824	CLA	O2A-CGA-CBA	2.10	118.24	111.83
18	J	1101	CLA	CHA-C1A-NA	-2.10	121.63	126.39
18	A	832	CLA	CAA-C2A-C3A	-2.10	107.32	113.00
18	B	814	CLA	C3B-C4B-NB	-2.10	108.65	110.53
30	4	302	CHL	CMD-C2D-C3D	2.10	128.88	124.68
30	1	5014	CHL	C1-O2A-CGA	2.10	122.80	116.07
18	1	5008	CLA	C2D-C1D-ND	2.10	112.20	110.13
24	F	306	LMG	O7-C10-O9	-2.10	118.80	123.70
18	3	307	CLA	O2A-CGA-CBA	2.10	118.24	111.83
18	A	816	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
18	4	315	CLA	CHA-C1A-NA	-2.10	121.64	126.39
21	F	305	BCR	C31-C1-C6	-2.10	106.95	110.24
18	4	311	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
21	A	855	BCR	C35-C13-C12	2.10	121.29	118.09
18	B	838	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
26	2	327	DGD	O2G-C1B-O1B	-2.10	118.81	123.70
30	4	318	CHL	C4C-CHD-C1D	2.09	123.56	116.07
18	3	319	CLA	O2A-CGA-CBA	2.09	118.21	111.83
18	A	814	CLA	CHA-C1A-NA	-2.09	121.65	126.39
30	2	314	CHL	CMD-C2D-C3D	2.09	128.86	124.68
30	4	313	CHL	CMD-C2D-C3D	2.09	128.86	124.68
18	3	309	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
18	A	830	CLA	CMA-C3A-C4A	2.09	117.39	111.77

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	F	302	CLA	C1D-ND-C4D	-2.09	104.84	106.31
31	2	304	XAT	O24-C25-C38	-2.09	112.71	115.05
30	3	310	CHL	CMD-C2D-C3D	2.09	128.86	124.68
21	I	102	BCR	C35-C13-C12	2.09	121.28	118.09
18	A	833	CLA	CHA-C1A-NA	-2.09	121.66	126.39
18	L	305	CLA	C2D-C1D-ND	2.09	112.19	110.13
21	A	855	BCR	C38-C26-C27	2.09	118.05	113.60
18	A	816	CLA	CHA-C1A-NA	-2.09	121.66	126.39
18	B	824	CLA	CHA-C1A-NA	-2.09	121.66	126.39
18	B	831	CLA	CAA-C2A-C3A	-2.09	107.36	113.00
18	4	307	CLA	C1-O2A-CGA	2.09	121.70	116.65
18	B	838	CLA	CHA-C1A-NA	-2.09	121.67	126.39
18	A	820	CLA	CHA-C1A-NA	-2.08	121.67	126.39
18	A	835	CLA	C2D-C1D-ND	2.08	112.19	110.13
21	B	846	BCR	C12-C13-C14	-2.08	115.73	119.01
18	A	829	CLA	CHA-C1A-NA	-2.08	121.67	126.39
18	A	809	CLA	C2D-C1D-ND	2.08	112.19	110.13
30	2	319	CHL	CMD-C2D-C3D	2.08	128.84	124.68
18	A	807	CLA	C2D-C1D-ND	2.08	112.19	110.13
18	A	839	CLA	C1-O2A-CGA	2.08	121.69	116.65
18	A	803	CLA	C1D-ND-C4D	-2.08	104.85	106.31
18	B	830	CLA	CHA-C1A-NA	-2.08	121.68	126.39
18	B	831	CLA	CHA-C1A-NA	-2.08	121.68	126.39
21	F	305	BCR	C30-C25-C26	-2.08	119.79	122.64
18	A	831	CLA	C1D-ND-C4D	-2.08	104.85	106.31
18	4	307	CLA	O2A-CGA-CBA	2.08	118.18	111.83
21	B	844	BCR	C30-C25-C26	-2.08	119.79	122.64
18	K	1401	CLA	CHA-C1A-NA	-2.08	121.68	126.39
18	B	816	CLA	O2A-CGA-CBA	2.08	118.17	111.83
18	4	309	CLA	CAC-C3C-C4C	2.08	127.50	124.79
26	1	5002	DGD	C2G-O2G-C1B	-2.08	112.82	117.80
18	A	822	CLA	CHA-C1A-NA	-2.08	121.68	126.39
18	1	5007	CLA	CMD-C2D-C3D	-2.08	122.92	127.69
18	A	811	CLA	CHA-C1A-NA	-2.08	121.69	126.39
18	B	811	CLA	CHA-C1A-NA	-2.08	121.69	126.39
18	B	832	CLA	C1D-ND-C4D	-2.08	104.85	106.31
18	F	302	CLA	C3B-C4B-NB	-2.08	108.67	110.53
30	4	316	CHL	C4C-CHD-C1D	2.08	123.50	116.07
18	A	840	CLA	CHA-C1A-NA	-2.08	121.69	126.39
21	A	845	BCR	C35-C13-C12	2.08	121.26	118.09
18	4	309	CLA	C2D-C1D-ND	2.08	112.18	110.13
18	A	808	CLA	O1D-CGD-CBD	-2.08	120.42	124.52

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	821	CLA	C1D-ND-C4D	-2.08	104.86	106.31
18	4	306	CLA	C1-O2A-CGA	2.07	121.67	116.65
18	3	317	CLA	C2D-C1D-ND	2.07	112.18	110.13
18	B	832	CLA	CHA-C1A-NA	-2.07	121.70	126.39
18	F	303	CLA	CHA-C1A-NA	-2.07	121.70	126.39
18	2	308	CLA	C2D-C1D-ND	2.07	112.18	110.13
21	3	305	BCR	C38-C26-C27	2.07	118.01	113.60
18	G	1602	CLA	CHA-C1A-NA	-2.07	121.70	126.39
18	A	806	CLA	C1-O2A-CGA	2.07	121.67	116.65
18	B	808	CLA	O2A-CGA-CBA	2.07	118.15	111.83
21	A	843	BCR	C2-C1-C6	2.07	113.45	110.44
31	4	304	XAT	C40-C33-C34	-2.07	119.46	122.82
18	A	812	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
21	3	306	BCR	C38-C26-C27	2.07	118.01	113.60
18	1	5017	CLA	CHA-C1A-NA	-2.07	121.70	126.39
18	A	815	CLA	C2D-C1D-ND	2.07	112.17	110.13
18	B	804	CLA	CAA-C2A-C3A	-2.07	107.41	113.00
18	3	314	CLA	O2A-CGA-CBA	2.07	118.14	111.83
18	1	5010	CLA	CHA-C1A-NA	-2.07	121.71	126.39
21	1	5005	BCR	C29-C28-C27	2.07	115.82	111.28
18	A	807	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
18	B	804	CLA	CMD-C2D-C3D	-2.07	122.95	127.69
18	B	829	CLA	C3B-C4B-NB	-2.07	108.69	110.53
18	F	301	CLA	CMD-C2D-C3D	-2.07	122.95	127.69
18	A	831	CLA	C2D-C1D-ND	2.07	112.17	110.13
18	B	805	CLA	C1D-ND-C4D	-2.07	104.86	106.31
18	A	830	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
30	4	314	CHL	CMD-C2D-C3D	2.06	128.81	124.68
18	B	818	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
18	B	813	CLA	CHA-C1A-NA	-2.06	121.72	126.39
18	A	833	CLA	C1D-ND-C4D	-2.06	104.86	106.31
18	A	817	CLA	C1-O2A-CGA	2.06	121.64	116.65
18	A	832	CLA	C2D-C1D-ND	2.06	112.17	110.13
18	A	818	CLA	CHA-C1A-NA	-2.06	121.72	126.39
29	3	303	LUT	C20-C13-C12	2.06	121.24	118.09
18	3	311	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
18	A	817	CLA	CAA-C2A-C3A	-2.06	107.43	113.00
30	2	316	CHL	C3D-C4D-ND	-2.06	109.63	112.94
18	B	801	CLA	CMD-C2D-C3D	-2.06	122.96	127.69
18	A	809	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
18	3	309	CLA	C1-O2A-CGA	2.06	121.64	116.65
18	1	5007	CLA	CHA-C1A-NA	-2.06	121.73	126.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	841	CLA	C1-O2A-CGA	2.06	121.63	116.65
18	A	822	CLA	CAA-C2A-C3A	-2.06	107.44	113.00
18	A	828	CLA	C6-C5-C3	-2.06	108.45	113.47
18	2	306	CLA	O1D-CGD-CBD	-2.06	120.46	124.52
18	A	840	CLA	C3B-C4B-NB	-2.06	108.69	110.53
30	1	5014	CHL	CMD-C2D-C3D	2.06	128.79	124.68
18	B	804	CLA	C1C-C2C-C3C	-2.06	104.82	106.98
21	I	102	BCR	C32-C1-C6	-2.06	107.02	110.24
21	L	307	BCR	C36-C18-C17	-2.06	119.48	122.82
21	I	101	BCR	C8-C7-C6	-2.06	121.50	127.00
18	A	830	CLA	C1D-ND-C4D	-2.06	104.87	106.31
18	A	812	CLA	CHA-C1A-NA	-2.06	121.73	126.39
18	A	823	CLA	CHA-C1A-NA	-2.06	121.73	126.39
18	B	835	CLA	CHA-C1A-NA	-2.06	121.73	126.39
21	A	845	BCR	C8-C7-C6	-2.06	121.51	127.00
21	L	303	BCR	C31-C1-C6	-2.06	107.02	110.24
18	1	5006	CLA	CHA-C1A-NA	-2.06	121.74	126.39
28	F	310	ZEX	C10-C11-C12	-2.06	117.24	123.20
18	3	307	CLA	CHA-C1A-NA	-2.06	121.74	126.39
18	4	311	CLA	CMD-C2D-C3D	-2.05	122.98	127.69
30	1	5016	CHL	CMD-C2D-C3D	2.05	128.79	124.68
18	L	301	CLA	CHA-C1A-NA	-2.05	121.74	126.39
30	2	319	CHL	C4C-CHD-C1D	2.05	123.42	116.07
18	B	820	CLA	CHA-C1A-NA	-2.05	121.74	126.39
18	A	831	CLA	CBB-CAB-C3B	-2.05	117.27	127.53
18	3	311	CLA	C1D-ND-C4D	-2.05	104.87	106.31
18	J	1101	CLA	C3B-C4B-NB	-2.05	108.70	110.53
18	B	837	CLA	C2D-C1D-ND	2.05	112.16	110.13
18	4	311	CLA	CHA-C1A-NA	-2.05	121.75	126.39
18	2	312	CLA	CMD-C2D-C3D	-2.05	122.99	127.69
30	2	318	CHL	CMD-C2D-C3D	2.05	128.78	124.68
30	4	317	CHL	CMD-C2D-C3D	2.05	128.78	124.68
18	2	312	CLA	C3B-C4B-NB	-2.05	108.70	110.53
18	A	803	CLA	O2A-CGA-CBA	2.05	118.08	111.83
22	A	849	LHG	O7-C7-O9	-2.05	118.91	123.70
18	H	1701	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
18	2	306	CLA	CAA-C2A-C1A	-2.05	105.26	111.97
21	B	847	BCR	C33-C5-C4	2.05	117.96	113.60
18	2	307	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
18	3	308	CLA	CHA-C1A-NA	-2.05	121.75	126.39
18	1	5018	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
18	4	311	CLA	O2A-CGA-CBA	2.05	118.08	111.83

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	J	1105	LUT	C19-C9-C8	2.05	121.22	118.09
18	1	5006	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
18	3	311	CLA	C1-O2A-CGA	2.05	121.61	116.65
21	A	846	BCR	C34-C9-C10	-2.05	119.50	122.82
18	B	833	CLA	C2D-C1D-ND	2.05	112.15	110.13
21	J	1104	BCR	C36-C18-C17	-2.05	119.50	122.82
18	A	820	CLA	C1D-ND-C4D	-2.05	104.88	106.31
18	A	836	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
18	F	301	CLA	CHA-C1A-NA	-2.05	121.76	126.39
18	G	1603	CLA	C2D-C1D-ND	2.05	112.15	110.13
18	3	314	CLA	C2D-C1D-ND	2.05	112.15	110.13
30	2	316	CHL	CMD-C2D-C3D	2.04	128.77	124.68
18	4	312	CLA	CHA-C1A-NA	-2.04	121.76	126.39
18	2	317	CLA	C1-O2A-CGA	2.04	121.60	116.65
18	B	820	CLA	C1D-ND-C4D	-2.04	104.88	106.31
18	1	5017	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
18	H	1701	CLA	O2A-CGA-CBA	2.04	118.07	111.83
18	2	311	CLA	C2D-C1D-ND	2.04	112.15	110.13
18	A	823	CLA	C1D-ND-C4D	-2.04	104.88	106.31
18	B	819	CLA	C2D-C1D-ND	2.04	112.15	110.13
18	B	818	CLA	CAA-C2A-C3A	-2.04	107.48	113.00
21	A	843	BCR	C38-C26-C25	-2.04	122.26	124.48
21	F	304	BCR	C15-C14-C13	-2.04	124.42	127.28
18	B	801	CLA	C2D-C1D-ND	2.04	112.15	110.13
18	B	835	CLA	C1D-ND-C4D	-2.04	104.88	106.31
30	3	312	CHL	CMD-C2D-C3D	2.04	128.76	124.68
18	A	818	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
18	B	816	CLA	C2D-C1D-ND	2.04	112.14	110.13
18	1	5011	CLA	CHA-C1A-NA	-2.04	121.77	126.39
18	A	814	CLA	C2D-C1D-ND	2.04	112.14	110.13
18	3	314	CLA	C1-O2A-CGA	2.04	121.59	116.65
18	B	826	CLA	C2D-C1D-ND	2.04	112.14	110.13
18	B	811	CLA	C1-O2A-CGA	2.04	121.58	116.65
18	B	805	CLA	CHA-C1A-NA	-2.04	121.78	126.39
18	A	819	CLA	CHA-C1A-NA	-2.04	121.78	126.39
18	B	838	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
18	B	814	CLA	C1D-ND-C4D	-2.04	104.88	106.31
29	J	1105	LUT	C10-C11-C12	-2.04	117.30	123.20
21	B	844	BCR	C37-C22-C23	2.04	121.20	118.09
18	3	315	CLA	CHA-C1A-NA	-2.04	121.78	126.39
18	B	817	CLA	C2D-C1D-ND	2.03	112.14	110.13
18	B	815	CLA	CHA-C1A-NA	-2.03	121.78	126.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	841	CLA	O2A-CGA-CBA	2.03	118.04	111.83
21	L	307	BCR	C27-C26-C25	-2.03	119.96	122.70
18	B	840	CLA	CHA-C1A-NA	-2.03	121.79	126.39
18	3	301	CLA	C2D-C1D-ND	2.03	112.14	110.13
18	1	5018	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
18	B	827	CLA	CHD-C1D-ND	-2.03	121.94	124.80
18	A	808	CLA	C1D-ND-C4D	-2.03	104.89	106.31
18	4	309	CLA	O2A-CGA-CBA	2.03	118.03	111.83
28	F	310	ZEX	C21-C26-C27	2.03	121.16	115.65
29	3	303	LUT	C8-C7-C6	-2.03	121.58	127.00
18	2	311	CLA	CMA-C3A-C4A	2.03	117.23	111.77
18	A	804	CLA	CAA-C2A-C3A	-2.03	107.52	113.00
18	A	834	CLA	C3B-C4B-NB	-2.03	108.72	110.53
29	1	5004	LUT	C3-C4-C5	-2.03	107.13	112.18
18	4	306	CLA	C1D-ND-C4D	-2.03	104.89	106.31
21	I	101	BCR	C38-C26-C27	2.03	117.92	113.60
18	2	313	CLA	CHA-C1A-NA	-2.03	121.80	126.39
21	2	305	BCR	C23-C24-C25	-2.03	121.58	127.00
24	1	5020	LMG	O7-C10-O9	-2.03	118.97	123.70
18	B	804	CLA	C2D-C1D-ND	2.03	112.13	110.13
18	B	810	CLA	C2D-C1D-ND	2.03	112.13	110.13
18	A	803	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
18	A	831	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
18	A	805	CLA	CMA-C3A-C4A	2.03	117.22	111.77
18	2	308	CLA	CAA-C2A-C3A	-2.03	107.52	113.00
18	1	5010	CLA	CBC-CAC-C3C	-2.03	106.93	112.42
18	B	822	CLA	C2D-C1D-ND	2.02	112.13	110.13
18	G	1603	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
18	B	829	CLA	C1-O2A-CGA	2.02	121.55	116.65
18	B	832	CLA	C1-O2A-CGA	2.02	121.55	116.65
18	B	810	CLA	C3B-C4B-NB	-2.02	108.72	110.53
18	L	305	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
21	L	307	BCR	C38-C26-C27	2.02	117.91	113.60
23	B	856	LMT	C3B-C4B-C5B	-2.02	106.56	110.23
18	3	307	CLA	C6-C5-C3	-2.02	108.54	113.47
18	1	5012	CLA	C2D-C1D-ND	2.02	112.13	110.13
18	B	817	CLA	CMC-C2C-C1C	2.02	128.19	125.03
18	B	837	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
18	B	806	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
18	H	1701	CLA	C1D-ND-C4D	-2.02	104.89	106.31
21	B	843	BCR	C38-C26-C25	-2.02	122.28	124.48
18	B	816	CLA	CHA-C1A-NA	-2.02	121.82	126.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	816	CLA	C3B-C4B-NB	-2.02	108.73	110.53
18	3	307	CLA	O2D-CGD-O1D	-2.02	119.92	123.85
18	B	840	CLA	C2D-C1D-ND	2.02	112.12	110.13
18	1	5009	CLA	C1-O2A-CGA	2.02	121.54	116.65
18	A	836	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
18	A	852	CLA	C1-O2A-CGA	2.02	121.53	116.65
18	3	301	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
18	B	835	CLA	C2D-C1D-ND	2.02	112.12	110.13
18	2	317	CLA	C3B-C4B-NB	-2.02	108.73	110.53
22	A	849	LHG	O8-C23-O10	-2.02	118.58	123.63
18	A	815	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
24	B	850	LMG	O8-C28-O10	-2.02	118.59	123.63
18	L	301	CLA	CAA-C2A-C3A	-2.01	107.55	113.00
21	A	844	BCR	C23-C24-C25	-2.01	121.62	127.00
18	A	825	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
18	4	306	CLA	C2D-C1D-ND	2.01	112.12	110.13
18	1	5007	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
18	B	815	CLA	C3B-C4B-NB	-2.01	108.73	110.53
18	2	313	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
24	B	850	LMG	O7-C10-O9	-2.01	119.00	123.70
29	4	303	LUT	C22-C23-C24	-2.01	108.20	111.18
18	B	807	CLA	CHA-C1A-NA	-2.01	121.83	126.39
18	B	812	CLA	C2D-C1D-ND	2.01	112.12	110.13
18	B	831	CLA	C1-O2A-CGA	2.01	121.52	116.65
30	2	315	CHL	CMD-C2D-C3D	2.01	128.70	124.68
18	A	813	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
18	A	832	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
18	3	319	CLA	CHA-C1A-NA	-2.01	121.84	126.39
18	J	1103	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
18	B	836	CLA	C2D-C1D-ND	2.01	112.11	110.13
18	G	1601	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
18	F	301	CLA	CAA-C2A-C3A	-2.01	107.57	113.00
29	J	1105	LUT	C35-C15-C14	-2.01	119.41	123.52
21	3	306	BCR	C27-C26-C25	-2.01	119.99	122.70
18	B	838	CLA	CAA-C2A-C3A	-2.01	107.57	113.00
18	J	1103	CLA	C2D-C1D-ND	2.01	112.11	110.13
18	B	841	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
18	B	821	CLA	CHA-C1A-NA	-2.01	121.85	126.39
18	A	840	CLA	C1D-ND-C4D	-2.01	104.91	106.31
18	L	305	CLA	CHA-C1A-NA	-2.00	121.85	126.39
18	1	5013	CLA	CHA-C1A-NA	-2.00	121.85	126.39
18	A	823	CLA	C3D-C2D-C1D	-2.00	103.09	105.83

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	5007	CLA	C3D-C2D-C1D	-2.00	103.09	105.83
18	3	315	CLA	O2A-CGA-CBA	2.00	117.94	111.83
18	A	827	CLA	CHA-C1A-NA	-2.00	121.86	126.39
18	4	307	CLA	C2D-C1D-ND	2.00	112.11	110.13
18	1	5010	CLA	O2A-CGA-CBA	2.00	117.94	111.83
18	4	307	CLA	CHA-C1A-NA	-2.00	121.86	126.39
18	B	808	CLA	C1-O2A-CGA	2.00	121.50	116.65
18	A	832	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
18	A	823	CLA	C2D-C1D-ND	2.00	112.11	110.13
18	L	301	CLA	C2D-C1D-ND	2.00	112.11	110.13
18	3	317	CLA	CHA-C1A-NA	-2.00	121.86	126.39

All (206) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	A	801	CL0	NC
17	A	801	CL0	NA
17	A	801	CL0	ND
18	A	802	CLA	ND
18	A	803	CLA	ND
18	A	804	CLA	ND
18	A	805	CLA	ND
18	A	806	CLA	ND
18	A	807	CLA	ND
18	A	808	CLA	ND
18	A	809	CLA	ND
18	A	810	CLA	ND
18	A	811	CLA	ND
18	A	812	CLA	ND
18	A	813	CLA	ND
18	A	814	CLA	ND
18	A	815	CLA	ND
18	A	816	CLA	ND
18	A	817	CLA	ND
18	A	818	CLA	ND
18	A	819	CLA	ND
18	A	820	CLA	ND
18	A	821	CLA	ND
18	A	822	CLA	ND
18	A	823	CLA	ND
18	A	824	CLA	ND
18	A	825	CLA	ND

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
18	A	826	CLA	ND
18	A	827	CLA	ND
18	A	828	CLA	ND
18	A	829	CLA	ND
18	A	830	CLA	ND
18	A	831	CLA	ND
18	A	832	CLA	ND
18	A	833	CLA	ND
18	A	834	CLA	ND
18	A	835	CLA	ND
18	A	836	CLA	ND
18	A	837	CLA	ND
18	A	838	CLA	ND
18	A	839	CLA	ND
18	A	840	CLA	ND
18	A	852	CLA	ND
18	A	853	CLA	ND
18	B	801	CLA	ND
18	B	803	CLA	ND
18	B	804	CLA	ND
18	B	805	CLA	ND
18	B	806	CLA	ND
18	B	807	CLA	ND
18	B	808	CLA	ND
18	B	809	CLA	ND
18	B	810	CLA	ND
18	B	811	CLA	ND
18	B	812	CLA	ND
18	B	813	CLA	ND
18	B	814	CLA	ND
18	B	815	CLA	ND
18	B	816	CLA	ND
18	B	817	CLA	ND
18	B	818	CLA	ND
18	B	819	CLA	ND
18	B	820	CLA	ND
18	B	821	CLA	ND
18	B	822	CLA	ND
18	B	823	CLA	ND
18	B	824	CLA	ND
18	B	825	CLA	ND
18	B	826	CLA	ND

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
18	B	827	CLA	ND
18	B	828	CLA	ND
18	B	829	CLA	ND
18	B	830	CLA	ND
18	B	831	CLA	ND
18	B	832	CLA	ND
18	B	833	CLA	ND
18	B	834	CLA	ND
18	B	835	CLA	ND
18	B	836	CLA	ND
18	B	837	CLA	ND
18	B	838	CLA	ND
18	B	839	CLA	ND
18	B	840	CLA	ND
18	B	841	CLA	ND
18	F	301	CLA	ND
18	F	302	CLA	ND
18	F	303	CLA	ND
18	G	1601	CLA	ND
18	G	1602	CLA	ND
18	G	1603	CLA	ND
18	H	1701	CLA	ND
18	J	1101	CLA	ND
18	J	1103	CLA	ND
18	K	1401	CLA	ND
18	K	1402	CLA	ND
18	K	1403	CLA	ND
18	K	1404	CLA	ND
18	L	301	CLA	ND
18	L	304	CLA	ND
18	L	305	CLA	ND
18	L	306	CLA	ND
18	1	5006	CLA	ND
18	1	5007	CLA	ND
18	1	5008	CLA	ND
18	1	5009	CLA	ND
18	1	5010	CLA	ND
18	1	5011	CLA	ND
18	1	5012	CLA	ND
18	1	5013	CLA	ND
18	1	5015	CLA	ND
18	1	5017	CLA	ND

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atom
18	1	5018	CLA	ND
18	2	306	CLA	ND
18	2	307	CLA	ND
18	2	308	CLA	ND
18	2	309	CLA	ND
18	2	310	CLA	ND
18	2	311	CLA	ND
18	2	312	CLA	ND
18	2	313	CLA	ND
18	2	317	CLA	ND
18	2	326	CLA	ND
18	3	301	CLA	ND
18	3	307	CLA	ND
18	3	308	CLA	ND
18	3	309	CLA	ND
18	3	311	CLA	ND
18	3	314	CLA	ND
18	3	315	CLA	ND
18	3	317	CLA	ND
18	3	318	CLA	ND
18	3	319	CLA	ND
18	4	305	CLA	ND
18	4	306	CLA	ND
18	4	307	CLA	ND
18	4	308	CLA	ND
18	4	309	CLA	ND
18	4	310	CLA	ND
18	4	311	CLA	ND
18	4	312	CLA	ND
18	4	315	CLA	ND
29	J	1105	LUT	C26
29	1	5004	LUT	C26
29	2	303	LUT	C26
29	3	304	LUT	C26
30	1	5014	CHL	NC
30	1	5014	CHL	NA
30	1	5014	CHL	ND
30	1	5016	CHL	NC
30	1	5016	CHL	C8
30	1	5016	CHL	NA
30	1	5016	CHL	ND
30	2	314	CHL	NC

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
30	2	314	CHL	C8
30	2	314	CHL	NA
30	2	314	CHL	ND
30	2	315	CHL	NC
30	2	315	CHL	C8
30	2	315	CHL	NA
30	2	315	CHL	ND
30	2	316	CHL	NC
30	2	316	CHL	NA
30	2	316	CHL	ND
30	2	318	CHL	NC
30	2	318	CHL	NA
30	2	318	CHL	ND
30	2	319	CHL	NC
30	2	319	CHL	C8
30	2	319	CHL	NA
30	2	319	CHL	ND
30	3	310	CHL	NC
30	3	310	CHL	C8
30	3	310	CHL	NA
30	3	310	CHL	ND
30	3	312	CHL	NC
30	3	312	CHL	NA
30	3	312	CHL	ND
30	3	313	CHL	NC
30	3	313	CHL	NA
30	3	313	CHL	ND
30	3	316	CHL	NC
30	3	316	CHL	NA
30	3	316	CHL	ND
30	4	302	CHL	NC
30	4	302	CHL	C8
30	4	302	CHL	NA
30	4	302	CHL	ND
30	4	313	CHL	NC
30	4	313	CHL	NA
30	4	313	CHL	ND
30	4	314	CHL	NC
30	4	314	CHL	NA
30	4	314	CHL	ND
30	4	316	CHL	NC
30	4	316	CHL	C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
30	4	316	CHL	NA
30	4	316	CHL	ND
30	4	317	CHL	NC
30	4	317	CHL	NA
30	4	317	CHL	ND
30	4	318	CHL	NC
30	4	318	CHL	C8
30	4	318	CHL	NA
30	4	318	CHL	ND
31	2	304	XAT	C6
31	4	304	XAT	C6

All (2665) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	802	CLA	C2-C1-O2A-CGA
18	A	802	CLA	C4-C3-C5-C6
18	A	803	CLA	C1A-C2A-CAA-CBA
18	A	803	CLA	C3A-C2A-CAA-CBA
18	A	803	CLA	C2B-C3B-CAB-CBB
18	A	803	CLA	C4B-C3B-CAB-CBB
18	A	803	CLA	CHA-CBD-CGD-O1D
18	A	803	CLA	CHA-CBD-CGD-O2D
18	A	804	CLA	C1A-C2A-CAA-CBA
18	A	804	CLA	C3A-C2A-CAA-CBA
18	A	804	CLA	C2-C1-O2A-CGA
18	A	804	CLA	CAD-CBD-CGD-O1D
18	A	804	CLA	CAD-CBD-CGD-O2D
18	A	805	CLA	C3A-C2A-CAA-CBA
18	A	805	CLA	CBD-CGD-O2D-CED
18	A	806	CLA	C2-C1-O2A-CGA
18	A	806	CLA	CBD-CGD-O2D-CED
18	A	807	CLA	C3A-C2A-CAA-CBA
18	A	807	CLA	CHA-CBD-CGD-O1D
18	A	807	CLA	CHA-CBD-CGD-O2D
18	A	808	CLA	CBD-CGD-O2D-CED
18	A	809	CLA	C2B-C3B-CAB-CBB
18	A	809	CLA	C4B-C3B-CAB-CBB
18	A	809	CLA	CBD-CGD-O2D-CED
18	A	810	CLA	C1A-C2A-CAA-CBA
18	A	810	CLA	C3A-C2A-CAA-CBA
18	A	811	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	811	CLA	C3A-C2A-CAA-CBA
18	A	813	CLA	C14-C13-C15-C16
18	A	814	CLA	CHA-CBD-CGD-O1D
18	A	814	CLA	CHA-CBD-CGD-O2D
18	A	814	CLA	CBD-CGD-O2D-CED
18	A	816	CLA	C3A-C2A-CAA-CBA
18	A	816	CLA	CBD-CGD-O2D-CED
18	A	818	CLA	C2-C1-O2A-CGA
18	A	818	CLA	CBD-CGD-O2D-CED
18	A	819	CLA	C2-C1-O2A-CGA
18	A	819	CLA	C2-C3-C5-C6
18	A	819	CLA	C4-C3-C5-C6
18	A	821	CLA	CBD-CGD-O2D-CED
18	A	823	CLA	C2-C1-O2A-CGA
18	A	824	CLA	C1A-C2A-CAA-CBA
18	A	824	CLA	C3A-C2A-CAA-CBA
18	A	825	CLA	C1A-C2A-CAA-CBA
18	A	825	CLA	C3A-C2A-CAA-CBA
18	A	826	CLA	C1A-C2A-CAA-CBA
18	A	826	CLA	C2-C1-O2A-CGA
18	A	828	CLA	CHA-CBD-CGD-O2D
18	A	830	CLA	C2B-C3B-CAB-CBB
18	A	830	CLA	C4B-C3B-CAB-CBB
18	A	831	CLA	CHA-CBD-CGD-O1D
18	A	831	CLA	CHA-CBD-CGD-O2D
18	A	831	CLA	C14-C13-C15-C16
18	A	832	CLA	C11-C10-C8-C9
18	A	833	CLA	C2B-C3B-CAB-CBB
18	A	833	CLA	C4B-C3B-CAB-CBB
18	A	834	CLA	C1A-C2A-CAA-CBA
18	A	834	CLA	C3A-C2A-CAA-CBA
18	A	834	CLA	CBD-CGD-O2D-CED
18	A	837	CLA	CBD-CGD-O2D-CED
18	A	839	CLA	CBD-CGD-O2D-CED
18	A	853	CLA	CBD-CGD-O2D-CED
18	A	853	CLA	C11-C12-C13-C14
18	B	801	CLA	CAD-CBD-CGD-O1D
18	B	801	CLA	CAD-CBD-CGD-O2D
18	B	803	CLA	CBD-CGD-O2D-CED
18	B	804	CLA	CBD-CGD-O2D-CED
18	B	805	CLA	C1A-C2A-CAA-CBA
18	B	805	CLA	C3A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	B	805	CLA	CBD-CGD-O2D-CED
18	B	806	CLA	C3A-C2A-CAA-CBA
18	B	807	CLA	C6-C7-C8-C9
18	B	809	CLA	C2B-C3B-CAB-CBB
18	B	809	CLA	C4B-C3B-CAB-CBB
18	B	809	CLA	CBD-CGD-O2D-CED
18	B	810	CLA	C2-C1-O2A-CGA
18	B	810	CLA	CBD-CGD-O2D-CED
18	B	811	CLA	C2-C1-O2A-CGA
18	B	811	CLA	CBD-CGD-O2D-CED
18	B	811	CLA	C6-C7-C8-C9
18	B	813	CLA	CBD-CGD-O2D-CED
18	B	816	CLA	CBD-CGD-O2D-CED
18	B	818	CLA	C2-C1-O2A-CGA
18	B	818	CLA	CBD-CGD-O2D-CED
18	B	818	CLA	C11-C10-C8-C9
18	B	820	CLA	C2B-C3B-CAB-CBB
18	B	820	CLA	C4B-C3B-CAB-CBB
18	B	821	CLA	CBA-CGA-O2A-C1
18	B	821	CLA	O1A-CGA-O2A-C1
18	B	824	CLA	C2B-C3B-CAB-CBB
18	B	824	CLA	C4B-C3B-CAB-CBB
18	B	825	CLA	C2-C1-O2A-CGA
18	B	826	CLA	C3A-C2A-CAA-CBA
18	B	826	CLA	CHA-CBD-CGD-O1D
18	B	826	CLA	CHA-CBD-CGD-O2D
18	B	828	CLA	C1A-C2A-CAA-CBA
18	B	829	CLA	C1A-C2A-CAA-CBA
18	B	829	CLA	C3A-C2A-CAA-CBA
18	B	830	CLA	CAD-CBD-CGD-O1D
18	B	830	CLA	CAD-CBD-CGD-O2D
18	B	832	CLA	C1A-C2A-CAA-CBA
18	B	832	CLA	C3A-C2A-CAA-CBA
18	B	832	CLA	C11-C10-C8-C9
18	B	833	CLA	C1A-C2A-CAA-CBA
18	B	833	CLA	C3A-C2A-CAA-CBA
18	B	833	CLA	CHA-CBD-CGD-O1D
18	B	833	CLA	CHA-CBD-CGD-O2D
18	B	835	CLA	C2-C1-O2A-CGA
18	B	835	CLA	CBD-CGD-O2D-CED
18	B	836	CLA	C1A-C2A-CAA-CBA
18	B	836	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	B	839	CLA	C2-C1-O2A-CGA
18	B	839	CLA	C4B-C3B-CAB-CBB
18	B	840	CLA	C1A-C2A-CAA-CBA
18	B	840	CLA	C3A-C2A-CAA-CBA
18	B	840	CLA	CBD-CGD-O2D-CED
18	F	301	CLA	C2-C1-O2A-CGA
18	F	301	CLA	CBD-CGD-O2D-CED
18	F	302	CLA	C1A-C2A-CAA-CBA
18	F	302	CLA	C3A-C2A-CAA-CBA
18	F	302	CLA	C2-C1-O2A-CGA
18	G	1601	CLA	CBD-CGD-O2D-CED
18	G	1602	CLA	CBA-CGA-O2A-C1
18	H	1701	CLA	CBD-CGD-O2D-CED
18	K	1402	CLA	C1A-C2A-CAA-CBA
18	K	1403	CLA	CHA-CBD-CGD-O1D
18	K	1403	CLA	CHA-CBD-CGD-O2D
18	K	1403	CLA	CBD-CGD-O2D-CED
18	L	301	CLA	CBD-CGD-O2D-CED
18	L	304	CLA	C1A-C2A-CAA-CBA
18	L	304	CLA	C2-C1-O2A-CGA
18	L	306	CLA	C1A-C2A-CAA-CBA
18	1	5007	CLA	CBA-CGA-O2A-C1
18	1	5007	CLA	CBD-CGD-O2D-CED
18	1	5008	CLA	C1A-C2A-CAA-CBA
18	1	5008	CLA	CBD-CGD-O2D-CED
18	1	5009	CLA	CHA-CBD-CGD-O1D
18	1	5009	CLA	CHA-CBD-CGD-O2D
18	1	5010	CLA	CBD-CGD-O2D-CED
18	1	5011	CLA	CBD-CGD-O2D-CED
18	1	5013	CLA	C2B-C3B-CAB-CBB
18	1	5013	CLA	C4B-C3B-CAB-CBB
18	1	5013	CLA	CBD-CGD-O2D-CED
18	1	5015	CLA	C2-C1-O2A-CGA
18	1	5018	CLA	CHA-CBD-CGD-O1D
18	1	5018	CLA	CHA-CBD-CGD-O2D
18	2	306	CLA	C3A-C2A-CAA-CBA
18	2	309	CLA	C3A-C2A-CAA-CBA
18	2	311	CLA	C1A-C2A-CAA-CBA
18	2	312	CLA	CBD-CGD-O2D-CED
18	2	313	CLA	C1A-C2A-CAA-CBA
18	2	326	CLA	CAD-CBD-CGD-O1D
18	2	326	CLA	CAD-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	3	301	CLA	C3A-C2A-CAA-CBA
18	3	307	CLA	C1A-C2A-CAA-CBA
18	3	307	CLA	C3A-C2A-CAA-CBA
18	3	308	CLA	C3-C5-C6-C7
18	3	309	CLA	C4-C3-C5-C6
18	3	314	CLA	C1A-C2A-CAA-CBA
18	3	315	CLA	C3A-C2A-CAA-CBA
18	3	317	CLA	C1A-C2A-CAA-CBA
18	3	317	CLA	C3A-C2A-CAA-CBA
18	3	317	CLA	C2-C1-O2A-CGA
18	3	317	CLA	CBD-CGD-O2D-CED
18	3	318	CLA	C1A-C2A-CAA-CBA
18	3	318	CLA	C3A-C2A-CAA-CBA
18	3	318	CLA	CBD-CGD-O2D-CED
18	3	319	CLA	C2-C1-O2A-CGA
18	3	319	CLA	CHA-CBD-CGD-O1D
18	3	319	CLA	CHA-CBD-CGD-O2D
18	3	319	CLA	CBD-CGD-O2D-CED
18	4	306	CLA	CHA-CBD-CGD-O1D
18	4	306	CLA	CHA-CBD-CGD-O2D
18	4	308	CLA	CHA-CBD-CGD-O1D
18	4	308	CLA	CHA-CBD-CGD-O2D
18	4	309	CLA	C1A-C2A-CAA-CBA
18	4	311	CLA	C1A-C2A-CAA-CBA
18	4	311	CLA	C3A-C2A-CAA-CBA
18	4	315	CLA	O1A-CGA-O2A-C1
18	4	315	CLA	CBD-CGD-O2D-CED
21	A	843	BCR	C11-C10-C9-C8
21	A	843	BCR	C11-C10-C9-C34
21	A	843	BCR	C10-C11-C12-C13
21	A	843	BCR	C11-C12-C13-C14
21	A	844	BCR	C11-C10-C9-C8
21	A	844	BCR	C11-C10-C9-C34
21	A	845	BCR	C11-C10-C9-C8
21	A	845	BCR	C11-C10-C9-C34
21	A	845	BCR	C17-C18-C19-C20
21	A	845	BCR	C36-C18-C19-C20
21	A	845	BCR	C21-C22-C23-C24
21	A	846	BCR	C11-C10-C9-C8
21	A	846	BCR	C11-C10-C9-C34
21	A	846	BCR	C10-C11-C12-C13
21	A	847	BCR	C11-C10-C9-C8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	A	847	BCR	C11-C10-C9-C34
21	A	847	BCR	C17-C18-C19-C20
21	A	847	BCR	C36-C18-C19-C20
21	A	847	BCR	C21-C22-C23-C24
21	A	847	BCR	C37-C22-C23-C24
21	A	855	BCR	C5-C6-C7-C8
21	A	855	BCR	C7-C8-C9-C10
21	A	855	BCR	C7-C8-C9-C34
21	A	855	BCR	C11-C10-C9-C8
21	A	855	BCR	C11-C10-C9-C34
21	B	802	BCR	C11-C10-C9-C8
21	B	802	BCR	C11-C10-C9-C34
21	B	843	BCR	C11-C10-C9-C8
21	B	843	BCR	C11-C10-C9-C34
21	B	843	BCR	C23-C24-C25-C26
21	B	843	BCR	C23-C24-C25-C30
21	B	844	BCR	C11-C10-C9-C8
21	B	844	BCR	C11-C10-C9-C34
21	B	844	BCR	C17-C18-C19-C20
21	B	844	BCR	C36-C18-C19-C20
21	B	844	BCR	C21-C22-C23-C24
21	B	844	BCR	C37-C22-C23-C24
21	B	845	BCR	C11-C12-C13-C14
21	B	846	BCR	C11-C10-C9-C8
21	B	846	BCR	C11-C10-C9-C34
21	B	847	BCR	C11-C10-C9-C8
21	B	847	BCR	C11-C10-C9-C34
21	B	847	BCR	C10-C11-C12-C13
21	B	847	BCR	C17-C18-C19-C20
21	B	847	BCR	C36-C18-C19-C20
21	F	304	BCR	C7-C8-C9-C34
21	F	304	BCR	C11-C10-C9-C8
21	F	304	BCR	C11-C10-C9-C34
21	F	304	BCR	C17-C18-C19-C20
21	F	304	BCR	C36-C18-C19-C20
21	F	305	BCR	C7-C8-C9-C10
21	F	305	BCR	C7-C8-C9-C34
21	F	305	BCR	C11-C10-C9-C8
21	F	305	BCR	C11-C10-C9-C34
21	F	305	BCR	C10-C11-C12-C13
21	G	1604	BCR	C17-C18-C19-C20
21	I	101	BCR	C7-C8-C9-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	I	101	BCR	C10-C11-C12-C13
21	I	101	BCR	C17-C18-C19-C20
21	I	101	BCR	C36-C18-C19-C20
21	I	102	BCR	C7-C8-C9-C10
21	I	102	BCR	C11-C10-C9-C8
21	I	102	BCR	C11-C10-C9-C34
21	I	102	BCR	C10-C11-C12-C13
21	I	102	BCR	C23-C24-C25-C26
21	I	102	BCR	C23-C24-C25-C30
21	J	1104	BCR	C7-C8-C9-C10
21	J	1104	BCR	C11-C10-C9-C8
21	J	1104	BCR	C11-C10-C9-C34
21	J	1104	BCR	C10-C11-C12-C13
21	J	1104	BCR	C21-C22-C23-C24
21	J	1104	BCR	C37-C22-C23-C24
21	K	1405	BCR	C11-C10-C9-C8
21	K	1405	BCR	C11-C10-C9-C34
21	K	1405	BCR	C21-C22-C23-C24
21	K	1405	BCR	C37-C22-C23-C24
21	L	302	BCR	C7-C8-C9-C10
21	L	302	BCR	C7-C8-C9-C34
21	L	302	BCR	C11-C10-C9-C8
21	L	302	BCR	C11-C10-C9-C34
21	L	303	BCR	C7-C8-C9-C10
21	L	307	BCR	C7-C8-C9-C10
21	L	307	BCR	C11-C10-C9-C8
21	L	307	BCR	C11-C10-C9-C34
21	L	307	BCR	C10-C11-C12-C13
21	L	307	BCR	C11-C12-C13-C14
21	L	307	BCR	C11-C12-C13-C35
21	2	305	BCR	C11-C10-C9-C8
21	2	305	BCR	C11-C10-C9-C34
21	2	305	BCR	C11-C12-C13-C14
21	3	305	BCR	C5-C6-C7-C8
21	3	305	BCR	C7-C8-C9-C10
21	3	305	BCR	C7-C8-C9-C34
21	3	305	BCR	C11-C10-C9-C8
21	3	305	BCR	C11-C10-C9-C34
21	3	305	BCR	C10-C11-C12-C13
21	3	306	BCR	C5-C6-C7-C8
21	3	306	BCR	C11-C10-C9-C8
21	3	306	BCR	C11-C10-C9-C34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	4	301	BCR	C5-C6-C7-C8
21	4	301	BCR	C17-C18-C19-C20
21	4	301	BCR	C21-C22-C23-C24
21	4	301	BCR	C37-C22-C23-C24
22	A	848	LHG	C3-O3-P-O5
22	A	848	LHG	C3-O3-P-O6
22	A	848	LHG	C4-O6-P-O3
22	A	848	LHG	C4-O6-P-O4
22	A	848	LHG	C4-O6-P-O5
22	A	848	LHG	O7-C5-C6-O8
22	A	849	LHG	C3-O3-P-O5
22	A	849	LHG	C4-O6-P-O3
22	A	849	LHG	C4-O6-P-O4
22	B	848	LHG	O1-C1-C2-O2
22	B	848	LHG	O1-C1-C2-C3
22	B	848	LHG	C3-O3-P-O5
22	B	848	LHG	C4-O6-P-O3
22	B	848	LHG	C8-C7-O7-C5
22	B	849	LHG	C1-C2-C3-O3
22	B	849	LHG	C3-O3-P-O4
22	B	849	LHG	C3-O3-P-O5
22	B	849	LHG	C3-O3-P-O6
22	B	849	LHG	C4-O6-P-O5
22	B	849	LHG	C8-C7-O7-C5
22	1	5019	LHG	C3-O3-P-O4
22	1	5019	LHG	C3-O3-P-O5
22	1	5019	LHG	C3-O3-P-O6
22	2	320	LHG	O1-C1-C2-C3
22	2	320	LHG	C4-O6-P-O3
23	G	1605	LMT	C2-C1-O1'-C1'
23	2	325	LMT	O5'-C1'-O1'-C1
23	2	325	LMT	C2-C1-O1'-C1'
24	A	851	LMG	O6-C1-O1-C7
24	A	851	LMG	O9-C10-O7-C8
24	B	850	LMG	O9-C10-O7-C8
24	B	850	LMG	C11-C10-O7-C8
24	B	851	LMG	O9-C10-O7-C8
24	B	851	LMG	C11-C10-O7-C8
24	F	306	LMG	C11-C10-O7-C8
24	F	308	LMG	O9-C10-O7-C8
24	F	308	LMG	C11-C10-O7-C8
24	G	1607	LMG	C2-C1-O1-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
24	G	1607	LMG	C11-C10-O7-C8
24	J	1102	LMG	C11-C10-O7-C8
24	1	5001	LMG	O9-C10-O7-C8
24	2	321	LMG	O9-C10-O7-C8
24	2	321	LMG	C11-C10-O7-C8
26	B	855	DGD	O1B-C1B-O2G-C2G
26	F	309	DGD	C2D-C1D-O3G-C3G
26	F	309	DGD	O6D-C1D-O3G-C3G
26	F	309	DGD	C4D-C5D-C6D-O5D
26	2	327	DGD	O1G-C1G-C2G-O2G
28	F	310	ZEX	C25-C26-C27-C28
29	J	1105	LUT	C21-C26-C27-C28
29	J	1105	LUT	C27-C28-C29-C30
29	J	1105	LUT	C27-C28-C29-C39
29	J	1105	LUT	C29-C30-C31-C32
29	1	5004	LUT	C21-C26-C27-C28
29	1	5004	LUT	C27-C28-C29-C30
29	1	5004	LUT	C27-C28-C29-C39
29	2	303	LUT	C21-C26-C27-C28
29	3	304	LUT	C21-C26-C27-C28
29	4	303	LUT	C25-C26-C27-C28
30	2	318	CHL	C1A-C2A-CAA-CBA
30	3	310	CHL	C1A-C2A-CAA-CBA
30	3	310	CHL	C3A-C2A-CAA-CBA
30	4	316	CHL	C3A-C2A-CAA-CBA
30	4	318	CHL	C2-C3-C5-C6
30	4	318	CHL	C4-C3-C5-C6
31	2	304	XAT	C1-C6-C7-C8
31	2	304	XAT	O4-C6-C7-C8
31	2	304	XAT	C7-C8-C9-C10
31	2	304	XAT	C7-C8-C9-C19
18	A	805	CLA	O1D-CGD-O2D-CED
18	A	826	CLA	O1D-CGD-O2D-CED
18	A	838	CLA	O1D-CGD-O2D-CED
18	B	807	CLA	O1D-CGD-O2D-CED
18	B	810	CLA	O1D-CGD-O2D-CED
18	B	823	CLA	O1D-CGD-O2D-CED
18	B	835	CLA	O1D-CGD-O2D-CED
18	2	310	CLA	O1D-CGD-O2D-CED
22	B	848	LHG	O9-C7-O7-C5
18	A	810	CLA	O1D-CGD-O2D-CED
18	A	840	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	B	803	CLA	O1D-CGD-O2D-CED
18	B	804	CLA	O1D-CGD-O2D-CED
18	F	303	CLA	O1D-CGD-O2D-CED
18	G	1602	CLA	O1D-CGD-O2D-CED
18	L	306	CLA	O1D-CGD-O2D-CED
18	3	308	CLA	O1D-CGD-O2D-CED
18	3	309	CLA	O1D-CGD-O2D-CED
18	4	310	CLA	O1D-CGD-O2D-CED
18	A	802	CLA	CBD-CGD-O2D-CED
18	A	804	CLA	CBD-CGD-O2D-CED
18	A	810	CLA	CBD-CGD-O2D-CED
18	A	811	CLA	CBD-CGD-O2D-CED
18	A	813	CLA	CBD-CGD-O2D-CED
18	A	815	CLA	CBD-CGD-O2D-CED
18	A	819	CLA	CBD-CGD-O2D-CED
18	A	820	CLA	CBD-CGD-O2D-CED
18	A	824	CLA	CBD-CGD-O2D-CED
18	A	826	CLA	CBD-CGD-O2D-CED
18	A	830	CLA	CBD-CGD-O2D-CED
18	A	838	CLA	CBD-CGD-O2D-CED
18	A	840	CLA	CBD-CGD-O2D-CED
18	A	852	CLA	CBD-CGD-O2D-CED
18	B	806	CLA	CBD-CGD-O2D-CED
18	B	807	CLA	CBD-CGD-O2D-CED
18	B	812	CLA	CBD-CGD-O2D-CED
18	B	815	CLA	CBD-CGD-O2D-CED
18	B	819	CLA	CBD-CGD-O2D-CED
18	B	820	CLA	CBD-CGD-O2D-CED
18	B	821	CLA	CBD-CGD-O2D-CED
18	B	823	CLA	CBD-CGD-O2D-CED
18	B	828	CLA	CBD-CGD-O2D-CED
18	B	831	CLA	CBD-CGD-O2D-CED
18	B	832	CLA	CBD-CGD-O2D-CED
18	B	833	CLA	CBD-CGD-O2D-CED
18	B	834	CLA	CBD-CGD-O2D-CED
18	F	302	CLA	CBD-CGD-O2D-CED
18	F	303	CLA	CBD-CGD-O2D-CED
18	G	1602	CLA	CBD-CGD-O2D-CED
18	G	1603	CLA	CBD-CGD-O2D-CED
18	J	1101	CLA	CBD-CGD-O2D-CED
18	J	1103	CLA	CBD-CGD-O2D-CED
18	K	1401	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	K	1404	CLA	CBD-CGD-O2D-CED
18	L	304	CLA	CBD-CGD-O2D-CED
18	L	306	CLA	CBD-CGD-O2D-CED
18	1	5006	CLA	CBD-CGD-O2D-CED
18	1	5015	CLA	CBD-CGD-O2D-CED
18	1	5017	CLA	CBD-CGD-O2D-CED
18	1	5018	CLA	CBD-CGD-O2D-CED
18	2	308	CLA	CBD-CGD-O2D-CED
18	2	309	CLA	CBD-CGD-O2D-CED
18	2	310	CLA	CBD-CGD-O2D-CED
18	2	311	CLA	CBD-CGD-O2D-CED
18	2	313	CLA	CBD-CGD-O2D-CED
18	2	317	CLA	CBD-CGD-O2D-CED
18	3	308	CLA	CBD-CGD-O2D-CED
18	3	309	CLA	CBD-CGD-O2D-CED
18	3	311	CLA	CBD-CGD-O2D-CED
18	3	314	CLA	CBD-CGD-O2D-CED
18	3	315	CLA	CBD-CGD-O2D-CED
18	4	305	CLA	CBD-CGD-O2D-CED
18	4	307	CLA	CBD-CGD-O2D-CED
18	4	309	CLA	CBD-CGD-O2D-CED
18	4	310	CLA	CBD-CGD-O2D-CED
18	4	311	CLA	CBD-CGD-O2D-CED
18	4	312	CLA	CBD-CGD-O2D-CED
18	B	835	CLA	O1A-CGA-O2A-C1
18	G	1603	CLA	O1A-CGA-O2A-C1
18	L	301	CLA	O1A-CGA-O2A-C1
18	3	308	CLA	O1A-CGA-O2A-C1
18	3	309	CLA	O1A-CGA-O2A-C1
24	1	5001	LMG	O10-C28-O8-C9
24	2	322	LMG	O10-C28-O8-C9
18	A	814	CLA	O1A-CGA-O2A-C1
18	G	1602	CLA	O1A-CGA-O2A-C1
18	1	5007	CLA	O1A-CGA-O2A-C1
18	A	814	CLA	CBA-CGA-O2A-C1
18	1	5013	CLA	CBA-CGA-O2A-C1
18	A	815	CLA	O1D-CGD-O2D-CED
18	A	820	CLA	O1D-CGD-O2D-CED
18	F	302	CLA	O1D-CGD-O2D-CED
18	J	1103	CLA	O1D-CGD-O2D-CED
18	K	1404	CLA	O1D-CGD-O2D-CED
18	1	5015	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	1	5017	CLA	O1D-CGD-O2D-CED
18	2	311	CLA	O1D-CGD-O2D-CED
18	4	305	CLA	O1D-CGD-O2D-CED
18	A	829	CLA	CBA-CGA-O2A-C1
18	3	309	CLA	CBA-CGA-O2A-C1
18	3	311	CLA	CBA-CGA-O2A-C1
18	4	315	CLA	CBA-CGA-O2A-C1
24	2	322	LMG	C29-C28-O8-C9
18	A	803	CLA	CBD-CGD-O2D-CED
18	A	831	CLA	CBD-CGD-O2D-CED
18	B	829	CLA	CBD-CGD-O2D-CED
18	A	822	CLA	O1A-CGA-O2A-C1
18	A	829	CLA	O1A-CGA-O2A-C1
18	A	853	CLA	O1A-CGA-O2A-C1
18	B	818	CLA	O1A-CGA-O2A-C1
18	B	831	CLA	O1A-CGA-O2A-C1
18	G	1601	CLA	O1A-CGA-O2A-C1
18	J	1103	CLA	O1A-CGA-O2A-C1
18	1	5011	CLA	O1A-CGA-O2A-C1
18	2	308	CLA	O1A-CGA-O2A-C1
18	2	312	CLA	O1A-CGA-O2A-C1
18	2	317	CLA	O1A-CGA-O2A-C1
18	2	326	CLA	O1A-CGA-O2A-C1
18	3	311	CLA	O1A-CGA-O2A-C1
18	3	317	CLA	O1A-CGA-O2A-C1
18	4	306	CLA	O1A-CGA-O2A-C1
18	4	307	CLA	O1A-CGA-O2A-C1
24	A	851	LMG	O10-C28-O8-C9
18	1	5013	CLA	O1A-CGA-O2A-C1
18	A	809	CLA	O1D-CGD-O2D-CED
18	A	814	CLA	O1D-CGD-O2D-CED
18	A	818	CLA	O1D-CGD-O2D-CED
18	A	834	CLA	O1D-CGD-O2D-CED
18	A	837	CLA	O1D-CGD-O2D-CED
18	B	828	CLA	O1D-CGD-O2D-CED
18	K	1401	CLA	O1D-CGD-O2D-CED
18	1	5010	CLA	O1D-CGD-O2D-CED
18	3	314	CLA	O1D-CGD-O2D-CED
18	4	307	CLA	O1D-CGD-O2D-CED
18	A	816	CLA	O1D-CGD-O2D-CED
18	A	821	CLA	O1D-CGD-O2D-CED
18	B	809	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	B	811	CLA	O1D-CGD-O2D-CED
18	B	816	CLA	O1D-CGD-O2D-CED
18	B	818	CLA	O1D-CGD-O2D-CED
18	B	836	CLA	O1D-CGD-O2D-CED
18	B	840	CLA	O1D-CGD-O2D-CED
18	F	301	CLA	O1D-CGD-O2D-CED
18	G	1601	CLA	O1D-CGD-O2D-CED
18	H	1701	CLA	O1D-CGD-O2D-CED
18	K	1403	CLA	O1D-CGD-O2D-CED
18	1	5007	CLA	O1D-CGD-O2D-CED
18	1	5008	CLA	O1D-CGD-O2D-CED
18	1	5011	CLA	O1D-CGD-O2D-CED
18	1	5013	CLA	O1D-CGD-O2D-CED
18	3	318	CLA	O1D-CGD-O2D-CED
18	4	315	CLA	O1D-CGD-O2D-CED
18	B	826	CLA	O1A-CGA-O2A-C1
18	3	315	CLA	O1A-CGA-O2A-C1
22	B	849	LHG	O9-C7-O7-C5
24	F	306	LMG	O9-C10-O7-C8
24	J	1102	LMG	O9-C10-O7-C8
18	3	319	CLA	O1D-CGD-O2D-CED
18	1	5012	CLA	O1A-CGA-O2A-C1
18	A	803	CLA	C3-C5-C6-C7
18	A	807	CLA	C3-C5-C6-C7
18	A	816	CLA	C3-C5-C6-C7
18	A	821	CLA	C3-C5-C6-C7
18	A	825	CLA	C3-C5-C6-C7
18	A	829	CLA	C3-C5-C6-C7
18	A	830	CLA	C3-C5-C6-C7
18	A	852	CLA	C3-C5-C6-C7
18	B	807	CLA	C3-C5-C6-C7
18	B	808	CLA	C3-C5-C6-C7
18	B	810	CLA	C3-C5-C6-C7
18	B	815	CLA	C3-C5-C6-C7
18	B	824	CLA	C3-C5-C6-C7
18	B	832	CLA	C3-C5-C6-C7
18	B	836	CLA	C3-C5-C6-C7
18	F	302	CLA	C3-C5-C6-C7
18	K	1402	CLA	C3-C5-C6-C7
18	1	5018	CLA	C3-C5-C6-C7
18	2	306	CLA	C3-C5-C6-C7
18	2	308	CLA	C3-C5-C6-C7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	2	309	CLA	C3-C5-C6-C7
18	3	311	CLA	C3-C5-C6-C7
18	3	319	CLA	C3-C5-C6-C7
18	4	308	CLA	C3-C5-C6-C7
30	3	310	CHL	C3-C5-C6-C7
18	A	839	CLA	O1D-CGD-O2D-CED
18	A	809	CLA	CBA-CGA-O2A-C1
18	A	822	CLA	CBA-CGA-O2A-C1
18	A	826	CLA	CBA-CGA-O2A-C1
18	A	853	CLA	CBA-CGA-O2A-C1
18	B	818	CLA	CBA-CGA-O2A-C1
18	B	831	CLA	CBA-CGA-O2A-C1
18	B	835	CLA	CBA-CGA-O2A-C1
18	G	1601	CLA	CBA-CGA-O2A-C1
18	G	1603	CLA	CBA-CGA-O2A-C1
18	J	1103	CLA	CBA-CGA-O2A-C1
18	L	301	CLA	CBA-CGA-O2A-C1
18	1	5011	CLA	CBA-CGA-O2A-C1
18	2	307	CLA	CBA-CGA-O2A-C1
18	2	308	CLA	CBA-CGA-O2A-C1
18	2	312	CLA	CBA-CGA-O2A-C1
18	2	317	CLA	CBA-CGA-O2A-C1
18	3	308	CLA	CBA-CGA-O2A-C1
18	3	317	CLA	CBA-CGA-O2A-C1
18	3	319	CLA	CBA-CGA-O2A-C1
18	4	307	CLA	CBA-CGA-O2A-C1
18	4	310	CLA	CBA-CGA-O2A-C1
18	4	311	CLA	CBA-CGA-O2A-C1
24	B	850	LMG	C29-C28-O8-C9
24	1	5001	LMG	C29-C28-O8-C9
24	1	5020	LMG	C29-C28-O8-C9
18	A	807	CLA	CBD-CGD-O2D-CED
18	A	825	CLA	CBD-CGD-O2D-CED
18	A	827	CLA	CBD-CGD-O2D-CED
18	A	828	CLA	CBD-CGD-O2D-CED
18	A	829	CLA	CBD-CGD-O2D-CED
18	A	832	CLA	CBD-CGD-O2D-CED
18	A	835	CLA	CBD-CGD-O2D-CED
18	B	827	CLA	CBD-CGD-O2D-CED
18	B	839	CLA	CBD-CGD-O2D-CED
18	1	5009	CLA	CBD-CGD-O2D-CED
18	2	307	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	4	308	CLA	CBD-CGD-O2D-CED
24	A	851	LMG	C11-C10-O7-C8
24	1	5001	LMG	C11-C10-O7-C8
26	B	855	DGD	C2B-C1B-O2G-C2G
18	A	806	CLA	O1D-CGD-O2D-CED
18	A	808	CLA	O1D-CGD-O2D-CED
18	A	853	CLA	O1D-CGD-O2D-CED
18	B	805	CLA	O1D-CGD-O2D-CED
18	B	813	CLA	O1D-CGD-O2D-CED
18	L	301	CLA	O1D-CGD-O2D-CED
18	1	5006	CLA	O1D-CGD-O2D-CED
18	2	308	CLA	O1D-CGD-O2D-CED
18	2	309	CLA	O1D-CGD-O2D-CED
18	2	312	CLA	O1D-CGD-O2D-CED
18	3	317	CLA	O1D-CGD-O2D-CED
18	4	312	CLA	O1D-CGD-O2D-CED
18	1	5018	CLA	O1D-CGD-O2D-CED
18	2	313	CLA	O1D-CGD-O2D-CED
18	A	805	CLA	C4-C3-C5-C6
18	A	808	CLA	C4-C3-C5-C6
18	A	810	CLA	C4-C3-C5-C6
18	A	815	CLA	C4-C3-C5-C6
18	A	816	CLA	C4-C3-C5-C6
18	A	822	CLA	C4-C3-C5-C6
18	A	831	CLA	C4-C3-C5-C6
18	A	838	CLA	C4-C3-C5-C6
18	A	853	CLA	C4-C3-C5-C6
18	B	819	CLA	C4-C3-C5-C6
18	B	822	CLA	C4-C3-C5-C6
18	B	823	CLA	C4-C3-C5-C6
18	B	829	CLA	C4-C3-C5-C6
18	B	833	CLA	C4-C3-C5-C6
18	H	1701	CLA	C4-C3-C5-C6
18	K	1402	CLA	C4-C3-C5-C6
18	1	5006	CLA	C4-C3-C5-C6
18	1	5010	CLA	C4-C3-C5-C6
18	2	312	CLA	C4-C3-C5-C6
18	3	319	CLA	C4-C3-C5-C6
18	4	307	CLA	C4-C3-C5-C6
19	A	841	PQN	C14-C13-C15-C16
18	A	802	CLA	C2-C3-C5-C6
18	A	805	CLA	C2-C3-C5-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	808	CLA	C2-C3-C5-C6
18	A	816	CLA	C2-C3-C5-C6
18	A	822	CLA	C2-C3-C5-C6
18	A	831	CLA	C2-C3-C5-C6
18	A	853	CLA	C2-C3-C5-C6
18	B	819	CLA	C2-C3-C5-C6
18	B	823	CLA	C2-C3-C5-C6
18	B	829	CLA	C2-C3-C5-C6
18	B	833	CLA	C2-C3-C5-C6
18	K	1402	CLA	C2-C3-C5-C6
18	1	5006	CLA	C2-C3-C5-C6
18	1	5010	CLA	C2-C3-C5-C6
18	3	309	CLA	C2-C3-C5-C6
18	3	319	CLA	C2-C3-C5-C6
18	4	307	CLA	C2-C3-C5-C6
19	A	841	PQN	C12-C13-C15-C16
18	2	306	CLA	CBD-CGD-O2D-CED
18	A	804	CLA	O1D-CGD-O2D-CED
18	A	830	CLA	O1D-CGD-O2D-CED
18	2	317	CLA	O1D-CGD-O2D-CED
18	A	829	CLA	C2A-CAA-CBA-CGA
18	A	840	CLA	C2A-CAA-CBA-CGA
18	F	303	CLA	O1A-CGA-O2A-C1
18	A	804	CLA	C3-C5-C6-C7
18	B	823	CLA	C3-C5-C6-C7
18	B	830	CLA	C3-C5-C6-C7
18	G	1603	CLA	C3-C5-C6-C7
18	L	301	CLA	C3-C5-C6-C7
18	2	312	CLA	C3-C5-C6-C7
18	3	315	CLA	C3-C5-C6-C7
24	2	324	LMG	O6-C1-O1-C7
18	A	802	CLA	CBA-CGA-O2A-C1
18	B	812	CLA	CBA-CGA-O2A-C1
18	B	822	CLA	CBA-CGA-O2A-C1
18	K	1403	CLA	CBA-CGA-O2A-C1
18	L	306	CLA	CBA-CGA-O2A-C1
18	2	326	CLA	CBA-CGA-O2A-C1
18	3	315	CLA	CBA-CGA-O2A-C1
18	4	306	CLA	CBA-CGA-O2A-C1
18	4	309	CLA	CBA-CGA-O2A-C1
24	A	851	LMG	C29-C28-O8-C9
26	B	855	DGD	C8A-C9A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
26	F	309	DGD	O6D-C5D-C6D-O5D
23	B	852	LMT	O5'-C5'-C6'-O6'
23	B	853	LMT	O5B-C5B-C6B-O6B
21	F	305	BCR	C13-C14-C15-C16
21	K	1405	BCR	C15-C16-C17-C18
21	3	306	BCR	C19-C20-C21-C22
18	A	809	CLA	O1A-CGA-O2A-C1
18	A	826	CLA	O1A-CGA-O2A-C1
18	B	810	CLA	O1A-CGA-O2A-C1
18	B	812	CLA	O1A-CGA-O2A-C1
18	L	304	CLA	O1A-CGA-O2A-C1
18	L	306	CLA	O1A-CGA-O2A-C1
18	2	307	CLA	O1A-CGA-O2A-C1
18	3	319	CLA	O1A-CGA-O2A-C1
18	4	309	CLA	O1A-CGA-O2A-C1
18	4	311	CLA	O1A-CGA-O2A-C1
24	B	850	LMG	O10-C28-O8-C9
24	F	306	LMG	O10-C28-O8-C9
26	1	5002	DGD	O1A-C1A-O1G-C1G
24	G	1607	LMG	O9-C10-O7-C8
18	A	824	CLA	O1D-CGD-O2D-CED
18	A	852	CLA	O1D-CGD-O2D-CED
18	B	819	CLA	O1D-CGD-O2D-CED
18	B	809	CLA	C5-C6-C7-C8
18	1	5012	CLA	CBA-CGA-O2A-C1
24	1	5001	LMG	C35-C36-C37-C38
24	1	5001	LMG	C38-C39-C40-C41
24	1	5020	LMG	O6-C5-C6-O5
23	A	850	LMT	C4B-C5B-C6B-O6B
18	B	832	CLA	O1D-CGD-O2D-CED
18	A	813	CLA	C3-C5-C6-C7
18	A	836	CLA	C3-C5-C6-C7
18	B	811	CLA	C3-C5-C6-C7
18	F	303	CLA	C3-C5-C6-C7
18	1	5006	CLA	C3-C5-C6-C7
18	A	836	CLA	CBD-CGD-O2D-CED
18	B	808	CLA	CBD-CGD-O2D-CED
18	B	826	CLA	CBD-CGD-O2D-CED
18	3	307	CLA	CBD-CGD-O2D-CED
24	A	851	LMG	C17-C18-C19-C20
24	2	324	LMG	C2-C1-O1-C7
18	A	811	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	819	CLA	O1D-CGD-O2D-CED
18	B	806	CLA	O1D-CGD-O2D-CED
18	B	834	CLA	O1D-CGD-O2D-CED
18	L	304	CLA	O1D-CGD-O2D-CED
18	3	311	CLA	O1D-CGD-O2D-CED
18	4	309	CLA	O1D-CGD-O2D-CED
18	A	805	CLA	CBA-CGA-O2A-C1
18	A	816	CLA	CBA-CGA-O2A-C1
18	A	820	CLA	CBA-CGA-O2A-C1
18	A	821	CLA	CBA-CGA-O2A-C1
18	B	826	CLA	CBA-CGA-O2A-C1
18	B	833	CLA	CBA-CGA-O2A-C1
18	F	303	CLA	CBA-CGA-O2A-C1
18	L	304	CLA	CBA-CGA-O2A-C1
18	2	309	CLA	CBA-CGA-O2A-C1
18	2	313	CLA	CBA-CGA-O2A-C1
26	1	5002	DGD	C2A-C1A-O1G-C1G
23	B	853	LMT	O5'-C5'-C6'-O6'
18	A	802	CLA	O1A-CGA-O2A-C1
18	A	805	CLA	O1A-CGA-O2A-C1
18	B	822	CLA	O1A-CGA-O2A-C1
18	K	1403	CLA	O1A-CGA-O2A-C1
18	4	310	CLA	O1A-CGA-O2A-C1
24	1	5020	LMG	O10-C28-O8-C9
23	G	1606	LMT	C4B-C5B-C6B-O6B
18	B	812	CLA	O1D-CGD-O2D-CED
23	G	1605	LMT	C3'-C4'-O1B-C1B
23	2	325	LMT	C4'-C5'-C6'-O6'
18	3	318	CLA	CBA-CGA-O2A-C1
23	2	325	LMT	O5'-C5'-C6'-O6'
18	B	820	CLA	O1D-CGD-O2D-CED
18	B	821	CLA	O1D-CGD-O2D-CED
18	B	831	CLA	O1D-CGD-O2D-CED
18	G	1603	CLA	O1D-CGD-O2D-CED
18	3	315	CLA	O1D-CGD-O2D-CED
18	A	805	CLA	C3-C5-C6-C7
18	B	833	CLA	C3-C5-C6-C7
18	A	817	CLA	CBD-CGD-O2D-CED
18	B	817	CLA	CBD-CGD-O2D-CED
18	B	822	CLA	CBD-CGD-O2D-CED
23	A	850	LMT	O5B-C5B-C6B-O6B
18	A	802	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	813	CLA	O1D-CGD-O2D-CED
18	B	815	CLA	O1D-CGD-O2D-CED
18	4	311	CLA	O1D-CGD-O2D-CED
18	B	810	CLA	CBA-CGA-O2A-C1
24	F	306	LMG	C29-C28-O8-C9
18	A	832	CLA	C4-C3-C5-C6
18	B	840	CLA	C4-C3-C5-C6
18	2	307	CLA	C4-C3-C5-C6
18	A	810	CLA	C2-C3-C5-C6
18	A	815	CLA	C2-C3-C5-C6
18	A	832	CLA	C2-C3-C5-C6
18	B	822	CLA	C2-C3-C5-C6
18	2	312	CLA	C2-C3-C5-C6
30	2	314	CHL	C2-C3-C5-C6
18	A	816	CLA	O1A-CGA-O2A-C1
18	A	821	CLA	O1A-CGA-O2A-C1
18	B	833	CLA	O1A-CGA-O2A-C1
23	G	1606	LMT	O5B-C5B-C6B-O6B
23	2	325	LMT	O5B-C5B-C6B-O6B
23	B	852	LMT	C4'-C5'-C6'-O6'
23	B	853	LMT	C4B-C5B-C6B-O6B
24	1	5020	LMG	C4-C5-C6-O5
18	A	833	CLA	C2A-CAA-CBA-CGA
18	2	311	CLA	C2A-CAA-CBA-CGA
18	B	833	CLA	O1D-CGD-O2D-CED
18	J	1101	CLA	O1D-CGD-O2D-CED
18	A	820	CLA	O1A-CGA-O2A-C1
18	2	313	CLA	O1A-CGA-O2A-C1
18	J	1101	CLA	C3-C5-C6-C7
23	B	853	LMT	O5'-C1'-O1'-C1
24	F	308	LMG	O6-C1-O1-C7
24	G	1607	LMG	O6-C1-O1-C7
24	2	322	LMG	O6-C1-O1-C7
23	J	1107	LMT	O5B-C5B-C6B-O6B
23	J	1107	LMT	O5'-C5'-C6'-O6'
26	F	309	DGD	O6E-C5E-C6E-O5E
18	A	803	CLA	O1D-CGD-O2D-CED
18	A	833	CLA	CBA-CGA-O2A-C1
18	B	815	CLA	CBA-CGA-O2A-C1
18	B	830	CLA	CBA-CGA-O2A-C1
17	A	801	CL0	CBD-CGD-O2D-CED
18	B	837	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	K	1402	CLA	CBD-CGD-O2D-CED
18	2	326	CLA	CBD-CGD-O2D-CED
18	K	1404	CLA	CBA-CGA-O2A-C1
18	B	829	CLA	O1D-CGD-O2D-CED
18	2	309	CLA	O1A-CGA-O2A-C1
23	4	319	LMT	O5B-C5B-C6B-O6B
24	2	324	LMG	C4-C5-C6-O5
18	1	5012	CLA	CBD-CGD-O2D-CED
18	1	5010	CLA	C3-C5-C6-C7
18	4	311	CLA	C3-C5-C6-C7
23	J	1107	LMT	C4'-C5'-C6'-O6'
21	I	101	BCR	C9-C10-C11-C12
21	L	302	BCR	C13-C14-C15-C16
18	A	833	CLA	O1A-CGA-O2A-C1
18	B	830	CLA	O1A-CGA-O2A-C1
22	2	320	LHG	C1-C2-C3-O3
18	A	831	CLA	O1D-CGD-O2D-CED
18	A	806	CLA	CBA-CGA-O2A-C1
18	A	808	CLA	CBA-CGA-O2A-C1
18	A	813	CLA	CBA-CGA-O2A-C1
18	A	819	CLA	CBA-CGA-O2A-C1
18	A	824	CLA	CBA-CGA-O2A-C1
18	A	827	CLA	CBA-CGA-O2A-C1
18	B	806	CLA	CBA-CGA-O2A-C1
18	B	823	CLA	CBA-CGA-O2A-C1
18	B	824	CLA	CBA-CGA-O2A-C1
18	B	834	CLA	CBA-CGA-O2A-C1
18	B	836	CLA	CBA-CGA-O2A-C1
18	B	841	CLA	CBA-CGA-O2A-C1
18	F	301	CLA	CBA-CGA-O2A-C1
18	J	1101	CLA	CBA-CGA-O2A-C1
18	K	1402	CLA	CBA-CGA-O2A-C1
18	1	5009	CLA	CBA-CGA-O2A-C1
26	J	1106	DGD	C2A-C1A-O1G-C1G
18	A	822	CLA	CBD-CGD-O2D-CED
23	B	853	LMT	C4'-C5'-C6'-O6'
26	J	1106	DGD	O6D-C5D-C6D-O5D
26	J	1106	DGD	C4D-C5D-C6D-O5D
18	A	807	CLA	O1D-CGD-O2D-CED
18	B	827	CLA	O1D-CGD-O2D-CED
18	B	839	CLA	O1D-CGD-O2D-CED
23	J	1107	LMT	C4B-C5B-C6B-O6B

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
30	2	314	CHL	C4-C3-C5-C6
18	A	838	CLA	C2-C3-C5-C6
18	B	840	CLA	C2-C3-C5-C6
18	H	1701	CLA	C2-C3-C5-C6
18	2	307	CLA	C2-C3-C5-C6
18	A	802	CLA	C14-C13-C15-C16
18	A	803	CLA	C11-C10-C8-C9
18	A	808	CLA	C6-C7-C8-C9
18	A	808	CLA	C11-C10-C8-C9
18	A	826	CLA	C6-C7-C8-C9
18	A	836	CLA	C11-C12-C13-C14
18	B	804	CLA	C14-C13-C15-C16
18	B	815	CLA	C14-C13-C15-C16
18	B	818	CLA	C11-C12-C13-C14
18	B	820	CLA	C14-C13-C15-C16
18	B	826	CLA	C6-C7-C8-C9
18	B	840	CLA	C11-C10-C8-C9
18	G	1603	CLA	C6-C7-C8-C9
18	L	305	CLA	C6-C7-C8-C9
18	1	5006	CLA	C6-C7-C8-C9
18	1	5010	CLA	C14-C13-C15-C16
18	1	5018	CLA	C6-C7-C8-C9
18	2	310	CLA	C6-C7-C8-C9
18	2	312	CLA	C6-C7-C8-C9
18	4	305	CLA	C6-C7-C8-C9
18	4	315	CLA	C14-C13-C15-C16
30	1	5016	CHL	C11-C10-C8-C9
18	A	829	CLA	O1D-CGD-O2D-CED
18	A	832	CLA	O1D-CGD-O2D-CED
18	2	307	CLA	O1D-CGD-O2D-CED
18	4	308	CLA	O1D-CGD-O2D-CED
23	B	853	LMT	C2'-C1'-O1'-C1
24	F	308	LMG	C2-C1-O1-C7
24	1	5001	LMG	C2-C1-O1-C7
18	3	318	CLA	O1A-CGA-O2A-C1
22	B	849	LHG	O2-C2-C3-O3
22	2	320	LHG	O2-C2-C3-O3
18	B	806	CLA	O1A-CGA-O2A-C1
18	1	5009	CLA	O1A-CGA-O2A-C1
21	A	843	BCR	C11-C12-C13-C35
21	A	844	BCR	C36-C18-C19-C20
21	A	845	BCR	C37-C22-C23-C24

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	A	846	BCR	C7-C8-C9-C34
21	A	847	BCR	C7-C8-C9-C34
21	B	845	BCR	C11-C12-C13-C35
21	B	847	BCR	C7-C8-C9-C34
21	F	305	BCR	C36-C18-C19-C20
21	G	1604	BCR	C36-C18-C19-C20
21	I	101	BCR	C7-C8-C9-C34
21	I	102	BCR	C7-C8-C9-C34
21	I	102	BCR	C37-C22-C23-C24
21	J	1104	BCR	C7-C8-C9-C34
21	J	1104	BCR	C11-C12-C13-C35
21	L	302	BCR	C36-C18-C19-C20
21	L	302	BCR	C37-C22-C23-C24
21	L	303	BCR	C7-C8-C9-C34
21	L	307	BCR	C7-C8-C9-C34
21	1	5005	BCR	C36-C18-C19-C20
21	1	5005	BCR	C37-C22-C23-C24
21	2	305	BCR	C11-C12-C13-C35
21	3	306	BCR	C37-C22-C23-C24
21	4	301	BCR	C7-C8-C9-C34
21	4	301	BCR	C11-C12-C13-C35
21	4	301	BCR	C36-C18-C19-C20
21	A	846	BCR	C7-C8-C9-C10
21	F	304	BCR	C7-C8-C9-C10
21	F	305	BCR	C17-C18-C19-C20
21	I	102	BCR	C21-C22-C23-C24
21	J	1104	BCR	C11-C12-C13-C14
21	L	302	BCR	C21-C22-C23-C24
21	1	5005	BCR	C21-C22-C23-C24
21	3	306	BCR	C21-C22-C23-C24
21	4	301	BCR	C7-C8-C9-C10
21	4	301	BCR	C11-C12-C13-C14
29	3	304	LUT	C27-C28-C29-C30
23	2	325	LMT	C4B-C5B-C6B-O6B
18	2	313	CLA	C2A-CAA-CBA-CGA
18	4	312	CLA	C2A-CAA-CBA-CGA
18	1	5009	CLA	O1D-CGD-O2D-CED
18	A	806	CLA	O1A-CGA-O2A-C1
18	A	824	CLA	O1A-CGA-O2A-C1
18	A	827	CLA	O1A-CGA-O2A-C1
18	B	824	CLA	O1A-CGA-O2A-C1
18	F	301	CLA	O1A-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	J	1101	CLA	O1A-CGA-O2A-C1
26	J	1106	DGD	O1A-C1A-O1G-C1G
23	G	1606	LMT	C5'-C4'-O1B-C1B
23	4	319	LMT	C4B-C5B-C6B-O6B
18	A	827	CLA	O1D-CGD-O2D-CED
18	B	808	CLA	CBA-CGA-O2A-C1
18	B	807	CLA	C8-C10-C11-C12
18	B	823	CLA	C5-C6-C7-C8
18	3	315	CLA	C10-C11-C12-C13
24	2	322	LMG	C10-C11-C12-C13
18	A	808	CLA	C2-C1-O2A-CGA
18	A	813	CLA	C2-C1-O2A-CGA
18	A	821	CLA	C2-C1-O2A-CGA
18	A	824	CLA	C2-C1-O2A-CGA
18	A	838	CLA	C2-C1-O2A-CGA
18	A	852	CLA	C2-C1-O2A-CGA
18	B	807	CLA	C2-C1-O2A-CGA
18	B	823	CLA	C2-C1-O2A-CGA
18	B	833	CLA	C2-C1-O2A-CGA
18	B	838	CLA	C2-C1-O2A-CGA
18	F	303	CLA	C2-C1-O2A-CGA
18	G	1603	CLA	C2-C1-O2A-CGA
18	J	1101	CLA	C2-C1-O2A-CGA
18	K	1403	CLA	C2-C1-O2A-CGA
18	L	306	CLA	C2-C1-O2A-CGA
18	1	5010	CLA	C2-C1-O2A-CGA
18	1	5011	CLA	C2-C1-O2A-CGA
18	2	310	CLA	C2-C1-O2A-CGA
18	2	312	CLA	C2-C1-O2A-CGA
18	2	313	CLA	C2-C1-O2A-CGA
18	2	317	CLA	C2-C1-O2A-CGA
18	2	326	CLA	C2-C1-O2A-CGA
18	3	308	CLA	C2-C1-O2A-CGA
18	4	306	CLA	C2-C1-O2A-CGA
18	4	310	CLA	C2-C1-O2A-CGA
18	A	819	CLA	O1A-CGA-O2A-C1
18	B	823	CLA	O1A-CGA-O2A-C1
18	A	828	CLA	O1D-CGD-O2D-CED
18	A	835	CLA	O1D-CGD-O2D-CED
18	L	305	CLA	CBD-CGD-O2D-CED
18	A	807	CLA	C5-C6-C7-C8
18	A	810	CLA	C13-C15-C16-C17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	831	CLA	C8-C10-C11-C12
18	A	853	CLA	C10-C11-C12-C13
18	B	801	CLA	C8-C10-C11-C12
18	B	809	CLA	C10-C11-C12-C13
18	B	830	CLA	C8-C10-C11-C12
18	F	303	CLA	C10-C11-C12-C13
18	G	1603	CLA	C10-C11-C12-C13
18	3	309	CLA	C5-C6-C7-C8
22	A	849	LHG	O1-C1-C2-O2
22	1	5019	LHG	O1-C1-C2-O2
18	A	805	CLA	C8-C10-C11-C12
18	A	826	CLA	C15-C16-C17-C18
18	B	803	CLA	C13-C15-C16-C17
18	A	822	CLA	C6-C7-C8-C10
18	3	315	CLA	C12-C13-C15-C16
18	A	818	CLA	CBA-CGA-O2A-C1
26	J	1106	DGD	CDA-CEA-CFA-CGA
18	A	820	CLA	C8-C10-C11-C12
18	A	831	CLA	C15-C16-C17-C18
18	A	832	CLA	C13-C15-C16-C17
21	A	843	BCR	C9-C10-C11-C12
21	A	846	BCR	C9-C10-C11-C12
21	A	846	BCR	C13-C14-C15-C16
21	B	846	BCR	C19-C20-C21-C22
18	A	817	CLA	C3-C5-C6-C7
18	A	806	CLA	C8-C10-C11-C12
18	A	827	CLA	C15-C16-C17-C18
18	B	807	CLA	C5-C6-C7-C8
18	B	819	CLA	C8-C10-C11-C12
18	G	1603	CLA	C13-C15-C16-C17
22	B	849	LHG	C7-C8-C9-C10
22	1	5019	LHG	C23-C24-C25-C26
24	A	851	LMG	C10-C11-C12-C13
24	F	307	LMG	C28-C29-C30-C31
24	1	5001	LMG	C28-C29-C30-C31
18	A	813	CLA	O1A-CGA-O2A-C1
18	B	808	CLA	O1A-CGA-O2A-C1
18	K	1402	CLA	O1A-CGA-O2A-C1
24	1	5020	LMG	C11-C10-O7-C8
26	F	309	DGD	C2B-C1B-O2G-C2G
18	A	806	CLA	C5-C6-C7-C8
18	A	812	CLA	C15-C16-C17-C18

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	817	CLA	C13-C15-C16-C17
18	A	822	CLA	C13-C15-C16-C17
18	B	811	CLA	C5-C6-C7-C8
18	B	819	CLA	C15-C16-C17-C18
18	B	822	CLA	C15-C16-C17-C18
18	B	824	CLA	C5-C6-C7-C8
18	B	831	CLA	C15-C16-C17-C18
18	H	1701	CLA	C8-C10-C11-C12
18	1	5015	CLA	C15-C16-C17-C18
18	1	5018	CLA	C5-C6-C7-C8
18	4	305	CLA	C8-C10-C11-C12
18	A	814	CLA	C2A-CAA-CBA-CGA
18	A	819	CLA	C2A-CAA-CBA-CGA
18	B	805	CLA	C2A-CAA-CBA-CGA
18	B	840	CLA	C2A-CAA-CBA-CGA
18	F	302	CLA	C2A-CAA-CBA-CGA
18	1	5018	CLA	C2A-CAA-CBA-CGA
18	2	308	CLA	C2A-CAA-CBA-CGA
18	3	309	CLA	C2A-CAA-CBA-CGA
18	4	310	CLA	C2A-CAA-CBA-CGA
30	1	5014	CHL	C2A-CAA-CBA-CGA
21	B	802	BCR	C10-C11-C12-C13
21	B	845	BCR	C10-C11-C12-C13
18	A	835	CLA	C5-C6-C7-C8
18	B	805	CLA	C13-C15-C16-C17
18	B	806	CLA	C15-C16-C17-C18
18	B	820	CLA	C15-C16-C17-C18
18	B	829	CLA	C15-C16-C17-C18
18	B	830	CLA	C10-C11-C12-C13
18	B	833	CLA	C5-C6-C7-C8
18	F	303	CLA	C5-C6-C7-C8
18	H	1701	CLA	C5-C6-C7-C8
18	K	1402	CLA	C8-C10-C11-C12
18	4	307	CLA	C8-C10-C11-C12
30	3	310	CHL	C8-C10-C11-C12
22	A	848	LHG	C7-C8-C9-C10
18	A	808	CLA	O1A-CGA-O2A-C1
18	B	834	CLA	O1A-CGA-O2A-C1
18	B	836	CLA	O1A-CGA-O2A-C1
18	A	824	CLA	C3-C5-C6-C7
18	F	301	CLA	C3-C5-C6-C7
23	B	852	LMT	O5'-C1'-O1'-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	825	CLA	O1D-CGD-O2D-CED
18	A	803	CLA	C8-C10-C11-C12
18	A	803	CLA	C15-C16-C17-C18
18	A	805	CLA	C5-C6-C7-C8
18	A	807	CLA	C15-C16-C17-C18
18	A	819	CLA	C8-C10-C11-C12
18	A	825	CLA	C5-C6-C7-C8
18	A	828	CLA	C5-C6-C7-C8
18	A	830	CLA	C15-C16-C17-C18
18	A	838	CLA	C8-C10-C11-C12
18	A	838	CLA	C13-C15-C16-C17
18	A	838	CLA	C15-C16-C17-C18
18	B	804	CLA	C13-C15-C16-C17
18	B	808	CLA	C8-C10-C11-C12
18	B	818	CLA	C10-C11-C12-C13
18	B	825	CLA	C10-C11-C12-C13
18	B	828	CLA	C10-C11-C12-C13
18	B	829	CLA	C10-C11-C12-C13
18	B	840	CLA	C10-C11-C12-C13
18	1	5006	CLA	C5-C6-C7-C8
18	1	5006	CLA	C15-C16-C17-C18
18	2	308	CLA	C13-C15-C16-C17
18	2	317	CLA	C5-C6-C7-C8
18	4	305	CLA	C10-C11-C12-C13
18	4	308	CLA	C10-C11-C12-C13
18	4	311	CLA	C8-C10-C11-C12
18	4	315	CLA	C13-C15-C16-C17
18	2	306	CLA	O1D-CGD-O2D-CED
18	B	815	CLA	O1A-CGA-O2A-C1
18	B	841	CLA	O1A-CGA-O2A-C1
22	A	849	LHG	C23-C24-C25-C26
22	B	849	LHG	C23-C24-C25-C26
18	A	836	CLA	C10-C11-C12-C13
18	B	822	CLA	C13-C15-C16-C17
18	1	5006	CLA	C8-C10-C11-C12
18	2	312	CLA	C8-C10-C11-C12
18	3	319	CLA	C10-C11-C12-C13
18	4	307	CLA	C10-C11-C12-C13
18	4	309	CLA	C8-C10-C11-C12
24	2	324	LMG	O6-C5-C6-O5
18	A	836	CLA	O1D-CGD-O2D-CED
18	3	307	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	817	CLA	C10-C11-C12-C13
18	A	833	CLA	C5-C6-C7-C8
18	B	814	CLA	C15-C16-C17-C18
18	B	826	CLA	C5-C6-C7-C8
18	B	840	CLA	C15-C16-C17-C18
18	G	1603	CLA	C5-C6-C7-C8
24	B	850	LMG	C10-C11-C12-C13
18	B	808	CLA	O1D-CGD-O2D-CED
18	B	814	CLA	C10-C11-C12-C13
18	F	302	CLA	C10-C11-C12-C13
18	L	301	CLA	C5-C6-C7-C8
19	A	841	PQN	C25-C26-C27-C28
18	A	834	CLA	CBA-CGA-O2A-C1
18	B	832	CLA	CBA-CGA-O2A-C1
18	1	5018	CLA	CBA-CGA-O2A-C1
26	2	327	DGD	C2B-C1B-O2G-C2G
18	B	826	CLA	O1D-CGD-O2D-CED
24	B	851	LMG	C10-C11-C12-C13
18	B	830	CLA	C15-C16-C17-C18
23	G	1606	LMT	C3'-C4'-O1B-C1B
29	1	5004	LUT	C29-C30-C31-C32
18	A	805	CLA	C15-C16-C17-C18
18	A	823	CLA	C15-C16-C17-C18
18	A	852	CLA	C10-C11-C12-C13
24	1	5020	LMG	O9-C10-O7-C8
26	F	309	DGD	O1B-C1B-O2G-C2G
26	2	327	DGD	O1B-C1B-O2G-C2G
18	B	818	CLA	C2A-CAA-CBA-CGA
18	2	307	CLA	C3-C5-C6-C7
18	B	817	CLA	O1D-CGD-O2D-CED
18	A	823	CLA	CBA-CGA-O2A-C1
18	F	302	CLA	CBA-CGA-O2A-C1
26	B	855	DGD	C2A-C1A-O1G-C1G
18	A	827	CLA	C5-C6-C7-C8
18	A	836	CLA	C5-C6-C7-C8
18	B	812	CLA	C5-C6-C7-C8
18	B	812	CLA	C10-C11-C12-C13
18	B	832	CLA	C8-C10-C11-C12
18	B	834	CLA	C8-C10-C11-C12
18	F	301	CLA	C13-C15-C16-C17
18	2	310	CLA	C10-C11-C12-C13
18	2	310	CLA	C15-C16-C17-C18

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	4	308	CLA	C8-C10-C11-C12
18	4	315	CLA	C10-C11-C12-C13
18	4	315	CLA	C15-C16-C17-C18
19	A	841	PQN	C18-C20-C21-C22
18	A	812	CLA	C3-C5-C6-C7
18	A	802	CLA	C10-C11-C12-C13
18	B	822	CLA	C5-C6-C7-C8
18	1	5006	CLA	C13-C15-C16-C17
18	2	312	CLA	C5-C6-C7-C8
18	A	802	CLA	C13-C15-C16-C17
18	A	836	CLA	C13-C15-C16-C17
18	B	820	CLA	C13-C15-C16-C17
18	B	837	CLA	C15-C16-C17-C18
18	B	839	CLA	C5-C6-C7-C8
18	B	841	CLA	C4-C3-C5-C6
18	L	301	CLA	C4-C3-C5-C6
18	4	305	CLA	C4-C3-C5-C6
23	B	852	LMT	C2B-C1B-O1B-C4'
18	B	806	CLA	C13-C15-C16-C17
18	1	5006	CLA	C10-C11-C12-C13
18	2	309	CLA	C15-C16-C17-C18
18	A	838	CLA	C3-C5-C6-C7
22	2	320	LHG	C8-C7-O7-C5
24	2	322	LMG	C11-C10-O7-C8
18	A	817	CLA	O1D-CGD-O2D-CED
22	2	320	LHG	O9-C7-O7-C5
24	2	322	LMG	O9-C10-O7-C8
23	B	852	LMT	C2'-C1'-O1'-C1
24	B	851	LMG	C2-C1-O1-C7
18	A	807	CLA	C13-C15-C16-C17
18	A	837	CLA	C8-C10-C11-C12
18	1	5010	CLA	C5-C6-C7-C8
18	B	841	CLA	C16-C17-C18-C19
18	B	837	CLA	C10-C11-C12-C13
23	B	852	LMT	O5B-C1B-O1B-C4'
21	G	1604	BCR	C11-C10-C9-C34
21	L	303	BCR	C11-C10-C9-C34
21	1	5005	BCR	C11-C10-C9-C34
23	G	1606	LMT	O5'-C5'-C6'-O6'
18	B	812	CLA	C8-C10-C11-C12
18	F	302	CLA	C8-C10-C11-C12
18	3	315	CLA	C8-C10-C11-C12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	A	844	BCR	C7-C8-C9-C34
21	A	846	BCR	C11-C12-C13-C35
21	A	855	BCR	C37-C22-C23-C24
21	B	844	BCR	C11-C12-C13-C35
21	K	1405	BCR	C11-C12-C13-C35
21	2	305	BCR	C37-C22-C23-C24
29	3	304	LUT	C27-C28-C29-C39
21	A	846	BCR	C11-C12-C13-C14
21	A	855	BCR	C21-C22-C23-C24
21	1	5005	BCR	C17-C18-C19-C20
21	2	305	BCR	C21-C22-C23-C24
18	A	807	CLA	C2A-CAA-CBA-CGA
18	B	829	CLA	C2A-CAA-CBA-CGA
18	G	1603	CLA	C2A-CAA-CBA-CGA
18	4	307	CLA	C2A-CAA-CBA-CGA
30	3	316	CHL	C2A-CAA-CBA-CGA
18	A	819	CLA	C10-C11-C12-C13
22	A	849	LHG	O1-C1-C2-C3
22	B	849	LHG	O1-C1-C2-C3
22	1	5019	LHG	O1-C1-C2-C3
18	K	1404	CLA	O1A-CGA-O2A-C1
21	3	305	BCR	C13-C14-C15-C16
17	A	801	CL0	C16-C17-C18-C19
18	A	819	CLA	C16-C17-C18-C20
18	A	823	CLA	C16-C17-C18-C20
18	B	839	CLA	C16-C17-C18-C20
18	G	1601	CLA	C6-C7-C8-C10
18	3	309	CLA	C6-C7-C8-C10
18	3	315	CLA	C16-C17-C18-C19
18	4	311	CLA	C11-C12-C13-C14
30	1	5016	CHL	C11-C12-C13-C15
18	B	822	CLA	O1D-CGD-O2D-CED
18	A	818	CLA	O1A-CGA-O2A-C1
18	A	834	CLA	O1A-CGA-O2A-C1
18	F	302	CLA	O1A-CGA-O2A-C1
18	B	840	CLA	C5-C6-C7-C8
23	G	1606	LMT	C4'-C5'-C6'-O6'
21	G	1604	BCR	C11-C10-C9-C8
21	L	303	BCR	C11-C10-C9-C8
21	1	5005	BCR	C11-C10-C9-C8
24	F	307	LMG	C11-C10-O7-C8
18	A	802	CLA	C8-C10-C11-C12

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	B	808	CLA	C15-C16-C17-C18
18	1	5009	CLA	C8-C10-C11-C12
18	4	312	CLA	CBA-CGA-O2A-C1
18	A	815	CLA	CBA-CGA-O2A-C1
18	B	837	CLA	CBA-CGA-O2A-C1
18	1	5015	CLA	CBA-CGA-O2A-C1
18	2	311	CLA	CBA-CGA-O2A-C1
18	A	808	CLA	C5-C6-C7-C8
18	A	816	CLA	C2-C1-O2A-CGA
18	A	820	CLA	C2-C1-O2A-CGA
18	A	829	CLA	C2-C1-O2A-CGA
18	A	836	CLA	C2-C1-O2A-CGA
18	B	817	CLA	C2-C1-O2A-CGA
18	B	829	CLA	C2-C1-O2A-CGA
18	B	834	CLA	C2-C1-O2A-CGA
18	B	840	CLA	C2-C1-O2A-CGA
18	J	1103	CLA	C2-C1-O2A-CGA
18	L	301	CLA	C2-C1-O2A-CGA
18	2	309	CLA	C2-C1-O2A-CGA
18	3	314	CLA	C2-C1-O2A-CGA
18	3	315	CLA	C2-C1-O2A-CGA
18	A	805	CLA	C16-C17-C18-C20
18	A	808	CLA	C16-C17-C18-C19
18	A	810	CLA	C16-C17-C18-C20
18	A	820	CLA	C11-C12-C13-C14
18	A	827	CLA	C16-C17-C18-C20
18	A	831	CLA	C16-C17-C18-C19
18	A	833	CLA	C6-C7-C8-C10
18	A	837	CLA	C16-C17-C18-C19
18	A	838	CLA	C16-C17-C18-C20
18	B	826	CLA	C16-C17-C18-C19
18	B	837	CLA	C16-C17-C18-C20
18	B	841	CLA	C16-C17-C18-C20
18	1	5010	CLA	C16-C17-C18-C19
18	3	315	CLA	C16-C17-C18-C20
18	3	319	CLA	C11-C12-C13-C14
18	4	308	CLA	C11-C12-C13-C14
18	A	823	CLA	O1A-CGA-O2A-C1
18	1	5018	CLA	O1A-CGA-O2A-C1
26	B	855	DGD	O1A-C1A-O1G-C1G
18	F	303	CLA	C13-C15-C16-C17
22	A	848	LHG	C27-C28-C29-C30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	1	5019	LHG	C28-C29-C30-C31
26	J	1106	DGD	C1B-C2B-C3B-C4B
18	2	308	CLA	C15-C16-C17-C18
22	B	849	LHG	C34-C35-C36-C37
18	B	832	CLA	O1A-CGA-O2A-C1
18	B	838	CLA	CBA-CGA-O2A-C1
22	A	848	LHG	C13-C14-C15-C16
23	B	852	LMT	C7-C8-C9-C10
24	F	307	LMG	O9-C10-O7-C8
22	B	849	LHG	O1-C1-C2-O2
23	B	853	LMT	C2-C1-O1'-C1'
24	F	308	LMG	C30-C31-C32-C33
17	A	801	CL0	O1D-CGD-O2D-CED
18	B	837	CLA	O1D-CGD-O2D-CED
18	K	1402	CLA	O1D-CGD-O2D-CED
18	B	801	CLA	C15-C16-C17-C18
18	A	824	CLA	C4B-C3B-CAB-CBB
18	A	826	CLA	C4B-C3B-CAB-CBB
18	A	831	CLA	C4B-C3B-CAB-CBB
18	A	852	CLA	C4B-C3B-CAB-CBB
18	H	1701	CLA	C4B-C3B-CAB-CBB
18	2	308	CLA	C4B-C3B-CAB-CBB
18	3	314	CLA	C4B-C3B-CAB-CBB
18	4	306	CLA	C4B-C3B-CAB-CBB
24	2	301	LMG	C2-C1-O1-C7
18	A	807	CLA	C16-C17-C18-C20
18	A	813	CLA	C16-C17-C18-C20
18	A	819	CLA	C16-C17-C18-C19
18	A	827	CLA	C16-C17-C18-C19
18	B	825	CLA	C16-C17-C18-C20
18	B	839	CLA	C16-C17-C18-C19
18	G	1601	CLA	C6-C7-C8-C9
18	3	309	CLA	C6-C7-C8-C9
18	A	816	CLA	C2A-CAA-CBA-CGA
18	B	814	CLA	C5-C6-C7-C8
18	B	823	CLA	C8-C10-C11-C12
18	F	301	CLA	C5-C6-C7-C8
18	A	823	CLA	C6-C7-C8-C10
18	2	308	CLA	C6-C7-C8-C10
24	2	322	LMG	C14-C15-C16-C17
23	G	1605	LMT	C5'-C4'-O1B-C1B
18	B	841	CLA	C15-C16-C17-C18

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	A	849	LHG	C13-C14-C15-C16
18	A	826	CLA	C3A-C2A-CAA-CBA
18	B	814	CLA	C3A-C2A-CAA-CBA
18	B	825	CLA	C3A-C2A-CAA-CBA
18	B	827	CLA	C3A-C2A-CAA-CBA
18	B	835	CLA	C4-C3-C5-C6
18	B	836	CLA	C3A-C2A-CAA-CBA
18	G	1602	CLA	C3A-C2A-CAA-CBA
18	J	1101	CLA	C3A-C2A-CAA-CBA
18	J	1103	CLA	C3A-C2A-CAA-CBA
18	K	1403	CLA	C3A-C2A-CAA-CBA
18	K	1404	CLA	C3A-C2A-CAA-CBA
18	L	304	CLA	C3A-C2A-CAA-CBA
18	L	306	CLA	C3A-C2A-CAA-CBA
18	1	5007	CLA	C3A-C2A-CAA-CBA
18	2	310	CLA	C3A-C2A-CAA-CBA
18	2	313	CLA	C3A-C2A-CAA-CBA
18	3	311	CLA	C3A-C2A-CAA-CBA
18	3	314	CLA	C3A-C2A-CAA-CBA
18	3	319	CLA	C3A-C2A-CAA-CBA
18	4	309	CLA	C3A-C2A-CAA-CBA
30	2	318	CHL	C3A-C2A-CAA-CBA
30	2	319	CHL	C3A-C2A-CAA-CBA
18	2	326	CLA	O1D-CGD-O2D-CED
24	2	322	LMG	C13-C14-C15-C16
18	A	820	CLA	C5-C6-C7-C8
18	A	825	CLA	C8-C10-C11-C12
18	A	831	CLA	C13-C15-C16-C17
18	B	805	CLA	C8-C10-C11-C12
18	B	805	CLA	C15-C16-C17-C18
18	B	837	CLA	C13-C15-C16-C17
18	1	5015	CLA	C8-C10-C11-C12
21	4	301	BCR	C19-C20-C21-C22
18	A	813	CLA	C16-C17-C18-C19
18	A	817	CLA	C16-C17-C18-C20
18	A	823	CLA	C16-C17-C18-C19
18	A	829	CLA	C16-C17-C18-C19
18	A	829	CLA	C16-C17-C18-C20
18	A	852	CLA	C16-C17-C18-C20
18	B	810	CLA	C16-C17-C18-C20
18	B	825	CLA	C16-C17-C18-C19
18	B	826	CLA	C16-C17-C18-C20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	F	301	CLA	C16-C17-C18-C19
18	L	305	CLA	C11-C12-C13-C15
18	2	312	CLA	C11-C12-C13-C14
18	4	311	CLA	C11-C12-C13-C15
23	B	852	LMT	C1-C2-C3-C4
22	1	5019	LHG	C25-C26-C27-C28
18	B	822	CLA	C3-C5-C6-C7
19	A	841	PQN	C13-C15-C16-C17
24	B	851	LMG	C28-C29-C30-C31
23	A	850	LMT	C2B-C1B-O1B-C4'
23	G	1606	LMT	C4-C5-C6-C7
24	1	5001	LMG	C37-C38-C39-C40
18	B	837	CLA	O1A-CGA-O2A-C1
17	A	801	CL0	C16-C17-C18-C20
18	A	808	CLA	C16-C17-C18-C20
18	A	810	CLA	C16-C17-C18-C19
30	1	5016	CHL	C11-C12-C13-C14
18	B	839	CLA	C2B-C3B-CAB-CBB
18	3	314	CLA	C2B-C3B-CAB-CBB
18	4	306	CLA	C2B-C3B-CAB-CBB
21	A	855	BCR	C1-C6-C7-C8
21	B	844	BCR	C1-C6-C7-C8
21	B	845	BCR	C1-C6-C7-C8
21	B	845	BCR	C5-C6-C7-C8
21	B	847	BCR	C1-C6-C7-C8
21	J	1104	BCR	C1-C6-C7-C8
21	J	1104	BCR	C5-C6-C7-C8
21	K	1405	BCR	C1-C6-C7-C8
21	K	1405	BCR	C5-C6-C7-C8
21	L	303	BCR	C23-C24-C25-C26
21	L	303	BCR	C23-C24-C25-C30
21	L	307	BCR	C1-C6-C7-C8
21	L	307	BCR	C5-C6-C7-C8
21	L	307	BCR	C23-C24-C25-C26
21	L	307	BCR	C23-C24-C25-C30
21	1	5005	BCR	C23-C24-C25-C26
21	1	5005	BCR	C23-C24-C25-C30
21	2	305	BCR	C1-C6-C7-C8
21	2	305	BCR	C5-C6-C7-C8
21	3	305	BCR	C1-C6-C7-C8
21	3	306	BCR	C1-C6-C7-C8
21	3	306	BCR	C23-C24-C25-C26

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	3	306	BCR	C23-C24-C25-C30
21	4	301	BCR	C1-C6-C7-C8
21	4	301	BCR	C23-C24-C25-C26
21	4	301	BCR	C23-C24-C25-C30
29	1	5003	LUT	C1-C6-C7-C8
29	1	5003	LUT	C5-C6-C7-C8
18	B	841	CLA	CBD-CGD-O2D-CED
26	1	5002	DGD	C2B-C1B-O2G-C2G
18	A	811	CLA	CBA-CGA-O2A-C1
18	B	805	CLA	CBA-CGA-O2A-C1
18	A	817	CLA	C5-C6-C7-C8
18	J	1101	CLA	C15-C16-C17-C18
23	B	852	LMT	C4-C5-C6-C7
18	A	802	CLA	C2A-CAA-CBA-CGA
30	4	316	CHL	C2A-CAA-CBA-CGA
18	A	815	CLA	O1A-CGA-O2A-C1
18	B	838	CLA	O1A-CGA-O2A-C1
18	1	5015	CLA	O1A-CGA-O2A-C1
18	2	311	CLA	O1A-CGA-O2A-C1
18	B	815	CLA	C4-C3-C5-C6
21	A	845	BCR	C10-C11-C12-C13
21	B	843	BCR	C10-C11-C12-C13
21	K	1405	BCR	C10-C11-C12-C13
18	A	840	CLA	C5-C6-C7-C8
18	J	1101	CLA	C8-C10-C11-C12
18	2	312	CLA	C10-C11-C12-C13
18	4	311	CLA	C5-C6-C7-C8
18	B	835	CLA	C2-C3-C5-C6
18	B	841	CLA	C2-C3-C5-C6
18	L	301	CLA	C2-C3-C5-C6
18	4	305	CLA	C2-C3-C5-C6
22	B	849	LHG	C11-C12-C13-C14
18	A	835	CLA	CBA-CGA-O2A-C1
18	A	840	CLA	CBA-CGA-O2A-C1
18	B	803	CLA	CBA-CGA-O2A-C1
18	B	828	CLA	CBA-CGA-O2A-C1
18	4	308	CLA	CBA-CGA-O2A-C1
18	A	815	CLA	C11-C10-C8-C9
18	B	809	CLA	C14-C13-C15-C16
18	3	315	CLA	C11-C10-C8-C9
23	G	1606	LMT	C2B-C1B-O1B-C4'
23	A	850	LMT	O5'-C1'-O1'-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
26	1	5002	DGD	O6D-C1D-O3G-C3G
23	G	1605	LMT	C1-C2-C3-C4
23	A	850	LMT	O5'-C5'-C6'-O6'
23	G	1606	LMT	C2'-C1'-O1'-C1
26	1	5002	DGD	C2D-C1D-O3G-C3G
18	A	804	CLA	C5-C6-C7-C8
22	A	848	LHG	C12-C13-C14-C15
24	2	301	LMG	O6-C1-O1-C7
21	B	845	BCR	C13-C14-C15-C16
21	F	305	BCR	C9-C10-C11-C12
18	A	822	CLA	C16-C17-C18-C19
18	A	831	CLA	C16-C17-C18-C20
18	A	838	CLA	C16-C17-C18-C19
18	1	5010	CLA	C16-C17-C18-C20
22	A	848	LHG	C8-C7-O7-C5
22	1	5019	LHG	C8-C7-O7-C5
26	J	1106	DGD	C2B-C1B-O2G-C2G
22	B	848	LHG	C24-C23-O8-C6
24	A	851	LMG	C28-C29-C30-C31
26	B	855	DGD	C2G-C1G-O1G-C1A
18	A	803	CLA	C10-C11-C12-C13
18	A	807	CLA	C8-C10-C11-C12
18	A	825	CLA	C15-C16-C17-C18
18	A	826	CLA	C10-C11-C12-C13
22	1	5019	LHG	O9-C7-O7-C5
26	J	1106	DGD	O1B-C1B-O2G-C2G
22	A	848	LHG	C28-C29-C30-C31
26	B	855	DGD	C2A-C3A-C4A-C5A
21	B	846	BCR	C7-C8-C9-C34
18	B	837	CLA	C3-C5-C6-C7
21	A	844	BCR	C17-C18-C19-C20
21	A	847	BCR	C7-C8-C9-C10
21	B	847	BCR	C7-C8-C9-C10
21	L	302	BCR	C17-C18-C19-C20
24	1	5020	LMG	C8-C7-O1-C1
18	B	821	CLA	C2A-CAA-CBA-CGA
18	A	817	CLA	C16-C17-C18-C19
18	A	833	CLA	C6-C7-C8-C9
18	B	804	CLA	C16-C17-C18-C19
18	B	804	CLA	C16-C17-C18-C20
18	B	810	CLA	C16-C17-C18-C19
18	F	301	CLA	C16-C17-C18-C20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	L	305	CLA	C11-C12-C13-C14
18	1	5008	CLA	C6-C7-C8-C9
18	1	5008	CLA	C6-C7-C8-C10
18	2	312	CLA	C11-C12-C13-C15
22	1	5019	LHG	C11-C10-C9-C8
18	1	5012	CLA	O1D-CGD-O2D-CED
18	A	810	CLA	C10-C11-C12-C13
18	A	812	CLA	C10-C11-C12-C13
18	B	826	CLA	C8-C10-C11-C12
22	A	849	LHG	C15-C16-C17-C18
18	A	811	CLA	O1A-CGA-O2A-C1
18	B	803	CLA	O1A-CGA-O2A-C1
18	A	803	CLA	C5-C6-C7-C8
18	A	812	CLA	C8-C10-C11-C12
18	A	840	CLA	C8-C10-C11-C12
18	B	818	CLA	C8-C10-C11-C12
18	G	1603	CLA	C8-C10-C11-C12
24	A	851	LMG	C11-C12-C13-C14
22	A	849	LHG	C9-C10-C11-C12
26	1	5002	DGD	O1B-C1B-O2G-C2G
18	A	820	CLA	C11-C12-C13-C15
18	B	805	CLA	C16-C17-C18-C20
18	4	308	CLA	C11-C12-C13-C15
18	J	1101	CLA	C5-C6-C7-C8
18	A	822	CLA	O1D-CGD-O2D-CED
18	L	305	CLA	O1D-CGD-O2D-CED
18	A	827	CLA	C3-C5-C6-C7
23	A	850	LMT	C2-C3-C4-C5
18	A	822	CLA	C10-C11-C12-C13
18	B	823	CLA	C15-C16-C17-C18
18	B	841	CLA	C8-C10-C11-C12
18	4	311	CLA	C10-C11-C12-C13
22	A	849	LHG	C11-C10-C9-C8
18	A	832	CLA	C2-C1-O2A-CGA
18	A	833	CLA	C2-C1-O2A-CGA
18	2	311	CLA	C2-C1-O2A-CGA
18	A	837	CLA	C16-C17-C18-C20
18	A	823	CLA	C8-C10-C11-C12
24	B	850	LMG	C11-C12-C13-C14
26	F	309	DGD	C5A-C6A-C7A-C8A
18	B	801	CLA	C3-C5-C6-C7
30	2	315	CHL	C3-C5-C6-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	B	815	CLA	C2-C3-C5-C6
18	B	828	CLA	C15-C16-C17-C18
18	A	810	CLA	C2A-CAA-CBA-CGA
18	A	853	CLA	C2A-CAA-CBA-CGA
18	L	306	CLA	C2A-CAA-CBA-CGA
18	1	5009	CLA	C2A-CAA-CBA-CGA
18	3	315	CLA	C2A-CAA-CBA-CGA
24	1	5020	LMG	C11-C12-C13-C14
18	A	832	CLA	C10-C11-C12-C13
18	B	815	CLA	C15-C16-C17-C18
22	2	320	LHG	O1-C1-C2-O2
18	A	835	CLA	O1A-CGA-O2A-C1
18	A	840	CLA	O1A-CGA-O2A-C1
18	B	805	CLA	O1A-CGA-O2A-C1
18	B	835	CLA	C3-C5-C6-C7
18	3	307	CLA	C3-C5-C6-C7
18	A	805	CLA	C1A-C2A-CAA-CBA
18	A	807	CLA	C1A-C2A-CAA-CBA
18	A	808	CLA	C1A-C2A-CAA-CBA
18	A	809	CLA	C1A-C2A-CAA-CBA
18	A	813	CLA	C1A-C2A-CAA-CBA
18	A	816	CLA	C1A-C2A-CAA-CBA
18	A	820	CLA	C1A-C2A-CAA-CBA
18	A	832	CLA	C1A-C2A-CAA-CBA
18	A	836	CLA	C1A-C2A-CAA-CBA
18	B	806	CLA	C1A-C2A-CAA-CBA
18	B	812	CLA	C1A-C2A-CAA-CBA
18	B	813	CLA	C1A-C2A-CAA-CBA
18	B	814	CLA	C1A-C2A-CAA-CBA
18	B	823	CLA	C1A-C2A-CAA-CBA
18	B	825	CLA	C1A-C2A-CAA-CBA
18	B	826	CLA	C1A-C2A-CAA-CBA
18	B	838	CLA	C1A-C2A-CAA-CBA
18	F	301	CLA	C1A-C2A-CAA-CBA
18	G	1602	CLA	C1A-C2A-CAA-CBA
18	G	1603	CLA	C1A-C2A-CAA-CBA
18	J	1101	CLA	C1A-C2A-CAA-CBA
18	J	1103	CLA	C1A-C2A-CAA-CBA
18	K	1403	CLA	C1A-C2A-CAA-CBA
18	K	1404	CLA	C1A-C2A-CAA-CBA
18	1	5006	CLA	C1A-C2A-CAA-CBA
18	1	5007	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	1	5013	CLA	C1A-C2A-CAA-CBA
18	2	306	CLA	C1A-C2A-CAA-CBA
18	2	308	CLA	C1A-C2A-CAA-CBA
18	2	309	CLA	C1A-C2A-CAA-CBA
18	2	310	CLA	C1A-C2A-CAA-CBA
18	3	301	CLA	C1A-C2A-CAA-CBA
18	3	309	CLA	C1A-C2A-CAA-CBA
18	3	311	CLA	C1A-C2A-CAA-CBA
18	3	315	CLA	C1A-C2A-CAA-CBA
18	3	319	CLA	C1A-C2A-CAA-CBA
18	4	305	CLA	C1A-C2A-CAA-CBA
18	A	813	CLA	C13-C15-C16-C17
18	A	822	CLA	C15-C16-C17-C18
18	A	852	CLA	C15-C16-C17-C18
22	1	5019	LHG	C13-C14-C15-C16
18	4	308	CLA	O1A-CGA-O2A-C1
26	B	855	DGD	C2B-C3B-C4B-C5B
23	A	850	LMT	O1'-C1-C2-C3
23	G	1605	LMT	O5'-C5'-C6'-O6'
22	A	848	LHG	C33-C34-C35-C36
26	2	327	DGD	C4A-C5A-C6A-C7A
18	A	803	CLA	C11-C12-C13-C15
18	A	804	CLA	C6-C7-C8-C10
18	A	804	CLA	C11-C12-C13-C15
18	A	805	CLA	C12-C13-C15-C16
18	A	826	CLA	C6-C7-C8-C10
18	A	827	CLA	C11-C12-C13-C15
18	A	831	CLA	C6-C7-C8-C10
18	A	832	CLA	C6-C7-C8-C10
18	A	853	CLA	C11-C12-C13-C15
18	B	804	CLA	C11-C10-C8-C7
18	B	814	CLA	C11-C12-C13-C15
18	B	819	CLA	C6-C7-C8-C10
18	B	820	CLA	C6-C7-C8-C10
18	B	823	CLA	C12-C13-C15-C16
18	B	825	CLA	C11-C12-C13-C15
18	B	829	CLA	C6-C7-C8-C10
18	B	829	CLA	C12-C13-C15-C16
18	B	839	CLA	C6-C7-C8-C10
18	B	840	CLA	C11-C10-C8-C7
18	F	303	CLA	C11-C10-C8-C7
18	J	1101	CLA	C11-C12-C13-C15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	K	1402	CLA	C6-C7-C8-C10
18	1	5015	CLA	C6-C7-C8-C10
18	2	310	CLA	C6-C7-C8-C10
18	2	310	CLA	C11-C12-C13-C15
18	2	312	CLA	C6-C7-C8-C10
18	3	315	CLA	C6-C7-C8-C10
18	3	315	CLA	C11-C12-C13-C15
19	B	842	PQN	C17-C18-C20-C21
30	2	314	CHL	C11-C10-C8-C7
18	A	853	CLA	C16-C17-C18-C19
18	B	841	CLA	C10-C11-C12-C13
18	B	828	CLA	O1A-CGA-O2A-C1
24	1	5001	LMG	O6-C5-C6-O5
24	F	306	LMG	C34-C35-C36-C37
22	B	849	LHG	C24-C23-O8-C6
23	G	1605	LMT	C5-C6-C7-C8
26	B	855	DGD	C7A-C8A-C9A-CAA
18	A	803	CLA	C13-C15-C16-C17
18	2	306	CLA	C10-C11-C12-C13
18	3	315	CLA	C2-C3-C5-C6
18	A	815	CLA	C5-C6-C7-C8
18	A	827	CLA	C10-C11-C12-C13
18	B	807	CLA	C13-C15-C16-C17
18	B	828	CLA	C2A-CAA-CBA-CGA
18	A	802	CLA	C11-C10-C8-C9
18	A	802	CLA	C11-C12-C13-C14
18	A	803	CLA	C11-C12-C13-C14
18	A	805	CLA	C11-C12-C13-C14
18	A	822	CLA	C6-C7-C8-C9
18	A	823	CLA	C11-C10-C8-C9
18	A	829	CLA	C14-C13-C15-C16
18	A	838	CLA	C6-C7-C8-C9
18	A	852	CLA	C6-C7-C8-C9
18	B	801	CLA	C6-C7-C8-C9
18	B	804	CLA	C11-C10-C8-C9
18	B	808	CLA	C11-C12-C13-C14
18	B	810	CLA	C6-C7-C8-C9
18	B	815	CLA	C11-C10-C8-C9
18	B	823	CLA	C14-C13-C15-C16
18	B	829	CLA	C6-C7-C8-C9
18	B	829	CLA	C14-C13-C15-C16
18	B	830	CLA	C14-C13-C15-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	B	837	CLA	C14-C13-C15-C16
18	B	840	CLA	C6-C7-C8-C9
18	K	1402	CLA	C6-C7-C8-C9
18	1	5009	CLA	C11-C12-C13-C14
18	2	310	CLA	C14-C13-C15-C16
18	2	312	CLA	C11-C10-C8-C9
18	4	307	CLA	C14-C13-C15-C16
22	1	5019	LHG	C33-C34-C35-C36
22	1	5019	LHG	C9-C10-C11-C12
23	B	852	LMT	C6-C7-C8-C9
22	A	848	LHG	C34-C35-C36-C37
24	2	321	LMG	O6-C5-C6-O5
23	A	850	LMT	C2'-C1'-O1'-C1
23	J	1107	LMT	C2'-C1'-O1'-C1
22	A	848	LHG	C4-C5-C6-O8
24	F	308	LMG	C7-C8-C9-O8
24	G	1607	LMG	O1-C7-C8-C9
24	2	322	LMG	O1-C7-C8-C9
26	2	327	DGD	O1G-C1G-C2G-C3G
22	A	849	LHG	C16-C17-C18-C19
22	A	848	LHG	C11-C12-C13-C14
17	A	801	CL0	CBA-CGA-O2A-C1
18	A	812	CLA	CBA-CGA-O2A-C1
18	A	831	CLA	CBA-CGA-O2A-C1
18	B	819	CLA	CBA-CGA-O2A-C1
23	B	852	LMT	O5B-C5B-C6B-O6B
24	B	851	LMG	O6-C5-C6-O5
24	2	322	LMG	O6-C5-C6-O5
18	A	825	CLA	C16-C17-C18-C20
18	3	307	CLA	C6-C7-C8-C10
22	1	5019	LHG	C29-C30-C31-C32
24	A	851	LMG	C15-C16-C17-C18
21	B	845	BCR	C11-C10-C9-C34
30	2	316	CHL	CHA-CBD-CGD-O1D
18	L	305	CLA	C3-C5-C6-C7
23	B	856	LMT	O5'-C5'-C6'-O6'
26	2	327	DGD	C2B-C3B-C4B-C5B
18	3	315	CLA	C4-C3-C5-C6
23	2	325	LMT	C11-C10-C9-C8
18	F	302	CLA	C13-C15-C16-C17
18	1	5009	CLA	C10-C11-C12-C13
21	A	844	BCR	C37-C22-C23-C24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	822	CLA	C16-C17-C18-C20
21	A	844	BCR	C7-C8-C9-C10
21	A	844	BCR	C21-C22-C23-C24
18	B	835	CLA	C5-C6-C7-C8
24	A	851	LMG	O6-C5-C6-O5
24	2	301	LMG	O6-C5-C6-O5
18	4	307	CLA	C13-C15-C16-C17
24	F	308	LMG	C10-C11-C12-C13
24	1	5001	LMG	C10-C11-C12-C13
26	F	309	DGD	C1A-C2A-C3A-C4A
18	A	825	CLA	CBA-CGA-O2A-C1
22	B	849	LHG	C26-C27-C28-C29
21	L	303	BCR	C10-C11-C12-C13
18	A	808	CLA	C10-C11-C12-C13
18	B	808	CLA	C5-C6-C7-C8
18	B	829	CLA	C13-C15-C16-C17
24	B	851	LMG	C12-C13-C14-C15
18	B	805	CLA	C16-C17-C18-C19
18	B	837	CLA	C16-C17-C18-C19
17	A	801	CL0	O1A-CGA-O2A-C1
18	A	829	CLA	C8-C10-C11-C12
18	B	827	CLA	CBA-CGA-O2A-C1
18	A	812	CLA	O1A-CGA-O2A-C1
24	B	850	LMG	C12-C13-C14-C15
22	A	848	LHG	C24-C25-C26-C27
18	A	824	CLA	C4-C3-C5-C6
18	F	302	CLA	C4-C3-C5-C6
22	B	849	LHG	C24-C25-C26-C27
18	B	814	CLA	CBA-CGA-O2A-C1
22	A	849	LHG	C26-C27-C28-C29
18	A	832	CLA	C2A-CAA-CBA-CGA
23	B	852	LMT	C5-C6-C7-C8
26	B	855	DGD	C6A-C7A-C8A-C9A
18	A	802	CLA	C5-C6-C7-C8
18	A	823	CLA	C10-C11-C12-C13
18	B	824	CLA	C2-C1-O2A-CGA
18	B	803	CLA	C16-C17-C18-C19
26	1	5002	DGD	C4A-C5A-C6A-C7A
23	G	1605	LMT	C9-C10-C11-C12
23	G	1606	LMT	O5B-C1B-O1B-C4'
18	B	801	CLA	C13-C15-C16-C17
18	A	840	CLA	C10-C11-C12-C13

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	J	1104	BCR	C9-C10-C11-C12
18	A	824	CLA	C6-C7-C8-C9
18	A	821	CLA	C4-C3-C5-C6
18	B	837	CLA	C4-C3-C5-C6
18	F	301	CLA	C4-C3-C5-C6
30	1	5016	CHL	C4-C3-C5-C6
18	A	806	CLA	C2-C3-C5-C6
30	4	302	CHL	C2-C3-C5-C6
18	B	807	CLA	CBA-CGA-O2A-C1
18	B	839	CLA	CBA-CGA-O2A-C1
22	A	848	LHG	O1-C1-C2-O2
23	A	850	LMT	C2-C1-O1'-C1'
18	4	312	CLA	O1A-CGA-O2A-C1
18	A	804	CLA	C11-C12-C13-C14
18	A	804	CLA	C14-C13-C15-C16
18	A	810	CLA	C11-C12-C13-C14
18	A	816	CLA	C6-C7-C8-C9
18	A	820	CLA	C11-C10-C8-C9
18	A	827	CLA	C11-C12-C13-C14
18	A	831	CLA	C6-C7-C8-C9
18	A	832	CLA	C6-C7-C8-C9
18	B	801	CLA	C11-C12-C13-C14
18	B	819	CLA	C6-C7-C8-C9
18	B	820	CLA	C6-C7-C8-C9
18	B	825	CLA	C11-C12-C13-C14
18	B	825	CLA	C14-C13-C15-C16
18	B	839	CLA	C6-C7-C8-C9
18	F	301	CLA	C14-C13-C15-C16
18	F	302	CLA	C6-C7-C8-C9
18	F	302	CLA	C11-C12-C13-C14
18	F	303	CLA	C11-C10-C8-C9
18	J	1101	CLA	C11-C12-C13-C14
18	1	5015	CLA	C6-C7-C8-C9
18	2	308	CLA	C6-C7-C8-C9
18	2	310	CLA	C11-C12-C13-C14
18	3	315	CLA	C6-C7-C8-C9
18	3	315	CLA	C11-C12-C13-C14
18	4	315	CLA	C6-C7-C8-C9
18	A	804	CLA	C8-C10-C11-C12
18	A	824	CLA	C5-C6-C7-C8
18	A	828	CLA	C8-C10-C11-C12
18	A	830	CLA	C13-C15-C16-C17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	853	CLA	C15-C16-C17-C18
18	B	805	CLA	C5-C6-C7-C8
18	F	301	CLA	C15-C16-C17-C18
18	B	801	CLA	C4B-C3B-CAB-CBB
18	L	305	CLA	C4B-C3B-CAB-CBB
18	1	5017	CLA	C4B-C3B-CAB-CBB
18	2	311	CLA	C4B-C3B-CAB-CBB
18	2	313	CLA	C4B-C3B-CAB-CBB
18	4	309	CLA	C4B-C3B-CAB-CBB
18	4	312	CLA	C4B-C3B-CAB-CBB
18	A	826	CLA	C5-C6-C7-C8
18	A	829	CLA	C5-C6-C7-C8
18	B	831	CLA	C5-C6-C7-C8
18	A	805	CLA	C16-C17-C18-C19
23	2	325	LMT	C2'-C1'-O1'-C1
26	J	1106	DGD	C2E-C1E-O5D-C6D
22	A	848	LHG	C35-C36-C37-C38
18	A	802	CLA	C6-C7-C8-C10
18	A	802	CLA	C11-C12-C13-C15
18	A	805	CLA	C11-C12-C13-C15
18	A	806	CLA	C6-C7-C8-C10
18	A	810	CLA	C11-C12-C13-C15
18	A	817	CLA	C11-C10-C8-C7
18	A	823	CLA	C11-C10-C8-C7
18	A	829	CLA	C12-C13-C15-C16
18	A	831	CLA	C12-C13-C15-C16
18	A	832	CLA	C11-C10-C8-C7
18	A	838	CLA	C6-C7-C8-C10
18	A	852	CLA	C6-C7-C8-C10
18	A	852	CLA	C11-C10-C8-C7
18	B	801	CLA	C6-C7-C8-C10
18	B	801	CLA	C11-C12-C13-C15
18	B	805	CLA	C11-C10-C8-C7
18	B	807	CLA	C6-C7-C8-C10
18	B	807	CLA	C11-C12-C13-C15
18	B	808	CLA	C11-C12-C13-C15
18	B	810	CLA	C6-C7-C8-C10
18	B	811	CLA	C6-C7-C8-C10
18	B	815	CLA	C11-C10-C8-C7
18	B	818	CLA	C11-C10-C8-C7
18	B	830	CLA	C12-C13-C15-C16
18	B	837	CLA	C12-C13-C15-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	B	840	CLA	C6-C7-C8-C10
18	F	301	CLA	C12-C13-C15-C16
18	1	5009	CLA	C11-C12-C13-C15
18	1	5018	CLA	C6-C7-C8-C10
18	2	309	CLA	C6-C7-C8-C10
18	4	305	CLA	C6-C7-C8-C10
18	4	307	CLA	C12-C13-C15-C16
18	4	308	CLA	C11-C10-C8-C7
18	4	315	CLA	C11-C10-C8-C7
23	A	850	LMT	O5B-C1B-O1B-C4'
22	2	320	LHG	C28-C29-C30-C31
18	A	853	CLA	C16-C17-C18-C20
18	A	831	CLA	O1A-CGA-O2A-C1
22	B	849	LHG	O10-C23-O8-C6
22	B	849	LHG	C35-C36-C37-C38
18	A	804	CLA	C4-C3-C5-C6
18	B	817	CLA	C3A-C2A-CAA-CBA
18	B	828	CLA	C3A-C2A-CAA-CBA
18	B	831	CLA	C4-C3-C5-C6
18	L	305	CLA	C3A-C2A-CAA-CBA
18	1	5008	CLA	C3A-C2A-CAA-CBA
18	2	317	CLA	C3A-C2A-CAA-CBA
18	2	326	CLA	C3A-C2A-CAA-CBA
18	4	310	CLA	C3A-C2A-CAA-CBA
18	4	315	CLA	C3A-C2A-CAA-CBA
30	4	302	CHL	C3A-C2A-CAA-CBA
18	A	808	CLA	C13-C15-C16-C17
19	A	841	PQN	C15-C16-C17-C18
18	F	301	CLA	C2-C3-C5-C6
23	G	1605	LMT	O1'-C1-C2-C3
21	B	847	BCR	C19-C20-C21-C22
21	F	304	BCR	C19-C20-C21-C22
21	I	101	BCR	C19-C20-C21-C22
21	I	102	BCR	C9-C10-C11-C12
21	J	1104	BCR	C19-C20-C21-C22
21	1	5005	BCR	C19-C20-C21-C22
29	1	5003	LUT	C29-C30-C31-C32
18	A	834	CLA	C4-C3-C5-C6
24	F	307	LMG	C10-C11-C12-C13
22	B	849	LHG	C33-C34-C35-C36
24	F	307	LMG	C7-C8-C9-O8
26	J	1106	DGD	O1G-C1G-C2G-C3G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
23	B	853	LMT	C6-C7-C8-C9
18	B	819	CLA	C3-C5-C6-C7
22	B	849	LHG	C9-C10-C11-C12
18	A	825	CLA	C16-C17-C18-C19
18	A	826	CLA	C16-C17-C18-C19
30	2	319	CHL	C1A-C2A-CAA-CBA
30	4	316	CHL	C1A-C2A-CAA-CBA
26	F	309	DGD	C4E-C5E-C6E-O5E
18	A	806	CLA	C4-C3-C5-C6
30	4	302	CHL	C4-C3-C5-C6
18	A	804	CLA	C2-C3-C5-C6
18	A	821	CLA	C2-C3-C5-C6
23	B	856	LMT	C1-C2-C3-C4
18	B	831	CLA	C8-C10-C11-C12
22	B	849	LHG	C13-C14-C15-C16
18	A	826	CLA	C16-C17-C18-C20
22	A	848	LHG	O9-C7-O7-C5
22	A	848	LHG	C23-C24-C25-C26
18	4	312	CLA	C2B-C3B-CAB-CBB
21	A	843	BCR	C1-C6-C7-C8
21	A	844	BCR	C23-C24-C25-C30
21	B	845	BCR	C23-C24-C25-C30
21	F	305	BCR	C23-C24-C25-C30
21	I	101	BCR	C1-C6-C7-C8
21	3	305	BCR	C23-C24-C25-C30
28	F	310	ZEX	C1-C6-C7-C8
29	3	303	LUT	C1-C6-C7-C8
18	B	826	CLA	C13-C15-C16-C17
26	F	309	DGD	C6A-C7A-C8A-C9A
18	A	852	CLA	C16-C17-C18-C19
30	2	315	CHL	C6-C7-C8-C10
18	A	831	CLA	C5-C6-C7-C8
24	B	851	LMG	O1-C7-C8-O7
24	F	307	LMG	O7-C8-C9-O8
24	F	308	LMG	O7-C8-C9-O8
24	2	322	LMG	O7-C8-C9-O8
22	B	849	LHG	C28-C29-C30-C31
18	A	826	CLA	C3-C5-C6-C7
18	B	819	CLA	O1A-CGA-O2A-C1
18	B	827	CLA	O1A-CGA-O2A-C1
18	A	806	CLA	C10-C11-C12-C13
18	B	831	CLA	C2-C3-C5-C6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	B	837	CLA	C2-C3-C5-C6
18	A	824	CLA	C6-C7-C8-C10
22	A	849	LHG	C11-C12-C13-C14
22	2	320	LHG	C7-C8-C9-C10
24	F	306	LMG	C28-C29-C30-C31
18	A	804	CLA	C6-C7-C8-C9
18	A	817	CLA	C11-C10-C8-C9
18	A	817	CLA	C11-C12-C13-C14
18	A	825	CLA	C11-C12-C13-C14
18	A	832	CLA	C11-C12-C13-C14
18	J	1101	CLA	C6-C7-C8-C9
18	1	5015	CLA	C14-C13-C15-C16
18	4	308	CLA	C11-C10-C8-C9
18	1	5018	CLA	C10-C11-C12-C13
18	A	853	CLA	C8-C10-C11-C12
18	B	814	CLA	O1A-CGA-O2A-C1
18	3	319	CLA	C5-C6-C7-C8
25	A	854	GOL	O2-C2-C3-O3
18	A	828	CLA	CBA-CGA-O2A-C1
18	B	824	CLA	C4-C3-C5-C6
21	A	847	BCR	C19-C20-C21-C22
21	B	847	BCR	C9-C10-C11-C12
21	I	102	BCR	C13-C14-C15-C16
30	1	5016	CHL	C2-C3-C5-C6
18	A	807	CLA	C16-C17-C18-C19
18	B	803	CLA	C16-C17-C18-C20
30	2	315	CHL	C6-C7-C8-C9
22	A	848	LHG	C11-C10-C9-C8
18	A	827	CLA	C8-C10-C11-C12
21	I	101	BCR	C11-C10-C9-C34
18	A	825	CLA	O1A-CGA-O2A-C1
22	A	849	LHG	C14-C15-C16-C17
22	A	848	LHG	O6-C4-C5-C6
22	2	320	LHG	O6-C4-C5-C6
18	3	307	CLA	C6-C7-C8-C9
18	3	319	CLA	C11-C12-C13-C15
18	B	839	CLA	O1A-CGA-O2A-C1
21	A	843	BCR	C37-C22-C23-C24
18	A	808	CLA	C6-C7-C8-C10
18	A	810	CLA	C11-C10-C8-C7
18	A	812	CLA	C6-C7-C8-C10
18	A	817	CLA	C11-C12-C13-C15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	819	CLA	C11-C12-C13-C15
18	A	825	CLA	C11-C12-C13-C15
18	A	826	CLA	C11-C10-C8-C7
18	A	832	CLA	C11-C12-C13-C15
18	B	822	CLA	C6-C7-C8-C10
18	B	826	CLA	C11-C10-C8-C7
18	B	831	CLA	C11-C12-C13-C15
18	B	832	CLA	C11-C10-C8-C7
18	F	302	CLA	C11-C12-C13-C15
18	1	5015	CLA	C12-C13-C15-C16
18	2	312	CLA	C11-C10-C8-C7
18	4	309	CLA	C11-C10-C8-C7
19	B	842	PQN	C16-C17-C18-C20
30	3	310	CHL	C6-C7-C8-C10
26	F	309	DGD	C1B-C2B-C3B-C4B
26	B	855	DGD	C4A-C5A-C6A-C7A
18	K	1402	CLA	C10-C11-C12-C13
21	B	844	BCR	C11-C12-C13-C14
21	B	846	BCR	C7-C8-C9-C10
21	K	1405	BCR	C11-C12-C13-C14
22	A	848	LHG	C29-C30-C31-C32
18	B	807	CLA	O1A-CGA-O2A-C1
24	2	322	LMG	C8-C7-O1-C1
18	B	832	CLA	C2A-CAA-CBA-CGA
22	A	848	LHG	C19-C20-C21-C22
18	A	816	CLA	C11-C10-C8-C9
18	K	1401	CLA	C2C-C3C-CAC-CBC
18	1	5009	CLA	C15-C16-C17-C18
18	1	5010	CLA	C13-C15-C16-C17
21	A	843	BCR	C19-C20-C21-C22
21	K	1405	BCR	C19-C20-C21-C22
18	4	306	CLA	CBD-CGD-O2D-CED
22	A	849	LHG	C19-C20-C21-C22
18	B	810	CLA	C8-C10-C11-C12
18	B	833	CLA	C8-C10-C11-C12
22	B	848	LHG	O10-C23-O8-C6
21	B	845	BCR	C11-C10-C9-C8
22	A	848	LHG	O6-C4-C5-O7
23	G	1606	LMT	O5'-C1'-O1'-C1
22	A	849	LHG	C4-C5-C6-O8
24	B	850	LMG	C7-C8-C9-O8
24	B	851	LMG	O1-C7-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
26	B	855	DGD	O1G-C1G-C2G-C3G
22	1	5019	LHG	C35-C36-C37-C38
18	B	804	CLA	C15-C16-C17-C18
18	A	806	CLA	C3-C5-C6-C7
18	A	828	CLA	O1A-CGA-O2A-C1
18	F	303	CLA	C8-C10-C11-C12
24	F	308	LMG	O8-C28-C29-C30
18	B	824	CLA	C2-C3-C5-C6
18	A	828	CLA	C13-C15-C16-C17
18	3	315	CLA	C13-C15-C16-C17
24	B	850	LMG	O7-C8-C9-O8
24	2	322	LMG	O1-C7-C8-O7
18	A	810	CLA	C11-C10-C8-C9
18	A	823	CLA	C11-C12-C13-C14
18	B	805	CLA	C11-C10-C8-C9
18	B	805	CLA	C14-C13-C15-C16
18	F	303	CLA	C16-C17-C18-C19
23	G	1605	LMT	C11-C10-C9-C8
22	A	848	LHG	C25-C26-C27-C28
22	B	849	LHG	C29-C30-C31-C32
23	4	319	LMT	C4'-C5'-C6'-O6'
26	B	855	DGD	C6B-C7B-C8B-C9B
26	J	1106	DGD	C3A-C4A-C5A-C6A
18	B	834	CLA	C11-C12-C13-C14
30	2	319	CHL	C4-C3-C5-C6
26	2	327	DGD	C2A-C3A-C4A-C5A
18	B	811	CLA	C10-C11-C12-C13
18	B	806	CLA	C16-C17-C18-C20
18	B	815	CLA	C16-C17-C18-C19
18	A	812	CLA	C13-C15-C16-C17
22	2	320	LHG	C23-C24-C25-C26
18	A	813	CLA	C10-C11-C12-C13
18	B	834	CLA	C3-C5-C6-C7
24	2	322	LMG	C15-C16-C17-C18
18	F	303	CLA	C15-C16-C17-C18
21	A	843	BCR	C36-C18-C19-C20
18	A	817	CLA	C1A-C2A-CAA-CBA
18	A	831	CLA	C1A-C2A-CAA-CBA
18	B	820	CLA	C1A-C2A-CAA-CBA
18	B	827	CLA	C1A-C2A-CAA-CBA
18	B	830	CLA	C1A-C2A-CAA-CBA
18	F	303	CLA	C4B-C3B-CAB-CBB

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	2	326	CLA	C1A-C2A-CAA-CBA
18	3	319	CLA	C4B-C3B-CAB-CBB
18	4	307	CLA	C4B-C3B-CAB-CBB
18	4	306	CLA	O1D-CGD-O2D-CED
18	B	820	CLA	CBA-CGA-O2A-C1
18	A	830	CLA	C4-C3-C5-C6
18	B	806	CLA	C4-C3-C5-C6
18	4	309	CLA	C10-C11-C12-C13
23	4	319	LMT	O1'-C1-C2-C3
18	B	841	CLA	CAA-CBA-CGA-O2A
26	2	327	DGD	O1G-C1A-C2A-C3A
21	B	802	BCR	C9-C10-C11-C12
29	4	303	LUT	C29-C30-C31-C32
18	A	853	CLA	C3-C5-C6-C7
22	A	848	LHG	C30-C31-C32-C33
30	2	315	CHL	C2A-CAA-CBA-CGA
18	A	836	CLA	C15-C16-C17-C18
22	B	849	LHG	O6-C4-C5-C6
18	A	834	CLA	C2-C3-C5-C6
18	A	808	CLA	C11-C12-C13-C15
18	A	810	CLA	C6-C7-C8-C10
18	A	828	CLA	C11-C12-C13-C15
18	A	832	CLA	C12-C13-C15-C16
18	A	836	CLA	C12-C13-C15-C16
18	A	837	CLA	C11-C10-C8-C7
18	B	815	CLA	C12-C13-C15-C16
18	B	817	CLA	C6-C7-C8-C10
18	B	828	CLA	C6-C7-C8-C10
18	B	837	CLA	C6-C7-C8-C10
18	B	841	CLA	C11-C12-C13-C15
18	G	1603	CLA	C6-C7-C8-C10
18	2	309	CLA	C12-C13-C15-C16
18	4	315	CLA	C11-C12-C13-C15
30	2	314	CHL	C6-C7-C8-C10
18	B	818	CLA	C16-C17-C18-C19
18	B	824	CLA	C6-C7-C8-C9
18	B	841	CLA	O1D-CGD-O2D-CED
23	B	853	LMT	C3-C4-C5-C6
18	B	818	CLA	C15-C16-C17-C18
18	B	827	CLA	C8-C10-C11-C12
18	B	828	CLA	C8-C10-C11-C12
19	B	842	PQN	C25-C26-C27-C28

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	K	1402	CLA	C5-C6-C7-C8
22	B	849	LHG	O6-C4-C5-O7
22	2	320	LHG	O6-C4-C5-O7
30	2	314	CHL	C3-C5-C6-C7
18	A	802	CLA	C6-C7-C8-C9
18	A	819	CLA	C11-C12-C13-C14
18	B	822	CLA	C6-C7-C8-C9
18	3	315	CLA	C14-C13-C15-C16
18	4	309	CLA	C11-C10-C8-C9
19	B	842	PQN	C16-C17-C18-C19
30	2	314	CHL	C6-C7-C8-C9
30	3	310	CHL	C6-C7-C8-C9
21	A	855	BCR	C19-C20-C21-C22
18	2	309	CLA	C16-C17-C18-C20
18	G	1603	CLA	C15-C16-C17-C18
22	1	5019	LHG	O7-C5-C6-O8
24	G	1607	LMG	O1-C7-C8-O7
18	B	832	CLA	C5-C6-C7-C8
18	2	309	CLA	C13-C15-C16-C17
24	A	851	LMG	C18-C19-C20-C21
22	1	5019	LHG	C4-C5-C6-O8
24	G	1607	LMG	C7-C8-C9-O8
24	2	322	LMG	C7-C8-C9-O8
18	A	818	CLA	CAD-CBD-CGD-O2D
18	B	806	CLA	CAD-CBD-CGD-O2D
18	B	831	CLA	CAD-CBD-CGD-O2D
18	B	836	CLA	CAD-CBD-CGD-O2D
30	2	319	CHL	CAD-CBD-CGD-O2D
18	B	811	CLA	CBA-CGA-O2A-C1
18	1	5009	CLA	C16-C17-C18-C20
18	A	827	CLA	C13-C15-C16-C17
18	B	837	CLA	C8-C10-C11-C12
18	A	818	CLA	CAD-CBD-CGD-O1D
18	A	823	CLA	CHA-CBD-CGD-O1D
18	A	823	CLA	CHA-CBD-CGD-O2D
18	A	828	CLA	CHA-CBD-CGD-O1D
18	B	806	CLA	CAD-CBD-CGD-O1D
18	B	831	CLA	CAD-CBD-CGD-O1D
18	B	836	CLA	CAD-CBD-CGD-O1D
18	4	309	CLA	CHA-CBD-CGD-O1D
18	4	309	CLA	CHA-CBD-CGD-O2D
21	B	843	BCR	C19-C20-C21-C22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	B	845	BCR	C19-C20-C21-C22
21	F	305	BCR	C19-C20-C21-C22
21	L	307	BCR	C19-C20-C21-C22
21	2	305	BCR	C19-C20-C21-C22
21	3	305	BCR	C9-C10-C11-C12
22	A	849	LHG	C3-O3-P-O6
22	B	848	LHG	C4-O6-P-O5
22	2	320	LHG	C4-O6-P-O5
29	1	5003	LUT	C25-C26-C27-C28
29	3	304	LUT	C25-C26-C27-C28
29	3	304	LUT	C29-C30-C31-C32
30	1	5016	CHL	CHA-CBD-CGD-O2D
30	2	316	CHL	CHA-CBD-CGD-O2D
30	2	319	CHL	CAD-CBD-CGD-O1D
30	4	318	CHL	CHA-CBD-CGD-O1D
30	4	318	CHL	CHA-CBD-CGD-O2D
23	G	1606	LMT	O1'-C1-C2-C3
18	2	308	CLA	C4-C3-C5-C6
18	A	824	CLA	C2B-C3B-CAB-CBB
18	A	831	CLA	C2B-C3B-CAB-CBB
18	A	852	CLA	C2B-C3B-CAB-CBB
18	F	303	CLA	C2B-C3B-CAB-CBB
18	H	1701	CLA	C2B-C3B-CAB-CBB
18	2	308	CLA	C2B-C3B-CAB-CBB
18	4	307	CLA	C2B-C3B-CAB-CBB
21	B	844	BCR	C5-C6-C7-C8
21	B	847	BCR	C5-C6-C7-C8
29	3	304	LUT	C1-C6-C7-C8
21	I	102	BCR	C36-C18-C19-C20
22	B	849	LHG	C2-C3-O3-P
18	B	832	CLA	C11-C12-C13-C14
18	B	811	CLA	O1A-CGA-O2A-C1
22	B	849	LHG	C12-C13-C14-C15
18	A	836	CLA	C8-C10-C11-C12
18	A	822	CLA	C8-C10-C11-C12
18	A	816	CLA	C11-C10-C8-C7
24	F	307	LMG	C9-C8-O7-C10
26	J	1106	DGD	C1G-C2G-O2G-C1B
21	B	845	BCR	C18-C19-C20-C21
21	K	1405	BCR	C18-C19-C20-C21
21	2	305	BCR	C18-C19-C20-C21
18	1	5012	CLA	CAA-CBA-CGA-O2A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	L	307	BCR	C9-C10-C11-C12
21	3	305	BCR	C19-C20-C21-C22
21	3	306	BCR	C15-C16-C17-C18
18	F	303	CLA	C16-C17-C18-C20
18	A	825	CLA	C13-C15-C16-C17
18	A	806	CLA	C6-C7-C8-C9
18	A	828	CLA	C6-C7-C8-C9
18	A	837	CLA	C11-C10-C8-C9
18	A	840	CLA	C11-C10-C8-C9
18	A	852	CLA	C11-C10-C8-C9
18	B	804	CLA	C11-C12-C13-C14
18	B	807	CLA	C11-C12-C13-C14
18	B	817	CLA	C6-C7-C8-C9
18	B	826	CLA	C11-C10-C8-C9
18	H	1701	CLA	C6-C7-C8-C9
18	2	309	CLA	C6-C7-C8-C9
18	2	309	CLA	C14-C13-C15-C16
23	A	850	LMT	C1-C2-C3-C4
18	B	804	CLA	C11-C12-C13-C15
18	B	826	CLA	C6-C7-C8-C10
18	H	1701	CLA	C6-C7-C8-C10
18	B	824	CLA	C6-C7-C8-C10
30	4	316	CHL	C11-C12-C13-C15
18	B	805	CLA	C10-C11-C12-C13
26	2	327	DGD	C2D-C1D-O3G-C3G
18	A	824	CLA	C2-C3-C5-C6
18	F	302	CLA	C2-C3-C5-C6
30	3	310	CHL	CBA-CGA-O2A-C1
22	1	5019	LHG	C34-C35-C36-C37
18	B	819	CLA	CAA-CBA-CGA-O2A
21	A	843	BCR	C15-C16-C17-C18
21	B	846	BCR	C13-C14-C15-C16
18	2	308	CLA	C16-C17-C18-C19
18	4	308	CLA	C2A-CAA-CBA-CGA
18	A	809	CLA	C2-C1-O2A-CGA
23	G	1605	LMT	C7-C8-C9-C10
18	A	835	CLA	C10-C11-C12-C13
18	2	308	CLA	C16-C17-C18-C20
18	A	828	CLA	C10-C11-C12-C13
21	B	845	BCR	C9-C10-C11-C12
21	L	303	BCR	C19-C20-C21-C22
29	3	303	LUT	C29-C30-C31-C32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
24	J	1102	LMG	C11-C12-C13-C14
22	1	5019	LHG	C11-C12-C13-C14
18	B	825	CLA	C4-C3-C5-C6
18	B	828	CLA	C4-C3-C5-C6
18	B	820	CLA	O1A-CGA-O2A-C1
23	B	852	LMT	C2-C1-O1'-C1'
24	2	321	LMG	O7-C10-C11-C12
18	A	808	CLA	C11-C12-C13-C14
18	A	830	CLA	C14-C13-C15-C16
18	B	828	CLA	C6-C7-C8-C9
18	B	834	CLA	C6-C7-C8-C9
18	4	315	CLA	C11-C10-C8-C9
18	4	315	CLA	C11-C12-C13-C14
18	L	305	CLA	CBA-CGA-O2A-C1
18	F	302	CLA	C15-C16-C17-C18
18	A	853	CLA	C4B-C3B-CAB-CBB
18	K	1403	CLA	C4B-C3B-CAB-CBB
18	2	309	CLA	C4B-C3B-CAB-CBB
18	3	308	CLA	C4B-C3B-CAB-CBB
18	4	315	CLA	C4B-C3B-CAB-CBB
24	A	851	LMG	C12-C13-C14-C15
18	1	5015	CLA	C16-C17-C18-C20
18	G	1601	CLA	C2A-CAA-CBA-CGA
18	K	1404	CLA	C2A-CAA-CBA-CGA
18	A	817	CLA	C4-C3-C5-C6
18	1	5015	CLA	C4-C3-C5-C6
18	B	828	CLA	CAA-CBA-CGA-O2A
18	F	302	CLA	CAA-CBA-CGA-O2A
22	A	849	LHG	O6-C4-C5-O7
18	3	301	CLA	CAA-CBA-CGA-O2A
22	1	5019	LHG	C30-C31-C32-C33
21	A	846	BCR	C19-C20-C21-C22
21	I	102	BCR	C19-C20-C21-C22
18	B	815	CLA	C16-C17-C18-C20
18	A	802	CLA	C12-C13-C15-C16
18	A	807	CLA	C12-C13-C15-C16
18	B	805	CLA	C6-C7-C8-C10
18	B	819	CLA	C11-C10-C8-C7
18	B	820	CLA	C12-C13-C15-C16
19	B	842	PQN	C21-C22-C23-C25
18	B	817	CLA	C5-C6-C7-C8
18	L	305	CLA	O1A-CGA-O2A-C1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	B	834	CLA	C10-C11-C12-C13
18	B	832	CLA	C11-C12-C13-C15
18	2	309	CLA	C16-C17-C18-C19
22	1	5019	LHG	C31-C32-C33-C34
18	B	825	CLA	C15-C16-C17-C18
18	A	838	CLA	O1A-CGA-O2A-C1
24	A	851	LMG	O7-C8-C9-O8
22	A	848	LHG	C17-C18-C19-C20
18	A	819	CLA	C3A-C2A-CAA-CBA
18	1	5018	CLA	C3A-C2A-CAA-CBA
18	B	806	CLA	C2-C3-C5-C6
30	2	319	CHL	C2-C3-C5-C6
21	A	845	BCR	C16-C17-C18-C36
21	A	847	BCR	C16-C17-C18-C36
21	B	802	BCR	C16-C17-C18-C36
21	B	843	BCR	C35-C13-C14-C15
21	B	843	BCR	C16-C17-C18-C36
21	F	305	BCR	C16-C17-C18-C36
21	G	1604	BCR	C16-C17-C18-C36
21	I	101	BCR	C35-C13-C14-C15
21	L	303	BCR	C16-C17-C18-C36
21	L	303	BCR	C20-C21-C22-C37
21	3	306	BCR	C35-C13-C14-C15
21	3	306	BCR	C16-C17-C18-C36
26	2	327	DGD	O6D-C1D-O3G-C3G
22	B	849	LHG	C30-C31-C32-C33
22	A	849	LHG	C17-C18-C19-C20
18	A	810	CLA	C2-C1-O2A-CGA
18	A	811	CLA	C2-C1-O2A-CGA
18	1	5009	CLA	C2-C1-O2A-CGA
21	L	307	BCR	C13-C14-C15-C16
22	2	320	LHG	C2-C3-O3-P
18	B	819	CLA	C10-C11-C12-C13
21	A	843	BCR	C17-C18-C19-C20
21	A	843	BCR	C21-C22-C23-C24
18	A	812	CLA	C4-C3-C5-C6
18	B	814	CLA	C4-C3-C5-C6
18	B	839	CLA	C4-C3-C5-C6
18	A	830	CLA	C2-C3-C5-C6
18	2	308	CLA	C2-C3-C5-C6
18	A	815	CLA	C16-C17-C18-C20
30	3	310	CHL	C5-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	3	301	CLA	CAA-CBA-CGA-O1A
22	A	848	LHG	C26-C27-C28-C29
18	A	804	CLA	O1A-CGA-O2A-C1
18	A	815	CLA	C14-C13-C15-C16
18	A	826	CLA	C14-C13-C15-C16
18	B	832	CLA	C6-C7-C8-C9
18	1	5006	CLA	C11-C12-C13-C14
19	B	842	PQN	C21-C22-C23-C24
24	2	322	LMG	C7-C8-O7-C10
24	2	322	LMG	C9-C8-O7-C10
18	A	819	CLA	C5-C6-C7-C8
18	B	825	CLA	O1D-CGD-O2D-CED
30	3	316	CHL	C1A-C2A-CAA-CBA
18	B	828	CLA	C2-C3-C5-C6
18	B	804	CLA	C2A-CAA-CBA-CGA
18	2	306	CLA	C2A-CAA-CBA-CGA
18	A	821	CLA	C1A-C2A-CAA-CBA
18	B	801	CLA	C1A-C2A-CAA-CBA
18	B	811	CLA	C1A-C2A-CAA-CBA
18	B	817	CLA	C1A-C2A-CAA-CBA
18	B	819	CLA	C1A-C2A-CAA-CBA
18	B	821	CLA	C1A-C2A-CAA-CBA
18	L	305	CLA	C1A-C2A-CAA-CBA
18	1	5018	CLA	C1A-C2A-CAA-CBA
18	2	317	CLA	C1A-C2A-CAA-CBA
18	4	310	CLA	C1A-C2A-CAA-CBA
21	A	845	BCR	C16-C17-C18-C19
21	A	847	BCR	C16-C17-C18-C19
21	B	802	BCR	C16-C17-C18-C19
21	B	843	BCR	C12-C13-C14-C15
21	B	843	BCR	C16-C17-C18-C19
21	F	305	BCR	C16-C17-C18-C19
21	G	1604	BCR	C16-C17-C18-C19
21	I	101	BCR	C12-C13-C14-C15
21	L	303	BCR	C16-C17-C18-C19
21	L	303	BCR	C20-C21-C22-C23
21	3	306	BCR	C12-C13-C14-C15
21	3	306	BCR	C16-C17-C18-C19
18	4	315	CLA	C16-C17-C18-C20
22	B	849	LHG	C31-C32-C33-C34
18	B	819	CLA	C5-C6-C7-C8
18	A	826	CLA	C2B-C3B-CAB-CBB

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	853	CLA	C2B-C3B-CAB-CBB
18	1	5017	CLA	C2B-C3B-CAB-CBB
18	2	309	CLA	C2B-C3B-CAB-CBB
18	2	311	CLA	C2B-C3B-CAB-CBB
18	2	313	CLA	C2B-C3B-CAB-CBB
18	3	319	CLA	C2B-C3B-CAB-CBB
18	4	315	CLA	C2B-C3B-CAB-CBB
21	A	843	BCR	C5-C6-C7-C8
21	A	844	BCR	C23-C24-C25-C26
21	A	846	BCR	C1-C6-C7-C8
21	A	846	BCR	C23-C24-C25-C30
21	A	847	BCR	C1-C6-C7-C8
21	B	845	BCR	C23-C24-C25-C26
21	B	846	BCR	C23-C24-C25-C30
21	F	305	BCR	C23-C24-C25-C26
21	G	1604	BCR	C23-C24-C25-C30
21	I	101	BCR	C5-C6-C7-C8
21	L	302	BCR	C1-C6-C7-C8
21	3	305	BCR	C23-C24-C25-C26
28	F	310	ZEX	C5-C6-C7-C8
29	2	303	LUT	C1-C6-C7-C8
29	3	303	LUT	C5-C6-C7-C8
29	4	303	LUT	C1-C6-C7-C8
22	A	849	LHG	C7-C8-C9-C10
18	1	5017	CLA	CAA-CBA-CGA-O1A
18	B	811	CLA	C8-C10-C11-C12
19	B	842	PQN	C26-C27-C28-C29
18	A	823	CLA	C3-C5-C6-C7
18	G	1601	CLA	C3-C5-C6-C7
18	K	1401	CLA	CAA-CBA-CGA-O1A
18	A	820	CLA	C4-C3-C5-C6
18	A	817	CLA	C2-C3-C5-C6
18	B	814	CLA	C2-C3-C5-C6
18	1	5017	CLA	CAA-CBA-CGA-O2A
18	A	812	CLA	C11-C10-C8-C7
18	A	829	CLA	C6-C7-C8-C10
18	A	830	CLA	C12-C13-C15-C16
18	A	836	CLA	C11-C12-C13-C15
18	B	804	CLA	C12-C13-C15-C16
18	B	834	CLA	C6-C7-C8-C10
18	B	839	CLA	C11-C10-C8-C7
26	2	327	DGD	C6A-C7A-C8A-C9A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	1	5015	CLA	C16-C17-C18-C19
18	B	819	CLA	C2A-CAA-CBA-CGA
18	L	305	CLA	C2A-CAA-CBA-CGA
30	3	313	CHL	C2A-CAA-CBA-CGA
26	B	855	DGD	C3A-C4A-C5A-C6A
22	2	320	LHG	O7-C5-C6-O8
24	A	851	LMG	O1-C7-C8-O7
24	G	1607	LMG	O7-C8-C9-O8
26	F	309	DGD	C2A-C3A-C4A-C5A
29	1	5003	LUT	C7-C8-C9-C19
18	K	1401	CLA	CAA-CBA-CGA-O2A
18	B	801	CLA	C4-C3-C5-C6
18	4	308	CLA	C4-C3-C5-C6
18	B	839	CLA	C2-C3-C5-C6
18	1	5015	CLA	C2-C3-C5-C6
18	B	840	CLA	C13-C15-C16-C17
18	1	5009	CLA	C13-C15-C16-C17
24	1	5020	LMG	O7-C10-C11-C12
18	A	838	CLA	CBA-CGA-O2A-C1
18	B	816	CLA	CBA-CGA-O2A-C1
18	B	830	CLA	C6-C7-C8-C9
18	B	841	CLA	C11-C12-C13-C14
18	G	1603	CLA	C11-C12-C13-C14
18	B	808	CLA	C13-C15-C16-C17
26	J	1106	DGD	C6B-C7B-C8B-C9B
21	K	1405	BCR	C9-C10-C11-C12
18	A	825	CLA	C10-C11-C12-C13
18	B	830	CLA	C4-C3-C5-C6
18	A	804	CLA	C10-C11-C12-C13
24	A	851	LMG	C7-C8-C9-O8
18	A	812	CLA	C2A-CAA-CBA-CGA
18	B	806	CLA	C2A-CAA-CBA-CGA
18	B	838	CLA	C2A-CAA-CBA-CGA
17	A	801	CL0	C5-C6-C7-C8
26	F	309	DGD	CCA-CDA-CEA-CFA
18	A	826	CLA	C4-C3-C5-C6
18	B	816	CLA	C4-C3-C5-C6
18	K	1404	CLA	CAA-CBA-CGA-O2A
18	B	828	CLA	C16-C17-C18-C19
18	A	810	CLA	C4B-C3B-CAB-CBB
18	B	828	CLA	C4B-C3B-CAB-CBB
23	2	325	LMT	C1-C2-C3-C4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	B	816	CLA	O1A-CGA-O2A-C1
18	L	301	CLA	C6-C7-C8-C10
18	4	315	CLA	C16-C17-C18-C19
30	1	5014	CHL	CHA-CBD-CGD-O1D
30	1	5014	CHL	CHA-CBD-CGD-O2D
30	2	315	CHL	CHA-CBD-CGD-O2D
30	3	310	CHL	CHA-CBD-CGD-O1D
30	3	310	CHL	CHA-CBD-CGD-O2D
30	3	312	CHL	CHA-CBD-CGD-O1D
30	4	314	CHL	CHA-CBD-CGD-O1D
30	4	314	CHL	CHA-CBD-CGD-O2D
18	1	5007	CLA	C2A-CAA-CBA-CGA
22	2	320	LHG	O8-C23-C24-C25
30	2	315	CHL	CAA-CBA-CGA-O2A
22	A	849	LHG	O6-C4-C5-C6
26	B	855	DGD	O1G-C1G-C2G-O2G
18	A	827	CLA	CAA-CBA-CGA-O2A
24	B	851	LMG	O6-C1-O1-C7
18	B	829	CLA	C8-C10-C11-C12
18	B	806	CLA	C12-C13-C15-C16
18	B	830	CLA	C6-C7-C8-C10
18	L	305	CLA	C11-C10-C8-C7
18	1	5006	CLA	C6-C7-C8-C10
18	B	803	CLA	C10-C11-C12-C13
18	A	810	CLA	C6-C7-C8-C9
18	A	831	CLA	C11-C12-C13-C14
18	A	836	CLA	C14-C13-C15-C16
18	B	805	CLA	C11-C12-C13-C14
18	B	828	CLA	C11-C10-C8-C9
18	B	837	CLA	C6-C7-C8-C9
18	F	301	CLA	C6-C7-C8-C9
18	1	5018	CLA	C11-C10-C8-C9
18	4	308	CLA	C6-C7-C8-C9
18	A	826	CLA	CAA-CBA-CGA-O2A
18	A	852	CLA	C2A-CAA-CBA-CGA
18	B	827	CLA	C2A-CAA-CBA-CGA
18	A	830	CLA	C2-C1-O2A-CGA
18	4	307	CLA	C2-C1-O2A-CGA
18	4	308	CLA	C2-C1-O2A-CGA
19	B	842	PQN	C26-C27-C28-C30
18	B	801	CLA	C3A-C2A-CAA-CBA
18	B	811	CLA	C3A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	B	819	CLA	C3A-C2A-CAA-CBA
26	1	5002	DGD	C1G-C2G-O2G-C1B
26	1	5002	DGD	C3G-C2G-O2G-C1B
21	F	304	BCR	C10-C11-C12-C13
21	L	302	BCR	C10-C11-C12-C13
18	1	5015	CLA	C5-C6-C7-C8
21	B	845	BCR	C15-C16-C17-C18
18	A	804	CLA	CBA-CGA-O2A-C1
18	A	802	CLA	C16-C17-C18-C19
30	2	319	CHL	C2A-CAA-CBA-CGA
26	B	855	DGD	CAB-CBB-CCB-CDB
26	B	855	DGD	O6D-C5D-C6D-O5D
26	1	5002	DGD	C2A-C3A-C4A-C5A
22	B	849	LHG	C4-C5-C6-O8
22	B	849	LHG	C27-C28-C29-C30
18	A	806	CLA	C2A-CAA-CBA-CGA
18	K	1402	CLA	CAA-CBA-CGA-O2A
30	2	318	CHL	CAA-CBA-CGA-O1A
21	A	845	BCR	C19-C20-C21-C22
26	J	1106	DGD	CCA-CDA-CEA-CFA
22	B	849	LHG	O7-C5-C6-O8
18	H	1701	CLA	C10-C11-C12-C13
18	A	812	CLA	C6-C7-C8-C9
18	A	819	CLA	C6-C7-C8-C9
18	A	828	CLA	C11-C12-C13-C14
18	A	832	CLA	C14-C13-C15-C16
18	B	831	CLA	C11-C12-C13-C14
30	2	314	CHL	C14-C13-C15-C16
18	A	804	CLA	C16-C17-C18-C19
18	A	806	CLA	CAA-CBA-CGA-O2A
18	B	824	CLA	CAA-CBA-CGA-O2A
18	1	5018	CLA	CAA-CBA-CGA-O2A
30	2	318	CHL	CAA-CBA-CGA-O2A
30	4	316	CHL	C11-C12-C13-C14
18	4	308	CLA	C2-C3-C5-C6
18	A	803	CLA	C11-C10-C8-C7
18	A	808	CLA	C11-C10-C8-C7
18	A	813	CLA	C12-C13-C15-C16
18	A	828	CLA	C12-C13-C15-C16
18	A	831	CLA	C11-C12-C13-C15
18	B	812	CLA	C6-C7-C8-C10
18	B	818	CLA	C11-C12-C13-C15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	B	828	CLA	C11-C10-C8-C7
18	B	829	CLA	C11-C10-C8-C7
18	B	832	CLA	C6-C7-C8-C10
18	K	1402	CLA	C11-C10-C8-C7
18	L	305	CLA	C6-C7-C8-C10
18	1	5010	CLA	C12-C13-C15-C16
18	4	315	CLA	C12-C13-C15-C16
30	1	5016	CHL	C11-C10-C8-C7
24	B	854	LMG	O6-C5-C6-O5
18	B	801	CLA	C2B-C3B-CAB-CBB
18	B	803	CLA	C2B-C3B-CAB-CBB
18	B	828	CLA	C2B-C3B-CAB-CBB
18	B	831	CLA	C2B-C3B-CAB-CBB
18	G	1601	CLA	C2B-C3B-CAB-CBB
18	G	1603	CLA	C2B-C3B-CAB-CBB
18	L	305	CLA	C2B-C3B-CAB-CBB
18	1	5015	CLA	C2B-C3B-CAB-CBB
18	4	309	CLA	C2B-C3B-CAB-CBB
21	A	846	BCR	C5-C6-C7-C8
21	A	846	BCR	C23-C24-C25-C26
21	A	847	BCR	C5-C6-C7-C8
21	B	846	BCR	C23-C24-C25-C26
21	B	847	BCR	C23-C24-C25-C30
21	G	1604	BCR	C23-C24-C25-C26
21	I	101	BCR	C23-C24-C25-C26
21	I	101	BCR	C23-C24-C25-C30
21	I	102	BCR	C1-C6-C7-C8
21	I	102	BCR	C5-C6-C7-C8
21	L	302	BCR	C5-C6-C7-C8
29	2	303	LUT	C5-C6-C7-C8
29	3	304	LUT	C5-C6-C7-C8
29	4	303	LUT	C5-C6-C7-C8
18	A	812	CLA	C2-C1-O2A-CGA
18	A	828	CLA	C2-C1-O2A-CGA
18	A	834	CLA	C2-C1-O2A-CGA
18	B	822	CLA	C2-C1-O2A-CGA
18	B	828	CLA	C2-C1-O2A-CGA
18	B	814	CLA	CAA-CBA-CGA-O2A
18	1	5013	CLA	CAA-CBA-CGA-O2A
24	1	5001	LMG	O7-C10-C11-C12
24	1	5020	LMG	C18-C19-C20-C21
18	A	819	CLA	C3-C5-C6-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	3	308	CLA	CAA-CBA-CGA-O2A
18	A	823	CLA	C2-C3-C5-C6
22	B	849	LHG	C25-C26-C27-C28
18	A	816	CLA	CAA-CBA-CGA-O2A
18	3	319	CLA	CAA-CBA-CGA-O2A
18	B	803	CLA	C8-C10-C11-C12
24	1	5001	LMG	O8-C28-C29-C30
26	2	327	DGD	O2G-C1B-C2B-C3B
30	3	313	CHL	CAA-CBA-CGA-O2A
18	2	313	CLA	CAA-CBA-CGA-O2A
18	3	307	CLA	CAA-CBA-CGA-O2A
18	A	812	CLA	C2-C3-C5-C6
18	2	309	CLA	C2A-CAA-CBA-CGA
30	3	316	CHL	CAA-CBA-CGA-O2A
18	A	812	CLA	C11-C10-C8-C9
21	B	847	BCR	C37-C22-C23-C24
21	J	1104	BCR	C36-C18-C19-C20
18	A	803	CLA	CAA-CBA-CGA-O2A
18	A	835	CLA	CAA-CBA-CGA-O2A
18	B	832	CLA	CAA-CBA-CGA-O2A
18	B	837	CLA	CAA-CBA-CGA-O2A
18	B	839	CLA	CAA-CBA-CGA-O2A
18	B	840	CLA	CAA-CBA-CGA-O2A
24	J	1102	LMG	O7-C10-C11-C12
24	A	851	LMG	O1-C7-C8-C9
18	A	832	CLA	C15-C16-C17-C18
18	B	829	CLA	C5-C6-C7-C8
18	A	820	CLA	C4B-C3B-CAB-CBB
18	A	832	CLA	C4B-C3B-CAB-CBB
18	A	835	CLA	C4B-C3B-CAB-CBB
18	B	818	CLA	C4B-C3B-CAB-CBB
18	B	821	CLA	C4B-C3B-CAB-CBB
18	B	831	CLA	C4B-C3B-CAB-CBB
18	B	837	CLA	C4B-C3B-CAB-CBB
18	F	303	CLA	C1A-C2A-CAA-CBA
18	G	1603	CLA	C4B-C3B-CAB-CBB
18	1	5015	CLA	C4B-C3B-CAB-CBB
18	2	307	CLA	C4B-C3B-CAB-CBB
18	A	804	CLA	C13-C15-C16-C17
18	A	813	CLA	CAA-CBA-CGA-O2A
18	A	839	CLA	CAA-CBA-CGA-O2A
18	2	306	CLA	CAA-CBA-CGA-O2A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	B	847	BCR	C21-C22-C23-C24
21	I	102	BCR	C17-C18-C19-C20
21	J	1104	BCR	C17-C18-C19-C20
21	A	845	BCR	C15-C16-C17-C18
21	B	802	BCR	C19-C20-C21-C22
18	B	811	CLA	C16-C17-C18-C20
18	B	834	CLA	C11-C12-C13-C15
18	A	812	CLA	C2C-C3C-CAC-CBC
18	B	811	CLA	CAA-CBA-CGA-O2A
18	L	305	CLA	CAA-CBA-CGA-O2A
30	3	312	CHL	C2A-CAA-CBA-CGA
24	F	307	LMG	C32-C33-C34-C35
18	A	822	CLA	C3-C5-C6-C7
18	A	804	CLA	CAA-CBA-CGA-O2A
18	A	823	CLA	C4-C3-C5-C6
24	2	321	LMG	O9-C10-C11-C12
18	B	814	CLA	C2-C1-O2A-CGA
26	F	309	DGD	O1G-C1A-C2A-C3A
18	A	829	CLA	C11-C12-C13-C15
18	A	835	CLA	C11-C12-C13-C15
18	A	839	CLA	C12-C13-C15-C16
18	B	805	CLA	C11-C12-C13-C15
18	B	809	CLA	C6-C7-C8-C10
18	B	810	CLA	C11-C12-C13-C15
18	F	301	CLA	C6-C7-C8-C10
18	1	5018	CLA	C11-C10-C8-C7
18	4	308	CLA	C6-C7-C8-C10
30	3	310	CHL	C12-C13-C15-C16
18	A	815	CLA	C16-C17-C18-C19
18	A	835	CLA	C16-C17-C18-C20
30	4	318	CHL	C2C-C3C-CAC-CBC
24	F	307	LMG	C7-C8-O7-C10
24	F	308	LMG	C7-C8-O7-C10
24	F	308	LMG	C9-C8-O7-C10
30	2	314	CHL	O2A-C1-C2-C3
18	A	803	CLA	C2A-CAA-CBA-CGA
18	A	817	CLA	C2A-CAA-CBA-CGA
18	B	808	CLA	C2A-CAA-CBA-CGA
18	B	808	CLA	C16-C17-C18-C20
26	B	855	DGD	C5A-C6A-C7A-C8A
18	B	815	CLA	CAA-CBA-CGA-O2A
30	4	316	CHL	C2C-C3C-CAC-CBC

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
26	2	327	DGD	C4B-C5B-C6B-C7B
18	B	822	CLA	C8-C10-C11-C12
18	B	826	CLA	C10-C11-C12-C13
22	2	320	LHG	C12-C13-C14-C15
18	A	852	CLA	C3A-C2A-CAA-CBA
18	K	1402	CLA	C3A-C2A-CAA-CBA
18	1	5018	CLA	CAA-CBA-CGA-O1A
30	3	310	CHL	O1A-CGA-O2A-C1
30	2	314	CHL	C5-C6-C7-C8
18	B	825	CLA	C2-C3-C5-C6
21	I	101	BCR	C11-C10-C9-C8
23	B	856	LMT	O5B-C5B-C6B-O6B
18	A	806	CLA	CAA-CBA-CGA-O1A
18	B	814	CLA	CAA-CBA-CGA-O1A
24	A	851	LMG	O7-C10-C11-C12
18	B	841	CLA	CAA-CBA-CGA-O1A
18	3	319	CLA	CAA-CBA-CGA-O1A
18	B	804	CLA	C8-C10-C11-C12
18	B	828	CLA	C13-C15-C16-C17
30	4	318	CHL	C5-C6-C7-C8
18	A	823	CLA	C6-C7-C8-C9
18	A	840	CLA	C6-C7-C8-C9
18	B	806	CLA	C14-C13-C15-C16
18	B	810	CLA	C11-C12-C13-C14
18	B	839	CLA	C11-C10-C8-C9
18	K	1402	CLA	C11-C10-C8-C9
18	A	803	CLA	CAA-CBA-CGA-O1A
18	A	816	CLA	CAA-CBA-CGA-O1A
18	B	840	CLA	CAA-CBA-CGA-O1A
18	K	1402	CLA	CAA-CBA-CGA-O1A
24	F	308	LMG	O10-C28-C29-C30
24	1	5001	LMG	O9-C10-C11-C12
30	3	316	CHL	CAA-CBA-CGA-O1A
18	B	824	CLA	CAA-CBA-CGA-O1A
18	B	839	CLA	CAA-CBA-CGA-O1A
18	2	313	CLA	CAA-CBA-CGA-O1A
30	3	313	CHL	CAA-CBA-CGA-O1A
18	B	817	CLA	C8-C10-C11-C12
18	A	813	CLA	CAA-CBA-CGA-O1A
30	2	315	CHL	C5-C6-C7-C8
18	B	810	CLA	C15-C16-C17-C18
26	F	309	DGD	C7A-C8A-C9A-CAA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	3	307	CLA	CAA-CBA-CGA-O1A
18	A	812	CLA	C4C-C3C-CAC-CBC
18	B	827	CLA	C10-C11-C12-C13
24	J	1102	LMG	C8-C7-O1-C1
26	2	327	DGD	C5D-C6D-O5D-C1E
18	A	835	CLA	CAA-CBA-CGA-O1A
18	2	306	CLA	CAA-CBA-CGA-O1A
18	3	308	CLA	CAA-CBA-CGA-O1A
24	J	1102	LMG	O9-C10-C11-C12
26	2	327	DGD	O1B-C1B-C2B-C3B
18	1	5008	CLA	CAA-CBA-CGA-O2A
30	4	302	CHL	CAA-CBA-CGA-O2A
30	4	316	CHL	C10-C11-C12-C13
30	4	313	CHL	C2A-CAA-CBA-CGA
18	B	832	CLA	CAA-CBA-CGA-O1A
18	L	305	CLA	CAA-CBA-CGA-O1A
24	1	5001	LMG	O10-C28-C29-C30
18	A	814	CLA	CAA-CBA-CGA-O2A
18	A	836	CLA	CAA-CBA-CGA-O2A
26	1	5002	DGD	C1A-C2A-C3A-C4A
26	F	309	DGD	CFA-CGA-CHA-CIA
18	1	5006	CLA	C2-C1-O2A-CGA
18	A	839	CLA	CAA-CBA-CGA-O1A
22	A	848	LHG	C10-C11-C12-C13
23	G	1606	LMT	C3-C4-C5-C6
18	B	837	CLA	CAA-CBA-CGA-O1A
18	A	820	CLA	CAA-CBA-CGA-O2A
18	B	803	CLA	CAA-CBA-CGA-O2A
18	B	813	CLA	CAA-CBA-CGA-O2A
22	A	849	LHG	O7-C7-C8-C9
24	F	306	LMG	C36-C37-C38-C39
26	B	855	DGD	C1B-C2B-C3B-C4B
18	B	811	CLA	CAA-CBA-CGA-O1A
18	B	815	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

218 monomers are involved in 749 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	2	312	CLA	7	0
18	2	326	CLA	3	0
18	3	309	CLA	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	829	CLA	6	0
18	A	806	CLA	6	0
18	A	839	CLA	5	0
24	1	5020	LMG	3	0
22	A	848	LHG	8	0
18	A	840	CLA	7	0
18	A	814	CLA	1	0
19	B	842	PQN	2	0
30	2	316	CHL	4	0
18	J	1101	CLA	8	0
18	K	1401	CLA	3	0
18	1	5012	CLA	3	0
21	B	846	BCR	3	0
18	2	317	CLA	2	0
21	A	846	BCR	7	0
18	4	315	CLA	3	0
18	G	1603	CLA	3	0
18	A	812	CLA	5	0
18	B	809	CLA	4	0
18	1	5011	CLA	2	0
18	B	805	CLA	8	0
18	4	307	CLA	2	0
18	A	810	CLA	7	0
21	I	101	BCR	2	0
24	2	301	LMG	1	0
23	2	325	LMT	1	0
18	1	5007	CLA	2	0
30	3	312	CHL	6	0
21	B	802	BCR	4	0
21	A	843	BCR	6	0
18	B	807	CLA	5	0
18	1	5018	CLA	3	0
18	4	311	CLA	3	0
21	3	306	BCR	3	0
18	1	5008	CLA	1	0
24	F	306	LMG	4	0
18	A	853	CLA	7	0
24	B	850	LMG	2	0
18	1	5010	CLA	5	0
21	L	302	BCR	1	0
18	B	835	CLA	4	0
18	A	804	CLA	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1	5019	LHG	3	0
21	L	307	BCR	3	0
24	A	851	LMG	6	0
18	B	801	CLA	10	0
17	A	801	CL0	7	0
18	A	852	CLA	6	0
18	B	838	CLA	7	0
29	3	303	LUT	3	0
18	L	305	CLA	1	0
18	2	307	CLA	3	0
18	A	828	CLA	7	0
21	B	847	BCR	2	0
30	2	319	CHL	1	0
18	B	834	CLA	5	0
29	4	303	LUT	2	0
24	F	307	LMG	1	0
18	B	841	CLA	8	0
18	A	813	CLA	6	0
18	B	804	CLA	7	0
28	F	310	ZEX	3	0
21	B	844	BCR	4	0
18	1	5015	CLA	3	0
18	1	5009	CLA	5	0
18	2	308	CLA	3	0
18	A	816	CLA	8	0
30	4	317	CHL	3	0
18	B	831	CLA	5	0
18	A	837	CLA	9	0
18	H	1701	CLA	6	0
18	F	302	CLA	4	0
18	B	839	CLA	6	0
18	B	819	CLA	6	0
18	2	313	CLA	4	0
24	2	322	LMG	2	0
18	B	830	CLA	6	0
18	G	1601	CLA	1	0
20	C	102	SF4	1	0
21	F	304	BCR	6	0
18	1	5017	CLA	2	0
21	A	855	BCR	5	0
18	4	309	CLA	1	0
22	2	320	LHG	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	805	CLA	5	0
18	B	816	CLA	4	0
18	B	820	CLA	4	0
18	A	823	CLA	10	0
26	2	327	DGD	5	0
30	2	318	CHL	5	0
21	K	1405	BCR	2	0
30	2	314	CHL	5	0
24	G	1607	LMG	1	0
18	A	807	CLA	5	0
21	1	5005	BCR	3	0
25	A	854	GOL	1	0
30	4	316	CHL	5	0
18	B	822	CLA	3	0
24	1	5001	LMG	6	0
18	3	315	CLA	2	0
18	2	311	CLA	2	0
18	3	307	CLA	7	0
18	A	824	CLA	4	0
30	3	313	CHL	1	0
18	B	811	CLA	7	0
18	A	831	CLA	4	0
31	2	304	XAT	7	0
18	B	810	CLA	4	0
18	K	1403	CLA	4	0
30	4	318	CHL	5	0
18	4	308	CLA	2	0
18	A	836	CLA	6	0
18	B	803	CLA	7	0
18	B	837	CLA	8	0
18	A	803	CLA	9	0
18	2	306	CLA	5	0
18	1	5013	CLA	2	0
22	B	849	LHG	4	0
30	1	5014	CHL	4	0
18	B	821	CLA	2	0
18	A	829	CLA	3	0
18	3	318	CLA	2	0
18	3	314	CLA	2	0
18	B	828	CLA	8	0
18	A	815	CLA	3	0
18	4	305	CLA	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	827	CLA	5	0
19	A	841	PQN	5	0
30	4	313	CHL	1	0
18	4	310	CLA	3	0
18	3	317	CLA	8	0
21	4	301	BCR	7	0
30	1	5016	CHL	6	0
18	B	815	CLA	5	0
18	B	833	CLA	5	0
21	F	305	BCR	5	0
24	2	321	LMG	2	0
18	A	802	CLA	11	0
18	A	827	CLA	2	0
18	A	809	CLA	3	0
21	A	847	BCR	6	0
29	2	303	LUT	5	0
30	4	314	CHL	1	0
18	3	301	CLA	1	0
18	L	306	CLA	1	0
18	B	812	CLA	4	0
18	L	304	CLA	3	0
18	B	826	CLA	10	0
18	L	301	CLA	2	0
18	B	836	CLA	6	0
18	1	5006	CLA	12	0
21	B	843	BCR	7	0
18	B	825	CLA	6	0
18	B	813	CLA	2	0
21	L	303	BCR	3	0
18	A	825	CLA	8	0
18	A	835	CLA	7	0
18	G	1602	CLA	1	0
18	4	306	CLA	2	0
21	3	305	BCR	3	0
18	K	1404	CLA	3	0
30	2	315	CHL	6	0
22	B	848	LHG	4	0
18	A	817	CLA	5	0
18	A	834	CLA	2	0
18	B	840	CLA	4	0
18	A	821	CLA	2	0
21	B	845	BCR	9	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	J	1104	BCR	5	0
29	J	1105	LUT	9	0
18	A	838	CLA	4	0
18	A	830	CLA	3	0
26	B	855	DGD	8	0
30	4	302	CHL	5	0
30	3	316	CHL	6	0
18	B	814	CLA	5	0
18	B	832	CLA	4	0
18	B	818	CLA	9	0
18	2	309	CLA	5	0
18	A	818	CLA	1	0
18	F	303	CLA	6	0
18	A	808	CLA	8	0
18	3	319	CLA	5	0
30	3	310	CHL	10	0
24	2	302	LMG	1	0
21	A	845	BCR	7	0
18	B	806	CLA	9	0
18	A	822	CLA	13	0
23	G	1606	LMT	1	0
23	B	853	LMT	1	0
18	F	301	CLA	2	0
31	4	304	XAT	6	0
18	3	311	CLA	4	0
18	A	833	CLA	3	0
21	G	1604	BCR	4	0
18	B	808	CLA	5	0
29	1	5004	LUT	6	0
18	A	811	CLA	10	0
23	B	856	LMT	2	0
21	A	844	BCR	2	0
18	2	310	CLA	4	0
18	A	820	CLA	3	0
26	J	1106	DGD	4	0
29	1	5003	LUT	8	0
21	I	102	BCR	2	0
21	2	305	BCR	10	0
18	K	1402	CLA	6	0
18	B	824	CLA	8	0
29	3	304	LUT	9	0
22	A	849	LHG	8	0

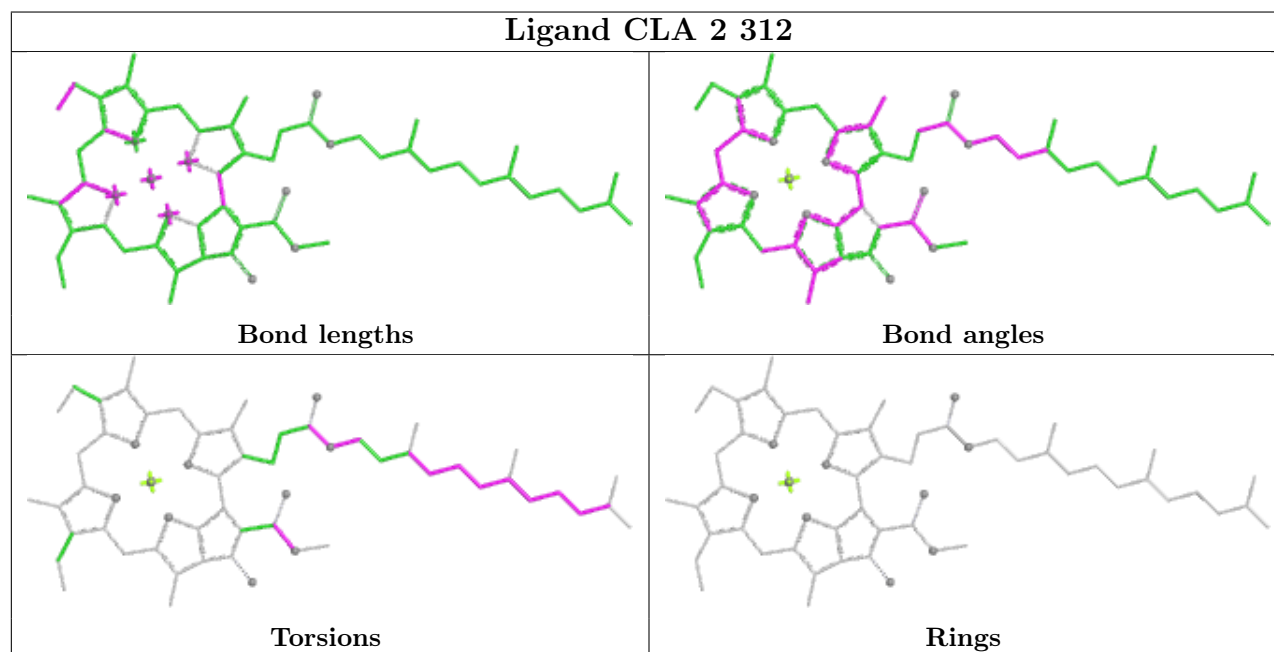
*Continued on next page...*



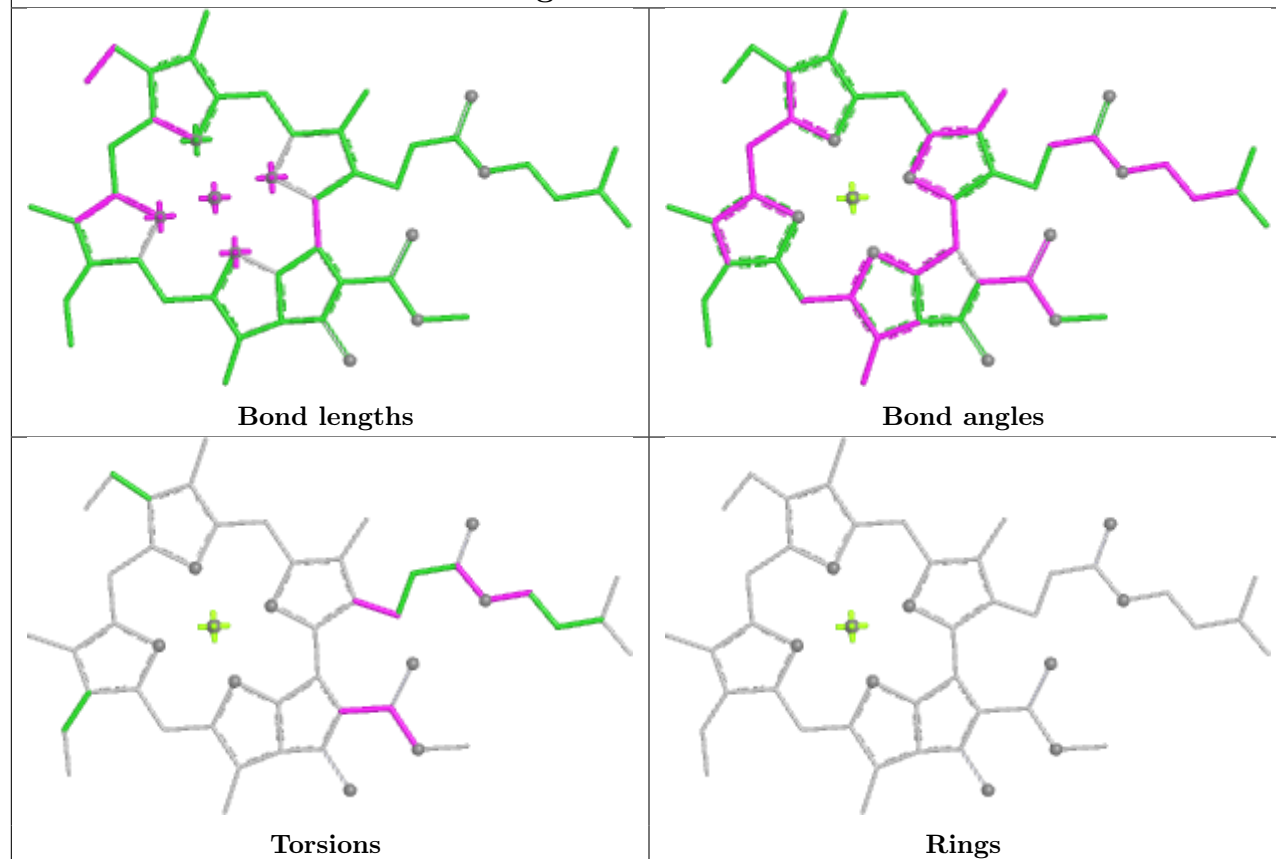
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	G	1605	LMT	2	0
18	A	826	CLA	6	0
18	A	819	CLA	12	0
18	A	832	CLA	7	0
18	B	823	CLA	7	0

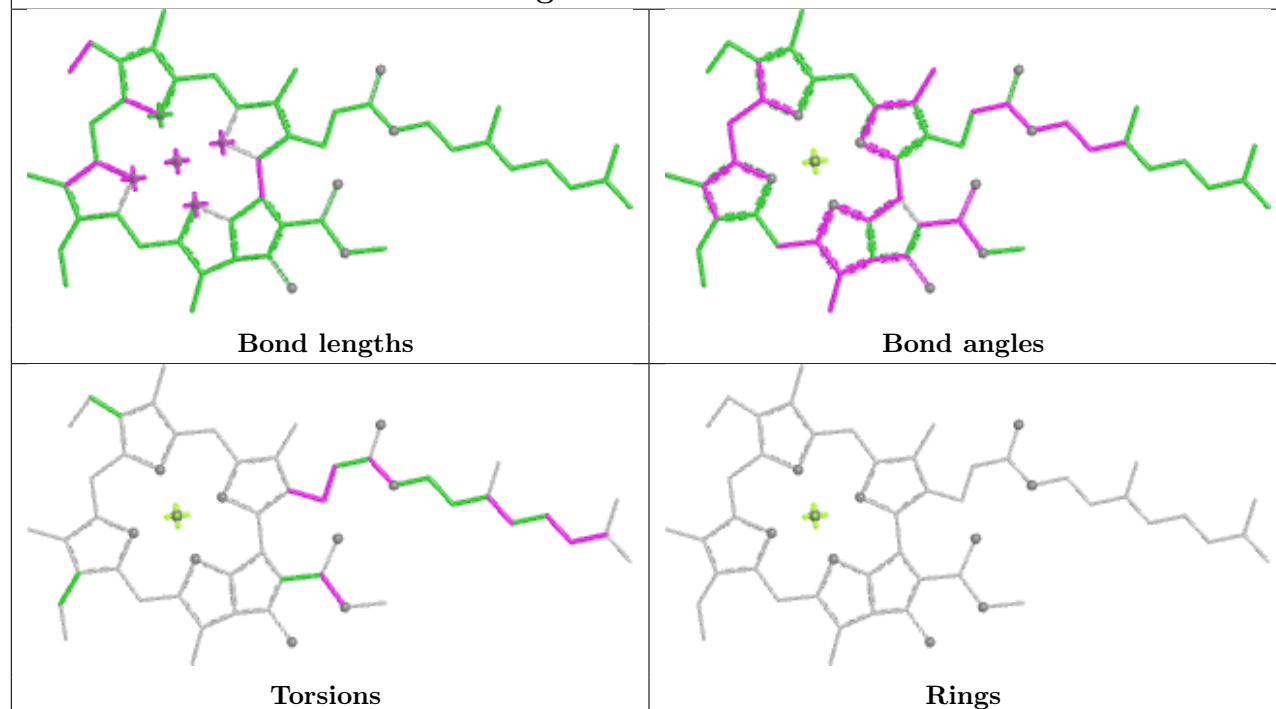
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

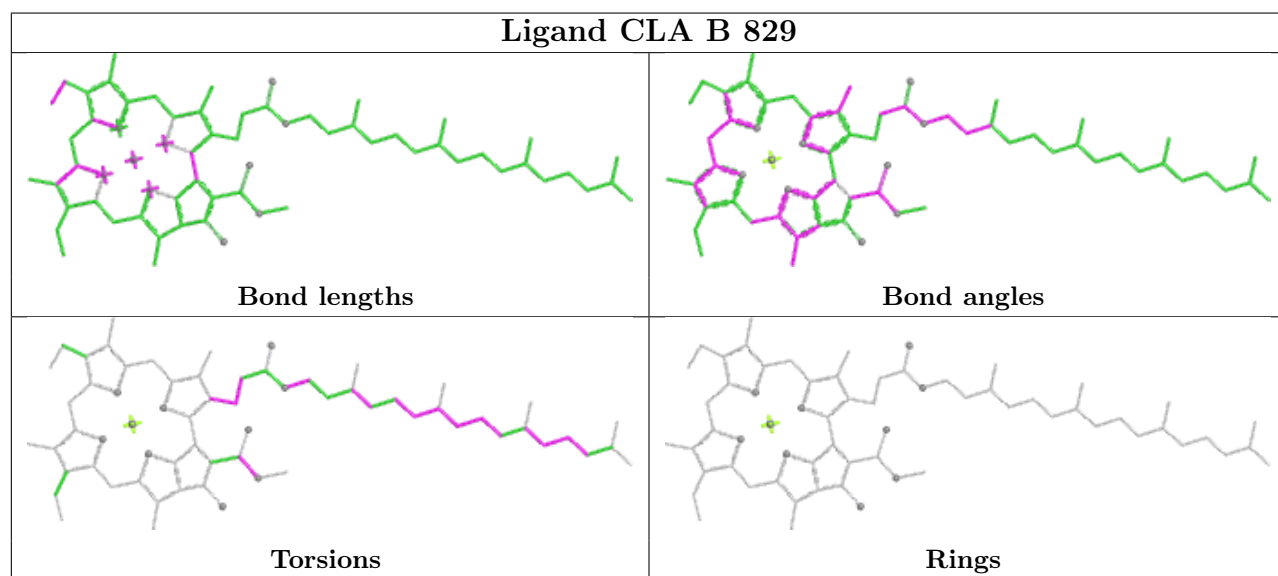
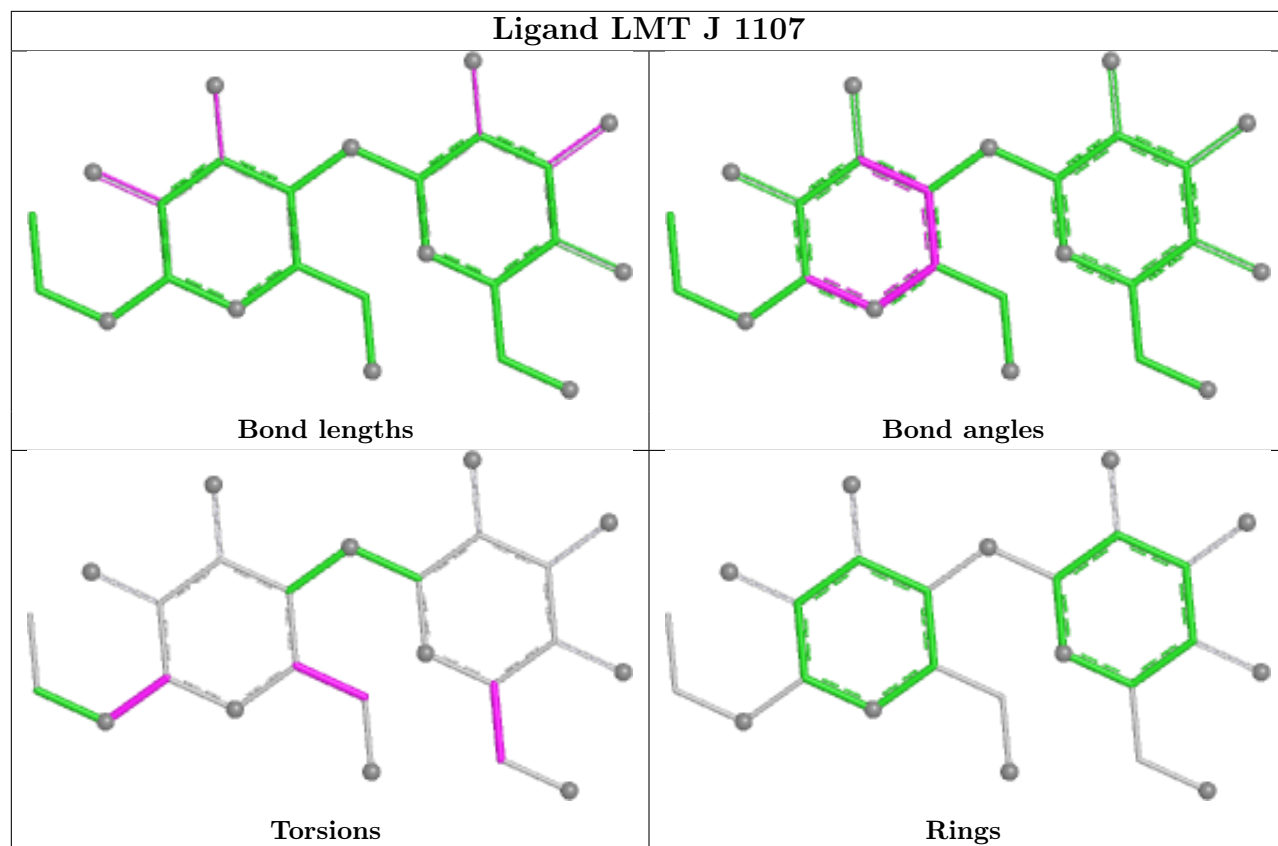


## Ligand CLA 2 326

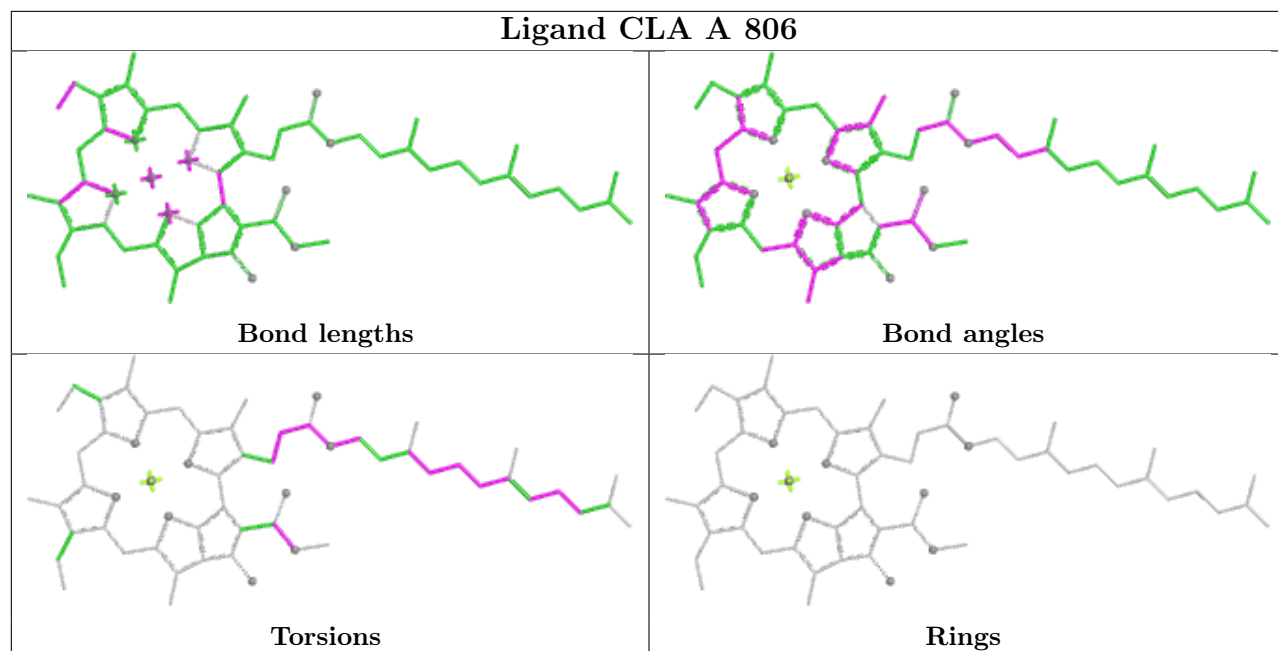


## Ligand CLA 3 309

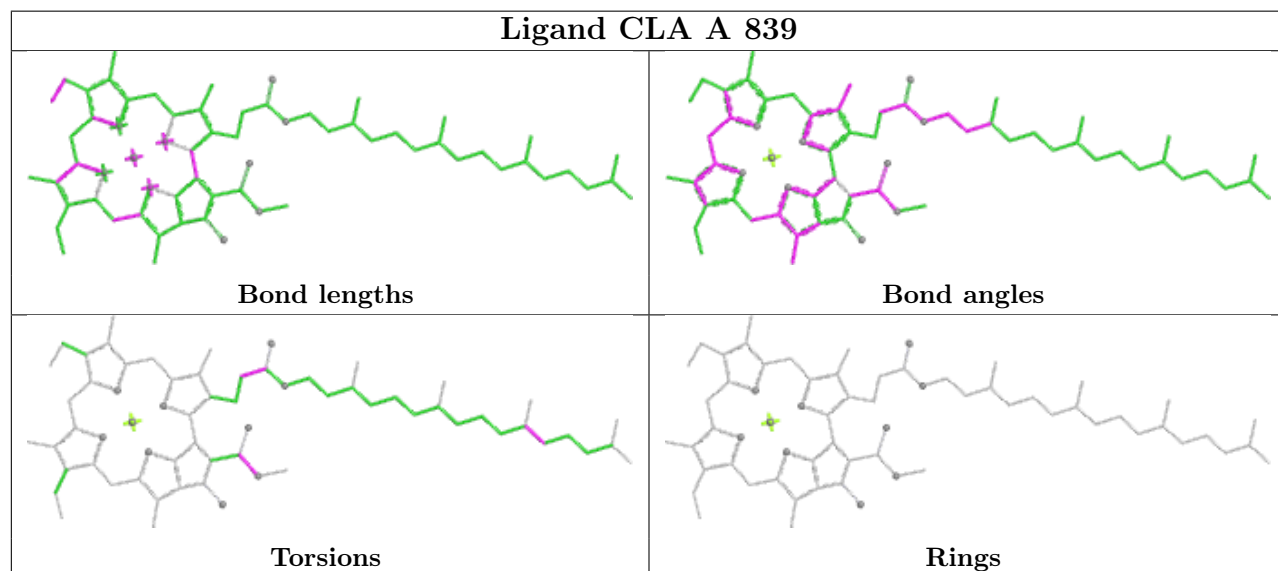




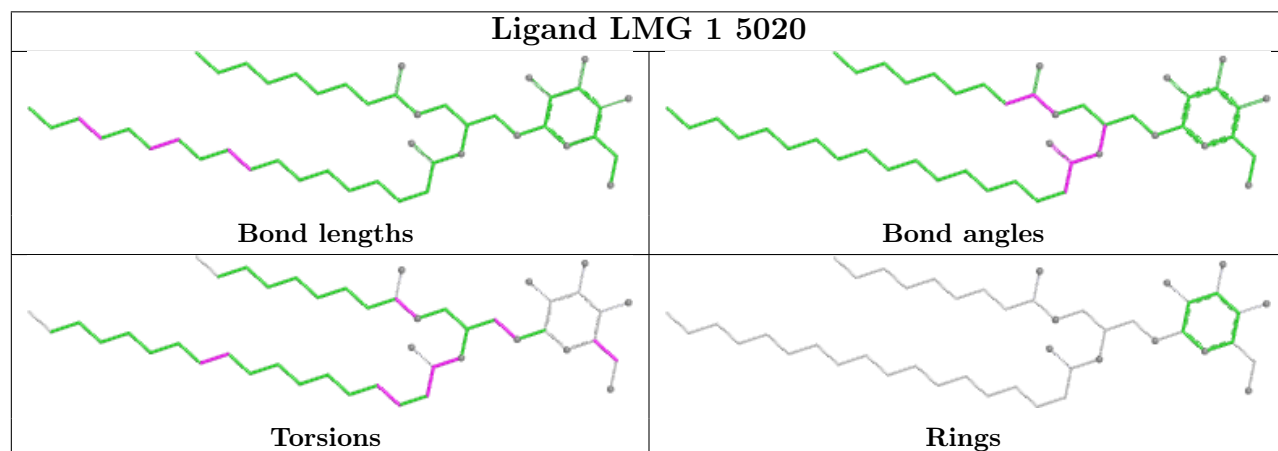
## Ligand CLA A 806

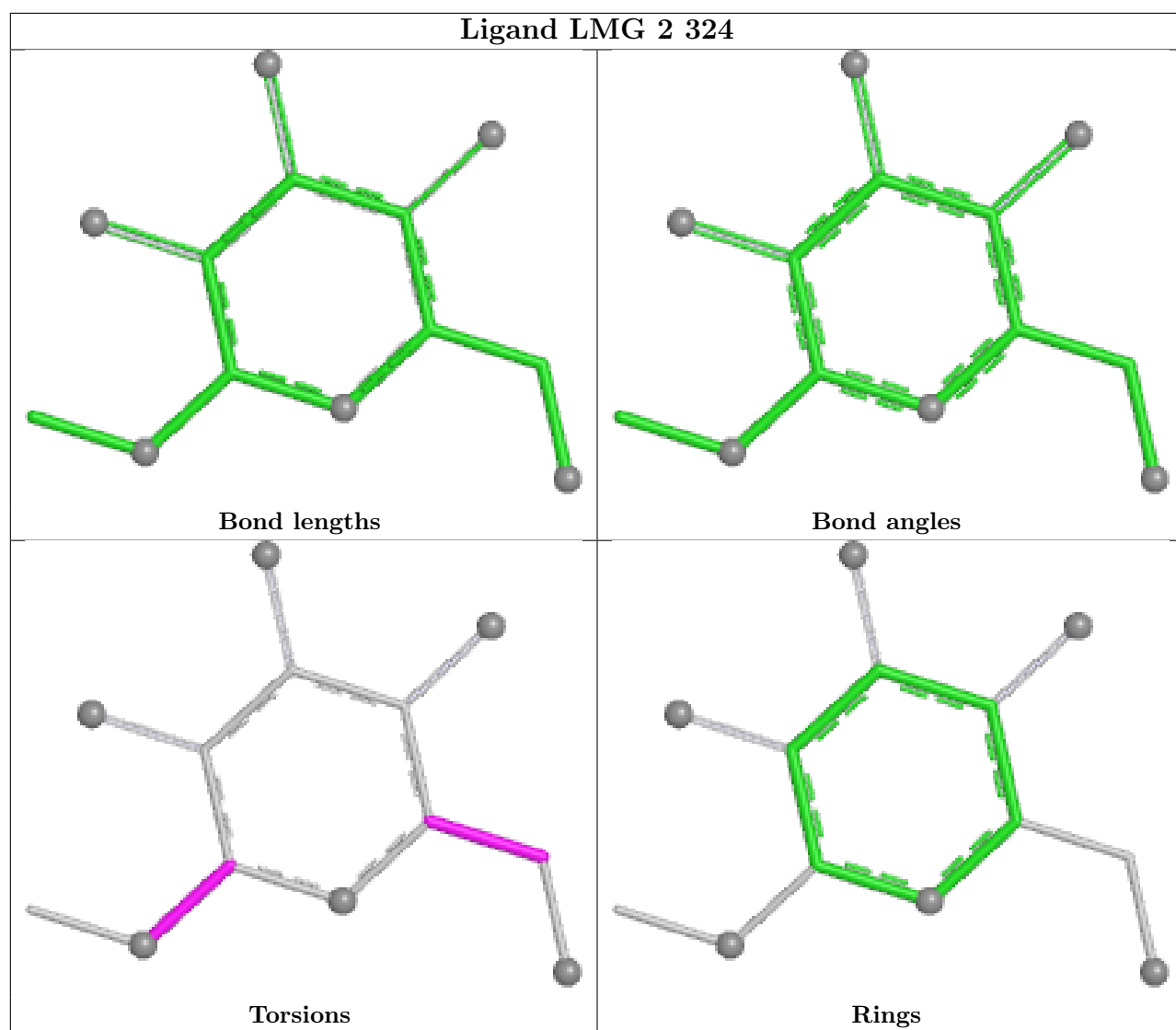


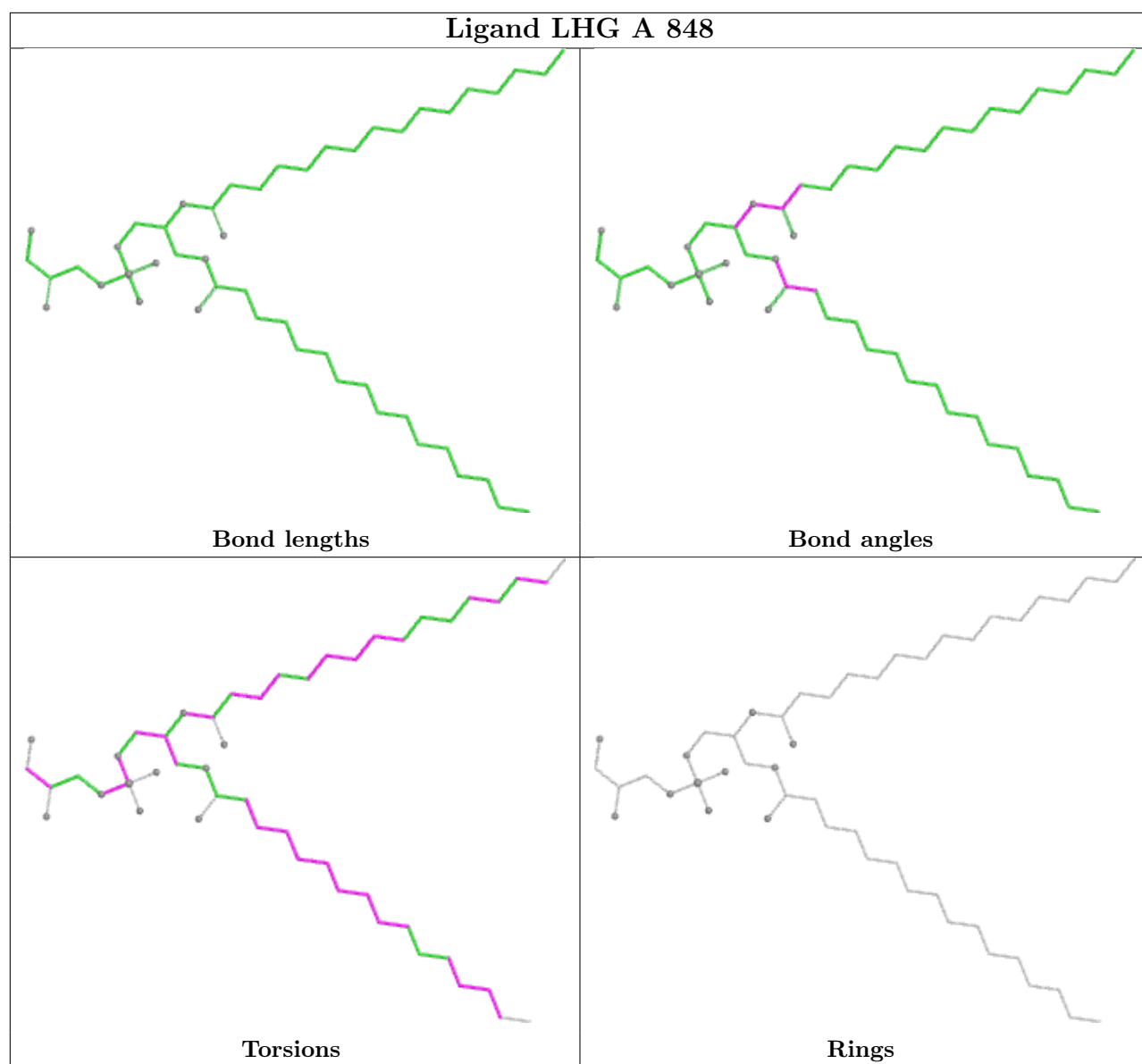
## Ligand CLA A 839



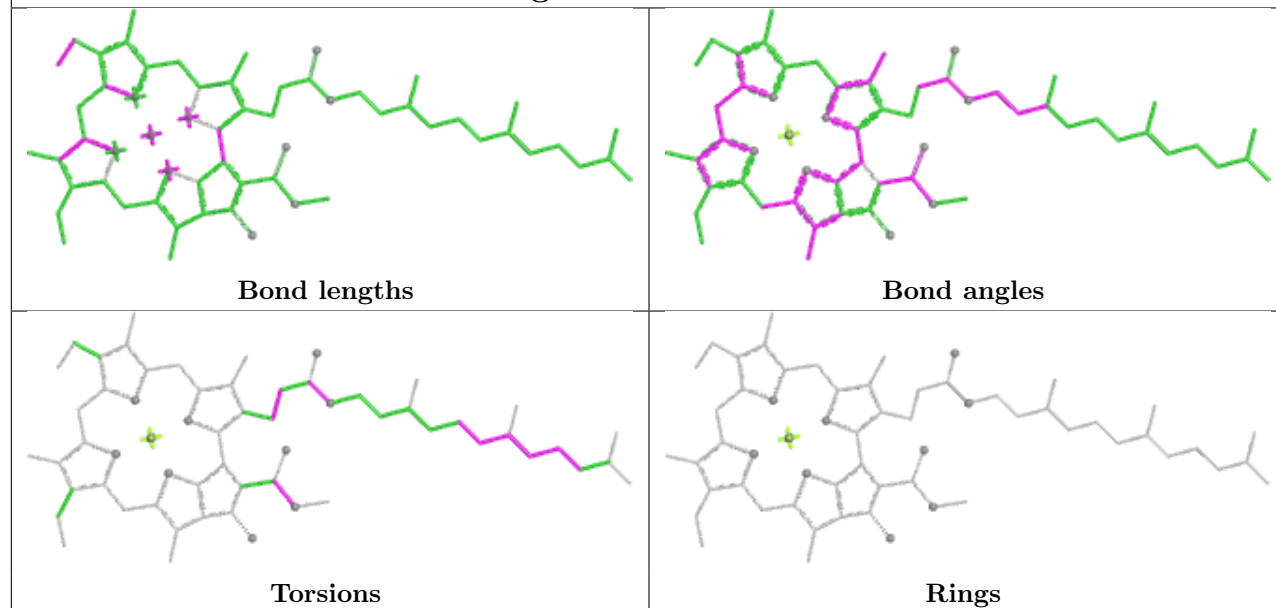
## Ligand LMG 1 5020



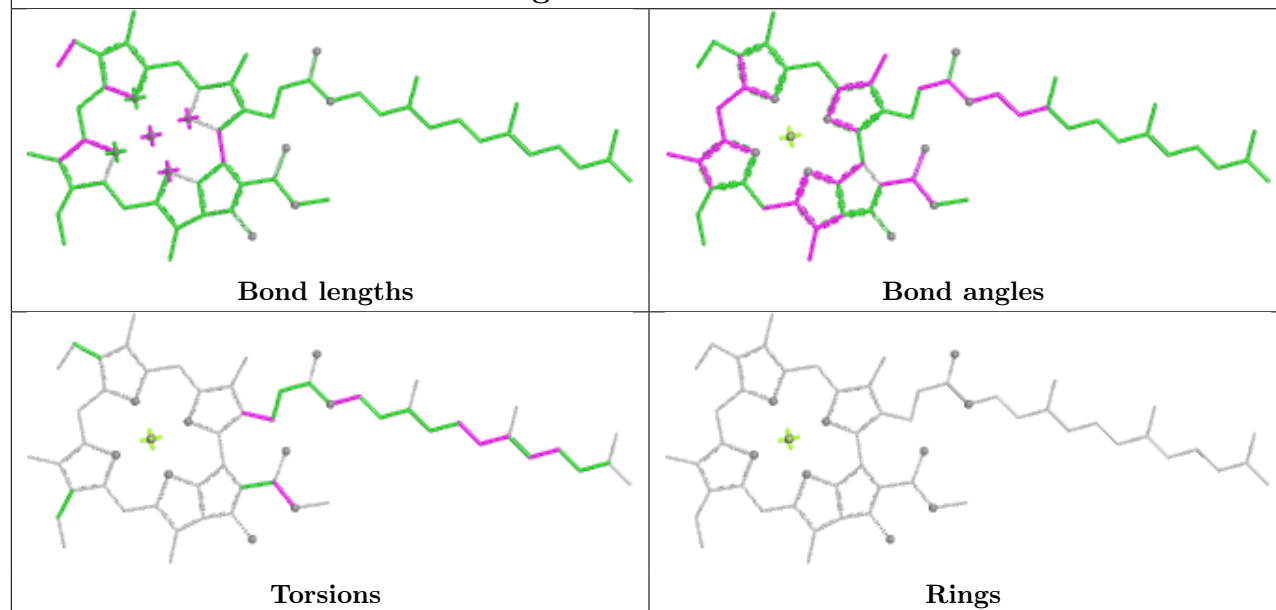




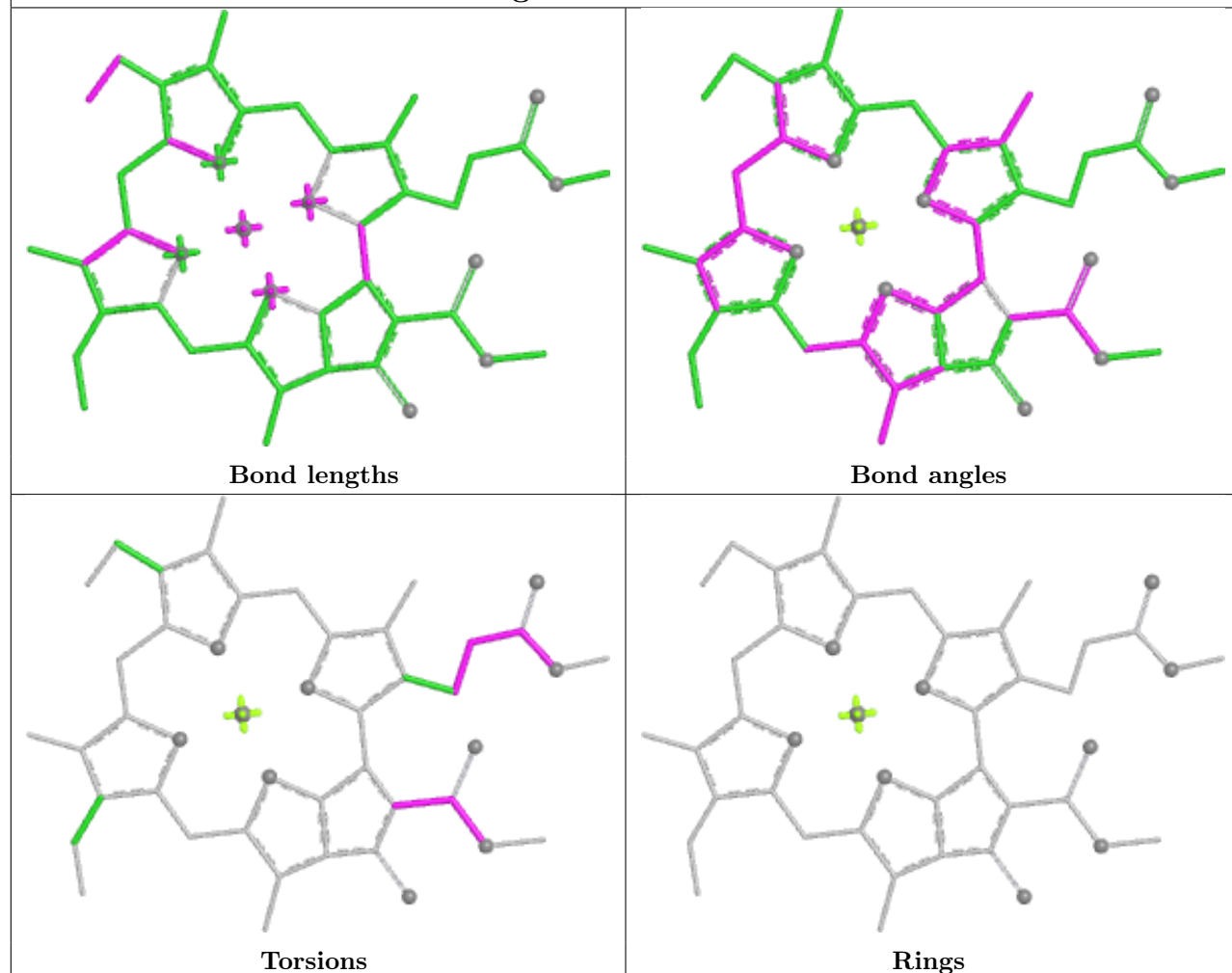
## Ligand CLA A 840



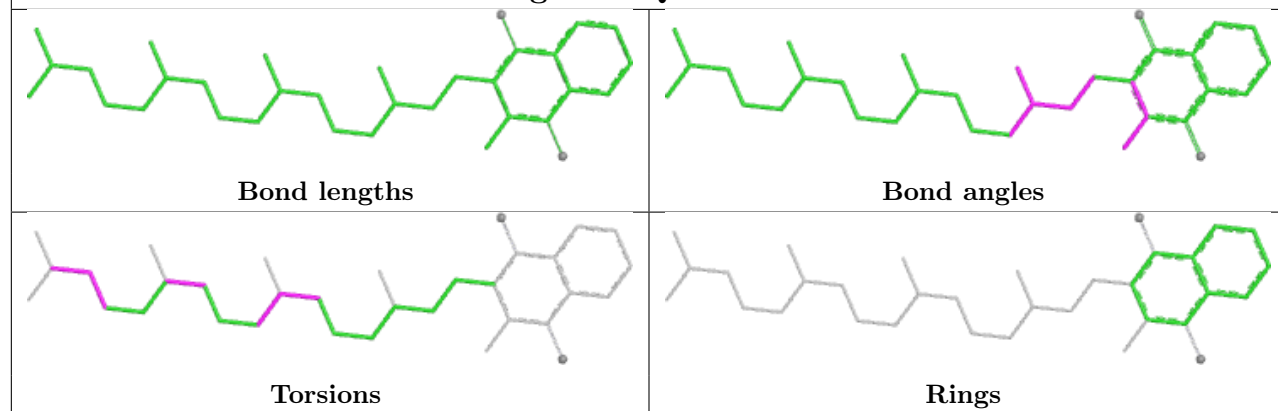
## Ligand CLA B 817



## Ligand CLA A 814

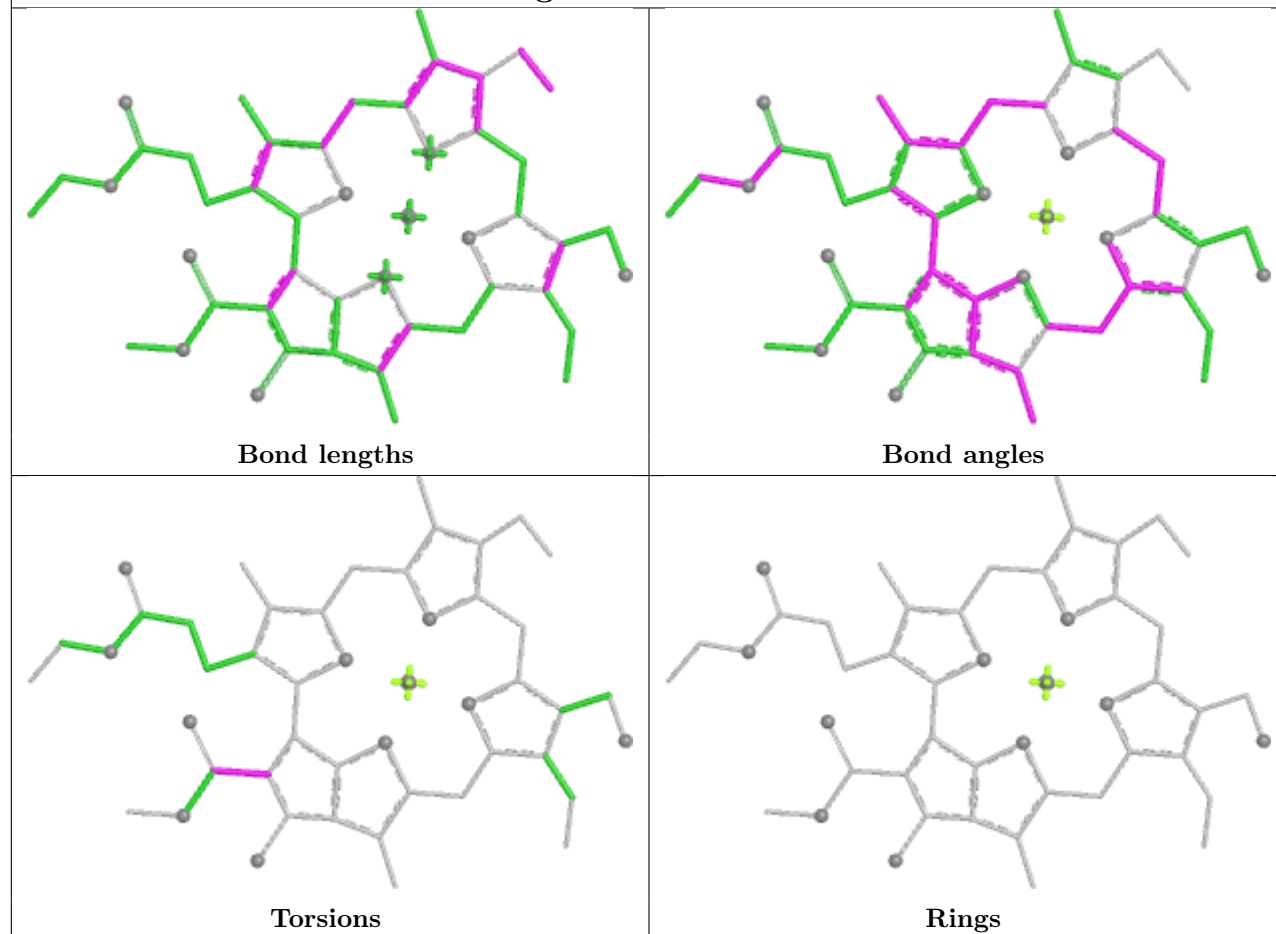


## Ligand PQN B 842

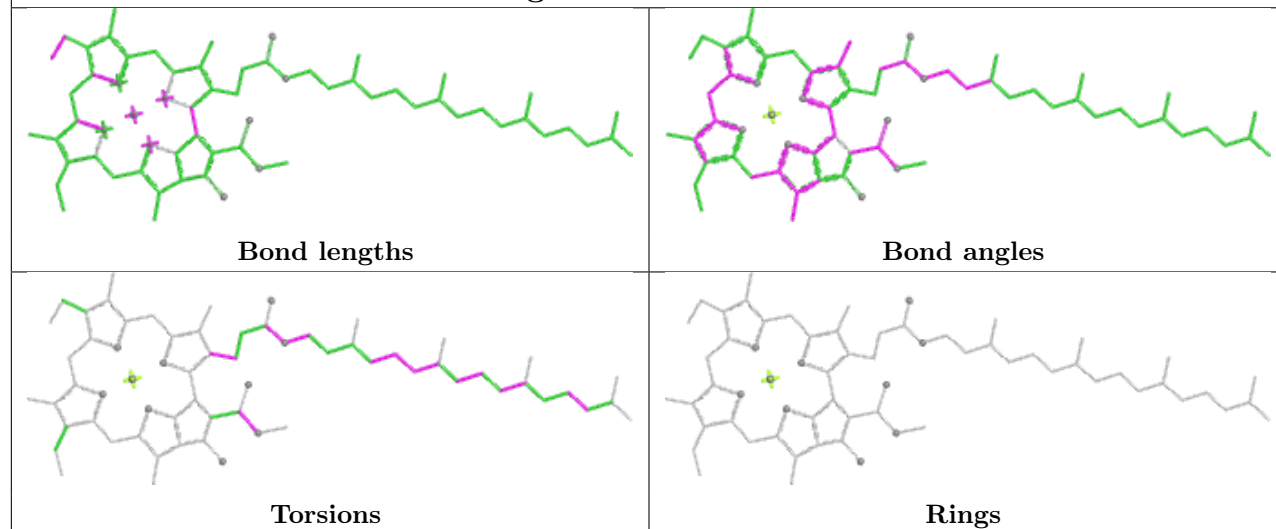




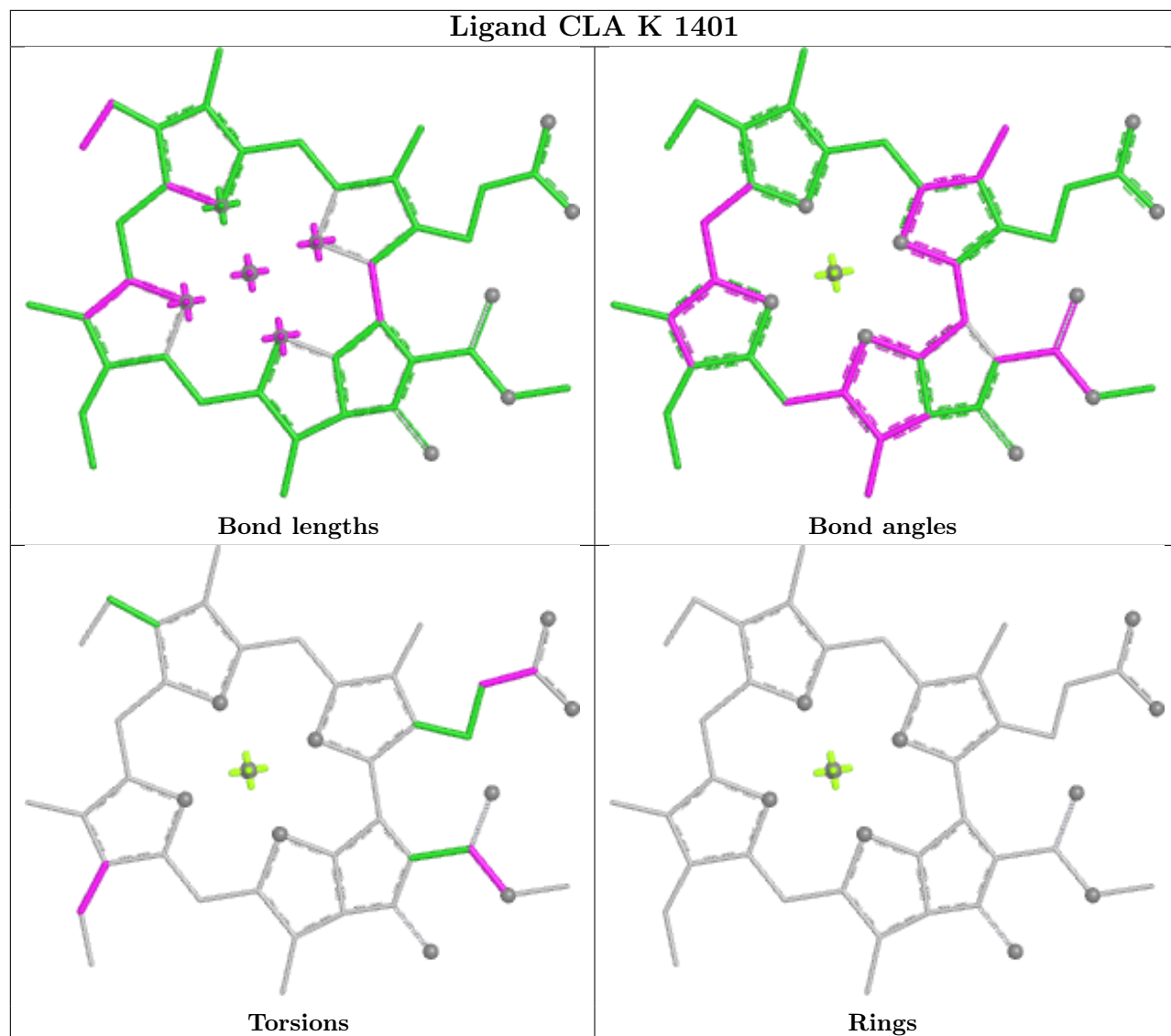
## Ligand CHL 2 316

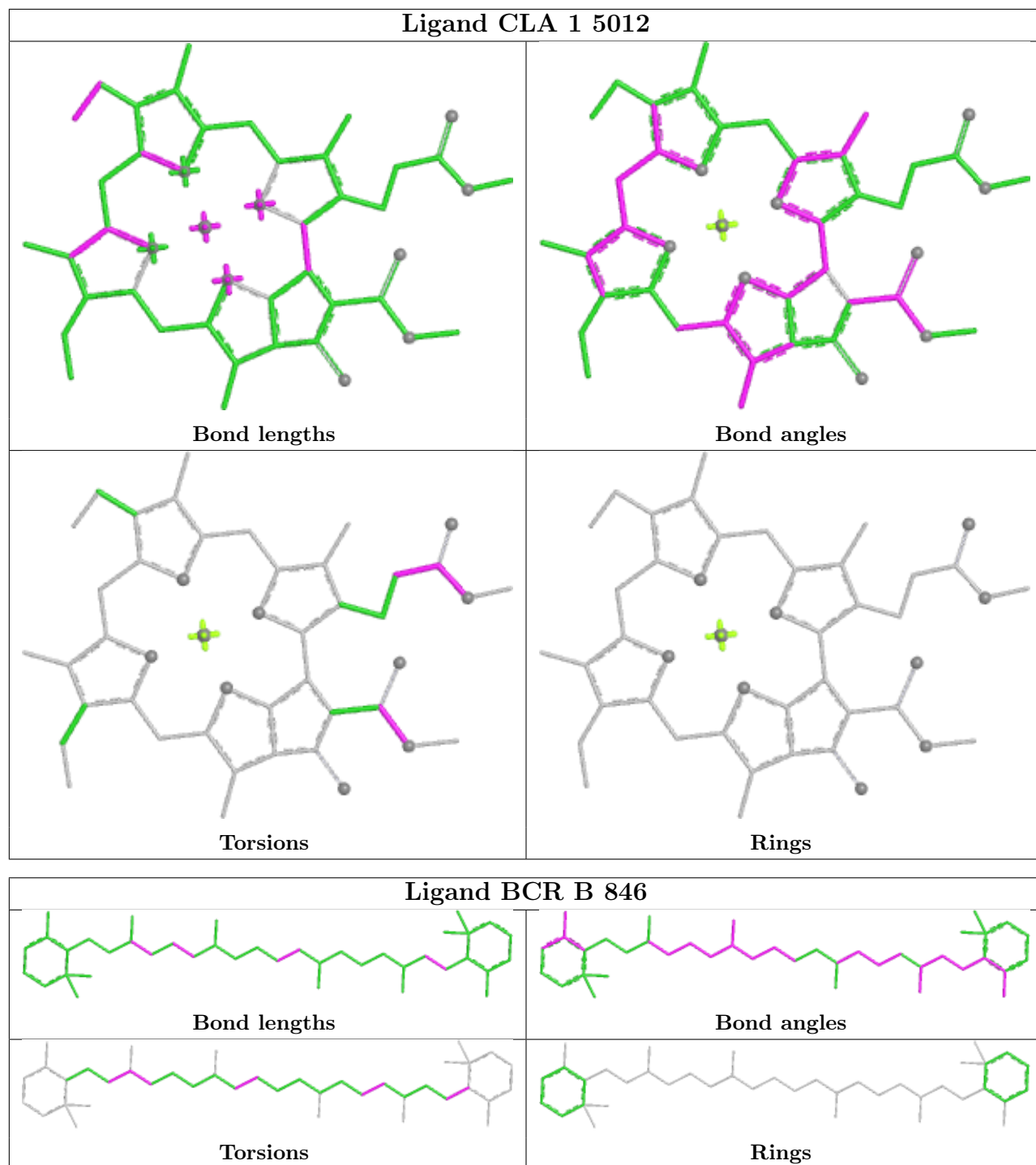


## Ligand CLA J 1101

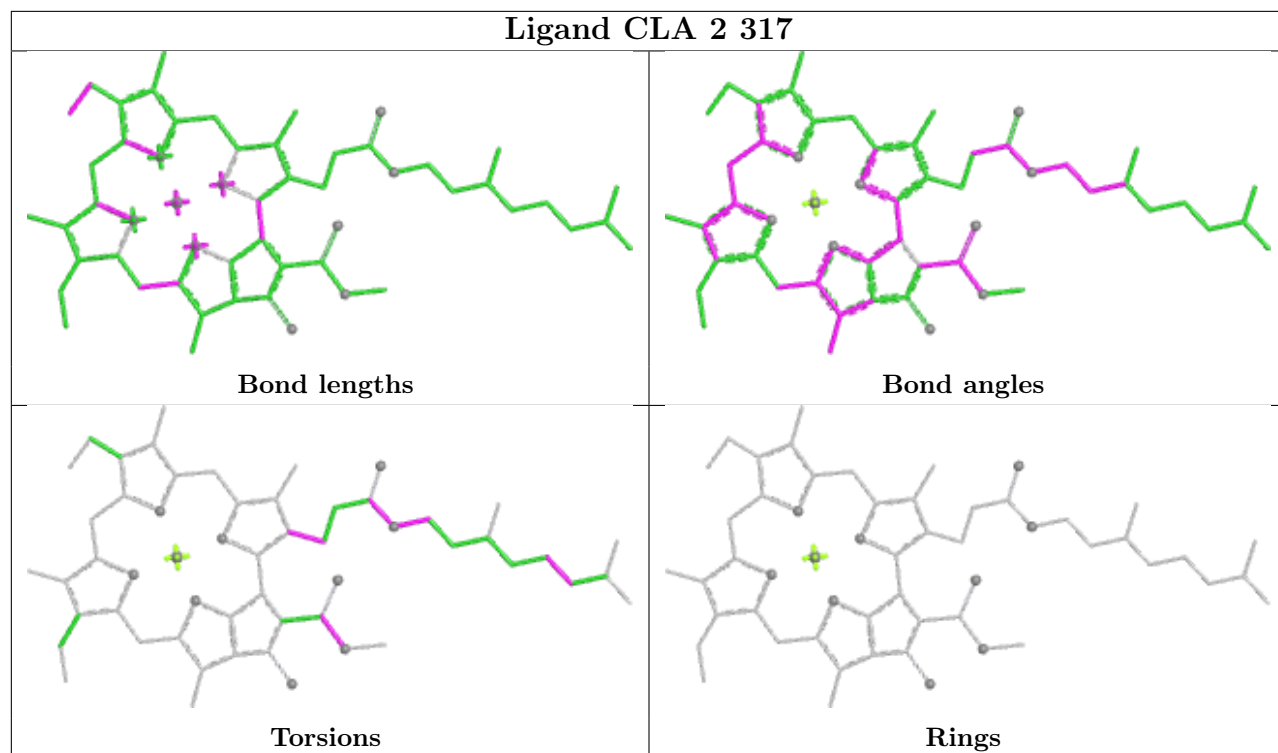


## Ligand CLA K 1401

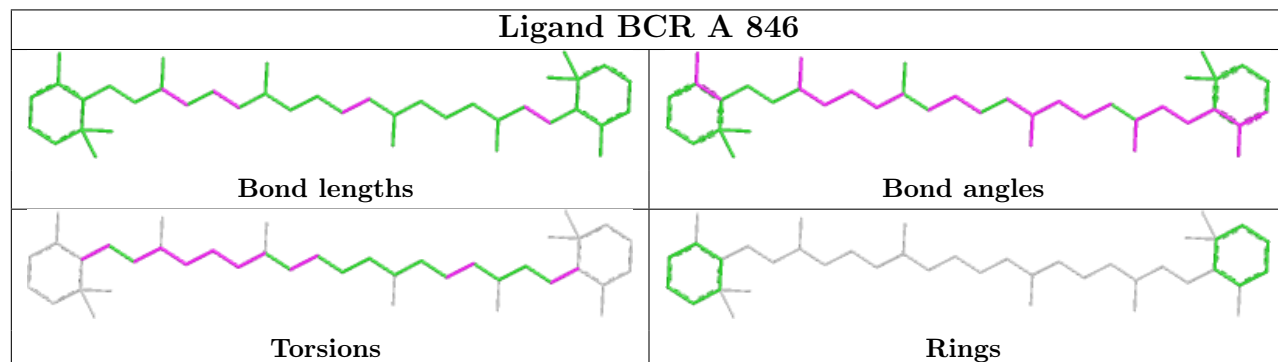




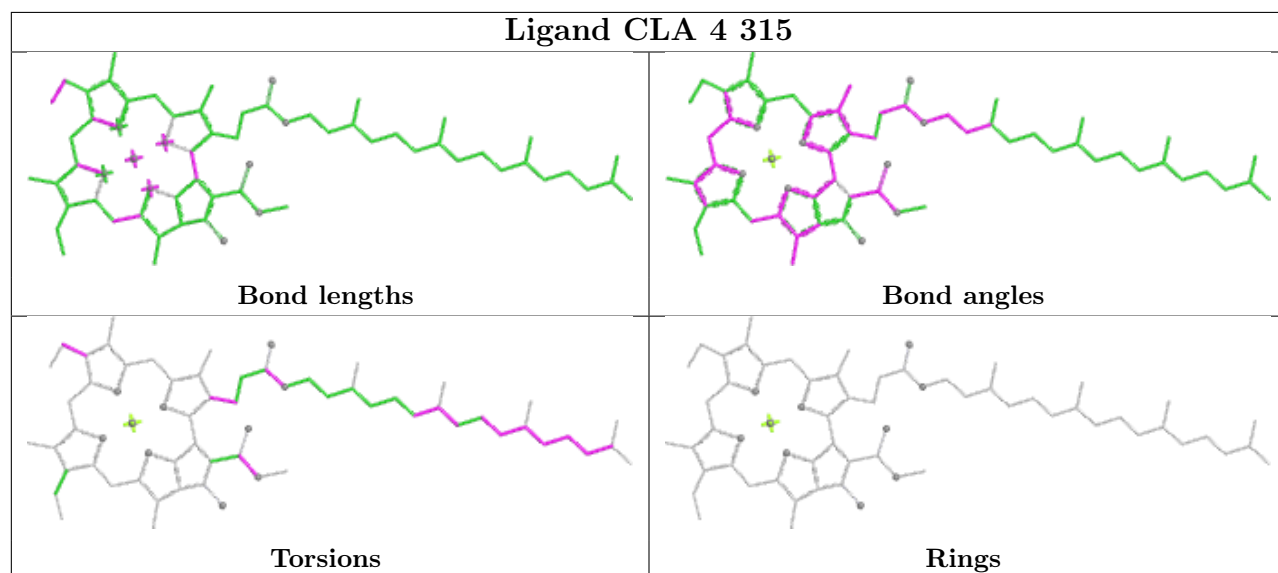
## Ligand CLA 2 317



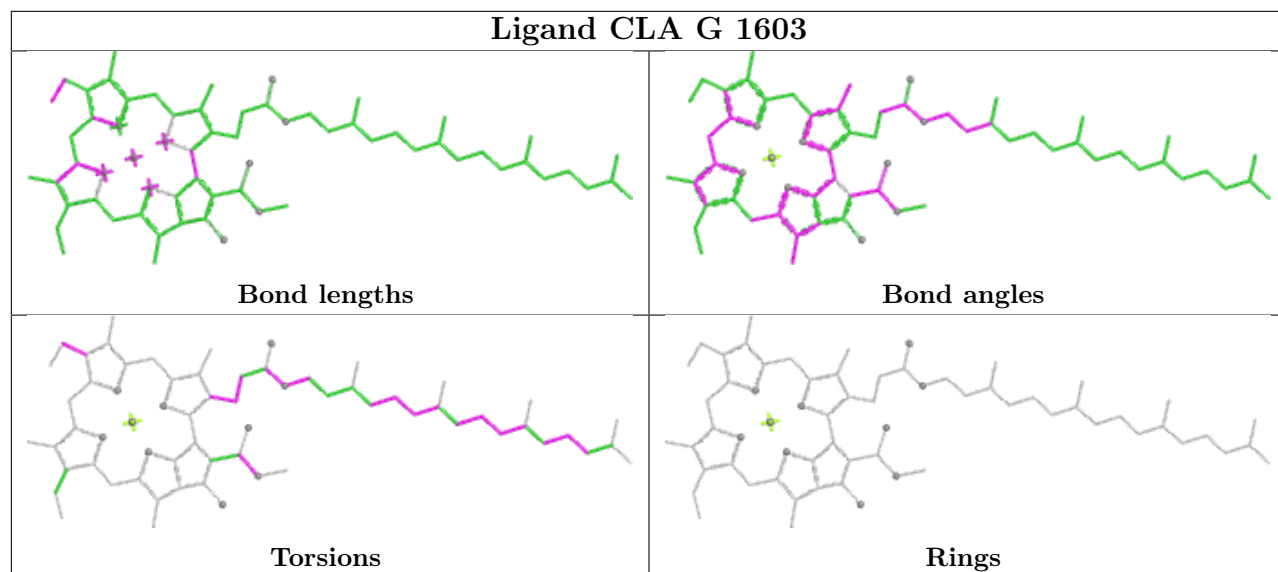
## Ligand BCR A 846



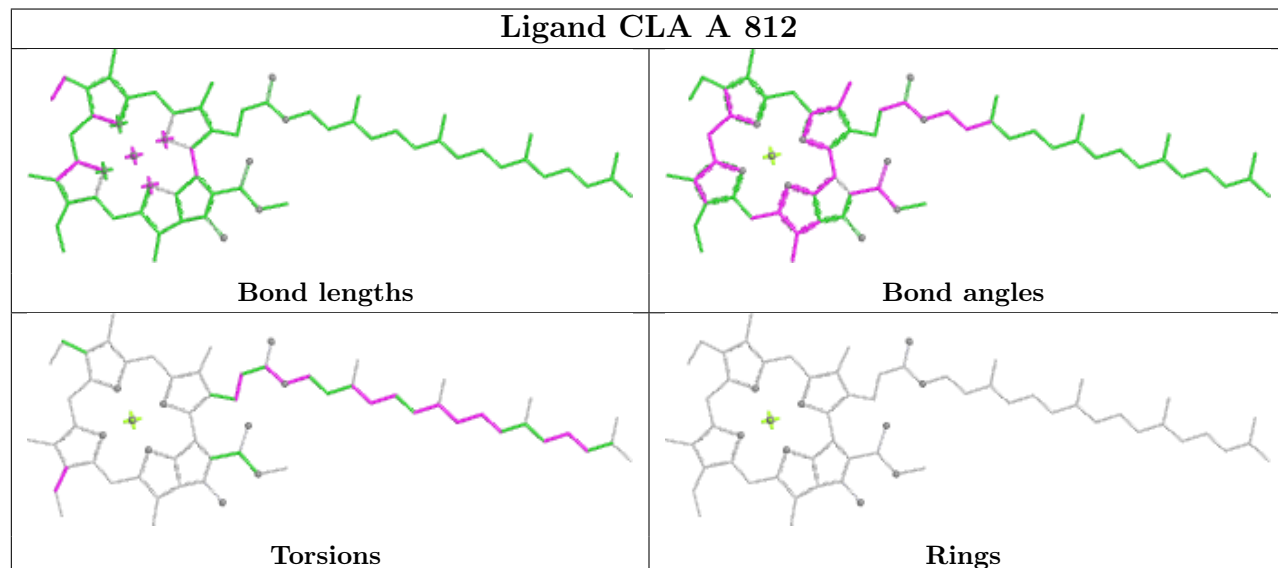
## Ligand CLA 4 315



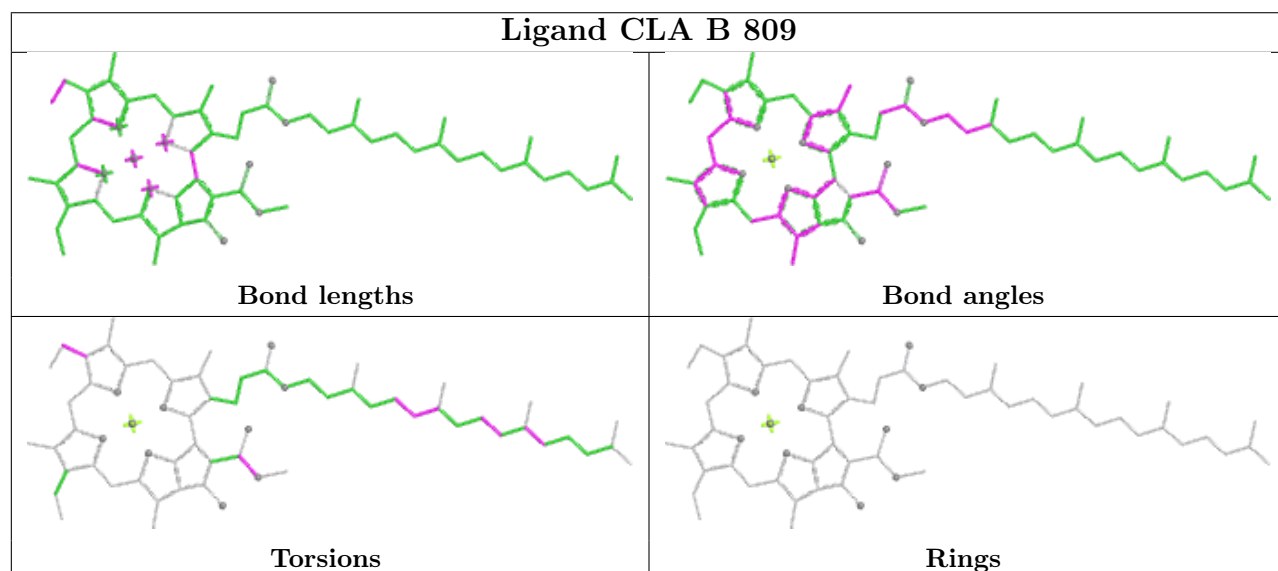
## Ligand CLA G 1603

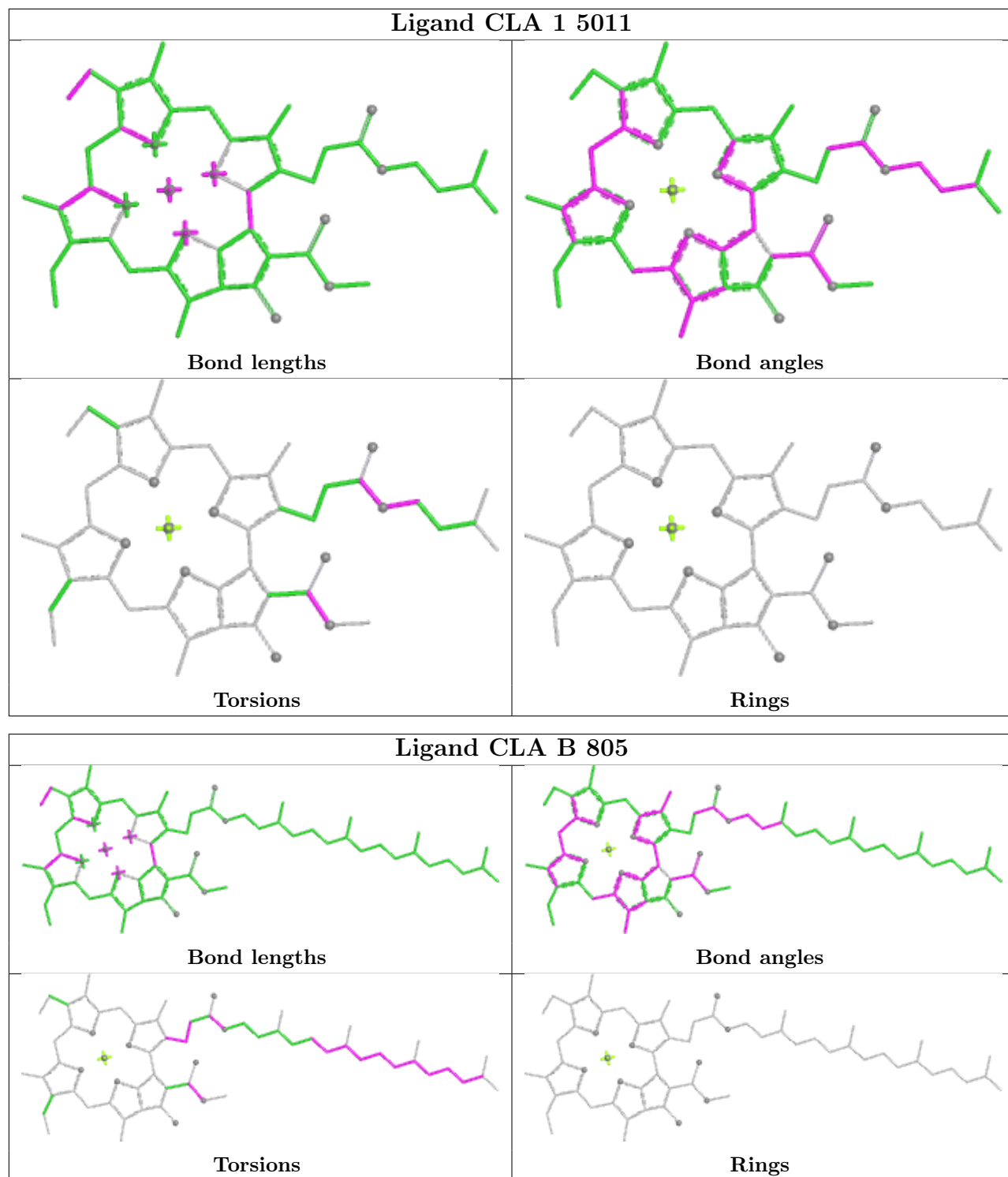


## Ligand CLA A 812

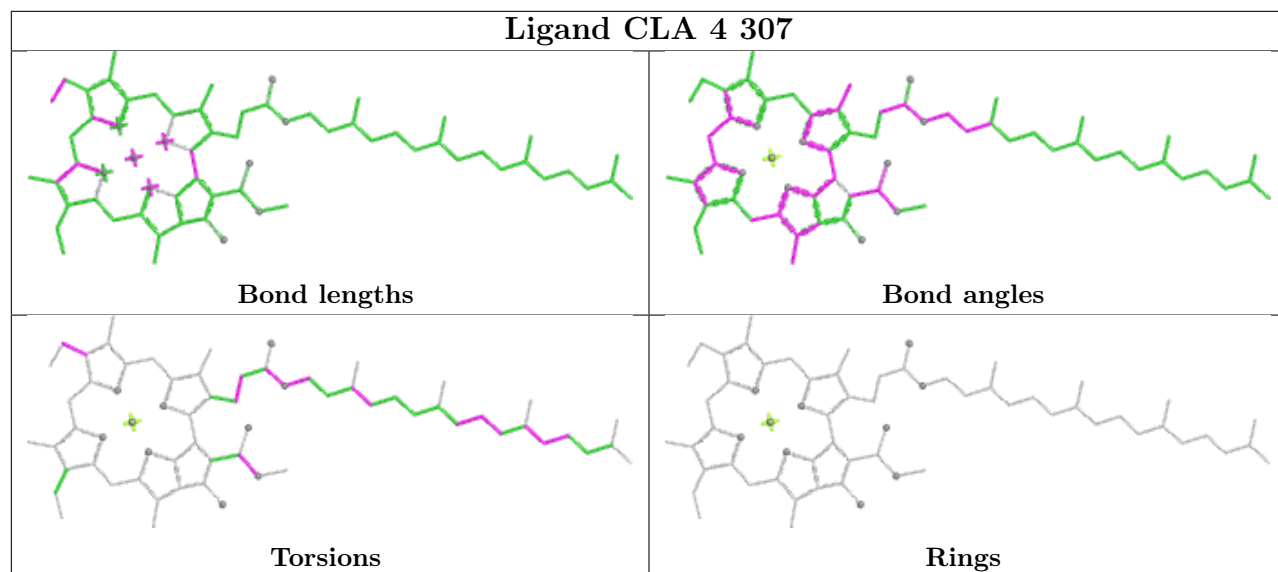


## Ligand CLA B 809

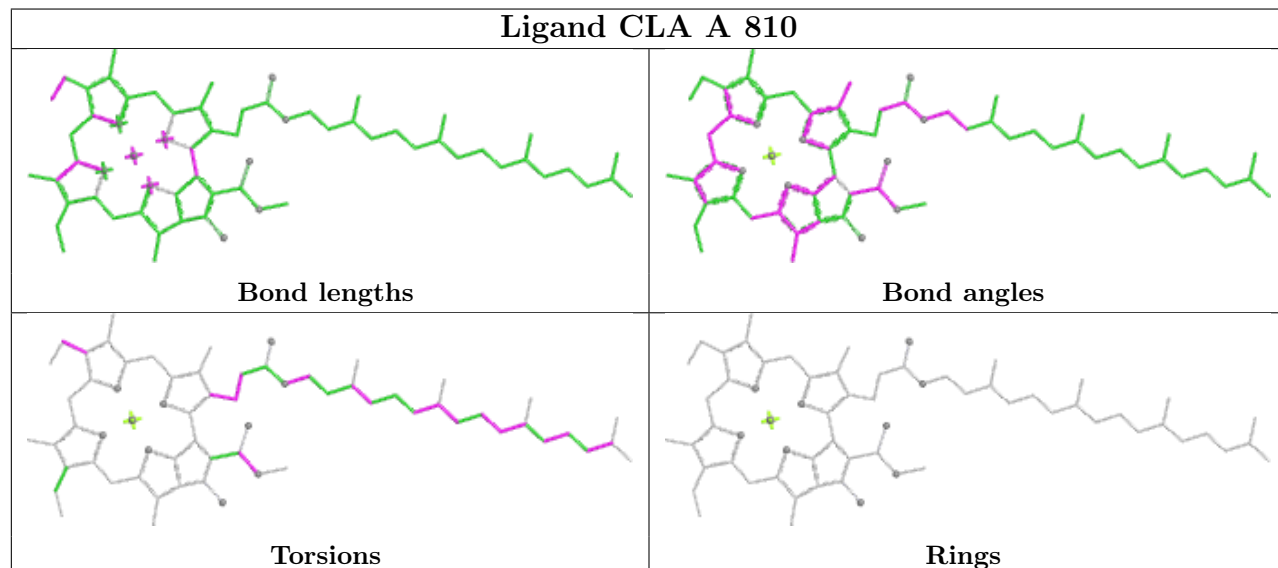




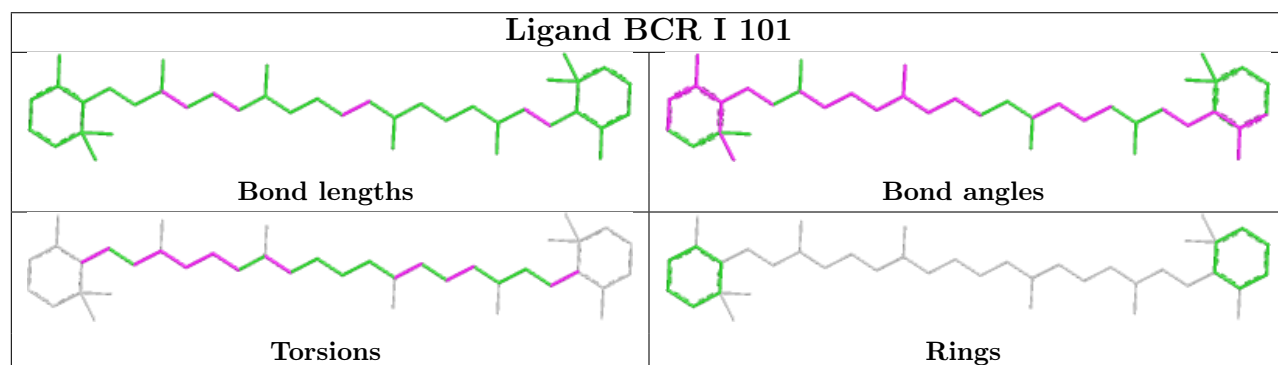
## Ligand CLA 4 307



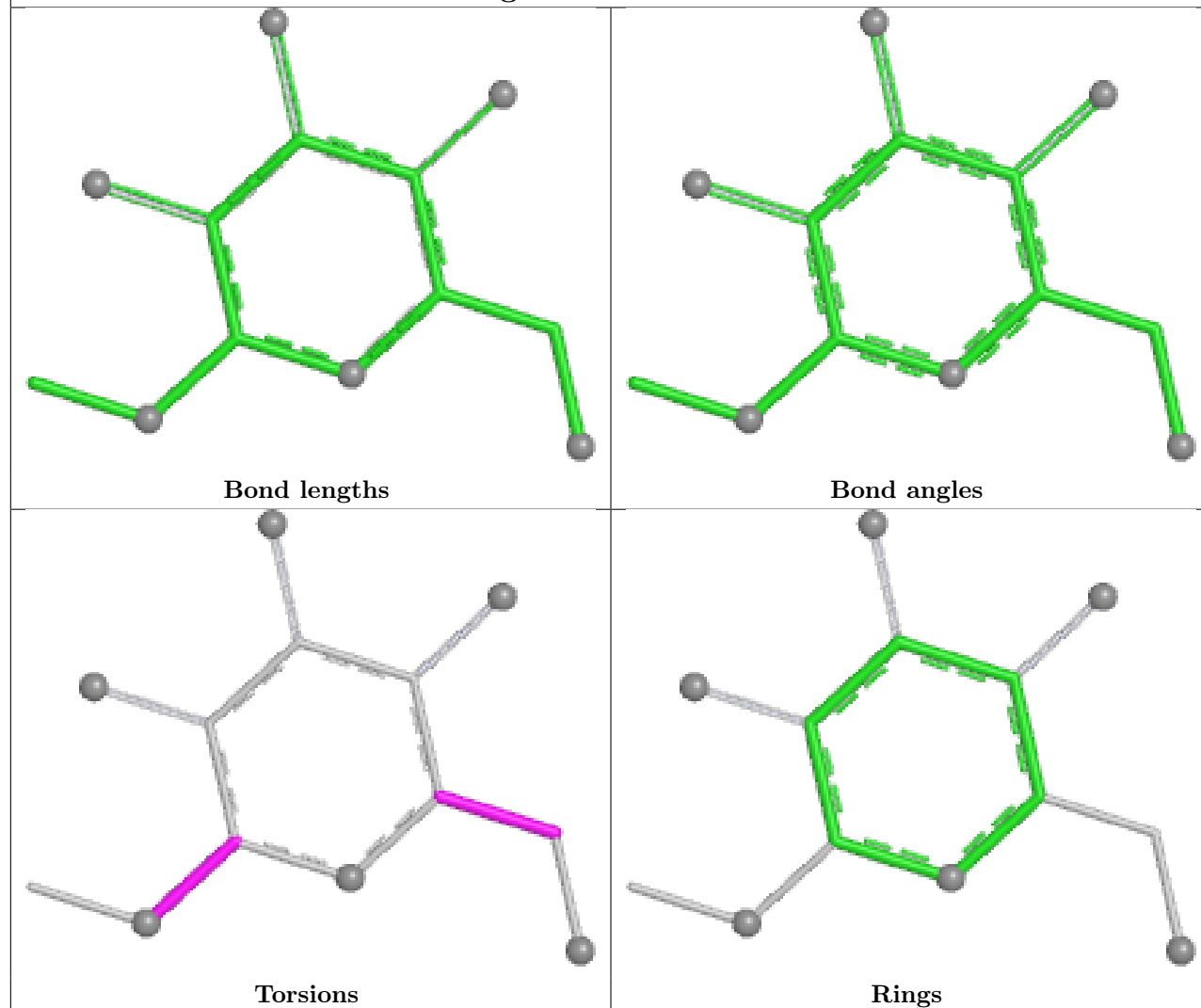
## Ligand CLA A 810



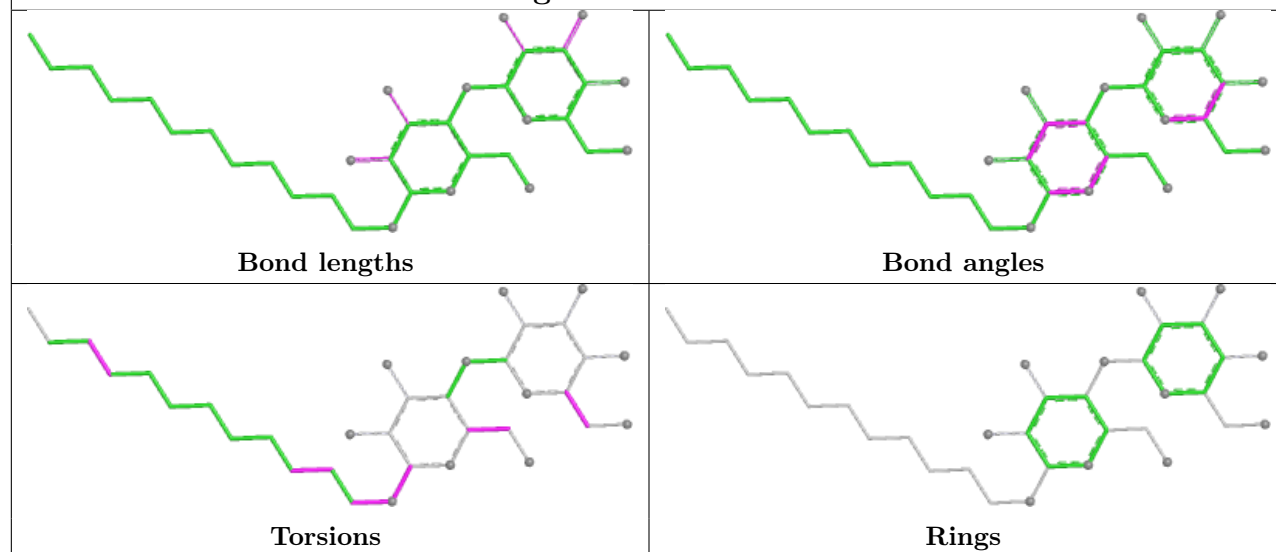
## Ligand BCR I 101



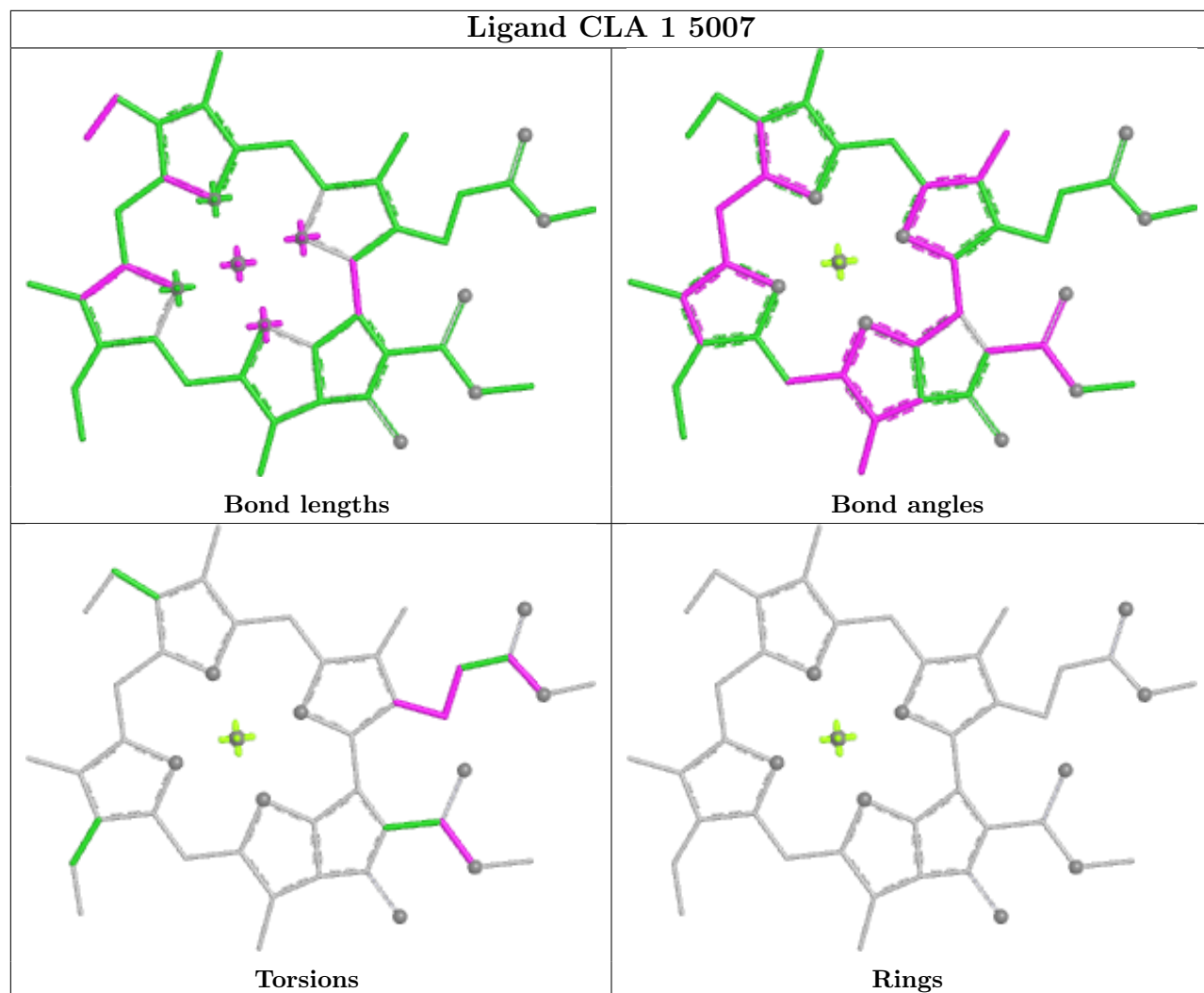
## Ligand LMG 2 301

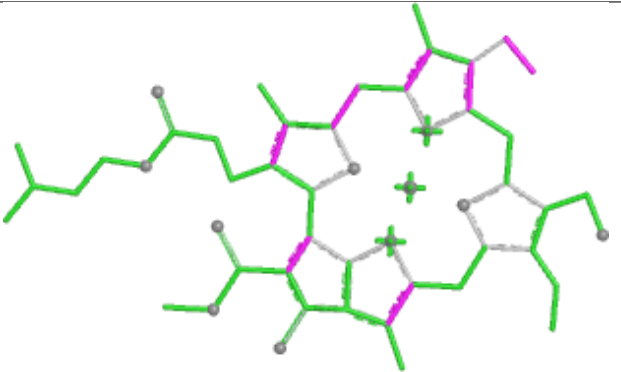
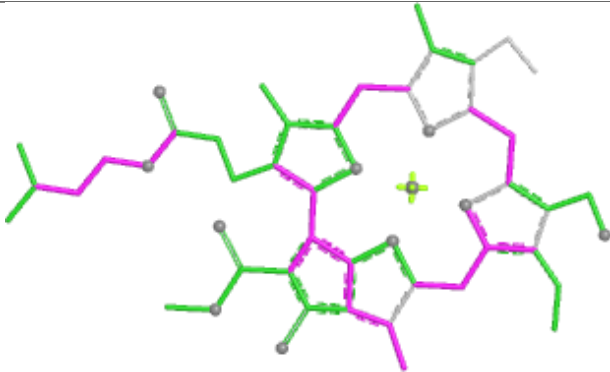
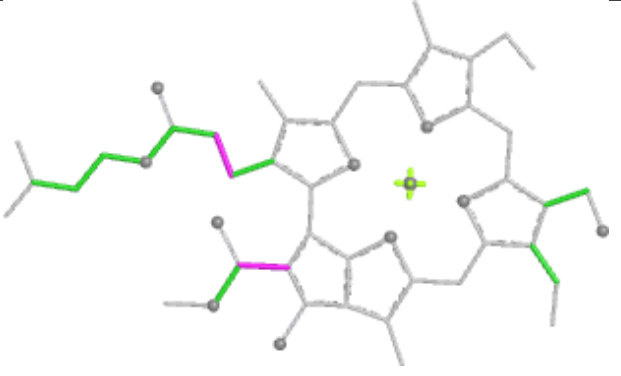
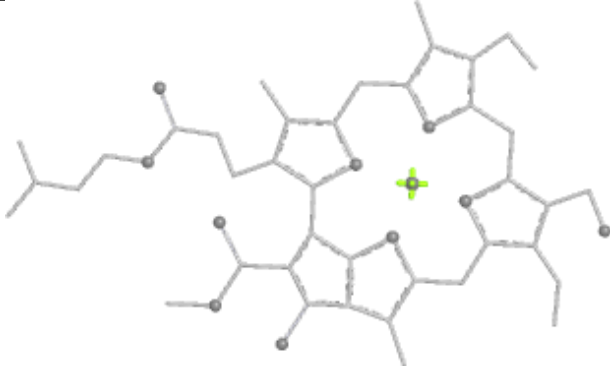


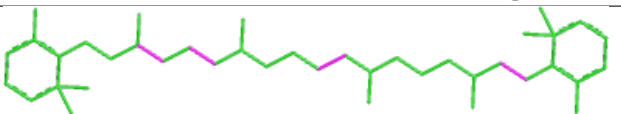
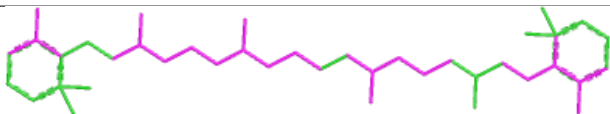
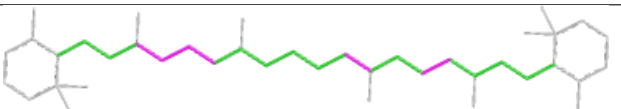
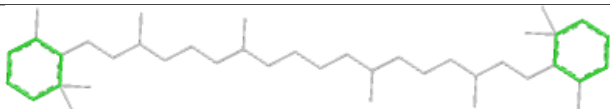
## Ligand LMT 2 325

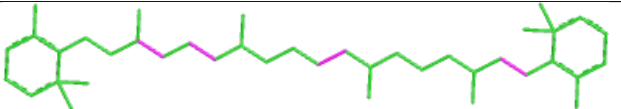
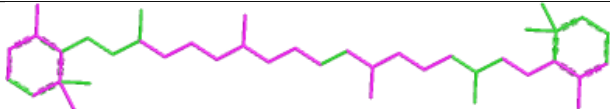
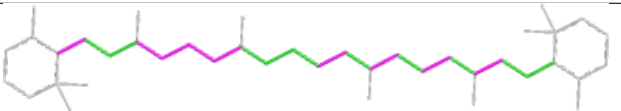
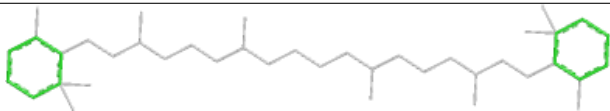


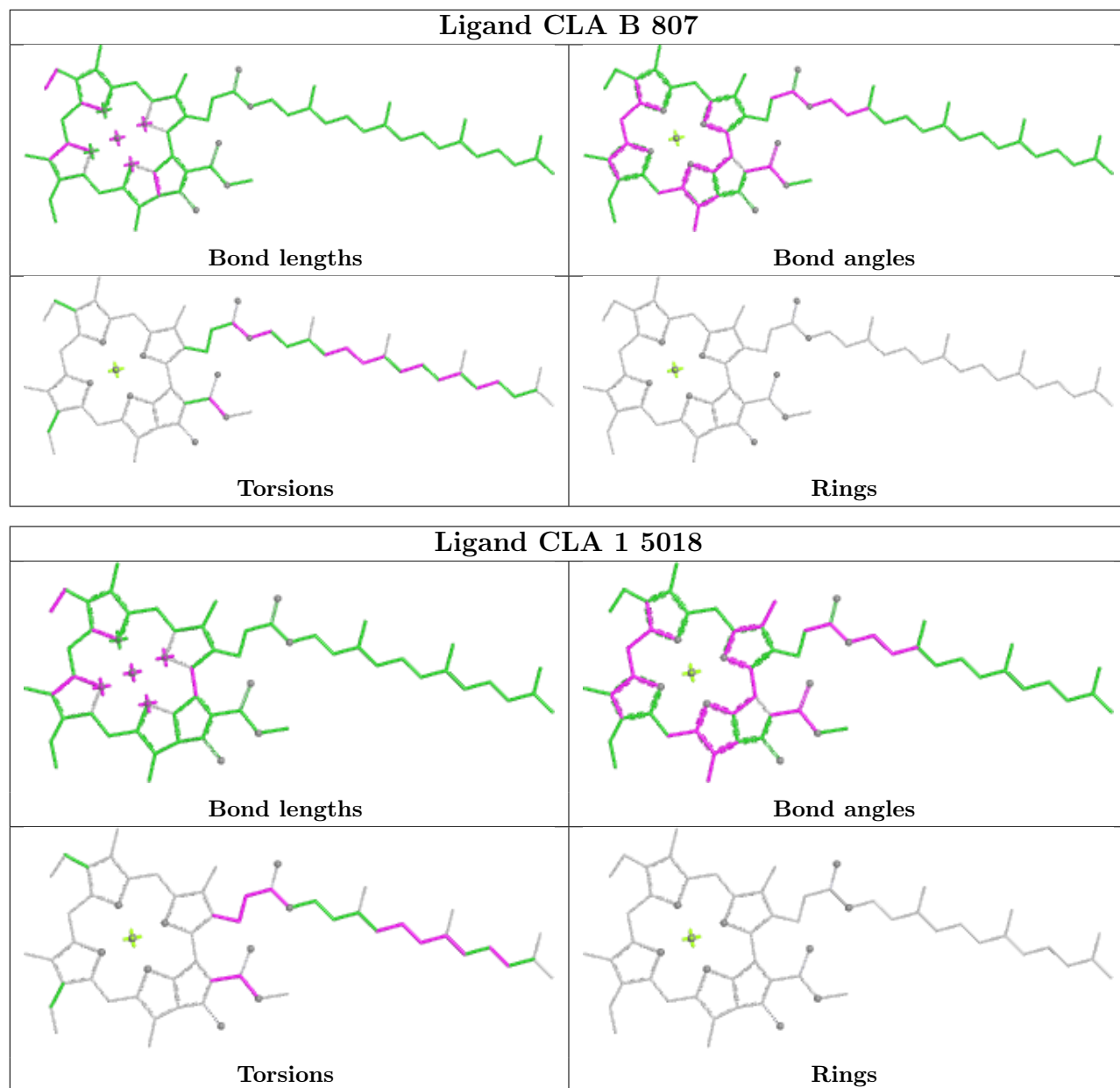




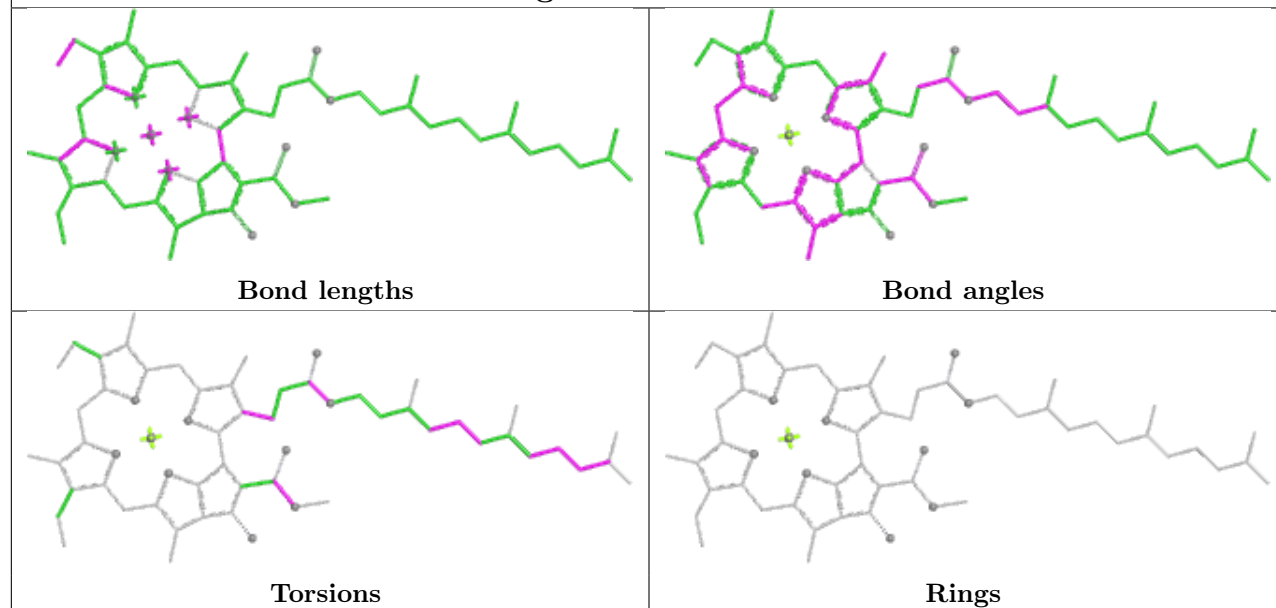
Ligand CHL 3 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

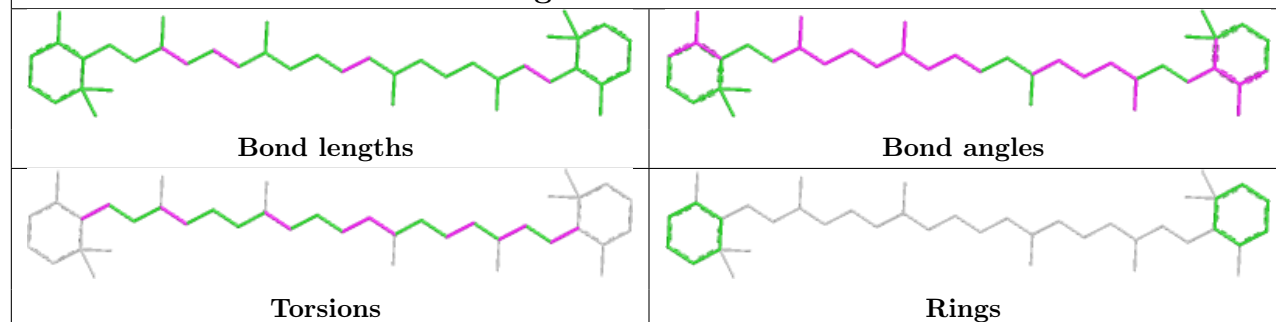
Ligand BCR A 843	
	
Bond lengths	Bond angles
	
Torsions	Rings



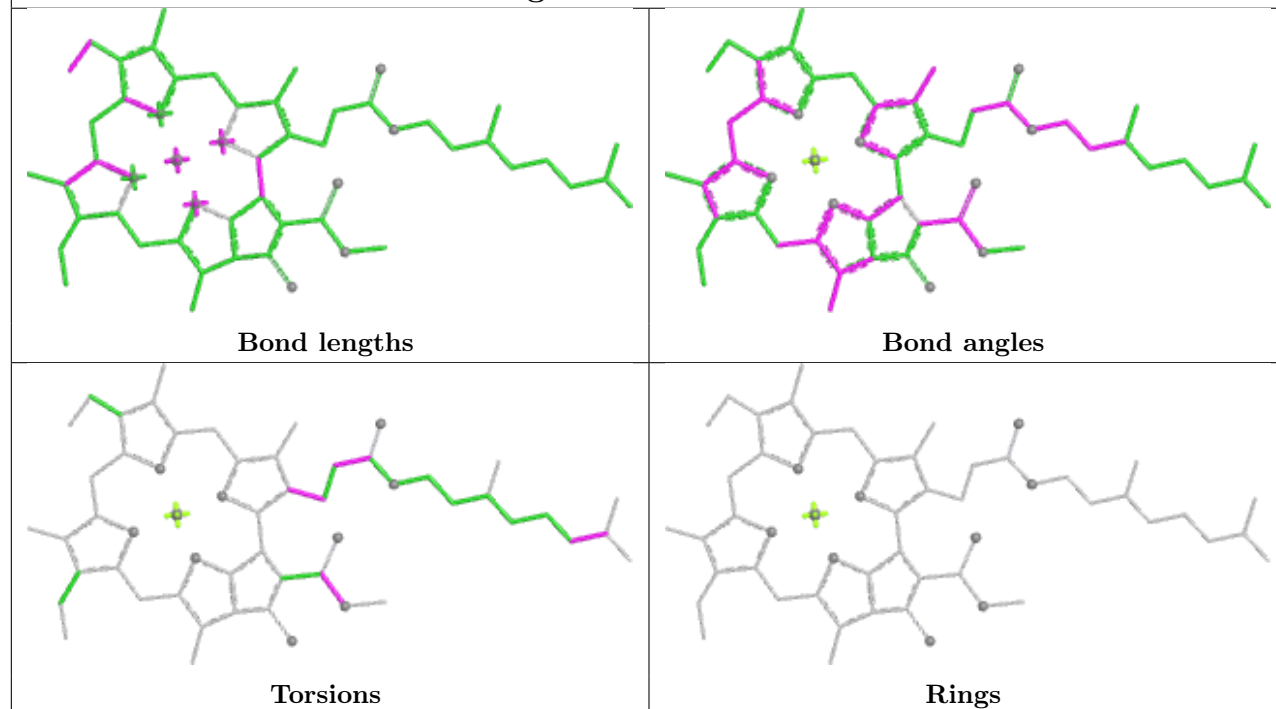
## Ligand CLA 4 311

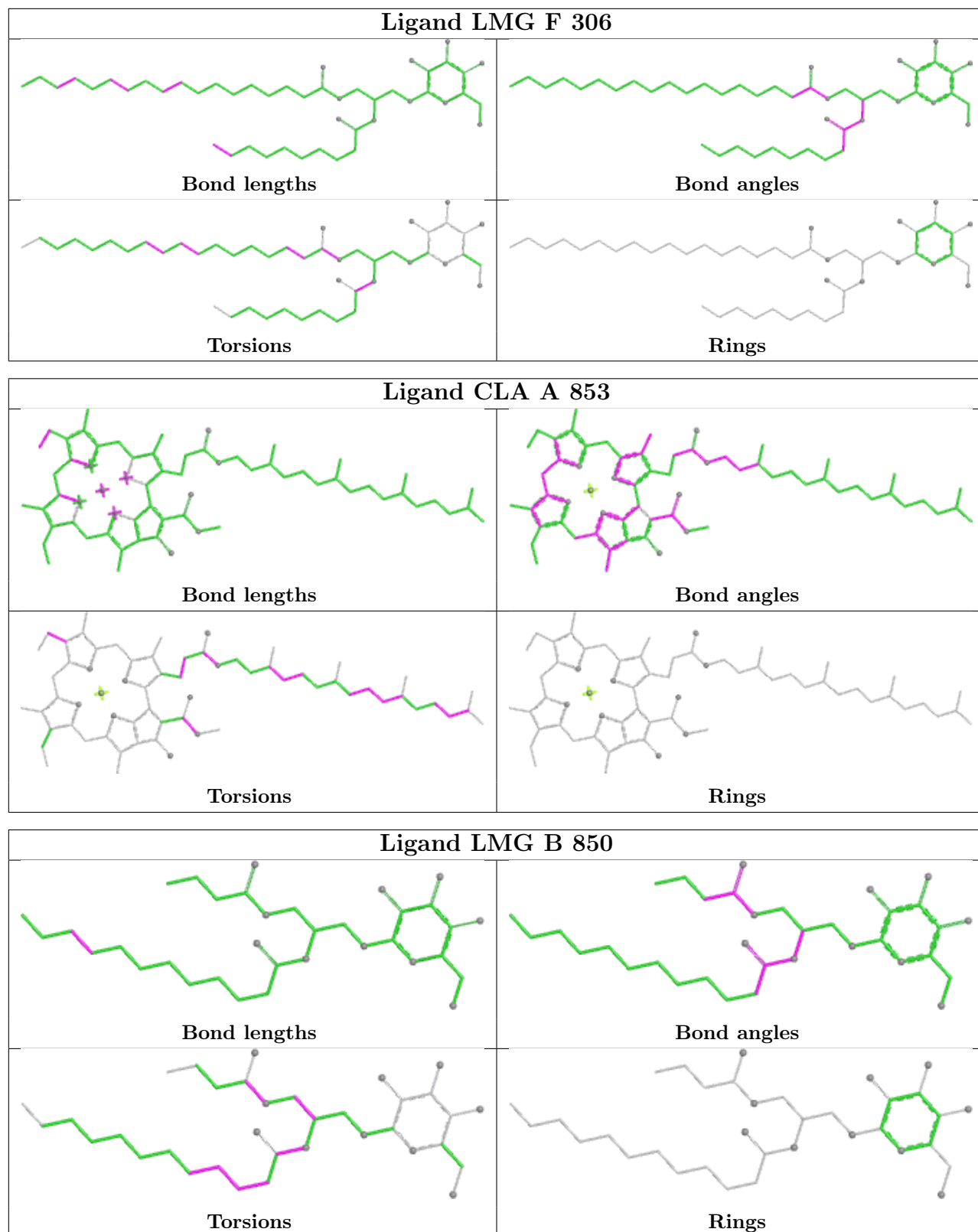


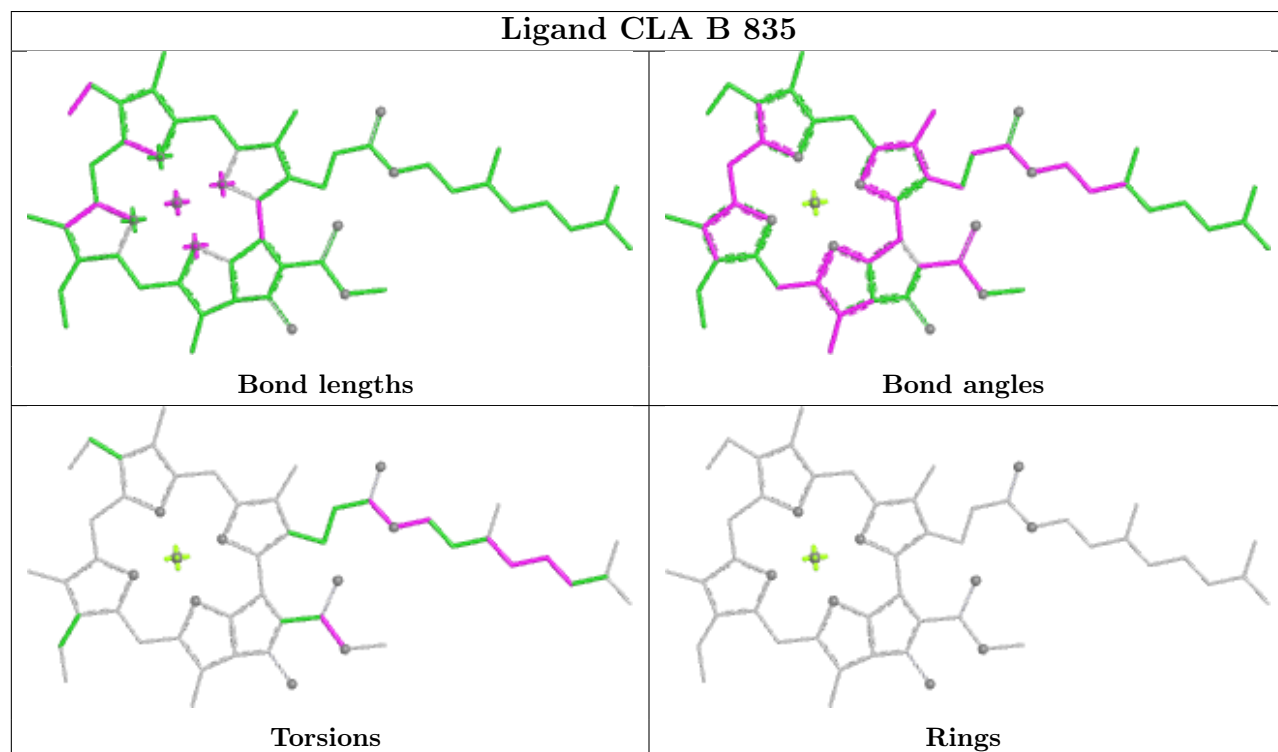
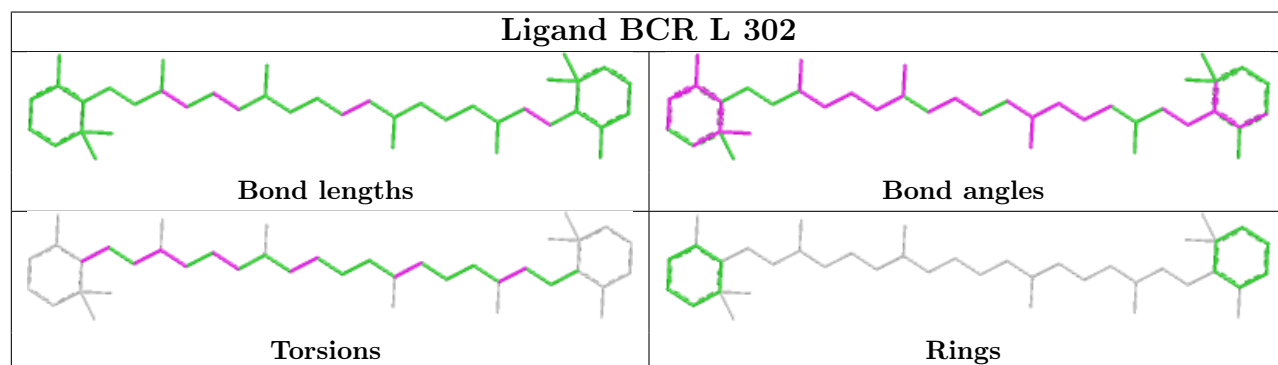
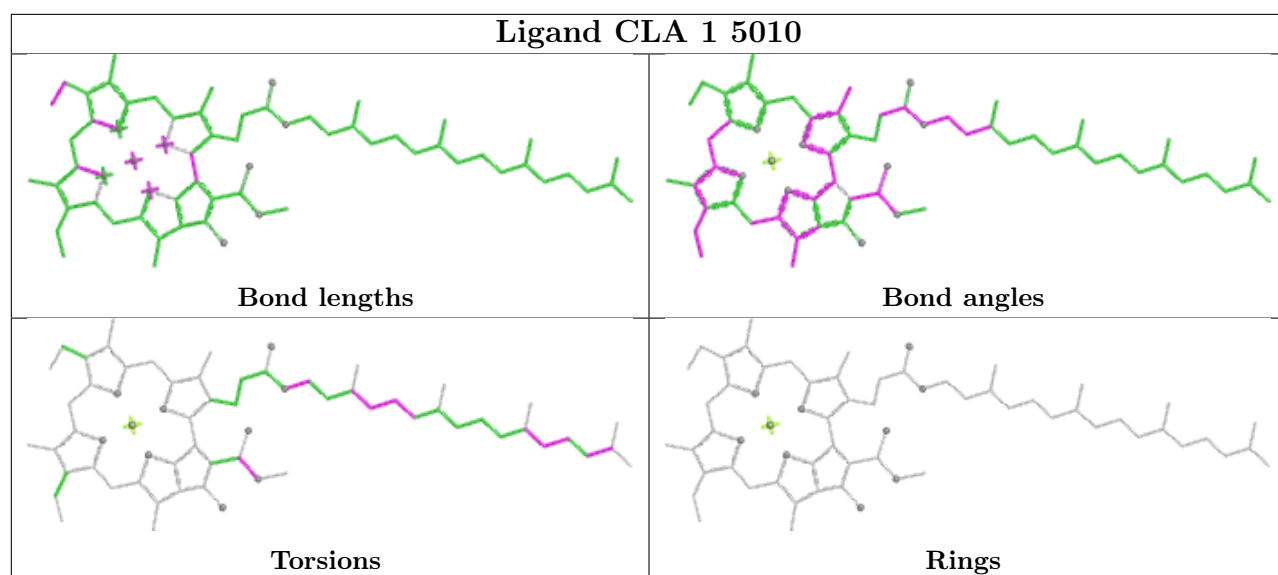
## Ligand BCR 3 306

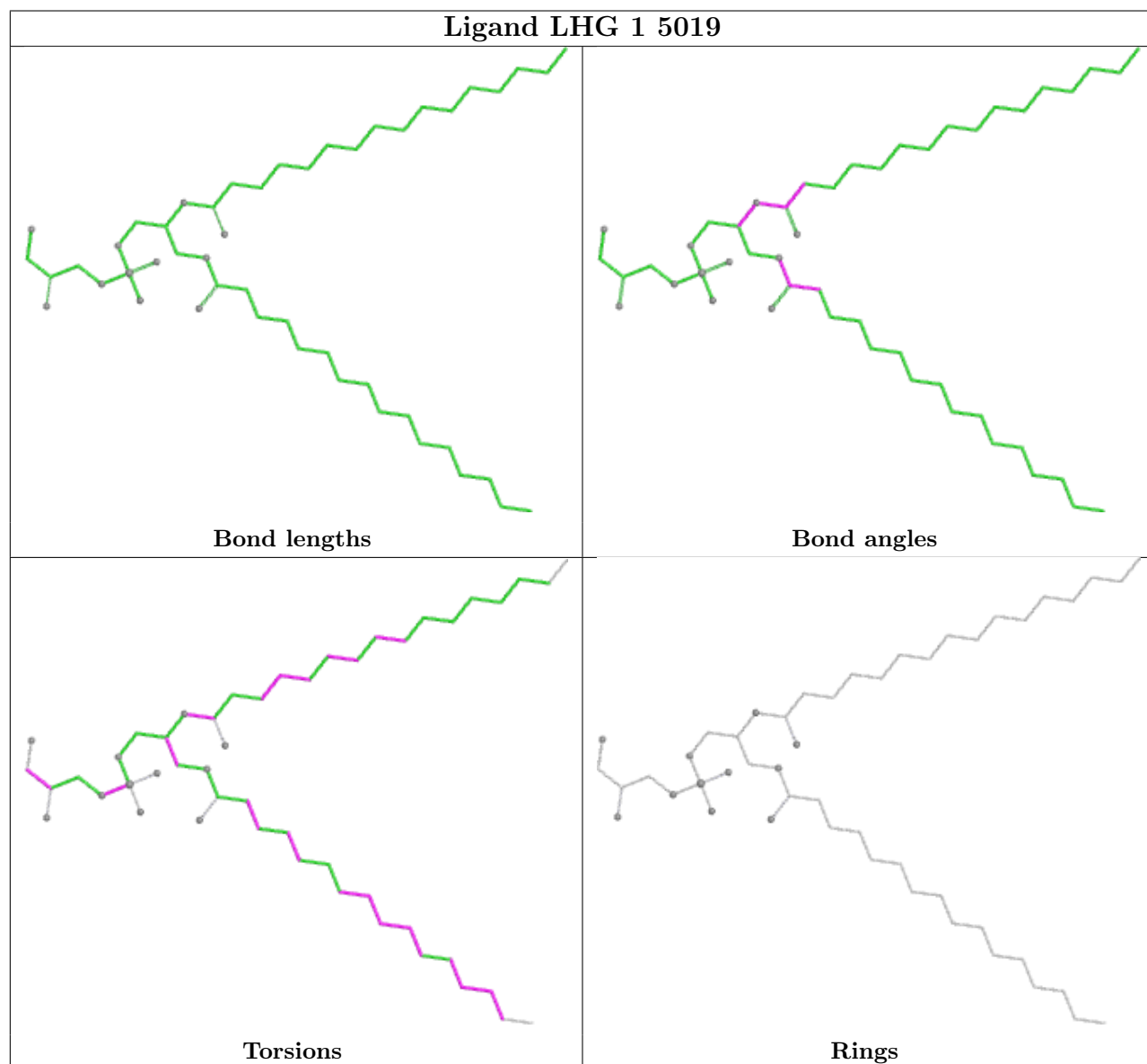
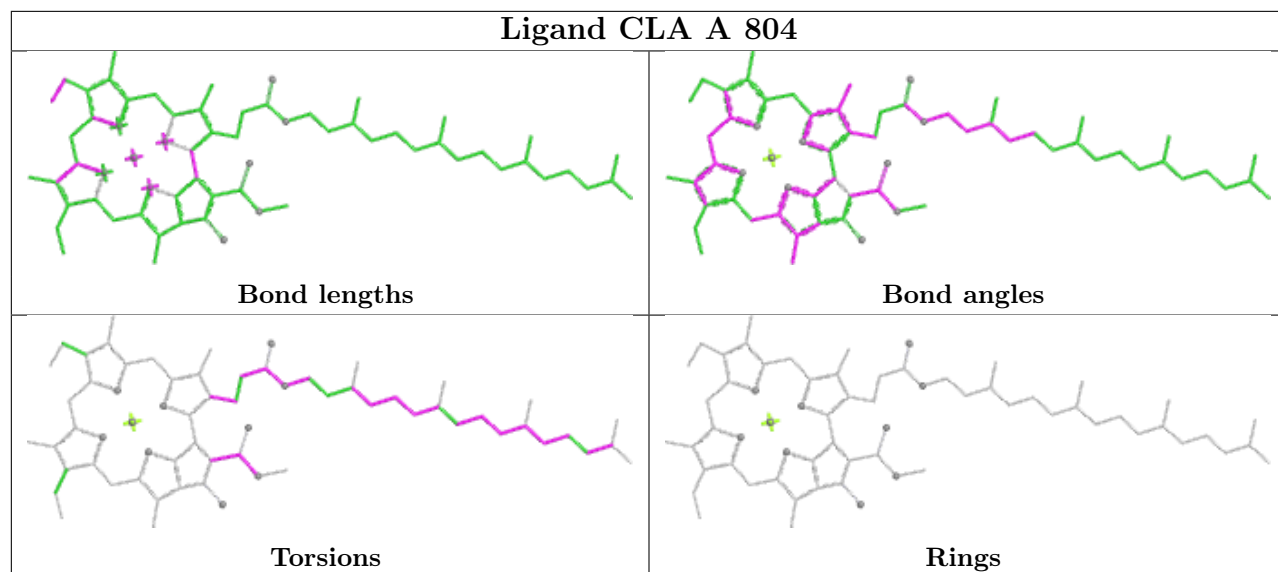


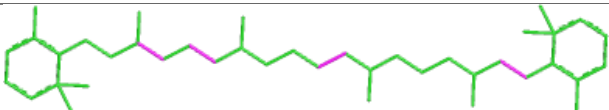
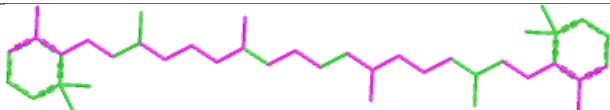
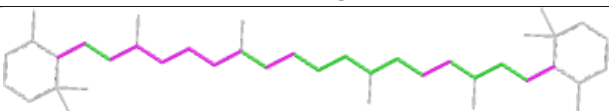
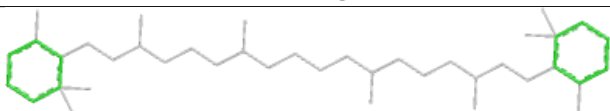
## Ligand CLA 1 5008

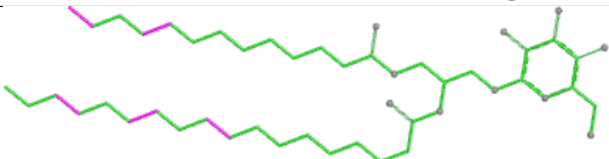
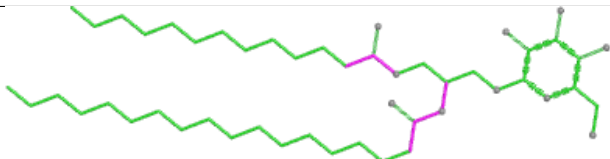
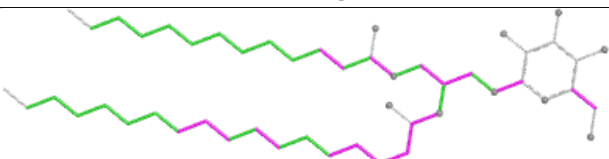
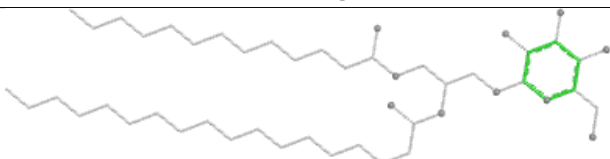


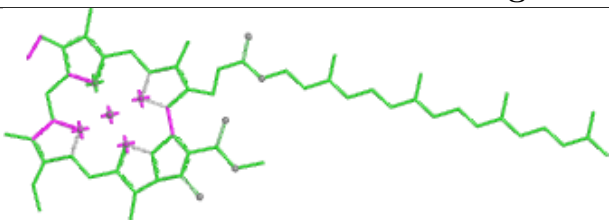
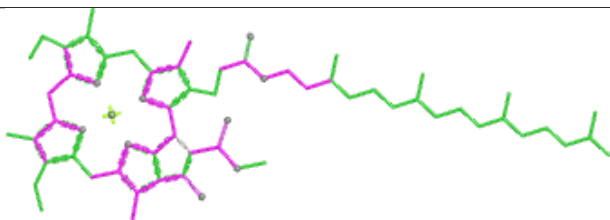
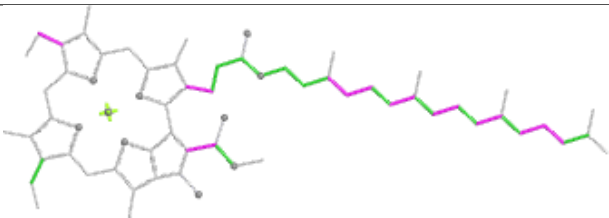
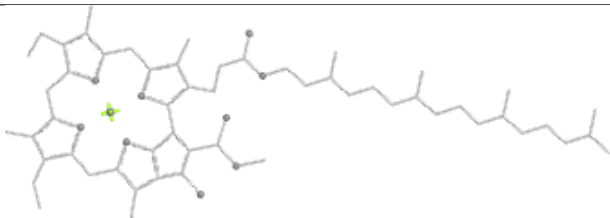




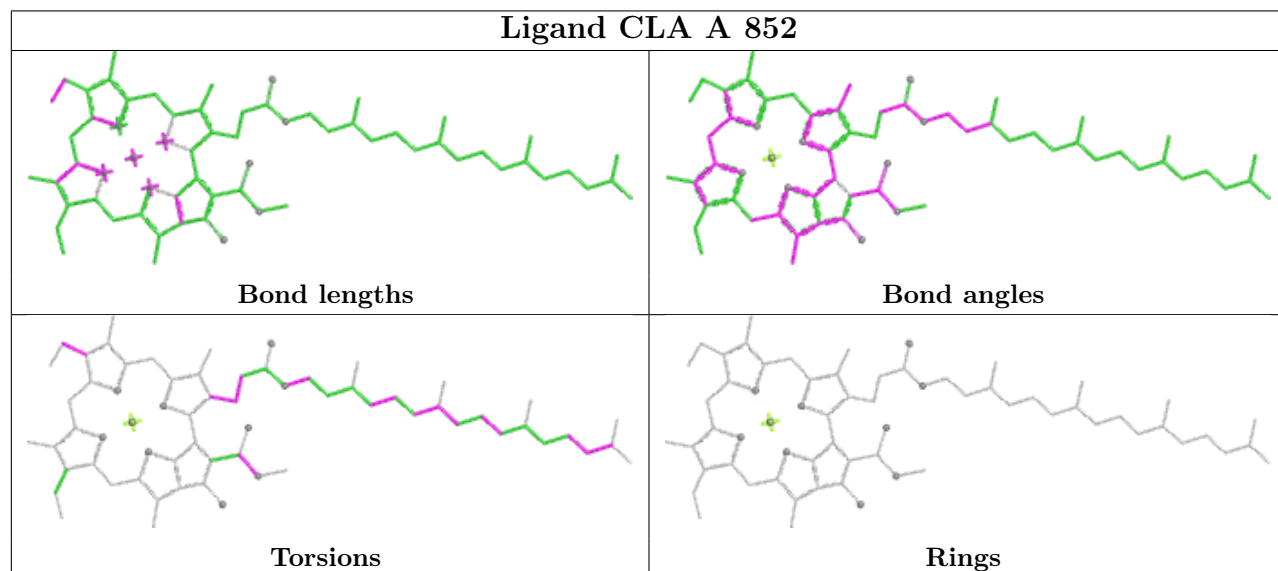
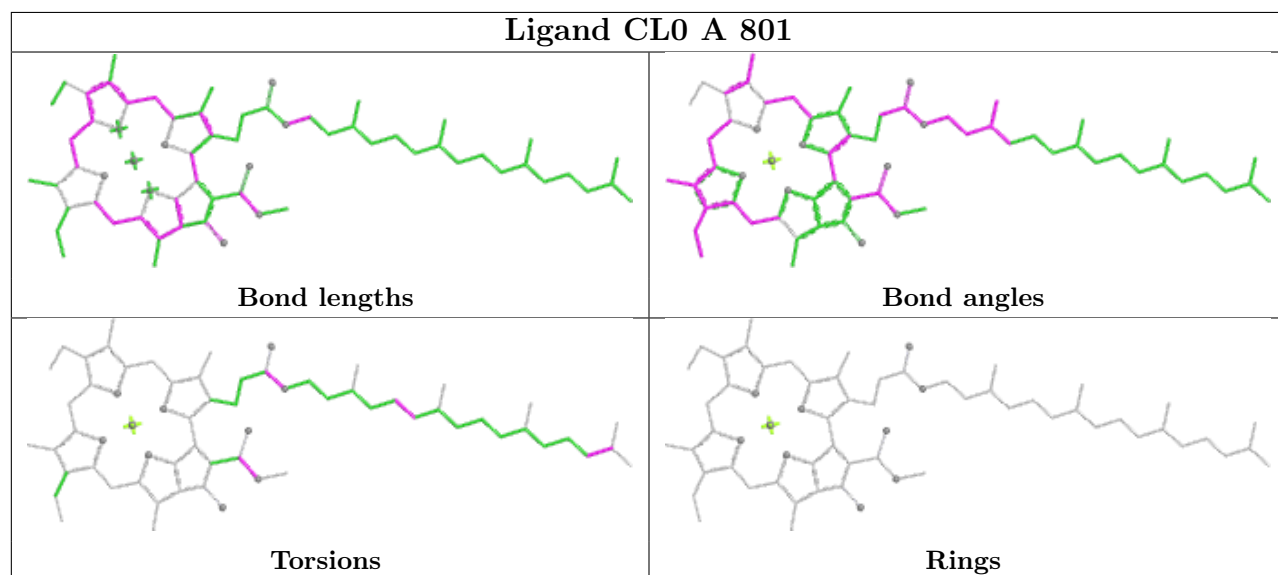
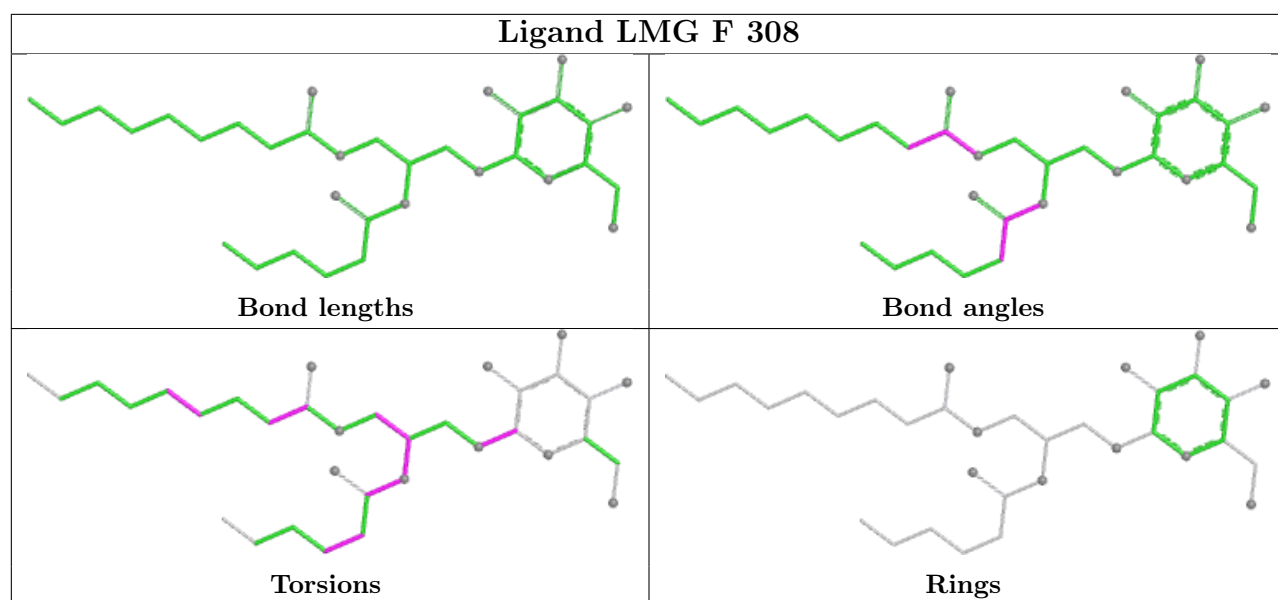


Ligand BCR L 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

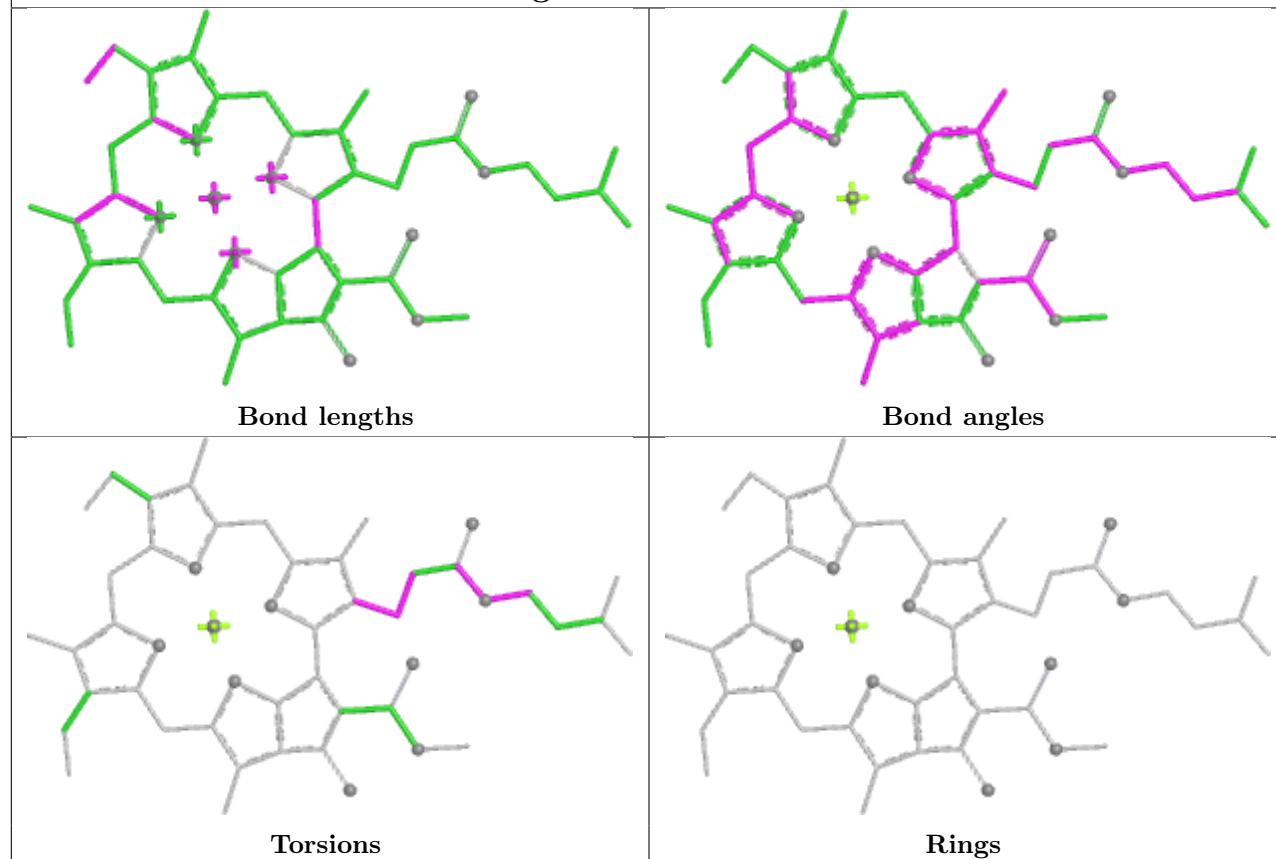
Ligand LMG A 851	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

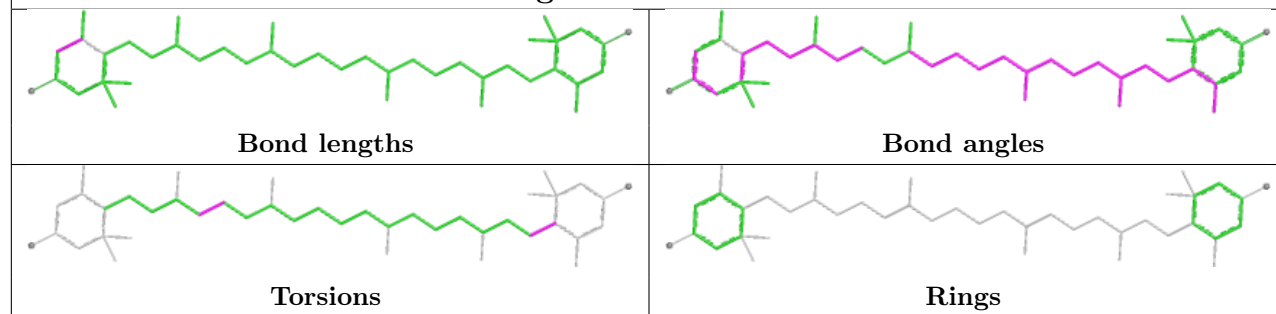




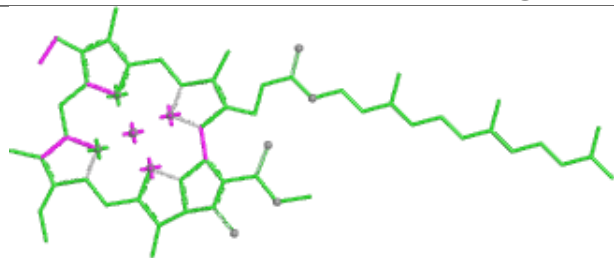
## Ligand CLA B 838



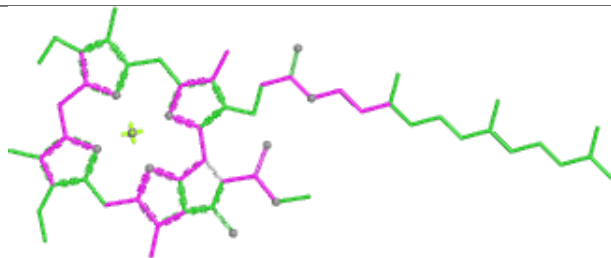
## Ligand LUT 3 303



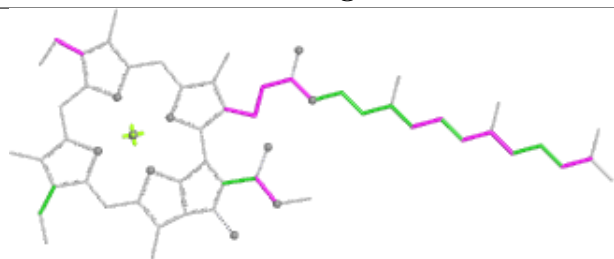
## Ligand CLA L 305



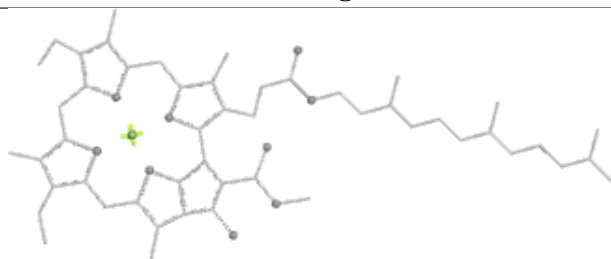
Bond lengths



Bond angles

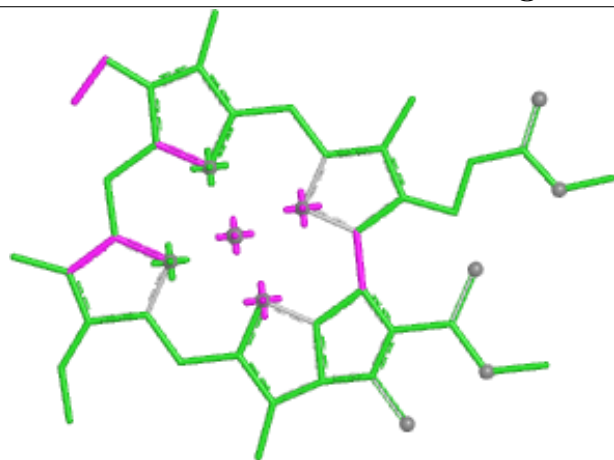


Torsions

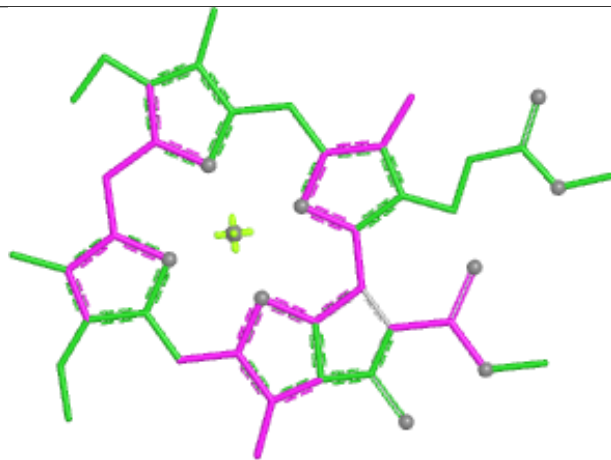


Rings

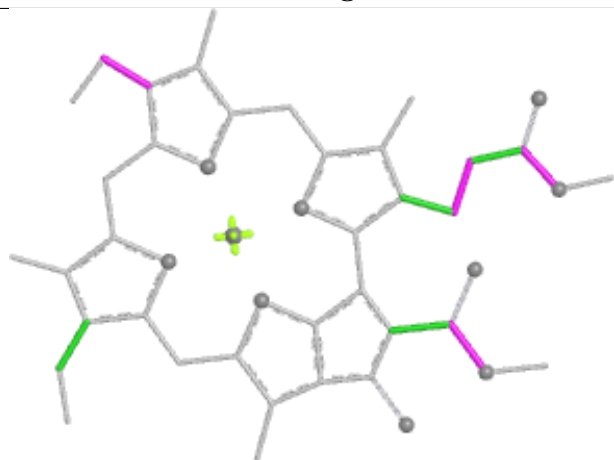
## Ligand CLA 4 312



Bond lengths



Bond angles

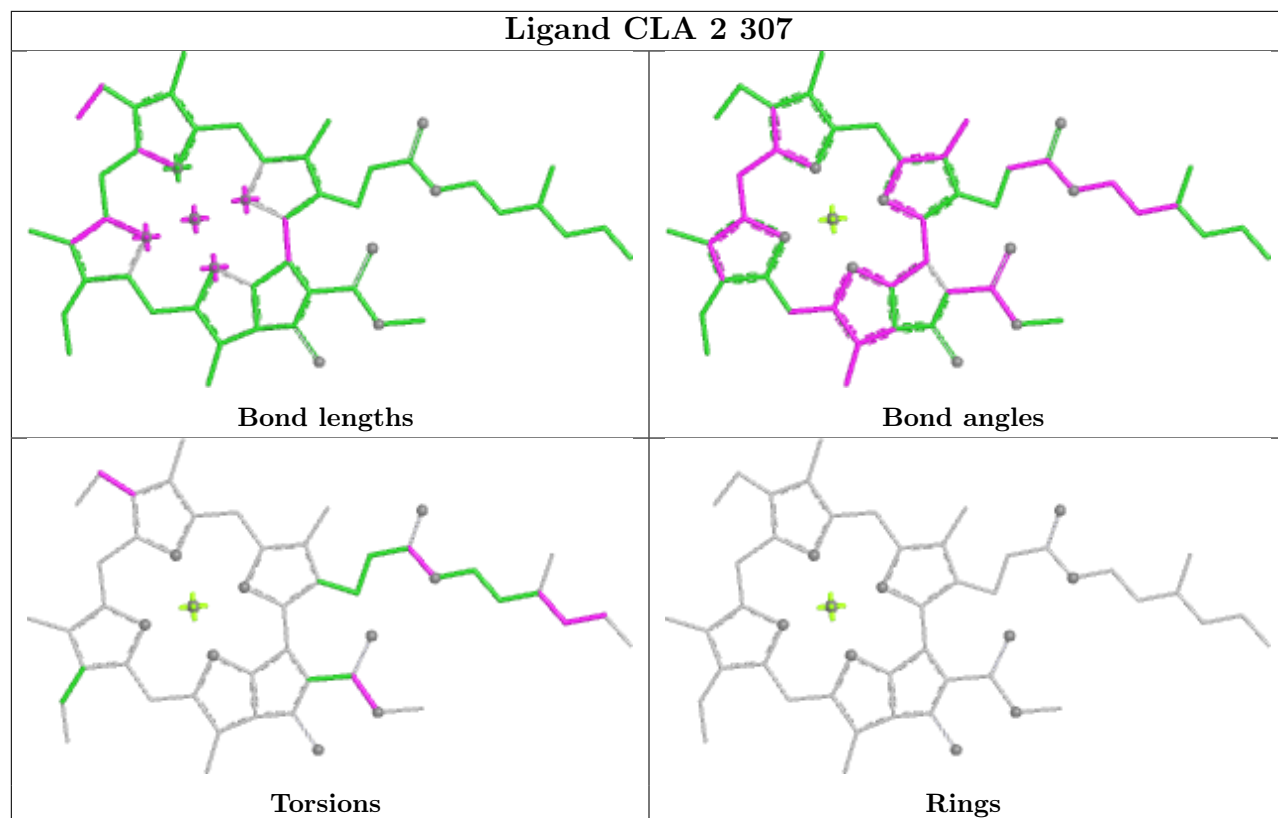


Torsions

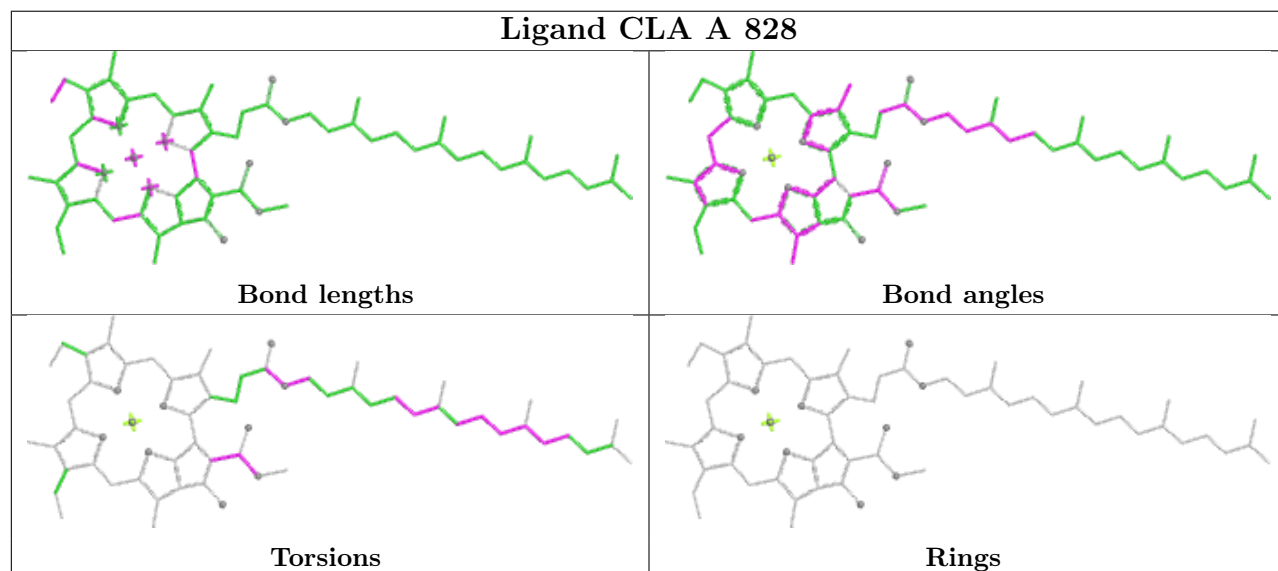


Rings

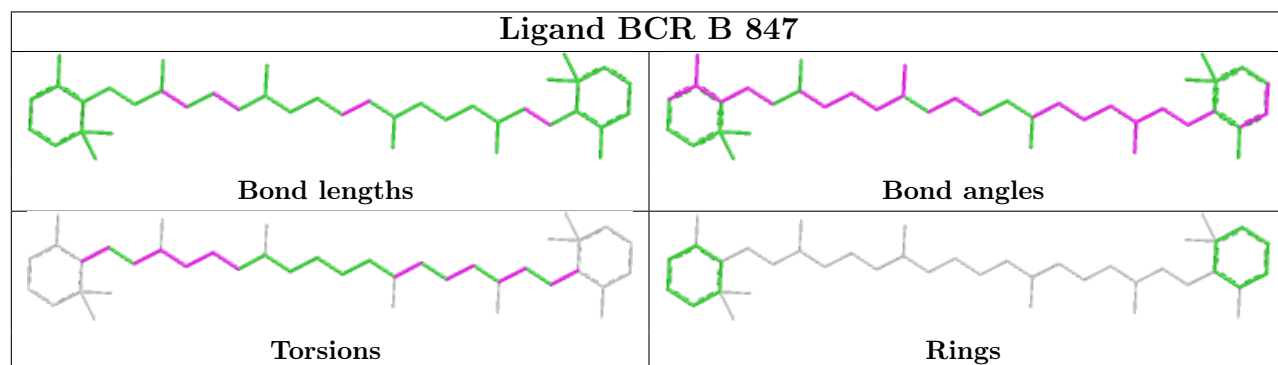
## Ligand CLA 2 307

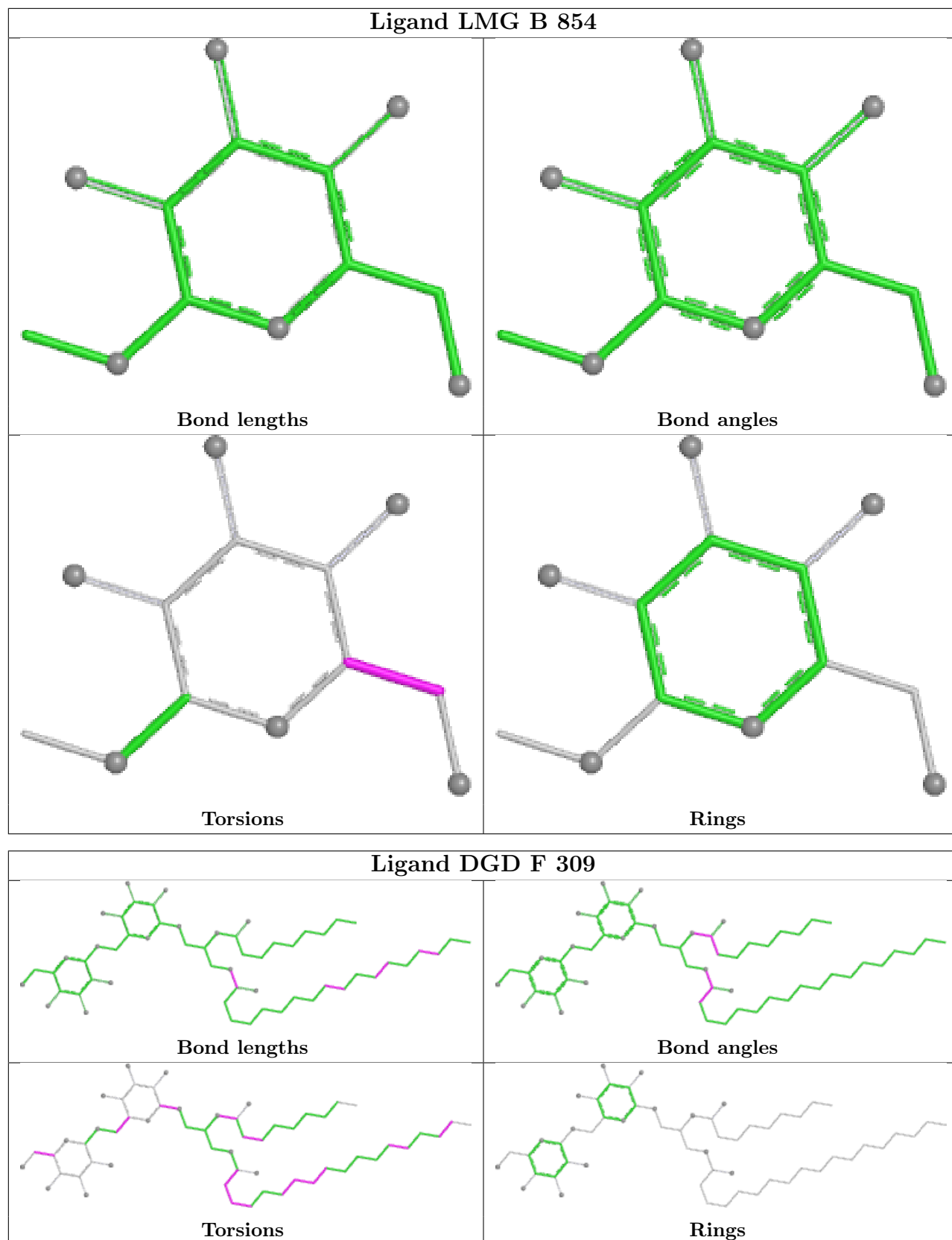


## Ligand CLA A 828

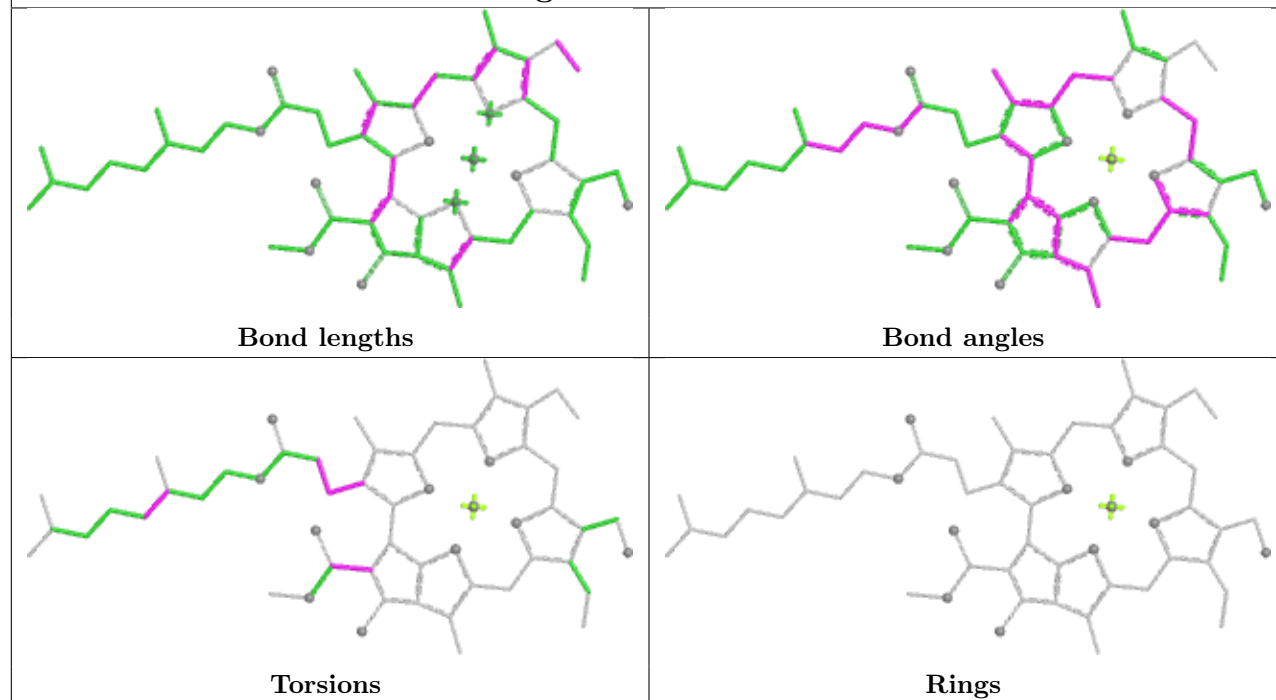


## Ligand BCR B 847

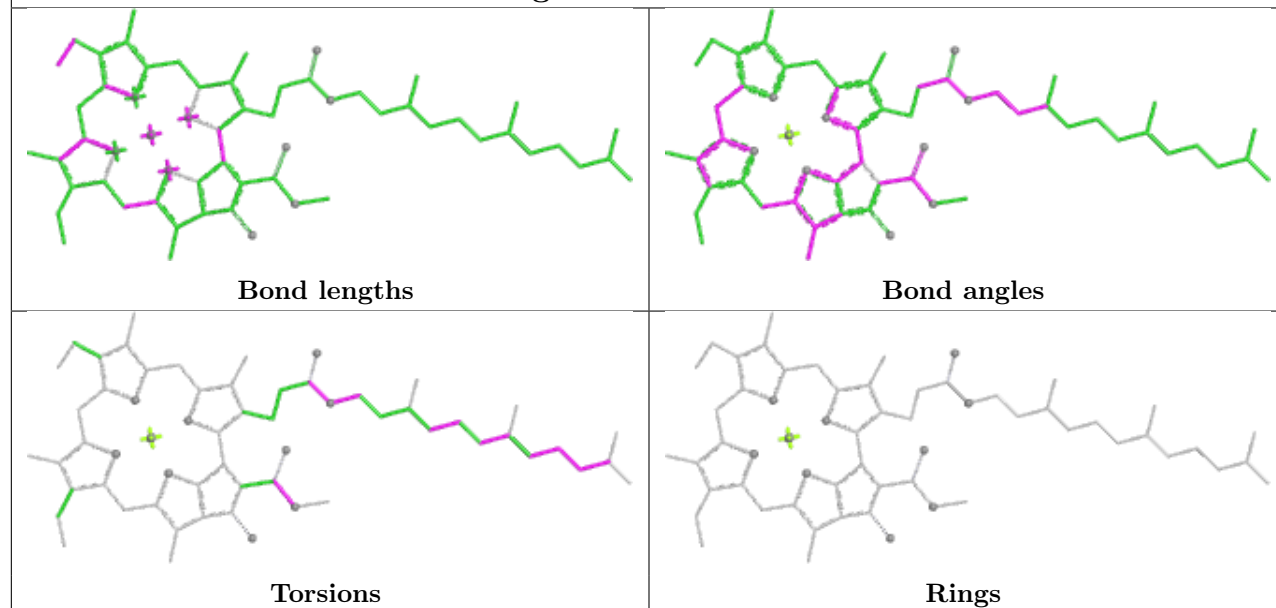




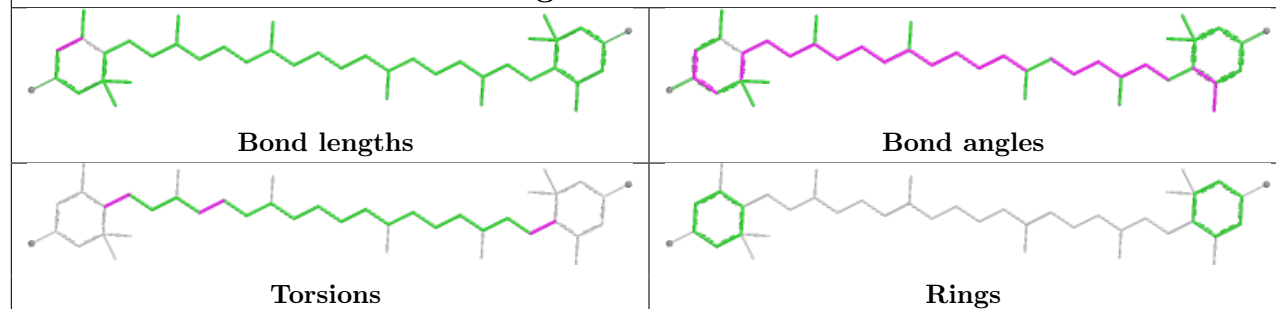
## Ligand CHL 2 319

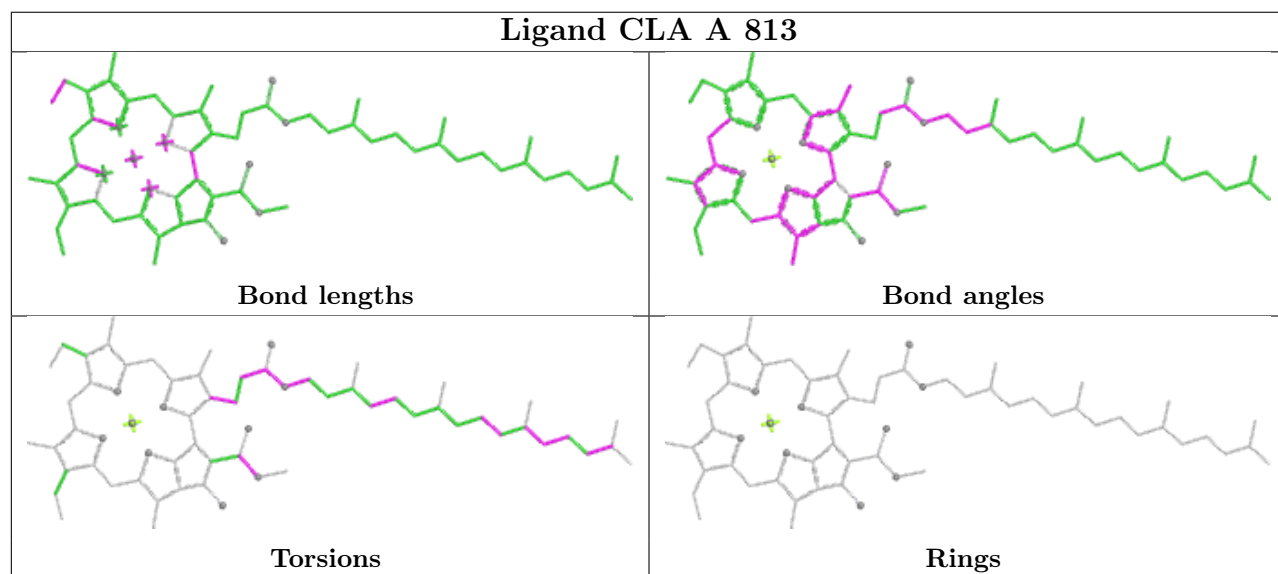
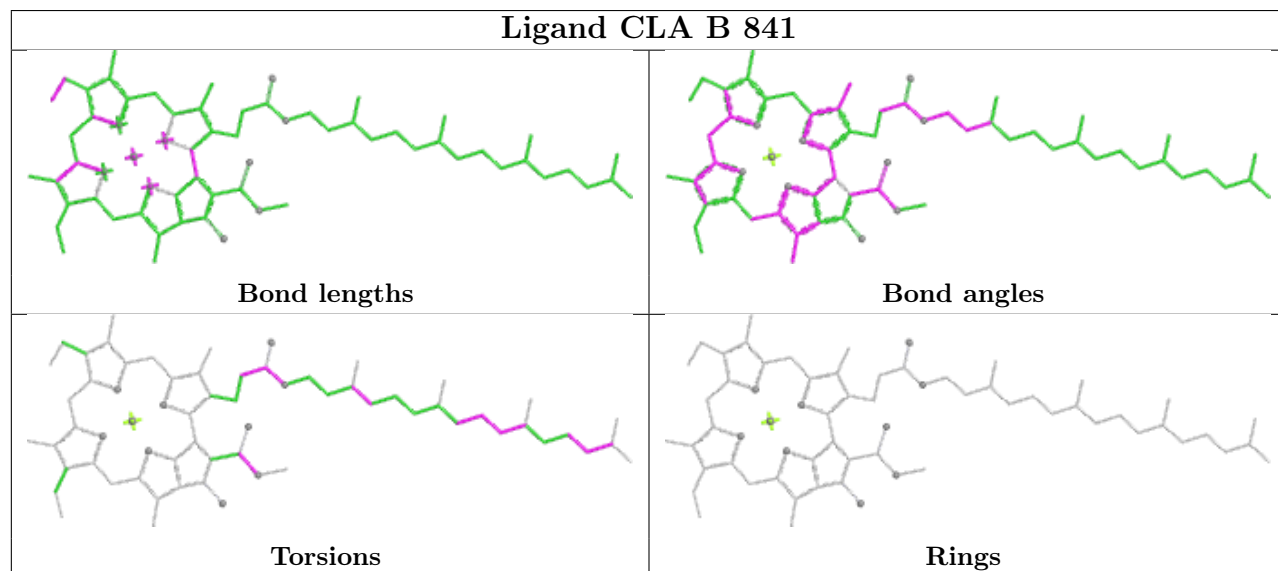
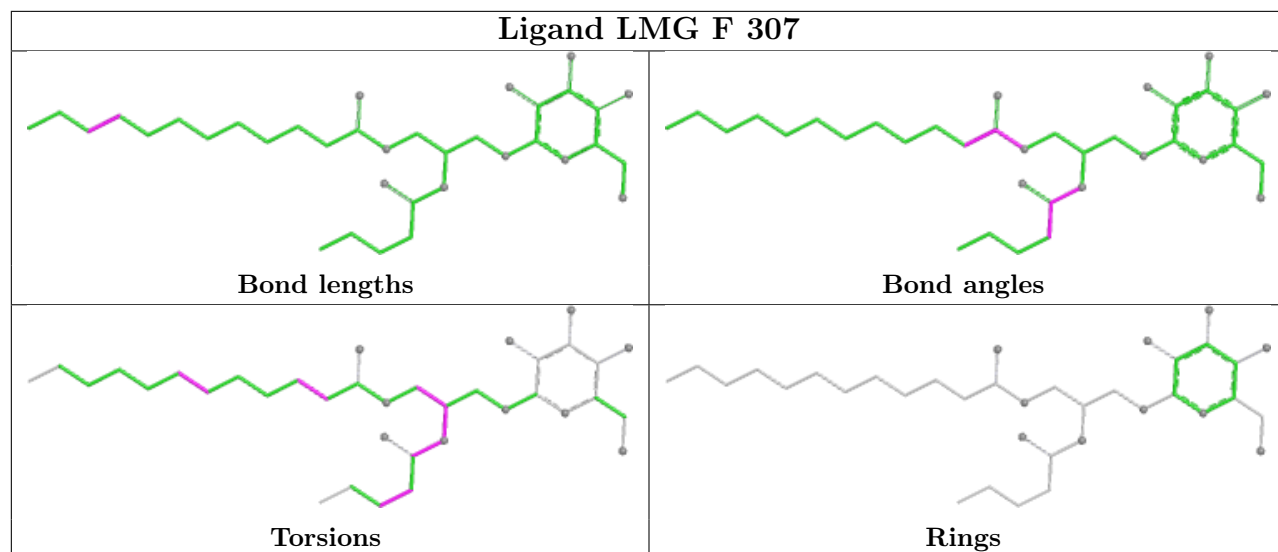


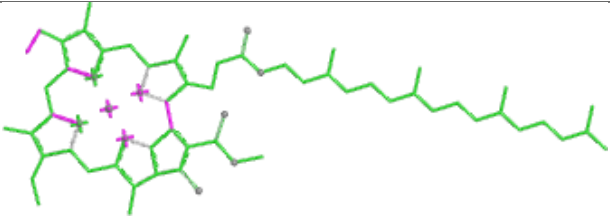
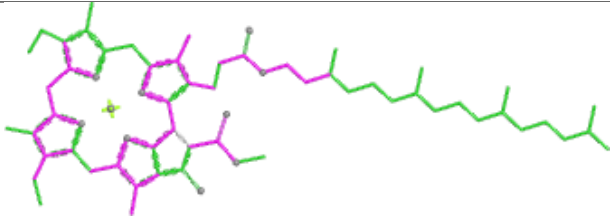
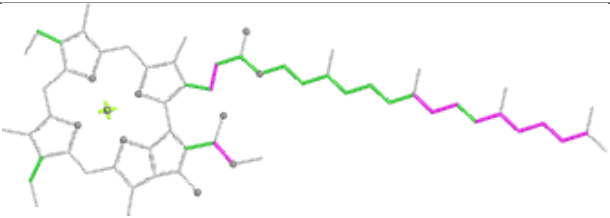
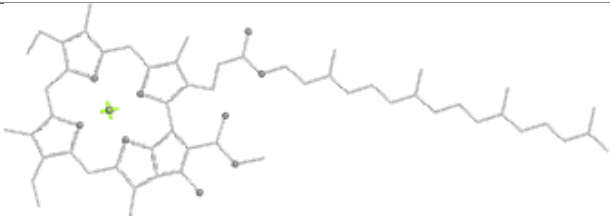
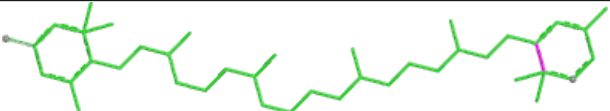
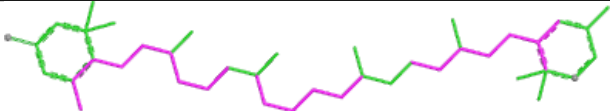
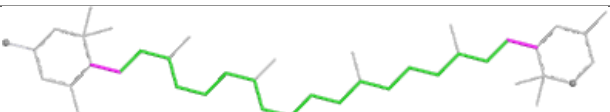
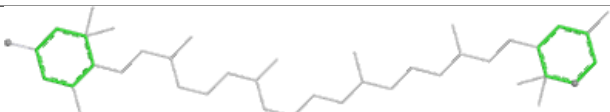
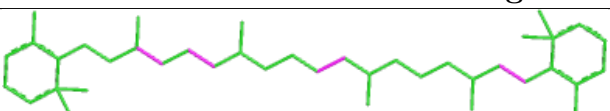
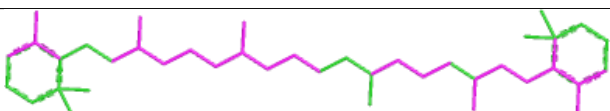

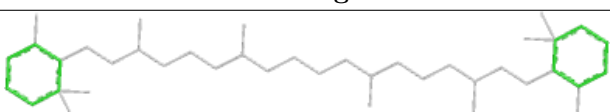
## Ligand CLA B 834



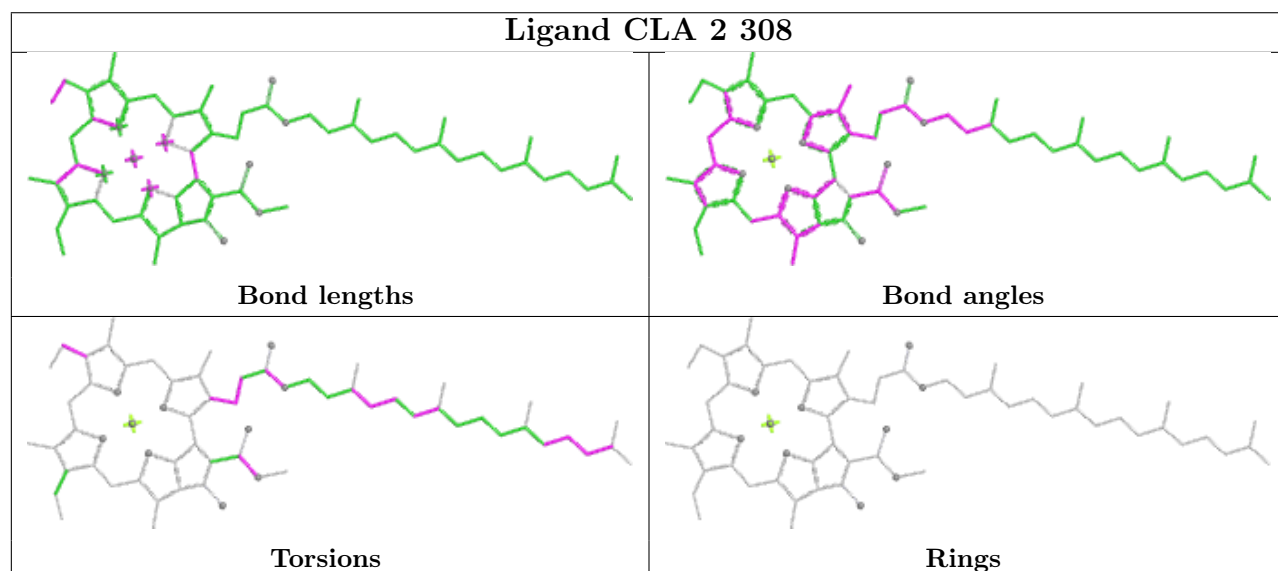
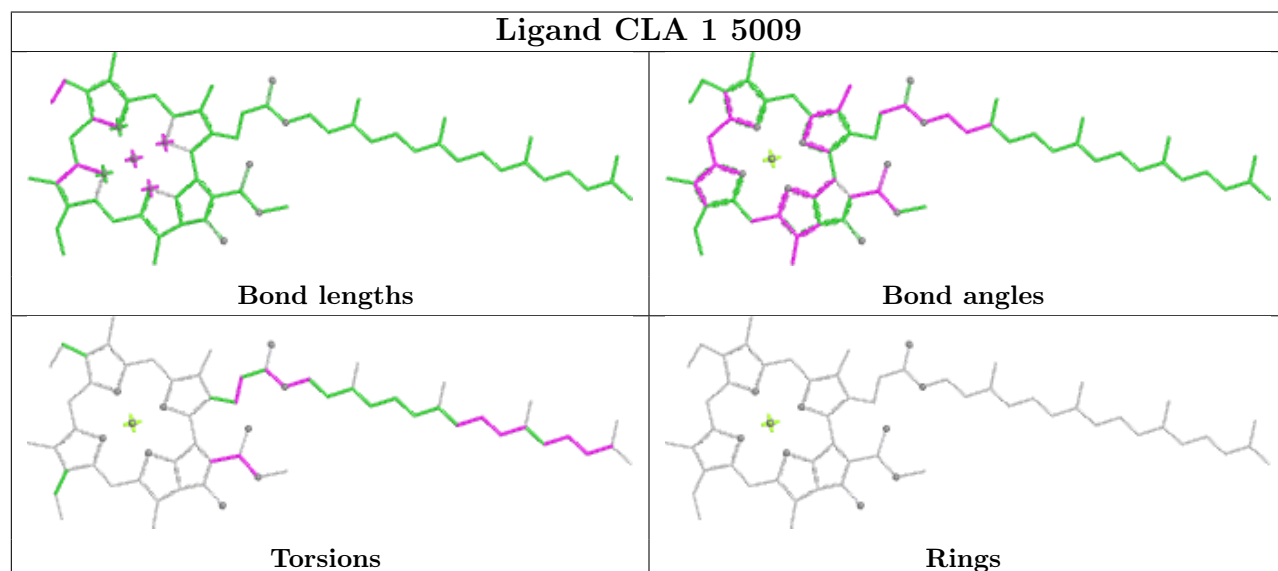
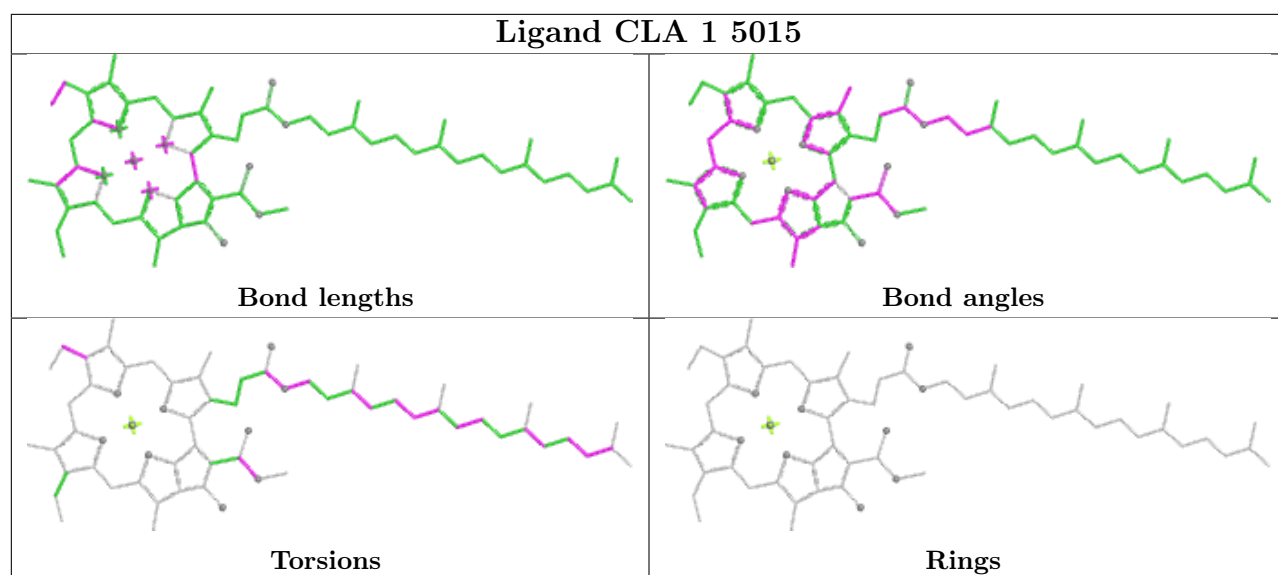
## Ligand LUT 4 303

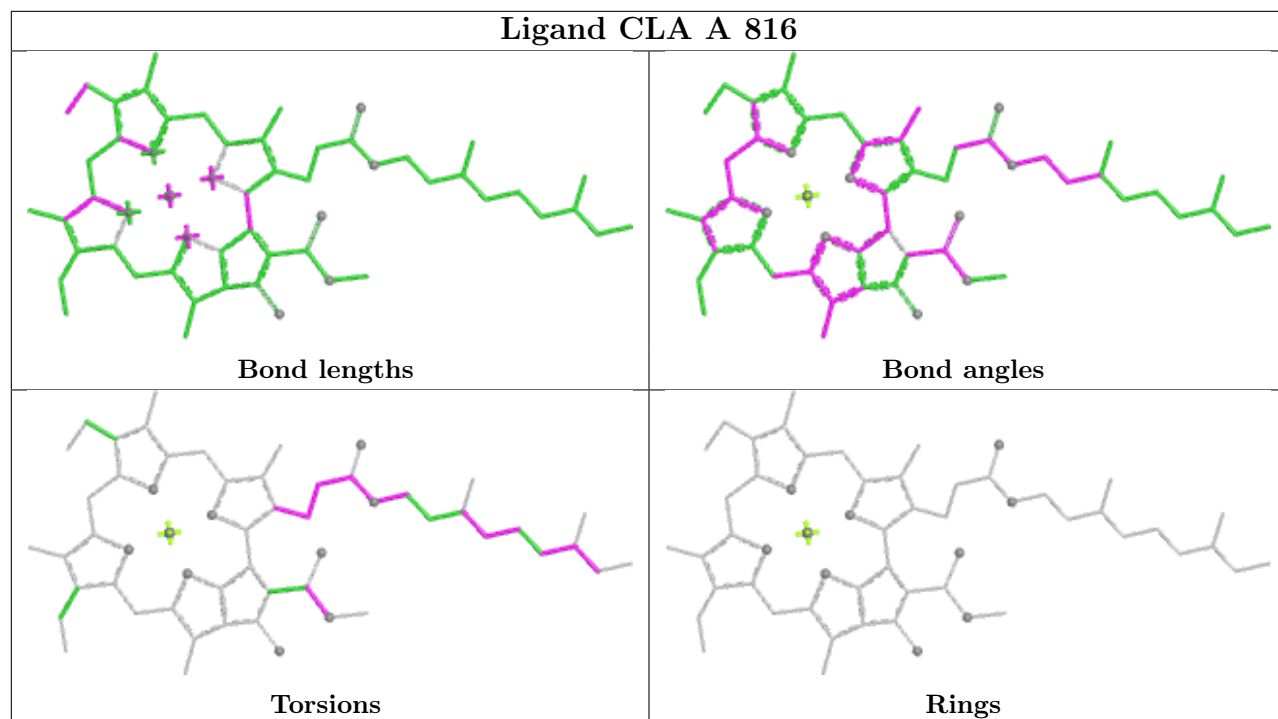




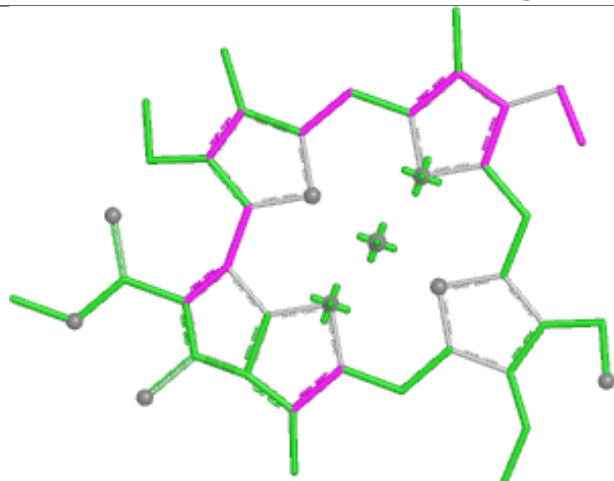
Ligand CLA B 804	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand ZEX F 310	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR B 844	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



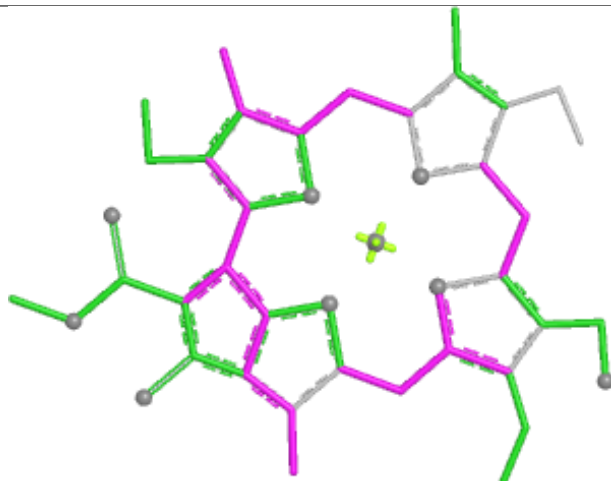




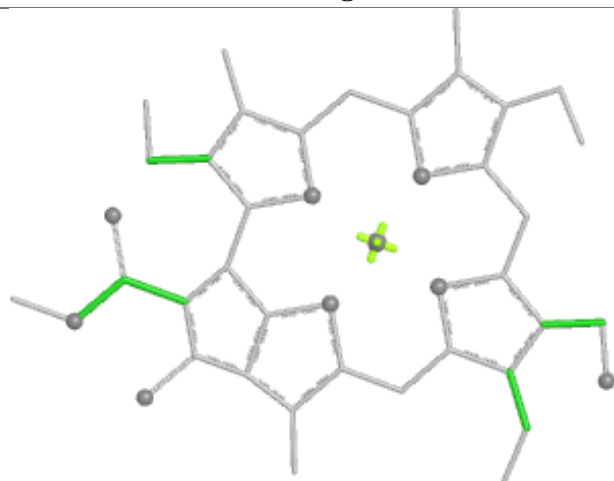
## Ligand CHL 4 317



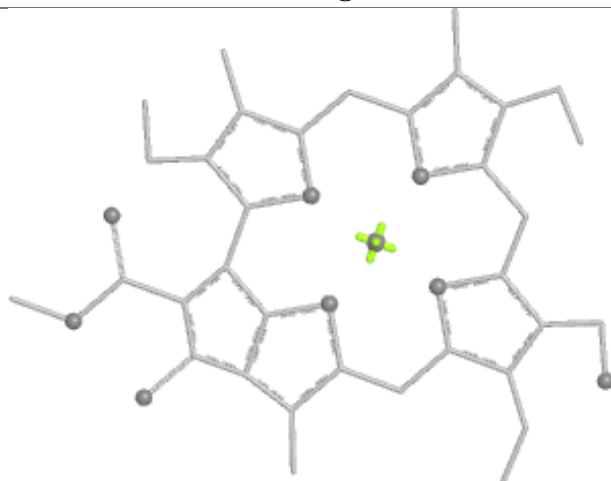
Bond lengths



Bond angles

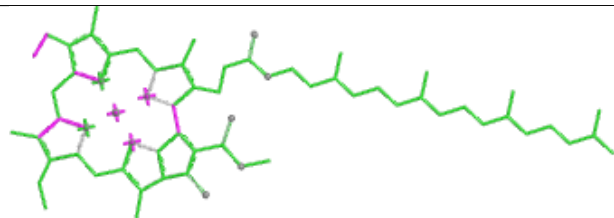


Torsions

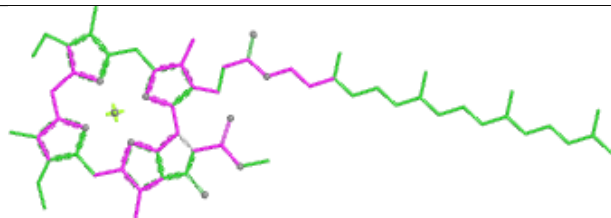


Rings

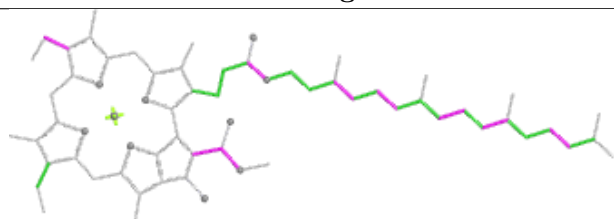
## Ligand CLA B 831



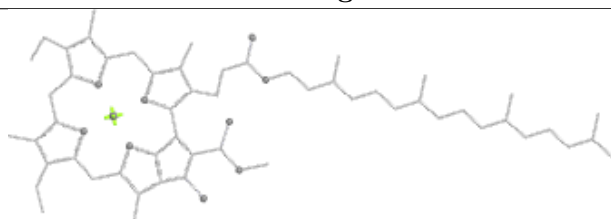
Bond lengths



Bond angles

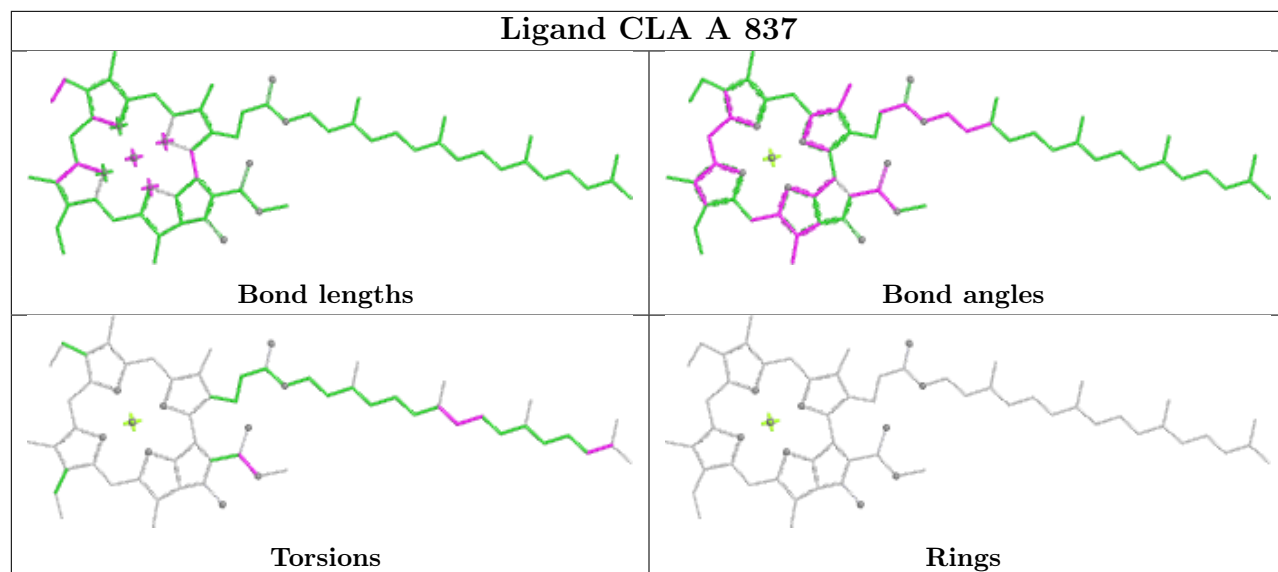


Torsions

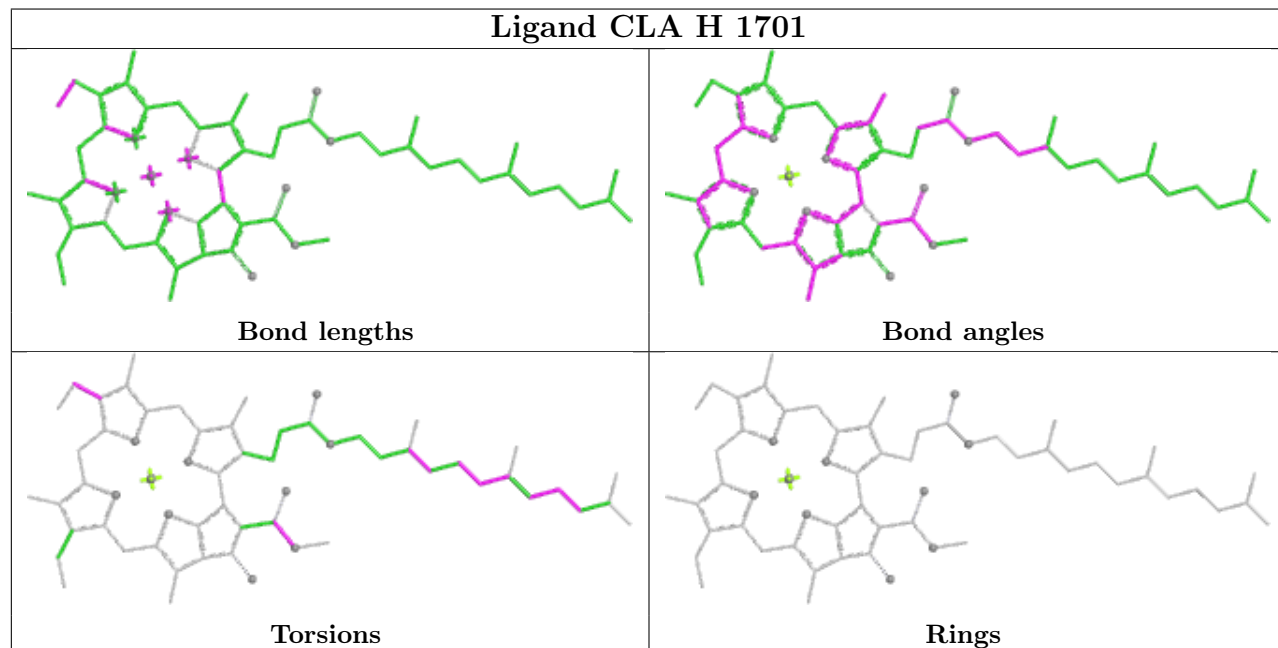


Rings

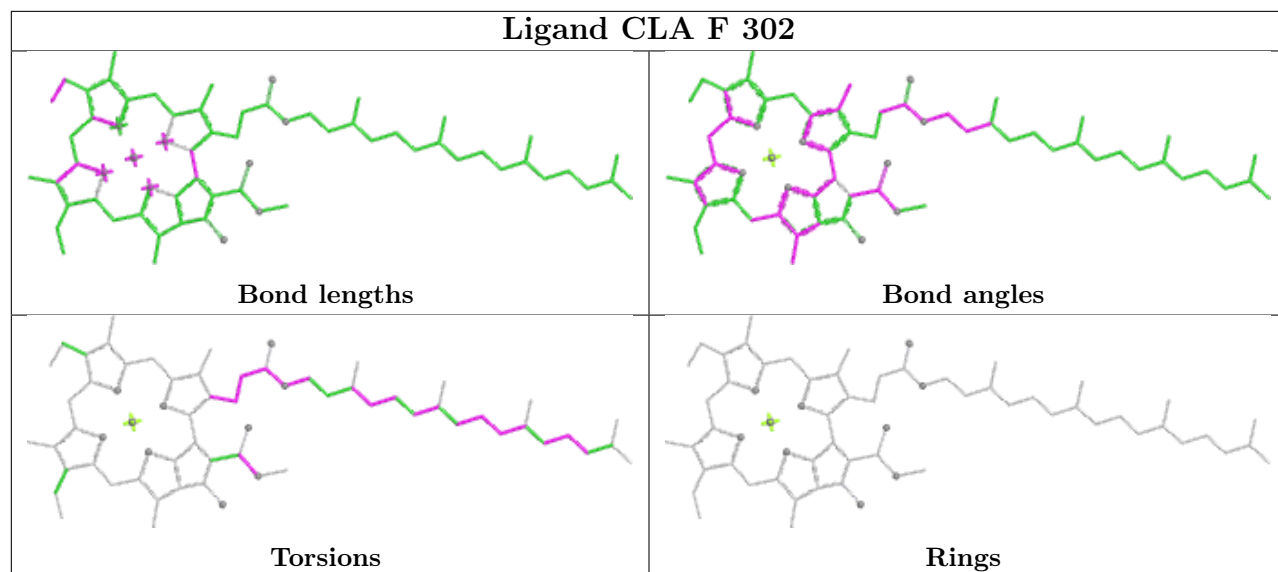
## Ligand CLA A 837



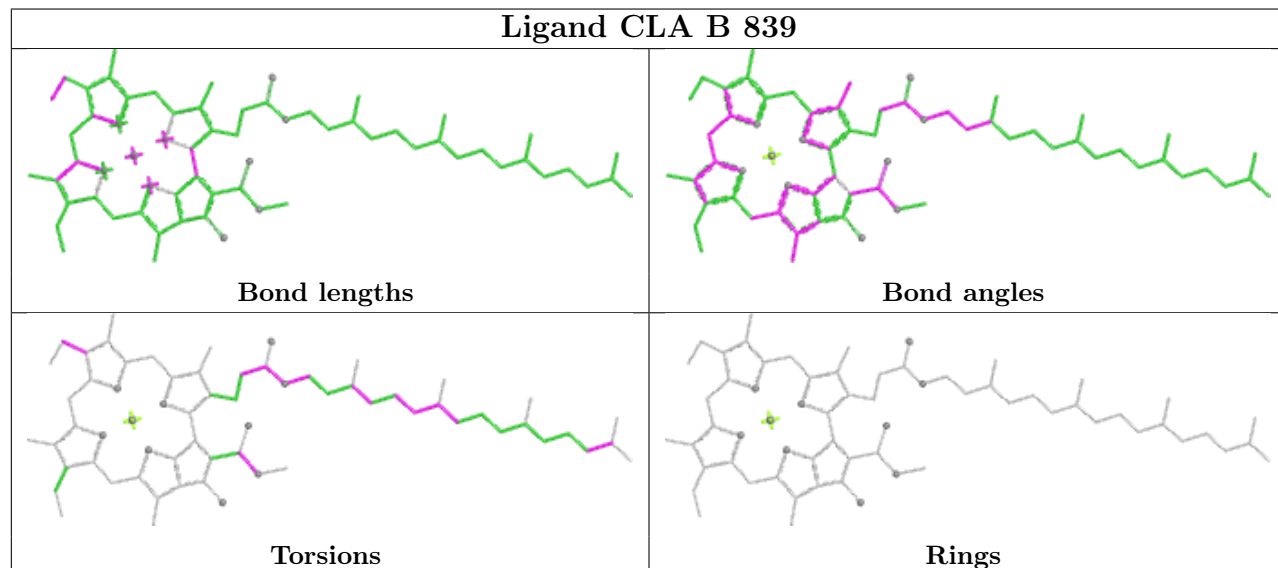
## Ligand CLA H 1701



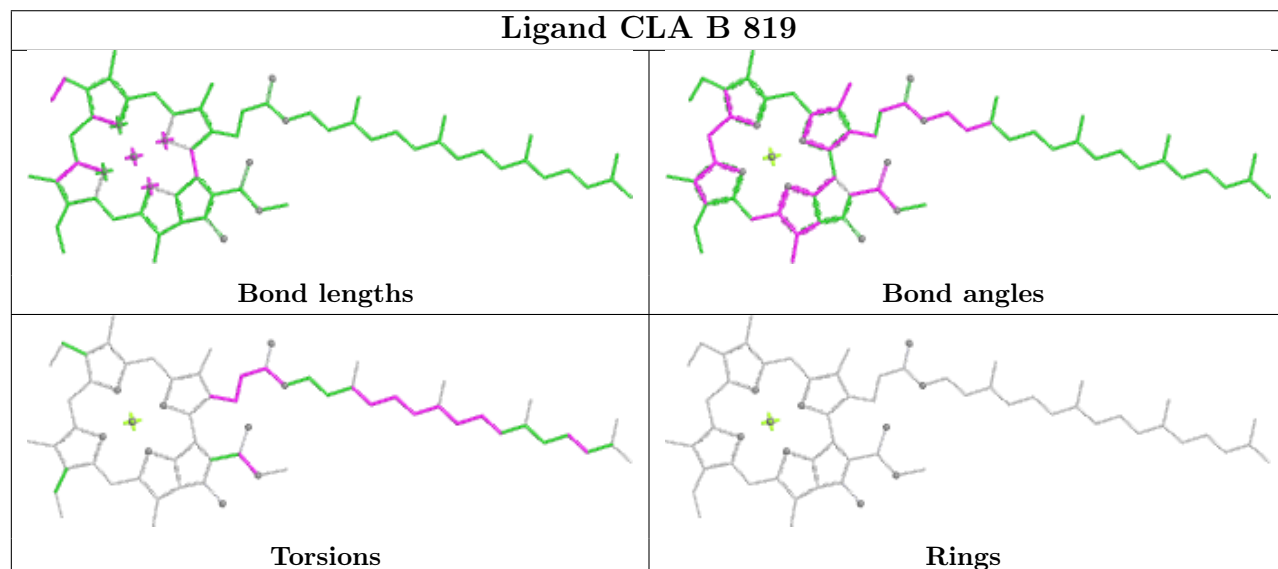
## Ligand CLA F 302



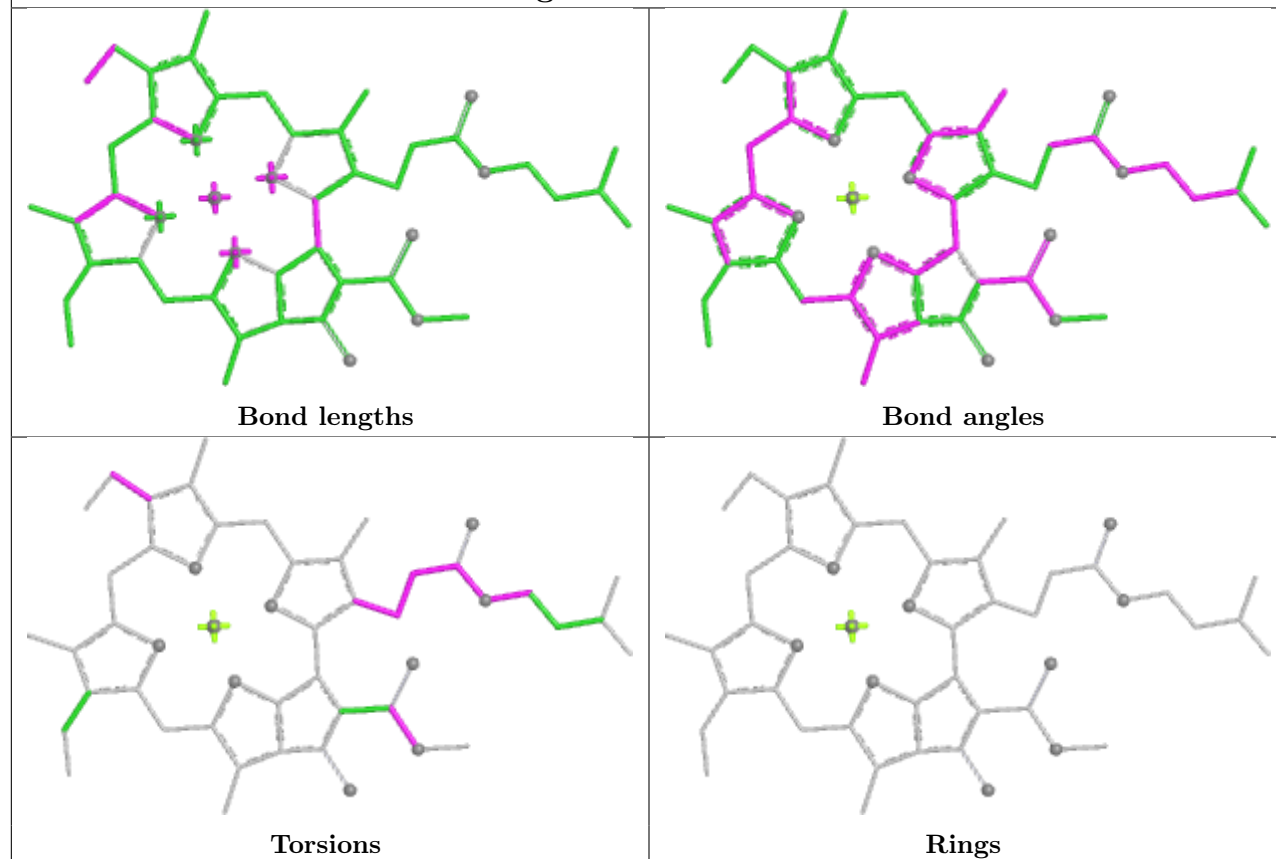
## Ligand CLA B 839



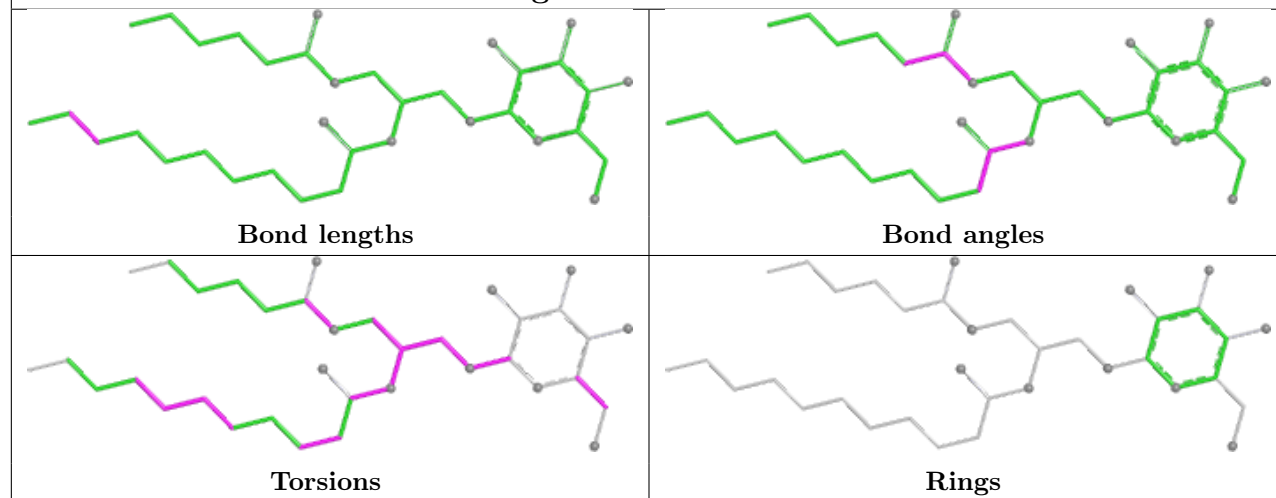
## Ligand CLA B 819



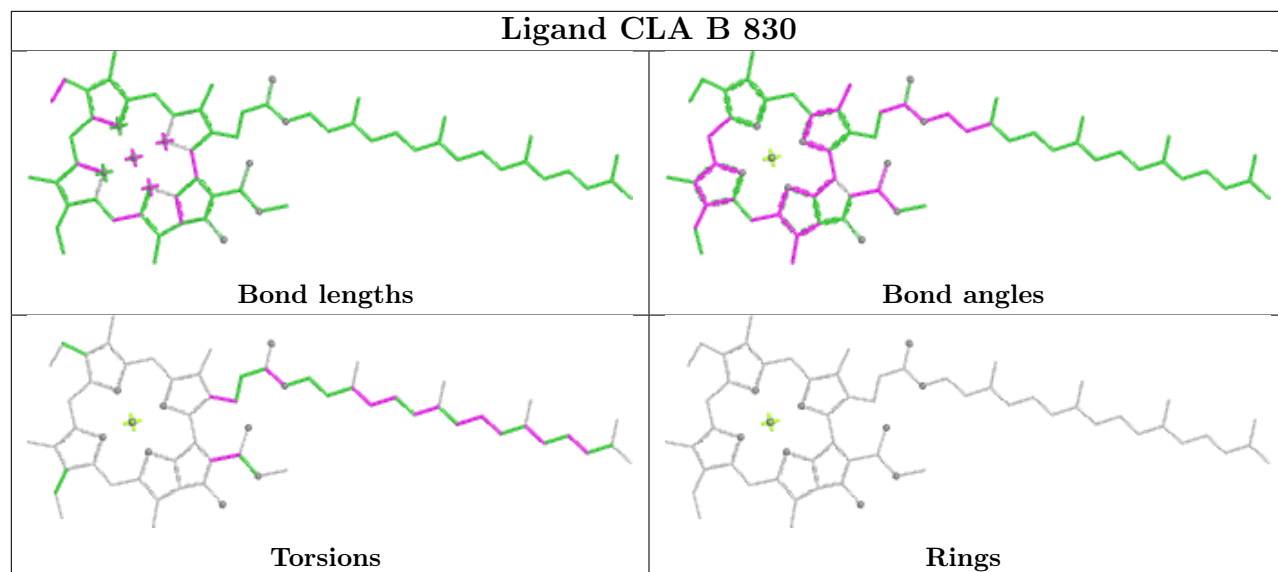
## Ligand CLA 2 313



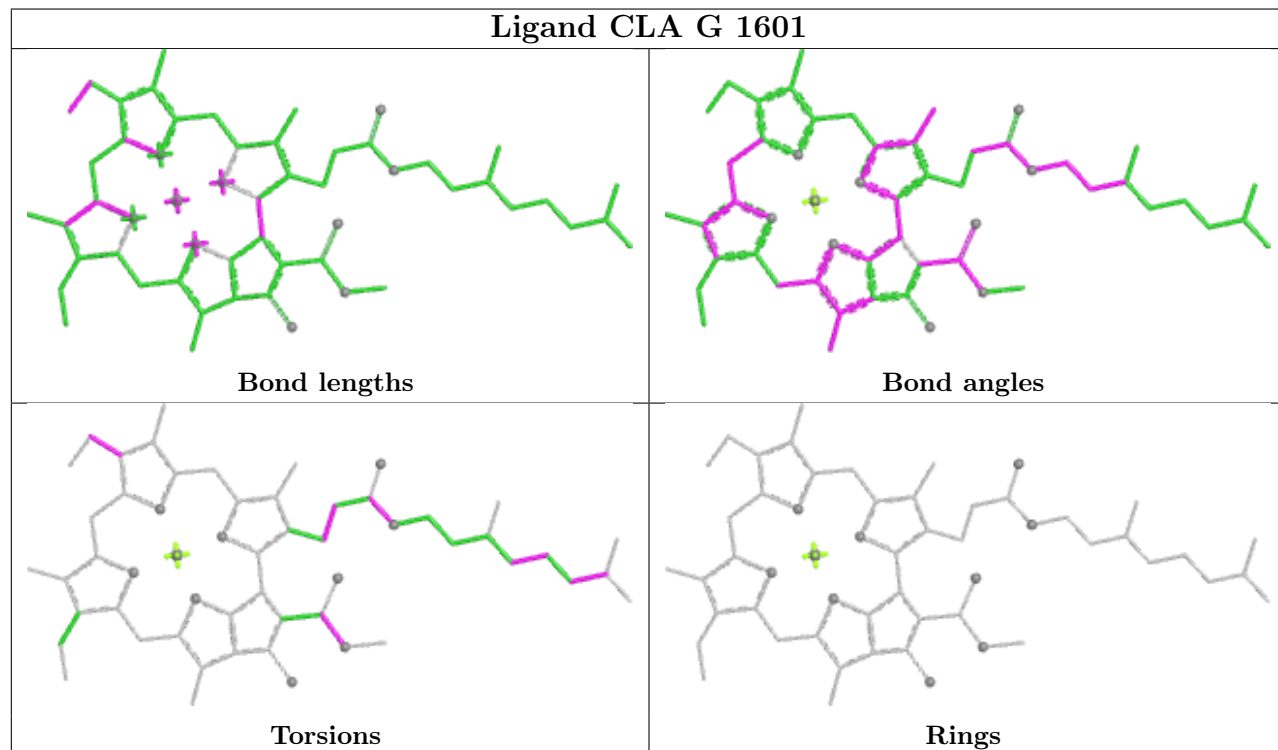
## Ligand LMG 2 322



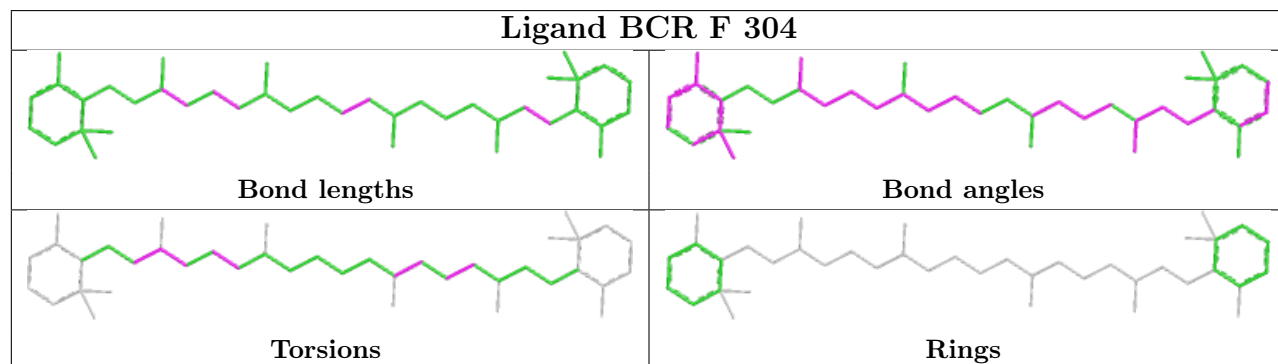
## Ligand CLA B 830

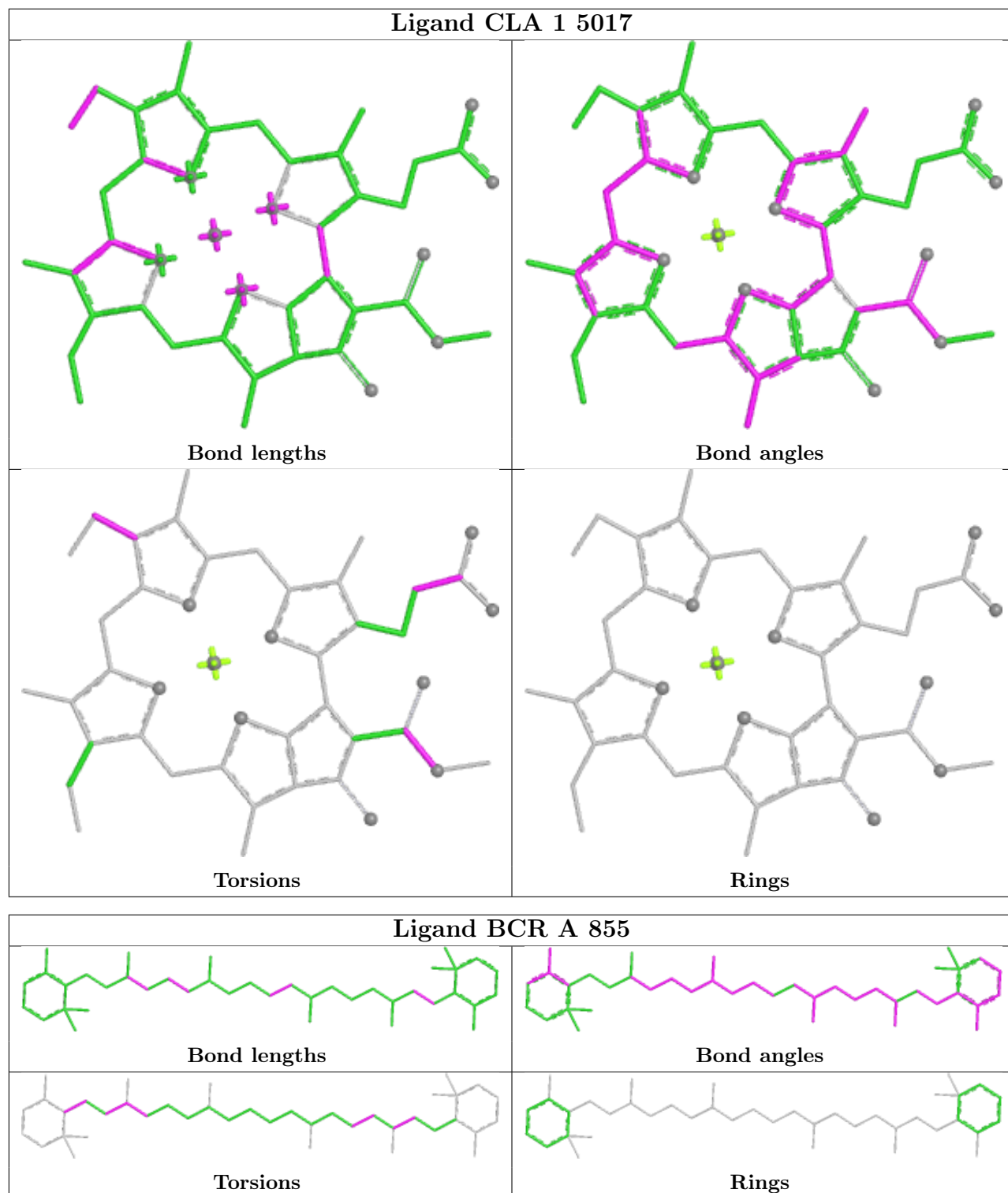


## Ligand CLA G 1601



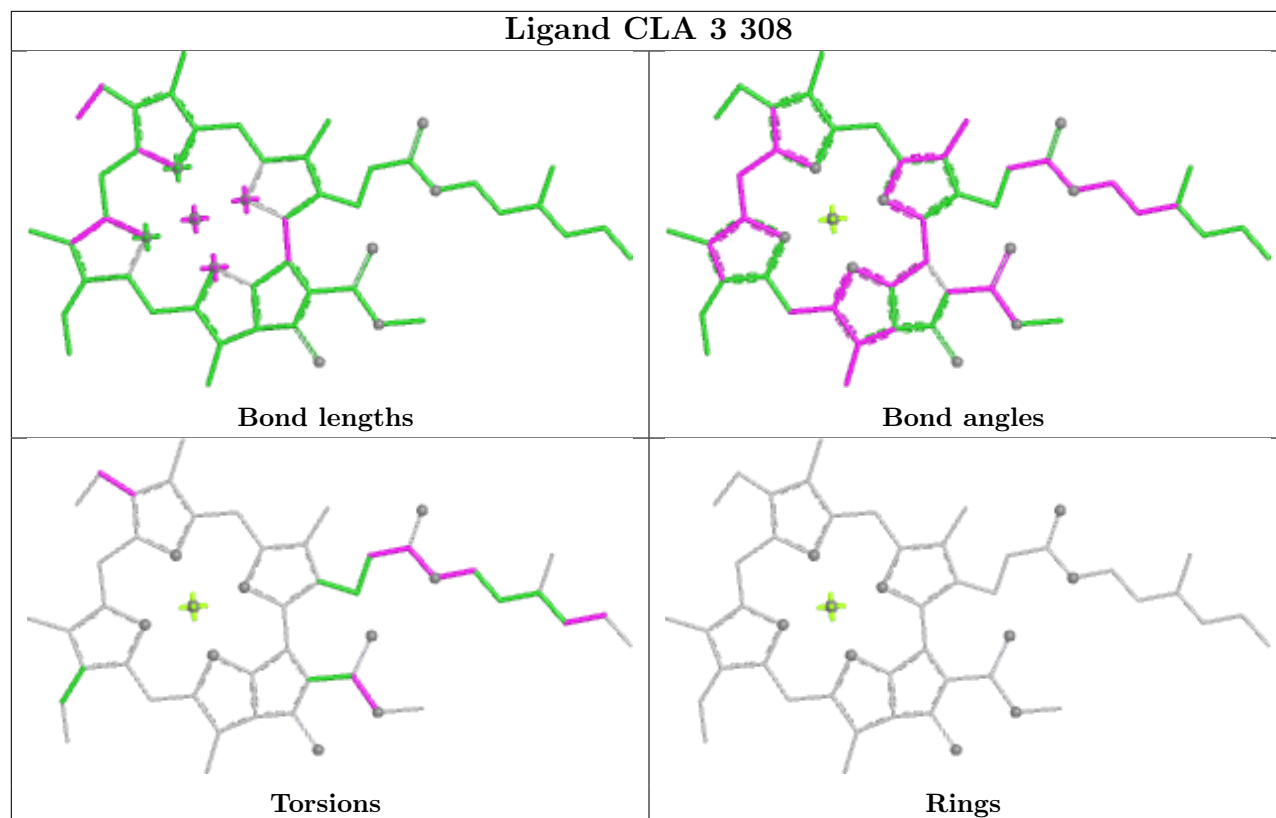
## Ligand BCR F 304



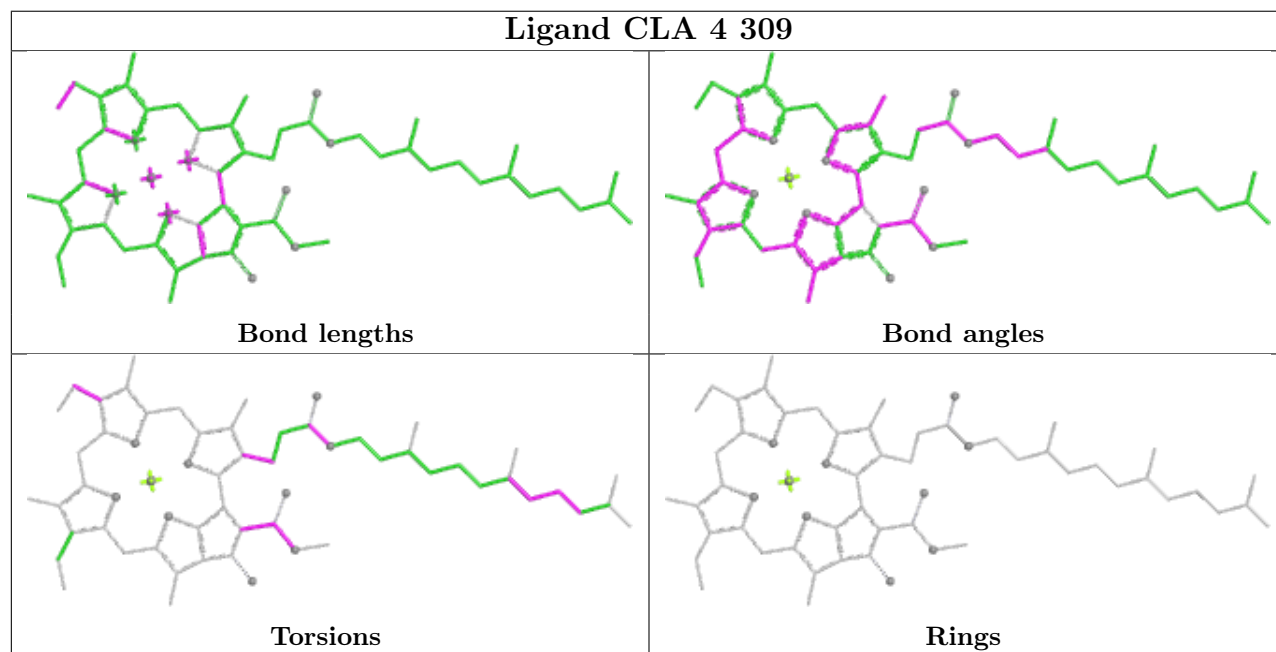




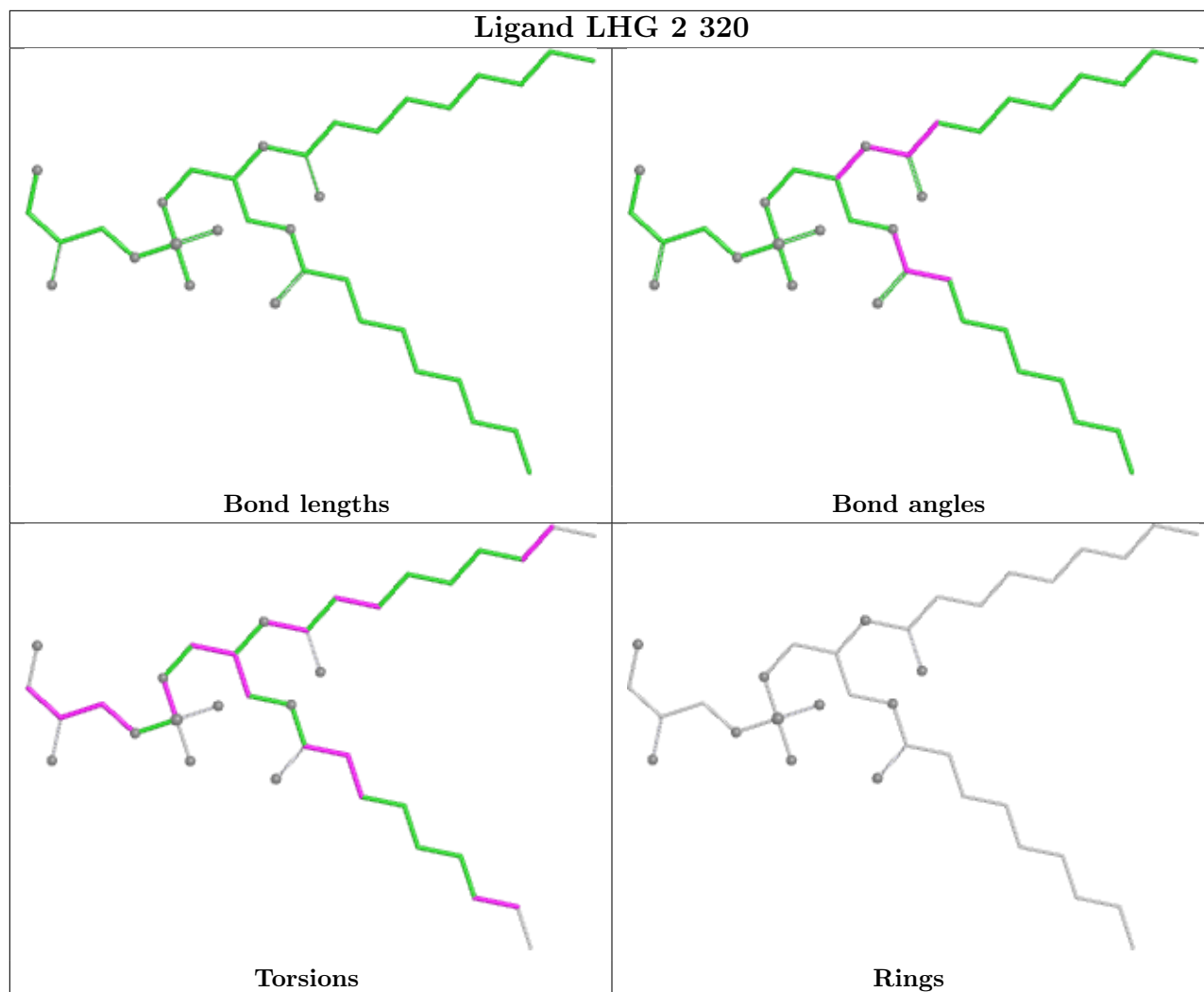
## Ligand CLA 3 308



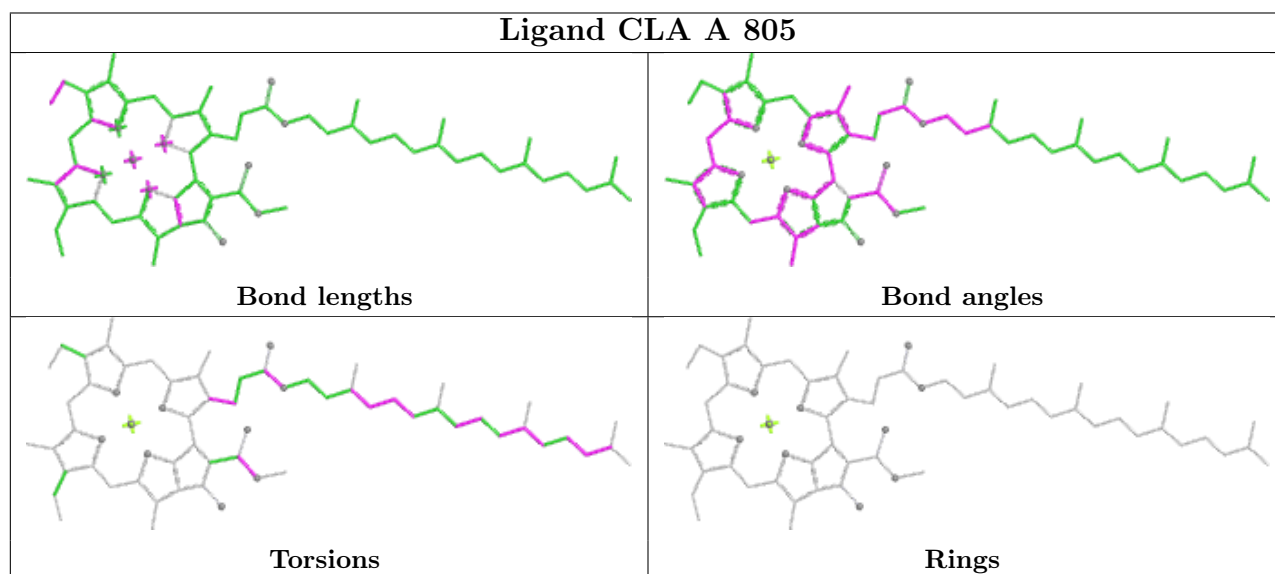
## Ligand CLA 4 309



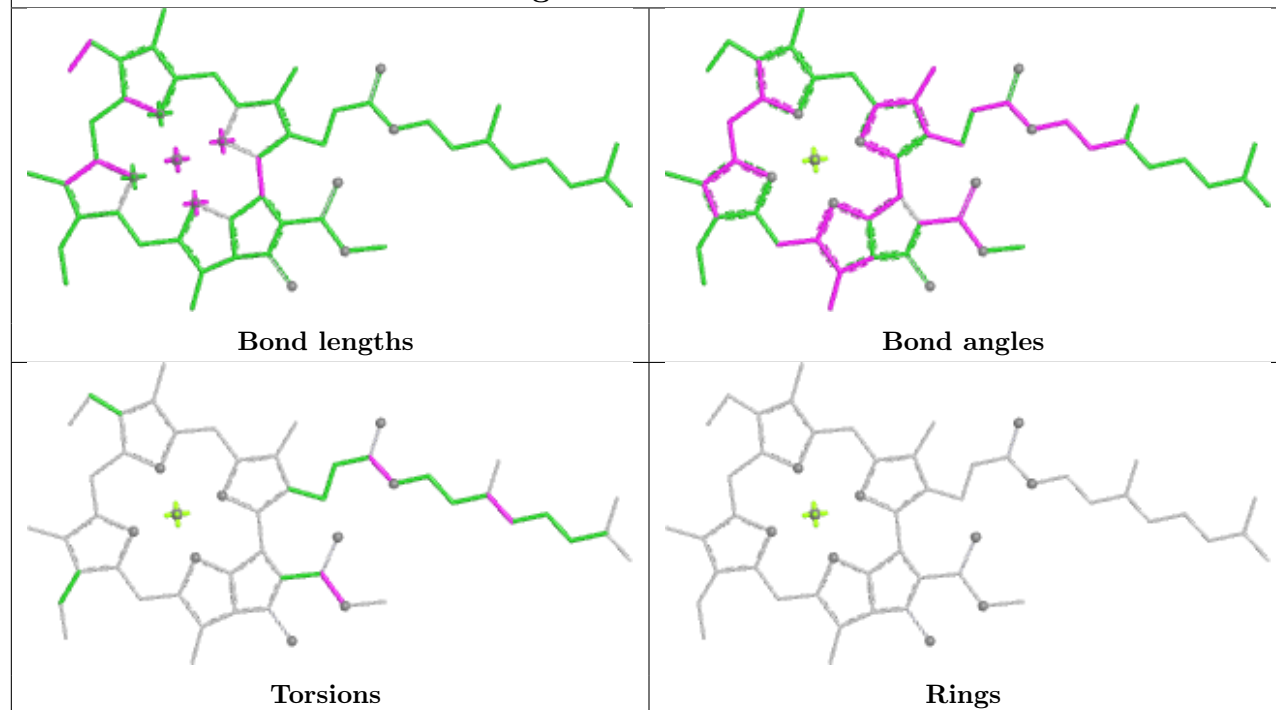
## Ligand LHG 2 320



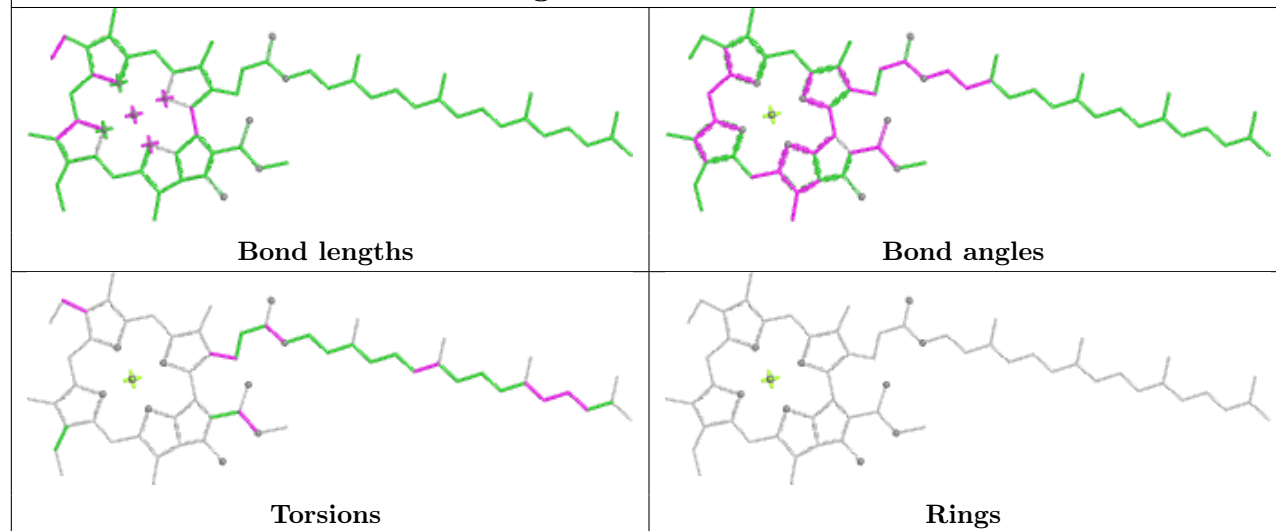
## Ligand CLA A 805

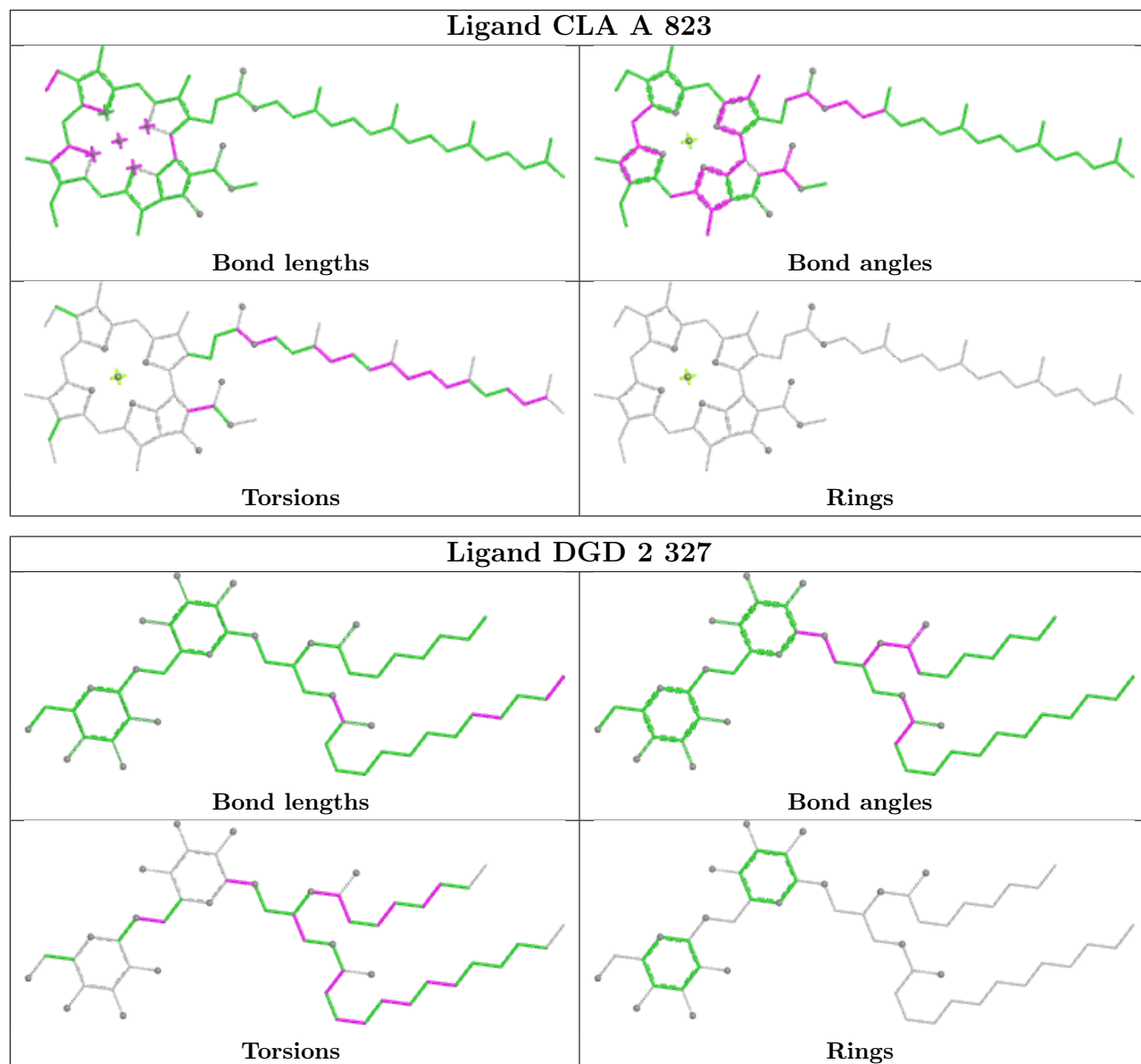


## Ligand CLA B 816

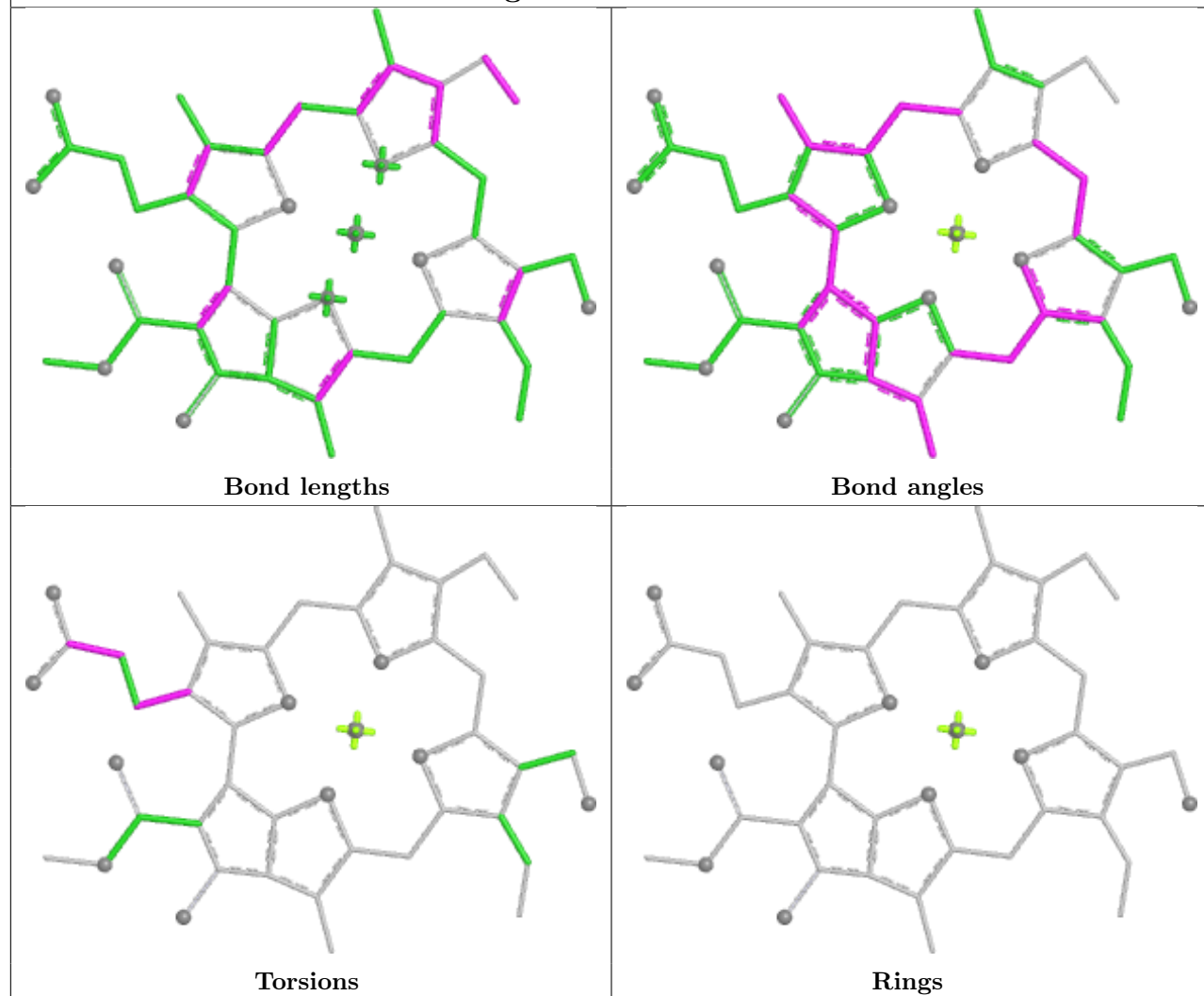


## Ligand CLA B 820

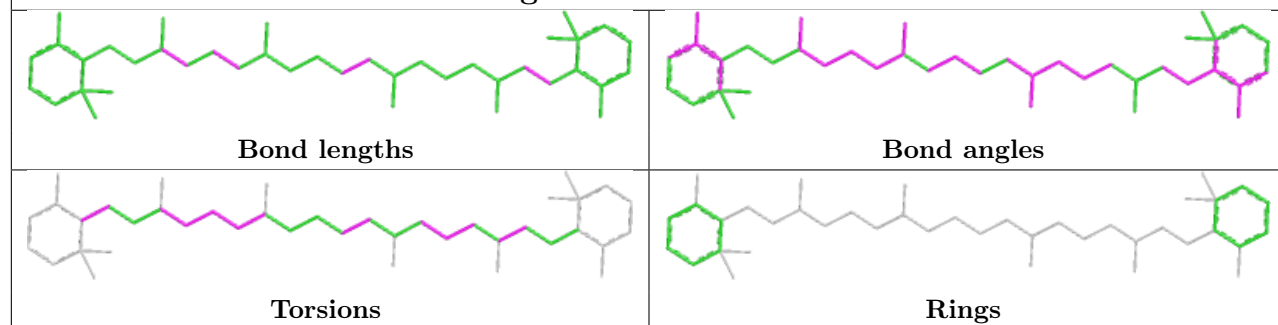




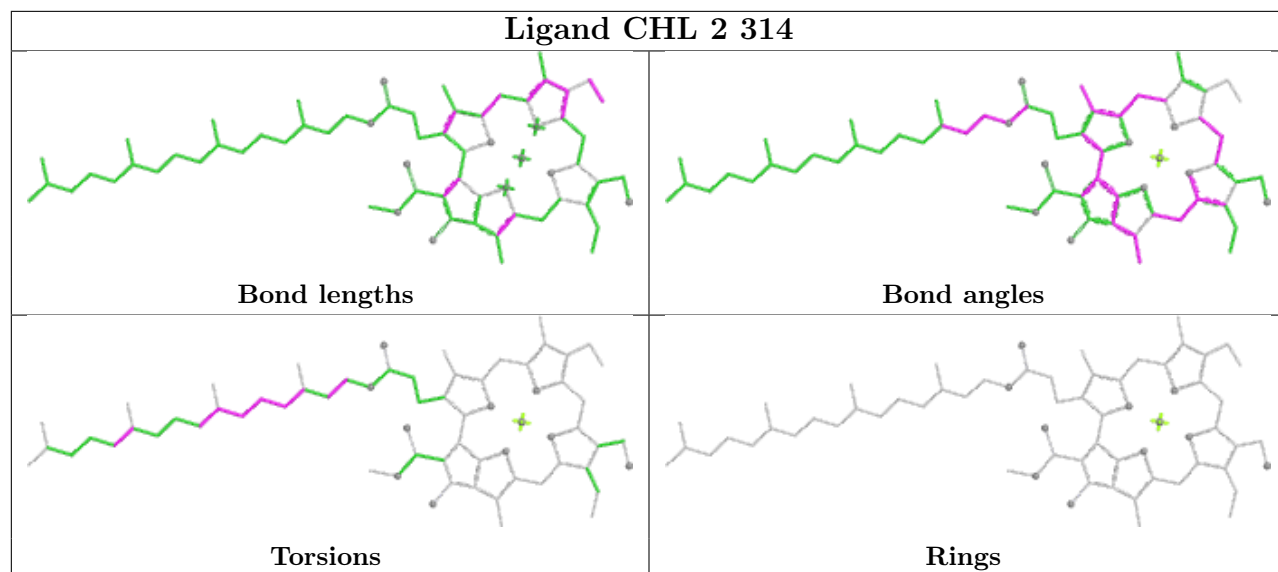
## Ligand CHL 2 318



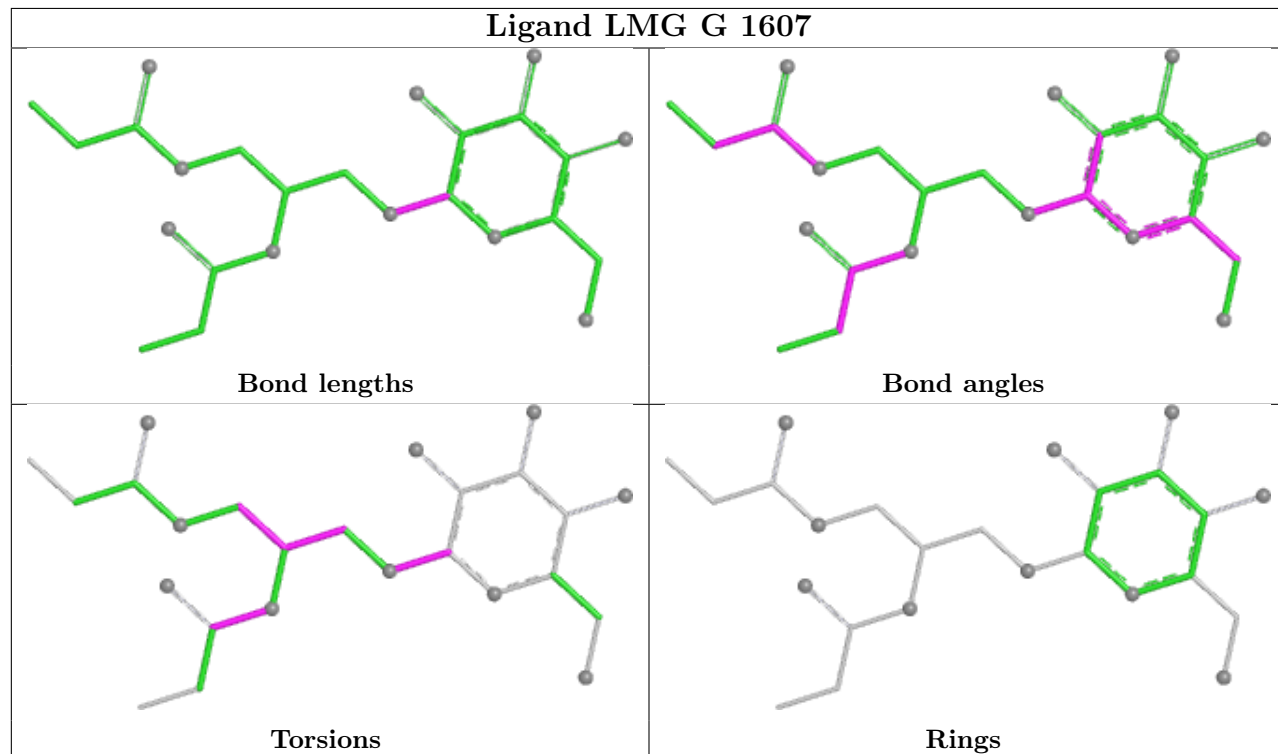
## Ligand BCR K 1405



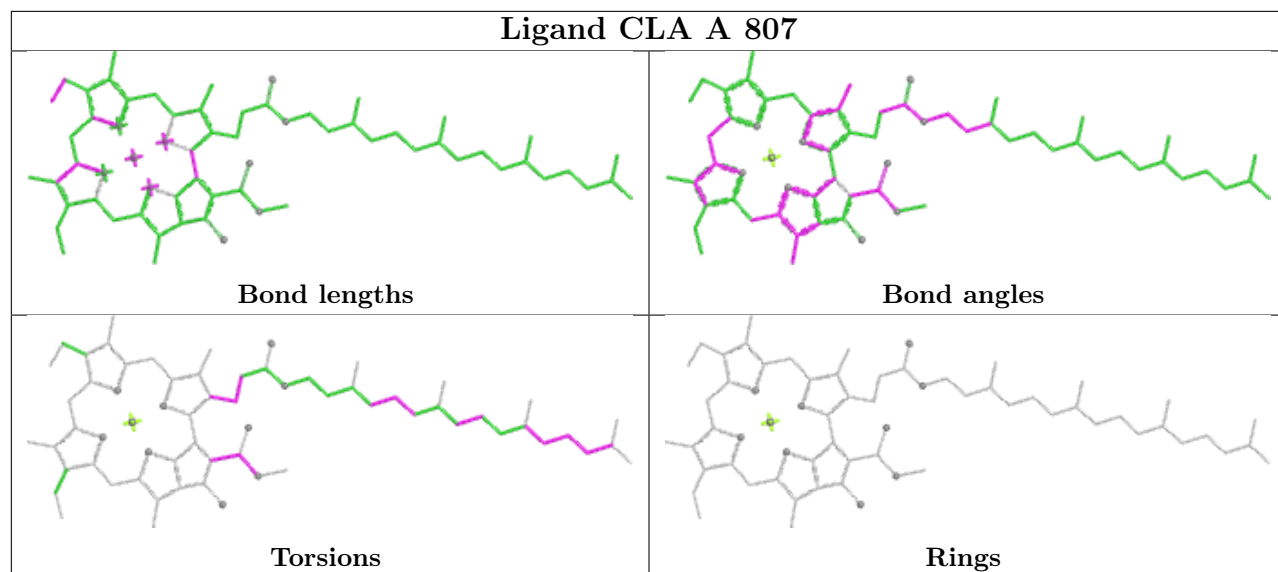
## Ligand CHL 2 314



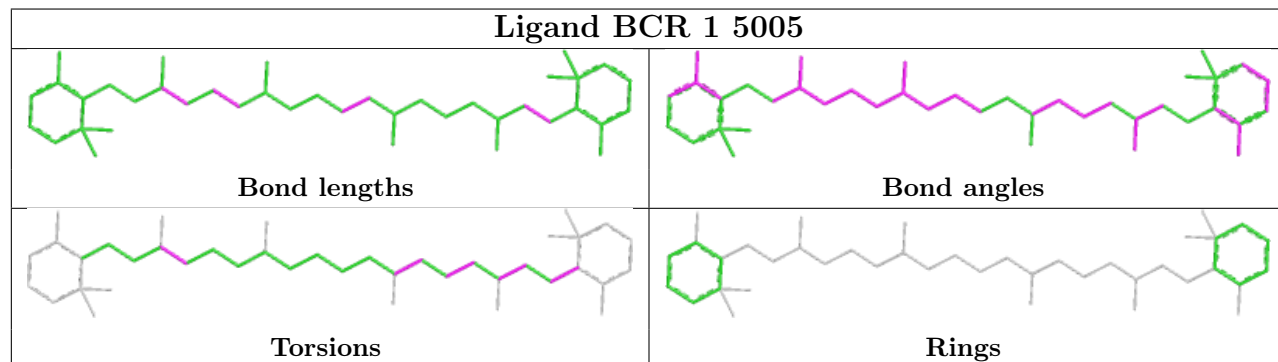
## Ligand LMG G 1607



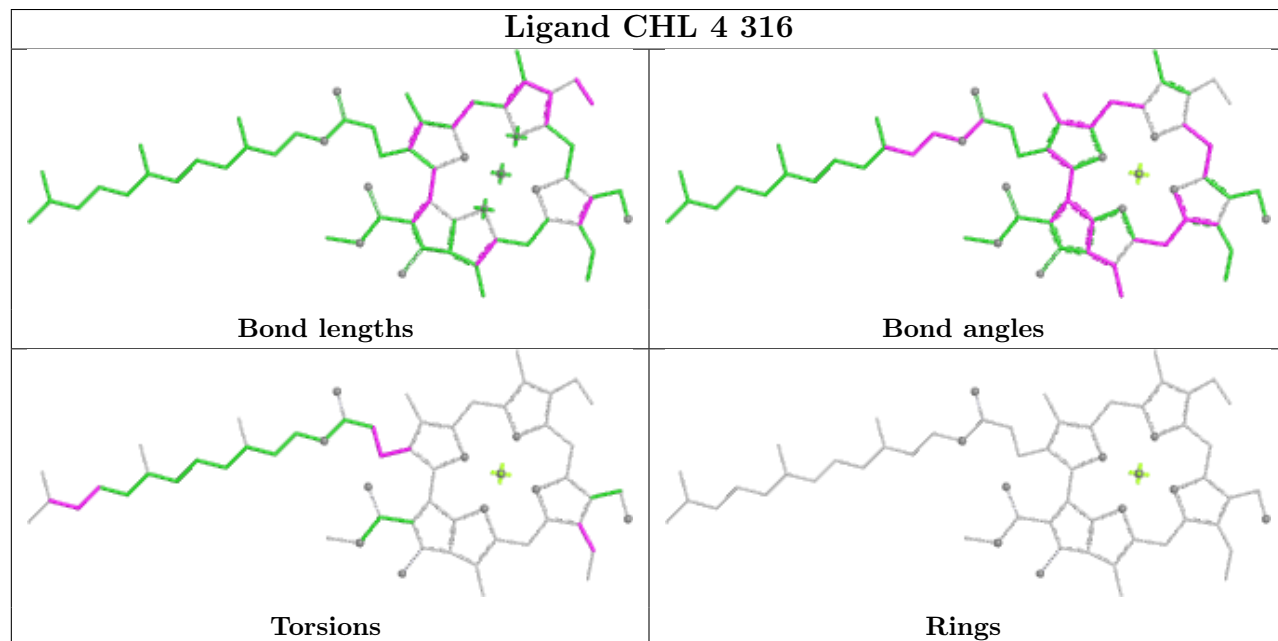
## Ligand CLA A 807

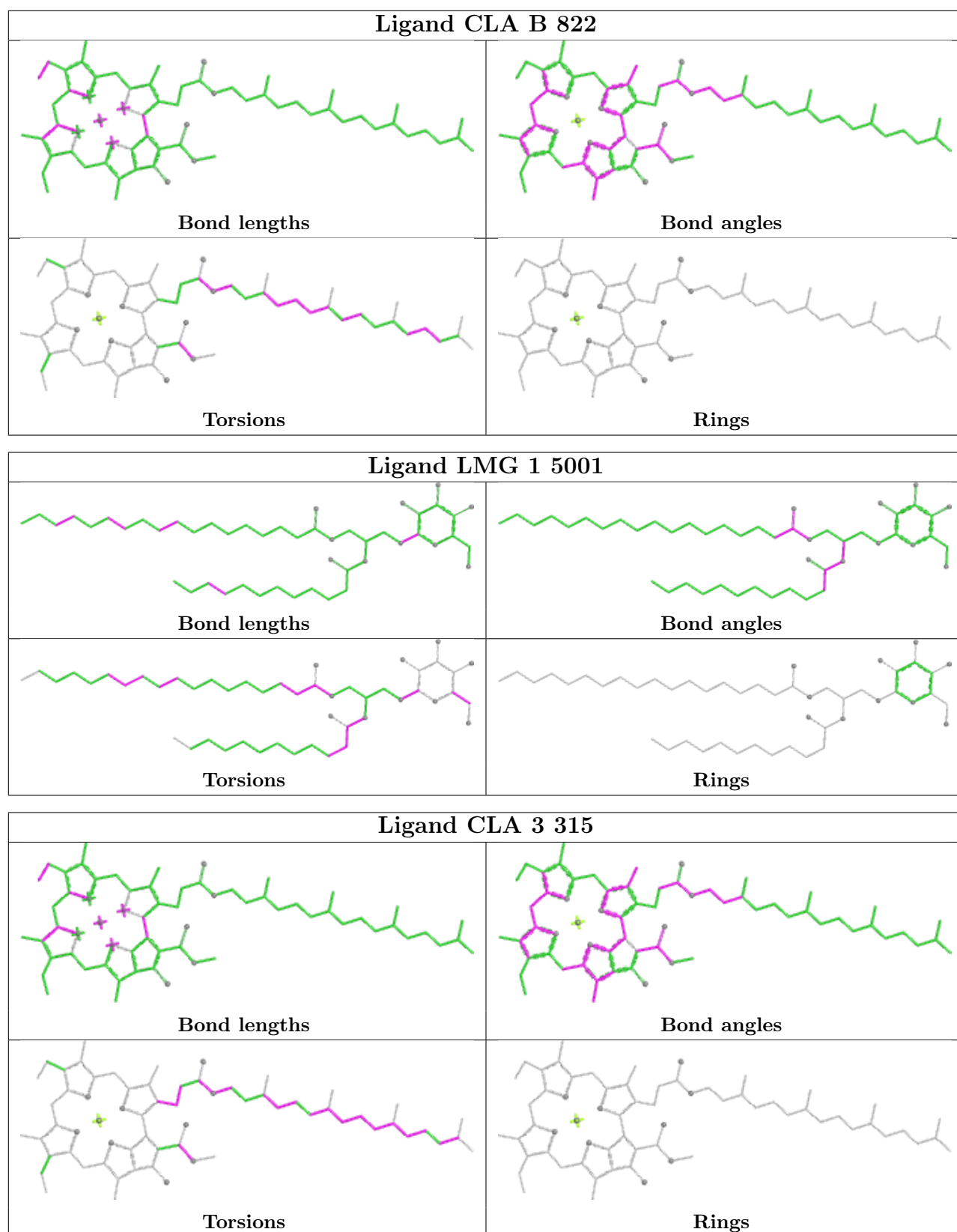


## Ligand BCR 1 5005



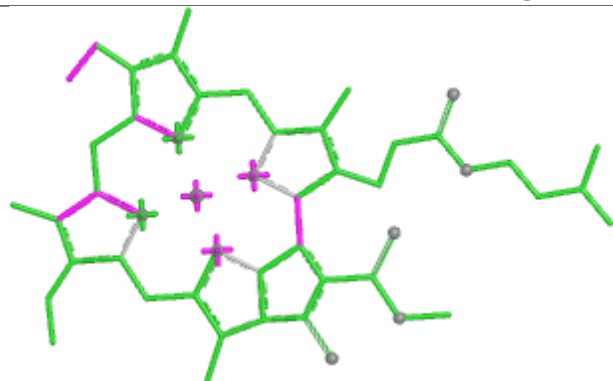
## Ligand CHL 4 316



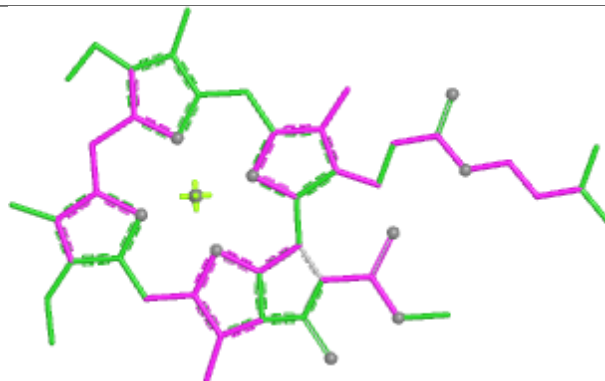




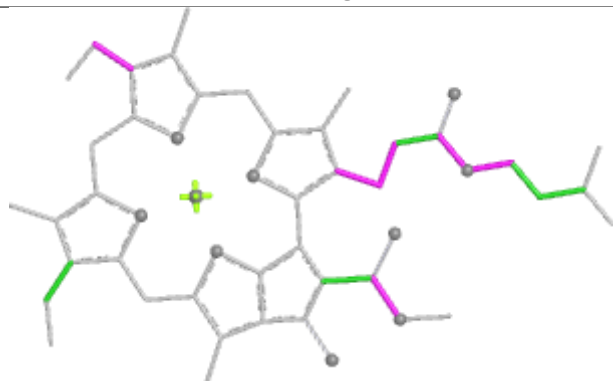
## Ligand CLA 2 311



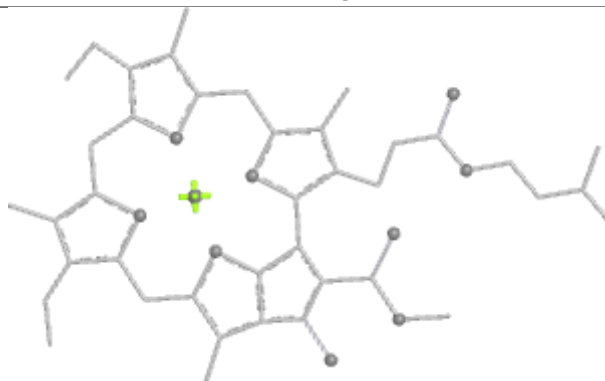
Bond lengths



Bond angles

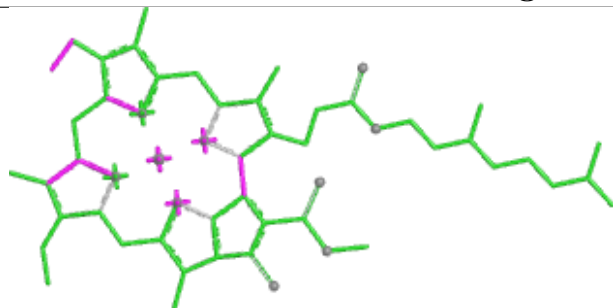


Torsions

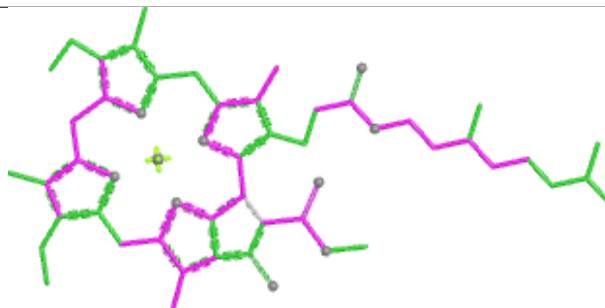


Rings

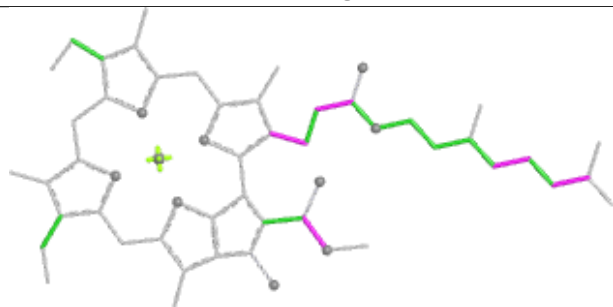
## Ligand CLA 3 307



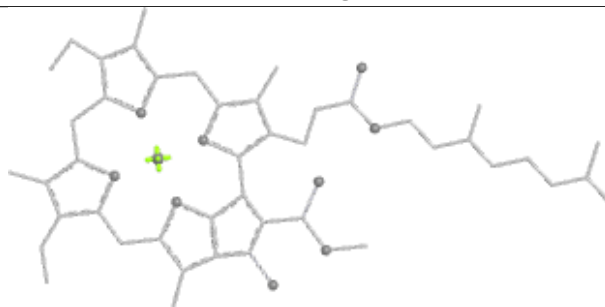
Bond lengths



Bond angles

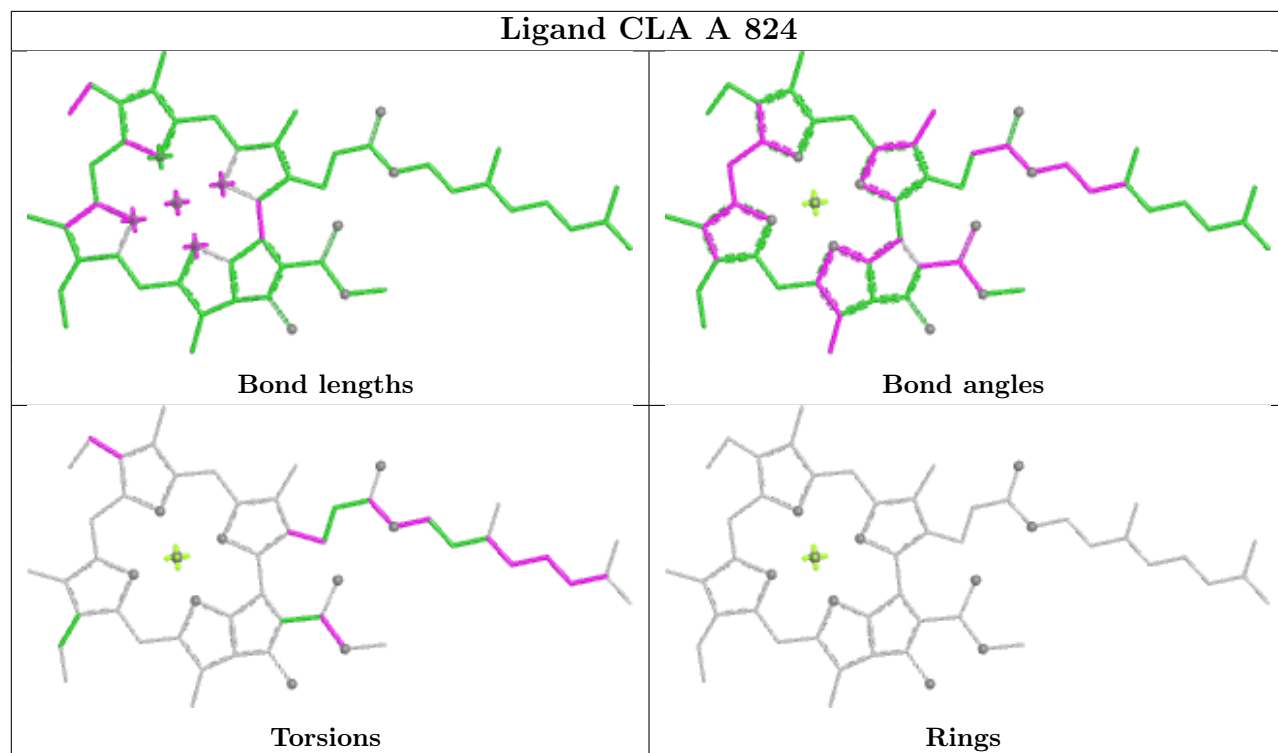


Torsions

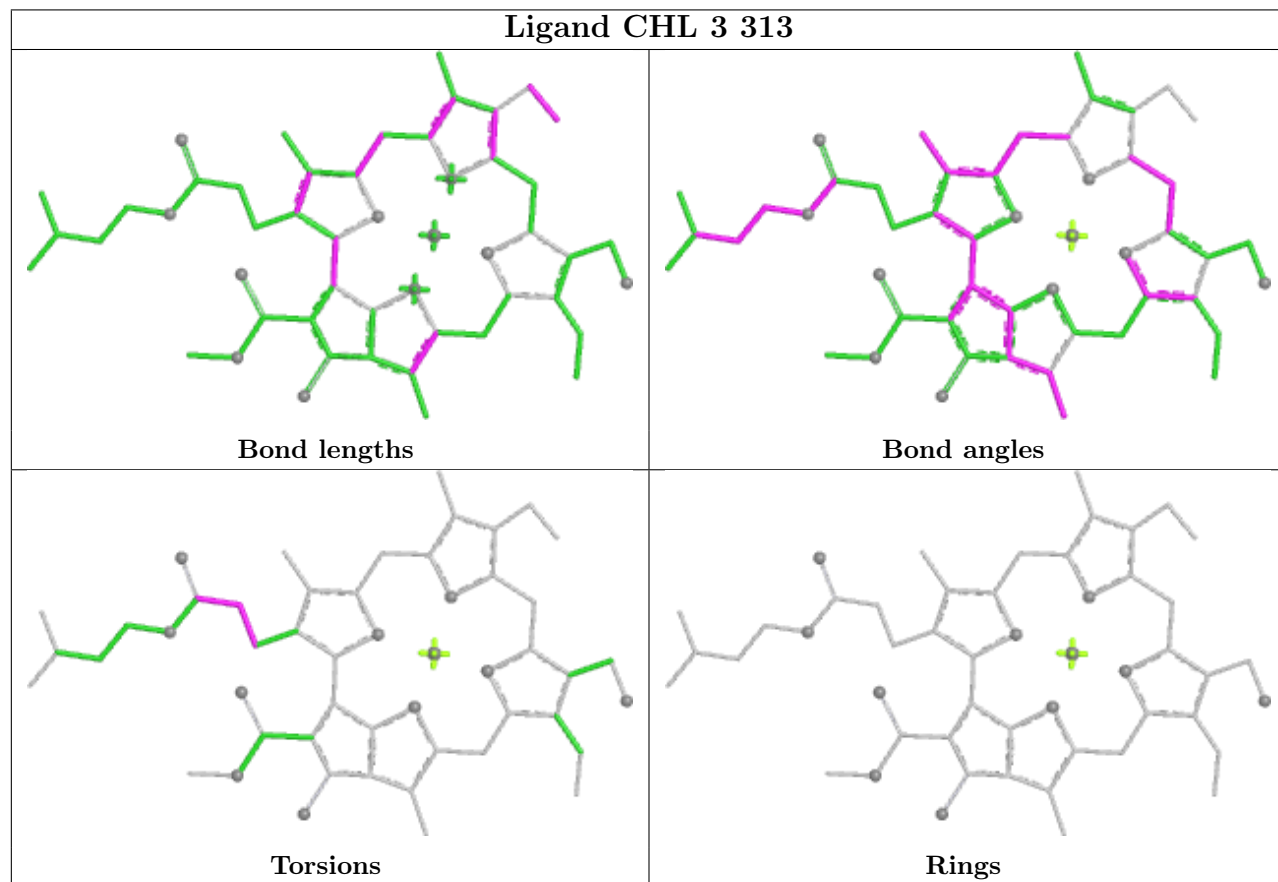


Rings

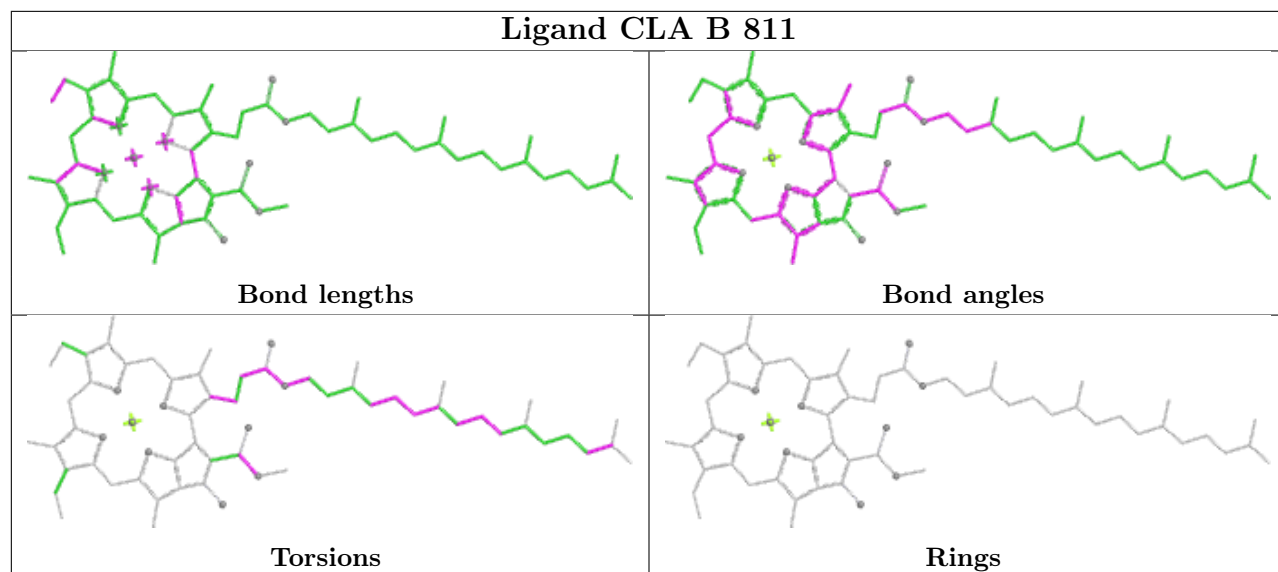
## Ligand CLA A 824



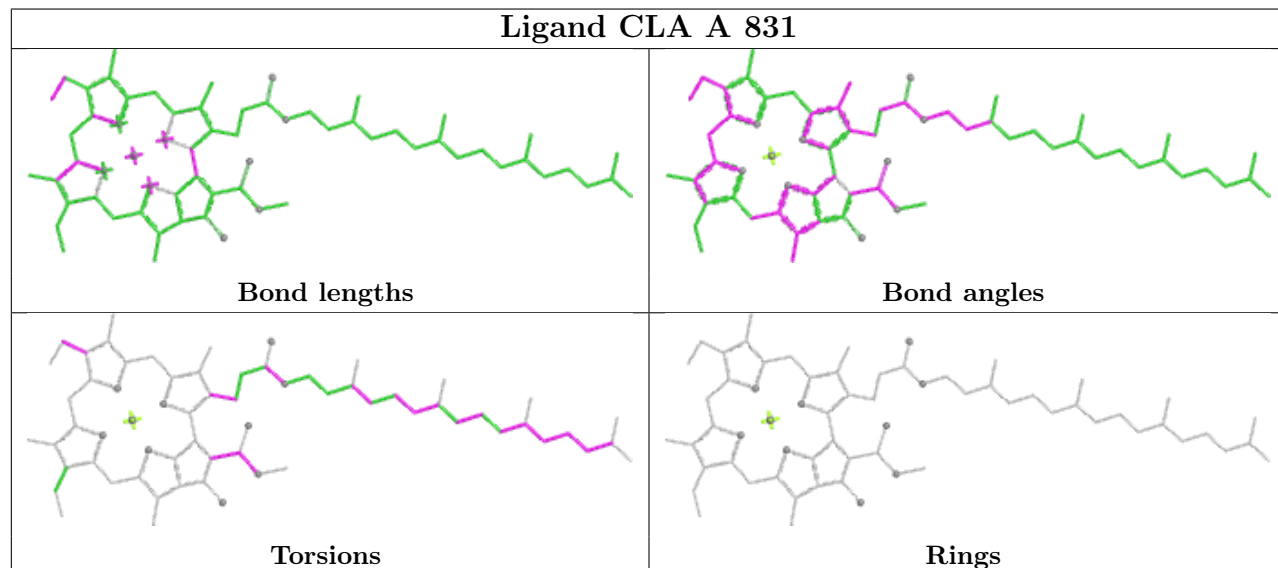
## Ligand CHL 3 313



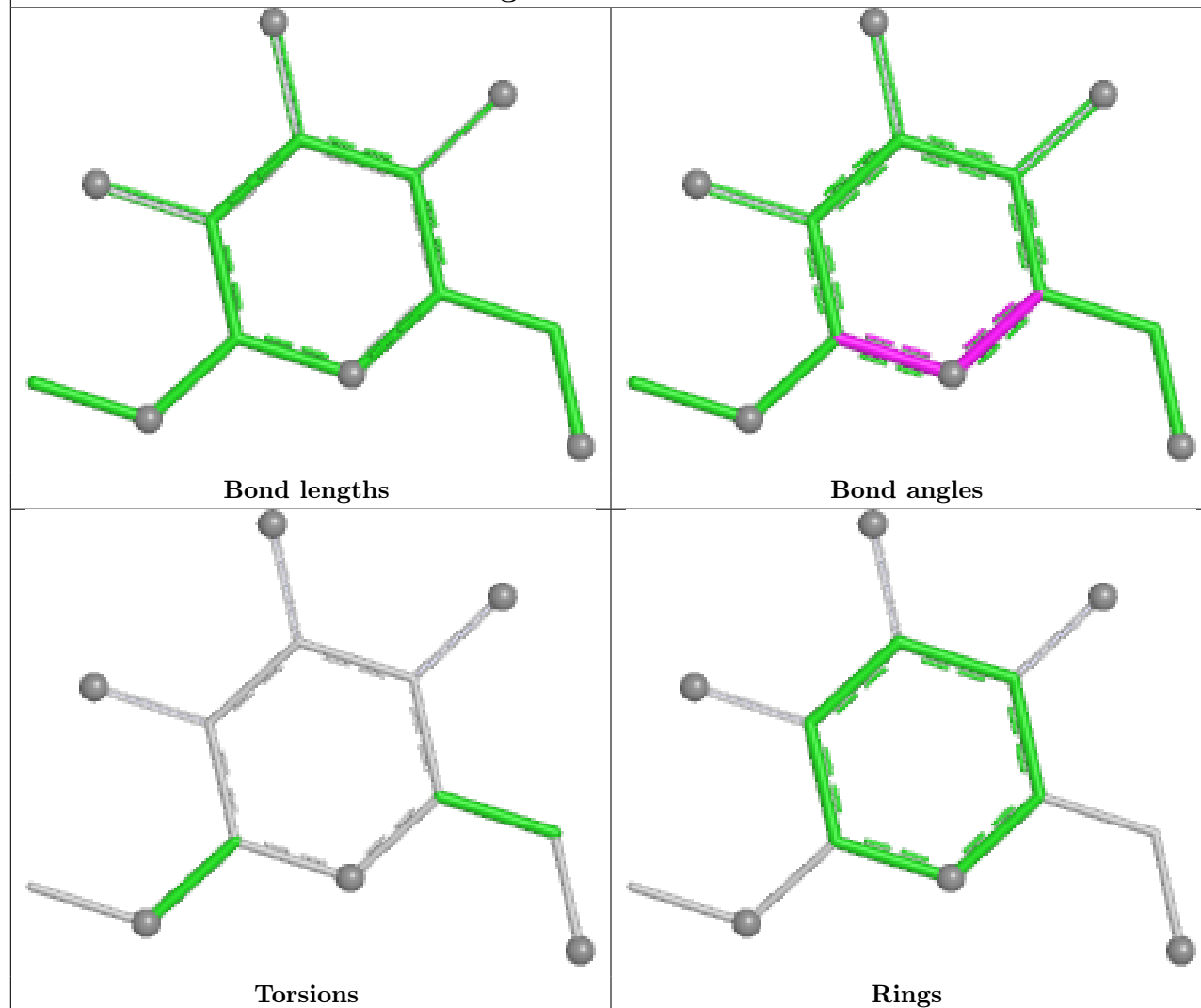
## Ligand CLA B 811



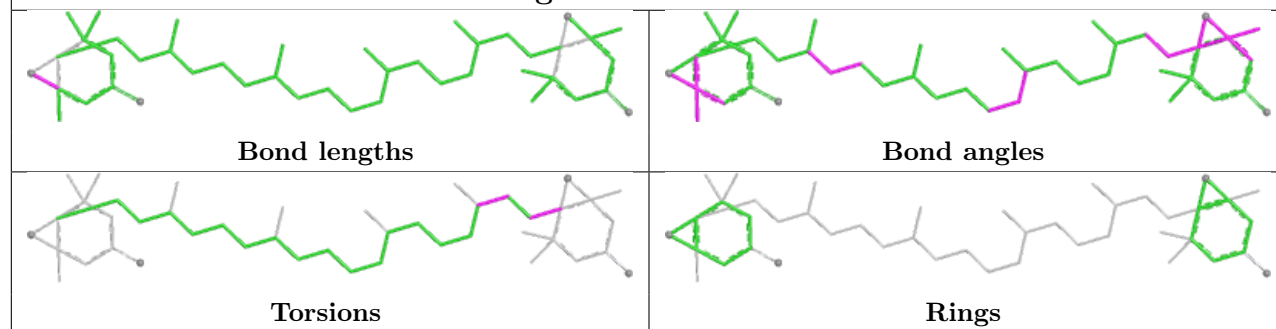
## Ligand CLA A 831



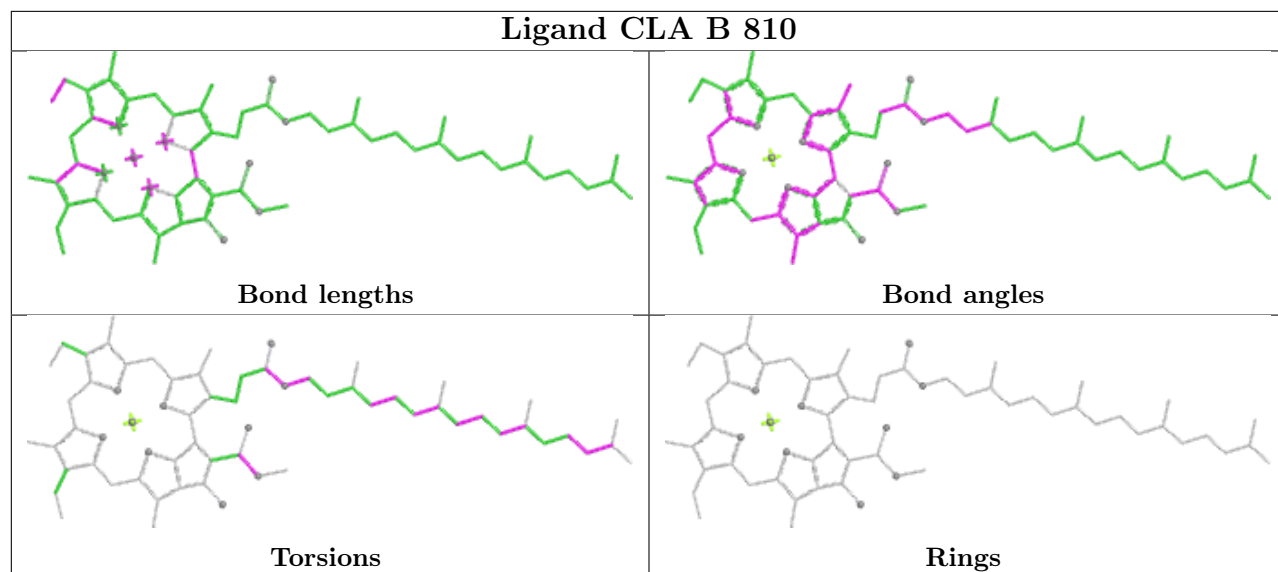
## Ligand LMG 2 323



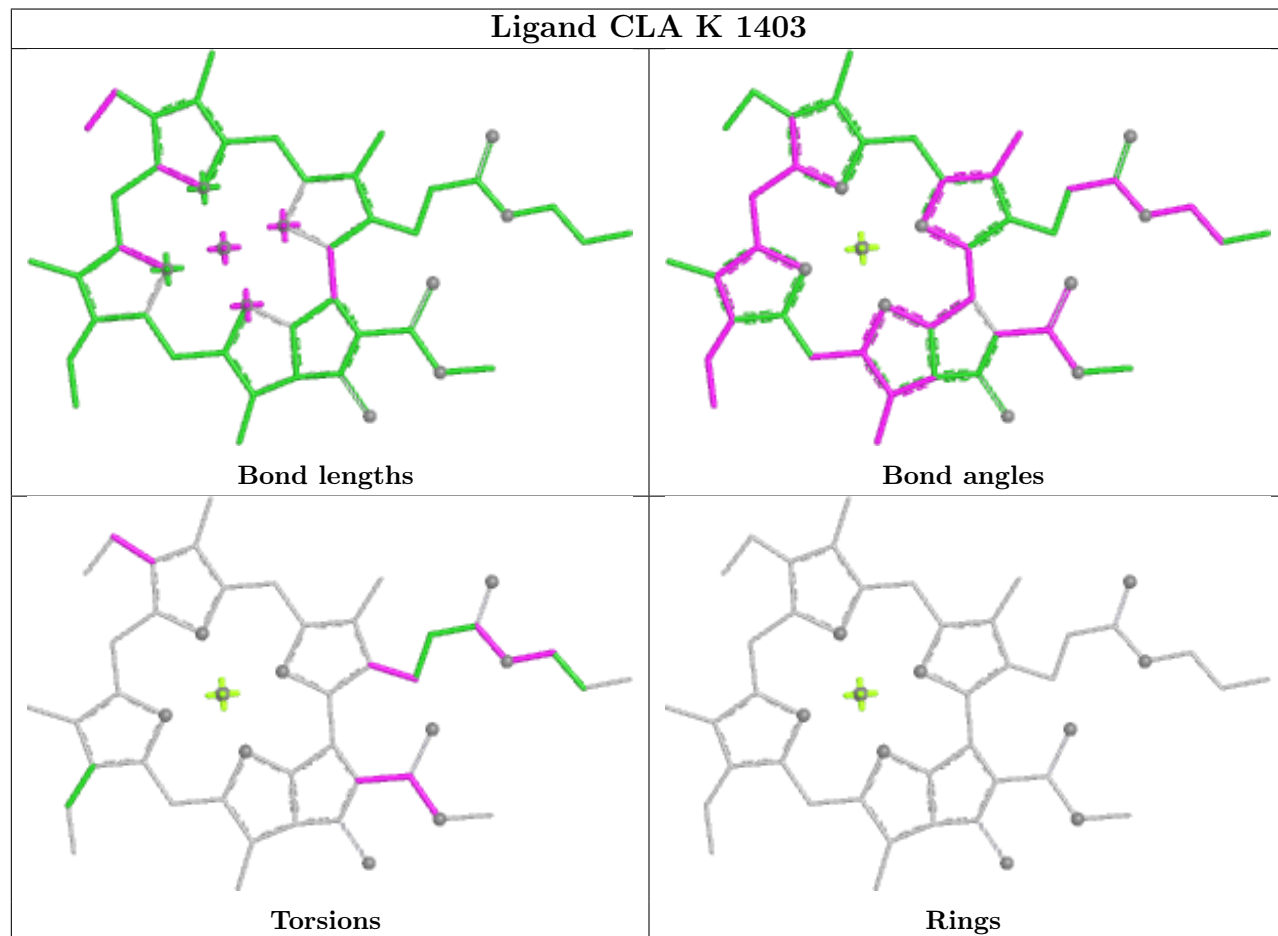
## Ligand XAT 2 304



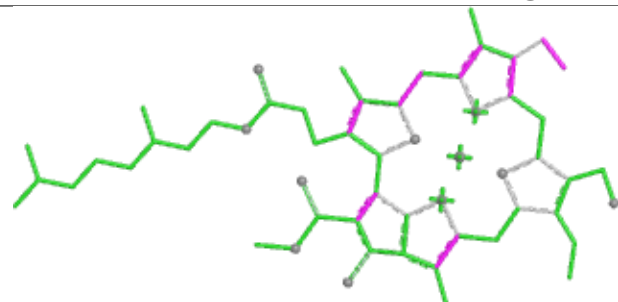
## Ligand CLA B 810



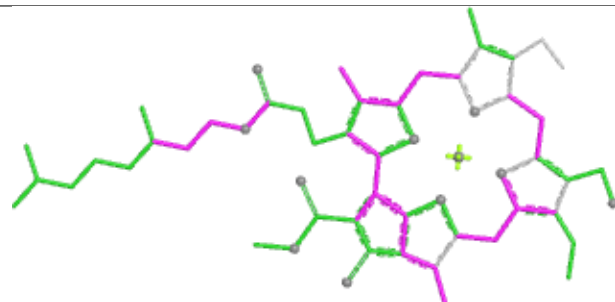
## Ligand CLA K 1403



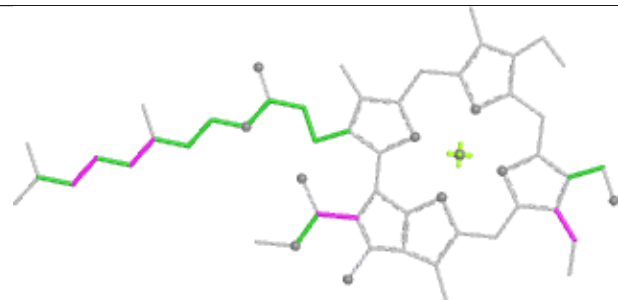
## Ligand CHL 4 318



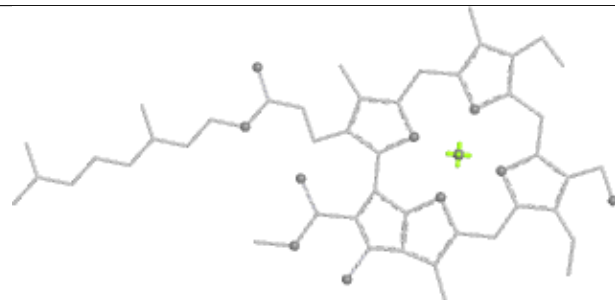
Bond lengths



Bond angles

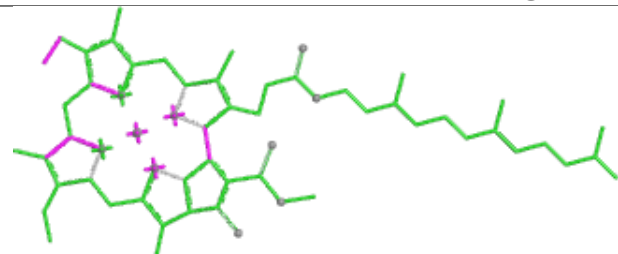


Torsions

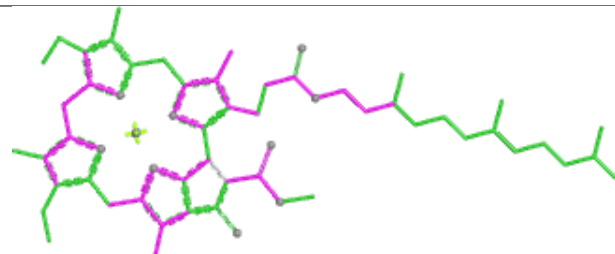


Rings

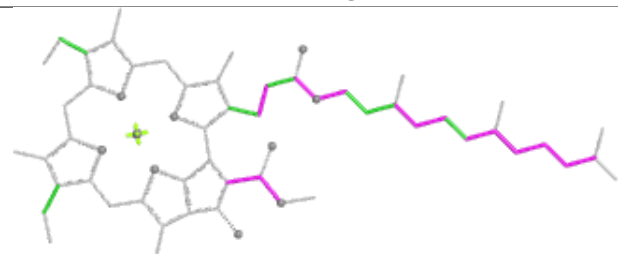
## Ligand CLA 4 308



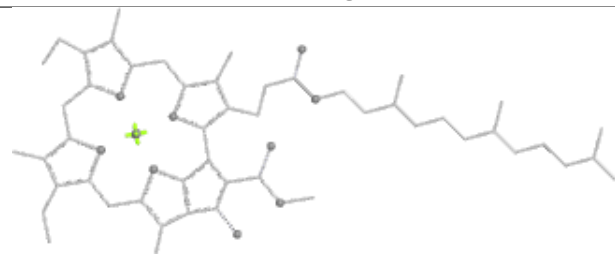
Bond lengths



Bond angles

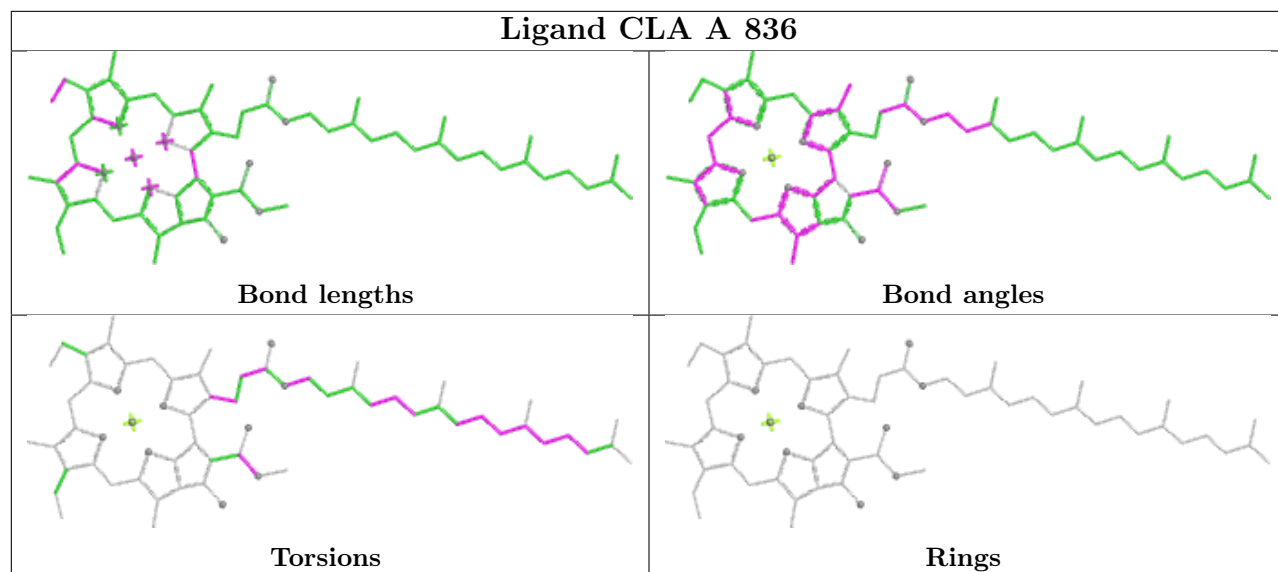


Torsions

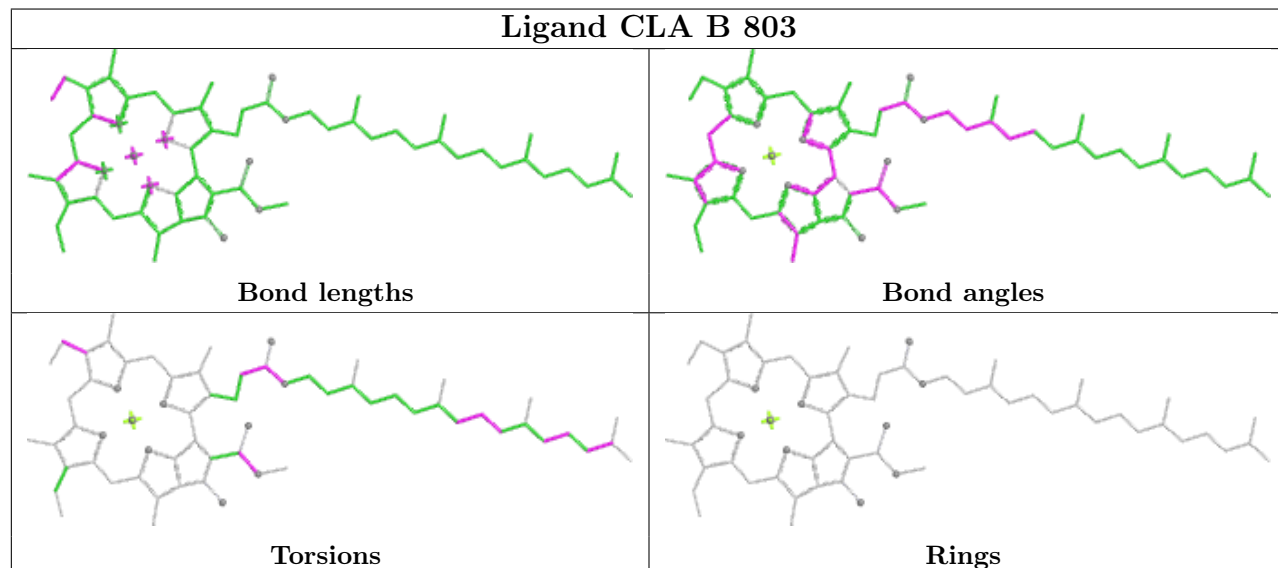


Rings

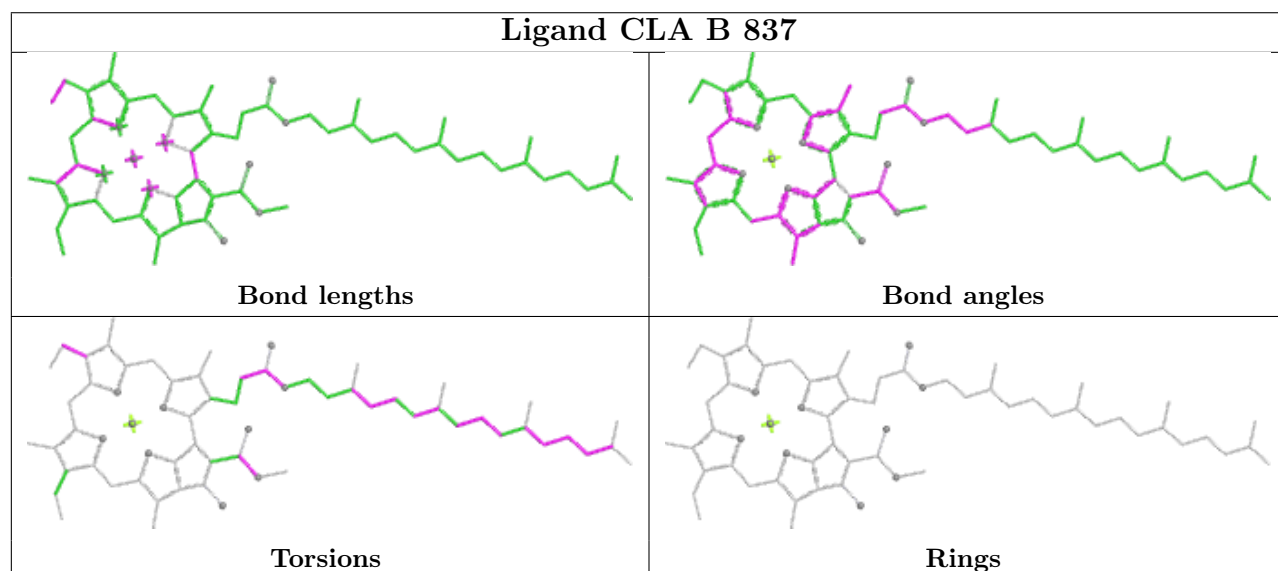
## Ligand CLA A 836



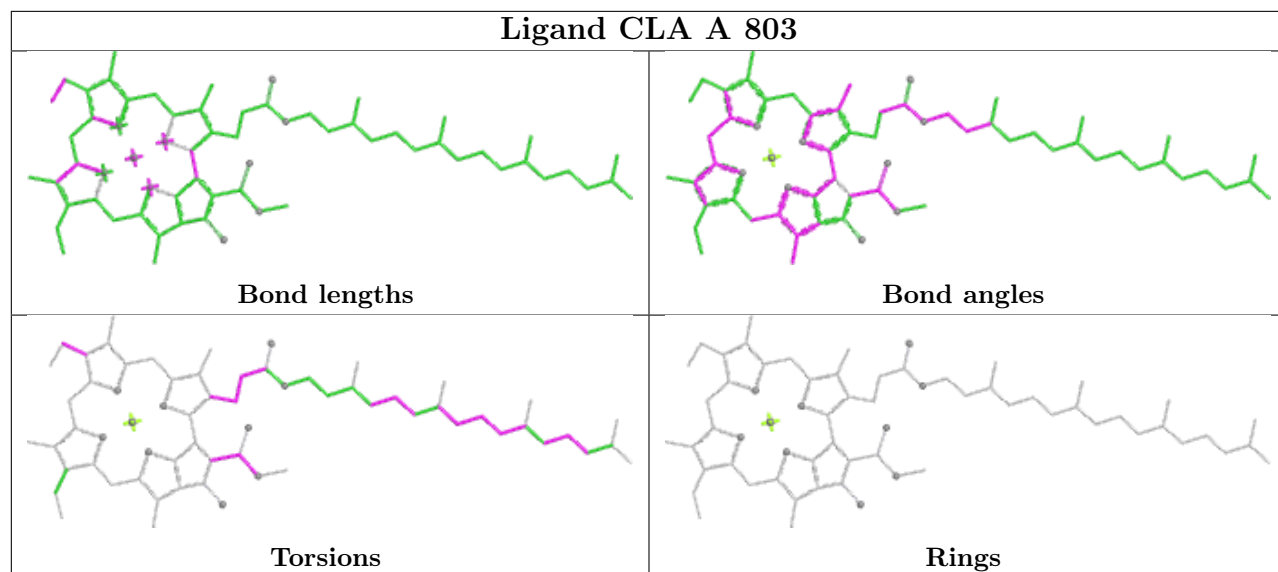
## Ligand CLA B 803



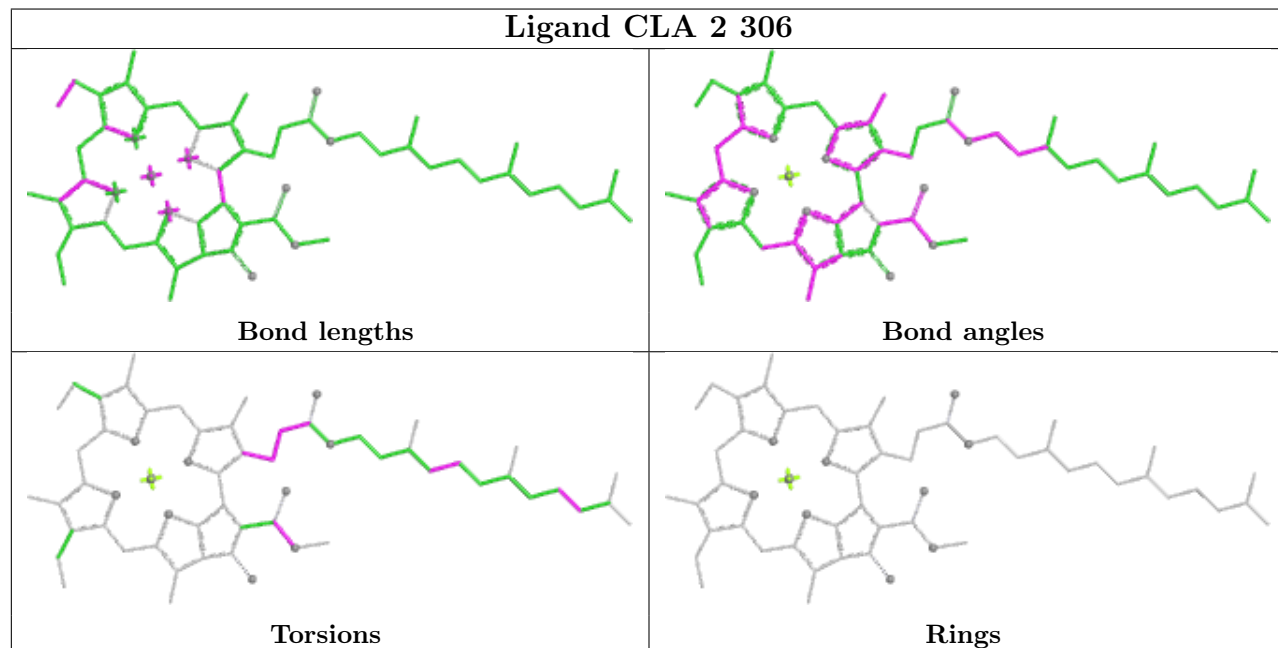
## Ligand CLA B 837



## Ligand CLA A 803

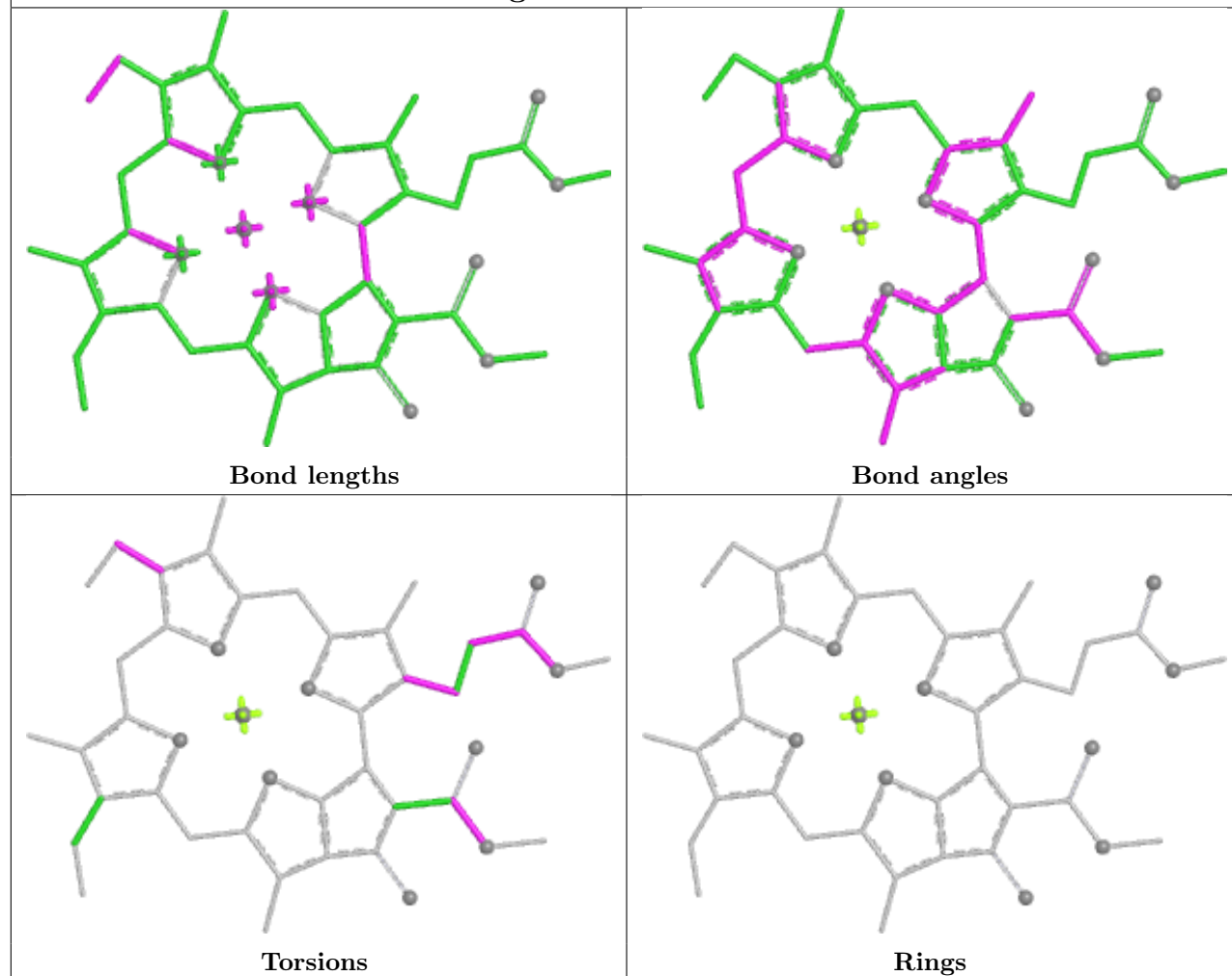


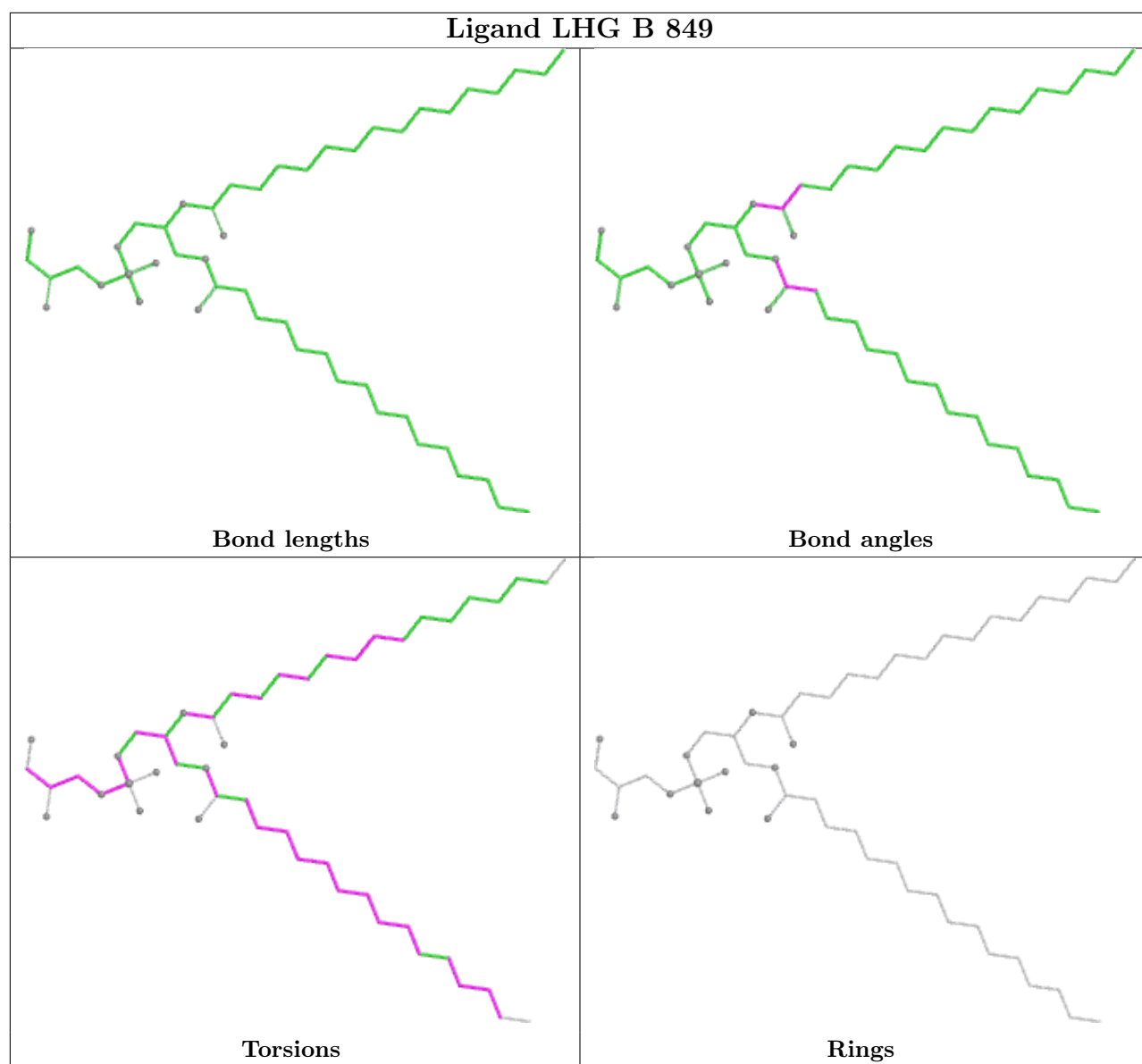
## Ligand CLA 2 306

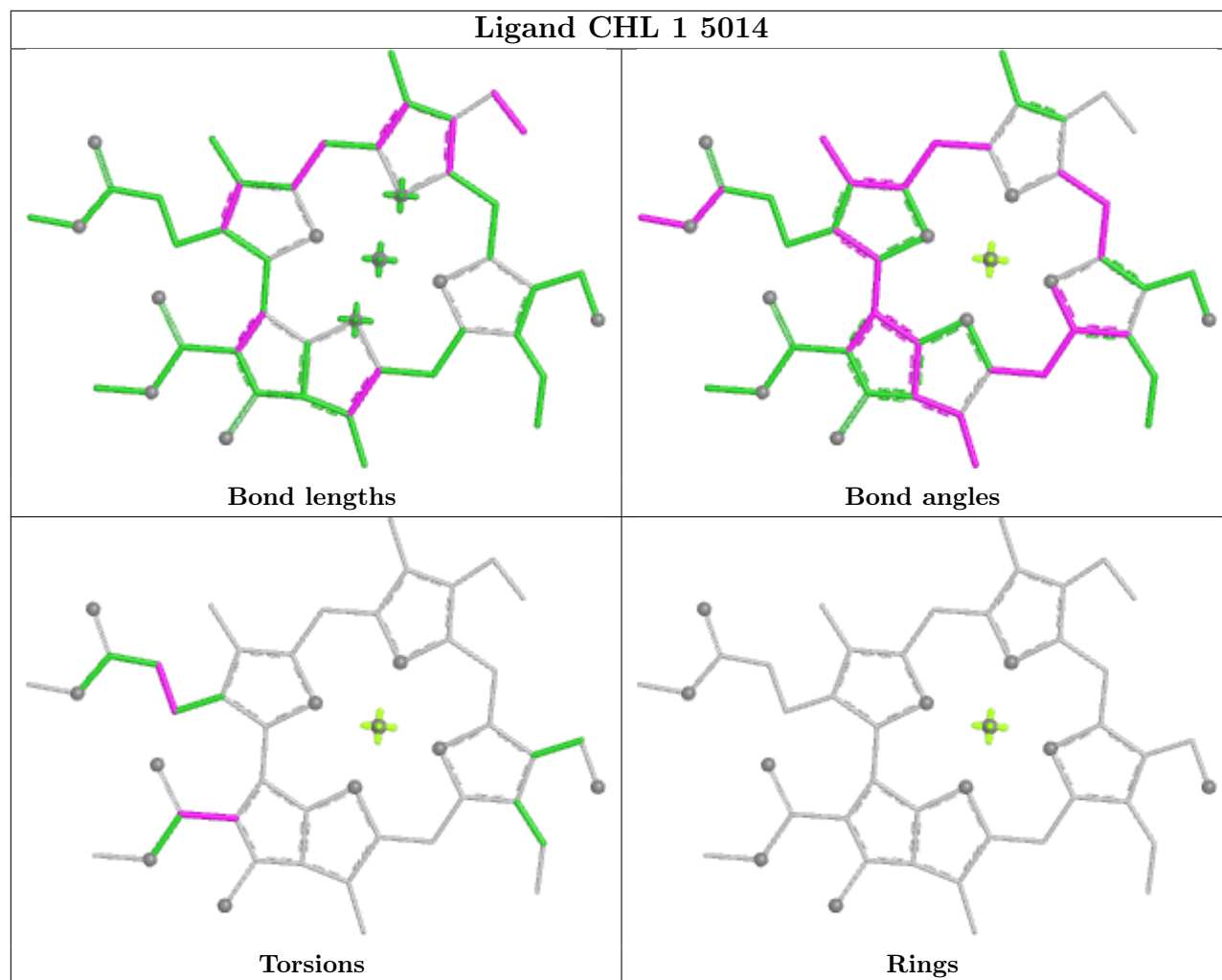




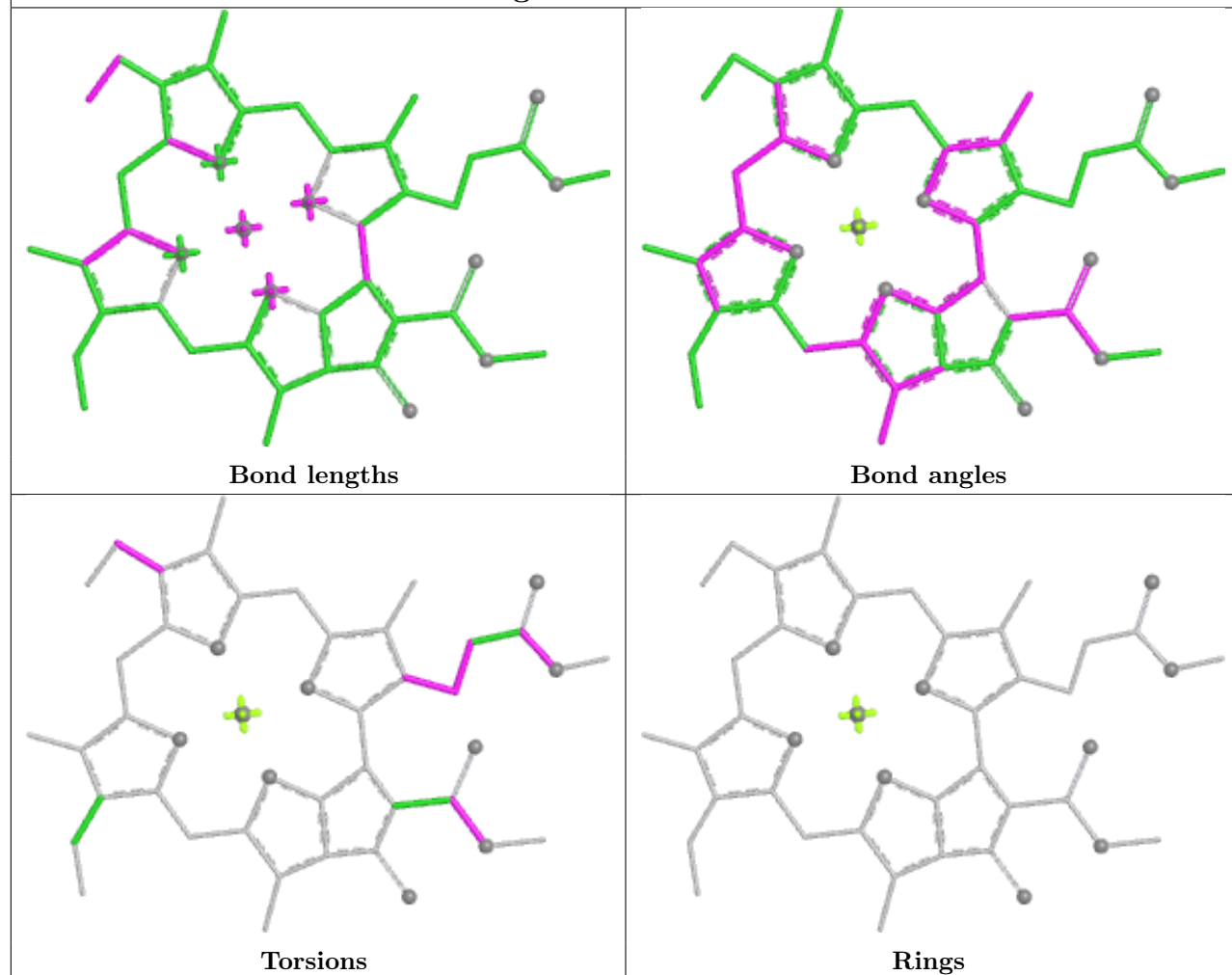
## Ligand CLA 1 5013



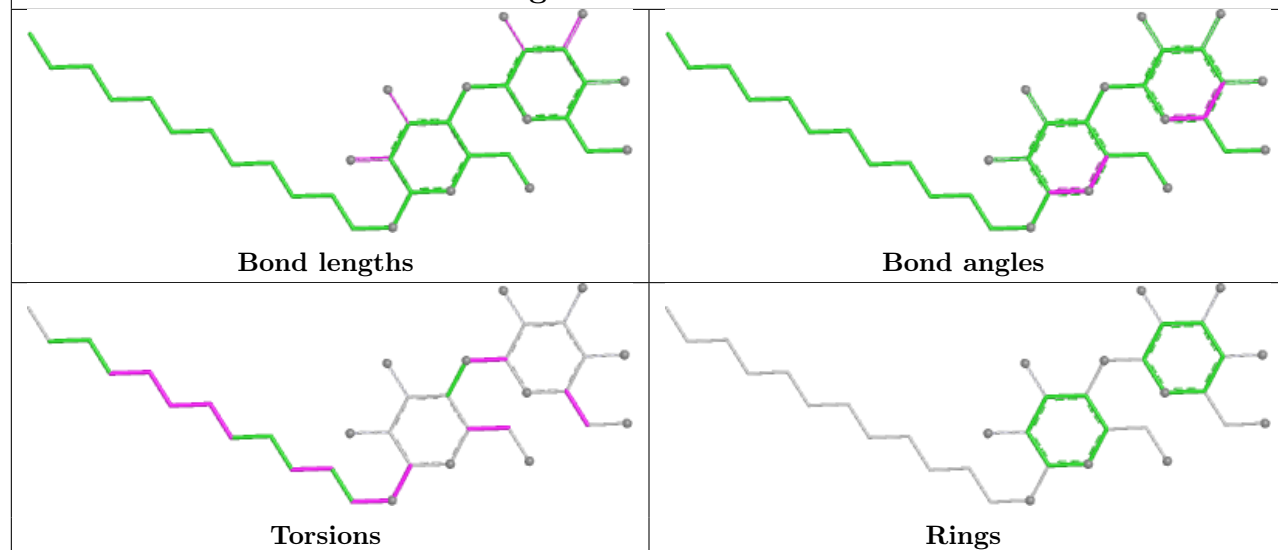




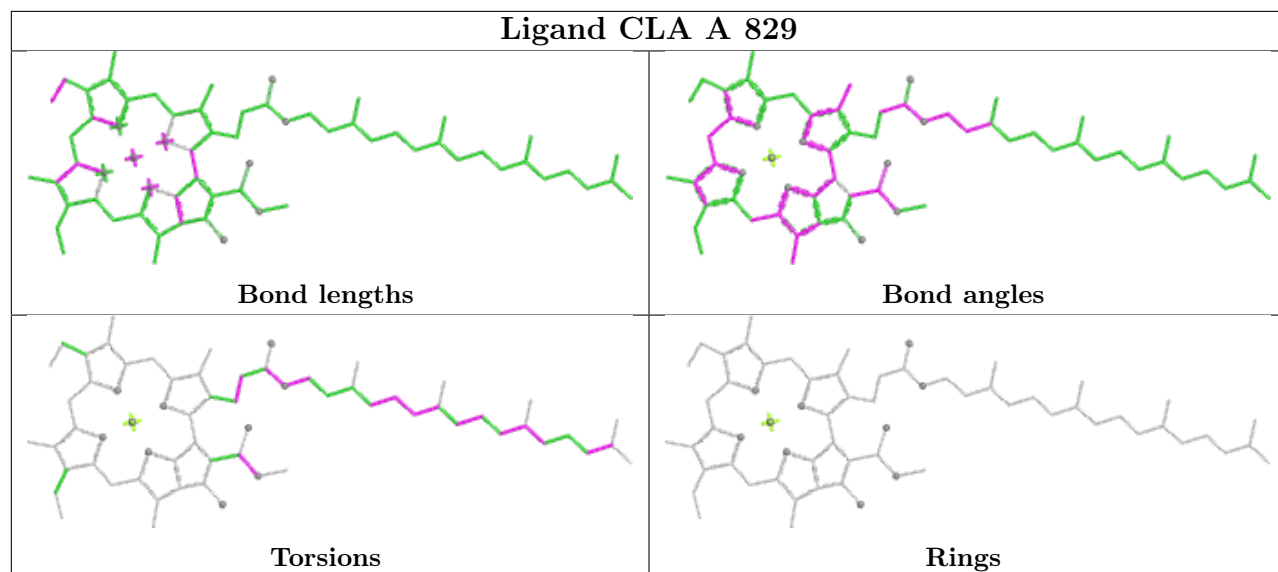
## Ligand CLA B 821



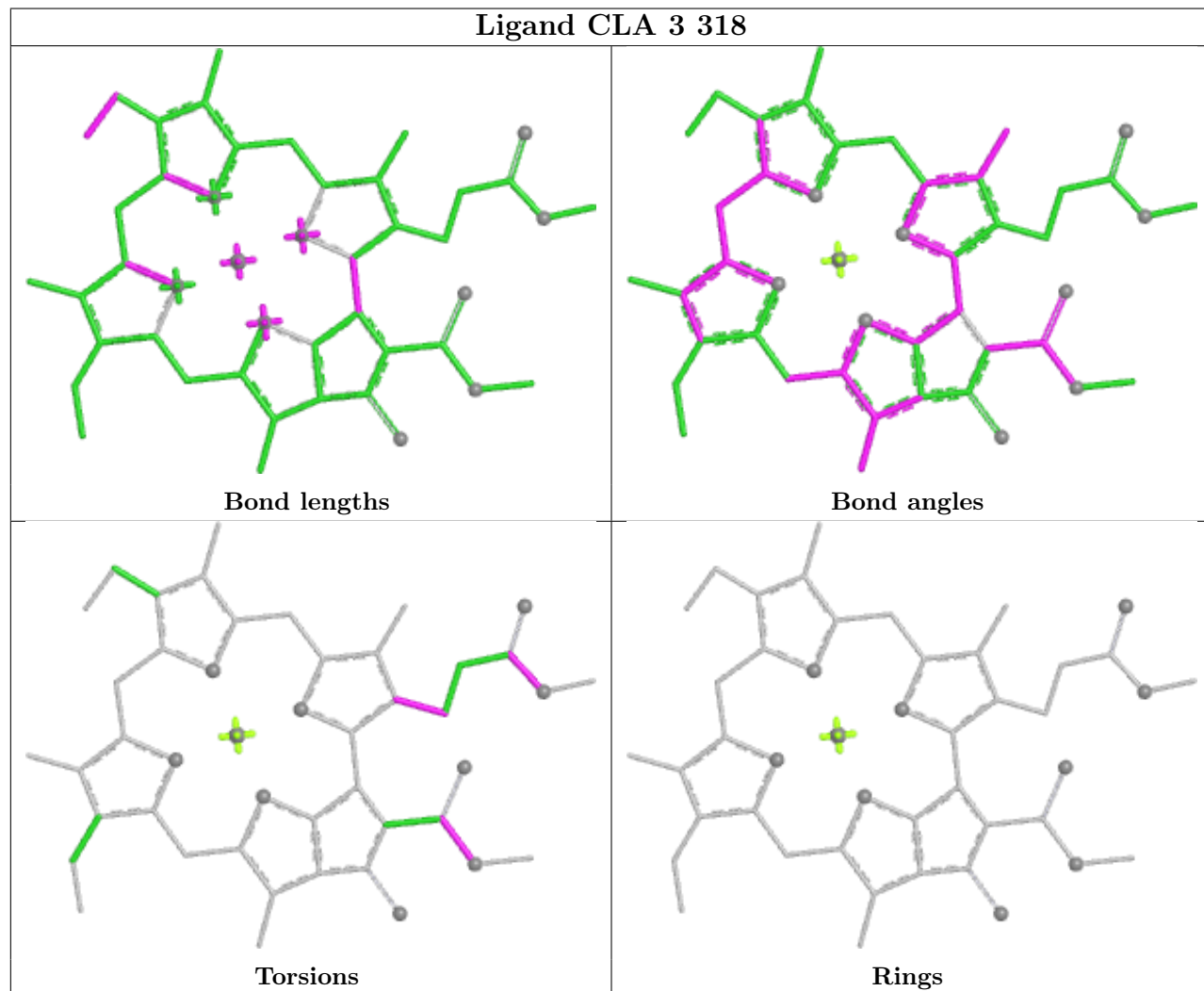
## Ligand LMT B 852



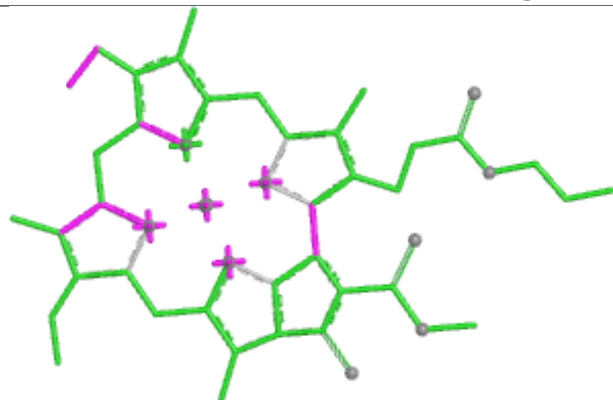
## Ligand CLA A 829



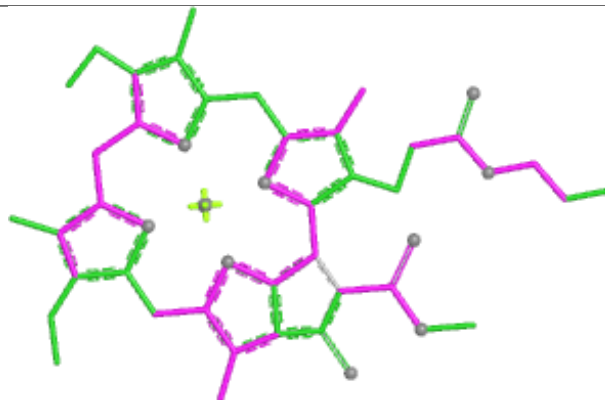
## Ligand CLA 3 318



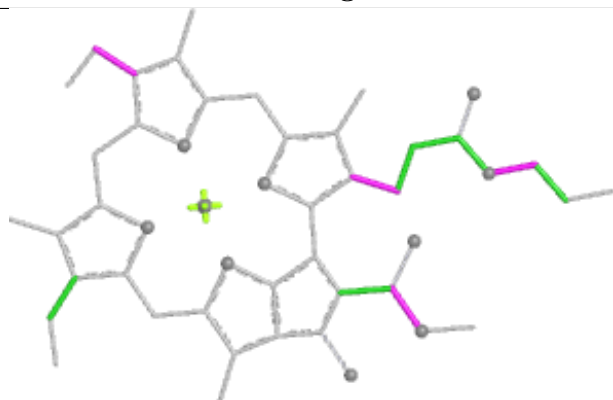
## Ligand CLA 3 314



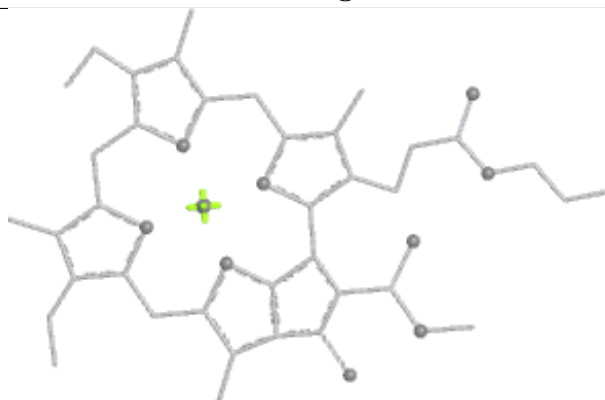
Bond lengths



Bond angles

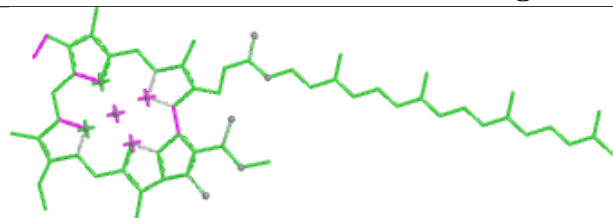


Torsions

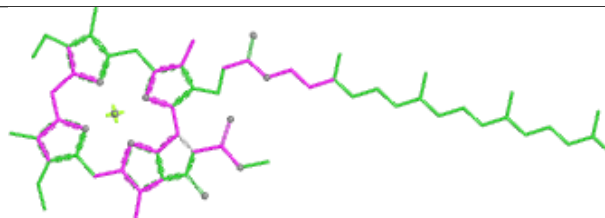


Rings

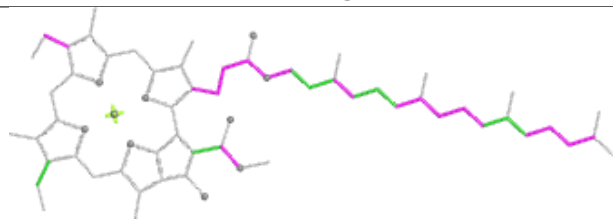
## Ligand CLA B 828



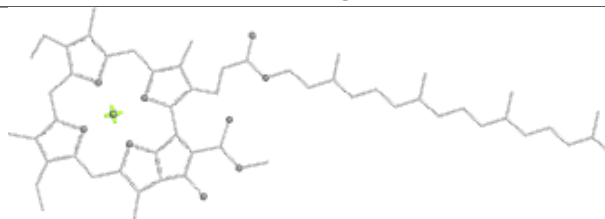
Bond lengths



Bond angles

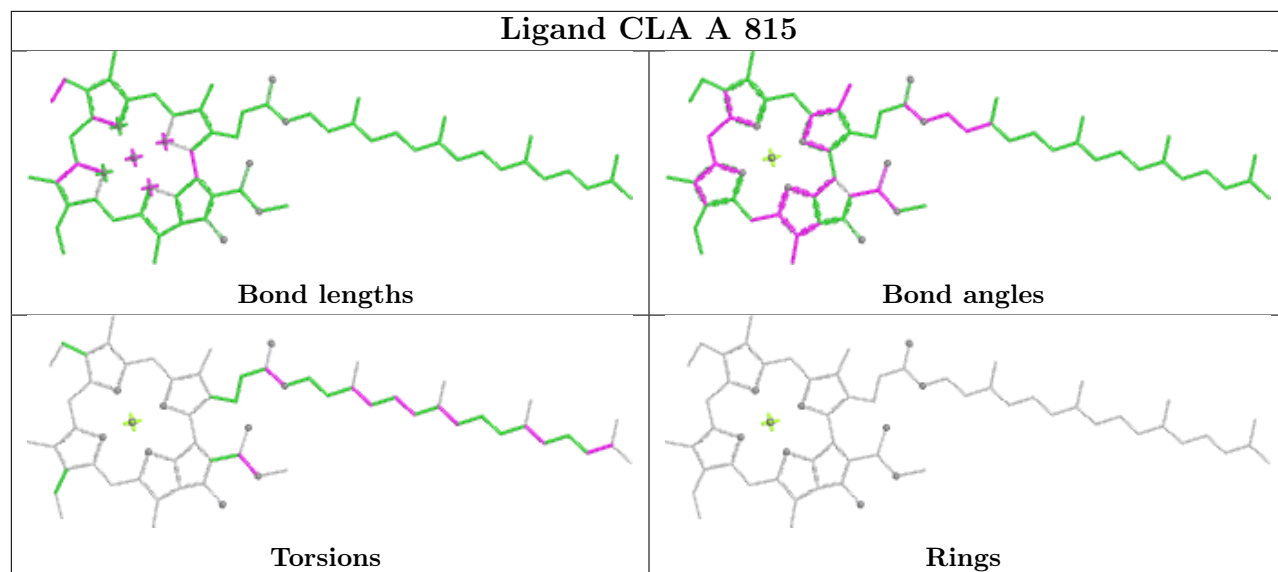


Torsions

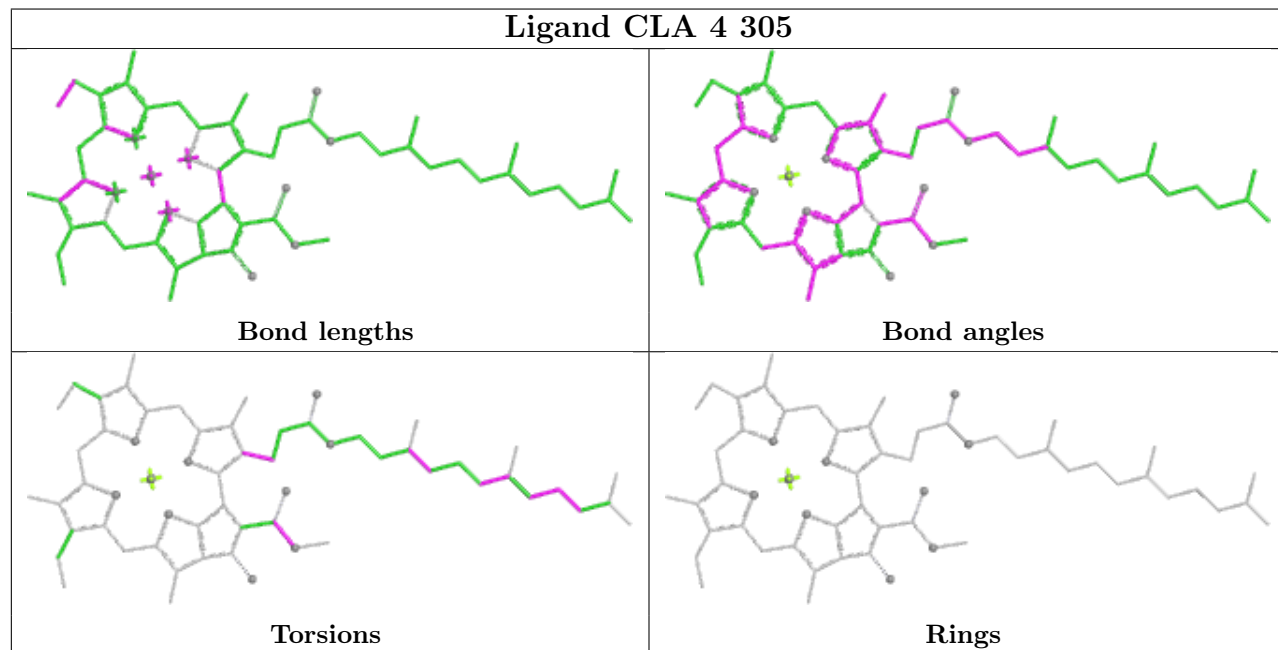


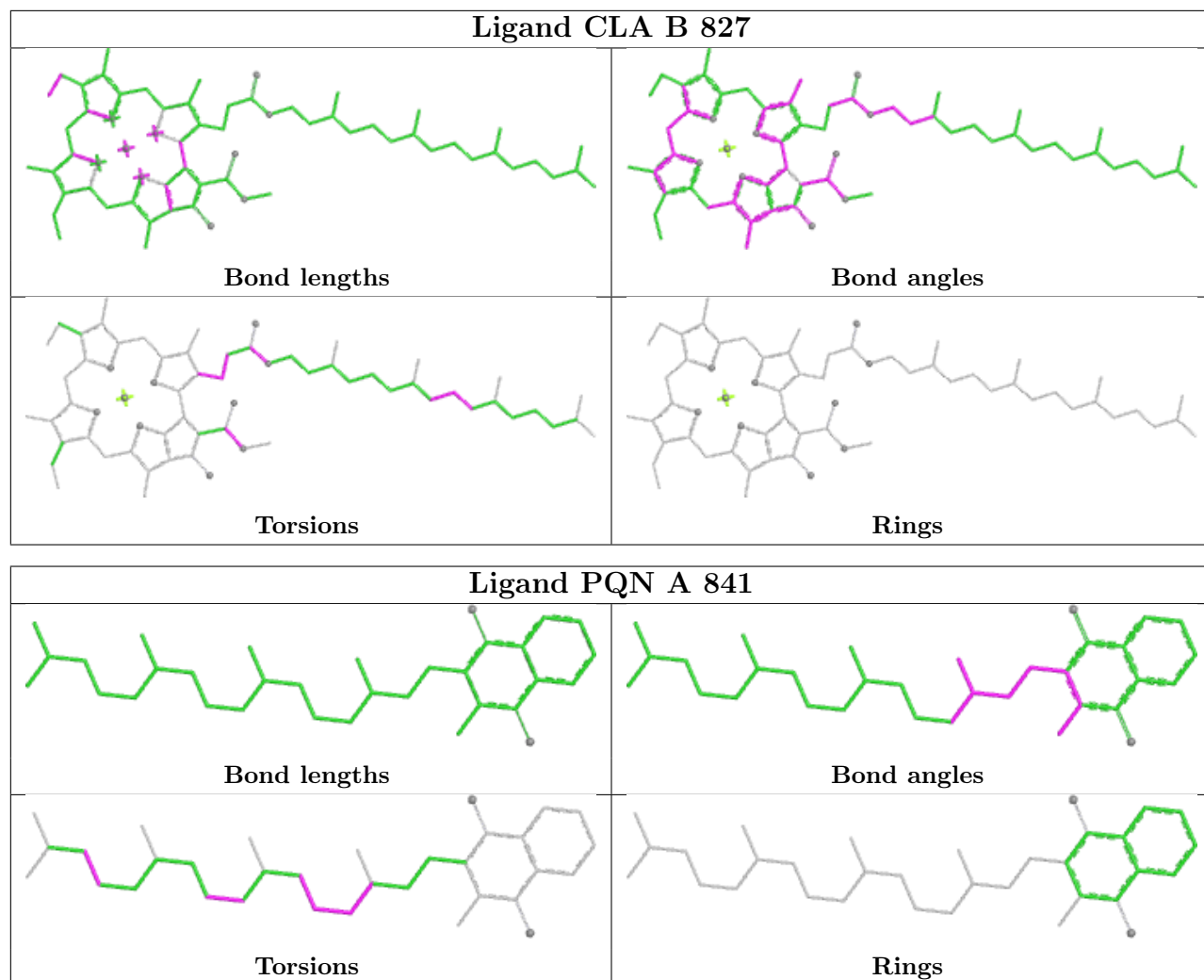
Rings

## Ligand CLA A 815



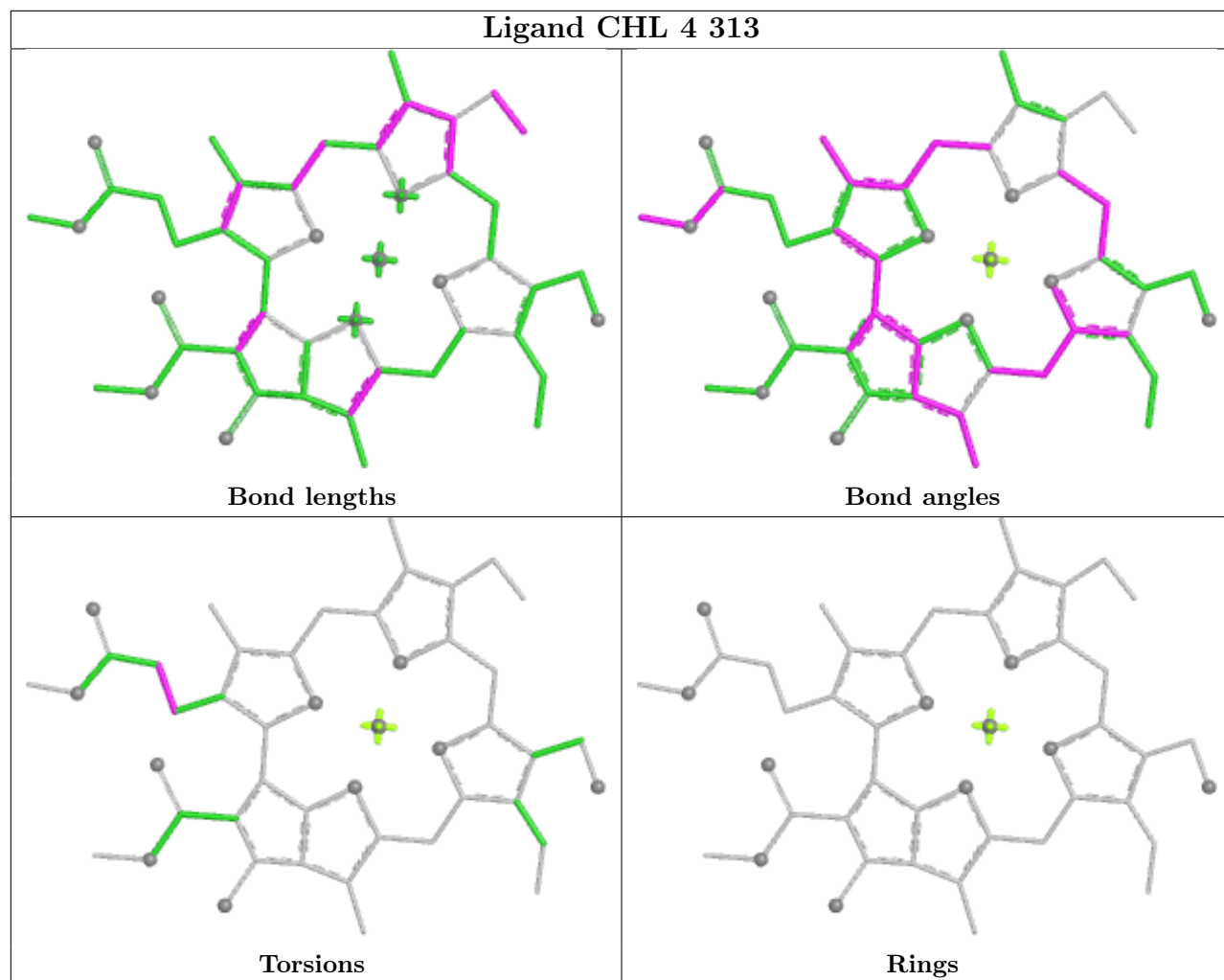
## Ligand CLA 4 305



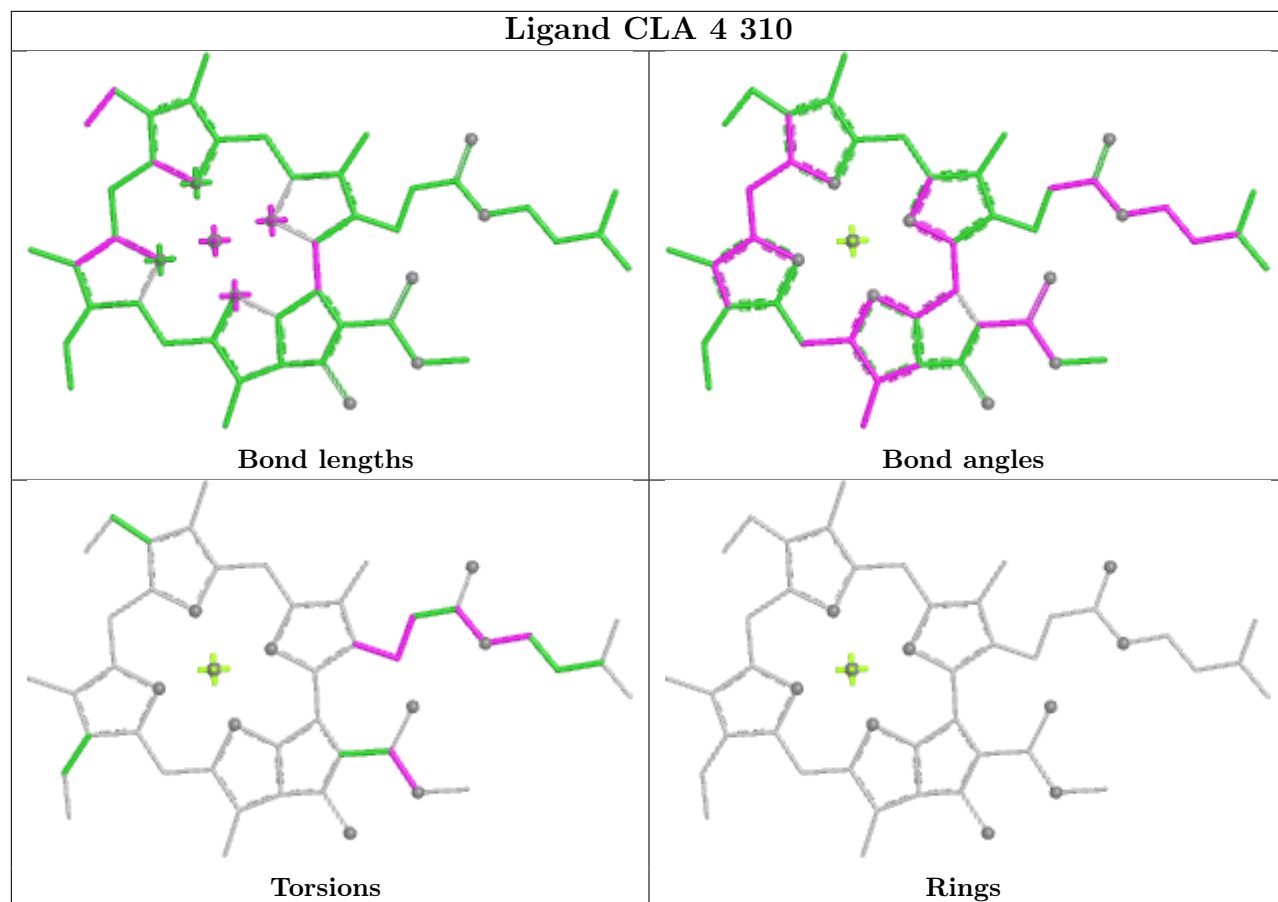




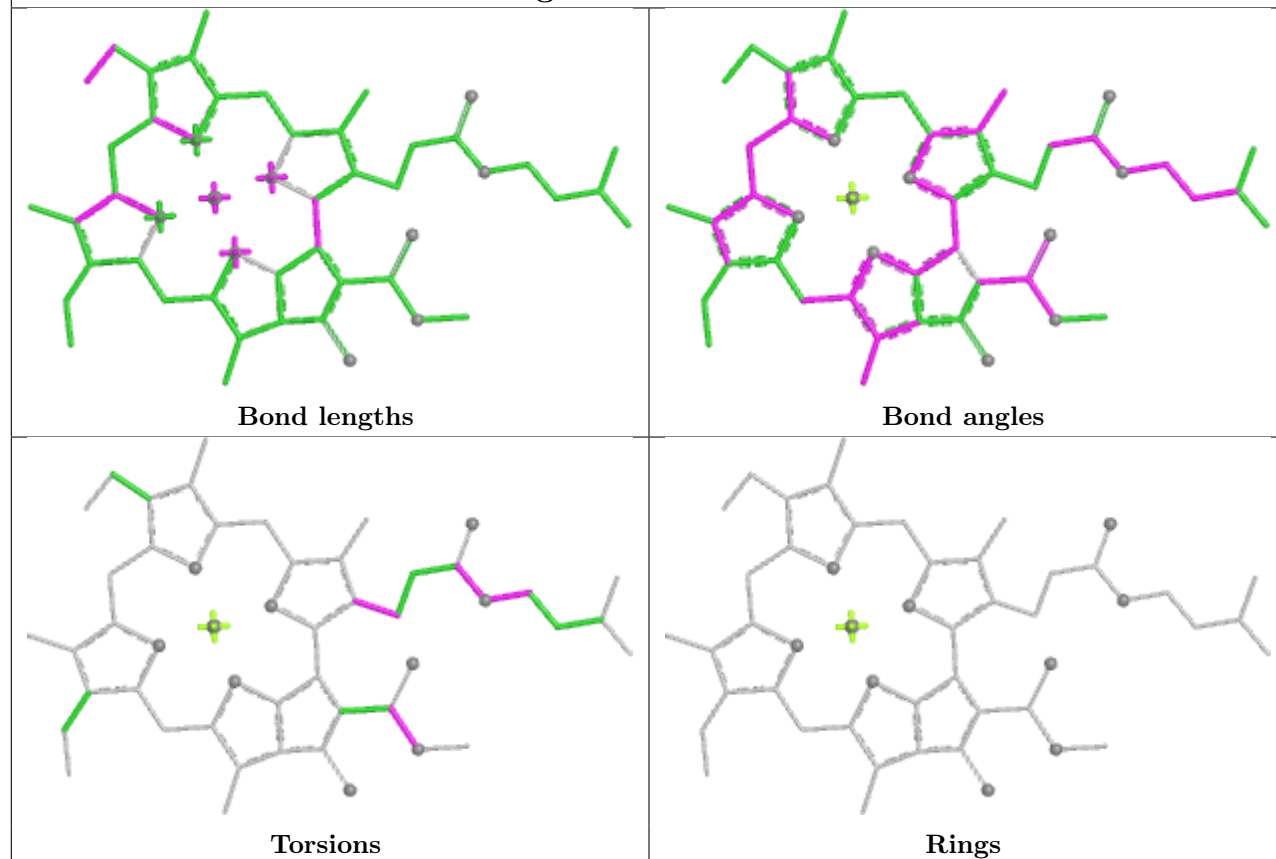
## Ligand CHL 4 313



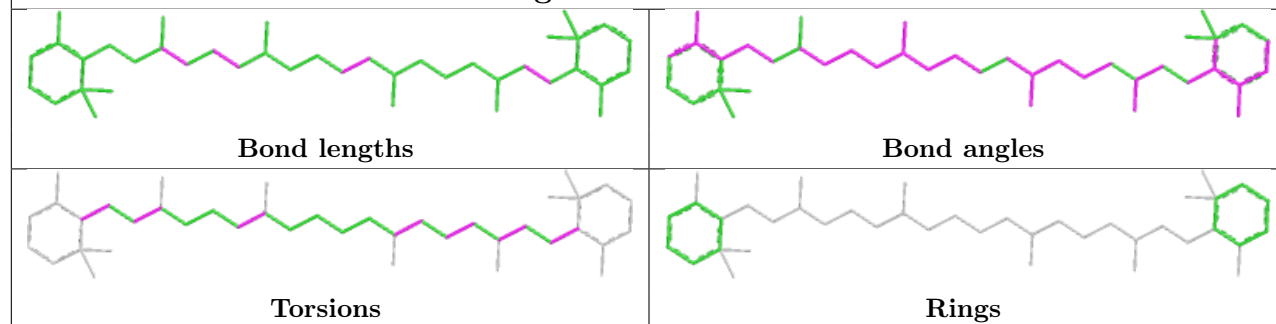
## Ligand CLA 4 310

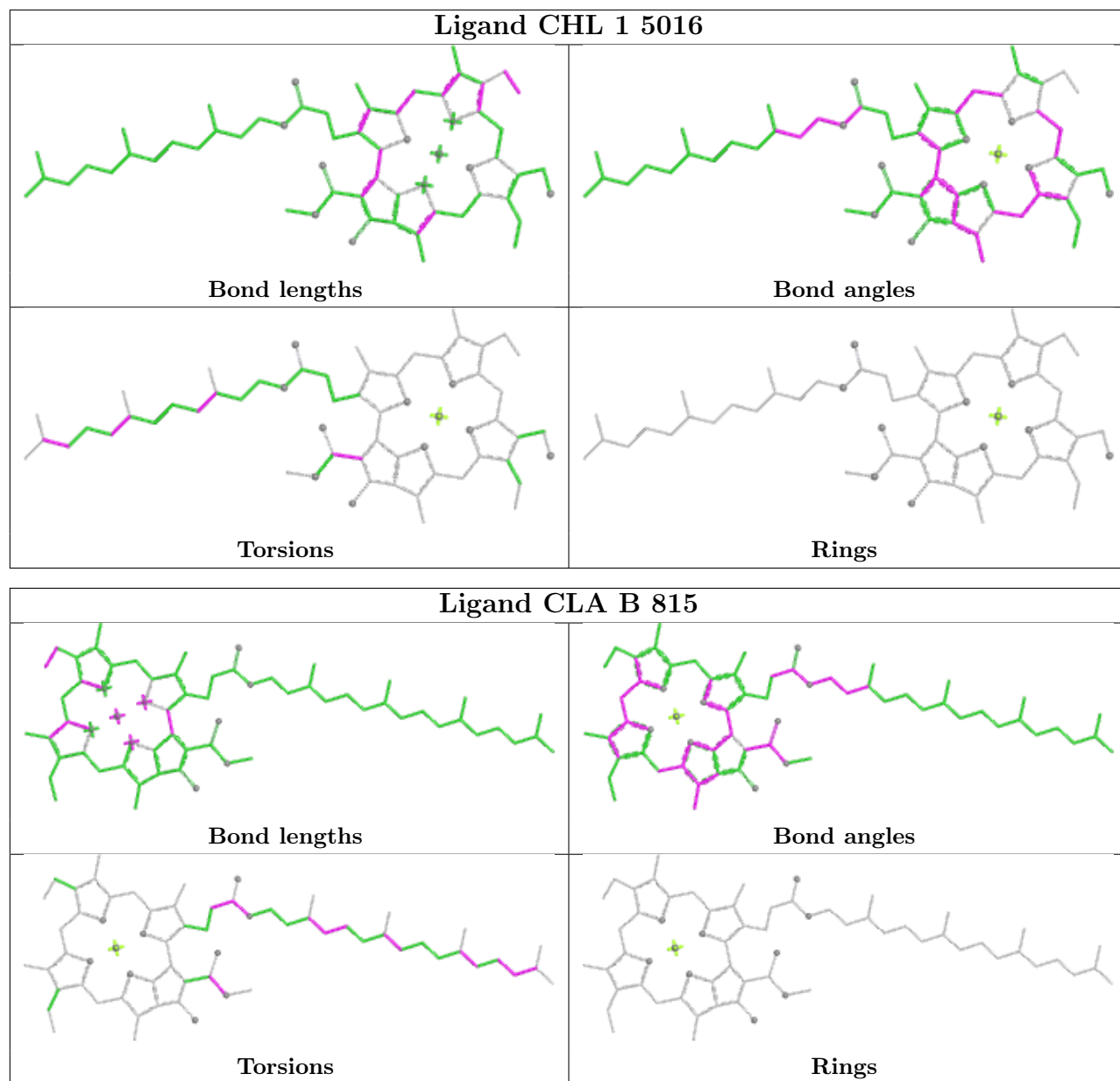


## Ligand CLA 3 317

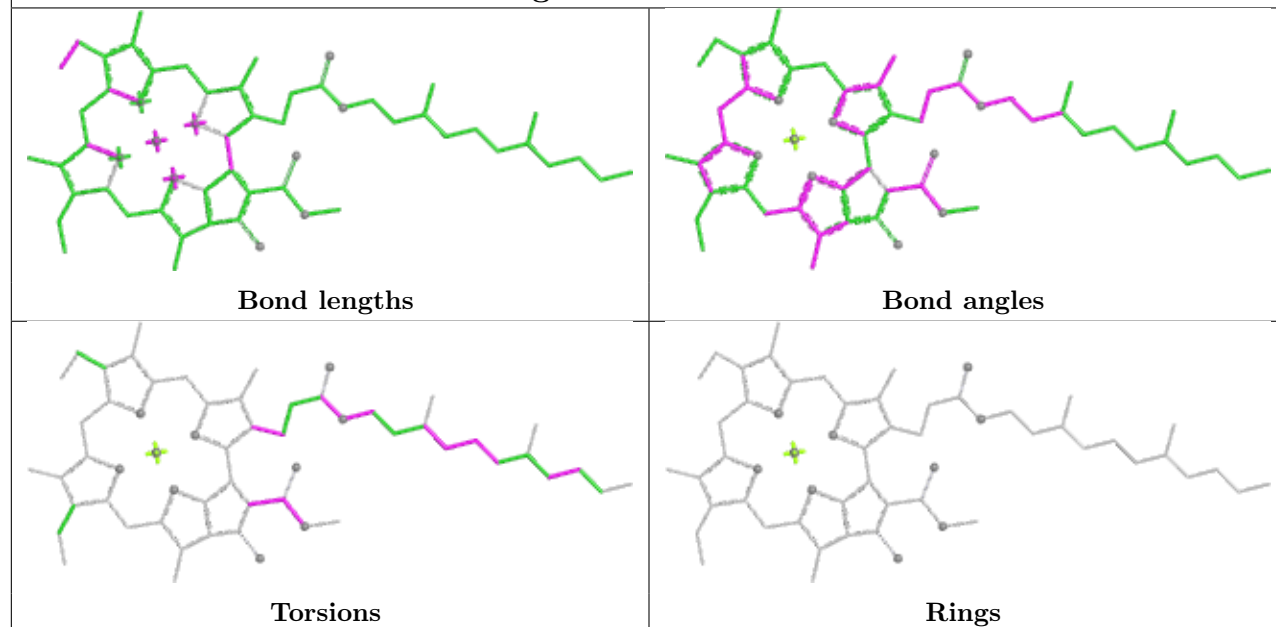


## Ligand BCR 4 301

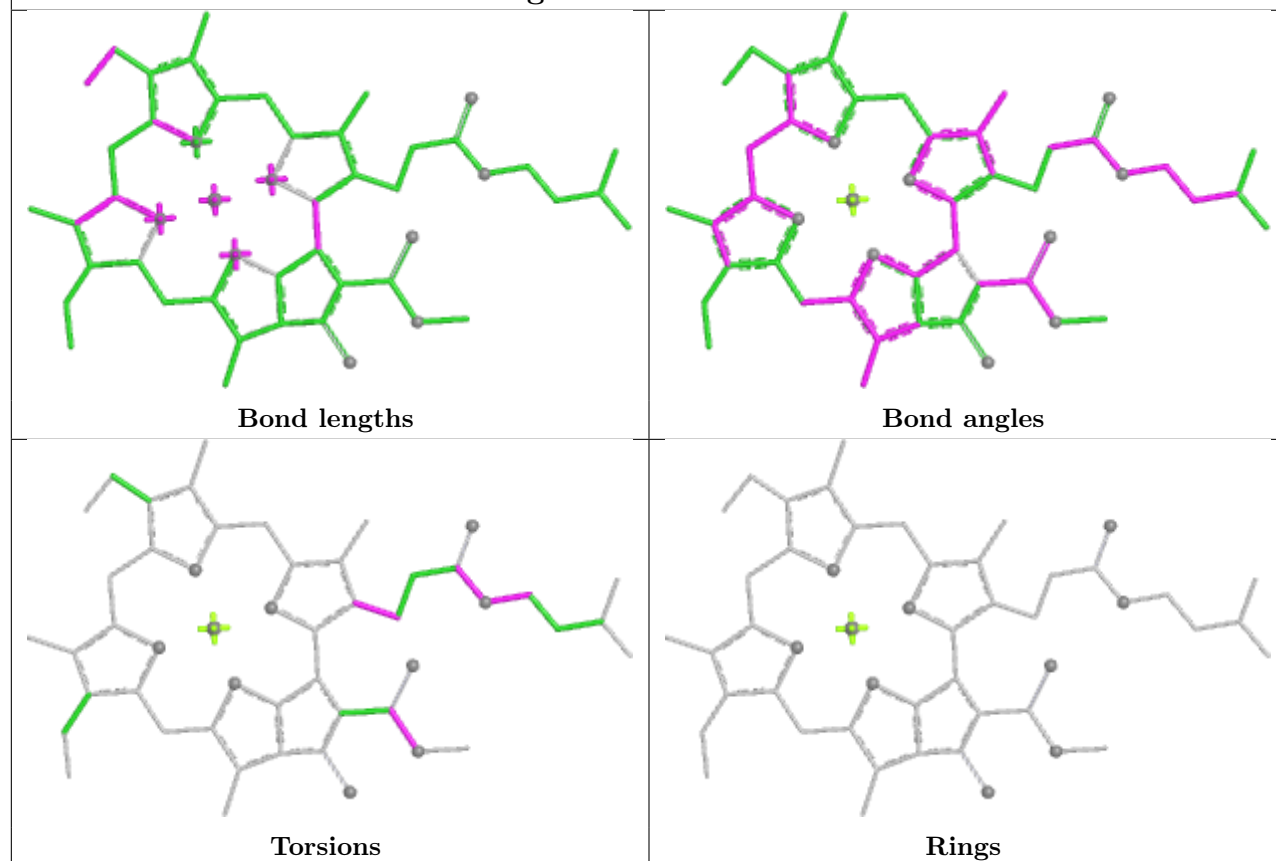


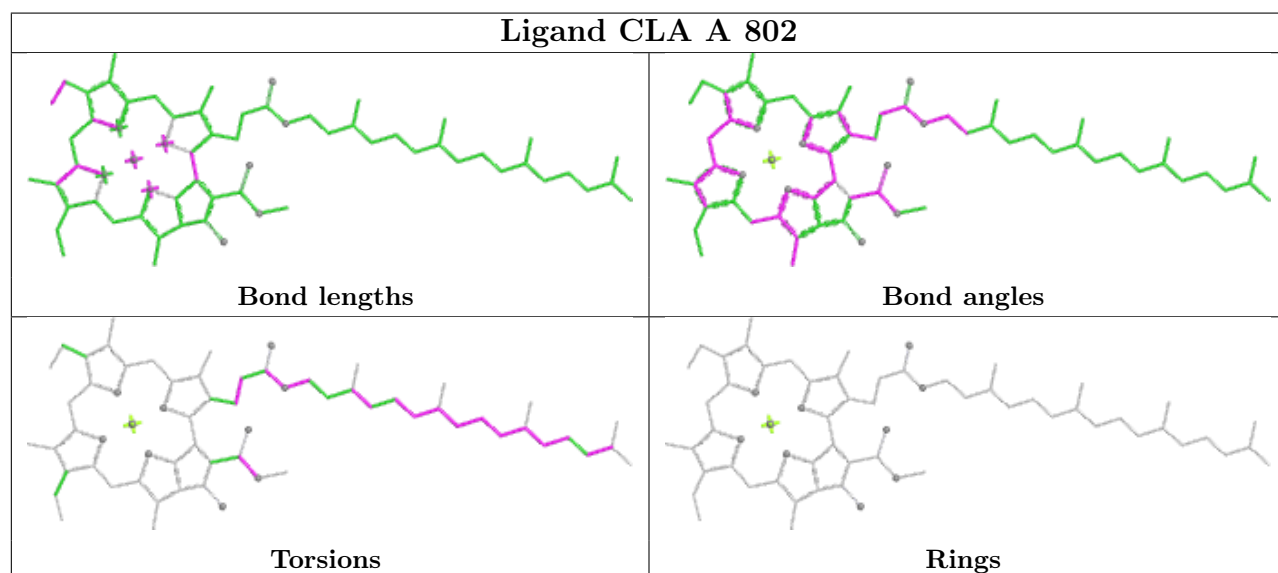
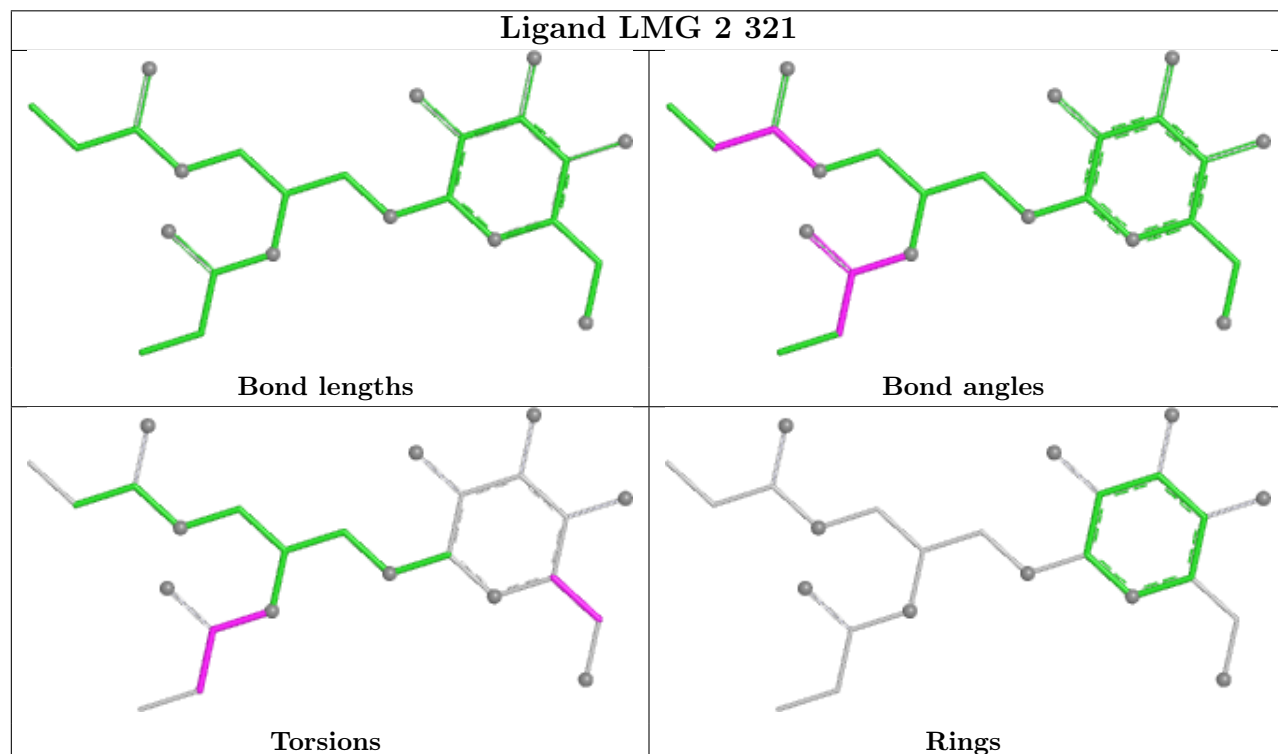
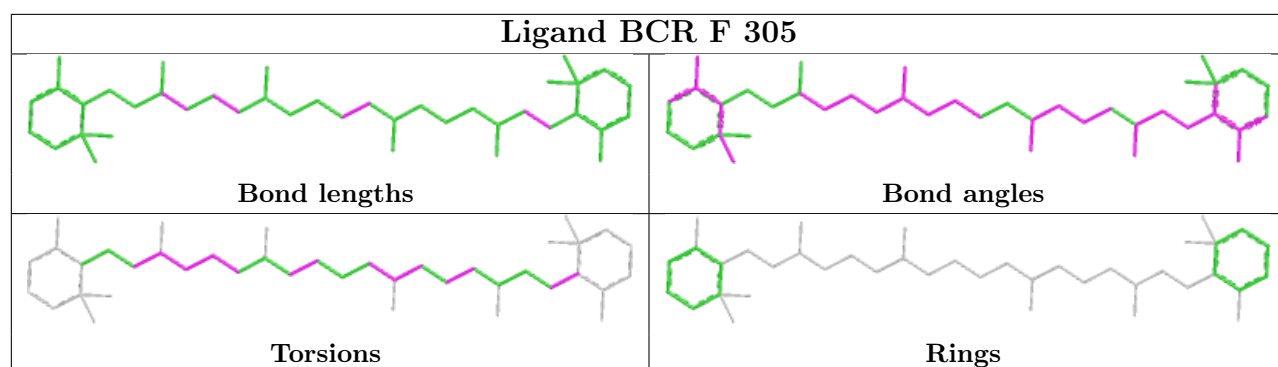


## Ligand CLA B 833

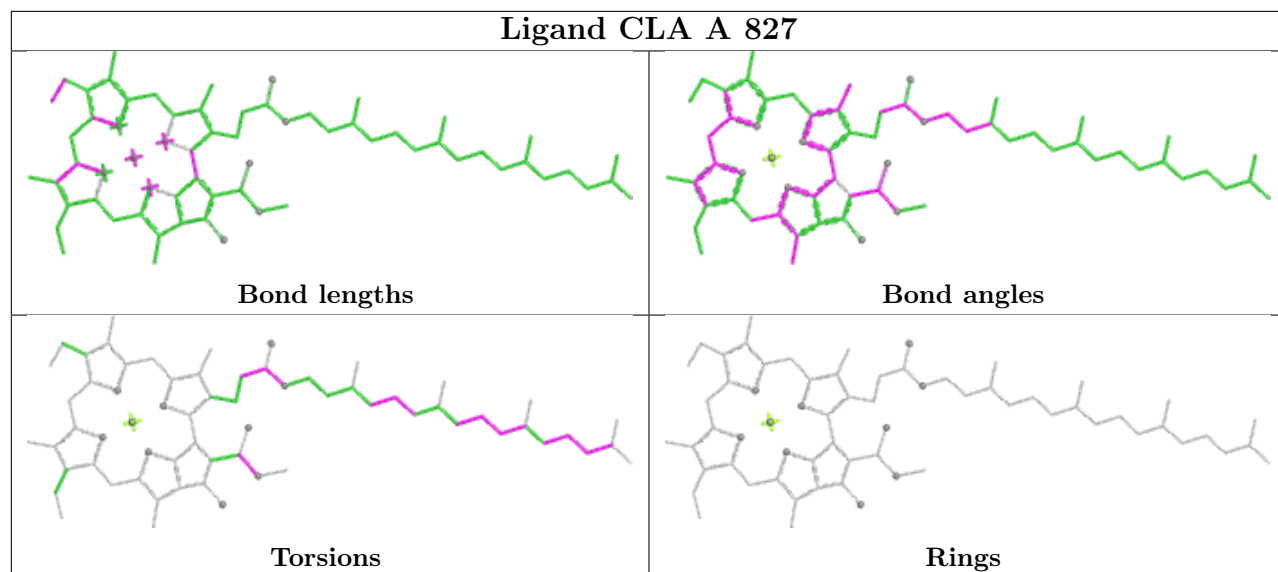


## Ligand CLA J 1103

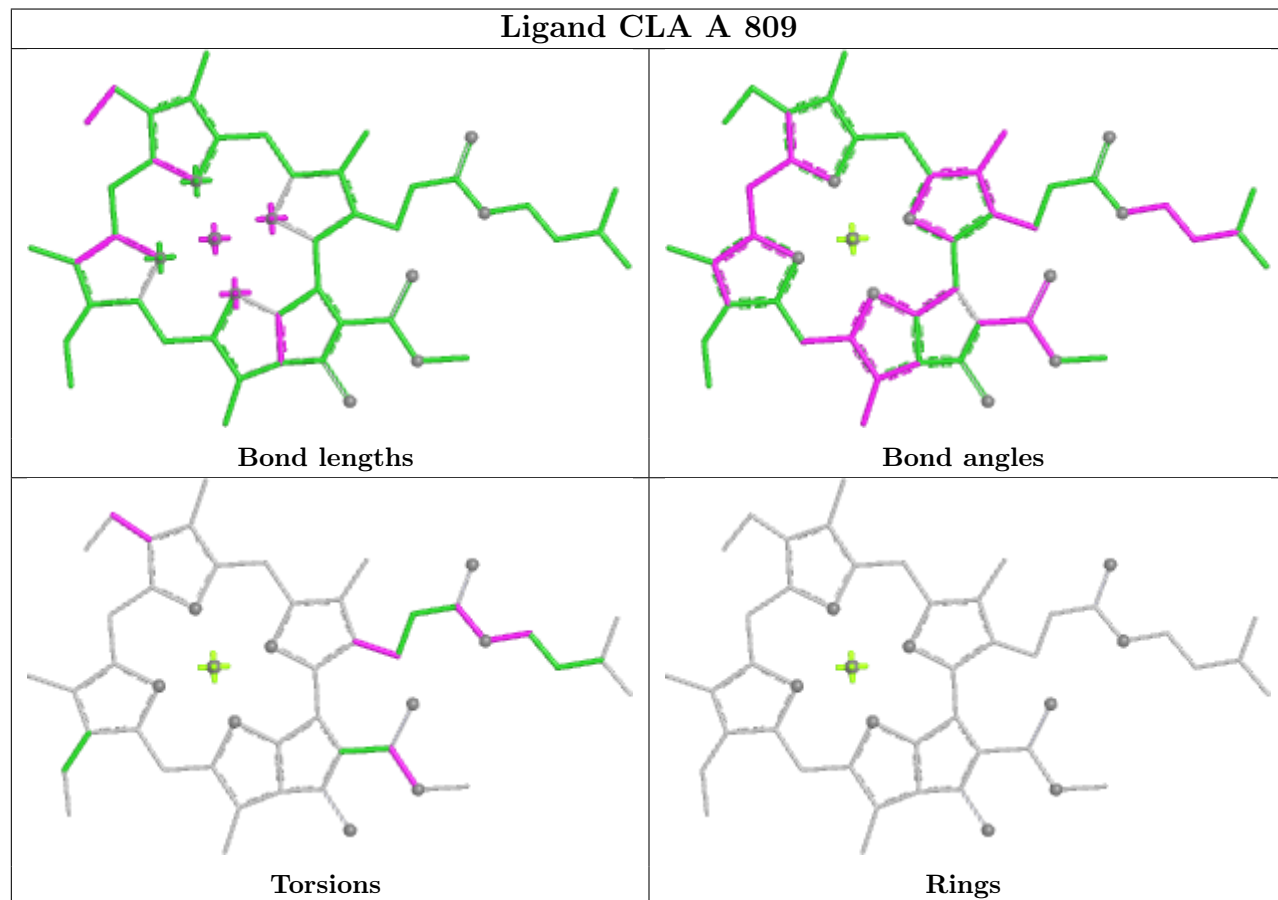


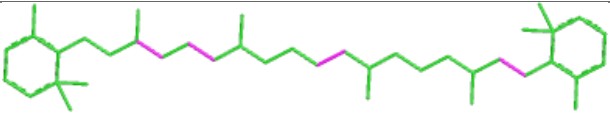
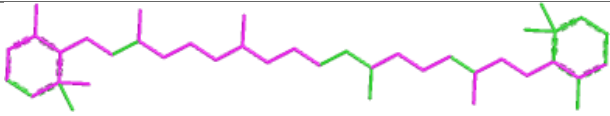
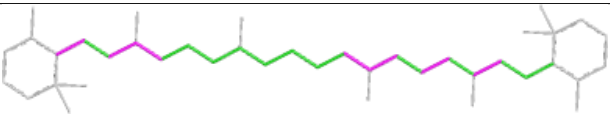
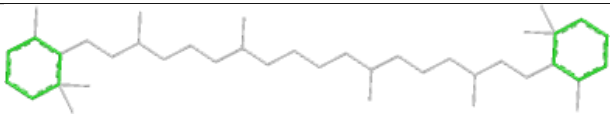

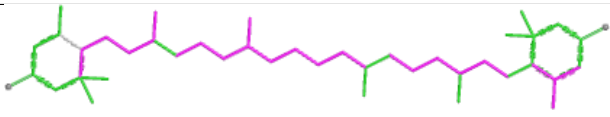
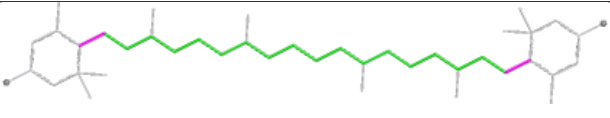
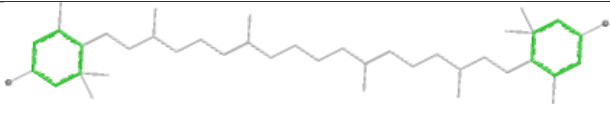
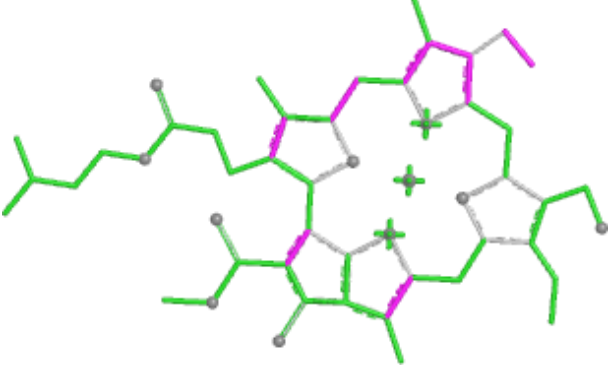
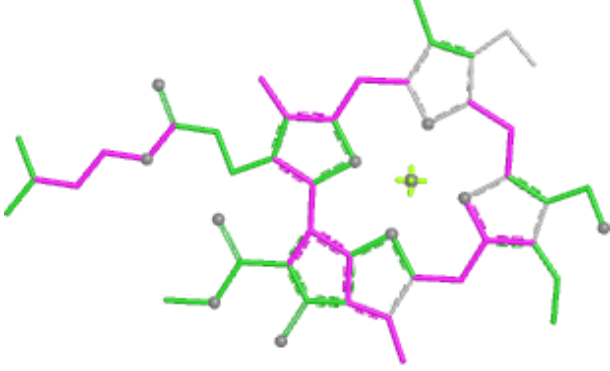
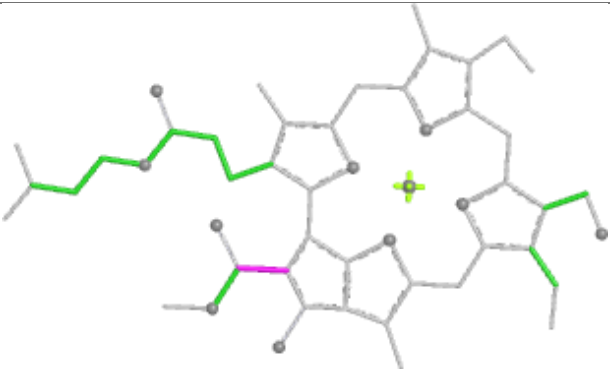
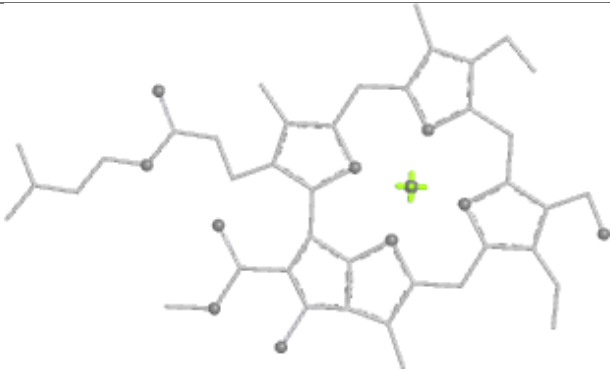


## Ligand CLA A 827



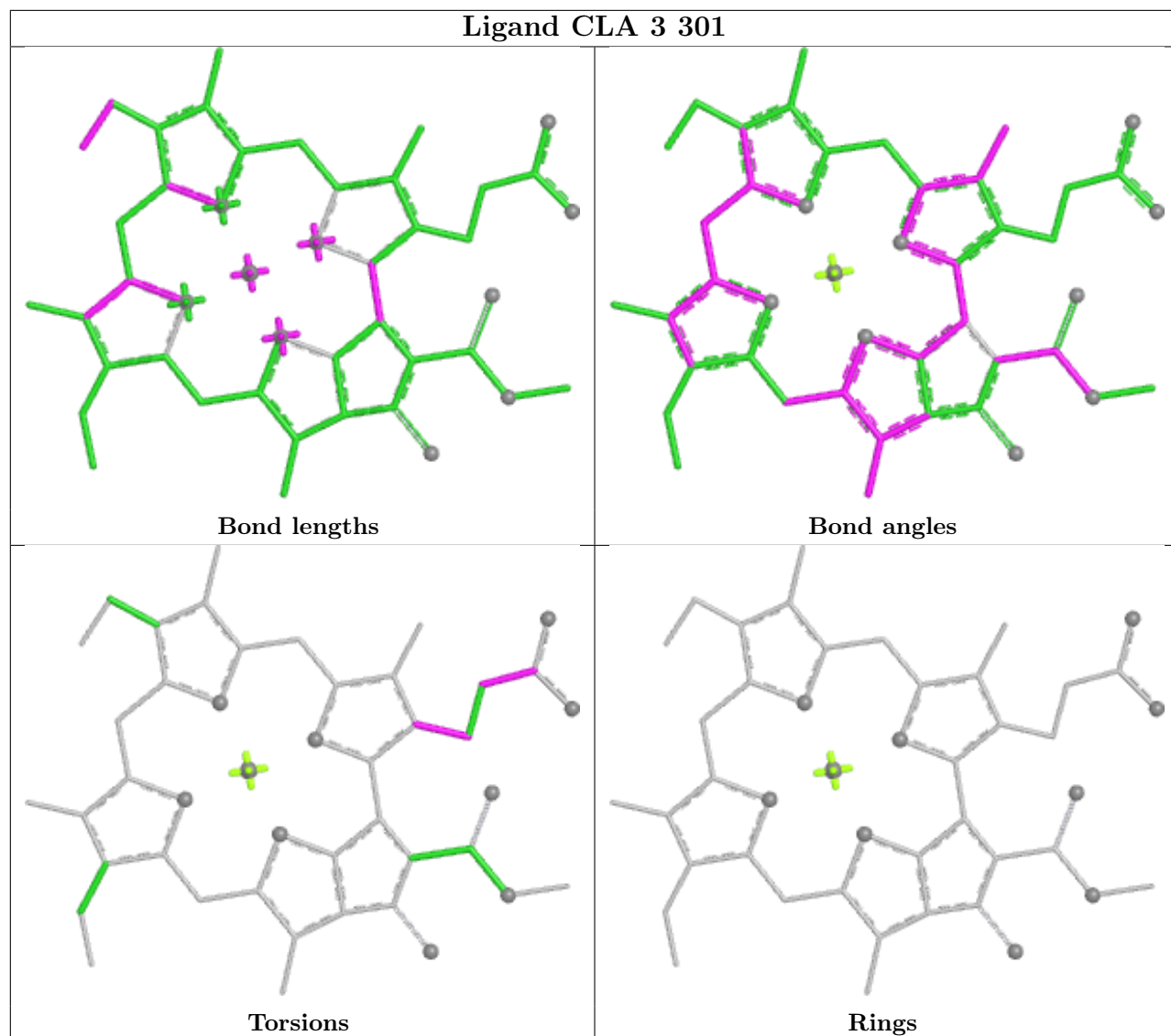
## Ligand CLA A 809



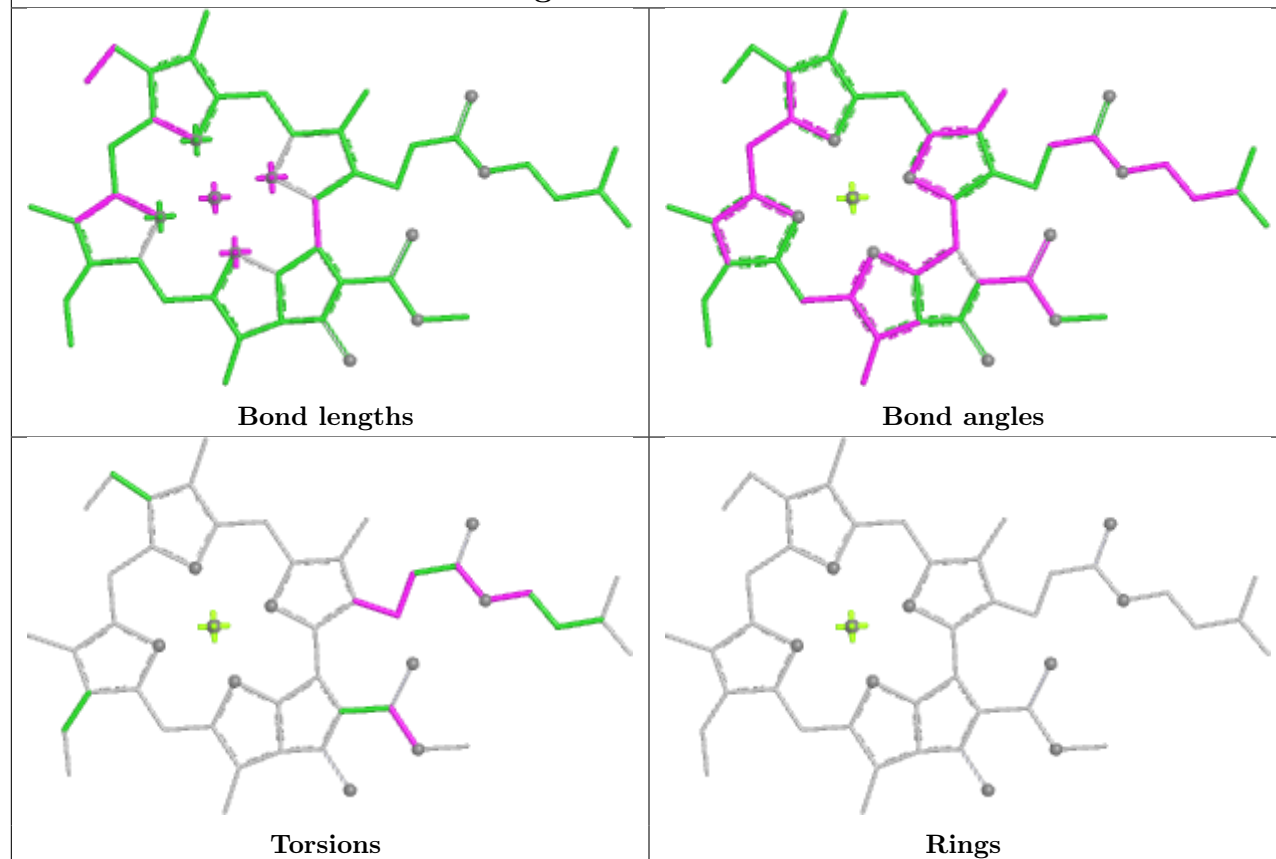
Ligand BCR A 847	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LUT 2 303	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CHL 4 314	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



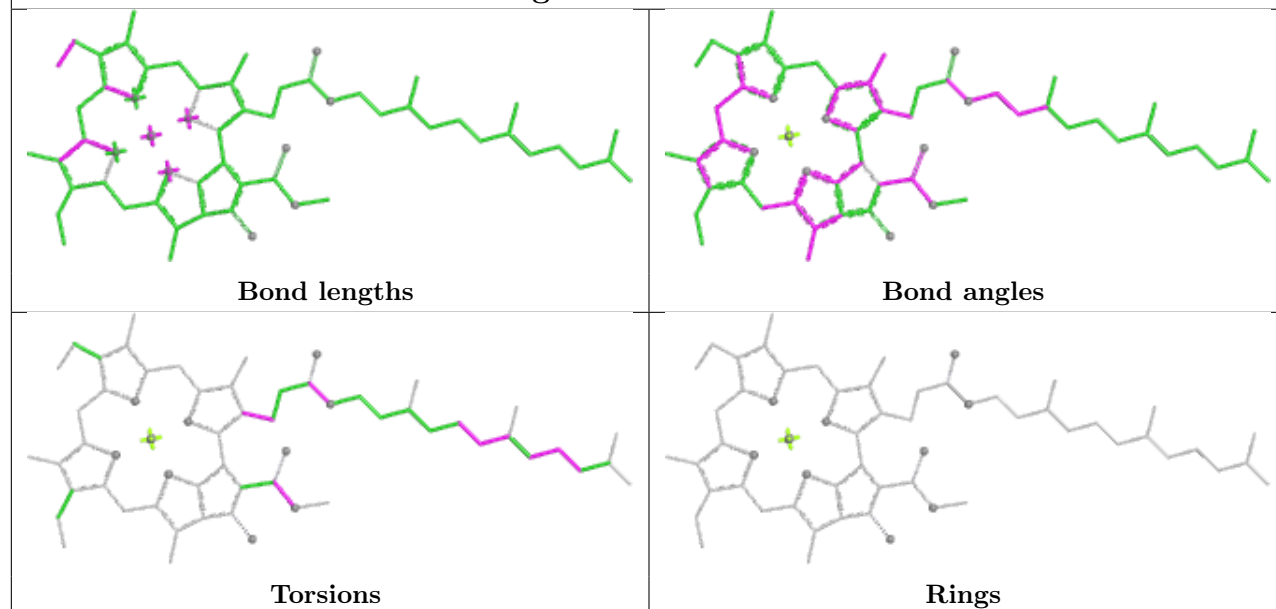
## Ligand CLA 3 301



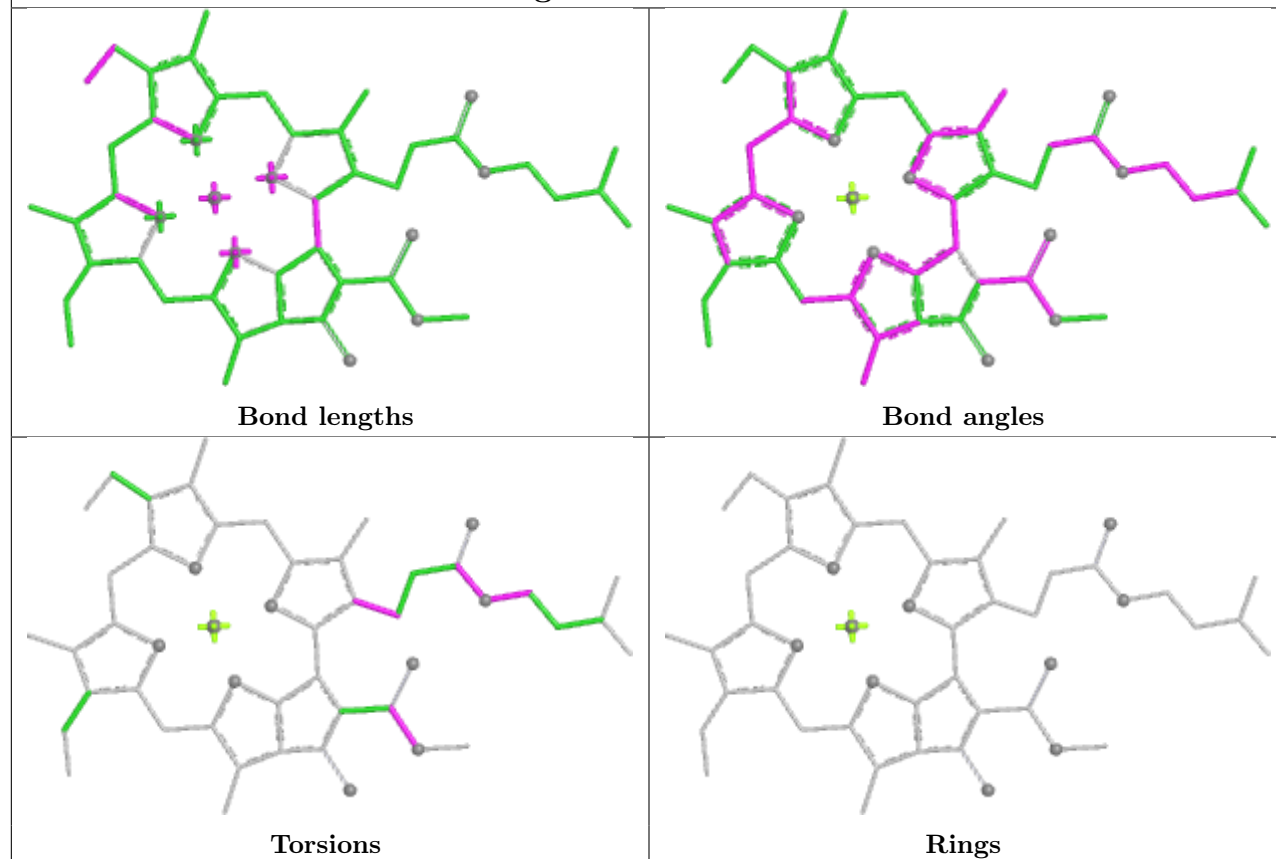
## Ligand CLA L 306



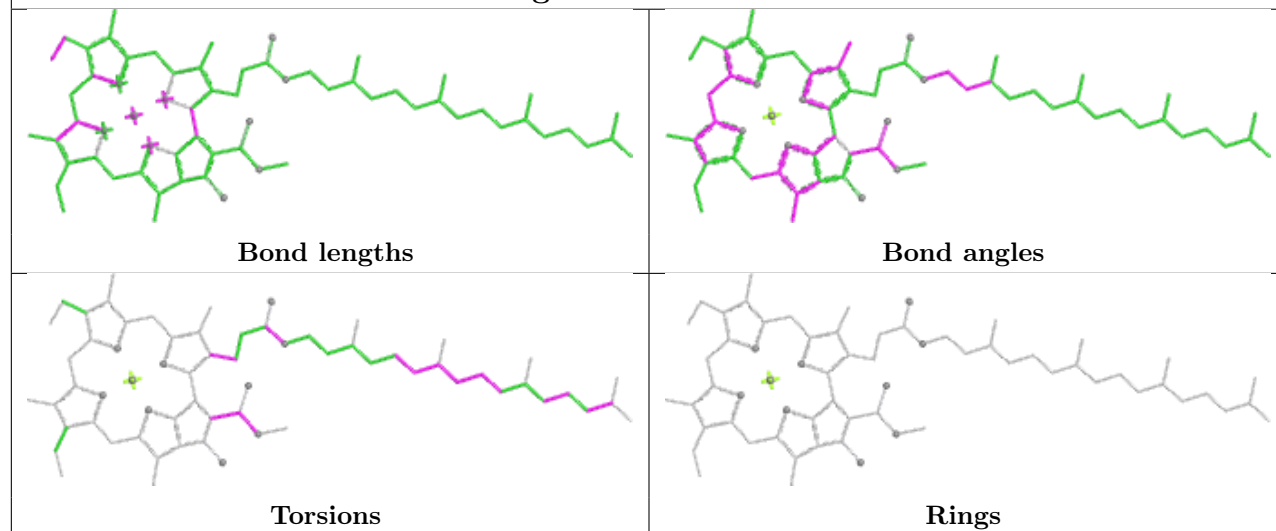
## Ligand CLA B 812



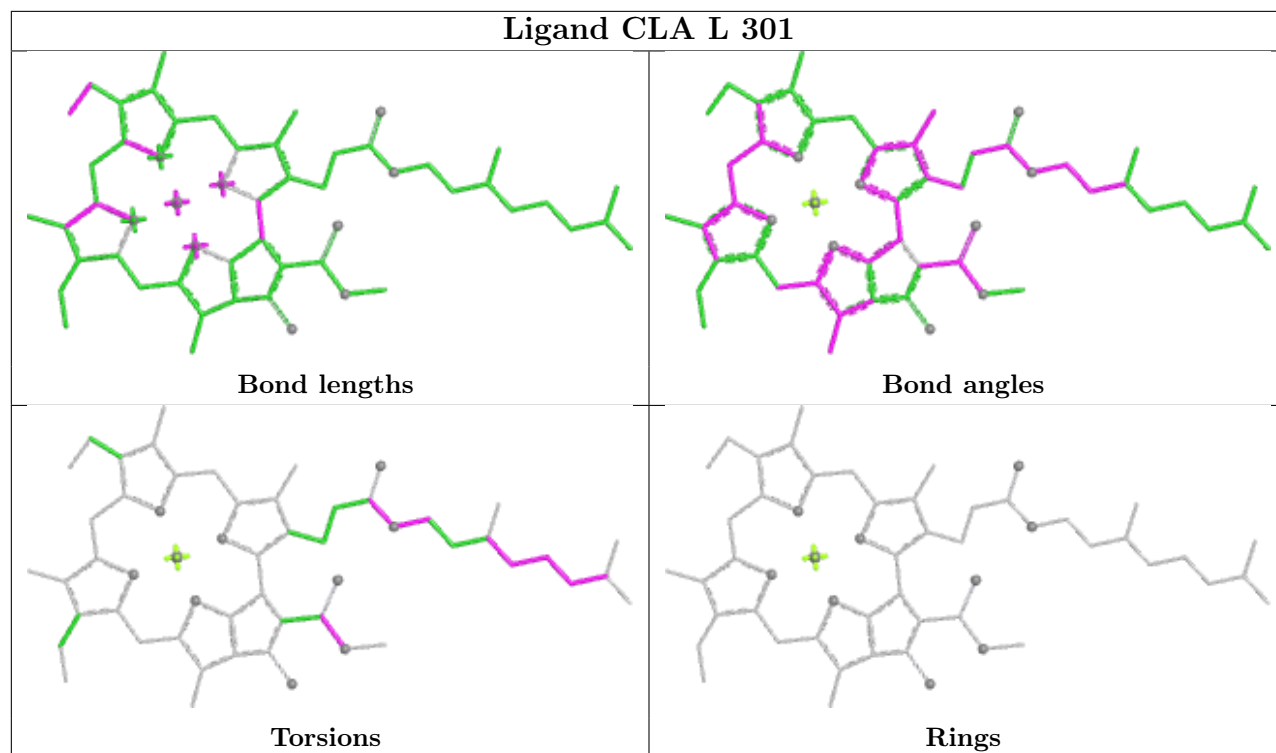
## Ligand CLA L 304



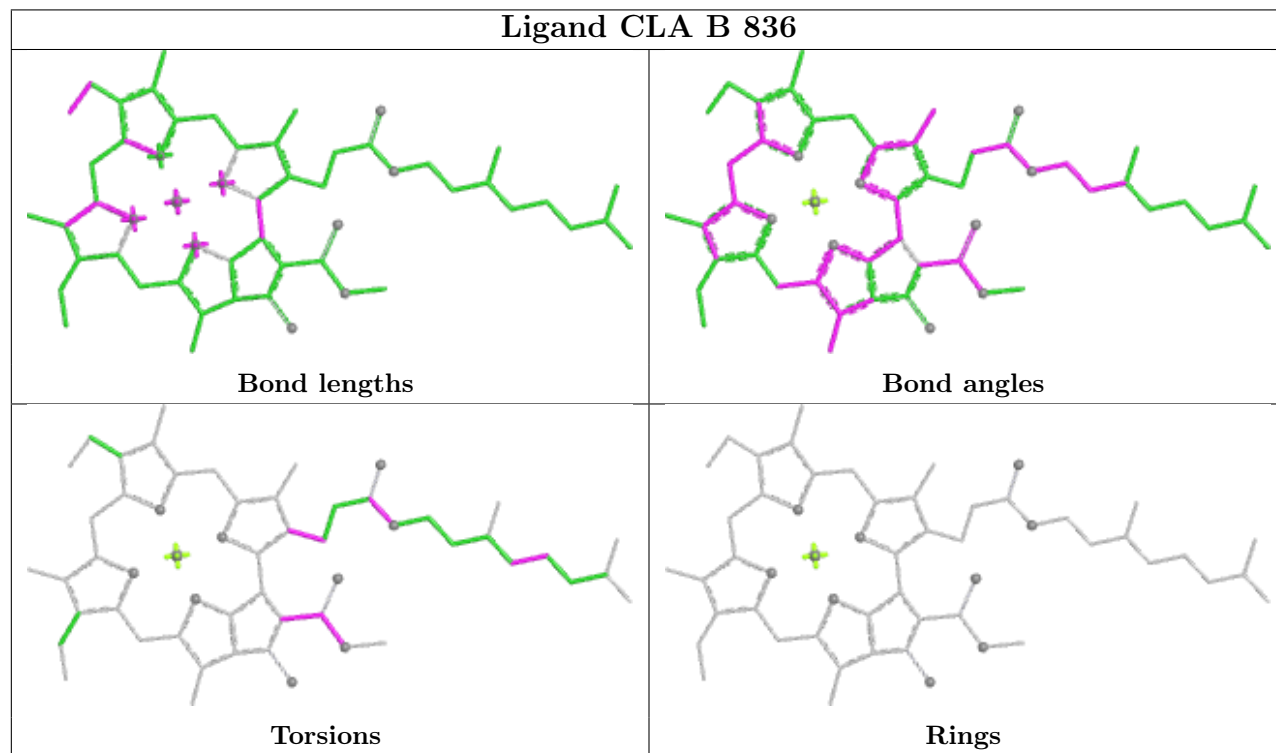
## Ligand CLA B 826

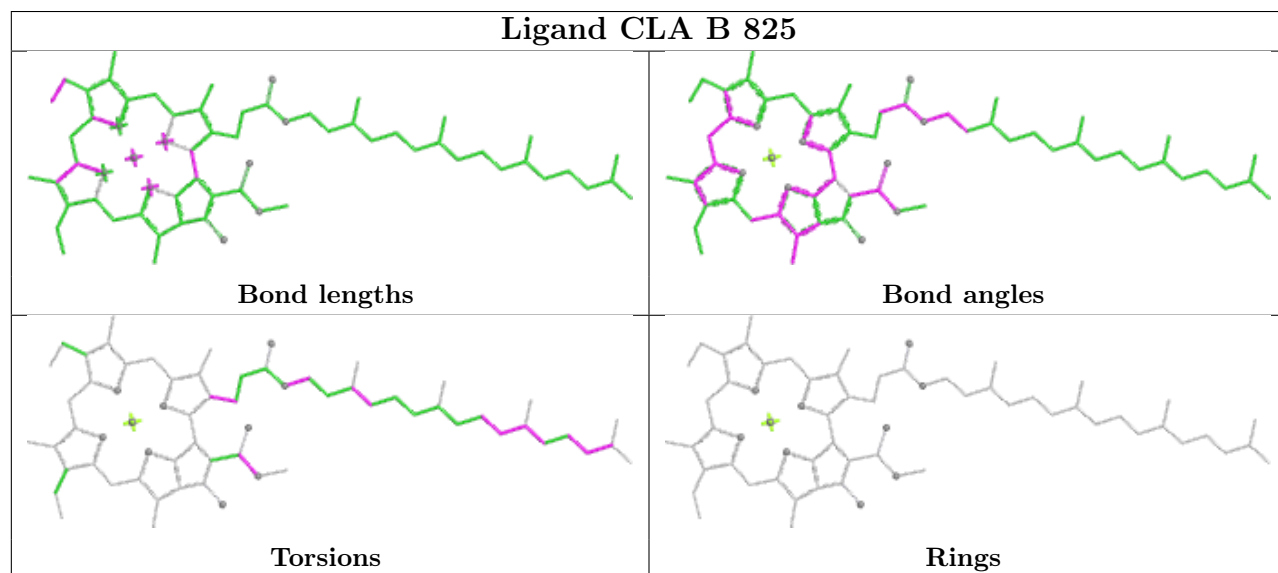
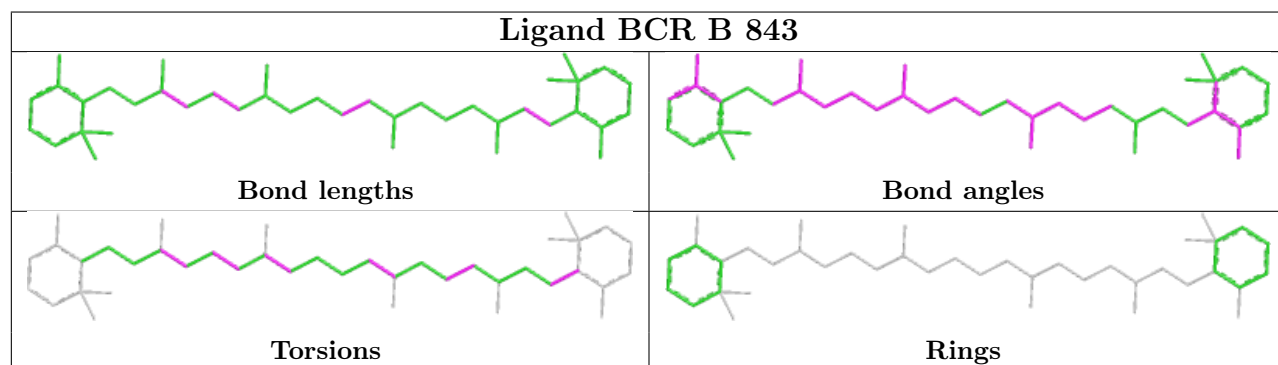
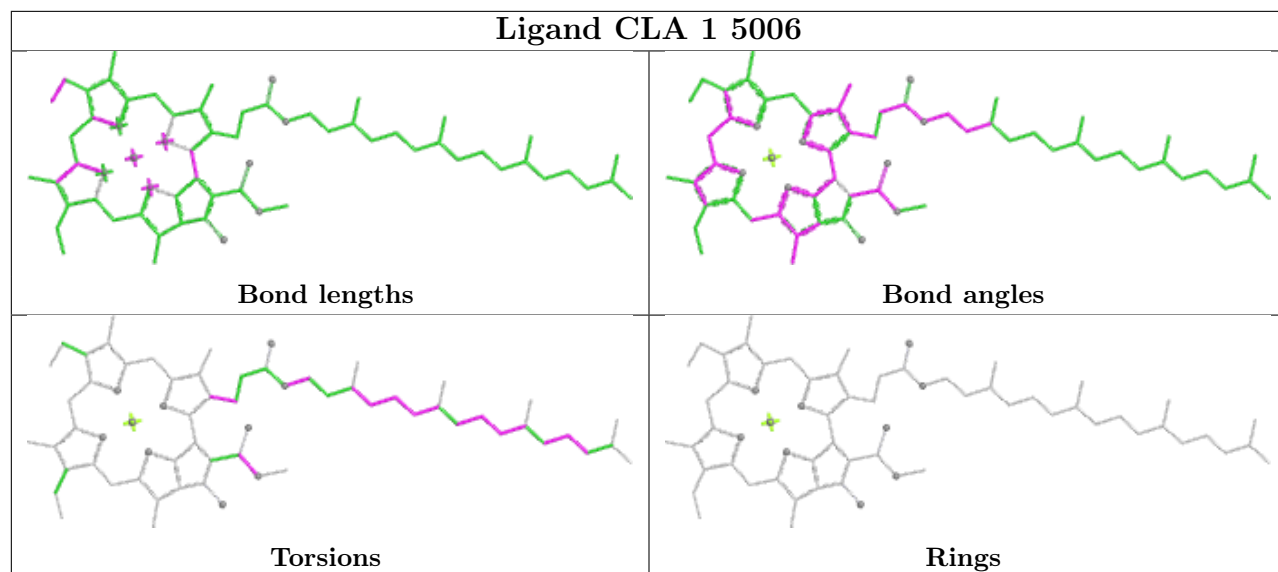


## Ligand CLA L 301

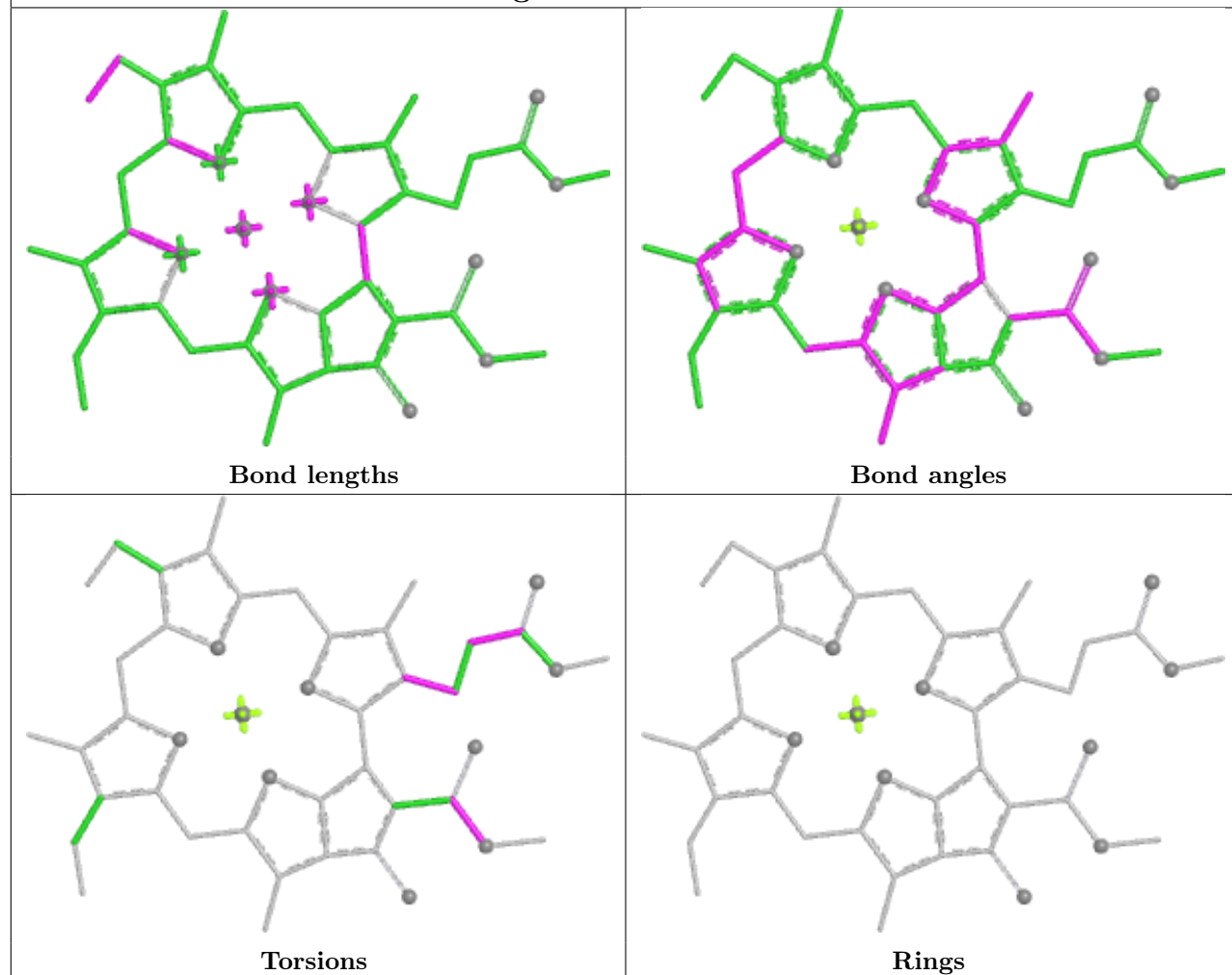


## Ligand CLA B 836

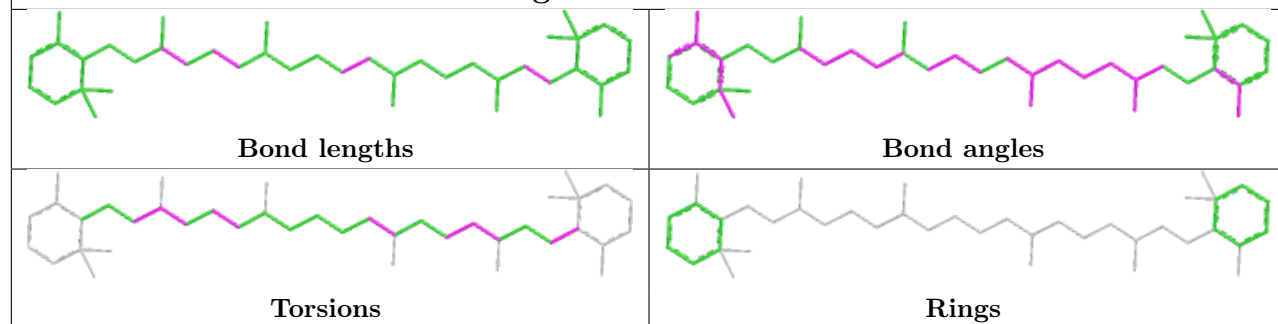


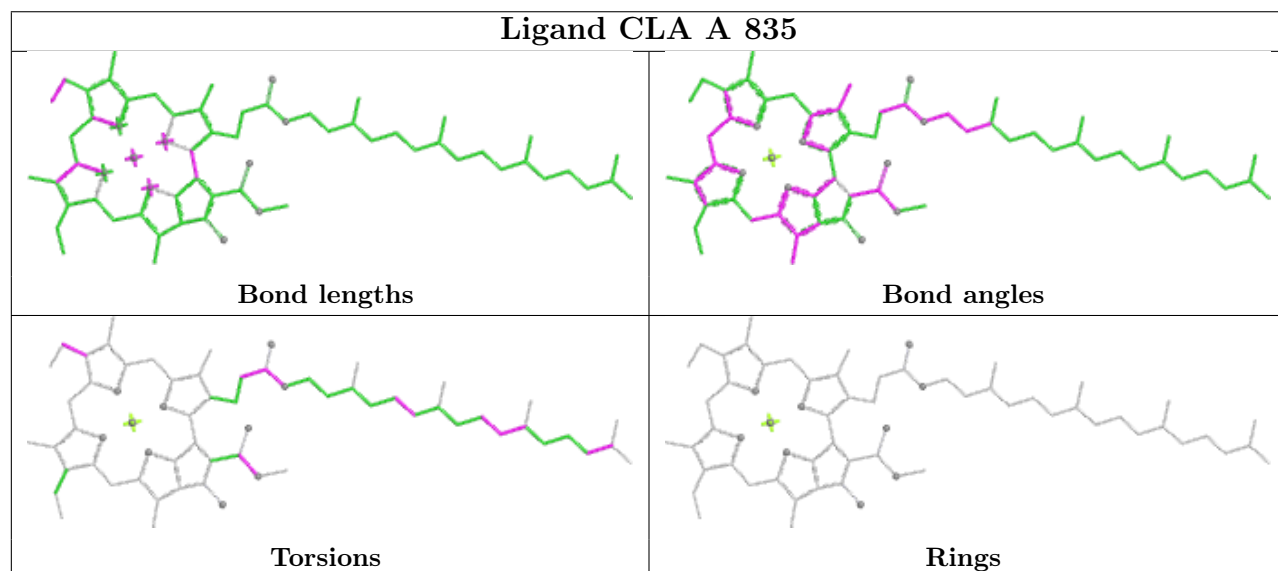
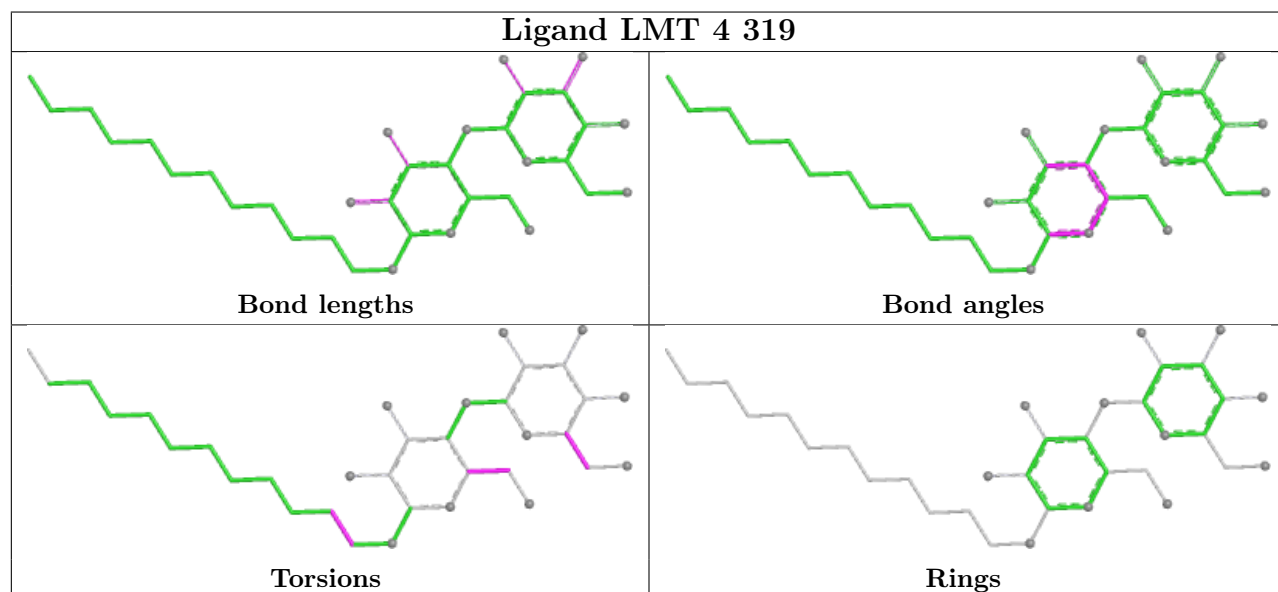
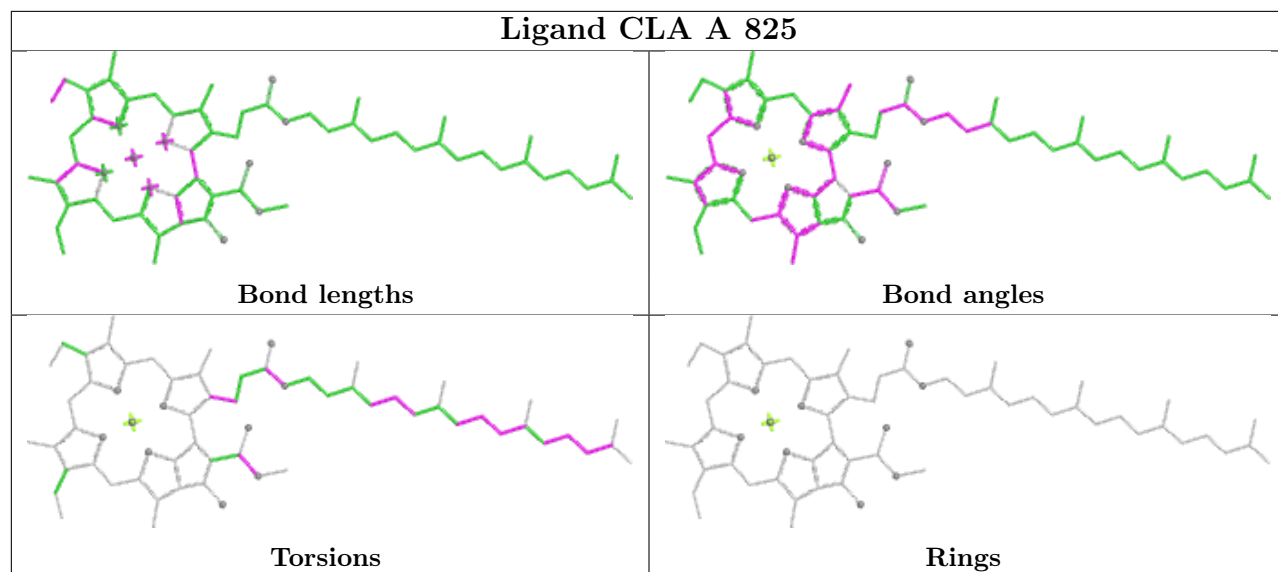


## Ligand CLA B 813

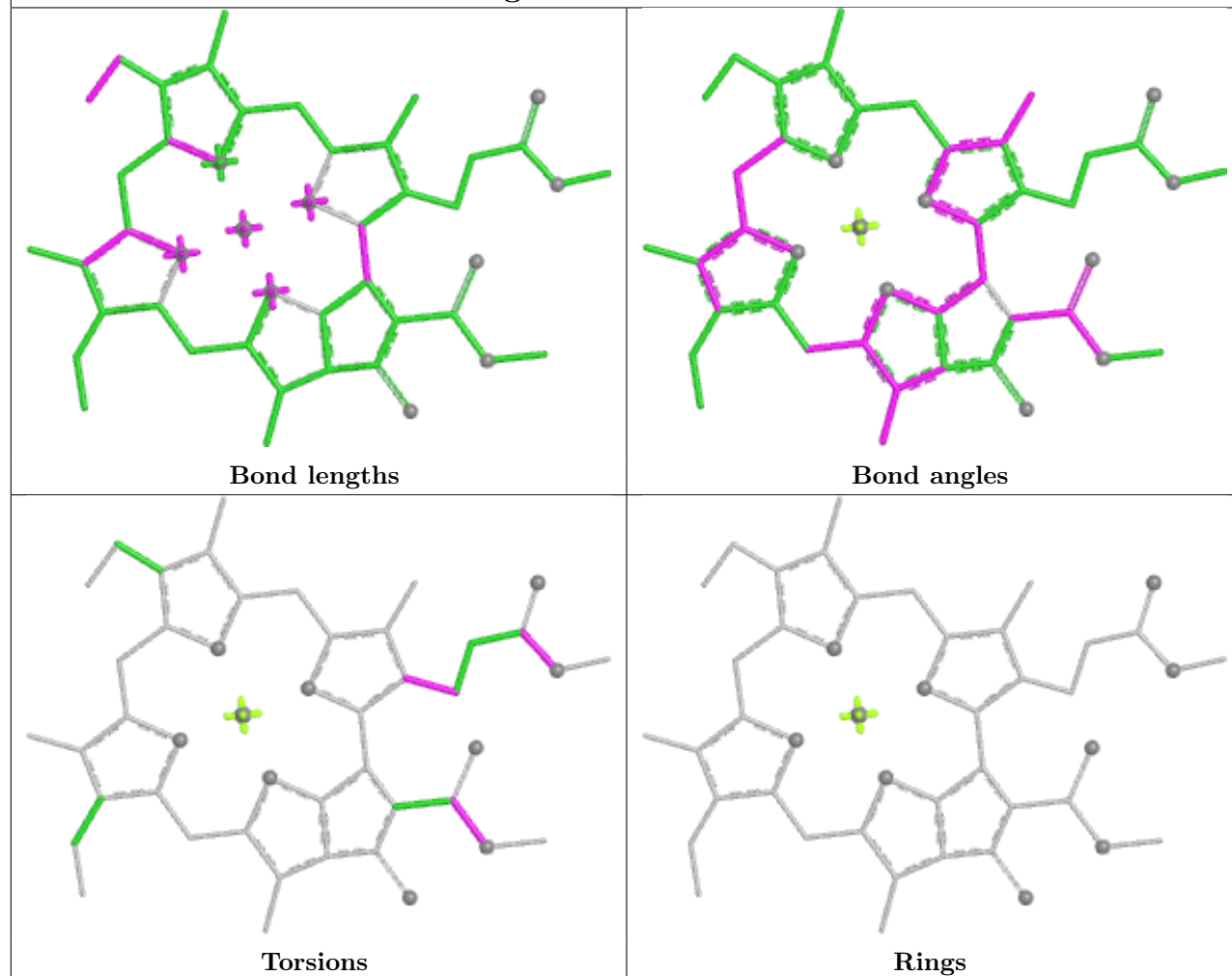


## Ligand BCR L 303



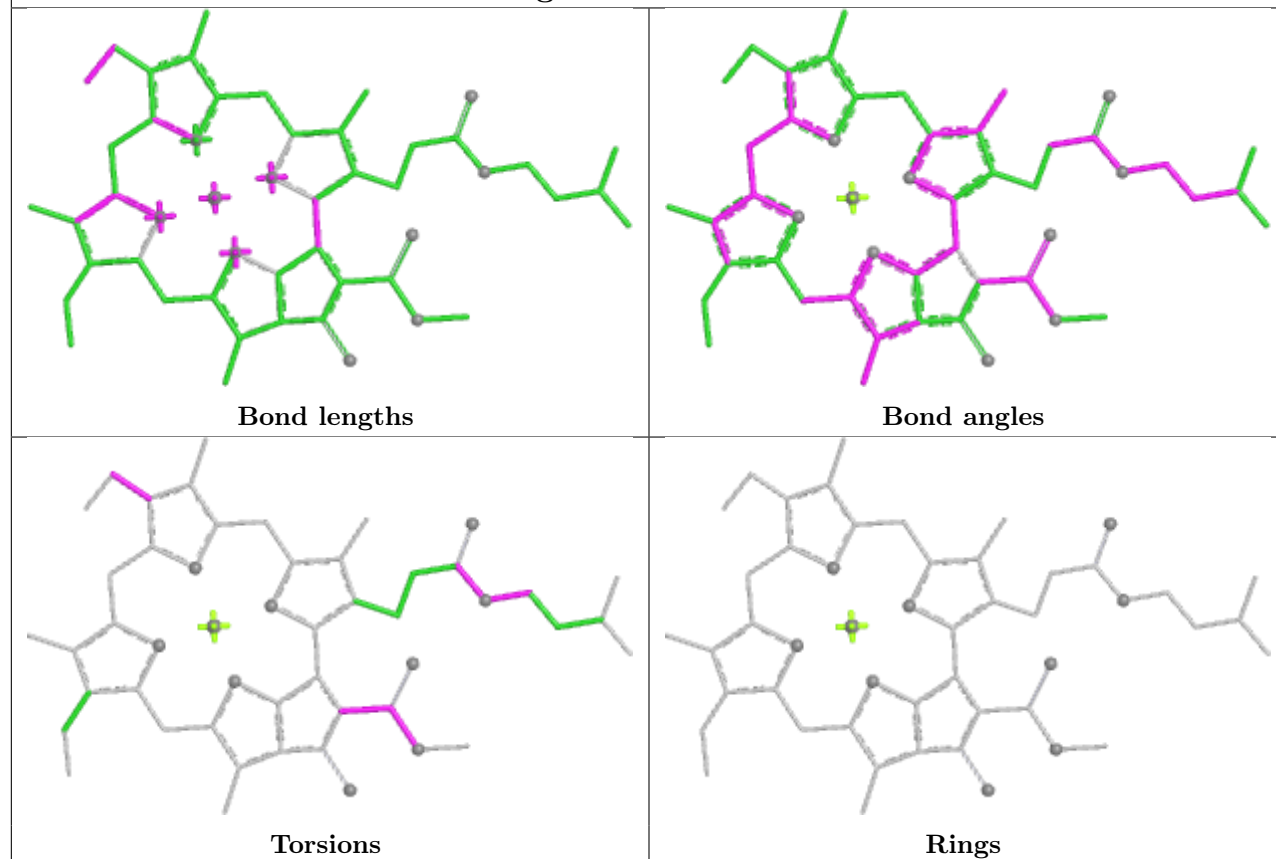


## Ligand CLA G 1602

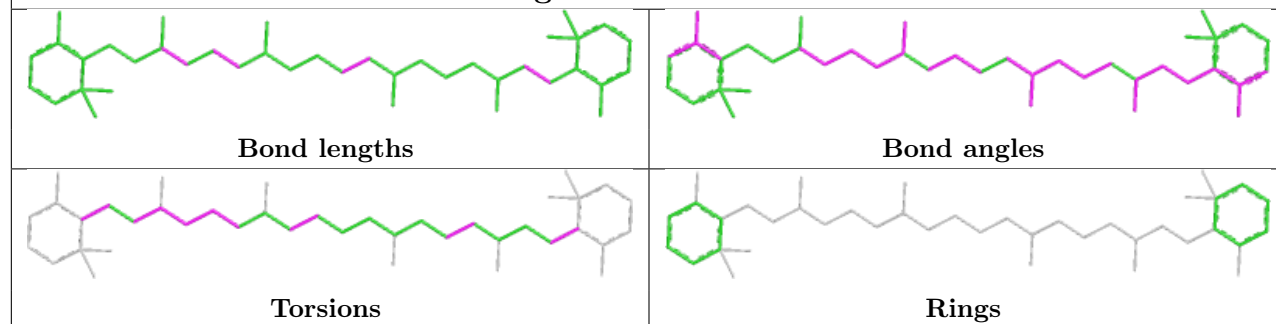


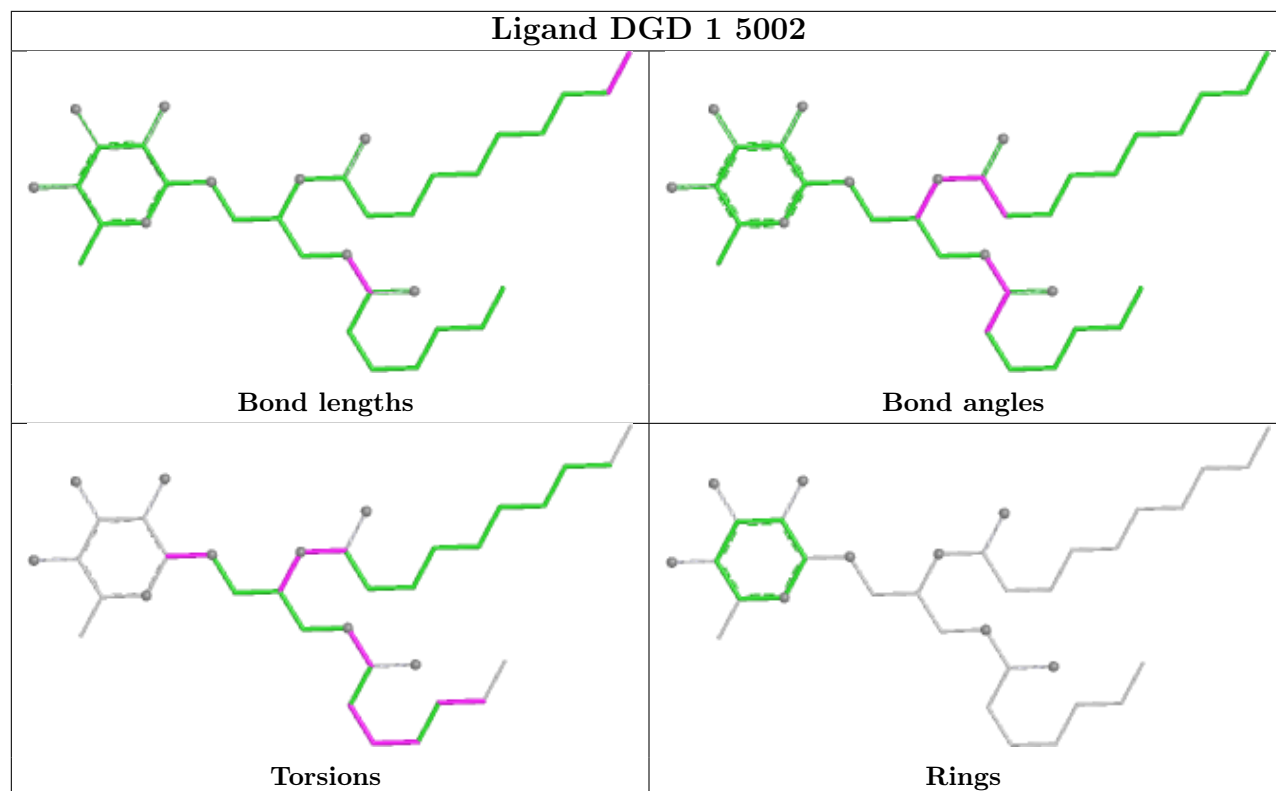


## Ligand CLA 4 306

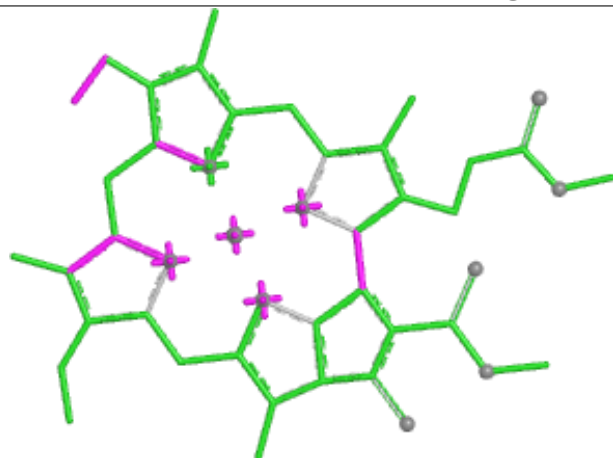


## Ligand BCR 3 305

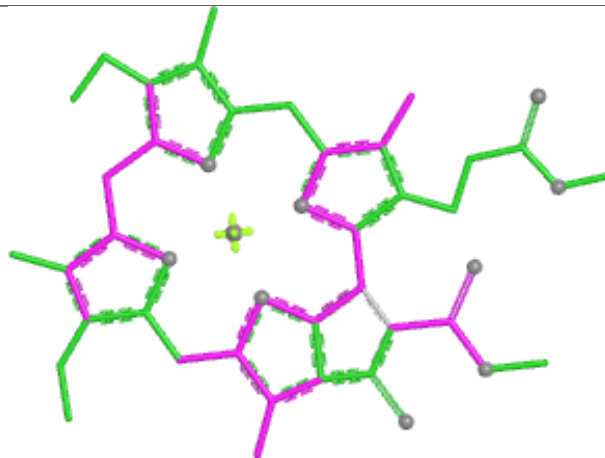




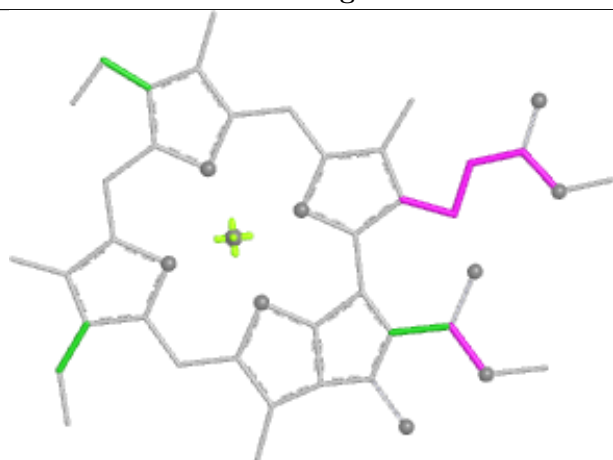
## Ligand CLA K 1404



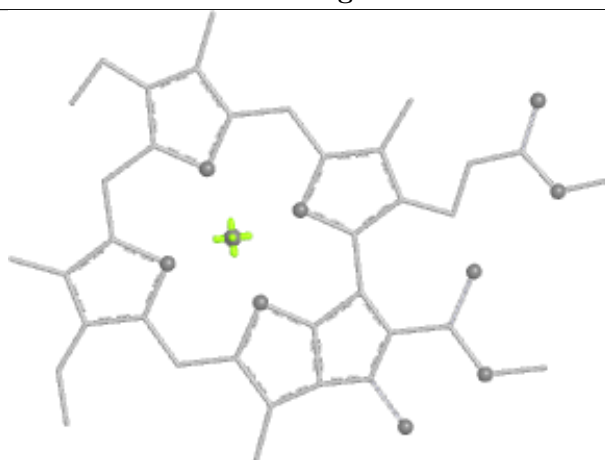
Bond lengths



Bond angles

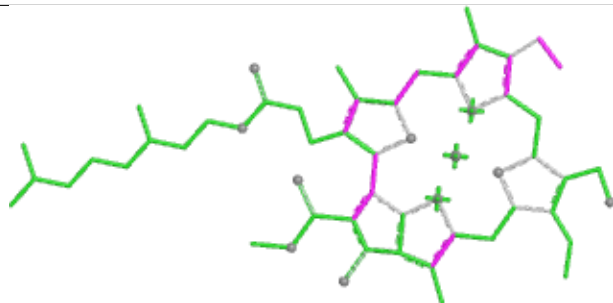


Torsions

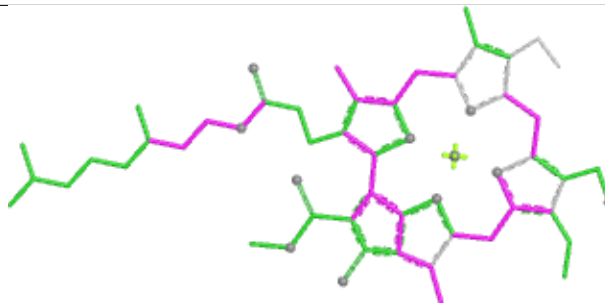


Rings

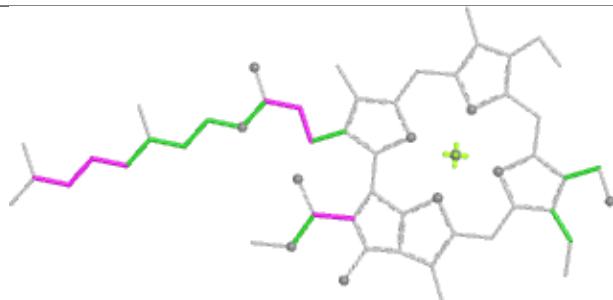
## Ligand CHL 2 315



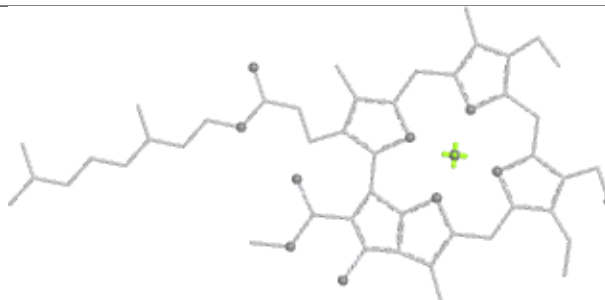
Bond lengths



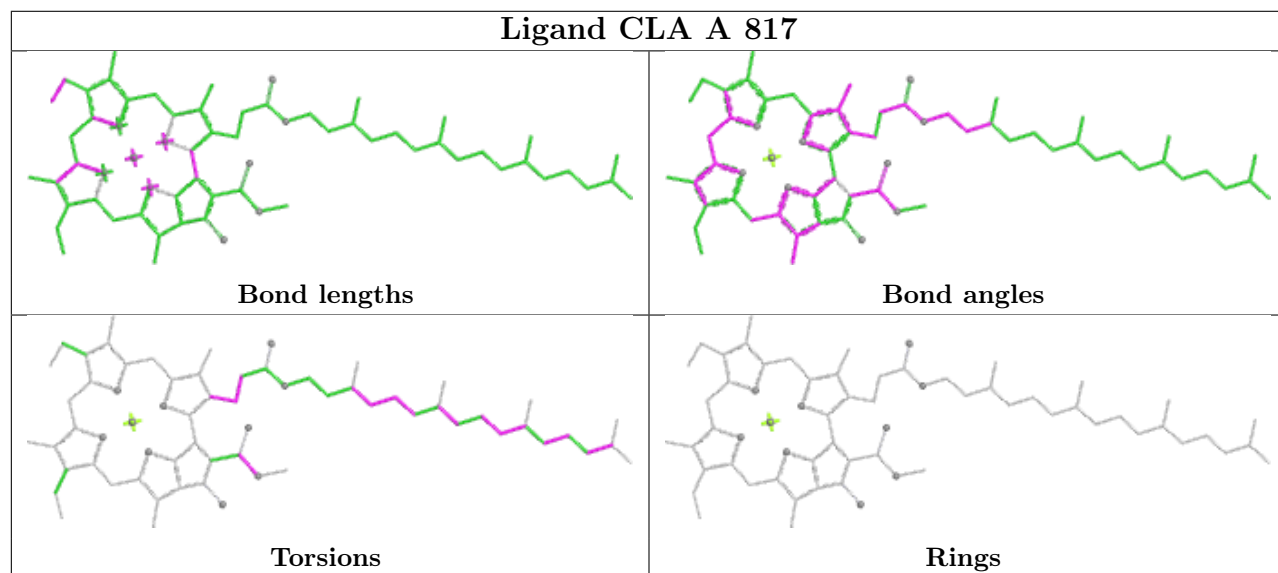
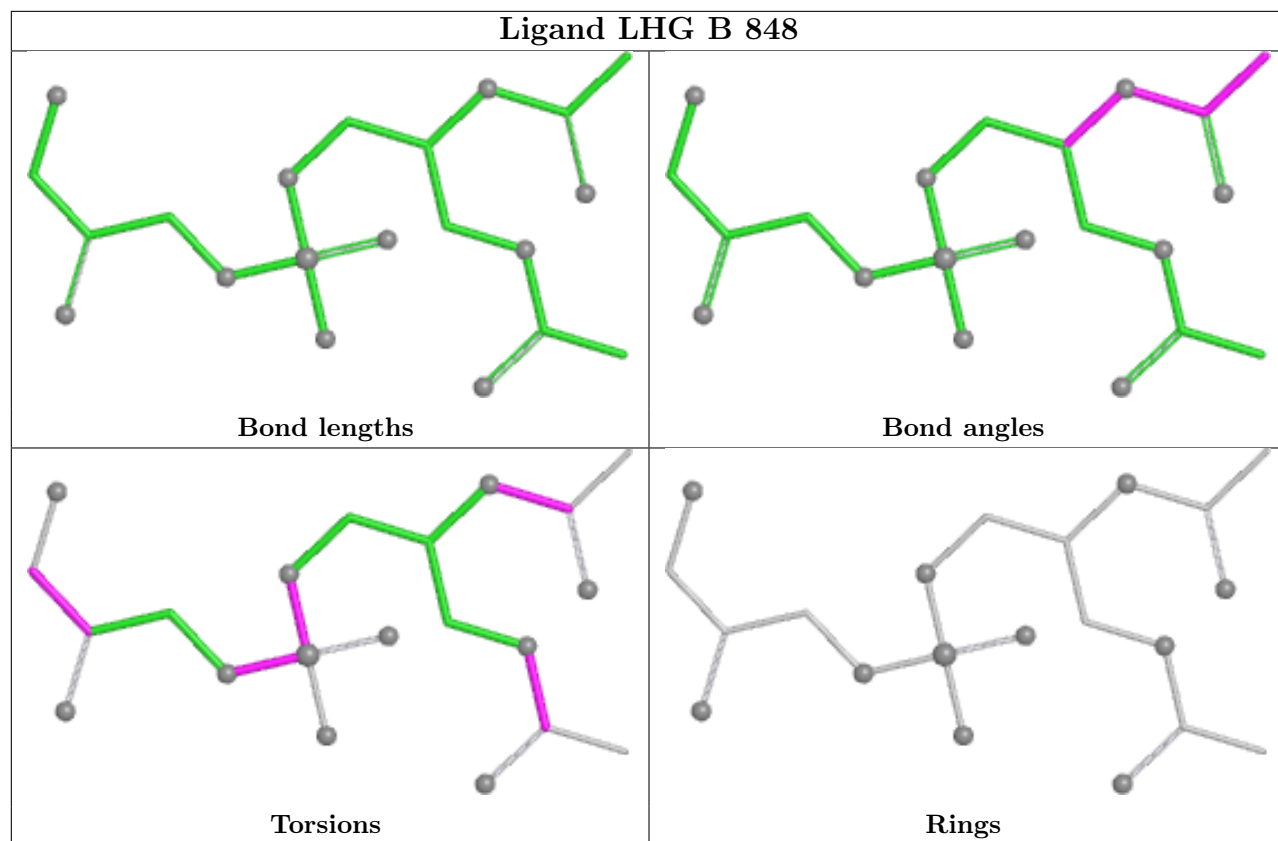
Bond angles



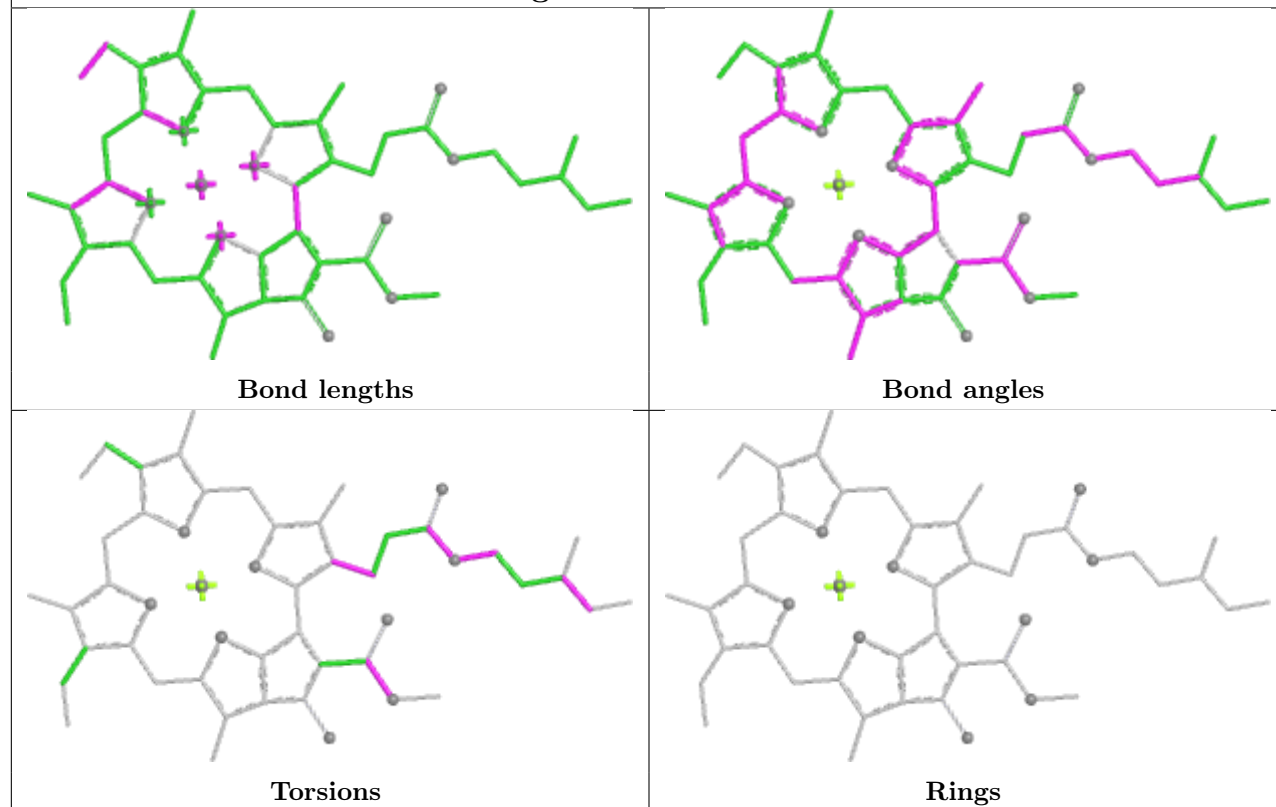
Torsions



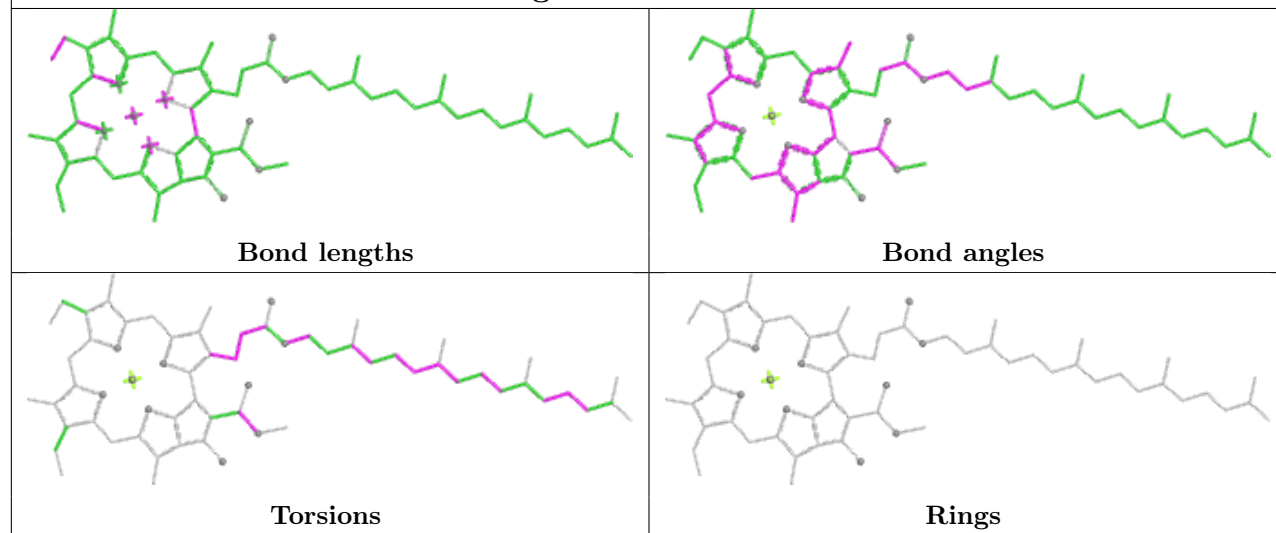
Rings

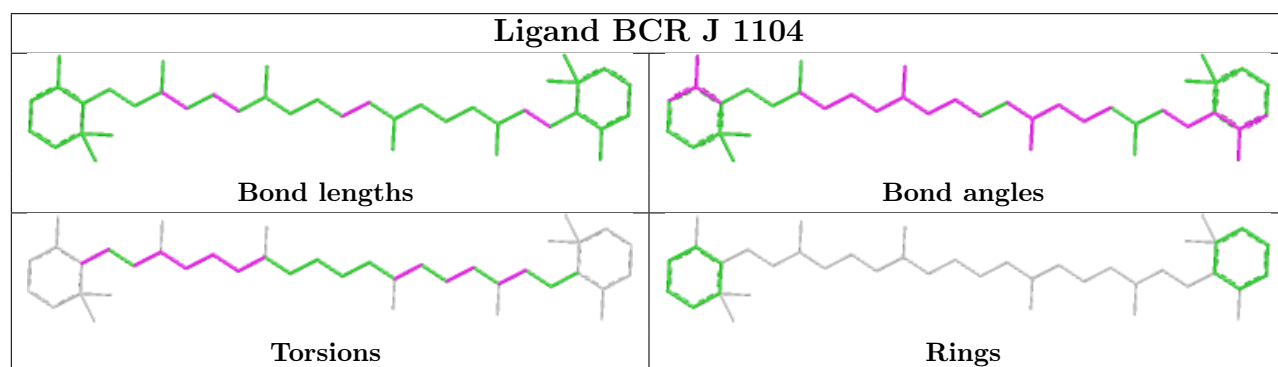
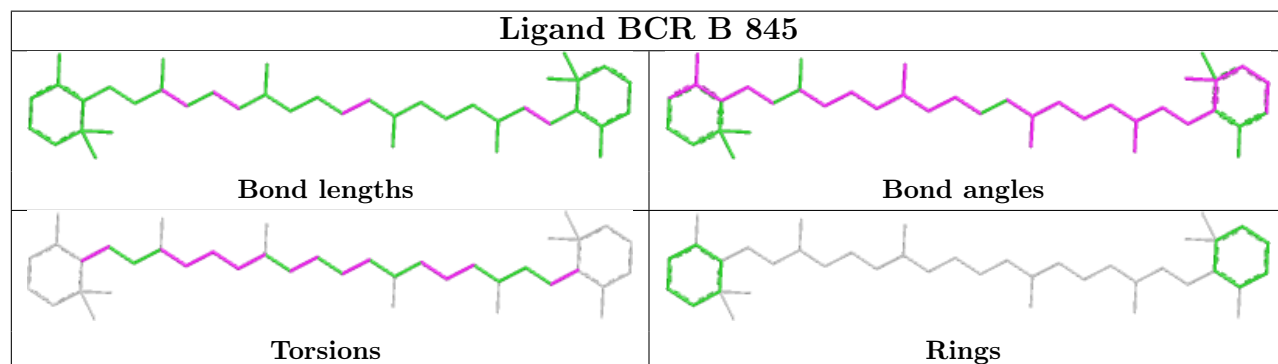
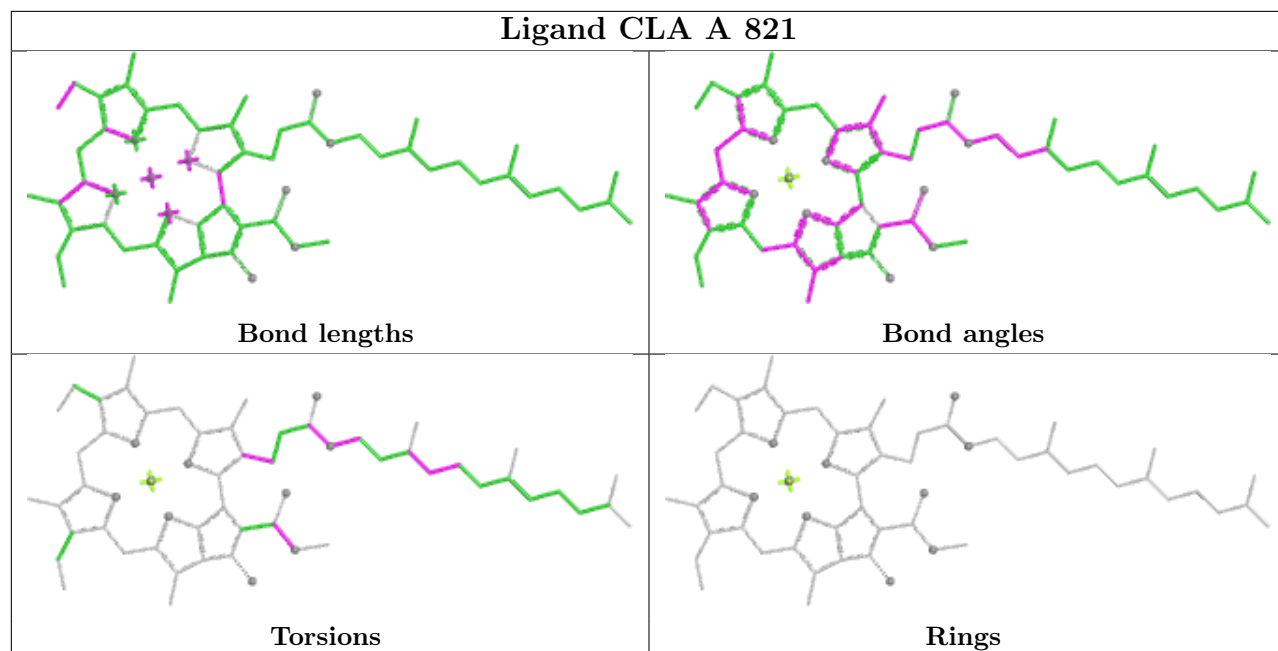


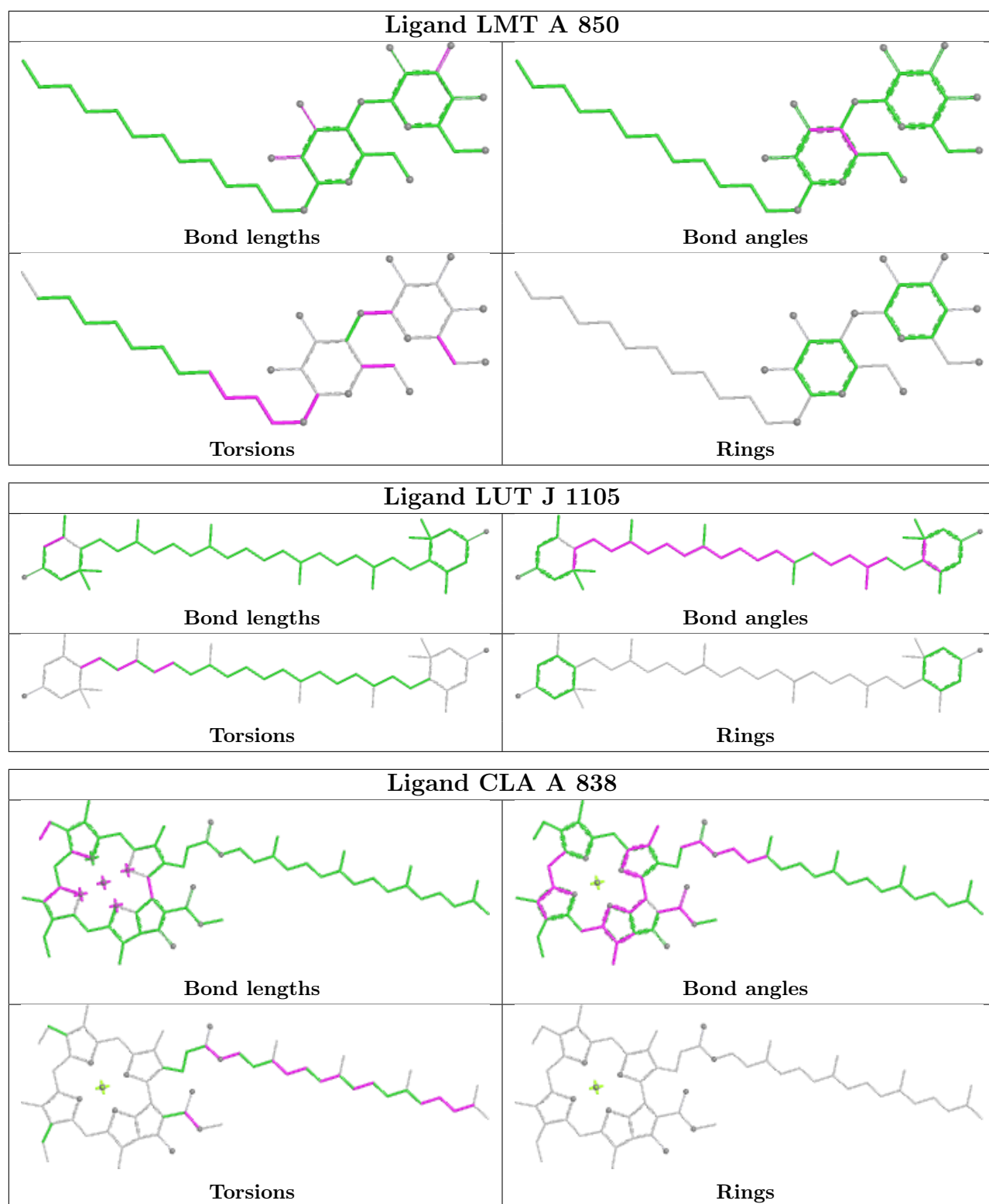
## Ligand CLA A 834



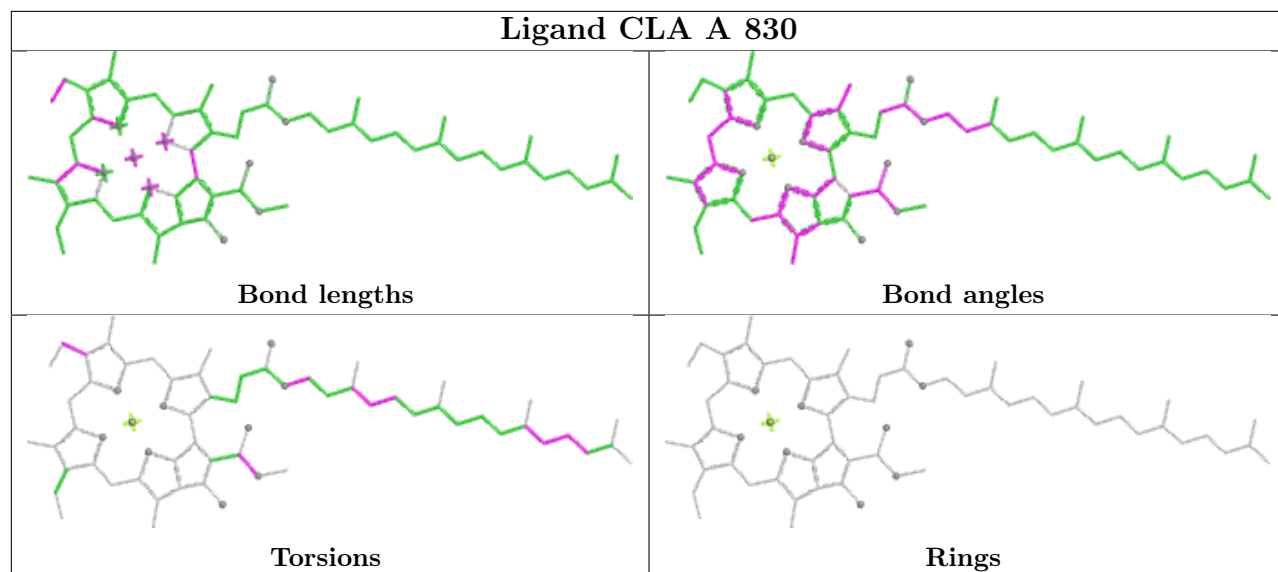
## Ligand CLA B 840



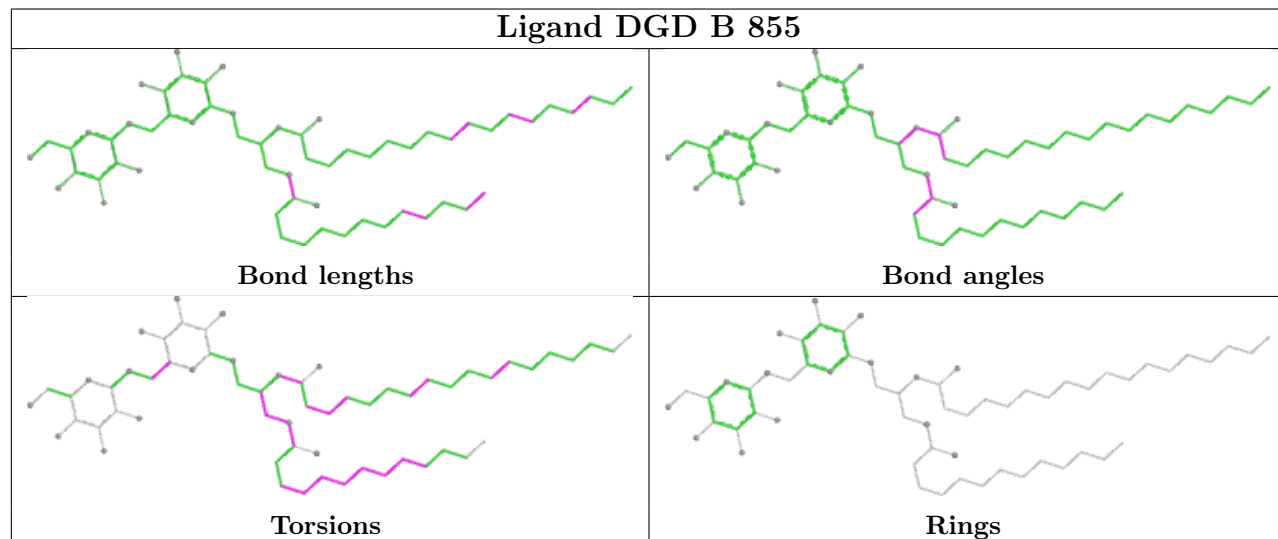




## Ligand CLA A 830

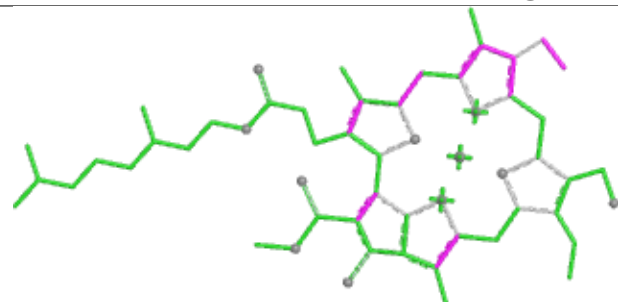


## Ligand DGD B 855

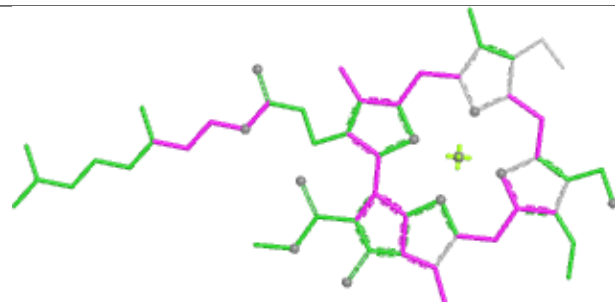




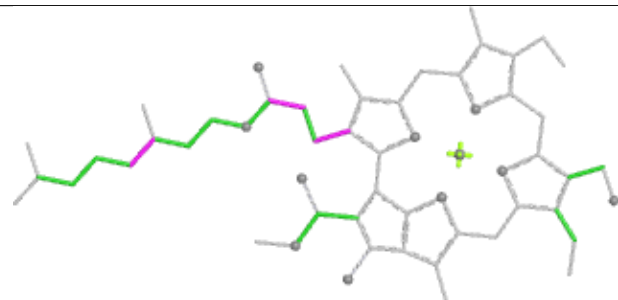
## Ligand CHL 4 302



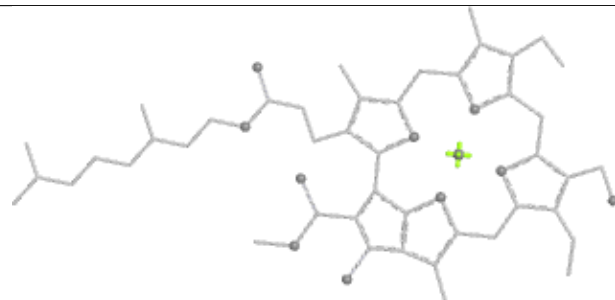
Bond lengths



Bond angles

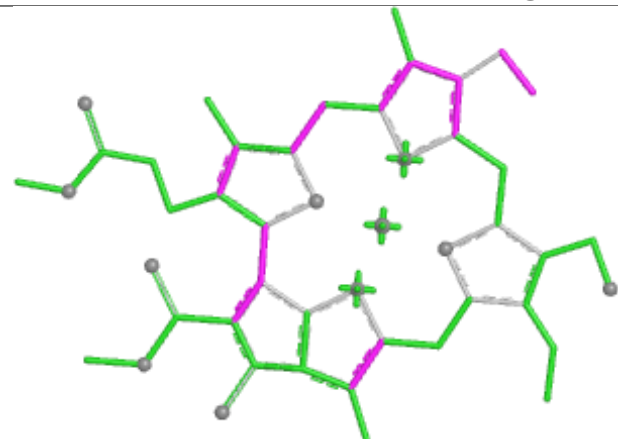


Torsions

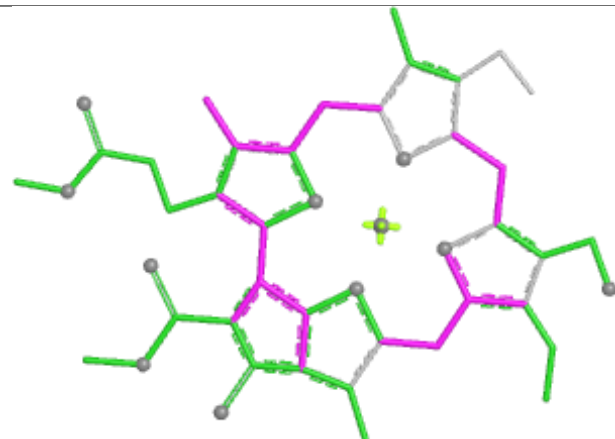


Rings

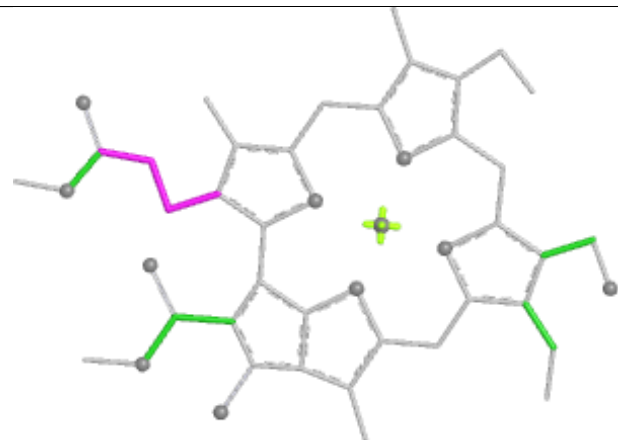
## Ligand CHL 3 316



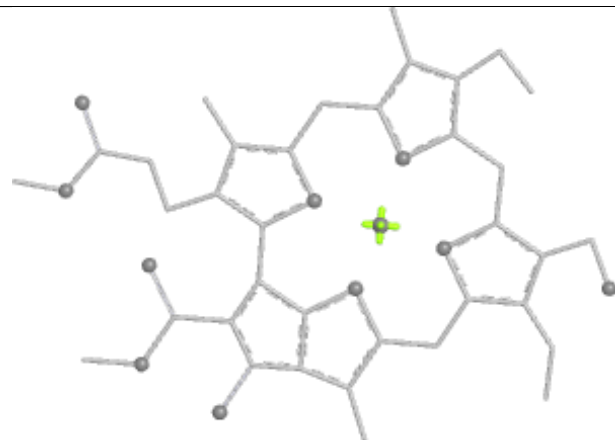
Bond lengths



Bond angles

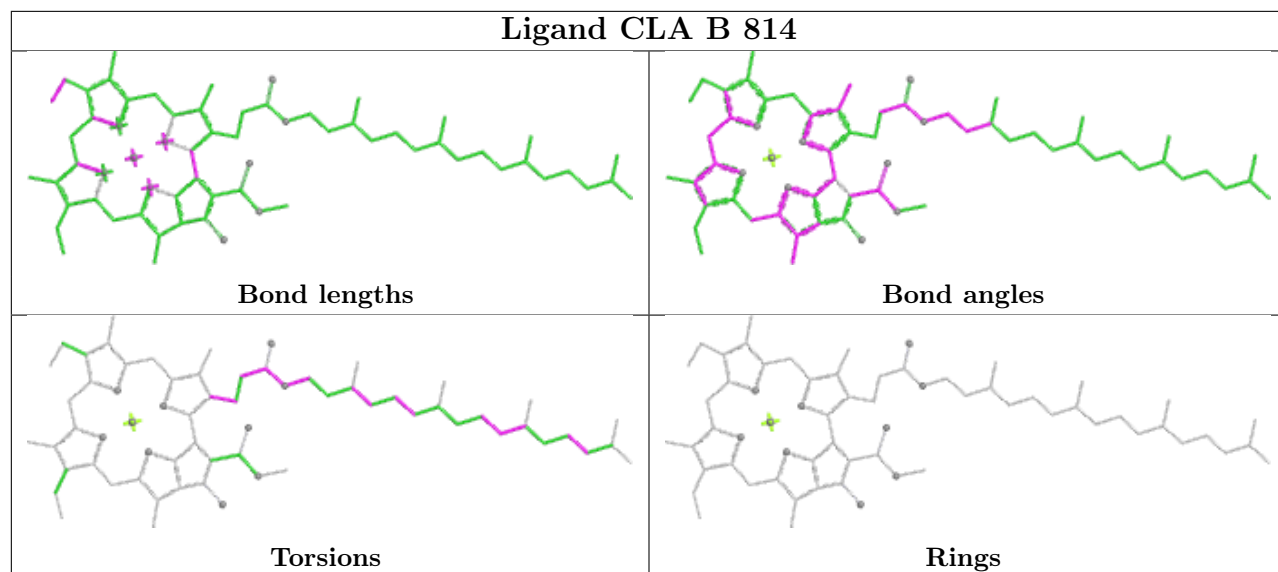


Torsions

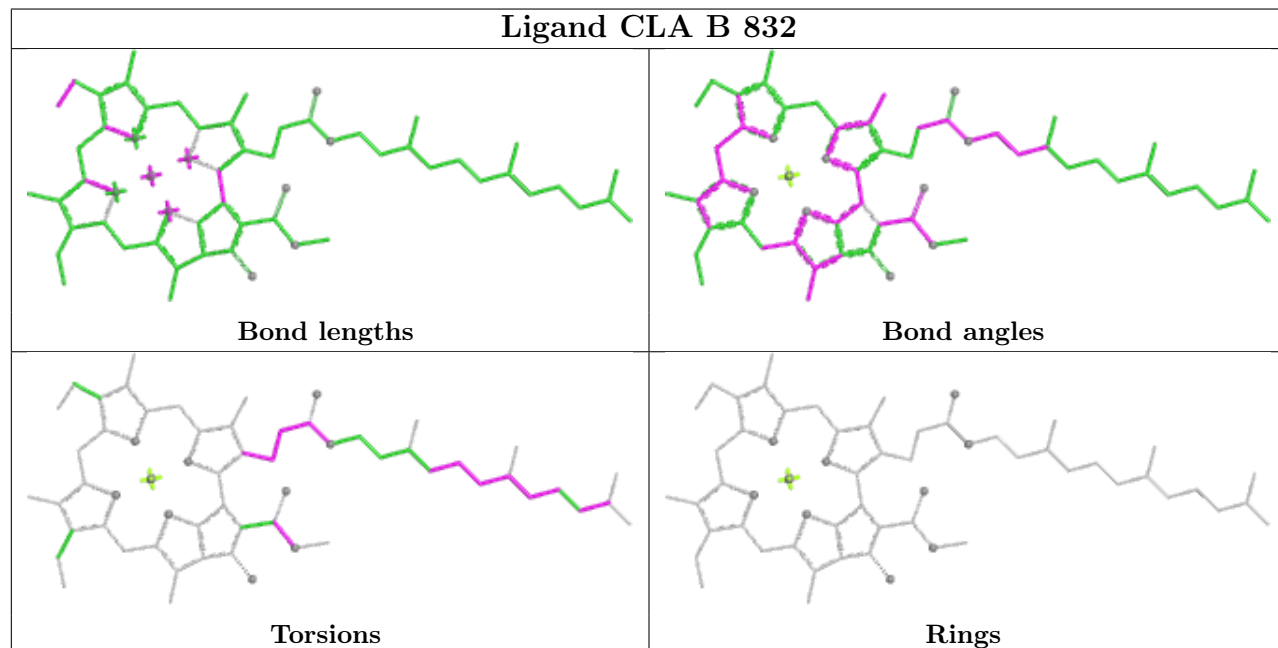


Rings

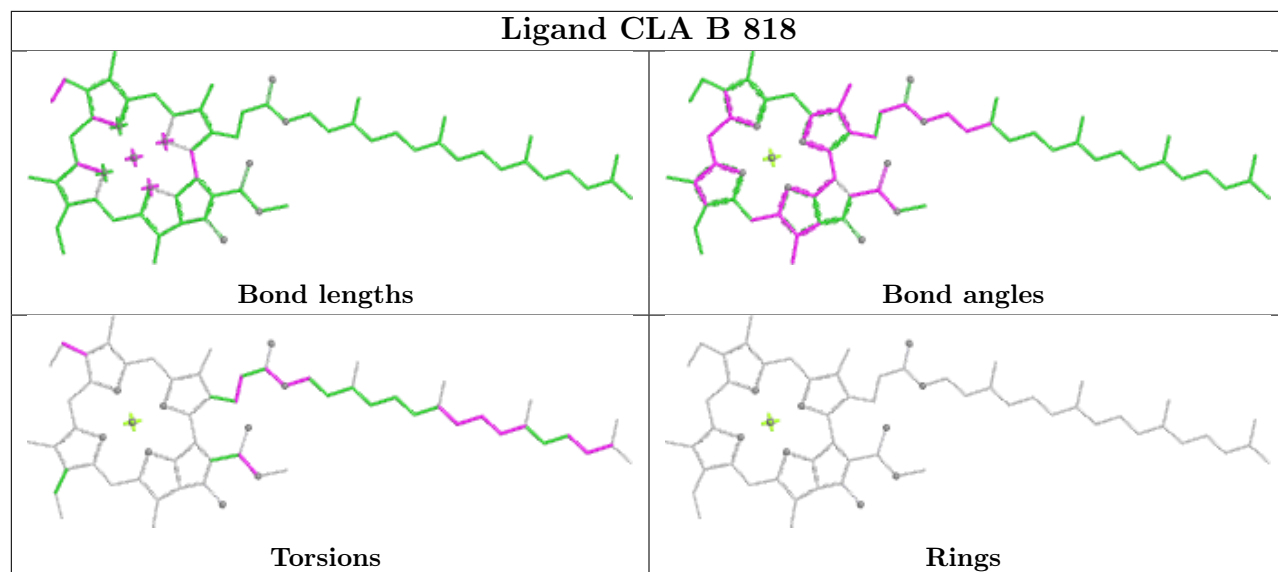
## Ligand CLA B 814



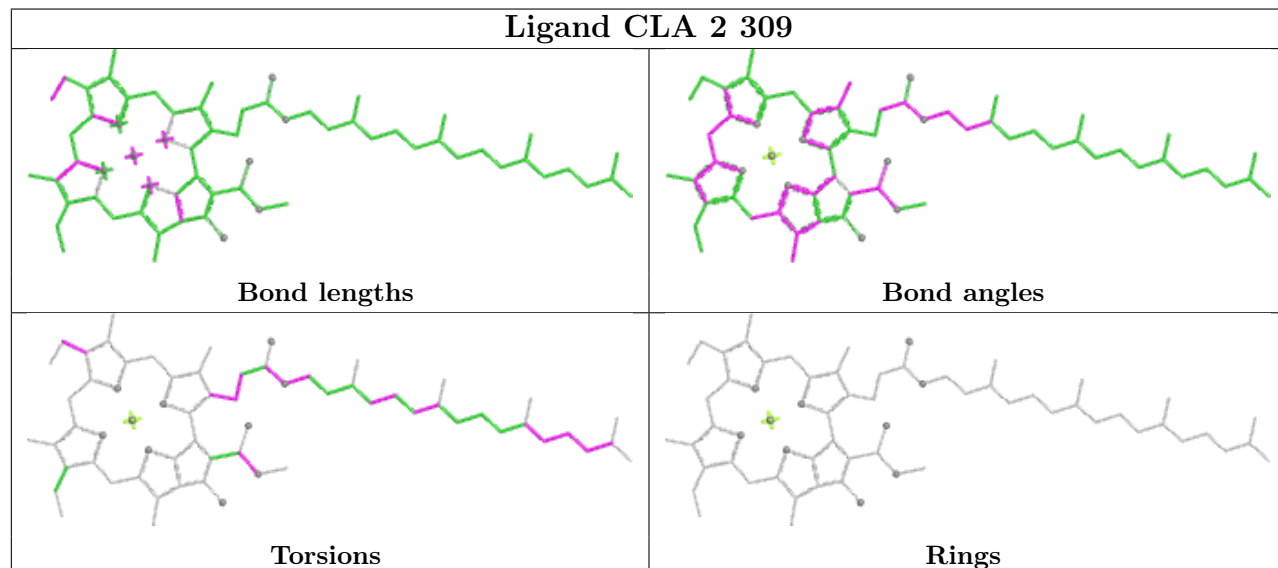
## Ligand CLA B 832



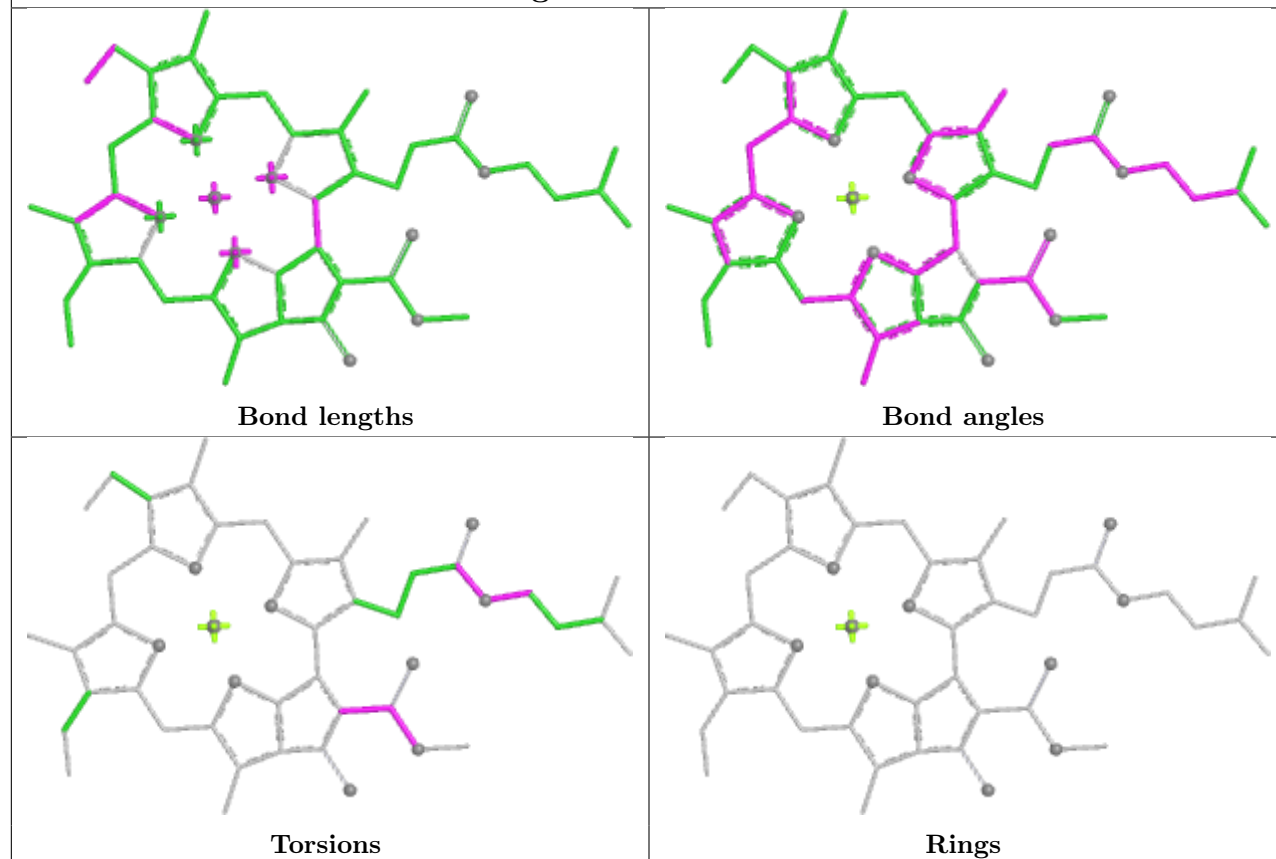
## Ligand CLA B 818



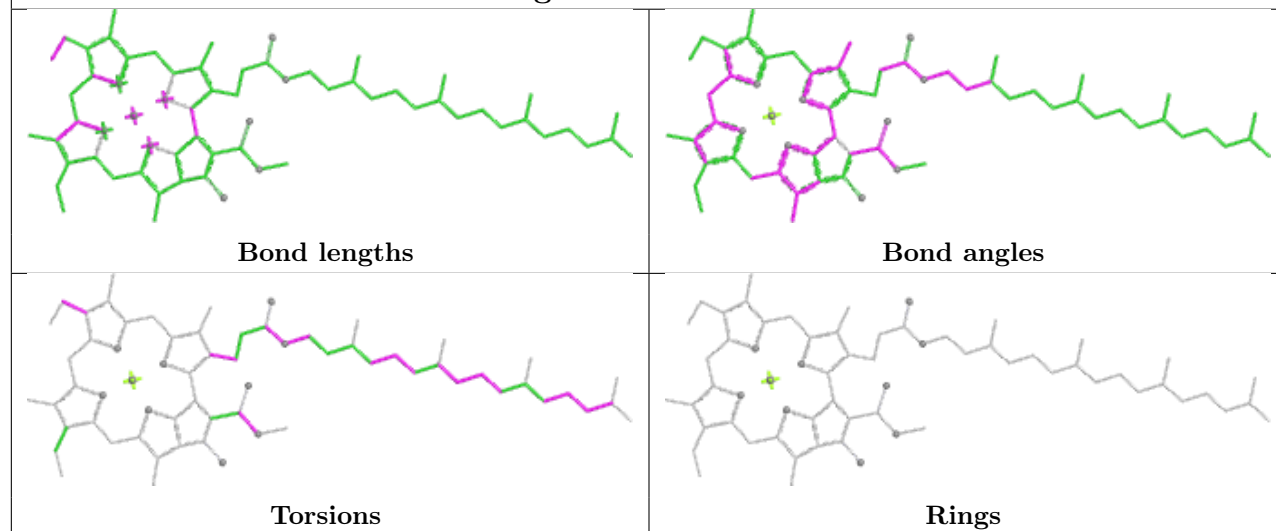
## Ligand CLA 2 309



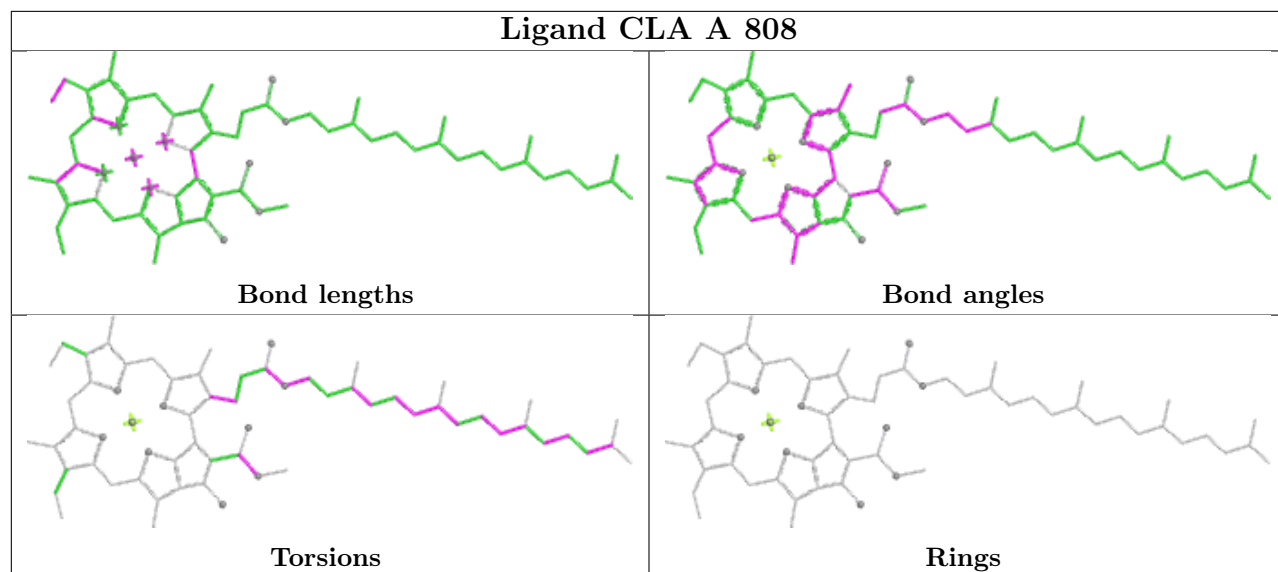
## Ligand CLA A 818



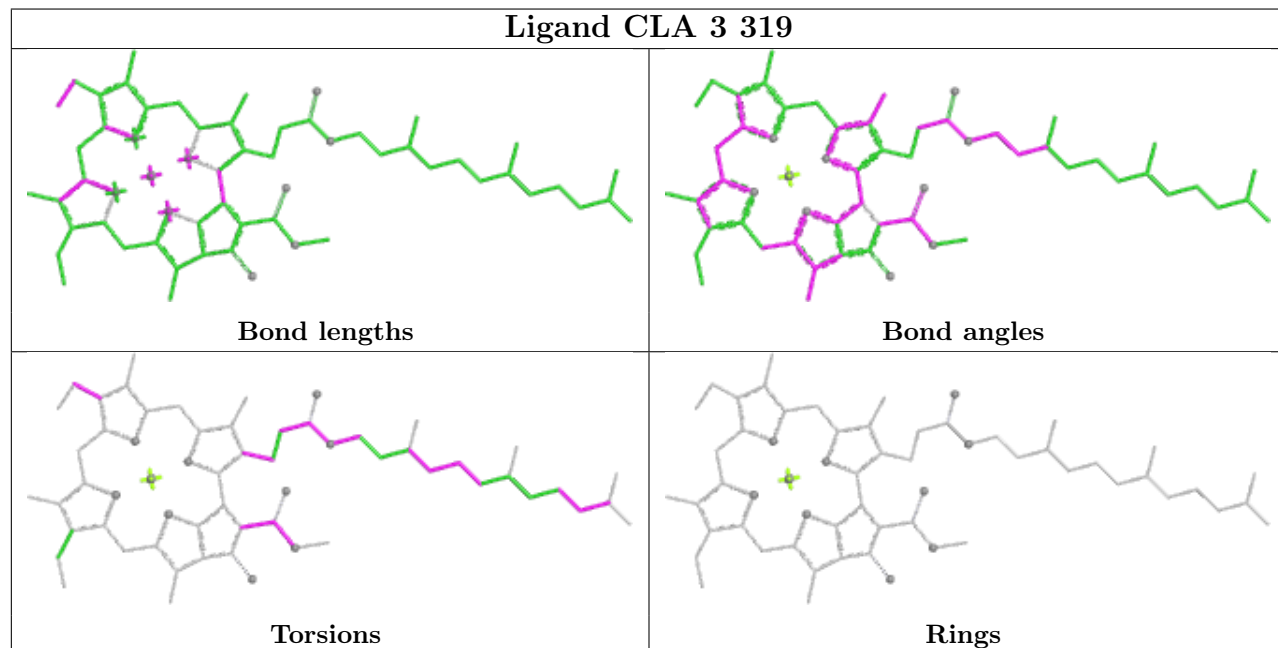
## Ligand CLA F 303

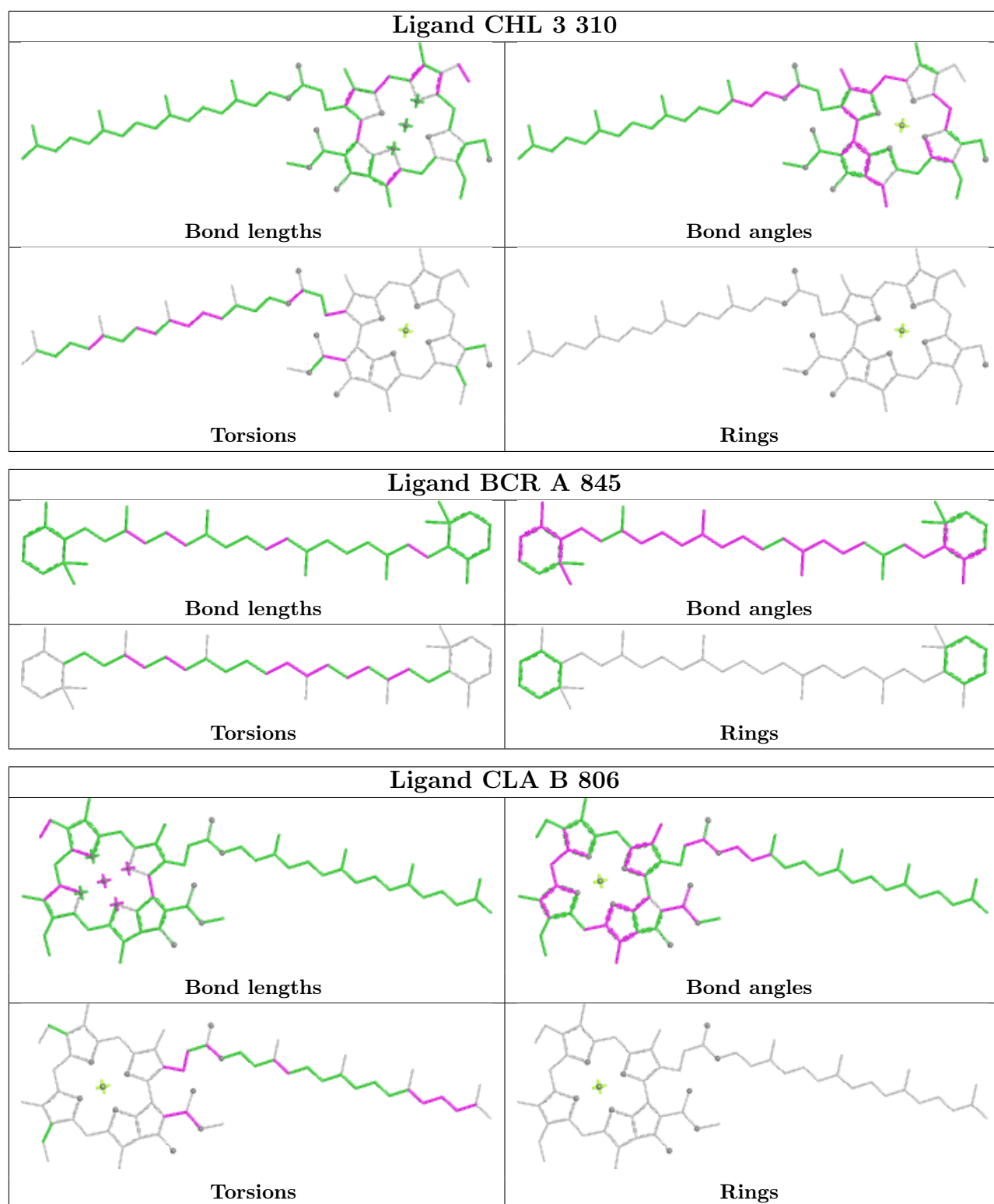


## Ligand CLA A 808

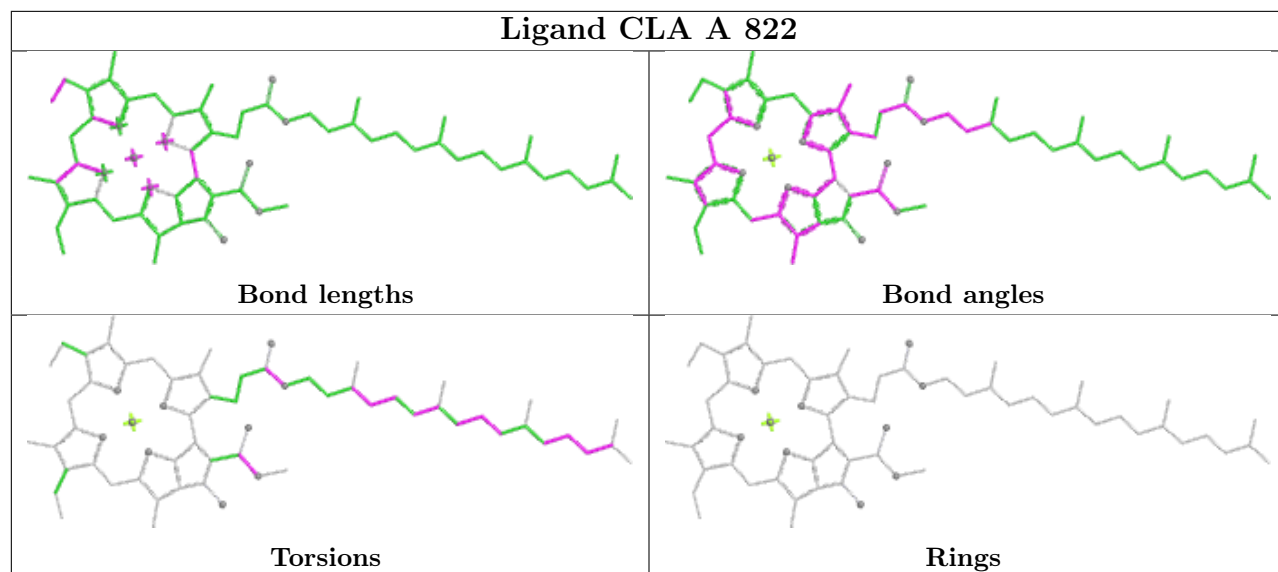


## Ligand CLA 3 319

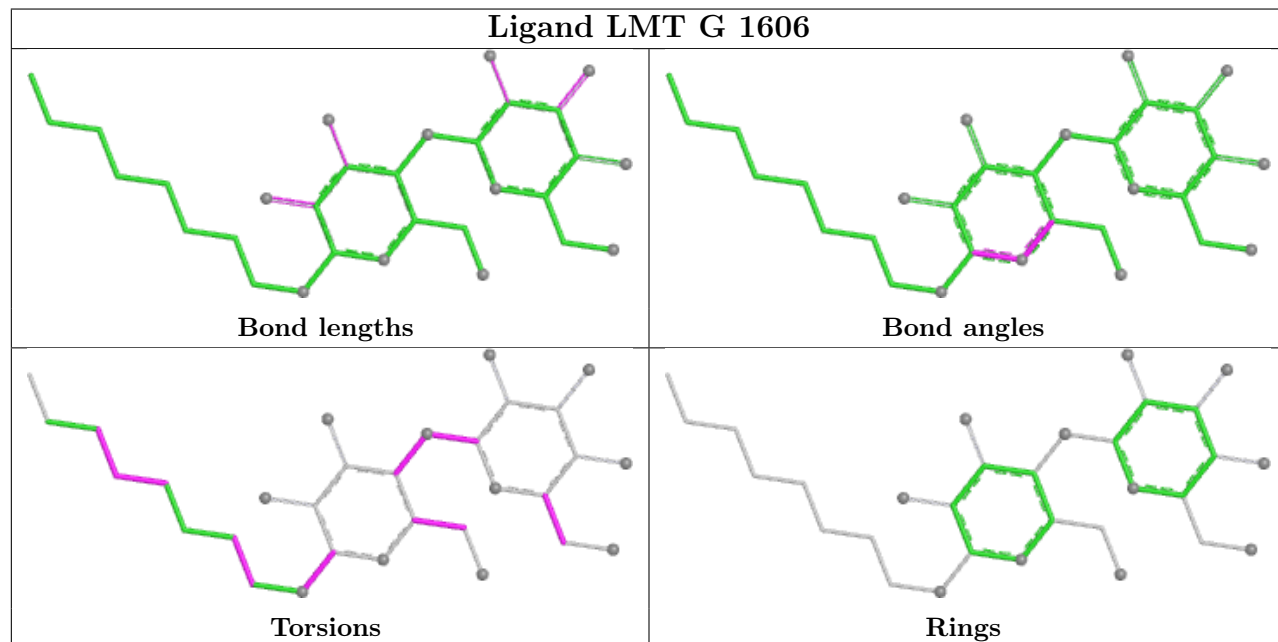


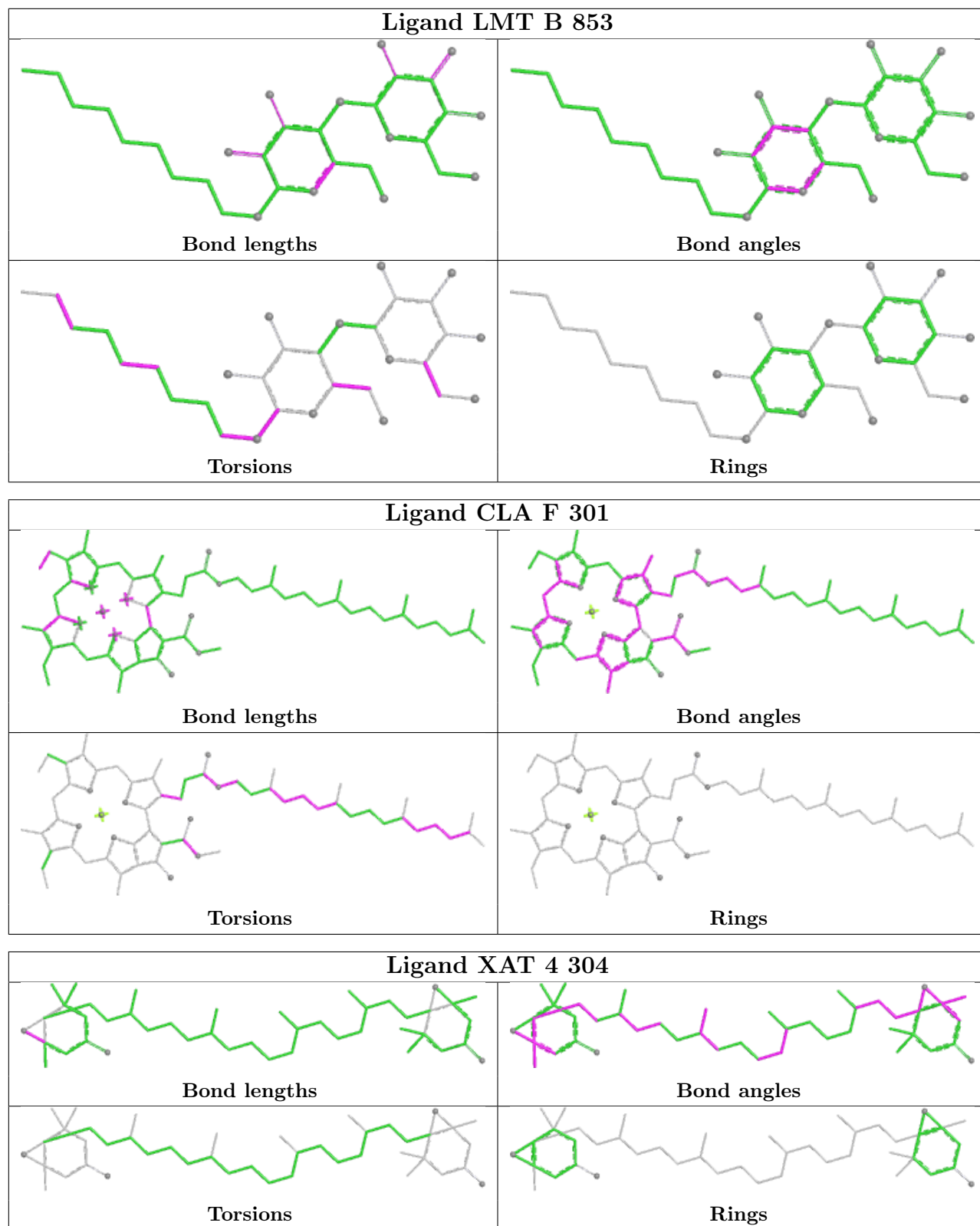


## Ligand CLA A 822



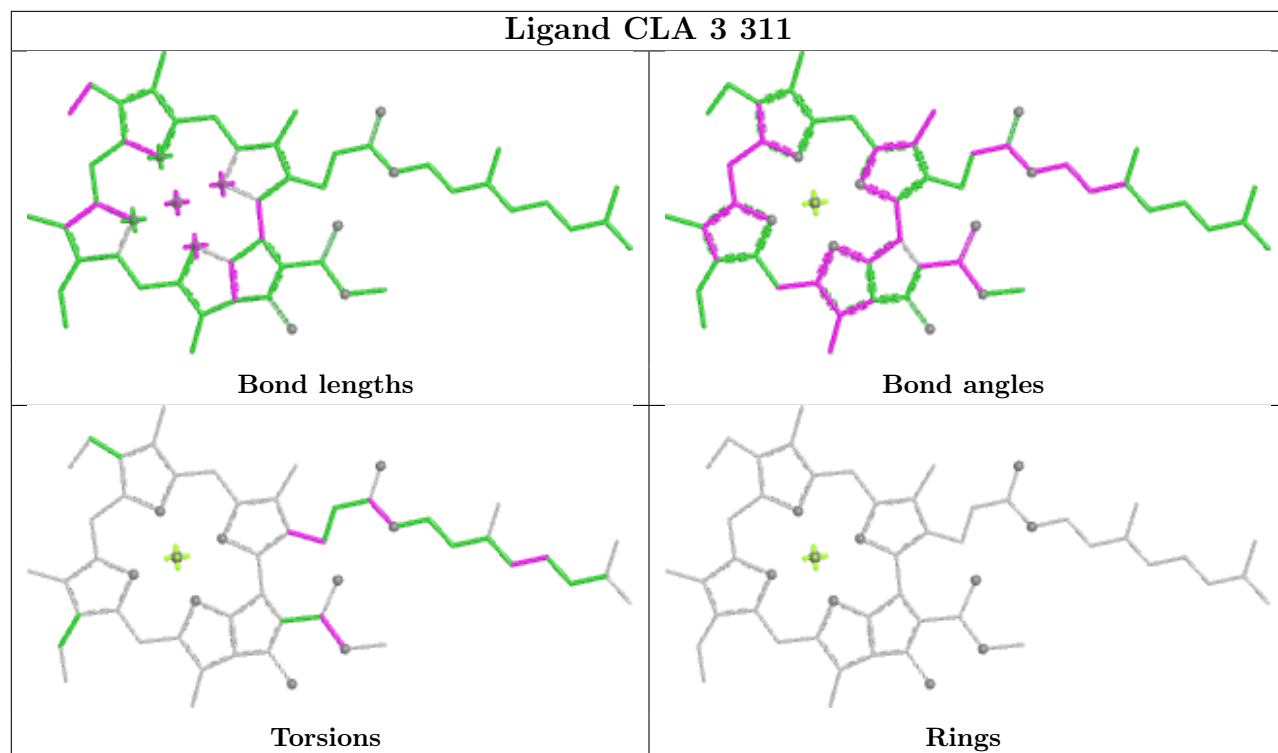
## Ligand LMT G 1606



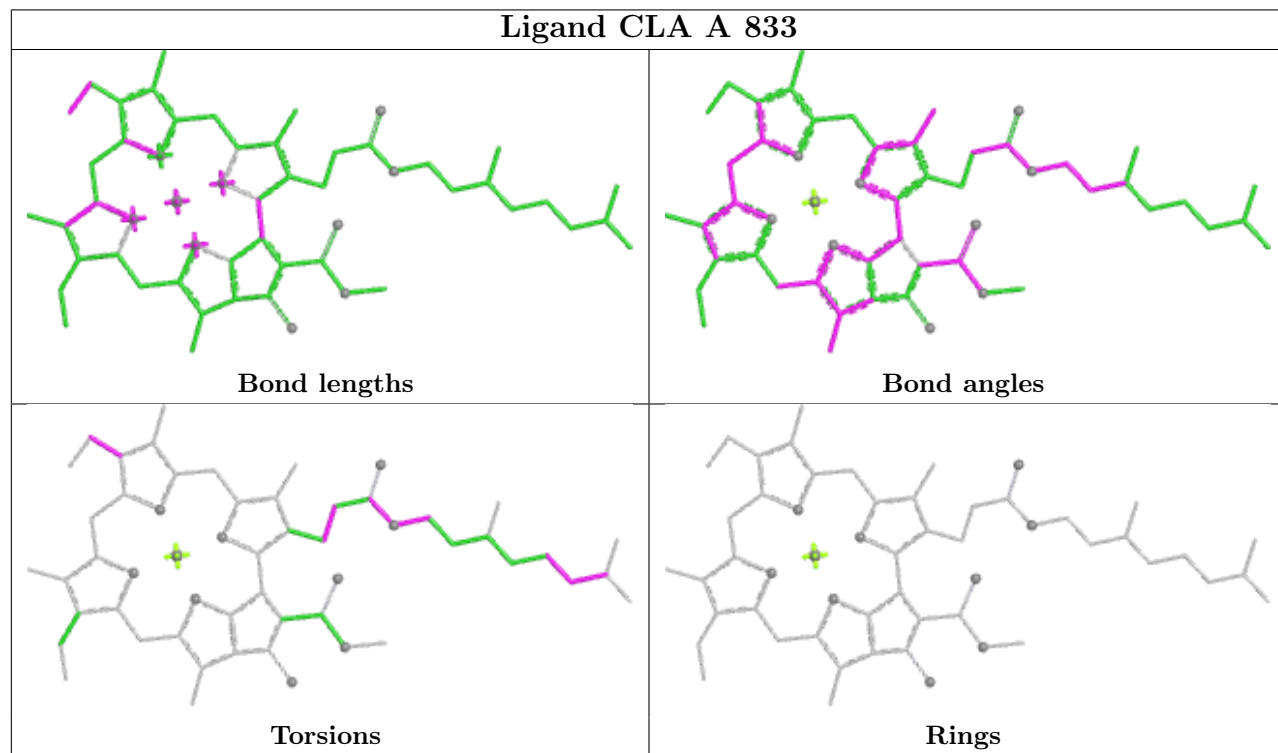


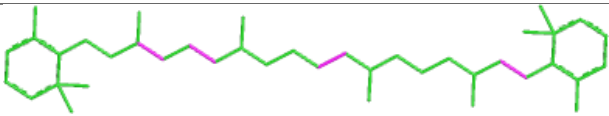
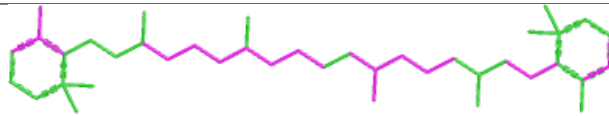
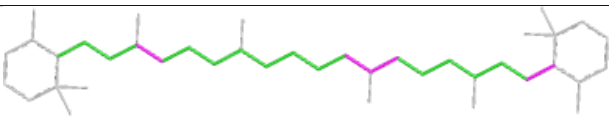
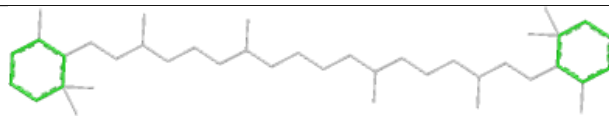


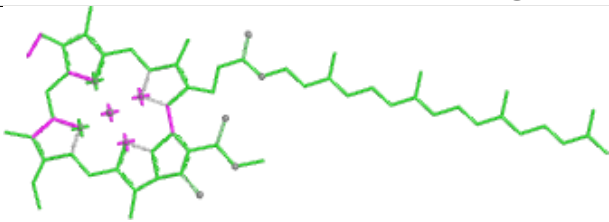
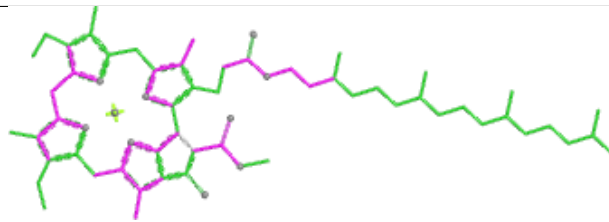
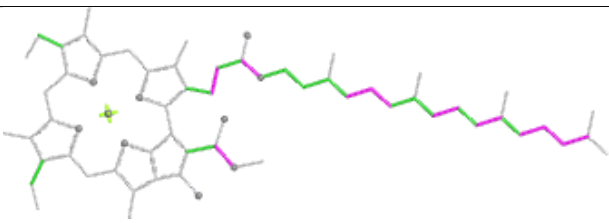
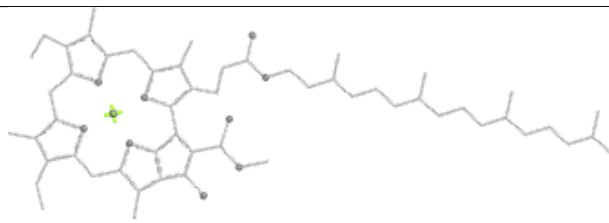
## Ligand CLA 3 311

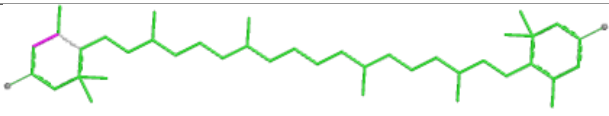
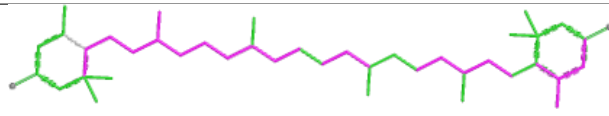
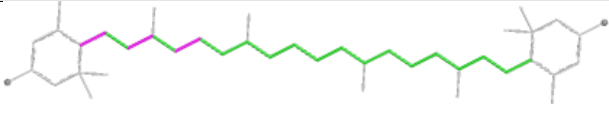
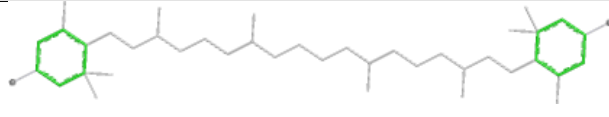


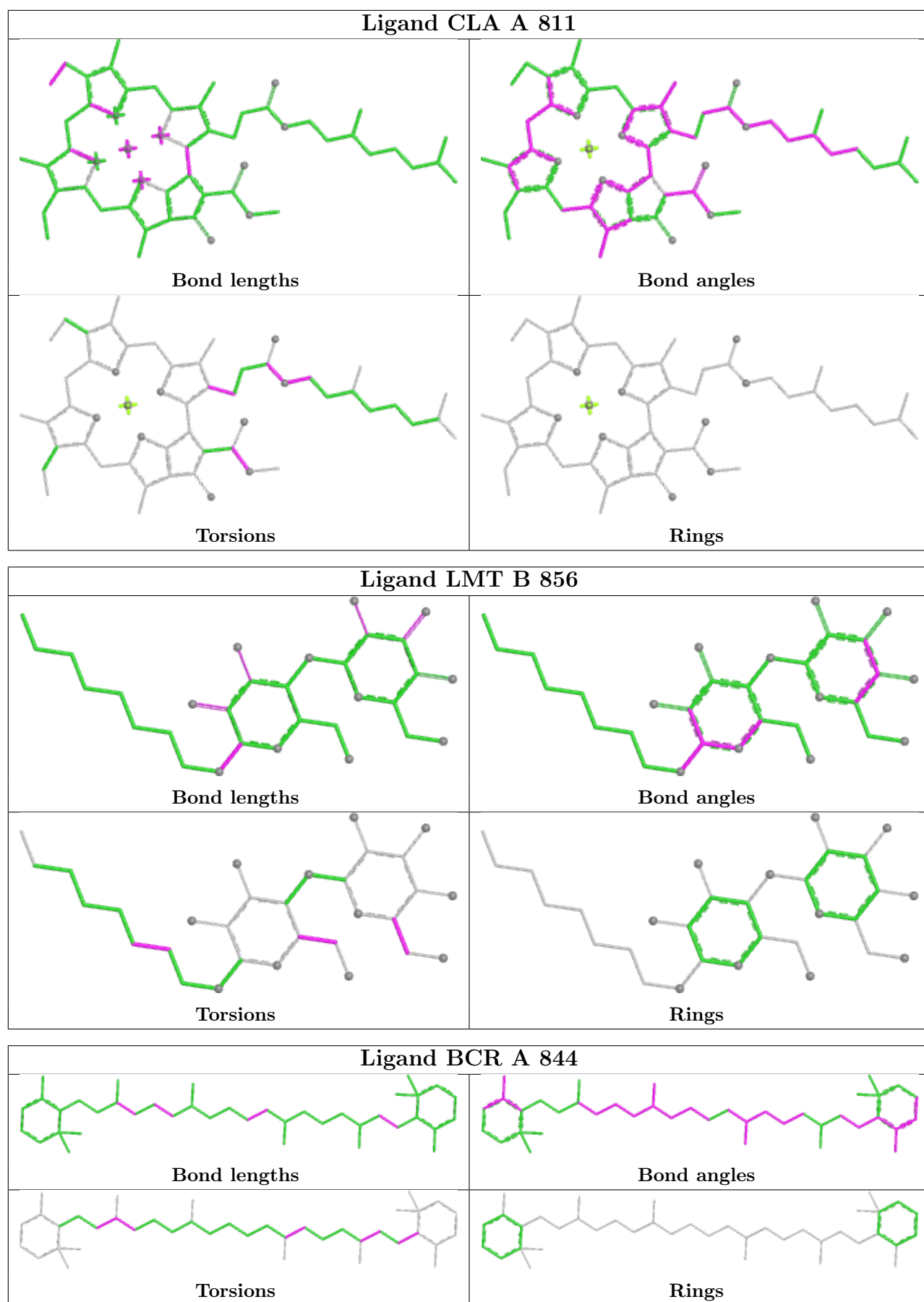
## Ligand CLA A 833



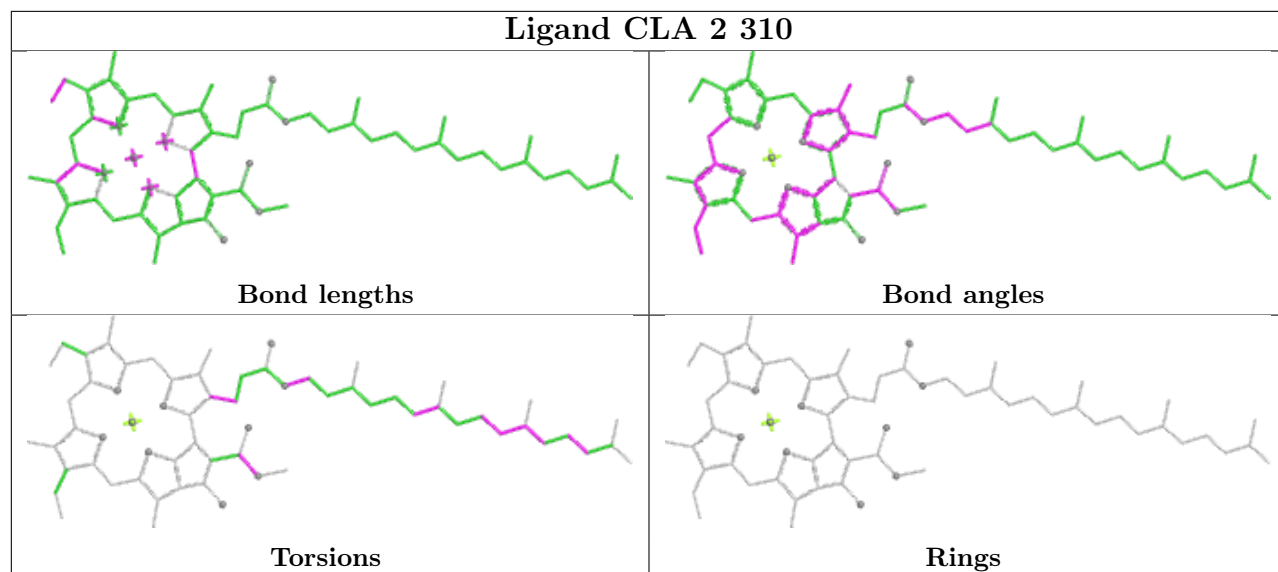
Ligand BCR G 1604	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

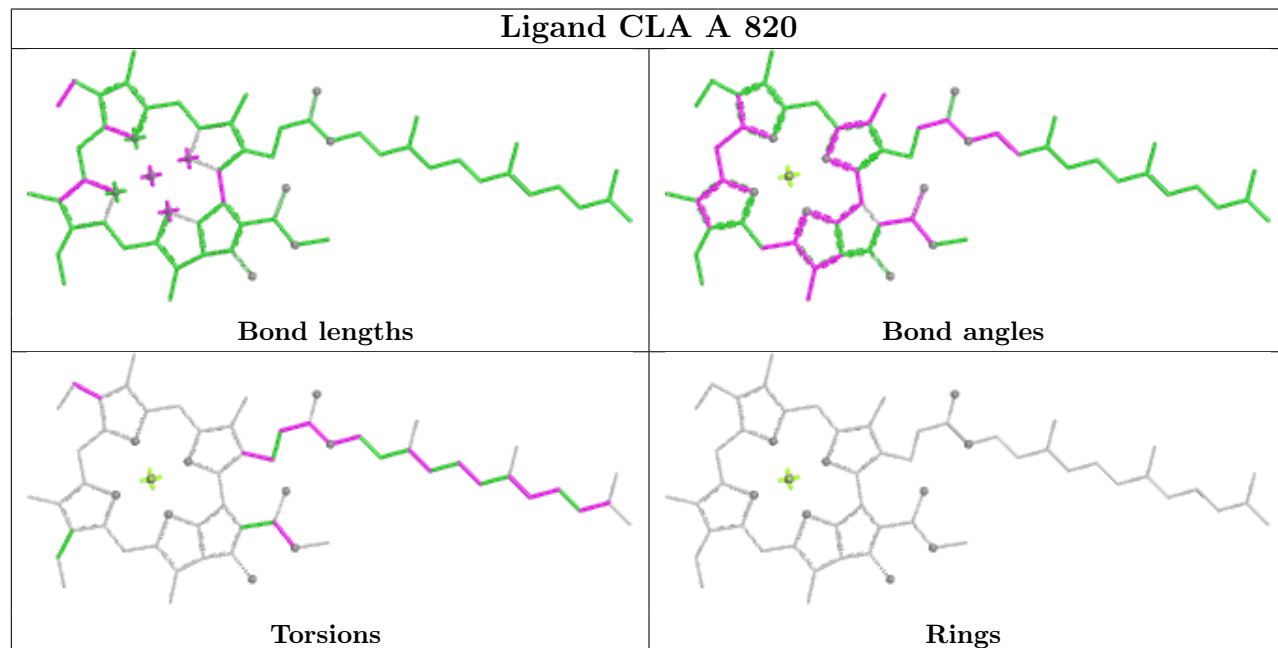
Ligand LUT 1 5004	
	
Bond lengths	Bond angles
	
Torsions	Rings



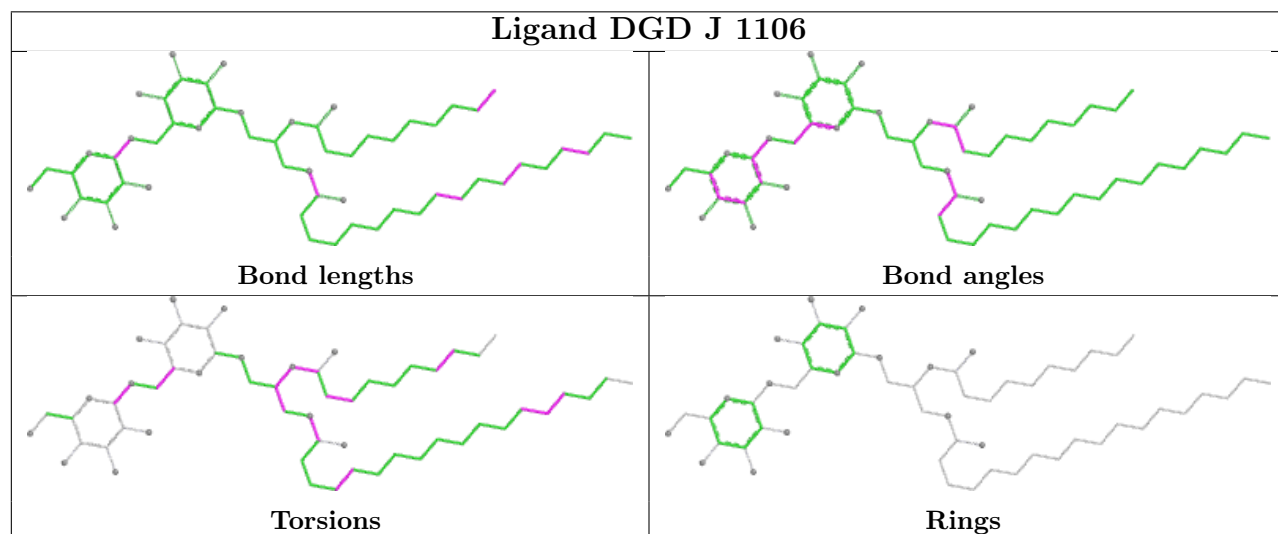
## Ligand CLA 2 310

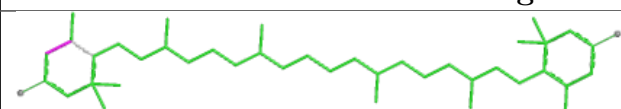
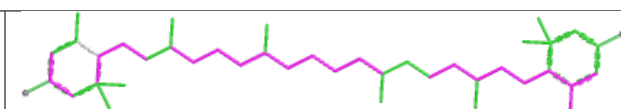
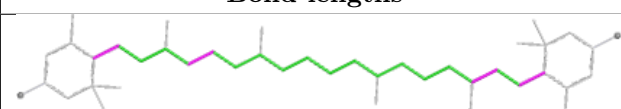
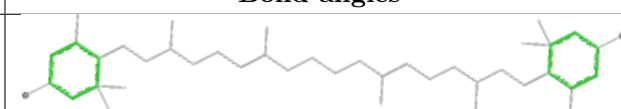



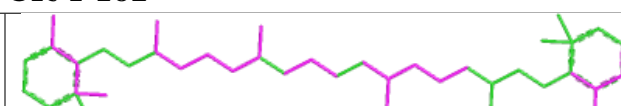
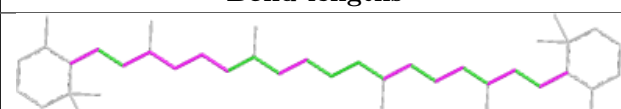
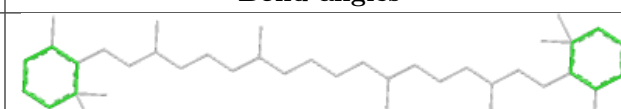
## Ligand CLA A 820

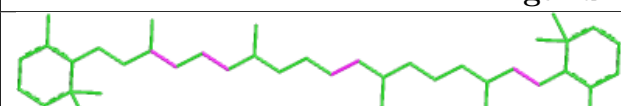
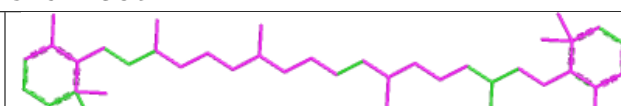

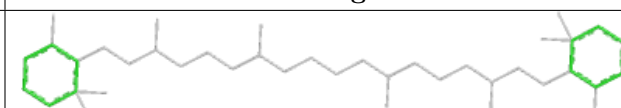


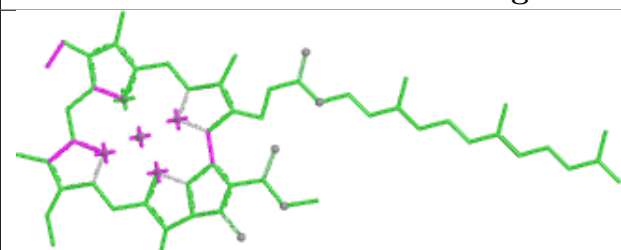
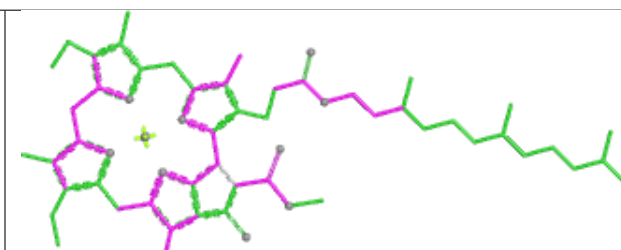
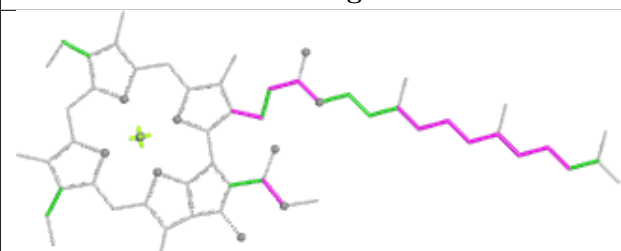
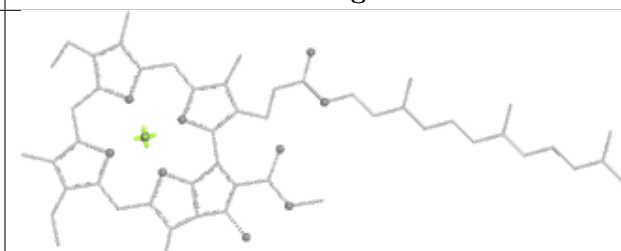
## Ligand DGD J 1106



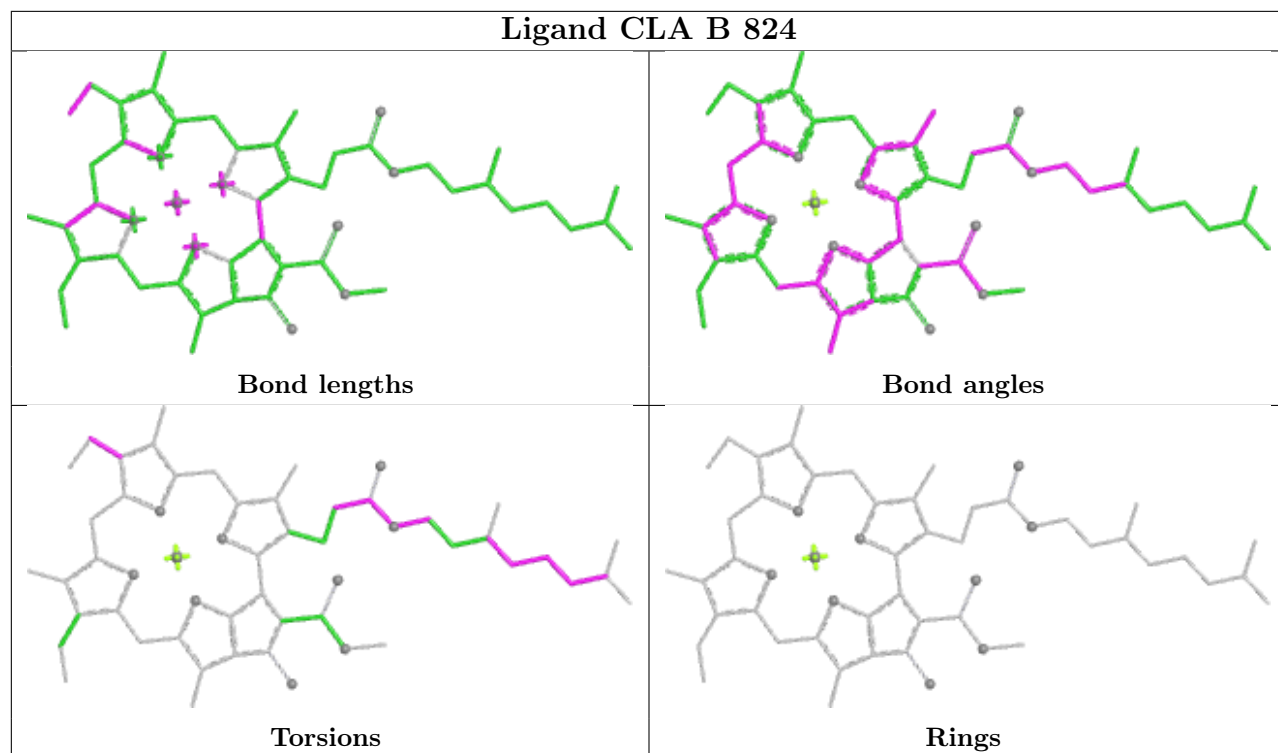
Ligand LUT 1 5003	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR I 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

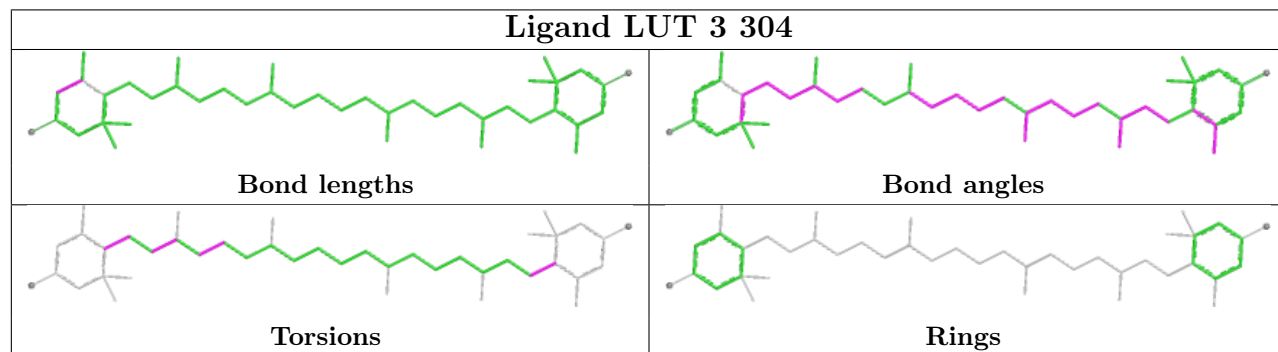
Ligand BCR 2 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

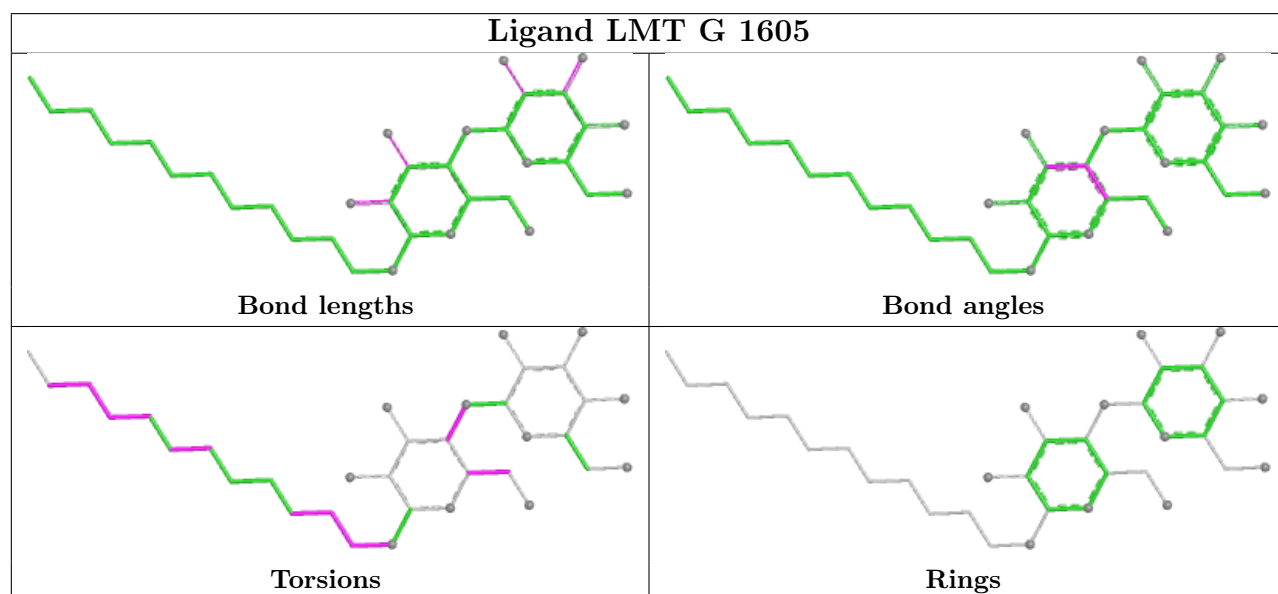
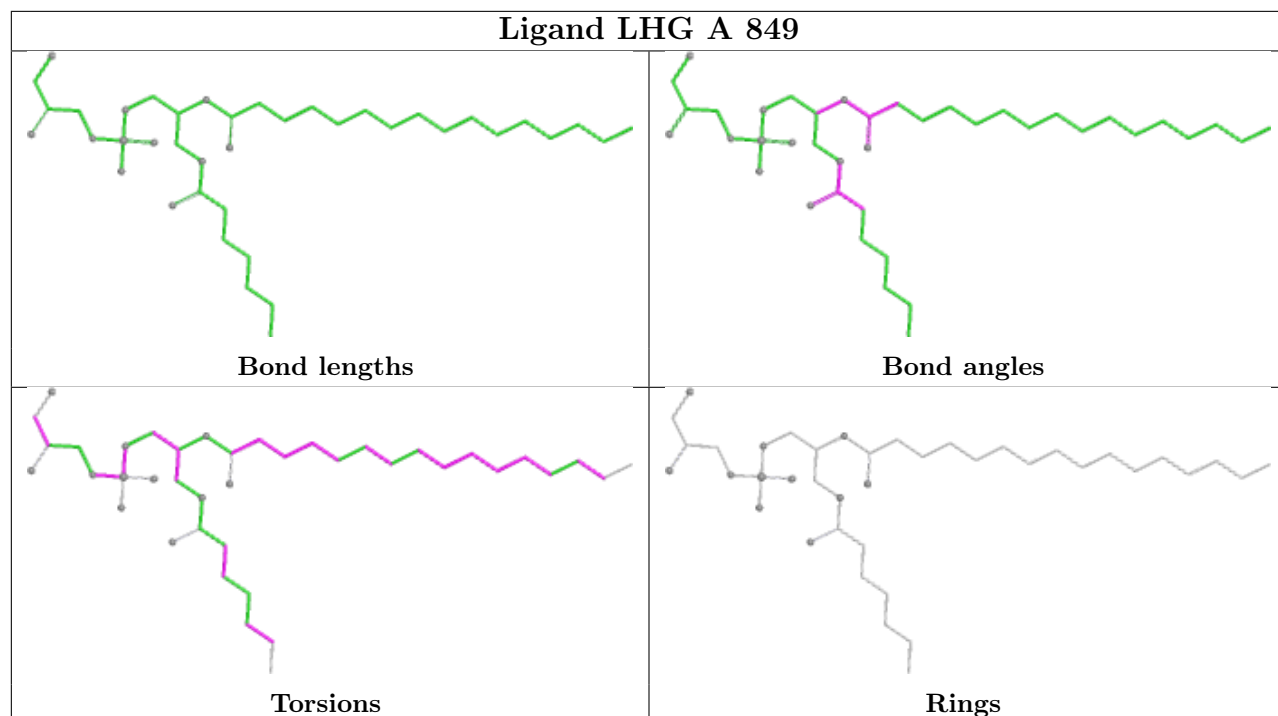
Ligand CLA K 1402	
	
Bond lengths	Bond angles
	
Torsions	Rings

## Ligand CLA B 824

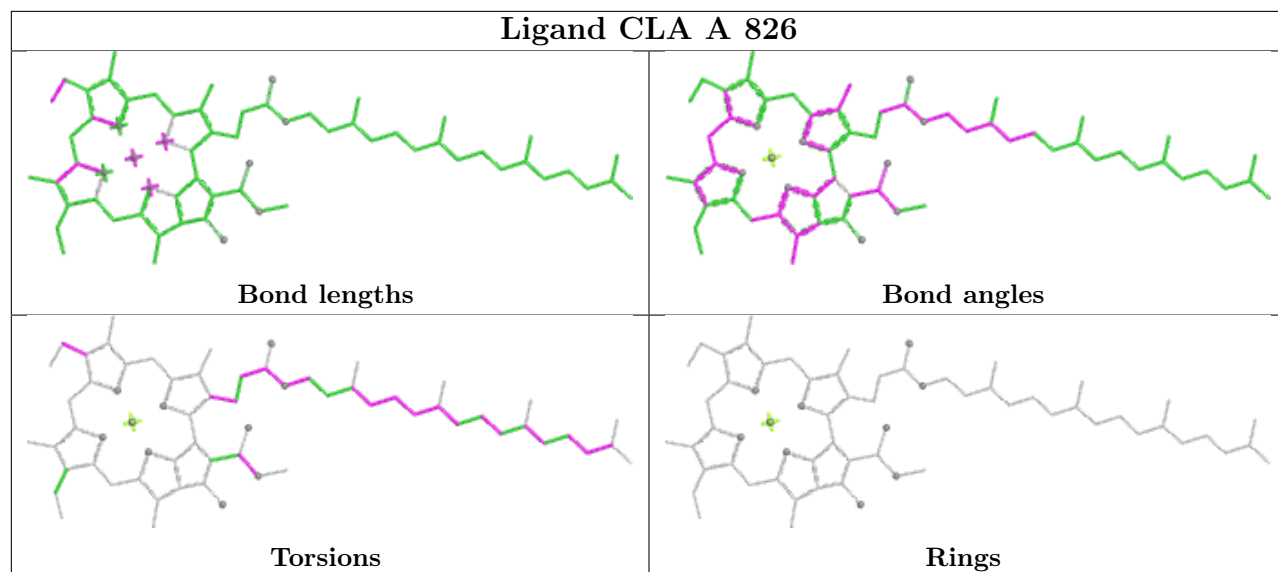


## Ligand LUT 3 304

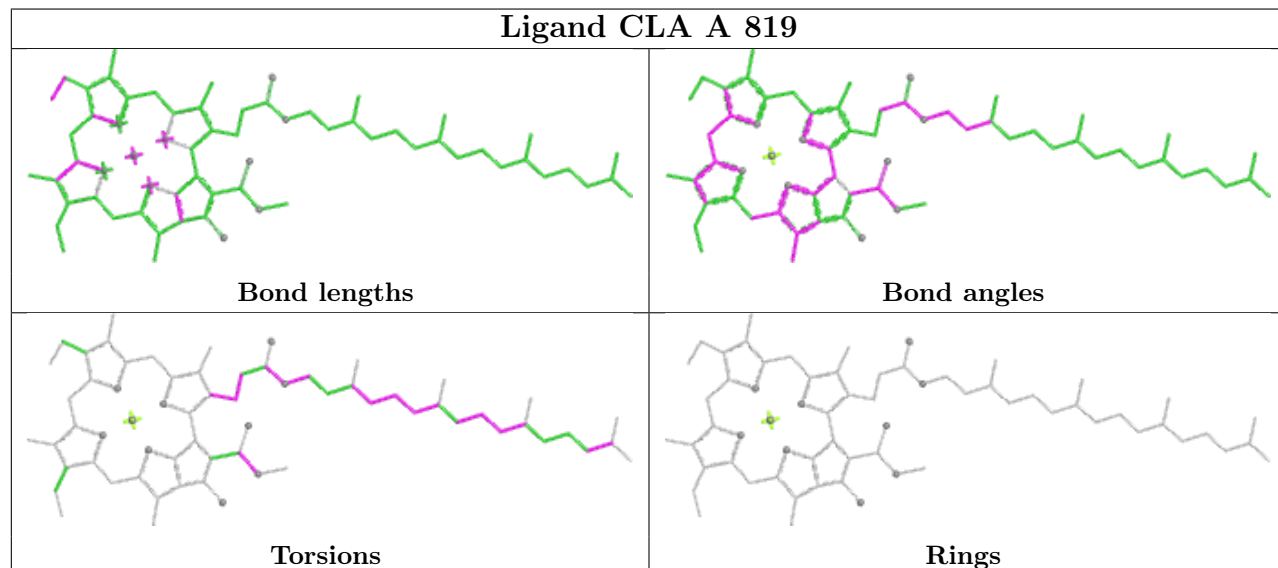




## Ligand CLA A 826

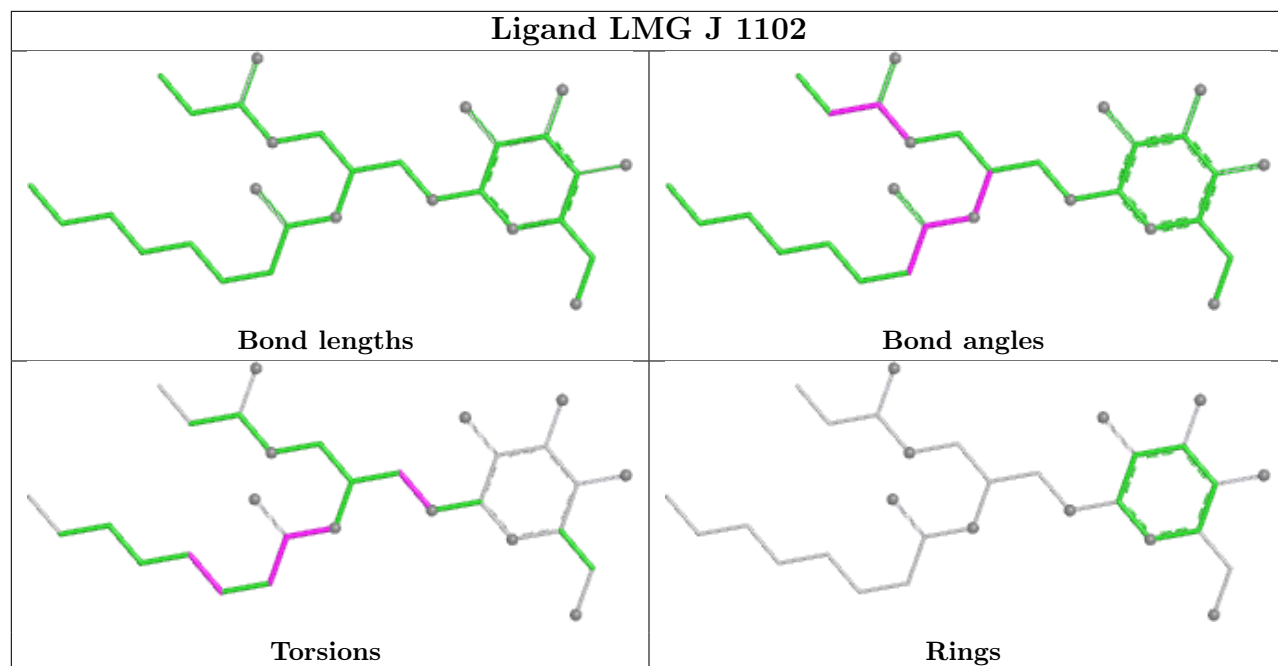


## Ligand CLA A 819

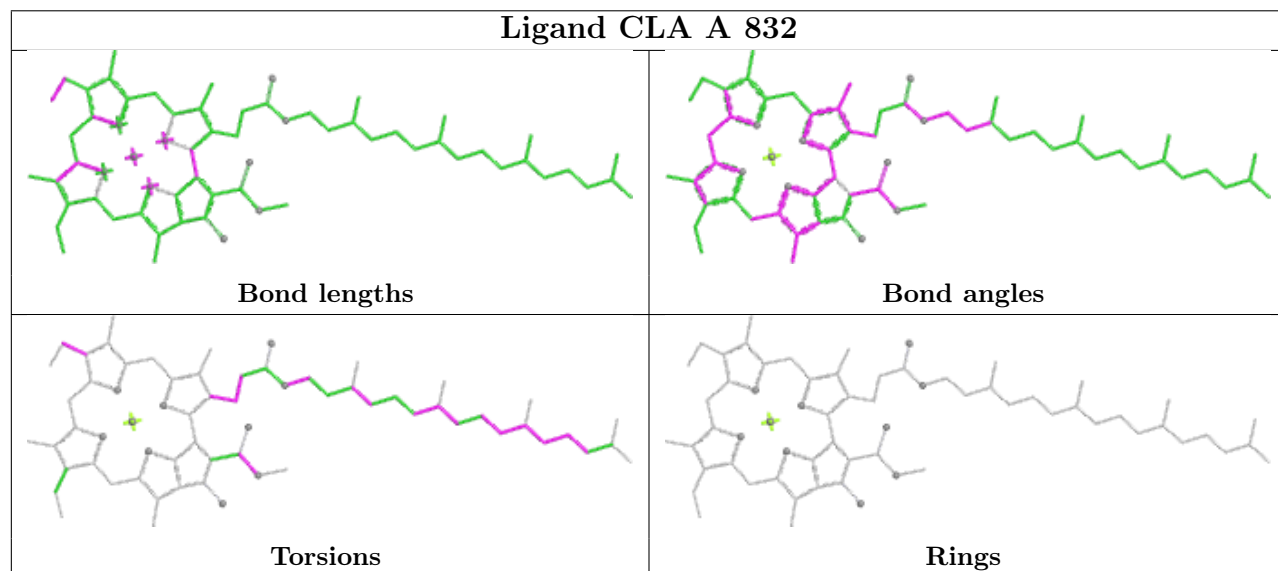


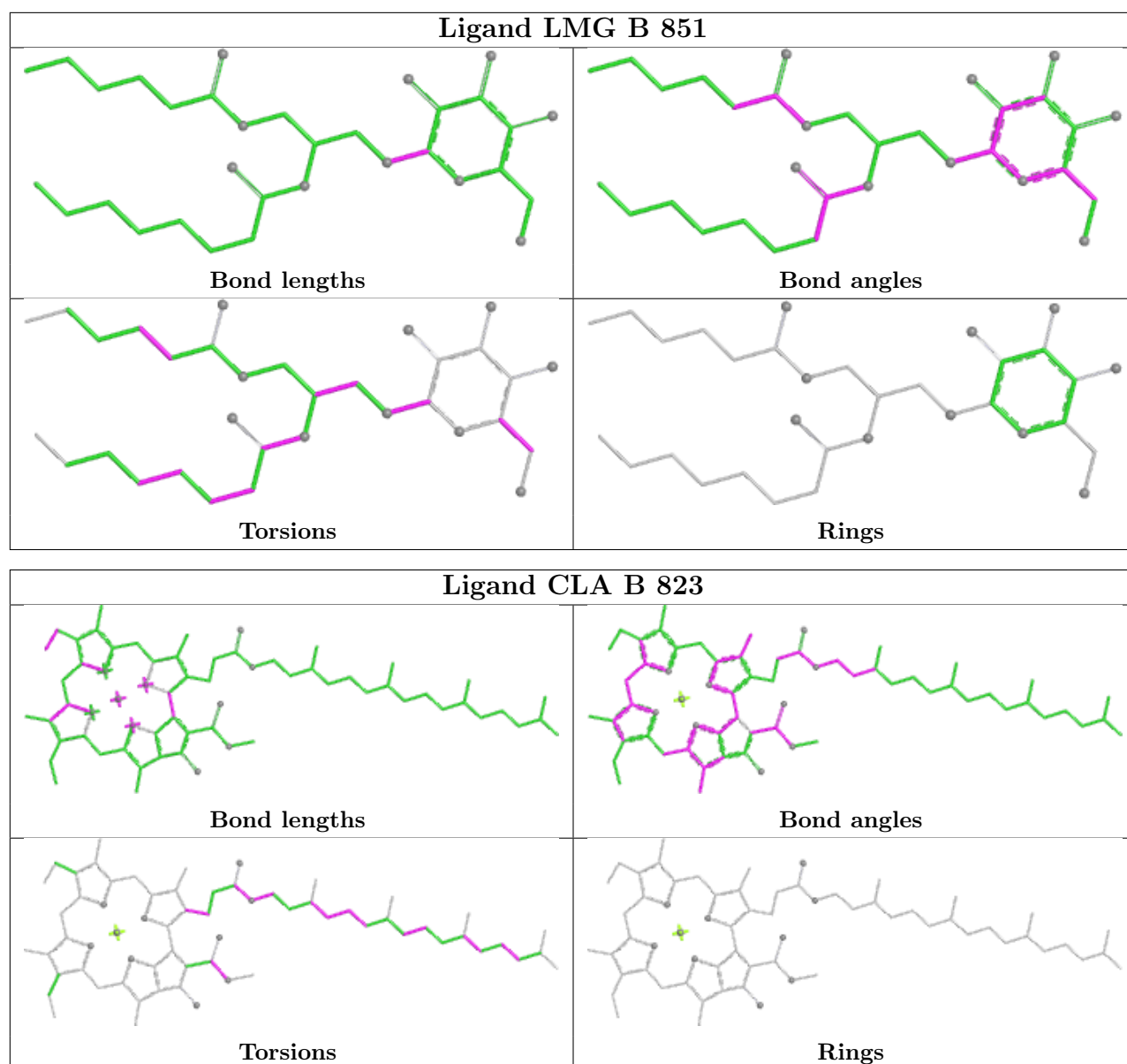


## Ligand LMG J 1102



## Ligand CLA A 832





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	743/743 (100%)	0.26	41 (5%) 30 15	68, 103, 151, 196	0
2	B	733/733 (100%)	0.42	68 (9%) 14 7	67, 101, 138, 182	0
3	C	80/80 (100%)	0.53	7 (8%) 15 8	77, 95, 158, 180	0
4	D	143/143 (100%)	0.60	17 (11%) 9 5	77, 105, 128, 151	0
5	E	66/66 (100%)	0.35	7 (10%) 11 6	85, 113, 168, 180	0
6	F	154/154 (100%)	0.06	6 (3%) 43 24	82, 105, 141, 156	0
7	G	97/97 (100%)	0.53	12 (12%) 8 5	109, 139, 165, 199	0
8	H	88/88 (100%)	0.36	8 (9%) 15 8	100, 132, 160, 169	0
9	I	30/30 (100%)	0.30	3 (10%) 12 7	97, 115, 132, 154	0
10	J	42/42 (100%)	-0.16	2 (4%) 35 19	82, 96, 138, 171	0
11	K	80/80 (100%)	0.22	3 (3%) 44 24	142, 177, 208, 219	0
12	L	157/157 (100%)	0.76	26 (16%) 4 3	96, 125, 173, 204	0
13	1	193/193 (100%)	0.77	27 (13%) 6 4	124, 156, 201, 228	0
14	2	208/208 (100%)	0.39	17 (8%) 17 9	106, 134, 168, 200	0
15	3	221/221 (100%)	0.91	40 (18%) 3 2	124, 161, 218, 248	0
16	4	198/198 (100%)	0.44	19 (9%) 13 7	110, 136, 174, 204	0
All	All	3233/3233 (100%)	0.43	303 (9%) 14 7	67, 118, 178, 248	0

All (303) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	566	GLY	11.9
2	B	565	GLY	10.5
15	3	87	GLU	9.8
3	C	35	LYS	9.7
2	B	294	ASN	8.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	295	PHE	8.0
12	L	111	VAL	7.2
3	C	34	CYS	7.0
2	B	296	GLY	7.0
13	1	161	PRO	6.9
15	3	177	ALA	6.9
7	G	114	LEU	6.1
15	3	86	PRO	6.0
12	L	115	VAL	5.8
13	1	171	SER	5.7
15	3	92	PHE	5.7
15	3	173	PHE	5.7
15	3	260	VAL	5.5
4	D	196	VAL	5.4
13	1	226	ILE	5.2
13	1	232	PRO	5.2
2	B	557	PHE	5.1
2	B	66	PHE	5.1
2	B	504	ASN	5.1
15	3	96	ARG	5.1
2	B	567	THR	5.0
13	1	225	THR	5.0
15	3	178	LYS	5.0
13	1	100	LEU	5.0
2	B	562	PRO	4.9
14	2	176	CYS	4.9
4	D	165	GLN	4.9
2	B	293	THR	4.9
13	1	60	GLY	4.8
2	B	554	GLY	4.8
4	D	199	ILE	4.7
12	L	116	LYS	4.7
12	L	62	GLY	4.7
16	4	64	GLY	4.7
12	L	114	PHE	4.6
15	3	97	TRP	4.6
2	B	136	TYR	4.5
15	3	176	TRP	4.5
2	B	297	ILE	4.5
1	A	374	HIS	4.4
2	B	292	ARG	4.4
2	B	154	TRP	4.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
8	H	115	SER	4.4
13	1	101	GLY	4.4
12	L	110	LEU	4.4
1	A	180	PHE	4.3
7	G	110	GLU	4.3
7	G	111	TYR	4.3
15	3	269	LEU	4.3
3	C	36	ALA	4.3
15	3	261	ALA	4.2
14	2	206	TRP	4.2
13	1	227	GLY	4.1
12	L	209	LEU	4.1
1	A	350	LEU	4.0
15	3	121	TYR	4.0
2	B	211	ASN	4.0
4	D	71	THR	4.0
2	B	395	ILE	4.0
2	B	413	GLU	4.0
16	4	174	GLN	3.9
4	D	197	SER	3.9
1	A	33	GLN	3.9
13	1	59	PHE	3.9
2	B	555	TYR	3.9
15	3	256	LEU	3.9
13	1	229	VAL	3.9
15	3	253	TYR	3.9
4	D	75	LEU	3.9
4	D	156	TYR	3.9
14	2	58	THR	3.9
8	H	80	SER	3.9
1	A	373	ALA	3.9
1	A	46	LYS	3.8
1	A	492	ILE	3.8
1	A	75	SER	3.8
12	L	128	GLN	3.8
15	3	271	SER	3.8
4	D	200	GLU	3.8
15	3	229	LYS	3.7
16	4	143	VAL	3.7
14	2	70	GLY	3.7
1	A	584	PRO	3.7
2	B	229	GLN	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	299	HIS	3.7
15	3	246	LEU	3.7
2	B	563	GLY	3.7
15	3	267	ASN	3.6
4	D	208	PRO	3.6
16	4	196	PRO	3.6
1	A	386	ALA	3.6
15	3	257	LEU	3.6
2	B	67	HIS	3.6
1	A	100	GLY	3.5
16	4	175	TYR	3.5
1	A	183	TRP	3.5
12	L	210	PRO	3.5
7	G	113	SER	3.5
12	L	172	GLN	3.5
1	A	264	GLU	3.5
2	B	568	CYS	3.5
16	4	139	SER	3.5
15	3	258	ASP	3.4
15	3	59	PHE	3.4
13	1	103	GLY	3.4
13	1	64	LEU	3.4
1	A	387	THR	3.4
5	E	98	ASN	3.4
2	B	552	ASP	3.4
7	G	115	LEU	3.4
11	K	91	LEU	3.4
13	1	172	LYS	3.4
2	B	571	SER	3.3
2	B	157	LEU	3.3
4	D	72	PRO	3.3
6	F	227	VAL	3.3
2	B	68	VAL	3.3
13	1	135	LEU	3.2
15	3	103	VAL	3.2
2	B	70	TRP	3.2
13	1	230	LEU	3.2
4	D	166	TYR	3.2
15	3	275	HIS	3.2
1	A	511	THR	3.2
14	2	127	THR	3.2
12	L	170	LYS	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
13	1	58	ASP	3.1
15	3	62	LYS	3.1
4	D	201	VAL	3.1
16	4	173	LYS	3.1
7	G	92	LEU	3.1
5	E	64	PRO	3.1
2	B	641	ASN	3.1
15	3	225	LEU	3.1
8	H	140	GLY	3.1
1	A	375	HIS	3.0
15	3	265	ASN	3.0
16	4	141	LEU	3.0
8	H	53	VAL	3.0
10	J	7	TYR	3.0
12	L	60	ILE	3.0
16	4	66	LEU	3.0
1	A	184	PHE	3.0
13	1	228	ASN	3.0
5	E	91	VAL	2.9
12	L	124	GLU	2.9
15	3	128	ILE	2.9
15	3	272	LEU	2.9
2	B	291	TYR	2.9
2	B	119	GLY	2.9
6	F	147	HIS	2.9
15	3	94	GLU	2.9
2	B	71	GLN	2.9
4	D	99	GLU	2.8
2	B	643	LEU	2.8
12	L	127	GLY	2.8
2	B	69	ALA	2.8
2	B	456	GLU	2.8
1	A	370	ILE	2.8
2	B	505	SER	2.8
1	A	249	ILE	2.8
16	4	59	GLY	2.8
15	3	255	ASN	2.8
1	A	277	TYR	2.8
13	1	153	LYS	2.7
14	2	227	LEU	2.7
4	D	206	LYS	2.7
12	L	133	ALA	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
14	2	169	ALA	2.7
1	A	583	GLY	2.7
5	E	109	LYS	2.7
1	A	162	LEU	2.7
9	I	30	LYS	2.6
2	B	298	GLY	2.6
16	4	226	GLY	2.6
2	B	699	ALA	2.6
14	2	230	LEU	2.6
15	3	247	VAL	2.6
3	C	33	GLY	2.6
2	B	172	GLU	2.6
12	L	186	THR	2.6
14	2	209	ALA	2.6
15	3	248	THR	2.6
1	A	322	GLY	2.6
7	G	104	GLY	2.6
2	B	616	LEU	2.6
16	4	140	THR	2.6
8	H	78	TYR	2.6
15	3	262	ASP	2.6
12	L	113	PRO	2.5
16	4	119	GLY	2.5
14	2	204	LEU	2.5
15	3	124	LYS	2.5
1	A	45	ALA	2.5
5	E	97	PRO	2.5
7	G	93	PRO	2.5
12	L	58	GLN	2.5
2	B	165	VAL	2.5
8	H	111	LEU	2.5
2	B	561	GLY	2.5
12	L	201	PHE	2.5
14	2	137	TRP	2.5
4	D	118	GLY	2.5
9	I	23	SER	2.4
11	K	47	ILE	2.4
16	4	144	ILE	2.4
14	2	248	ASP	2.4
16	4	227	LYS	2.4
4	D	102	VAL	2.4
13	1	56	PRO	2.4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	215	VAL	2.4
15	3	245	GLY	2.4
4	D	117	THR	2.4
16	4	122	ASN	2.4
2	B	300	SER	2.4
2	B	206	TYR	2.3
2	B	733	PHE	2.3
6	F	211	PHE	2.3
2	B	550	LYS	2.3
12	L	146	THR	2.3
2	B	559	CYS	2.3
12	L	63	ASP	2.3
16	4	52	LYS	2.3
1	A	261	SER	2.3
8	H	59	ASP	2.3
2	B	630	GLN	2.3
12	L	64	PRO	2.3
13	1	132	PRO	2.3
2	B	171	ALA	2.3
14	2	208	SER	2.3
7	G	58	LEU	2.3
2	B	642	SER	2.3
10	J	42	PHE	2.3
1	A	644	GLN	2.3
3	C	75	ARG	2.3
6	F	87	ASP	2.3
13	1	61	PHE	2.2
1	A	377	TYR	2.2
1	A	382	TYR	2.2
2	B	207	VAL	2.2
2	B	669	GLY	2.2
15	3	91	GLY	2.2
3	C	26	LEU	2.2
8	H	73	ASP	2.2
6	F	224	GLY	2.2
11	K	80	ALA	2.2
13	1	204	ALA	2.2
1	A	43	THR	2.2
16	4	67	THR	2.2
12	L	54	TYR	2.2
13	1	205	TYR	2.2
15	3	66	SER	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
13	1	157	LYS	2.2
2	B	581	PHE	2.2
14	2	168	TRP	2.2
1	A	187	HIS	2.2
7	G	112	VAL	2.2
12	L	97	LEU	2.2
2	B	640	MET	2.2
2	B	551	LYS	2.2
2	B	558	PRO	2.2
14	2	170	ASP	2.2
2	B	100	ALA	2.1
2	B	604	GLY	2.1
13	1	162	GLY	2.1
5	E	94	ASP	2.1
5	E	96	ASP	2.1
7	G	126	VAL	2.1
14	2	171	ILE	2.1
2	B	135	LEU	2.1
1	A	292	GLY	2.1
6	F	113	SER	2.1
15	3	84	SER	2.1
15	3	212	GLY	2.1
12	L	206	VAL	2.1
9	I	27	HIS	2.1
1	A	276	LYS	2.1
1	A	42	ARG	2.1
1	A	643	ALA	2.1
1	A	354	TRP	2.1
2	B	361	ILE	2.1
14	2	194	GLY	2.1
2	B	210	ASN	2.1
16	4	210	LEU	2.1
13	1	62	ASP	2.1
7	G	106	THR	2.1
1	A	587	GLY	2.1
1	A	40	PHE	2.1
1	A	513	LEU	2.0
2	B	570	ILE	2.0
1	A	67	HIS	2.0
2	B	560	ASP	2.0
3	C	50	GLY	2.0
2	B	214	SER	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
12	L	125	ILE	2.0
1	A	582	ASP	2.0
2	B	204	GLY	2.0
1	A	611	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	LMT	J	1107	25/35	0.21	0.17	151,182,201,206	0
23	LMT	2	325	35/35	0.24	0.17	157,224,241,245	0
18	CLA	K	1404	46/65	0.43	0.17	170,208,235,242	0
24	LMG	2	302	13/55	0.51	0.24	130,165,187,190	0
23	LMT	G	1606	31/35	0.53	0.15	144,198,232,237	0
24	LMG	2	301	13/55	0.56	0.14	148,168,192,202	0
23	LMT	A	850	35/35	0.57	0.18	79,146,165,174	0
26	DGD	1	5002	35/66	0.64	0.27	125,209,233,236	0
24	LMG	A	851	50/55	0.65	0.17	136,173,197,203	0
23	LMT	B	852	35/35	0.65	0.13	114,212,231,232	0
24	LMG	2	323	13/55	0.68	0.16	126,164,190,192	0
24	LMG	4	320	13/55	0.68	0.15	166,194,213,219	0
24	LMG	B	850	35/55	0.68	0.21	74,146,176,185	0
18	CLA	3	314	48/65	0.69	0.17	159,194,205,208	0
18	CLA	K	1403	48/65	0.70	0.14	166,197,226,242	0
21	BCR	2	305	40/40	0.71	0.26	131,154,181,186	0
18	CLA	H	1701	60/65	0.72	0.19	148,175,199,206	0
24	LMG	1	5001	49/55	0.73	0.26	91,156,219,221	0
24	LMG	2	321	25/55	0.74	0.15	114,144,164,168	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
18	CLA	K	1402	60/65	0.74	0.16	100,164,183,192	0
18	CLA	J	1103	50/65	0.75	0.17	92,155,195,209	0
24	LMG	2	324	13/55	0.76	0.11	159,183,205,212	0
24	LMG	F	307	36/55	0.76	0.21	125,159,194,197	0
25	GOL	4	321	6/6	0.76	0.19	135,146,153,158	0
22	LHG	B	849	49/49	0.76	0.21	101,139,196,220	0
18	CLA	1	5015	65/65	0.77	0.20	140,176,193,202	0
24	LMG	B	851	33/55	0.77	0.20	133,208,223,227	0
23	LMT	B	856	31/35	0.77	0.12	138,156,173,179	0
30	CHL	3	313	51/66	0.77	0.17	185,220,249,260	0
21	BCR	L	302	40/40	0.78	0.16	118,167,216,221	0
24	LMG	J	1102	30/55	0.78	0.14	103,123,146,159	0
18	CLA	K	1401	45/65	0.79	0.14	133,166,181,194	0
21	BCR	K	1405	40/40	0.79	0.17	138,166,194,201	0
24	LMG	2	322	36/55	0.79	0.14	111,177,212,217	0
21	BCR	3	306	40/40	0.80	0.17	134,160,182,188	0
30	CHL	3	312	51/66	0.80	0.12	141,157,177,183	0
24	LMG	G	1607	25/55	0.80	0.19	130,194,215,220	0
23	LMT	B	853	32/35	0.81	0.13	121,153,174,179	0
24	LMG	B	854	13/55	0.82	0.14	131,170,201,202	0
23	LMT	G	1605	35/35	0.82	0.12	116,177,214,218	0
18	CLA	G	1603	65/65	0.82	0.23	127,161,197,202	0
23	LMT	4	319	35/35	0.82	0.14	95,179,207,207	0
24	LMG	1	5020	46/55	0.83	0.18	88,157,201,209	0
18	CLA	1	5006	65/65	0.83	0.16	137,169,186,193	0
18	CLA	G	1602	46/65	0.83	0.11	132,158,180,206	0
26	DGD	F	309	57/66	0.83	0.21	105,158,186,192	0
22	LHG	1	5019	49/49	0.83	0.21	112,135,168,176	0
30	CHL	2	315	56/66	0.83	0.12	109,151,170,175	0
21	BCR	1	5005	40/40	0.83	0.15	135,175,224,229	0
18	CLA	A	840	60/65	0.83	0.13	101,147,196,206	0
18	CLA	3	308	52/65	0.84	0.12	165,202,217,224	0
24	LMG	F	308	34/55	0.84	0.13	102,163,181,202	0
26	DGD	2	327	51/66	0.84	0.16	99,129,165,174	0
30	CHL	4	317	43/66	0.84	0.12	125,162,177,190	0
30	CHL	2	319	56/66	0.85	0.15	117,147,181,192	0
29	LUT	4	303	42/42	0.85	0.19	106,128,148,160	0
29	LUT	2	303	42/42	0.85	0.19	114,132,145,159	0
30	CHL	4	313	47/66	0.85	0.13	104,133,160,176	0
30	CHL	2	318	46/66	0.85	0.12	117,142,157,175	0
21	BCR	A	846	40/40	0.86	0.20	72,100,129,147	0
18	CLA	2	311	50/65	0.86	0.10	116,139,154,158	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
18	CLA	3	319	60/65	0.86	0.17	118,140,186,194	0
21	BCR	L	307	40/40	0.86	0.15	102,130,153,164	0
29	LUT	1	5003	42/42	0.87	0.15	117,157,181,193	0
18	CLA	1	5011	50/65	0.87	0.12	146,167,182,191	0
29	LUT	3	303	42/42	0.87	0.13	145,166,176,181	0
21	BCR	G	1604	40/40	0.87	0.14	106,133,171,173	0
18	CLA	B	835	55/65	0.87	0.14	99,115,163,178	0
18	CLA	1	5018	60/65	0.87	0.18	88,137,192,196	0
18	CLA	L	304	50/65	0.87	0.14	123,151,170,179	0
18	CLA	L	306	50/65	0.87	0.14	101,134,155,170	0
18	CLA	B	808	65/65	0.87	0.16	87,100,144,165	0
18	CLA	1	5007	46/65	0.87	0.12	122,149,167,180	0
30	CHL	4	316	61/66	0.87	0.19	121,144,165,172	0
29	LUT	J	1105	42/42	0.87	0.16	89,122,148,163	0
31	XAT	2	304	44/44	0.87	0.16	106,124,144,150	0
18	CLA	1	5013	46/65	0.88	0.16	118,159,175,202	0
18	CLA	B	834	60/65	0.88	0.15	82,106,129,140	0
21	BCR	3	305	40/40	0.88	0.18	120,134,155,161	0
18	CLA	4	311	60/65	0.88	0.14	117,134,155,167	0
18	CLA	A	803	65/65	0.88	0.17	67,91,146,172	0
21	BCR	B	843	40/40	0.88	0.23	104,121,144,166	0
18	CLA	A	836	65/65	0.88	0.14	80,107,169,181	0
18	CLA	2	317	55/65	0.88	0.17	91,126,157,174	0
18	CLA	1	5012	46/65	0.88	0.12	117,149,168,183	0
18	CLA	3	309	55/65	0.88	0.13	132,175,204,219	0
22	LHG	A	849	40/49	0.89	0.14	88,125,152,155	0
30	CHL	2	316	48/66	0.89	0.17	107,124,145,160	0
18	CLA	A	833	55/65	0.89	0.14	113,137,165,171	0
18	CLA	4	312	46/65	0.89	0.14	115,145,160,175	0
25	GOL	A	854	6/6	0.89	0.13	124,136,142,142	0
29	LUT	1	5004	42/42	0.89	0.17	105,145,165,174	0
18	CLA	B	805	65/65	0.89	0.15	89,123,175,194	0
26	DGD	B	855	61/66	0.89	0.17	70,100,132,155	0
24	LMG	F	306	47/55	0.89	0.11	96,131,158,169	0
30	CHL	1	5016	61/66	0.89	0.12	114,154,166,171	0
18	CLA	3	307	55/65	0.90	0.12	148,169,183,191	0
21	BCR	B	845	40/40	0.90	0.17	92,121,179,183	0
21	BCR	B	846	40/40	0.90	0.20	73,106,123,130	0
21	BCR	B	847	40/40	0.90	0.20	73,99,115,120	0
18	CLA	G	1601	55/65	0.90	0.10	120,147,172,177	0
18	CLA	A	814	46/65	0.90	0.13	127,143,167,179	0
18	CLA	1	5017	45/65	0.90	0.11	159,182,206,210	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
21	BCR	L	303	40/40	0.90	0.18	90,108,127,135	0
30	CHL	3	310	66/66	0.90	0.16	107,148,166,194	0
18	CLA	B	816	55/65	0.90	0.13	107,133,154,171	0
18	CLA	4	310	50/65	0.90	0.14	125,146,176,189	0
28	ZEX	F	310	42/42	0.90	0.16	104,141,157,167	0
18	CLA	2	306	60/65	0.90	0.13	115,134,164,175	0
18	CLA	A	825	65/65	0.90	0.15	85,116,136,143	0
18	CLA	A	806	60/65	0.90	0.12	79,112,152,161	0
18	CLA	2	307	52/65	0.91	0.12	120,144,157,159	0
18	CLA	B	822	65/65	0.91	0.15	95,114,160,165	0
21	BCR	A	855	40/40	0.91	0.20	128,148,176,177	0
18	CLA	B	823	65/65	0.91	0.17	87,114,150,162	0
18	CLA	B	826	65/65	0.91	0.15	67,88,122,124	0
30	CHL	1	5014	47/66	0.91	0.13	139,168,192,198	0
18	CLA	A	815	65/65	0.91	0.15	135,149,171,179	0
18	CLA	A	829	65/65	0.91	0.14	78,118,173,180	0
18	CLA	B	839	65/65	0.91	0.16	82,101,124,130	0
21	BCR	I	102	40/40	0.91	0.20	83,115,133,139	0
21	BCR	J	1104	40/40	0.91	0.16	67,92,114,125	0
26	DGD	J	1106	58/66	0.91	0.13	67,115,186,193	0
18	CLA	3	318	46/65	0.91	0.10	140,158,170,172	0
18	CLA	F	302	65/65	0.91	0.17	73,107,198,210	0
27	CA	B	857	1/1	0.91	0.07	123,123,123,123	0
30	CHL	4	314	51/66	0.91	0.17	120,144,159,172	0
27	CA	3	302	1/1	0.91	0.09	129,129,129,129	0
18	CLA	B	810	65/65	0.91	0.15	87,116,141,161	0
18	CLA	A	832	65/65	0.91	0.14	92,120,139,165	0
18	CLA	B	818	65/65	0.92	0.18	82,102,119,128	0
18	CLA	4	305	60/65	0.92	0.11	119,141,161,167	0
18	CLA	A	810	65/65	0.92	0.11	70,97,115,128	0
18	CLA	2	310	65/65	0.92	0.14	107,128,155,166	0
18	CLA	1	5008	55/65	0.92	0.14	114,142,159,162	0
30	CHL	2	314	66/66	0.92	0.12	99,128,151,165	0
18	CLA	2	312	60/65	0.92	0.11	122,139,161,183	0
21	BCR	A	847	40/40	0.92	0.16	63,75,103,105	0
18	CLA	F	303	65/65	0.92	0.13	83,116,145,166	0
22	LHG	B	848	21/49	0.92	0.12	88,113,140,155	0
18	CLA	A	816	56/65	0.92	0.15	93,129,143,150	0
18	CLA	A	824	55/65	0.92	0.15	82,99,124,135	0
18	CLA	B	811	65/65	0.92	0.15	82,109,139,151	0
30	CHL	3	316	47/66	0.92	0.13	135,159,171,181	0
18	CLA	3	311	55/65	0.92	0.15	113,139,155,160	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
18	CLA	L	305	60/65	0.92	0.14	93,121,133,146	0
18	CLA	3	315	65/65	0.92	0.13	115,153,164,191	0
18	CLA	3	317	50/65	0.92	0.14	111,145,156,171	0
18	CLA	B	801	65/65	0.92	0.17	63,84,96,109	0
31	XAT	4	304	44/44	0.92	0.13	92,127,146,156	0
21	BCR	A	844	40/40	0.93	0.20	87,115,169,186	0
21	BCR	A	845	40/40	0.93	0.12	79,99,155,162	0
18	CLA	A	838	65/65	0.93	0.14	64,84,119,134	0
18	CLA	A	809	50/65	0.93	0.14	97,128,146,159	0
18	CLA	A	852	65/65	0.93	0.14	70,91,105,112	0
18	CLA	A	853	65/65	0.93	0.14	84,105,130,138	0
21	BCR	B	844	40/40	0.93	0.15	81,109,151,165	0
18	CLA	A	820	60/65	0.93	0.12	121,148,178,189	0
18	CLA	B	827	65/65	0.93	0.14	74,94,112,120	0
18	CLA	B	828	65/65	0.93	0.16	72,100,128,141	0
21	BCR	F	305	40/40	0.93	0.14	76,98,116,120	0
29	LUT	3	304	42/42	0.93	0.17	116,146,169,173	0
18	CLA	2	313	50/65	0.93	0.09	121,134,153,157	0
18	CLA	B	829	65/65	0.93	0.16	78,93,111,127	0
18	CLA	B	832	60/65	0.93	0.15	70,99,137,153	0
18	CLA	L	301	55/65	0.93	0.15	89,120,136,145	0
18	CLA	B	833	58/65	0.93	0.12	65,87,107,117	0
18	CLA	A	821	60/65	0.93	0.12	122,149,190,193	0
18	CLA	A	823	65/65	0.93	0.16	82,110,130,137	0
18	CLA	B	837	65/65	0.93	0.12	68,88,105,114	0
18	CLA	B	838	50/65	0.93	0.13	69,91,103,126	0
18	CLA	A	834	51/65	0.93	0.14	81,106,134,147	0
18	CLA	1	5009	65/65	0.93	0.11	91,137,151,157	0
21	BCR	4	301	40/40	0.93	0.20	120,140,157,165	0
30	CHL	4	302	56/66	0.93	0.12	109,129,143,148	0
18	CLA	B	840	65/65	0.93	0.14	74,97,120,127	0
18	CLA	4	306	50/65	0.93	0.11	118,145,159,169	0
18	CLA	B	841	65/65	0.93	0.12	72,107,126,133	0
18	CLA	A	811	55/65	0.93	0.13	102,127,140,151	0
18	CLA	B	812	60/65	0.93	0.11	94,128,153,169	0
18	CLA	4	315	65/65	0.93	0.16	107,134,164,176	0
18	CLA	A	822	65/65	0.94	0.13	78,93,121,129	0
18	CLA	A	826	65/65	0.94	0.12	66,88,109,121	0
18	CLA	B	815	65/65	0.94	0.10	96,116,136,155	0
22	LHG	2	320	35/49	0.94	0.14	101,131,149,160	0
18	CLA	2	308	65/65	0.94	0.12	113,132,152,167	0
21	BCR	F	304	40/40	0.94	0.14	67,85,100,105	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
18	CLA	A	835	65/65	0.94	0.13	89,114,148,162	0
18	CLA	4	308	60/65	0.94	0.10	92,118,142,153	0
21	BCR	I	101	40/40	0.94	0.14	85,108,125,129	0
18	CLA	B	830	65/65	0.94	0.13	77,98,128,139	0
18	CLA	B	831	65/65	0.94	0.14	69,88,115,121	0
18	CLA	B	817	60/65	0.94	0.15	110,133,148,156	0
18	CLA	A	813	65/65	0.94	0.13	104,133,165,180	0
21	BCR	A	843	40/40	0.94	0.18	86,116,155,162	0
18	CLA	B	820	65/65	0.94	0.14	84,106,123,152	0
18	CLA	J	1101	65/65	0.94	0.10	65,87,114,129	0
18	CLA	B	821	46/65	0.94	0.12	110,126,143,155	0
18	CLA	B	836	55/65	0.94	0.12	74,92,108,115	0
18	CLA	A	831	65/65	0.94	0.14	81,104,128,146	0
21	BCR	B	802	40/40	0.94	0.16	72,100,119,128	0
22	LHG	A	848	49/49	0.94	0.15	63,90,107,112	0
18	CLA	A	807	65/65	0.94	0.13	66,84,106,119	0
18	CLA	B	825	65/65	0.95	0.12	77,94,120,134	0
18	CLA	A	828	65/65	0.95	0.13	64,79,99,118	0
18	CLA	B	813	46/65	0.95	0.09	107,126,142,166	0
18	CLA	A	817	65/65	0.95	0.18	84,115,134,143	0
18	CLA	B	803	65/65	0.95	0.14	64,81,98,107	0
18	CLA	F	301	65/65	0.95	0.10	65,87,105,109	0
18	CLA	A	830	65/65	0.95	0.13	77,95,108,122	0
18	CLA	B	806	65/65	0.95	0.12	76,92,112,121	0
18	CLA	A	802	65/65	0.95	0.11	62,77,96,111	0
18	CLA	B	809	65/65	0.95	0.13	79,108,122,129	0
18	CLA	A	812	65/65	0.95	0.13	92,113,130,139	0
18	CLA	4	307	65/65	0.95	0.12	109,135,157,165	0
17	CLO	A	801	65/65	0.95	0.14	65,86,99,118	0
18	CLA	4	309	60/65	0.95	0.12	83,123,138,143	0
18	CLA	B	824	55/65	0.95	0.12	82,105,123,133	0
18	CLA	1	5010	65/65	0.95	0.12	89,146,162,180	0
18	CLA	2	326	50/65	0.95	0.11	94,114,150,160	0
30	CHL	4	318	56/66	0.95	0.12	109,134,178,182	0
18	CLA	3	301	45/65	0.95	0.11	120,138,174,192	0
19	PQN	B	842	33/33	0.95	0.13	67,84,105,120	0
18	CLA	B	814	65/65	0.96	0.11	84,107,122,131	0
18	CLA	A	827	65/65	0.96	0.14	81,99,115,120	0
18	CLA	A	839	65/65	0.96	0.10	61,82,97,106	0
18	CLA	B	807	65/65	0.96	0.10	73,93,108,115	0
18	CLA	2	309	65/65	0.96	0.12	99,121,132,145	0
18	CLA	A	819	65/65	0.96	0.11	78,111,133,145	0

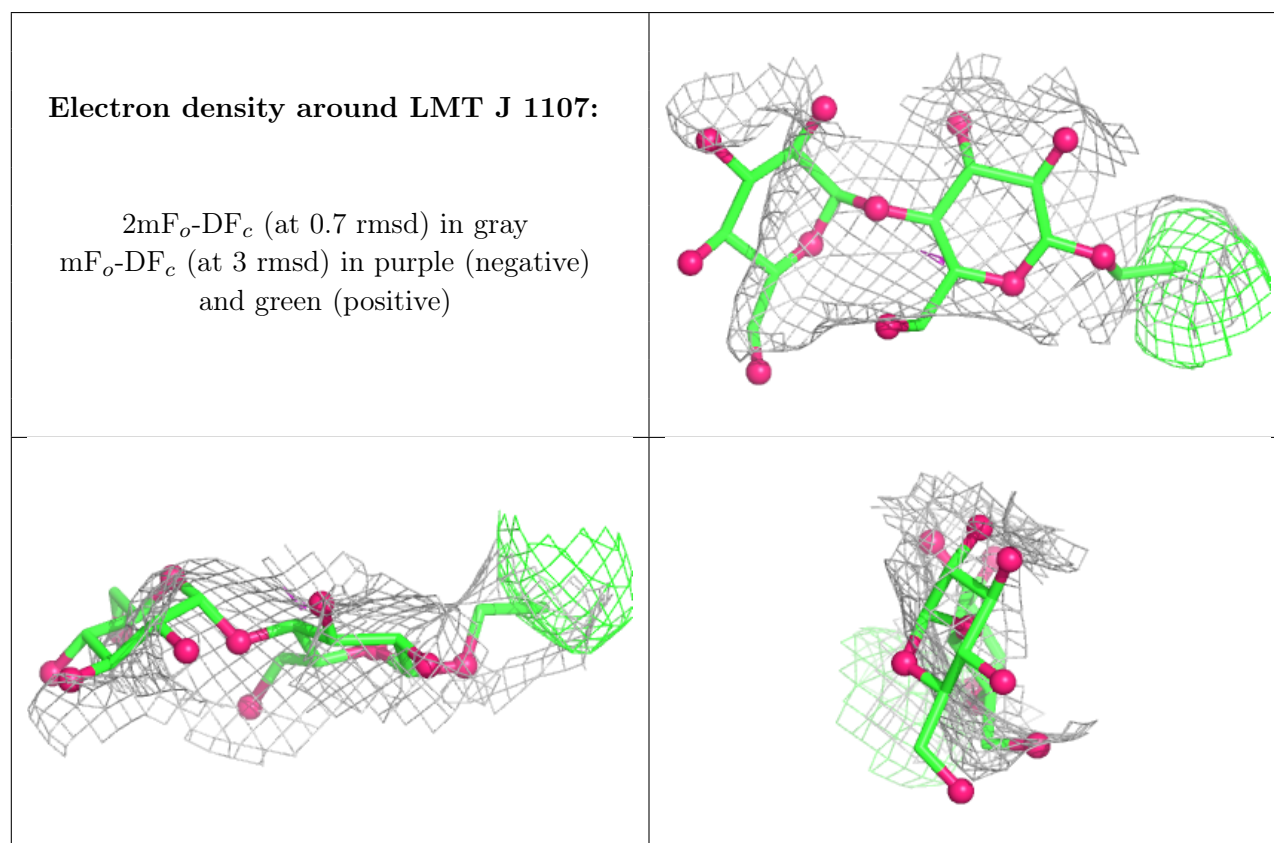
*Continued on next page...*



Continued from previous page...

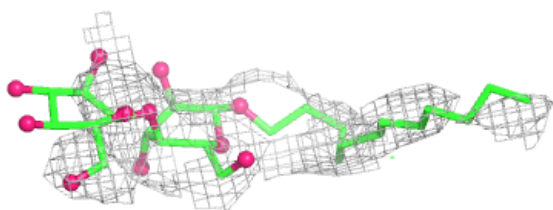
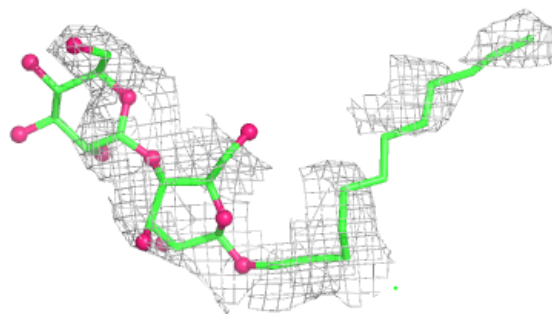
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
19	PQN	A	841	33/33	0.96	0.14	63,82,97,104	0
18	CLA	B	819	65/65	0.96	0.14	82,104,123,132	0
18	CLA	A	804	65/65	0.96	0.11	78,91,114,138	0
18	CLA	A	805	65/65	0.96	0.10	65,86,103,115	0
18	CLA	A	808	65/65	0.96	0.10	67,85,132,144	0
18	CLA	A	837	65/65	0.96	0.10	63,77,94,114	0
18	CLA	B	804	65/65	0.96	0.12	69,90,105,117	0
18	CLA	A	818	50/65	0.97	0.11	101,128,151,163	0
20	SF4	A	842	8/8	0.98	0.08	70,71,119,144	0
20	SF4	C	102	8/8	0.98	0.06	79,89,122,145	0
20	SF4	C	101	8/8	0.99	0.05	69,86,120,124	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.



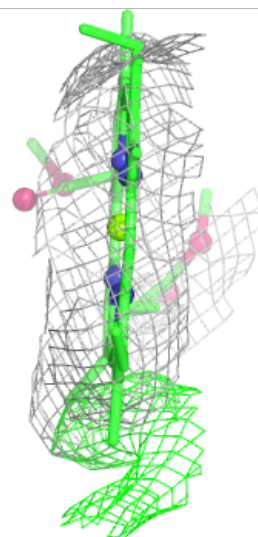
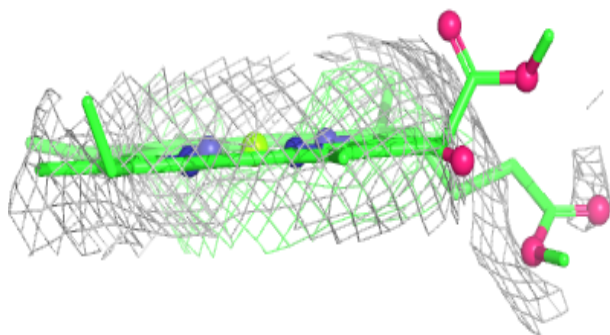
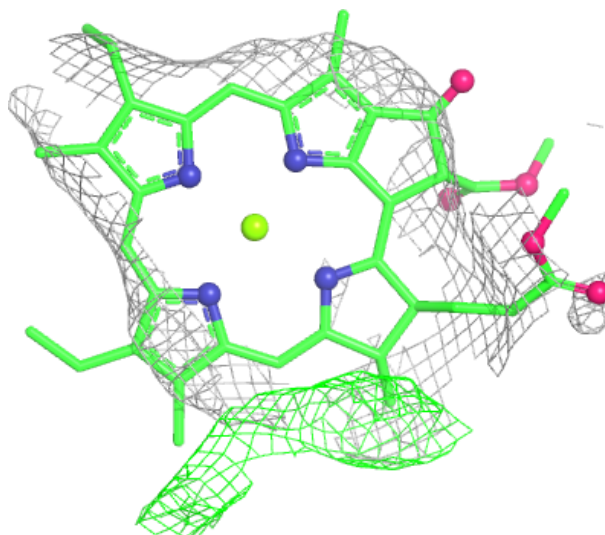
**Electron density around LMT 2 325:**

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



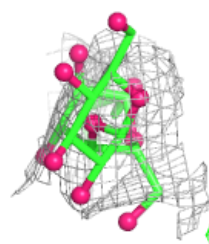
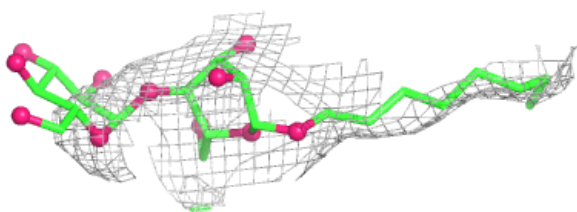
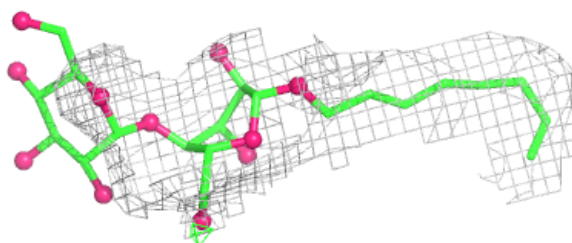
**Electron density around CLA K 1404:**

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

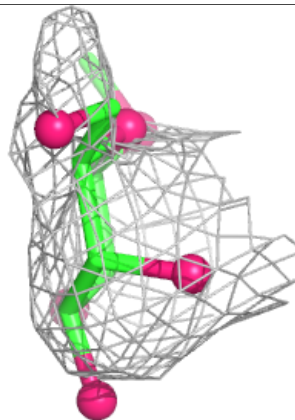
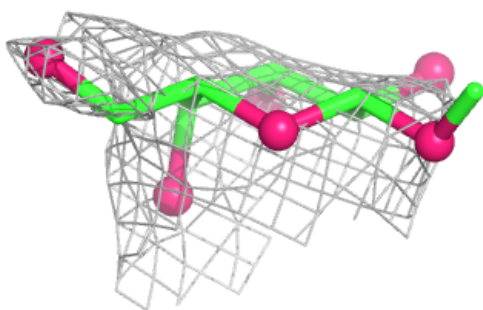
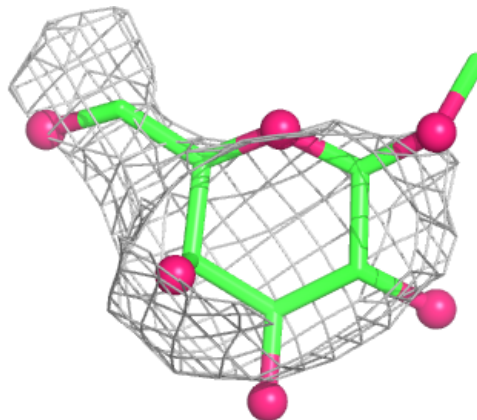


**Electron density around LMT G 1606:**

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

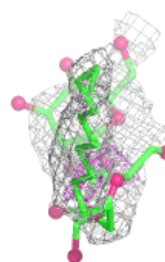
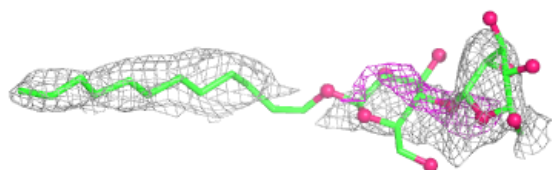
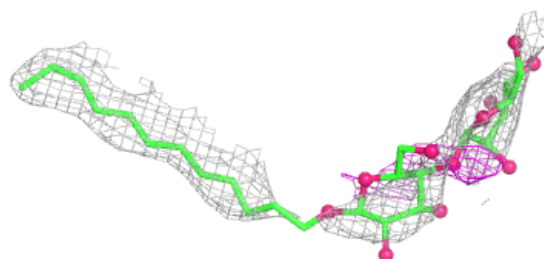
**Electron density around LMG 2 301:**

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

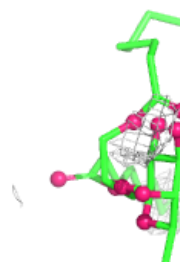
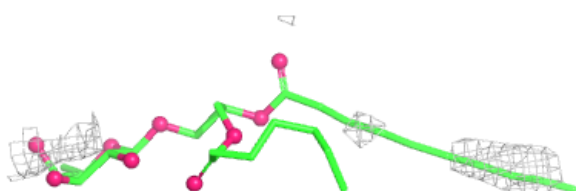
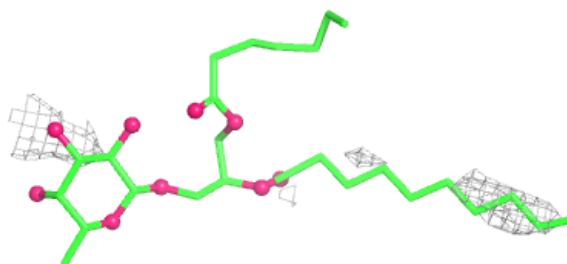


**Electron density around LMT A 850:**

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

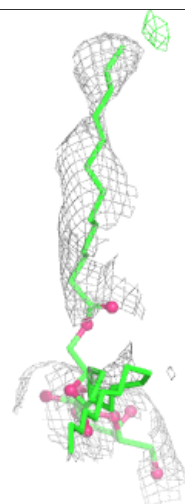
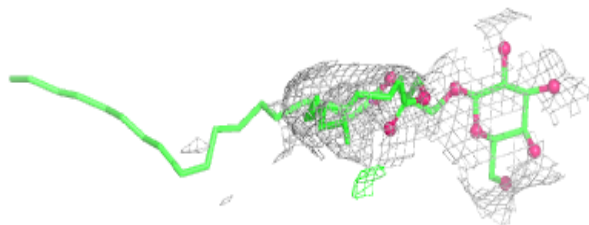
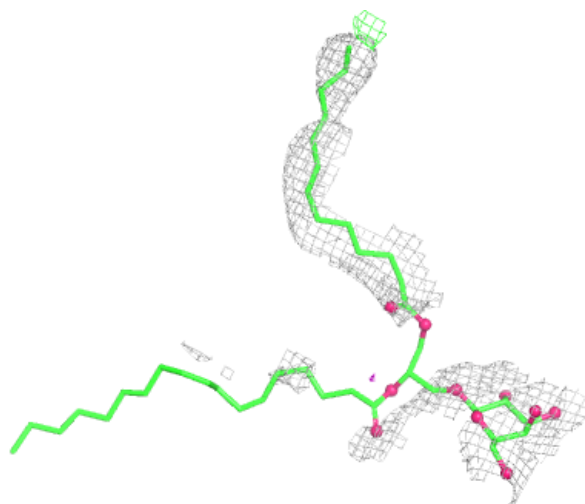
**Electron density around DGD 1 5002:**

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



**Electron density around LMG A 851:**

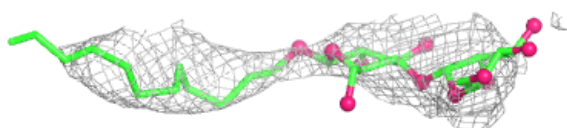
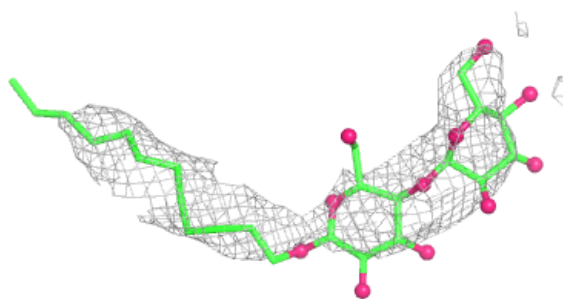
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



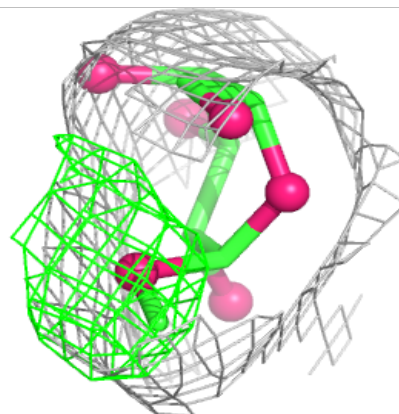
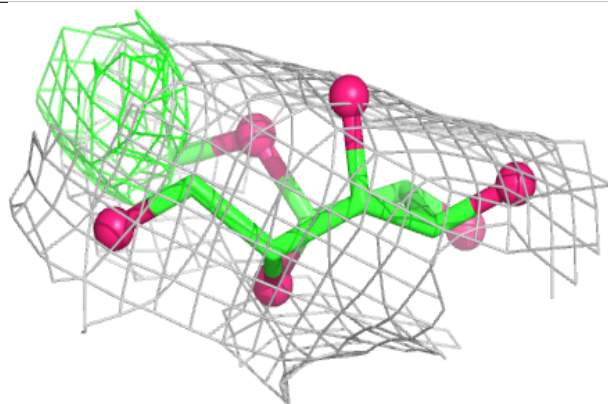
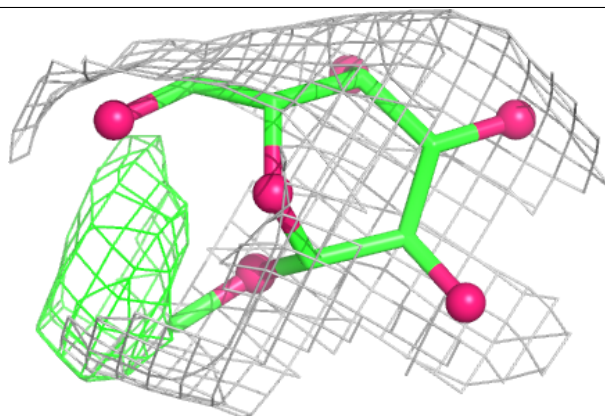


**Electron density around LMT B 852:**

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

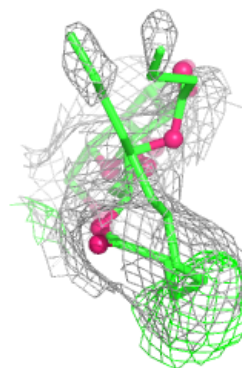
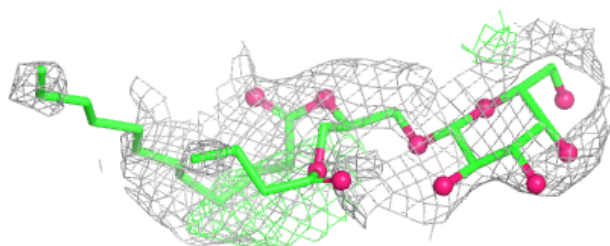
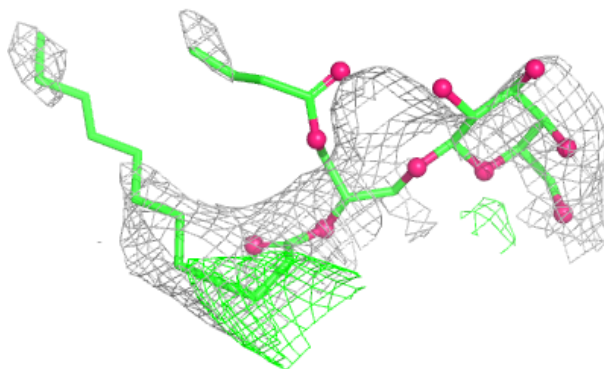
**Electron density around LMG 2 323:**

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

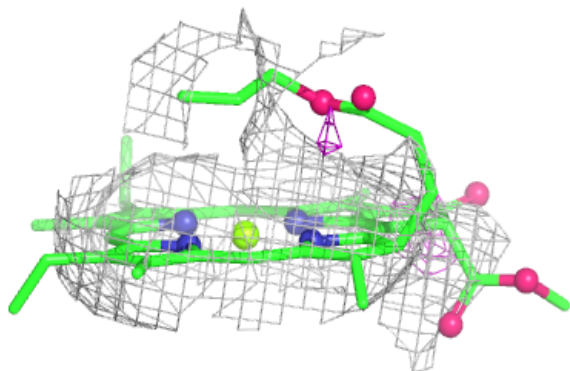
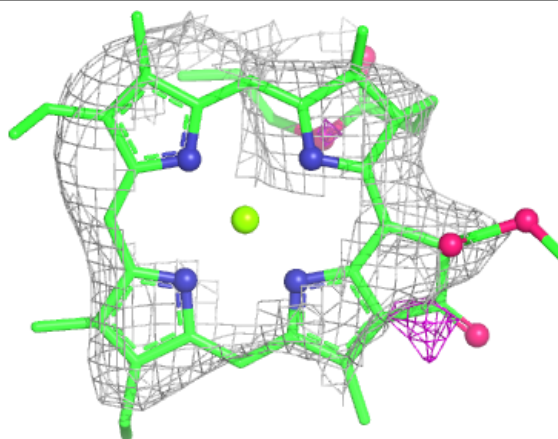


**Electron density around LMG B 850:**

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

**Electron density around CLA 3 314:**

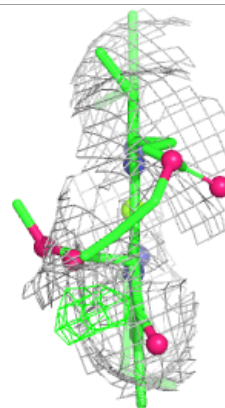
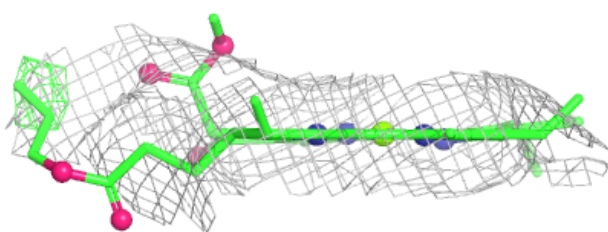
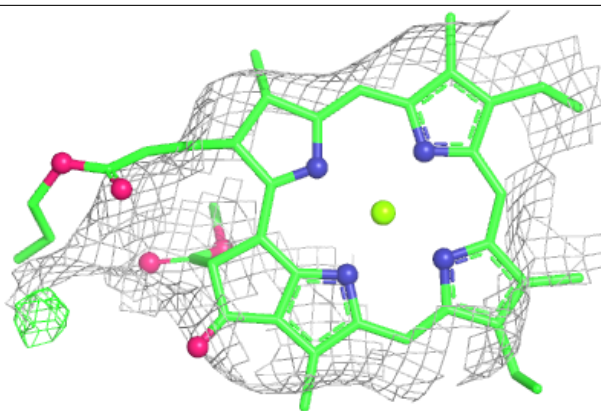
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



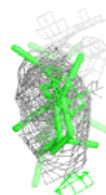
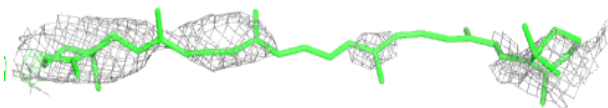
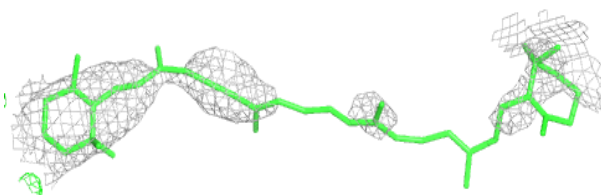


**Electron density around CLA K 1403:**

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

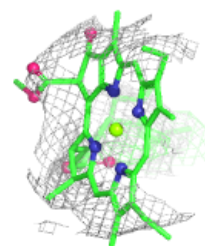
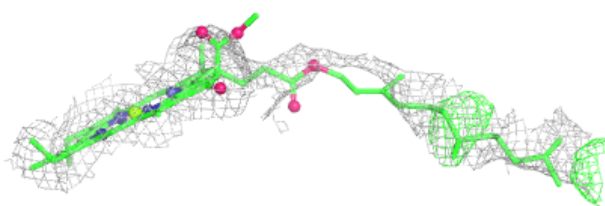
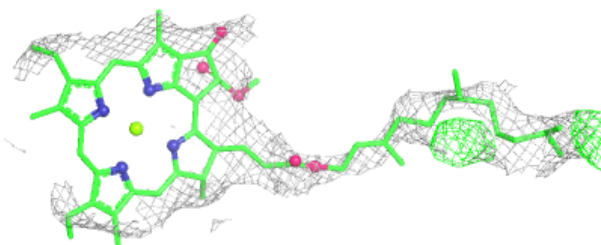
**Electron density around BCR 2 305:**

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



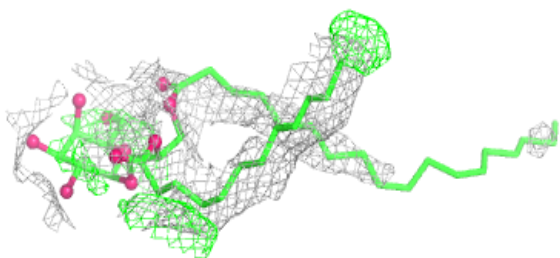
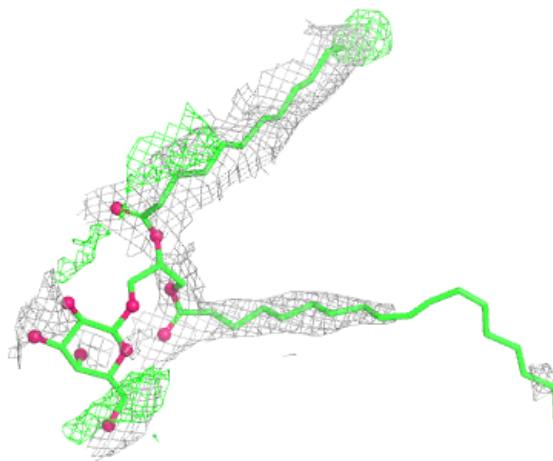
**Electron density around CLA H 1701:**

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



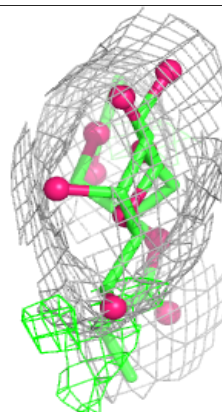
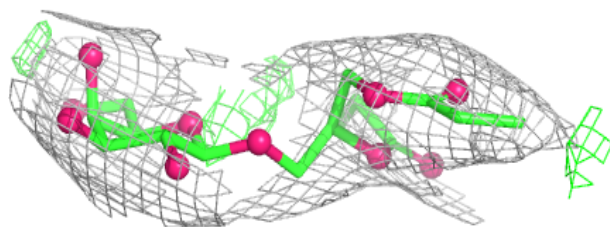
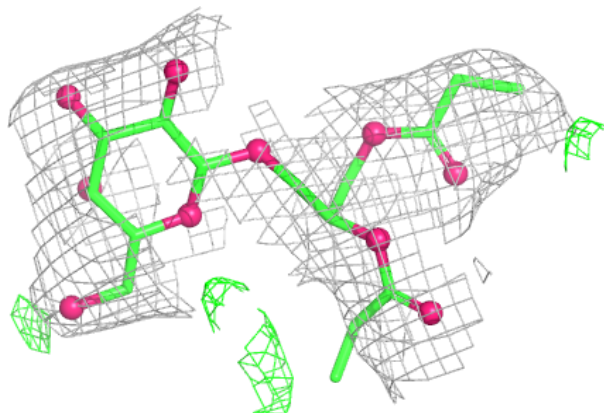
**Electron density around LMG 1 5001:**

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

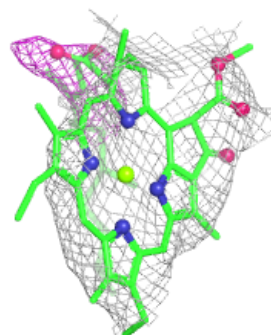
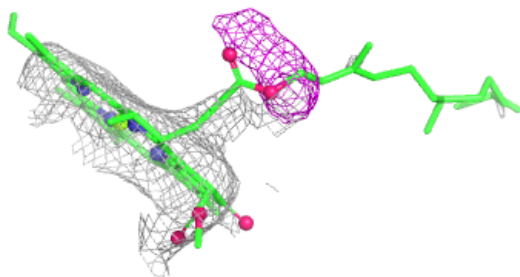
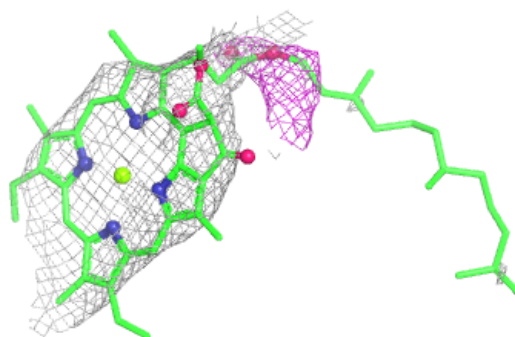


**Electron density around LMG 2 321:**

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

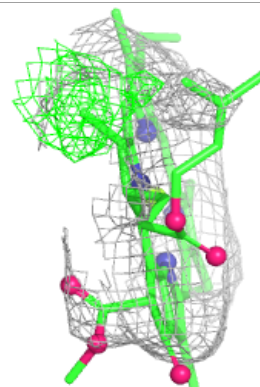
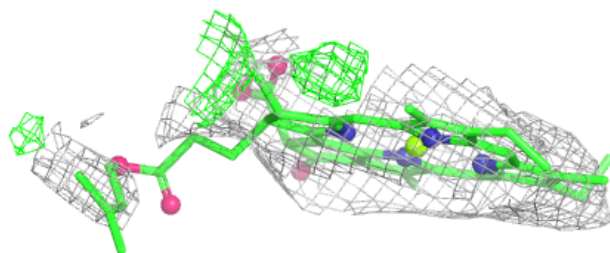
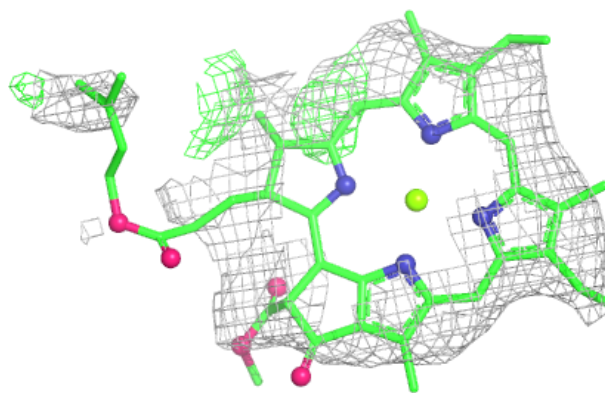
**Electron density around CLA K 1402:**

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



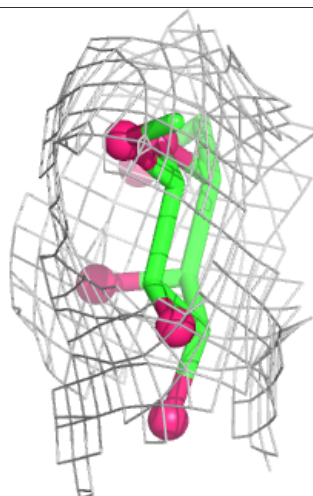
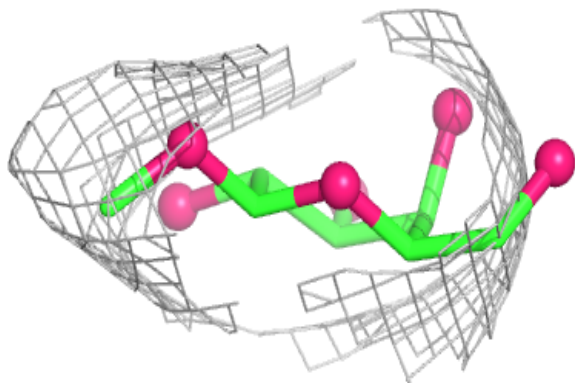
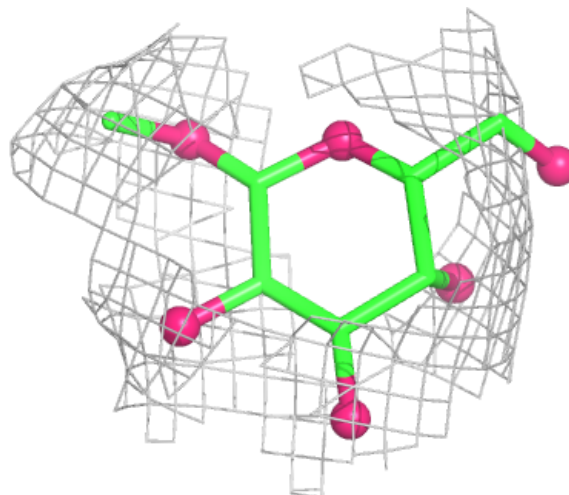
**Electron density around CLA J 1103:**

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



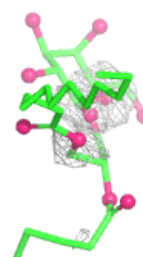
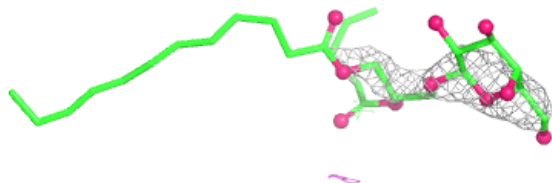
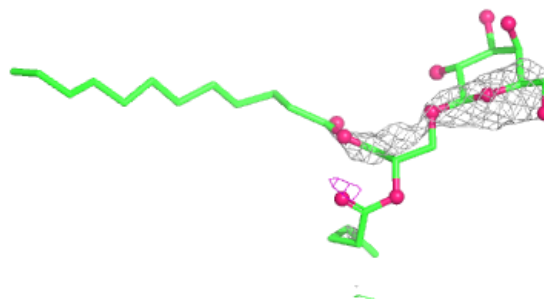
**Electron density around LMG 2 324:**

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

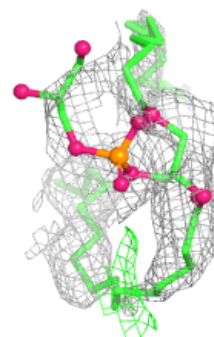
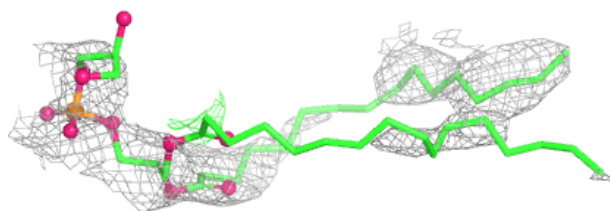
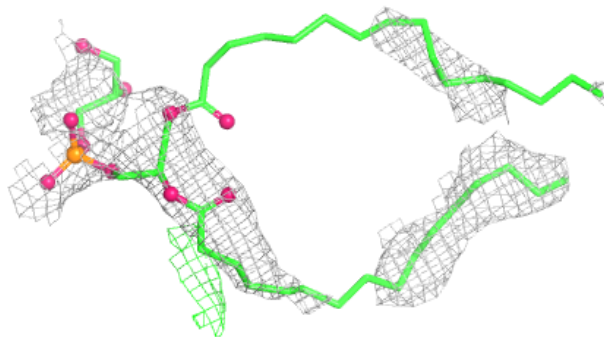


**Electron density around LMG F 307:**

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

**Electron density around LHG B 849:**

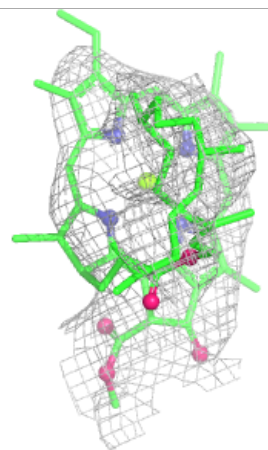
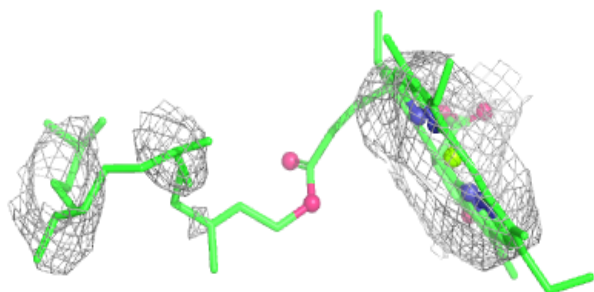
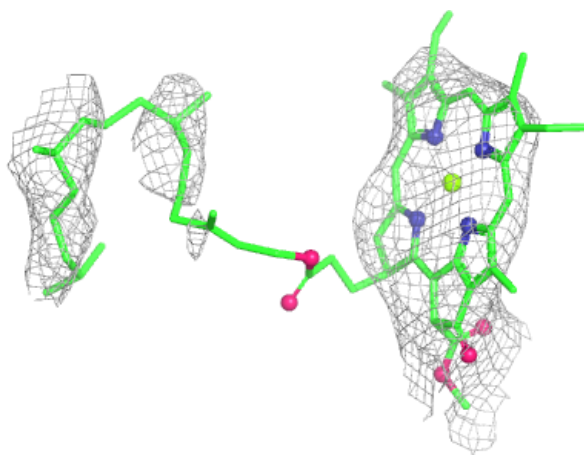
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA 1 5015:**

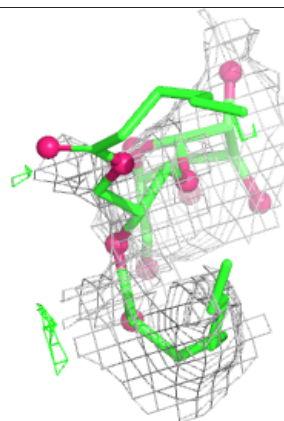
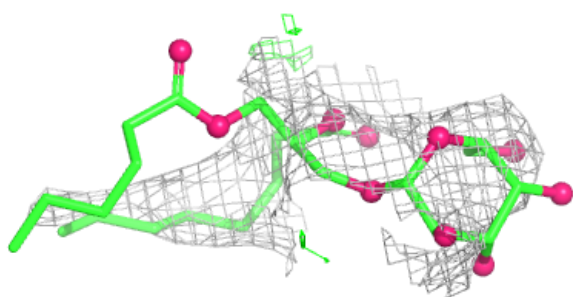
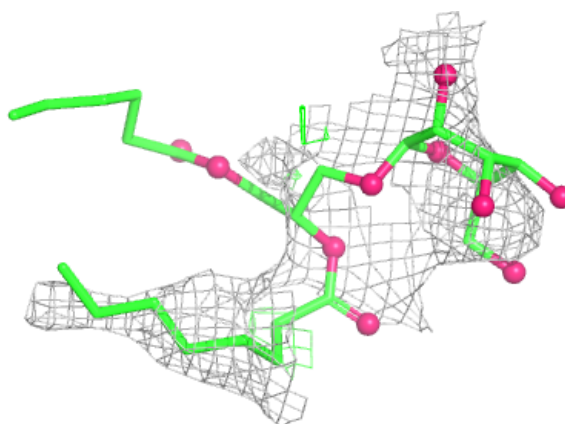
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



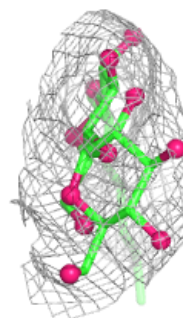
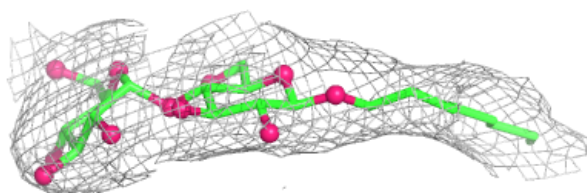
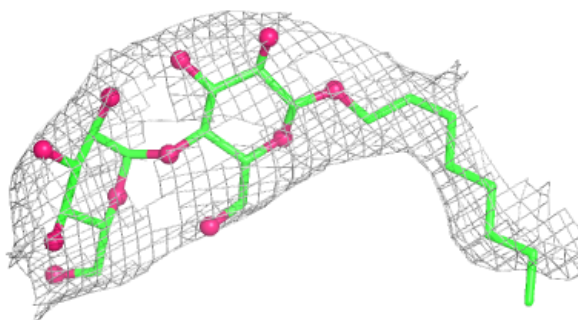


**Electron density around LMG B 851:**

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

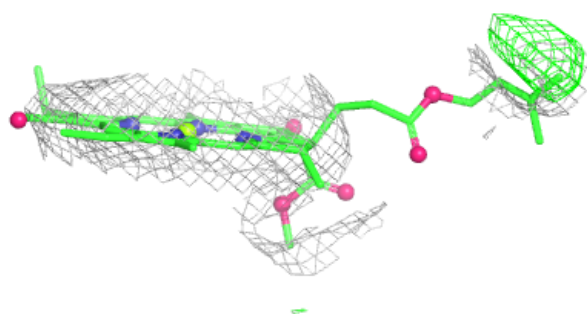
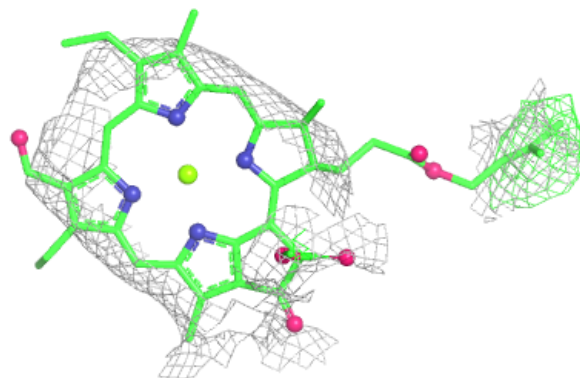
**Electron density around LMT B 856:**

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

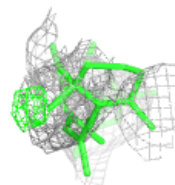
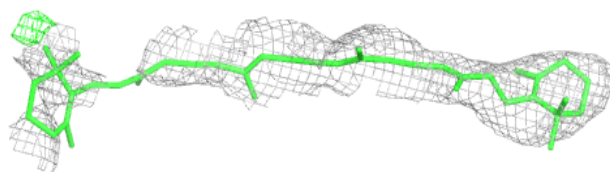
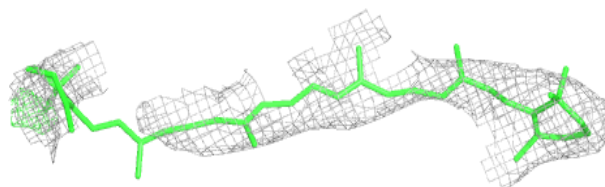


**Electron density around CHL 3 313:**

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

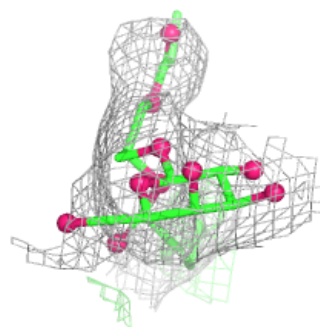
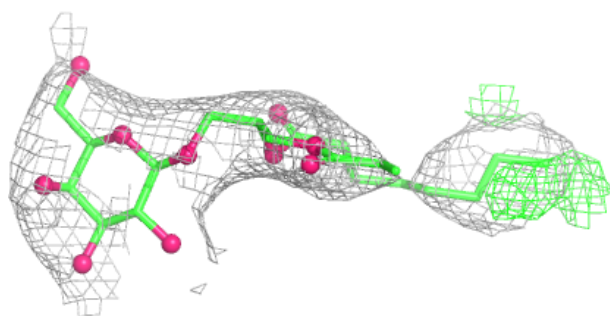
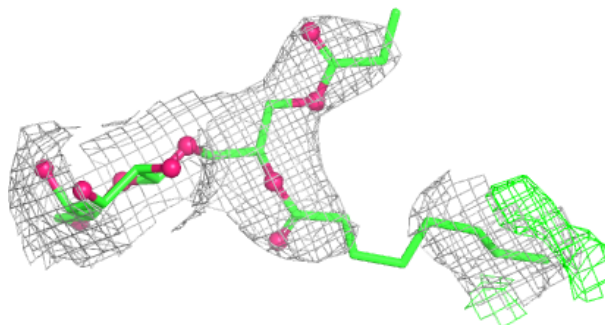
**Electron density around BCR L 302:**

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



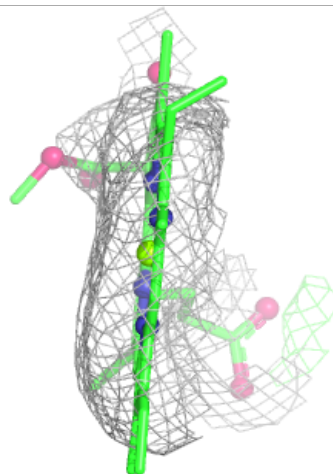
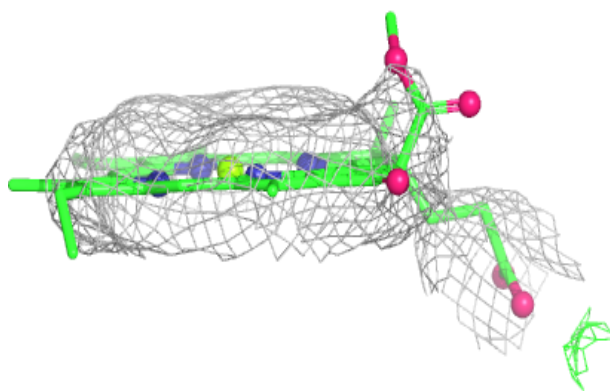
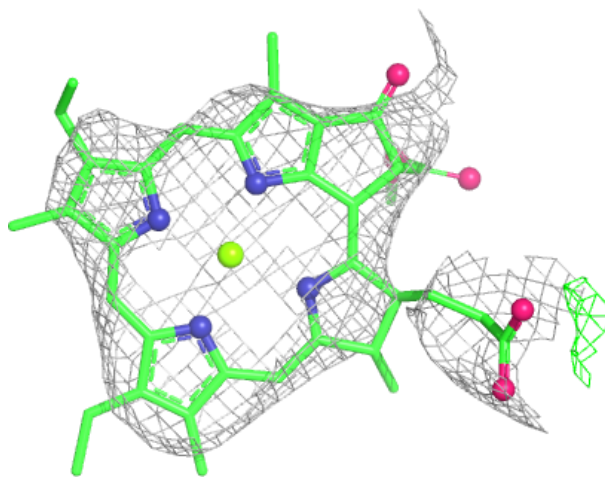
**Electron density around LMG J 1102:**

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



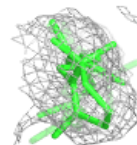
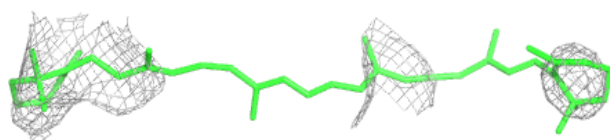
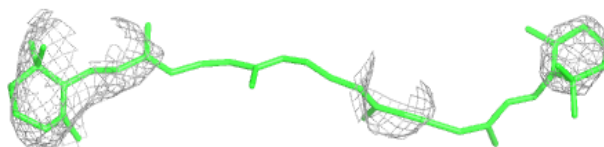
**Electron density around CLA K 1401:**

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

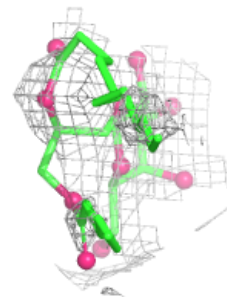
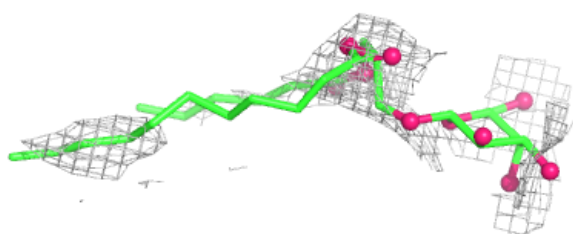


**Electron density around BCR K 1405:**

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

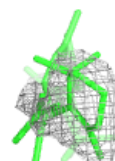
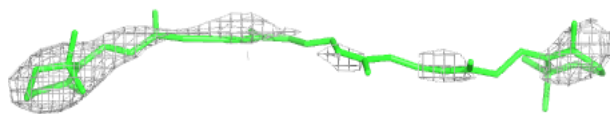
**Electron density around LMG 2 322:**

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



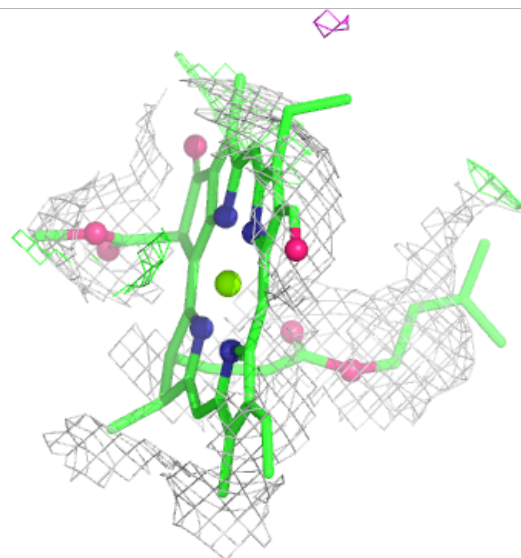
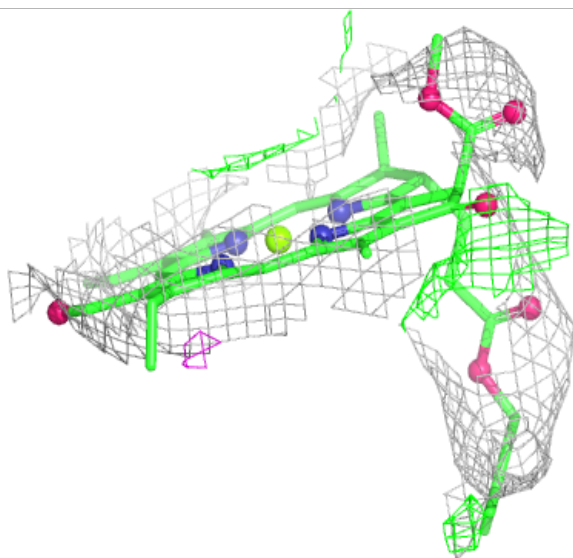
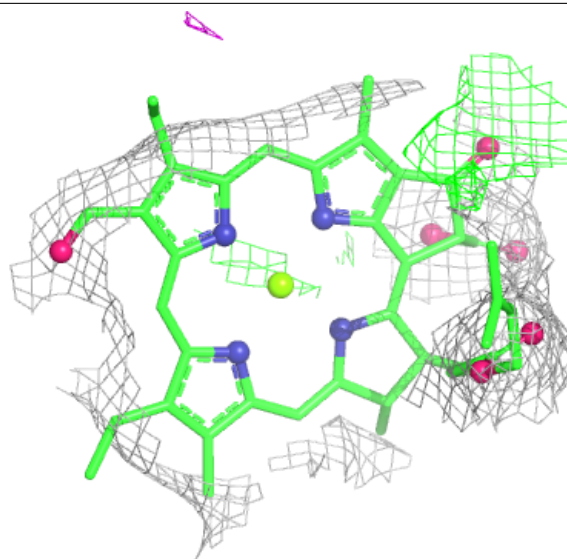
**Electron density around BCR 3 306:**

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



**Electron density around CHL 3 312:**

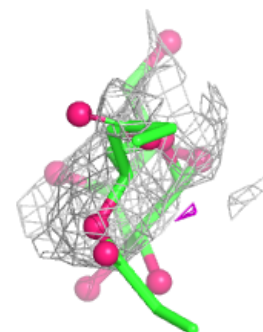
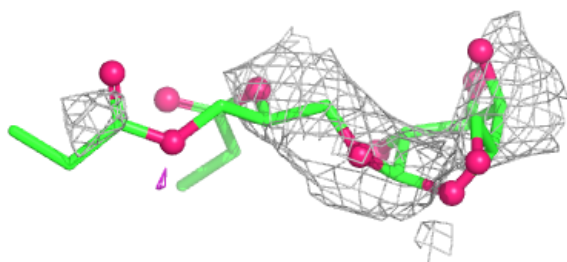
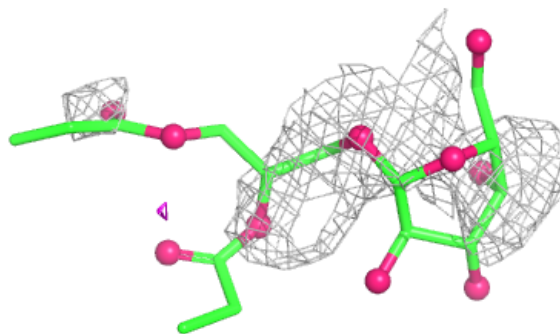
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



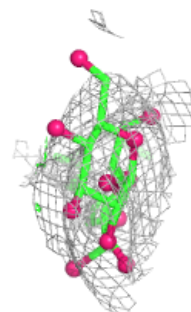
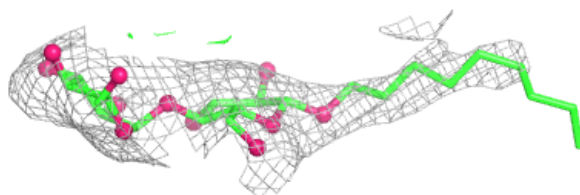
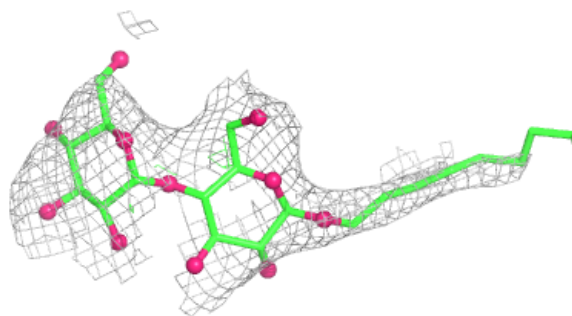


**Electron density around LMG G 1607:**

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

**Electron density around LMT B 853:**

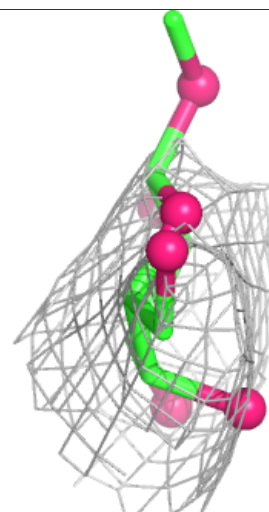
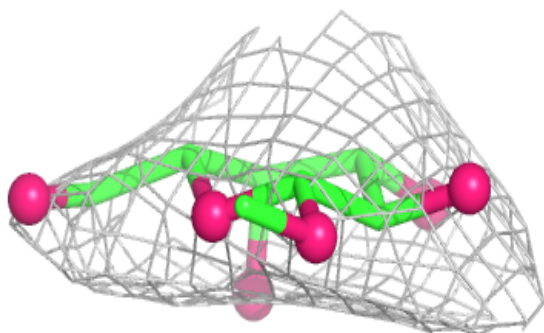
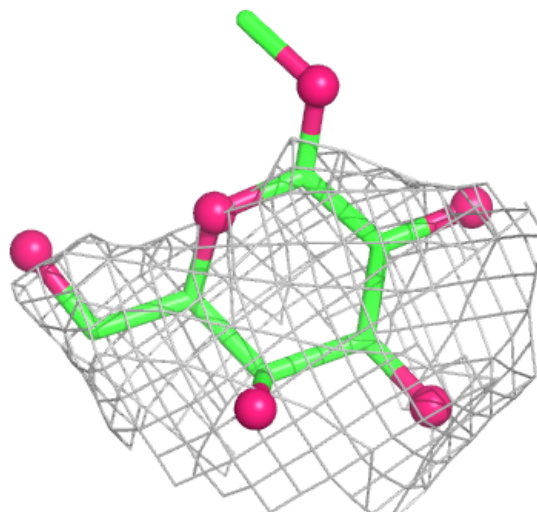
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





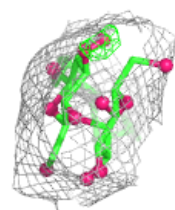
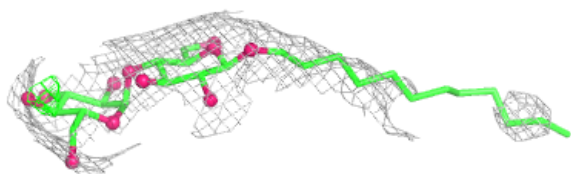
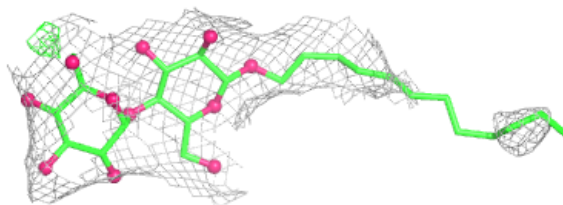
**Electron density around LMG B 854:**

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

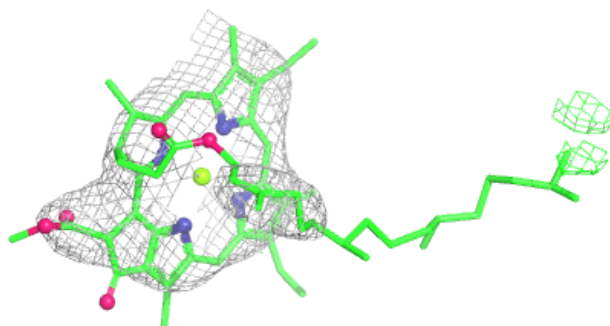
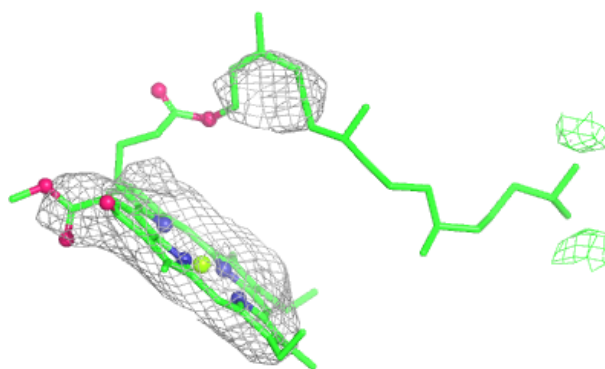


**Electron density around LMT G 1605:**

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

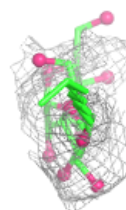
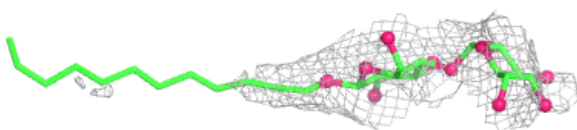
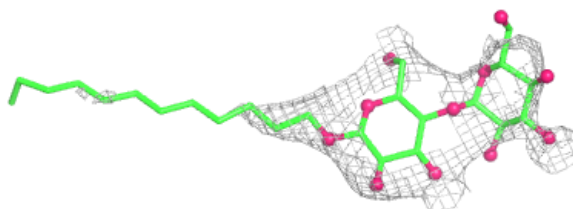
**Electron density around CLA G 1603:**

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

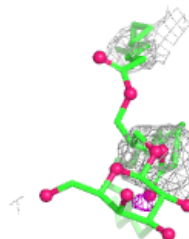
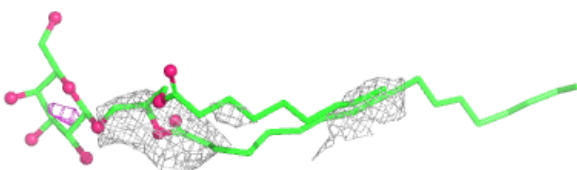
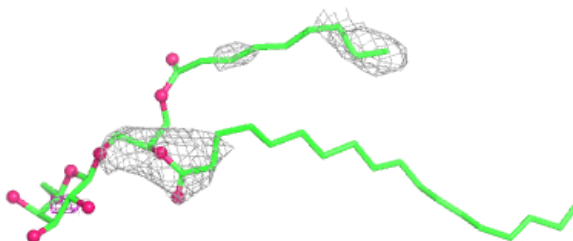


**Electron density around LMT 4 319:**

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

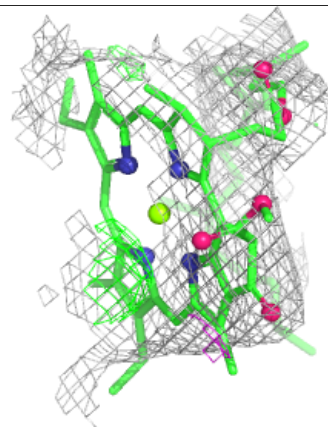
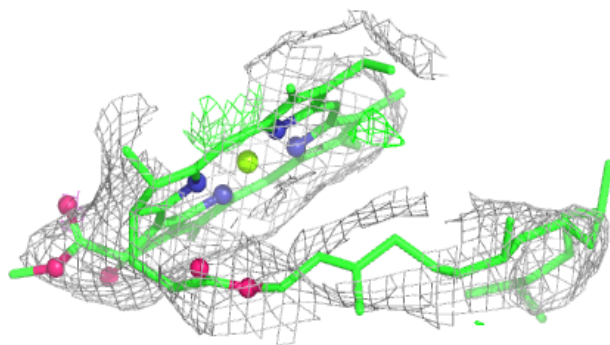
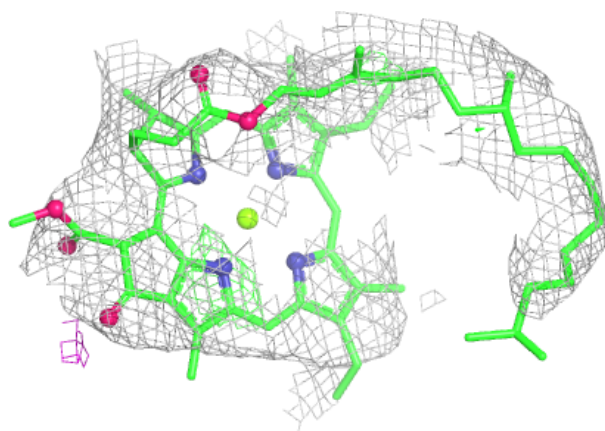
**Electron density around LMG 1 5020:**

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



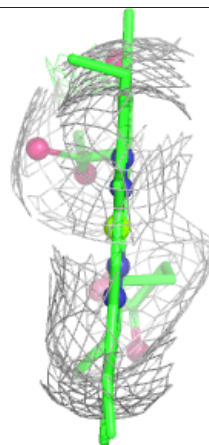
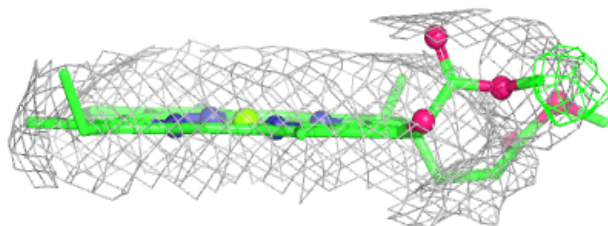
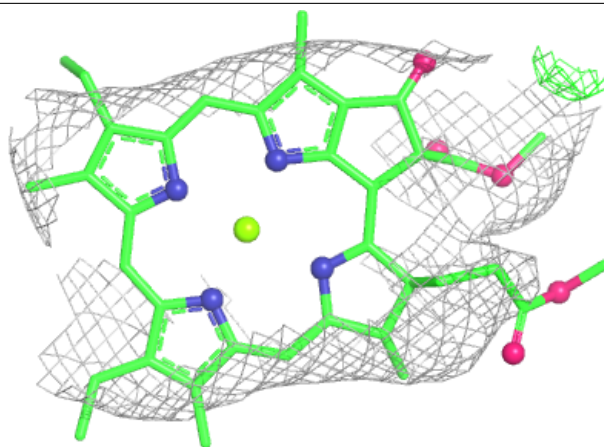
**Electron density around CLA 1 5006:**

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



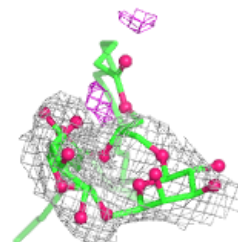
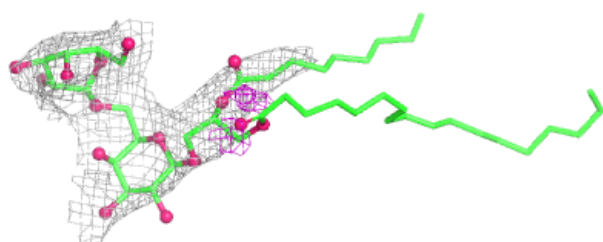
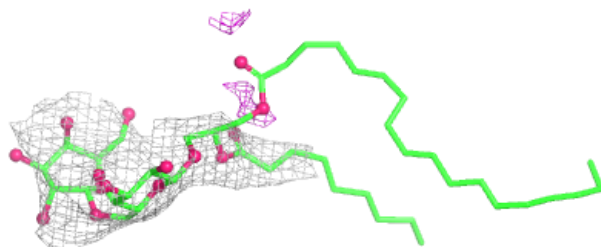
**Electron density around CLA G 1602:**

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

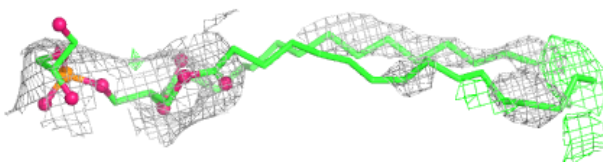


**Electron density around DGD F 309:**

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

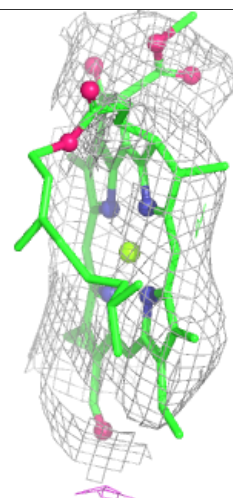
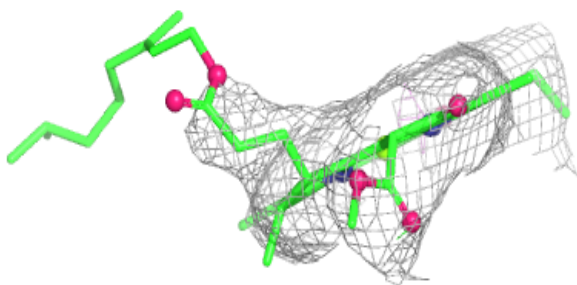
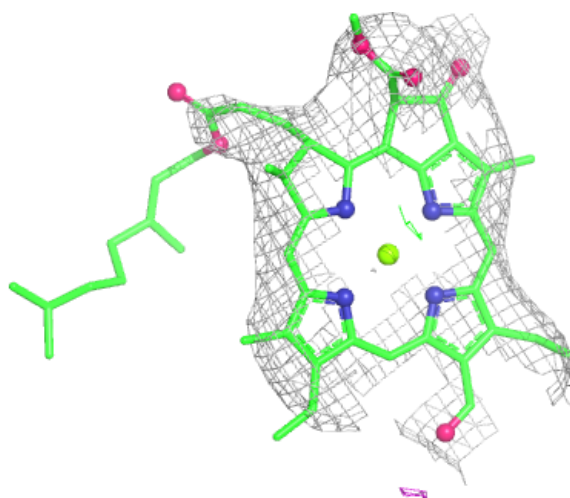
**Electron density around LHG 1 5019:**

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



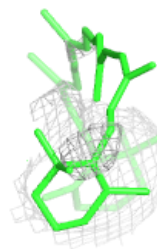
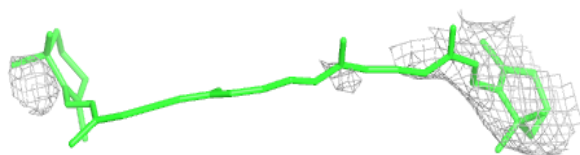
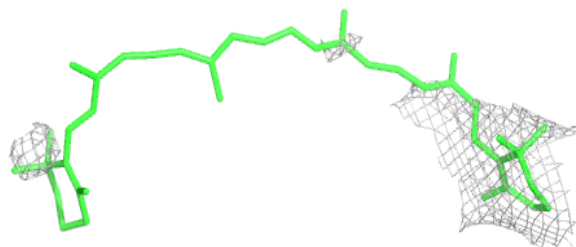
**Electron density around CHL 2 315:**

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



**Electron density around BCR 1 5005:**

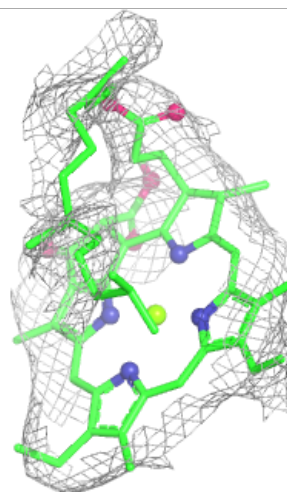
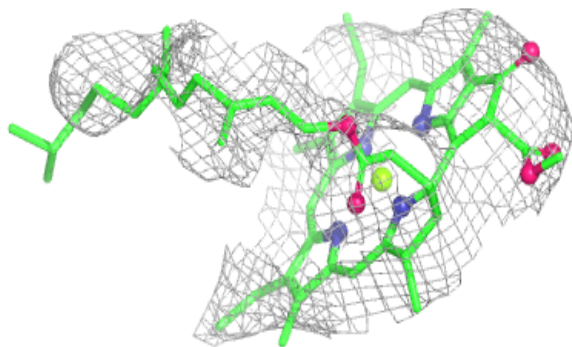
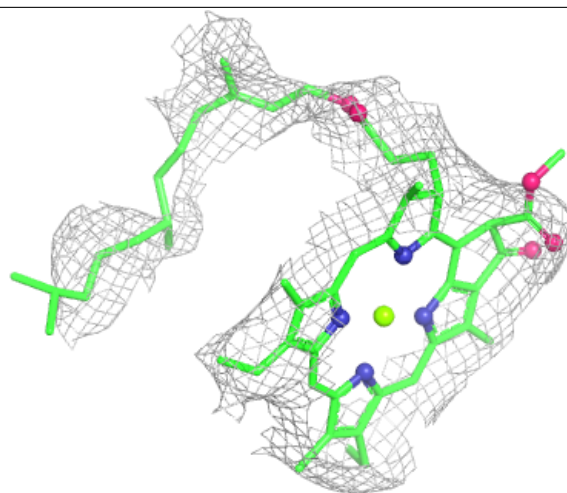
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





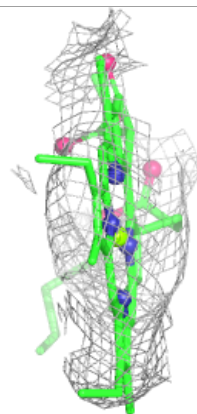
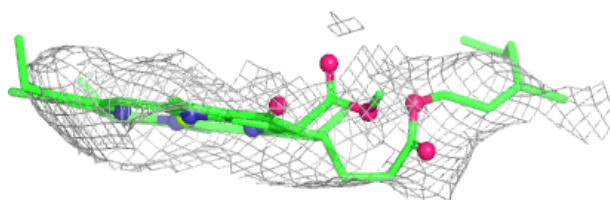
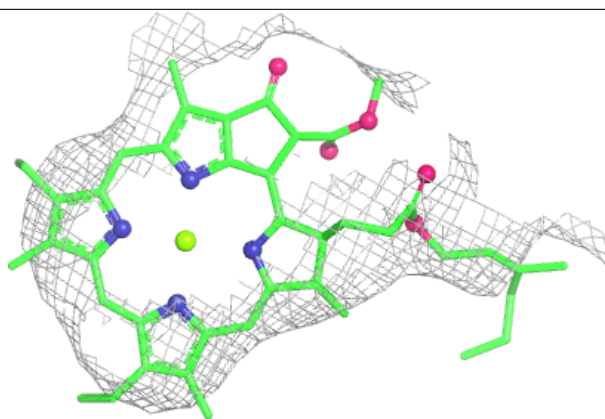
**Electron density around CLA A 840:**

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

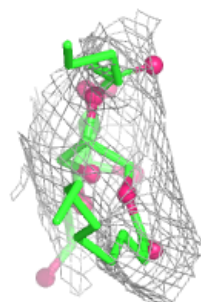
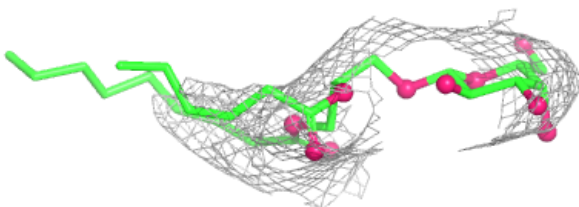
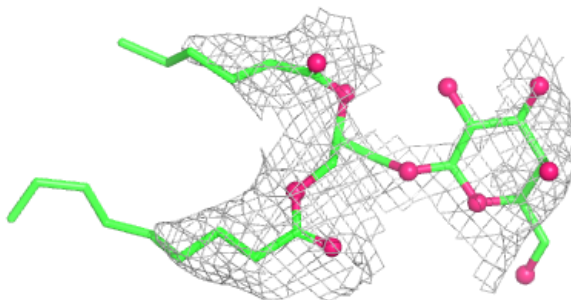


**Electron density around CLA 3 308:**

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

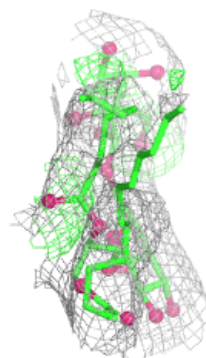
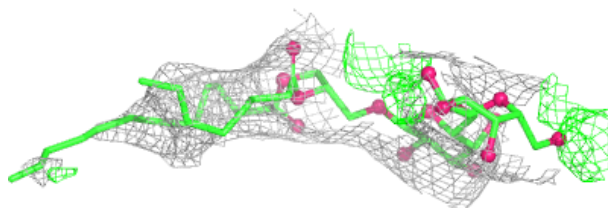
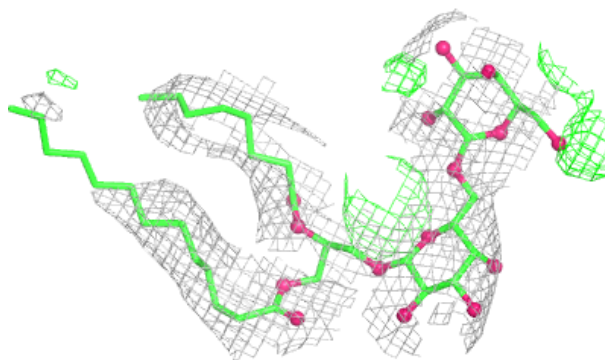
**Electron density around LMG F 308:**

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



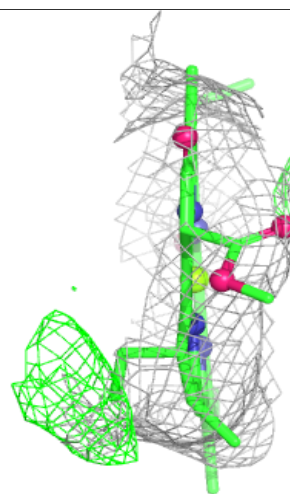
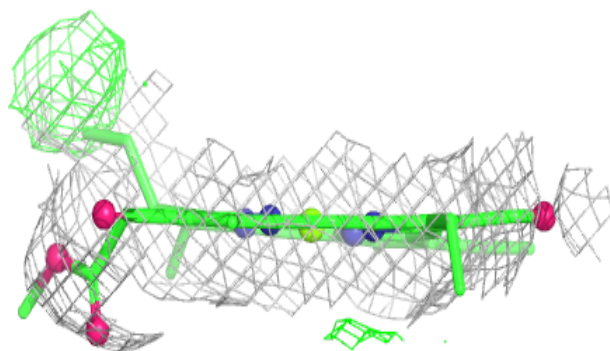
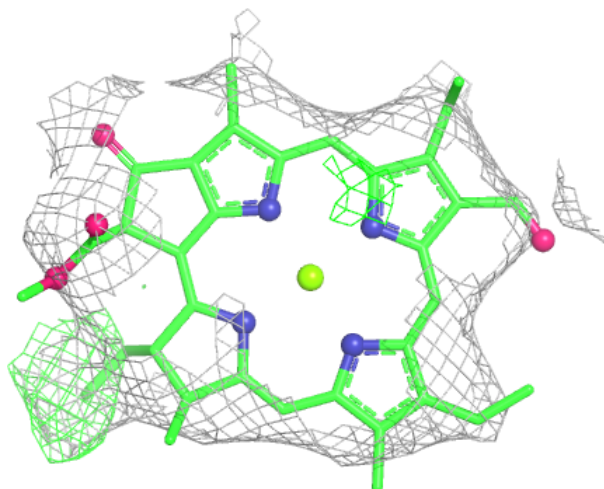
**Electron density around DGD 2 327:**

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



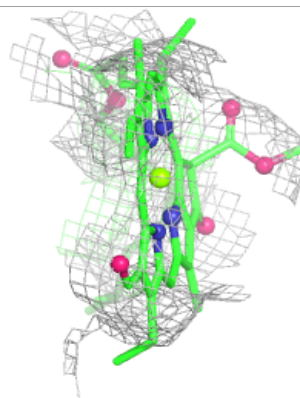
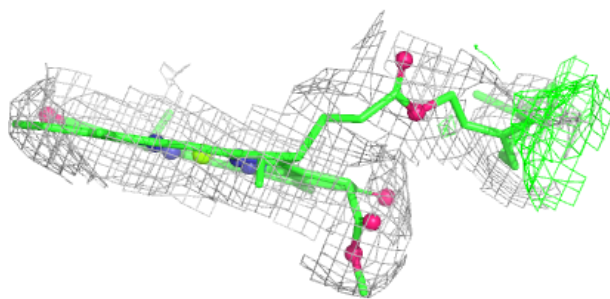
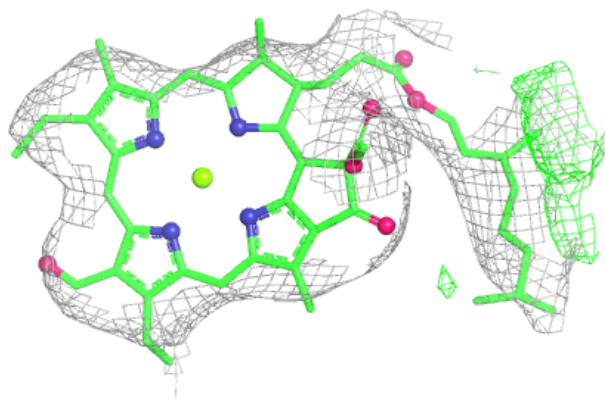
**Electron density around CHL 4 317:**

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

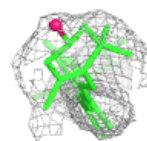
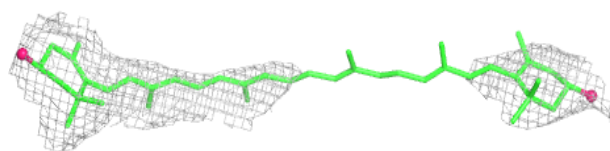
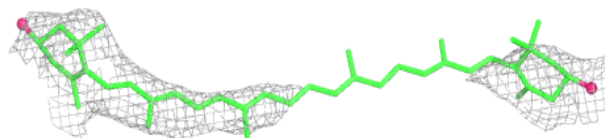


**Electron density around CHL 2 319:**

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

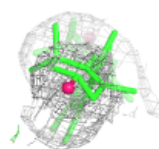
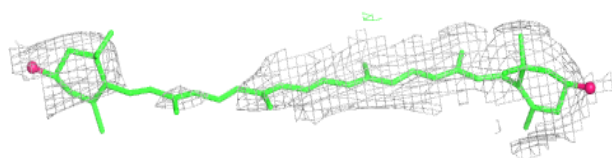
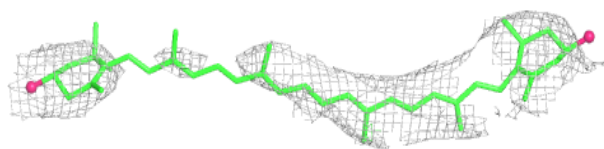
**Electron density around LUT 4 303:**

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

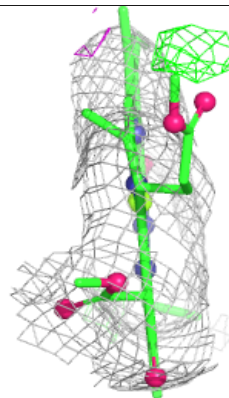
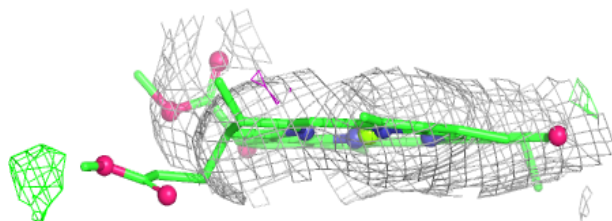
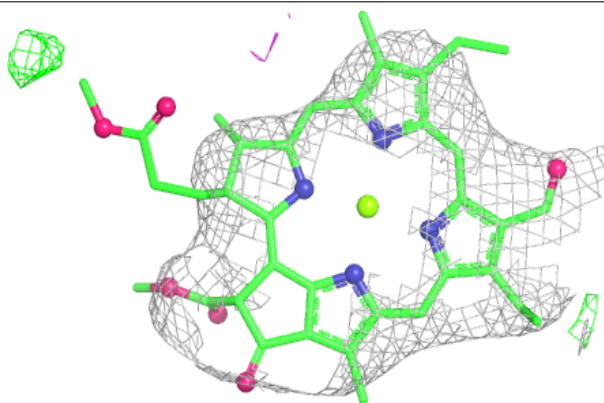


**Electron density around LUT 2 303:**

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

**Electron density around CHL 4 313:**

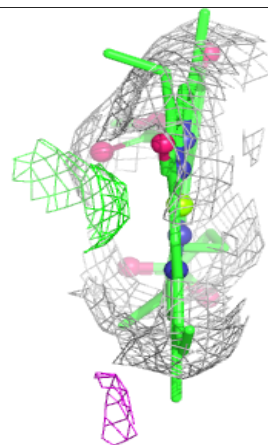
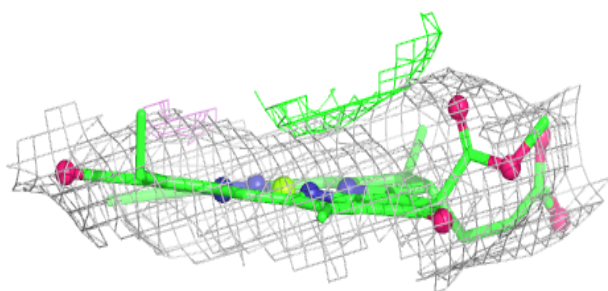
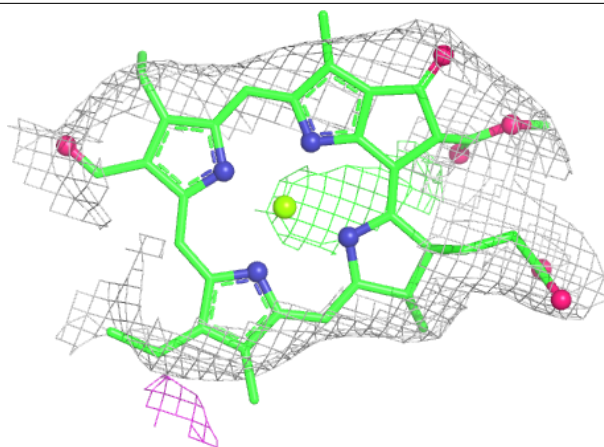
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



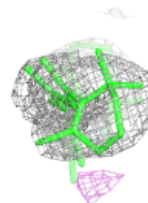
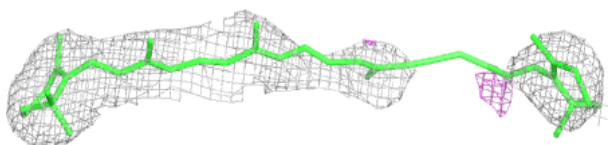
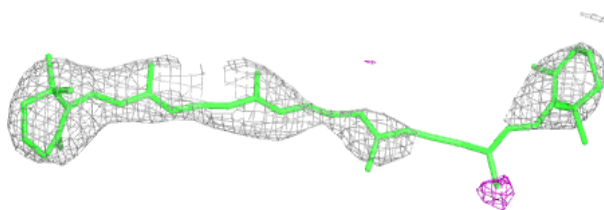


**Electron density around CHL 2 318:**

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

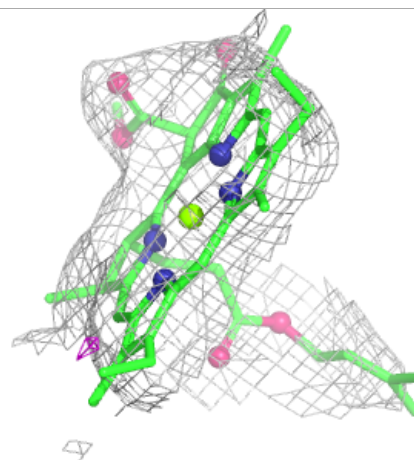
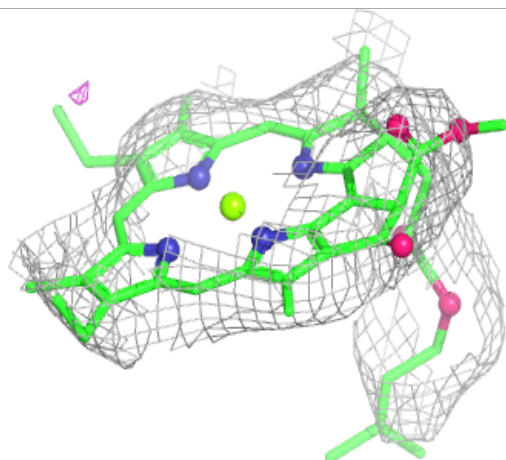
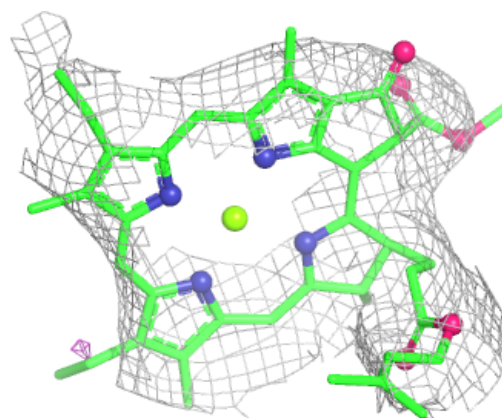
**Electron density around BCR A 846:**

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



**Electron density around CLA 2 311:**

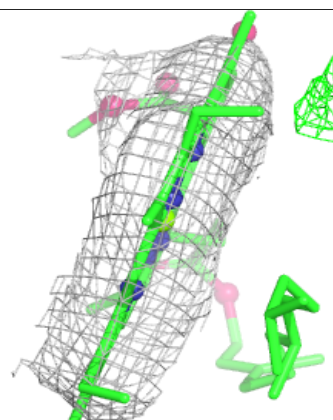
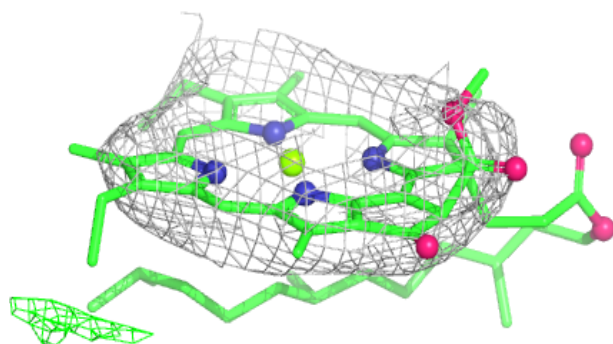
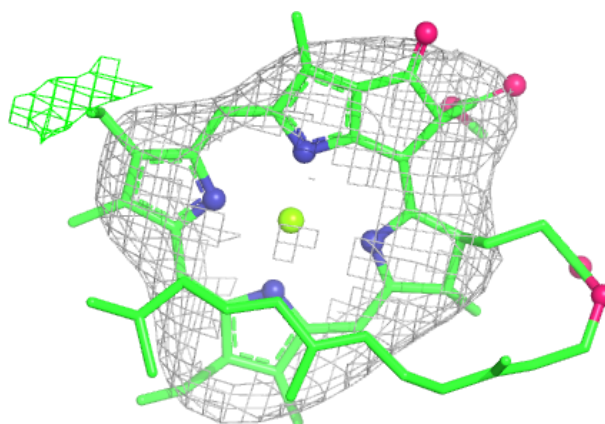
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



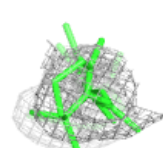
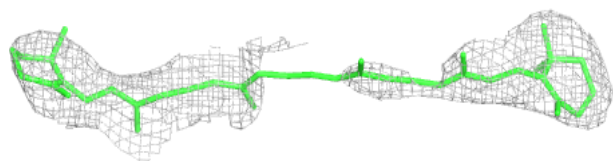
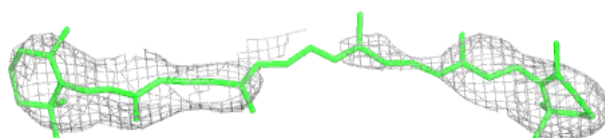


**Electron density around CLA 3 319:**

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

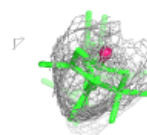
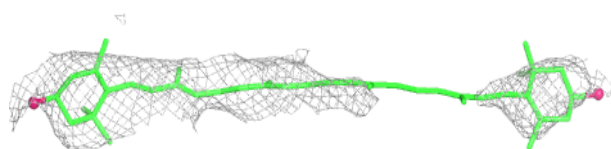
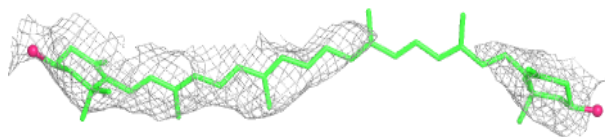
**Electron density around BCR L 307:**

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

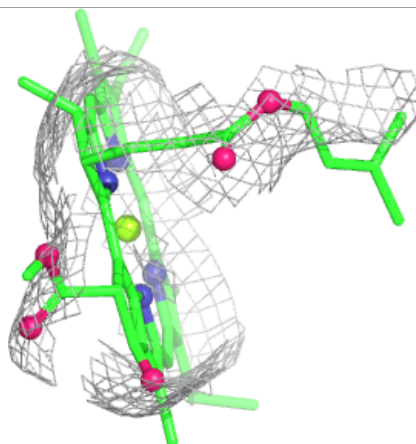
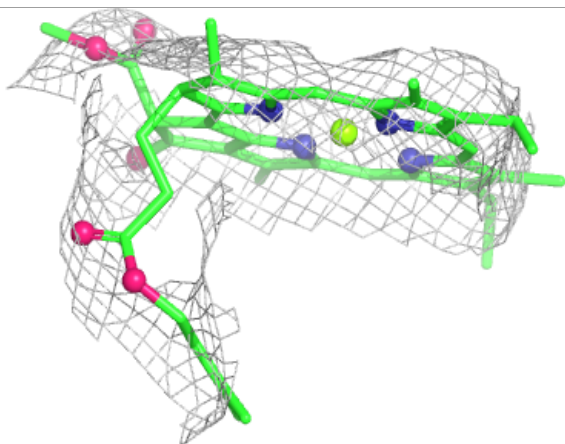
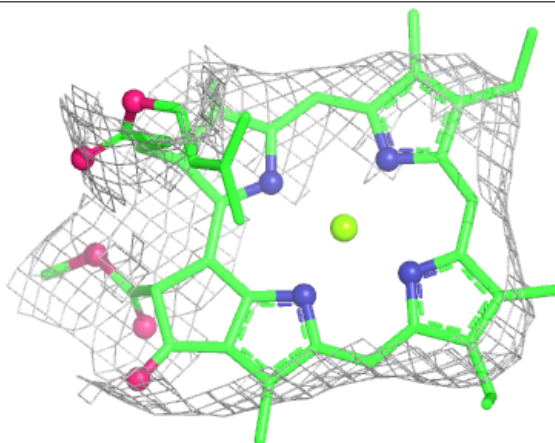


**Electron density around LUT 1 5003:**

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

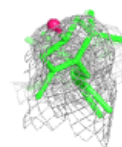
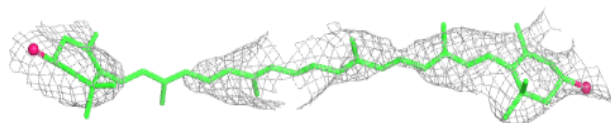
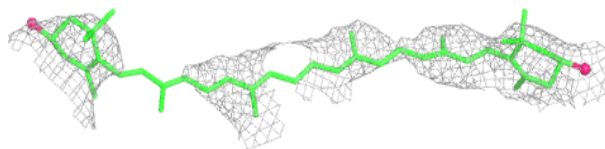
**Electron density around CLA 1 5011:**

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

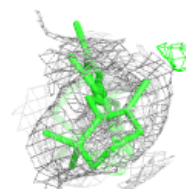
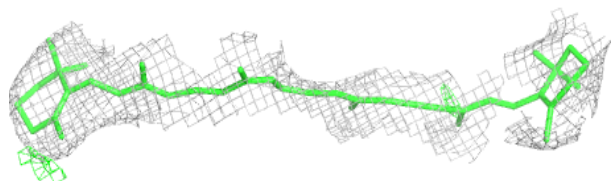
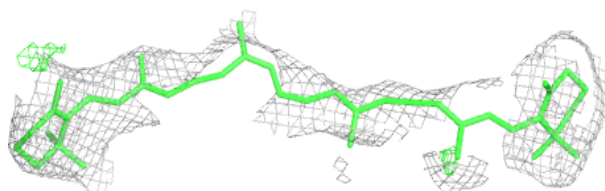


**Electron density around LUT 3 303:**

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

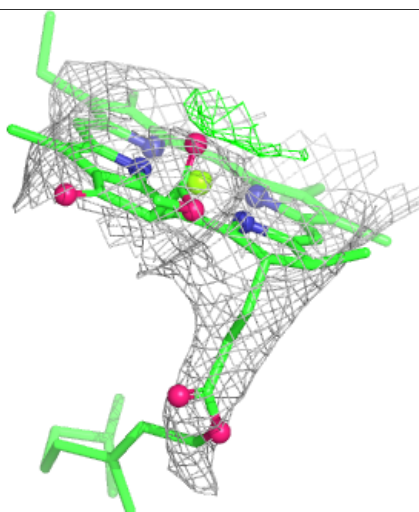
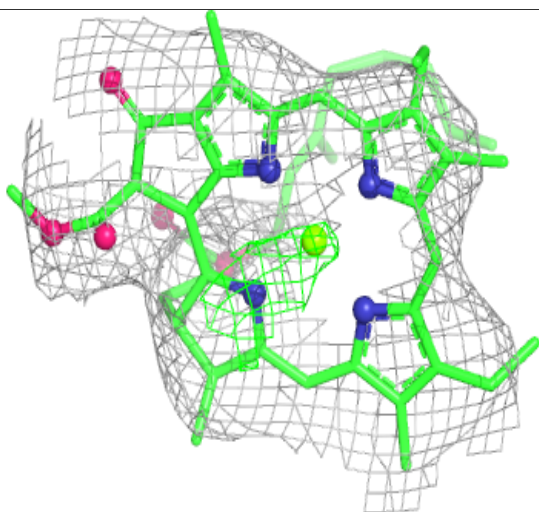
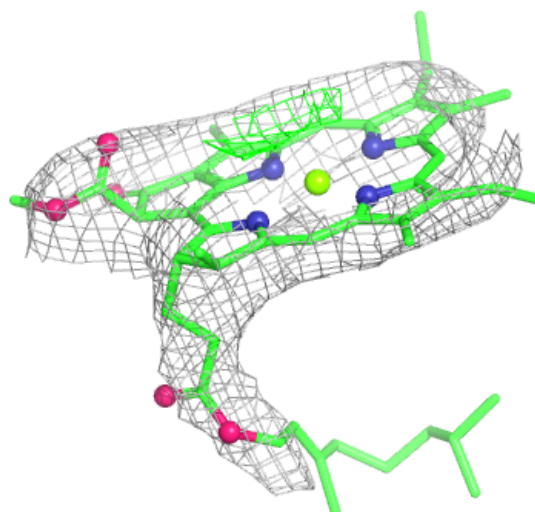
**Electron density around BCR G 1604:**

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



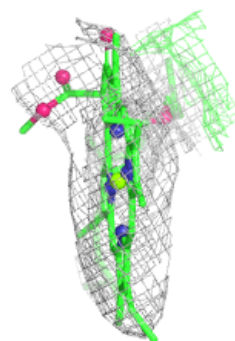
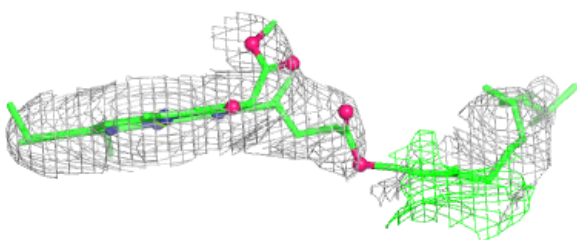
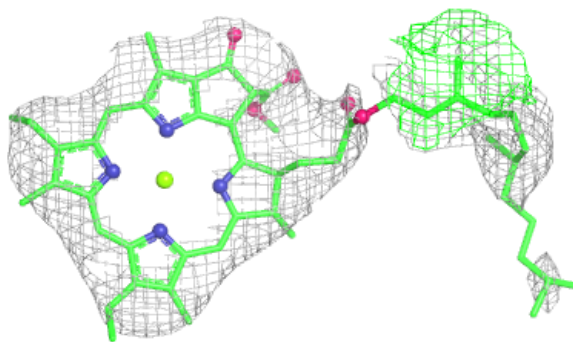
**Electron density around CLA B 835:**

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



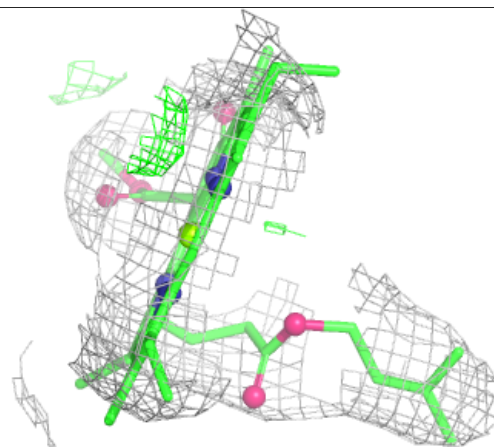
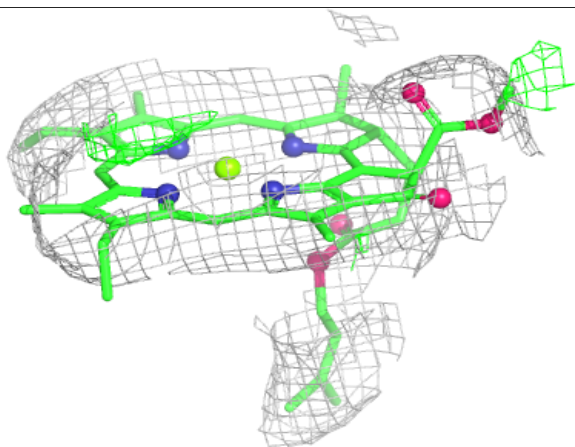
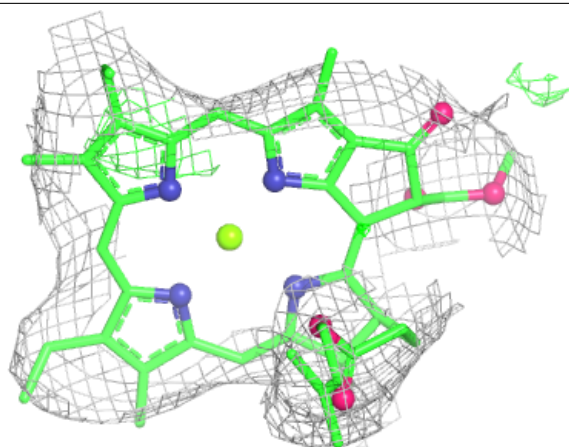
**Electron density around CLA 1 5018:**

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



**Electron density around CLA L 304:**

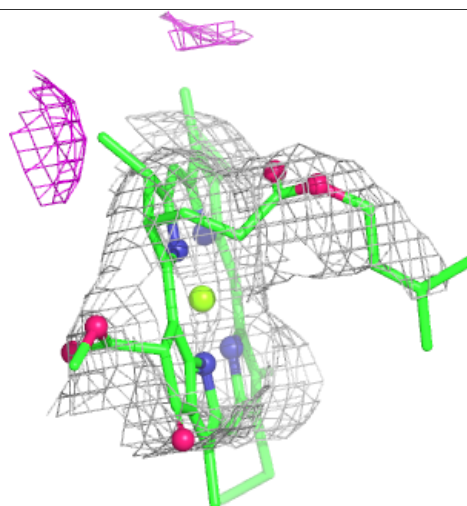
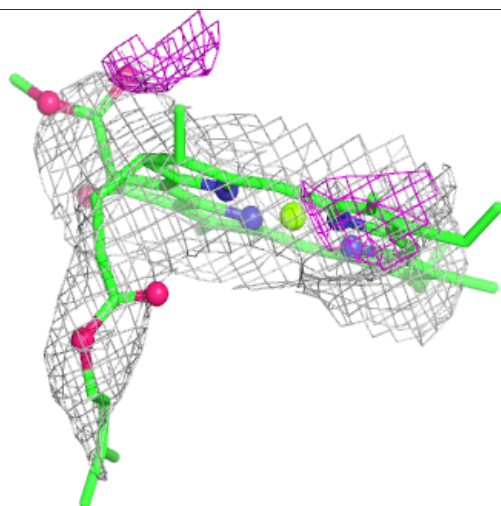
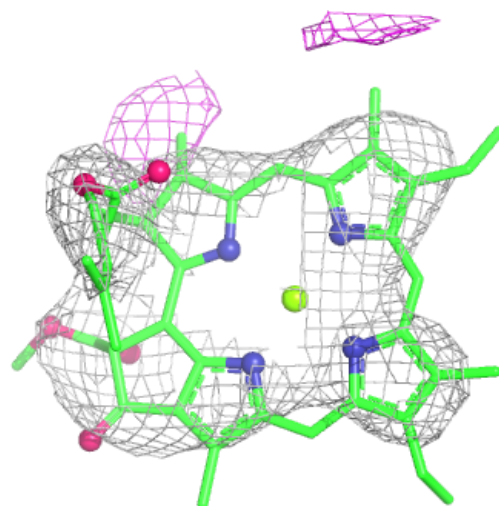
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





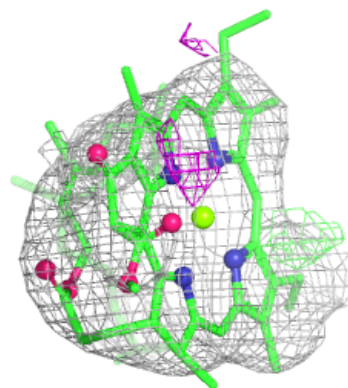
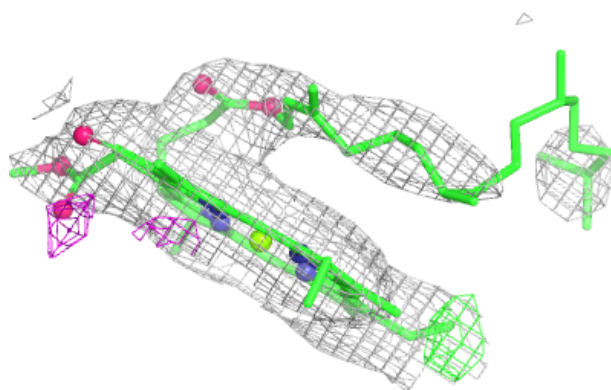
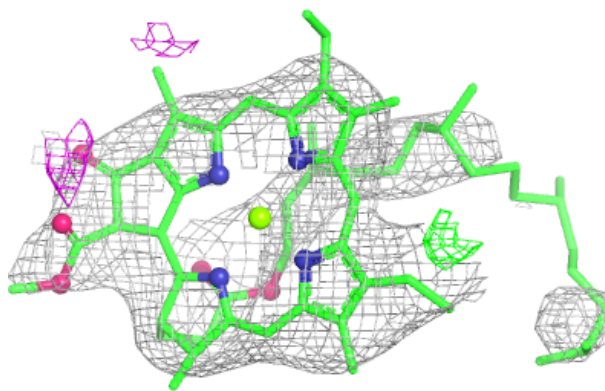
**Electron density around CLA L 306:**

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



**Electron density around CLA B 808:**

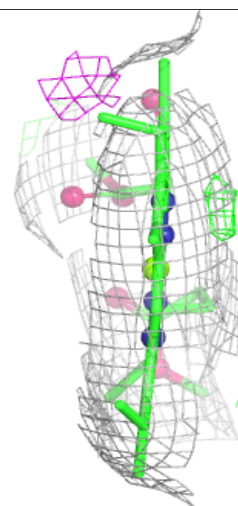
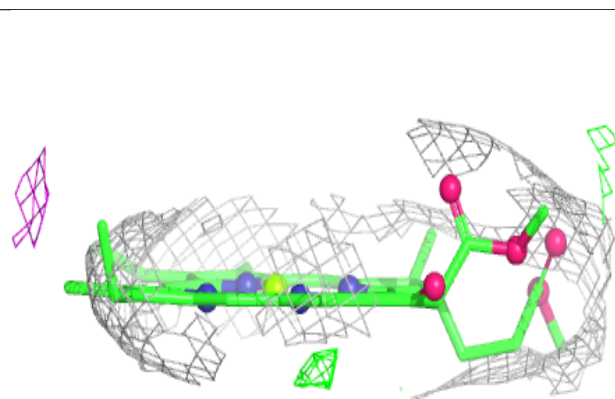
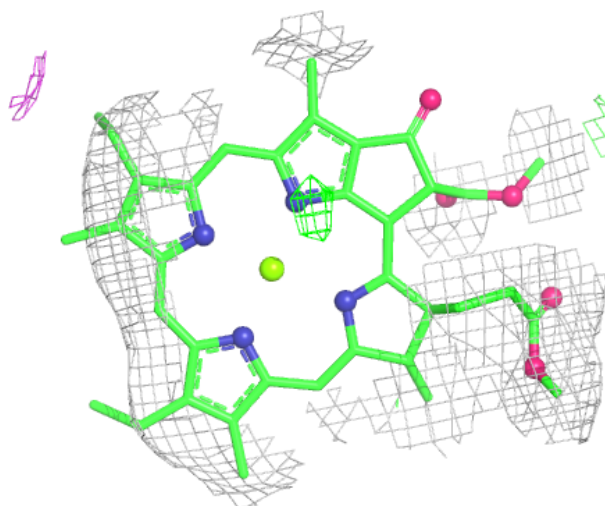
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





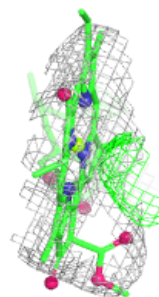
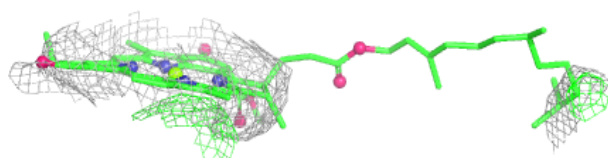
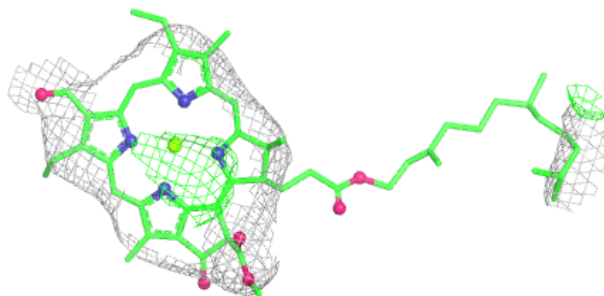
**Electron density around CLA 1 5007:**

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

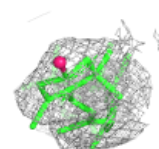
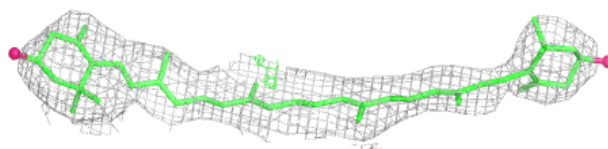


**Electron density around CHL 4 316:**

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

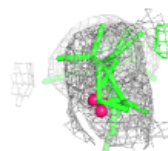
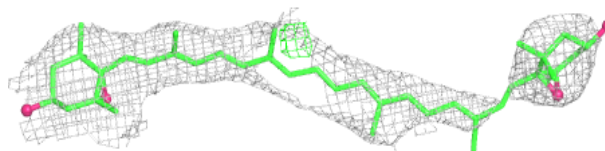
**Electron density around LUT J 1105:**

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



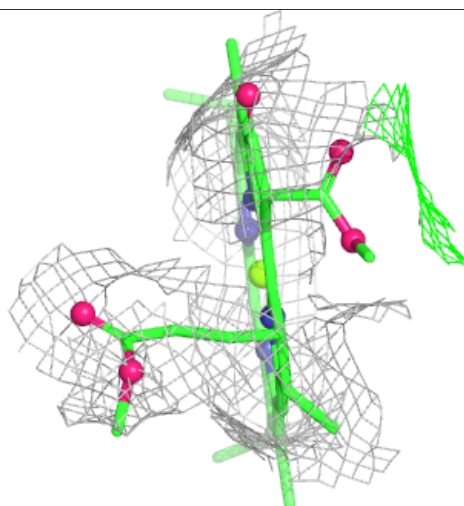
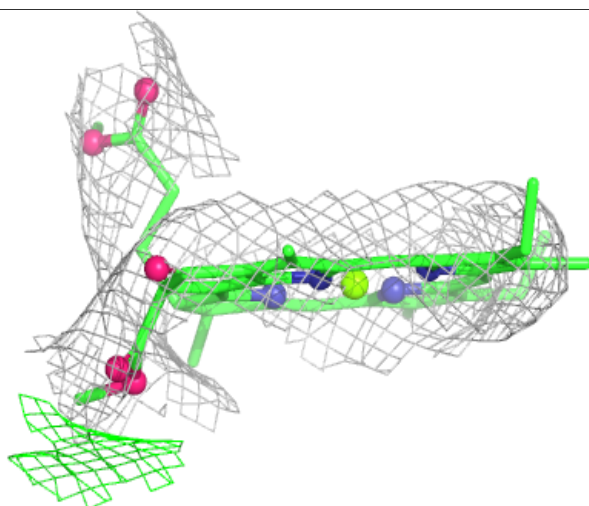
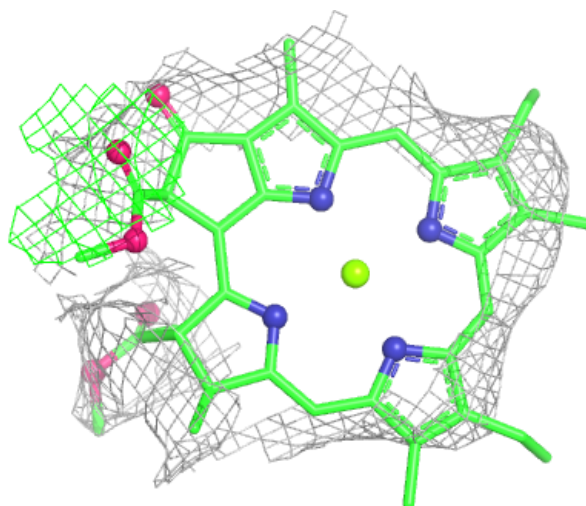
**Electron density around XAT 2 304:**

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



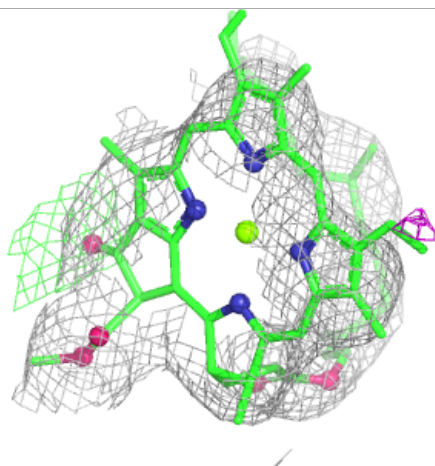
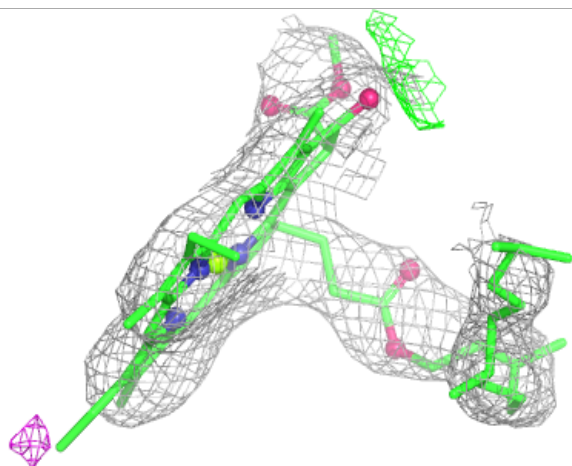
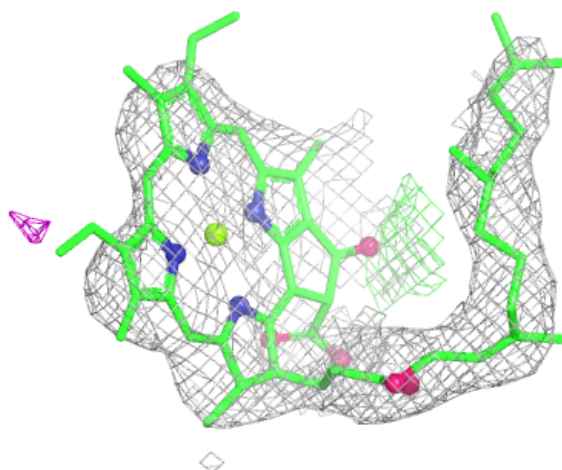
**Electron density around CLA 1 5013:**

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



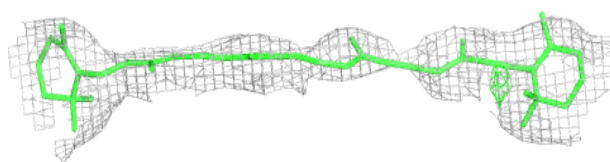
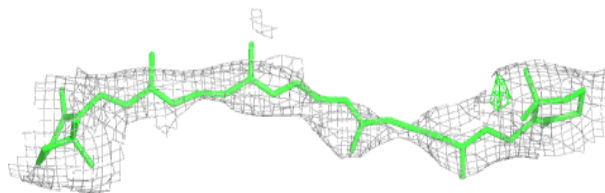
**Electron density around CLA B 834:**

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

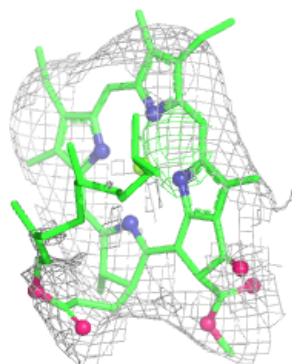
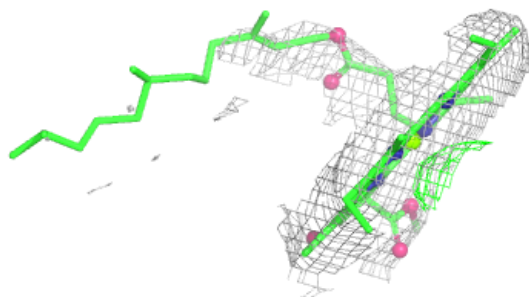
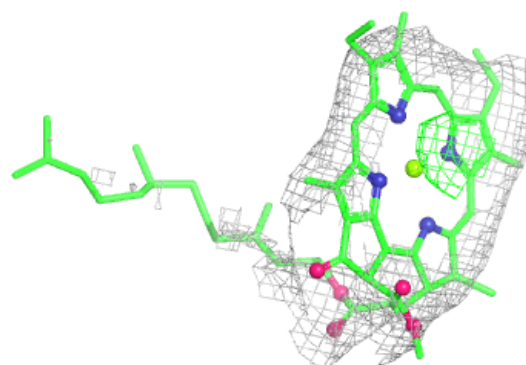


**Electron density around BCR 3 305:**

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

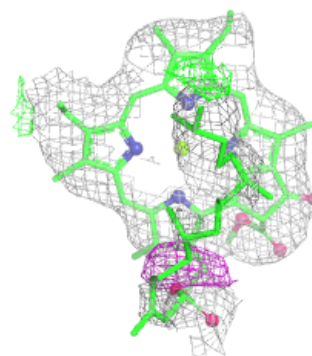
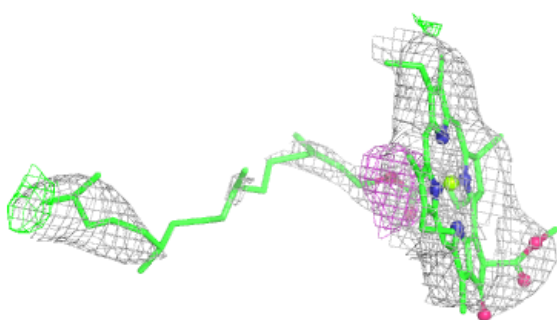
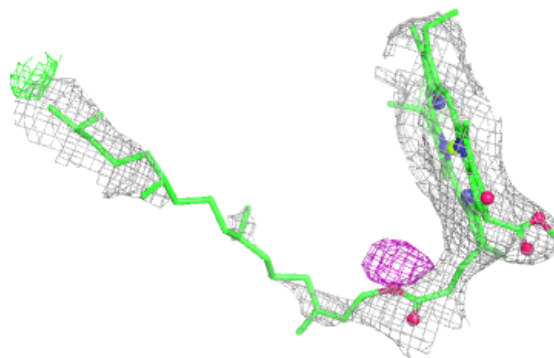
**Electron density around CLA 4 311:**

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

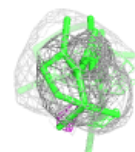
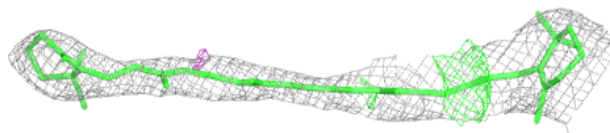
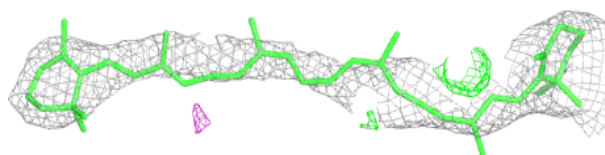


**Electron density around CLA A 803:**

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

**Electron density around BCR B 843:**

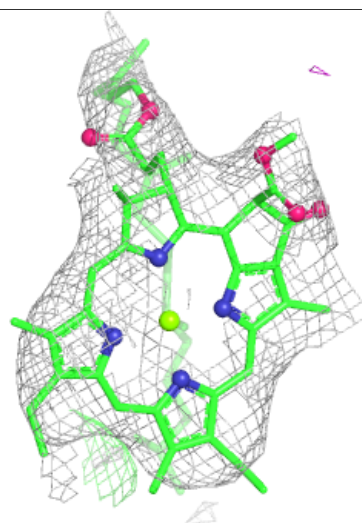
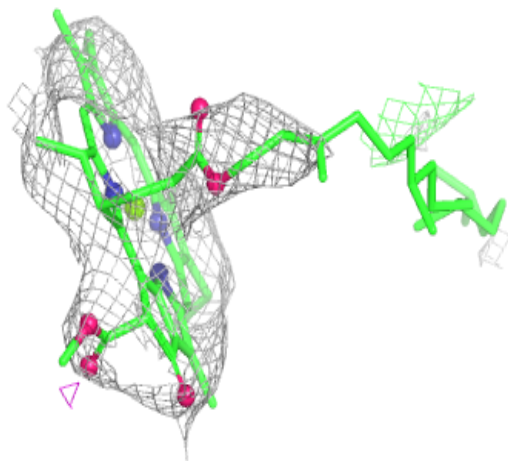
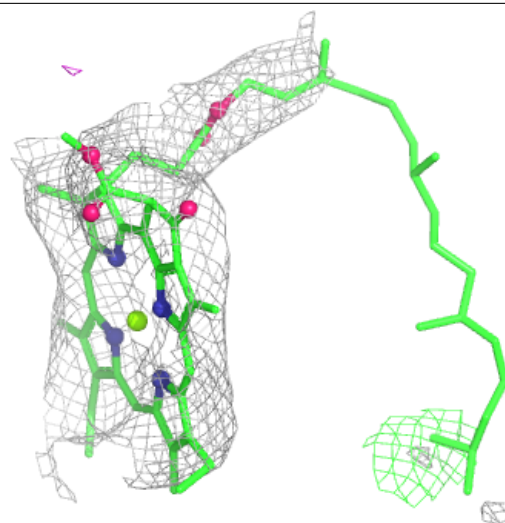
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA A 836:**

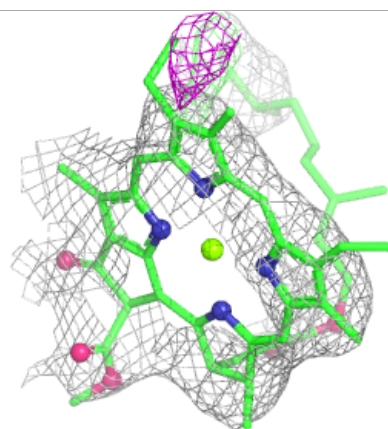
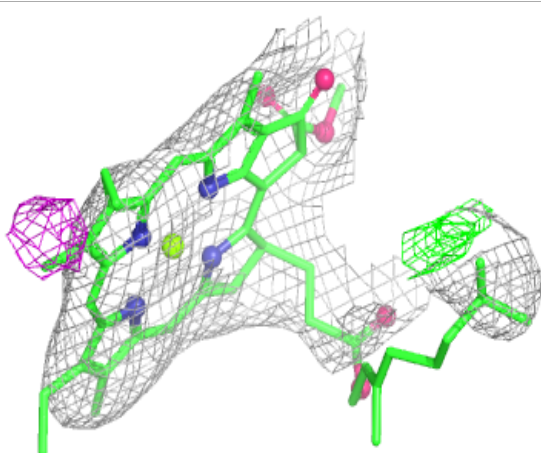
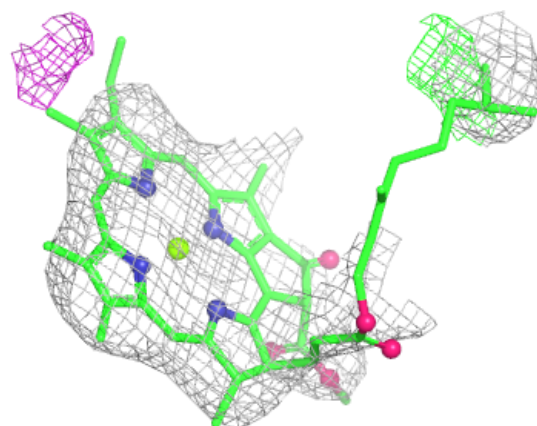
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





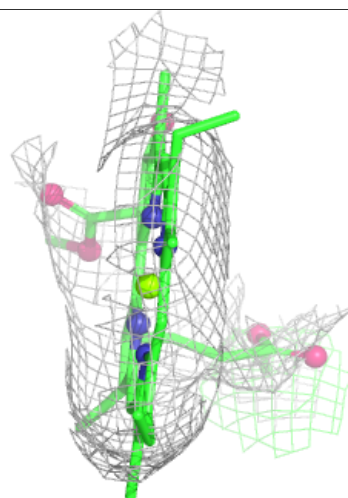
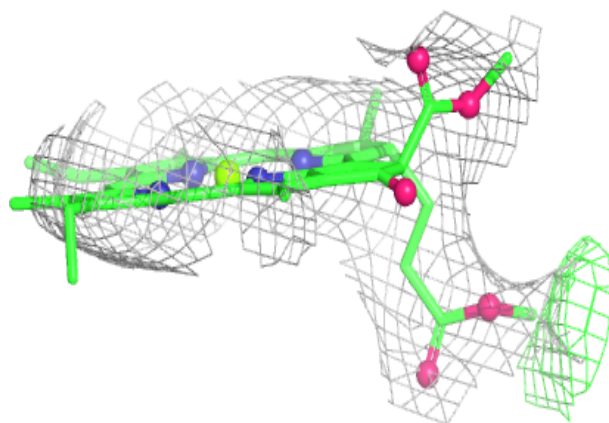
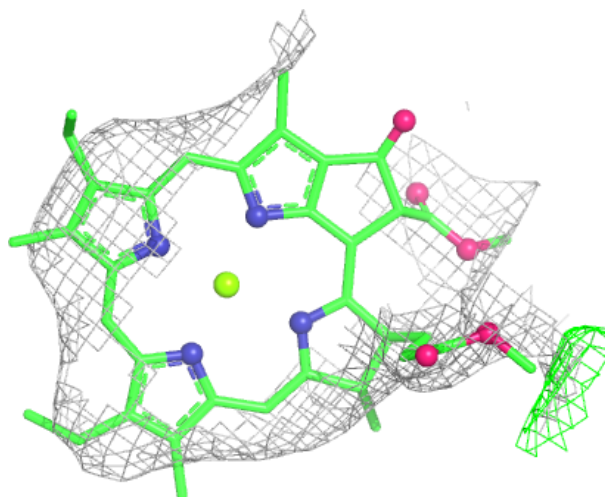
**Electron density around CLA 2 317:**

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



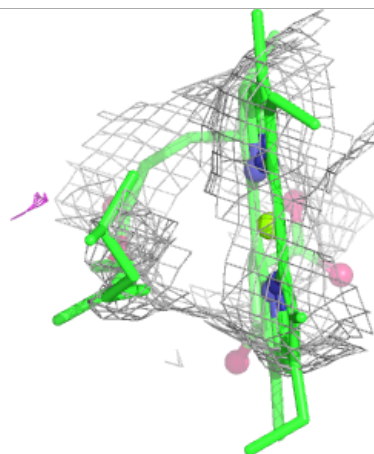
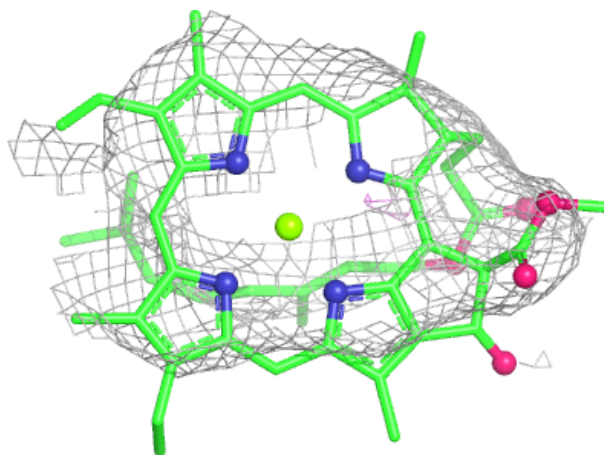
**Electron density around CLA 1 5012:**

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



**Electron density around CLA 3 309:**

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

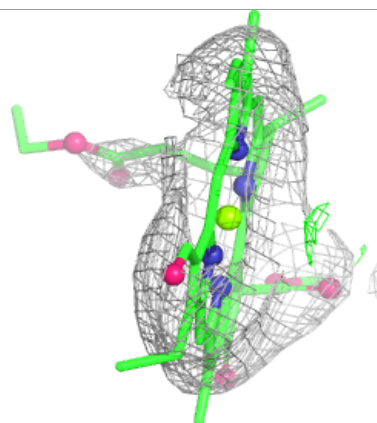
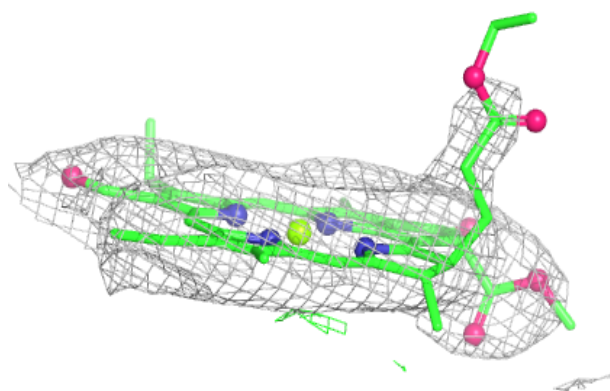
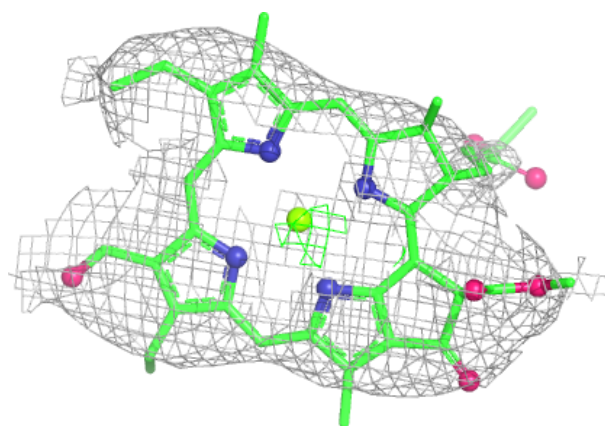


**Electron density around LHG A 849:**

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

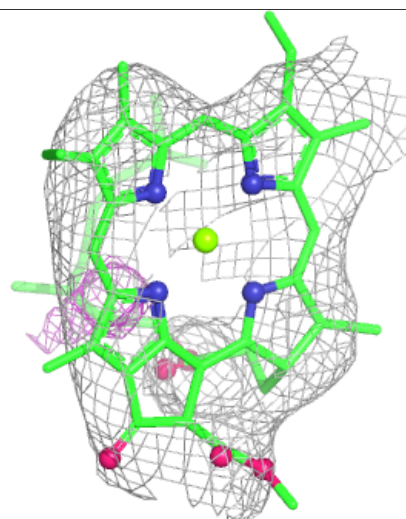
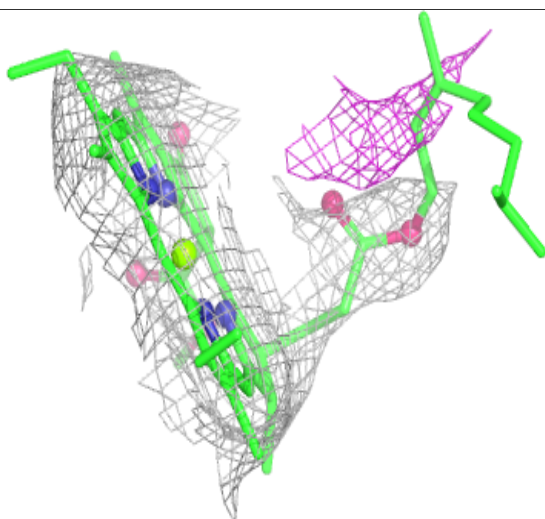
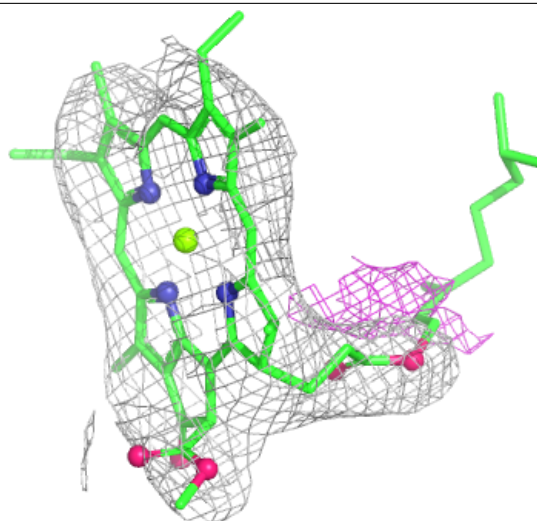
**Electron density around CHL 2 316:**

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



**Electron density around CLA A 833:**

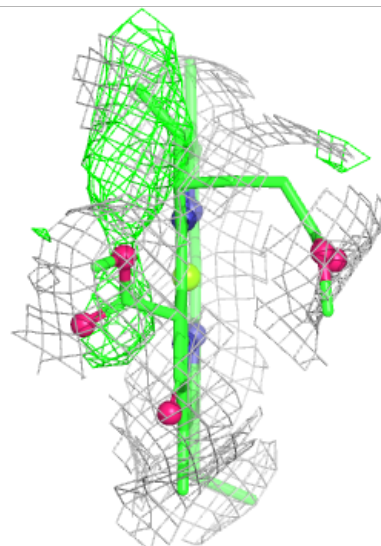
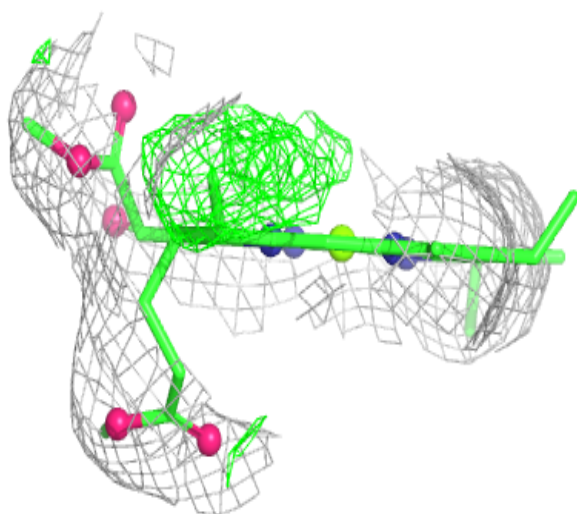
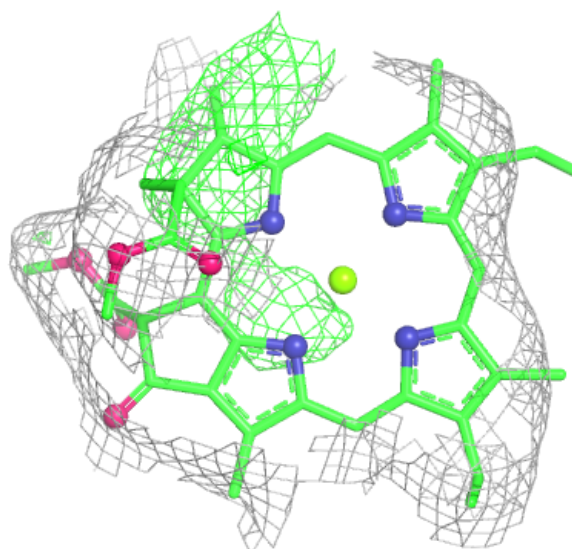
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





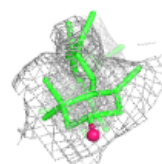
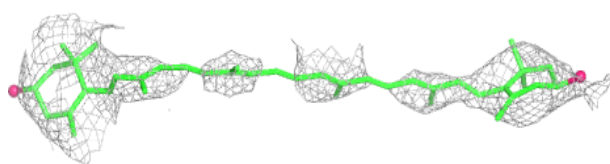
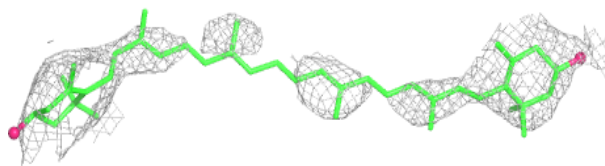
**Electron density around CLA 4 312:**

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

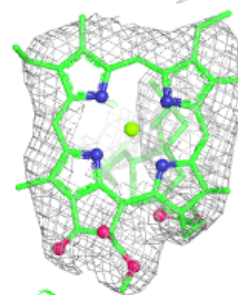
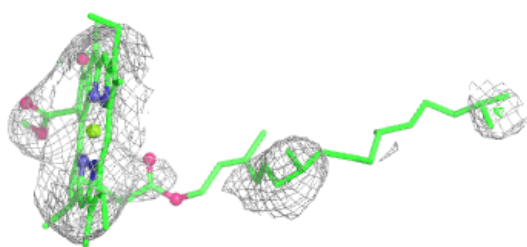
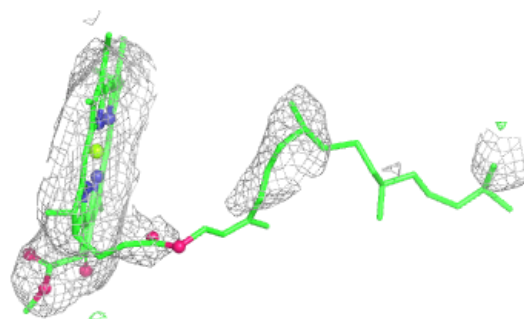


**Electron density around LUT 1 5004:**

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

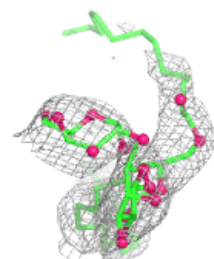
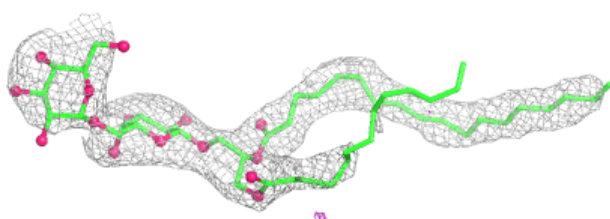
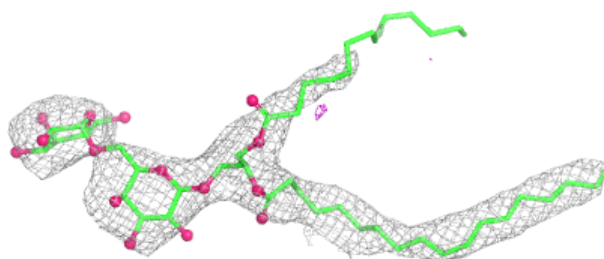
**Electron density around CLA B 805:**

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

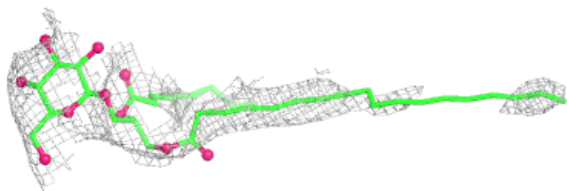


**Electron density around DGD B 855:**

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

**Electron density around LMG F 306:**

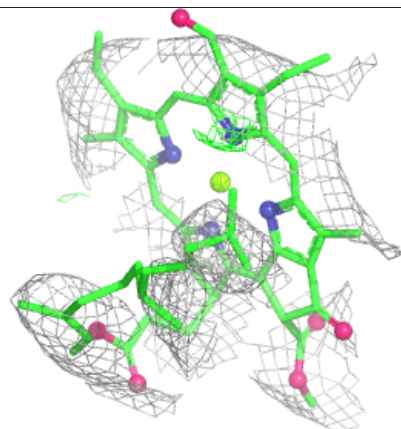
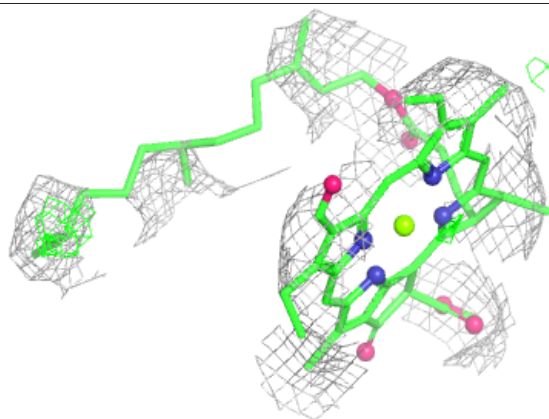
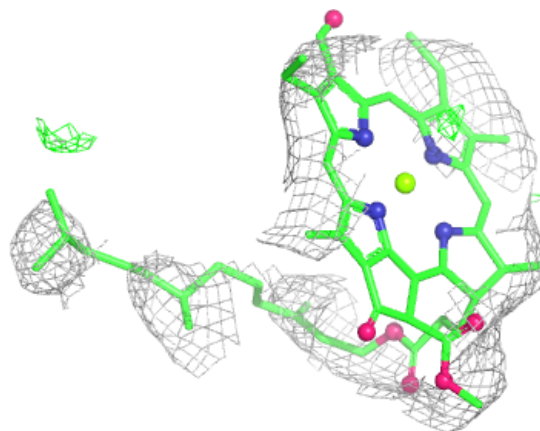
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





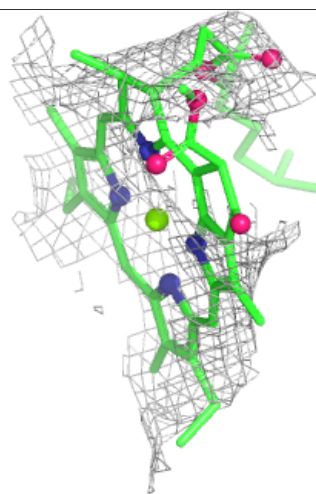
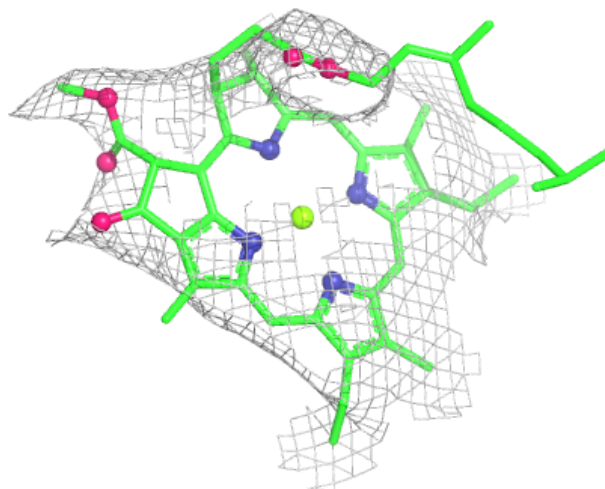
**Electron density around CHL 1 5016:**

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



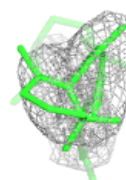
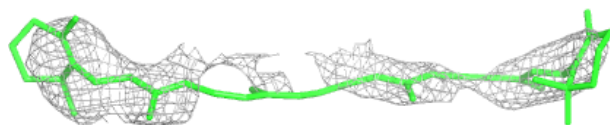
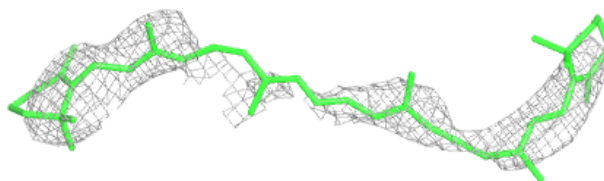
**Electron density around CLA 3 307:**

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

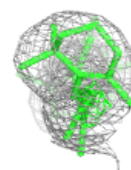
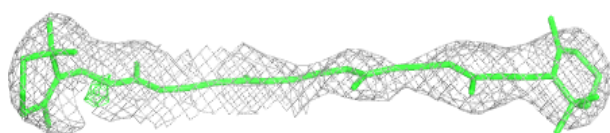
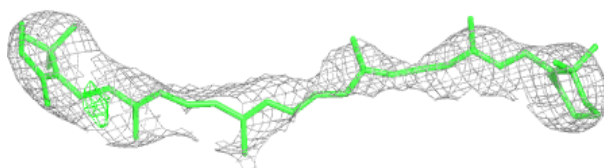


**Electron density around BCR B 845:**

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

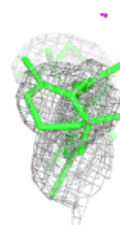
**Electron density around BCR B 846:**

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

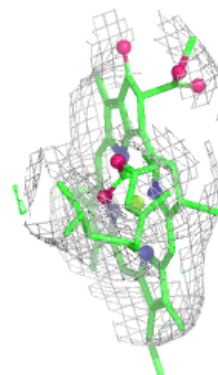
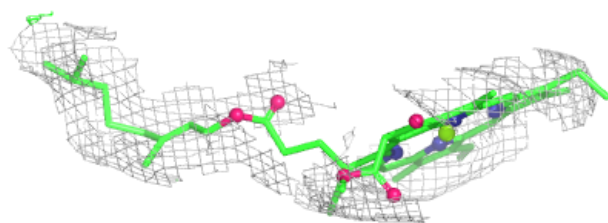
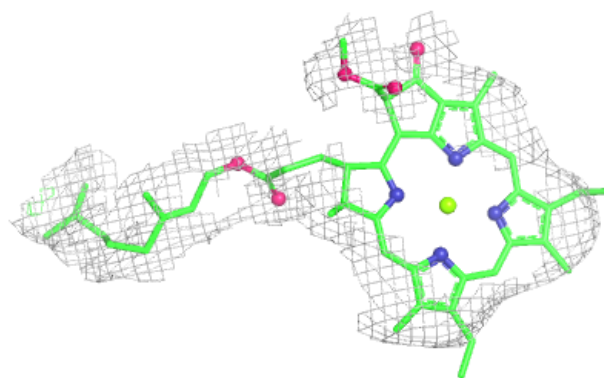


**Electron density around BCR B 847:**

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

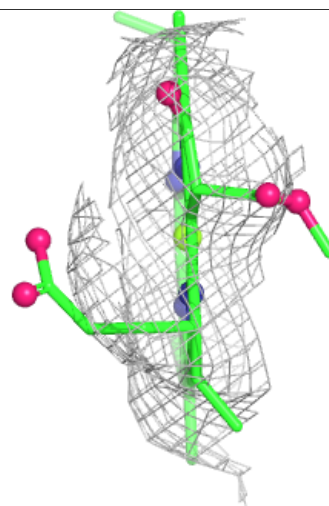
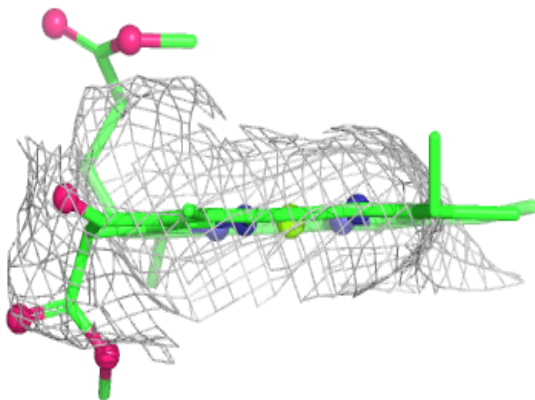
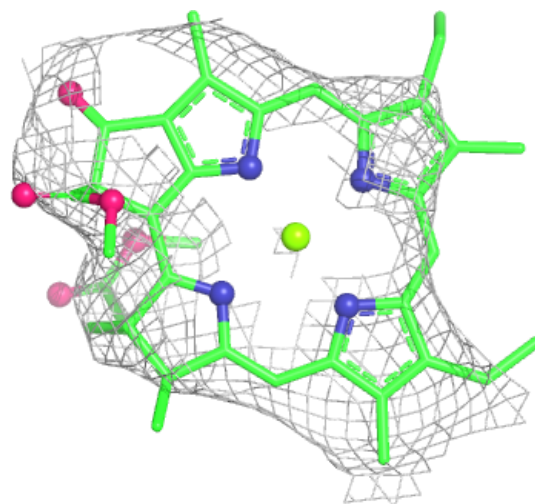
**Electron density around CLA G 1601:**

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



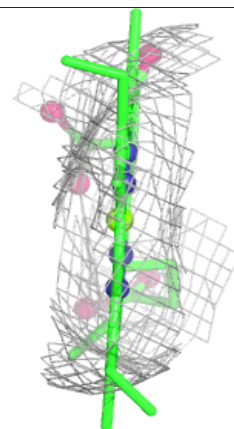
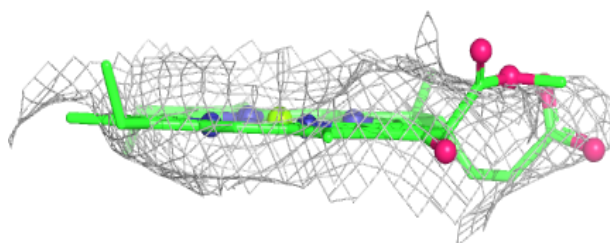
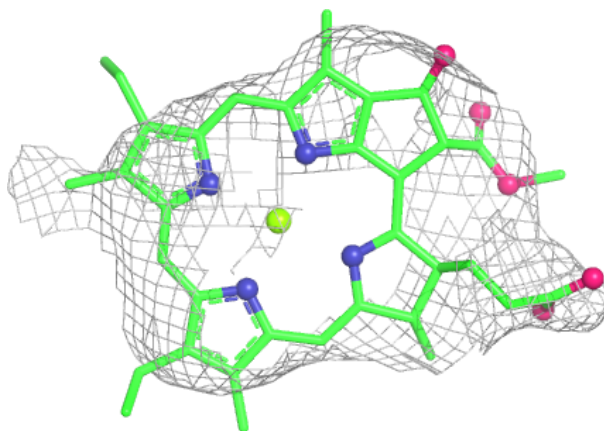
**Electron density around CLA A 814:**

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

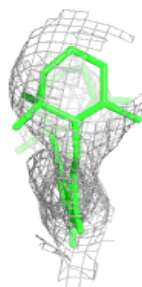
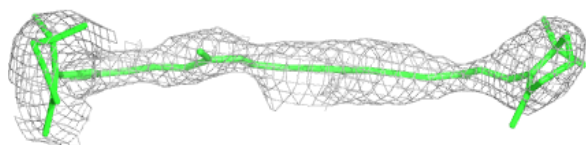
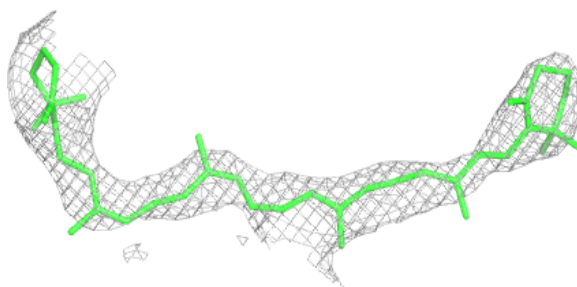


**Electron density around CLA 1 5017:**

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

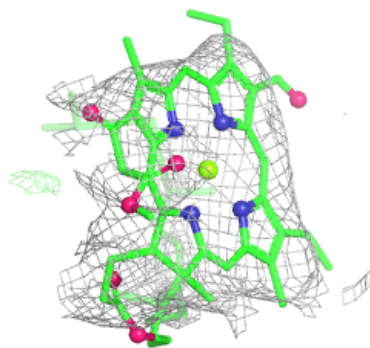
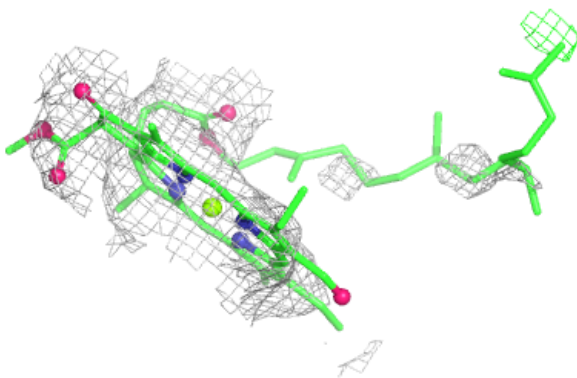
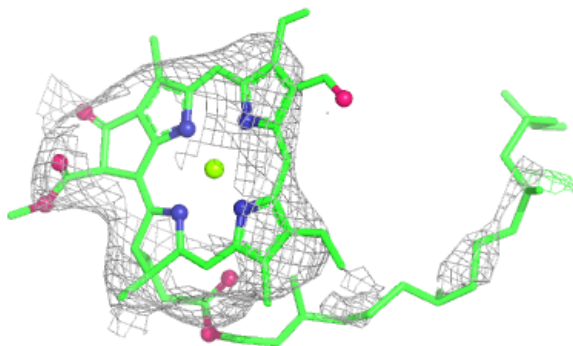
**Electron density around BCR L 303:**

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



**Electron density around CHL 3 310:**

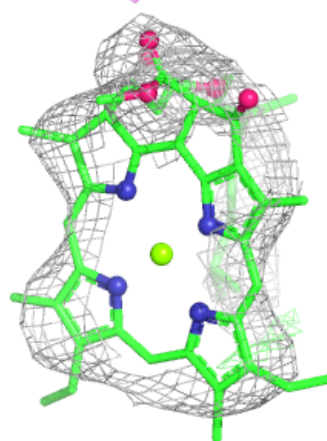
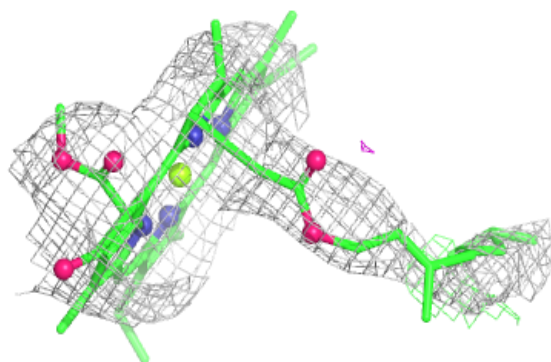
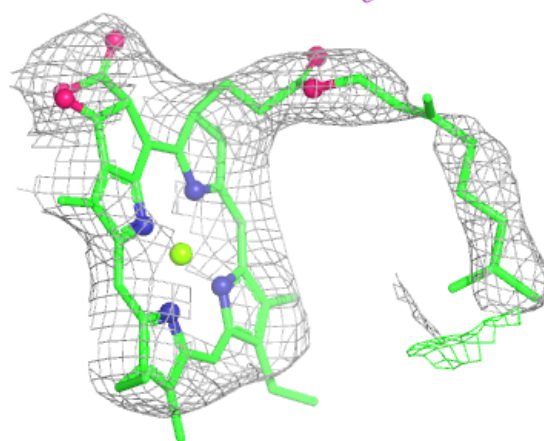
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA B 816:**

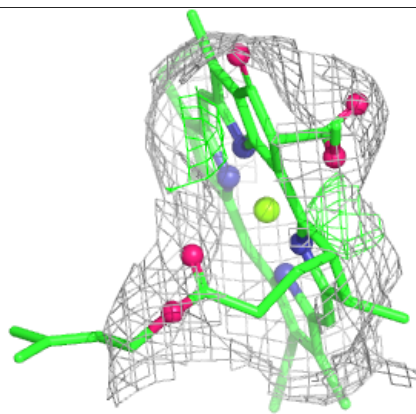
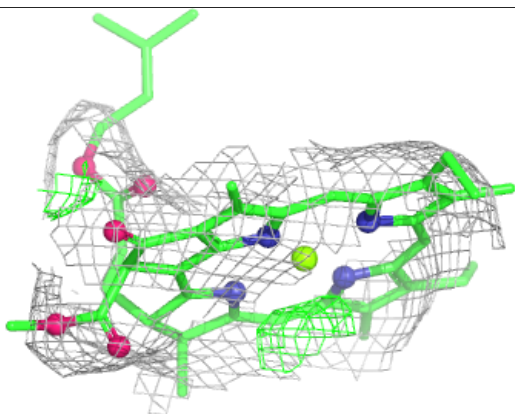
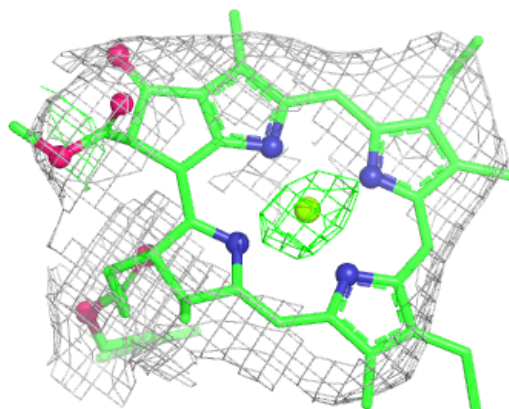
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



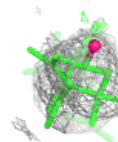
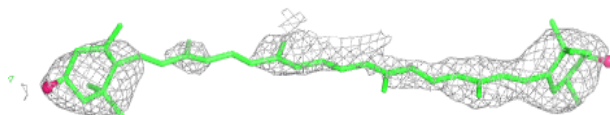
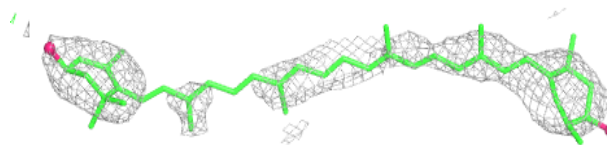


**Electron density around CLA 4 310:**

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

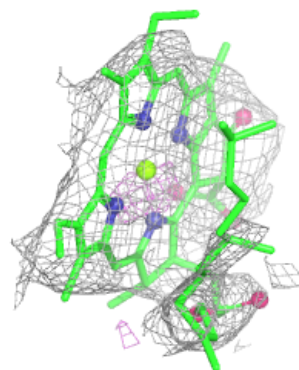
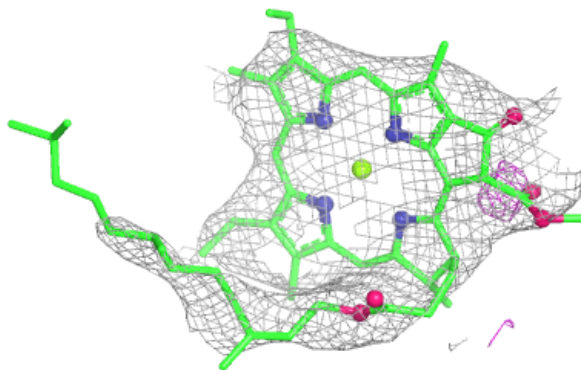
**Electron density around ZEX F 310:**

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

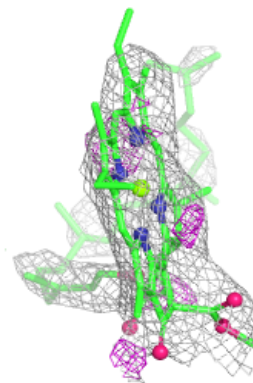
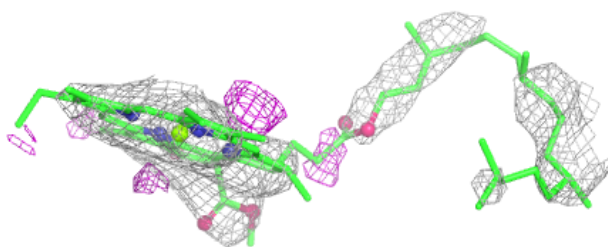
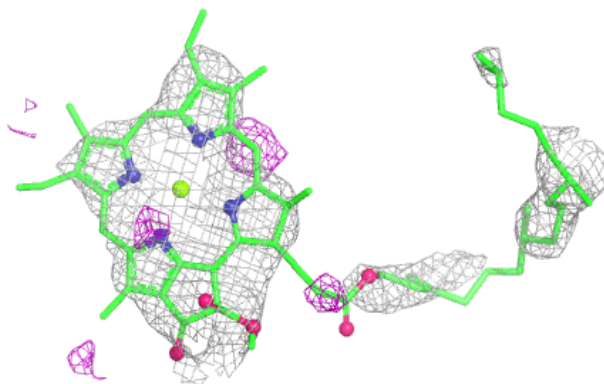


**Electron density around CLA 2 306:**

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

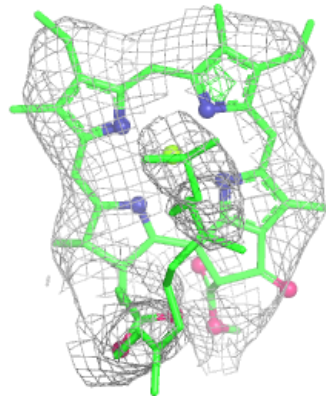
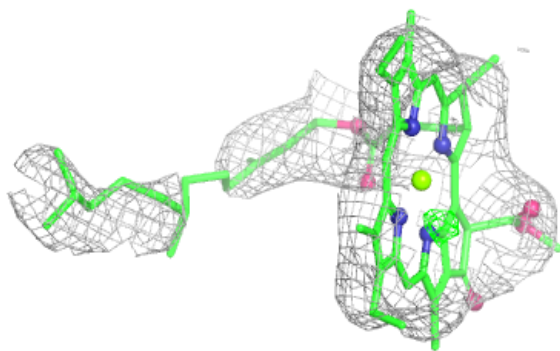
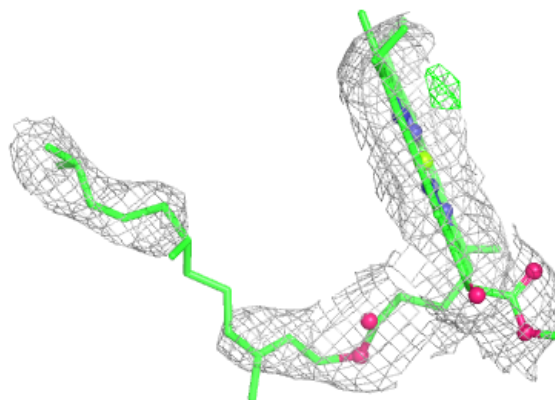
**Electron density around CLA A 825:**

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



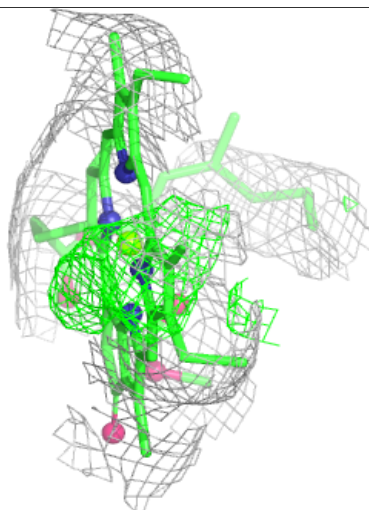
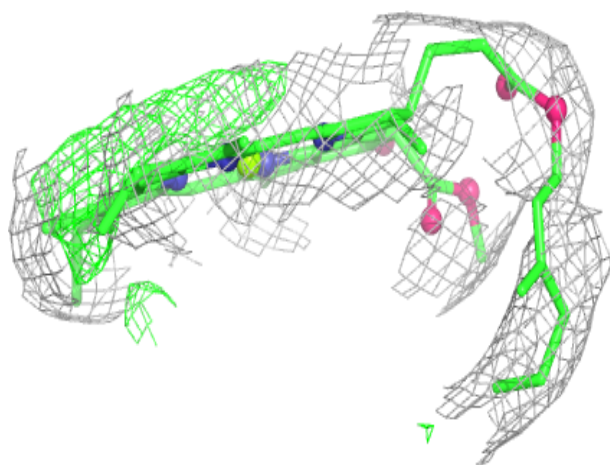
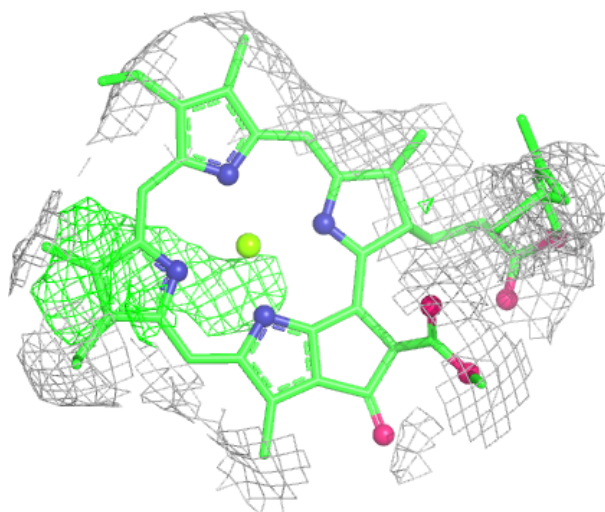
**Electron density around CLA A 806:**

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



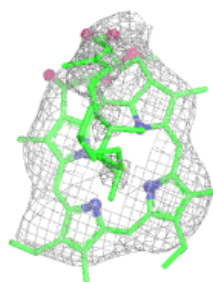
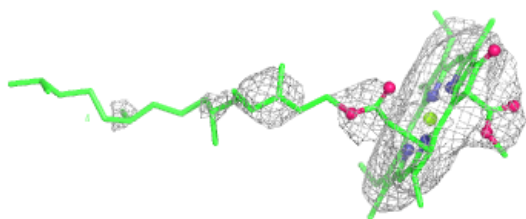
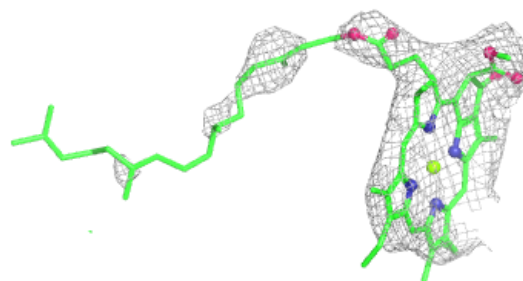
**Electron density around CLA 2 307:**

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

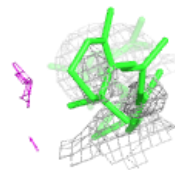
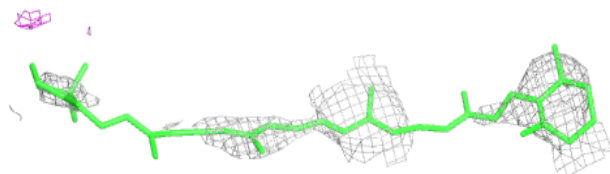
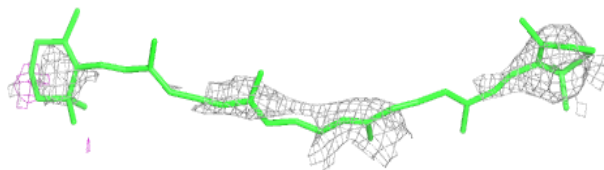


**Electron density around CLA B 822:**

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

**Electron density around BCR A 855:**

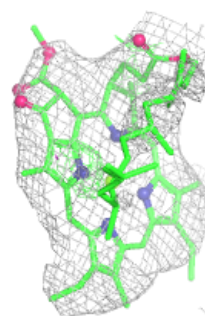
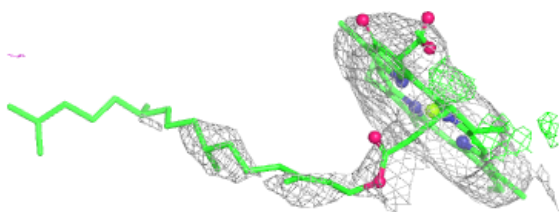
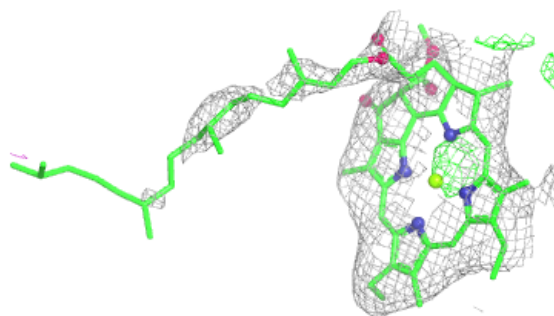
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



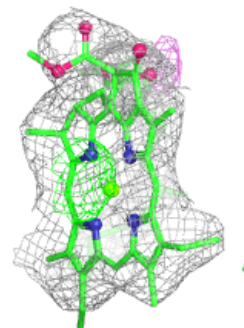
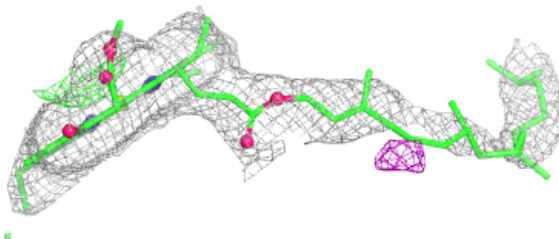
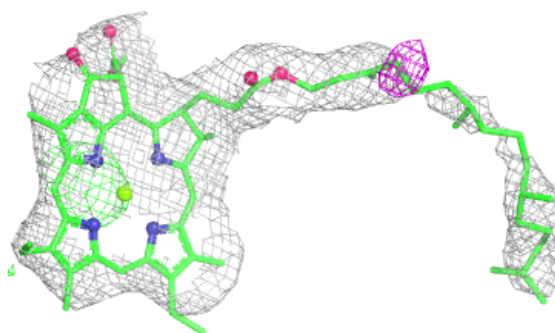


**Electron density around CLA B 823:**

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

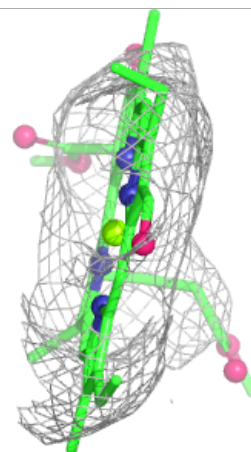
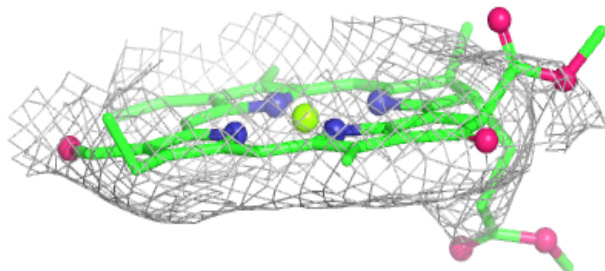
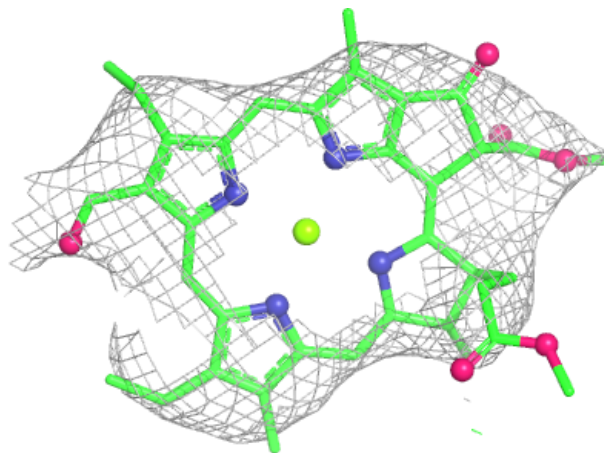
**Electron density around CLA B 826:**

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



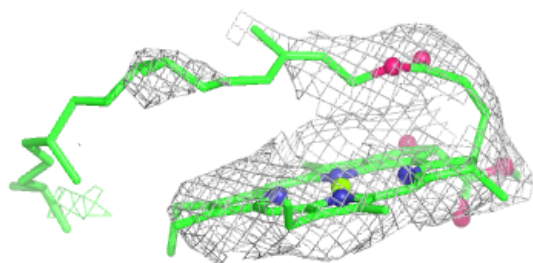
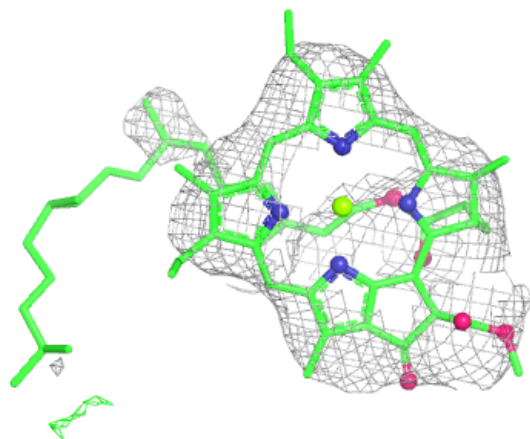
**Electron density around CHL 1 5014:**

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



**Electron density around CLA A 815:**

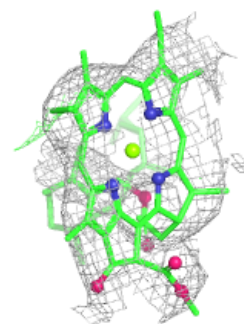
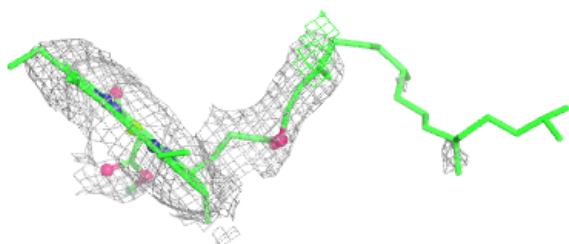
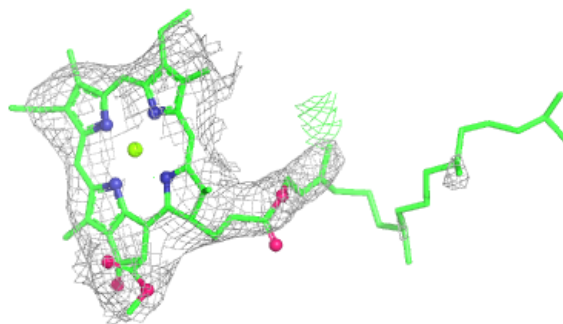
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



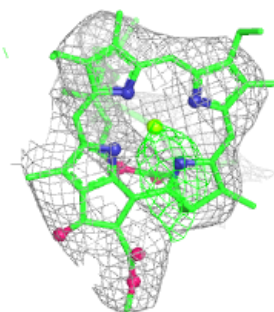
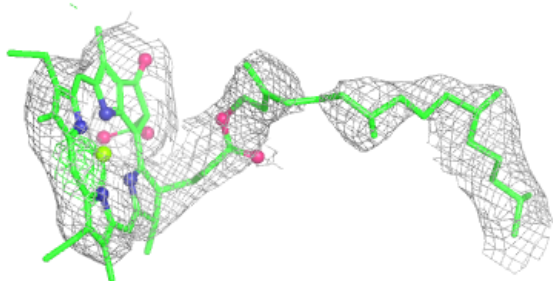
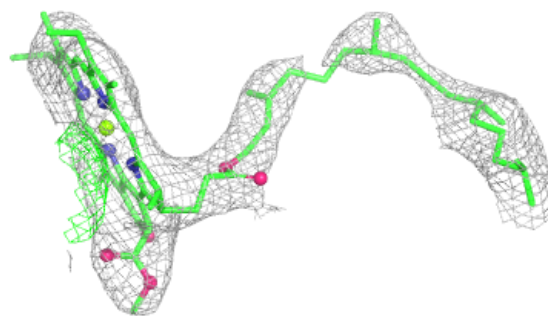


**Electron density around CLA A 829:**

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

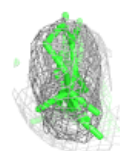
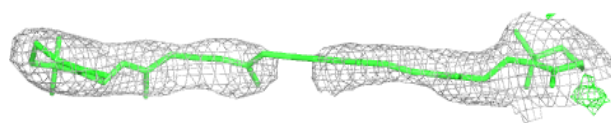
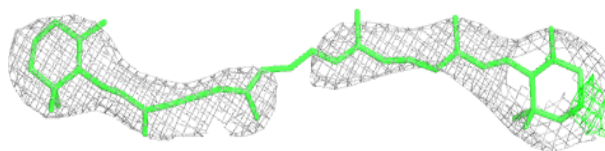
**Electron density around CLA B 839:**

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

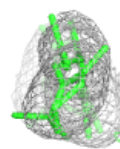
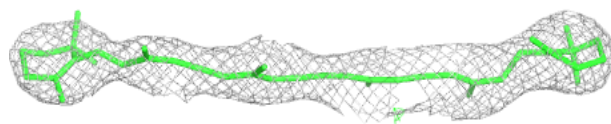
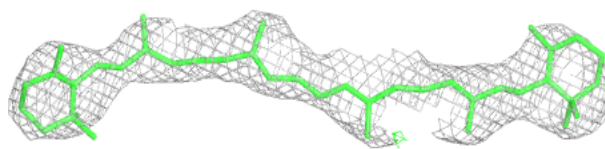


**Electron density around BCR I 102:**

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

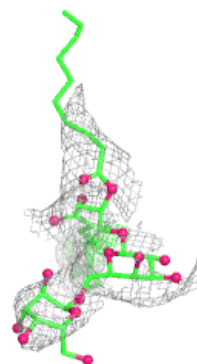
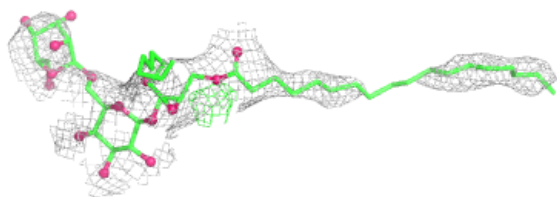
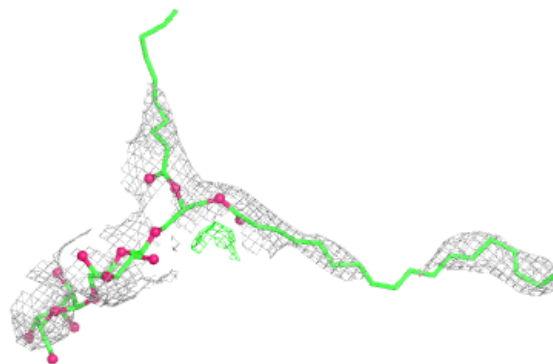
**Electron density around BCR J 1104:**

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

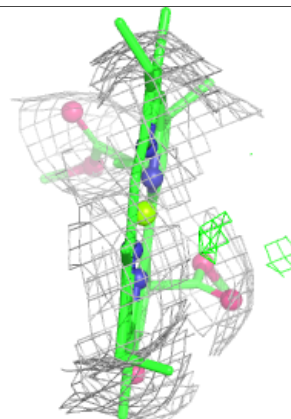
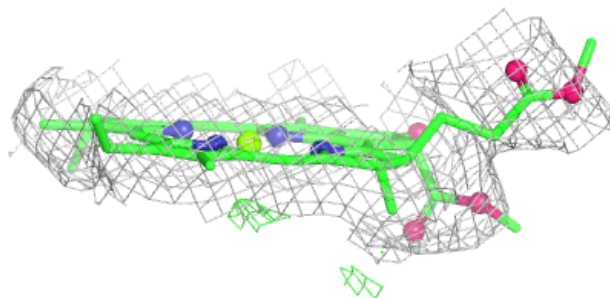
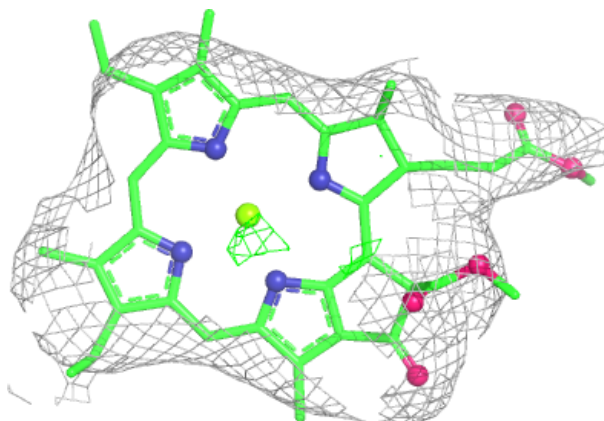


**Electron density around DGD J 1106:**

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

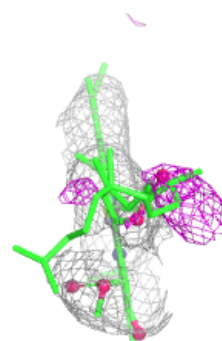
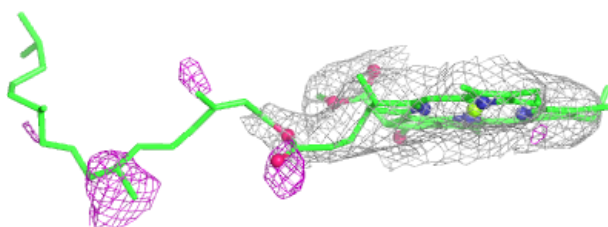
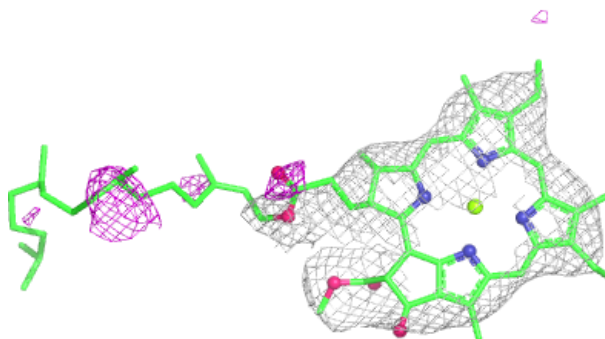
**Electron density around CLA 3 318:**

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

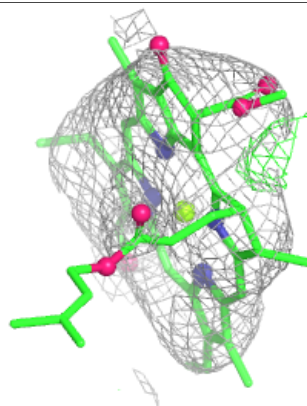
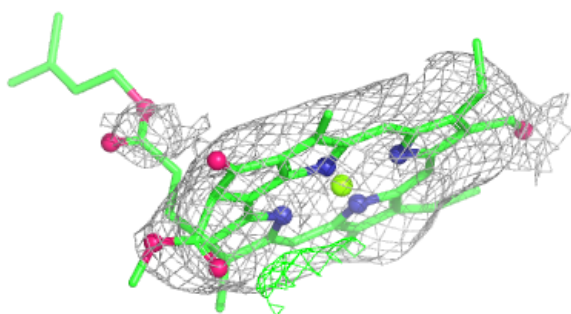
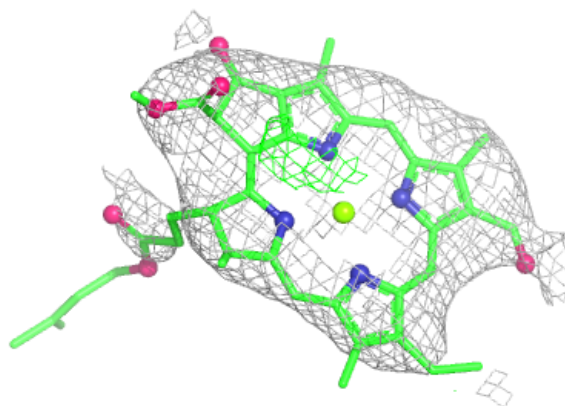


**Electron density around CLA F 302:**

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

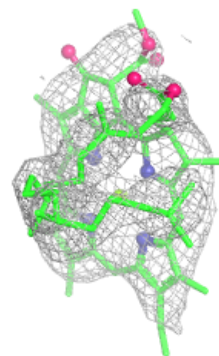
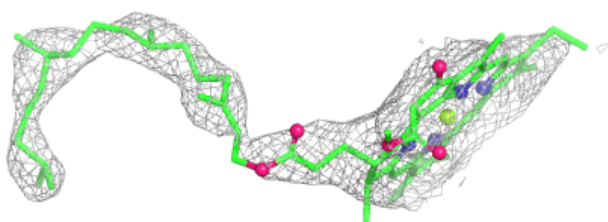
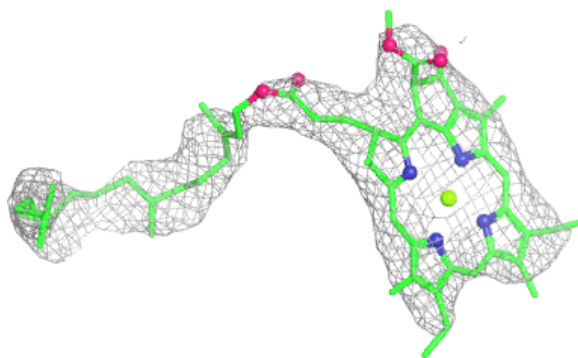
**Electron density around CHL 4 314:**

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

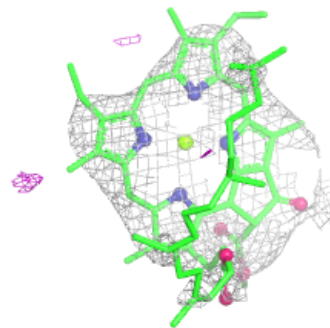
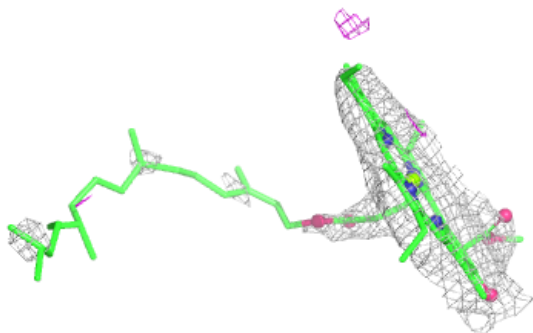
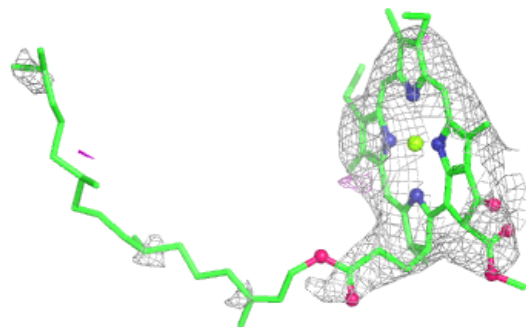


**Electron density around CLA B 810:**

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

**Electron density around CLA A 832:**

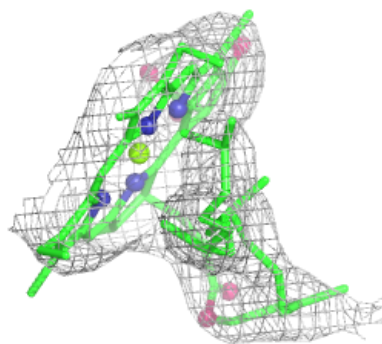
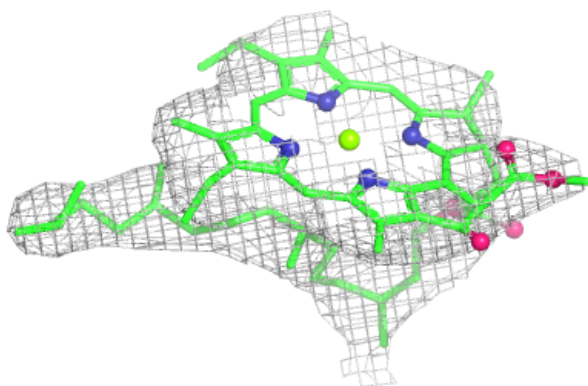
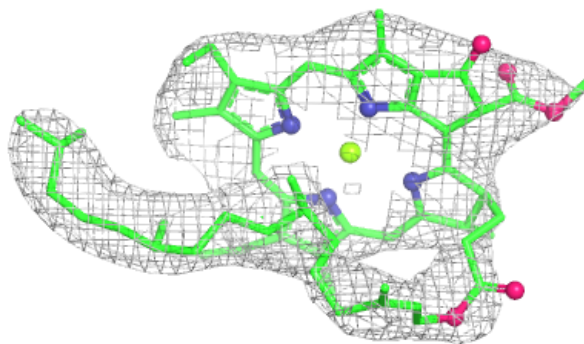
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



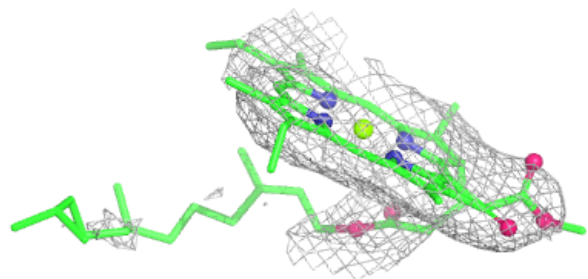
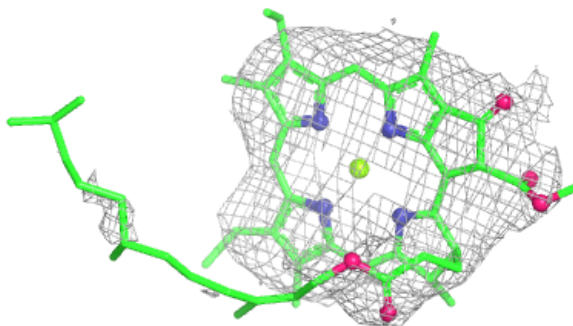


**Electron density around CLA B 818:**

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

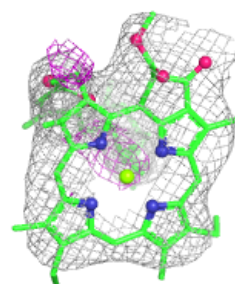
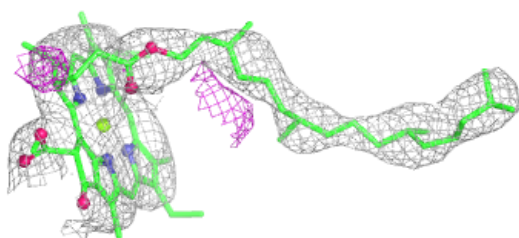
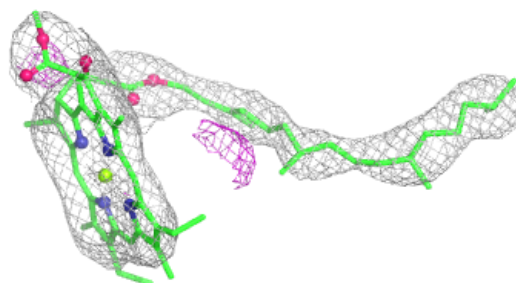
**Electron density around CLA 4 305:**

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



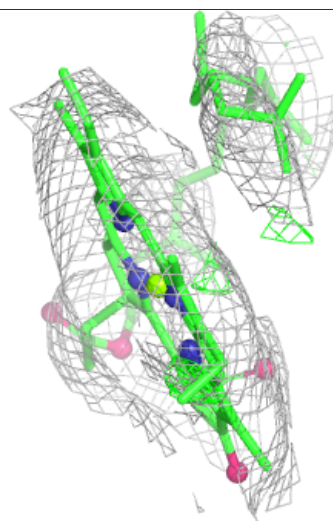
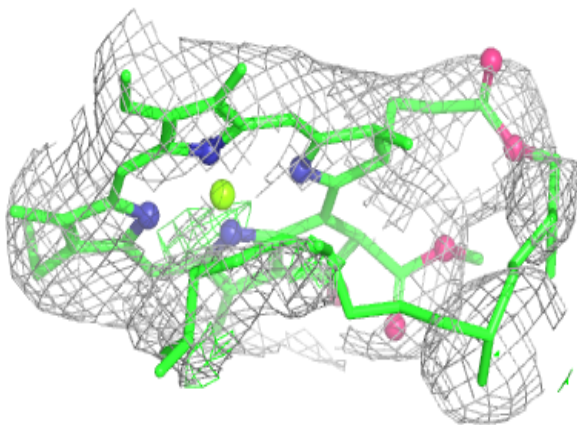
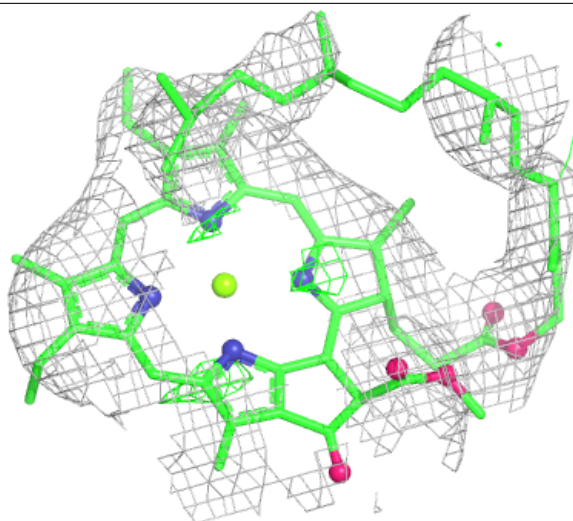
**Electron density around CLA A 810:**

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



**Electron density around CLA 2 310:**

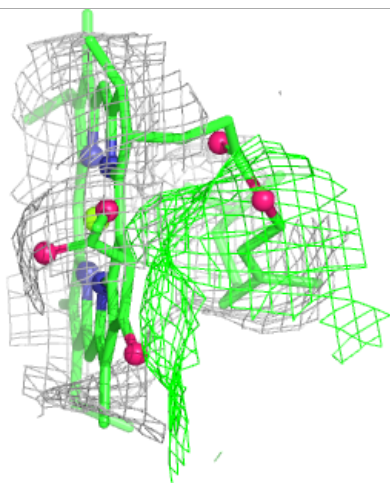
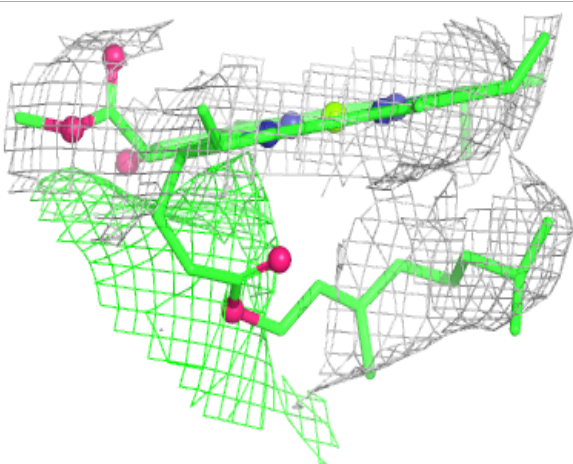
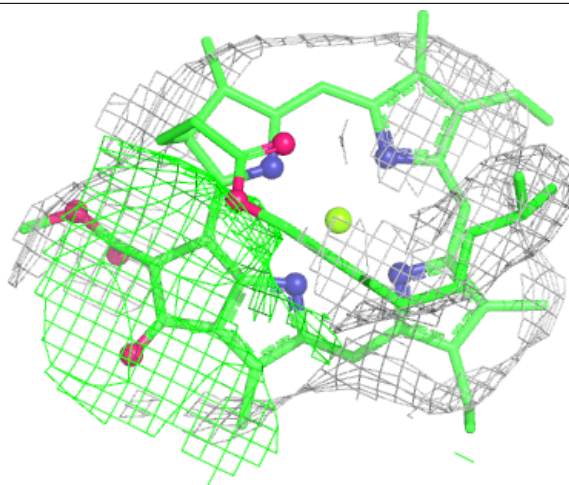
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





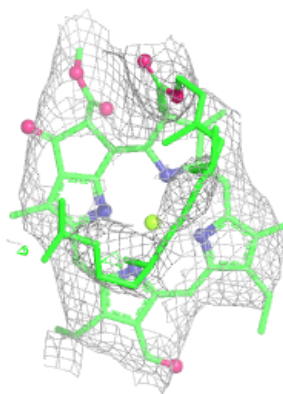
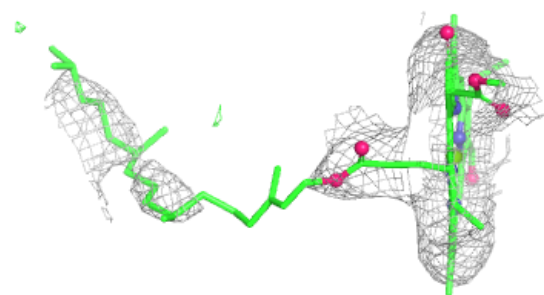
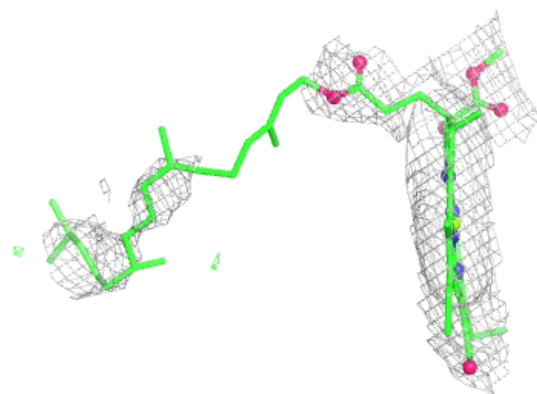
**Electron density around CLA 1 5008:**

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

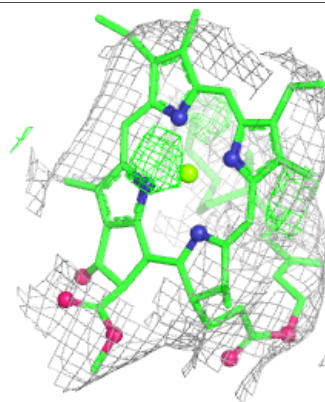
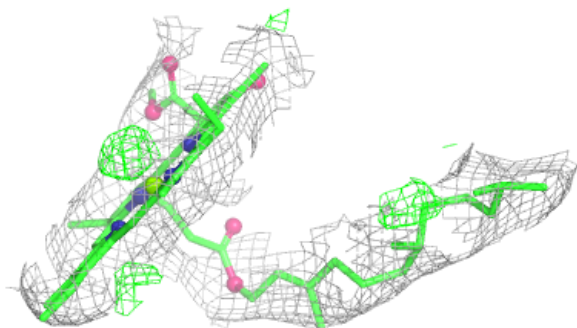
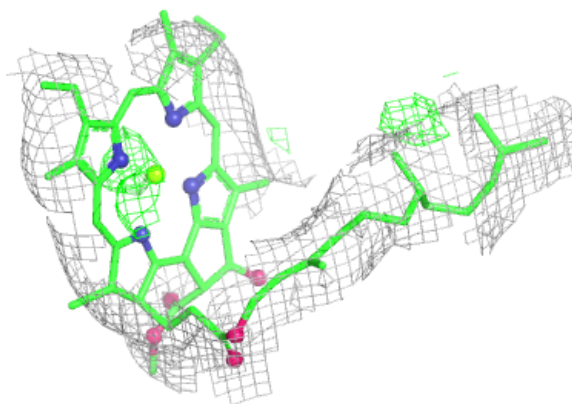


**Electron density around CHL 2 314:**

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

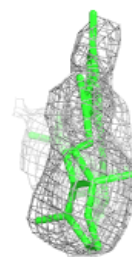
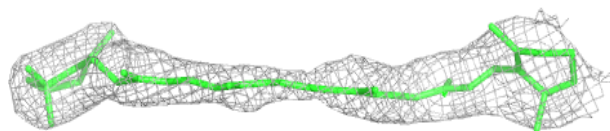
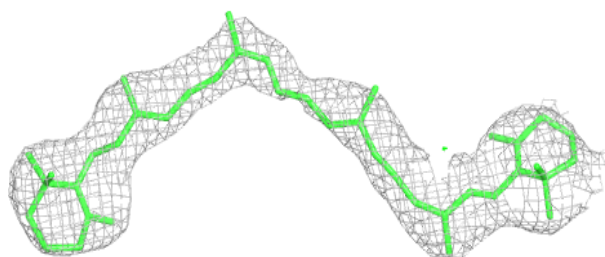
**Electron density around CLA 2 312:**

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

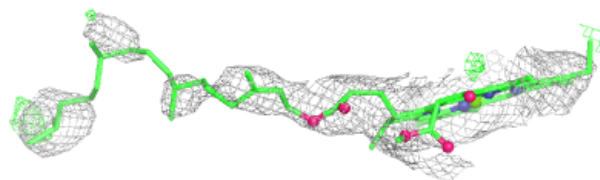
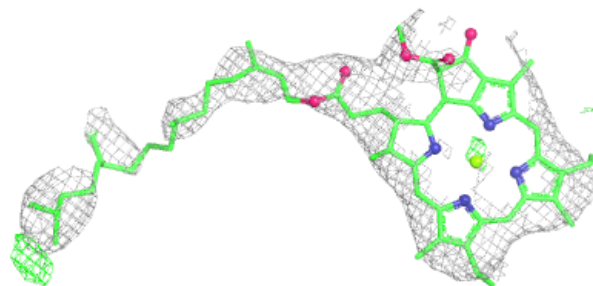


**Electron density around BCR A 847:**

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

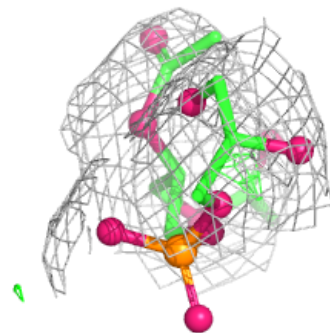
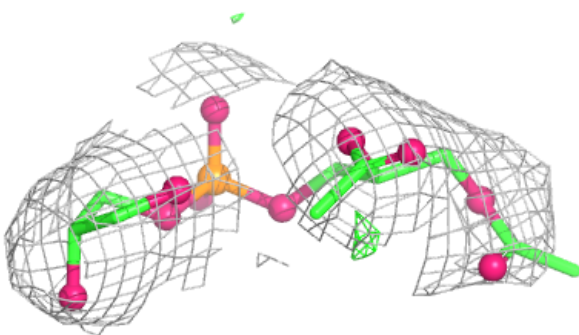
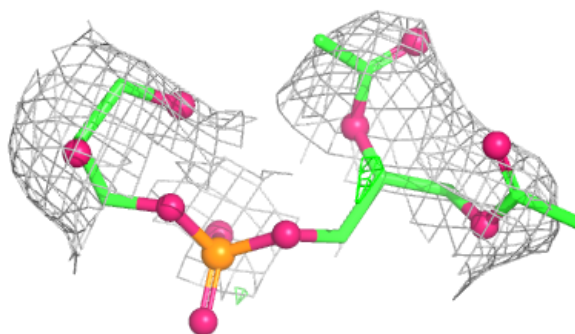
**Electron density around CLA F 303:**

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



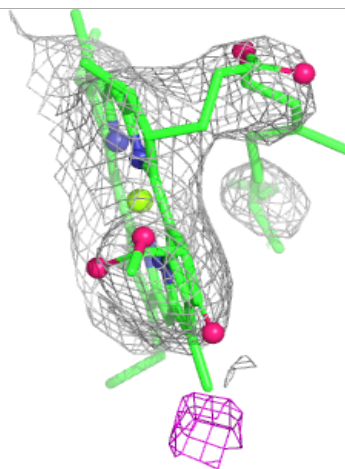
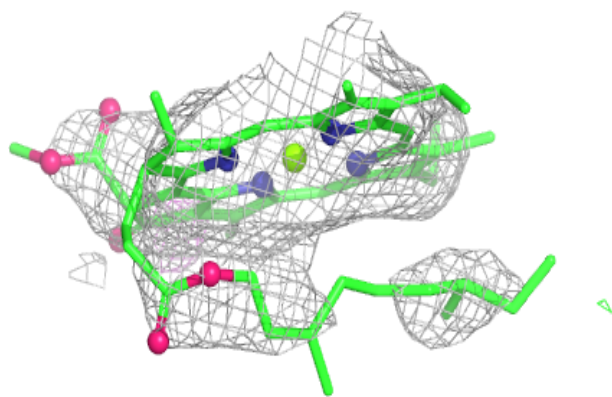
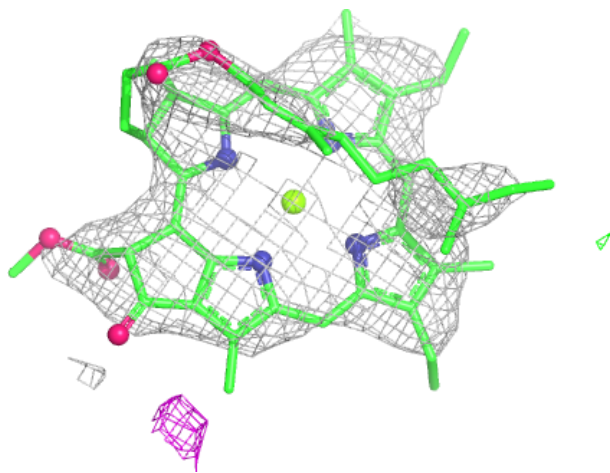
**Electron density around LHG B 848:**

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



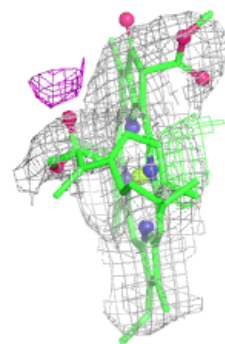
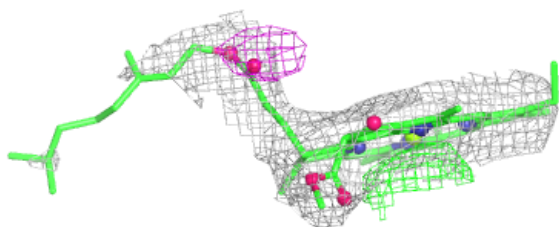
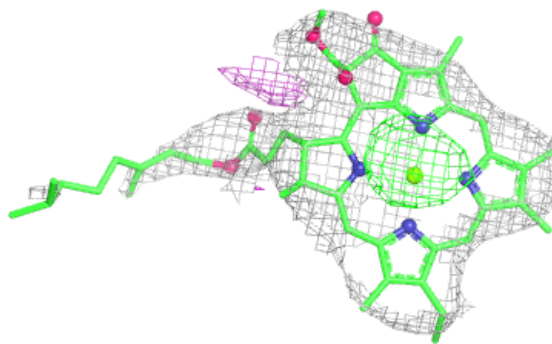
**Electron density around CLA A 816:**

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



**Electron density around CLA A 824:**

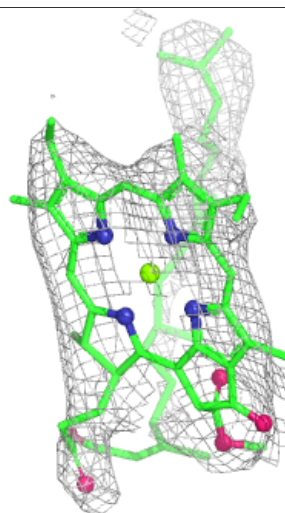
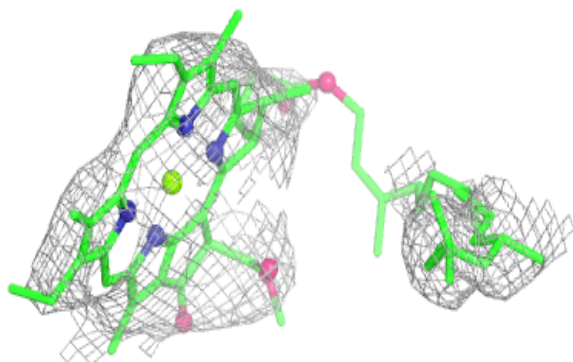
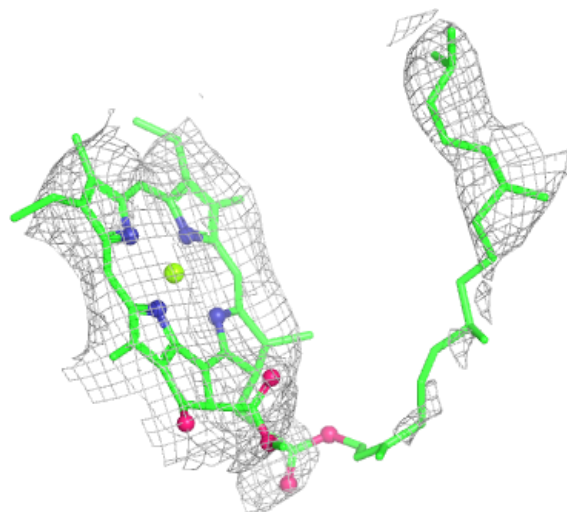
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





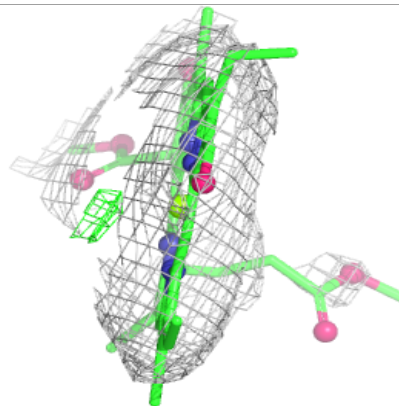
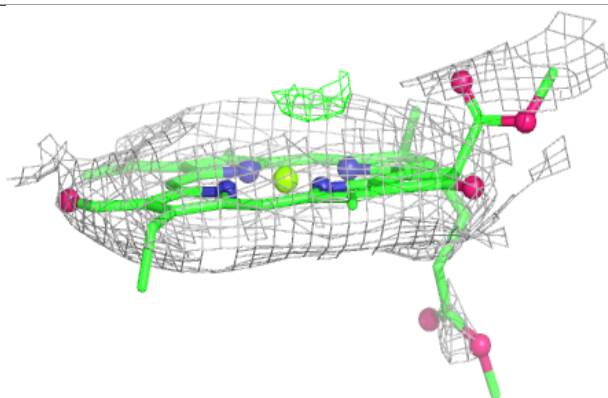
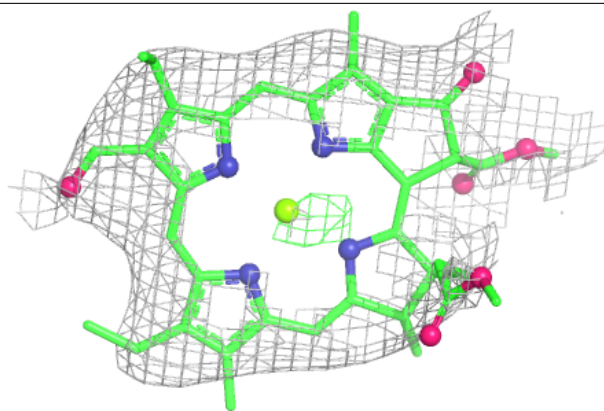
**Electron density around CLA B 811:**

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



**Electron density around CHL 3 316:**

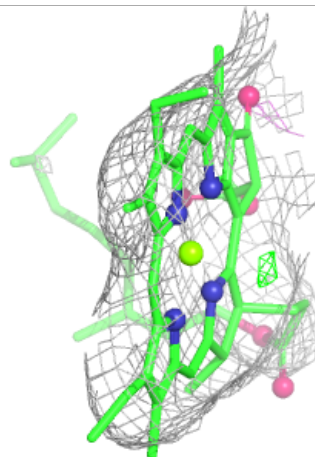
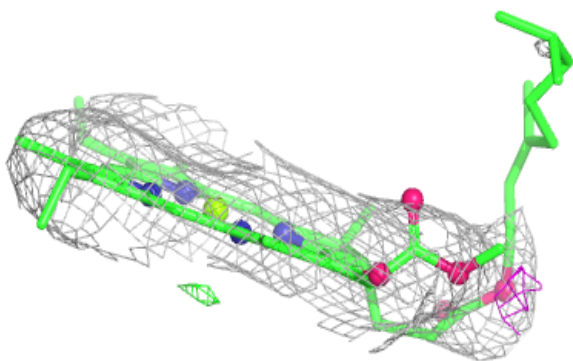
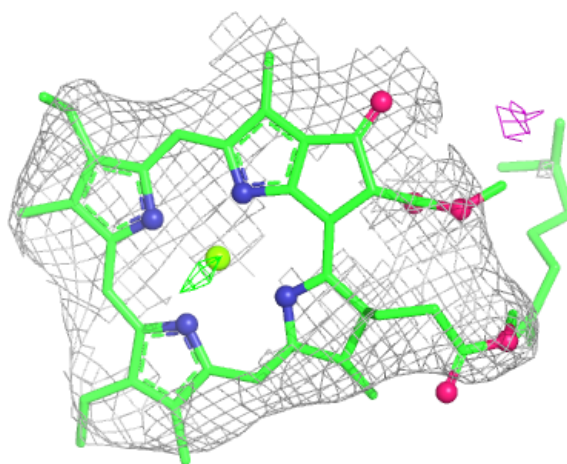
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





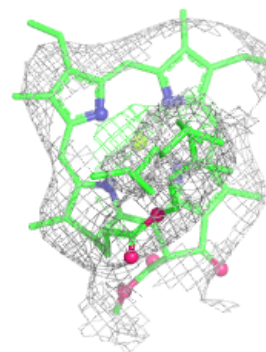
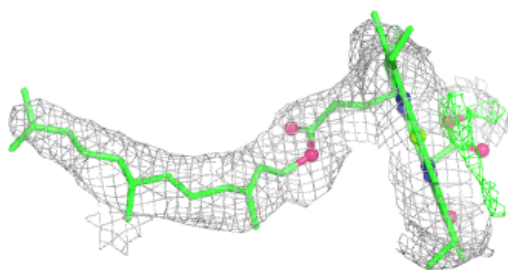
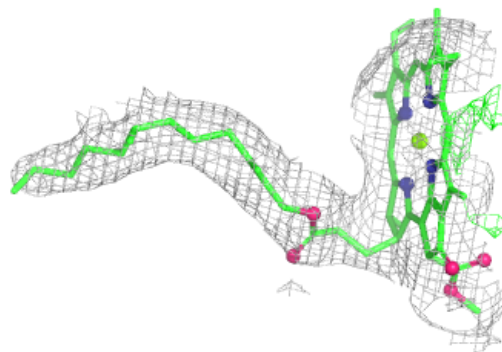
**Electron density around CLA 3 311:**

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



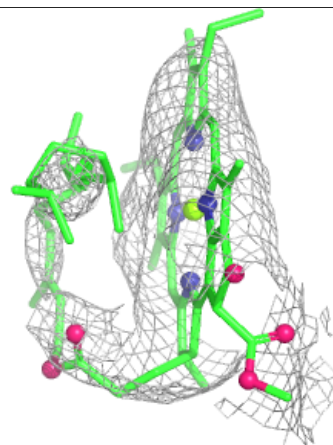
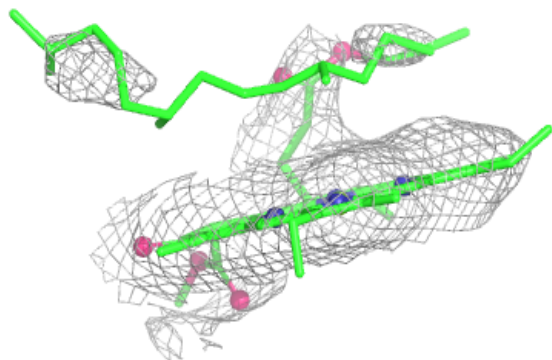
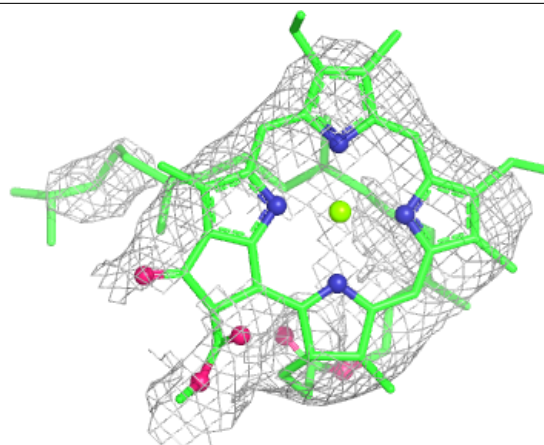
**Electron density around CLA L 305:**

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



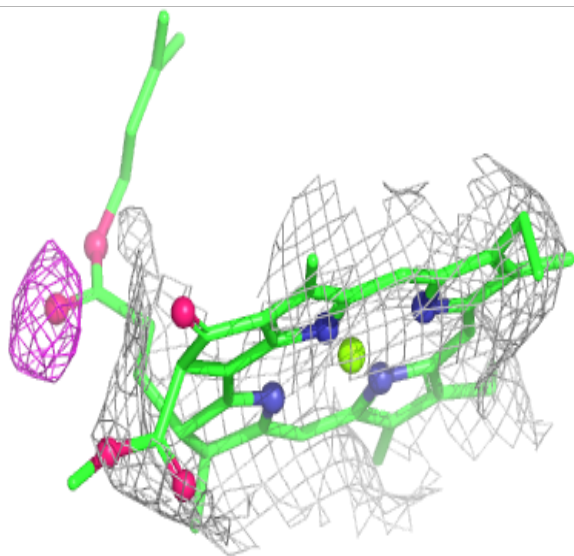
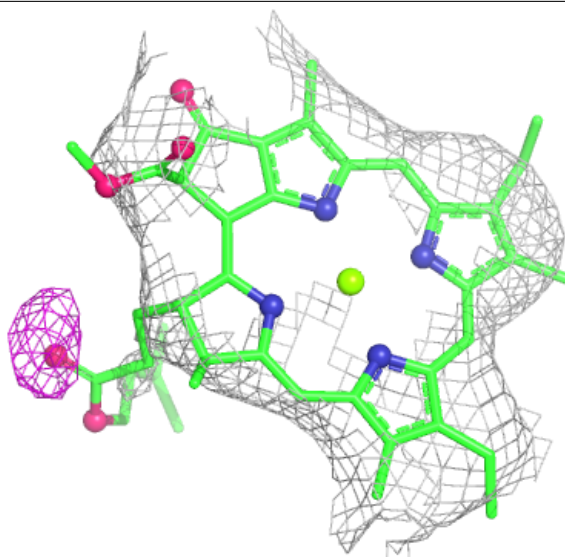
**Electron density around CLA 3 315:**

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



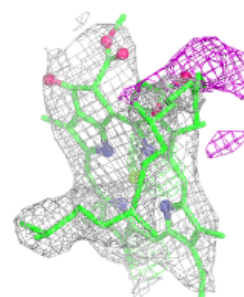
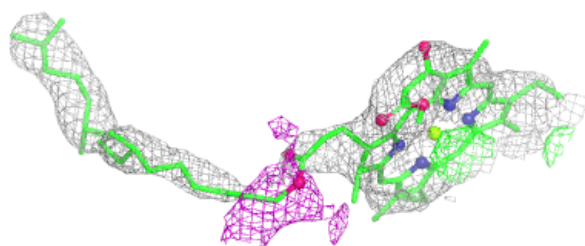
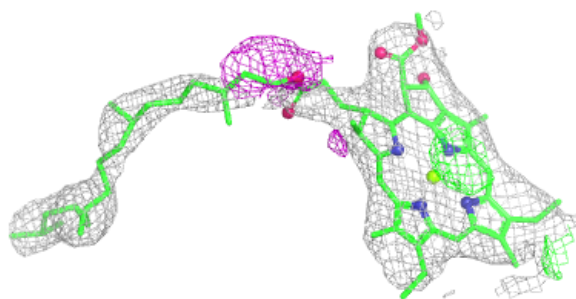
**Electron density around CLA 3 317:**

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

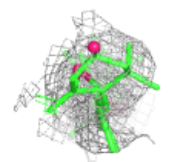
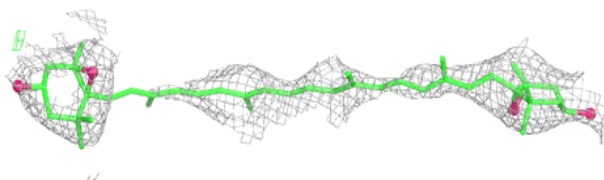
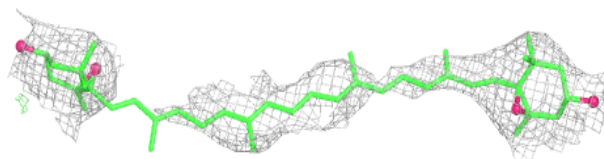


**Electron density around CLA B 801:**

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

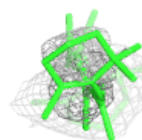
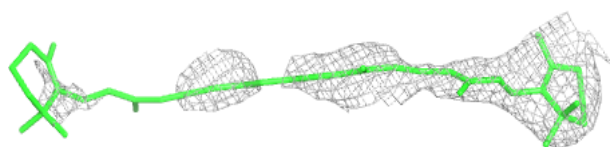
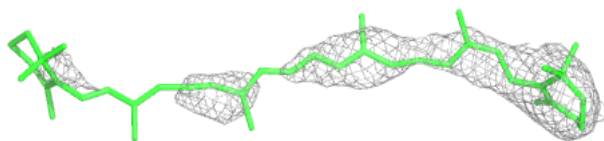
**Electron density around XAT 4 304:**

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

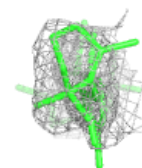
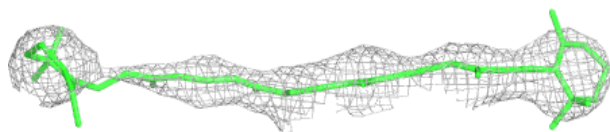


**Electron density around BCR A 844:**

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

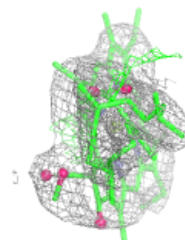
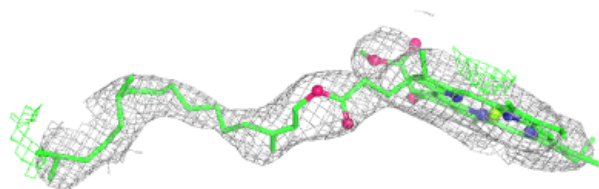
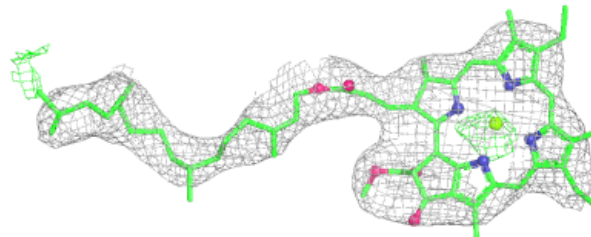
**Electron density around BCR A 845:**

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



**Electron density around CLA A 838:**

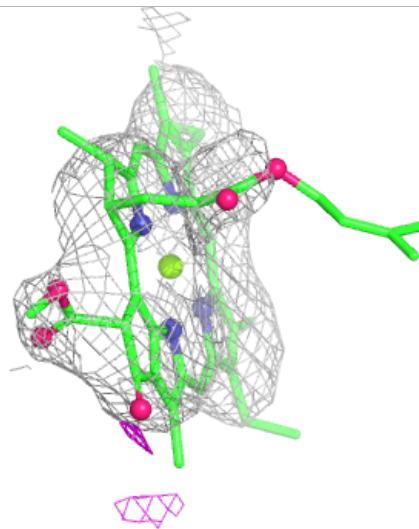
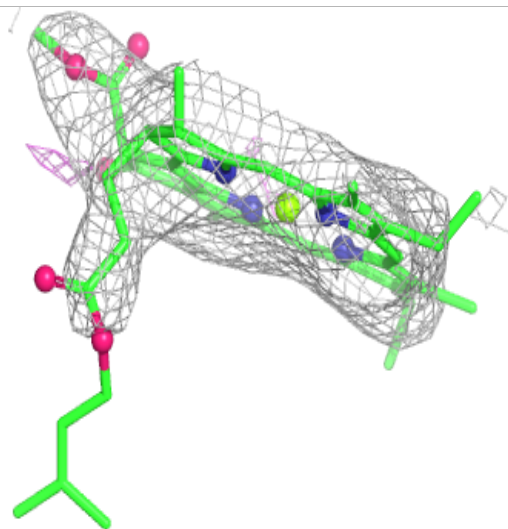
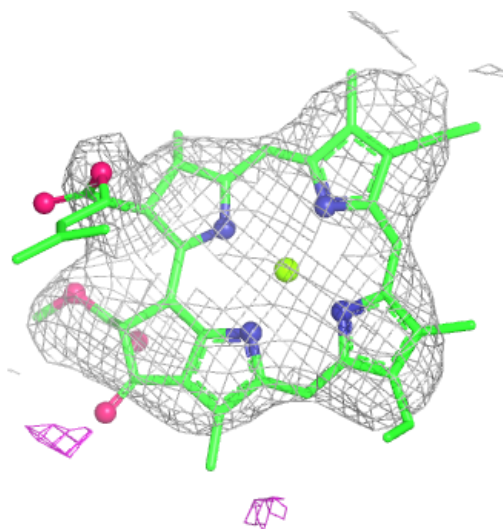
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA A 809:**

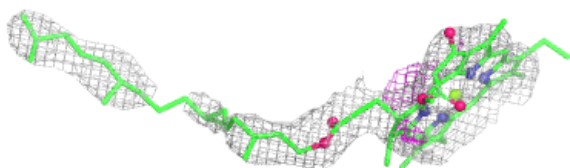
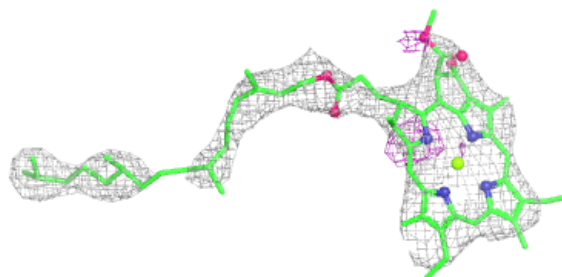
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



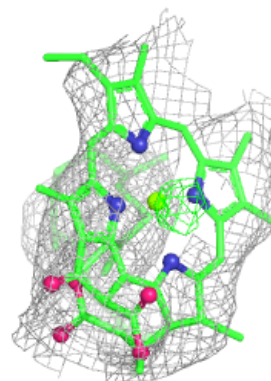
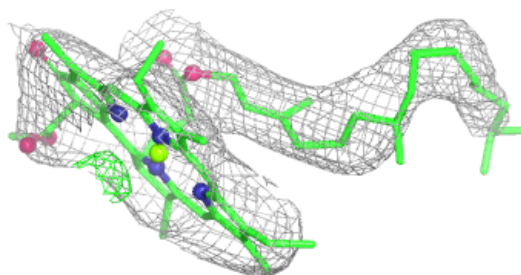
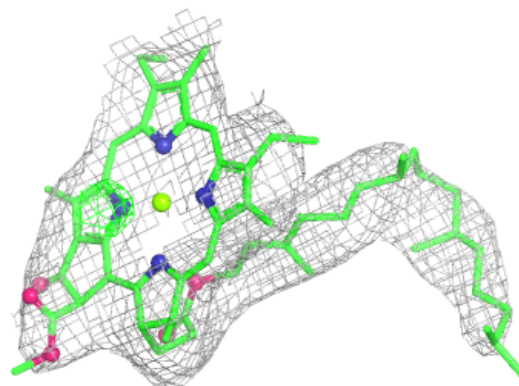


**Electron density around CLA A 852:**

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

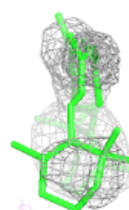
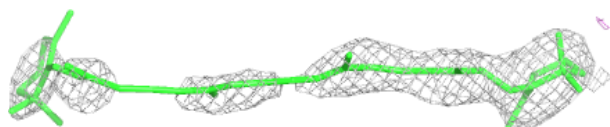
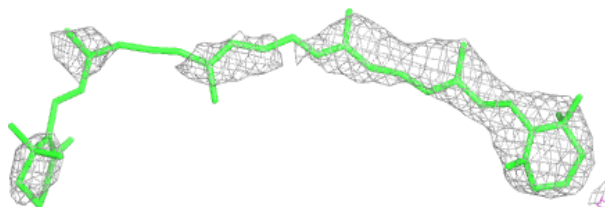
**Electron density around CLA A 853:**

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

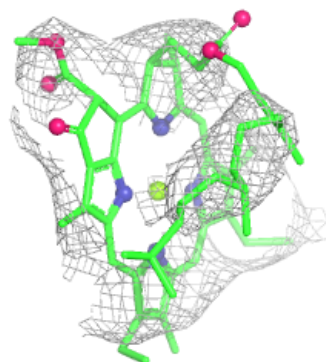
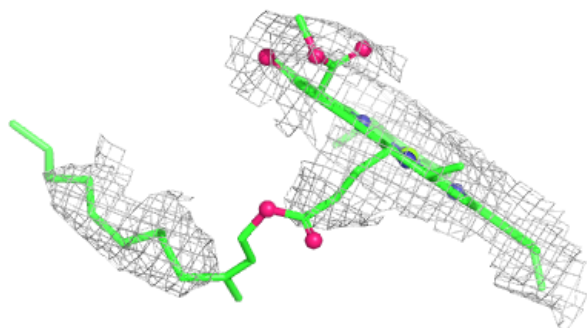
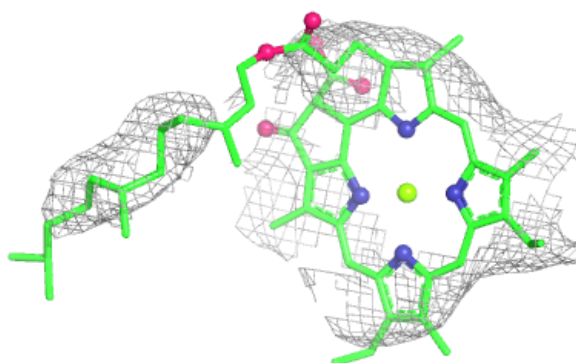


**Electron density around BCR B 844:**

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

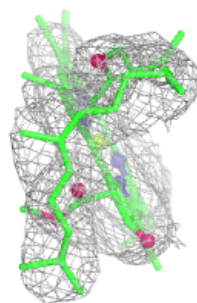
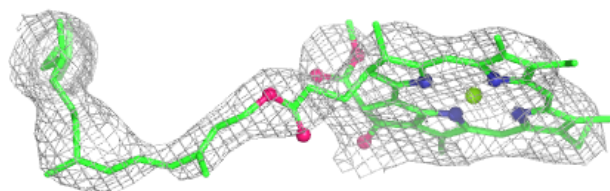
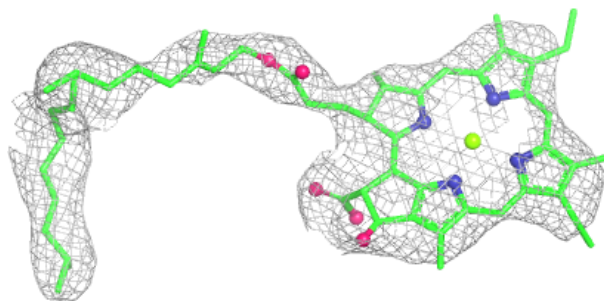
**Electron density around CLA A 820:**

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

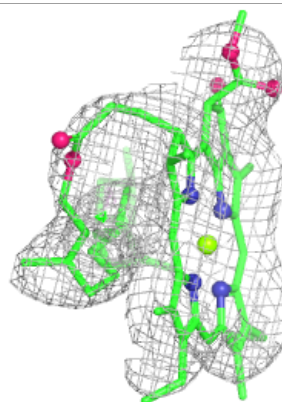
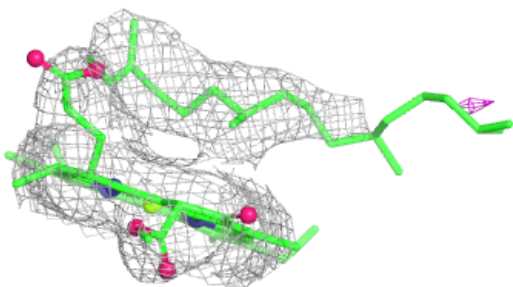
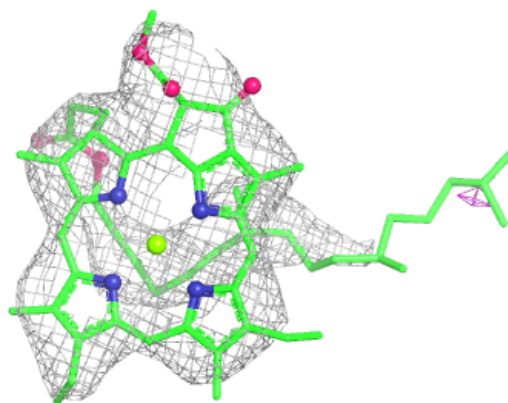


**Electron density around CLA B 827:**

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

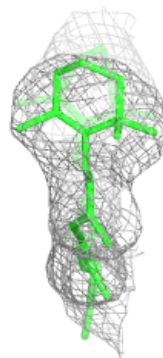
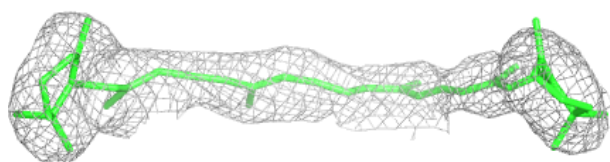
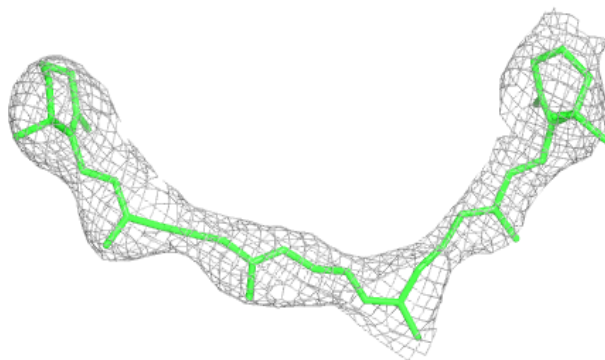
**Electron density around CLA B 828:**

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

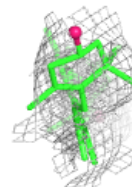
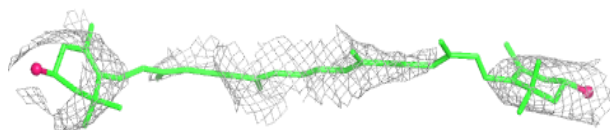
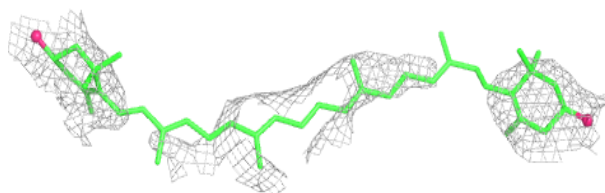


**Electron density around BCR F 305:**

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

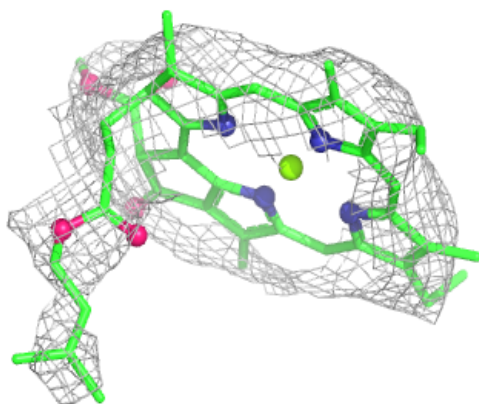
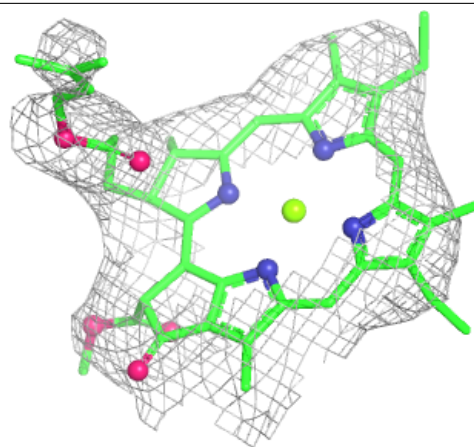
**Electron density around LUT 3 304:**

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



**Electron density around CLA 2 313:**

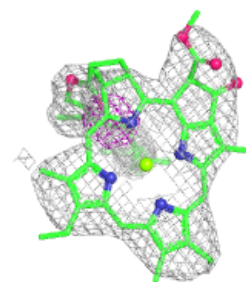
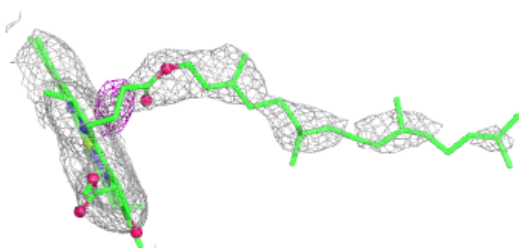
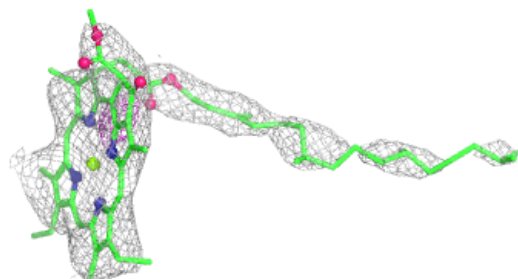
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



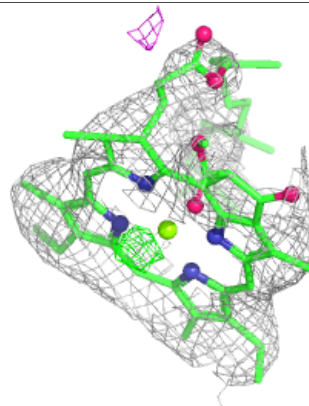
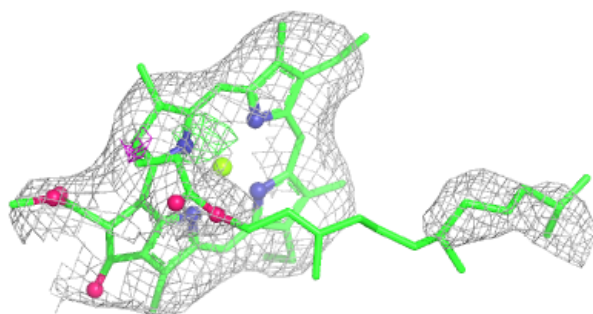
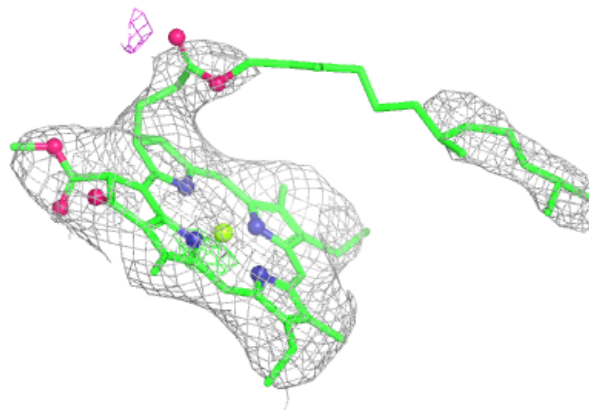


**Electron density around CLA B 829:**

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

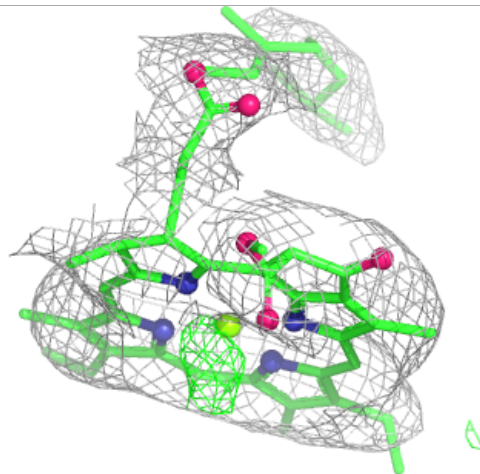
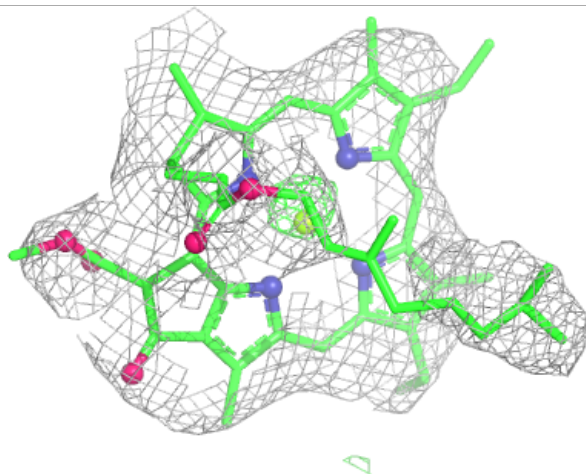
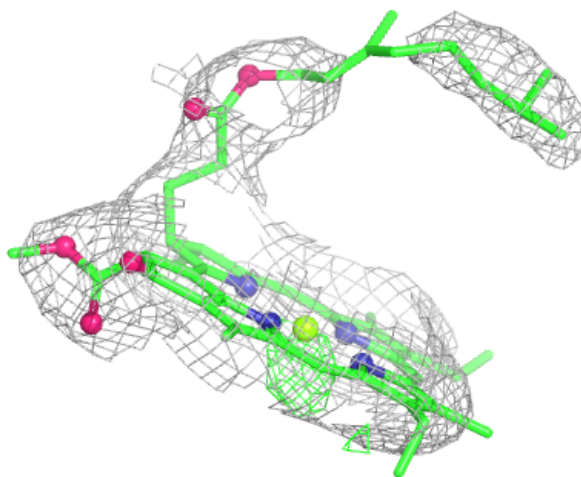
**Electron density around CLA B 832:**

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



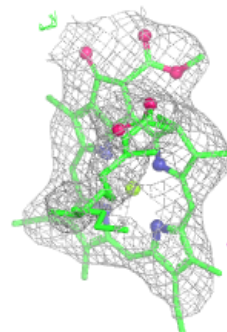
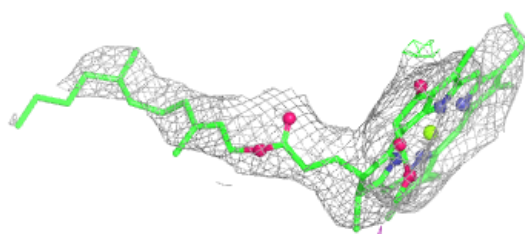
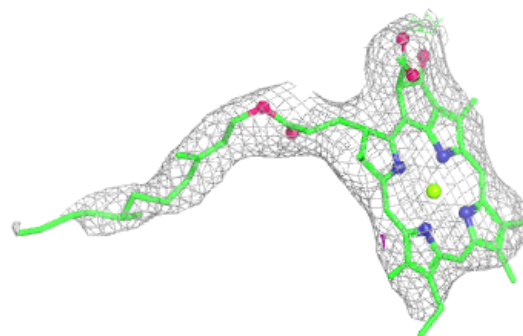
**Electron density around CLA L 301:**

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



**Electron density around CLA B 833:**

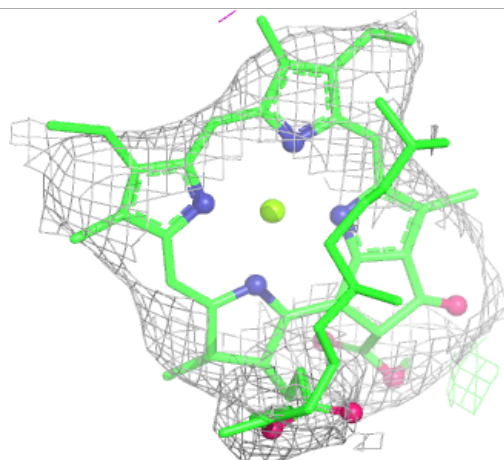
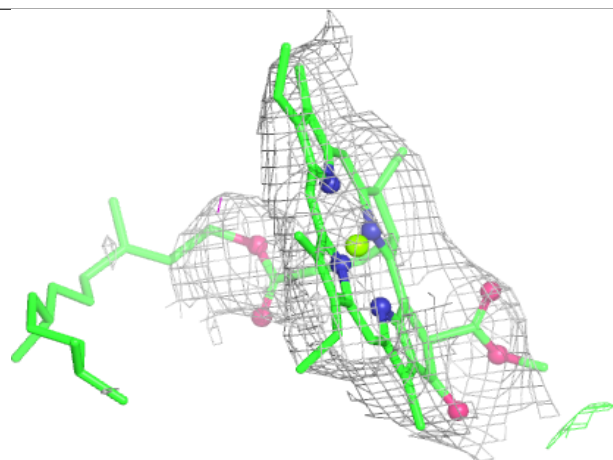
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





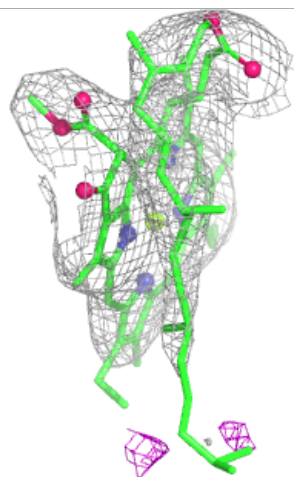
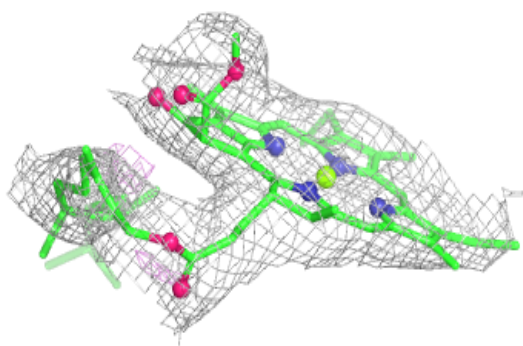
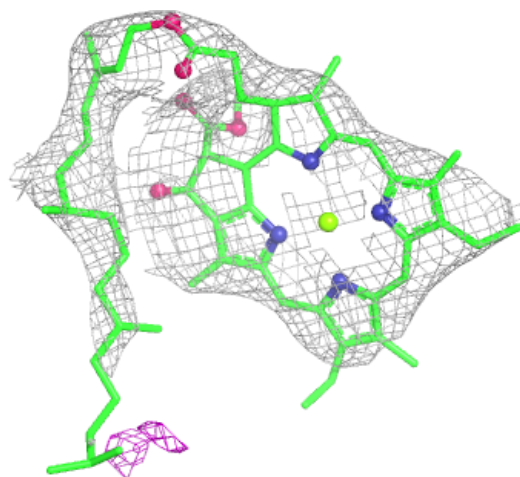
**Electron density around CLA A 821:**

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



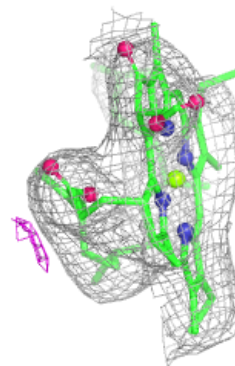
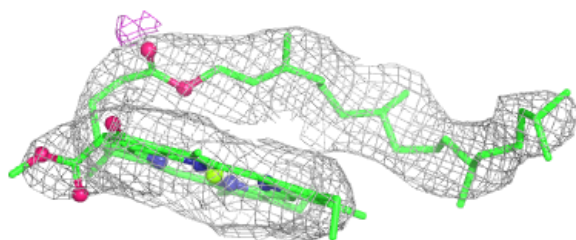
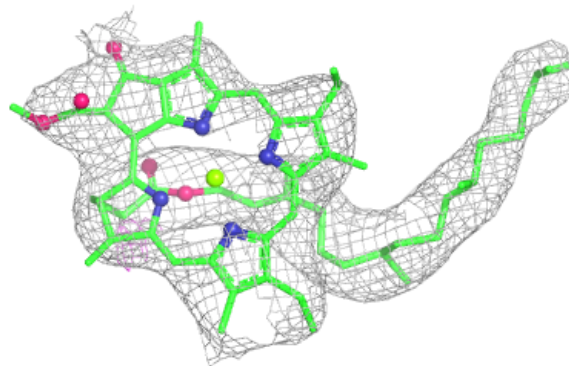
**Electron density around CLA A 823:**

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



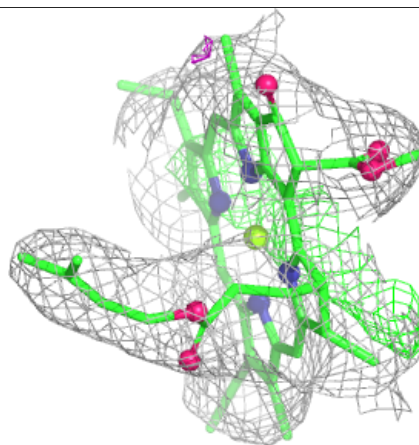
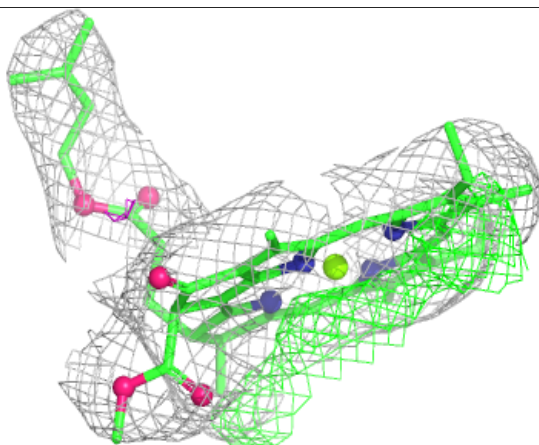
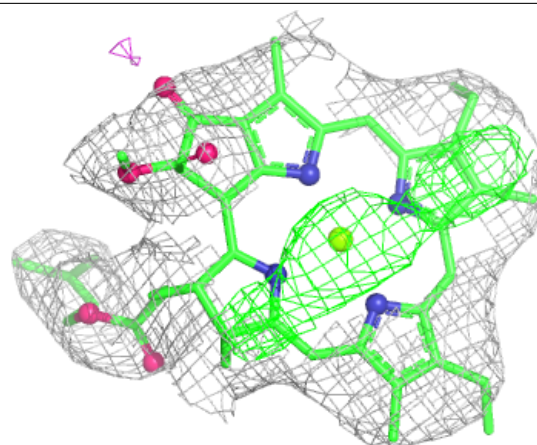
**Electron density around CLA B 837:**

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



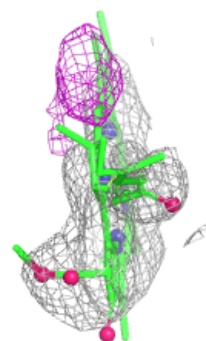
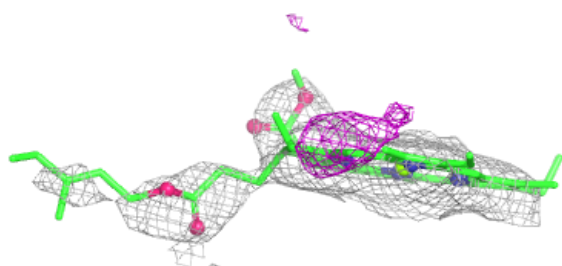
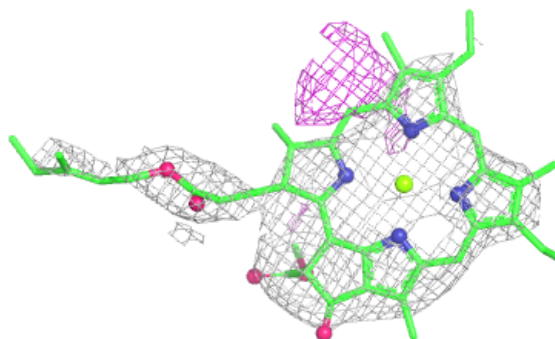
**Electron density around CLA B 838:**

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

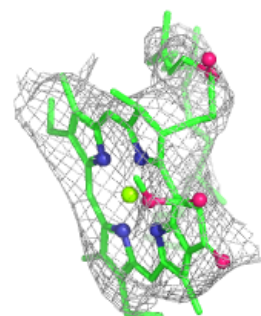
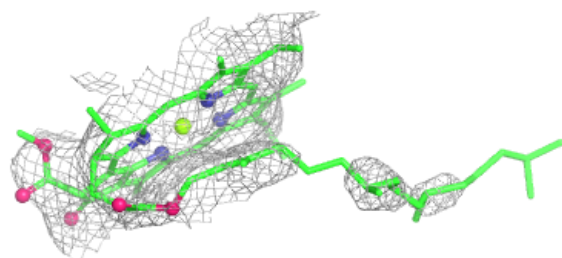
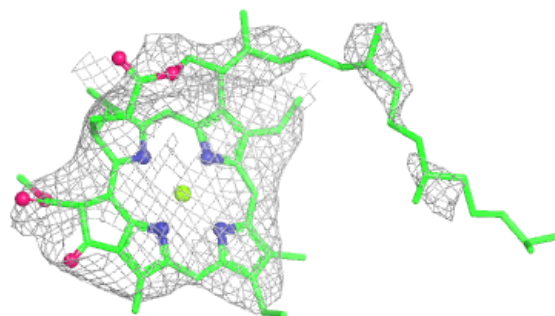


**Electron density around CLA A 834:**

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

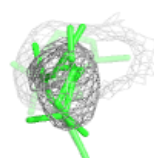
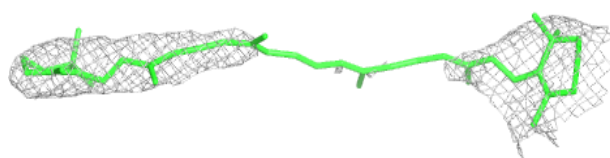
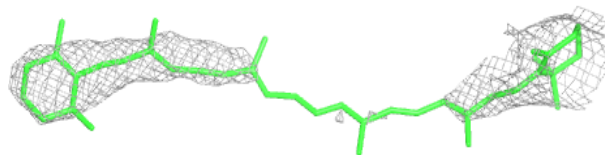
**Electron density around CLA 1 5009:**

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



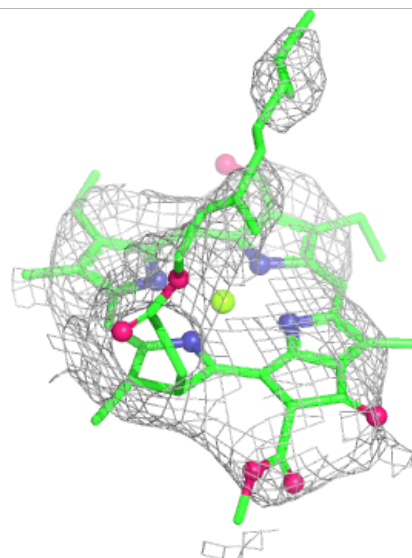
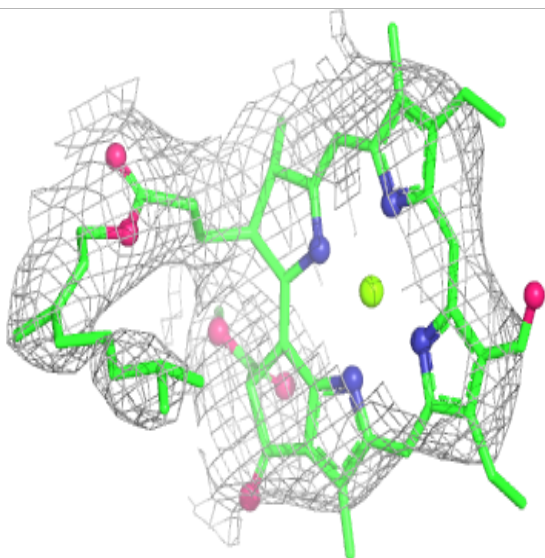
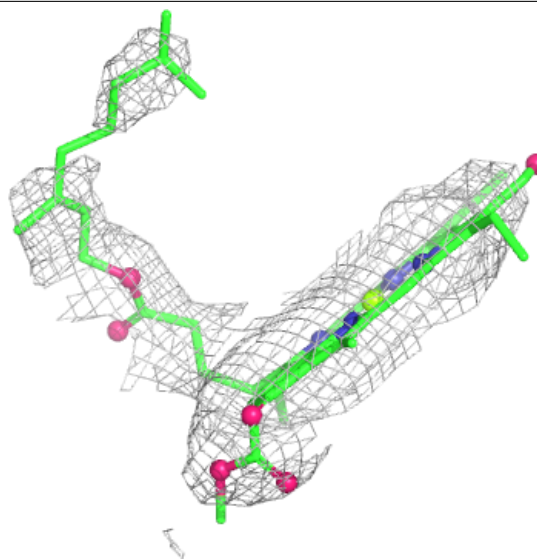
**Electron density around BCR 4 301:**

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



**Electron density around CHL 4 302:**

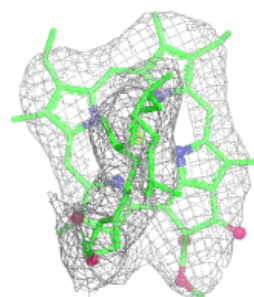
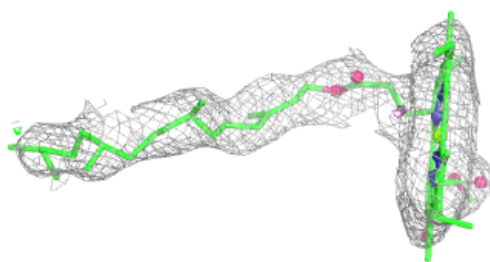
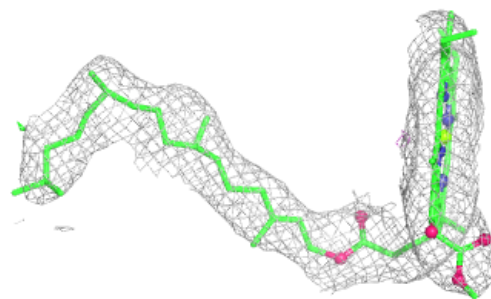
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA B 840:**

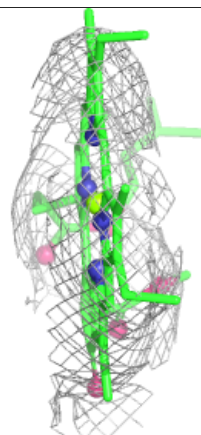
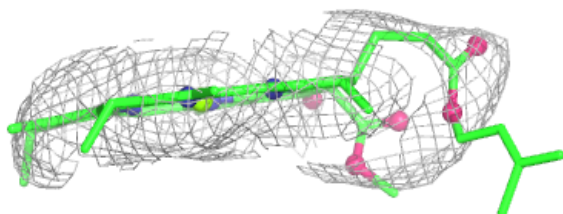
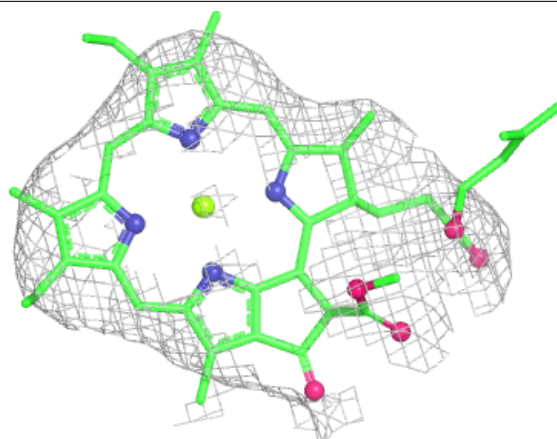
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



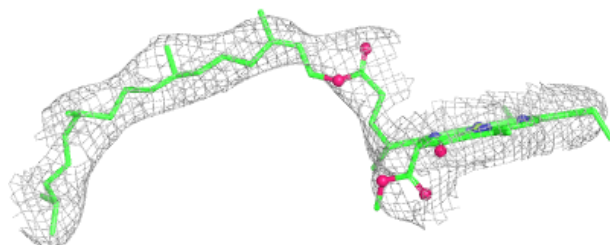
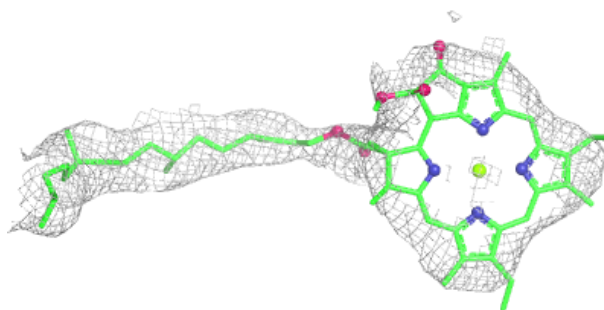


**Electron density around CLA 4 306:**

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

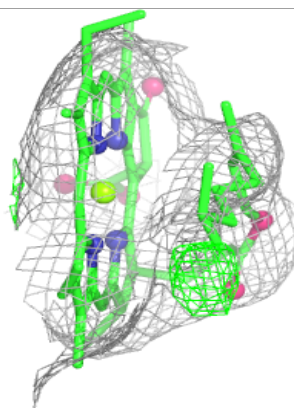
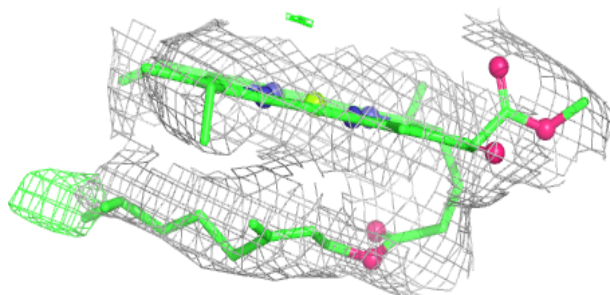
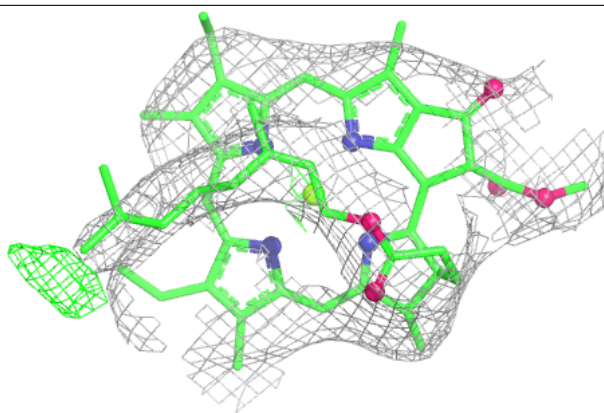
**Electron density around CLA B 841:**

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



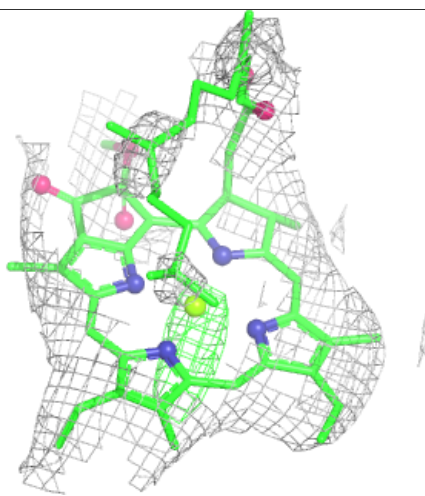
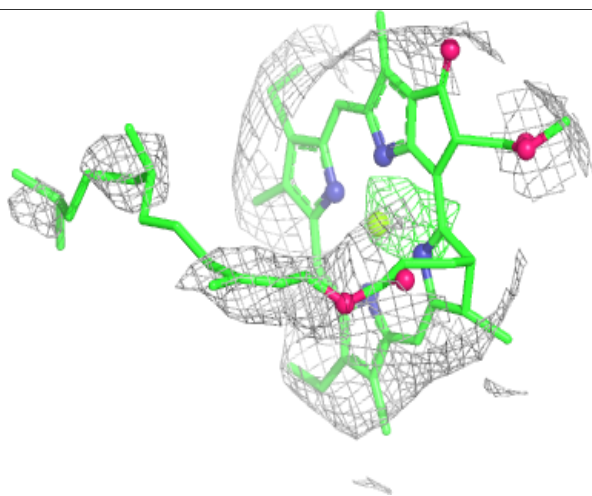
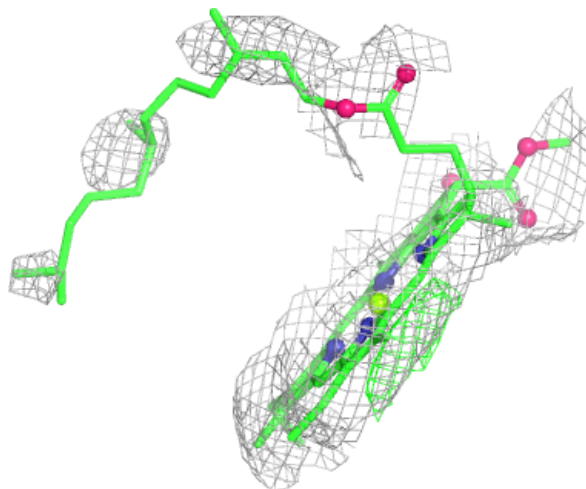
**Electron density around CLA A 811:**

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



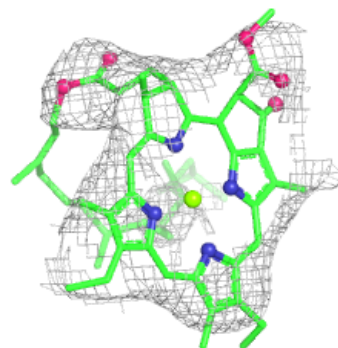
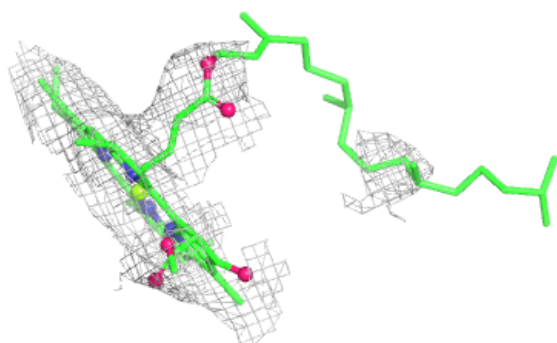
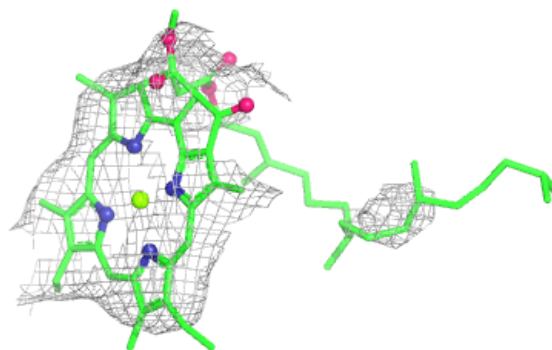
**Electron density around CLA B 812:**

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

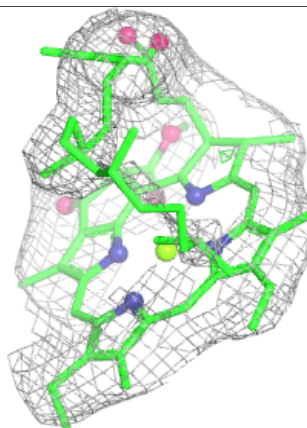
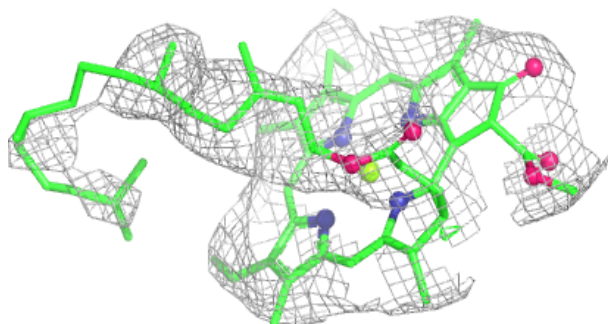
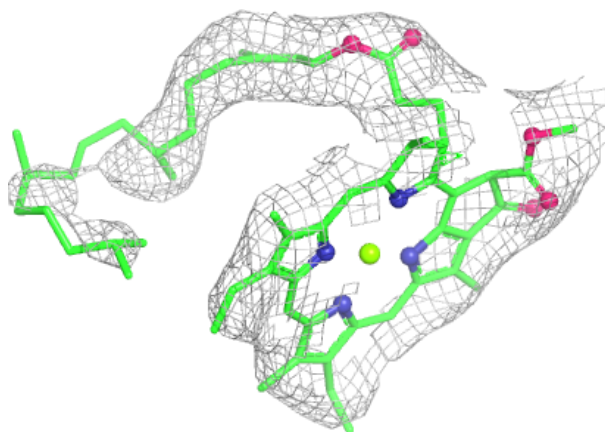


**Electron density around CLA 4 315:**

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

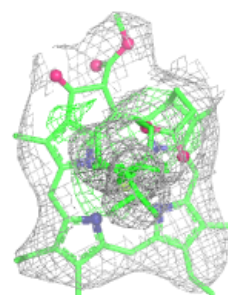
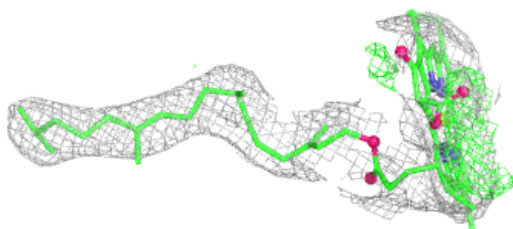
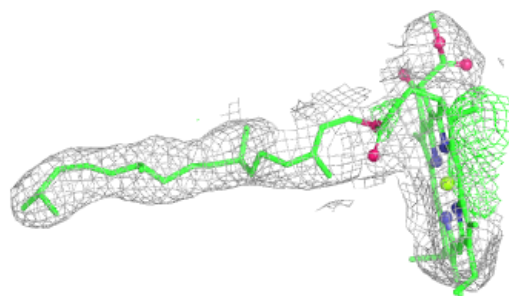
**Electron density around CLA A 822:**

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

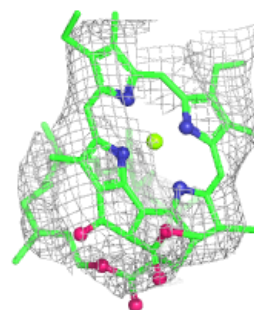
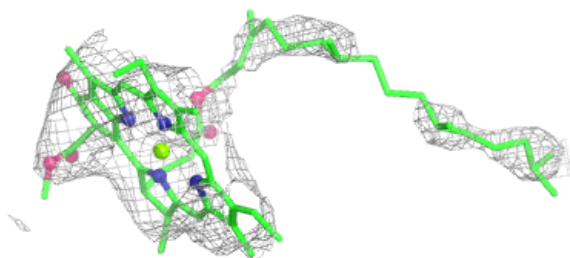
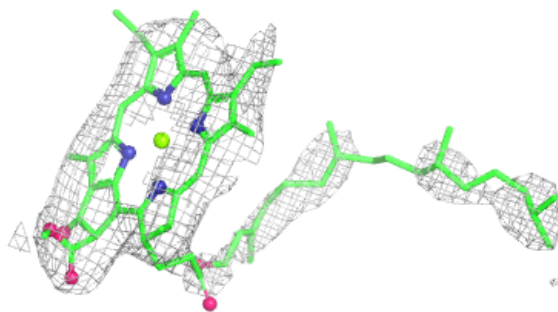


**Electron density around CLA A 826:**

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

**Electron density around CLA B 815:**

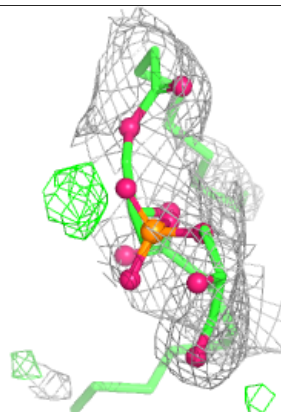
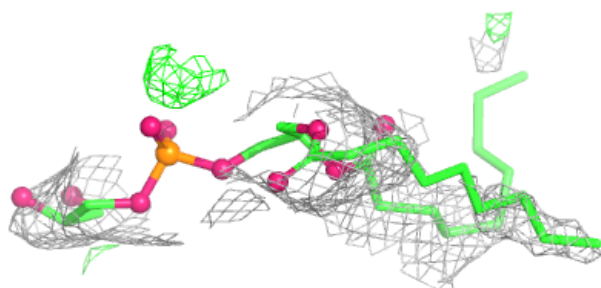
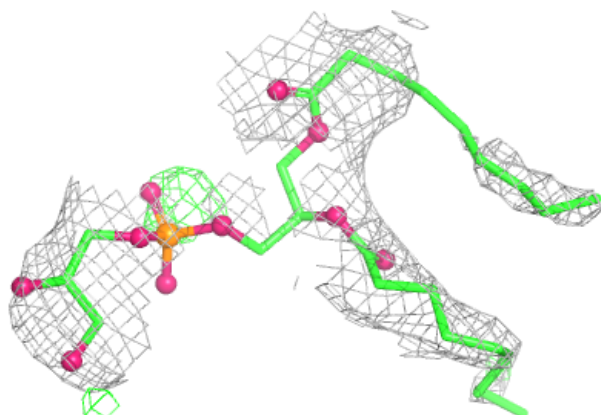
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



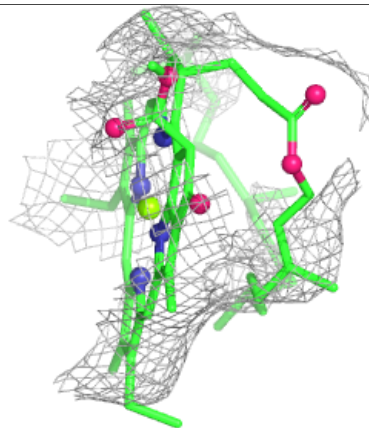
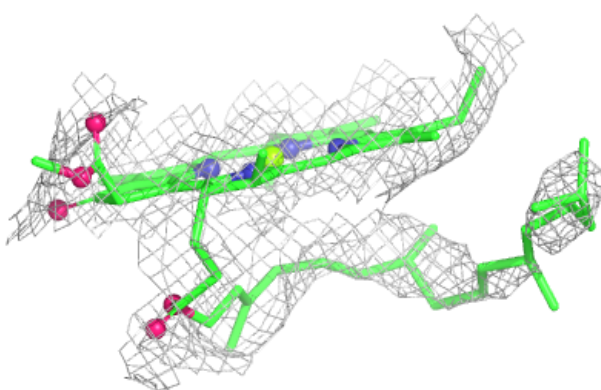
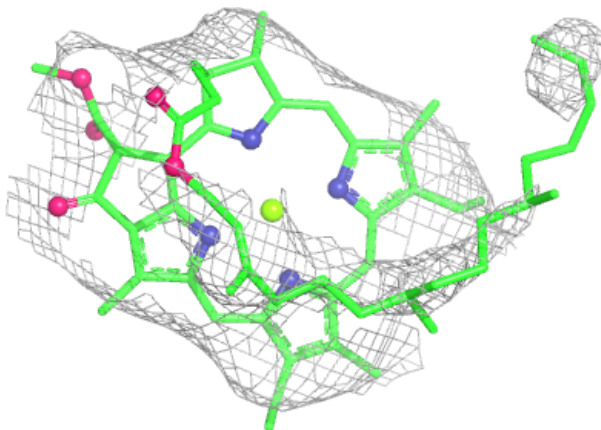


**Electron density around LHG 2 320:**

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

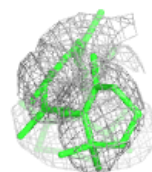
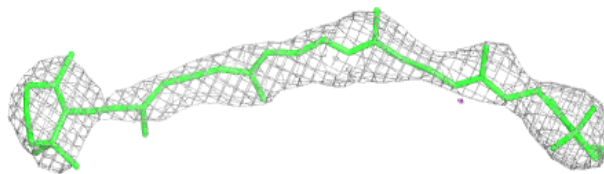
**Electron density around CLA 2 308:**

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

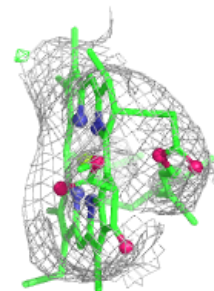
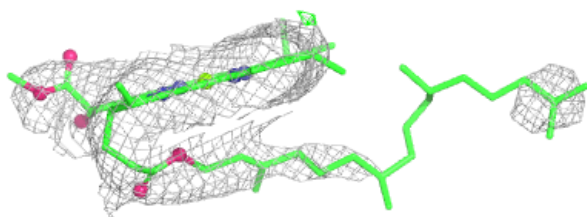
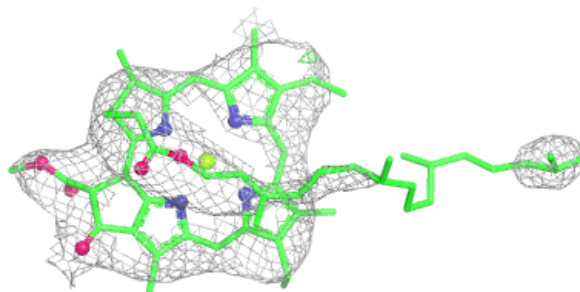


**Electron density around BCR F 304:**

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

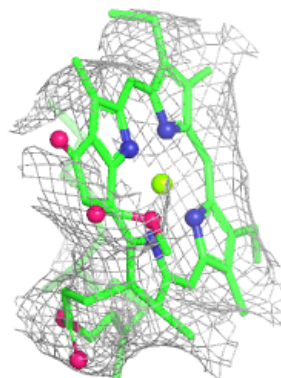
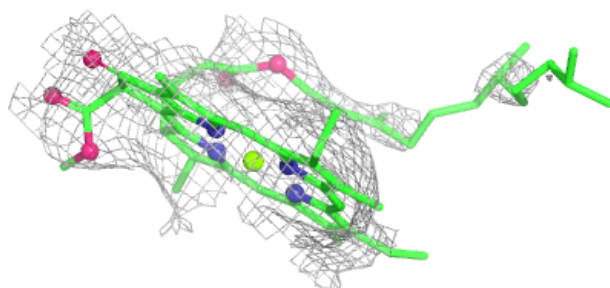
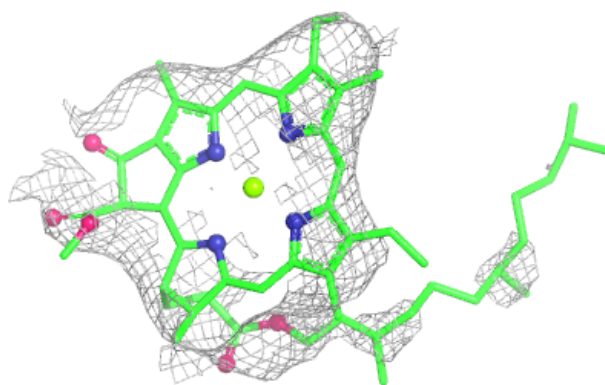
**Electron density around CLA A 835:**

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

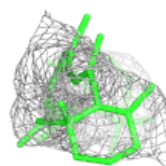
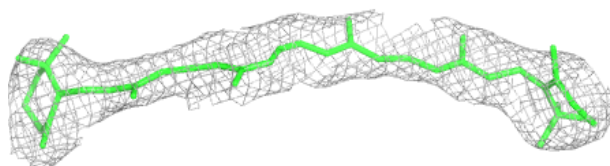
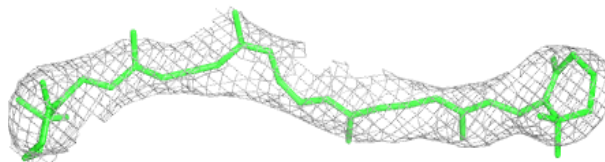


**Electron density around CLA 4 308:**

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

**Electron density around BCR I 101:**

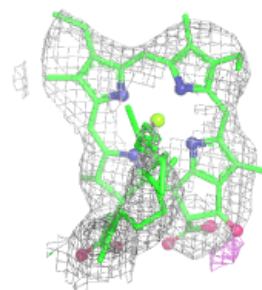
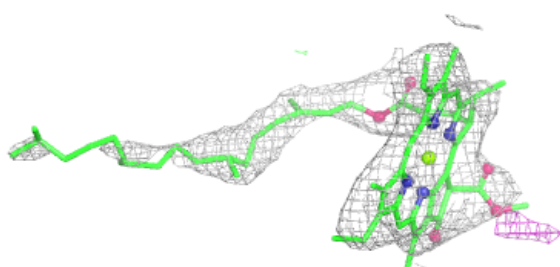
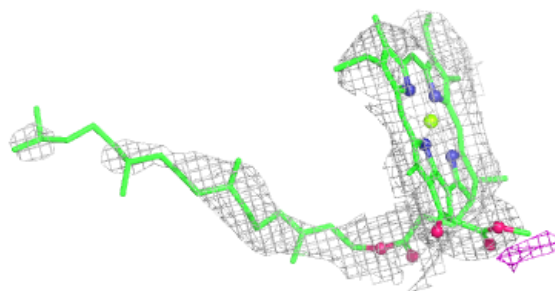
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



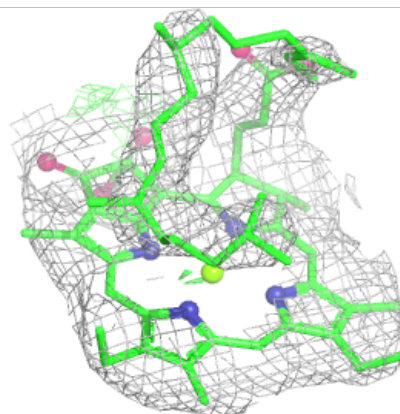
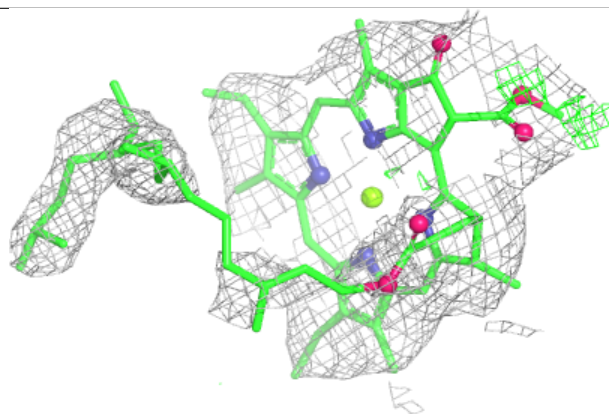
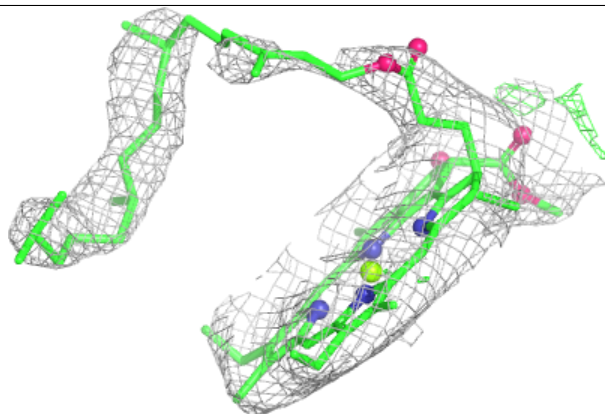


**Electron density around CLA B 830:**

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

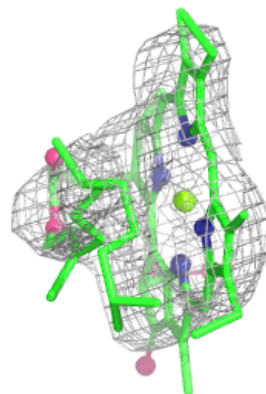
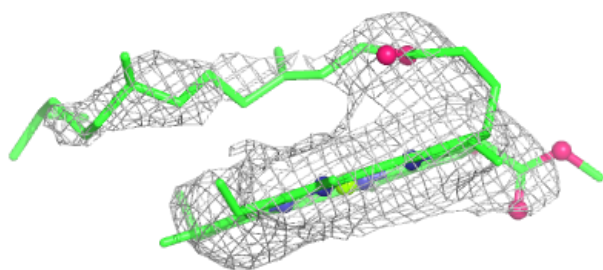
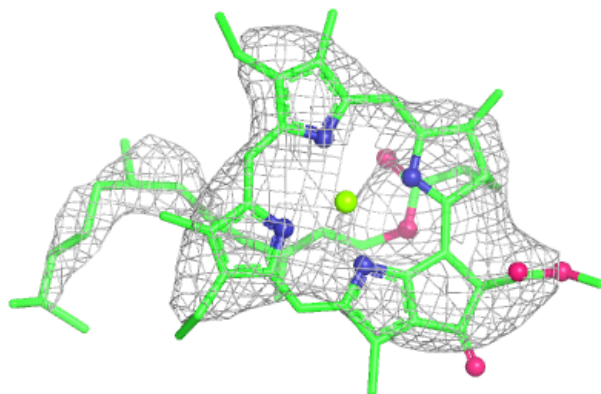
**Electron density around CLA B 831:**

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

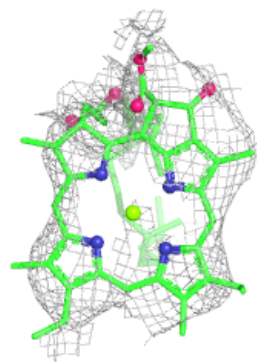
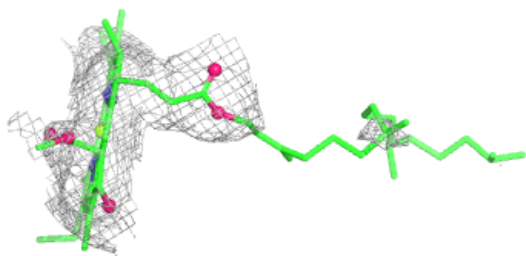
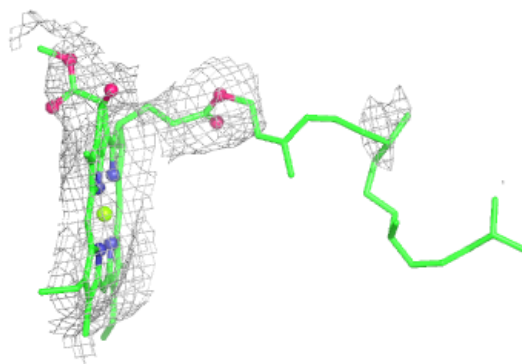


**Electron density around CLA B 817:**

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

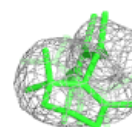
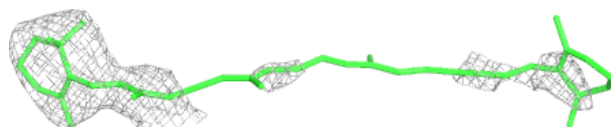
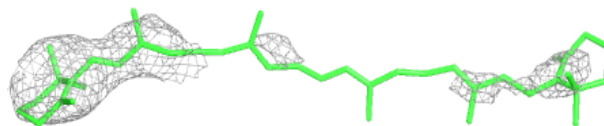
**Electron density around CLA A 813:**

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



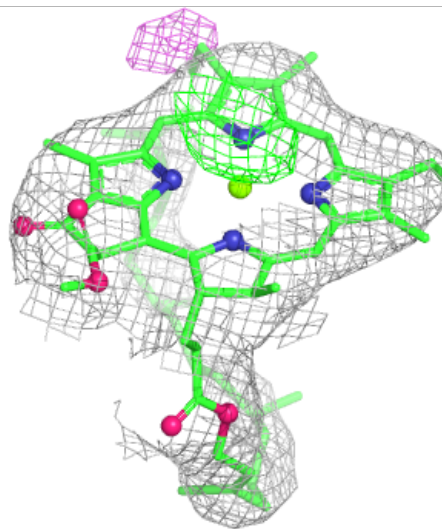
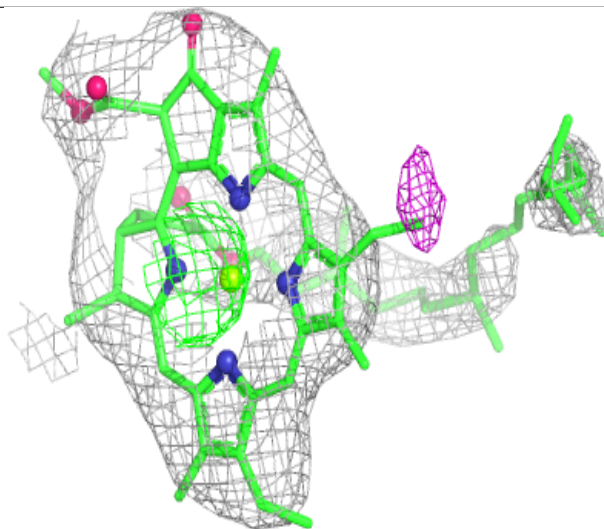
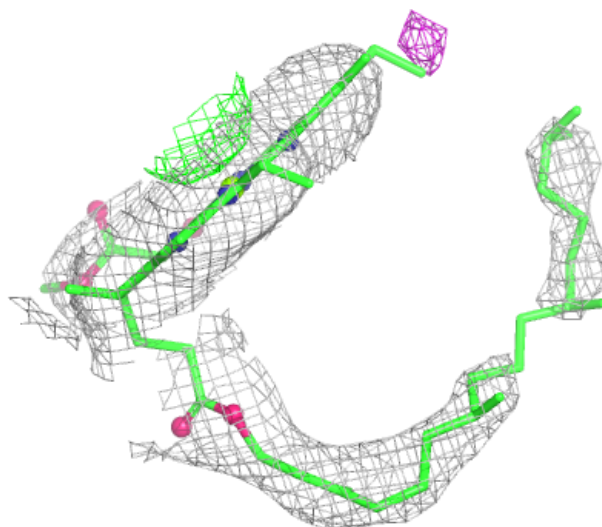
**Electron density around BCR A 843:**

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



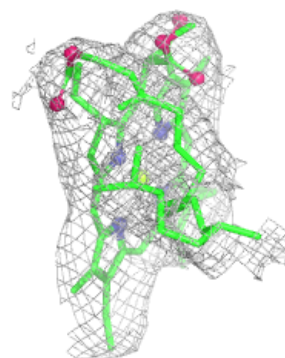
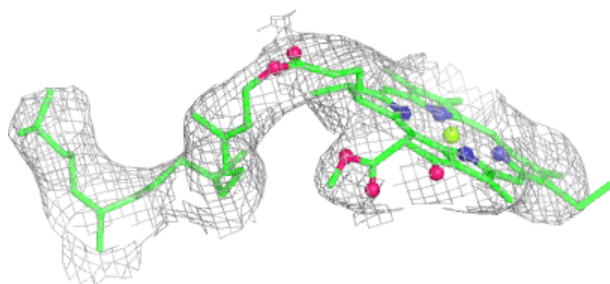
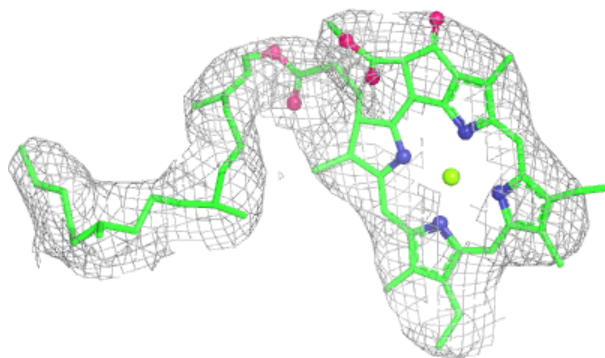
**Electron density around CLA B 820:**

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



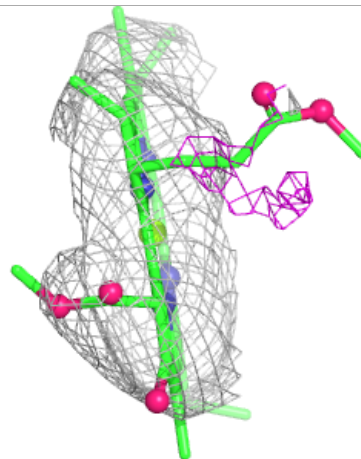
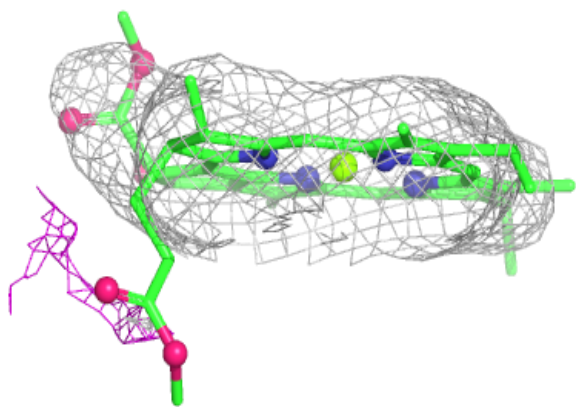
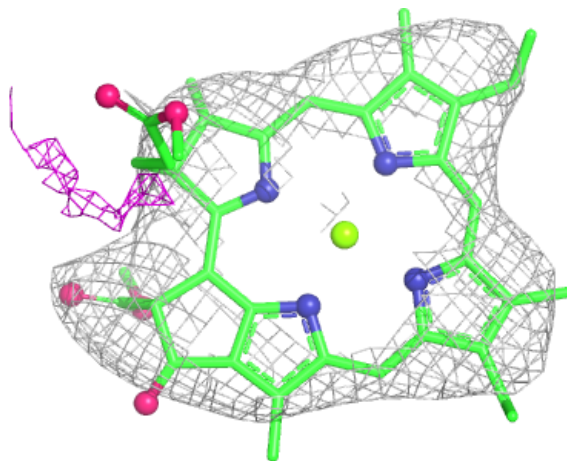
**Electron density around CLA J 1101:**

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



**Electron density around CLA B 821:**

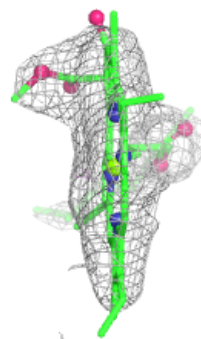
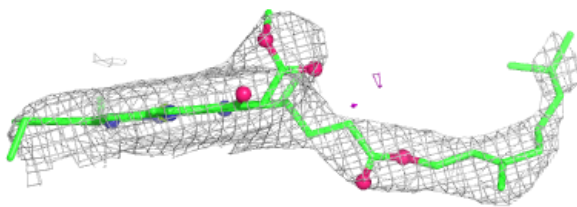
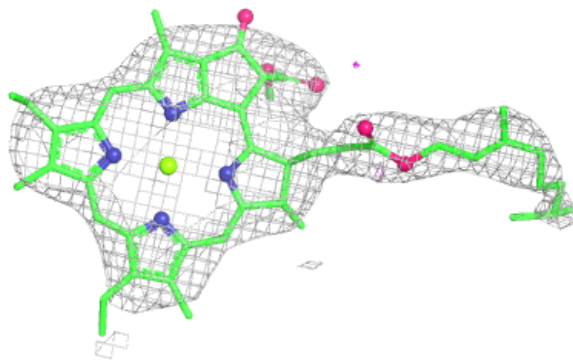
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



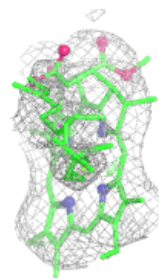
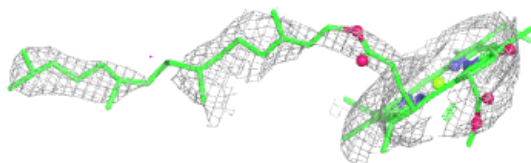
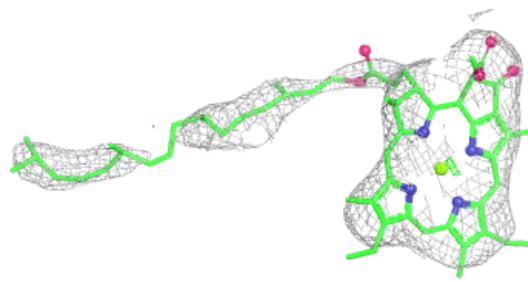


**Electron density around CLA B 836:**

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

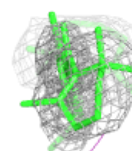
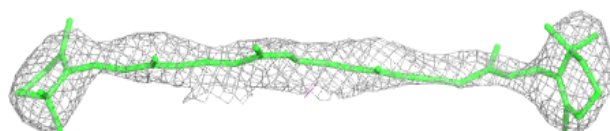
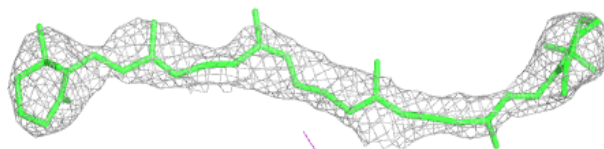
**Electron density around CLA A 831:**

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

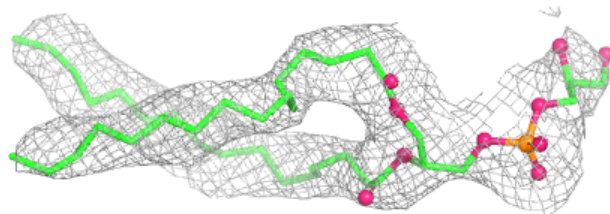
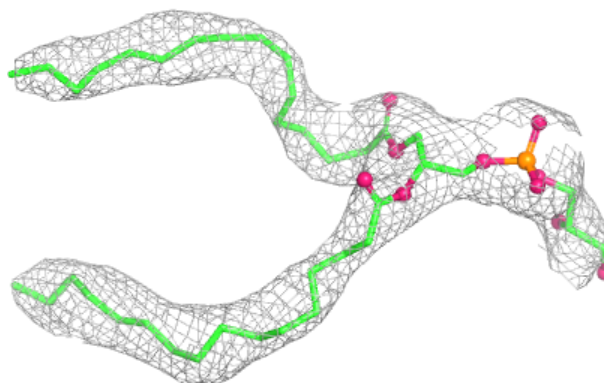


**Electron density around BCR B 802:**

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

**Electron density around LHG A 848:**

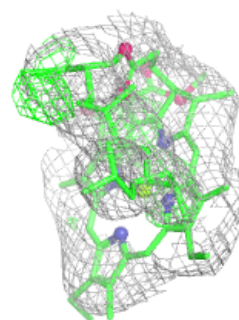
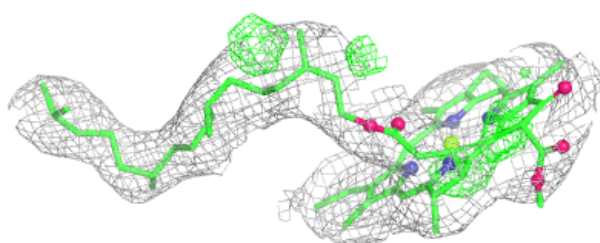
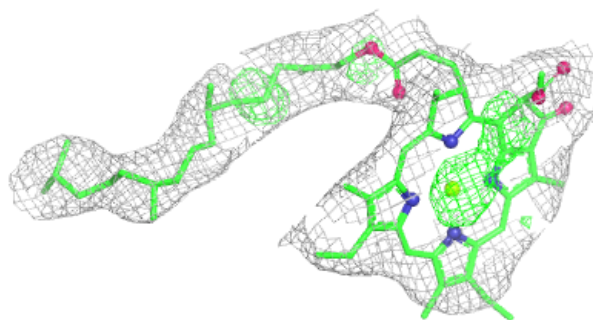
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



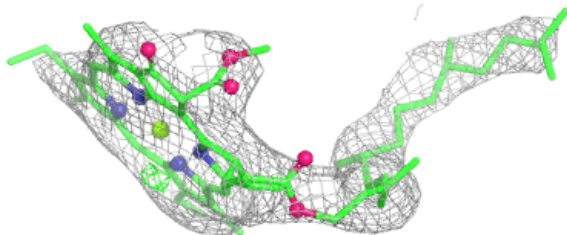
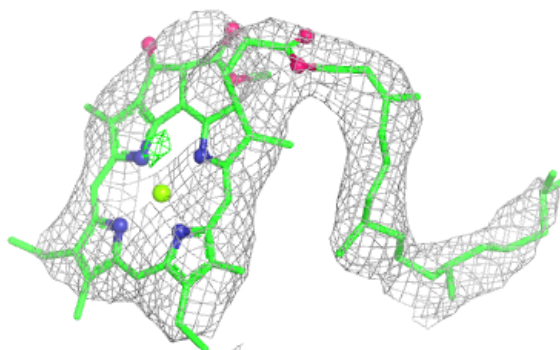


**Electron density around CLA A 807:**

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

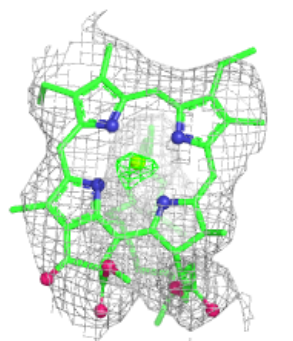
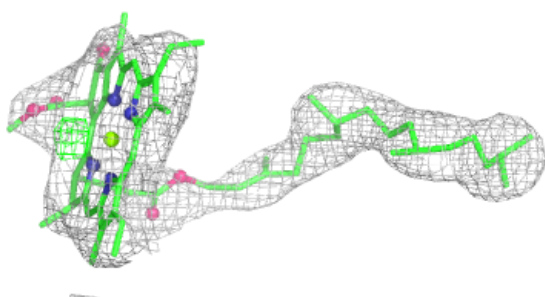
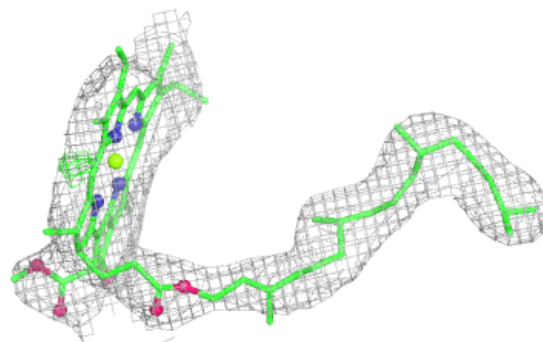
**Electron density around CLA B 825:**

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



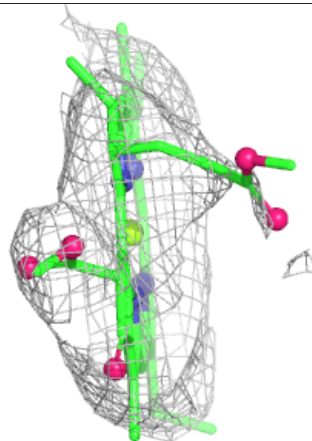
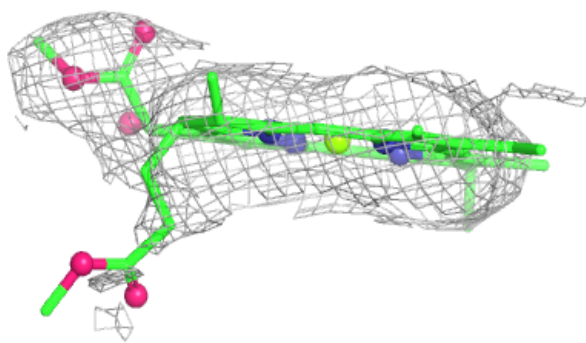
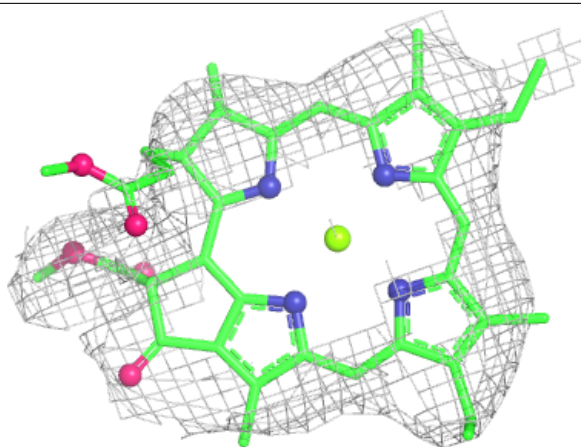
**Electron density around CLA A 828:**

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



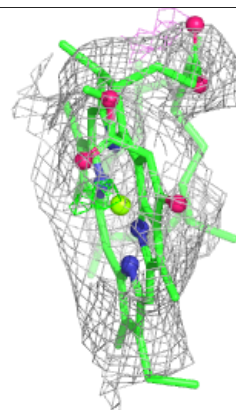
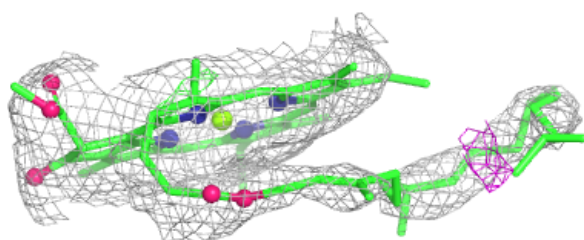
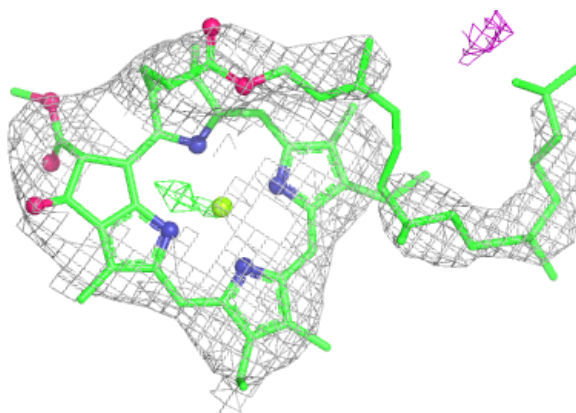
**Electron density around CLA B 813:**

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

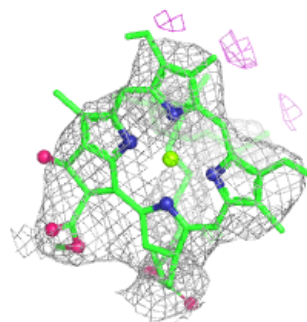
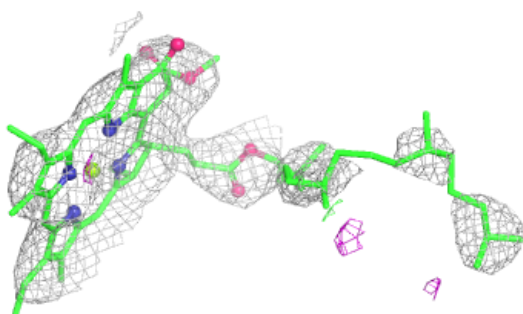
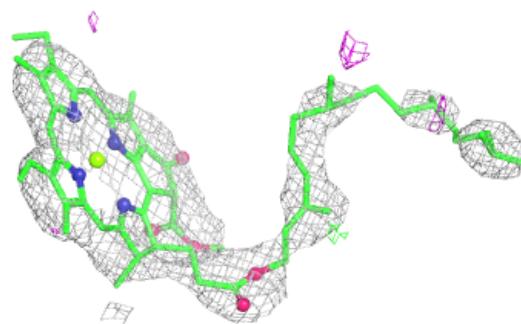


**Electron density around CLA A 817:**

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

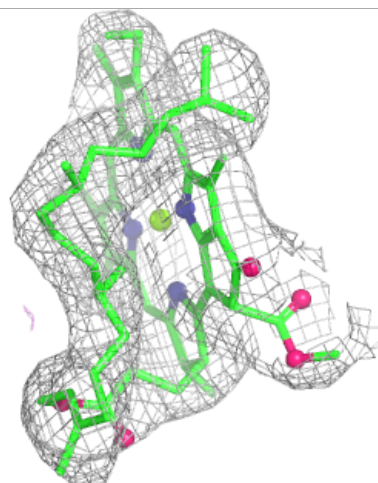
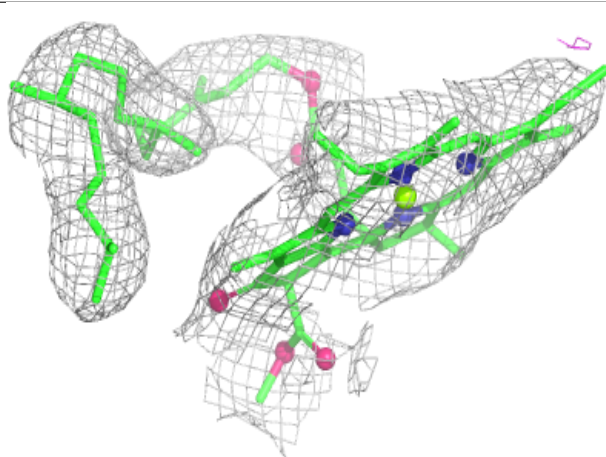
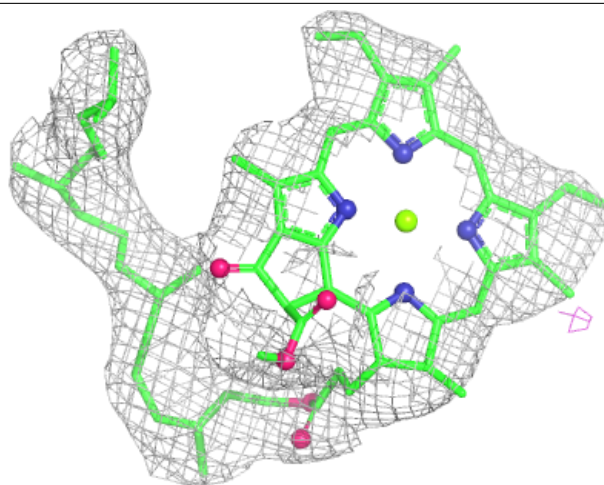
**Electron density around CLA B 803:**

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



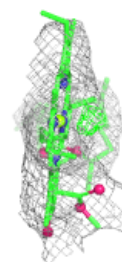
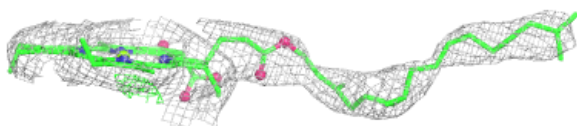
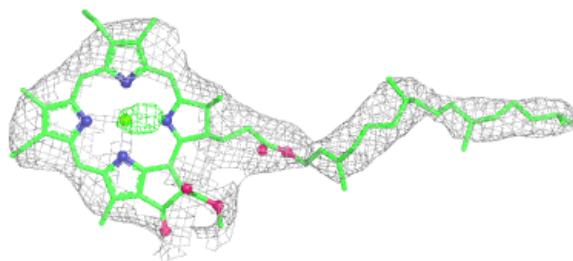
**Electron density around CLA F 301:**

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



**Electron density around CLA A 830:**

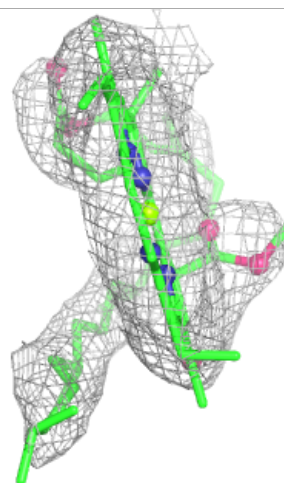
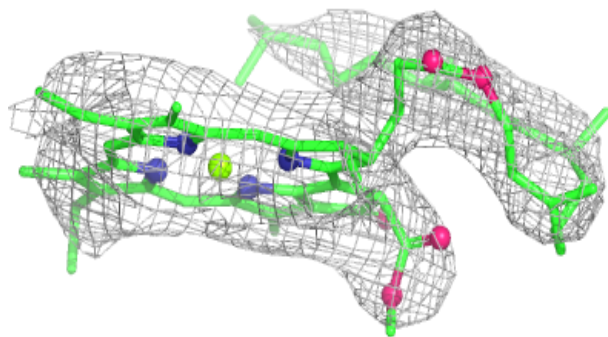
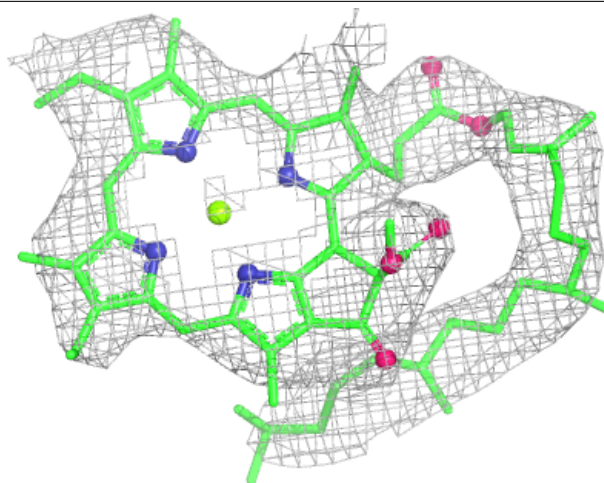
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





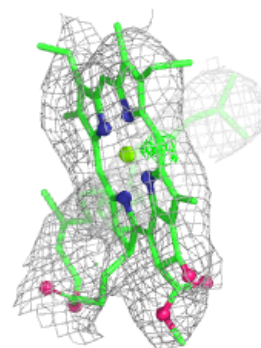
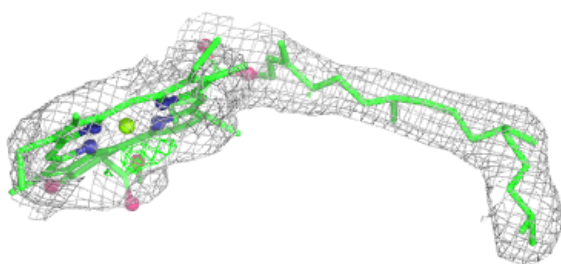
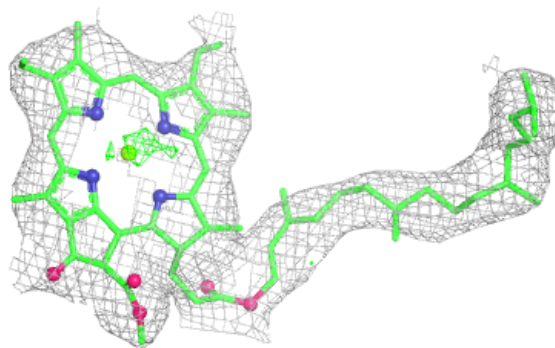
**Electron density around CLA B 806:**

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



**Electron density around CLA A 802:**

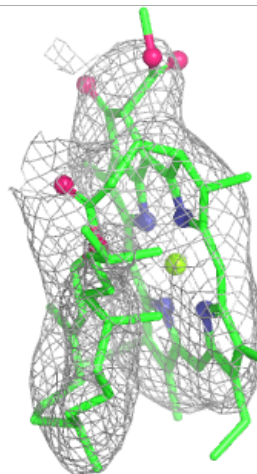
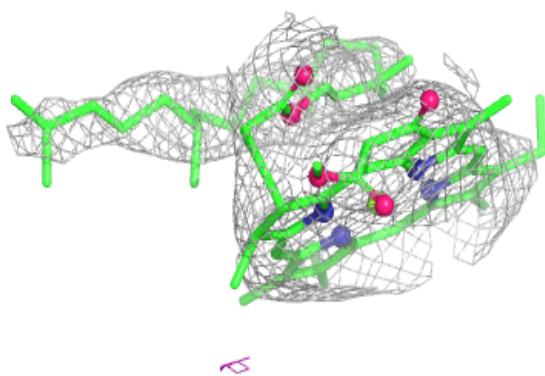
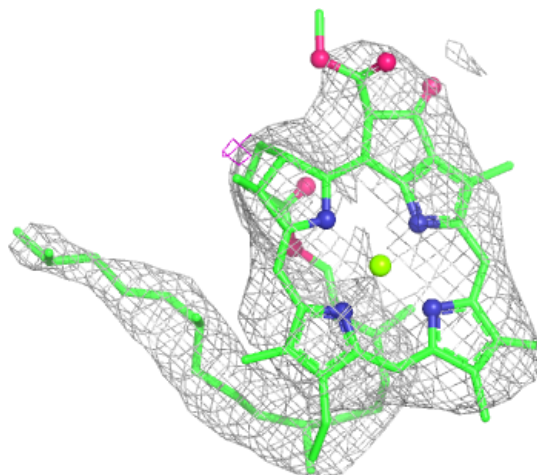
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





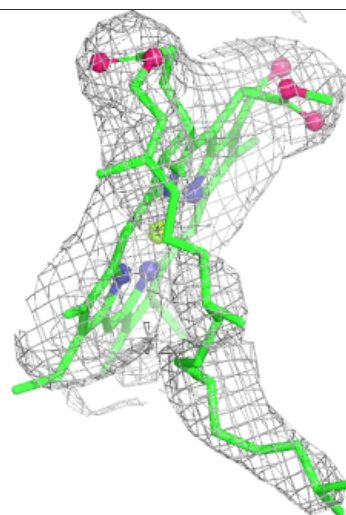
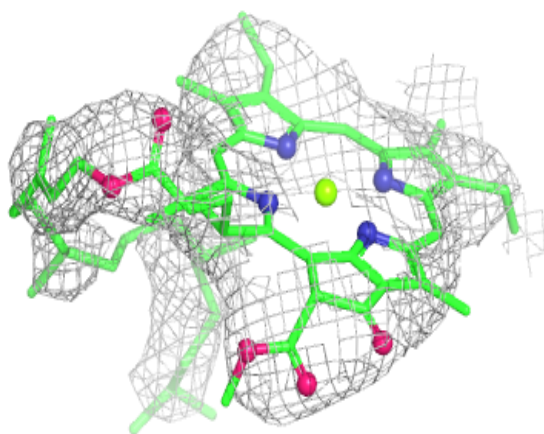
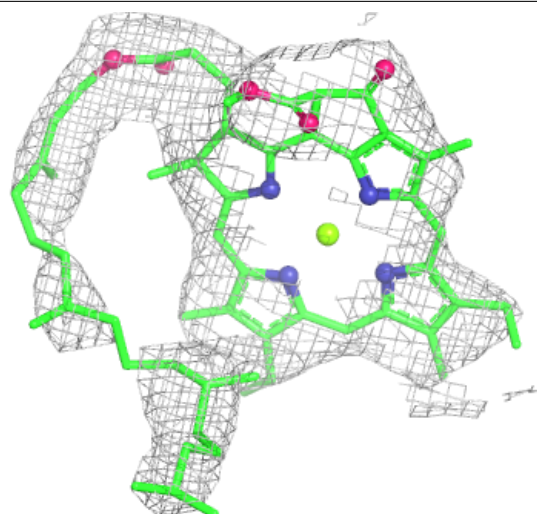
**Electron density around CLA B 809:**

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



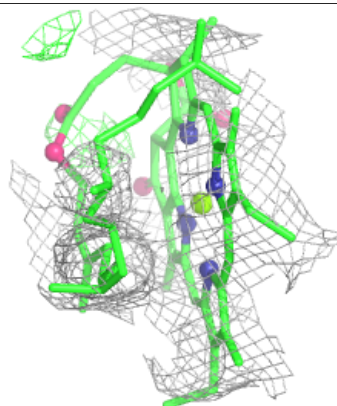
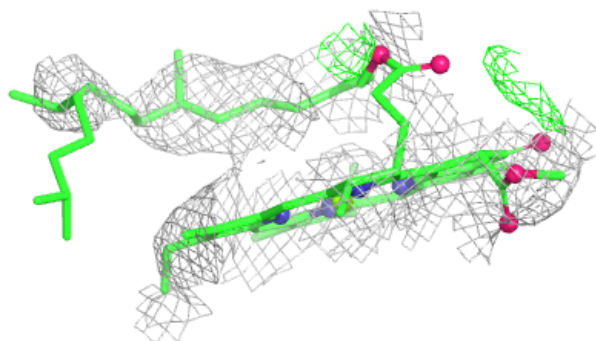
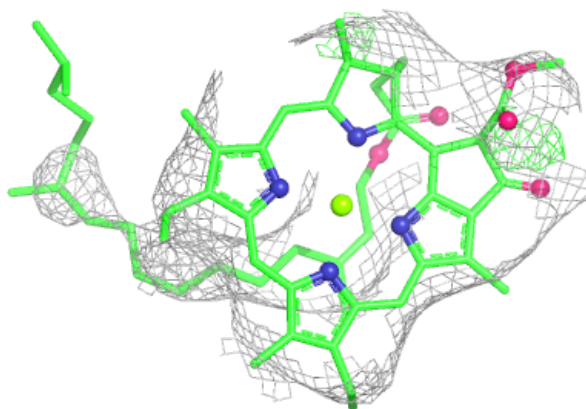
**Electron density around CLA A 812:**

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

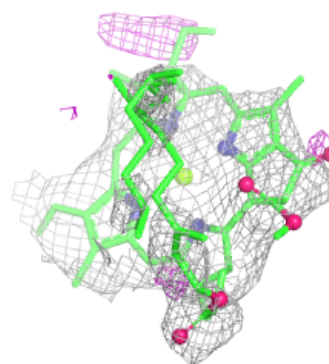
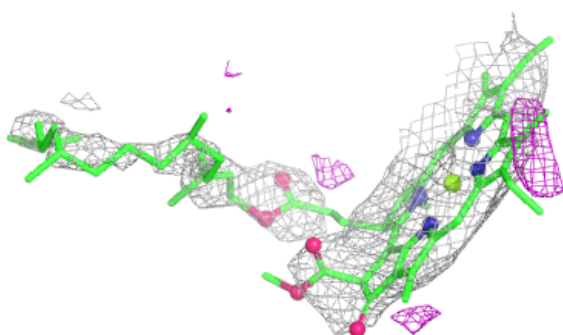
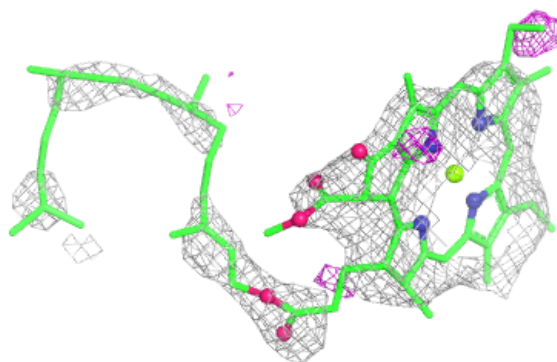


**Electron density around CLA 4 307:**

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

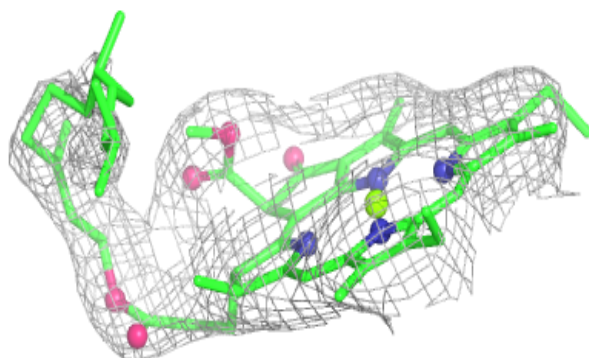
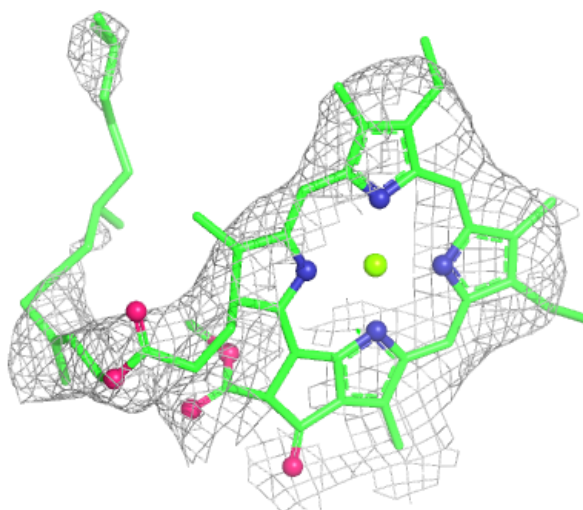
**Electron density around CL0 A 801:**

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



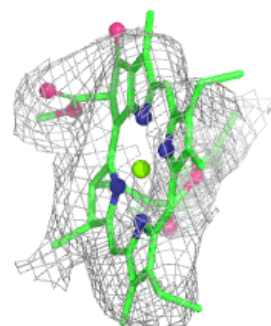
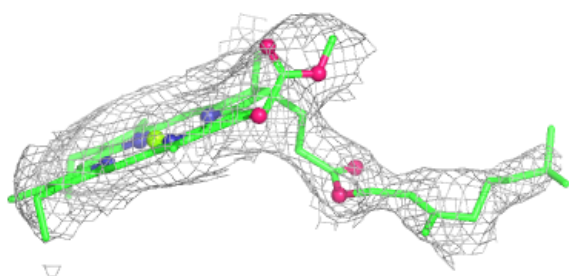
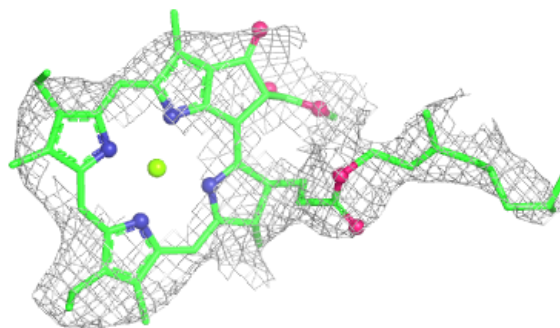
**Electron density around CLA 4 309:**

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



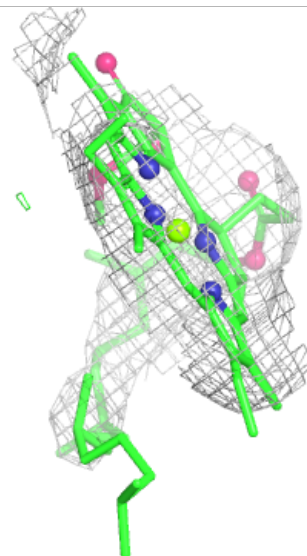
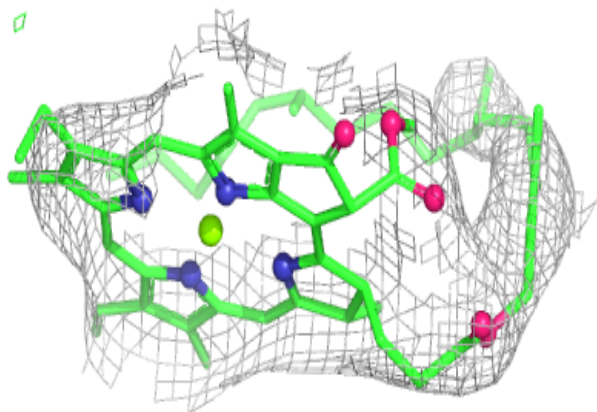
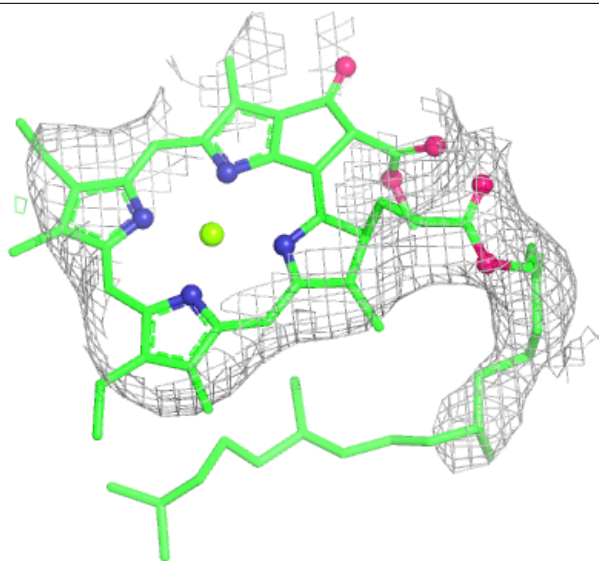
**Electron density around CLA B 824:**

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



**Electron density around CLA 1 5010:**

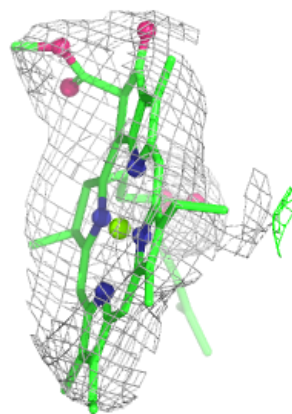
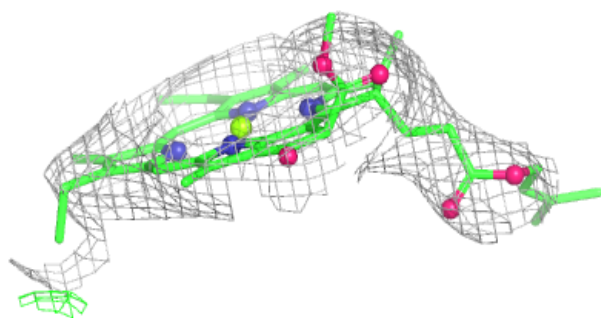
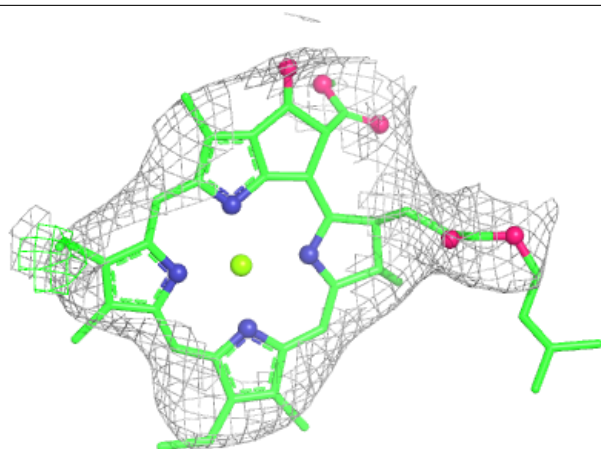
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





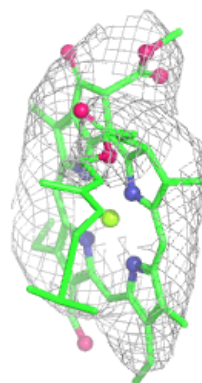
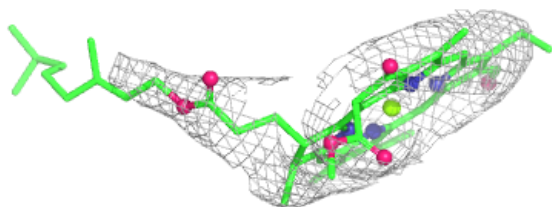
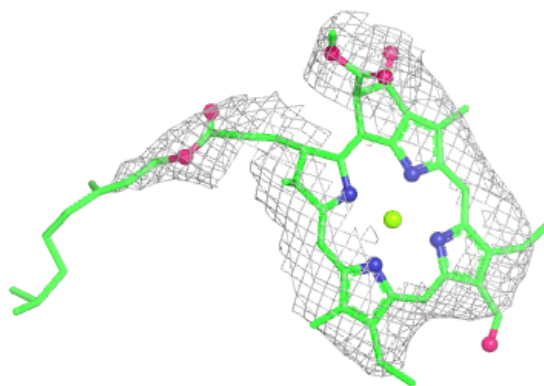
**Electron density around CLA 2 326:**

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



**Electron density around CHL 4 318:**

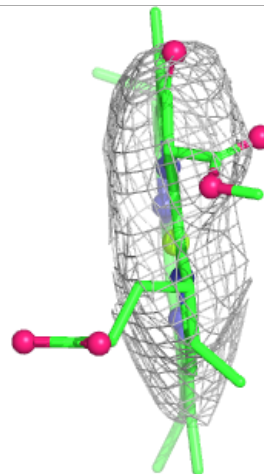
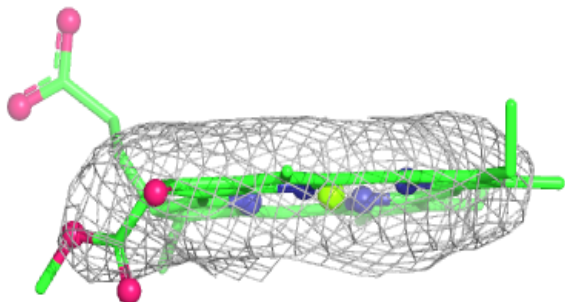
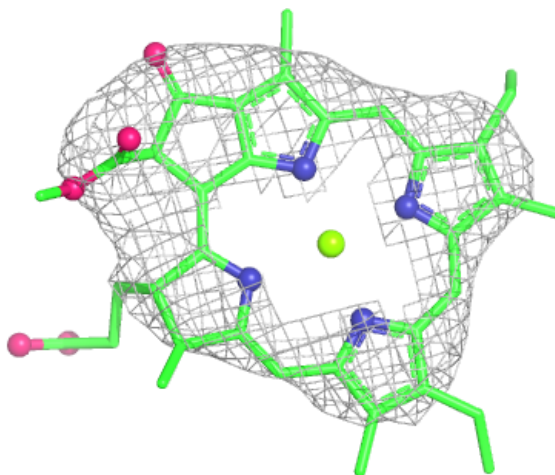
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





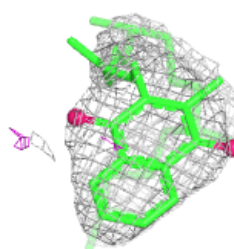
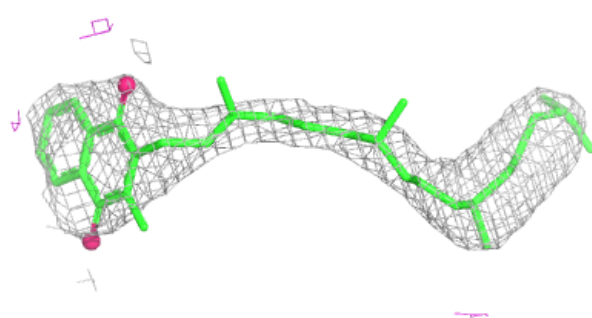
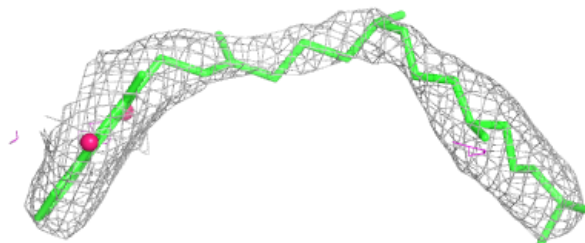
**Electron density around CLA 3 301:**

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

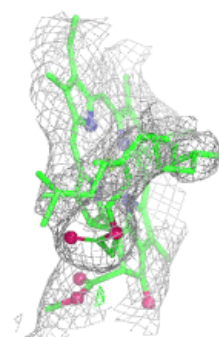
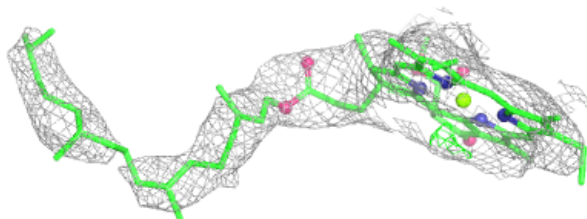
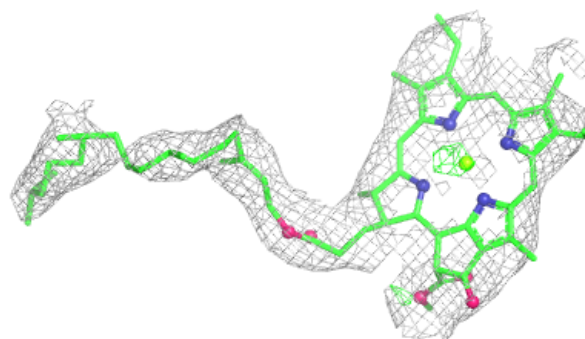


**Electron density around PQN B 842:**

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

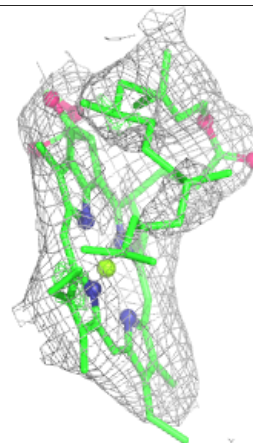
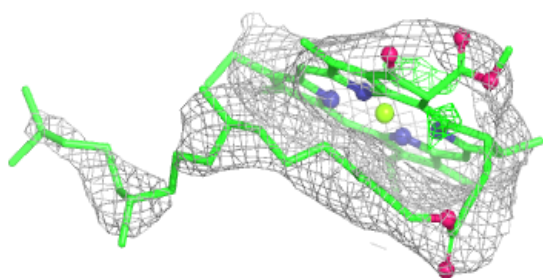
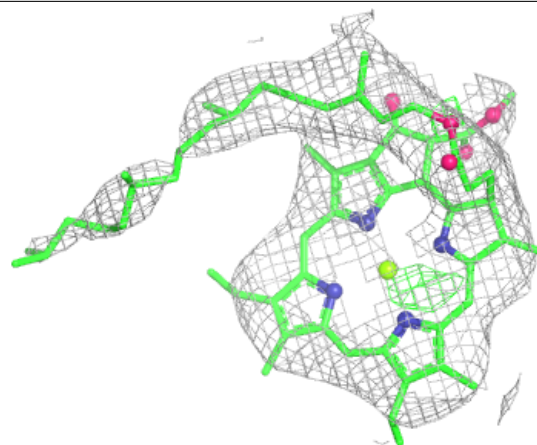
**Electron density around CLA B 814:**

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



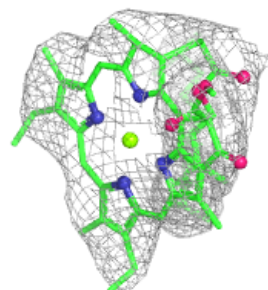
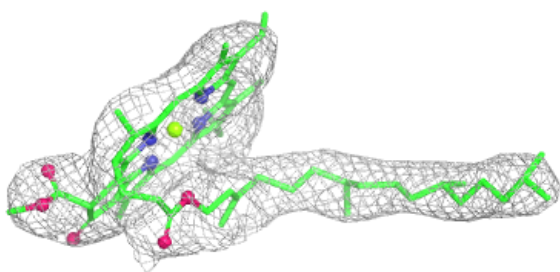
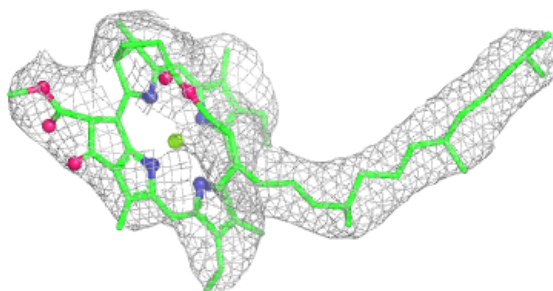
**Electron density around CLA A 827:**

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

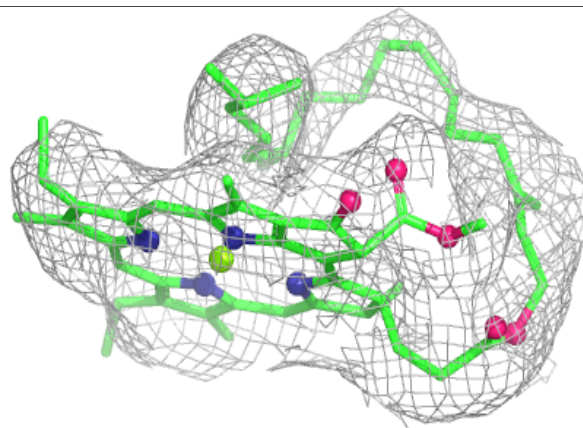
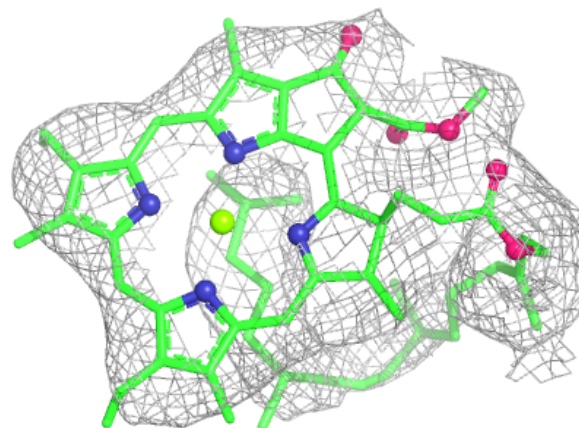


**Electron density around CLA A 839:**

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

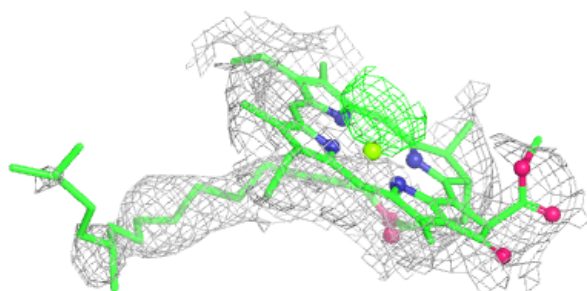
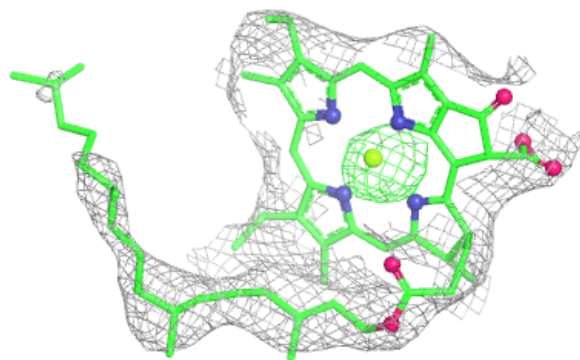
**Electron density around CLA B 807:**

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

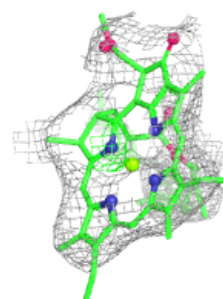
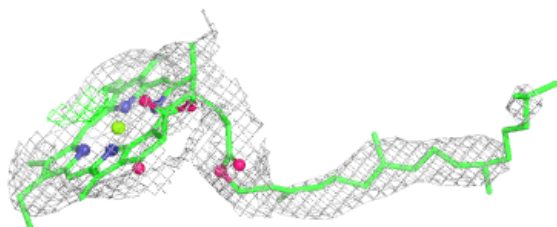
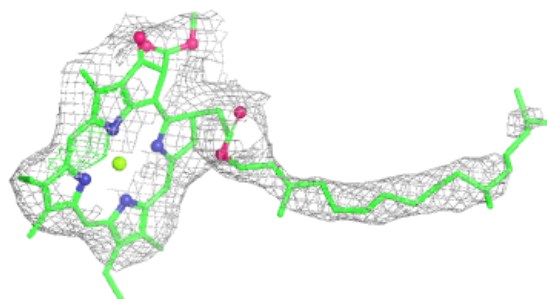


**Electron density around CLA 2 309:**

$2mF_o-DF_c$  (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:**

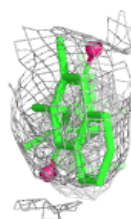
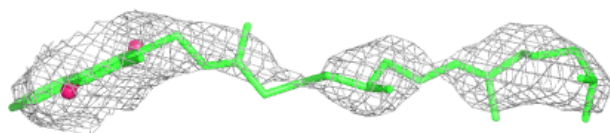
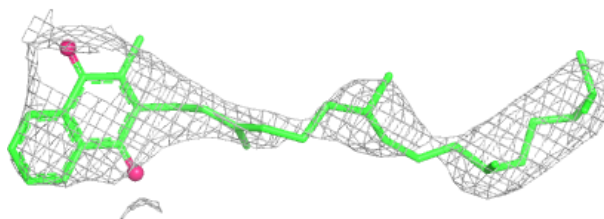
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



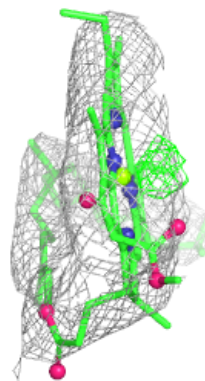
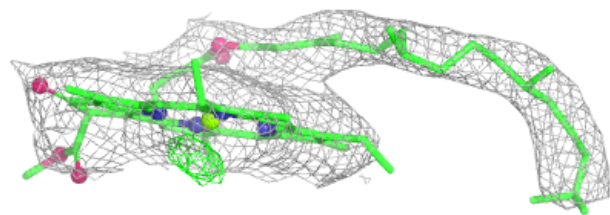
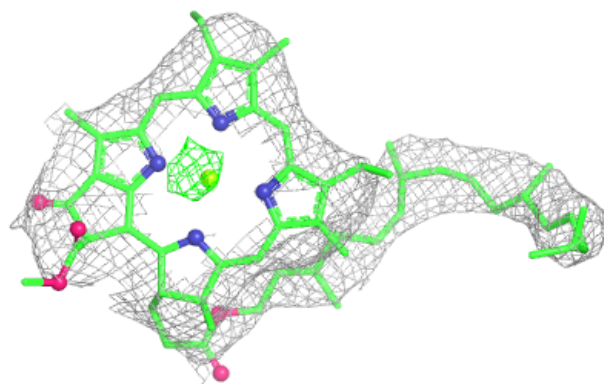


**Electron density around PQN A 841:**

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

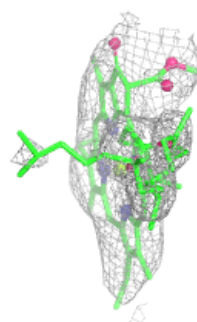
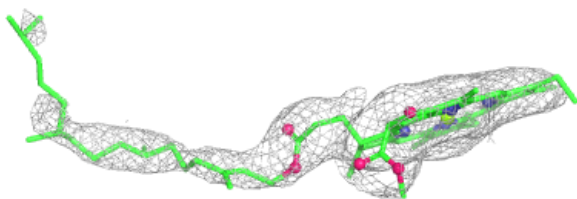
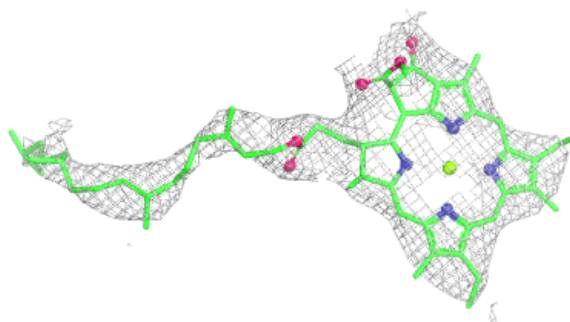
**Electron density around CLA B 819:**

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



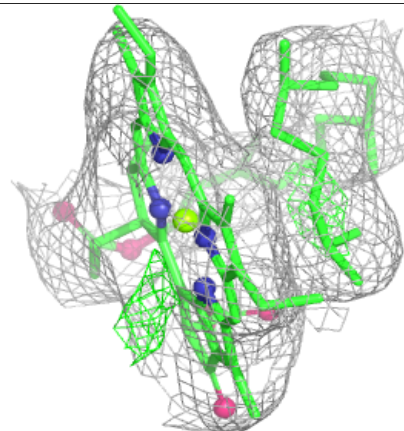
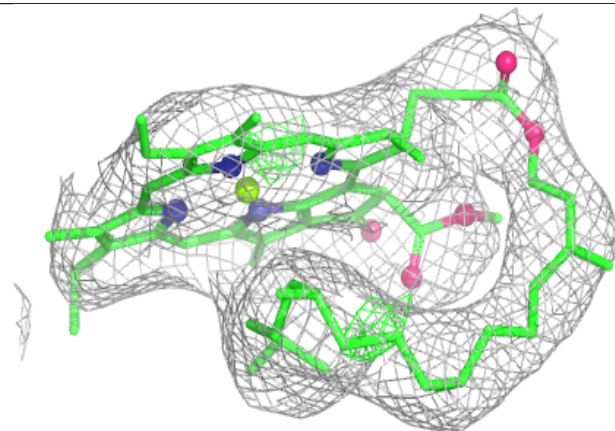
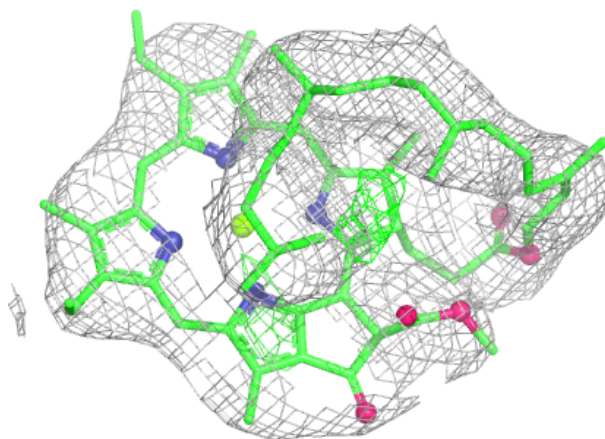
**Electron density around CLA A 804:**

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



**Electron density around CLA A 805:**

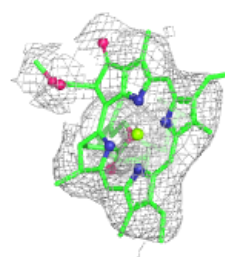
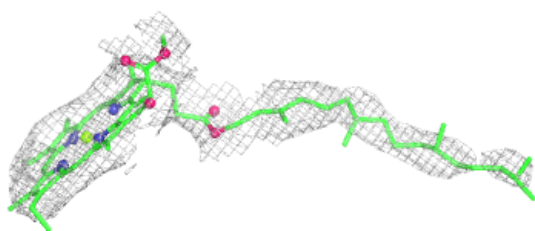
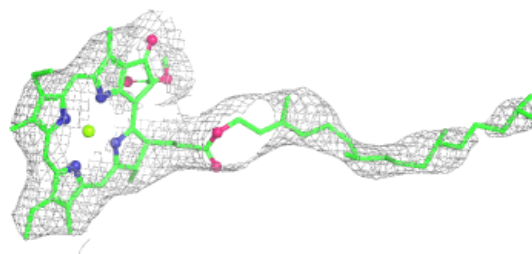
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



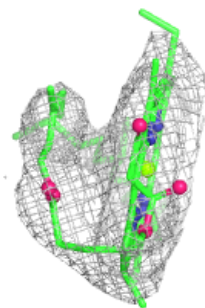
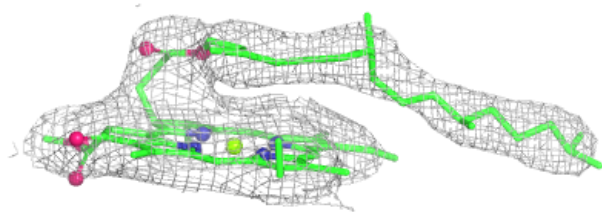
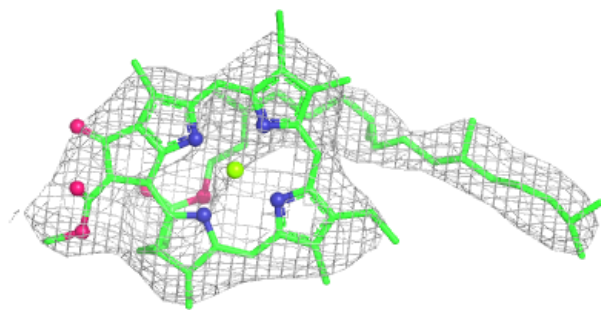


**Electron density around CLA A 808:**

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

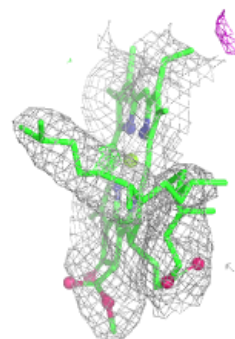
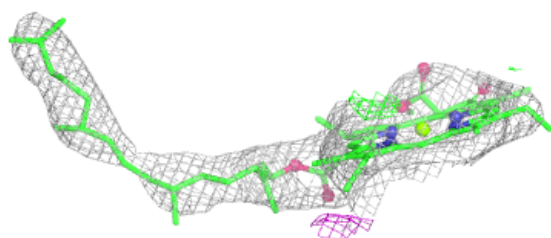
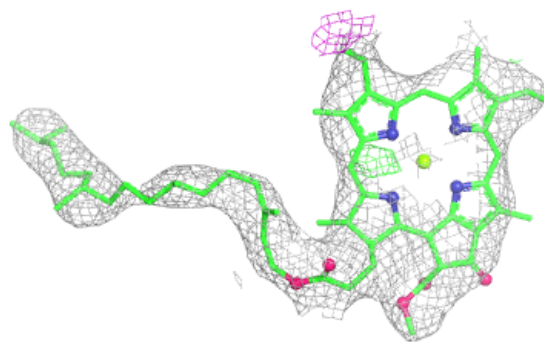
**Electron density around CLA A 837:**

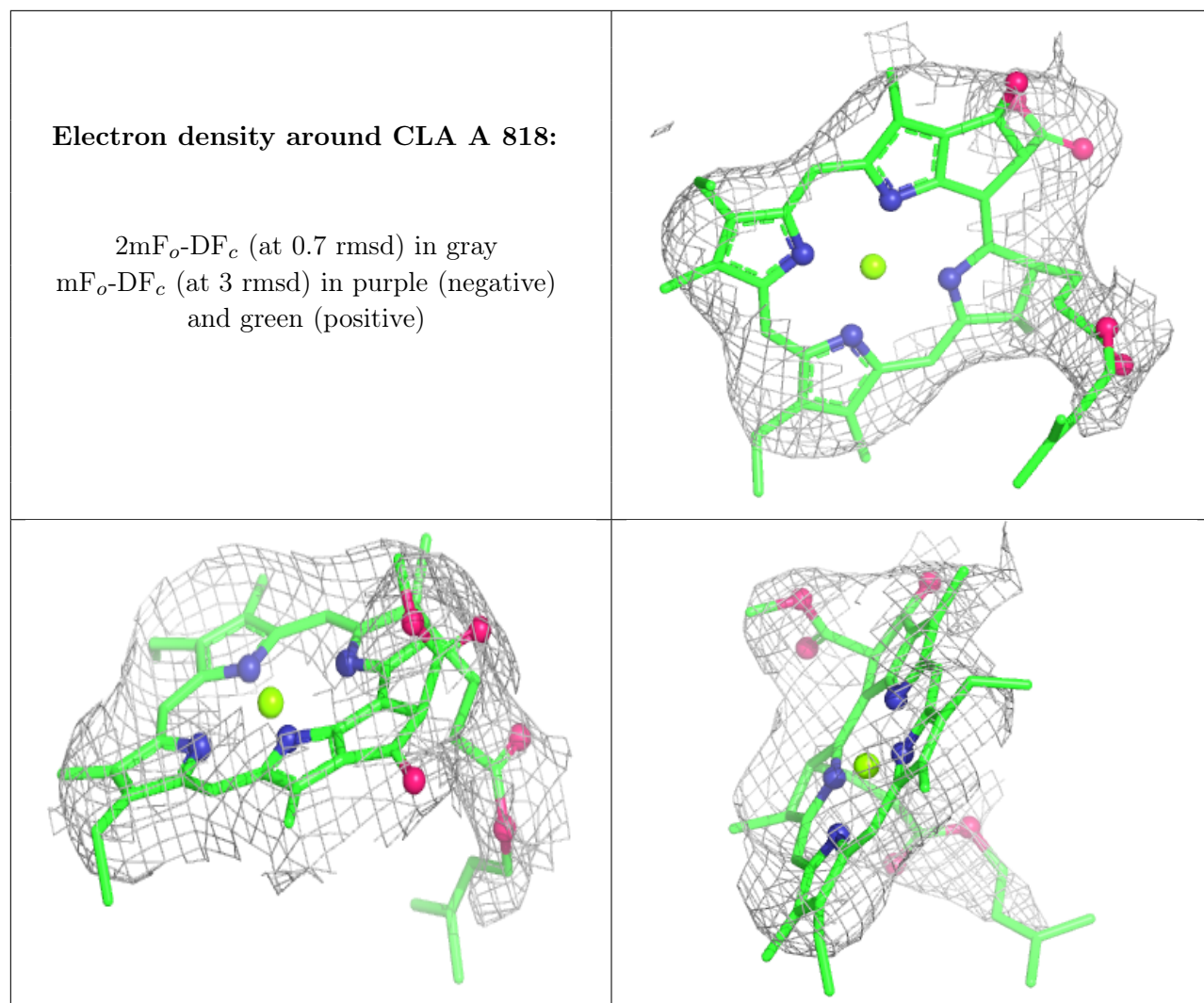
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 804:**

$2mF_o-DF_c$  (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.