



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:22 AM UTC

PDB ID : 5L8R / pdb_00005l8r
Title : The structure of plant photosystem I super-complex at 2.6 angstrom resolution.
Authors : Mazor, Y.; Borovikova, A.; Caspy, I.; Nelson, N.
Deposited on : 2016-06-08
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

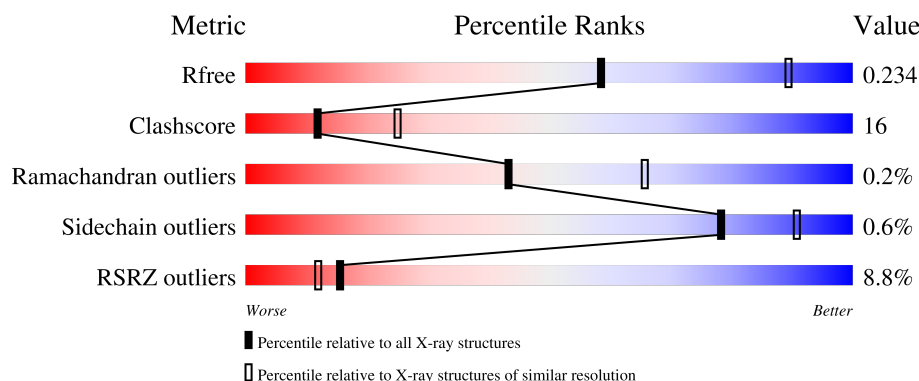
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



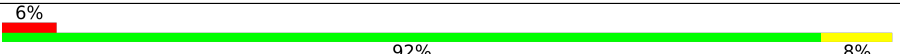
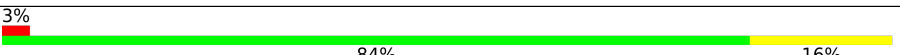
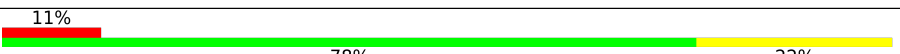
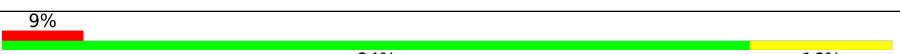
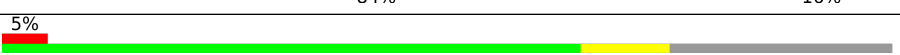
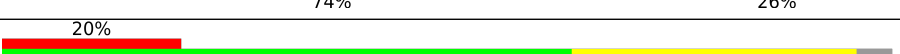
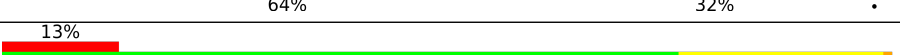
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	1	193	19% 72% 28% .
2	2	269	4% 55% 22% 23%
3	3	275	13% 60% 21% 20%
4	4	198	7% 74% 26%
5	A	758	6% 78% 19% .

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

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	LUT	1	502	X	-	-	-
17	LUT	2	501	X	-	-	-
17	LUT	3	302	X	-	-	-
17	LUT	J	1109	X	-	-	-
19	CLA	1	504	X	-	-	-
19	CLA	1	506	X	-	-	-
19	CLA	1	507	X	-	-	-
19	CLA	1	509	X	-	-	-
19	CLA	1	510	X	-	-	-
19	CLA	1	511	X	-	-	-
19	CLA	1	513	X	-	-	-
19	CLA	1	515	X	-	-	-
19	CLA	1	516	X	-	-	-
19	CLA	2	504	X	-	-	-
19	CLA	2	505	X	-	-	-
19	CLA	2	506	X	-	-	-
19	CLA	2	507	X	-	-	-
19	CLA	2	508	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	2	509	X	-	-	-
19	CLA	2	510	X	-	-	-
19	CLA	2	511	X	-	-	-
19	CLA	2	514	X	-	-	-
19	CLA	3	305	X	-	-	-
19	CLA	3	306	X	-	-	-
19	CLA	3	307	X	-	-	-
19	CLA	3	308	X	-	-	-
19	CLA	3	310	X	-	-	-
19	CLA	3	311	X	-	-	-
19	CLA	3	312	X	-	-	-
19	CLA	3	313	X	-	-	-
19	CLA	3	315	X	-	-	-
19	CLA	3	316	X	-	-	-
19	CLA	3	317	X	-	-	-
19	CLA	4	304	X	-	-	-
19	CLA	4	305	X	-	-	-
19	CLA	4	306	X	-	-	-
19	CLA	4	307	X	-	-	-
19	CLA	4	309	X	-	-	-
19	CLA	4	310	X	-	-	-
19	CLA	4	311	X	-	-	-
19	CLA	4	315	X	-	-	-
19	CLA	4	318	X	-	-	-
19	CLA	A	802	X	-	-	-
19	CLA	A	803	X	-	-	-
19	CLA	A	804	X	-	-	-
19	CLA	A	805	X	-	-	-
19	CLA	A	806	X	-	-	-
19	CLA	A	807	X	-	-	-
19	CLA	A	808	X	-	-	-
19	CLA	A	809	X	-	-	-
19	CLA	A	810	X	-	-	-
19	CLA	A	811	X	-	-	-
19	CLA	A	813	X	-	-	-
19	CLA	A	814	X	-	-	-
19	CLA	A	815	X	-	-	-
19	CLA	A	816	X	-	-	-
19	CLA	A	817	X	-	-	-
19	CLA	A	818	X	-	-	-
19	CLA	A	819	X	-	-	-
19	CLA	A	820	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	821	X	-	-	-
19	CLA	A	822	X	-	-	-
19	CLA	A	823	X	-	-	-
19	CLA	A	824	X	-	-	-
19	CLA	A	825	X	-	-	-
19	CLA	A	826	X	-	-	-
19	CLA	A	827	X	-	-	-
19	CLA	A	828	X	-	-	-
19	CLA	A	829	X	-	-	-
19	CLA	A	830	X	-	-	-
19	CLA	A	831	X	-	-	-
19	CLA	A	832	X	-	-	-
19	CLA	A	833	X	-	-	-
19	CLA	A	835	X	-	-	-
19	CLA	A	837	X	-	-	-
19	CLA	A	838	X	-	-	-
19	CLA	A	839	X	-	-	-
19	CLA	A	840	X	-	-	-
19	CLA	A	841	X	-	-	-
19	CLA	A	842	X	-	-	-
19	CLA	A	854	X	-	-	-
19	CLA	A	855	X	-	-	-
19	CLA	B	803	X	-	-	-
19	CLA	B	804	X	-	-	-
19	CLA	B	805	X	-	-	-
19	CLA	B	806	X	-	-	-
19	CLA	B	807	X	-	-	-
19	CLA	B	808	X	-	-	-
19	CLA	B	809	X	-	-	-
19	CLA	B	810	X	-	-	-
19	CLA	B	811	X	-	-	-
19	CLA	B	812	X	-	-	-
19	CLA	B	813	X	-	-	-
19	CLA	B	814	X	-	-	-
19	CLA	B	815	X	-	-	-
19	CLA	B	816	X	-	-	-
19	CLA	B	817	X	-	-	-
19	CLA	B	818	X	-	-	-
19	CLA	B	819	X	-	-	-
19	CLA	B	820	X	-	-	-
19	CLA	B	821	X	-	-	-
19	CLA	B	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	823	X	-	-	-
19	CLA	B	824	X	-	-	-
19	CLA	B	825	X	-	-	-
19	CLA	B	826	X	-	-	-
19	CLA	B	827	X	-	-	-
19	CLA	B	828	X	-	-	-
19	CLA	B	829	X	-	-	-
19	CLA	B	831	X	-	-	-
19	CLA	B	832	X	-	-	-
19	CLA	B	833	X	-	-	-
19	CLA	B	834	X	-	-	-
19	CLA	B	836	X	-	-	-
19	CLA	B	837	X	-	-	-
19	CLA	B	838	X	-	-	-
19	CLA	B	839	X	-	-	-
19	CLA	F	302	X	-	-	-
19	CLA	G	201	X	-	-	-
19	CLA	G	203	X	-	-	-
19	CLA	G	204	X	-	-	-
19	CLA	H	1000	X	-	-	-
19	CLA	J	1101	X	-	-	-
19	CLA	J	1102	X	-	-	-
19	CLA	J	1105	X	-	-	-
19	CLA	K	1001	X	-	-	-
19	CLA	K	1002	X	-	-	-
19	CLA	K	1003	X	-	-	-
19	CLA	K	1004	X	-	-	-
19	CLA	L	301	X	-	-	-
19	CLA	L	303	X	-	-	-
19	CLA	L	304	X	-	-	-
19	CLA	L	305	X	-	-	-
20	CHL	1	512	X	-	-	-
20	CHL	1	514	X	-	-	-
20	CHL	1	521	X	-	-	-
20	CHL	2	512	X	-	-	-
20	CHL	2	513	X	-	-	-
20	CHL	2	515	X	-	-	-
20	CHL	2	516	X	-	-	-
20	CHL	2	526	X	-	-	-
20	CHL	3	314	X	-	-	-
20	CHL	4	313	X	-	-	-
20	CHL	4	314	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CHL	4	316	X	-	-	-
20	CHL	4	317	X	-	-	-
23	XAT	4	303	X	-	-	-
27	CL0	A	801	X	-	-	-
28	SF4	C	102	-	-	X	-

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 37583 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Lhca1.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	221	Total	C	N	O	S	0	0	0
			1699	1114	277	303	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	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 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

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

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	ARG	GLY	conflict	UNP P05310
A	176	ALA	GLY	conflict	UNP P05310
A	194	VAL	ALA	conflict	UNP P05310
A	220	GLY	ARG	conflict	UNP P05310
A	371	ILE	VAL	conflict	UNP P05310
A	374	HIS	GLN	conflict	UNP P05310
A	378	ALA	SER	conflict	UNP P05310
A	390	GLY	ALA	conflict	UNP P05310
A	509	THR	ALA	conflict	UNP P05310
A	522	SER	ALA	conflict	UNP P05310
A	525	GLY	ASN	conflict	UNP P05310
A	608	ALA	SER	conflict	UNP P05310
A	627	SER	THR	conflict	UNP P05310
A	639	GLY	ALA	conflict	UNP P05310

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

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

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

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

- Molecule 8 is a protein called PsuD.

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

- Molecule 9 is a protein called Putative uncharacterized protein.

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	64	PRO	-	expression tag	UNP E1C9K6
E	65	PRO	-	expression tag	UNP E1C9K6
E	79	GLN	LYS	conflict	UNP E1C9K6
E	125	VAL	ILE	conflict	UNP E1C9K6
E	126	GLU	VAL	conflict	UNP E1C9K6
E	129	LYS	GLU	conflict	UNP E1C9K6

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	F	154	Total	C	N	O	S	0	0	0
			1213	786	210	215	2			

There are 7 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

- Molecule 11 is a protein called PsaG.

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

- Molecule 12 is a protein called Photosystem I reaction center subunit VI.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	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	-	expression tag	UNP A0A0M3KL10
H	140	GLY	-	expression tag	UNP A0A0M3KL10

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	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 15 is a protein called Photosystem I reaction center subunit X psaK.

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

There is a discrepancy between the modelled and reference sequences:

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

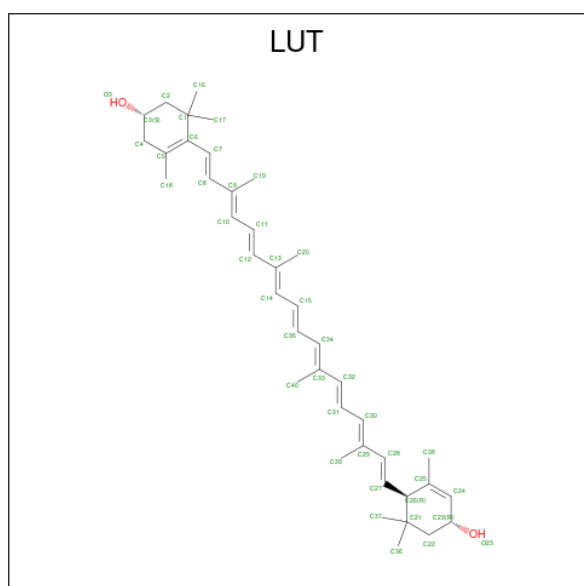
- Molecule 16 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	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 17 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



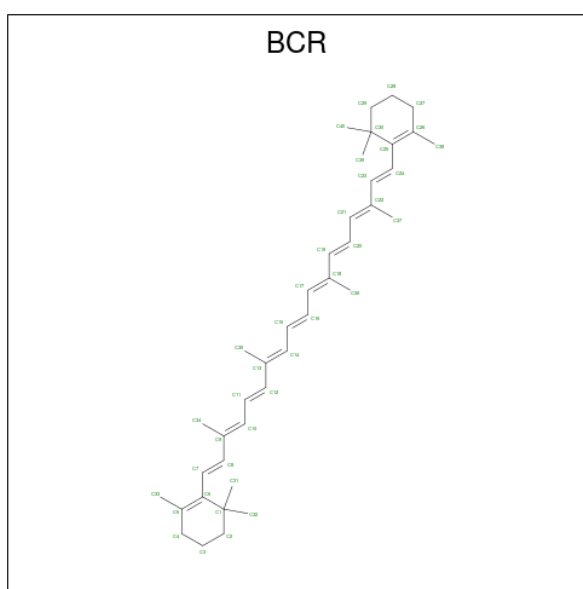
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	1	1	Total	C	O	0	0
			42	40	2		
17	1	1	Total	C	O	0	0
			42	40	2		
17	2	1	Total	C	O	0	0
			42	40	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	3	1	Total	C	O	0	0
			42	40	2		
17	3	1	Total	C	O	0	0
			42	40	2		
17	4	1	Total	C	O	0	0
			42	40	2		
17	J	1	Total	C	O	0	0
			42	40	2		

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



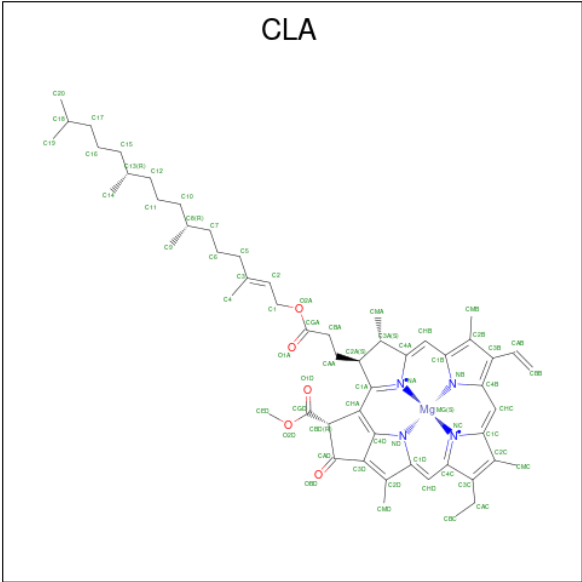
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	1	1	Total	C	0	0
			19	19		
18	2	1	Total	C	0	0
			40	40		
18	3	1	Total	C	0	0
			40	40		
18	3	1	Total	C	0	0
			40	40		
18	4	1	Total	C	0	0
			40	40		
18	A	1	Total	C	0	0
			40	40		
18	A	1	Total	C	0	0
			40	40		

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

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
19	3	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	4	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
19	4	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
19	4	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
19	4	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
19	4	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
19	4	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
19	4	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	4	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	A	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	A	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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

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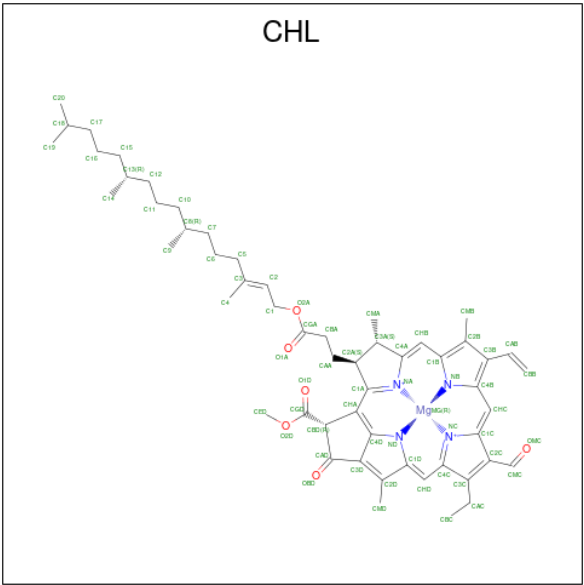
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	B	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	F	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	F	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	G	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
19	G	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
19	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	H	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
19	J	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	J	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
19	J	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
19	K	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
19	K	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
19	K	1	Total 27	C 22	Mg 1	N 4		0	0
19	K	1	Total 27	C 22	Mg 1	N 4		0	0
19	L	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
19	L	1	Total 50	C 40	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	L	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

- Molecule 20 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



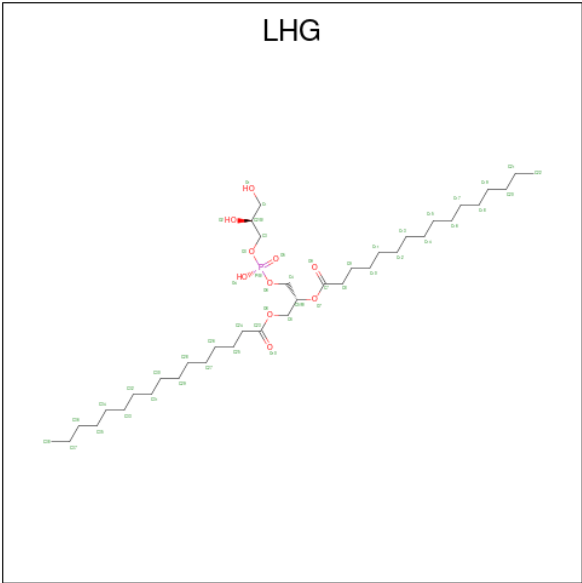
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	1	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
20	1	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
20	1	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
20	2	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
20	2	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
20	2	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
20	2	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
20	2	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
20	3	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		

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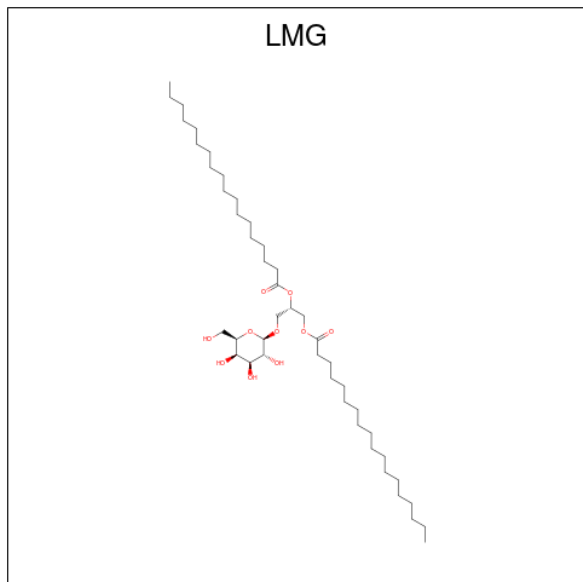
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	4	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
20	4	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
20	4	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
20	4	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		

- Molecule 21 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	1	1	Total	C	O	P	0	0
			49	38	10	1		
21	1	1	Total	C	O	P	0	0
			42	31	10	1		
21	2	1	Total	C	O	P	0	0
			35	24	10	1		
21	A	1	Total	C	O	P	0	0
			40	29	10	1		
21	A	1	Total	C	O	P	0	0
			49	38	10	1		
21	B	1	Total	C	O	P	0	0
			21	10	10	1		
21	B	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 22 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



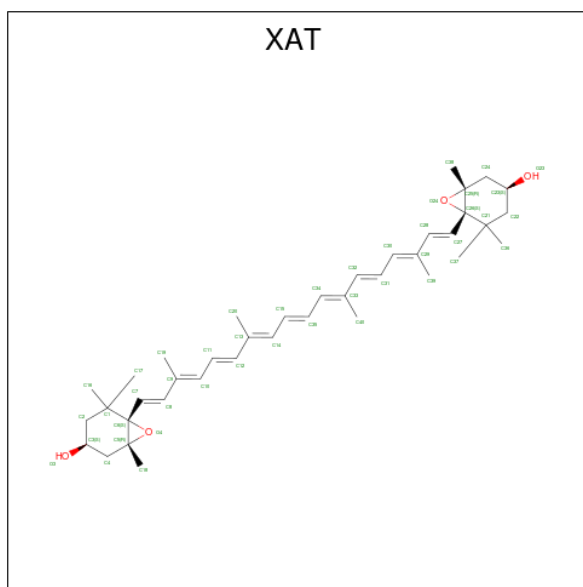
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	1	1	Total	C	O	0	0
			46	36	10		
22	1	1	Total	C	O	0	0
			13	7	6		
22	2	1	Total	C	O	0	0
			25	15	10		
22	2	1	Total	C	O	0	0
			36	26	10		
22	2	1	Total	C	O	0	0
			13	7	6		
22	2	1	Total	C	O	0	0
			13	7	6		
22	2	1	Total	C	O	0	0
			13	7	6		
22	2	1	Total	C	O	0	0
			13	7	6		
22	4	1	Total	C	O	0	0
			13	7	6		
22	4	1	Total	C	O	0	0
			45	35	10		
22	A	1	Total	C	O	0	0
			50	40	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			35	25	10		
22	B	1	Total	C	O	0	0
			33	23	10		
22	F	1	Total	C	O	0	0
			47	37	10		
22	F	1	Total	C	O	0	0
			36	26	10		
22	G	1	Total	C	O	0	0
			50	40	10		
22	G	1	Total	C	O	0	0
			25	15	10		
22	J	1	Total	C	O	0	0
			30	20	10		
22	J	1	Total	C	O	0	0
			34	24	10		

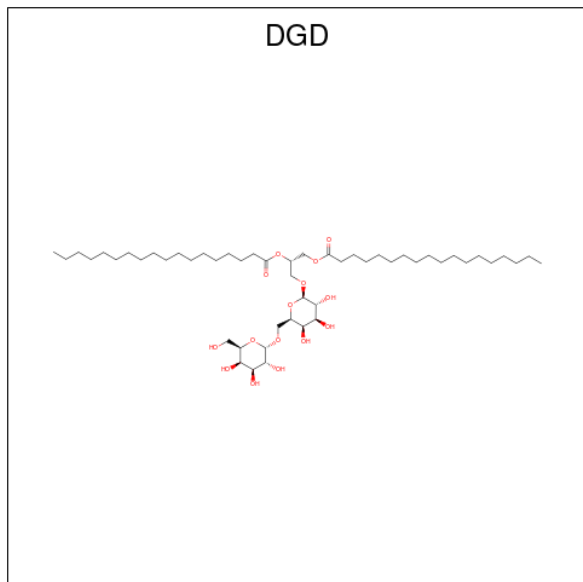
- Molecule 23 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	2	1	Total	C	O	0	0
			44	40	4		
23	4	1	Total	C	O	0	0
			44	40	4		

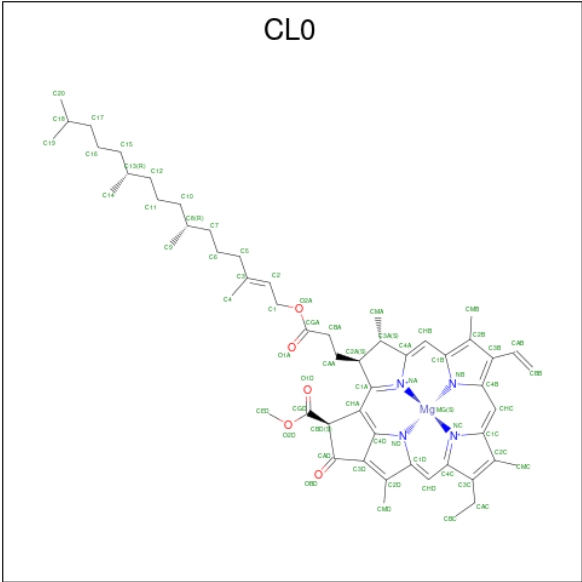
- Molecule 24 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).

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



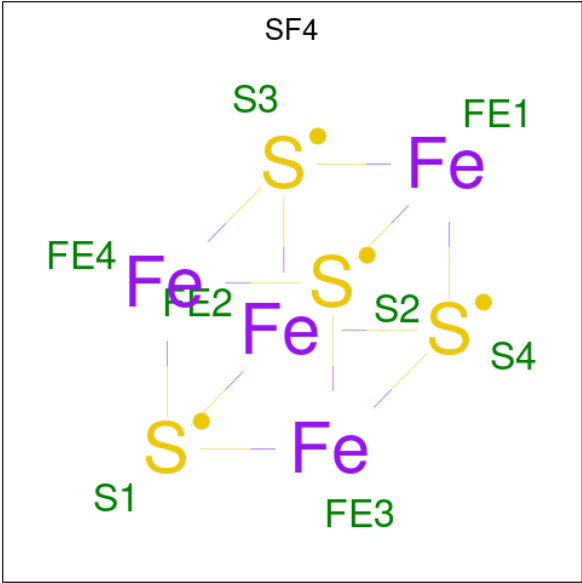
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	4	1	Total	C	O	0	0
			51	36	15		
26	B	1	Total	C	O	0	0
			41	26	15		
26	B	1	Total	C	O	0	0
			61	46	15		
26	G	1	Total	C	O	0	0
			47	32	15		
26	J	1	Total	C	O	0	0
			58	43	15		

- Molecule 27 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



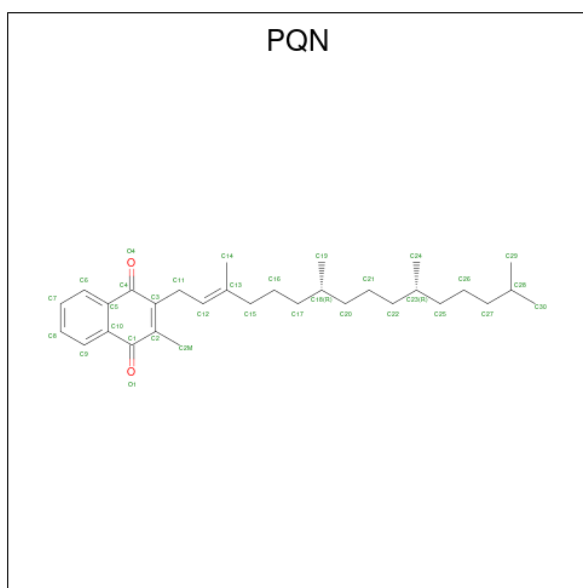
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



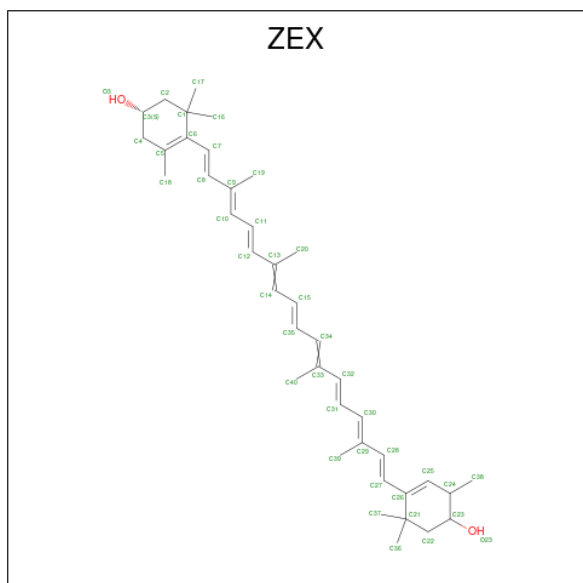
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	Fe	S	0	0
			8	4	4		
28	C	1	Total	Fe	S	0	0
			8	4	4		
28	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 29 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 30 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: $C_{40}H_{56}O_2$).



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

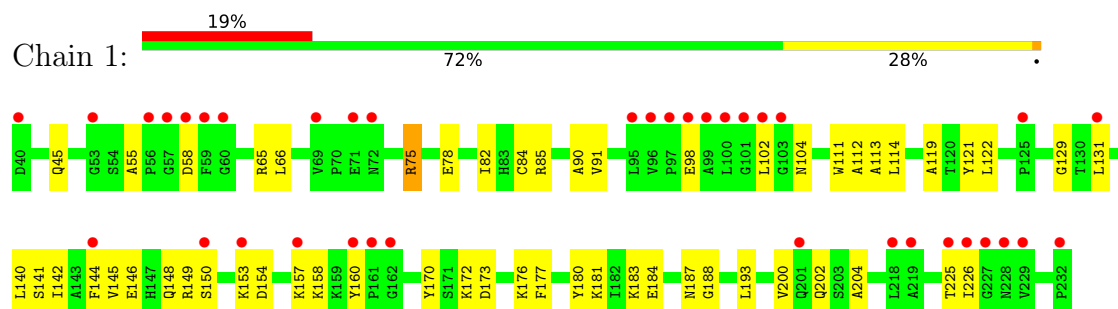
- Molecule 31 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	2	7	Total	O		0	0
			7	7			
31	3	3	Total	O		0	0
			3	3			
31	4	13	Total	O		0	0
			13	13			
31	A	49	Total	O		0	0
			49	49			
31	B	73	Total	O		0	0
			73	73			
31	C	19	Total	O		0	0
			19	19			
31	D	14	Total	O		0	0
			14	14			
31	E	10	Total	O		0	0
			10	10			
31	F	9	Total	O		0	0
			9	9			
31	G	3	Total	O		0	0
			3	3			
31	H	1	Total	O		0	0
			1	1			
31	J	4	Total	O		0	0
			4	4			
31	L	4	Total	O		0	0
			4	4			

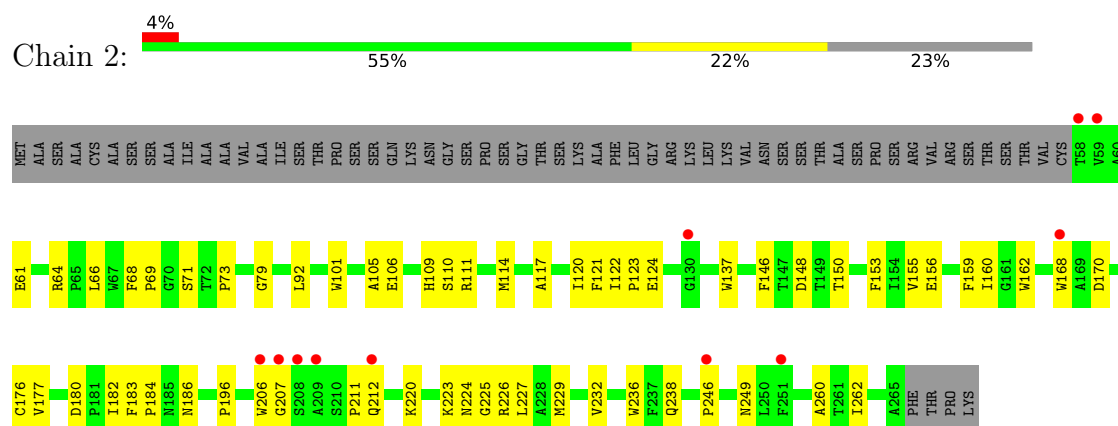
3 Residue-property plots

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.

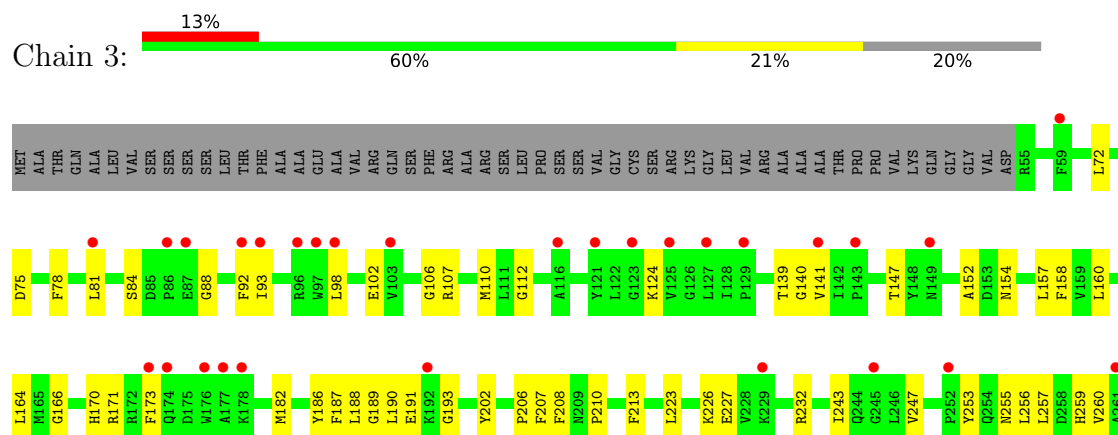
• Molecule 1: Lhca1

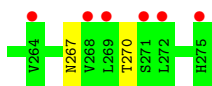


• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

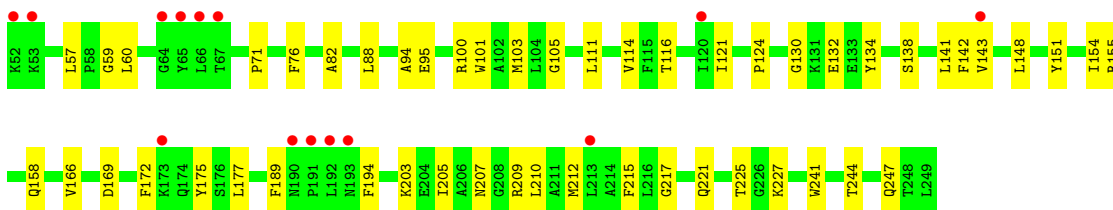
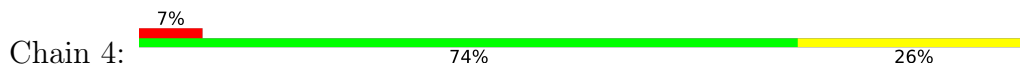


• Molecule 3: Chlorophyll a-b binding protein 3, chloroplastic

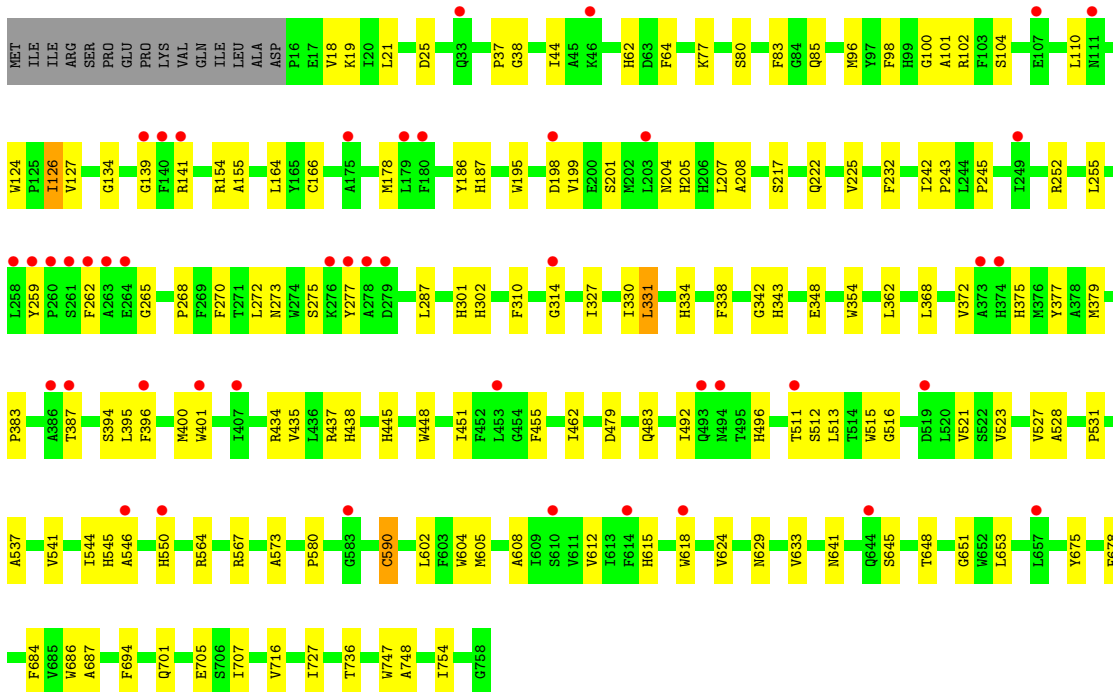
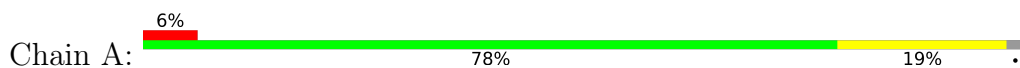




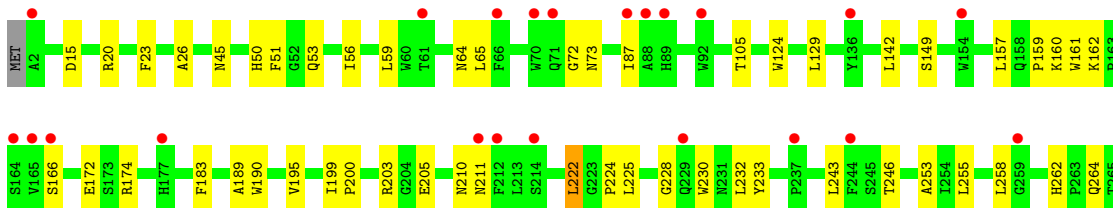
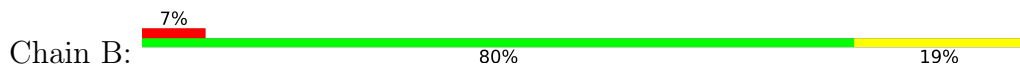
- Molecule 4: Chlorophyll a-b binding protein P4, chloroplastic

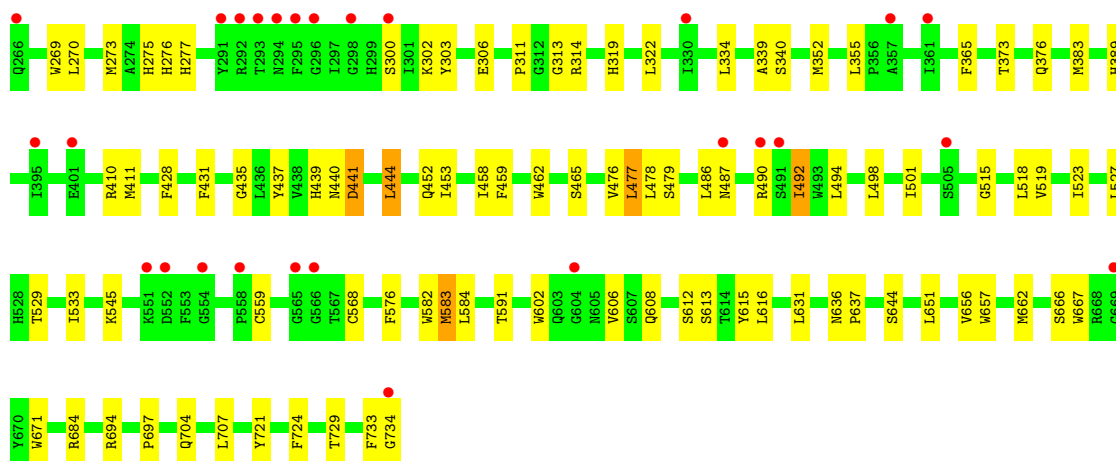


- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

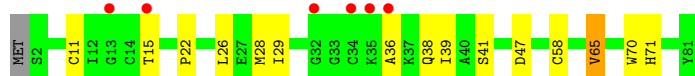
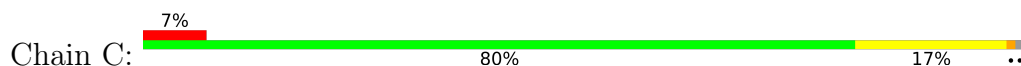


- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

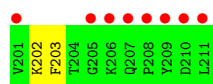
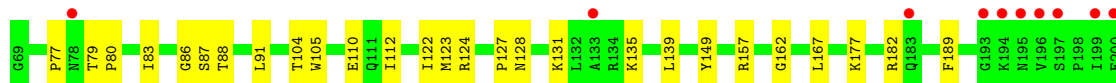
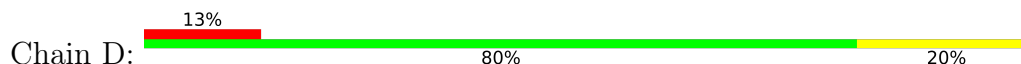




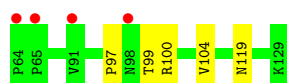
• Molecule 7: Photosystem I iron-sulfur center



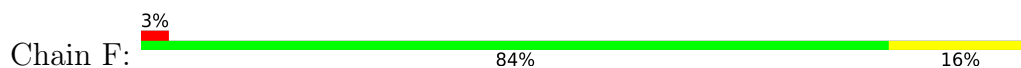
• Molecule 8: Psad



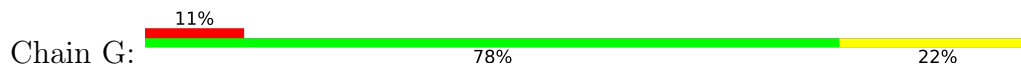
• Molecule 9: Putative uncharacterized protein

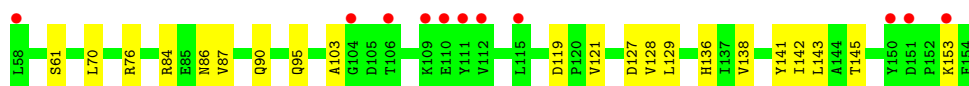


• Molecule 10: Photosystem I reaction center subunit III

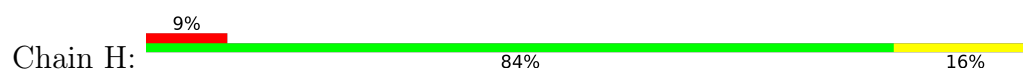


• Molecule 11: Psag





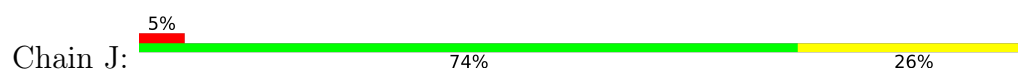
- Molecule 12: Photosystem I reaction center subunit VI



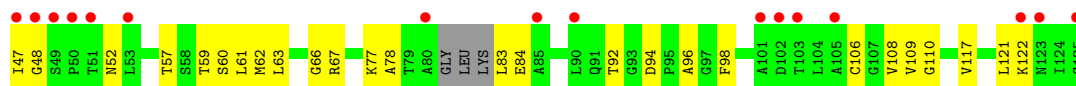
- Molecule 13: Photosystem I reaction center subunit VIII



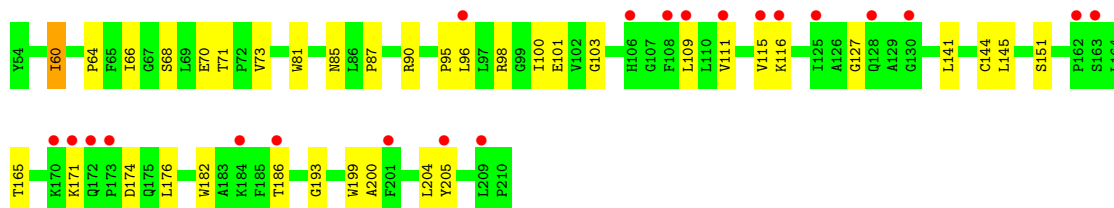
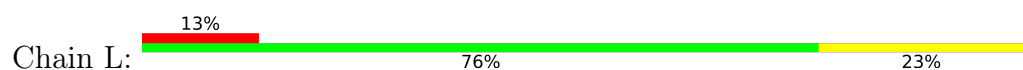
- Molecule 14: Photosystem I reaction center subunit IX



- Molecule 15: Photosystem I reaction center subunit X psaK



- Molecule 16: Putative uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	189.61Å 200.99Å 212.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.91 – 2.60 39.91 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.91-2.60) 93.4 (39.91-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.210 , 0.232 0.213 , 0.234	Depositor DCC
R_{free} test set	4925 reflections (1.73%)	wwPDB-VP
Wilson B-factor (Å ²)	60.7	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	37583	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.15	0/1558	0.32	0/2125
2	2	0.16	0/1679	0.35	0/2302
3	3	0.15	0/1753	0.34	0/2382
4	4	0.17	0/1608	0.33	0/2191
5	A	0.17	0/6057	0.37	0/8264
6	B	0.18	0/6069	0.37	0/8286
7	C	0.21	0/625	0.44	0/846
8	D	0.18	0/1163	0.43	0/1572
9	E	0.13	0/540	0.36	0/734
10	F	0.17	0/1241	0.36	0/1679
11	G	0.12	0/776	0.31	0/1054
12	H	0.15	0/693	0.36	0/942
13	I	0.14	0/238	0.32	0/324
14	J	0.25	0/349	0.40	0/476
15	K	0.12	0/520	0.30	0/707
16	L	0.14	0/1207	0.33	0/1651
All	All	0.17	0/26076	0.36	0/35535

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	1	1508	0	1489	56	0
2	2	1620	0	1557	56	0
3	3	1699	0	1648	65	0
4	4	1559	0	1527	51	0
5	A	5858	0	5719	145	0
6	B	5857	0	5653	135	0
7	C	612	0	592	11	0
8	D	1132	0	1141	21	0
9	E	528	0	528	3	0
10	F	1213	0	1241	19	0
11	G	757	0	743	21	0
12	H	673	0	667	13	0
13	I	232	0	253	2	0
14	J	338	0	345	16	0
15	K	515	0	513	23	0
16	L	1174	0	1183	34	0
17	1	84	0	110	11	0
17	2	42	0	55	7	0
17	3	84	0	110	20	0
17	4	42	0	55	3	0
17	J	42	0	55	8	0
18	1	19	0	24	4	0
18	2	40	0	55	11	0
18	3	80	0	109	12	0
18	4	40	0	55	9	0
18	A	240	0	329	20	0
18	B	280	0	384	27	0
18	F	40	0	55	1	0
18	G	40	0	55	3	0
18	I	80	0	110	11	0
18	J	40	0	55	4	0
18	K	40	0	55	7	0
18	L	120	0	165	6	0
19	1	608	0	563	50	0
19	2	512	0	479	32	0
19	3	623	0	526	59	0
19	4	631	0	599	53	0
19	A	2653	0	2772	218	0
19	B	2350	0	2461	178	0
19	F	130	0	144	10	0
19	G	231	0	225	24	0
19	H	60	0	59	2	0
19	J	160	0	143	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	K	159	0	96	10	0
19	L	215	0	185	8	0
20	1	164	0	134	20	0
20	2	263	0	210	30	0
20	3	47	0	30	9	0
20	4	202	0	150	18	0
21	1	91	0	131	18	0
21	2	35	0	40	9	0
21	A	89	0	127	9	0
21	B	70	0	86	8	0
22	1	59	0	76	4	0
22	2	126	0	117	10	0
22	4	58	0	71	4	0
22	A	50	0	73	4	0
22	B	68	0	76	6	0
22	F	83	0	109	10	0
22	G	75	0	90	6	0
22	J	64	0	68	3	0
23	2	44	0	56	4	0
23	4	44	0	56	9	0
24	2	35	0	46	0	0
24	3	31	0	34	2	0
24	4	35	0	45	2	0
24	A	35	0	46	3	0
24	B	98	0	114	8	0
24	G	66	0	80	5	0
24	J	25	0	23	1	0
25	3	1	0	0	0	0
25	B	1	0	0	0	0
26	4	51	0	60	6	0
26	B	102	0	123	14	0
26	G	47	0	52	1	0
26	J	58	0	77	6	0
27	A	65	0	72	6	0
28	A	8	0	0	1	0
28	C	16	0	0	2	0
29	A	33	0	46	3	0
29	B	33	0	46	8	0
30	F	42	0	56	5	0
31	2	7	0	0	0	0
31	3	3	0	0	0	0
31	4	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	A	49	0	0	1	0
31	B	73	0	0	2	0
31	C	19	0	0	0	0
31	D	14	0	0	0	0
31	E	10	0	0	0	0
31	F	9	0	0	2	0
31	G	3	0	0	1	0
31	H	1	0	0	0	0
31	J	4	0	0	0	0
31	L	4	0	0	1	0
All	All	37583	0	37507	1186	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 16.

All (1186) 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)
17:4:302:LUT:H373	19:4:304:CLA:H11	1.35	1.07
19:A:832:CLA:HBB1	19:A:833:CLA:H2	1.48	0.95
17:3:301:LUT:H32	19:3:305:CLA:HBB1	1.45	0.94
19:J:1105:CLA:HHC	19:J:1105:CLA:HBB1	1.55	0.86
5:A:379:MET:HE1	19:A:827:CLA:HAB	1.59	0.84
19:A:839:CLA:H111	19:A:839:CLA:HAB	1.58	0.84
5:A:310:PHE:HE1	19:A:821:CLA:HAB	1.42	0.83
5:A:401:TRP:CD1	19:A:828:CLA:HAB	2.16	0.81
6:B:694:ARG:NH1	16:L:151:SER:O	2.14	0.80
1:1:98:GLU:HG2	1:1:104:ASN:HA	1.62	0.79
5:A:270:PHE:HA	19:K:1001:CLA:HAC2	1.63	0.79
5:A:126:ILE:HB	17:J:1109:LUT:H182	1.66	0.77
3:3:141:VAL:HG21	17:3:302:LUT:H22	1.65	0.77
4:4:134:TYR:HE1	19:4:309:CLA:HAA2	1.48	0.77
19:A:855:CLA:H141	18:L:302:BCR:H17C	1.67	0.76
18:2:503:BCR:H332	26:4:319:DGD:HB32	1.68	0.76
19:2:511:CLA:HBA1	3:3:160:LEU:HD13	1.67	0.76
6:B:613:SER:O	31:B:901:HOH:O	2.04	0.76
20:4:314:CHL:HHC	20:4:314:CHL:HBB1	1.68	0.75
17:3:301:LUT:H28	19:3:305:CLA:H52	1.66	0.75
6:B:410:ARG:HH22	22:B:844:LMG:HC62	1.50	0.75
19:B:823:CLA:HAB	19:B:830:CLA:HMD2	1.69	0.74
3:3:107:ARG:HB3	19:3:305:CLA:HBC3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:826:CLA:H2	19:A:836:CLA:HMA2	1.69	0.74
3:3:139:THR:HG23	19:3:310:CLA:HED3	1.69	0.74
23:4:303:XAT:H183	19:4:309:CLA:C3B	2.18	0.74
19:1:510:CLA:HHC	19:1:510:CLA:HBB1	1.68	0.74
21:1:520:LHG:H101	19:B:822:CLA:H43	1.67	0.74
19:A:805:CLA:H61	18:A:849:BCR:H24C	1.70	0.74
16:L:145:LEU:HB3	16:L:186:THR:HG22	1.69	0.73
19:4:305:CLA:HBB1	19:4:310:CLA:H143	1.70	0.73
2:2:223:LYS:NZ	21:2:517:LHG:O5	2.17	0.73
23:4:303:XAT:H32	19:4:307:CLA:HAB	1.72	0.72
16:L:60:ILE:HA	16:L:70:GLU:HG3	1.71	0.72
19:A:811:CLA:HHC	19:A:811:CLA:HBB1	1.70	0.72
20:1:514:CHL:HBA1	21:1:520:LHG:HC92	1.70	0.72
5:A:400:MET:HE2	5:A:612:VAL:HG11	1.72	0.72
2:2:236:TRP:HZ3	20:2:512:CHL:HHB	1.53	0.72
5:A:255:LEU:O	5:A:259:TYR:N	2.14	0.72
4:4:134:TYR:CE1	19:4:309:CLA:HAA2	2.23	0.72
19:B:804:CLA:H201	19:B:839:CLA:H51	1.71	0.72
18:A:856:BCR:H353	18:K:1005:BCR:H323	1.71	0.71
19:A:835:CLA:HMB3	18:A:851:BCR:HC31	1.73	0.71
5:A:716:VAL:HG21	19:A:839:CLA:HMB2	1.71	0.71
19:B:805:CLA:HBB1	21:B:843:LHG:H223	1.72	0.71
19:B:833:CLA:H61	19:B:834:CLA:H12	1.73	0.71
5:A:590:CYS:HB3	28:A:843:SF4:S2	2.31	0.71
19:F:303:CLA:HAB	22:F:304:LMG:H382	1.71	0.70
17:2:501:LUT:H362	19:2:511:CLA:HBC1	1.74	0.70
20:2:512:CHL:HAA2	20:2:512:CHL:HBD	1.72	0.70
6:B:431:PHE:HZ	18:B:856:BCR:H11C	1.57	0.70
19:B:816:CLA:H2	18:B:851:BCR:HC42	1.72	0.70
4:4:203:LYS:HG3	19:4:310:CLA:HED2	1.74	0.70
12:H:78:TYR:OH	16:L:101:GLU:OE1	2.09	0.70
6:B:166:SER:HA	11:G:95:GLN:HE22	1.56	0.70
6:B:224:PRO:HB3	6:B:232:LEU:HD12	1.72	0.70
1:1:141:SER:HB2	18:1:503:BCR:H363	1.73	0.70
19:4:305:CLA:HMA1	19:4:305:CLA:H12	1.72	0.70
18:3:303:BCR:H351	20:3:314:CHL:HMB1	1.73	0.69
4:4:100:ARG:NH1	20:4:314:CHL:OBD	2.25	0.69
5:A:252:ARG:NH2	5:A:262:PHE:O	2.25	0.69
6:B:487:ASN:HB3	11:G:153:LYS:HB2	1.73	0.69
2:2:120:ILE:HG13	23:2:502:XAT:H163	1.73	0.69
1:1:153:LYS:HD3	1:1:158:LYS:HD2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:516:CLA:HBA2	30:F:301:ZEX:H41	1.75	0.69
18:2:503:BCR:H17C	20:2:513:CHL:HMB2	1.75	0.69
5:A:604:TRP:CH2	19:A:803:CLA:HAB	2.28	0.69
11:G:61:SER:HB3	19:G:202:CLA:HED2	1.75	0.68
19:B:812:CLA:HBD	24:G:208:LMT:H1'	1.75	0.68
19:B:838:CLA:H152	18:I:101:BCR:H11C	1.75	0.68
1:1:85:ARG:NE	1:1:184:GLU:OE2	2.23	0.68
5:A:362:LEU:HD21	19:A:830:CLA:HAB	1.76	0.68
10:F:78:ASP:N	10:F:82:LEU:O	2.26	0.68
15:K:92:THR:HG22	15:K:94:ASP:H	1.57	0.68
17:3:302:LUT:H32	19:3:308:CLA:HAB	1.76	0.68
17:1:501:LUT:H30	19:1:504:CLA:H52	1.74	0.68
17:3:301:LUT:H31	18:3:304:BCR:H363	1.75	0.68
5:A:648:THR:HG23	5:A:651:GLY:H	1.59	0.68
19:B:809:CLA:HAB	19:B:810:CLA:O1A	1.93	0.67
2:2:110:SER:HB3	2:2:225:GLY:HA3	1.75	0.67
2:2:111:ARG:NH1	20:2:513:CHL:OBD	2.26	0.67
5:A:199:VAL:HG11	19:A:825:CLA:HAC2	1.77	0.67
19:B:830:CLA:H191	22:F:304:LMG:H451	1.76	0.67
19:1:508:CLA:H2A	19:1:508:CLA:HED2	1.76	0.67
5:A:387:THR:HG21	5:A:523:VAL:HB	1.77	0.67
21:1:520:LHG:HC32	19:B:840:CLA:HBC1	1.76	0.67
22:2:524:LMG:HC1	10:F:201:PRO:HB3	1.75	0.67
6:B:440:ASN:HB3	6:B:452:GLN:HE21	1.60	0.67
6:B:666:SER:HB3	6:B:671:TRP:HE1	1.60	0.67
19:A:835:CLA:HHC	19:A:835:CLA:HBB1	1.77	0.67
22:4:322:LMG:H152	22:4:322:LMG:H352	1.78	0.66
5:A:678:PHE:HD2	5:A:747:TRP:HZ3	1.44	0.66
19:A:832:CLA:H171	18:I:102:BCR:H11C	1.76	0.66
3:3:190:LEU:HD22	18:3:304:BCR:HC31	1.76	0.66
19:A:804:CLA:HBB1	19:A:811:CLA:H122	1.78	0.66
6:B:523:ILE:HG21	19:B:835:CLA:HAB	1.77	0.66
2:2:92:LEU:HA	14:J:1:MET:HE3	1.78	0.66
5:A:567:ARG:NH2	8:D:88:THR:O	2.29	0.65
10:F:207:VAL:HB	19:J:1102:CLA:HED2	1.79	0.65
24:B:847:LMT:H11	22:F:304:LMG:H301	1.78	0.65
3:3:98:LEU:HD13	19:3:308:CLA:H11	1.78	0.65
20:1:512:CHL:HHC	20:1:512:CHL:HBB1	1.77	0.65
19:B:832:CLA:H91	19:J:1102:CLA:HMA3	1.78	0.65
19:A:809:CLA:HBB1	18:J:1108:BCR:HC8	1.77	0.65
19:B:819:CLA:H3A	19:B:819:CLA:CGA	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:806:CLA:H152	19:A:829:CLA:HBB2	1.78	0.65
5:A:686:TRP:CD2	27:A:801:CL0:H5	2.32	0.64
3:3:107:ARG:NH1	20:3:314:CHL:OBD	2.29	0.64
3:3:187:PHE:CE2	20:3:314:CHL:HBB2	2.33	0.64
19:A:855:CLA:H202	18:I:102:BCR:H391	1.80	0.64
19:B:815:CLA:H161	18:B:850:BCR:H363	1.80	0.64
6:B:458:ILE:HG21	10:F:151:SER:HB3	1.80	0.64
5:A:208:ALA:HB2	5:A:314:GLY:HA3	1.80	0.64
19:B:807:CLA:H152	19:B:828:CLA:HBB2	1.78	0.63
15:K:59:THR:HA	15:K:110:GLY:HA3	1.79	0.63
19:A:824:CLA:HMA1	19:A:842:CLA:HAB	1.79	0.63
19:B:836:CLA:HMA3	19:B:837:CLA:HED2	1.80	0.63
19:B:825:CLA:H91	22:F:304:LMG:H422	1.80	0.63
5:A:684:PHE:CG	18:A:852:BCR:H363	2.33	0.63
6:B:26:ALA:HB2	26:B:854:DGD:HA32	1.81	0.63
6:B:51:PHE:CE1	19:B:812:CLA:HBB1	2.33	0.63
19:B:840:CLA:HED1	18:B:852:BCR:H353	1.79	0.63
19:A:820:CLA:HAB	18:K:1005:BCR:H341	1.81	0.63
19:J:1105:CLA:HBA1	19:J:1105:CLA:CGD	2.29	0.63
19:B:833:CLA:H142	19:B:834:CLA:H51	1.79	0.63
2:2:155:VAL:HG22	19:4:311:CLA:HAA2	1.81	0.62
5:A:629:ASN:HB2	5:A:633:VAL:H	1.64	0.62
19:A:838:CLA:HMC2	19:L:301:CLA:HBC2	1.81	0.62
11:G:70:LEU:HD12	26:G:207:DGD:HB41	1.81	0.62
19:A:841:CLA:H18	19:J:1101:CLA:H193	1.81	0.62
2:2:150:THR:HG23	22:2:519:LMG:HC61	1.81	0.62
19:G:202:CLA:OBD	24:G:209:LMT:O3'	2.18	0.62
5:A:204:ASN:HB3	19:A:820:CLA:HMD2	1.80	0.62
6:B:275:HIS:HB3	19:B:818:CLA:HMB2	1.82	0.62
16:L:109:LEU:O	31:L:401:HOH:O	2.16	0.62
19:B:823:CLA:HBB1	19:B:830:CLA:H13	1.82	0.62
29:B:841:PQN:H28	18:I:102:BCR:H343	1.81	0.62
2:2:220:LYS:O	2:2:224:ASN:ND2	2.28	0.61
3:3:166:GLY:O	3:3:170:HIS:ND1	2.27	0.61
5:A:83:PHE:CE1	19:A:810:CLA:HBB1	2.34	0.61
19:B:825:CLA:HAA2	19:B:826:CLA:OBD	2.00	0.61
16:L:85:ASN:HB3	19:L:303:CLA:HAC1	1.80	0.61
19:3:305:CLA:H41	19:3:306:CLA:HMA2	1.82	0.61
19:A:809:CLA:H91	17:J:1109:LUT:H391	1.81	0.61
18:B:849:BCR:H402	19:G:201:CLA:C1D	2.30	0.61
14:J:16:THR:HG21	17:J:1109:LUT:H371	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:150:SER:HB2	20:1:514:CHL:HMA1	1.80	0.61
1:1:204:ALA:O	26:B:801:DGD:HE3	2.00	0.61
19:A:808:CLA:H171	19:J:1101:CLA:H93	1.83	0.61
6:B:365:PHE:HD2	6:B:734:GLY:HA2	1.65	0.61
19:H:1000:CLA:H121	16:L:81:TRP:HE1	1.64	0.61
4:4:225:THR:HG23	4:4:227:LYS:H	1.64	0.61
19:A:827:CLA:CAB	19:A:834:CLA:HMA2	2.30	0.61
20:4:317:CHL:HHC	20:4:317:CHL:HBB1	1.83	0.61
5:A:434:ARG:HH11	19:A:831:CLA:HED2	1.65	0.61
6:B:189:ALA:HA	19:B:816:CLA:HAB	1.81	0.61
3:3:226:LYS:NZ	19:3:306:CLA:O1A	2.33	0.61
19:4:307:CLA:H91	19:4:308:CLA:H142	1.83	0.61
6:B:15:ASP:HB3	6:B:20:ARG:HB2	1.81	0.61
19:B:823:CLA:H52	19:B:824:CLA:H142	1.81	0.61
3:3:92:PHE:HB3	19:3:309:CLA:H11	1.83	0.60
19:3:305:CLA:H43	19:3:306:CLA:HBA1	1.83	0.60
6:B:486:LEU:HD12	6:B:494:LEU:HD13	1.82	0.60
19:B:811:CLA:CAC	18:I:101:BCR:H10C	2.31	0.60
17:1:502:LUT:H28	17:1:502:LUT:H361	1.82	0.60
2:2:162:TRP:HH2	18:2:503:BCR:H321	1.66	0.60
15:K:67:ARG:HH12	15:K:96:ALA:HB3	1.64	0.60
23:2:502:XAT:H203	19:2:508:CLA:HBC3	1.82	0.60
2:2:232:VAL:HG11	23:2:502:XAT:H12	1.84	0.60
21:1:520:LHG:H211	19:G:204:CLA:H203	1.83	0.60
19:3:309:CLA:HED2	19:3:315:CLA:H2	1.82	0.60
20:1:514:CHL:HHC	20:1:514:CHL:HBB1	1.83	0.60
8:D:83:ILE:HB	8:D:122:ILE:HB	1.84	0.60
19:3:310:CLA:HMA3	19:3:316:CLA:C2C	2.32	0.60
19:3:310:CLA:HBA1	19:3:316:CLA:C1D	2.32	0.60
21:1:517:LHG:H223	19:4:318:CLA:HMA2	1.84	0.59
15:K:67:ARG:HE	19:K:1004:CLA:C4B	2.14	0.59
19:A:842:CLA:H3A	22:A:847:LMG:H372	1.83	0.59
6:B:431:PHE:CZ	18:B:856:BCR:H11C	2.36	0.59
3:3:107:ARG:NE	3:3:227:GLU:OE2	2.32	0.59
19:A:824:CLA:H43	18:A:851:BCR:H351	1.83	0.59
6:B:721:TYR:HB2	19:B:803:CLA:HED2	1.83	0.59
19:3:315:CLA:HBB1	19:3:315:CLA:HMB3	1.85	0.59
19:4:308:CLA:O1D	19:4:308:CLA:H12	2.01	0.59
5:A:102:ARG:NH2	24:A:846:LMT:O6'	2.35	0.59
19:B:827:CLA:CGA	19:B:827:CLA:H3A	2.32	0.59
19:B:840:CLA:HED3	18:B:852:BCR:H11C	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:70:TRP:CD1	7:C:71:HIS:H	2.20	0.59
20:2:513:CHL:HHC	20:2:513:CHL:HBB1	1.83	0.59
19:4:308:CLA:HBB1	19:4:308:CLA:HMB3	1.85	0.59
5:A:462:ILE:HG22	19:A:833:CLA:HBC2	1.85	0.59
1:1:119:ALA:H	1:1:129:GLY:HA3	1.67	0.59
18:4:301:BCR:H373	20:4:316:CHL:HHB	1.85	0.59
5:A:245:PRO:HG3	19:A:814:CLA:HED2	1.83	0.59
19:G:201:CLA:HHC	19:G:201:CLA:HBB1	1.84	0.59
20:1:521:CHL:H11	4:4:151:TYR:HB2	1.85	0.59
19:A:821:CLA:HBB1	19:A:821:CLA:HMB3	1.85	0.59
6:B:373:THR:HG23	6:B:591:THR:HG21	1.84	0.59
19:4:307:CLA:HMB1	19:4:307:CLA:HBB1	1.84	0.58
6:B:51:PHE:HE1	19:B:812:CLA:HBB1	1.68	0.58
6:B:174:ARG:HB2	19:B:814:CLA:HBC2	1.85	0.58
17:4:302:LUT:C37	19:4:304:CLA:H51	2.33	0.58
11:G:76:ARG:NH1	11:G:119:ASP:OD1	2.37	0.58
20:4:316:CHL:HHC	20:4:316:CHL:HBB1	1.85	0.58
5:A:124:TRP:HE1	24:A:846:LMT:H4'	1.68	0.58
3:3:102:GLU:OE2	3:3:232:ARG:NE	2.26	0.58
3:3:267:ASN:OD1	3:3:270:THR:OG1	2.20	0.58
18:4:301:BCR:H403	18:4:301:BCR:H23C	1.84	0.58
5:A:37:PRO:HA	19:J:1101:CLA:HBC1	1.86	0.58
4:4:244:THR:HG21	19:4:311:CLA:HED3	1.86	0.58
19:A:839:CLA:H92	18:B:856:BCR:H16C	1.84	0.58
6:B:411:MET:HE1	19:B:830:CLA:C1D	2.34	0.58
12:H:55:PHE:HA	12:H:63:THR:HG23	1.85	0.58
6:B:465:SER:O	6:B:479:SER:HB2	2.03	0.58
8:D:157:ARG:HB2	8:D:167:LEU:HD11	1.84	0.58
1:1:154:ASP:HB3	1:1:157:LYS:H	1.68	0.58
19:A:806:CLA:HED1	19:A:830:CLA:H2	1.86	0.58
6:B:105:THR:HG21	12:H:129:PRO:HG3	1.85	0.58
20:2:516:CHL:HHC	20:2:516:CHL:HBB1	1.86	0.57
19:B:823:CLA:CMA	19:B:840:CLA:HED2	2.34	0.57
1:1:84:CYS:HB3	1:1:188:GLY:HA3	1.86	0.57
19:B:806:CLA:HHC	19:B:806:CLA:HBB1	1.86	0.57
19:A:827:CLA:HBA1	18:A:851:BCR:H14C	1.87	0.57
6:B:314:ARG:NH1	22:B:844:LMG:O10	2.34	0.57
16:L:95:PRO:HG3	16:L:98:ARG:HH11	1.69	0.57
2:2:168:TRP:CE3	19:2:514:CLA:HMA1	2.40	0.57
5:A:375:HIS:ND1	19:A:818:CLA:OBD	2.38	0.57
19:A:804:CLA:HBD	19:A:811:CLA:H12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:1109:LUT:H28	17:J:1109:LUT:H361	1.86	0.56
19:1:508:CLA:H43	19:1:508:CLA:HED3	1.86	0.56
5:A:178:MET:HE1	19:A:813:CLA:H71	1.86	0.56
5:A:372:VAL:HG22	19:A:819:CLA:H42	1.86	0.56
19:B:809:CLA:O1A	19:B:827:CLA:HBD	2.05	0.56
6:B:59:LEU:HG	19:B:808:CLA:HBB2	1.88	0.56
5:A:201:SER:O	5:A:205:HIS:ND1	2.21	0.56
19:A:855:CLA:H171	16:L:141:LEU:HD11	1.87	0.56
6:B:45:ASN:OD1	21:B:843:LHG:O1	2.23	0.56
17:3:302:LUT:H27	19:3:308:CLA:H101	1.87	0.56
26:B:801:DGD:HB32	26:B:801:DGD:HG31	1.88	0.56
17:1:501:LUT:H32	19:1:504:CLA:CAB	2.36	0.56
5:A:275:SER:OG	15:K:122:LYS:NZ	2.33	0.56
14:J:16:THR:HG22	19:J:1101:CLA:H8	1.86	0.56
20:2:512:CHL:HBB1	20:2:512:CHL:HMB3	1.87	0.56
5:A:77:LYS:NZ	19:A:811:CLA:OBD	2.35	0.56
5:A:310:PHE:CE1	19:A:821:CLA:HAB	2.32	0.56
5:A:707:ILE:HD13	19:A:839:CLA:HMD1	1.87	0.55
19:A:824:CLA:H18	18:A:850:BCR:H363	1.87	0.55
19:B:819:CLA:H8	19:B:819:CLA:CAB	2.36	0.55
20:2:515:CHL:HHC	20:2:515:CHL:HBB1	1.88	0.55
19:A:818:CLA:H101	19:A:818:CLA:HMC2	1.88	0.55
18:B:802:BCR:H362	19:B:804:CLA:H122	1.87	0.55
19:B:805:CLA:HMA1	21:B:843:LHG:H262	1.89	0.55
18:B:856:BCR:H362	19:F:302:CLA:O2A	2.06	0.55
20:3:314:CHL:HHC	20:3:314:CHL:HBB1	1.87	0.55
6:B:657:TRP:CD2	19:B:803:CLA:HMA2	2.41	0.55
6:B:365:PHE:CD2	6:B:734:GLY:HA2	2.40	0.55
8:D:112:ILE:O	8:D:149:TYR:OH	2.22	0.55
19:G:204:CLA:HMC1	22:G:206:LMG:H361	1.89	0.55
20:1:521:CHL:HBC3	20:1:521:CHL:HHD	1.89	0.55
3:3:160:LEU:HD21	19:3:316:CLA:HED3	1.88	0.55
19:A:822:CLA:H62	19:A:823:CLA:H12	1.88	0.55
7:C:70:TRP:CG	7:C:71:HIS:H	2.24	0.55
5:A:496:HIS:HE1	19:A:834:CLA:NA	2.05	0.55
19:A:805:CLA:HHC	19:A:805:CLA:HBB1	1.89	0.55
2:2:120:ILE:HG12	2:2:137:TRP:CG	2.42	0.55
17:3:302:LUT:H7	19:3:310:CLA:HMB2	1.88	0.55
5:A:678:PHE:HD2	5:A:747:TRP:CZ3	2.25	0.55
19:B:812:CLA:HBA2	24:G:208:LMT:H22	1.88	0.55
19:G:204:CLA:H193	22:G:206:LMG:H401	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:124:LYS:HG3	3:3:253:TYR:HE2	1.72	0.54
3:3:152:ALA:HB3	3:3:157:LEU:HG	1.89	0.54
19:4:318:CLA:H101	30:F:301:ZEX:H163	1.89	0.54
5:A:64:PHE:CD2	19:A:805:CLA:HMC2	2.42	0.54
19:A:854:CLA:HAB	6:B:582:TRP:CH2	2.42	0.54
1:1:90:ALA:HB1	17:1:502:LUT:H27	1.89	0.54
17:3:301:LUT:H34	19:3:305:CLA:HBB2	1.88	0.54
19:A:805:CLA:H203	19:A:813:CLA:H62	1.89	0.54
19:B:818:CLA:HBA2	19:B:826:CLA:HBB2	1.90	0.54
1:1:66:LEU:HD12	17:1:502:LUT:H41	1.89	0.54
20:4:314:CHL:HBB2	20:4:317:CHL:OMC	2.08	0.54
5:A:330:ILE:O	5:A:334:HIS:ND1	2.34	0.54
19:A:803:CLA:H161	18:B:802:BCR:H321	1.88	0.54
19:A:806:CLA:HMD1	21:A:853:LHG:H221	1.90	0.54
19:A:810:CLA:H11	19:A:812:CLA:H43	1.90	0.54
19:A:811:CLA:H102	19:J:1101:CLA:HBB2	1.90	0.54
19:A:824:CLA:H161	21:A:845:LHG:H161	1.89	0.54
29:B:841:PQN:H301	26:B:854:DGD:HA91	1.90	0.54
11:G:142:ILE:HG12	22:G:206:LMG:H111	1.90	0.54
19:B:817:CLA:H11	19:G:204:CLA:HED1	1.90	0.54
5:A:343:HIS:HE1	21:A:845:LHG:HC11	1.73	0.54
6:B:462:TRP:NE1	6:B:476:VAL:HG11	2.21	0.54
6:B:636:ASN:HB2	6:B:637:PRO:HD2	1.90	0.54
19:A:827:CLA:H152	19:A:834:CLA:H121	1.89	0.54
1:1:183:LYS:HA	19:1:510:CLA:OBD	2.08	0.54
20:2:526:CHL:HHC	20:2:526:CHL:HBB1	1.89	0.54
19:4:309:CLA:HMA1	20:4:316:CHL:HBC2	1.90	0.54
15:K:67:ARG:NH2	15:K:94:ASP:OD1	2.41	0.54
1:1:183:LYS:HA	19:1:510:CLA:O1D	2.08	0.54
4:4:82:ALA:HB1	4:4:88:LEU:HD13	1.90	0.54
19:A:809:CLA:H193	19:A:811:CLA:H112	1.89	0.53
19:A:809:CLA:CBB	18:J:1108:BCR:HC8	2.38	0.53
12:H:77:PRO:HG3	16:L:90:ARG:CZ	2.38	0.53
14:J:10:VAL:HG13	14:J:12:PRO:HD2	1.90	0.53
15:K:63:LEU:O	15:K:67:ARG:HB2	2.09	0.53
5:A:327:ILE:HG23	19:A:821:CLA:HED3	1.90	0.53
21:B:842:LHG:O3	21:B:842:LHG:O1	2.18	0.53
1:1:184:GLU:HB2	19:1:504:CLA:CHB	2.39	0.53
6:B:515:GLY:O	6:B:519:VAL:HG23	2.08	0.53
19:4:304:CLA:H42	19:4:305:CLA:HBA1	1.90	0.53
5:A:139:GLY:HA2	10:F:109:TYR:HE1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:653:LEU:HD22	6:B:651:LEU:HD21	1.89	0.53
19:B:822:CLA:HBB1	19:B:822:CLA:HHC	1.90	0.53
2:2:120:ILE:HG13	23:2:502:XAT:C16	2.39	0.53
22:2:518:LMG:H111	22:J:1103:LMG:H291	1.89	0.53
1:1:180:TYR:HA	1:1:183:LYS:HB2	1.89	0.53
19:1:510:CLA:H2A	19:1:510:CLA:O2D	2.08	0.53
19:A:802:CLA:HMD3	6:B:533:ILE:HG12	1.91	0.53
6:B:545:LYS:NZ	31:B:907:HOH:O	2.37	0.53
29:B:841:PQN:H303	26:B:854:DGD:HA72	1.90	0.53
17:3:301:LUT:H34	19:3:305:CLA:CBB	2.39	0.53
23:4:303:XAT:H183	19:4:309:CLA:C4B	2.38	0.53
5:A:18:VAL:O	31:A:901:HOH:O	2.18	0.53
5:A:232:PHE:HD2	5:A:242:ILE:HG23	1.74	0.53
19:B:821:CLA:HMC3	18:B:850:BCR:H313	1.89	0.53
24:B:846:LMT:H41	24:G:208:LMT:H32	1.89	0.53
9:E:104:VAL:HG22	9:E:119:ASN:ND2	2.23	0.53
6:B:444:LEU:HD22	6:B:615:TYR:CZ	2.43	0.53
22:B:844:LMG:H141	22:F:305:LMG:H111	1.91	0.53
2:2:122:ILE:HB	2:2:123:PRO:HD3	1.90	0.53
3:3:81:LEU:HD13	19:A:812:CLA:H52	1.91	0.53
5:A:195:TRP:CE2	19:A:813:CLA:HBC3	2.43	0.53
5:A:375:HIS:HB3	19:A:818:CLA:HED2	1.91	0.53
2:2:68:PHE:CD2	2:2:71:SER:HB3	2.43	0.52
4:4:241:TRP:CE3	19:4:311:CLA:HMA2	2.44	0.52
3:3:112:GLY:HA2	17:3:302:LUT:H181	1.91	0.52
7:C:58:CYS:HA	28:C:102:SF4:S2	2.49	0.52
19:F:302:CLA:H61	18:F:306:BCR:H393	1.91	0.52
5:A:331:LEU:HD12	5:A:343:HIS:HB3	1.91	0.52
19:A:807:CLA:HBA1	19:A:809:CLA:H12	1.91	0.52
19:K:1001:CLA:C3B	18:K:1005:BCR:H12C	2.39	0.52
4:4:217:GLY:O	4:4:221:GLN:HB2	2.10	0.52
5:A:604:TRP:HH2	19:A:803:CLA:HAB	1.74	0.52
18:A:852:BCR:H362	19:A:854:CLA:H52	1.91	0.52
6:B:302:LYS:O	6:B:306:GLU:HG2	2.10	0.52
5:A:544:ILE:HD12	27:A:801:CL0:H63	1.92	0.52
6:B:222:LEU:O	24:B:855:LMT:O2B	2.28	0.52
19:B:823:CLA:HMA1	19:B:840:CLA:HED2	1.91	0.52
5:A:205:HIS:CG	19:A:813:CLA:HMC1	2.45	0.52
19:A:832:CLA:H112	29:B:841:PQN:H202	1.90	0.52
6:B:65:LEU:HD21	18:B:851:BCR:H291	1.91	0.52
26:4:319:DGD:HG31	26:4:319:DGD:O1A	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:303:TYR:HE2	19:B:822:CLA:HED3	1.74	0.52
6:B:64:ASN:HB3	19:B:809:CLA:HED1	1.92	0.52
19:1:516:CLA:C4D	22:F:304:LMG:H121	2.40	0.52
5:A:155:ALA:HB2	5:A:383:PRO:HD2	1.92	0.52
5:A:272:LEU:HD13	19:K:1001:CLA:HMD1	1.92	0.52
5:A:455:PHE:HB3	19:A:833:CLA:HBB2	1.91	0.52
19:A:812:CLA:C4C	19:A:812:CLA:H42	2.40	0.52
6:B:527:LEU:HD12	19:B:837:CLA:HED3	1.92	0.52
2:2:162:TRP:CH2	18:2:503:BCR:H321	2.45	0.51
6:B:72:GLY:HA2	6:B:87:ILE:HB	1.92	0.51
19:F:303:CLA:H193	22:F:305:LMG:H371	1.91	0.51
20:1:521:CHL:HHC	20:1:521:CHL:HBB1	1.91	0.51
19:2:508:CLA:OBD	19:2:514:CLA:H2	2.09	0.51
21:2:517:LHG:HC12	20:2:526:CHL:HBC1	1.92	0.51
8:D:131:LYS:NZ	12:H:63:THR:O	2.41	0.51
20:1:521:CHL:C2D	18:4:301:BCR:HC22	2.41	0.51
5:A:195:TRP:CZ2	19:A:813:CLA:HBC3	2.44	0.51
2:2:226:ARG:HA	2:2:229:MET:HE3	1.92	0.51
6:B:340:SER:HA	19:B:826:CLA:H41	1.91	0.51
6:B:704:GLN:HG3	26:B:854:DGD:HA22	1.91	0.51
19:L:303:CLA:HAA2	18:L:306:BCR:H352	1.91	0.51
1:1:121:TYR:CE1	19:1:509:CLA:H2	2.46	0.51
3:3:173:PHE:HB2	19:3:315:CLA:CMA	2.41	0.51
22:G:206:LMG:H201	22:G:206:LMG:H152	1.92	0.51
4:4:124:PRO:HG2	4:4:132:GLU:HG3	1.92	0.51
4:4:194:PHE:HD2	19:4:304:CLA:H12	1.74	0.51
5:A:80:SER:OG	5:A:186:TYR:HB2	2.11	0.51
15:K:57:THR:O	15:K:61:LEU:HB2	2.11	0.51
19:1:511:CLA:HED3	4:4:143:VAL:HB	1.93	0.51
20:1:512:CHL:HED1	22:G:210:LMG:HC71	1.93	0.51
3:3:186:TYR:CZ	24:3:318:LMT:H6D	2.46	0.51
3:3:213:PHE:HB2	19:3:305:CLA:HBA1	1.93	0.51
17:3:301:LUT:C31	18:3:304:BCR:H363	2.41	0.51
19:B:832:CLA:HMA3	26:J:1106:DGD:HA62	1.93	0.51
19:2:508:CLA:HBC1	20:2:512:CHL:HBB2	1.92	0.51
3:3:107:ARG:HB2	20:3:314:CHL:HED1	1.92	0.51
3:3:187:PHE:CZ	20:3:314:CHL:HBB2	2.45	0.51
23:4:303:XAT:H362	22:4:322:LMG:H381	1.93	0.51
19:B:806:CLA:H122	19:B:806:CLA:HBD	1.93	0.51
19:B:811:CLA:HAC2	18:I:101:BCR:H10C	1.92	0.51
2:2:69:PRO:HD2	20:2:526:CHL:O1D	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:259:HIS:CD2	19:3:307:CLA:HAA2	2.46	0.50
4:4:76:PHE:HB3	19:4:307:CLA:CAD	2.42	0.50
1:1:146:GLU:HG2	20:1:514:CHL:NB	2.26	0.50
17:3:301:LUT:C32	19:3:305:CLA:HMC1	2.41	0.50
19:A:818:CLA:C4A	19:A:818:CLA:H12	2.42	0.50
19:A:824:CLA:H12	18:A:850:BCR:H15C	1.93	0.50
1:1:75:ARG:NH2	20:1:514:CHL:O1A	2.42	0.50
19:1:507:CLA:HBC1	21:1:517:LHG:H152	1.94	0.50
6:B:195:VAL:HA	6:B:199:ILE:HD12	1.93	0.50
5:A:435:VAL:HA	5:A:438:HIS:CE1	2.46	0.50
6:B:222:LEU:HB2	24:B:855:LMT:H3B	1.92	0.50
19:B:825:CLA:H51	19:B:836:CLA:HBA1	1.92	0.50
11:G:76:ARG:HG2	19:G:203:CLA:CAB	2.42	0.50
19:J:1102:CLA:HBB1	19:J:1102:CLA:HMB1	1.93	0.50
1:1:75:ARG:NH1	19:1:508:CLA:O1A	2.45	0.50
19:3:315:CLA:H12	19:3:317:CLA:CBB	2.41	0.50
4:4:215:PHE:CG	23:4:303:XAT:H12	2.46	0.50
4:4:101:TRP:CE2	20:4:314:CHL:HED3	2.47	0.50
5:A:379:MET:HE3	19:A:827:CLA:HMC3	1.93	0.50
18:A:852:BCR:H24C	19:B:832:CLA:HMC1	1.92	0.50
5:A:252:ARG:HH22	5:A:265:GLY:HA2	1.75	0.50
19:A:808:CLA:H203	19:J:1101:CLA:HMA3	1.94	0.50
19:A:841:CLA:HAC2	18:B:856:BCR:H342	1.94	0.50
19:J:1105:CLA:HHC	19:J:1105:CLA:CBB	2.34	0.50
3:3:158:PHE:CD1	19:3:313:CLA:HBD	2.47	0.50
4:4:94:ALA:HB2	19:4:315:CLA:HED2	1.92	0.50
4:4:100:ARG:HA	4:4:103:MET:HE3	1.92	0.50
17:4:302:LUT:H371	19:4:304:CLA:H51	1.94	0.50
19:B:825:CLA:HMA1	18:B:853:BCR:H14C	1.94	0.50
1:1:45:GLN:HG2	4:4:158:GLN:HE22	1.76	0.49
3:3:106:GLY:O	3:3:110:MET:HG3	2.11	0.49
4:4:148:LEU:HB3	18:4:301:BCR:H16C	1.94	0.49
5:A:629:ASN:HD22	5:A:633:VAL:HB	1.76	0.49
11:G:138:VAL:HG22	22:G:206:LMG:H231	1.94	0.49
16:L:98:ARG:NH1	16:L:176:LEU:HB2	2.26	0.49
19:1:508:CLA:H52	19:B:840:CLA:C4B	2.42	0.49
17:2:501:LUT:H10	19:2:504:CLA:H61	1.94	0.49
3:3:256:LEU:O	3:3:260:VAL:HG23	2.11	0.49
19:A:802:CLA:H203	19:A:841:CLA:H2	1.94	0.49
19:A:819:CLA:H72	19:A:829:CLA:H91	1.93	0.49
19:G:201:CLA:H193	19:G:204:CLA:H121	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:19:PHE:CZ	19:J:1102:CLA:HBC2	2.46	0.49
1:1:65:ARG:HH21	22:1:518:LMG:HC3	1.77	0.49
22:1:518:LMG:H122	22:1:518:LMG:HC92	1.95	0.49
5:A:139:GLY:HA2	10:F:109:TYR:CE1	2.47	0.49
5:A:546:ALA:O	5:A:550:HIS:HD2	1.94	0.49
19:B:834:CLA:O1A	19:G:204:CLA:HBB	2.12	0.49
1:1:202:GLN:HG3	26:B:801:DGD:HA32	1.94	0.49
20:2:512:CHL:HAB	20:2:515:CHL:HBB2	1.93	0.49
4:4:241:TRP:CD2	19:4:311:CLA:HMA2	2.47	0.49
11:G:84:ARG:NH2	11:G:127:ASP:OD2	2.45	0.49
15:K:77:LYS:O	15:K:84:GLU:N	2.44	0.49
1:1:183:LYS:HG3	19:1:510:CLA:CGD	2.43	0.49
19:3:306:CLA:HHC	19:3:306:CLA:HBB1	1.93	0.49
4:4:138:SER:HA	4:4:141:LEU:HD12	1.95	0.49
21:A:845:LHG:H261	18:A:850:BCR:H373	1.94	0.49
6:B:311:PRO:C	6:B:313:GLY:H	2.21	0.49
19:3:308:CLA:HMB2	19:3:308:CLA:H43	1.95	0.49
4:4:210:LEU:HA	26:4:319:DGD:HA31	1.94	0.49
27:A:801:CL0:H12	19:A:854:CLA:CAD	2.43	0.49
18:L:302:BCR:C36	19:L:304:CLA:HAB	2.42	0.49
4:4:169:ASP:HB3	4:4:172:PHE:O	2.13	0.49
6:B:190:TRP:NE1	19:B:819:CLA:O1D	2.37	0.49
6:B:697:PRO:HB3	19:B:838:CLA:C1C	2.43	0.49
14:J:34:PRO:O	26:J:1106:DGD:O2D	2.28	0.49
19:A:837:CLA:H201	19:L:304:CLA:H102	1.95	0.49
4:4:57:LEU:HB3	4:4:60:LEU:HB3	1.95	0.49
5:A:701:GLN:O	5:A:705:GLU:HG3	2.13	0.49
5:A:747:TRP:CG	18:A:852:BCR:HC41	2.48	0.49
6:B:428:PHE:CE2	19:B:836:CLA:HAB	2.47	0.49
19:B:838:CLA:HBB2	29:B:841:PQN:H141	1.95	0.49
5:A:301:HIS:CD2	19:A:818:CLA:HMB1	2.48	0.49
22:B:845:LMG:H132	24:B:847:LMT:H2'	1.94	0.49
8:D:91:LEU:HD12	16:L:66:ILE:HD13	1.95	0.49
2:2:153:PHE:CE1	22:2:519:LMG:H321	2.47	0.48
3:3:210:PRO:HD2	17:3:301:LUT:H23	1.95	0.48
14:J:12:PRO:HB2	17:J:1109:LUT:H372	1.94	0.48
15:K:117:VAL:O	15:K:121:LEU:HG	2.13	0.48
20:1:514:CHL:HBA2	21:1:520:LHG:H121	1.95	0.48
5:A:38:GLY:HA3	5:A:44:ILE:HG22	1.95	0.48
5:A:521:VAL:HG12	5:A:528:ALA:HB3	1.95	0.48
1:1:170:TYR:CE2	17:1:501:LUT:H221	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:306:CLA:H12	19:3:306:CLA:HMA3	1.95	0.48
19:A:824:CLA:H61	19:A:824:CLA:H41	1.61	0.48
19:A:855:CLA:H71	19:B:838:CLA:H43	1.95	0.48
3:3:193:GLY:HA3	3:3:207:PHE:CD2	2.49	0.48
6:B:26:ALA:HA	19:B:829:CLA:H42	1.94	0.48
14:J:31:ARG:HD2	17:J:1109:LUT:H41	1.96	0.48
2:2:148:ASP:OD1	4:4:247:GLN:NE2	2.46	0.48
18:2:503:BCR:C33	26:4:319:DGD:HB32	2.42	0.48
6:B:224:PRO:HG2	6:B:233:TYR:CZ	2.48	0.48
6:B:486:LEU:O	6:B:490:ARG:HG3	2.13	0.48
6:B:631:LEU:HD22	6:B:724:PHE:HA	1.95	0.48
4:4:209:ARG:HA	4:4:212:MET:HE3	1.95	0.48
6:B:339:ALA:HB2	18:B:853:BCR:H372	1.95	0.48
12:H:123:LEU:HB3	12:H:125:ILE:HG22	1.94	0.48
3:3:72:LEU:HD23	19:3:308:CLA:HED1	1.96	0.48
18:A:850:BCR:H15C	18:A:850:BCR:H351	1.65	0.48
19:B:805:CLA:HBC1	26:B:854:DGD:HA92	1.95	0.48
24:B:846:LMT:H91	24:G:208:LMT:H61	1.94	0.48
2:2:66:LEU:HD11	2:2:73:PRO:HD3	1.95	0.48
20:2:526:CHL:HED1	3:3:171:ARG:HA	1.96	0.48
18:4:301:BCR:H271	19:4:309:CLA:C1B	2.44	0.48
19:B:805:CLA:H62	19:B:805:CLA:H102	1.57	0.48
15:K:47:ILE:HG12	15:K:48:GLY:H	1.78	0.48
1:1:173:ASP:HB3	1:1:176:LYS:HB3	1.95	0.48
19:A:809:CLA:HBB1	19:A:809:CLA:HMB3	1.95	0.48
19:A:842:CLA:HMA3	22:A:847:LMG:H392	1.95	0.48
6:B:142:LEU:HD11	18:B:851:BCR:H402	1.95	0.48
3:3:171:ARG:NH2	3:3:182:MET:O	2.46	0.48
3:3:202:TYR:HA	19:3:305:CLA:O1D	2.14	0.48
19:4:318:CLA:HAC2	30:F:301:ZEX:H372	1.96	0.48
3:3:141:VAL:HG22	19:3:316:CLA:HMC3	1.96	0.47
4:4:95:GLU:HB2	19:4:307:CLA:CHB	2.44	0.47
4:4:175:TYR:HB3	20:4:317:CHL:C3D	2.44	0.47
19:A:824:CLA:H122	19:A:824:CLA:H202	1.96	0.47
10:F:173:TRP:CD1	10:F:210:GLY:HA3	2.49	0.47
1:1:183:LYS:O	1:1:187:ASN:ND2	2.43	0.47
2:2:262:ILE:HD11	19:2:506:CLA:H42	1.96	0.47
18:2:503:BCR:H333	19:4:310:CLA:HHC	1.96	0.47
5:A:516:GLY:O	5:A:531:PRO:HG3	2.14	0.47
19:A:803:CLA:H122	18:B:802:BCR:H352	1.95	0.47
19:A:818:CLA:H61	19:A:818:CLA:NC	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:842:CLA:H8	22:A:847:LMG:H332	1.95	0.47
7:C:29:ILE:HG22	8:D:182:ARG:HB3	1.96	0.47
14:J:16:THR:HG22	19:J:1101:CLA:C8	2.44	0.47
19:4:306:CLA:H171	19:4:306:CLA:H13	1.62	0.47
19:B:837:CLA:H43	18:B:853:BCR:H10C	1.95	0.47
19:B:839:CLA:HBA2	19:B:839:CLA:H3A	1.58	0.47
11:G:136:HIS:CE1	18:G:205:BCR:H16C	2.49	0.47
17:1:502:LUT:H31	19:1:508:CLA:HBC3	1.96	0.47
2:2:101:TRP:CH2	2:2:168:TRP:HZ3	2.32	0.47
22:2:518:LMG:H112	22:2:518:LMG:HC8	1.66	0.47
4:4:148:LEU:HB3	18:4:301:BCR:C16	2.45	0.47
5:A:448:TRP:HH2	19:A:837:CLA:H151	1.79	0.47
19:A:821:CLA:H52	19:A:825:CLA:HBB1	1.95	0.47
6:B:159:PRO:HA	6:B:162:LYS:HG2	1.97	0.47
6:B:225:LEU:HA	6:B:230:TRP:CD1	2.49	0.47
6:B:411:MET:HE2	6:B:411:MET:HA	1.96	0.47
19:B:819:CLA:H72	19:B:819:CLA:H112	1.57	0.47
19:B:831:CLA:H93	19:B:831:CLA:H111	1.78	0.47
19:F:303:CLA:H41	19:F:303:CLA:H61	1.66	0.47
19:2:506:CLA:HMA1	19:2:511:CLA:HBC3	1.96	0.47
19:2:507:CLA:CGA	19:2:507:CLA:H3A	2.42	0.47
19:A:805:CLA:H143	19:A:805:CLA:H161	1.69	0.47
19:A:837:CLA:HHC	19:A:837:CLA:HBB1	1.95	0.47
6:B:523:ILE:CG2	19:B:835:CLA:HAB	2.44	0.47
6:B:684:ARG:HE	16:L:68:SER:HB2	1.79	0.47
9:E:97:PRO:C	9:E:99:THR:H	2.22	0.47
16:L:96:LEU:O	16:L:100:ILE:HG12	2.14	0.47
16:L:98:ARG:NH1	16:L:174:ASP:OD1	2.47	0.47
19:4:306:CLA:C4C	19:4:306:CLA:H42	2.45	0.47
5:A:83:PHE:CZ	19:A:810:CLA:HBB1	2.49	0.47
5:A:437:ARG:HG2	8:D:87:SER:HB3	1.95	0.47
6:B:159:PRO:C	6:B:161:TRP:H	2.23	0.47
16:L:103:GLY:O	16:L:193:GLY:HA2	2.15	0.47
20:1:512:CHL:HBB2	19:1:515:CLA:HBB2	1.95	0.47
3:3:124:LYS:HG3	3:3:253:TYR:CE2	2.50	0.47
5:A:302:HIS:HB2	19:A:818:CLA:CHB	2.45	0.47
5:A:394:SER:HB3	19:A:828:CLA:HMA1	1.95	0.47
5:A:479:ASP:O	5:A:483:GLN:NE2	2.48	0.47
5:A:512:SER:H	5:A:515:TRP:HD1	1.62	0.47
19:A:827:CLA:C3B	19:A:834:CLA:HMA2	2.43	0.47
19:A:842:CLA:H61	19:A:842:CLA:H41	1.71	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:662:MET:HE2	29:B:841:PQN:H2M2	1.97	0.47
19:B:813:CLA:HMB1	19:B:813:CLA:HBB1	1.95	0.47
7:C:15:THR:HG22	7:C:28:MET:HG3	1.97	0.47
10:F:113:SER:OG	10:F:115:PRO:HD2	2.14	0.47
10:F:203:ALA:O	10:F:207:VAL:HG13	2.15	0.47
1:1:177:PHE:CE2	1:1:181:LYS:HE3	2.49	0.47
19:1:507:CLA:H203	19:4:318:CLA:H52	1.96	0.47
19:3:313:CLA:H12	19:3:313:CLA:H3A	1.97	0.47
5:A:100:GLY:HA2	5:A:104:SER:OG	2.15	0.47
5:A:527:VAL:HG21	5:A:624:VAL:O	2.15	0.47
19:A:832:CLA:H143	19:A:832:CLA:H111	1.67	0.47
6:B:486:LEU:HG	6:B:490:ARG:HE	1.79	0.47
19:B:833:CLA:H111	19:B:834:CLA:H2	1.97	0.47
3:3:139:THR:HB	3:3:141:VAL:HG23	1.95	0.47
5:A:225:VAL:HG13	5:A:245:PRO:HB3	1.95	0.47
6:B:228:GLY:HA3	11:G:143:LEU:HB3	1.97	0.47
6:B:729:THR:O	6:B:733:PHE:N	2.43	0.47
24:B:846:LMT:H52	24:B:846:LMT:H82	1.67	0.47
7:C:65:VAL:HG22	28:C:102:SF4:S1	2.55	0.47
8:D:105:TRP:HE1	8:D:123:MET:HG3	1.80	0.47
19:1:516:CLA:C3D	22:F:304:LMG:H121	2.45	0.47
4:4:130:GLY:HA2	20:4:316:CHL:HBC3	1.97	0.47
11:G:142:ILE:HA	11:G:145:THR:HG22	1.96	0.47
15:K:47:ILE:HA	15:K:52:ASN:HD22	1.79	0.47
18:2:503:BCR:H372	20:2:513:CHL:HMA2	1.95	0.46
3:3:140:GLY:HA2	3:3:147:THR:HA	1.96	0.46
4:4:221:GLN:O	4:4:225:THR:HG22	2.14	0.46
19:A:808:CLA:H41	19:A:808:CLA:H61	1.43	0.46
19:A:822:CLA:HHC	19:A:822:CLA:HBB1	1.97	0.46
6:B:492:ILE:HG23	19:B:817:CLA:HED2	1.97	0.46
19:B:820:CLA:H141	19:B:820:CLA:H162	1.66	0.46
14:J:28:GLU:HG3	19:J:1105:CLA:NB	2.29	0.46
15:K:60:SER:HA	15:K:63:LEU:HD12	1.96	0.46
1:1:66:LEU:HA	21:B:842:LHG:HC12	1.97	0.46
17:1:502:LUT:H182	19:1:507:CLA:H2	1.97	0.46
21:1:517:LHG:H162	19:4:318:CLA:HED1	1.97	0.46
2:2:68:PHE:HD2	2:2:71:SER:HB3	1.79	0.46
19:A:817:CLA:H143	19:A:817:CLA:H161	1.72	0.46
19:A:821:CLA:HBA1	19:A:825:CLA:C3B	2.45	0.46
18:A:856:BCR:H11C	18:K:1005:BCR:H323	1.97	0.46
19:B:828:CLA:H3A	19:B:828:CLA:HBA2	1.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:512:CHL:HMD3	22:2:519:LMG:HC72	1.96	0.46
3:3:189:GLY:C	3:3:191:GLU:H	2.24	0.46
5:A:100:GLY:O	5:A:104:SER:HB2	2.15	0.46
19:A:811:CLA:H161	19:A:811:CLA:H141	1.63	0.46
19:A:839:CLA:H171	19:A:840:CLA:H43	1.98	0.46
19:B:804:CLA:H202	19:B:804:CLA:H162	1.73	0.46
19:K:1001:CLA:C1B	18:K:1005:BCR:H14C	2.46	0.46
2:2:227:LEU:HD13	19:2:510:CLA:HBC1	1.98	0.46
5:A:268:PRO:HB3	5:A:273:ASN:HB2	1.96	0.46
19:A:802:CLA:H71	19:A:841:CLA:HMC3	1.97	0.46
19:A:825:CLA:HBA1	19:A:829:CLA:H191	1.97	0.46
19:A:826:CLA:HAB	18:A:851:BCR:C23	2.46	0.46
6:B:172:GLU:OE1	6:B:172:GLU:N	2.46	0.46
6:B:694:ARG:HG2	19:B:838:CLA:HED3	1.97	0.46
14:J:22:LEU:HD21	19:J:1102:CLA:C3B	2.46	0.46
1:1:91:VAL:HG11	17:1:501:LUT:H12	1.96	0.46
5:A:395:LEU:HD11	19:A:829:CLA:HED3	1.97	0.46
19:B:814:CLA:H141	19:B:814:CLA:H162	1.72	0.46
19:B:840:CLA:HED1	18:B:852:BCR:C35	2.45	0.46
11:G:84:ARG:HA	11:G:84:ARG:HD3	1.73	0.46
13:I:14:LEU:C	13:I:17:PRO:HD2	2.41	0.46
19:1:508:CLA:HBA1	19:1:508:CLA:H3A	1.73	0.46
19:1:508:CLA:HMD2	21:1:520:LHG:H181	1.98	0.46
4:4:116:THR:HA	4:4:121:ILE:O	2.16	0.46
6:B:459:PHE:HB3	19:B:835:CLA:H42	1.98	0.46
29:A:844:PQN:H141	29:A:844:PQN:H161	1.68	0.46
6:B:23:PHE:CE2	26:B:854:DGD:HG11	2.50	0.46
6:B:576:PHE:CE1	19:B:829:CLA:HAC2	2.51	0.46
8:D:80:PRO:HB3	8:D:124:ARG:HH21	1.80	0.46
8:D:189:PHE:HB3	9:E:100:ARG:HH12	1.79	0.46
1:1:75:ARG:NH2	21:1:520:LHG:O8	2.48	0.46
1:1:200:VAL:HG13	30:F:301:ZEX:H173	1.98	0.46
17:3:301:LUT:H382	19:3:305:CLA:C4D	2.45	0.46
19:4:318:CLA:H3A	19:4:318:CLA:HBA2	1.69	0.46
5:A:354:TRP:HB3	19:A:805:CLA:HAC1	1.98	0.46
5:A:537:ALA:O	5:A:541:VAL:HG23	2.15	0.46
19:A:825:CLA:HBB1	19:A:825:CLA:HMB1	1.98	0.46
19:A:830:CLA:H41	21:A:853:LHG:H101	1.96	0.46
19:G:204:CLA:H142	19:G:204:CLA:H111	1.69	0.46
15:K:63:LEU:HD21	18:K:1005:BCR:H17C	1.98	0.46
1:1:78:GLU:CD	1:1:158:LYS:HE3	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:508:CLA:H71	18:B:852:BCR:H321	1.98	0.46
21:1:520:LHG:H223	19:G:204:CLA:H192	1.98	0.46
2:2:137:TRP:HH2	2:2:236:TRP:HA	1.81	0.46
2:2:238:GLN:OE1	17:2:501:LUT:H24	2.16	0.46
17:2:501:LUT:H392	19:2:506:CLA:HBB1	1.98	0.46
21:2:517:LHG:HC42	18:3:303:BCR:HC22	1.98	0.46
3:3:84:SER:OG	19:3:308:CLA:HAA2	2.16	0.46
19:4:312:CLA:HBC1	26:4:319:DGD:O5D	2.15	0.46
19:A:825:CLA:H193	19:A:825:CLA:H161	1.71	0.46
19:B:823:CLA:HAB	19:B:830:CLA:CMD	2.42	0.46
19:B:829:CLA:H193	19:B:839:CLA:HMA2	1.98	0.46
10:F:154:GLN:HE21	19:F:303:CLA:HED2	1.79	0.46
16:L:182:TRP:O	16:L:186:THR:HG23	2.16	0.46
2:2:148:ASP:HB2	22:2:519:LMG:C6	2.46	0.46
19:A:811:CLA:H3A	19:A:811:CLA:HBA2	1.39	0.46
19:A:813:CLA:H41	19:A:813:CLA:H61	1.71	0.46
19:A:854:CLA:HAB	6:B:582:TRP:CZ2	2.51	0.46
19:A:854:CLA:H91	19:A:854:CLA:H111	1.81	0.46
6:B:183:PHE:CE1	19:B:814:CLA:H92	2.50	0.46
6:B:243:LEU:HB2	6:B:246:THR:OG1	2.15	0.46
19:G:204:CLA:HBD	31:G:302:HOH:O	2.16	0.46
1:1:146:GLU:OE2	1:1:149:ARG:NH2	2.49	0.45
19:1:508:CLA:H62	19:1:508:CLA:H41	1.34	0.45
2:2:186:ASN:HB3	20:2:516:CHL:C2D	2.46	0.45
21:2:517:LHG:O4	21:2:517:LHG:HC11	2.16	0.45
3:3:166:GLY:C	3:3:170:HIS:HD1	2.20	0.45
5:A:736:THR:HG23	21:A:853:LHG:H342	1.98	0.45
19:A:824:CLA:CAB	19:A:824:CLA:H191	2.46	0.45
23:4:303:XAT:H31	23:4:303:XAT:H391	1.81	0.45
6:B:365:PHE:HB3	6:B:602:TRP:CZ3	2.52	0.45
21:B:843:LHG:H211	21:B:843:LHG:H182	1.79	0.45
1:1:142:ILE:HD13	18:1:503:BCR:H361	1.98	0.45
3:3:243:ILE:HG13	19:3:307:CLA:HAC2	1.99	0.45
4:4:155:ARG:NH2	4:4:166:VAL:O	2.45	0.45
20:4:314:CHL:HHC	20:4:314:CHL:CBB	2.42	0.45
5:A:479:ASP:HA	5:A:483:GLN:HG2	1.97	0.45
5:A:496:HIS:HE1	19:A:834:CLA:C4A	2.29	0.45
6:B:50:HIS:HE1	19:B:806:CLA:H161	1.81	0.45
18:2:503:BCR:H17C	20:2:513:CHL:CMB	2.45	0.45
3:3:247:VAL:HG12	3:3:267:ASN:HD21	1.81	0.45
4:4:111:LEU:HA	4:4:114:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:806:CLA:H192	19:A:806:CLA:H162	1.67	0.45
19:A:855:CLA:H143	19:A:855:CLA:H112	1.61	0.45
19:B:822:CLA:H61	19:B:822:CLA:H41	1.65	0.45
7:C:47:ASP:OD2	8:D:135:LYS:NZ	2.37	0.45
10:F:197:ILE:HG12	14:J:10:VAL:HG23	1.98	0.45
14:J:12:PRO:O	14:J:16:THR:HG23	2.16	0.45
15:K:52:ASN:HA	19:K:1001:CLA:OBD	2.16	0.45
1:1:140:LEU:HD11	11:G:70:LEU:HD13	1.97	0.45
2:2:207:GLY:CA	19:2:504:CLA:HAA2	2.47	0.45
20:2:526:CHL:H41	20:2:526:CHL:H62	1.59	0.45
5:A:368:LEU:HD11	19:A:819:CLA:H62	1.98	0.45
19:A:830:CLA:H162	19:A:841:CLA:HMA3	1.98	0.45
19:A:842:CLA:CHB	21:A:845:LHG:HC62	2.47	0.45
19:B:812:CLA:H93	19:B:812:CLA:H112	1.74	0.45
8:D:110:GLU:HA	8:D:123:MET:O	2.16	0.45
8:D:177:LYS:O	8:D:182:ARG:NH1	2.49	0.45
11:G:84:ARG:HA	11:G:87:VAL:HG12	1.99	0.45
18:G:205:BCR:H15C	18:G:205:BCR:H351	1.80	0.45
19:L:304:CLA:H91	19:L:304:CLA:H112	1.81	0.45
1:1:85:ARG:HB3	19:1:504:CLA:HBC2	1.98	0.45
20:2:515:CHL:HED2	4:4:241:TRP:CH2	2.51	0.45
6:B:276:HIS:HB2	19:B:818:CLA:C1B	2.47	0.45
6:B:462:TRP:HE1	6:B:476:VAL:HG11	1.81	0.45
19:B:837:CLA:C1D	19:B:840:CLA:H203	2.47	0.45
19:B:838:CLA:H111	19:B:839:CLA:H13	1.99	0.45
16:L:87:PRO:O	16:L:98:ARG:HD2	2.16	0.45
1:1:55:ALA:HB3	1:1:58:ASP:HB2	1.98	0.45
3:3:139:THR:CG2	19:3:310:CLA:HED3	2.44	0.45
20:3:314:CHL:CHA	20:3:314:CHL:HBA1	2.47	0.45
4:4:105:GLY:HA2	23:4:303:XAT:H181	1.98	0.45
5:A:85:GLN:HG2	19:A:805:CLA:HMA2	1.98	0.45
19:A:802:CLA:H42	19:A:854:CLA:HBB1	1.98	0.45
19:A:832:CLA:H193	19:A:832:CLA:H161	1.70	0.45
19:A:839:CLA:H193	10:F:177:VAL:HG12	1.99	0.45
19:A:855:CLA:H152	16:L:141:LEU:HD21	1.98	0.45
6:B:383:MET:HE1	18:B:853:BCR:H361	1.99	0.45
6:B:529:THR:HG21	6:B:582:TRP:CE2	2.52	0.45
6:B:608:GLN:O	6:B:612:SER:HB2	2.17	0.45
2:2:117:ALA:HB1	17:2:501:LUT:H32	1.99	0.45
19:4:315:CLA:H143	19:4:315:CLA:H161	1.71	0.45
19:A:821:CLA:H91	19:A:821:CLA:H111	1.88	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:507:CLA:H2A	19:1:507:CLA:HED2	1.99	0.45
21:1:520:LHG:H132	21:1:520:LHG:H161	1.53	0.45
2:2:159:PHE:HB3	18:2:503:BCR:C16	2.46	0.45
19:A:827:CLA:H161	19:A:827:CLA:H122	1.74	0.45
6:B:435:GLY:HA3	19:B:832:CLA:HAB	1.99	0.45
19:B:807:CLA:H92	19:B:807:CLA:H61	1.84	0.45
19:B:838:CLA:C15	18:I:101:BCR:H11C	2.44	0.45
1:1:180:TYR:HD1	1:1:183:LYS:HD3	1.81	0.45
3:3:193:GLY:HA2	3:3:206:PRO:HD2	1.99	0.45
4:4:130:GLY:HA2	20:4:316:CHL:CBC	2.48	0.45
5:A:101:ALA:HB2	5:A:164:LEU:HB2	1.99	0.45
19:A:828:CLA:H162	19:A:828:CLA:H202	1.61	0.45
19:A:855:CLA:H111	19:B:838:CLA:H61	1.98	0.45
10:F:219:ARG:NH1	31:F:403:HOH:O	2.49	0.45
15:K:67:ARG:HH21	19:K:1004:CLA:C1C	2.30	0.45
19:1:513:CLA:H161	19:1:513:CLA:H203	1.75	0.44
22:1:518:LMG:H151	19:4:318:CLA:HMD3	2.00	0.44
19:A:802:CLA:H92	6:B:431:PHE:HE1	1.82	0.44
19:A:838:CLA:H8	19:A:838:CLA:H52	1.58	0.44
19:B:817:CLA:H3A	19:B:817:CLA:HBA2	1.73	0.44
19:B:819:CLA:H192	19:B:819:CLA:H161	1.72	0.44
1:1:85:ARG:HB3	19:1:504:CLA:CBC	2.48	0.44
3:3:75:ASP:HA	19:3:308:CLA:O1D	2.17	0.44
17:3:302:LUT:C7	19:3:310:CLA:HMB2	2.46	0.44
19:4:307:CLA:HED2	19:4:307:CLA:H2A	1.99	0.44
10:F:188:ASP:OD1	10:F:189:LYS:N	2.48	0.44
18:I:102:BCR:H24C	16:L:145:LEU:CD2	2.46	0.44
2:2:180:ASP:HB3	2:2:183:PHE:O	2.17	0.44
6:B:160:LYS:O	19:B:812:CLA:HED3	2.17	0.44
19:B:820:CLA:H112	19:B:820:CLA:H142	1.63	0.44
19:B:825:CLA:C1B	18:B:853:BCR:H363	2.48	0.44
11:G:128:VAL:HG21	19:G:203:CLA:HMA3	1.99	0.44
11:G:141:TYR:OH	19:G:204:CLA:H2	2.18	0.44
18:I:102:BCR:H19C	16:L:144:CYS:HB3	1.99	0.44
16:L:165:THR:HG22	16:L:171:LYS:HD2	1.99	0.44
1:1:121:TYR:CD1	19:1:509:CLA:H2	2.53	0.44
1:1:160:TYR:CD2	1:1:181:LYS:HE2	2.52	0.44
2:2:61:GLU:CG	2:2:64:ARG:HB3	2.47	0.44
17:2:501:LUT:H27	19:2:506:CLA:HMB1	1.99	0.44
22:2:519:LMG:C10	19:J:1105:CLA:H11	2.47	0.44
3:3:164:LEU:C	18:3:303:BCR:H363	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:85:GLN:HG2	19:A:805:CLA:CMA	2.47	0.44
5:A:207:LEU:O	5:A:310:PHE:HB3	2.16	0.44
5:A:338:PHE:CD2	21:A:845:LHG:HC42	2.53	0.44
19:A:828:CLA:H152	18:J:1108:BCR:H16C	2.00	0.44
19:B:809:CLA:CGA	19:B:809:CLA:C1A	2.96	0.44
19:B:834:CLA:H62	19:B:834:CLA:H41	1.67	0.44
1:1:193:LEU:HD22	21:1:517:LHG:H141	1.99	0.44
3:3:256:LEU:HD23	3:3:257:LEU:HD23	1.98	0.44
19:3:317:CLA:HHC	19:3:317:CLA:HBB1	1.98	0.44
4:4:138:SER:OG	24:4:320:LMT:H6E	2.17	0.44
5:A:124:TRP:HB3	17:J:1109:LUT:H183	1.99	0.44
27:A:801:CL0:H10	27:A:801:CL0:H72	1.58	0.44
10:F:148:LEU:HD22	10:F:159:GLU:HB3	1.99	0.44
22:F:304:LMG:H151	22:F:304:LMG:H122	1.66	0.44
12:H:85:PHE:CE1	18:L:307:BCR:H11C	2.53	0.44
2:2:236:TRP:CZ3	20:2:512:CHL:HHB	2.42	0.44
3:3:223:LEU:C	19:3:305:CLA:HMA1	2.43	0.44
17:3:302:LUT:H24	19:3:308:CLA:H2	2.00	0.44
19:A:822:CLA:H111	19:A:822:CLA:H93	1.75	0.44
6:B:203:ARG:NH2	6:B:253:ALA:O	2.41	0.44
6:B:459:PHE:CE2	19:F:303:CLA:HBB1	2.52	0.44
19:B:833:CLA:HBA2	19:B:834:CLA:HMB2	1.98	0.44
18:1:503:BCR:H383	19:1:515:CLA:HAA1	2.00	0.44
20:2:513:CHL:HBB2	20:2:516:CHL:CMC	2.48	0.44
3:3:171:ARG:HD3	20:3:314:CHL:CBB	2.47	0.44
5:A:18:VAL:HG13	5:A:198:ASP:OD2	2.17	0.44
5:A:225:VAL:HG11	19:A:814:CLA:O1D	2.18	0.44
2:2:114:MET:SD	19:2:504:CLA:HAB	2.57	0.44
4:4:203:LYS:HD3	19:4:305:CLA:HAA2	2.00	0.44
19:4:306:CLA:H41	19:4:306:CLA:H61	1.63	0.44
5:A:166:CYS:SG	19:A:816:CLA:HAA2	2.58	0.44
5:A:252:ARG:HD2	19:A:815:CLA:HED2	2.00	0.44
19:A:806:CLA:H162	19:A:806:CLA:H122	1.47	0.44
6:B:270:LEU:HD23	6:B:273:MET:HE3	2.00	0.44
19:B:825:CLA:HED2	19:B:826:CLA:HBD	1.98	0.44
15:K:66:GLY:HA3	15:K:106:CYS:SG	2.58	0.44
16:L:73:VAL:HG12	19:L:301:CLA:O1A	2.18	0.44
1:1:183:LYS:CA	19:1:510:CLA:O1D	2.66	0.44
20:1:514:CHL:H11	21:1:520:LHG:H261	1.98	0.44
5:A:348:GLU:OE1	5:A:348:GLU:N	2.45	0.44
27:A:801:CL0:H49	27:A:801:CL0:H41	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:59:LEU:HD21	19:B:808:CLA:H111	2.00	0.44
19:B:840:CLA:H62	19:B:840:CLA:H41	1.62	0.44
29:B:841:PQN:H292	29:B:841:PQN:H262	1.70	0.44
10:F:162:THR:HB	10:F:163:PRO:HD3	1.99	0.44
15:K:92:THR:HG21	15:K:98:PHE:O	2.18	0.44
19:1:504:CLA:H51	19:1:505:CLA:HMA2	1.99	0.43
19:A:806:CLA:H41	19:A:806:CLA:H61	1.74	0.43
6:B:56:ILE:HD11	21:B:843:LHG:H361	2.00	0.43
6:B:210:ASN:OD1	6:B:211:ASN:N	2.50	0.43
1:1:153:LYS:HA	1:1:158:LYS:HD2	2.00	0.43
2:2:124:GLU:HG2	2:2:246:PRO:HD2	1.99	0.43
19:2:505:CLA:H61	19:2:505:CLA:H41	1.67	0.43
19:3:306:CLA:H2A	19:3:306:CLA:O2A	2.17	0.43
19:3:308:CLA:H141	19:3:308:CLA:H161	1.79	0.43
5:A:580:PRO:HB3	5:A:727:ILE:HB	2.01	0.43
5:A:641:ASN:O	5:A:645:SER:HB2	2.18	0.43
19:A:807:CLA:C1C	24:A:846:LMT:H101	2.48	0.43
19:A:828:CLA:H3A	19:A:828:CLA:HBA2	1.64	0.43
17:2:501:LUT:H173	19:2:504:CLA:H12	2.00	0.43
22:4:322:LMG:H121	31:F:405:HOH:O	2.18	0.43
5:A:96:MET:HE1	19:A:808:CLA:HMA2	2.01	0.43
5:A:675:TYR:O	5:A:748:ALA:HB1	2.18	0.43
6:B:53:GLN:HG2	19:B:806:CLA:HMA2	2.00	0.43
6:B:439:HIS:CD2	6:B:453:ILE:HG13	2.53	0.43
19:B:808:CLA:H161	19:B:808:CLA:H203	1.73	0.43
19:B:815:CLA:H91	19:B:815:CLA:H112	1.78	0.43
1:1:183:LYS:HG2	19:1:505:CLA:HBD	2.01	0.43
19:2:504:CLA:H3A	19:2:504:CLA:HBA2	1.49	0.43
19:2:509:CLA:HMA3	20:2:515:CHL:C2C	2.48	0.43
19:3:307:CLA:HHC	19:3:307:CLA:HBB1	2.00	0.43
19:3:313:CLA:H91	19:3:313:CLA:H111	1.74	0.43
5:A:252:ARG:HH22	5:A:265:GLY:CA	2.30	0.43
5:A:334:HIS:HB3	21:A:845:LHG:O1	2.18	0.43
19:A:802:CLA:H111	18:A:852:BCR:H23C	2.00	0.43
19:A:804:CLA:HBB1	19:A:811:CLA:C12	2.46	0.43
19:A:809:CLA:HBB1	18:J:1108:BCR:C8	2.47	0.43
6:B:410:ARG:HD3	19:B:830:CLA:OBD	2.18	0.43
6:B:583:MET:HE2	6:B:583:MET:HB3	1.95	0.43
19:B:803:CLA:O2D	19:B:803:CLA:HAA2	2.19	0.43
11:G:129:LEU:O	18:G:205:BCR:H362	2.19	0.43
19:2:511:CLA:HBB1	20:2:526:CHL:H202	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:301:BCR:H403	18:4:301:BCR:C23	2.49	0.43
5:A:217:SER:HB3	18:A:848:BCR:H14C	1.99	0.43
19:A:855:CLA:H41	19:A:855:CLA:H61	1.63	0.43
19:B:818:CLA:H192	19:B:818:CLA:H162	1.72	0.43
19:B:819:CLA:H41	19:B:819:CLA:H61	1.67	0.43
1:1:78:GLU:O	1:1:82:ILE:HG12	2.19	0.43
19:2:507:CLA:H193	19:2:507:CLA:H162	1.68	0.43
19:A:804:CLA:H3A	19:A:804:CLA:HBA2	1.39	0.43
19:A:812:CLA:HBA1	19:A:812:CLA:HBD	2.01	0.43
6:B:255:LEU:HD11	19:B:816:CLA:HBC1	2.00	0.43
19:B:819:CLA:H8	19:B:819:CLA:HAB	2.00	0.43
19:B:820:CLA:H41	19:B:820:CLA:H61	1.74	0.43
19:G:201:CLA:HHC	19:G:201:CLA:CBB	2.49	0.43
1:1:91:VAL:HG11	17:1:501:LUT:H10	2.01	0.43
21:1:517:LHG:H182	19:4:318:CLA:HED1	2.00	0.43
19:2:507:CLA:H62	19:2:507:CLA:H41	1.78	0.43
17:3:302:LUT:H3	19:3:310:CLA:HMA2	1.99	0.43
5:A:541:VAL:HG11	5:A:615:HIS:CG	2.53	0.43
19:A:802:CLA:O1A	19:A:802:CLA:H2	2.18	0.43
19:A:817:CLA:H62	19:A:817:CLA:H41	1.46	0.43
19:B:805:CLA:H3A	21:B:843:LHG:H291	2.00	0.43
15:K:47:ILE:HG12	15:K:48:GLY:N	2.33	0.43
21:1:517:LHG:H382	21:1:517:LHG:H352	1.85	0.43
2:2:146:PHE:HE1	4:4:241:TRP:CD2	2.36	0.43
2:2:153:PHE:CD1	20:2:512:CHL:HAC2	2.54	0.43
19:3:305:CLA:H71	19:3:306:CLA:HMA1	1.99	0.43
5:A:379:MET:HE1	19:A:827:CLA:CAB	2.38	0.43
5:A:396:PHE:O	5:A:400:MET:HG2	2.19	0.43
19:A:833:CLA:H11	18:L:302:BCR:C11	2.48	0.43
19:B:834:CLA:HMD2	19:G:204:CLA:HAB	2.01	0.43
22:J:1104:LMG:H341	26:J:1106:DGD:HB51	2.01	0.43
26:J:1106:DGD:HAS1	26:J:1106:DGD:HAH2	1.58	0.43
1:1:184:GLU:HB2	19:1:504:CLA:C1B	2.49	0.43
19:1:510:CLA:C1C	21:1:517:LHG:HC42	2.48	0.43
5:A:268:PRO:HB2	5:A:277:TYR:CE2	2.54	0.43
5:A:287:LEU:HD22	5:A:513:LEU:HD12	2.00	0.43
5:A:608:ALA:O	5:A:612:VAL:HG23	2.19	0.43
6:B:166:SER:OG	11:G:103:ALA:O	2.34	0.43
19:B:830:CLA:H102	19:B:830:CLA:H61	1.84	0.43
18:B:856:BCR:H403	10:F:167:PHE:HB2	2.01	0.43
7:C:11:CYS:SG	7:C:39:ILE:HG13	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:2:519:LMG:HC8	22:2:519:LMG:HC1	1.87	0.43
20:4:316:CHL:HBC3	20:4:316:CHL:OMC	2.19	0.43
5:A:62:HIS:HB2	19:A:830:CLA:HBA1	2.00	0.43
19:A:854:CLA:O1A	19:A:854:CLA:H3A	2.18	0.43
6:B:303:TYR:CE2	19:B:822:CLA:HED3	2.54	0.43
6:B:352:MET:HG2	19:B:819:CLA:O1A	2.19	0.43
19:B:803:CLA:HBA2	19:B:803:CLA:H3A	1.79	0.43
10:F:213:TRP:CG	10:F:214:PRO:HD3	2.53	0.43
19:G:203:CLA:HMB1	19:G:203:CLA:HBB1	2.00	0.43
1:1:144:PHE:O	1:1:148:GLN:HG2	2.18	0.42
2:2:61:GLU:HB3	2:2:79:GLY:HA3	2.01	0.42
20:2:526:CHL:H112	20:2:526:CHL:H71	1.66	0.42
19:4:306:CLA:H203	19:4:310:CLA:HAC2	2.00	0.42
19:4:309:CLA:H3A	19:4:309:CLA:HBA2	1.40	0.42
5:A:62:HIS:CD2	19:A:805:CLA:HBB2	2.54	0.42
19:A:824:CLA:H202	19:A:824:CLA:H8	2.00	0.42
19:A:840:CLA:H93	10:F:203:ALA:HB1	2.01	0.42
6:B:437:TYR:CZ	6:B:518:LEU:HB3	2.54	0.42
19:B:825:CLA:H141	19:B:825:CLA:H162	1.73	0.42
8:D:162:GLY:HA2	12:H:60:LEU:HD11	2.01	0.42
20:1:521:CHL:HED1	4:4:154:ILE:C	2.44	0.42
4:4:71:PRO:HB2	4:4:205:ILE:HD12	2.01	0.42
19:B:811:CLA:H3A	19:B:811:CLA:HBA1	1.77	0.42
19:B:832:CLA:H111	19:B:832:CLA:H72	1.92	0.42
19:G:201:CLA:H61	19:G:201:CLA:H41	1.49	0.42
19:H:1000:CLA:H61	19:H:1000:CLA:H41	1.77	0.42
19:1:516:CLA:H141	26:B:801:DGD:HA61	2.01	0.42
4:4:142:PHE:CD1	24:4:320:LMT:H62	2.54	0.42
5:A:134:GLY:O	5:A:141:ARG:HA	2.19	0.42
5:A:451:ILE:HD11	18:B:802:BCR:H402	2.01	0.42
19:A:803:CLA:HED2	19:B:803:CLA:C3B	2.49	0.42
19:A:808:CLA:H3A	19:A:808:CLA:HBA2	1.30	0.42
19:A:812:CLA:HHC	19:A:812:CLA:HBB1	2.01	0.42
19:A:831:CLA:H61	19:A:831:CLA:H102	1.46	0.42
19:B:816:CLA:H61	19:B:816:CLA:H92	1.81	0.42
19:B:819:CLA:H172	19:B:826:CLA:HMA2	2.01	0.42
19:B:826:CLA:H93	19:B:826:CLA:H111	1.74	0.42
19:B:830:CLA:HMC1	19:B:840:CLA:H142	2.01	0.42
19:B:840:CLA:H3A	19:B:840:CLA:HBA1	1.81	0.42
19:1:508:CLA:H141	19:1:508:CLA:H162	1.77	0.42
22:1:518:LMG:H352	19:4:318:CLA:C1D	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:514:CLA:HBA1	19:2:514:CLA:H3A	1.80	0.42
19:3:305:CLA:C4	19:3:306:CLA:HBA1	2.48	0.42
19:A:828:CLA:C1C	18:A:852:BCR:HC21	2.49	0.42
19:A:838:CLA:H61	19:A:838:CLA:H41	1.55	0.42
19:A:841:CLA:HAC1	29:A:844:PQN:H171	2.01	0.42
19:B:838:CLA:H161	18:I:101:BCR:H353	2.01	0.42
19:B:840:CLA:H91	19:B:840:CLA:H111	1.79	0.42
24:B:855:LMT:H52	19:G:202:CLA:HBC3	2.00	0.42
3:3:78:PHE:HB3	19:3:308:CLA:CAD	2.50	0.42
19:A:824:CLA:H201	18:A:850:BCR:H17C	2.02	0.42
19:A:830:CLA:H171	19:A:830:CLA:H13	1.83	0.42
6:B:376:GLN:HA	6:B:376:GLN:OE1	2.19	0.42
19:B:805:CLA:H3A	19:B:805:CLA:HBA2	1.50	0.42
19:B:806:CLA:HBC2	19:B:829:CLA:HMA1	2.01	0.42
19:B:811:CLA:H92	19:B:811:CLA:H61	1.74	0.42
22:J:1104:LMG:H112	24:J:1107:LMT:H2'	2.02	0.42
18:K:1005:BCR:H351	18:K:1005:BCR:H15C	1.90	0.42
2:2:69:PRO:HB2	3:3:182:MET:HE1	2.02	0.42
2:2:238:GLN:HB3	2:2:249:ASN:ND2	2.34	0.42
19:2:510:CLA:C4C	21:2:517:LHG:HC62	2.49	0.42
3:3:154:ASN:HA	3:3:157:LEU:HD12	2.01	0.42
3:3:208:PHE:HB3	19:3:305:CLA:HMD1	2.01	0.42
4:4:203:LYS:O	4:4:207:ASN:ND2	2.38	0.42
19:A:821:CLA:HBA1	19:A:825:CLA:CAB	2.50	0.42
6:B:656:VAL:HG22	19:B:839:CLA:HMB2	2.01	0.42
19:B:806:CLA:H3A	19:B:806:CLA:HBA1	1.47	0.42
19:B:807:CLA:HMA2	19:B:829:CLA:C4B	2.50	0.42
19:B:832:CLA:O1D	14:J:35:ASP:HA	2.20	0.42
19:G:204:CLA:H93	19:G:204:CLA:H61	1.83	0.42
2:2:176:CYS:SG	4:4:59:GLY:HA2	2.59	0.42
18:3:303:BCR:C35	20:3:314:CHL:HAB	2.50	0.42
20:4:313:CHL:HHC	20:4:313:CHL:HBB1	2.01	0.42
20:4:314:CHL:HBB2	20:4:317:CHL:CMC	2.48	0.42
5:A:455:PHE:C	19:A:833:CLA:HBB2	2.45	0.42
5:A:645:SER:O	5:A:651:GLY:HA3	2.20	0.42
5:A:686:TRP:CG	27:A:801:CL0:H5	2.53	0.42
19:A:809:CLA:H161	19:A:811:CLA:H142	2.01	0.42
19:A:832:CLA:C1C	19:A:833:CLA:H93	2.49	0.42
6:B:149:SER:OG	19:B:815:CLA:H191	2.19	0.42
6:B:441:ASP:OD2	6:B:616:LEU:N	2.44	0.42
19:B:829:CLA:C14	26:B:854:DGD:HAW1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:829:CLA:H141	19:B:829:CLA:H161	1.65	0.42
8:D:86:GLY:HA2	16:L:64:PRO:O	2.20	0.42
12:H:65:GLY:HA2	12:H:67:TRP:CH2	2.54	0.42
19:J:1101:CLA:HBB1	19:J:1101:CLA:HMB1	2.02	0.42
15:K:62:MET:HG2	15:K:109:VAL:HB	2.02	0.42
1:1:102:LEU:HD11	1:1:122:LEU:HD23	2.02	0.42
18:1:503:BCR:H381	19:1:509:CLA:H12	2.02	0.42
21:1:520:LHG:HC81	21:1:520:LHG:HC5	1.44	0.42
2:2:109:HIS:HE1	19:2:508:CLA:ND	2.17	0.42
5:A:694:PHE:HB2	19:A:802:CLA:HBC2	2.01	0.42
19:A:821:CLA:H41	19:A:821:CLA:H62	1.56	0.42
19:A:828:CLA:H112	19:A:828:CLA:H71	1.67	0.42
29:A:844:PQN:H261	29:A:844:PQN:H303	1.80	0.42
19:B:804:CLA:H141	19:B:804:CLA:H161	1.64	0.42
19:B:835:CLA:HMB2	19:B:837:CLA:HED1	2.02	0.42
7:C:26:LEU:HA	7:C:41:SER:O	2.19	0.42
8:D:202:LYS:HE2	8:D:203:PHE:CZ	2.54	0.42
26:J:1106:DGD:HD61	26:J:1106:DGD:HE2	1.75	0.42
15:K:78:ALA:HB2	15:K:83:LEU:HD23	2.02	0.42
2:2:148:ASP:HB2	22:2:519:LMG:HC62	2.01	0.42
2:2:182:ILE:O	2:2:184:PRO:HD3	2.20	0.42
2:2:238:GLN:HE21	19:2:506:CLA:C1A	2.33	0.42
20:2:526:CHL:H93	20:2:526:CHL:H51	2.02	0.42
5:A:25:ASP:HA	5:A:187:HIS:O	2.19	0.42
5:A:252:ARG:HH22	5:A:265:GLY:N	2.18	0.42
8:D:104:THR:HA	8:D:128:ASN:O	2.20	0.42
14:J:28:GLU:HG3	19:J:1105:CLA:C4B	2.50	0.42
2:2:106:GLU:HB2	19:2:507:CLA:CHB	2.50	0.42
21:2:517:LHG:HC82	20:2:526:CHL:C1C	2.50	0.42
5:A:564:ARG:HA	5:A:573:ALA:HB2	2.02	0.42
19:A:825:CLA:H93	19:A:825:CLA:H61	1.86	0.42
6:B:478:LEU:HD21	19:B:833:CLA:HED2	2.01	0.42
6:B:576:PHE:HE1	19:B:829:CLA:HAC2	1.83	0.42
6:B:644:SER:OG	19:B:810:CLA:HBC1	2.20	0.42
15:K:47:ILE:HG13	15:K:52:ASN:HD22	1.84	0.42
16:L:98:ARG:HH12	16:L:176:LEU:HB2	1.84	0.42
1:1:113:ALA:HA	19:G:204:CLA:HAC2	2.02	0.41
1:1:183:LYS:N	19:1:510:CLA:O1D	2.53	0.41
2:2:211:PRO:O	2:2:212:GLN:HB2	2.20	0.41
3:3:267:ASN:HB3	19:3:307:CLA:CAD	2.50	0.41
5:A:394:SER:HB3	19:A:828:CLA:CMA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:754:ILE:HD12	5:A:754:ILE:HA	1.87	0.41
19:A:807:CLA:H12	19:A:809:CLA:O1A	2.20	0.41
19:A:830:CLA:H41	19:A:830:CLA:H62	1.76	0.41
19:B:823:CLA:HBB2	19:B:840:CLA:H51	2.02	0.41
8:D:77:PRO:C	8:D:79:THR:H	2.28	0.41
12:H:73:ASP:HB2	16:L:171:LYS:HE2	2.01	0.41
16:L:116:LYS:HD3	19:L:305:CLA:HMB2	2.02	0.41
19:2:506:CLA:H161	19:2:506:CLA:H192	1.69	0.41
19:2:508:CLA:HMB3	19:2:508:CLA:HBB1	2.02	0.41
5:A:379:MET:HE2	5:A:511:THR:HG22	2.02	0.41
19:A:824:CLA:H191	19:A:824:CLA:HAB	2.02	0.41
19:A:831:CLA:HMA1	16:L:71:THR:HG21	2.01	0.41
19:A:837:CLA:HBB2	19:A:838:CLA:HBC3	2.01	0.41
6:B:410:ARG:HH22	22:B:844:LMG:C6	2.26	0.41
19:B:808:CLA:H101	19:B:808:CLA:H62	1.55	0.41
19:B:819:CLA:HBB2	19:B:824:CLA:C19	2.49	0.41
19:B:829:CLA:H143	19:B:829:CLA:H111	1.83	0.41
12:H:60:LEU:HA	12:H:63:THR:HB	2.02	0.41
20:1:521:CHL:C1D	18:4:301:BCR:HC22	2.49	0.41
19:2:510:CLA:HBB2	18:3:303:BCR:HC7	2.02	0.41
3:3:110:MET:HB3	17:3:301:LUT:C35	2.50	0.41
19:A:802:CLA:H91	19:A:802:CLA:H112	1.72	0.41
6:B:124:TRP:HB3	6:B:129:LEU:HD12	2.02	0.41
6:B:707:LEU:HD23	26:B:854:DGD:HA21	2.02	0.41
7:C:22:PRO:C	8:D:139:LEU:HD23	2.46	0.41
21:2:517:LHG:H122	21:2:517:LHG:HC92	1.76	0.41
3:3:182:MET:HA	3:3:182:MET:HE2	2.01	0.41
3:3:186:TYR:CZ	3:3:188:LEU:HA	2.56	0.41
17:3:302:LUT:H35	17:3:302:LUT:H401	1.94	0.41
19:4:304:CLA:H92	19:4:304:CLA:H61	1.83	0.41
19:A:812:CLA:HED2	19:A:813:CLA:HBC1	2.03	0.41
6:B:355:LEU:HD13	19:B:818:CLA:HAA1	2.03	0.41
19:B:836:CLA:H111	19:F:302:CLA:H191	2.02	0.41
7:C:36:ALA:O	7:C:38:GLN:HG2	2.20	0.41
19:J:1101:CLA:H143	17:J:1109:LUT:H34	2.03	0.41
3:3:213:PHE:HB2	19:3:305:CLA:CBA	2.49	0.41
5:A:19:LYS:HD2	5:A:21:LEU:HD21	2.01	0.41
5:A:127:VAL:HG22	19:B:832:CLA:OBD	2.20	0.41
19:A:823:CLA:O1A	19:K:1003:CLA:HHD	2.20	0.41
6:B:666:SER:C	6:B:667:TRP:HD1	2.29	0.41
19:B:808:CLA:H91	19:B:808:CLA:H112	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:820:CLA:H172	19:B:823:CLA:H92	2.01	0.41
19:B:829:CLA:C3D	26:B:854:DGD:HB62	2.51	0.41
19:F:302:CLA:H152	19:F:302:CLA:H112	1.82	0.41
1:1:111:TRP:CZ2	19:1:515:CLA:HAC1	2.56	0.41
19:1:507:CLA:H203	19:1:507:CLA:H162	1.74	0.41
20:1:521:CHL:OBD	4:4:155:ARG:NH1	2.54	0.41
5:A:629:ASN:ND2	5:A:633:VAL:HB	2.34	0.41
19:A:813:CLA:H141	19:A:813:CLA:H161	1.82	0.41
6:B:262:HIS:CE1	6:B:264:GLN:HB3	2.54	0.41
6:B:334:LEU:HD23	6:B:389:HIS:CE1	2.56	0.41
19:B:810:CLA:H43	18:I:101:BCR:C22	2.51	0.41
22:B:845:LMG:HC8	22:B:845:LMG:H112	1.69	0.41
30:F:301:ZEX:H31	30:F:301:ZEX:H401	1.85	0.41
3:3:188:LEU:HD12	18:3:303:BCR:H343	2.02	0.41
17:3:301:LUT:H32	19:3:305:CLA:CBB	2.32	0.41
4:4:212:MET:HG2	23:4:303:XAT:C15	2.51	0.41
5:A:222:GLN:NE2	19:A:819:CLA:O1D	2.54	0.41
5:A:232:PHE:CD2	5:A:243:PRO:HD2	2.56	0.41
19:A:802:CLA:H71	19:A:841:CLA:CMC	2.50	0.41
19:A:818:CLA:H3A	19:A:818:CLA:HBA2	1.43	0.41
19:A:819:CLA:H71	19:A:819:CLA:C3B	2.50	0.41
6:B:73:ASN:ND2	6:B:87:ILE:HG13	2.36	0.41
6:B:200:PRO:HB3	6:B:205:GLU:HB2	2.02	0.41
26:J:1106:DGD:HB31	26:J:1106:DGD:HB62	1.80	0.41
16:L:199:TRP:CG	18:L:306:BCR:H10C	2.56	0.41
2:2:196:PRO:HB3	20:2:513:CHL:HBC2	2.01	0.41
19:3:308:CLA:H41	19:3:308:CLA:H62	1.55	0.41
23:4:303:XAT:H162	20:4:316:CHL:CBB	2.50	0.41
19:4:309:CLA:H12	20:4:316:CHL:C3D	2.51	0.41
5:A:98:PHE:CG	19:A:807:CLA:HBC3	2.55	0.41
5:A:310:PHE:CZ	19:A:819:CLA:H142	2.55	0.41
5:A:687:ALA:HB3	19:A:802:CLA:HBB2	2.02	0.41
19:A:819:CLA:H52	19:A:819:CLA:HMB2	2.03	0.41
19:A:826:CLA:H62	19:A:826:CLA:H41	1.78	0.41
19:A:842:CLA:H8	19:A:842:CLA:H51	1.93	0.41
18:A:856:BCR:C18	15:K:108:VAL:HG11	2.50	0.41
6:B:53:GLN:HG2	19:B:806:CLA:CMA	2.51	0.41
6:B:258:LEU:HD12	6:B:269:TRP:CG	2.55	0.41
6:B:273:MET:O	6:B:277:HIS:ND1	2.53	0.41
19:B:830:CLA:HAB	19:B:837:CLA:CBB	2.51	0.41
16:L:204:LEU:HD23	16:L:205:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:120:ILE:HG22	2:2:121:PHE:CD1	2.56	0.41
2:2:206:TRP:C	19:2:504:CLA:HBA1	2.45	0.41
18:2:503:BCR:HC7	18:2:503:BCR:H331	1.85	0.41
21:2:517:LHG:HC42	18:3:303:BCR:HC31	2.03	0.41
20:2:526:CHL:H3A	19:3:317:CLA:O1D	2.21	0.41
3:3:93:ILE:HG22	3:3:93:ILE:O	2.21	0.41
3:3:255:ASN:ND2	19:3:307:CLA:O1D	2.47	0.41
18:3:304:BCR:H15C	18:3:304:BCR:H351	1.80	0.41
5:A:445:HIS:CD2	19:A:831:CLA:HMB1	2.56	0.41
19:A:817:CLA:H142	19:A:817:CLA:H112	1.72	0.41
19:A:837:CLA:H102	19:A:837:CLA:H13	1.92	0.41
19:A:840:CLA:H161	19:A:840:CLA:H121	1.91	0.41
19:A:841:CLA:H12	19:J:1101:CLA:O1A	2.21	0.41
6:B:498:LEU:HA	6:B:501:ILE:HG22	2.02	0.41
19:B:815:CLA:H2	18:B:851:BCR:H362	2.03	0.41
19:B:819:CLA:H93	19:B:824:CLA:H42	2.03	0.41
19:B:823:CLA:H61	19:B:823:CLA:H93	1.69	0.41
19:B:836:CLA:H193	19:B:836:CLA:H162	1.89	0.41
12:H:82:GLN:O	12:H:85:PHE:HB3	2.21	0.41
13:I:26:LEU:O	13:I:30:LYS:HG3	2.20	0.41
16:L:111:VAL:HG21	16:L:200:ALA:HB3	2.03	0.41
1:1:112:ALA:HB1	1:1:131:LEU:HD22	2.03	0.41
1:1:225:THR:HG22	1:1:226:ILE:N	2.36	0.41
18:2:503:BCR:HC32	26:4:319:DGD:O2E	2.21	0.41
21:2:517:LHG:HC42	18:3:303:BCR:C2	2.50	0.41
4:4:177:LEU:HD11	4:4:189:PHE:HE2	1.86	0.41
18:4:301:BCR:H271	19:4:309:CLA:NB	2.36	0.41
19:4:315:CLA:H203	19:4:315:CLA:H162	1.80	0.41
5:A:377:TYR:OH	19:A:836:CLA:HBC3	2.21	0.41
6:B:59:LEU:HG	19:B:808:CLA:CBB	2.50	0.41
19:B:820:CLA:H203	19:B:820:CLA:H161	1.73	0.41
19:B:825:CLA:H93	19:B:825:CLA:H61	1.72	0.41
8:D:79:THR:HG23	8:D:127:PRO:HB2	2.03	0.41
16:L:115:VAL:HG13	16:L:127:GLY:O	2.21	0.41
19:1:508:CLA:HBD	20:1:514:CHL:HBD	2.03	0.40
19:1:508:CLA:CBC	20:1:514:CHL:HAC1	2.52	0.40
3:3:226:LYS:HD3	19:3:306:CLA:HAA2	2.02	0.40
19:3:308:CLA:H112	19:3:308:CLA:H143	1.82	0.40
4:4:244:THR:HB	4:4:247:GLN:OE1	2.21	0.40
5:A:545:HIS:HE1	5:A:615:HIS:CD2	2.38	0.40
19:A:805:CLA:H202	19:A:805:CLA:H162	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:824:CLA:HHB	19:A:842:CLA:HAB	2.02	0.40
6:B:662:MET:HE2	29:B:841:PQN:C2M	2.51	0.40
19:B:809:CLA:H111	19:B:809:CLA:H142	1.87	0.40
19:F:303:CLA:ND	22:F:304:LMG:H302	2.36	0.40
14:J:32:PHE:CE2	19:J:1105:CLA:HMA1	2.56	0.40
19:J:1101:CLA:H162	19:J:1101:CLA:H122	1.81	0.40
17:1:501:LUT:H35	17:1:501:LUT:H401	1.94	0.40
19:1:504:CLA:H93	19:1:504:CLA:H111	1.72	0.40
19:3:305:CLA:H3A	19:3:305:CLA:HBA2	1.40	0.40
24:3:318:LMT:O6B	24:3:318:LMT:O4'	2.24	0.40
4:4:175:TYR:CD2	20:4:317:CHL:HAA2	2.55	0.40
19:4:307:CLA:HMD1	19:4:312:CLA:CBB	2.51	0.40
19:4:318:CLA:H203	19:4:318:CLA:H161	1.85	0.40
19:A:804:CLA:H161	19:A:804:CLA:H143	1.79	0.40
19:A:822:CLA:H72	19:A:823:CLA:C1B	2.51	0.40
6:B:300:SER:H	11:G:90:GLN:HE21	1.68	0.40
6:B:411:MET:HE1	19:B:830:CLA:CHD	2.51	0.40
6:B:477:LEU:C	6:B:479:SER:H	2.29	0.40
6:B:684:ARG:NE	16:L:68:SER:HB2	2.36	0.40
11:G:86:ASN:HB3	19:G:201:CLA:HED1	2.03	0.40
19:K:1002:CLA:H41	19:K:1002:CLA:H61	1.47	0.40
1:1:145:VAL:O	1:1:148:GLN:HB2	2.22	0.40
19:1:504:CLA:HMB2	19:1:505:CLA:HAA1	2.02	0.40
2:2:156:GLU:O	2:2:160:ILE:HB	2.22	0.40
2:2:170:ASP:HB2	2:2:177:VAL:HG11	2.03	0.40
19:2:510:CLA:H92	19:2:510:CLA:H62	1.85	0.40
5:A:496:HIS:CE1	19:A:834:CLA:NA	2.89	0.40
5:A:602:LEU:HD21	19:A:830:CLA:HBC1	2.04	0.40
19:A:808:CLA:H92	19:A:808:CLA:H62	1.85	0.40
22:A:847:LMG:H352	22:A:847:LMG:H321	1.68	0.40
6:B:583:MET:HE3	6:B:584:LEU:N	2.36	0.40
19:B:814:CLA:C14	19:B:819:CLA:H2	2.50	0.40
12:H:94:THR:HG21	16:L:96:LEU:HD12	2.03	0.40
20:1:512:CHL:OMC	19:1:515:CLA:HAB	2.21	0.40
2:2:105:ALA:O	2:2:109:HIS:HD2	2.04	0.40
19:4:306:CLA:H72	19:4:306:CLA:CHC	2.51	0.40
19:4:310:CLA:H102	19:4:310:CLA:H62	1.82	0.40
22:4:322:LMG:H152	22:4:322:LMG:C35	2.49	0.40
5:A:110:LEU:HD12	5:A:154:ARG:HH11	1.87	0.40
5:A:270:PHE:O	19:K:1001:CLA:HHD	2.22	0.40
5:A:648:THR:HG23	5:A:651:GLY:N	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:833:CLA:H141	19:A:833:CLA:H161	1.69	0.40
6:B:319:HIS:HB3	6:B:322:LEU:HD12	2.04	0.40
6:B:477:LEU:HD13	19:B:833:CLA:HMD2	2.03	0.40
19:B:805:CLA:H162	19:B:805:CLA:H141	1.75	0.40
19:B:811:CLA:H11	19:B:811:CLA:H51	1.89	0.40
19:1:504:CLA:HAC1	19:1:513:CLA:O1A	2.22	0.40
19:1:508:CLA:H11	19:B:840:CLA:HAB	2.04	0.40
3:3:88:GLY:HA3	5:A:21:LEU:HA	2.02	0.40
3:3:223:LEU:HA	3:3:226:LYS:HD2	2.03	0.40
5:A:492:ILE:HD12	19:A:836:CLA:HBA1	2.04	0.40
19:A:854:CLA:H43	6:B:441:ASP:HB3	2.04	0.40
6:B:477:LEU:H	6:B:477:LEU:HG	1.68	0.40
26:B:801:DGD:HD62	26:B:801:DGD:HE2	1.78	0.40
19:B:825:CLA:CMA	18:B:853:BCR:H14C	2.51	0.40
19:B:839:CLA:H162	19:B:839:CLA:H122	1.81	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	191/193 (99%)	184 (96%)	6 (3%)	1 (0%)	24	46
2	2	206/269 (77%)	196 (95%)	9 (4%)	1 (0%)	24	46
3	3	219/275 (80%)	207 (94%)	12 (6%)	0	100	100
4	4	196/198 (99%)	194 (99%)	2 (1%)	0	100	100
5	A	741/758 (98%)	710 (96%)	30 (4%)	1 (0%)	48	70
6	B	731/734 (100%)	710 (97%)	18 (2%)	3 (0%)	30	51
7	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
8	D	141/143 (99%)	135 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	E	64/66 (97%)	60 (94%)	4 (6%)	0	100	100
10	F	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
11	G	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
12	H	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
13	I	28/40 (70%)	27 (96%)	1 (4%)	0	100	100
14	J	40/42 (95%)	37 (92%)	3 (8%)	0	100	100
15	K	73/80 (91%)	67 (92%)	6 (8%)	0	100	100
16	L	155/157 (99%)	149 (96%)	6 (4%)	0	100	100
All	All	3196/3375 (95%)	3075 (96%)	115 (4%)	6 (0%)	43	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	172	LYS
6	B	222	LEU
6	B	559	CYS
2	2	260	ALA
6	B	492	ILE
5	A	342	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	158/158 (100%)	156 (99%)	2 (1%)	61	82
2	2	167/216 (77%)	167 (100%)	0	100	100
3	3	169/213 (79%)	169 (100%)	0	100	100
4	4	164/164 (100%)	164 (100%)	0	100	100
5	A	604/618 (98%)	599 (99%)	5 (1%)	73	88
6	B	598/599 (100%)	591 (99%)	7 (1%)	63	83
7	C	69/70 (99%)	68 (99%)	1 (1%)	59	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	D	122/122 (100%)	122 (100%)	0	100	100
9	E	58/58 (100%)	58 (100%)	0	100	100
10	F	126/127 (99%)	126 (100%)	0	100	100
11	G	82/82 (100%)	81 (99%)	1 (1%)	63	83
12	H	71/71 (100%)	71 (100%)	0	100	100
13	I	26/36 (72%)	26 (100%)	0	100	100
14	J	35/35 (100%)	35 (100%)	0	100	100
15	K	51/58 (88%)	51 (100%)	0	100	100
16	L	124/124 (100%)	123 (99%)	1 (1%)	73	88
All	All	2624/2751 (95%)	2607 (99%)	17 (1%)	78	91

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	75	ARG
1	1	114	LEU
5	A	126	ILE
5	A	331	LEU
5	A	590	CYS
5	A	605	MET
5	A	618	TRP
6	B	157	LEU
6	B	441	ASP
6	B	444	LEU
6	B	477	LEU
6	B	568	CYS
6	B	583	MET
6	B	606	VAL
7	C	65	VAL
11	G	121	VAL
16	L	60	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	228	ASN
2	2	109	HIS
2	2	186	ASN

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Mol	Chain	Res	Type
3	3	174	GLN
4	4	74	ASN
4	4	235	GLN
4	4	243	ASN
5	A	33	GLN
5	A	62	HIS
5	A	222	GLN
5	A	273	ASN
5	A	301	HIS
5	A	303	HIS
5	A	325	HIS
5	A	374	HIS
5	A	445	HIS
5	A	456	HIS
5	A	496	HIS
5	A	545	HIS
5	A	550	HIS
5	A	615	HIS
5	A	721	GLN
6	B	178	HIS
6	B	196	HIS
6	B	266	GLN
6	B	368	GLN
6	B	452	GLN
8	D	168	HIS
9	E	119	ASN
10	F	193	GLN
11	G	95	GLN
12	H	82	GLN
15	K	52	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 242 ligands modelled in this entry, 2 are monoatomic - leaving 240 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$
19	CLA	A	810	-	54,58,73	1.55	10 (18%)	64,95,113	1.96	13 (20%)
19	CLA	A	808	5	69,73,73	1.35	6 (8%)	82,113,113	1.78	13 (15%)
23	XAT	4	303	-	41,47,47	0.60	0	54,74,74	2.50	12 (22%)
19	CLA	3	316	-	50,54,73	1.61	9 (18%)	59,90,113	1.95	12 (20%)
22	LMG	G	206	-	50,50,55	1.18	5 (10%)	58,58,63	1.08	3 (5%)
18	BCR	A	849	-	41,41,41	0.65	0	56,56,56	3.37	16 (28%)
19	CLA	A	830	-	69,73,73	1.36	7 (10%)	82,113,113	1.71	16 (19%)
18	BCR	B	849	-	41,41,41	0.77	0	56,56,56	3.81	21 (37%)
19	CLA	B	825	31	69,73,73	1.36	7 (10%)	82,113,113	1.82	17 (20%)
19	CLA	A	839	-	69,73,73	1.35	6 (8%)	82,113,113	1.64	12 (14%)
19	CLA	3	308	-	69,73,73	1.38	8 (11%)	82,113,113	1.76	16 (19%)
19	CLA	B	839	-	69,73,73	1.37	6 (8%)	82,113,113	1.70	14 (17%)
17	LUT	2	501	-	42,43,43	2.44	1 (2%)	51,60,60	1.60	9 (17%)
22	LMG	F	305	-	36,36,55	0.78	1 (2%)	44,44,63	1.11	3 (6%)
19	CLA	B	830	-	69,73,73	1.36	9 (13%)	82,113,113	1.70	13 (15%)
19	CLA	A	828	-	69,73,73	1.35	7 (10%)	82,113,113	1.80	13 (15%)
19	CLA	4	304	4	64,68,73	1.44	7 (10%)	76,107,113	1.94	18 (23%)
19	CLA	B	835	-	59,63,73	1.46	7 (11%)	70,101,113	1.78	13 (18%)
19	CLA	4	309	-	54,58,73	1.51	7 (12%)	64,95,113	1.99	16 (25%)
22	LMG	G	210	-	25,25,55	0.55	0	33,33,63	1.19	4 (12%)
19	CLA	K	1002	-	64,68,73	1.43	8 (12%)	76,107,113	1.80	15 (19%)
19	CLA	K	1003	-	27,35,73	2.10	9 (33%)	32,60,113	2.18	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	836	-	55,59,73	1.53	7 (12%)	64,96,113	1.90	14 (21%)
18	BCR	A	856	-	41,41,41	0.69	0	56,56,56	3.37	13 (23%)
18	BCR	B	802	-	41,41,41	0.70	0	56,56,56	4.08	18 (32%)
22	LMG	2	520	-	13,13,55	0.59	0	18,18,63	0.87	1 (5%)
18	BCR	B	852	-	41,41,41	0.62	0	56,56,56	3.02	14 (25%)
19	CLA	B	804	-	69,73,73	1.38	7 (10%)	82,113,113	1.83	15 (18%)
22	LMG	J	1104	-	34,34,55	0.47	0	42,42,63	1.23	5 (11%)
29	PQN	B	841	-	34,34,34	0.38	0	43,45,45	1.14	3 (6%)
19	CLA	A	816	-	50,54,73	1.60	7 (14%)	59,90,113	1.95	13 (22%)
19	CLA	A	842	21	64,68,73	1.41	8 (12%)	76,107,113	1.81	15 (19%)
19	CLA	2	507	2	69,73,73	1.37	6 (8%)	82,113,113	1.78	14 (17%)
19	CLA	A	806	5	69,73,73	1.36	7 (10%)	82,113,113	1.70	14 (17%)
19	CLA	B	806	-	69,73,73	1.34	5 (7%)	82,113,113	1.72	13 (15%)
19	CLA	F	302	-	69,73,73	1.39	9 (13%)	82,113,113	1.72	16 (19%)
19	CLA	A	821	-	69,73,73	1.36	6 (8%)	82,113,113	1.63	14 (17%)
19	CLA	B	821	-	50,54,73	1.60	7 (14%)	59,90,113	1.95	12 (20%)
20	CHL	1	512	-	41,55,74	1.62	8 (19%)	35,91,114	2.01	11 (31%)
22	LMG	2	518	-	25,25,55	0.60	0	33,33,63	1.02	3 (9%)
19	CLA	2	506	-	69,73,73	1.38	8 (11%)	82,113,113	1.82	16 (19%)
19	CLA	B	828	-	69,73,73	1.34	8 (11%)	82,113,113	1.70	12 (14%)
19	CLA	H	1000	-	64,68,73	1.43	8 (12%)	76,107,113	1.78	14 (18%)
18	BCR	G	205	-	41,41,41	0.74	0	56,56,56	3.17	11 (19%)
19	CLA	3	309	-	59,63,73	1.51	8 (13%)	70,101,113	1.84	15 (21%)
19	CLA	A	814	-	69,73,73	1.38	8 (11%)	82,113,113	1.77	15 (18%)
19	CLA	B	838	31	69,73,73	1.37	6 (8%)	82,113,113	1.70	16 (19%)
24	LMT	2	523	-	36,36,36	1.10	4 (11%)	47,47,47	1.01	2 (4%)
19	CLA	G	203	11	50,54,73	1.62	8 (16%)	59,90,113	1.89	11 (18%)
19	CLA	4	308	4	64,68,73	1.40	6 (9%)	76,107,113	1.87	15 (19%)
18	BCR	I	102	-	41,41,41	0.67	0	56,56,56	3.21	13 (23%)
19	CLA	B	824	31	69,73,73	1.36	8 (11%)	82,113,113	1.84	15 (18%)
21	LHG	1	520	-	41,41,48	0.45	0	44,47,54	1.17	4 (9%)
19	CLA	G	202	-	59,63,73	1.50	8 (13%)	70,101,113	1.82	15 (21%)
21	LHG	A	853	-	48,48,48	0.40	0	51,54,54	1.06	3 (5%)
19	CLA	A	827	-	69,73,73	1.37	8 (11%)	82,113,113	1.73	15 (18%)
22	LMG	2	522	-	13,13,55	0.58	0	18,18,63	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	1	511	-	50,54,73	1.60	7 (14%)	59,90,113	1.91	12 (20%)
19	CLA	A	819	-	69,73,73	1.36	7 (10%)	82,113,113	1.69	13 (15%)
22	LMG	2	525	-	13,13,55	0.63	0	18,18,63	0.70	0
19	CLA	2	509	-	54,58,73	1.53	6 (11%)	64,95,113	1.83	12 (18%)
22	LMG	F	304	-	47,47,55	1.08	4 (8%)	55,55,63	1.10	2 (3%)
22	LMG	2	519	-	36,36,55	0.71	1 (2%)	44,44,63	1.25	7 (15%)
22	LMG	4	322	-	45,45,55	1.04	4 (8%)	53,53,63	1.09	4 (7%)
19	CLA	A	820	-	54,58,73	1.56	8 (14%)	64,95,113	1.90	13 (20%)
19	CLA	A	840	31	69,73,73	1.34	7 (10%)	82,113,113	1.75	14 (17%)
19	CLA	B	840	21	69,73,73	1.37	6 (8%)	82,113,113	1.71	14 (17%)
19	CLA	B	818	-	69,73,73	1.37	8 (11%)	82,113,113	1.70	15 (18%)
20	CHL	1	521	1	50,64,74	1.53	8 (16%)	46,102,114	2.04	11 (23%)
19	CLA	A	829	-	69,73,73	1.35	7 (10%)	82,113,113	1.71	14 (17%)
19	CLA	B	829	-	69,73,73	1.39	8 (11%)	82,113,113	1.66	11 (13%)
19	CLA	2	508	-	59,63,73	1.45	7 (11%)	70,101,113	1.90	16 (22%)
19	CLA	A	813	-	69,73,73	1.34	7 (10%)	82,113,113	1.78	16 (19%)
19	CLA	A	835	5	59,63,73	1.50	8 (13%)	70,101,113	1.80	14 (20%)
19	CLA	1	508	-	69,73,73	1.37	7 (10%)	82,113,113	1.74	13 (15%)
19	CLA	A	825	31	69,73,73	1.40	8 (11%)	82,113,113	1.78	13 (15%)
22	LMG	2	521	-	13,13,55	0.60	0	18,18,63	0.76	0
18	BCR	B	851	-	41,41,41	0.68	0	56,56,56	2.72	15 (26%)
19	CLA	3	306	-	56,60,73	1.52	7 (12%)	65,97,113	1.89	13 (20%)
22	LMG	B	845	-	33,33,55	0.58	1 (3%)	41,41,63	1.25	5 (12%)
19	CLA	J	1102	31	49,53,73	1.59	7 (14%)	58,89,113	1.96	12 (20%)
20	CHL	2	526	2	60,74,74	1.44	9 (15%)	58,114,114	1.70	12 (20%)
22	LMG	A	847	-	50,50,55	1.16	5 (10%)	58,58,63	0.99	2 (3%)
19	CLA	A	822	-	64,68,73	1.44	7 (10%)	76,107,113	1.77	15 (19%)
24	LMT	A	846	-	36,36,36	1.12	4 (11%)	47,47,47	1.14	2 (4%)
19	CLA	B	827	-	69,73,73	1.35	8 (11%)	82,113,113	1.74	13 (15%)
19	CLA	4	307	4	64,68,73	1.41	7 (10%)	76,107,113	1.82	15 (19%)
24	LMT	B	847	-	33,33,36	1.19	4 (12%)	44,44,47	0.97	1 (2%)
19	CLA	1	507	1	69,73,73	1.37	7 (10%)	82,113,113	1.77	14 (17%)
19	CLA	B	826	-	69,73,73	1.39	9 (13%)	82,113,113	1.72	13 (15%)
21	LHG	A	845	19	39,39,48	0.43	0	42,45,54	1.27	4 (9%)
22	LMG	4	321	-	13,13,55	0.57	0	18,18,63	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	3	313	3	64,68,73	1.42	7 (10%)	76,107,113	1.78	15 (19%)
17	LUT	J	1109	-	42,43,43	2.37	1 (2%)	51,60,60	1.95	6 (11%)
19	CLA	3	310	31	54,58,73	1.52	7 (12%)	64,95,113	2.10	14 (21%)
19	CLA	3	317	-	50,54,73	1.61	8 (16%)	59,90,113	1.90	13 (22%)
19	CLA	B	832	-	62,66,73	1.43	6 (9%)	73,104,113	1.86	16 (21%)
19	CLA	4	310	-	64,68,73	1.43	9 (14%)	76,107,113	1.76	13 (17%)
20	CHL	4	313	-	41,55,74	1.82	8 (19%)	35,91,114	2.16	11 (31%)
22	LMG	2	524	-	13,13,55	0.57	0	18,18,63	0.82	0
19	CLA	3	307	-	59,63,73	1.48	7 (11%)	70,101,113	1.92	18 (25%)
19	CLA	4	311	-	50,54,73	1.60	6 (12%)	59,90,113	1.95	11 (18%)
18	BCR	L	306	-	41,41,41	0.69	0	56,56,56	3.09	11 (19%)
19	CLA	A	823	-	64,68,73	1.44	8 (12%)	76,107,113	1.75	15 (19%)
19	CLA	B	813	-	50,54,73	1.62	7 (14%)	59,90,113	1.96	13 (22%)
26	DGD	G	207	-	48,48,67	0.62	1 (2%)	62,62,81	1.07	4 (6%)
28	SF4	C	102	7	0,12,12	-	-	-	-	-
28	SF4	C	101	7	0,12,12	-	-	-	-	-
18	BCR	J	1108	-	41,41,41	0.62	0	56,56,56	2.96	14 (25%)
19	CLA	1	516	1	64,68,73	1.44	7 (10%)	76,107,113	1.79	16 (21%)
19	CLA	2	514	2	59,63,73	1.47	7 (11%)	70,101,113	1.85	12 (17%)
19	CLA	B	836	-	69,73,73	1.36	6 (8%)	82,113,113	1.65	13 (15%)
21	LHG	B	843	-	48,48,48	0.40	0	51,54,54	1.02	2 (3%)
19	CLA	G	204	31	69,73,73	1.35	8 (11%)	82,113,113	1.79	15 (18%)
30	ZEX	F	301	-	43,43,43	0.68	0	51,60,60	1.82	9 (17%)
19	CLA	B	810	6	69,73,73	1.36	7 (10%)	82,113,113	1.72	13 (15%)
24	LMT	G	208	-	36,36,36	1.13	4 (11%)	47,47,47	0.99	2 (4%)
18	BCR	1	503	-	19,19,41	0.68	0	26,26,56	3.30	9 (34%)
18	BCR	A	850	-	41,41,41	0.66	0	56,56,56	3.29	14 (25%)
18	BCR	A	851	-	41,41,41	0.68	0	56,56,56	3.31	14 (25%)
19	CLA	4	305	4	54,58,73	1.57	8 (14%)	64,95,113	1.94	16 (25%)
19	CLA	L	303	16	54,58,73	1.53	7 (12%)	64,95,113	1.92	13 (20%)
19	CLA	G	201	-	69,73,73	1.37	7 (10%)	82,113,113	1.81	17 (20%)
24	LMT	B	846	-	36,36,36	1.11	5 (13%)	47,47,47	1.05	3 (6%)
18	BCR	L	302	-	41,41,41	0.83	0	56,56,56	3.25	14 (25%)
19	CLA	A	817	-	69,73,73	1.37	6 (8%)	82,113,113	1.64	13 (15%)
19	CLA	A	854	31	69,73,73	1.34	7 (10%)	82,113,113	1.78	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	1	515	-	49,53,73	1.64	8 (16%)	58,89,113	1.84	10 (17%)
17	LUT	4	302	-	42,43,43	2.55	1 (2%)	51,60,60	1.72	10 (19%)
19	CLA	B	834	31	59,63,73	1.49	8 (13%)	70,101,113	1.81	15 (21%)
18	BCR	B	856	-	41,41,41	0.67	0	56,56,56	3.14	14 (25%)
19	CLA	L	304	-	64,68,73	1.40	6 (9%)	76,107,113	1.79	14 (18%)
19	CLA	A	812	-	59,63,73	1.48	7 (11%)	70,101,113	1.83	15 (21%)
19	CLA	3	312	-	52,56,73	1.58	8 (15%)	61,92,113	2.01	16 (26%)
19	CLA	B	817	-	64,68,73	1.43	8 (12%)	76,107,113	1.80	13 (17%)
19	CLA	L	305	31	54,58,73	1.57	9 (16%)	64,95,113	1.86	15 (23%)
18	BCR	A	848	-	41,41,41	0.65	0	56,56,56	3.36	18 (32%)
18	BCR	3	304	-	41,41,41	0.70	0	56,56,56	3.51	13 (23%)
19	CLA	4	315	4	69,73,73	1.37	7 (10%)	82,113,113	1.72	14 (17%)
19	CLA	A	833	-	69,73,73	1.36	9 (13%)	82,113,113	1.73	16 (19%)
20	CHL	2	515	-	40,54,74	1.61	8 (20%)	34,90,114	2.18	10 (29%)
21	LHG	1	517	-	48,48,48	0.42	0	51,54,54	1.11	4 (7%)
19	CLA	A	841	-	69,73,73	1.37	8 (11%)	82,113,113	1.68	15 (18%)
19	CLA	B	823	-	59,63,73	1.49	7 (11%)	70,101,113	1.83	11 (15%)
19	CLA	2	505	2	56,60,73	1.52	8 (14%)	65,97,113	1.90	15 (23%)
19	CLA	A	818	-	60,64,73	1.48	9 (15%)	71,102,113	1.79	14 (19%)
19	CLA	A	809	5	69,73,73	1.35	7 (10%)	82,113,113	1.73	15 (18%)
18	BCR	B	850	-	41,41,41	0.67	0	56,56,56	3.09	11 (19%)
19	CLA	3	315	3	54,58,73	1.52	6 (11%)	64,95,113	1.90	13 (20%)
19	CLA	A	826	31	59,63,73	1.48	7 (11%)	70,101,113	1.84	15 (21%)
17	LUT	1	501	-	42,43,43	2.49	2 (4%)	51,60,60	1.42	9 (17%)
18	BCR	I	101	-	41,41,41	0.74	0	56,56,56	3.57	16 (28%)
20	CHL	4	317	4	37,51,74	1.91	8 (21%)	30,86,114	2.10	9 (30%)
18	BCR	L	307	-	41,41,41	0.71	0	56,56,56	3.42	15 (26%)
19	CLA	4	306	-	69,73,73	1.39	7 (10%)	82,113,113	1.74	17 (20%)
19	CLA	A	838	-	69,73,73	1.38	6 (8%)	82,113,113	1.72	15 (18%)
17	LUT	1	502	-	42,43,43	2.46	1 (2%)	51,60,60	1.66	7 (13%)
29	PQN	A	844	-	34,34,34	0.41	0	43,45,45	1.26	5 (11%)
26	DGD	B	801	-	42,42,67	0.62	0	56,56,81	1.17	6 (10%)
19	CLA	B	819	-	69,73,73	1.34	6 (8%)	82,113,113	1.74	15 (18%)
19	CLA	A	834	-	69,73,73	1.34	6 (8%)	82,113,113	1.69	14 (17%)
19	CLA	B	837	-	54,58,73	1.53	8 (14%)	64,95,113	1.82	14 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	2	503	-	41,41,41	0.89	1 (2%)	56,56,56	3.32	14 (25%)
19	CLA	B	833	-	64,68,73	1.41	8 (12%)	76,107,113	1.73	11 (14%)
26	DGD	4	319	-	52,52,67	0.80	2 (3%)	66,66,81	1.42	9 (13%)
19	CLA	A	804	-	69,73,73	1.34	8 (11%)	82,113,113	1.77	13 (15%)
26	DGD	B	854	-	62,62,67	1.09	5 (8%)	76,76,81	1.01	3 (3%)
19	CLA	B	807	6	69,73,73	1.36	6 (8%)	82,113,113	1.69	14 (17%)
19	CLA	A	831	-	69,73,73	1.37	6 (8%)	82,113,113	1.70	14 (17%)
19	CLA	B	831	-	64,68,73	1.41	8 (12%)	76,107,113	1.71	14 (18%)
19	CLA	B	822	-	69,73,73	1.37	7 (10%)	82,113,113	1.75	14 (17%)
19	CLA	J	1101	-	69,73,73	1.35	6 (8%)	82,113,113	1.80	15 (18%)
19	CLA	4	312	4	54,58,73	1.53	7 (12%)	64,95,113	1.95	16 (25%)
19	CLA	4	318	-	69,73,73	1.34	7 (10%)	82,113,113	1.75	15 (18%)
19	CLA	A	803	31	69,73,73	1.35	8 (11%)	82,113,113	1.74	13 (15%)
18	BCR	A	852	-	41,41,41	0.64	0	56,56,56	2.98	14 (25%)
18	BCR	B	853	-	41,41,41	0.64	0	56,56,56	3.13	14 (25%)
20	CHL	1	514	1	55,69,74	1.48	8 (14%)	52,108,114	1.73	10 (19%)
19	CLA	A	824	-	69,73,73	1.36	6 (8%)	82,113,113	1.67	14 (17%)
19	CLA	K	1001	-	49,53,73	1.63	8 (16%)	58,89,113	1.99	14 (24%)
19	CLA	L	301	-	59,63,73	1.48	7 (11%)	70,101,113	1.83	15 (21%)
19	CLA	1	506	-	59,63,73	1.47	7 (11%)	70,101,113	1.88	15 (21%)
19	CLA	3	311	-	45,49,73	1.70	8 (17%)	54,84,113	2.00	15 (27%)
22	LMG	B	844	-	35,35,55	0.80	1 (2%)	43,43,63	1.09	3 (6%)
19	CLA	B	816	-	59,63,73	1.49	7 (11%)	70,101,113	1.84	13 (18%)
19	CLA	B	811	-	69,73,73	1.39	9 (13%)	82,113,113	1.74	15 (18%)
19	CLA	F	303	10	69,73,73	1.35	6 (8%)	82,113,113	1.72	14 (17%)
19	CLA	A	805	-	69,73,73	1.36	7 (10%)	82,113,113	1.73	13 (15%)
26	DGD	J	1106	-	59,59,67	1.02	4 (6%)	73,73,81	1.06	4 (5%)
19	CLA	2	504	2	64,68,73	1.42	7 (10%)	76,107,113	1.88	15 (19%)
19	CLA	1	505	1	50,54,73	1.60	8 (16%)	59,90,113	1.93	13 (22%)
19	CLA	1	509	-	54,58,73	1.54	7 (12%)	64,95,113	1.91	17 (26%)
19	CLA	A	855	-	69,73,73	1.35	8 (11%)	82,113,113	1.72	15 (18%)
22	LMG	1	519	-	13,13,55	0.56	0	18,18,63	0.90	1 (5%)
23	XAT	2	502	-	41,47,47	0.63	0	54,74,74	1.70	11 (20%)
19	CLA	B	814	-	69,73,73	1.37	8 (11%)	82,113,113	1.72	14 (17%)
22	LMG	J	1103	-	30,30,55	0.52	0	38,38,63	1.06	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	815	-	49,53,73	1.64	7 (14%)	58,89,113	1.89	14 (24%)
24	LMT	G	209	-	32,32,36	1.21	5 (15%)	43,43,47	0.98	1 (2%)
19	CLA	1	513	-	69,73,73	1.36	6 (8%)	82,113,113	1.74	15 (18%)
19	CLA	B	815	-	69,73,73	1.36	6 (8%)	82,113,113	1.76	12 (14%)
24	LMT	B	855	-	32,32,36	1.21	6 (18%)	43,43,47	0.98	2 (4%)
19	CLA	A	832	-	69,73,73	1.37	6 (8%)	82,113,113	1.68	12 (14%)
19	CLA	3	305	-	59,63,73	1.48	8 (13%)	70,101,113	1.97	17 (24%)
28	SF4	A	843	6,5	0,12,12	-	-	-		
19	CLA	B	805	-	69,73,73	1.36	8 (11%)	82,113,113	1.70	12 (14%)
19	CLA	1	510	-	50,54,73	1.64	7 (14%)	59,90,113	2.25	14 (23%)
19	CLA	J	1105	-	54,58,73	1.56	7 (12%)	64,95,113	2.17	18 (28%)
19	CLA	B	812	-	64,68,73	1.43	8 (12%)	76,107,113	1.71	14 (18%)
17	LUT	3	301	-	42,43,43	2.51	1 (2%)	51,60,60	1.45	6 (11%)
19	CLA	B	803	-	69,73,73	1.36	6 (8%)	82,113,113	1.71	10 (12%)
17	LUT	3	302	-	42,43,43	2.40	1 (2%)	51,60,60	1.46	9 (17%)
19	CLA	B	808	-	69,73,73	1.38	7 (10%)	82,113,113	1.68	14 (17%)
20	CHL	4	314	31	45,59,74	2.01	8 (17%)	40,96,114	2.18	14 (35%)
21	LHG	2	517	19	34,34,48	0.46	0	37,40,54	1.08	2 (5%)
19	CLA	B	820	31	69,73,73	1.37	7 (10%)	82,113,113	1.63	14 (17%)
18	BCR	F	306	-	41,41,41	0.66	0	56,56,56	3.13	9 (16%)
19	CLA	A	807	-	64,68,73	1.45	8 (12%)	76,107,113	1.76	13 (17%)
20	CHL	2	513	-	42,56,74	1.70	9 (21%)	36,92,114	2.02	10 (27%)
18	BCR	4	301	-	41,41,41	0.67	0	56,56,56	3.43	16 (28%)
19	CLA	A	811	-	69,73,73	1.35	6 (8%)	82,113,113	1.76	15 (18%)
24	LMT	4	320	-	36,36,36	1.13	4 (11%)	47,47,47	0.96	3 (6%)
19	CLA	2	511	-	54,58,73	1.54	7 (12%)	64,95,113	1.96	16 (25%)
19	CLA	A	802	-	69,73,73	1.33	8 (11%)	82,113,113	1.76	18 (21%)
20	CHL	4	316	-	55,69,74	1.55	10 (18%)	52,108,114	1.76	11 (21%)
24	LMT	3	318	-	32,32,36	1.14	3 (9%)	43,43,47	1.20	5 (11%)
19	CLA	1	504	1	69,73,73	1.37	7 (10%)	82,113,113	1.76	17 (20%)
19	CLA	2	510	21	64,68,73	1.43	8 (12%)	76,107,113	1.77	13 (17%)
19	CLA	A	837	-	69,73,73	1.37	8 (11%)	82,113,113	1.70	14 (17%)
27	CL0	A	801	-	58,73,73	2.42	7 (12%)	60,113,113	2.78	18 (30%)
24	LMT	J	1107	-	26,26,36	1.30	4 (15%)	37,37,47	1.09	2 (5%)
18	BCR	3	303	-	41,41,41	0.66	0	56,56,56	3.29	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	809	-	69,73,73	1.37	8 (11%)	82,113,113	1.69	13 (15%)
20	CHL	2	512	-	41,55,74	2.27	10 (24%)	35,91,114	2.15	12 (34%)
20	CHL	2	516	2	50,64,74	1.46	8 (16%)	46,102,114	1.97	13 (28%)
20	CHL	3	314	-	41,55,74	1.75	8 (19%)	35,91,114	1.98	10 (28%)
19	CLA	K	1004	-	27,35,73	2.09	9 (33%)	32,60,113	2.08	6 (18%)
21	LHG	B	842	19	20,20,48	0.59	0	23,26,54	1.59	3 (13%)
18	BCR	K	1005	-	41,41,41	0.70	0	56,56,56	3.26	12 (21%)
22	LMG	1	518	-	46,46,55	1.03	3 (6%)	54,54,63	1.04	2 (3%)

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
19	CLA	A	810	-	1/1/12/20	6/21/97/115	-
19	CLA	A	808	5	1/1/15/20	19/39/115/115	-
23	XAT	4	303	-	2/2/12/26	0/31/93/93	0/4/4/4
19	CLA	3	316	-	1/1/11/20	9/17/93/115	-
22	LMG	G	206	-	-	17/45/65/70	0/1/1/1
18	BCR	A	849	-	-	11/29/63/63	0/2/2/2
19	CLA	A	830	-	1/1/15/20	14/39/115/115	-
19	CLA	B	825	31	1/1/15/20	22/39/115/115	-
18	BCR	B	849	-	-	10/29/63/63	0/2/2/2
19	CLA	A	839	-	1/1/15/20	10/39/115/115	-
19	CLA	3	308	-	1/1/15/20	18/39/115/115	-
19	CLA	B	839	-	1/1/15/20	20/39/115/115	-
17	LUT	2	501	-	1/1/12/27	5/29/67/67	0/2/2/2
22	LMG	F	305	-	-	10/31/51/70	0/1/1/1
19	CLA	B	830	-	-	12/39/115/115	-
19	CLA	A	828	-	1/1/15/20	20/39/115/115	-
19	CLA	4	304	4	1/1/14/20	10/33/109/115	-
19	CLA	B	835	-	-	13/27/103/115	-
19	CLA	4	309	-	1/1/12/20	9/21/97/115	-
22	LMG	G	210	-	-	10/20/40/70	0/1/1/1
19	CLA	K	1002	-	1/1/14/20	19/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	K	1003	-	1/1/5/20	-	-
19	CLA	A	836	-	-	7/23/99/115	-
18	BCR	K	1005	-	-	12/29/63/63	0/2/2/2
18	BCR	A	856	-	-	13/29/63/63	0/2/2/2
18	BCR	B	802	-	-	5/29/63/63	0/2/2/2
22	LMG	2	520	-	-	0/4/24/70	0/1/1/1
19	CLA	B	804	-	1/1/15/20	10/39/115/115	-
18	BCR	B	852	-	-	11/29/63/63	0/2/2/2
22	LMG	J	1104	-	-	11/29/49/70	0/1/1/1
29	PQN	B	841	-	-	12/23/43/43	0/2/2/2
19	CLA	A	816	-	1/1/11/20	10/17/93/115	-
19	CLA	A	842	21	1/1/14/20	10/33/109/115	-
19	CLA	2	507	2	1/1/15/20	12/39/115/115	-
19	CLA	A	806	5	1/1/15/20	21/39/115/115	-
19	CLA	B	806	-	1/1/15/20	15/39/115/115	-
19	CLA	F	302	-	1/1/15/20	13/39/115/115	-
19	CLA	A	821	-	1/1/15/20	17/39/115/115	-
19	CLA	B	821	-	1/1/11/20	8/17/93/115	-
20	CHL	1	512	-	3/3/16/26	3/17/115/137	-
22	LMG	2	518	-	-	6/20/40/70	0/1/1/1
19	CLA	2	506	-	1/1/15/20	12/39/115/115	-
19	CLA	B	828	-	1/1/15/20	18/39/115/115	-
19	CLA	H	1000	-	1/1/14/20	8/33/109/115	-
18	BCR	G	205	-	-	10/29/63/63	0/2/2/2
19	CLA	3	309	-	-	11/27/103/115	-
19	CLA	A	814	-	1/1/15/20	16/39/115/115	-
19	CLA	B	838	31	1/1/15/20	12/39/115/115	-
24	LMT	2	523	-	-	10/21/61/61	0/2/2/2
19	CLA	G	203	11	1/1/11/20	6/17/93/115	-
19	CLA	4	308	4	-	13/33/109/115	-
19	CLA	B	824	31	1/1/15/20	15/39/115/115	-
18	BCR	I	102	-	-	14/29/63/63	0/2/2/2
21	LHG	1	520	-	-	23/46/46/53	-
19	CLA	G	202	-	-	11/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LHG	A	853	-	-	30/53/53/53	-
19	CLA	A	827	-	1/1/15/20	14/39/115/115	-
22	LMG	2	522	-	-	4/4/24/70	0/1/1/1
19	CLA	1	511	-	1/1/11/20	9/17/93/115	-
19	CLA	A	819	-	1/1/15/20	13/39/115/115	-
22	LMG	2	525	-	-	0/4/24/70	0/1/1/1
19	CLA	2	509	-	1/1/12/20	9/21/97/115	-
22	LMG	F	304	-	-	10/42/62/70	0/1/1/1
22	LMG	2	519	-	-	17/31/51/70	0/1/1/1
22	LMG	4	322	-	-	14/40/60/70	0/1/1/1
19	CLA	A	820	-	1/1/12/20	8/21/97/115	-
19	CLA	A	840	31	1/1/15/20	16/39/115/115	-
19	CLA	B	840	21	-	16/39/115/115	-
19	CLA	B	818	-	1/1/15/20	18/39/115/115	-
20	CHL	1	521	1	4/4/18/26	6/27/125/137	-
19	CLA	A	829	-	1/1/15/20	19/39/115/115	-
19	CLA	B	829	-	1/1/15/20	18/39/115/115	-
19	CLA	2	508	-	1/1/13/20	7/27/103/115	-
19	CLA	A	813	-	1/1/15/20	9/39/115/115	-
19	CLA	A	835	5	1/1/13/20	8/27/103/115	-
19	CLA	A	825	31	1/1/15/20	15/39/115/115	-
19	CLA	1	508	-	-	20/39/115/115	-
22	LMG	2	521	-	-	0/4/24/70	0/1/1/1
18	BCR	B	851	-	-	11/29/63/63	0/2/2/2
19	CLA	3	306	-	1/1/12/20	8/24/100/115	-
22	LMG	B	845	-	-	12/28/48/70	0/1/1/1
19	CLA	J	1102	31	1/1/11/20	2/15/91/115	-
20	CHL	2	526	2	4/4/20/26	8/39/137/137	-
22	LMG	A	847	-	-	16/45/65/70	0/1/1/1
19	CLA	A	822	-	1/1/14/20	14/33/109/115	-
24	LMT	A	846	-	-	8/21/61/61	0/2/2/2
19	CLA	B	827	-	1/1/15/20	15/39/115/115	-
19	CLA	4	307	4	1/1/14/20	15/33/109/115	-
24	LMT	B	847	-	-	6/18/58/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	1	507	1	1/1/15/20	13/39/115/115	-
19	CLA	B	826	-	1/1/15/20	5/39/115/115	-
21	LHG	A	845	19	-	25/44/44/53	-
22	LMG	4	321	-	-	0/4/24/70	0/1/1/1
19	CLA	3	313	3	1/1/14/20	16/33/109/115	-
17	LUT	J	1109	-	1/1/12/27	6/29/67/67	0/2/2/2
19	CLA	3	310	31	1/1/12/20	8/21/97/115	-
19	CLA	3	317	-	1/1/11/20	6/17/93/115	-
19	CLA	B	832	-	1/1/13/20	11/31/107/115	-
19	CLA	4	310	-	1/1/14/20	11/33/109/115	-
20	CHL	4	313	-	3/3/16/26	2/17/115/137	-
22	LMG	2	524	-	-	1/4/24/70	0/1/1/1
19	CLA	3	307	-	1/1/13/20	11/27/103/115	-
19	CLA	4	311	-	1/1/11/20	5/17/93/115	-
19	CLA	B	813	-	1/1/11/20	3/17/93/115	-
19	CLA	A	823	-	1/1/14/20	14/33/109/115	-
18	BCR	L	306	-	-	7/29/63/63	0/2/2/2
26	DGD	G	207	-	-	10/36/76/95	0/2/2/2
28	SF4	C	102	7	-	-	0/6/5/5
28	SF4	C	101	7	-	-	0/6/5/5
19	CLA	2	514	2	1/1/13/20	7/27/103/115	-
19	CLA	1	516	1	1/1/14/20	12/33/109/115	-
19	CLA	B	836	-	1/1/15/20	9/39/115/115	-
18	BCR	J	1108	-	-	8/29/63/63	0/2/2/2
21	LHG	B	843	-	-	27/53/53/53	-
19	CLA	G	204	31	1/1/15/20	19/39/115/115	-
30	ZEX	F	301	-	-	1/29/67/67	0/2/2/2
19	CLA	B	810	6	1/1/15/20	12/39/115/115	-
24	LMT	G	208	-	-	9/21/61/61	0/2/2/2
18	BCR	1	503	-	-	7/11/28/63	0/1/1/2
18	BCR	A	850	-	-	4/29/63/63	0/2/2/2
18	BCR	A	851	-	-	13/29/63/63	0/2/2/2
19	CLA	4	305	4	1/1/12/20	7/21/97/115	-
19	CLA	L	303	16	1/1/12/20	9/21/97/115	-
19	CLA	G	201	-	1/1/15/20	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LMT	B	846	-	-	11/21/61/61	0/2/2/2
19	CLA	A	817	-	1/1/15/20	16/39/115/115	-
18	BCR	L	302	-	-	6/29/63/63	0/2/2/2
19	CLA	A	854	31	1/1/15/20	15/39/115/115	-
19	CLA	1	515	-	1/1/11/20	5/15/91/115	-
17	LUT	4	302	-	-	2/29/67/67	0/2/2/2
19	CLA	B	834	31	1/1/13/20	12/27/103/115	-
19	CLA	L	304	-	1/1/14/20	9/33/109/115	-
18	BCR	B	856	-	-	13/29/63/63	0/2/2/2
19	CLA	A	812	-	-	11/27/103/115	-
19	CLA	3	312	-	1/1/11/20	6/19/95/115	-
19	CLA	B	817	-	1/1/14/20	7/33/109/115	-
19	CLA	L	305	31	1/1/12/20	8/21/97/115	-
18	BCR	A	848	-	-	10/29/63/63	0/2/2/2
19	CLA	4	315	4	1/1/15/20	16/39/115/115	-
19	CLA	A	833	-	1/1/15/20	19/39/115/115	-
20	CHL	2	515	-	3/3/16/26	4/15/113/137	-
18	BCR	3	304	-	-	16/29/63/63	0/2/2/2
21	LHG	1	517	-	-	26/53/53/53	-
19	CLA	A	841	-	1/1/15/20	6/39/115/115	-
19	CLA	B	823	-	1/1/13/20	13/27/103/115	-
19	CLA	2	505	2	1/1/12/20	8/24/100/115	-
19	CLA	A	818	-	1/1/13/20	14/29/105/115	-
19	CLA	A	809	5	1/1/15/20	17/39/115/115	-
19	CLA	A	826	31	1/1/13/20	11/27/103/115	-
19	CLA	3	315	3	1/1/12/20	7/21/97/115	-
18	BCR	B	850	-	-	10/29/63/63	0/2/2/2
17	LUT	1	501	-	-	4/29/67/67	0/2/2/2
20	CHL	4	317	4	3/3/15/26	0/12/110/137	-
18	BCR	L	307	-	-	11/29/63/63	0/2/2/2
19	CLA	4	306	-	1/1/15/20	16/39/115/115	-
19	CLA	A	838	-	1/1/15/20	12/39/115/115	-
17	LUT	1	502	-	1/1/12/27	8/29/67/67	0/2/2/2
29	PQN	A	844	-	-	7/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	DGD	B	801	-	-	21/30/70/95	0/2/2/2
19	CLA	B	819	-	1/1/15/20	18/39/115/115	-
19	CLA	B	837	-	1/1/12/20	5/21/97/115	-
19	CLA	A	834	-	-	19/39/115/115	-
19	CLA	B	833	-	1/1/14/20	10/33/109/115	-
18	BCR	2	503	-	-	11/29/63/63	0/2/2/2
26	DGD	4	319	-	-	17/40/80/95	0/2/2/2
19	CLA	A	804	-	1/1/15/20	22/39/115/115	-
26	DGD	B	854	-	-	19/50/90/95	0/2/2/2
19	CLA	B	807	6	1/1/15/20	13/39/115/115	-
19	CLA	A	831	-	1/1/15/20	12/39/115/115	-
19	CLA	B	831	-	1/1/14/20	16/33/109/115	-
19	CLA	B	822	-	1/1/15/20	18/39/115/115	-
19	CLA	J	1101	-	1/1/15/20	13/39/115/115	-
19	CLA	4	312	4	-	7/21/97/115	-
19	CLA	4	318	-	1/1/15/20	11/39/115/115	-
19	CLA	A	803	31	1/1/15/20	7/39/115/115	-
18	BCR	A	852	-	-	11/29/63/63	0/2/2/2
20	CHL	1	514	1	4/4/19/26	8/33/131/137	-
18	BCR	B	853	-	-	10/29/63/63	0/2/2/2
19	CLA	A	824	-	1/1/15/20	15/39/115/115	-
19	CLA	K	1001	-	1/1/11/20	9/15/91/115	-
19	CLA	L	301	-	1/1/13/20	6/27/103/115	-
19	CLA	1	506	-	1/1/13/20	7/27/103/115	-
19	CLA	3	311	-	1/1/10/20	6/10/86/115	-
22	LMG	B	844	-	-	13/30/50/70	0/1/1/1
19	CLA	B	816	-	1/1/13/20	7/27/103/115	-
19	CLA	B	811	-	1/1/15/20	15/39/115/115	-
19	CLA	F	303	10	-	20/39/115/115	-
19	CLA	A	805	-	1/1/15/20	25/39/115/115	-
26	DGD	J	1106	-	-	14/47/87/95	0/2/2/2
19	CLA	2	504	2	1/1/14/20	9/33/109/115	-
19	CLA	1	505	1	-	6/17/93/115	-
19	CLA	1	509	-	1/1/12/20	6/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	855	-	1/1/15/20	16/39/115/115	-
22	LMG	1	519	-	-	1/4/24/70	0/1/1/1
23	XAT	2	502	-	-	6/31/93/93	0/4/4/4
19	CLA	B	814	-	1/1/15/20	16/39/115/115	-
22	LMG	J	1103	-	-	4/25/45/70	0/1/1/1
19	CLA	A	815	-	1/1/11/20	5/15/91/115	-
24	LMT	G	209	-	-	13/17/57/61	0/2/2/2
19	CLA	1	513	-	1/1/15/20	17/39/115/115	-
19	CLA	B	815	-	1/1/15/20	10/39/115/115	-
24	LMT	B	855	-	-	3/17/57/61	0/2/2/2
19	CLA	A	832	-	1/1/15/20	13/39/115/115	-
19	CLA	3	305	-	1/1/13/20	16/27/103/115	-
28	SF4	A	843	6,5	-	-	0/6/5/5
19	CLA	B	805	-	1/1/15/20	18/39/115/115	-
19	CLA	1	510	-	1/1/11/20	7/17/93/115	-
19	CLA	J	1105	-	1/1/12/20	10/21/97/115	-
19	CLA	B	812	-	1/1/14/20	13/33/109/115	-
17	LUT	3	301	-	-	3/29/67/67	0/2/2/2
19	CLA	B	803	-	1/1/15/20	8/39/115/115	-
17	LUT	3	302	-	1/1/12/27	9/29/67/67	0/2/2/2
19	CLA	B	808	-	1/1/15/20	19/39/115/115	-
20	CHL	4	314	31	3/3/17/26	4/21/119/137	-
21	LHG	2	517	19	-	14/39/39/53	-
19	CLA	B	820	31	1/1/15/20	18/39/115/115	-
18	BCR	F	306	-	-	8/29/63/63	0/2/2/2
19	CLA	A	807	-	1/1/14/20	17/33/109/115	-
20	CHL	2	513	-	3/3/16/26	1/18/116/137	-
18	BCR	4	301	-	-	13/29/63/63	0/2/2/2
19	CLA	A	811	-	1/1/15/20	16/39/115/115	-
24	LMT	4	320	-	-	4/21/61/61	0/2/2/2
19	CLA	2	511	-	1/1/12/20	10/21/97/115	-
19	CLA	A	802	-	1/1/15/20	17/39/115/115	-
20	CHL	4	316	-	4/4/19/26	9/33/131/137	-
24	LMT	3	318	-	-	4/17/57/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	1	504	1	1/1/15/20	9/39/115/115	-
19	CLA	2	510	21	1/1/14/20	12/33/109/115	-
19	CLA	A	837	-	1/1/15/20	6/39/115/115	-
27	CL0	A	801	-	3/3/20/25	9/37/135/135	-
24	LMT	J	1107	-	-	8/11/51/61	0/2/2/2
19	CLA	B	809	-	1/1/15/20	7/39/115/115	-
18	BCR	3	303	-	-	11/29/63/63	0/2/2/2
20	CHL	2	512	-	3/3/16/26	2/17/115/137	-
20	CHL	2	516	2	4/4/18/26	6/27/125/137	-
20	CHL	3	314	-	3/3/16/26	3/17/115/137	-
19	CLA	K	1004	-	1/1/5/20	-	-
21	LHG	B	842	19	-	12/23/23/53	-
18	BCR	I	101	-	-	10/29/63/63	0/2/2/2
22	LMG	1	518	-	-	12/41/61/70	0/1/1/1

All (1241) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	302	LUT	C24-C25	15.66	1.51	1.33
17	3	301	LUT	C24-C25	15.47	1.51	1.33
17	1	501	LUT	C24-C25	15.26	1.51	1.33
17	1	502	LUT	C24-C25	15.22	1.51	1.33
17	2	501	LUT	C24-C25	15.02	1.51	1.33
17	3	302	LUT	C24-C25	14.85	1.50	1.33
17	J	1109	LUT	C24-C25	14.60	1.50	1.33
20	2	512	CHL	C3A-C2A	-11.15	1.45	1.54
27	A	801	CL0	C1A-CHA	9.67	1.51	1.40
27	A	801	CL0	C1D-C2D	9.18	1.50	1.39
20	4	314	CHL	C3A-C2A	-8.89	1.47	1.54
27	A	801	CL0	C1B-C2B	8.79	1.49	1.39
20	4	313	CHL	C3B-C4B	6.83	1.48	1.41
19	F	302	CLA	MG-NA	6.73	2.22	2.06
19	A	825	CLA	MG-NA	6.73	2.22	2.06
19	3	309	CLA	MG-NA	6.72	2.22	2.06
19	4	305	CLA	MG-NA	6.71	2.22	2.06
19	B	838	CLA	MG-NA	6.71	2.22	2.06
19	4	310	CLA	MG-NA	6.67	2.22	2.06
19	L	305	CLA	MG-NA	6.65	2.22	2.06
19	K	1002	CLA	MG-NA	6.64	2.22	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	G	202	CLA	MG-NA	6.63	2.22	2.06
19	3	307	CLA	MG-NA	6.62	2.22	2.06
19	3	311	CLA	MG-NA	6.62	2.22	2.06
19	A	815	CLA	MG-NA	6.60	2.22	2.06
19	1	515	CLA	MG-NA	6.60	2.22	2.06
19	K	1003	CLA	MG-NA	6.59	2.21	2.06
19	A	823	CLA	MG-NA	6.58	2.21	2.06
19	1	516	CLA	MG-NA	6.58	2.21	2.06
19	K	1004	CLA	MG-NA	6.58	2.21	2.06
19	A	835	CLA	MG-NA	6.57	2.21	2.06
19	B	826	CLA	MG-NA	6.57	2.21	2.06
19	2	505	CLA	MG-NA	6.57	2.21	2.06
19	A	812	CLA	MG-NA	6.56	2.21	2.06
19	B	813	CLA	MG-NA	6.56	2.21	2.06
20	4	317	CHL	C3A-C2A	-6.55	1.49	1.54
19	A	822	CLA	MG-NA	6.55	2.21	2.06
19	1	505	CLA	MG-NA	6.54	2.21	2.06
19	K	1001	CLA	MG-NA	6.54	2.21	2.06
19	B	834	CLA	MG-NA	6.53	2.21	2.06
19	G	203	CLA	MG-NA	6.53	2.21	2.06
19	B	808	CLA	MG-NA	6.52	2.21	2.06
19	4	308	CLA	MG-NA	6.52	2.21	2.06
19	3	317	CLA	MG-NA	6.52	2.21	2.06
19	B	818	CLA	MG-NA	6.52	2.21	2.06
19	A	807	CLA	MG-NA	6.51	2.21	2.06
19	A	818	CLA	MG-NA	6.50	2.21	2.06
19	L	304	CLA	MG-NA	6.50	2.21	2.06
19	1	513	CLA	MG-NA	6.50	2.21	2.06
19	3	312	CLA	MG-NA	6.50	2.21	2.06
19	G	201	CLA	MG-NA	6.50	2.21	2.06
19	B	839	CLA	MG-NA	6.50	2.21	2.06
19	4	306	CLA	MG-NA	6.49	2.21	2.06
19	A	817	CLA	MG-NA	6.49	2.21	2.06
19	2	510	CLA	MG-NA	6.48	2.21	2.06
19	B	829	CLA	MG-NA	6.48	2.21	2.06
19	H	1000	CLA	MG-NA	6.48	2.21	2.06
19	A	841	CLA	MG-NA	6.48	2.21	2.06
19	2	506	CLA	MG-NA	6.47	2.21	2.06
19	A	816	CLA	MG-NA	6.47	2.21	2.06
19	3	313	CLA	MG-NA	6.47	2.21	2.06
19	G	204	CLA	MG-NA	6.47	2.21	2.06
19	A	836	CLA	MG-NA	6.47	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	303	CLA	MG-NA	6.46	2.21	2.06
19	A	838	CLA	MG-NA	6.46	2.21	2.06
19	1	509	CLA	MG-NA	6.46	2.21	2.06
19	1	508	CLA	MG-NA	6.46	2.21	2.06
19	B	816	CLA	MG-NA	6.46	2.21	2.06
19	B	817	CLA	MG-NA	6.46	2.21	2.06
19	A	814	CLA	MG-NA	6.45	2.21	2.06
19	2	508	CLA	MG-NA	6.45	2.21	2.06
19	A	820	CLA	MG-NA	6.45	2.21	2.06
19	3	308	CLA	MG-NA	6.45	2.21	2.06
19	2	507	CLA	MG-NA	6.45	2.21	2.06
19	B	812	CLA	MG-NA	6.44	2.21	2.06
19	A	831	CLA	MG-NA	6.44	2.21	2.06
19	A	842	CLA	MG-NA	6.44	2.21	2.06
19	A	832	CLA	MG-NA	6.44	2.21	2.06
19	1	504	CLA	MG-NA	6.44	2.21	2.06
19	2	511	CLA	MG-NA	6.44	2.21	2.06
19	A	824	CLA	MG-NA	6.43	2.21	2.06
19	4	304	CLA	MG-NA	6.43	2.21	2.06
19	B	824	CLA	MG-NA	6.42	2.21	2.06
19	1	506	CLA	MG-NA	6.42	2.21	2.06
19	A	837	CLA	MG-NA	6.41	2.21	2.06
19	A	827	CLA	MG-NA	6.41	2.21	2.06
19	L	301	CLA	MG-NA	6.41	2.21	2.06
19	B	814	CLA	MG-NA	6.41	2.21	2.06
19	A	808	CLA	MG-NA	6.40	2.21	2.06
19	B	821	CLA	MG-NA	6.40	2.21	2.06
19	4	307	CLA	MG-NA	6.40	2.21	2.06
19	F	303	CLA	MG-NA	6.39	2.21	2.06
20	1	514	CHL	C3A-C2A	-6.38	1.49	1.54
19	3	316	CLA	MG-NA	6.38	2.21	2.06
19	A	809	CLA	MG-NA	6.38	2.21	2.06
19	B	811	CLA	MG-NA	6.38	2.21	2.06
19	A	811	CLA	MG-NA	6.38	2.21	2.06
19	B	804	CLA	MG-NA	6.38	2.21	2.06
19	B	822	CLA	MG-NA	6.38	2.21	2.06
19	B	805	CLA	MG-NA	6.37	2.21	2.06
19	B	810	CLA	MG-NA	6.37	2.21	2.06
19	B	835	CLA	MG-NA	6.37	2.21	2.06
19	A	829	CLA	MG-NA	6.36	2.21	2.06
19	B	809	CLA	MG-NA	6.36	2.21	2.06
19	1	511	CLA	MG-NA	6.35	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	507	CLA	MG-NA	6.35	2.21	2.06
19	B	840	CLA	MG-NA	6.35	2.21	2.06
19	B	823	CLA	MG-NA	6.34	2.21	2.06
19	A	833	CLA	MG-NA	6.34	2.21	2.06
19	4	315	CLA	MG-NA	6.34	2.21	2.06
19	A	819	CLA	MG-NA	6.33	2.21	2.06
19	A	839	CLA	MG-NA	6.32	2.21	2.06
19	B	837	CLA	MG-NA	6.32	2.21	2.06
19	B	828	CLA	MG-NA	6.32	2.21	2.06
19	A	830	CLA	MG-NA	6.32	2.21	2.06
19	4	318	CLA	MG-NA	6.31	2.21	2.06
19	2	514	CLA	MG-NA	6.31	2.21	2.06
19	B	832	CLA	MG-NA	6.31	2.21	2.06
19	A	840	CLA	MG-NA	6.29	2.21	2.06
19	B	825	CLA	MG-NA	6.29	2.21	2.06
19	A	805	CLA	MG-NA	6.28	2.21	2.06
19	B	815	CLA	MG-NA	6.28	2.21	2.06
19	3	305	CLA	MG-NA	6.28	2.21	2.06
19	J	1102	CLA	MG-NA	6.28	2.21	2.06
19	J	1101	CLA	MG-NA	6.28	2.21	2.06
19	A	803	CLA	MG-NA	6.27	2.21	2.06
19	4	312	CLA	MG-NA	6.27	2.21	2.06
19	2	509	CLA	MG-NA	6.27	2.21	2.06
19	A	828	CLA	MG-NA	6.27	2.21	2.06
19	3	315	CLA	MG-NA	6.27	2.21	2.06
19	A	810	CLA	MG-NA	6.26	2.21	2.06
19	3	306	CLA	MG-NA	6.25	2.21	2.06
19	B	807	CLA	MG-NA	6.25	2.21	2.06
19	A	855	CLA	MG-NA	6.25	2.21	2.06
19	B	831	CLA	MG-NA	6.25	2.21	2.06
19	A	834	CLA	MG-NA	6.25	2.21	2.06
19	B	827	CLA	MG-NA	6.25	2.21	2.06
19	B	830	CLA	MG-NA	6.24	2.21	2.06
19	1	510	CLA	MG-NA	6.24	2.21	2.06
19	A	826	CLA	MG-NA	6.24	2.21	2.06
19	B	820	CLA	MG-NA	6.23	2.21	2.06
19	A	821	CLA	MG-NA	6.22	2.21	2.06
19	B	836	CLA	MG-NA	6.21	2.21	2.06
19	B	803	CLA	MG-NA	6.20	2.21	2.06
19	2	504	CLA	MG-NA	6.17	2.20	2.06
19	A	813	CLA	MG-NA	6.15	2.20	2.06
19	A	806	CLA	MG-NA	6.15	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	819	CLA	MG-NA	6.14	2.20	2.06
19	B	806	CLA	MG-NA	6.12	2.20	2.06
19	J	1105	CLA	MG-NA	6.12	2.20	2.06
19	A	804	CLA	MG-NA	6.11	2.20	2.06
20	2	526	CHL	C3A-C2A	-6.10	1.49	1.54
19	4	311	CLA	MG-NA	6.09	2.20	2.06
19	4	309	CLA	MG-NA	6.09	2.20	2.06
19	3	310	CLA	MG-NA	6.01	2.20	2.06
19	B	833	CLA	MG-NA	6.01	2.20	2.06
19	A	854	CLA	MG-NA	5.93	2.20	2.06
20	3	314	CHL	C3B-C4B	5.88	1.47	1.41
19	A	802	CLA	MG-NA	5.86	2.20	2.06
27	A	801	CL0	C3B-C2B	5.72	1.48	1.40
20	4	317	CHL	C3B-C4B	5.61	1.46	1.41
20	1	521	CHL	C3B-C4B	5.52	1.46	1.41
20	2	516	CHL	C3B-C4B	5.47	1.46	1.41
20	4	313	CHL	C3A-C2A	-5.46	1.50	1.54
20	4	316	CHL	C3B-C4B	5.37	1.46	1.41
20	2	513	CHL	C3A-C2A	-5.33	1.50	1.54
20	4	316	CHL	C2C-C3C	5.32	1.41	1.36
20	2	526	CHL	C3B-C4B	5.29	1.46	1.41
20	4	314	CHL	C3B-C4B	5.27	1.46	1.41
20	1	512	CHL	C3B-C4B	5.24	1.46	1.41
20	2	513	CHL	C3B-C4B	5.24	1.46	1.41
20	3	314	CHL	C3A-C2A	-5.09	1.50	1.54
20	2	515	CHL	C3B-C4B	4.98	1.46	1.41
20	1	514	CHL	C3B-C4B	4.95	1.46	1.41
20	1	512	CHL	C3A-C2A	-4.90	1.50	1.54
20	1	521	CHL	C3A-C2A	-4.55	1.50	1.54
19	J	1105	CLA	CBB-CAB	4.51	1.52	1.30
20	2	516	CHL	C3A-C2A	-4.48	1.50	1.54
19	F	302	CLA	CBB-CAB	4.45	1.51	1.30
19	2	510	CLA	CBB-CAB	4.44	1.51	1.30
19	4	306	CLA	CBB-CAB	4.44	1.51	1.30
19	B	810	CLA	CBB-CAB	4.43	1.51	1.30
19	A	806	CLA	CBB-CAB	4.43	1.51	1.30
19	4	307	CLA	CBB-CAB	4.43	1.51	1.30
19	1	516	CLA	CBB-CAB	4.43	1.51	1.30
19	2	509	CLA	CBB-CAB	4.43	1.51	1.30
19	4	311	CLA	CBB-CAB	4.42	1.51	1.30
19	A	826	CLA	CBB-CAB	4.42	1.51	1.30
19	3	315	CLA	CBB-CAB	4.42	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	807	CLA	CBB-CAB	4.42	1.51	1.30
19	3	307	CLA	CBB-CAB	4.42	1.51	1.30
19	3	312	CLA	CBB-CAB	4.42	1.51	1.30
19	G	203	CLA	CBB-CAB	4.42	1.51	1.30
19	1	509	CLA	CBB-CAB	4.42	1.51	1.30
19	K	1001	CLA	CBB-CAB	4.41	1.51	1.30
19	A	820	CLA	CBB-CAB	4.41	1.51	1.30
19	L	303	CLA	CBB-CAB	4.41	1.51	1.30
19	A	825	CLA	CBB-CAB	4.41	1.51	1.30
19	3	306	CLA	CBB-CAB	4.41	1.51	1.30
19	J	1102	CLA	CBB-CAB	4.41	1.51	1.30
19	A	819	CLA	CBB-CAB	4.41	1.51	1.30
19	B	826	CLA	CBB-CAB	4.41	1.51	1.30
19	3	316	CLA	CBB-CAB	4.41	1.51	1.30
19	A	808	CLA	CBB-CAB	4.41	1.51	1.30
19	B	813	CLA	CBB-CAB	4.41	1.51	1.30
19	4	305	CLA	CBB-CAB	4.41	1.51	1.30
19	A	835	CLA	CBB-CAB	4.41	1.51	1.30
19	A	833	CLA	CBB-CAB	4.41	1.51	1.30
19	3	311	CLA	CBB-CAB	4.40	1.51	1.30
19	1	513	CLA	CBB-CAB	4.40	1.51	1.30
19	1	515	CLA	CBB-CAB	4.40	1.51	1.30
19	4	308	CLA	CBB-CAB	4.40	1.51	1.30
19	1	510	CLA	CBB-CAB	4.40	1.51	1.30
19	L	305	CLA	CBB-CAB	4.40	1.51	1.30
19	3	313	CLA	CBB-CAB	4.40	1.51	1.30
19	B	836	CLA	CBB-CAB	4.40	1.51	1.30
19	H	1000	CLA	CBB-CAB	4.40	1.51	1.30
19	K	1002	CLA	CBB-CAB	4.40	1.51	1.30
19	1	508	CLA	CBB-CAB	4.40	1.51	1.30
19	A	815	CLA	CBB-CAB	4.40	1.51	1.30
19	B	817	CLA	CBB-CAB	4.39	1.51	1.30
19	2	507	CLA	CBB-CAB	4.39	1.51	1.30
19	2	505	CLA	CBB-CAB	4.39	1.51	1.30
19	4	309	CLA	CBB-CAB	4.39	1.51	1.30
19	G	201	CLA	CBB-CAB	4.39	1.51	1.30
19	A	830	CLA	CBB-CAB	4.39	1.51	1.30
19	B	819	CLA	CBB-CAB	4.39	1.51	1.30
19	A	807	CLA	CBB-CAB	4.39	1.51	1.30
19	B	815	CLA	CBB-CAB	4.39	1.51	1.30
19	4	304	CLA	CBB-CAB	4.39	1.51	1.30
19	A	813	CLA	CBB-CAB	4.39	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	G	202	CLA	CBB-CAB	4.39	1.51	1.30
19	A	836	CLA	CBB-CAB	4.39	1.51	1.30
19	2	504	CLA	CBB-CAB	4.39	1.51	1.30
19	3	309	CLA	CBB-CAB	4.39	1.51	1.30
19	A	818	CLA	CBB-CAB	4.39	1.51	1.30
19	1	505	CLA	CBB-CAB	4.38	1.51	1.30
19	B	840	CLA	CBB-CAB	4.38	1.51	1.30
19	A	811	CLA	CBB-CAB	4.38	1.51	1.30
19	A	842	CLA	CBB-CAB	4.38	1.51	1.30
19	1	511	CLA	CBB-CAB	4.38	1.51	1.30
19	A	812	CLA	CBB-CAB	4.38	1.51	1.30
19	A	816	CLA	CBB-CAB	4.38	1.51	1.30
19	2	506	CLA	CBB-CAB	4.38	1.51	1.30
19	B	839	CLA	CBB-CAB	4.38	1.51	1.30
19	2	508	CLA	CBB-CAB	4.38	1.51	1.30
19	L	301	CLA	CBB-CAB	4.38	1.51	1.30
19	A	814	CLA	CBB-CAB	4.38	1.51	1.30
19	A	831	CLA	CBB-CAB	4.38	1.51	1.30
19	3	308	CLA	CBB-CAB	4.38	1.51	1.30
19	2	514	CLA	CBB-CAB	4.38	1.51	1.30
19	B	820	CLA	CBB-CAB	4.38	1.51	1.30
19	B	832	CLA	CBB-CAB	4.38	1.51	1.30
19	4	310	CLA	CBB-CAB	4.38	1.51	1.30
19	B	838	CLA	CBB-CAB	4.38	1.51	1.30
19	L	304	CLA	CBB-CAB	4.38	1.51	1.30
19	1	504	CLA	CBB-CAB	4.38	1.51	1.30
19	1	507	CLA	CBB-CAB	4.38	1.51	1.30
19	B	821	CLA	CBB-CAB	4.38	1.51	1.30
19	B	825	CLA	CBB-CAB	4.38	1.51	1.30
19	B	822	CLA	CBB-CAB	4.37	1.51	1.30
19	B	816	CLA	CBB-CAB	4.37	1.51	1.30
19	B	824	CLA	CBB-CAB	4.37	1.51	1.30
19	4	315	CLA	CBB-CAB	4.37	1.51	1.30
19	B	830	CLA	CBB-CAB	4.37	1.51	1.30
19	B	833	CLA	CBB-CAB	4.37	1.51	1.30
19	B	818	CLA	CBB-CAB	4.37	1.51	1.30
19	B	827	CLA	CBB-CAB	4.37	1.51	1.30
19	B	831	CLA	CBB-CAB	4.37	1.51	1.30
19	A	824	CLA	CBB-CAB	4.37	1.51	1.30
19	4	318	CLA	CBB-CAB	4.36	1.51	1.30
19	A	822	CLA	CBB-CAB	4.36	1.51	1.30
19	A	841	CLA	CBB-CAB	4.36	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	809	CLA	CBB-CAB	4.36	1.51	1.30
19	F	303	CLA	CBB-CAB	4.36	1.51	1.30
19	1	506	CLA	CBB-CAB	4.35	1.51	1.30
19	A	855	CLA	CBB-CAB	4.35	1.51	1.30
19	A	839	CLA	CBB-CAB	4.35	1.51	1.30
19	B	811	CLA	CBB-CAB	4.35	1.51	1.30
19	A	829	CLA	CBB-CAB	4.35	1.51	1.30
19	A	803	CLA	CBB-CAB	4.35	1.51	1.30
19	A	823	CLA	CBB-CAB	4.35	1.51	1.30
19	A	817	CLA	CBB-CAB	4.35	1.51	1.30
19	2	511	CLA	CBB-CAB	4.35	1.51	1.30
19	B	834	CLA	CBB-CAB	4.34	1.51	1.30
19	B	829	CLA	CBB-CAB	4.34	1.51	1.30
19	A	810	CLA	CBB-CAB	4.34	1.51	1.30
19	G	204	CLA	CBB-CAB	4.34	1.51	1.30
19	A	821	CLA	CBB-CAB	4.34	1.51	1.30
19	A	828	CLA	CBB-CAB	4.34	1.51	1.30
19	A	827	CLA	CBB-CAB	4.33	1.51	1.30
19	J	1101	CLA	CBB-CAB	4.33	1.51	1.30
19	B	804	CLA	CBB-CAB	4.33	1.51	1.30
19	A	838	CLA	CBB-CAB	4.33	1.51	1.30
19	A	832	CLA	CBB-CAB	4.33	1.51	1.30
19	B	814	CLA	CBB-CAB	4.33	1.51	1.30
19	A	809	CLA	CBB-CAB	4.33	1.51	1.30
19	A	854	CLA	CBB-CAB	4.32	1.51	1.30
19	A	802	CLA	CBB-CAB	4.32	1.51	1.30
19	3	310	CLA	CBB-CAB	4.32	1.51	1.30
19	B	837	CLA	CBB-CAB	4.32	1.51	1.30
19	B	803	CLA	CBB-CAB	4.32	1.51	1.30
19	B	808	CLA	CBB-CAB	4.32	1.51	1.30
19	1	510	CLA	MG-ND	-4.32	1.97	2.05
19	A	837	CLA	CBB-CAB	4.32	1.51	1.30
19	B	812	CLA	CBB-CAB	4.32	1.51	1.30
19	B	805	CLA	CBB-CAB	4.31	1.51	1.30
19	A	840	CLA	CBB-CAB	4.31	1.51	1.30
19	B	835	CLA	CBB-CAB	4.30	1.51	1.30
19	4	312	CLA	CBB-CAB	4.30	1.51	1.30
19	B	823	CLA	CBB-CAB	4.29	1.51	1.30
19	B	806	CLA	CBB-CAB	4.29	1.51	1.30
19	A	834	CLA	CBB-CAB	4.28	1.50	1.30
19	B	828	CLA	CBB-CAB	4.27	1.50	1.30
19	A	804	CLA	CBB-CAB	4.25	1.50	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	305	CLA	CBB-CAB	4.24	1.50	1.30
19	3	317	CLA	CBB-CAB	4.23	1.50	1.30
19	A	805	CLA	CBB-CAB	4.17	1.50	1.30
20	4	314	CHL	C3B-C2B	-4.04	1.34	1.40
19	B	826	CLA	MG-ND	-3.91	1.98	2.05
19	4	311	CLA	MG-ND	-3.87	1.98	2.05
19	J	1105	CLA	MG-ND	-3.83	1.98	2.05
26	J	1106	DGD	CAA-C9A	-3.81	1.32	1.51
19	B	804	CLA	MG-ND	-3.81	1.98	2.05
19	A	820	CLA	MG-ND	-3.80	1.98	2.05
26	B	854	DGD	CAB-C9B	-3.78	1.33	1.51
19	A	825	CLA	MG-ND	-3.78	1.98	2.05
26	J	1106	DGD	CDA-CCA	-3.75	1.33	1.51
26	4	319	DGD	CAA-C9A	-3.74	1.33	1.51
22	F	304	LMG	C40-C39	-3.73	1.33	1.51
19	B	824	CLA	MG-ND	-3.73	1.98	2.05
19	3	311	CLA	MG-ND	-3.73	1.98	2.05
22	F	304	LMG	C43-C42	-3.73	1.33	1.51
19	A	827	CLA	MG-ND	-3.72	1.98	2.05
22	4	322	LMG	C40-C39	-3.71	1.33	1.51
19	B	829	CLA	MG-ND	-3.71	1.98	2.05
19	A	814	CLA	MG-ND	-3.71	1.98	2.05
19	A	818	CLA	MG-ND	-3.71	1.98	2.05
22	1	518	LMG	C19-C18	-3.70	1.33	1.51
19	J	1101	CLA	MG-ND	-3.70	1.98	2.05
22	G	206	LMG	C40-C39	-3.70	1.33	1.51
22	A	847	LMG	C19-C18	-3.69	1.33	1.51
22	F	304	LMG	C37-C36	-3.69	1.33	1.51
22	A	847	LMG	C25-C24	-3.69	1.33	1.51
19	4	304	CLA	MG-ND	-3.69	1.98	2.05
26	J	1106	DGD	CGA-CFA	-3.68	1.33	1.51
19	3	305	CLA	MG-ND	-3.68	1.98	2.05
19	A	839	CLA	MG-ND	-3.68	1.98	2.05
19	3	310	CLA	MG-ND	-3.68	1.98	2.05
22	4	322	LMG	C37-C36	-3.68	1.33	1.51
22	A	847	LMG	C22-C21	-3.68	1.33	1.51
19	4	305	CLA	MG-ND	-3.68	1.98	2.05
22	G	206	LMG	C37-C36	-3.67	1.33	1.51
19	A	830	CLA	MG-ND	-3.67	1.98	2.05
19	A	854	CLA	MG-ND	-3.67	1.98	2.05
19	A	831	CLA	MG-ND	-3.67	1.98	2.05
26	B	854	DGD	CGB-CFB	-3.67	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	835	CLA	MG-ND	-3.67	1.98	2.05
19	B	822	CLA	MG-ND	-3.67	1.98	2.05
22	F	305	LMG	C37-C36	-3.66	1.33	1.51
22	1	518	LMG	C22-C21	-3.66	1.33	1.51
19	B	814	CLA	MG-ND	-3.66	1.98	2.05
22	A	847	LMG	C37-C36	-3.66	1.33	1.51
19	J	1105	CLA	C1C-NC	-3.66	1.32	1.37
19	A	807	CLA	MG-ND	-3.65	1.98	2.05
26	B	854	DGD	CAA-C9A	-3.65	1.33	1.51
19	H	1000	CLA	MG-ND	-3.65	1.98	2.05
19	A	802	CLA	MG-ND	-3.65	1.98	2.05
19	A	809	CLA	MG-ND	-3.65	1.98	2.05
19	4	306	CLA	MG-ND	-3.64	1.98	2.05
19	B	818	CLA	MG-ND	-3.64	1.98	2.05
22	G	206	LMG	C22-C21	-3.64	1.33	1.51
19	3	316	CLA	MG-ND	-3.64	1.98	2.05
19	A	822	CLA	MG-ND	-3.64	1.98	2.05
19	B	807	CLA	MG-ND	-3.64	1.98	2.05
22	1	518	LMG	C25-C24	-3.64	1.33	1.51
26	B	854	DGD	CDB-CCB	-3.63	1.33	1.51
19	3	309	CLA	MG-ND	-3.63	1.98	2.05
19	A	815	CLA	MG-ND	-3.63	1.98	2.05
19	B	803	CLA	MG-ND	-3.63	1.98	2.05
22	G	206	LMG	C19-C18	-3.63	1.33	1.51
19	A	832	CLA	MG-ND	-3.63	1.98	2.05
19	B	837	CLA	MG-ND	-3.62	1.98	2.05
19	1	515	CLA	MG-ND	-3.62	1.98	2.05
19	B	816	CLA	MG-ND	-3.62	1.98	2.05
19	A	803	CLA	MG-ND	-3.61	1.98	2.05
22	B	844	LMG	C19-C18	-3.61	1.33	1.51
19	B	833	CLA	MG-ND	-3.61	1.98	2.05
19	A	817	CLA	MG-ND	-3.61	1.98	2.05
19	B	820	CLA	MG-ND	-3.60	1.98	2.05
19	2	505	CLA	MG-ND	-3.60	1.98	2.05
19	B	806	CLA	MG-ND	-3.60	1.98	2.05
19	2	514	CLA	MG-ND	-3.60	1.98	2.05
19	3	317	CLA	MG-ND	-3.60	1.98	2.05
19	1	511	CLA	MG-ND	-3.60	1.98	2.05
19	B	813	CLA	MG-ND	-3.59	1.98	2.05
19	3	312	CLA	MG-ND	-3.59	1.98	2.05
19	L	305	CLA	MG-ND	-3.59	1.98	2.05
19	B	825	CLA	MG-ND	-3.58	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	810	CLA	MG-ND	-3.58	1.98	2.05
19	B	808	CLA	MG-ND	-3.58	1.98	2.05
19	B	827	CLA	MG-ND	-3.58	1.98	2.05
20	2	513	CHL	C3B-C2B	-3.58	1.35	1.40
19	3	315	CLA	MG-ND	-3.58	1.98	2.05
19	1	504	CLA	MG-ND	-3.58	1.98	2.05
20	2	512	CHL	C1A-CHA	-3.57	1.35	1.40
19	2	506	CLA	MG-ND	-3.57	1.98	2.05
19	2	511	CLA	MG-ND	-3.57	1.98	2.05
19	A	828	CLA	MG-ND	-3.57	1.98	2.05
19	4	312	CLA	MG-ND	-3.57	1.98	2.05
19	A	836	CLA	MG-ND	-3.57	1.98	2.05
19	A	838	CLA	MG-ND	-3.57	1.98	2.05
20	2	515	CHL	CBB-CAB	3.57	1.51	1.29
19	G	203	CLA	MG-ND	-3.56	1.98	2.05
19	B	811	CLA	MG-ND	-3.56	1.98	2.05
19	A	821	CLA	MG-ND	-3.56	1.98	2.05
20	2	515	CHL	C3A-C2A	-3.55	1.51	1.54
27	A	801	CL0	CBB-CAB	3.55	1.51	1.29
19	4	308	CLA	MG-ND	-3.55	1.98	2.05
19	A	806	CLA	MG-ND	-3.55	1.98	2.05
19	1	516	CLA	MG-ND	-3.54	1.98	2.05
19	3	308	CLA	MG-ND	-3.54	1.98	2.05
19	2	510	CLA	MG-ND	-3.54	1.98	2.05
19	2	504	CLA	MG-ND	-3.54	1.98	2.05
19	4	315	CLA	MG-ND	-3.54	1.98	2.05
19	K	1001	CLA	MG-ND	-3.54	1.98	2.05
19	B	840	CLA	MG-ND	-3.53	1.98	2.05
19	B	831	CLA	MG-ND	-3.53	1.98	2.05
19	3	306	CLA	MG-ND	-3.53	1.98	2.05
19	L	301	CLA	MG-ND	-3.53	1.98	2.05
19	B	821	CLA	MG-ND	-3.53	1.98	2.05
20	1	514	CHL	CBB-CAB	3.53	1.51	1.29
19	A	808	CLA	MG-ND	-3.51	1.98	2.05
19	1	508	CLA	MG-ND	-3.51	1.98	2.05
19	B	835	CLA	MG-ND	-3.51	1.98	2.05
19	B	834	CLA	MG-ND	-3.51	1.98	2.05
19	A	816	CLA	MG-ND	-3.50	1.98	2.05
20	2	526	CHL	CBB-CAB	3.50	1.51	1.29
19	1	506	CLA	MG-ND	-3.49	1.98	2.05
19	A	812	CLA	MG-ND	-3.49	1.98	2.05
19	B	819	CLA	MG-ND	-3.48	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	824	CLA	MG-ND	-3.48	1.98	2.05
19	A	805	CLA	MG-ND	-3.48	1.98	2.05
19	1	513	CLA	MG-ND	-3.48	1.98	2.05
19	B	817	CLA	MG-ND	-3.47	1.98	2.05
19	K	1003	CLA	MG-ND	-3.47	1.98	2.05
20	4	317	CHL	CBB-CAB	3.47	1.51	1.29
19	A	833	CLA	MG-ND	-3.47	1.98	2.05
19	1	507	CLA	MG-ND	-3.46	1.98	2.05
19	K	1002	CLA	MG-ND	-3.46	1.98	2.05
19	A	819	CLA	MG-ND	-3.46	1.98	2.05
19	4	318	CLA	MG-ND	-3.46	1.98	2.05
20	4	313	CHL	CBB-CAB	3.46	1.51	1.29
19	G	202	CLA	MG-ND	-3.45	1.98	2.05
20	2	516	CHL	CBB-CAB	3.45	1.51	1.29
19	A	804	CLA	MG-ND	-3.45	1.98	2.05
19	A	842	CLA	MG-ND	-3.45	1.98	2.05
19	1	505	CLA	MG-ND	-3.45	1.99	2.05
19	2	507	CLA	MG-ND	-3.45	1.99	2.05
19	A	813	CLA	MG-ND	-3.44	1.99	2.05
19	A	823	CLA	MG-ND	-3.44	1.99	2.05
20	1	521	CHL	C1A-CHA	-3.44	1.36	1.40
19	3	313	CLA	MG-ND	-3.43	1.99	2.05
20	1	512	CHL	CBB-CAB	3.43	1.50	1.29
19	B	815	CLA	MG-ND	-3.41	1.99	2.05
19	A	810	CLA	MG-ND	-3.40	1.99	2.05
19	1	510	CLA	C1C-NC	-3.40	1.32	1.37
19	1	509	CLA	MG-ND	-3.39	1.99	2.05
19	2	509	CLA	MG-ND	-3.39	1.99	2.05
19	4	310	CLA	MG-ND	-3.39	1.99	2.05
19	B	830	CLA	MG-ND	-3.39	1.99	2.05
19	B	809	CLA	MG-ND	-3.38	1.99	2.05
19	G	204	CLA	MG-ND	-3.38	1.99	2.05
19	G	201	CLA	MG-ND	-3.37	1.99	2.05
19	B	836	CLA	MG-ND	-3.37	1.99	2.05
19	L	303	CLA	MG-ND	-3.36	1.99	2.05
19	3	306	CLA	C1C-NC	-3.36	1.32	1.37
19	F	302	CLA	MG-ND	-3.36	1.99	2.05
19	J	1102	CLA	MG-ND	-3.35	1.99	2.05
19	B	812	CLA	MG-ND	-3.35	1.99	2.05
19	B	823	CLA	MG-ND	-3.35	1.99	2.05
19	A	837	CLA	MG-ND	-3.35	1.99	2.05
19	4	307	CLA	MG-ND	-3.35	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	834	CLA	MG-ND	-3.35	1.99	2.05
19	A	811	CLA	MG-ND	-3.35	1.99	2.05
19	B	832	CLA	MG-ND	-3.34	1.99	2.05
20	1	521	CHL	CBB-CAB	3.34	1.50	1.29
20	4	316	CHL	CBB-CAB	3.34	1.50	1.29
19	A	826	CLA	MG-ND	-3.33	1.99	2.05
19	A	840	CLA	MG-ND	-3.33	1.99	2.05
19	2	508	CLA	MG-ND	-3.31	1.99	2.05
19	F	303	CLA	MG-ND	-3.31	1.99	2.05
19	3	307	CLA	MG-ND	-3.31	1.99	2.05
19	A	829	CLA	MG-ND	-3.31	1.99	2.05
20	4	316	CHL	C3B-C2B	-3.30	1.35	1.40
19	K	1004	CLA	MG-ND	-3.30	1.99	2.05
20	4	316	CHL	C3A-C2A	-3.29	1.51	1.54
20	2	515	CHL	C2C-C3C	3.28	1.39	1.36
19	B	805	CLA	MG-ND	-3.28	1.99	2.05
19	B	838	CLA	MG-ND	-3.27	1.99	2.05
19	A	855	CLA	MG-ND	-3.26	1.99	2.05
19	A	841	CLA	MG-ND	-3.23	1.99	2.05
19	B	815	CLA	C1C-NC	-3.23	1.32	1.37
20	3	314	CHL	CBB-CAB	3.22	1.49	1.29
20	4	314	CHL	CHB-C4A	-3.21	1.34	1.38
19	4	309	CLA	MG-ND	-3.21	1.99	2.05
19	L	304	CLA	MG-ND	-3.20	1.99	2.05
19	B	839	CLA	MG-ND	-3.20	1.99	2.05
20	2	513	CHL	CBB-CAB	3.18	1.49	1.29
19	G	201	CLA	C1C-NC	-3.18	1.32	1.37
19	4	306	CLA	C1C-NC	-3.18	1.32	1.37
19	K	1004	CLA	C4D-C3D	-3.14	1.40	1.46
19	B	821	CLA	C1C-NC	-3.14	1.32	1.37
19	3	310	CLA	C1C-NC	-3.13	1.32	1.37
19	3	305	CLA	C1C-NC	-3.13	1.33	1.37
19	B	828	CLA	MG-ND	-3.12	1.99	2.05
19	4	311	CLA	C1C-NC	-3.11	1.33	1.37
20	4	314	CHL	CBB-CAB	3.11	1.48	1.29
19	B	831	CLA	C1C-NC	-3.11	1.33	1.37
19	A	807	CLA	C1C-NC	-3.10	1.33	1.37
19	B	832	CLA	C1C-NC	-3.10	1.33	1.37
20	3	314	CHL	CHB-C4A	-3.10	1.34	1.38
19	A	805	CLA	C1C-NC	-3.10	1.33	1.37
19	3	316	CLA	C1C-NC	-3.09	1.33	1.37
19	G	202	CLA	C1C-NC	-3.09	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	826	CLA	C1C-NC	-3.08	1.33	1.37
19	A	838	CLA	C1C-NC	-3.08	1.33	1.37
19	K	1003	CLA	C4D-C3D	-3.07	1.40	1.46
19	4	315	CLA	C1C-NC	-3.07	1.33	1.37
19	L	303	CLA	C1C-NC	-3.07	1.33	1.37
19	B	822	CLA	C1C-NC	-3.06	1.33	1.37
19	A	828	CLA	C1C-NC	-3.06	1.33	1.37
20	3	314	CHL	C3B-C2B	-3.05	1.36	1.40
19	4	308	CLA	C1C-NC	-3.05	1.33	1.37
20	2	512	CHL	CBB-CAB	3.05	1.48	1.29
19	A	831	CLA	C1C-NC	-3.04	1.33	1.37
19	4	318	CLA	C1C-NC	-3.04	1.33	1.37
19	3	311	CLA	C1C-NC	-3.03	1.33	1.37
19	B	840	CLA	C1C-NC	-3.03	1.33	1.37
19	A	841	CLA	C1C-NC	-3.02	1.33	1.37
19	4	307	CLA	C1C-NC	-3.02	1.33	1.37
19	A	813	CLA	C1C-NC	-3.02	1.33	1.37
19	H	1000	CLA	C1C-NC	-3.01	1.33	1.37
19	1	508	CLA	C1C-NC	-3.01	1.33	1.37
19	2	510	CLA	C1C-NC	-3.01	1.33	1.37
19	4	304	CLA	C1C-NC	-3.01	1.33	1.37
19	3	313	CLA	C1C-NC	-3.01	1.33	1.37
19	A	808	CLA	C1C-NC	-3.01	1.33	1.37
20	2	512	CHL	CHB-C4A	-3.00	1.35	1.38
19	2	504	CLA	C1C-NC	-3.00	1.33	1.37
19	A	822	CLA	C1C-NC	-3.00	1.33	1.37
19	A	832	CLA	C1C-NC	-3.00	1.33	1.37
19	A	855	CLA	C1C-NC	-3.00	1.33	1.37
19	B	803	CLA	C1C-NC	-2.99	1.33	1.37
19	B	805	CLA	C1C-NC	-2.99	1.33	1.37
19	B	810	CLA	C1C-NC	-2.99	1.33	1.37
19	A	823	CLA	C1C-NC	-2.99	1.33	1.37
19	A	816	CLA	C1C-NC	-2.98	1.33	1.37
19	B	820	CLA	C1C-NC	-2.98	1.33	1.37
19	2	511	CLA	C1C-NC	-2.98	1.33	1.37
19	A	812	CLA	C1C-NC	-2.98	1.33	1.37
19	2	514	CLA	C1C-NC	-2.97	1.33	1.37
19	K	1001	CLA	C1C-NC	-2.97	1.33	1.37
19	B	839	CLA	C1C-NC	-2.96	1.33	1.37
19	B	826	CLA	C1C-NC	-2.96	1.33	1.37
19	3	308	CLA	C1C-NC	-2.95	1.33	1.37
19	A	854	CLA	C1C-NC	-2.95	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	828	CLA	C1C-NC	-2.95	1.33	1.37
19	A	837	CLA	C1C-NC	-2.95	1.33	1.37
19	4	305	CLA	C1C-NC	-2.95	1.33	1.37
19	A	811	CLA	C1C-NC	-2.95	1.33	1.37
19	A	821	CLA	C1C-NC	-2.95	1.33	1.37
20	4	316	CHL	CHB-C4A	-2.95	1.35	1.38
19	A	839	CLA	C1C-NC	-2.94	1.33	1.37
19	2	509	CLA	C1C-NC	-2.94	1.33	1.37
19	B	807	CLA	C1C-NC	-2.94	1.33	1.37
19	B	813	CLA	C1C-NC	-2.94	1.33	1.37
19	A	827	CLA	C1C-NC	-2.94	1.33	1.37
19	A	814	CLA	C1C-NC	-2.94	1.33	1.37
19	4	309	CLA	C1C-NC	-2.93	1.33	1.37
19	2	507	CLA	C1C-NC	-2.93	1.33	1.37
19	B	823	CLA	C1C-NC	-2.93	1.33	1.37
19	4	312	CLA	C1C-NC	-2.93	1.33	1.37
19	B	835	CLA	C1C-NC	-2.92	1.33	1.37
19	B	812	CLA	C1C-NC	-2.92	1.33	1.37
19	B	816	CLA	C1C-NC	-2.92	1.33	1.37
19	1	505	CLA	C1C-NC	-2.92	1.33	1.37
19	B	808	CLA	C1C-NC	-2.92	1.33	1.37
19	G	204	CLA	C1C-NC	-2.92	1.33	1.37
19	1	507	CLA	C1C-NC	-2.92	1.33	1.37
19	B	811	CLA	C1C-NC	-2.92	1.33	1.37
19	1	515	CLA	C1C-NC	-2.92	1.33	1.37
22	2	519	LMG	C19-C18	-2.91	1.33	1.51
19	B	827	CLA	C1C-NC	-2.91	1.33	1.37
19	J	1102	CLA	C1C-NC	-2.91	1.33	1.37
19	A	809	CLA	C1C-NC	-2.91	1.33	1.37
19	B	804	CLA	C1C-NC	-2.91	1.33	1.37
19	1	504	CLA	C1C-NC	-2.90	1.33	1.37
19	B	806	CLA	C1C-NC	-2.90	1.33	1.37
19	A	810	CLA	C1C-NC	-2.89	1.33	1.37
19	A	817	CLA	C1C-NC	-2.89	1.33	1.37
19	B	809	CLA	C1C-NC	-2.89	1.33	1.37
19	B	817	CLA	C1C-NC	-2.89	1.33	1.37
19	A	824	CLA	C1C-NC	-2.89	1.33	1.37
19	2	506	CLA	C1C-NC	-2.89	1.33	1.37
19	B	814	CLA	C1C-NC	-2.89	1.33	1.37
20	4	317	CHL	CHB-C4A	-2.89	1.35	1.38
19	1	516	CLA	C1C-NC	-2.88	1.33	1.37
19	G	203	CLA	C1C-NC	-2.88	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	833	CLA	C1C-NC	-2.88	1.33	1.37
19	L	304	CLA	C1C-NC	-2.88	1.33	1.37
19	3	307	CLA	C1C-NC	-2.88	1.33	1.37
19	2	505	CLA	C1C-NC	-2.88	1.33	1.37
19	3	315	CLA	C1C-NC	-2.87	1.33	1.37
19	B	836	CLA	C1C-NC	-2.87	1.33	1.37
19	A	834	CLA	C1C-NC	-2.87	1.33	1.37
19	K	1002	CLA	C1C-NC	-2.87	1.33	1.37
19	B	819	CLA	C1C-NC	-2.86	1.33	1.37
19	B	829	CLA	C1C-NC	-2.86	1.33	1.37
19	A	835	CLA	C1C-NC	-2.86	1.33	1.37
19	1	509	CLA	C1C-NC	-2.86	1.33	1.37
19	A	820	CLA	C1C-NC	-2.86	1.33	1.37
19	L	301	CLA	C1C-NC	-2.85	1.33	1.37
19	A	815	CLA	C1C-NC	-2.84	1.33	1.37
19	2	508	CLA	C1C-NC	-2.84	1.33	1.37
19	B	825	CLA	C1C-NC	-2.84	1.33	1.37
19	1	511	CLA	C1C-NC	-2.84	1.33	1.37
19	A	840	CLA	C1C-NC	-2.84	1.33	1.37
19	3	309	CLA	C1C-NC	-2.83	1.33	1.37
19	3	312	CLA	C1C-NC	-2.83	1.33	1.37
19	B	818	CLA	C1C-NC	-2.83	1.33	1.37
20	4	317	CHL	C1D-C2D	2.83	1.42	1.39
19	B	838	CLA	C1C-NC	-2.83	1.33	1.37
20	2	526	CHL	C1D-C2D	2.83	1.42	1.39
19	A	806	CLA	C1C-NC	-2.83	1.33	1.37
19	F	303	CLA	C1C-NC	-2.83	1.33	1.37
19	A	836	CLA	C1C-NC	-2.82	1.33	1.37
19	A	802	CLA	C1C-NC	-2.82	1.33	1.37
19	3	317	CLA	C1C-NC	-2.82	1.33	1.37
19	B	834	CLA	C1C-NC	-2.82	1.33	1.37
19	A	819	CLA	C1C-NC	-2.81	1.33	1.37
19	A	842	CLA	C1C-NC	-2.81	1.33	1.37
19	1	513	CLA	C1C-NC	-2.81	1.33	1.37
19	A	833	CLA	C1C-NC	-2.81	1.33	1.37
19	F	302	CLA	C1C-NC	-2.81	1.33	1.37
19	J	1101	CLA	C1C-NC	-2.81	1.33	1.37
19	4	310	CLA	C1C-NC	-2.80	1.33	1.37
20	2	515	CHL	C1D-C2D	2.80	1.42	1.39
19	A	830	CLA	C1C-NC	-2.80	1.33	1.37
19	1	506	CLA	C1C-NC	-2.79	1.33	1.37
19	A	829	CLA	C1C-NC	-2.78	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	305	CLA	C1C-NC	-2.78	1.33	1.37
19	K	1003	CLA	C3B-C4B	2.78	1.46	1.40
20	4	313	CHL	CHB-C4A	-2.78	1.35	1.38
20	1	514	CHL	C1B-C2B	2.78	1.42	1.39
20	2	526	CHL	C1B-C2B	2.77	1.42	1.39
20	2	513	CHL	CHB-C4A	-2.77	1.35	1.38
20	1	521	CHL	C1B-C2B	2.77	1.42	1.39
19	K	1004	CLA	C3B-C4B	2.76	1.46	1.40
20	1	514	CHL	C1D-C2D	2.76	1.42	1.39
19	A	818	CLA	C1C-NC	-2.76	1.33	1.37
19	B	824	CLA	C1C-NC	-2.75	1.33	1.37
20	4	313	CHL	C1D-C2D	2.75	1.42	1.39
20	4	316	CHL	C1D-C2D	2.74	1.42	1.39
20	2	515	CHL	C1B-C2B	2.73	1.42	1.39
20	2	513	CHL	C1D-C2D	2.73	1.42	1.39
20	3	314	CHL	C1D-C2D	2.72	1.42	1.39
20	1	521	CHL	C1D-C2D	2.71	1.42	1.39
20	2	512	CHL	C3B-C4B	2.71	1.44	1.41
20	2	526	CHL	C1A-CHA	-2.70	1.36	1.40
19	A	825	CLA	C1C-NC	-2.70	1.33	1.37
19	B	830	CLA	C1C-NC	-2.69	1.33	1.37
20	2	516	CHL	C1D-C2D	2.68	1.42	1.39
19	A	803	CLA	C1C-NC	-2.68	1.33	1.37
19	B	837	CLA	C1C-NC	-2.68	1.33	1.37
19	A	804	CLA	C1C-NC	-2.68	1.33	1.37
20	4	316	CHL	C1B-C2B	2.68	1.42	1.39
19	K	1004	CLA	C2D-C1D	2.67	1.47	1.42
20	1	512	CHL	CHB-C4A	-2.67	1.35	1.38
20	4	314	CHL	C1D-C2D	2.67	1.42	1.39
19	K	1003	CLA	C2D-C1D	2.65	1.47	1.42
20	2	516	CHL	C1B-C2B	2.63	1.42	1.39
20	1	512	CHL	C1B-C2B	2.62	1.42	1.39
24	B	855	LMT	O3'-C3'	-2.61	1.36	1.43
20	1	512	CHL	C1D-C2D	2.60	1.42	1.39
20	2	516	CHL	CHB-C4A	-2.59	1.35	1.38
20	4	317	CHL	C1B-C2B	2.59	1.42	1.39
24	4	320	LMT	O3'-C3'	-2.59	1.36	1.43
20	1	521	CHL	C3B-C2B	-2.57	1.36	1.40
20	2	526	CHL	CHB-C4A	-2.57	1.35	1.38
20	4	313	CHL	C1B-C2B	2.57	1.42	1.39
20	2	516	CHL	C1A-CHA	-2.55	1.37	1.40
20	2	515	CHL	CHB-C4A	-2.55	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	513	CHL	C1B-C2B	2.53	1.42	1.39
24	B	846	LMT	O3'-C3'	-2.53	1.36	1.43
20	4	313	CHL	C3B-C2B	-2.53	1.36	1.40
27	A	801	CL0	C3A-C2A	-2.52	1.52	1.54
20	1	521	CHL	CHB-C4A	-2.51	1.35	1.38
20	2	512	CHL	C3D-C2D	-2.51	1.35	1.39
20	1	514	CHL	CHB-C4A	-2.51	1.35	1.38
24	G	208	LMT	O3'-C3'	-2.49	1.36	1.43
24	B	847	LMT	O3'-C3'	-2.49	1.36	1.43
24	3	318	LMT	O3'-C3'	-2.47	1.36	1.43
20	4	317	CHL	C3B-C2B	-2.46	1.37	1.40
19	B	829	CLA	C1B-NB	-2.46	1.34	1.37
20	4	314	CHL	C1B-C2B	2.45	1.42	1.39
19	A	830	CLA	C1B-NB	-2.42	1.34	1.37
19	2	514	CLA	C1B-NB	-2.41	1.34	1.37
19	1	510	CLA	C1B-NB	-2.40	1.34	1.37
19	F	302	CLA	C1B-NB	-2.40	1.34	1.37
24	G	209	LMT	O3'-C3'	-2.40	1.37	1.43
24	A	846	LMT	O3'-C3'	-2.39	1.37	1.43
26	B	854	DGD	CDA-CCA	-2.38	1.33	1.50
22	4	322	LMG	C19-C18	-2.38	1.33	1.50
19	4	309	CLA	C1B-NB	-2.38	1.34	1.37
26	G	207	DGD	CAB-C9B	-2.37	1.33	1.50
26	J	1106	DGD	CAB-C9B	-2.37	1.33	1.50
24	J	1107	LMT	O3'-C3'	-2.37	1.37	1.43
26	4	319	DGD	CDA-CCA	-2.37	1.33	1.50
24	B	847	LMT	O2'-C2'	-2.37	1.37	1.43
22	A	847	LMG	C40-C39	-2.37	1.33	1.50
22	F	304	LMG	C19-C18	-2.37	1.33	1.50
20	2	512	CHL	C1B-C2B	2.37	1.42	1.39
19	3	310	CLA	C1B-NB	-2.37	1.34	1.37
19	A	808	CLA	C1B-NB	-2.37	1.34	1.37
19	B	831	CLA	C1B-NB	-2.37	1.34	1.37
27	A	801	CL0	C3B-C4B	2.36	1.43	1.41
19	B	811	CLA	C1C-C2C	2.36	1.49	1.44
19	3	315	CLA	C1B-NB	-2.36	1.34	1.37
19	A	802	CLA	C1B-NB	-2.36	1.34	1.37
19	B	820	CLA	C1B-NB	-2.36	1.34	1.37
19	A	805	CLA	C1B-NB	-2.36	1.34	1.37
22	G	206	LMG	C43-C42	-2.36	1.33	1.50
19	1	515	CLA	C1B-NB	-2.36	1.34	1.37
19	B	810	CLA	C1B-NB	-2.35	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	317	CLA	C1B-NB	-2.35	1.34	1.37
19	3	313	CLA	C1B-NB	-2.35	1.34	1.37
19	4	306	CLA	C1B-NB	-2.35	1.34	1.37
19	A	826	CLA	C1B-NB	-2.35	1.34	1.37
22	4	322	LMG	C43-C42	-2.34	1.33	1.50
20	3	314	CHL	C1B-C2B	2.34	1.42	1.39
19	J	1101	CLA	C1B-NB	-2.34	1.34	1.37
19	4	311	CLA	C1B-NB	-2.34	1.34	1.37
19	B	836	CLA	C1B-NB	-2.34	1.34	1.37
19	B	816	CLA	C1B-NB	-2.34	1.34	1.37
19	B	830	CLA	C1B-NB	-2.34	1.34	1.37
19	A	840	CLA	C1B-NB	-2.34	1.34	1.37
19	A	854	CLA	C1B-NB	-2.34	1.34	1.37
19	B	804	CLA	C1B-NB	-2.34	1.34	1.37
19	B	828	CLA	C1B-NB	-2.34	1.34	1.37
20	2	526	CHL	C3B-C2B	-2.34	1.37	1.40
19	2	510	CLA	C1B-NB	-2.33	1.34	1.37
19	A	813	CLA	C1B-NB	-2.33	1.34	1.37
19	A	841	CLA	CHC-C1C	2.33	1.43	1.38
19	A	825	CLA	MG-NC	2.33	2.11	2.06
19	A	816	CLA	C1B-NB	-2.33	1.34	1.37
19	A	855	CLA	C1B-NB	-2.33	1.34	1.37
19	K	1003	CLA	C2C-C1C	2.33	1.48	1.43
19	3	308	CLA	C1B-NB	-2.33	1.34	1.37
19	4	308	CLA	C1B-NB	-2.33	1.34	1.37
19	L	304	CLA	C1B-NB	-2.33	1.34	1.37
19	A	803	CLA	C1B-NB	-2.32	1.34	1.37
19	B	815	CLA	C1B-NB	-2.32	1.34	1.37
19	J	1105	CLA	C1B-NB	-2.32	1.34	1.37
19	A	829	CLA	C1B-NB	-2.32	1.34	1.37
19	2	509	CLA	C1B-NB	-2.32	1.34	1.37
19	4	304	CLA	C1B-NB	-2.32	1.34	1.37
19	1	506	CLA	C1B-NB	-2.32	1.34	1.37
19	B	835	CLA	C1B-NB	-2.32	1.34	1.37
19	B	806	CLA	C1B-NB	-2.32	1.34	1.37
20	2	512	CHL	C1D-C2D	2.32	1.42	1.39
19	B	813	CLA	C1B-NB	-2.32	1.34	1.37
19	B	822	CLA	C1B-NB	-2.32	1.34	1.37
19	1	509	CLA	C1B-NB	-2.31	1.34	1.37
19	B	807	CLA	C1B-NB	-2.31	1.34	1.37
19	B	811	CLA	C1B-NB	-2.31	1.34	1.37
19	A	836	CLA	C1B-NB	-2.31	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	309	CLA	C4B-NB	-2.31	1.34	1.37
19	A	833	CLA	C1B-NB	-2.31	1.34	1.37
19	H	1000	CLA	C1B-NB	-2.31	1.34	1.37
19	B	825	CLA	C1B-NB	-2.31	1.34	1.37
19	2	504	CLA	C1B-NB	-2.31	1.34	1.37
19	A	821	CLA	C1B-NB	-2.31	1.34	1.37
19	1	504	CLA	C1B-NB	-2.31	1.34	1.37
19	A	819	CLA	C1B-NB	-2.31	1.34	1.37
19	L	303	CLA	C1B-NB	-2.31	1.34	1.37
19	3	316	CLA	C1B-NB	-2.30	1.34	1.37
19	B	827	CLA	C1B-NB	-2.30	1.34	1.37
19	3	305	CLA	C1B-NB	-2.30	1.34	1.37
19	A	815	CLA	C1B-NB	-2.30	1.34	1.37
19	A	828	CLA	C4B-NB	-2.30	1.34	1.37
19	4	318	CLA	C1B-NB	-2.30	1.34	1.37
19	A	825	CLA	C1B-NB	-2.30	1.34	1.37
19	4	307	CLA	C1B-NB	-2.30	1.34	1.37
19	1	516	CLA	C1B-NB	-2.30	1.34	1.37
19	B	814	CLA	C1B-NB	-2.30	1.34	1.37
19	B	833	CLA	C1B-NB	-2.30	1.34	1.37
19	A	809	CLA	C1B-NB	-2.29	1.34	1.37
19	L	301	CLA	C1B-NB	-2.29	1.34	1.37
19	B	826	CLA	C1B-NB	-2.29	1.34	1.37
19	4	315	CLA	C1B-NB	-2.29	1.34	1.37
19	A	818	CLA	C1B-NB	-2.29	1.34	1.37
19	A	814	CLA	C1B-NB	-2.29	1.34	1.37
19	A	811	CLA	C1B-NB	-2.29	1.34	1.37
24	2	523	LMT	O3'-C3'	-2.29	1.37	1.43
19	1	508	CLA	C1B-NB	-2.28	1.34	1.37
19	B	815	CLA	C4B-NB	-2.28	1.34	1.37
19	A	812	CLA	C1B-NB	-2.28	1.34	1.37
19	A	837	CLA	C1B-NB	-2.28	1.34	1.37
19	B	808	CLA	C1B-NB	-2.28	1.34	1.37
19	L	305	CLA	C1B-NB	-2.28	1.34	1.37
24	B	855	LMT	O2B-C2B	-2.28	1.37	1.43
20	1	512	CHL	C3B-C2B	-2.28	1.37	1.40
19	A	842	CLA	C1B-NB	-2.28	1.34	1.37
19	A	804	CLA	C1B-NB	-2.28	1.34	1.37
19	2	507	CLA	C1B-NB	-2.28	1.34	1.37
19	A	807	CLA	C1B-NB	-2.28	1.34	1.37
19	A	810	CLA	C1B-NB	-2.28	1.34	1.37
19	K	1002	CLA	C1B-NB	-2.28	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	508	CLA	C1B-NB	-2.28	1.34	1.37
19	4	312	CLA	C1B-NB	-2.28	1.34	1.37
19	B	818	CLA	C1B-NB	-2.28	1.34	1.37
19	G	203	CLA	C1B-NB	-2.28	1.34	1.37
19	A	806	CLA	C1B-NB	-2.28	1.34	1.37
19	1	513	CLA	C1B-NB	-2.27	1.34	1.37
19	2	506	CLA	C1B-NB	-2.27	1.34	1.37
19	A	841	CLA	C1B-NB	-2.27	1.34	1.37
19	A	823	CLA	C1B-NB	-2.27	1.34	1.37
19	3	309	CLA	C1B-NB	-2.27	1.34	1.37
19	3	311	CLA	C1B-NB	-2.27	1.34	1.37
19	G	201	CLA	C1B-NB	-2.27	1.34	1.37
24	A	846	LMT	O3B-C3B	-2.27	1.37	1.43
19	A	820	CLA	C1B-NB	-2.27	1.34	1.37
19	K	1003	CLA	C2B-C1B	2.27	1.45	1.40
19	B	834	CLA	C1B-NB	-2.27	1.34	1.37
19	4	310	CLA	C1B-NB	-2.26	1.34	1.37
19	4	305	CLA	C1B-NB	-2.26	1.34	1.37
19	B	809	CLA	C1B-NB	-2.26	1.34	1.37
19	1	507	CLA	C1B-NB	-2.26	1.34	1.37
19	3	310	CLA	C4B-NB	-2.26	1.34	1.37
19	B	803	CLA	C1B-NB	-2.26	1.34	1.37
19	B	830	CLA	CHD-C1D	2.26	1.42	1.38
19	A	808	CLA	C4B-NB	-2.26	1.34	1.37
19	J	1102	CLA	C1B-NB	-2.26	1.34	1.37
19	K	1001	CLA	C1B-NB	-2.26	1.34	1.37
19	A	827	CLA	C1B-NB	-2.26	1.34	1.37
19	A	822	CLA	C1B-NB	-2.26	1.34	1.37
19	A	832	CLA	C1B-NB	-2.26	1.34	1.37
19	2	511	CLA	C1B-NB	-2.26	1.34	1.37
19	4	311	CLA	C4B-NB	-2.25	1.34	1.37
19	A	831	CLA	C1B-NB	-2.25	1.34	1.37
19	B	838	CLA	C1B-NB	-2.25	1.34	1.37
19	K	1004	CLA	C2C-C1C	2.25	1.48	1.43
19	A	838	CLA	C1B-NB	-2.25	1.34	1.37
19	B	805	CLA	C1B-NB	-2.25	1.34	1.37
19	4	315	CLA	C4B-NB	-2.25	1.34	1.37
19	A	835	CLA	C1B-NB	-2.25	1.34	1.37
19	J	1105	CLA	C4B-NB	-2.25	1.34	1.37
19	1	511	CLA	C1B-NB	-2.25	1.34	1.37
19	2	504	CLA	C4B-NB	-2.25	1.34	1.37
19	3	307	CLA	C1B-NB	-2.25	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	834	CLA	C1B-NB	-2.25	1.34	1.37
19	B	821	CLA	C1B-NB	-2.24	1.34	1.37
20	3	314	CHL	CHA-CBD	2.24	1.54	1.51
24	J	1107	LMT	O2B-C2B	-2.24	1.37	1.43
19	B	839	CLA	C1B-NB	-2.24	1.34	1.37
19	G	202	CLA	C1B-NB	-2.24	1.34	1.37
19	A	836	CLA	MG-NC	2.24	2.11	2.06
19	B	804	CLA	C1A-CHA	2.24	1.52	1.43
19	B	831	CLA	C4B-NB	-2.24	1.34	1.37
19	B	833	CLA	C4B-NB	-2.24	1.34	1.37
20	2	512	CHL	CHA-CBD	2.24	1.54	1.51
19	B	825	CLA	C4B-NB	-2.24	1.34	1.37
19	K	1003	CLA	C1C-NC	-2.24	1.33	1.38
19	1	505	CLA	C1B-NB	-2.24	1.34	1.37
19	A	824	CLA	C1B-NB	-2.24	1.34	1.37
19	B	832	CLA	C1B-NB	-2.23	1.34	1.37
19	B	837	CLA	C1B-NB	-2.23	1.34	1.37
19	B	832	CLA	C4B-NB	-2.23	1.34	1.37
19	B	819	CLA	C1B-NB	-2.23	1.34	1.37
19	A	854	CLA	C4B-NB	-2.23	1.34	1.37
19	B	812	CLA	C1B-NB	-2.23	1.34	1.37
19	3	306	CLA	C1B-NB	-2.23	1.34	1.37
19	A	814	CLA	C4B-NB	-2.23	1.34	1.37
19	B	823	CLA	C1B-NB	-2.23	1.34	1.37
19	K	1004	CLA	C2B-C1B	2.22	1.45	1.40
19	B	817	CLA	C1B-NB	-2.22	1.34	1.37
19	G	204	CLA	C1B-NB	-2.22	1.34	1.37
24	G	208	LMT	O1'-C1'	-2.22	1.36	1.40
19	A	821	CLA	C4B-NB	-2.22	1.34	1.37
20	4	317	CHL	CHA-CBD	2.22	1.54	1.51
20	1	514	CHL	CHA-CBD	2.22	1.54	1.51
19	4	304	CLA	C4B-NB	-2.22	1.35	1.37
19	A	817	CLA	C1B-NB	-2.21	1.35	1.37
19	B	814	CLA	C4B-NB	-2.21	1.35	1.37
19	B	840	CLA	C1B-NB	-2.21	1.35	1.37
24	3	318	LMT	O2'-C2'	-2.21	1.37	1.43
19	1	513	CLA	C4B-NB	-2.21	1.35	1.37
19	3	312	CLA	C1B-NB	-2.21	1.35	1.37
20	2	513	CHL	C1A-CHA	-2.21	1.37	1.40
19	K	1004	CLA	C1C-NC	-2.21	1.33	1.38
19	B	810	CLA	C4B-NB	-2.21	1.35	1.37
19	3	309	CLA	MG-NC	2.20	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	512	CHL	CBD-CAD	-2.20	1.45	1.53
19	2	505	CLA	C1B-NB	-2.20	1.35	1.37
19	B	824	CLA	C1B-NB	-2.20	1.35	1.37
19	2	506	CLA	C1A-CHA	2.20	1.52	1.43
19	4	307	CLA	C4B-NB	-2.20	1.35	1.37
19	3	310	CLA	C1A-CHA	2.20	1.52	1.43
19	A	832	CLA	C4B-NB	-2.20	1.35	1.37
19	A	815	CLA	C4B-NB	-2.20	1.35	1.37
19	4	308	CLA	C4B-NB	-2.20	1.35	1.37
19	4	304	CLA	C1A-CHA	2.20	1.52	1.43
24	B	855	LMT	O4'-C4B	-2.20	1.37	1.43
19	A	855	CLA	C4B-NB	-2.19	1.35	1.37
24	B	855	LMT	O2'-C2'	-2.19	1.37	1.43
19	H	1000	CLA	C1A-CHA	2.19	1.52	1.43
19	1	510	CLA	C4B-NB	-2.19	1.35	1.37
19	1	508	CLA	C4B-NB	-2.19	1.35	1.37
24	B	846	LMT	O3B-C3B	-2.19	1.37	1.43
19	3	309	CLA	C1A-CHA	2.19	1.52	1.43
19	1	504	CLA	C4B-NB	-2.19	1.35	1.37
19	2	509	CLA	C4B-NB	-2.19	1.35	1.37
19	3	313	CLA	C4B-NB	-2.19	1.35	1.37
19	B	827	CLA	C4B-NB	-2.19	1.35	1.37
19	3	316	CLA	C4B-NB	-2.19	1.35	1.37
19	1	510	CLA	C3D-C4D	-2.19	1.39	1.44
19	1	515	CLA	C4B-NB	-2.19	1.35	1.37
19	A	836	CLA	C4B-NB	-2.18	1.35	1.37
20	2	515	CHL	CHA-CBD	2.18	1.54	1.51
19	4	318	CLA	C4B-NB	-2.18	1.35	1.37
19	B	804	CLA	C4B-NB	-2.18	1.35	1.37
19	2	507	CLA	C4B-NB	-2.18	1.35	1.37
19	A	828	CLA	C1B-NB	-2.18	1.35	1.37
19	4	306	CLA	C4B-NB	-2.18	1.35	1.37
19	A	833	CLA	C4B-NB	-2.18	1.35	1.37
20	1	512	CHL	CHA-CBD	2.18	1.54	1.51
19	3	306	CLA	C4B-NB	-2.18	1.35	1.37
19	A	816	CLA	C4B-NB	-2.18	1.35	1.37
19	F	303	CLA	C1B-NB	-2.18	1.35	1.37
19	A	840	CLA	C4B-NB	-2.18	1.35	1.37
19	B	819	CLA	C4B-NB	-2.18	1.35	1.37
20	2	513	CHL	CHA-CBD	2.18	1.54	1.51
19	3	308	CLA	C4B-NB	-2.18	1.35	1.37
19	B	829	CLA	C4B-NB	-2.18	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	807	CLA	C4B-NB	-2.18	1.35	1.37
19	A	839	CLA	C1B-NB	-2.18	1.35	1.37
19	J	1102	CLA	C4B-NB	-2.17	1.35	1.37
19	1	505	CLA	C1A-CHA	2.17	1.52	1.43
24	G	209	LMT	O1'-C1'	-2.17	1.36	1.40
19	B	820	CLA	C4B-NB	-2.17	1.35	1.37
19	2	510	CLA	C1A-CHA	2.17	1.52	1.43
19	B	826	CLA	MG-NC	2.17	2.11	2.06
19	B	826	CLA	C4B-NB	-2.17	1.35	1.37
19	2	506	CLA	C4B-NB	-2.17	1.35	1.37
19	B	837	CLA	C3D-C4D	-2.17	1.39	1.44
19	B	835	CLA	C4B-NB	-2.17	1.35	1.37
19	J	1101	CLA	C4B-NB	-2.17	1.35	1.37
19	1	509	CLA	C4B-NB	-2.16	1.35	1.37
19	2	508	CLA	C4B-NB	-2.16	1.35	1.37
19	A	813	CLA	C4B-NB	-2.16	1.35	1.37
19	A	838	CLA	C4B-NB	-2.16	1.35	1.37
19	F	302	CLA	C1C-C2C	2.16	1.48	1.44
19	2	514	CLA	C4B-NB	-2.16	1.35	1.37
19	2	510	CLA	C4B-NB	-2.16	1.35	1.37
19	4	312	CLA	C4B-NB	-2.16	1.35	1.37
24	B	855	LMT	O3B-C3B	-2.16	1.37	1.43
19	B	807	CLA	C4B-NB	-2.16	1.35	1.37
19	B	824	CLA	C4B-NB	-2.16	1.35	1.37
19	1	508	CLA	C1A-CHA	2.16	1.52	1.43
19	B	812	CLA	C1C-C2C	2.16	1.48	1.44
19	F	302	CLA	C4B-NB	-2.16	1.35	1.37
19	A	802	CLA	C4B-NB	-2.15	1.35	1.37
19	3	312	CLA	C1A-CHA	2.15	1.52	1.43
20	1	514	CHL	C1A-CHA	-2.15	1.37	1.40
19	A	803	CLA	C4B-NB	-2.15	1.35	1.37
19	B	803	CLA	C4B-NB	-2.15	1.35	1.37
24	G	208	LMT	O3B-C3B	-2.15	1.37	1.43
19	G	204	CLA	C4B-NB	-2.15	1.35	1.37
19	1	516	CLA	C1A-CHA	2.15	1.51	1.43
19	1	506	CLA	MG-NC	2.15	2.11	2.06
19	A	835	CLA	MG-NC	2.15	2.11	2.06
19	B	813	CLA	C4B-NB	-2.14	1.35	1.37
19	B	837	CLA	C4B-NB	-2.14	1.35	1.37
19	B	812	CLA	C4B-NB	-2.14	1.35	1.37
19	A	818	CLA	MG-NC	2.14	2.11	2.06
19	A	825	CLA	C1A-CHA	2.14	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	823	CLA	C4B-NB	-2.14	1.35	1.37
19	2	511	CLA	C4B-NB	-2.14	1.35	1.37
19	3	315	CLA	C4B-NB	-2.14	1.35	1.37
19	A	831	CLA	C4B-NB	-2.14	1.35	1.37
19	B	808	CLA	C4B-NB	-2.14	1.35	1.37
19	A	820	CLA	C1A-CHA	2.14	1.51	1.43
24	2	523	LMT	O2B-C2B	-2.14	1.37	1.43
19	B	826	CLA	C3D-C4D	-2.14	1.39	1.44
19	A	819	CLA	C4B-NB	-2.14	1.35	1.37
19	B	836	CLA	C4B-NB	-2.14	1.35	1.37
19	B	830	CLA	C4B-NB	-2.14	1.35	1.37
19	2	508	CLA	C1A-CHA	2.14	1.51	1.43
19	3	313	CLA	C1A-CHA	2.14	1.51	1.43
19	L	305	CLA	MG-NC	2.13	2.11	2.06
19	A	833	CLA	C1C-C2C	2.13	1.48	1.44
19	B	824	CLA	C1A-CHA	2.13	1.51	1.43
22	B	845	LMG	O1-C1	2.13	1.43	1.40
19	A	839	CLA	C4B-NB	-2.13	1.35	1.37
19	A	817	CLA	C4B-NB	-2.13	1.35	1.37
19	F	303	CLA	C4B-NB	-2.13	1.35	1.37
19	4	305	CLA	C1A-CHA	2.13	1.51	1.43
19	2	504	CLA	C1A-CHA	2.13	1.51	1.43
19	L	303	CLA	C4B-NB	-2.13	1.35	1.37
19	K	1003	CLA	MG-NC	2.13	2.11	2.06
19	B	816	CLA	C1A-CHA	2.13	1.51	1.43
19	B	809	CLA	C4B-NB	-2.13	1.35	1.37
19	1	507	CLA	C4B-NB	-2.12	1.35	1.37
19	A	820	CLA	C4B-NB	-2.12	1.35	1.37
19	K	1002	CLA	C4B-NB	-2.12	1.35	1.37
19	B	811	CLA	C3D-C4D	-2.12	1.39	1.44
19	3	312	CLA	C4B-NB	-2.12	1.35	1.37
24	G	209	LMT	O3B-C3B	-2.12	1.37	1.43
19	B	805	CLA	C4B-NB	-2.12	1.35	1.37
19	B	817	CLA	C4B-NB	-2.12	1.35	1.37
19	B	828	CLA	C4B-NB	-2.12	1.35	1.37
19	B	816	CLA	C4B-NB	-2.12	1.35	1.37
19	A	818	CLA	C1A-CHA	2.12	1.51	1.43
24	B	846	LMT	O2B-C2B	-2.12	1.37	1.43
19	A	842	CLA	C4B-NB	-2.12	1.35	1.37
19	B	834	CLA	CHC-C1C	2.12	1.42	1.38
19	A	811	CLA	C1A-CHA	2.12	1.51	1.43
19	L	303	CLA	C1A-CHA	2.12	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	847	LMT	O2B-C2B	-2.12	1.37	1.43
19	4	310	CLA	C1C-C2C	2.12	1.48	1.44
19	2	505	CLA	C1A-CHA	2.12	1.51	1.43
19	A	812	CLA	C1A-CHA	2.12	1.51	1.43
19	1	506	CLA	C4B-NB	-2.12	1.35	1.37
19	H	1000	CLA	C4B-NB	-2.12	1.35	1.37
19	A	818	CLA	C4B-NB	-2.12	1.35	1.37
19	3	311	CLA	C4B-NB	-2.12	1.35	1.37
24	4	320	LMT	O2'-C2'	-2.12	1.37	1.43
19	K	1002	CLA	MG-NC	2.11	2.11	2.06
19	K	1004	CLA	MG-NC	2.11	2.11	2.06
24	B	846	LMT	O2'-C2'	-2.11	1.37	1.43
19	B	834	CLA	C1C-C2C	2.11	1.48	1.44
19	4	310	CLA	C1A-CHA	2.11	1.51	1.43
19	A	827	CLA	C4B-NB	-2.11	1.35	1.37
19	G	202	CLA	C4B-NB	-2.11	1.35	1.37
19	A	805	CLA	C1C-C2C	2.11	1.48	1.44
19	A	835	CLA	C4B-NB	-2.11	1.35	1.37
24	B	847	LMT	O3B-C3B	-2.11	1.37	1.43
19	3	309	CLA	C4B-NB	-2.11	1.35	1.37
19	B	822	CLA	C4B-NB	-2.11	1.35	1.37
19	L	301	CLA	C4B-NB	-2.11	1.35	1.37
19	A	834	CLA	C4B-NB	-2.11	1.35	1.37
19	2	506	CLA	MG-NC	2.11	2.11	2.06
19	3	312	CLA	MG-NC	2.10	2.11	2.06
19	A	826	CLA	C4B-NB	-2.10	1.35	1.37
19	G	201	CLA	C1A-CHA	2.10	1.51	1.43
24	J	1107	LMT	O3B-C3B	-2.10	1.37	1.43
19	B	814	CLA	MG-NC	2.10	2.11	2.06
24	G	209	LMT	O2B-C2B	-2.10	1.37	1.43
19	A	810	CLA	C1C-C2C	2.10	1.48	1.44
19	B	839	CLA	C4B-NB	-2.10	1.35	1.37
19	B	833	CLA	C3D-C4D	-2.10	1.39	1.44
19	1	505	CLA	C4B-NB	-2.10	1.35	1.37
19	A	809	CLA	C4B-NB	-2.10	1.35	1.37
19	A	823	CLA	C1A-CHA	2.10	1.51	1.43
20	4	316	CHL	C1A-CHA	-2.10	1.37	1.40
19	A	810	CLA	C4B-NB	-2.10	1.35	1.37
24	4	320	LMT	O2B-C2B	-2.10	1.37	1.43
19	B	821	CLA	C1A-CHA	2.10	1.51	1.43
19	K	1002	CLA	C1A-CHA	2.10	1.51	1.43
24	G	209	LMT	O2'-C2'	-2.10	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	516	CHL	CHA-CBD	2.10	1.54	1.51
19	A	825	CLA	C4B-NB	-2.10	1.35	1.37
19	B	811	CLA	C4B-NB	-2.10	1.35	1.37
19	K	1001	CLA	C4B-NB	-2.10	1.35	1.37
24	4	320	LMT	O3B-C3B	-2.10	1.37	1.43
19	1	507	CLA	C3D-C4D	-2.10	1.39	1.44
19	A	823	CLA	C4B-NB	-2.10	1.35	1.37
19	B	834	CLA	C4B-NB	-2.10	1.35	1.37
19	3	317	CLA	C1C-C2C	2.09	1.48	1.44
20	4	313	CHL	CHA-CBD	2.09	1.54	1.51
19	B	813	CLA	C1A-CHA	2.09	1.51	1.43
19	4	310	CLA	C4B-NB	-2.09	1.35	1.37
19	B	840	CLA	C4B-NB	-2.09	1.35	1.37
19	G	202	CLA	C1A-CHA	2.09	1.51	1.43
19	A	822	CLA	C4B-NB	-2.09	1.35	1.37
19	G	203	CLA	C4B-NB	-2.09	1.35	1.37
19	A	815	CLA	C1A-CHA	2.09	1.51	1.43
19	1	515	CLA	MG-NC	2.09	2.11	2.06
19	J	1105	CLA	C3D-C4D	-2.09	1.39	1.44
20	4	316	CHL	CHA-CBD	2.09	1.54	1.51
19	B	822	CLA	C1A-CHA	2.09	1.51	1.43
19	L	305	CLA	C4B-NB	-2.09	1.35	1.37
19	G	203	CLA	C1A-CHA	2.09	1.51	1.43
24	A	846	LMT	O2B-C2B	-2.09	1.37	1.43
19	1	516	CLA	C4B-NB	-2.09	1.35	1.37
24	B	846	LMT	O1'-C1'	-2.09	1.36	1.40
19	1	504	CLA	C1A-CHA	2.09	1.51	1.43
17	1	501	LUT	C1-C6	-2.08	1.51	1.53
19	H	1000	CLA	MG-NC	2.08	2.11	2.06
19	B	818	CLA	C1A-CHA	2.08	1.51	1.43
19	A	806	CLA	C4B-NB	-2.08	1.35	1.37
19	A	820	CLA	MG-NC	2.08	2.11	2.06
19	3	317	CLA	C4B-NB	-2.08	1.35	1.37
19	A	802	CLA	C1A-CHA	2.08	1.51	1.43
19	A	816	CLA	C1A-CHA	2.08	1.51	1.43
24	2	523	LMT	O3B-C3B	-2.08	1.37	1.43
19	B	818	CLA	C4B-NB	-2.08	1.35	1.37
19	A	812	CLA	C4B-NB	-2.08	1.35	1.37
19	2	505	CLA	MG-NC	2.08	2.11	2.06
24	B	855	LMT	O1'-C1'	-2.08	1.36	1.40
20	4	314	CHL	CHA-CBD	2.08	1.54	1.51
19	A	824	CLA	C4B-NB	-2.08	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	825	CLA	C1A-CHA	2.08	1.51	1.43
19	B	829	CLA	CHD-C1D	2.07	1.42	1.38
19	A	814	CLA	C1A-CHA	2.07	1.51	1.43
19	A	835	CLA	C1A-CHA	2.07	1.51	1.43
19	L	304	CLA	C4B-NB	-2.07	1.35	1.37
19	3	305	CLA	C4B-NB	-2.07	1.35	1.37
19	L	301	CLA	C1C-C2C	2.07	1.48	1.44
19	A	803	CLA	MG-NC	2.07	2.11	2.06
19	B	828	CLA	CHD-C1D	2.07	1.42	1.38
19	B	823	CLA	C3D-C4D	-2.07	1.39	1.44
19	3	307	CLA	C4B-NB	-2.07	1.35	1.37
19	3	311	CLA	MG-NC	2.07	2.11	2.06
19	A	818	CLA	C1C-C2C	2.07	1.48	1.44
24	J	1107	LMT	O2'-C2'	-2.07	1.37	1.43
19	B	814	CLA	CHD-C1D	2.07	1.42	1.38
19	B	810	CLA	C1A-CHA	2.07	1.51	1.43
19	3	305	CLA	C1C-C2C	2.07	1.48	1.44
19	B	828	CLA	C1A-CHA	2.07	1.51	1.43
19	1	511	CLA	C4B-NB	-2.06	1.35	1.37
19	4	305	CLA	C4B-NB	-2.06	1.35	1.37
19	A	829	CLA	C4B-NB	-2.06	1.35	1.37
19	A	805	CLA	C4B-NB	-2.06	1.35	1.37
19	A	837	CLA	MG-NC	2.06	2.11	2.06
19	A	827	CLA	C1A-CHA	2.06	1.51	1.43
19	2	511	CLA	C1A-CHA	2.06	1.51	1.43
19	A	827	CLA	C1C-C2C	2.06	1.48	1.44
24	G	208	LMT	O2'-C2'	-2.06	1.37	1.43
19	G	204	CLA	MG-NC	2.06	2.11	2.06
19	3	316	CLA	C1A-CHA	2.06	1.51	1.43
19	A	841	CLA	C1C-C2C	2.06	1.48	1.44
24	3	318	LMT	O3B-C3B	-2.06	1.37	1.43
19	A	814	CLA	MG-NC	2.06	2.11	2.06
19	L	305	CLA	C1A-CHA	2.06	1.51	1.43
19	3	316	CLA	CHD-C1D	2.06	1.42	1.38
19	A	804	CLA	C4B-NB	-2.06	1.35	1.37
19	A	833	CLA	C1A-CHA	2.05	1.51	1.43
19	A	810	CLA	CHC-C1C	2.05	1.42	1.38
19	A	823	CLA	C1C-C2C	2.05	1.48	1.44
19	L	305	CLA	C1C-C2C	2.05	1.48	1.44
19	A	819	CLA	C1A-CHA	2.05	1.51	1.43
19	B	821	CLA	C4B-NB	-2.05	1.35	1.37
19	B	824	CLA	C1C-C2C	2.05	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	318	CLA	C1A-CHA	2.05	1.51	1.43
19	2	505	CLA	C4B-NB	-2.05	1.35	1.37
19	A	855	CLA	C3D-C4D	-2.05	1.39	1.44
19	B	831	CLA	C1C-C2C	2.05	1.48	1.44
20	2	526	CHL	CHA-CBD	2.05	1.54	1.51
19	G	201	CLA	C4B-NB	-2.05	1.35	1.37
19	A	842	CLA	C1A-CHA	2.05	1.51	1.43
19	A	833	CLA	CHC-C1C	2.05	1.42	1.38
19	3	305	CLA	C3D-C4D	-2.04	1.39	1.44
19	A	830	CLA	C4B-NB	-2.04	1.35	1.37
19	B	830	CLA	MG-NC	2.04	2.11	2.06
19	3	317	CLA	C1A-CHA	2.04	1.51	1.43
19	2	514	CLA	C1A-CHA	2.04	1.51	1.43
19	4	306	CLA	C1A-CHA	2.04	1.51	1.43
19	K	1001	CLA	MG-NC	2.04	2.11	2.06
19	4	309	CLA	C1A-CHA	2.04	1.51	1.43
19	A	804	CLA	C1A-CHA	2.04	1.51	1.43
19	B	827	CLA	C1A-CHA	2.04	1.51	1.43
19	A	828	CLA	C1A-CHA	2.04	1.51	1.43
19	3	311	CLA	C1A-CHA	2.04	1.51	1.43
19	3	316	CLA	MG-NC	2.04	2.11	2.06
19	B	830	CLA	C3D-C4D	-2.04	1.39	1.44
19	B	808	CLA	C1C-C2C	2.03	1.48	1.44
19	G	203	CLA	MG-NC	2.03	2.11	2.06
19	4	315	CLA	CHD-C1D	2.03	1.42	1.38
19	B	820	CLA	CHD-C1D	2.03	1.42	1.38
19	2	510	CLA	MG-NC	2.03	2.11	2.06
19	B	817	CLA	CHD-C1D	2.03	1.42	1.38
19	B	831	CLA	C1A-CHA	2.03	1.51	1.43
19	A	806	CLA	C1A-CHA	2.03	1.51	1.43
19	4	305	CLA	MG-NC	2.03	2.11	2.06
19	A	837	CLA	C1C-C2C	2.03	1.48	1.44
19	B	826	CLA	C1A-CHA	2.03	1.51	1.43
19	A	804	CLA	C1C-C2C	2.03	1.48	1.44
19	A	829	CLA	C1A-CHA	2.03	1.51	1.43
19	K	1001	CLA	C3D-C4D	-2.02	1.39	1.44
19	A	854	CLA	MG-NC	2.02	2.11	2.06
19	B	817	CLA	C1C-C2C	2.02	1.48	1.44
19	4	307	CLA	C3D-C4D	-2.02	1.39	1.44
18	2	503	BCR	C40-C30	-2.02	1.49	1.53
19	A	826	CLA	C1C-C2C	2.02	1.48	1.44
19	B	837	CLA	C1A-CHA	2.02	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	807	CLA	CHD-C1D	2.02	1.42	1.38
19	3	307	CLA	C1A-CHA	2.02	1.51	1.43
19	A	841	CLA	C4B-NB	-2.02	1.35	1.37
19	B	818	CLA	MG-NC	2.02	2.11	2.06
19	B	805	CLA	C1A-CHA	2.02	1.51	1.43
19	3	306	CLA	C1A-CHA	2.02	1.51	1.43
19	A	855	CLA	MG-NC	2.02	2.11	2.06
19	4	312	CLA	C1A-CHA	2.02	1.51	1.43
19	A	802	CLA	C3D-C4D	-2.02	1.39	1.44
19	G	204	CLA	C1A-CHA	2.02	1.51	1.43
19	A	840	CLA	MG-NC	2.02	2.11	2.06
19	A	809	CLA	C1A-CHA	2.02	1.51	1.43
19	1	509	CLA	MG-NC	2.02	2.11	2.06
19	B	833	CLA	CHD-C1D	2.02	1.42	1.38
24	A	846	LMT	O2'-C2'	-2.02	1.38	1.43
19	B	835	CLA	MG-NC	2.02	2.11	2.06
19	1	515	CLA	C3D-C4D	-2.01	1.39	1.44
19	B	809	CLA	MG-NC	2.01	2.11	2.06
24	2	523	LMT	O2'-C2'	-2.01	1.38	1.43
19	1	505	CLA	MG-NC	2.01	2.11	2.06
19	A	810	CLA	MG-NC	2.01	2.11	2.06
19	4	310	CLA	MG-NC	2.01	2.11	2.06
19	F	302	CLA	C1A-CHA	2.01	1.51	1.43
19	A	810	CLA	C1A-CHA	2.01	1.51	1.43
19	B	829	CLA	C3D-C4D	-2.01	1.39	1.44
19	B	812	CLA	CHC-C1C	2.01	1.42	1.38
19	B	805	CLA	C3D-C4D	-2.01	1.39	1.44
19	A	807	CLA	C1A-CHA	2.01	1.51	1.43
19	B	838	CLA	C4B-NB	-2.01	1.35	1.37
19	A	813	CLA	C1C-C2C	2.01	1.48	1.44
19	A	822	CLA	C1C-C2C	2.01	1.48	1.44
19	F	302	CLA	MG-NC	2.01	2.11	2.06
19	1	511	CLA	C3D-C4D	-2.00	1.39	1.44
19	B	809	CLA	C1A-CHA	2.00	1.51	1.43
19	A	842	CLA	MG-NC	2.00	2.11	2.06
19	J	1102	CLA	MG-NC	2.00	2.11	2.06
19	G	202	CLA	C1C-C2C	2.00	1.48	1.44
19	B	827	CLA	MG-NC	2.00	2.11	2.06
19	B	811	CLA	CHC-C1C	2.00	1.42	1.38
19	A	837	CLA	C1A-CHA	2.00	1.51	1.43
19	A	803	CLA	C1C-C2C	2.00	1.48	1.44
19	3	308	CLA	MG-NC	2.00	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	308	CLA	C3D-C4D	-2.00	1.39	1.44
19	A	830	CLA	MG-NC	2.00	2.11	2.06

All (2748) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	802	BCR	C16-C15-C14	18.74	161.87	123.52
18	B	849	BCR	C21-C20-C19	15.46	168.01	123.20
18	I	101	BCR	C16-C15-C14	15.14	154.50	123.52
18	3	304	BCR	C21-C20-C19	15.07	166.87	123.20
27	A	801	CL0	C1B-CHB-C4A	14.70	130.78	121.32
18	A	856	BCR	C21-C20-C19	14.61	165.52	123.20
18	A	850	BCR	C21-C20-C19	14.15	164.19	123.20
18	3	304	BCR	C16-C15-C14	13.98	152.13	123.52
18	3	303	BCR	C16-C15-C14	13.92	152.00	123.52
18	A	849	BCR	C21-C20-C19	13.72	162.95	123.20
18	2	503	BCR	C16-C15-C14	13.70	151.55	123.52
18	A	849	BCR	C11-C10-C9	13.68	146.47	127.28
18	A	850	BCR	C16-C15-C14	13.51	151.15	123.52
18	L	302	BCR	C16-C15-C14	13.36	150.85	123.52
18	G	205	BCR	C16-C15-C14	13.36	150.85	123.52
18	B	802	BCR	C11-C10-C9	13.25	145.86	127.28
18	4	301	BCR	C16-C15-C14	13.19	150.51	123.52
18	L	307	BCR	C16-C15-C14	12.89	149.89	123.52
18	A	856	BCR	C16-C15-C14	12.84	149.78	123.52
18	L	302	BCR	C21-C20-C19	12.83	160.37	123.20
18	K	1005	BCR	C16-C15-C14	12.80	149.70	123.52
18	G	205	BCR	C21-C20-C19	12.78	160.23	123.20
18	A	848	BCR	C21-C20-C19	12.67	159.91	123.20
18	L	307	BCR	C11-C10-C9	12.58	144.92	127.28
18	B	802	BCR	C21-C20-C19	12.57	159.62	123.20
18	L	307	BCR	C21-C20-C19	12.41	159.15	123.20
18	I	102	BCR	C16-C15-C14	12.40	148.90	123.52
18	A	848	BCR	C11-C10-C9	12.37	144.62	127.28
18	B	849	BCR	C11-C10-C9	12.29	144.52	127.28
18	2	503	BCR	C11-C10-C9	12.22	144.41	127.28
18	K	1005	BCR	C11-C10-C9	12.21	144.41	127.28
18	I	102	BCR	C21-C20-C19	12.07	158.19	123.20
18	4	301	BCR	C21-C20-C19	12.03	158.05	123.20
18	A	851	BCR	C11-C10-C9	12.02	144.13	127.28
18	B	853	BCR	C11-C10-C9	11.91	143.98	127.28
18	A	851	BCR	C16-C15-C14	11.80	147.66	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	4	303	XAT	O4-C5-C18	-11.76	101.90	115.05
18	4	301	BCR	C11-C10-C9	11.73	143.73	127.28
18	J	1108	BCR	C21-C20-C19	11.72	157.16	123.20
18	F	306	BCR	C16-C15-C14	11.68	147.42	123.52
18	B	850	BCR	C16-C15-C14	11.68	147.42	123.52
18	F	306	BCR	C21-C20-C19	11.67	157.00	123.20
18	I	101	BCR	C11-C10-C9	11.62	143.57	127.28
18	K	1005	BCR	C21-C20-C19	11.56	156.69	123.20
18	L	306	BCR	C21-C20-C19	11.52	156.57	123.20
18	B	856	BCR	C21-C20-C19	11.41	156.27	123.20
18	A	848	BCR	C16-C15-C14	11.41	146.86	123.52
18	A	851	BCR	C21-C20-C19	11.37	156.15	123.20
18	B	851	BCR	C16-C15-C14	11.34	146.73	123.52
19	3	310	CLA	C4A-NA-C1A	11.28	111.83	106.68
18	I	101	BCR	C21-C20-C19	11.20	155.65	123.20
18	B	853	BCR	C16-C15-C14	11.15	146.34	123.52
18	3	303	BCR	C11-C10-C9	11.09	142.83	127.28
18	2	503	BCR	C21-C20-C19	11.05	155.21	123.20
18	B	850	BCR	C21-C20-C19	11.01	155.09	123.20
18	1	503	BCR	C21-C20-C19	10.95	154.92	123.20
18	L	306	BCR	C11-C10-C9	10.81	142.44	127.28
18	A	856	BCR	C11-C10-C9	10.77	142.38	127.28
18	3	303	BCR	C21-C20-C19	10.71	154.22	123.20
18	A	852	BCR	C21-C20-C19	10.66	154.09	123.20
18	B	856	BCR	C11-C10-C9	10.66	142.22	127.28
18	B	856	BCR	C16-C15-C14	10.61	145.23	123.52
18	3	304	BCR	C11-C10-C9	10.50	142.01	127.28
18	B	852	BCR	C11-C10-C9	10.48	141.98	127.28
18	I	102	BCR	C11-C10-C9	10.38	141.84	127.28
18	A	849	BCR	C16-C15-C14	10.38	144.75	123.52
18	A	852	BCR	C16-C15-C14	10.33	144.66	123.52
19	A	828	CLA	C4A-NA-C1A	10.31	111.38	106.68
18	F	306	BCR	C11-C10-C9	10.28	141.69	127.28
19	2	504	CLA	C4A-NA-C1A	10.26	111.36	106.68
18	L	306	BCR	C16-C15-C14	10.22	144.42	123.52
18	B	852	BCR	C16-C15-C14	10.18	144.35	123.52
17	J	1109	LUT	C21-C26-C27	10.16	124.51	112.83
18	B	852	BCR	C21-C20-C19	10.10	152.45	123.20
19	B	803	CLA	C4A-NA-C1A	9.99	111.23	106.68
18	B	850	BCR	C11-C10-C9	9.97	141.26	127.28
18	B	852	BCR	C20-C19-C18	9.86	153.39	126.36
18	B	851	BCR	C11-C10-C9	9.70	140.88	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	804	CLA	C4A-NA-C1A	9.69	111.10	106.68
18	A	852	BCR	C20-C19-C18	9.67	152.88	126.36
18	B	853	BCR	C20-C19-C18	9.65	152.82	126.36
18	J	1108	BCR	C16-C15-C14	9.64	143.25	123.52
19	3	305	CLA	C4A-NA-C1A	9.64	111.08	106.68
19	4	318	CLA	C4A-NA-C1A	9.62	111.07	106.68
19	4	304	CLA	C4A-NA-C1A	9.60	111.06	106.68
19	2	508	CLA	C4A-NA-C1A	9.56	111.04	106.68
18	I	101	BCR	C20-C19-C18	9.56	152.58	126.36
18	1	503	BCR	C20-C19-C18	9.54	152.53	126.36
18	F	306	BCR	C20-C19-C18	9.51	152.43	126.36
19	A	803	CLA	C4A-NA-C1A	9.50	111.01	106.68
18	B	849	BCR	C16-C15-C14	9.50	142.96	123.52
19	B	810	CLA	C4A-NA-C1A	9.49	111.01	106.68
19	2	506	CLA	C4A-NA-C1A	9.47	111.00	106.68
19	A	840	CLA	C4A-NA-C1A	9.46	110.99	106.68
18	B	853	BCR	C21-C20-C19	9.44	150.57	123.20
19	B	824	CLA	C4A-NA-C1A	9.44	110.99	106.68
18	3	303	BCR	C20-C19-C18	9.44	152.25	126.36
19	3	312	CLA	C4A-NA-C1A	9.43	110.98	106.68
19	3	315	CLA	C4A-NA-C1A	9.43	110.98	106.68
19	A	808	CLA	C4A-NA-C1A	9.42	110.97	106.68
19	H	1000	CLA	C4A-NA-C1A	9.41	110.97	106.68
19	4	309	CLA	C4A-NA-C1A	9.40	110.97	106.68
19	G	201	CLA	C4A-NA-C1A	9.36	110.95	106.68
19	A	802	CLA	C4A-NA-C1A	9.35	110.94	106.68
19	A	810	CLA	C4A-NA-C1A	9.34	110.94	106.68
19	A	854	CLA	C4A-NA-C1A	9.33	110.93	106.68
19	J	1105	CLA	C4A-NA-C1A	9.32	110.93	106.68
19	A	804	CLA	C4A-NA-C1A	9.32	110.93	106.68
19	B	806	CLA	C4A-NA-C1A	9.30	110.92	106.68
19	B	815	CLA	C4A-NA-C1A	9.30	110.92	106.68
19	B	825	CLA	C4A-NA-C1A	9.30	110.92	106.68
19	L	303	CLA	C4A-NA-C1A	9.30	110.92	106.68
19	2	514	CLA	C4A-NA-C1A	9.29	110.92	106.68
19	B	827	CLA	C4A-NA-C1A	9.29	110.92	106.68
19	A	811	CLA	C4A-NA-C1A	9.28	110.92	106.68
19	4	315	CLA	C4A-NA-C1A	9.26	110.91	106.68
19	B	828	CLA	C4A-NA-C1A	9.26	110.91	106.68
19	J	1102	CLA	C4A-NA-C1A	9.26	110.90	106.68
18	J	1108	BCR	C11-C10-C9	9.21	140.20	127.28
19	2	510	CLA	C4A-NA-C1A	9.21	110.88	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	856	BCR	C20-C19-C18	9.20	151.60	126.36
19	A	820	CLA	C4A-NA-C1A	9.18	110.87	106.68
19	3	306	CLA	C4A-NA-C1A	9.17	110.86	106.68
19	4	311	CLA	C4A-NA-C1A	9.14	110.85	106.68
18	G	205	BCR	C11-C10-C9	9.11	140.06	127.28
19	A	842	CLA	C4A-NA-C1A	9.11	110.83	106.68
19	1	504	CLA	C4A-NA-C1A	9.10	110.83	106.68
19	4	308	CLA	C4A-NA-C1A	9.09	110.82	106.68
19	A	829	CLA	C4A-NA-C1A	9.08	110.82	106.68
18	A	852	BCR	C11-C10-C9	9.05	139.97	127.28
19	2	511	CLA	C4A-NA-C1A	9.05	110.81	106.68
19	A	816	CLA	C4A-NA-C1A	9.05	110.81	106.68
18	L	302	BCR	C11-C10-C9	9.04	139.96	127.28
19	3	316	CLA	C4A-NA-C1A	9.04	110.80	106.68
19	A	806	CLA	C4A-NA-C1A	9.04	110.80	106.68
19	B	822	CLA	C4A-NA-C1A	9.03	110.80	106.68
18	A	851	BCR	C20-C19-C18	9.03	151.11	126.36
19	B	816	CLA	C4A-NA-C1A	9.01	110.79	106.68
18	B	850	BCR	C20-C19-C18	9.00	151.05	126.36
19	1	505	CLA	C4A-NA-C1A	8.99	110.78	106.68
19	1	516	CLA	C4A-NA-C1A	8.99	110.78	106.68
19	1	506	CLA	C4A-NA-C1A	8.99	110.78	106.68
19	B	821	CLA	C4A-NA-C1A	8.98	110.78	106.68
19	A	841	CLA	C4A-NA-C1A	8.92	110.75	106.68
27	A	801	CL0	O2D-CGD-CBD	8.90	120.72	110.95
19	3	313	CLA	C4A-NA-C1A	8.89	110.74	106.68
20	1	521	CHL	C1B-CHB-C4A	8.89	127.04	121.32
18	I	102	BCR	C20-C19-C18	8.88	150.71	126.36
18	L	306	BCR	C20-C19-C18	8.88	150.70	126.36
19	A	825	CLA	C4A-NA-C1A	8.86	110.72	106.68
19	B	805	CLA	C4A-NA-C1A	8.86	110.72	106.68
19	A	813	CLA	C4A-NA-C1A	8.86	110.72	106.68
19	A	827	CLA	C4A-NA-C1A	8.85	110.72	106.68
19	A	809	CLA	C4A-NA-C1A	8.84	110.71	106.68
19	G	204	CLA	C4A-NA-C1A	8.83	110.71	106.68
19	K	1003	CLA	C4A-NA-C1A	8.82	110.70	106.68
19	A	839	CLA	C4A-NA-C1A	8.80	110.69	106.68
19	2	507	CLA	C4A-NA-C1A	8.77	110.68	106.68
19	1	508	CLA	C4A-NA-C1A	8.76	110.67	106.68
19	B	832	CLA	C4A-NA-C1A	8.76	110.67	106.68
19	A	807	CLA	C4A-NA-C1A	8.71	110.65	106.68
19	L	305	CLA	C4A-NA-C1A	8.71	110.65	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	K	1001	CLA	C4A-NA-C1A	8.70	110.65	106.68
19	B	814	CLA	C4A-NA-C1A	8.70	110.65	106.68
19	B	840	CLA	C4A-NA-C1A	8.69	110.64	106.68
19	1	507	CLA	C4A-NA-C1A	8.68	110.64	106.68
19	J	1101	CLA	C4A-NA-C1A	8.68	110.64	106.68
19	A	812	CLA	C4A-NA-C1A	8.66	110.63	106.68
19	A	834	CLA	C4A-NA-C1A	8.66	110.63	106.68
19	A	832	CLA	C4A-NA-C1A	8.65	110.63	106.68
19	K	1002	CLA	C4A-NA-C1A	8.65	110.63	106.68
19	L	304	CLA	C4A-NA-C1A	8.65	110.63	106.68
19	B	807	CLA	C4A-NA-C1A	8.64	110.62	106.68
19	A	837	CLA	C4A-NA-C1A	8.64	110.62	106.68
19	G	203	CLA	C4A-NA-C1A	8.64	110.62	106.68
19	B	813	CLA	C4A-NA-C1A	8.63	110.61	106.68
19	F	302	CLA	C4A-NA-C1A	8.62	110.61	106.68
18	4	301	BCR	C20-C19-C18	8.61	149.98	126.36
19	A	818	CLA	C4A-NA-C1A	8.61	110.61	106.68
19	F	303	CLA	C4A-NA-C1A	8.59	110.60	106.68
19	A	814	CLA	C4A-NA-C1A	8.57	110.59	106.68
19	A	831	CLA	C4A-NA-C1A	8.56	110.59	106.68
19	B	826	CLA	C4A-NA-C1A	8.55	110.58	106.68
19	G	202	CLA	C4A-NA-C1A	8.54	110.58	106.68
19	1	513	CLA	C4A-NA-C1A	8.54	110.57	106.68
19	B	833	CLA	C4A-NA-C1A	8.53	110.57	106.68
19	3	311	CLA	C4A-NA-C1A	8.53	110.57	106.68
19	A	815	CLA	C4A-NA-C1A	8.52	110.57	106.68
19	B	836	CLA	C4A-NA-C1A	8.51	110.56	106.68
19	A	855	CLA	C4A-NA-C1A	8.51	110.56	106.68
19	A	824	CLA	C4A-NA-C1A	8.50	110.56	106.68
19	A	838	CLA	C4A-NA-C1A	8.49	110.55	106.68
18	J	1108	BCR	C20-C19-C18	8.49	149.65	126.36
19	A	826	CLA	C4A-NA-C1A	8.49	110.55	106.68
19	B	831	CLA	C4A-NA-C1A	8.49	110.55	106.68
19	3	317	CLA	C4A-NA-C1A	8.48	110.55	106.68
19	B	823	CLA	C4A-NA-C1A	8.48	110.55	106.68
19	A	819	CLA	C4A-NA-C1A	8.47	110.54	106.68
19	4	305	CLA	C4A-NA-C1A	8.47	110.54	106.68
19	1	509	CLA	C4A-NA-C1A	8.46	110.54	106.68
19	A	836	CLA	C4A-NA-C1A	8.45	110.54	106.68
19	3	307	CLA	C4A-NA-C1A	8.45	110.53	106.68
19	3	309	CLA	C4A-NA-C1A	8.45	110.53	106.68
19	K	1004	CLA	C4A-NA-C1A	8.44	110.53	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	509	CLA	C4A-NA-C1A	8.44	110.53	106.68
19	B	809	CLA	C4A-NA-C1A	8.42	110.52	106.68
19	4	306	CLA	C4A-NA-C1A	8.42	110.52	106.68
19	2	505	CLA	C4A-NA-C1A	8.41	110.51	106.68
19	B	818	CLA	C4A-NA-C1A	8.40	110.51	106.68
19	A	835	CLA	C4A-NA-C1A	8.37	110.50	106.68
18	L	307	BCR	C20-C19-C18	8.36	149.29	126.36
18	A	850	BCR	C11-C10-C9	8.36	139.00	127.28
19	4	312	CLA	C4A-NA-C1A	8.35	110.49	106.68
19	A	817	CLA	C4A-NA-C1A	8.35	110.49	106.68
19	4	310	CLA	C4A-NA-C1A	8.31	110.47	106.68
19	A	822	CLA	C4A-NA-C1A	8.31	110.47	106.68
19	A	830	CLA	C4A-NA-C1A	8.29	110.46	106.68
19	1	511	CLA	C4A-NA-C1A	8.27	110.45	106.68
19	A	821	CLA	C4A-NA-C1A	8.27	110.45	106.68
19	A	823	CLA	C4A-NA-C1A	8.27	110.45	106.68
19	B	839	CLA	C4A-NA-C1A	8.27	110.45	106.68
19	3	308	CLA	C4A-NA-C1A	8.24	110.44	106.68
19	B	834	CLA	C4A-NA-C1A	8.22	110.43	106.68
19	A	805	CLA	C4A-NA-C1A	8.21	110.42	106.68
18	B	849	BCR	C15-C14-C13	8.20	138.77	127.28
19	4	307	CLA	C4A-NA-C1A	8.18	110.41	106.68
19	B	817	CLA	C4A-NA-C1A	8.18	110.41	106.68
19	B	837	CLA	C4A-NA-C1A	8.17	110.41	106.68
19	B	820	CLA	C4A-NA-C1A	8.11	110.38	106.68
19	L	301	CLA	C4A-NA-C1A	8.10	110.37	106.68
19	B	808	CLA	C4A-NA-C1A	8.09	110.37	106.68
19	B	835	CLA	C4A-NA-C1A	8.08	110.37	106.68
19	A	833	CLA	C4A-NA-C1A	8.07	110.36	106.68
19	B	812	CLA	C4A-NA-C1A	7.97	110.31	106.68
19	B	819	CLA	C4A-NA-C1A	7.96	110.31	106.68
19	1	510	CLA	C4A-NA-C1A	7.90	110.28	106.68
23	4	303	XAT	C18-C5-C4	7.89	123.10	114.24
19	1	515	CLA	C4A-NA-C1A	7.88	110.28	106.68
19	B	838	CLA	C4A-NA-C1A	7.87	110.27	106.68
19	B	829	CLA	C4A-NA-C1A	7.79	110.23	106.68
19	B	830	CLA	C4A-NA-C1A	7.77	110.22	106.68
17	1	502	LUT	C21-C26-C27	7.75	121.73	112.83
18	A	848	BCR	C20-C19-C18	7.71	147.49	126.36
18	B	802	BCR	C15-C14-C13	-7.65	116.55	127.28
20	2	515	CHL	C1B-CHB-C4A	7.57	126.19	121.32
19	B	811	CLA	C4A-NA-C1A	7.54	110.12	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	510	CLA	O2D-CGD-CBD	7.37	124.11	111.23
18	K	1005	BCR	C20-C19-C18	7.27	146.28	126.36
18	B	851	BCR	C21-C20-C19	7.25	144.20	123.20
20	2	526	CHL	C1B-CHB-C4A	7.25	125.98	121.32
20	2	516	CHL	C1B-CHB-C4A	7.22	125.97	121.32
18	A	850	BCR	C20-C19-C18	7.08	145.77	126.36
18	G	205	BCR	C20-C19-C18	6.95	145.43	126.36
18	L	302	BCR	C20-C19-C18	6.88	145.23	126.36
19	1	510	CLA	O2D-CGD-O1D	-6.81	110.60	123.85
18	B	849	BCR	C12-C13-C14	6.73	129.59	119.01
20	4	313	CHL	C1B-CHB-C4A	6.71	125.64	121.32
18	2	503	BCR	C20-C19-C18	6.61	144.50	126.36
18	A	849	BCR	C20-C19-C18	6.50	144.20	126.36
19	1	507	CLA	CMD-C2D-C1D	6.47	136.13	124.73
18	B	802	BCR	C20-C19-C18	6.33	143.71	126.36
18	A	856	BCR	C20-C19-C18	6.23	143.44	126.36
19	K	1001	CLA	CMD-C2D-C1D	6.22	135.68	124.73
20	2	513	CHL	C1B-CHB-C4A	6.13	125.27	121.32
19	B	811	CLA	CMD-C2D-C1D	6.10	135.47	124.73
20	4	314	CHL	C1C-CHC-C4B	6.09	137.85	116.07
26	4	319	DGD	C3G-O3G-C1D	-6.01	100.92	113.80
18	3	304	BCR	C20-C19-C18	6.00	142.81	126.36
20	4	314	CHL	C1A-CHA-C4D	6.00	128.99	118.98
19	4	307	CLA	CMD-C2D-C1D	5.99	135.27	124.73
17	4	302	LUT	C21-C26-C27	5.91	119.62	112.83
19	A	810	CLA	CMD-C2D-C1D	5.88	135.09	124.73
19	2	507	CLA	CMD-C2D-C1D	5.87	135.07	124.73
19	A	805	CLA	CMD-C2D-C1D	5.86	135.05	124.73
19	J	1102	CLA	CMD-C2D-C1D	5.85	135.03	124.73
19	J	1105	CLA	CMD-C2D-C1D	5.85	135.03	124.73
19	4	304	CLA	CMD-C2D-C1D	5.84	135.02	124.73
19	A	822	CLA	CMD-C2D-C1D	5.84	135.01	124.73
19	B	833	CLA	CMD-C2D-C1D	5.83	135.00	124.73
19	B	838	CLA	CMD-C2D-C1D	5.81	134.96	124.73
19	A	808	CLA	CMD-C2D-C1D	5.80	134.94	124.73
20	2	512	CHL	C1C-CHC-C4B	5.77	136.73	116.07
19	B	823	CLA	CMD-C2D-C1D	5.77	134.88	124.73
19	G	202	CLA	CMD-C2D-C1D	5.75	134.86	124.73
18	B	849	BCR	C36-C18-C19	-5.74	109.32	118.09
19	A	827	CLA	CMD-C2D-C1D	5.72	134.80	124.73
19	B	813	CLA	CMD-C2D-C1D	5.71	134.78	124.73
19	1	515	CLA	CMD-C2D-C1D	5.70	134.77	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	306	CLA	CMD-C2D-C1D	5.70	134.76	124.73
19	1	513	CLA	CMD-C2D-C1D	5.70	134.76	124.73
19	B	817	CLA	CMD-C2D-C1D	5.69	134.75	124.73
19	3	310	CLA	CMD-C2D-C1D	5.68	134.73	124.73
19	2	505	CLA	CMD-C2D-C1D	5.68	134.73	124.73
19	A	807	CLA	CMD-C2D-C1D	5.67	134.71	124.73
19	J	1105	CLA	CMA-C3A-C4A	5.67	127.01	111.77
19	3	309	CLA	CMD-C2D-C1D	5.65	134.68	124.73
19	G	203	CLA	CMD-C2D-C1D	5.65	134.68	124.73
19	1	511	CLA	CMD-C2D-C1D	5.65	134.67	124.73
19	A	804	CLA	CMD-C2D-C1D	5.64	134.66	124.73
19	3	307	CLA	CMD-C2D-C1D	5.64	134.66	124.73
19	B	808	CLA	CMD-C2D-C1D	5.64	134.66	124.73
19	A	816	CLA	CMD-C2D-C1D	5.64	134.66	124.73
19	B	819	CLA	CMD-C2D-C1D	5.63	134.65	124.73
19	B	814	CLA	CMD-C2D-C1D	5.63	134.64	124.73
19	J	1101	CLA	CMD-C2D-C1D	5.63	134.64	124.73
19	2	504	CLA	CMD-C2D-C1D	5.62	134.63	124.73
19	A	825	CLA	CMD-C2D-C1D	5.62	134.63	124.73
19	B	830	CLA	CMD-C2D-C1D	5.61	134.60	124.73
19	B	812	CLA	CMD-C2D-C1D	5.60	134.60	124.73
19	F	303	CLA	CMD-C2D-C1D	5.60	134.59	124.73
19	2	508	CLA	CMD-C2D-C1D	5.60	134.58	124.73
19	B	821	CLA	CMD-C2D-C1D	5.59	134.58	124.73
19	B	805	CLA	CMD-C2D-C1D	5.59	134.58	124.73
18	B	849	BCR	C19-C18-C17	5.59	127.80	119.01
19	B	825	CLA	CMD-C2D-C1D	5.59	134.57	124.73
19	K	1002	CLA	CMD-C2D-C1D	5.58	134.56	124.73
19	A	838	CLA	CMD-C2D-C1D	5.58	134.56	124.73
19	3	311	CLA	CMD-C2D-C1D	5.58	134.55	124.73
19	4	305	CLA	CMD-C2D-C1D	5.57	134.54	124.73
19	A	842	CLA	CMD-C2D-C1D	5.57	134.54	124.73
19	A	835	CLA	CMD-C2D-C1D	5.57	134.53	124.73
19	A	814	CLA	CMD-C2D-C1D	5.56	134.52	124.73
19	B	839	CLA	CMD-C2D-C1D	5.56	134.51	124.73
19	G	204	CLA	CMD-C2D-C1D	5.55	134.51	124.73
19	4	312	CLA	CMD-C2D-C1D	5.55	134.50	124.73
19	1	516	CLA	CMD-C2D-C1D	5.55	134.50	124.73
19	H	1000	CLA	CMD-C2D-C1D	5.55	134.49	124.73
19	B	840	CLA	CMD-C2D-C1D	5.54	134.49	124.73
19	3	316	CLA	CMD-C2D-C1D	5.54	134.48	124.73
19	4	315	CLA	CMD-C2D-C1D	5.54	134.48	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	806	CLA	CMD-C2D-C1D	5.53	134.47	124.73
19	B	834	CLA	CMD-C2D-C1D	5.51	134.44	124.73
19	1	509	CLA	CMD-C2D-C1D	5.51	134.43	124.73
19	L	303	CLA	CMD-C2D-C1D	5.48	134.38	124.73
19	L	301	CLA	CMD-C2D-C1D	5.48	134.38	124.73
19	A	813	CLA	CMD-C2D-C1D	5.48	134.38	124.73
19	4	318	CLA	CMD-C2D-C1D	5.47	134.36	124.73
19	A	832	CLA	CMD-C2D-C1D	5.47	134.36	124.73
19	B	818	CLA	CMD-C2D-C1D	5.46	134.35	124.73
19	3	313	CLA	CMD-C2D-C1D	5.46	134.35	124.73
19	A	819	CLA	CMD-C2D-C1D	5.46	134.35	124.73
19	G	201	CLA	CMD-C2D-C1D	5.46	134.35	124.73
23	2	502	XAT	C18-C5-C4	5.46	120.37	114.24
19	B	824	CLA	CMD-C2D-C1D	5.45	134.33	124.73
19	B	836	CLA	CMD-C2D-C1D	5.45	134.32	124.73
19	3	312	CLA	CMD-C2D-C1D	5.44	134.31	124.73
19	4	309	CLA	CMD-C2D-C1D	5.44	134.31	124.73
19	A	831	CLA	CMD-C2D-C1D	5.43	134.29	124.73
19	1	505	CLA	CMD-C2D-C1D	5.43	134.29	124.73
19	4	306	CLA	CMD-C2D-C1D	5.42	134.28	124.73
19	B	809	CLA	CMD-C2D-C1D	5.42	134.28	124.73
19	2	509	CLA	CMD-C2D-C1D	5.42	134.27	124.73
19	3	317	CLA	CMD-C2D-C1D	5.42	134.26	124.73
19	A	830	CLA	CMD-C2D-C1D	5.42	134.26	124.73
19	A	836	CLA	CMD-C2D-C1D	5.41	134.25	124.73
19	A	815	CLA	CMD-C2D-C1D	5.41	134.25	124.73
19	B	807	CLA	CMD-C2D-C1D	5.41	134.25	124.73
19	B	837	CLA	CMD-C2D-C1D	5.39	134.22	124.73
19	3	308	CLA	CMD-C2D-C1D	5.39	134.21	124.73
19	B	835	CLA	CMD-C2D-C1D	5.39	134.21	124.73
19	1	504	CLA	CMD-C2D-C1D	5.37	134.19	124.73
19	L	305	CLA	CMD-C2D-C1D	5.37	134.18	124.73
19	1	508	CLA	CMD-C2D-C1D	5.36	134.18	124.73
19	A	824	CLA	CMD-C2D-C1D	5.36	134.17	124.73
19	A	833	CLA	CMD-C2D-C1D	5.35	134.16	124.73
19	L	304	CLA	CMD-C2D-C1D	5.35	134.14	124.73
19	B	827	CLA	CMD-C2D-C1D	5.35	134.14	124.73
19	4	308	CLA	CMD-C2D-C1D	5.34	134.13	124.73
19	A	829	CLA	CMD-C2D-C1D	5.33	134.12	124.73
20	1	512	CHL	C1C-CHC-C4B	5.33	135.14	116.07
19	A	837	CLA	CMD-C2D-C1D	5.33	134.11	124.73
19	A	812	CLA	CMD-C2D-C1D	5.32	134.10	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	F	301	ZEX	C28-C27-C26	-5.32	118.38	126.94
19	2	511	CLA	CMD-C2D-C1D	5.31	134.09	124.73
23	4	303	XAT	C38-C25-C24	5.31	120.20	114.24
19	B	815	CLA	CMD-C2D-C1D	5.29	134.05	124.73
19	A	834	CLA	CMD-C2D-C1D	5.28	134.02	124.73
19	B	826	CLA	CMD-C2D-C1D	5.28	134.02	124.73
19	B	832	CLA	O2D-CGD-CBD	5.27	120.44	111.23
19	A	821	CLA	CMD-C2D-C1D	5.27	134.01	124.73
19	4	310	CLA	CMD-C2D-C1D	5.27	134.00	124.73
17	3	301	LUT	C21-C26-C27	5.26	118.88	112.83
19	A	855	CLA	CMD-C2D-C1D	5.26	133.99	124.73
19	B	828	CLA	CMD-C2D-C1D	5.26	133.99	124.73
19	A	823	CLA	CMD-C2D-C1D	5.25	133.97	124.73
19	A	811	CLA	CMD-C2D-C1D	5.24	133.96	124.73
19	A	840	CLA	CMD-C2D-C1D	5.24	133.96	124.73
19	A	818	CLA	CMD-C2D-C1D	5.23	133.94	124.73
19	2	510	CLA	CMD-C2D-C1D	5.21	133.91	124.73
19	B	822	CLA	CMD-C2D-C1D	5.20	133.88	124.73
19	A	817	CLA	CMD-C2D-C1D	5.19	133.87	124.73
21	B	842	LHG	O7-C7-C8	5.18	120.33	111.09
19	B	832	CLA	CMD-C2D-C1D	5.16	133.82	124.73
19	B	831	CLA	CMD-C2D-C1D	5.14	133.78	124.73
19	3	315	CLA	CMD-C2D-C1D	5.14	133.77	124.73
19	A	820	CLA	CMD-C2D-C1D	5.12	133.75	124.73
19	4	311	CLA	CMD-C2D-C1D	5.12	133.74	124.73
19	A	806	CLA	CMD-C2D-C1D	5.09	133.70	124.73
19	A	826	CLA	CMD-C2D-C1D	5.09	133.70	124.73
20	4	316	CHL	C1C-CHC-C4B	5.09	134.29	116.07
19	1	506	CLA	CMD-C2D-C1D	5.07	133.66	124.73
20	2	512	CHL	C1A-CHA-C4D	5.05	127.41	118.98
19	2	506	CLA	CMD-C2D-C1D	5.04	133.61	124.73
20	3	314	CHL	C1C-CHC-C4B	5.04	134.09	116.07
20	4	317	CHL	C1C-CHC-C4B	5.04	134.09	116.07
19	3	305	CLA	CMD-C2D-C1D	5.03	133.58	124.73
19	3	305	CLA	O2D-CGD-CBD	5.02	120.01	111.23
19	B	829	CLA	CMD-C2D-C1D	5.02	133.57	124.73
19	A	814	CLA	O2D-CGD-CBD	5.00	119.97	111.23
20	1	514	CHL	C1C-CHC-C4B	4.96	133.82	116.07
19	B	816	CLA	CMD-C2D-C1D	4.96	133.46	124.73
19	B	820	CLA	CMD-C2D-C1D	4.95	133.44	124.73
19	2	514	CLA	CMD-C2D-C1D	4.93	133.42	124.73
19	A	828	CLA	CMD-C2D-C1D	4.93	133.42	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	F	302	CLA	CMD-C2D-C1D	4.86	133.28	124.73
19	A	809	CLA	CMD-C2D-C1D	4.83	133.23	124.73
19	B	810	CLA	CMD-C2D-C1D	4.81	133.20	124.73
17	2	501	LUT	C21-C26-C27	4.80	118.34	112.83
17	3	302	LUT	C21-C26-C27	4.80	118.34	112.83
20	2	512	CHL	CHA-C1A-C2A	-4.80	122.05	133.31
23	2	502	XAT	C38-C25-C24	4.78	119.61	114.24
20	1	514	CHL	C1B-CHB-C4A	4.76	124.39	121.32
19	B	804	CLA	CMD-C2D-C1D	4.75	133.10	124.73
19	A	854	CLA	CMD-C2D-C1D	4.74	133.08	124.73
18	I	101	BCR	C1-C6-C5	-4.72	116.18	122.64
19	A	841	CLA	CMD-C2D-C1D	4.71	133.02	124.73
21	1	520	LHG	O7-C7-C8	4.71	121.66	111.48
19	A	825	CLA	O2D-CGD-CBD	4.70	119.44	111.23
19	A	830	CLA	O2D-CGD-CBD	4.68	119.42	111.23
20	4	313	CHL	C1C-CHC-C4B	4.68	132.81	116.07
19	A	833	CLA	O2D-CGD-CBD	4.68	119.41	111.23
30	F	301	ZEX	C15-C14-C13	-4.66	120.74	127.28
18	1	503	BCR	C38-C26-C25	-4.65	119.41	124.48
19	4	304	CLA	O2A-C1-C2	4.64	125.97	108.11
19	B	829	CLA	O2D-CGD-CBD	4.63	119.33	111.23
19	A	813	CLA	O2D-CGD-CBD	4.61	119.29	111.23
20	2	513	CHL	C1C-CHC-C4B	4.61	132.55	116.07
19	A	839	CLA	CMD-C2D-C1D	4.59	132.81	124.73
21	A	845	LHG	O7-C7-C8	4.58	121.39	111.48
19	B	803	CLA	CMD-C2D-C1D	4.56	132.77	124.73
20	2	526	CHL	C1C-CHC-C4B	4.55	132.35	116.07
22	B	845	LMG	O7-C10-C11	4.53	121.28	111.48
20	2	515	CHL	C1C-CHC-C4B	4.52	132.23	116.07
19	B	815	CLA	O2D-CGD-CBD	4.51	119.11	111.23
30	F	301	ZEX	C7-C8-C9	-4.48	119.60	126.23
19	4	308	CLA	O2A-C1-C2	4.47	125.31	108.11
22	F	304	LMG	O7-C10-C11	4.46	121.13	111.48
27	A	801	CL0	C1C-CHC-C4B	4.46	132.01	116.07
20	2	516	CHL	C1C-CHC-C4B	4.45	132.00	116.07
26	G	207	DGD	O2G-C1B-C2B	4.45	121.11	111.48
22	G	206	LMG	O7-C10-C11	4.44	121.09	111.48
20	3	314	CHL	C1A-CHA-C4D	4.40	126.33	118.98
18	B	849	BCR	C35-C13-C14	-4.40	115.69	122.82
19	B	804	CLA	O2D-CGD-CBD	4.36	118.85	111.23
19	A	808	CLA	O2D-CGD-CBD	4.35	118.84	111.23
19	A	803	CLA	CMD-C2D-C1D	4.34	132.37	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	J	1101	CLA	O2D-CGD-CBD	4.32	118.78	111.23
20	1	512	CHL	C1A-CHA-C4D	4.31	126.18	118.98
19	L	301	CLA	O2A-C1-C2	4.30	124.64	108.11
19	B	824	CLA	O2D-CGD-CBD	4.28	118.72	111.23
19	A	804	CLA	O2D-CGD-CBD	4.27	118.69	111.23
19	B	830	CLA	O2D-CGD-CBD	4.26	118.68	111.23
19	2	507	CLA	O2D-CGD-CBD	4.24	118.64	111.23
18	B	849	BCR	C20-C19-C18	4.22	137.93	126.36
19	2	511	CLA	O2D-CGD-CBD	4.22	118.60	111.23
19	B	817	CLA	O2A-C1-C2	4.22	124.34	108.11
19	1	504	CLA	O2D-CGD-CBD	4.21	118.59	111.23
20	4	317	CHL	C1A-CHA-C4D	4.21	126.00	118.98
20	2	513	CHL	C3D-C4D-CHA	4.20	114.92	108.54
19	A	802	CLA	CMD-C2D-C1D	4.19	132.11	124.73
19	A	809	CLA	O2A-C1-C2	4.18	124.21	108.11
20	1	521	CHL	C1C-CHC-C4B	4.18	131.04	116.07
19	4	307	CLA	O2D-CGD-CBD	4.17	118.53	111.23
19	A	854	CLA	O2D-CGD-CBD	4.16	118.50	111.23
20	4	316	CHL	C1A-CHA-C4D	4.16	125.92	118.98
22	F	305	LMG	O7-C10-C11	4.15	120.47	111.48
19	4	312	CLA	O2D-CGD-CBD	4.14	118.47	111.23
19	3	308	CLA	O2D-CGD-CBD	4.13	118.45	111.23
19	L	301	CLA	O2D-CGD-CBD	4.13	118.45	111.23
20	2	515	CHL	C3D-C4D-CHA	4.12	114.81	108.54
18	3	304	BCR	C39-C30-C25	-4.12	103.78	110.24
17	2	501	LUT	C26-C27-C28	-4.12	118.17	124.58
18	A	852	BCR	C15-C14-C13	4.11	133.04	127.28
19	2	507	CLA	O2A-C1-C2	4.10	123.89	108.11
19	B	825	CLA	O2D-CGD-CBD	4.10	118.40	111.23
19	1	506	CLA	O2A-C1-C2	4.10	123.88	108.11
22	J	1104	LMG	O7-C10-C11	4.09	120.34	111.48
30	F	301	ZEX	C31-C30-C29	-4.09	121.54	127.28
20	2	516	CHL	C3D-C4D-CHA	4.09	114.75	108.54
20	1	521	CHL	C3D-C4D-CHA	4.08	114.73	108.54
19	3	307	CLA	O2A-C1-C2	4.08	123.79	108.11
19	B	819	CLA	O2A-C1-C2	4.07	123.77	108.11
20	1	514	CHL	C3D-C4D-CHA	4.07	114.72	108.54
23	4	303	XAT	C7-C8-C9	-4.06	119.22	125.53
20	1	512	CHL	C3D-C4D-CHA	4.06	114.70	108.54
19	4	305	CLA	O2A-C1-C2	4.04	123.65	108.11
22	1	518	LMG	O7-C10-C11	4.04	120.21	111.48
22	2	519	LMG	O7-C10-C11	4.03	120.20	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	818	CLA	O2D-CGD-CBD	4.02	118.25	111.23
18	B	849	BCR	C11-C12-C13	-4.01	115.38	126.36
18	L	306	BCR	C15-C14-C13	4.01	132.90	127.28
20	4	316	CHL	C1B-CHB-C4A	4.01	123.90	121.32
17	1	501	LUT	C21-C26-C27	4.00	117.43	112.83
19	B	838	CLA	O2A-C1-C2	3.99	123.47	108.11
20	4	313	CHL	C3D-C4D-CHA	3.99	114.60	108.54
17	2	501	LUT	C7-C8-C9	-3.99	120.34	126.23
20	4	316	CHL	C1-O2A-CGA	3.98	126.30	116.65
19	B	821	CLA	O2D-CGD-CBD	3.98	118.19	111.23
19	3	308	CLA	O2A-C1-C2	3.98	123.42	108.11
18	A	851	BCR	C38-C26-C25	-3.97	120.15	124.48
18	4	301	BCR	C38-C26-C25	-3.97	120.16	124.48
19	A	809	CLA	O2D-CGD-CBD	3.97	118.16	111.23
27	A	801	CL0	C1-C2-C3	-3.96	119.71	126.20
19	4	308	CLA	O2D-CGD-CBD	3.95	118.13	111.23
20	4	316	CHL	CHA-C1A-C2A	-3.93	124.07	133.31
19	A	802	CLA	C1-C2-C3	3.93	132.63	126.20
21	1	517	LHG	O7-C7-C8	3.90	119.93	111.48
23	2	502	XAT	C18-C5-C6	-3.90	115.88	122.30
21	B	843	LHG	O7-C7-C8	3.90	119.92	111.48
20	4	317	CHL	C3D-C4D-CHA	3.90	114.47	108.54
20	2	526	CHL	C3D-C4D-CHA	3.90	114.46	108.54
19	A	855	CLA	O2A-C1-C2	3.89	123.09	108.11
19	B	806	CLA	O2D-CGD-CBD	3.89	118.04	111.23
19	B	811	CLA	O2A-C1-C2	3.89	123.06	108.11
19	B	817	CLA	O2D-CGD-CBD	3.88	118.02	111.23
19	B	813	CLA	O2D-CGD-CBD	3.88	118.01	111.23
26	B	801	DGD	O2G-C1B-C2B	3.88	119.87	111.48
20	4	314	CHL	C3D-C4D-CHA	3.87	114.42	108.54
19	A	805	CLA	O2D-CGD-CBD	3.87	117.99	111.23
20	4	314	CHL	CHA-C1A-C2A	-3.86	124.25	133.31
19	1	508	CLA	O2A-C1-C2	3.86	122.95	108.11
18	L	302	BCR	C40-C30-C25	-3.85	104.20	110.24
19	A	831	CLA	O2D-CGD-CBD	3.85	117.95	111.23
19	G	204	CLA	O2D-CGD-CBD	3.84	117.95	111.23
19	B	820	CLA	O2D-CGD-CBD	3.84	117.94	111.23
19	G	201	CLA	O2D-CGD-CBD	3.84	117.94	111.23
19	3	309	CLA	O2D-CGD-CBD	3.84	117.94	111.23
20	4	316	CHL	C3D-C4D-CHA	3.83	114.37	108.54
19	B	807	CLA	O2A-C1-C2	3.83	122.86	108.11
19	2	506	CLA	O2D-CGD-CBD	3.83	117.93	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	510	CLA	CMD-C2D-C1D	3.83	131.47	124.73
19	3	313	CLA	O2D-CGD-CBD	3.83	117.92	111.23
19	A	826	CLA	O2D-CGD-CBD	3.83	117.92	111.23
19	B	805	CLA	O2D-CGD-CBD	3.82	117.91	111.23
19	B	837	CLA	O2A-C1-C2	3.82	122.81	108.11
19	F	302	CLA	O2D-CGD-CBD	3.82	117.91	111.23
19	1	509	CLA	O2A-C1-C2	3.82	122.80	108.11
19	3	316	CLA	O2D-CGD-CBD	3.81	117.90	111.23
19	A	834	CLA	O2A-C1-C2	3.81	122.78	108.11
19	B	809	CLA	O2D-CGD-CBD	3.81	117.89	111.23
19	B	810	CLA	O2A-C1-C2	3.80	122.74	108.11
19	B	816	CLA	O2D-CGD-CBD	3.78	117.84	111.23
19	A	810	CLA	O2D-CGD-CBD	3.78	117.84	111.23
19	3	309	CLA	O2A-C1-C2	3.78	122.65	108.11
19	B	804	CLA	O2A-C1-C2	3.77	122.63	108.11
21	2	517	LHG	O7-C7-C8	3.77	119.64	111.48
19	B	808	CLA	O2A-C1-C2	3.77	122.62	108.11
19	B	834	CLA	C3B-C4B-NB	-3.77	107.16	110.53
17	4	302	LUT	C37-C21-C26	3.76	115.25	109.55
19	3	312	CLA	O2A-C1-C2	3.76	122.04	109.44
20	1	514	CHL	CHA-C1A-C2A	-3.76	124.47	133.31
18	4	301	BCR	C30-C25-C24	3.76	125.85	115.65
20	3	314	CHL	C3D-C4D-CHA	3.75	114.24	108.54
19	2	514	CLA	O2D-CGD-CBD	3.75	117.79	111.23
19	J	1101	CLA	O2A-C1-C2	3.75	122.53	108.11
19	4	318	CLA	O2D-CGD-CBD	3.74	117.77	111.23
19	1	511	CLA	O2D-CGD-CBD	3.74	117.76	111.23
19	L	304	CLA	C1D-ND-C4D	-3.72	103.70	106.31
19	L	304	CLA	O2A-C1-C2	3.71	122.40	108.11
19	A	835	CLA	O2A-C1-C2	3.71	122.39	108.11
19	K	1004	CLA	C1B-NB-C4B	3.71	108.92	106.31
19	A	807	CLA	O2A-C1-C2	3.71	122.37	108.11
19	G	203	CLA	O2D-CGD-CBD	3.69	117.69	111.23
23	4	303	XAT	O4-C5-C4	-3.69	110.04	113.49
19	A	834	CLA	O2D-CGD-CBD	3.68	117.66	111.23
29	A	844	PQN	C14-C13-C15	3.68	121.61	115.23
20	2	526	CHL	CHA-C1A-C2A	-3.67	124.68	133.31
19	B	839	CLA	O2A-C1-C2	3.67	122.25	108.11
19	B	826	CLA	O2A-C1-C2	3.67	122.24	108.11
19	A	828	CLA	O2D-CGD-CBD	3.67	117.65	111.23
19	B	826	CLA	O2D-CGD-CBD	3.66	117.64	111.23
19	4	311	CLA	O2D-CGD-CBD	3.66	117.63	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	856	BCR	C2-C1-C6	3.66	115.75	110.44
20	2	512	CHL	C4D-CHA-CBD	-3.66	105.28	108.97
20	2	512	CHL	CMA-C3A-C4A	3.66	122.49	114.61
20	1	521	CHL	CHA-C1A-C2A	-3.66	124.72	133.31
19	A	806	CLA	O2A-C1-C2	3.65	122.17	108.11
19	A	828	CLA	O2A-C1-C2	3.65	122.17	108.11
19	4	305	CLA	O2D-CGD-CBD	3.65	117.62	111.23
19	B	824	CLA	O2A-C1-C2	3.65	122.16	108.11
19	3	315	CLA	O2A-C1-C2	3.65	122.16	108.11
21	A	853	LHG	O7-C7-C8	3.65	119.37	111.48
19	A	840	CLA	O2D-CGD-CBD	3.65	117.60	111.23
26	B	801	DGD	O3G-C1D-C2D	3.65	113.81	108.27
18	A	851	BCR	C40-C30-C25	-3.65	104.53	110.24
22	B	844	LMG	O7-C10-C11	3.64	119.36	111.48
19	A	829	CLA	O2D-CGD-CBD	3.64	117.60	111.23
18	3	304	BCR	C30-C25-C24	3.64	125.53	115.65
20	4	314	CHL	C4D-CHA-CBD	-3.64	105.30	108.97
17	4	302	LUT	C7-C8-C9	-3.63	120.86	126.23
19	F	303	CLA	C1D-ND-C4D	-3.63	103.76	106.31
19	2	510	CLA	O2A-C1-C2	3.63	122.08	108.11
30	F	301	ZEX	C21-C26-C25	-3.63	120.03	122.84
19	B	816	CLA	O2A-C1-C2	3.63	122.08	108.11
19	3	307	CLA	C1D-ND-C4D	-3.63	103.77	106.31
19	A	831	CLA	O2A-C1-C2	3.63	122.07	108.11
19	1	505	CLA	O2D-CGD-CBD	3.63	117.57	111.23
18	B	851	BCR	C20-C19-C18	3.63	136.31	126.36
19	A	836	CLA	O2D-CGD-CBD	3.62	117.57	111.23
19	B	811	CLA	O2D-CGD-CBD	3.62	117.57	111.23
18	J	1108	BCR	C15-C14-C13	3.62	132.36	127.28
19	B	823	CLA	O2A-C1-C2	3.62	122.04	108.11
19	A	817	CLA	O2A-C1-C2	3.62	122.02	108.11
19	H	1000	CLA	O2A-C1-C2	3.62	122.02	108.11
19	2	511	CLA	O2A-C1-C2	3.61	122.02	108.11
20	1	512	CHL	CHA-C1A-C2A	-3.61	124.82	133.31
18	2	503	BCR	C8-C7-C6	3.61	136.65	127.00
19	L	304	CLA	O2D-CGD-CBD	3.61	117.54	111.23
22	J	1103	LMG	O7-C10-C11	3.60	119.27	111.48
19	4	306	CLA	O2D-CGD-CBD	3.60	117.53	111.23
19	A	804	CLA	O2A-C1-C2	3.59	121.94	108.11
20	4	317	CHL	CHA-C1A-C2A	-3.59	124.87	133.31
19	K	1003	CLA	C1B-NB-C4B	3.59	108.83	106.31
19	L	305	CLA	O2D-CGD-CBD	3.59	117.50	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	J	1106	DGD	O2G-C1B-C2B	3.58	119.24	111.48
22	A	847	LMG	O7-C10-C11	3.58	119.23	111.48
19	A	827	CLA	O2A-C1-C2	3.58	121.89	108.11
19	A	803	CLA	O2D-CGD-CBD	3.58	117.49	111.23
19	A	841	CLA	O2D-CGD-CBD	3.58	117.49	111.23
19	A	812	CLA	O2A-C1-C2	3.58	121.88	108.11
19	B	833	CLA	O2D-CGD-CBD	3.58	117.48	111.23
19	1	507	CLA	O2D-CGD-CBD	3.57	117.47	111.23
21	1	517	LHG	C5-O7-C7	-3.57	109.26	117.80
19	A	818	CLA	O2A-C1-C2	3.57	121.83	108.11
19	4	310	CLA	O2A-C1-C2	3.56	121.83	108.11
19	L	303	CLA	O2D-CGD-CBD	3.56	117.46	111.23
18	B	802	BCR	C19-C18-C17	3.56	124.61	119.01
18	2	503	BCR	C40-C30-C25	-3.55	104.67	110.24
19	3	317	CLA	O2D-CGD-CBD	3.55	117.44	111.23
19	3	308	CLA	CMA-C3A-C4A	3.55	121.32	111.77
19	3	312	CLA	O2D-CGD-CBD	3.55	117.44	111.23
18	B	802	BCR	C35-C13-C14	-3.55	117.06	122.82
19	A	811	CLA	O2A-C1-C2	3.55	121.77	108.11
19	B	814	CLA	O2D-CGD-CBD	3.55	117.43	111.23
19	A	838	CLA	O2D-CGD-CBD	3.55	117.43	111.23
20	1	514	CHL	C1-C2-C3	-3.54	120.39	126.20
19	A	824	CLA	O2A-C1-C2	3.54	121.74	108.11
19	1	507	CLA	O2A-C1-C2	3.54	121.73	108.11
19	K	1001	CLA	O2D-CGD-CBD	3.54	117.42	111.23
19	B	808	CLA	O2D-CGD-CBD	3.54	117.41	111.23
19	A	826	CLA	O2A-C1-C2	3.52	121.67	108.11
19	J	1105	CLA	O2D-CGD-CBD	3.52	117.38	111.23
19	4	307	CLA	O2A-C1-C2	3.52	121.64	108.11
20	2	513	CHL	CHA-C1A-C2A	-3.52	125.05	133.31
19	4	306	CLA	O2A-C1-C2	3.52	121.64	108.11
20	4	313	CHL	C1A-CHA-C4D	3.51	124.84	118.98
19	2	505	CLA	O2D-CGD-CBD	3.51	117.37	111.23
19	A	832	CLA	O2A-C1-C2	3.51	121.62	108.11
17	1	502	LUT	C7-C8-C9	-3.51	121.04	126.23
20	2	516	CHL	CHA-C1A-C2A	-3.51	125.06	133.31
19	B	815	CLA	O2A-C1-C2	3.51	121.60	108.11
19	4	304	CLA	O2D-CGD-CBD	3.50	117.36	111.23
18	3	304	BCR	C30-C25-C26	-3.50	117.85	122.64
19	A	825	CLA	O2A-C1-C2	3.50	121.58	108.11
18	B	802	BCR	C36-C18-C19	-3.50	112.74	118.09
20	1	514	CHL	C3C-C4C-NC	-3.49	106.11	114.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	504	CLA	O2D-CGD-CBD	3.49	117.33	111.23
19	G	202	CLA	O2D-CGD-CBD	3.49	117.32	111.23
19	B	819	CLA	O2D-CGD-CBD	3.49	117.32	111.23
29	B	841	PQN	C11-C12-C13	-3.49	120.83	126.83
19	1	509	CLA	O2D-CGD-CBD	3.48	117.32	111.23
19	4	312	CLA	CAA-CBA-CGA	-3.48	103.33	113.21
18	A	849	BCR	C15-C14-C13	3.47	132.15	127.28
19	A	816	CLA	O2D-CGD-CBD	3.47	117.30	111.23
19	A	807	CLA	O2D-CGD-CBD	3.47	117.30	111.23
20	4	317	CHL	C3C-C4C-NC	-3.47	106.17	114.65
19	B	819	CLA	O2A-CGA-CBA	3.47	122.41	111.83
20	1	512	CHL	C4D-CHA-CBD	-3.47	105.47	108.97
19	1	504	CLA	O2A-C1-C2	3.46	121.43	108.11
19	A	805	CLA	O2A-C1-C2	3.46	121.42	108.11
19	J	1102	CLA	C1D-ND-C4D	-3.46	103.89	106.31
19	A	832	CLA	O2D-CGD-CBD	3.46	117.28	111.23
19	2	508	CLA	O2A-C1-C2	3.46	121.41	108.11
19	A	836	CLA	O2A-C1-C2	3.46	121.41	108.11
19	A	821	CLA	O2D-CGD-CBD	3.45	117.27	111.23
19	A	820	CLA	O2D-CGD-CBD	3.45	117.26	111.23
18	I	101	BCR	C40-C30-C25	-3.45	104.83	110.24
19	A	823	CLA	O2D-CGD-CBD	3.45	117.26	111.23
19	B	805	CLA	O2A-C1-C2	3.44	121.36	108.11
19	2	506	CLA	O2A-C1-C2	3.44	121.35	108.11
19	B	812	CLA	C3B-C4B-NB	-3.44	107.46	110.53
20	2	526	CHL	C3C-C4C-NC	-3.44	106.25	114.65
19	A	811	CLA	O2D-CGD-CBD	3.43	117.23	111.23
19	3	305	CLA	O1D-CGD-CBD	-3.43	117.75	124.52
19	A	817	CLA	O2D-CGD-CBD	3.43	117.22	111.23
19	3	305	CLA	O2A-C1-C2	3.43	121.30	108.11
19	3	317	CLA	C3B-C4B-NB	-3.43	107.47	110.53
20	4	317	CHL	C1B-CHB-C4A	3.42	123.53	121.32
19	4	315	CLA	O2D-CGD-CBD	3.42	117.22	111.23
19	B	839	CLA	O2D-CGD-CBD	3.42	117.21	111.23
19	2	505	CLA	O2A-C1-C2	3.41	121.25	108.11
19	B	822	CLA	O2D-CGD-CBD	3.41	117.20	111.23
19	B	836	CLA	O2D-CGD-CBD	3.41	117.19	111.23
19	3	308	CLA	O2A-CGA-CBA	3.41	122.22	111.83
19	1	510	CLA	C3B-C4B-NB	-3.40	107.49	110.53
19	K	1002	CLA	O2A-C1-C2	3.40	121.20	108.11
19	A	842	CLA	O2A-C1-C2	3.40	121.20	108.11
19	A	838	CLA	O2A-C1-C2	3.40	121.20	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	314	CHL	C3C-C4C-NC	-3.40	106.35	114.65
19	2	509	CLA	O2A-C1-C2	3.40	121.17	108.11
19	4	309	CLA	CAA-CBA-CGA	-3.40	103.57	113.21
19	3	305	CLA	C3B-C4B-NB	-3.39	107.50	110.53
19	B	830	CLA	O2A-C1-C2	3.39	121.17	108.11
19	2	510	CLA	O2D-CGD-CBD	3.39	117.16	111.23
19	A	837	CLA	O2D-CGD-CBD	3.39	117.16	111.23
19	B	835	CLA	O2A-C1-C2	3.38	121.13	108.11
19	A	819	CLA	O2D-CGD-CBD	3.38	117.14	111.23
18	B	850	BCR	C40-C30-C25	-3.38	104.94	110.24
19	A	802	CLA	O2D-CGD-CBD	3.38	117.14	111.23
19	B	835	CLA	O2D-CGD-CBD	3.37	117.13	111.23
19	2	509	CLA	O2D-CGD-CBD	3.37	117.13	111.23
19	1	516	CLA	O2A-C1-C2	3.37	121.09	108.11
19	4	309	CLA	O2D-CGD-CBD	3.37	117.13	111.23
18	B	802	BCR	C12-C13-C14	3.37	124.31	119.01
18	L	302	BCR	C36-C18-C19	-3.37	112.94	118.09
19	3	311	CLA	O2D-CGD-CBD	3.37	117.12	111.23
19	B	814	CLA	O2A-C1-C2	3.37	121.07	108.11
19	B	828	CLA	O2A-C1-C2	3.36	121.05	108.11
19	G	202	CLA	O2A-C1-C2	3.36	121.05	108.11
26	B	854	DGD	O2G-C1B-C2B	3.36	118.75	111.48
19	A	814	CLA	O2A-C1-C2	3.36	121.04	108.11
18	3	303	BCR	C38-C26-C25	-3.36	120.82	124.48
22	4	322	LMG	O7-C10-C11	3.36	118.75	111.48
19	A	810	CLA	O2A-C1-C2	3.36	121.03	108.11
19	B	832	CLA	C1D-ND-C4D	-3.36	103.96	106.31
19	A	822	CLA	O2A-C1-C2	3.35	121.01	108.11
18	B	851	BCR	C38-C26-C25	-3.35	120.83	124.48
19	A	812	CLA	O2D-CGD-CBD	3.35	117.08	111.23
19	B	812	CLA	O2A-C1-C2	3.35	120.98	108.11
19	3	315	CLA	O2D-CGD-CBD	3.34	117.07	111.23
18	A	851	BCR	C2-C1-C6	3.34	115.29	110.44
19	1	513	CLA	O2D-CGD-CBD	3.34	117.07	111.23
20	3	314	CHL	CHA-C1A-C2A	-3.34	125.47	133.31
19	F	303	CLA	O2A-C1-C2	3.34	120.96	108.11
19	B	838	CLA	C1D-ND-C4D	-3.34	103.97	106.31
19	A	810	CLA	C3B-C4B-NB	-3.34	107.55	110.53
19	2	514	CLA	O2A-C1-C2	3.33	120.92	108.11
19	A	819	CLA	O2A-C1-C2	3.33	120.92	108.11
19	3	306	CLA	O2D-CGD-CBD	3.33	117.05	111.23
19	1	516	CLA	O2D-CGD-CBD	3.32	117.04	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	808	CLA	O2A-C1-C2	3.32	120.89	108.11
20	1	521	CHL	C3C-C4C-NC	-3.32	106.53	114.65
18	A	848	BCR	C40-C30-C25	-3.32	105.04	110.24
19	A	803	CLA	O2A-C1-C2	3.32	120.87	108.11
19	A	824	CLA	C3B-C4B-NB	-3.32	107.57	110.53
19	B	827	CLA	O2A-CGA-CBA	3.31	121.94	111.83
19	B	837	CLA	O2D-CGD-CBD	3.31	117.02	111.23
18	F	306	BCR	C40-C30-C25	-3.31	105.05	110.24
18	L	302	BCR	C19-C18-C17	3.31	124.22	119.01
19	A	841	CLA	C3B-C4B-NB	-3.30	107.58	110.53
19	B	827	CLA	O2D-CGD-CBD	3.29	116.99	111.23
19	B	807	CLA	O2D-CGD-CBD	3.29	116.99	111.23
19	2	506	CLA	CMA-C3A-C4A	3.29	120.62	111.77
19	A	826	CLA	C1D-ND-C4D	-3.29	104.00	106.31
19	1	515	CLA	O2D-CGD-CBD	3.29	116.98	111.23
18	A	848	BCR	C15-C14-C13	3.29	131.89	127.28
19	A	841	CLA	C1D-ND-C4D	-3.29	104.01	106.31
18	K	1005	BCR	C40-C30-C25	-3.28	105.09	110.24
26	4	319	DGD	O2G-C1B-C2B	3.28	118.58	111.48
19	A	833	CLA	O2A-C1-C2	3.28	120.73	108.11
18	B	856	BCR	C27-C26-C25	-3.28	118.28	122.70
20	2	516	CHL	C3C-C4C-NC	-3.27	106.66	114.65
19	J	1105	CLA	C3B-C4B-NB	-3.27	107.61	110.53
19	B	811	CLA	C3B-C4B-NB	-3.26	107.62	110.53
18	B	853	BCR	C39-C30-C25	-3.26	105.13	110.24
19	B	823	CLA	C1D-ND-C4D	-3.26	104.02	106.31
19	A	818	CLA	O2D-CGD-CBD	3.26	116.93	111.23
19	A	820	CLA	O2A-C1-C2	3.26	120.66	108.11
18	B	853	BCR	C15-C14-C13	3.26	131.85	127.28
19	A	833	CLA	C3B-C4B-NB	-3.26	107.62	110.53
19	A	822	CLA	C3B-C4B-NB	-3.26	107.62	110.53
19	B	831	CLA	O2D-CGD-CBD	3.26	116.92	111.23
19	4	315	CLA	O2A-C1-C2	3.26	120.64	108.11
19	K	1002	CLA	O2D-CGD-CBD	3.25	116.91	111.23
20	3	314	CHL	C1B-CHB-C4A	3.25	123.41	121.32
19	H	1000	CLA	O2D-CGD-CBD	3.24	116.90	111.23
19	A	842	CLA	O2D-CGD-CBD	3.24	116.89	111.23
19	B	822	CLA	O2A-C1-C2	3.24	120.56	108.11
19	B	827	CLA	O2A-C1-C2	3.23	120.55	108.11
18	G	205	BCR	C36-C18-C19	-3.23	113.15	118.09
18	A	850	BCR	C40-C30-C25	-3.23	105.18	110.24
19	B	804	CLA	C3B-C4B-NB	-3.23	107.65	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	831	CLA	O2A-C1-C2	3.23	120.53	108.11
19	A	830	CLA	O2A-C1-C2	3.22	120.50	108.11
19	B	838	CLA	O2D-CGD-CBD	3.22	116.86	111.23
20	4	313	CHL	C3C-C4C-NC	-3.22	106.78	114.65
19	B	828	CLA	O2D-CGD-CBD	3.22	116.85	111.23
17	J	1109	LUT	C26-C27-C28	3.21	129.58	124.58
18	B	852	BCR	C40-C30-C25	-3.21	105.21	110.24
19	2	504	CLA	O2A-C1-C2	3.21	120.47	108.11
21	B	842	LHG	C5-O7-C7	-3.21	112.18	117.85
29	B	841	PQN	C14-C13-C15	3.21	120.79	115.23
19	B	834	CLA	O2D-CGD-CBD	3.20	116.83	111.23
20	4	313	CHL	CHA-C1A-C2A	-3.20	125.79	133.31
19	B	810	CLA	O2D-CGD-CBD	3.20	116.82	111.23
19	A	835	CLA	O2D-CGD-CBD	3.19	116.81	111.23
20	2	513	CHL	C3C-C4C-NC	-3.19	106.85	114.65
19	1	506	CLA	O2A-CGA-CBA	3.19	121.56	111.83
20	2	515	CHL	C1A-CHA-C4D	3.18	124.29	118.98
17	3	302	LUT	C15-C14-C13	3.18	131.74	127.28
20	2	513	CHL	C1A-CHA-C4D	3.18	124.29	118.98
19	J	1105	CLA	CAC-C3C-C2C	3.18	133.40	127.56
19	1	513	CLA	O2A-C1-C2	3.18	120.34	108.11
19	A	811	CLA	C3B-C4B-NB	-3.18	107.69	110.53
19	A	823	CLA	O2A-C1-C2	3.17	120.33	108.11
18	L	307	BCR	C40-C30-C25	-3.17	105.27	110.24
20	2	516	CHL	C1-C2-C3	-3.17	121.00	126.20
21	A	845	LHG	O8-C23-C24	3.17	121.51	111.83
20	1	514	CHL	C1A-CHA-C4D	3.17	124.28	118.98
18	A	856	BCR	C40-C30-C25	-3.17	105.27	110.24
19	A	822	CLA	O2D-CGD-CBD	3.17	116.77	111.23
19	4	310	CLA	C1D-ND-C4D	-3.17	104.09	106.31
21	A	845	LHG	C5-O7-C7	-3.17	110.21	117.80
19	G	204	CLA	C1D-ND-C4D	-3.17	104.09	106.31
18	L	302	BCR	C38-C26-C25	-3.16	121.03	124.48
20	2	515	CHL	C3C-C4C-NC	-3.16	106.92	114.65
20	4	314	CHL	C3C-C4C-NC	-3.16	106.92	114.65
19	A	805	CLA	C3B-C4B-NB	-3.15	107.72	110.53
19	4	310	CLA	C3B-C4B-NB	-3.14	107.72	110.53
19	B	833	CLA	O2A-C1-C2	3.14	120.19	108.11
18	G	205	BCR	C19-C18-C17	3.13	123.94	119.01
18	L	307	BCR	C1-C6-C5	-3.13	118.36	122.64
18	2	503	BCR	C38-C26-C25	-3.13	121.07	124.48
18	L	307	BCR	C38-C26-C25	-3.13	121.07	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2	502	XAT	C38-C25-C26	-3.13	117.16	122.30
19	A	827	CLA	O2D-CGD-CBD	3.13	116.69	111.23
19	1	515	CLA	C3B-C4B-NB	-3.12	107.74	110.53
19	1	508	CLA	O2D-CGD-CBD	3.12	116.68	111.23
19	B	840	CLA	O2A-C1-C2	3.12	120.11	108.11
19	K	1002	CLA	CMA-C3A-C4A	3.11	120.14	111.77
18	B	851	BCR	C40-C30-C39	-3.11	99.72	108.63
20	2	512	CHL	C3D-C4D-CHA	3.11	113.27	108.54
19	A	837	CLA	C3B-C4B-NB	-3.11	107.75	110.53
20	2	516	CHL	C1-O2A-CGA	3.11	124.17	116.65
19	A	855	CLA	C1D-ND-C4D	-3.10	104.13	106.31
19	4	311	CLA	C3B-C4B-NB	-3.10	107.76	110.53
19	G	201	CLA	CMA-C3A-C4A	3.10	120.11	111.77
19	B	823	CLA	O2D-CGD-CBD	3.10	116.64	111.23
19	K	1003	CLA	C1C-NC-C4C	-3.09	105.27	106.68
19	B	836	CLA	O2A-C1-C2	3.09	120.01	108.11
19	A	829	CLA	O2A-C1-C2	3.09	120.01	108.11
19	A	855	CLA	O2D-CGD-CBD	3.09	116.63	111.23
19	A	815	CLA	CMA-C3A-C4A	3.09	120.07	111.77
18	L	306	BCR	C40-C30-C25	-3.09	105.41	110.24
19	3	310	CLA	O2A-C1-C2	3.08	119.98	108.11
22	B	844	LMG	O8-C28-C29	3.08	121.23	111.83
19	A	816	CLA	CMA-C3A-C4A	3.08	120.06	111.77
20	4	314	CHL	C1B-CHB-C4A	-3.08	119.34	121.32
19	2	508	CLA	O2D-CGD-CBD	3.08	116.61	111.23
19	3	311	CLA	CMA-C3A-C4A	3.08	120.05	111.77
20	2	515	CHL	CHA-C1A-C2A	-3.08	126.08	133.31
19	B	835	CLA	C3B-C4B-NB	-3.08	107.78	110.53
19	2	508	CLA	C1D-ND-C4D	-3.08	104.15	106.31
19	A	839	CLA	O2A-C1-C2	3.08	119.94	108.11
19	B	822	CLA	C3B-C4B-NB	-3.07	107.79	110.53
19	A	826	CLA	C3B-C4B-NB	-3.07	107.79	110.53
19	2	507	CLA	CMA-C3A-C4A	3.07	120.02	111.77
19	2	508	CLA	CBC-CAC-C3C	-3.07	104.10	112.42
19	3	307	CLA	O2D-CGD-CBD	3.07	116.59	111.23
19	3	313	CLA	O2A-C1-C2	3.07	119.91	108.11
18	B	851	BCR	C30-C25-C26	-3.07	118.45	122.64
19	4	308	CLA	C1D-ND-C4D	-3.06	104.16	106.31
18	B	849	BCR	C30-C25-C26	-3.06	118.45	122.64
19	B	838	CLA	C3B-C4B-NB	-3.06	107.80	110.53
18	B	849	BCR	C38-C26-C25	-3.06	121.14	124.48
19	B	825	CLA	C1D-ND-C4D	-3.06	104.17	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	J	1105	CLA	C4B-CHC-C1C	3.06	133.44	126.25
26	4	319	DGD	C3G-C2G-C1G	-3.06	104.66	111.78
19	1	506	CLA	O2D-CGD-CBD	3.06	116.57	111.23
18	F	306	BCR	C38-C26-C25	-3.05	121.16	124.48
18	I	102	BCR	C39-C30-C25	-3.05	105.46	110.24
19	B	829	CLA	O2A-C1-C2	3.05	119.84	108.11
18	4	301	BCR	C24-C25-C26	-3.05	114.54	121.56
18	I	101	BCR	C1-C6-C7	3.05	123.91	115.65
19	3	310	CLA	O2D-CGD-CBD	3.05	116.56	111.23
19	A	804	CLA	C3B-C4B-NB	-3.04	107.81	110.53
18	B	849	BCR	C30-C25-C24	3.04	123.90	115.65
19	B	832	CLA	O2A-C1-C2	3.04	119.81	108.11
18	A	852	BCR	C39-C30-C25	-3.04	105.48	110.24
20	1	512	CHL	CMA-C3A-C4A	3.04	121.15	114.61
27	A	801	CL0	CBC-CAC-C3C	-3.03	108.53	112.87
19	A	823	CLA	C3B-C4B-NB	-3.03	107.82	110.53
19	A	837	CLA	O2A-C1-C2	3.03	119.75	108.11
19	B	808	CLA	C3B-C4B-NB	-3.03	107.83	110.53
18	B	802	BCR	C8-C9-C10	3.02	123.76	119.01
19	J	1102	CLA	O2D-CGD-CBD	3.02	116.51	111.23
19	B	824	CLA	C1-O2A-CGA	3.02	123.96	116.65
20	1	512	CHL	C3C-C4C-NC	-3.02	107.28	114.65
19	J	1101	CLA	CHD-C1D-ND	-3.02	120.56	124.80
22	G	210	LMG	O8-C28-C29	3.02	120.30	111.15
19	3	307	CLA	CMA-C3A-C4A	3.01	119.88	111.77
19	F	302	CLA	C3B-C4B-NB	-3.01	107.84	110.53
19	A	837	CLA	C1D-ND-C4D	-3.01	104.20	106.31
22	B	845	LMG	O8-C28-C29	3.01	121.02	111.83
19	F	302	CLA	O2A-C1-C2	3.01	119.69	108.11
19	B	824	CLA	CMA-C3A-C4A	3.01	119.86	111.77
19	B	839	CLA	C1D-ND-C4D	-3.01	104.20	106.31
19	1	513	CLA	CMA-C3A-C4A	3.01	119.86	111.77
19	1	513	CLA	C1D-ND-C4D	-3.01	104.20	106.31
19	B	817	CLA	C3B-C4B-NB	-3.01	107.85	110.53
19	L	303	CLA	CMA-C3A-C4A	3.00	119.84	111.77
19	4	310	CLA	O2D-CGD-CBD	3.00	116.48	111.23
27	A	801	CL0	O2D-CGD-O1D	-3.00	118.00	123.85
19	A	838	CLA	C3B-C4B-NB	-3.00	107.85	110.53
18	4	301	BCR	C23-C24-C25	3.00	135.01	127.00
21	B	843	LHG	O8-C23-C24	3.00	120.98	111.83
19	G	201	CLA	C1D-ND-C4D	-3.00	104.21	106.31
18	B	802	BCR	C38-C26-C25	-3.00	121.21	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	846	LMT	C1'-O5'-C5'	-2.99	107.87	113.72
30	F	301	ZEX	C15-C35-C34	-2.99	117.40	123.52
18	I	102	BCR	C40-C30-C25	-2.99	105.55	110.24
27	A	801	CL0	CHA-C1A-C2A	-2.99	126.28	133.31
19	B	809	CLA	O2A-C1-C2	2.99	119.61	108.11
19	B	834	CLA	CMA-C3A-C4A	2.99	119.80	111.77
19	A	814	CLA	CMA-C3A-C4A	2.99	119.80	111.77
19	1	507	CLA	CMD-C2D-C3D	-2.99	120.84	127.69
19	B	812	CLA	O2D-CGD-CBD	2.99	116.45	111.23
19	B	840	CLA	C3B-C4B-NB	-2.98	107.87	110.53
18	B	851	BCR	C36-C18-C19	-2.98	113.53	118.09
19	B	839	CLA	C3B-C4B-NB	-2.98	107.87	110.53
19	A	834	CLA	C1D-ND-C4D	-2.98	104.22	106.31
20	2	512	CHL	C3C-C4C-NC	-2.98	107.37	114.65
24	2	523	LMT	C1'-O5'-C5'	-2.98	107.90	113.72
22	2	518	LMG	O8-C28-C29	2.98	120.19	111.15
27	A	801	CL0	O2A-C1-C2	2.98	119.56	108.11
19	F	302	CLA	C1D-ND-C4D	-2.98	104.22	106.31
22	F	305	LMG	O8-C28-C29	2.97	120.91	111.83
19	3	306	CLA	O2A-CGA-CBA	2.97	120.90	111.83
19	F	303	CLA	O2D-CGD-CBD	2.97	116.43	111.23
24	J	1107	LMT	C3'-C4'-C5'	-2.97	104.34	110.93
18	B	851	BCR	C19-C18-C17	2.97	123.68	119.01
19	3	305	CLA	C1D-ND-C4D	-2.97	104.23	106.31
19	A	813	CLA	C1D-ND-C4D	-2.97	104.23	106.31
26	B	854	DGD	O1G-C1A-C2A	2.97	120.89	111.83
20	2	516	CHL	C1A-CHA-C4D	2.96	123.93	118.98
27	A	801	CL0	C4C-CHD-C1D	2.96	126.67	116.07
19	K	1001	CLA	CMA-C3A-C4A	2.96	119.74	111.77
19	B	820	CLA	O2A-C1-C2	2.96	119.51	108.11
19	2	506	CLA	O2A-CGA-CBA	2.96	120.86	111.83
19	4	304	CLA	O2A-CGA-CBA	2.96	120.86	111.83
18	B	802	BCR	C34-C9-C10	-2.96	118.02	122.82
19	B	817	CLA	O2A-CGA-CBA	2.96	120.85	111.83
19	B	819	CLA	C3B-C4B-NB	-2.96	107.89	110.53
19	A	829	CLA	C3B-C4B-NB	-2.95	107.89	110.53
20	1	514	CHL	C4D-CHA-CBD	-2.95	105.99	108.97
19	B	809	CLA	C3B-C4B-NB	-2.95	107.89	110.53
19	B	834	CLA	C1D-ND-C4D	-2.95	104.24	106.31
19	L	303	CLA	O2A-C1-C2	2.95	119.46	108.11
19	4	310	CLA	CMA-C3A-C4A	2.95	119.70	111.77
19	B	835	CLA	C1D-ND-C4D	-2.95	104.24	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	813	CLA	CMA-C3A-C4A	2.95	119.69	111.77
19	3	312	CLA	CMA-C3A-C4A	2.94	119.69	111.77
19	B	828	CLA	C1D-ND-C4D	-2.94	104.25	106.31
19	A	819	CLA	CMA-C3A-C4A	2.94	119.69	111.77
19	A	836	CLA	CMA-C3A-C4A	2.94	119.68	111.77
19	4	318	CLA	O2A-C1-C2	2.94	119.42	108.11
17	3	301	LUT	C7-C8-C9	-2.94	121.89	126.23
18	I	101	BCR	C38-C26-C25	-2.94	121.28	124.48
19	A	815	CLA	O2D-CGD-CBD	2.94	116.36	111.23
19	B	819	CLA	C1D-ND-C4D	-2.93	104.25	106.31
18	K	1005	BCR	C1-C6-C5	-2.93	118.63	122.64
19	L	305	CLA	O2A-C1-C2	2.93	119.40	108.11
19	1	510	CLA	CAA-CBA-CGA	-2.93	104.88	113.21
18	1	503	BCR	C40-C30-C25	-2.93	105.65	110.24
20	4	316	CHL	C3C-C4C-NC	-2.93	107.50	114.65
19	3	309	CLA	CMA-C3A-C4A	2.93	119.64	111.77
19	A	840	CLA	O2A-C1-C2	2.92	119.36	108.11
19	A	835	CLA	CMA-C3A-C4A	2.92	119.62	111.77
19	4	312	CLA	C3B-C4B-NB	-2.92	107.92	110.53
19	A	841	CLA	O2A-C1-C2	2.92	119.34	108.11
19	A	823	CLA	CMA-C3A-C4A	2.92	119.61	111.77
19	4	307	CLA	O2A-CGA-CBA	2.91	120.71	111.83
19	G	204	CLA	C3B-C4B-NB	-2.91	107.93	110.53
19	A	824	CLA	O2D-CGD-CBD	2.91	116.32	111.23
19	A	803	CLA	C2D-C1D-ND	2.91	113.00	110.13
18	B	852	BCR	C15-C14-C13	2.91	131.35	127.28
22	F	304	LMG	O8-C28-C29	2.90	120.69	111.83
19	B	816	CLA	CMA-C3A-C4A	2.90	119.58	111.77
19	B	837	CLA	CHD-C1D-ND	-2.90	120.72	124.80
19	4	306	CLA	C3B-C4B-NB	-2.90	107.94	110.53
19	B	830	CLA	C1D-ND-C4D	-2.90	104.28	106.31
18	I	102	BCR	C38-C26-C25	-2.90	121.33	124.48
19	B	820	CLA	C3B-C4B-NB	-2.89	107.95	110.53
20	2	526	CHL	C1A-CHA-C4D	2.89	123.80	118.98
19	B	805	CLA	C3B-C4B-NB	-2.88	107.96	110.53
18	3	303	BCR	C40-C30-C25	-2.88	105.72	110.24
19	1	506	CLA	CMA-C3A-C4A	2.88	119.51	111.77
19	4	307	CLA	CMA-C3A-C4A	2.88	119.51	111.77
18	B	856	BCR	C40-C30-C25	-2.88	105.73	110.24
19	4	312	CLA	CMA-C3A-C4A	2.88	119.50	111.77
24	A	846	LMT	C3'-C4'-C5'	-2.88	104.56	110.93
19	A	802	CLA	C3B-C4B-NB	-2.87	107.96	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	305	CLA	O2A-CGA-CBA	2.87	120.60	111.83
19	B	816	CLA	C3B-C4B-NB	-2.87	107.97	110.53
20	1	521	CHL	C4C-CHD-C1D	2.87	126.34	116.07
18	B	850	BCR	C15-C14-C13	2.87	131.30	127.28
19	4	309	CLA	O2A-C1-C2	2.87	119.15	108.11
19	L	303	CLA	C1D-ND-C4D	-2.87	104.30	106.31
17	3	302	LUT	C7-C8-C9	-2.87	122.00	126.23
18	A	856	BCR	C30-C25-C26	-2.86	118.72	122.64
17	1	501	LUT	C7-C8-C9	-2.86	122.00	126.23
19	B	833	CLA	CHD-C1D-ND	-2.86	120.77	124.80
19	A	803	CLA	C3B-C4B-NB	-2.86	107.98	110.53
18	A	850	BCR	C39-C30-C25	-2.86	105.76	110.24
19	B	826	CLA	OBD-CAD-C3D	-2.86	121.73	128.42
19	1	506	CLA	C3B-C4B-NB	-2.86	107.98	110.53
19	B	812	CLA	CMA-C3A-C4A	2.85	119.44	111.77
19	A	825	CLA	CAC-C3C-C4C	2.85	128.50	124.79
19	A	839	CLA	C3B-C4B-NB	-2.85	107.98	110.53
19	L	301	CLA	O2A-CGA-CBA	2.85	120.53	111.83
18	A	851	BCR	C15-C14-C13	2.85	131.28	127.28
19	A	842	CLA	C1D-ND-C4D	-2.85	104.31	106.31
19	1	504	CLA	CMA-C3A-C4A	2.85	119.43	111.77
17	4	302	LUT	C38-C25-C24	-2.85	116.62	123.36
19	A	803	CLA	C1D-ND-C4D	-2.85	104.31	106.31
19	B	827	CLA	C1D-ND-C4D	-2.84	104.32	106.31
18	B	852	BCR	C35-C13-C12	2.84	122.43	118.09
20	2	526	CHL	C1-O2A-CGA	2.84	123.53	116.65
19	G	204	CLA	CMA-C3A-C4A	2.84	119.39	111.77
18	A	856	BCR	C27-C26-C25	-2.83	118.87	122.70
19	B	822	CLA	CMA-C3A-C4A	2.83	119.39	111.77
19	A	821	CLA	O2A-C1-C2	2.83	119.01	108.11
19	1	506	CLA	C1D-ND-C4D	-2.83	104.33	106.31
19	B	840	CLA	C1D-ND-C4D	-2.83	104.33	106.31
19	A	806	CLA	O2A-CGA-CBA	2.83	120.46	111.83
19	J	1105	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
19	A	818	CLA	C3B-C4B-NB	-2.83	108.01	110.53
19	B	806	CLA	CHD-C1D-ND	-2.83	120.83	124.80
19	B	833	CLA	C3B-C4B-NB	-2.82	108.01	110.53
19	1	505	CLA	CMA-C3A-C4A	2.82	119.34	111.77
19	B	819	CLA	CHD-C1D-ND	-2.81	120.85	124.80
27	A	801	CL0	O2A-CGA-CBA	2.81	120.39	111.83
19	B	807	CLA	CHD-C1D-ND	-2.81	120.85	124.80
18	B	851	BCR	C23-C24-C25	-2.81	119.50	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	G	204	CLA	C2D-C1D-ND	2.81	112.90	110.13
19	1	510	CLA	C4B-CHC-C1C	2.80	132.84	126.25
24	J	1107	LMT	C1'-O5'-C5'	-2.80	108.25	113.72
19	4	309	CLA	C1D-ND-C4D	-2.80	104.34	106.31
19	A	825	CLA	CMA-C3A-C4A	2.80	119.30	111.77
23	4	303	XAT	O24-C25-C38	-2.80	111.92	115.05
19	3	315	CLA	C1D-ND-C4D	-2.80	104.35	106.31
19	A	806	CLA	CAA-C2A-C3A	-2.80	105.43	113.00
19	B	803	CLA	O2A-C1-C2	2.80	118.88	108.11
19	A	809	CLA	C1-O2A-CGA	2.80	123.42	116.65
19	2	511	CLA	C3B-C4B-NB	-2.79	108.04	110.53
19	B	818	CLA	C3B-C4B-NB	-2.79	108.04	110.53
19	B	803	CLA	O2D-CGD-CBD	2.79	116.11	111.23
27	A	801	CL0	C6-C5-C3	-2.79	106.67	113.47
19	4	318	CLA	C1D-ND-C4D	-2.79	104.36	106.31
18	A	850	BCR	C15-C14-C13	-2.79	123.37	127.28
22	2	519	LMG	O8-C28-C29	2.79	120.34	111.83
24	B	846	LMT	C3'-C4'-C5'	-2.79	104.75	110.93
19	A	822	CLA	CMA-C3A-C4A	2.79	119.27	111.77
18	B	849	BCR	C8-C9-C10	2.79	123.39	119.01
19	B	812	CLA	C1D-ND-C4D	-2.78	104.36	106.31
20	3	314	CHL	C4D-CHA-CBD	-2.78	106.16	108.97
24	3	318	LMT	C3B-C4B-C5B	-2.78	105.19	110.23
19	A	832	CLA	CHD-C1D-ND	-2.78	120.89	124.80
19	4	309	CLA	C3B-C4B-NB	-2.77	108.05	110.53
19	B	823	CLA	C3B-C4B-NB	-2.77	108.05	110.53
19	G	202	CLA	C1D-ND-C4D	-2.77	104.37	106.31
19	1	511	CLA	C3B-C4B-NB	-2.77	108.06	110.53
26	J	1106	DGD	O1G-C1A-C2A	2.77	120.28	111.83
20	4	314	CHL	C1-C2-C3	-2.77	122.28	126.76
19	B	811	CLA	CMD-C2D-C3D	-2.77	121.34	127.69
24	3	318	LMT	O1'-C1'-C2'	2.77	112.48	108.27
19	A	812	CLA	C3B-C4B-NB	-2.77	108.06	110.53
19	A	812	CLA	CMA-C3A-C4A	2.77	119.21	111.77
19	A	824	CLA	CMA-C3A-C4A	2.77	119.21	111.77
19	B	834	CLA	O2A-C1-C2	2.77	118.76	108.11
19	A	817	CLA	C3B-C4B-NB	-2.77	108.06	110.53
19	J	1105	CLA	C1D-ND-C4D	-2.76	104.37	106.31
19	F	303	CLA	C3B-C4B-NB	-2.76	108.06	110.53
18	A	849	BCR	C40-C30-C25	-2.76	105.91	110.24
19	K	1002	CLA	O2A-CGA-CBA	2.76	120.26	111.83
19	1	510	CLA	CMA-C3A-C4A	2.76	119.20	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	805	CLA	C4B-CHC-C1C	2.76	132.74	126.25
19	A	815	CLA	C3B-C4B-NB	-2.76	108.06	110.53
18	A	849	BCR	C35-C13-C12	2.76	122.31	118.09
19	1	505	CLA	C1D-ND-C4D	-2.76	104.38	106.31
19	3	313	CLA	O2A-CGA-CBA	2.76	120.24	111.83
19	G	201	CLA	C3B-C4B-NB	-2.76	108.07	110.53
19	A	855	CLA	CAC-C3C-C4C	2.75	128.37	124.79
18	A	848	BCR	C35-C13-C12	2.75	122.29	118.09
20	4	313	CHL	C4D-CHA-CBD	-2.75	106.19	108.97
19	A	836	CLA	C1D-ND-C4D	-2.75	104.38	106.31
19	A	839	CLA	O2D-CGD-CBD	2.75	116.04	111.23
19	A	855	CLA	CMA-C3A-C4A	2.75	119.16	111.77
19	A	813	CLA	C3B-C4B-NB	-2.75	108.08	110.53
19	A	837	CLA	CMA-C3A-C4A	2.75	119.15	111.77
19	4	307	CLA	C1D-ND-C4D	-2.74	104.39	106.31
19	A	814	CLA	CHD-C1D-ND	-2.74	120.94	124.80
19	A	854	CLA	C1D-ND-C4D	-2.74	104.39	106.31
19	A	835	CLA	C3B-C4B-NB	-2.74	108.08	110.53
19	A	832	CLA	C3B-C4B-NB	-2.74	108.08	110.53
19	A	813	CLA	O2A-C1-C2	2.74	118.64	108.11
19	3	307	CLA	C3B-C4B-NB	-2.74	108.09	110.53
19	B	809	CLA	C1D-ND-C4D	-2.74	104.39	106.31
19	3	316	CLA	CHD-C1D-ND	-2.73	120.95	124.80
19	G	204	CLA	CHD-C1D-ND	-2.73	120.95	124.80
19	B	818	CLA	O2A-C1-C2	2.73	118.63	108.11
19	L	305	CLA	CMA-C3A-C4A	2.73	119.12	111.77
18	G	205	BCR	C38-C26-C25	-2.73	121.50	124.48
19	A	807	CLA	CMA-C3A-C4A	2.73	119.11	111.77
19	4	311	CLA	CHD-C1D-ND	-2.73	120.97	124.80
20	2	515	CHL	C4D-CHA-CBD	-2.73	106.22	108.97
17	3	302	LUT	C11-C10-C9	2.73	131.10	127.28
20	4	314	CHL	CMA-C3A-C4A	2.73	120.48	114.61
19	B	806	CLA	C3B-C4B-NB	-2.73	108.10	110.53
19	B	817	CLA	C1D-ND-C4D	-2.72	104.40	106.31
30	F	301	ZEX	C27-C28-C29	-2.72	122.21	126.23
19	A	813	CLA	CHD-C1D-ND	-2.72	120.97	124.80
19	A	822	CLA	CHD-C1D-ND	-2.72	120.97	124.80
19	B	836	CLA	CHD-C1D-ND	-2.72	120.97	124.80
19	1	509	CLA	C1D-ND-C4D	-2.72	104.40	106.31
19	4	309	CLA	C3B-C2B-C1B	-2.72	103.96	107.17
19	2	508	CLA	CMA-C3A-C4A	2.72	119.08	111.77
19	A	841	CLA	C2D-C1D-ND	2.72	112.82	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	F	302	CLA	C2D-C1D-ND	2.72	112.82	110.13
19	B	811	CLA	C1D-ND-C4D	-2.72	104.41	106.31
19	G	201	CLA	C4B-CHC-C1C	2.72	132.63	126.25
17	3	301	LUT	C26-C27-C28	-2.72	120.35	124.58
17	4	302	LUT	C31-C32-C33	-2.71	118.92	126.36
19	B	803	CLA	C3B-C4B-NB	-2.71	108.11	110.53
20	4	313	CHL	CMA-C3A-C4A	2.71	120.45	114.61
19	B	832	CLA	C3B-C4B-NB	-2.71	108.11	110.53
19	A	854	CLA	O2A-CGA-CBA	2.71	120.10	111.83
19	A	819	CLA	CHD-C1D-ND	-2.71	120.99	124.80
19	A	811	CLA	CMA-C3A-C4A	2.71	119.05	111.77
20	4	316	CHL	C4D-CHA-CBD	-2.71	106.24	108.97
19	L	301	CLA	CHD-C1D-ND	-2.71	120.99	124.80
19	4	304	CLA	OBD-CAD-C3D	-2.71	122.09	128.42
19	B	808	CLA	CMA-C3A-C4A	2.71	119.05	111.77
19	1	510	CLA	CAC-C3C-C4C	2.71	128.31	124.79
18	3	303	BCR	C29-C28-C27	2.71	117.23	111.28
19	A	840	CLA	C1D-ND-C4D	-2.71	104.41	106.31
19	B	821	CLA	C3B-C4B-NB	-2.71	108.11	110.53
19	B	804	CLA	CAC-C3C-C4C	2.71	128.31	124.79
19	A	829	CLA	C1D-ND-C4D	-2.71	104.41	106.31
20	1	521	CHL	C4D-CHA-CBD	-2.70	106.24	108.97
17	1	501	LUT	C31-C32-C33	-2.70	118.95	126.36
19	A	835	CLA	CHD-C1D-ND	-2.70	121.00	124.80
19	A	822	CLA	C1D-ND-C4D	-2.70	104.42	106.31
19	1	511	CLA	CHD-C1D-ND	-2.70	121.00	124.80
19	3	317	CLA	CHD-C1D-ND	-2.70	121.00	124.80
19	B	825	CLA	O2A-C1-C2	2.70	118.50	108.11
18	A	849	BCR	C39-C30-C25	-2.70	106.01	110.24
19	B	811	CLA	C4B-CHC-C1C	2.70	132.59	126.25
19	G	203	CLA	CMA-C3A-C4A	2.70	119.02	111.77
19	L	304	CLA	CMA-C3A-C4A	2.70	119.02	111.77
19	1	508	CLA	CAC-C3C-C4C	2.69	128.29	124.79
20	2	513	CHL	C4D-CHA-CBD	-2.69	106.25	108.97
19	B	823	CLA	CHD-C1D-ND	-2.69	121.01	124.80
18	I	101	BCR	C31-C1-C6	-2.69	106.02	110.24
19	4	310	CLA	C2D-C1D-ND	2.69	112.79	110.13
19	2	505	CLA	CMA-C3A-C4A	2.69	119.00	111.77
19	B	814	CLA	CMA-C3A-C4A	2.69	119.00	111.77
19	1	507	CLA	O2A-CGA-CBA	2.69	120.03	111.83
19	B	826	CLA	CHA-C4D-ND	2.68	138.09	132.55
18	B	856	BCR	C39-C30-C25	-2.68	106.04	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	513	CLA	C3B-C4B-NB	-2.68	108.14	110.53
18	G	205	BCR	C39-C30-C25	-2.68	106.04	110.24
19	1	516	CLA	CMA-C3A-C4A	2.68	118.97	111.77
23	4	303	XAT	C26-C27-C28	-2.68	120.33	125.99
18	B	851	BCR	C35-C13-C12	2.68	122.18	118.09
19	2	511	CLA	CMA-C3A-C4A	2.68	118.97	111.77
19	B	804	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
19	B	829	CLA	O2A-CGA-CBA	2.67	119.99	111.83
26	G	207	DGD	O1G-C1A-C2A	2.67	119.99	111.83
19	L	304	CLA	C2D-C1D-ND	2.67	112.77	110.13
17	4	302	LUT	C22-C23-C24	-2.67	107.21	111.18
19	L	304	CLA	C3B-C4B-NB	-2.67	108.14	110.53
24	G	208	LMT	C3'-C4'-C5'	-2.67	105.01	110.93
19	4	305	CLA	CMA-C3A-C4A	2.67	118.95	111.77
19	2	509	CLA	C1D-ND-C4D	-2.67	104.44	106.31
19	A	824	CLA	C1D-ND-C4D	-2.67	104.44	106.31
19	4	312	CLA	CHD-C1D-ND	-2.67	121.05	124.80
18	4	301	BCR	C39-C30-C25	-2.67	106.06	110.24
19	4	310	CLA	C4B-CHC-C1C	2.67	132.52	126.25
19	A	854	CLA	O2A-CGA-O1A	-2.67	116.96	123.63
19	4	304	CLA	C3B-C4B-NB	-2.66	108.15	110.53
24	G	209	LMT	C1'-O5'-C5'	-2.66	108.52	113.72
19	3	311	CLA	C3B-C4B-NB	-2.66	108.15	110.53
19	1	507	CLA	C1D-ND-C4D	-2.66	104.44	106.31
19	3	307	CLA	C2D-C1D-ND	2.66	112.76	110.13
19	3	312	CLA	CHD-C1D-ND	-2.66	121.06	124.80
19	B	815	CLA	O2A-CGA-CBA	2.66	119.94	111.83
22	G	210	LMG	O7-C10-C11	2.66	120.69	110.93
19	A	818	CLA	CMA-C3A-C4A	2.66	118.91	111.77
17	1	502	LUT	C31-C32-C33	-2.66	119.08	126.36
19	A	855	CLA	O2A-CGA-CBA	2.65	119.92	111.83
26	4	319	DGD	O1G-C1A-C2A	2.65	119.92	111.83
19	G	201	CLA	CHD-C1D-ND	-2.65	121.07	124.80
19	B	823	CLA	CMD-C2D-C3D	-2.65	121.61	127.69
19	B	834	CLA	C4B-CHC-C1C	2.65	132.47	126.25
19	2	505	CLA	O2A-CGA-CBA	2.65	119.91	111.83
19	B	819	CLA	CAA-C2A-C1A	-2.65	103.30	111.97
19	A	806	CLA	O2D-CGD-CBD	2.65	115.86	111.23
29	A	844	PQN	C2M-C2-C3	-2.65	120.10	124.45
20	4	317	CHL	CMA-C3A-C4A	2.65	120.31	114.61
19	B	832	CLA	C2D-C1D-ND	2.65	112.74	110.13
19	A	821	CLA	C3B-C4B-NB	-2.64	108.17	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	807	CLA	O2A-CGA-CBA	2.64	119.90	111.83
19	A	842	CLA	O2A-CGA-CBA	2.64	119.90	111.83
19	2	504	CLA	CHD-C1D-ND	-2.64	121.08	124.80
19	A	827	CLA	C3B-C4B-NB	-2.64	108.17	110.53
19	B	829	CLA	CAC-C3C-C4C	2.64	128.23	124.79
19	1	516	CLA	C1D-ND-C4D	-2.64	104.46	106.31
18	2	503	BCR	C32-C1-C6	-2.64	106.11	110.24
17	1	501	LUT	C38-C25-C24	-2.64	117.12	123.36
22	1	518	LMG	O8-C28-C29	2.64	119.87	111.83
19	A	810	CLA	C1D-ND-C4D	-2.64	104.46	106.31
19	A	831	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
19	A	805	CLA	C1D-ND-C4D	-2.63	104.46	106.31
22	2	518	LMG	O7-C10-C11	2.63	120.60	110.93
19	A	842	CLA	CMA-C3A-C4A	2.63	118.85	111.77
19	A	823	CLA	CHD-C1D-ND	-2.63	121.10	124.80
19	2	504	CLA	C1D-ND-C4D	-2.63	104.47	106.31
19	B	831	CLA	C1D-ND-C4D	-2.63	104.47	106.31
19	2	505	CLA	CHD-C1D-ND	-2.63	121.10	124.80
19	A	810	CLA	CMA-C3A-C4A	2.63	118.85	111.77
19	3	308	CLA	CHD-C1D-ND	-2.63	121.10	124.80
18	B	802	BCR	C40-C30-C25	-2.63	106.12	110.24
26	4	319	DGD	O3G-C1D-C2D	2.63	112.26	108.27
19	G	202	CLA	CMA-C3A-C4A	2.63	118.83	111.77
19	B	836	CLA	C1D-ND-C4D	-2.62	104.47	106.31
19	2	505	CLA	C3B-C4B-NB	-2.62	108.19	110.53
20	4	317	CHL	C4D-CHA-CBD	-2.62	106.32	108.97
19	A	827	CLA	CMA-C3A-C4A	2.62	118.82	111.77
19	A	840	CLA	CMA-C3A-C4A	2.62	118.82	111.77
19	A	822	CLA	C4B-CHC-C1C	2.62	132.41	126.25
19	B	809	CLA	CMA-C3A-C4A	2.62	118.81	111.77
19	B	839	CLA	CHD-C1D-ND	-2.62	121.12	124.80
17	2	501	LUT	C38-C25-C24	-2.62	117.17	123.36
19	4	306	CLA	CMA-C3A-C4A	2.61	118.80	111.77
19	1	504	CLA	C3B-C4B-NB	-2.61	108.20	110.53
19	B	827	CLA	CHD-C1D-ND	-2.61	121.12	124.80
19	A	833	CLA	C1D-ND-C4D	-2.61	104.48	106.31
19	B	812	CLA	CHD-C1D-ND	-2.61	121.12	124.80
19	3	317	CLA	CMA-C3A-C4A	2.61	118.80	111.77
19	A	837	CLA	C4B-CHC-C1C	2.61	132.39	126.25
19	A	817	CLA	CMA-C3A-C4A	2.61	118.79	111.77
19	3	309	CLA	CHA-C4D-ND	2.61	137.93	132.55
19	B	814	CLA	CHD-C1D-ND	-2.61	121.13	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	507	CLA	C1D-ND-C4D	-2.61	104.48	106.31
19	B	825	CLA	C3B-C4B-NB	-2.61	108.20	110.53
19	A	838	CLA	CMA-C3A-C4A	2.61	118.78	111.77
19	4	306	CLA	C4B-CHC-C1C	2.61	132.38	126.25
19	B	822	CLA	C4B-CHC-C1C	2.61	132.38	126.25
19	F	302	CLA	O2A-CGA-CBA	2.60	119.78	111.83
19	B	809	CLA	O2A-CGA-CBA	2.60	119.77	111.83
20	4	314	CHL	C1A-CHA-CBD	-2.60	125.70	132.36
19	B	831	CLA	C4B-CHC-C1C	2.60	132.36	126.25
19	4	305	CLA	C3B-C4B-NB	-2.60	108.21	110.53
19	4	304	CLA	CHA-C4D-ND	2.60	137.91	132.55
19	4	305	CLA	CHA-C4D-ND	2.60	137.91	132.55
18	B	850	BCR	C35-C13-C12	2.60	122.06	118.09
19	B	829	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
19	B	838	CLA	CMA-C3A-C4A	2.60	118.75	111.77
19	1	510	CLA	OBD-CAD-C3D	-2.59	122.35	128.42
23	4	303	XAT	C31-C30-C29	-2.59	123.64	127.28
19	B	833	CLA	CMD-C2D-C3D	-2.59	121.74	127.69
19	B	806	CLA	C1-O2A-CGA	2.59	122.93	116.65
18	A	848	BCR	C38-C26-C25	-2.59	121.66	124.48
19	A	805	CLA	CMD-C2D-C3D	-2.58	121.76	127.69
19	B	826	CLA	C3B-C4B-NB	-2.58	108.22	110.53
19	4	315	CLA	C1D-ND-C4D	-2.58	104.50	106.31
24	B	846	LMT	C1'-O5'-C5'	-2.58	108.67	113.72
19	2	506	CLA	CAA-CBA-CGA	-2.58	105.87	113.21
22	J	1103	LMG	O8-C28-C29	2.58	118.99	111.15
19	A	825	CLA	CHD-C1D-ND	-2.58	121.17	124.80
19	K	1001	CLA	CMD-C2D-C3D	-2.58	121.77	127.69
19	B	840	CLA	CMA-C3A-C4A	2.58	118.71	111.77
19	A	820	CLA	C3B-C4B-NB	-2.58	108.23	110.53
27	A	801	CL0	CMB-C2B-C3B	2.58	129.84	124.68
19	3	312	CLA	C3B-C4B-NB	-2.58	108.23	110.53
19	B	810	CLA	O2A-CGA-CBA	2.58	119.70	111.83
19	L	305	CLA	C1D-ND-C4D	-2.58	104.50	106.31
19	G	204	CLA	C3D-C2D-C1D	-2.58	102.31	105.83
19	L	301	CLA	C3B-C4B-NB	-2.58	108.23	110.53
19	B	835	CLA	O2A-CGA-CBA	2.57	119.68	111.83
19	B	828	CLA	CHD-C1D-ND	-2.57	121.18	124.80
19	1	509	CLA	O2A-CGA-CBA	2.57	119.68	111.83
20	4	314	CHL	C3D-C4D-ND	-2.57	108.81	112.94
18	A	848	BCR	C10-C11-C12	-2.57	115.75	123.20
19	B	824	CLA	CHD-C1D-ND	-2.57	121.19	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	842	CLA	CHD-C1D-ND	-2.56	121.19	124.80
18	K	1005	BCR	C40-C30-C29	2.56	118.79	108.95
19	1	515	CLA	CMD-C2D-C3D	-2.56	121.81	127.69
19	4	307	CLA	CMD-C2D-C3D	-2.56	121.81	127.69
19	3	313	CLA	CMA-C3A-C4A	2.56	118.66	111.77
19	A	838	CLA	C4B-CHC-C1C	2.56	132.27	126.25
19	A	810	CLA	CHD-C1D-ND	-2.56	121.20	124.80
18	B	849	BCR	C40-C30-C29	2.56	118.77	108.95
19	J	1105	CLA	O2A-C1-C2	2.56	117.95	108.11
19	A	811	CLA	O2A-CGA-CBA	2.56	119.63	111.83
19	K	1001	CLA	CHD-C1D-ND	-2.56	121.20	124.80
18	B	852	BCR	C37-C22-C23	2.56	121.99	118.09
19	J	1102	CLA	C2D-C1D-ND	2.56	112.66	110.13
22	A	847	LMG	O8-C28-C29	2.55	119.62	111.83
20	1	521	CHL	C1-O2A-CGA	2.55	122.83	116.65
20	4	316	CHL	CMA-C3A-C4A	2.55	120.11	114.61
18	B	802	BCR	C40-C30-C29	2.55	118.75	108.95
19	A	805	CLA	CHD-C1D-ND	-2.55	121.21	124.80
19	4	308	CLA	C2D-C1D-ND	2.55	112.65	110.13
19	1	507	CLA	CHD-C1D-ND	-2.55	121.21	124.80
19	3	306	CLA	CHD-C1D-ND	-2.55	121.21	124.80
19	B	826	CLA	O2A-CGA-CBA	2.55	119.61	111.83
19	G	202	CLA	CHD-C1D-ND	-2.55	121.21	124.80
19	K	1002	CLA	CHD-C1D-ND	-2.55	121.21	124.80
19	B	814	CLA	CAC-C3C-C4C	2.55	128.11	124.79
18	A	849	BCR	C40-C30-C29	2.55	118.74	108.95
19	3	306	CLA	C4B-CHC-C1C	2.55	132.24	126.25
19	1	507	CLA	CMA-C3A-C4A	2.55	118.62	111.77
18	A	848	BCR	C12-C13-C14	-2.55	115.00	119.01
19	3	306	CLA	O2A-C1-C2	2.55	117.92	108.11
18	G	205	BCR	C40-C30-C29	2.55	118.73	108.95
19	A	826	CLA	O2A-CGA-CBA	2.55	119.60	111.83
18	A	852	BCR	C40-C30-C29	2.55	118.73	108.95
19	1	507	CLA	CHA-C4D-ND	2.55	137.80	132.55
19	4	304	CLA	CMA-C3A-C4A	2.55	118.62	111.77
18	3	303	BCR	C40-C30-C29	2.55	118.72	108.95
18	F	306	BCR	C40-C30-C29	2.54	118.72	108.95
18	L	306	BCR	C40-C30-C29	2.54	118.72	108.95
19	K	1002	CLA	C3B-C4B-NB	-2.54	108.26	110.53
18	I	101	BCR	C40-C30-C29	2.54	118.72	108.95
18	B	852	BCR	C40-C30-C29	2.54	118.72	108.95
19	A	815	CLA	CHD-C1D-ND	-2.54	121.22	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	505	CLA	C3B-C4B-NB	-2.54	108.26	110.53
19	A	834	CLA	C3B-C4B-NB	-2.54	108.26	110.53
18	B	852	BCR	C39-C30-C25	-2.54	106.26	110.24
18	A	856	BCR	C40-C30-C29	2.54	118.70	108.95
19	2	510	CLA	CHA-C4D-ND	2.54	137.79	132.55
19	B	836	CLA	C3B-C4B-NB	-2.54	108.26	110.53
18	A	848	BCR	C40-C30-C29	2.54	118.70	108.95
18	A	851	BCR	C40-C30-C29	2.54	118.69	108.95
18	L	302	BCR	C40-C30-C29	2.54	118.69	108.95
19	F	303	CLA	CHD-C1D-ND	-2.54	121.23	124.80
19	1	515	CLA	CHA-C4D-ND	2.54	137.78	132.55
18	B	853	BCR	C40-C30-C29	2.54	118.69	108.95
18	B	852	BCR	C38-C26-C25	-2.54	121.72	124.48
19	A	812	CLA	C1D-ND-C4D	-2.54	104.53	106.31
18	L	307	BCR	C40-C30-C29	2.53	118.68	108.95
19	A	827	CLA	C1D-ND-C4D	-2.53	104.53	106.31
19	A	838	CLA	C1D-ND-C4D	-2.53	104.53	106.31
19	A	808	CLA	CHA-C4D-ND	2.53	137.78	132.55
19	2	514	CLA	O2A-CGA-CBA	2.53	119.56	111.83
18	B	850	BCR	C40-C30-C29	2.53	118.68	108.95
19	A	806	CLA	CHD-C1D-ND	-2.53	121.24	124.80
19	B	818	CLA	CAC-C3C-C4C	2.53	128.09	124.79
17	3	301	LUT	C38-C25-C24	-2.53	117.36	123.36
19	A	816	CLA	C1D-ND-C4D	-2.53	104.53	106.31
18	B	851	BCR	C40-C30-C29	2.53	118.67	108.95
19	A	819	CLA	C1D-ND-C4D	-2.53	104.54	106.31
19	A	830	CLA	CHA-C4D-ND	2.53	137.77	132.55
20	1	521	CHL	C1A-CHA-C4D	2.53	123.20	118.98
19	B	817	CLA	CHD-C1D-ND	-2.53	121.24	124.80
19	B	834	CLA	O2A-CGA-CBA	2.53	119.55	111.83
18	1	503	BCR	C40-C30-C29	2.53	118.66	108.95
19	B	816	CLA	C1D-ND-C4D	-2.53	104.54	106.31
19	A	832	CLA	O2A-CGA-CBA	2.53	119.54	111.83
18	3	304	BCR	C40-C30-C29	2.53	118.65	108.95
19	A	836	CLA	CHD-C1D-ND	-2.53	121.25	124.80
18	A	850	BCR	C40-C30-C29	2.53	118.65	108.95
19	A	842	CLA	C3B-C4B-NB	-2.52	108.28	110.53
18	J	1108	BCR	C40-C30-C29	2.52	118.64	108.95
19	B	836	CLA	O2A-CGA-CBA	2.52	119.52	111.83
19	4	308	CLA	CHA-C4D-ND	2.52	137.75	132.55
19	A	820	CLA	CMA-C3A-C4A	2.52	118.55	111.77
19	A	833	CLA	CMA-C3A-C4A	2.52	118.54	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	819	CLA	CMA-C3A-C4A	2.52	118.54	111.77
18	I	102	BCR	C40-C30-C29	2.52	118.62	108.95
19	B	812	CLA	C4B-CHC-C1C	2.52	132.17	126.25
18	4	301	BCR	C40-C30-C29	2.52	118.62	108.95
19	3	310	CLA	C1D-ND-C4D	-2.52	104.55	106.31
19	A	803	CLA	CHD-C1D-ND	-2.52	121.26	124.80
19	1	515	CLA	CMA-C3A-C4A	2.52	118.54	111.77
19	3	309	CLA	CAC-C3C-C4C	2.52	128.06	124.79
24	B	847	LMT	C1'-O5'-C5'	-2.52	108.81	113.72
23	2	502	XAT	O4-C5-C18	-2.51	112.24	115.05
19	3	310	CLA	CHD-C1D-ND	-2.51	121.27	124.80
19	4	318	CLA	CHD-C1D-ND	-2.51	121.27	124.80
17	2	501	LUT	C22-C23-C24	-2.51	107.45	111.18
19	4	307	CLA	CHD-C1D-ND	-2.51	121.27	124.80
19	A	840	CLA	C3B-C4B-NB	-2.51	108.29	110.53
19	B	808	CLA	CHD-C1D-ND	-2.51	121.27	124.80
19	B	824	CLA	CHA-C4D-ND	2.51	137.73	132.55
19	A	823	CLA	C1D-ND-C4D	-2.51	104.55	106.31
17	J	1109	LUT	C37-C21-C22	-2.51	104.73	109.41
19	B	804	CLA	CMA-C3A-C4A	2.51	118.52	111.77
19	B	825	CLA	CMA-C3A-C4A	2.51	118.52	111.77
18	B	856	BCR	C40-C30-C29	2.51	118.58	108.95
19	A	826	CLA	CMA-C3A-C4A	2.51	118.51	111.77
17	4	302	LUT	C19-C9-C8	2.51	121.92	118.09
19	2	505	CLA	CHA-C4D-ND	2.51	137.72	132.55
19	A	827	CLA	CHA-C4D-ND	2.51	137.72	132.55
19	A	807	CLA	C4B-CHC-C1C	2.51	132.14	126.25
19	A	809	CLA	CMA-C3A-C4A	2.50	118.50	111.77
19	B	818	CLA	CMA-C3A-C4A	2.50	118.50	111.77
18	J	1108	BCR	C2-C1-C6	2.50	114.08	110.44
19	B	831	CLA	C2D-C1D-ND	2.50	112.60	110.13
19	G	202	CLA	CHA-C4D-ND	2.50	137.71	132.55
19	1	507	CLA	C3B-C4B-NB	-2.50	108.30	110.53
19	1	509	CLA	C3B-C4B-NB	-2.50	108.30	110.53
19	B	811	CLA	CHA-C4D-ND	2.50	137.71	132.55
19	2	514	CLA	C3B-C4B-NB	-2.50	108.30	110.53
19	B	825	CLA	C1-O2A-CGA	2.50	122.70	116.65
18	A	849	BCR	C36-C18-C19	-2.50	114.27	118.09
19	B	838	CLA	C2D-C1D-ND	2.50	112.60	110.13
19	K	1004	CLA	C1C-NC-C4C	-2.50	105.54	106.68
19	2	507	CLA	CMD-C2D-C3D	-2.50	121.96	127.69
19	B	808	CLA	C1D-ND-C4D	-2.50	104.56	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2	502	XAT	C20-C13-C14	-2.50	118.77	122.82
19	A	813	CLA	C2D-C1D-ND	2.50	112.60	110.13
18	B	849	BCR	C34-C9-C10	-2.50	118.77	122.82
19	B	823	CLA	O2A-CGA-CBA	2.49	119.44	111.83
19	B	807	CLA	C1D-ND-C4D	-2.49	104.56	106.31
19	A	833	CLA	CHD-C1D-ND	-2.49	121.29	124.80
19	A	823	CLA	C4B-CHC-C1C	2.49	132.11	126.25
19	B	826	CLA	C3D-C2D-C1D	-2.49	102.43	105.83
19	K	1001	CLA	C1D-ND-C4D	-2.49	104.56	106.31
19	1	508	CLA	CHA-C4D-ND	2.49	137.69	132.55
18	A	848	BCR	C8-C9-C10	2.49	122.93	119.01
18	A	849	BCR	C19-C18-C17	2.49	122.93	119.01
19	F	303	CLA	CMA-C3A-C4A	2.49	118.47	111.77
19	4	309	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
19	G	202	CLA	C3B-C4B-NB	-2.49	108.31	110.53
18	B	852	BCR	C12-C13-C14	-2.49	115.09	119.01
23	4	303	XAT	O4-C6-C7	-2.49	109.75	116.88
19	B	838	CLA	CHD-C1D-ND	-2.49	121.30	124.80
19	K	1001	CLA	CHA-C4D-ND	2.49	137.68	132.55
19	H	1000	CLA	CHA-C4D-ND	2.49	137.68	132.55
19	A	831	CLA	C3B-C4B-NB	-2.49	108.31	110.53
19	4	305	CLA	CHD-C1D-ND	-2.49	121.30	124.80
19	A	828	CLA	C3B-C4B-NB	-2.49	108.31	110.53
19	A	811	CLA	C1D-ND-C4D	-2.49	104.57	106.31
19	B	814	CLA	CHA-C4D-ND	2.49	137.68	132.55
19	B	808	CLA	C4B-CHC-C1C	2.48	132.09	126.25
19	4	315	CLA	CHD-C1D-ND	-2.48	121.31	124.80
19	B	829	CLA	CHA-C4D-ND	2.48	137.68	132.55
18	A	852	BCR	C2-C1-C6	2.48	114.05	110.44
19	A	825	CLA	CHA-C4D-ND	2.48	137.67	132.55
19	A	818	CLA	CHD-C1D-ND	-2.48	121.31	124.80
19	B	830	CLA	C3B-C4B-NB	-2.48	108.31	110.53
19	1	516	CLA	C3B-C4B-NB	-2.48	108.32	110.53
19	L	303	CLA	CHD-C1D-ND	-2.48	121.31	124.80
19	4	306	CLA	C1D-ND-C4D	-2.48	104.57	106.31
19	A	818	CLA	O2A-CGA-CBA	2.48	119.39	111.83
20	1	512	CHL	C1B-CHB-C4A	2.48	122.92	121.32
19	A	819	CLA	C3B-C4B-NB	-2.48	108.32	110.53
19	B	814	CLA	O2A-CGA-CBA	2.48	119.39	111.83
19	4	318	CLA	O2A-CGA-CBA	2.48	119.39	111.83
18	3	303	BCR	C10-C11-C12	-2.48	116.03	123.20
19	A	854	CLA	C2D-C1D-ND	2.47	112.58	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	805	CLA	C4B-CHC-C1C	2.47	132.06	126.25
18	B	856	BCR	C34-C9-C10	-2.47	118.81	122.82
19	4	308	CLA	C3D-C2D-C1D	-2.47	102.46	105.83
19	A	820	CLA	CHA-C4D-ND	2.47	137.65	132.55
19	4	306	CLA	CHD-C1D-ND	-2.47	121.32	124.80
19	B	817	CLA	C4B-CHC-C1C	2.47	132.06	126.25
19	B	809	CLA	C4B-CHC-C1C	2.47	132.06	126.25
19	3	307	CLA	O2A-CGA-CBA	2.47	119.36	111.83
19	B	821	CLA	CHA-C4D-ND	2.47	137.64	132.55
19	L	304	CLA	CHD-C1D-ND	-2.47	121.33	124.80
19	A	838	CLA	CHD-C1D-ND	-2.47	121.33	124.80
18	A	851	BCR	C32-C1-C6	-2.47	106.38	110.24
30	F	301	ZEX	C35-C34-C33	-2.47	123.82	127.28
19	A	817	CLA	C1D-ND-C4D	-2.47	104.58	106.31
19	1	505	CLA	CHA-C4D-ND	2.46	137.63	132.55
20	4	314	CHL	C1-O2A-CGA	2.46	122.62	116.65
19	A	810	CLA	CMD-C2D-C3D	-2.46	122.04	127.69
19	1	506	CLA	C2D-C1D-ND	2.46	112.56	110.13
19	A	831	CLA	CHD-C1D-ND	-2.46	121.34	124.80
19	A	841	CLA	CHD-C1D-ND	-2.46	121.34	124.80
21	1	517	LHG	O8-C23-C24	2.46	119.34	111.83
20	3	314	CHL	CMA-C3A-C4A	2.46	119.91	114.61
19	A	805	CLA	CHA-C4D-ND	2.46	137.62	132.55
19	G	203	CLA	CHA-C4D-ND	2.46	137.62	132.55
19	B	838	CLA	O2A-CGA-CBA	2.46	119.33	111.83
19	A	854	CLA	CMA-C3A-C4A	2.46	118.38	111.77
19	4	310	CLA	CHA-C4D-ND	2.46	137.62	132.55
21	1	520	LHG	O8-C23-C24	2.46	119.33	111.83
18	2	503	BCR	C40-C30-C29	2.46	118.39	108.95
19	A	824	CLA	C4B-CHC-C1C	2.46	132.03	126.25
17	J	1109	LUT	C31-C32-C33	-2.46	119.62	126.36
19	A	804	CLA	C1D-ND-C4D	-2.46	104.59	106.31
20	4	313	CHL	C1-O2A-CGA	2.46	123.94	116.07
19	G	203	CLA	CHD-C1D-ND	-2.46	121.34	124.80
19	2	507	CLA	CHA-C4D-ND	2.46	137.62	132.55
19	B	817	CLA	CMD-C2D-C3D	-2.45	122.06	127.69
19	3	305	CLA	O2A-CGA-CBA	2.45	119.31	111.83
19	3	315	CLA	O2A-CGA-CBA	2.45	119.31	111.83
19	2	505	CLA	C1D-ND-C4D	-2.45	104.59	106.31
19	3	313	CLA	C1D-ND-C4D	-2.45	104.59	106.31
19	1	504	CLA	CHD-C1D-ND	-2.45	121.35	124.80
19	2	514	CLA	CAC-C3C-C4C	2.45	127.98	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	804	CLA	CHA-C4D-ND	2.45	137.60	132.55
19	B	805	CLA	C1D-ND-C4D	-2.45	104.59	106.31
19	1	513	CLA	CHD-C1D-ND	-2.45	121.36	124.80
19	4	307	CLA	CHA-C4D-ND	2.45	137.60	132.55
19	A	831	CLA	CHA-C4D-ND	2.45	137.60	132.55
19	4	318	CLA	C2D-C1D-ND	2.45	112.55	110.13
29	B	841	PQN	C2M-C2-C3	-2.45	120.43	124.45
19	B	824	CLA	C3B-C4B-NB	-2.45	108.35	110.53
19	F	302	CLA	CMA-C3A-C4A	2.45	118.34	111.77
19	B	820	CLA	CHA-C4D-ND	2.44	137.59	132.55
19	1	511	CLA	CAC-C3C-C4C	2.44	127.97	124.79
19	B	809	CLA	CHA-C4D-ND	2.44	137.59	132.55
18	B	802	BCR	C39-C30-C25	-2.44	106.41	110.24
19	B	825	CLA	O2A-CGA-CBA	2.44	119.28	111.83
19	J	1102	CLA	CHD-C1D-ND	-2.44	121.37	124.80
19	A	829	CLA	O2A-CGA-CBA	2.44	119.28	111.83
19	B	835	CLA	CHD-C1D-ND	-2.44	121.37	124.80
19	A	832	CLA	CMA-C3A-C4A	2.44	118.33	111.77
18	B	851	BCR	C30-C25-C24	2.44	122.27	115.65
19	A	835	CLA	C4B-CHC-C1C	2.44	131.99	126.25
19	A	822	CLA	CHA-C4D-ND	2.44	137.58	132.55
19	L	301	CLA	CHA-C4D-ND	2.44	137.58	132.55
19	B	834	CLA	C2D-C1D-ND	2.44	112.54	110.13
19	1	516	CLA	CHA-C4D-ND	2.44	137.58	132.55
19	B	832	CLA	O1D-CGD-CBD	-2.44	119.71	124.52
19	2	510	CLA	O2A-CGA-CBA	2.44	119.26	111.83
19	A	841	CLA	CMA-C3A-C4A	2.44	118.32	111.77
19	4	312	CLA	O2A-CGA-CBA	2.43	119.25	111.83
19	1	513	CLA	C2D-C1D-ND	2.43	112.53	110.13
19	A	811	CLA	C4B-CHC-C1C	2.43	131.97	126.25
19	B	835	CLA	C2D-C1D-ND	2.43	112.53	110.13
19	B	818	CLA	CHA-C4D-ND	2.43	137.56	132.55
19	2	505	CLA	C3D-C2D-C1D	-2.43	102.51	105.83
18	B	851	BCR	C29-C28-C27	2.43	116.62	111.28
19	B	806	CLA	O2A-C1-C2	2.43	117.46	108.11
19	1	504	CLA	CHA-C4D-ND	2.43	137.56	132.55
19	3	311	CLA	CHA-C4D-ND	2.43	137.56	132.55
19	A	839	CLA	O2A-CGA-CBA	2.43	119.24	111.83
19	B	825	CLA	C2D-C1D-ND	2.43	112.53	110.13
19	2	506	CLA	C3B-C4B-NB	-2.43	108.36	110.53
18	L	306	BCR	C38-C26-C25	-2.43	121.84	124.48
18	A	851	BCR	C37-C22-C23	2.43	121.79	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	813	CLA	CHA-C4D-ND	2.42	137.55	132.55
19	J	1101	CLA	CHA-C4D-ND	2.42	137.55	132.55
21	A	853	LHG	O8-C23-C24	2.42	119.23	111.83
19	A	810	CLA	CHA-C4D-ND	2.42	137.55	132.55
22	J	1104	LMG	C7-O1-C1	-2.42	108.60	113.80
19	A	802	CLA	CAA-C2A-C1A	-2.42	104.03	111.97
19	B	826	CLA	CHA-C1A-NA	-2.42	120.91	126.39
19	B	835	CLA	C3D-C2D-C1D	-2.42	102.53	105.83
19	1	508	CLA	C1D-ND-C4D	-2.42	104.61	106.31
19	B	815	CLA	C1D-ND-C4D	-2.42	104.61	106.31
18	B	853	BCR	C34-C9-C10	-2.42	118.89	122.82
19	B	825	CLA	CHA-C4D-ND	2.42	137.54	132.55
19	2	508	CLA	C2D-C1D-ND	2.42	112.52	110.13
19	A	803	CLA	C1-O2A-CGA	2.42	122.51	116.65
19	A	854	CLA	CHA-C1A-NA	-2.42	120.91	126.39
22	G	206	LMG	O8-C28-C29	2.42	119.21	111.83
19	A	811	CLA	CHA-C4D-ND	2.42	137.54	132.55
19	A	804	CLA	CHD-C1D-ND	-2.42	121.40	124.80
19	4	308	CLA	CMA-C3A-C4A	2.42	118.27	111.77
19	2	504	CLA	C4B-CHC-C1C	2.42	131.93	126.25
19	B	826	CLA	CMA-C3A-C4A	2.42	118.27	111.77
19	4	304	CLA	C1-C2-C3	2.42	130.15	126.20
19	A	828	CLA	CHD-C1D-ND	-2.41	121.40	124.80
18	J	1108	BCR	C12-C13-C14	-2.41	115.21	119.01
19	2	504	CLA	CHA-C4D-ND	2.41	137.53	132.55
19	A	829	CLA	CHD-C1D-ND	-2.41	121.41	124.80
19	3	317	CLA	C4B-CHC-C1C	2.41	131.92	126.25
19	J	1102	CLA	C3B-C4B-NB	-2.41	108.38	110.53
19	J	1105	CLA	CHA-C4D-ND	2.41	137.53	132.55
19	A	821	CLA	CHD-C1D-ND	-2.41	121.41	124.80
19	4	304	CLA	C4B-CHC-C1C	2.41	131.92	126.25
19	A	830	CLA	CHD-C1D-ND	-2.41	121.41	124.80
19	L	301	CLA	C1-O2A-CGA	2.41	122.49	116.65
19	A	840	CLA	CHA-C4D-ND	2.41	137.53	132.55
19	A	822	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
19	A	802	CLA	CHD-C1D-ND	-2.41	121.41	124.80
17	1	501	LUT	C22-C23-C24	-2.41	107.60	111.18
19	A	854	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
17	3	302	LUT	C31-C32-C33	-2.41	119.75	126.36
19	B	807	CLA	CHA-C4D-ND	2.41	137.52	132.55
19	4	318	CLA	C3B-C4B-NB	-2.41	108.38	110.53
19	L	301	CLA	C1D-ND-C4D	-2.41	104.62	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	309	CLA	CHD-C1D-ND	-2.41	121.41	124.80
19	2	514	CLA	CHA-C4D-ND	2.41	137.52	132.55
19	B	803	CLA	CHA-C4D-ND	2.41	137.52	132.55
18	L	302	BCR	C23-C24-C25	2.41	133.43	127.00
19	F	303	CLA	C2D-C1D-ND	2.41	112.51	110.13
19	1	504	CLA	C1D-ND-C4D	-2.41	104.62	106.31
19	B	804	CLA	C3D-C2D-C1D	-2.41	102.55	105.83
19	4	315	CLA	C3B-C4B-NB	-2.41	108.38	110.53
21	A	853	LHG	C5-O7-C7	-2.41	112.04	117.80
19	A	807	CLA	CHA-C4D-ND	2.41	137.51	132.55
19	B	822	CLA	CHA-C4D-ND	2.41	137.51	132.55
19	A	826	CLA	CHD-C1D-ND	-2.40	121.42	124.80
19	A	806	CLA	C1D-ND-C4D	-2.40	104.62	106.31
19	B	840	CLA	CHD-C1D-ND	-2.40	121.42	124.80
19	4	312	CLA	O2A-C1-C2	2.40	117.36	108.11
19	A	836	CLA	O2A-CGA-CBA	2.40	119.16	111.83
19	B	837	CLA	O2A-CGA-CBA	2.40	119.16	111.83
23	4	303	XAT	C38-C25-C26	-2.40	118.35	122.30
19	A	812	CLA	C4B-CHC-C1C	2.40	131.90	126.25
19	A	808	CLA	C3D-C2D-C1D	-2.40	102.55	105.83
18	L	307	BCR	C39-C30-C25	-2.40	106.48	110.24
19	K	1001	CLA	C3D-C2D-C1D	-2.40	102.56	105.83
19	A	808	CLA	C1D-ND-C4D	-2.40	104.63	106.31
26	4	319	DGD	C2G-O2G-C1B	2.40	123.54	117.80
19	B	831	CLA	C3B-C4B-NB	-2.40	108.39	110.53
19	F	302	CLA	C4B-CHC-C1C	2.40	131.89	126.25
19	2	511	CLA	O2A-CGA-CBA	2.40	119.15	111.83
19	K	1002	CLA	C1D-ND-C4D	-2.40	104.63	106.31
19	2	507	CLA	CHD-C1D-ND	-2.40	121.43	124.80
19	A	830	CLA	O2A-CGA-CBA	2.40	119.15	111.83
19	A	826	CLA	C4B-CHC-C1C	2.40	131.89	126.25
24	4	320	LMT	C3'-C4'-C5'	-2.40	105.61	110.93
19	B	820	CLA	CAC-C3C-C4C	2.40	127.91	124.79
18	J	1108	BCR	C35-C13-C12	2.40	121.75	118.09
18	J	1108	BCR	C37-C22-C23	2.40	121.75	118.09
19	B	811	CLA	CMA-C3A-C4A	2.40	118.22	111.77
19	H	1000	CLA	CHD-C1D-ND	-2.40	121.43	124.80
19	4	312	CLA	CHA-C4D-ND	2.40	137.49	132.55
19	B	821	CLA	CMA-C3A-C4A	2.40	118.21	111.77
19	A	821	CLA	C4B-CHC-C1C	2.40	131.88	126.25
19	A	833	CLA	O2A-CGA-CBA	2.40	119.14	111.83
18	K	1005	BCR	C30-C25-C26	-2.40	119.36	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	503	BCR	C33-C5-C6	-2.40	121.87	124.48
19	3	307	CLA	CHD-C1D-ND	-2.40	121.43	124.80
19	A	829	CLA	CMA-C3A-C4A	2.39	118.21	111.77
18	L	306	BCR	C30-C25-C26	-2.39	119.36	122.64
19	A	807	CLA	CMD-C2D-C3D	-2.39	122.20	127.69
19	2	509	CLA	C4B-CHC-C1C	2.39	131.88	126.25
19	A	810	CLA	C4B-CHC-C1C	2.39	131.88	126.25
19	A	828	CLA	C1D-ND-C4D	-2.39	104.63	106.31
19	4	304	CLA	C3D-C2D-C1D	-2.39	102.57	105.83
22	G	210	LMG	C9-C8-C7	-2.39	106.21	111.78
21	2	517	LHG	O8-C23-C24	2.39	119.12	111.83
19	B	828	CLA	O2A-CGA-CBA	2.39	119.12	111.83
19	2	504	CLA	C3B-C4B-NB	-2.39	108.40	110.53
19	3	306	CLA	CMD-C2D-C3D	-2.39	122.21	127.69
19	L	305	CLA	CHA-C4D-ND	2.39	137.48	132.55
19	3	307	CLA	C4B-CHC-C1C	2.39	131.87	126.25
19	B	816	CLA	O2A-CGA-CBA	2.39	119.12	111.83
19	3	309	CLA	CHD-C1D-ND	-2.39	121.44	124.80
19	A	802	CLA	O2A-CGA-CBA	2.39	119.12	111.83
19	A	820	CLA	CAC-C3C-C4C	2.39	127.90	124.79
19	B	811	CLA	CAC-C3C-C4C	2.39	127.90	124.79
19	B	837	CLA	CHA-C4D-ND	2.39	137.48	132.55
19	A	812	CLA	CHA-C4D-ND	2.39	137.47	132.55
18	A	856	BCR	C8-C9-C10	2.39	122.76	119.01
19	B	830	CLA	CMD-C2D-C3D	-2.39	122.22	127.69
19	1	511	CLA	CMD-C2D-C3D	-2.39	122.22	127.69
18	K	1005	BCR	C38-C26-C25	-2.39	121.88	124.48
19	A	808	CLA	CMA-C3A-C4A	2.39	118.18	111.77
19	A	803	CLA	C3D-C2D-C1D	-2.39	102.58	105.83
19	B	808	CLA	CHA-C4D-ND	2.39	137.47	132.55
19	1	513	CLA	O2A-CGA-CBA	2.38	119.11	111.83
26	4	319	DGD	O5D-C1E-C2E	2.38	111.89	108.27
19	1	509	CLA	CHA-C4D-ND	2.38	137.47	132.55
19	3	308	CLA	C4B-CHC-C1C	2.38	131.85	126.25
19	3	308	CLA	C1D-ND-C4D	-2.38	104.64	106.31
19	A	804	CLA	CMD-C2D-C3D	-2.38	122.23	127.69
19	L	305	CLA	C3B-C4B-NB	-2.38	108.40	110.53
19	H	1000	CLA	CMA-C3A-C4A	2.38	118.17	111.77
19	1	515	CLA	C4B-CHC-C1C	2.38	131.84	126.25
19	B	806	CLA	CMD-C2D-C3D	-2.38	122.23	127.69
19	4	306	CLA	O2A-CGA-CBA	2.38	119.09	111.83
19	B	811	CLA	CAA-CBA-CGA	-2.38	106.45	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	839	CLA	CMA-C3A-C4A	2.38	118.17	111.77
18	I	101	BCR	C35-C13-C14	-2.38	118.96	122.82
19	1	507	CLA	C4B-CHC-C1C	2.38	131.84	126.25
18	B	853	BCR	C27-C26-C25	-2.38	119.49	122.70
18	B	850	BCR	C39-C30-C25	-2.38	106.52	110.24
20	2	526	CHL	C4D-CHA-CBD	-2.38	106.57	108.97
19	B	835	CLA	CHA-C4D-ND	2.37	137.45	132.55
19	A	816	CLA	C3B-C4B-NB	-2.37	108.41	110.53
19	A	803	CLA	CMA-C3A-C4A	2.37	118.15	111.77
19	B	823	CLA	CHA-C4D-ND	2.37	137.44	132.55
19	A	855	CLA	C3B-C4B-NB	-2.37	108.41	110.53
19	K	1001	CLA	C3B-C4B-NB	-2.37	108.41	110.53
20	2	526	CHL	C1-C2-C3	-2.37	122.31	126.20
19	F	302	CLA	CHD-C1D-ND	-2.37	121.46	124.80
19	3	307	CLA	C3D-C2D-C1D	-2.37	102.59	105.83
19	1	508	CLA	C1-O2A-CGA	2.37	122.39	116.65
19	3	311	CLA	C3D-C2D-C1D	-2.37	102.59	105.83
19	2	506	CLA	CAC-C3C-C4C	2.37	127.87	124.79
19	A	804	CLA	C4B-CHC-C1C	2.37	131.82	126.25
19	B	806	CLA	C1D-ND-C4D	-2.37	104.65	106.31
19	A	833	CLA	CHA-C4D-ND	2.37	137.44	132.55
19	2	509	CLA	CHD-C1D-ND	-2.37	121.47	124.80
19	A	830	CLA	C3B-C4B-NB	-2.37	108.42	110.53
19	3	306	CLA	C1D-ND-C4D	-2.37	104.65	106.31
18	J	1108	BCR	C30-C25-C26	-2.37	119.40	122.64
19	K	1003	CLA	CHD-C1D-ND	-2.37	121.50	124.84
19	B	804	CLA	O2A-CGA-CBA	2.37	119.05	111.83
19	1	513	CLA	C3D-C2D-C1D	-2.37	102.60	105.83
19	B	840	CLA	C3D-C2D-C1D	-2.37	102.60	105.83
19	A	802	CLA	CHA-C4D-ND	2.37	137.43	132.55
18	A	850	BCR	C34-C9-C10	-2.37	118.98	122.82
20	2	516	CHL	CMA-C3A-C4A	2.37	119.71	114.61
19	A	837	CLA	C2D-C1D-ND	2.37	112.47	110.13
19	3	307	CLA	CHA-C4D-ND	2.37	137.43	132.55
19	G	203	CLA	CMD-C2D-C3D	-2.37	122.26	127.69
19	A	831	CLA	CMA-C3A-C4A	2.37	118.13	111.77
19	A	855	CLA	CHD-C1D-ND	-2.37	121.47	124.80
20	2	526	CHL	C4C-CHD-C1D	2.36	124.53	116.07
19	A	822	CLA	O2A-CGA-CBA	2.36	119.05	111.83
24	3	318	LMT	O5B-C1B-C2B	2.36	115.23	110.37
19	A	842	CLA	CHA-C4D-ND	2.36	137.43	132.55
19	B	831	CLA	C3D-C2D-C1D	-2.36	102.61	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	813	CLA	CHD-C1D-ND	-2.36	121.48	124.80
19	B	820	CLA	CHD-C1D-ND	-2.36	121.48	124.80
26	B	801	DGD	C3A-C2A-C1A	-2.36	105.03	113.69
19	3	315	CLA	CHA-C4D-ND	2.36	137.43	132.55
19	2	506	CLA	C4B-CHC-C1C	2.36	131.80	126.25
19	F	302	CLA	C6-C7-C8	-2.36	108.11	115.97
19	B	830	CLA	CMA-C3A-C4A	2.36	118.12	111.77
19	J	1105	CLA	CMD-C2D-C3D	-2.36	122.27	127.69
19	B	821	CLA	C1D-ND-C4D	-2.36	104.66	106.31
19	A	832	CLA	CHA-C4D-ND	2.36	137.42	132.55
19	G	202	CLA	O2A-CGA-CBA	2.36	119.03	111.83
19	A	827	CLA	C3D-C2D-C1D	-2.36	102.61	105.83
19	B	838	CLA	CMD-C2D-C3D	-2.36	122.28	127.69
17	1	501	LUT	C26-C27-C28	-2.36	120.91	124.58
19	4	306	CLA	CAC-C3C-C4C	2.36	127.86	124.79
19	1	506	CLA	C4B-CHC-C1C	2.36	131.79	126.25
19	B	805	CLA	CHD-C1D-ND	-2.36	121.48	124.80
19	J	1102	CLA	CMD-C2D-C3D	-2.36	122.28	127.69
19	A	813	CLA	C3D-C2D-C1D	-2.36	102.61	105.83
18	3	304	BCR	C27-C26-C25	-2.36	119.52	122.70
19	1	511	CLA	C4B-CHC-C1C	2.36	131.79	126.25
19	2	507	CLA	C4B-CHC-C1C	2.36	131.79	126.25
19	B	825	CLA	CHD-C1D-ND	-2.36	121.49	124.80
19	A	821	CLA	CHA-C4D-ND	2.36	137.41	132.55
19	G	204	CLA	O2A-C1-C2	2.36	117.17	108.11
19	A	808	CLA	C3B-C4B-NB	-2.35	108.43	110.53
19	A	836	CLA	CHA-C4D-ND	2.35	137.41	132.55
19	B	819	CLA	C4B-CHC-C1C	2.35	131.78	126.25
19	B	806	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
19	3	305	CLA	CHA-C4D-ND	2.35	137.41	132.55
19	A	827	CLA	C4B-CHC-C1C	2.35	131.78	126.25
19	B	839	CLA	C4B-CHC-C1C	2.35	131.78	126.25
19	B	805	CLA	CHA-C4D-ND	2.35	137.40	132.55
18	B	802	BCR	C37-C22-C23	2.35	121.68	118.09
19	B	839	CLA	C2D-C1D-ND	2.35	112.45	110.13
18	A	848	BCR	C30-C25-C24	2.35	122.03	115.65
19	4	304	CLA	CHD-C1D-ND	-2.35	121.50	124.80
18	I	101	BCR	C8-C9-C10	2.35	122.70	119.01
19	A	834	CLA	CHD-C1D-ND	-2.35	121.50	124.80
19	A	828	CLA	O2A-CGA-CBA	2.35	119.00	111.83
19	2	509	CLA	O2A-CGA-CBA	2.35	119.00	111.83
18	B	802	BCR	C30-C25-C26	-2.35	119.43	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	305	CLA	CMA-C3A-C4A	2.35	118.08	111.77
18	A	850	BCR	C27-C26-C25	-2.35	119.53	122.70
19	A	816	CLA	CHA-C4D-ND	2.35	137.39	132.55
19	1	504	CLA	CAA-C2A-C3A	-2.35	106.66	113.00
18	B	849	BCR	C8-C7-C6	2.35	133.27	127.00
19	A	835	CLA	CHA-C4D-ND	2.35	137.39	132.55
19	L	305	CLA	CHD-C1D-ND	-2.35	121.50	124.80
19	B	824	CLA	C3D-C2D-C1D	-2.34	102.63	105.83
19	B	813	CLA	C1D-ND-C4D	-2.34	104.67	106.31
19	K	1004	CLA	C4D-ND-C1D	-2.34	104.67	106.31
19	A	820	CLA	O2A-CGA-CBA	2.34	118.98	111.83
19	2	506	CLA	CHA-C4D-ND	2.34	137.38	132.55
19	4	312	CLA	CMD-C2D-C3D	-2.34	122.31	127.69
19	A	826	CLA	CAA-C2A-C1A	-2.34	104.30	111.97
19	B	825	CLA	C4B-CHC-C1C	2.34	131.76	126.25
19	1	510	CLA	CHA-C4D-ND	2.34	137.38	132.55
19	4	307	CLA	C4B-CHC-C1C	2.34	131.75	126.25
19	A	830	CLA	C1D-ND-C4D	-2.34	104.67	106.31
19	B	813	CLA	CMD-C2D-C3D	-2.34	122.32	127.69
19	4	315	CLA	CHA-C4D-ND	2.34	137.38	132.55
19	A	815	CLA	CHA-C4D-ND	2.34	137.38	132.55
18	A	856	BCR	C34-C9-C10	-2.34	119.03	122.82
19	2	514	CLA	C4B-CHC-C1C	2.34	131.75	126.25
19	B	813	CLA	CAC-C3C-C4C	2.34	127.83	124.79
19	2	511	CLA	CHA-C4D-ND	2.34	137.37	132.55
19	B	823	CLA	C4B-CHC-C1C	2.34	131.74	126.25
19	A	834	CLA	CHA-C4D-ND	2.34	137.37	132.55
18	J	1108	BCR	C40-C30-C25	-2.34	106.58	110.24
19	3	312	CLA	CHA-C4D-ND	2.34	137.37	132.55
19	4	310	CLA	C3D-C2D-C1D	-2.34	102.64	105.83
19	3	317	CLA	CHA-C4D-ND	2.33	137.37	132.55
19	4	305	CLA	C1-O2A-CGA	2.33	122.30	116.65
19	4	305	CLA	C4B-CHC-C1C	2.33	131.74	126.25
19	B	809	CLA	CMD-C2D-C3D	-2.33	122.34	127.69
18	A	848	BCR	C39-C30-C25	-2.33	106.58	110.24
19	4	315	CLA	CMA-C3A-C4A	2.33	118.04	111.77
19	B	822	CLA	C1D-ND-C4D	-2.33	104.67	106.31
19	A	808	CLA	C2D-C1D-ND	2.33	112.44	110.13
19	B	817	CLA	CHA-C4D-ND	2.33	137.36	132.55
20	2	516	CHL	C4D-CHA-CBD	-2.33	106.62	108.97
19	4	318	CLA	C3D-C2D-C1D	-2.33	102.65	105.83
19	3	312	CLA	C4B-CHC-C1C	2.33	131.72	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	838	CLA	CHA-C4D-ND	2.33	137.35	132.55
19	B	833	CLA	CHA-C4D-ND	2.33	137.35	132.55
19	1	505	CLA	C4B-CHC-C1C	2.33	131.72	126.25
17	1	502	LUT	C38-C25-C24	-2.33	117.85	123.36
17	2	501	LUT	C15-C35-C34	-2.33	118.75	123.52
19	B	834	CLA	C3D-C2D-C1D	-2.33	102.65	105.83
19	3	309	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
19	4	311	CLA	C3B-C2B-C1B	-2.33	104.43	107.17
19	B	813	CLA	C4B-CHC-C1C	2.33	131.72	126.25
19	A	820	CLA	CHD-C1D-ND	-2.33	121.53	124.80
19	A	824	CLA	CHA-C4D-ND	2.33	137.35	132.55
19	G	204	CLA	O2A-CGA-CBA	2.33	118.92	111.83
19	2	511	CLA	C1D-ND-C4D	-2.32	104.68	106.31
18	4	301	BCR	C29-C28-C27	2.32	116.39	111.28
19	4	306	CLA	CHA-C4D-ND	2.32	137.34	132.55
19	A	842	CLA	C2D-C1D-ND	2.32	112.43	110.13
18	A	849	BCR	C8-C9-C10	2.32	122.66	119.01
19	B	821	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
19	B	838	CLA	CHA-C4D-ND	2.32	137.34	132.55
19	2	508	CLA	C3D-C2D-C1D	-2.32	102.66	105.83
19	K	1002	CLA	CAC-C3C-C4C	2.32	127.81	124.79
19	A	830	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
19	B	828	CLA	C3B-C4B-NB	-2.32	108.46	110.53
19	B	814	CLA	C4B-CHC-C1C	2.32	131.71	126.25
19	B	827	CLA	C2D-C1D-ND	2.32	112.42	110.13
19	A	804	CLA	CHA-C4D-ND	2.32	137.34	132.55
19	K	1001	CLA	CAC-C3C-C4C	2.32	127.81	124.79
19	4	312	CLA	C1D-ND-C4D	-2.32	104.68	106.31
19	G	201	CLA	CHA-C1A-NA	-2.32	121.14	126.39
18	K	1005	BCR	C37-C22-C23	2.32	121.63	118.09
22	1	519	LMG	O1-C1-C2	2.32	110.81	108.14
19	J	1101	CLA	O2A-CGA-CBA	2.32	118.91	111.83
19	3	307	CLA	CAC-C3C-C4C	2.32	127.81	124.79
18	L	307	BCR	C34-C9-C10	-2.32	119.06	122.82
19	1	511	CLA	CHA-C4D-ND	2.32	137.33	132.55
19	3	306	CLA	CMA-C3A-C4A	2.32	118.00	111.77
19	B	815	CLA	CHA-C4D-ND	2.32	137.33	132.55
19	3	315	CLA	C3B-C4B-NB	-2.32	108.46	110.53
19	B	803	CLA	C1D-ND-C4D	-2.32	104.69	106.31
18	A	851	BCR	C39-C30-C25	-2.32	106.61	110.24
19	A	813	CLA	CHA-C1A-NA	-2.32	121.15	126.39
19	J	1101	CLA	C6-C7-C8	-2.32	108.27	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	836	CLA	C4B-CHC-C1C	2.32	131.69	126.25
23	2	502	XAT	C39-C29-C30	-2.32	119.06	122.82
19	A	837	CLA	CHD-C1D-ND	-2.32	121.54	124.80
19	4	305	CLA	CHA-C1A-NA	-2.32	121.15	126.39
19	3	305	CLA	C4B-CHC-C1C	2.32	131.69	126.25
19	B	806	CLA	CMA-C3A-C4A	2.31	118.00	111.77
19	A	809	CLA	C1D-ND-C4D	-2.31	104.69	106.31
21	1	520	LHG	O7-C7-O9	-2.31	118.30	123.70
19	3	313	CLA	CHA-C4D-ND	2.31	137.32	132.55
19	A	811	CLA	CAC-C3C-C4C	2.31	127.80	124.79
19	3	316	CLA	CHA-C4D-ND	2.31	137.32	132.55
19	2	510	CLA	C1D-ND-C4D	-2.31	104.69	106.31
18	I	102	BCR	C34-C9-C10	-2.31	119.07	122.82
17	3	302	LUT	C38-C25-C24	-2.31	117.89	123.36
19	L	303	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
19	A	825	CLA	C1-O2A-CGA	2.31	122.25	116.65
19	A	817	CLA	C4B-CHC-C1C	2.31	131.68	126.25
26	B	801	DGD	C1G-O1G-C1A	2.31	125.57	117.12
19	A	812	CLA	CHD-C1D-ND	-2.31	121.55	124.80
19	B	815	CLA	C4B-CHC-C1C	2.31	131.68	126.25
18	I	101	BCR	C8-C7-C6	2.31	133.17	127.00
19	1	513	CLA	CHA-C4D-ND	2.31	137.31	132.55
19	A	817	CLA	CHD-C1D-ND	-2.31	121.55	124.80
19	B	811	CLA	CHD-C1D-ND	-2.31	121.55	124.80
19	B	818	CLA	O2A-CGA-CBA	2.31	118.88	111.83
19	3	317	CLA	C1D-ND-C4D	-2.31	104.69	106.31
19	A	818	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
18	I	102	BCR	C32-C1-C6	-2.31	106.62	110.24
19	B	821	CLA	CHD-C1D-ND	-2.31	121.56	124.80
19	A	813	CLA	CHA-C4D-ND	2.31	137.31	132.55
19	A	831	CLA	O2A-CGA-CBA	2.31	118.87	111.83
19	A	818	CLA	C4B-CHC-C1C	2.31	131.67	126.25
19	A	836	CLA	C4B-CHC-C1C	2.31	131.67	126.25
19	J	1102	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
19	A	855	CLA	C2D-C1D-ND	2.31	112.41	110.13
19	1	516	CLA	CHD-C1D-ND	-2.31	121.56	124.80
19	2	507	CLA	O2A-CGA-CBA	2.31	118.86	111.83
19	2	509	CLA	CHA-C4D-ND	2.31	137.31	132.55
19	4	311	CLA	C4B-CHC-C1C	2.30	131.67	126.25
19	B	818	CLA	C4B-CHC-C1C	2.30	131.67	126.25
19	K	1002	CLA	CHA-C1A-NA	-2.30	121.17	126.39
19	K	1002	CLA	CHA-C4D-ND	2.30	137.30	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	856	BCR	C19-C18-C17	2.30	122.63	119.01
19	B	805	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
19	2	508	CLA	CHA-C4D-ND	2.30	137.30	132.55
19	B	840	CLA	C2D-C1D-ND	2.30	112.41	110.13
19	1	509	CLA	C4B-CHC-C1C	2.30	131.66	126.25
19	4	307	CLA	C3B-C4B-NB	-2.30	108.47	110.53
19	B	839	CLA	O2A-CGA-CBA	2.30	118.86	111.83
19	L	301	CLA	C4B-CHC-C1C	2.30	131.66	126.25
19	3	311	CLA	CHA-C1A-NA	-2.30	121.18	126.39
19	B	831	CLA	CHA-C4D-ND	2.30	137.30	132.55
19	1	504	CLA	C4B-CHC-C1C	2.30	131.66	126.25
19	3	313	CLA	CHD-C1D-ND	-2.30	121.56	124.80
19	B	811	CLA	C1-O2A-CGA	2.30	122.22	116.65
20	1	512	CHL	C1-O2A-CGA	2.30	123.43	116.07
19	B	837	CLA	C3B-C4B-NB	-2.30	108.48	110.53
19	2	510	CLA	C4B-CHC-C1C	2.30	131.66	126.25
19	4	318	CLA	CHA-C4D-ND	2.30	137.29	132.55
19	3	309	CLA	O2A-CGA-CBA	2.30	118.84	111.83
19	4	304	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
19	1	506	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
19	J	1105	CLA	C3D-C2D-C1D	-2.30	102.70	105.83
19	4	312	CLA	O2D-CGD-O1D	-2.30	119.38	123.85
19	A	817	CLA	CHA-C4D-ND	2.30	137.29	132.55
19	A	825	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
17	3	301	LUT	C22-C23-C24	-2.30	107.78	111.18
19	F	303	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
19	G	202	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
19	2	508	CLA	CHD-C1D-ND	-2.29	121.57	124.80
19	G	201	CLA	O2A-C1-C2	2.29	116.94	108.11
19	2	506	CLA	C3D-C2D-C1D	-2.29	102.70	105.83
19	A	826	CLA	CAA-CBA-CGA	-2.29	106.69	113.21
19	3	316	CLA	CMA-C3A-C4A	2.29	117.94	111.77
18	A	851	BCR	C10-C11-C12	-2.29	116.56	123.20
18	L	306	BCR	C39-C30-C25	-2.29	106.65	110.24
19	B	818	CLA	CHA-C1A-NA	-2.29	121.20	126.39
19	B	808	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
19	A	818	CLA	CHA-C4D-ND	2.29	137.28	132.55
18	B	849	BCR	C37-C22-C23	2.29	121.59	118.09
19	B	838	CLA	C4B-CHC-C1C	2.29	131.63	126.25
19	A	806	CLA	C3B-C4B-NB	-2.29	108.48	110.53
19	3	313	CLA	C4B-CHC-C1C	2.29	131.63	126.25
19	A	809	CLA	O2A-CGA-CBA	2.29	118.82	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	819	CLA	O2A-CGA-CBA	2.29	118.82	111.83
19	2	504	CLA	C1-O2A-CGA	2.29	122.19	116.65
19	B	810	CLA	CHA-C4D-ND	2.29	137.27	132.55
19	J	1102	CLA	CHA-C4D-ND	2.29	137.27	132.55
19	B	814	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
19	2	511	CLA	CHD-C1D-ND	-2.29	121.58	124.80
19	A	815	CLA	C4B-CHC-C1C	2.29	131.62	126.25
19	B	834	CLA	CHD-C1D-ND	-2.29	121.58	124.80
19	A	823	CLA	CHA-C4D-ND	2.29	137.27	132.55
19	F	303	CLA	C4B-CHC-C1C	2.29	131.62	126.25
18	K	1005	BCR	C39-C30-C25	-2.29	106.66	110.24
19	4	308	CLA	CHA-C1A-NA	-2.29	121.22	126.39
18	A	852	BCR	C34-C9-C8	2.29	121.58	118.09
19	A	809	CLA	CHA-C1A-NA	-2.28	121.22	126.39
18	B	850	BCR	C38-C26-C25	-2.28	121.99	124.48
19	B	836	CLA	CHA-C4D-ND	2.28	137.26	132.55
19	L	305	CLA	O2A-CGA-CBA	2.28	118.80	111.83
19	B	821	CLA	C4B-CHC-C1C	2.28	131.62	126.25
19	B	831	CLA	O2A-CGA-CBA	2.28	118.79	111.83
19	G	202	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
19	B	830	CLA	CHD-C1D-ND	-2.28	121.59	124.80
26	B	801	DGD	O1G-C1G-C2G	2.28	114.97	108.40
19	A	816	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
19	4	308	CLA	C1-O2A-CGA	2.28	122.17	116.65
19	L	304	CLA	O2A-CGA-CBA	2.28	118.78	111.83
19	B	840	CLA	CHA-C1A-NA	-2.28	121.23	126.39
19	J	1105	CLA	CMC-C2C-C1C	-2.28	121.47	125.03
24	4	320	LMT	O5B-C5B-C4B	2.28	113.80	109.70
19	1	516	CLA	O2A-CGA-CBA	2.28	118.78	111.83
19	2	506	CLA	C1D-ND-C4D	-2.28	104.72	106.31
19	A	854	CLA	CHD-C1D-ND	-2.28	121.60	124.80
19	3	315	CLA	C2D-C1D-ND	2.28	112.38	110.13
19	A	829	CLA	CHA-C4D-ND	2.28	137.24	132.55
27	A	801	CL0	O1D-CGD-CBD	-2.27	121.27	124.72
19	A	829	CLA	C2D-C1D-ND	2.27	112.38	110.13
19	B	833	CLA	O2A-CGA-CBA	2.27	118.77	111.83
19	A	841	CLA	C4B-CHC-C1C	2.27	131.59	126.25
20	2	515	CHL	C4C-CHD-C1D	2.27	124.20	116.07
18	L	307	BCR	C8-C9-C10	2.27	122.58	119.01
19	3	310	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
19	1	509	CLA	CMA-C3A-C4A	2.27	117.88	111.77
19	A	837	CLA	O2A-CGA-CBA	2.27	118.76	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	309	CLA	C1D-ND-C4D	-2.27	104.72	106.31
19	A	837	CLA	CHA-C4D-ND	2.27	137.24	132.55
19	B	819	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
18	I	101	BCR	C12-C13-C14	2.27	122.58	119.01
19	1	506	CLA	CAC-C3C-C4C	2.27	127.74	124.79
19	1	506	CLA	CHA-C4D-ND	2.27	137.23	132.55
18	1	503	BCR	C39-C30-C25	-2.27	106.69	110.24
19	2	510	CLA	C3D-C2D-C1D	-2.27	102.73	105.83
19	A	839	CLA	CHD-C1D-ND	-2.27	121.61	124.80
19	2	505	CLA	C2D-C1D-ND	2.27	112.37	110.13
19	A	824	CLA	C2D-C1D-ND	2.27	112.37	110.13
19	3	311	CLA	C4B-CHC-C1C	2.27	131.58	126.25
19	3	311	CLA	C1D-ND-C4D	-2.27	104.72	106.31
19	B	830	CLA	CAC-C3C-C4C	2.27	127.74	124.79
19	A	838	CLA	C3D-C2D-C1D	-2.27	102.74	105.83
19	2	509	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
19	K	1001	CLA	C4B-CHC-C1C	2.27	131.58	126.25
19	B	816	CLA	CHA-C4D-ND	2.27	137.22	132.55
19	B	829	CLA	CHD-C1D-ND	-2.27	121.61	124.80
18	3	304	BCR	C36-C18-C19	-2.27	114.63	118.09
19	G	201	CLA	C2D-C1D-ND	2.27	112.37	110.13
19	A	816	CLA	CAC-C3C-C4C	2.27	127.74	124.79
24	4	320	LMT	C1'-O5'-C5'	-2.26	109.30	113.72
19	B	803	CLA	C4B-CHC-C1C	2.26	131.57	126.25
19	K	1002	CLA	C4B-CHC-C1C	2.26	131.57	126.25
18	A	856	BCR	C36-C18-C19	-2.26	114.63	118.09
19	3	316	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
19	3	306	CLA	CHA-C4D-ND	2.26	137.22	132.55
19	A	808	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
20	2	516	CHL	C4C-CHD-C1D	2.26	124.16	116.07
19	4	311	CLA	CAC-C3C-C4C	2.26	127.73	124.79
19	3	310	CLA	CHA-C4D-ND	2.26	137.22	132.55
19	A	823	CLA	O2A-CGA-CBA	2.26	118.73	111.83
19	A	807	CLA	C1D-ND-C4D	-2.26	104.72	106.31
19	K	1003	CLA	C4D-ND-C1D	-2.26	104.72	106.31
20	2	513	CHL	C4C-CHD-C1D	2.26	124.16	116.07
19	3	312	CLA	CAC-C3C-C4C	2.26	127.73	124.79
19	A	814	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
19	2	506	CLA	C2D-C1D-ND	2.26	112.36	110.13
19	A	814	CLA	CHA-C4D-ND	2.26	137.21	132.55
19	2	505	CLA	C4B-CHC-C1C	2.26	131.56	126.25
22	4	322	LMG	C9-C8-C7	-2.26	106.52	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	F	302	CLA	CHA-C4D-ND	2.26	137.21	132.55
23	2	502	XAT	C7-C8-C9	-2.26	122.03	125.53
19	J	1102	CLA	C4B-CHC-C1C	2.26	131.55	126.25
17	1	501	LUT	C15-C14-C13	2.25	130.44	127.28
22	4	322	LMG	O8-C28-C29	2.25	118.70	111.83
22	B	845	LMG	O6-C5-C6	2.25	112.02	106.44
19	3	305	CLA	CHD-C1D-ND	-2.25	121.63	124.80
19	A	835	CLA	O2A-CGA-CBA	2.25	118.70	111.83
19	A	838	CLA	O2A-CGA-CBA	2.25	118.70	111.83
19	L	305	CLA	CHA-C1A-NA	-2.25	121.29	126.39
19	B	810	CLA	C4B-CHC-C1C	2.25	131.54	126.25
19	B	812	CLA	CHA-C4D-ND	2.25	137.19	132.55
19	B	839	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
19	1	510	CLA	CGD-CBD-CAD	2.25	118.14	110.85
18	A	850	BCR	C11-C12-C13	-2.25	120.19	126.36
18	3	303	BCR	C37-C22-C23	2.25	121.53	118.09
19	A	832	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
19	3	307	CLA	OBD-CAD-C3D	-2.25	123.16	128.42
19	A	842	CLA	C3D-C2D-C1D	-2.25	102.76	105.83
19	1	505	CLA	C2D-C1D-ND	2.25	112.35	110.13
19	4	308	CLA	CHD-C1D-ND	-2.25	121.64	124.80
19	A	816	CLA	CHD-C1D-ND	-2.25	121.64	124.80
19	A	812	CLA	CHA-C1A-NA	-2.25	121.30	126.39
19	J	1105	CLA	CMC-C2C-C3C	2.25	132.23	126.15
19	1	511	CLA	C1D-ND-C4D	-2.25	104.73	106.31
19	B	838	CLA	C3D-C2D-C1D	-2.25	102.76	105.83
19	3	315	CLA	C4B-CHC-C1C	2.25	131.53	126.25
19	A	802	CLA	C2D-C1D-ND	2.25	112.35	110.13
20	3	314	CHL	C1-O2A-CGA	2.25	123.27	116.07
19	G	202	CLA	C4B-CHC-C1C	2.25	131.53	126.25
19	4	309	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
19	A	802	CLA	C3D-C2D-C1D	-2.25	102.76	105.83
19	B	828	CLA	CHA-C4D-ND	2.25	137.19	132.55
19	A	819	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
19	B	829	CLA	C3B-C4B-NB	-2.25	108.53	110.53
19	J	1101	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
19	2	514	CLA	CHD-C1D-ND	-2.25	121.64	124.80
18	A	849	BCR	C34-C9-C10	-2.24	119.18	122.82
19	B	815	CLA	C3B-C4B-NB	-2.24	108.53	110.53
20	1	514	CHL	C1-O2A-CGA	2.24	122.08	116.65
19	A	806	CLA	CHA-C4D-ND	2.24	137.18	132.55
19	3	317	CLA	C3D-C2D-C1D	-2.24	102.77	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	304	CLA	C3D-C2D-C1D	-2.24	102.77	105.83
19	A	819	CLA	C4B-CHC-C1C	2.24	131.52	126.25
19	B	832	CLA	C4B-CHC-C1C	2.24	131.52	126.25
19	B	809	CLA	O2D-CGD-O1D	-2.24	119.48	123.85
24	3	318	LMT	O5'-C1'-C2'	-2.24	105.76	110.37
19	G	201	CLA	CAC-C3C-C4C	2.24	127.71	124.79
18	2	503	BCR	C8-C9-C10	2.24	122.54	119.01
19	F	303	CLA	CHA-C4D-ND	2.24	137.18	132.55
19	4	315	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
19	A	832	CLA	C4B-CHC-C1C	2.24	131.52	126.25
19	A	821	CLA	O2A-CGA-CBA	2.24	118.67	111.83
19	K	1002	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
19	A	833	CLA	C2D-C1D-ND	2.24	112.34	110.13
19	B	825	CLA	CAA-CBA-CGA	-2.24	106.84	113.21
19	1	509	CLA	CHD-C1D-ND	-2.24	121.65	124.80
19	B	815	CLA	CHD-C1D-ND	-2.24	121.65	124.80
19	B	816	CLA	CHD-C1D-ND	-2.24	121.65	124.80
19	4	309	CLA	CHA-C4D-ND	2.24	137.17	132.55
19	A	854	CLA	C3D-C2D-C1D	-2.24	102.78	105.83
19	3	316	CLA	CAC-C3C-C4C	2.24	127.70	124.79
19	1	505	CLA	CHD-C1D-ND	-2.24	121.65	124.80
19	A	831	CLA	C4B-CHC-C1C	2.24	131.51	126.25
21	1	517	LHG	O7-C7-O9	-2.24	118.47	123.70
19	A	809	CLA	C3D-C2D-C1D	-2.24	102.78	105.83
18	3	304	BCR	C19-C18-C17	2.24	122.53	119.01
19	4	312	CLA	CBC-CAC-C3C	-2.24	106.36	112.42
19	4	311	CLA	CHA-C4D-ND	2.24	137.16	132.55
19	2	504	CLA	C3D-C2D-C1D	-2.23	102.78	105.83
19	A	817	CLA	C1-O2A-CGA	2.23	122.06	116.65
19	2	504	CLA	CAC-C3C-C4C	2.23	127.70	124.79
19	B	816	CLA	C2D-C1D-ND	2.23	112.34	110.13
18	A	852	BCR	C35-C13-C12	2.23	121.50	118.09
19	G	201	CLA	C3D-C2D-C1D	-2.23	102.78	105.83
19	B	807	CLA	O2A-CGA-CBA	2.23	118.64	111.83
19	B	816	CLA	C4B-CHC-C1C	2.23	131.50	126.25
18	I	102	BCR	C23-C24-C25	2.23	132.96	127.00
19	4	308	CLA	CAC-C3C-C4C	2.23	127.69	124.79
19	1	509	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
18	L	302	BCR	C30-C25-C26	-2.23	119.59	122.64
19	B	812	CLA	C2D-C1D-ND	2.23	112.33	110.13
19	1	515	CLA	CHA-C1A-NA	-2.23	121.34	126.39
18	B	853	BCR	C32-C1-C6	-2.23	106.75	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	310	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
18	3	303	BCR	C34-C9-C10	-2.23	119.21	122.82
19	A	855	CLA	C4B-CHC-C1C	2.23	131.49	126.25
19	4	304	CLA	CHA-C1A-NA	-2.23	121.35	126.39
19	A	809	CLA	CHA-C4D-ND	2.23	137.14	132.55
19	B	839	CLA	CHA-C4D-ND	2.23	137.14	132.55
19	4	311	CLA	O1D-CGD-CBD	-2.23	120.13	124.52
19	L	303	CLA	CHA-C4D-ND	2.23	137.14	132.55
19	B	804	CLA	CHD-C1D-ND	-2.22	121.67	124.80
19	2	504	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
19	B	830	CLA	CHA-C4D-ND	2.22	137.14	132.55
19	A	803	CLA	CHA-C1A-NA	-2.22	121.36	126.39
19	A	809	CLA	C2D-C1D-ND	2.22	112.33	110.13
19	A	827	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
19	B	817	CLA	CAC-C3C-C4C	2.22	127.68	124.79
19	B	825	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
19	1	508	CLA	CHA-C1A-NA	-2.22	121.36	126.39
19	B	812	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
19	3	308	CLA	CAC-C3C-C4C	2.22	127.68	124.79
19	J	1105	CLA	C2D-C1D-ND	2.22	112.33	110.13
19	B	820	CLA	C4B-CHC-C1C	2.22	131.47	126.25
19	A	842	CLA	C4B-CHC-C1C	2.22	131.47	126.25
17	3	301	LUT	C1-C2-C3	-2.22	108.72	113.59
18	B	856	BCR	C31-C1-C6	-2.22	106.76	110.24
19	A	808	CLA	CHD-C1D-ND	-2.22	121.68	124.80
18	4	301	BCR	C34-C9-C10	-2.22	119.22	122.82
19	2	504	CLA	C2D-C1D-ND	2.22	112.32	110.13
19	3	310	CLA	C2D-C1D-ND	2.22	112.32	110.13
19	4	305	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
17	4	302	LUT	C39-C29-C30	-2.22	119.22	122.82
19	A	828	CLA	C2D-C1D-ND	2.22	112.32	110.13
19	B	807	CLA	C3D-C2D-C1D	-2.22	102.81	105.83
19	3	308	CLA	CHA-C4D-ND	2.22	137.12	132.55
19	A	831	CLA	C1D-ND-C4D	-2.22	104.76	106.31
18	4	301	BCR	C30-C25-C26	-2.22	119.61	122.64
19	A	807	CLA	CHD-C1D-ND	-2.22	121.69	124.80
18	A	849	BCR	C10-C11-C12	-2.21	116.78	123.20
19	A	824	CLA	O2A-CGA-CBA	2.21	118.59	111.83
18	A	852	BCR	C37-C22-C23	2.21	121.47	118.09
19	A	803	CLA	CHA-C4D-ND	2.21	137.12	132.55
18	B	856	BCR	C32-C1-C6	-2.21	106.77	110.24
19	B	832	CLA	O2A-CGA-CBA	2.21	118.58	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	1104	LMG	C30-C29-C28	-2.21	105.58	113.69
19	B	812	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
19	B	815	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
19	B	804	CLA	CHA-C1A-NA	-2.21	121.38	126.39
19	A	821	CLA	C1D-ND-C4D	-2.21	104.76	106.31
19	J	1101	CLA	O2D-CGD-O1D	-2.21	119.54	123.85
19	1	507	CLA	CAC-C3C-C4C	2.21	127.67	124.79
19	3	309	CLA	CHA-C1A-NA	-2.21	121.38	126.39
18	B	802	BCR	C8-C7-C6	2.21	132.90	127.00
19	G	204	CLA	C4B-CHC-C1C	2.21	131.44	126.25
19	2	508	CLA	C1-O2A-CGA	2.21	122.00	116.65
26	4	319	DGD	C1D-C2D-C3D	-2.21	105.36	110.01
19	A	833	CLA	C4B-CHC-C1C	2.21	131.44	126.25
19	3	311	CLA	CHD-C1D-ND	-2.21	121.69	124.80
19	A	835	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
18	B	849	BCR	C35-C13-C12	-2.21	114.72	118.09
19	A	839	CLA	CHA-C4D-ND	2.21	137.10	132.55
19	A	839	CLA	C4B-CHC-C1C	2.21	131.44	126.25
19	B	814	CLA	CHA-C1A-NA	-2.20	121.40	126.39
19	J	1101	CLA	C3D-C2D-C1D	-2.20	102.82	105.83
19	G	203	CLA	C4B-CHC-C1C	2.20	131.43	126.25
27	A	801	CL0	CMA-C3A-C4A	-2.20	109.86	114.61
19	B	831	CLA	CHD-C1D-ND	-2.20	121.70	124.80
18	G	205	BCR	C37-C22-C23	2.20	121.45	118.09
19	A	814	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
19	A	802	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
19	3	307	CLA	CHA-C1A-NA	-2.20	121.41	126.39
19	1	513	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
19	A	840	CLA	C4B-CHC-C1C	2.20	131.42	126.25
19	1	516	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
17	4	302	LUT	C11-C10-C9	2.20	130.36	127.28
19	A	836	CLA	C3B-C4B-NB	-2.20	108.57	110.53
26	J	1106	DGD	C3A-C2A-C1A	-2.20	105.63	113.69
20	2	515	CHL	CMA-C3A-C4A	2.20	119.35	114.61
19	2	510	CLA	CMA-C3A-C4A	2.20	117.68	111.77
19	L	305	CLA	C4B-CHC-C1C	2.20	131.42	126.25
19	A	811	CLA	CHD-C1D-ND	-2.20	121.71	124.80
19	A	819	CLA	C1-O2A-CGA	2.20	121.97	116.65
19	A	830	CLA	CMA-C3A-C4A	2.20	117.68	111.77
17	3	302	LUT	C39-C29-C30	-2.20	119.25	122.82
19	A	835	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
19	3	305	CLA	C2D-C1D-ND	2.20	112.30	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	F	303	CLA	O2A-CGA-CBA	2.20	118.53	111.83
19	G	204	CLA	CHA-C1A-NA	-2.20	121.42	126.39
19	A	839	CLA	C1D-ND-C4D	-2.20	104.77	106.31
19	A	819	CLA	CHA-C4D-ND	2.20	137.08	132.55
22	4	322	LMG	O7-C10-O9	-2.20	118.57	123.70
19	B	834	CLA	CHA-C4D-ND	2.20	137.08	132.55
19	3	313	CLA	C3B-C4B-NB	-2.20	108.57	110.53
19	A	822	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
19	A	834	CLA	C1-O2A-CGA	2.20	121.96	116.65
19	1	505	CLA	CHA-C1A-NA	-2.19	121.42	126.39
19	B	825	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
21	1	520	LHG	O8-C6-C5	2.19	114.72	108.40
19	H	1000	CLA	CMD-C2D-C3D	-2.19	122.66	127.69
19	B	830	CLA	O2D-CGD-O1D	-2.19	119.58	123.85
18	B	853	BCR	C10-C11-C12	-2.19	116.84	123.20
19	F	302	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
19	1	516	CLA	C2D-C1D-ND	2.19	112.30	110.13
19	2	509	CLA	C3B-C4B-NB	-2.19	108.57	110.53
19	G	202	CLA	C2D-C1D-ND	2.19	112.30	110.13
19	1	505	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
19	A	802	CLA	CAA-C2A-C3A	-2.19	107.08	113.00
19	J	1102	CLA	CMA-C3A-C4A	2.19	117.66	111.77
19	B	822	CLA	CAA-CBA-CGA	-2.19	106.99	113.21
19	1	508	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
19	A	828	CLA	C4B-CHC-C1C	2.19	131.40	126.25
19	1	508	CLA	CHD-C1D-ND	-2.19	121.72	124.80
19	A	814	CLA	O2A-CGA-CBA	2.19	118.51	111.83
19	A	827	CLA	C2D-C1D-ND	2.19	112.29	110.13
19	2	511	CLA	C4B-CHC-C1C	2.19	131.39	126.25
19	A	855	CLA	CHA-C4D-ND	2.19	137.06	132.55
19	B	806	CLA	CHA-C4D-ND	2.19	137.06	132.55
19	1	516	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
19	A	814	CLA	C3D-C2D-C1D	-2.19	102.85	105.83
19	B	832	CLA	CHD-C1D-ND	-2.19	121.73	124.80
19	3	313	CLA	CMD-C2D-C3D	-2.19	122.68	127.69
18	A	850	BCR	C38-C26-C27	2.19	118.25	113.60
19	A	814	CLA	C4B-CHC-C1C	2.18	131.38	126.25
19	H	1000	CLA	C3D-C2D-C1D	-2.18	102.85	105.83
19	A	854	CLA	C4B-CHC-C1C	2.18	131.38	126.25
19	1	509	CLA	C1-O2A-CGA	2.18	121.94	116.65
18	A	849	BCR	C12-C13-C14	-2.18	115.57	119.01
18	L	302	BCR	C8-C9-C10	2.18	122.44	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	815	CLA	C3D-C2D-C1D	-2.18	102.85	105.83
19	3	310	CLA	C3B-C4B-NB	-2.18	108.58	110.53
18	1	503	BCR	C37-C22-C23	2.18	121.42	118.09
19	B	826	CLA	C4B-CHC-C1C	2.18	131.38	126.25
19	A	818	CLA	C2D-C1D-ND	2.18	112.29	110.13
19	B	824	CLA	C2D-C1D-ND	2.18	112.29	110.13
19	B	824	CLA	C4B-CHC-C1C	2.18	131.38	126.25
29	A	844	PQN	C12-C11-C3	-2.18	106.71	112.08
19	B	836	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
18	A	852	BCR	C40-C30-C25	-2.18	106.82	110.24
19	2	507	CLA	C3B-C4B-NB	-2.18	108.58	110.53
19	1	504	CLA	CAC-C3C-C4C	2.18	127.63	124.79
19	H	1000	CLA	O2A-CGA-CBA	2.18	118.48	111.83
18	A	848	BCR	C37-C22-C23	2.18	121.42	118.09
19	1	511	CLA	CMA-C3A-C4A	2.18	117.63	111.77
19	A	833	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
19	B	810	CLA	C2D-C1D-ND	2.18	112.28	110.13
19	A	836	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
19	A	826	CLA	CHA-C4D-ND	2.18	137.04	132.55
19	A	828	CLA	CHA-C4D-ND	2.18	137.04	132.55
19	B	810	CLA	C1D-ND-C4D	-2.18	104.78	106.31
19	A	814	CLA	CHA-C1A-NA	-2.18	121.46	126.39
19	L	303	CLA	C3B-C4B-NB	-2.18	108.58	110.53
18	A	848	BCR	C38-C26-C27	2.18	118.24	113.60
19	2	510	CLA	C2D-C1D-ND	2.18	112.28	110.13
19	1	509	CLA	CAC-C3C-C4C	2.18	127.62	124.79
19	B	822	CLA	O2A-CGA-CBA	2.18	118.48	111.83
18	I	102	BCR	C37-C22-C23	2.18	121.42	118.09
19	4	304	CLA	C1D-ND-C4D	-2.18	104.78	106.31
19	B	835	CLA	CHA-C1A-NA	-2.18	121.46	126.39
17	1	502	LUT	C11-C12-C13	-2.18	120.39	126.36
19	B	827	CLA	CHA-C4D-ND	2.18	137.04	132.55
19	A	841	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
19	3	312	CLA	CMD-C2D-C3D	-2.18	122.70	127.69
19	4	306	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
19	4	305	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
19	A	824	CLA	CHD-C1D-ND	-2.18	121.74	124.80
19	4	305	CLA	CAC-C3C-C4C	2.17	127.62	124.79
19	A	842	CLA	CMD-C2D-C3D	-2.17	122.70	127.69
19	A	808	CLA	C4B-CHC-C1C	2.17	131.36	126.25
19	4	306	CLA	CHA-C1A-NA	-2.17	121.47	126.39
19	1	516	CLA	C4B-CHC-C1C	2.17	131.36	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	838	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
19	3	313	CLA	CHA-C1A-NA	-2.17	121.47	126.39
19	1	515	CLA	C1D-ND-C4D	-2.17	104.79	106.31
19	B	832	CLA	CAA-CBA-CGA	-2.17	107.04	113.21
19	3	311	CLA	CAC-C3C-C4C	2.17	127.61	124.79
19	L	303	CLA	C4B-CHC-C1C	2.17	131.35	126.25
19	B	819	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
23	2	502	XAT	C40-C33-C34	-2.17	119.30	122.82
19	A	813	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
19	4	311	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
20	4	314	CHL	C4D-ND-C1D	2.17	106.87	105.22
18	B	856	BCR	C8-C7-C6	2.17	132.79	127.00
20	1	512	CHL	CMD-C2D-C3D	2.17	129.02	124.68
19	A	827	CLA	O2A-CGA-CBA	2.17	118.45	111.83
19	B	818	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
19	B	832	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
19	1	513	CLA	C4B-CHC-C1C	2.17	131.35	126.25
19	B	817	CLA	CMA-C3A-C4A	2.17	117.60	111.77
19	B	826	CLA	C2D-C1D-ND	2.17	112.27	110.13
19	4	318	CLA	CMA-C3A-C4A	2.17	117.60	111.77
17	2	501	LUT	C31-C30-C29	2.17	130.32	127.28
19	A	838	CLA	C2D-C1D-ND	2.17	112.27	110.13
19	A	824	CLA	C3D-C2D-C1D	-2.17	102.88	105.83
19	A	820	CLA	C4B-CHC-C1C	2.17	131.34	126.25
19	B	840	CLA	C4B-CHC-C1C	2.17	131.34	126.25
19	A	810	CLA	C3D-C2D-C1D	-2.17	102.88	105.83
22	2	519	LMG	C1-C2-C3	-2.17	105.45	110.01
18	L	306	BCR	C32-C1-C6	-2.16	106.85	110.24
26	J	1106	DGD	C2G-O2G-C1B	2.16	122.97	117.80
19	L	301	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
19	L	305	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
19	1	511	CLA	CHA-C1A-NA	-2.16	121.49	126.39
22	B	844	LMG	O8-C28-O10	-2.16	118.22	123.63
19	A	823	CLA	C2D-C1D-ND	2.16	112.27	110.13
19	4	308	CLA	O2A-CGA-CBA	2.16	118.43	111.83
19	A	841	CLA	CHA-C4D-ND	2.16	137.01	132.55
19	4	318	CLA	C4B-CHC-C1C	2.16	131.33	126.25
19	A	816	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
19	A	814	CLA	C1D-ND-C4D	-2.16	104.80	106.31
19	3	315	CLA	CHD-C1D-ND	-2.16	121.76	124.80
27	A	801	CL0	C4C-C3C-C2C	-2.16	104.84	113.37
20	3	314	CHL	C3D-C4D-ND	-2.16	109.47	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	810	CLA	CHA-C1A-NA	-2.16	121.50	126.39
19	2	508	CLA	C4B-CHC-C1C	2.16	131.32	126.25
17	2	501	LUT	C31-C32-C33	-2.16	120.44	126.36
19	L	301	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
23	4	303	XAT	C39-C29-C30	-2.16	119.32	122.82
19	B	837	CLA	CHA-C1A-NA	-2.16	121.50	126.39
19	B	835	CLA	C4B-CHC-C1C	2.16	131.32	126.25
19	B	807	CLA	C3B-C4B-NB	-2.16	108.60	110.53
19	J	1101	CLA	C1-O2A-CGA	2.16	121.87	116.65
19	2	514	CLA	CHA-C1A-NA	-2.16	121.51	126.39
19	B	813	CLA	CHA-C1A-NA	-2.16	121.51	126.39
19	3	307	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
17	3	302	LUT	C19-C9-C8	2.16	121.38	118.09
18	A	849	BCR	C37-C22-C23	2.16	121.38	118.09
19	A	830	CLA	CMD-C2D-C3D	-2.16	122.75	127.69
19	4	310	CLA	CHD-C1D-ND	-2.16	121.77	124.80
19	A	827	CLA	CHD-C1D-ND	-2.16	121.77	124.80
21	B	842	LHG	O7-C7-O9	-2.16	118.83	122.99
18	J	1108	BCR	C39-C30-C25	-2.16	106.86	110.24
19	3	310	CLA	C4B-CHC-C1C	2.16	131.31	126.25
19	B	824	CLA	O2A-CGA-CBA	2.16	118.41	111.83
19	K	1002	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
19	G	203	CLA	CHA-C1A-NA	-2.16	121.51	126.39
19	H	1000	CLA	CHA-C1A-NA	-2.16	121.51	126.39
19	L	305	CLA	C2D-C1D-ND	2.15	112.26	110.13
19	B	815	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
19	A	826	CLA	C2D-C1D-ND	2.15	112.26	110.13
19	3	317	CLA	CHA-C1A-NA	-2.15	121.52	126.39
19	B	820	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
19	A	840	CLA	O2A-CGA-CBA	2.15	118.40	111.83
19	A	831	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
19	A	837	CLA	C3D-C2D-C1D	-2.15	102.89	105.83
19	2	508	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
19	B	813	CLA	C3D-C2D-C1D	-2.15	102.89	105.83
19	A	834	CLA	C2D-C1D-ND	2.15	112.25	110.13
19	A	815	CLA	CHA-C1A-NA	-2.15	121.52	126.39
19	2	505	CLA	CMD-C2D-C3D	-2.15	122.76	127.69
19	K	1001	CLA	CHA-C1A-NA	-2.15	121.52	126.39
19	B	827	CLA	C4B-CHC-C1C	2.15	131.30	126.25
19	A	838	CLA	CHA-C1A-NA	-2.15	121.53	126.39
22	2	519	LMG	O8-C28-O10	-2.15	118.25	123.63
18	3	304	BCR	C24-C25-C26	-2.15	116.61	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	814	CLA	C3B-C4B-NB	-2.15	108.61	110.53
20	1	521	CHL	CMD-C2D-C3D	2.15	128.97	124.68
19	4	309	CLA	C4B-CHC-C1C	2.15	131.30	126.25
19	B	821	CLA	CAC-C3C-C4C	2.15	127.58	124.79
19	B	819	CLA	CHA-C4D-ND	2.15	136.98	132.55
24	B	846	LMT	O5B-C5B-C4B	2.15	113.57	109.70
19	A	815	CLA	C1D-ND-C4D	-2.15	104.81	106.31
19	B	825	CLA	CAA-C2A-C1A	-2.15	104.94	111.97
19	A	823	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
19	B	834	CLA	CHA-C1A-NA	-2.14	121.53	126.39
19	3	311	CLA	CAA-C2A-C3A	-2.14	111.31	116.23
19	2	510	CLA	CHA-C1A-NA	-2.14	121.53	126.39
19	A	828	CLA	C1-O2A-CGA	2.14	121.84	116.65
19	3	312	CLA	C1D-ND-C4D	-2.14	104.81	106.31
19	B	808	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
20	4	313	CHL	C4C-CHD-C1D	2.14	123.74	116.07
22	2	519	LMG	O1-C1-C2	2.14	111.53	108.27
19	B	833	CLA	C1D-ND-C4D	-2.14	104.81	106.31
19	A	841	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
19	G	203	CLA	C3B-C4B-NB	-2.14	108.62	110.53
19	G	201	CLA	C1-O2A-CGA	2.14	121.83	116.65
19	A	823	CLA	CAC-C3C-C4C	2.14	127.58	124.79
19	1	513	CLA	CHA-C1A-NA	-2.14	121.54	126.39
19	G	204	CLA	CHA-C4D-ND	2.14	136.97	132.55
19	3	317	CLA	C2D-C1D-ND	2.14	112.24	110.13
19	A	822	CLA	C2D-C1D-ND	2.14	112.24	110.13
19	B	827	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
19	B	824	CLA	CHA-C1A-NA	-2.14	121.55	126.39
19	4	312	CLA	C4B-CHC-C1C	2.14	131.28	126.25
17	1	501	LUT	C18-C5-C6	-2.14	122.15	124.48
19	A	814	CLA	C3B-C4B-NB	-2.14	108.62	110.53
19	4	307	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
19	3	316	CLA	C3B-C4B-NB	-2.14	108.62	110.53
19	B	813	CLA	C3B-C4B-NB	-2.14	108.62	110.53
19	A	841	CLA	C1-O2A-CGA	2.14	121.82	116.65
19	A	836	CLA	CHA-C1A-NA	-2.14	121.55	126.39
21	A	845	LHG	O8-C23-O10	-2.14	118.28	123.63
19	A	835	CLA	CHA-C1A-NA	-2.14	121.55	126.39
19	G	202	CLA	CHA-C1A-NA	-2.14	121.56	126.39
19	B	814	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
19	3	308	CLA	CHA-C1A-NA	-2.14	121.56	126.39
19	A	802	CLA	CHA-C1A-NA	-2.14	121.56	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	804	CLA	O2A-CGA-CBA	2.14	118.34	111.83
22	B	845	LMG	O7-C10-O9	-2.13	118.72	123.70
19	B	804	CLA	CAA-C2A-C3A	-2.13	107.23	113.00
20	1	512	CHL	C3D-C4D-ND	-2.13	109.52	112.94
30	F	301	ZEX	C21-C26-C27	2.13	121.43	115.65
19	A	809	CLA	C3B-C4B-NB	-2.13	108.63	110.53
19	1	509	CLA	CHA-C1A-NA	-2.13	121.56	126.39
17	J	1109	LUT	C39-C29-C30	-2.13	119.36	122.82
20	1	521	CHL	CMA-C3A-C4A	2.13	119.20	114.61
19	B	810	CLA	CMA-C3A-C4A	2.13	117.50	111.77
19	B	840	CLA	CHA-C4D-ND	2.13	136.94	132.55
18	A	856	BCR	C37-C22-C23	2.13	121.34	118.09
18	4	301	BCR	C37-C22-C23	2.13	121.34	118.09
19	A	829	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
20	2	512	CHL	C1-O2A-CGA	2.13	122.89	116.07
19	B	808	CLA	C1-O2A-CGA	2.13	121.80	116.65
24	2	523	LMT	O5B-C5B-C4B	2.13	113.53	109.70
19	A	806	CLA	C4B-CHC-C1C	2.13	131.25	126.25
19	1	516	CLA	CHA-C1A-NA	-2.13	121.57	126.39
19	A	802	CLA	C4B-CHC-C1C	2.13	131.25	126.25
19	3	308	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
19	A	812	CLA	O2A-CGA-CBA	2.13	118.32	111.83
19	B	818	CLA	CHD-C1D-ND	-2.13	121.81	124.80
20	4	313	CHL	CMD-C2D-C3D	2.13	128.93	124.68
24	G	208	LMT	C1'-O5'-C5'	-2.13	109.57	113.72
19	2	511	CLA	CHA-C1A-NA	-2.12	121.58	126.39
19	B	831	CLA	CMA-C3A-C4A	2.12	117.48	111.77
19	B	828	CLA	CMD-C2D-C3D	-2.12	122.82	127.69
19	3	308	CLA	C3B-C4B-NB	-2.12	108.63	110.53
19	H	1000	CLA	C3B-C4B-NB	-2.12	108.63	110.53
19	B	820	CLA	C6-C7-C8	-2.12	108.91	115.97
18	2	503	BCR	C36-C18-C19	-2.12	114.84	118.09
17	4	302	LUT	C20-C13-C12	2.12	121.33	118.09
19	4	315	CLA	C4B-CHC-C1C	2.12	131.24	126.25
19	2	511	CLA	C3D-C2D-C1D	-2.12	102.93	105.83
19	B	810	CLA	C3D-C2D-C1D	-2.12	102.93	105.83
19	B	818	CLA	C3D-C2D-C1D	-2.12	102.93	105.83
19	A	854	CLA	C11-C12-C13	-2.12	108.91	115.97
19	3	311	CLA	C2D-C1D-ND	2.12	112.23	110.13
19	A	834	CLA	O2A-CGA-CBA	2.12	118.30	111.83
19	L	303	CLA	O2A-CGA-CBA	2.12	118.30	111.83
19	B	830	CLA	C4B-CHC-C1C	2.12	131.24	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	830	CLA	C1-C2-C3	-2.12	122.72	126.20
19	3	305	CLA	OBD-CAD-C3D	-2.12	123.46	128.42
19	A	813	CLA	C1-O2A-CGA	2.12	121.78	116.65
22	J	1104	LMG	C9-C8-C7	-2.12	106.84	111.78
19	B	837	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
19	3	309	CLA	C4B-CHC-C1C	2.12	131.23	126.25
20	2	516	CHL	CMD-C2D-C3D	2.12	128.92	124.68
19	3	310	CLA	CHA-C1A-NA	-2.12	121.59	126.39
18	F	306	BCR	C39-C30-C25	-2.12	106.92	110.24
18	I	101	BCR	C39-C30-C25	-2.12	106.92	110.24
17	2	501	LUT	C39-C29-C28	2.12	121.32	118.09
18	4	301	BCR	C8-C7-C6	2.12	132.66	127.00
18	L	302	BCR	C39-C30-C25	-2.12	106.92	110.24
19	B	828	CLA	C2D-C1D-ND	2.12	112.22	110.13
19	K	1001	CLA	C2D-C1D-ND	2.12	112.22	110.13
19	B	803	CLA	C2A-C3A-C4A	2.12	105.29	101.87
19	4	310	CLA	CHA-C1A-NA	-2.12	121.60	126.39
19	A	832	CLA	C1D-ND-C4D	-2.12	104.83	106.31
19	4	309	CLA	O2A-CGA-CBA	2.11	118.28	111.83
19	A	809	CLA	CHD-C1D-ND	-2.11	121.83	124.80
22	G	206	LMG	O7-C10-O9	-2.11	118.76	123.70
19	B	837	CLA	CMD-C2D-C3D	-2.11	122.84	127.69
22	2	518	LMG	O7-C10-O9	-2.11	118.76	123.70
19	A	825	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
19	K	1003	CLA	C1C-CHC-C4B	2.11	131.62	126.04
19	H	1000	CLA	C1D-ND-C4D	-2.11	104.83	106.31
19	J	1101	CLA	C11-C12-C13	-2.11	108.94	115.97
19	K	1004	CLA	C3A-C2A-C1A	-2.11	101.69	104.67
18	B	856	BCR	C28-C27-C26	-2.11	110.29	114.06
19	A	854	CLA	CHA-C4D-ND	2.11	136.90	132.55
19	4	312	CLA	CAC-C3C-C4C	2.11	127.53	124.79
18	J	1108	BCR	C29-C28-C27	2.11	115.92	111.28
22	2	520	LMG	O1-C1-C2	2.11	110.57	108.14
19	A	825	CLA	CHA-C1A-NA	-2.11	121.61	126.39
19	A	827	CLA	CHA-C1A-NA	-2.11	121.61	126.39
19	L	304	CLA	CHA-C4D-ND	2.11	136.90	132.55
19	3	311	CLA	CMD-C2D-C3D	-2.11	122.86	127.69
19	B	803	CLA	CHA-C1A-NA	-2.11	121.62	126.39
19	1	516	CLA	CAC-C3C-C4C	2.11	127.53	124.79
19	A	831	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
19	1	504	CLA	CMD-C2D-C3D	-2.11	122.86	127.69
22	J	1104	LMG	O8-C28-C29	2.11	118.26	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	804	CLA	C4B-CHC-C1C	2.11	131.20	126.25
18	2	503	BCR	C19-C18-C17	2.11	122.32	119.01
20	4	314	CHL	CMD-C2D-C3D	2.11	128.89	124.68
26	G	207	DGD	O3G-C3G-C2G	-2.11	105.69	110.82
19	1	504	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
19	A	807	CLA	C3B-C4B-NB	-2.11	108.65	110.53
19	4	306	CLA	CMD-C2D-C3D	-2.11	122.86	127.69
19	A	802	CLA	CBC-CAC-C3C	-2.11	106.71	112.42
18	B	852	BCR	C10-C11-C12	-2.10	117.10	123.20
19	4	306	CLA	C2D-C1D-ND	2.10	112.21	110.13
19	A	826	CLA	CMD-C2D-C3D	-2.10	122.86	127.69
19	G	201	CLA	CHA-C4D-ND	2.10	136.89	132.55
19	A	805	CLA	O2A-CGA-CBA	2.10	118.25	111.83
19	A	828	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
19	B	839	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
19	G	201	CLA	CMD-C2D-C3D	-2.10	122.87	127.69
19	2	506	CLA	CHA-C1A-NA	-2.10	121.63	126.39
19	1	505	CLA	CMD-C2D-C3D	-2.10	122.87	127.69
19	B	816	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
19	B	818	CLA	C1D-ND-C4D	-2.10	104.84	106.31
19	A	804	CLA	C3B-C2B-C1B	-2.10	104.69	107.17
19	G	204	CLA	C16-C15-C13	-2.10	108.99	115.97
18	I	102	BCR	C35-C13-C12	2.10	121.30	118.09
19	4	304	CLA	C2D-C1D-ND	2.10	112.20	110.13
19	B	807	CLA	C2D-C1D-ND	2.10	112.20	110.13
19	A	812	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
19	3	309	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
19	A	806	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
19	B	810	CLA	CHD-C1D-ND	-2.10	121.85	124.80
19	A	812	CLA	CAC-C3C-C4C	2.10	127.52	124.79
18	1	503	BCR	C23-C24-C25	2.10	132.60	127.00
19	B	819	CLA	C2D-C1D-ND	2.10	112.20	110.13
19	3	313	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
19	A	806	CLA	C2D-C1D-ND	2.09	112.20	110.13
19	A	817	CLA	C2D-C1D-ND	2.09	112.20	110.13
19	B	832	CLA	CHA-C4D-ND	2.09	136.87	132.55
19	L	304	CLA	C4B-CHC-C1C	2.09	131.17	126.25
19	2	507	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
19	4	315	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
19	2	505	CLA	CHA-C1A-NA	-2.09	121.65	126.39
19	A	821	CLA	CMD-C2D-C3D	-2.09	122.89	127.69
19	3	308	CLA	C3D-C2D-C1D	-2.09	102.98	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	815	CLA	CMD-C2D-C3D	-2.09	122.90	127.69
18	3	303	BCR	C8-C9-C10	2.09	122.30	119.01
19	B	820	CLA	CHA-C1A-NA	-2.09	121.66	126.39
26	B	801	DGD	O3G-C3G-C2G	2.09	115.90	110.82
20	2	512	CHL	C3D-C4D-ND	-2.09	109.59	112.94
19	3	305	CLA	CHA-C1A-NA	-2.09	121.66	126.39
18	A	848	BCR	C30-C25-C26	-2.09	119.78	122.64
19	A	840	CLA	C2D-C1D-ND	2.09	112.19	110.13
20	2	513	CHL	CMD-C2D-C3D	2.09	128.86	124.68
22	2	519	LMG	O7-C10-O9	-2.09	118.82	123.70
19	A	834	CLA	C4B-CHC-C1C	2.09	131.16	126.25
19	B	833	CLA	C4B-CHC-C1C	2.09	131.16	126.25
19	B	805	CLA	CAC-C3C-C4C	2.09	127.50	124.79
19	2	509	CLA	CHA-C1A-NA	-2.08	121.67	126.39
19	F	303	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
19	B	827	CLA	C3B-C4B-NB	-2.08	108.67	110.53
19	B	834	CLA	CMD-C2D-C3D	-2.08	122.91	127.69
19	G	201	CLA	C4D-CHA-C1A	2.08	123.73	121.24
19	A	817	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
19	B	806	CLA	C4B-CHC-C1C	2.08	131.14	126.25
20	2	512	CHL	CMB-C2B-C3B	2.08	128.84	124.68
19	B	840	CLA	CMD-C2D-C3D	-2.08	122.92	127.69
19	A	806	CLA	CHA-C1A-NA	-2.08	121.68	126.39
19	B	836	CLA	C2D-C1D-ND	2.08	112.19	110.13
18	A	850	BCR	C38-C26-C25	-2.08	122.21	124.48
19	A	813	CLA	C4B-CHC-C1C	2.08	131.14	126.25
19	A	830	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
19	B	836	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
19	3	312	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
19	A	820	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
19	3	306	CLA	C2C-C1C-NC	2.08	112.17	109.98
19	1	508	CLA	C4B-CHC-C1C	2.08	131.13	126.25
18	B	851	BCR	C37-C22-C23	2.08	121.26	118.09
19	3	315	CLA	CHA-C1A-NA	-2.08	121.69	126.39
19	B	811	CLA	O2A-CGA-CBA	2.08	118.17	111.83
19	1	509	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
23	2	502	XAT	O4-C6-C7	-2.08	110.93	116.88
19	2	510	CLA	C3B-C4B-NB	-2.08	108.68	110.53
19	3	316	CLA	CHA-C1A-NA	-2.08	121.69	126.39
19	1	510	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
19	B	822	CLA	CMD-C2D-C3D	-2.08	122.93	127.69
19	J	1105	CLA	CAA-CBA-CGA	-2.08	107.32	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	850	BCR	C30-C25-C26	-2.08	119.80	122.64
22	B	845	LMG	C1-O6-C5	2.07	117.77	113.72
20	2	526	CHL	CMA-C3A-C4A	2.07	119.08	114.61
19	H	1000	CLA	C1-O2A-CGA	2.07	121.67	116.65
19	1	509	CLA	C2D-C1D-ND	2.07	112.18	110.13
19	L	301	CLA	C2D-C1D-ND	2.07	112.18	110.13
20	1	514	CHL	CMD-C2D-C3D	2.07	128.83	124.68
19	B	840	CLA	C1-O2A-CGA	2.07	121.67	116.65
29	A	844	PQN	C21-C20-C18	-2.07	109.07	115.97
19	A	833	CLA	O2D-CGD-O1D	-2.07	119.81	123.85
19	3	312	CLA	O2A-CGA-CBA	2.07	118.15	111.83
19	4	309	CLA	C2D-C1D-ND	2.07	112.18	110.13
19	A	834	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
26	B	854	DGD	O6D-C5D-C6D	2.07	110.80	106.69
18	3	304	BCR	C37-C22-C23	2.07	121.25	118.09
19	3	312	CLA	C1-O2A-CGA	2.07	121.66	116.65
19	3	310	CLA	O2A-CGA-CBA	2.07	118.15	111.83
19	L	305	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
19	A	855	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
19	4	315	CLA	CHA-C1A-NA	-2.07	121.71	126.39
19	J	1105	CLA	CHD-C1D-ND	-2.07	121.89	124.80
19	B	807	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
18	B	849	BCR	C40-C30-C25	-2.07	107.00	110.24
19	3	307	CLA	CAA-CBA-CGA	-2.07	107.34	113.21
19	B	827	CLA	CMD-C2D-C3D	-2.07	122.95	127.69
19	3	312	CLA	CHA-C1A-NA	-2.07	121.71	126.39
19	A	804	CLA	CHA-C1A-NA	-2.07	121.71	126.39
19	A	822	CLA	CHA-C1A-NA	-2.07	121.71	126.39
18	B	853	BCR	C29-C28-C27	-2.07	106.73	111.28
19	A	829	CLA	CMD-C2D-C3D	-2.07	122.95	127.69
19	A	824	CLA	CMD-C2D-C3D	-2.07	122.95	127.69
19	2	504	CLA	CAA-C2A-C1A	-2.07	105.21	111.97
19	1	506	CLA	CHD-C1D-ND	-2.07	121.90	124.80
19	A	811	CLA	C2D-C1D-ND	2.07	112.17	110.13
24	B	855	LMT	C1'-O5'-C5'	-2.07	109.69	113.72
19	A	818	CLA	CHA-C1A-NA	-2.06	121.72	126.39
19	K	1003	CLA	C3A-C2A-C1A	-2.06	101.76	104.67
26	G	207	DGD	O2G-C1B-O1B	-2.06	118.88	123.70
18	B	850	BCR	C37-C22-C23	2.06	121.24	118.09
18	L	307	BCR	C30-C25-C26	-2.06	119.82	122.64
19	3	316	CLA	C1D-ND-C4D	-2.06	104.87	106.31
19	3	316	CLA	C3D-C2D-C1D	-2.06	103.02	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	805	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
18	A	848	BCR	C2-C1-C6	2.06	113.43	110.44
19	4	305	CLA	CMA-C3A-C2A	2.06	121.95	113.98
19	1	508	CLA	CAA-CBA-CGA	-2.06	107.36	113.21
19	3	317	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
19	1	504	CLA	CHA-C1A-NA	-2.06	121.73	126.39
19	B	829	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
19	B	832	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
20	2	516	CHL	C1C-C2C-CMC	2.06	130.51	126.80
19	3	305	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
18	1	503	BCR	C30-C25-C24	2.06	121.23	115.65
19	A	809	CLA	C4B-CHC-C1C	2.06	131.08	126.25
19	3	308	CLA	O1D-CGD-CBD	-2.06	120.46	124.52
19	1	504	CLA	O2A-CGA-CBA	2.06	118.10	111.83
19	A	821	CLA	CHA-C1A-NA	-2.06	121.74	126.39
19	A	840	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
19	4	307	CLA	CAC-C3C-C4C	2.06	127.46	124.79
19	A	812	CLA	C3D-C2D-C1D	-2.06	103.03	105.83
29	A	844	PQN	C11-C3-C2	-2.06	121.37	124.89
18	L	307	BCR	C1-C6-C7	2.05	121.22	115.65
19	B	809	CLA	CHD-C1D-ND	-2.05	121.91	124.80
19	4	309	CLA	CAC-C3C-C4C	2.05	127.46	124.79
19	2	511	CLA	CMD-C2D-C3D	-2.05	122.98	127.69
19	3	306	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
19	A	816	CLA	C4B-CHC-C1C	2.05	131.07	126.25
18	L	307	BCR	C30-C25-C24	2.05	121.22	115.65
19	L	301	CLA	O2D-CGD-O1D	-2.05	119.85	123.85
18	A	852	BCR	C8-C9-C10	-2.05	115.78	119.01
19	1	507	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
19	A	820	CLA	CHA-C1A-NA	-2.05	121.74	126.39
19	4	318	CLA	CMD-C2D-C3D	-2.05	122.98	127.69
19	A	821	CLA	CAC-C3C-C4C	2.05	127.46	124.79
20	4	317	CHL	C3D-C4D-ND	-2.05	109.65	112.94
19	A	833	CLA	CMD-C2D-C3D	-2.05	122.99	127.69
19	A	841	CLA	O2A-CGA-CBA	2.05	118.09	111.83
19	A	830	CLA	C4B-CHC-C1C	2.05	131.07	126.25
19	A	811	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
19	J	1101	CLA	C1D-ND-C4D	-2.05	104.87	106.31
19	1	504	CLA	C2D-C1D-ND	2.05	112.15	110.13
19	B	808	CLA	C2D-C1D-ND	2.05	112.15	110.13
19	A	823	CLA	CHA-C1A-NA	-2.05	121.75	126.39
19	A	813	CLA	O2A-CGA-CBA	2.05	118.08	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	513	CHL	C1-O2A-CGA	2.05	122.49	116.67
19	B	812	CLA	CAA-C2A-C3A	-2.05	107.47	113.00
19	A	840	CLA	CHD-C1D-ND	-2.05	121.92	124.80
19	A	839	CLA	C2D-C1D-ND	2.05	112.15	110.13
19	A	837	CLA	CMD-C2D-C3D	-2.05	123.00	127.69
19	2	511	CLA	CMA-C3A-C2A	2.05	121.89	113.98
19	2	506	CLA	CHD-C1D-ND	-2.05	121.92	124.80
19	F	302	CLA	CHA-C1A-NA	-2.05	121.76	126.39
19	3	305	CLA	C1-O2A-CGA	2.04	121.60	116.65
19	A	811	CLA	CMD-C2D-C3D	-2.04	123.00	127.69
18	2	503	BCR	C34-C9-C10	-2.04	119.50	122.82
19	B	832	CLA	CMA-C3A-C4A	2.04	117.27	111.77
19	A	855	CLA	CMD-C2D-C3D	-2.04	123.00	127.69
19	A	834	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
19	A	813	CLA	CMD-C2D-C3D	-2.04	123.01	127.69
24	3	318	LMT	C1'-O5'-C5'	-2.04	109.73	113.72
18	A	852	BCR	C12-C13-C14	-2.04	115.80	119.01
23	2	502	XAT	C6-C7-C8	-2.04	121.68	125.99
19	A	839	CLA	O2D-CGD-O1D	-2.04	119.88	123.85
19	A	830	CLA	C2D-C1D-ND	2.04	112.14	110.13
20	2	512	CHL	CMD-C2D-C3D	2.04	128.76	124.68
19	4	315	CLA	CAC-C3C-C4C	2.04	127.44	124.79
19	B	807	CLA	CHA-C1A-NA	-2.04	121.78	126.39
19	A	854	CLA	C3B-C2B-C1B	-2.04	104.77	107.17
19	J	1101	CLA	C11-C10-C8	-2.04	109.19	115.97
27	A	801	CL0	C4-C3-C5	2.04	118.76	115.23
19	B	820	CLA	C11-C10-C8	-2.04	109.20	115.97
19	A	829	CLA	C4B-CHC-C1C	2.04	131.03	126.25
18	L	302	BCR	C37-C22-C23	2.04	121.20	118.09
19	A	836	CLA	C3D-C2D-C1D	-2.03	103.05	105.83
19	4	304	CLA	C5-C3-C2	2.03	125.73	121.17
22	F	305	LMG	O7-C10-O9	-2.03	118.95	123.70
20	2	515	CHL	CMD-C2D-C3D	2.03	128.75	124.68
19	2	508	CLA	O2A-CGA-CBA	2.03	118.03	111.83
19	B	837	CLA	C1D-ND-C4D	-2.03	104.89	106.31
19	2	508	CLA	CHA-C1A-NA	-2.03	121.79	126.39
19	B	821	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
19	G	203	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
26	4	319	DGD	C1D-O6D-C5D	-2.03	109.75	113.72
22	G	210	LMG	C7-O1-C1	-2.03	109.44	113.80
20	4	316	CHL	CMD-C2D-C3D	2.03	128.74	124.68
19	A	802	CLA	C5-C3-C2	2.03	125.72	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	840	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
19	B	828	CLA	C4B-CHC-C1C	2.03	131.02	126.25
19	B	820	CLA	O2A-CGA-CBA	2.03	118.02	111.83
19	B	807	CLA	C4B-CHC-C1C	2.03	131.02	126.25
19	2	514	CLA	C1D-ND-C4D	-2.03	104.89	106.31
19	B	824	CLA	CMD-C2D-C3D	-2.03	123.04	127.69
18	A	851	BCR	C34-C9-C10	-2.03	119.53	122.82
19	B	838	CLA	CHA-C1A-NA	-2.03	121.80	126.39
17	J	1109	LUT	C19-C9-C8	2.03	121.19	118.09
18	F	306	BCR	C15-C14-C13	2.03	130.12	127.28
18	B	849	BCR	C40-C30-C39	-2.03	102.83	108.63
19	A	810	CLA	C2D-C1D-ND	2.03	112.13	110.13
20	2	512	CHL	C1A-CHA-CBD	-2.03	127.17	132.36
18	B	853	BCR	C28-C27-C26	-2.03	110.44	114.06
20	2	526	CHL	CMD-C2D-C3D	2.03	128.73	124.68
19	4	308	CLA	CBC-CAC-C3C	-2.03	106.93	112.42
19	A	802	CLA	C6-C5-C3	-2.03	108.53	113.47
19	2	507	CLA	C2D-C1D-ND	2.02	112.13	110.13
18	I	101	BCR	C37-C22-C23	2.02	121.18	118.09
18	L	307	BCR	C37-C22-C23	2.02	121.18	118.09
19	L	303	CLA	CHA-C1A-NA	-2.02	121.81	126.39
23	4	303	XAT	C6-C7-C8	-2.02	121.72	125.99
19	A	825	CLA	O2D-CGD-O1D	-2.02	119.91	123.85
19	B	822	CLA	CHA-C1A-NA	-2.02	121.82	126.39
19	4	306	CLA	C1-O2A-CGA	2.02	121.54	116.65
18	B	853	BCR	C40-C30-C25	-2.02	107.08	110.24
19	3	315	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
19	B	837	CLA	C4B-CHC-C1C	2.02	130.99	126.25
19	A	842	CLA	CHA-C1A-NA	-2.02	121.82	126.39
19	B	837	CLA	CMA-C3A-C4A	2.02	117.19	111.77
19	3	309	CLA	C3B-C4B-NB	-2.02	108.73	110.53
22	2	519	LMG	C4-C3-C2	-2.02	107.29	110.83
17	1	502	LUT	C40-C33-C32	2.01	121.17	118.09
19	A	835	CLA	C1D-ND-C4D	-2.01	104.90	106.31
27	A	801	CL0	C1-O2A-CGA	2.01	121.52	116.65
19	A	833	CLA	C3B-C2B-C1B	-2.01	104.80	107.17
19	B	831	CLA	CHA-C1A-NA	-2.01	121.84	126.39
19	A	815	CLA	CAC-C3C-C4C	2.01	127.41	124.79
18	G	205	BCR	C34-C9-C10	-2.01	119.56	122.82
17	3	302	LUT	C20-C13-C12	2.01	121.16	118.09
18	B	852	BCR	C8-C9-C10	2.01	122.17	119.01
19	A	816	CLA	C2D-C1D-ND	2.01	112.11	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	307	CLA	C11-C10-C8	-2.01	109.29	115.97
19	B	838	CLA	C1-O2A-CGA	2.01	121.51	116.65
19	A	805	CLA	CAC-C3C-C4C	2.01	127.40	124.79
19	A	807	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
19	1	506	CLA	CHA-C1A-NA	-2.01	121.84	126.39
19	A	818	CLA	C1D-ND-C4D	-2.01	104.90	106.31
19	2	511	CLA	C2D-C1D-ND	2.01	112.11	110.13
20	4	316	CHL	C1C-C2C-CMC	-2.01	123.18	126.80
17	1	501	LUT	C20-C13-C12	2.01	121.15	118.09
19	L	304	CLA	CMD-C2D-C3D	-2.01	123.09	127.69
19	B	822	CLA	CHD-C1D-ND	-2.01	121.98	124.80
19	F	302	CLA	C1-O2A-CGA	2.01	121.50	116.65
19	4	318	CLA	CHA-C1A-NA	-2.00	121.85	126.39
18	4	301	BCR	C8-C9-C10	2.00	122.16	119.01
17	1	502	LUT	C19-C9-C8	2.00	121.15	118.09
19	A	815	CLA	C2D-C1D-ND	2.00	112.11	110.13
24	B	855	LMT	C3B-C4B-C5B	-2.00	106.60	110.23
27	A	801	CL0	CAA-C2A-C3A	-2.00	107.59	113.00
19	A	805	CLA	O2D-CGD-O1D	-2.00	119.95	123.85
19	K	1004	CLA	C1C-CHC-C4B	2.00	131.32	126.04
18	K	1005	BCR	C1-C6-C7	2.00	121.08	115.65
19	1	510	CLA	CHD-C1D-ND	-2.00	121.99	124.80
19	A	821	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
19	3	313	CLA	C1-C2-C3	2.00	129.47	126.20

All (182) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	1	502	LUT	C26
17	2	501	LUT	C26
17	3	302	LUT	C26
17	J	1109	LUT	C26
19	1	504	CLA	ND
19	1	506	CLA	ND
19	1	507	CLA	ND
19	1	509	CLA	ND
19	1	510	CLA	ND
19	1	511	CLA	ND
19	1	513	CLA	ND
19	1	515	CLA	ND
19	1	516	CLA	ND
19	2	504	CLA	ND

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Mol	Chain	Res	Type	Atom
19	2	505	CLA	ND
19	2	506	CLA	ND
19	2	507	CLA	ND
19	2	508	CLA	ND
19	2	509	CLA	ND
19	2	510	CLA	ND
19	2	511	CLA	ND
19	2	514	CLA	ND
19	3	305	CLA	ND
19	3	306	CLA	ND
19	3	307	CLA	ND
19	3	308	CLA	ND
19	3	310	CLA	ND
19	3	311	CLA	ND
19	3	312	CLA	ND
19	3	313	CLA	ND
19	3	315	CLA	ND
19	3	316	CLA	ND
19	3	317	CLA	ND
19	4	304	CLA	ND
19	4	305	CLA	ND
19	4	306	CLA	ND
19	4	307	CLA	ND
19	4	309	CLA	ND
19	4	310	CLA	ND
19	4	311	CLA	ND
19	4	315	CLA	ND
19	4	318	CLA	ND
19	A	802	CLA	ND
19	A	803	CLA	ND
19	A	804	CLA	ND
19	A	805	CLA	ND
19	A	806	CLA	ND
19	A	807	CLA	ND
19	A	808	CLA	ND
19	A	809	CLA	ND
19	A	810	CLA	ND
19	A	811	CLA	ND
19	A	813	CLA	ND
19	A	814	CLA	ND
19	A	815	CLA	ND
19	A	816	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A	817	CLA	ND
19	A	818	CLA	ND
19	A	819	CLA	ND
19	A	820	CLA	ND
19	A	821	CLA	ND
19	A	822	CLA	ND
19	A	823	CLA	ND
19	A	824	CLA	ND
19	A	825	CLA	ND
19	A	826	CLA	ND
19	A	827	CLA	ND
19	A	828	CLA	ND
19	A	829	CLA	ND
19	A	830	CLA	ND
19	A	831	CLA	ND
19	A	832	CLA	ND
19	A	833	CLA	ND
19	A	835	CLA	ND
19	A	837	CLA	ND
19	A	838	CLA	ND
19	A	839	CLA	ND
19	A	840	CLA	ND
19	A	841	CLA	ND
19	A	842	CLA	ND
19	A	854	CLA	ND
19	A	855	CLA	ND
19	B	803	CLA	ND
19	B	804	CLA	ND
19	B	805	CLA	ND
19	B	806	CLA	ND
19	B	807	CLA	ND
19	B	808	CLA	ND
19	B	809	CLA	ND
19	B	810	CLA	ND
19	B	811	CLA	ND
19	B	812	CLA	ND
19	B	813	CLA	ND
19	B	814	CLA	ND
19	B	815	CLA	ND
19	B	816	CLA	ND
19	B	817	CLA	ND
19	B	818	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B	819	CLA	ND
19	B	820	CLA	ND
19	B	821	CLA	ND
19	B	822	CLA	ND
19	B	823	CLA	ND
19	B	824	CLA	ND
19	B	825	CLA	ND
19	B	826	CLA	ND
19	B	827	CLA	ND
19	B	828	CLA	ND
19	B	829	CLA	ND
19	B	831	CLA	ND
19	B	832	CLA	ND
19	B	833	CLA	ND
19	B	834	CLA	ND
19	B	836	CLA	ND
19	B	837	CLA	ND
19	B	838	CLA	ND
19	B	839	CLA	ND
19	F	302	CLA	ND
19	G	201	CLA	ND
19	G	203	CLA	ND
19	G	204	CLA	ND
19	H	1000	CLA	ND
19	J	1101	CLA	ND
19	J	1102	CLA	ND
19	J	1105	CLA	ND
19	K	1001	CLA	ND
19	K	1002	CLA	ND
19	K	1003	CLA	ND
19	K	1004	CLA	ND
19	L	301	CLA	ND
19	L	303	CLA	ND
19	L	304	CLA	ND
19	L	305	CLA	ND
20	1	512	CHL	ND
20	1	512	CHL	NA
20	1	512	CHL	NC
20	1	514	CHL	C8
20	1	514	CHL	ND
20	1	514	CHL	NA
20	1	514	CHL	NC

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Mol	Chain	Res	Type	Atom
20	1	521	CHL	C8
20	1	521	CHL	ND
20	1	521	CHL	NA
20	1	521	CHL	NC
20	2	512	CHL	ND
20	2	512	CHL	NA
20	2	512	CHL	NC
20	2	513	CHL	ND
20	2	513	CHL	NA
20	2	513	CHL	NC
20	2	515	CHL	ND
20	2	515	CHL	NA
20	2	515	CHL	NC
20	2	516	CHL	C8
20	2	516	CHL	ND
20	2	516	CHL	NA
20	2	516	CHL	NC
20	2	526	CHL	C8
20	2	526	CHL	ND
20	2	526	CHL	NA
20	2	526	CHL	NC
20	3	314	CHL	ND
20	3	314	CHL	NA
20	3	314	CHL	NC
20	4	313	CHL	ND
20	4	313	CHL	NA
20	4	313	CHL	NC
20	4	314	CHL	ND
20	4	314	CHL	NA
20	4	314	CHL	NC
20	4	316	CHL	C8
20	4	316	CHL	ND
20	4	316	CHL	NA
20	4	316	CHL	NC
20	4	317	CHL	ND
20	4	317	CHL	NA
20	4	317	CHL	NC
23	4	303	XAT	C6
23	4	303	XAT	C5
27	A	801	CL0	ND
27	A	801	CL0	NA
27	A	801	CL0	NC

All (2581) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	1	502	LUT	C21-C26-C27-C28
17	1	502	LUT	C27-C28-C29-C30
17	1	502	LUT	C27-C28-C29-C39
17	2	501	LUT	C21-C26-C27-C28
17	2	501	LUT	C31-C32-C33-C34
17	3	302	LUT	C25-C26-C27-C28
17	3	302	LUT	C27-C28-C29-C30
17	3	302	LUT	C27-C28-C29-C39
17	4	302	LUT	C21-C26-C27-C28
17	J	1109	LUT	C21-C26-C27-C28
17	J	1109	LUT	C25-C26-C27-C28
17	J	1109	LUT	C27-C28-C29-C30
18	1	503	BCR	C36-C18-C19-C20
18	1	503	BCR	C23-C24-C25-C26
18	1	503	BCR	C23-C24-C25-C30
18	2	503	BCR	C11-C10-C9-C8
18	2	503	BCR	C11-C10-C9-C34
18	2	503	BCR	C13-C14-C15-C16
18	2	503	BCR	C21-C22-C23-C24
18	2	503	BCR	C37-C22-C23-C24
18	3	303	BCR	C1-C6-C7-C8
18	3	303	BCR	C5-C6-C7-C8
18	3	303	BCR	C11-C10-C9-C8
18	3	303	BCR	C11-C10-C9-C34
18	3	303	BCR	C13-C14-C15-C16
18	3	303	BCR	C21-C22-C23-C24
18	3	304	BCR	C1-C6-C7-C8
18	3	304	BCR	C5-C6-C7-C8
18	3	304	BCR	C11-C10-C9-C8
18	3	304	BCR	C11-C10-C9-C34
18	3	304	BCR	C10-C11-C12-C13
18	4	301	BCR	C11-C10-C9-C8
18	4	301	BCR	C11-C10-C9-C34
18	4	301	BCR	C10-C11-C12-C13
18	4	301	BCR	C17-C18-C19-C20
18	4	301	BCR	C21-C22-C23-C24
18	4	301	BCR	C37-C22-C23-C24
18	A	848	BCR	C11-C10-C9-C8
18	A	848	BCR	C11-C10-C9-C34
18	A	849	BCR	C11-C10-C9-C8
18	A	849	BCR	C11-C10-C9-C34
18	A	849	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
18	A	849	BCR	C17-C18-C19-C20
18	A	850	BCR	C21-C22-C23-C24
18	A	850	BCR	C37-C22-C23-C24
18	A	851	BCR	C11-C10-C9-C8
18	A	851	BCR	C11-C10-C9-C34
18	A	851	BCR	C10-C11-C12-C13
18	A	851	BCR	C13-C14-C15-C16
18	A	851	BCR	C15-C16-C17-C18
18	A	851	BCR	C17-C18-C19-C20
18	A	852	BCR	C7-C8-C9-C10
18	A	852	BCR	C17-C18-C19-C20
18	A	852	BCR	C36-C18-C19-C20
18	A	852	BCR	C21-C22-C23-C24
18	A	852	BCR	C37-C22-C23-C24
18	A	856	BCR	C1-C6-C7-C8
18	A	856	BCR	C5-C6-C7-C8
18	A	856	BCR	C11-C10-C9-C8
18	A	856	BCR	C11-C10-C9-C34
18	A	856	BCR	C10-C11-C12-C13
18	A	856	BCR	C11-C12-C13-C14
18	A	856	BCR	C11-C12-C13-C35
18	B	802	BCR	C11-C10-C9-C8
18	B	802	BCR	C11-C10-C9-C34
18	B	849	BCR	C11-C10-C9-C8
18	B	849	BCR	C11-C10-C9-C34
18	B	849	BCR	C23-C24-C25-C26
18	B	849	BCR	C23-C24-C25-C30
18	B	850	BCR	C17-C18-C19-C20
18	B	850	BCR	C21-C22-C23-C24
18	B	850	BCR	C37-C22-C23-C24
18	B	852	BCR	C11-C10-C9-C8
18	B	852	BCR	C11-C10-C9-C34
18	B	853	BCR	C11-C10-C9-C8
18	B	853	BCR	C11-C10-C9-C34
18	B	853	BCR	C10-C11-C12-C13
18	B	853	BCR	C11-C12-C13-C14
18	B	853	BCR	C11-C12-C13-C35
18	B	853	BCR	C21-C22-C23-C24
18	B	856	BCR	C7-C8-C9-C10
18	B	856	BCR	C11-C10-C9-C8
18	B	856	BCR	C11-C10-C9-C34
18	B	856	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
18	B	856	BCR	C36-C18-C19-C20
18	B	856	BCR	C21-C22-C23-C24
18	B	856	BCR	C37-C22-C23-C24
18	F	306	BCR	C17-C18-C19-C20
18	F	306	BCR	C36-C18-C19-C20
18	G	205	BCR	C10-C11-C12-C13
18	I	101	BCR	C1-C6-C7-C8
18	I	101	BCR	C5-C6-C7-C8
18	I	101	BCR	C11-C10-C9-C8
18	I	101	BCR	C11-C10-C9-C34
18	I	101	BCR	C10-C11-C12-C13
18	I	101	BCR	C17-C18-C19-C20
18	I	102	BCR	C11-C10-C9-C8
18	I	102	BCR	C11-C10-C9-C34
18	I	102	BCR	C11-C12-C13-C14
18	I	102	BCR	C11-C12-C13-C35
18	I	102	BCR	C23-C24-C25-C26
18	J	1108	BCR	C11-C12-C13-C14
18	J	1108	BCR	C11-C12-C13-C35
18	K	1005	BCR	C11-C10-C9-C8
18	K	1005	BCR	C11-C10-C9-C34
18	K	1005	BCR	C15-C16-C17-C18
18	K	1005	BCR	C19-C20-C21-C22
18	L	306	BCR	C11-C10-C9-C8
18	L	306	BCR	C11-C10-C9-C34
18	L	306	BCR	C10-C11-C12-C13
18	L	307	BCR	C11-C10-C9-C8
18	L	307	BCR	C11-C10-C9-C34
18	L	307	BCR	C17-C18-C19-C20
18	L	307	BCR	C36-C18-C19-C20
18	L	307	BCR	C21-C22-C23-C24
18	L	307	BCR	C37-C22-C23-C24
19	1	505	CLA	C1A-C2A-CAA-CBA
19	1	505	CLA	C3A-C2A-CAA-CBA
19	1	505	CLA	CBA-CGA-O2A-C1
19	1	505	CLA	CBD-CGD-O2D-CED
19	1	506	CLA	C1A-C2A-CAA-CBA
19	1	510	CLA	C1A-C2A-CAA-CBA
19	1	510	CLA	C3A-C2A-CAA-CBA
19	1	510	CLA	CBA-CGA-O2A-C1
19	1	510	CLA	CBD-CGD-O2D-CED
19	1	516	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	1	516	CLA	C6-C7-C8-C9
19	2	504	CLA	C3A-C2A-CAA-CBA
19	2	505	CLA	C2-C3-C5-C6
19	2	505	CLA	C4-C3-C5-C6
19	2	505	CLA	C3-C5-C6-C7
19	2	507	CLA	C3A-C2A-CAA-CBA
19	2	508	CLA	C2-C1-O2A-CGA
19	2	509	CLA	C1A-C2A-CAA-CBA
19	2	511	CLA	C1A-C2A-CAA-CBA
19	2	511	CLA	C2B-C3B-CAB-CBB
19	2	511	CLA	C4B-C3B-CAB-CBB
19	2	514	CLA	C2-C1-O2A-CGA
19	3	305	CLA	C1A-C2A-CAA-CBA
19	3	305	CLA	C3A-C2A-CAA-CBA
19	3	305	CLA	CBD-CGD-O2D-CED
19	3	306	CLA	C2-C1-O2A-CGA
19	3	307	CLA	CBD-CGD-O2D-CED
19	3	308	CLA	C2-C1-O2A-CGA
19	3	308	CLA	CBD-CGD-O2D-CED
19	3	310	CLA	CBD-CGD-O2D-CED
19	3	312	CLA	C1A-C2A-CAA-CBA
19	3	313	CLA	C1A-C2A-CAA-CBA
19	3	313	CLA	C2-C1-O2A-CGA
19	3	315	CLA	CBD-CGD-O2D-CED
19	4	304	CLA	C6-C7-C8-C9
19	4	306	CLA	CBD-CGD-O2D-CED
19	4	307	CLA	CHA-CBD-CGD-O2D
19	4	308	CLA	CBD-CGD-O2D-CED
19	4	309	CLA	C1A-C2A-CAA-CBA
19	4	309	CLA	C3A-C2A-CAA-CBA
19	4	312	CLA	C2-C1-O2A-CGA
19	4	318	CLA	C2-C1-O2A-CGA
19	A	802	CLA	C2-C1-O2A-CGA
19	A	804	CLA	C1A-C2A-CAA-CBA
19	A	804	CLA	C3A-C2A-CAA-CBA
19	A	805	CLA	CAD-CBD-CGD-O1D
19	A	805	CLA	CAD-CBD-CGD-O2D
19	A	806	CLA	CBD-CGD-O2D-CED
19	A	807	CLA	C2-C1-O2A-CGA
19	A	808	CLA	C3A-C2A-CAA-CBA
19	A	808	CLA	CHA-CBD-CGD-O1D
19	A	808	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	A	809	CLA	CBD-CGD-O2D-CED
19	A	811	CLA	C1A-C2A-CAA-CBA
19	A	811	CLA	C3A-C2A-CAA-CBA
19	A	812	CLA	C1A-C2A-CAA-CBA
19	A	812	CLA	C3A-C2A-CAA-CBA
19	A	815	CLA	C1A-C2A-CAA-CBA
19	A	817	CLA	CBD-CGD-O2D-CED
19	A	818	CLA	C3A-C2A-CAA-CBA
19	A	821	CLA	C2-C1-O2A-CGA
19	A	821	CLA	C2-C3-C5-C6
19	A	821	CLA	C4-C3-C5-C6
19	A	821	CLA	C11-C10-C8-C9
19	A	823	CLA	CBD-CGD-O2D-CED
19	A	824	CLA	C4-C3-C5-C6
19	A	825	CLA	CHA-CBD-CGD-O1D
19	A	825	CLA	CHA-CBD-CGD-O2D
19	A	828	CLA	C6-C7-C8-C9
19	A	830	CLA	CHA-CBD-CGD-O1D
19	A	830	CLA	CHA-CBD-CGD-O2D
19	A	833	CLA	CHA-CBD-CGD-O1D
19	A	833	CLA	CHA-CBD-CGD-O2D
19	A	840	CLA	C2-C1-O2A-CGA
19	A	840	CLA	CBD-CGD-O2D-CED
19	A	840	CLA	C4-C3-C5-C6
19	A	842	CLA	CBD-CGD-O2D-CED
19	A	842	CLA	C2-C3-C5-C6
19	A	842	CLA	C4-C3-C5-C6
19	B	804	CLA	CBD-CGD-O2D-CED
19	B	805	CLA	C1A-C2A-CAA-CBA
19	B	805	CLA	C3A-C2A-CAA-CBA
19	B	806	CLA	C3A-C2A-CAA-CBA
19	B	806	CLA	CAD-CBD-CGD-O1D
19	B	806	CLA	CAD-CBD-CGD-O2D
19	B	807	CLA	CBD-CGD-O2D-CED
19	B	807	CLA	C6-C7-C8-C9
19	B	808	CLA	C11-C10-C8-C9
19	B	809	CLA	CBD-CGD-O2D-CED
19	B	810	CLA	C2-C1-O2A-CGA
19	B	810	CLA	CBD-CGD-O2D-CED
19	B	811	CLA	CBD-CGD-O2D-CED
19	B	812	CLA	CBD-CGD-O2D-CED
19	B	818	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
19	B	819	CLA	CBD-CGD-O2D-CED
19	B	822	CLA	C2-C1-O2A-CGA
19	B	823	CLA	C3A-C2A-CAA-CBA
19	B	824	CLA	C2-C1-O2A-CGA
19	B	824	CLA	CHA-CBD-CGD-O1D
19	B	824	CLA	CHA-CBD-CGD-O2D
19	B	825	CLA	C1A-C2A-CAA-CBA
19	B	825	CLA	C3A-C2A-CAA-CBA
19	B	825	CLA	CHA-CBD-CGD-O1D
19	B	825	CLA	CHA-CBD-CGD-O2D
19	B	827	CLA	C1A-C2A-CAA-CBA
19	B	827	CLA	C3A-C2A-CAA-CBA
19	B	828	CLA	C1A-C2A-CAA-CBA
19	B	828	CLA	C3A-C2A-CAA-CBA
19	B	829	CLA	CAD-CBD-CGD-O1D
19	B	829	CLA	CAD-CBD-CGD-O2D
19	B	831	CLA	C1A-C2A-CAA-CBA
19	B	831	CLA	C3A-C2A-CAA-CBA
19	B	832	CLA	CHA-CBD-CGD-O1D
19	B	832	CLA	CHA-CBD-CGD-O2D
19	B	834	CLA	C2-C1-O2A-CGA
19	B	834	CLA	CBD-CGD-O2D-CED
19	B	834	CLA	C4-C3-C5-C6
19	B	835	CLA	C2B-C3B-CAB-CBB
19	B	835	CLA	C4B-C3B-CAB-CBB
19	B	837	CLA	C2-C1-O2A-CGA
19	B	839	CLA	C1A-C2A-CAA-CBA
19	B	839	CLA	C3A-C2A-CAA-CBA
19	B	839	CLA	CBD-CGD-O2D-CED
19	F	302	CLA	C2-C1-O2A-CGA
19	G	201	CLA	C1A-C2A-CAA-CBA
19	G	203	CLA	CBA-CGA-O2A-C1
19	G	204	CLA	C2-C1-O2A-CGA
19	J	1105	CLA	C1A-C2A-CAA-CBA
19	J	1105	CLA	C2-C1-O2A-CGA
19	K	1001	CLA	CAD-CBD-CGD-O1D
19	K	1001	CLA	CAD-CBD-CGD-O2D
19	K	1001	CLA	CBD-CGD-O2D-CED
19	K	1002	CLA	C1A-C2A-CAA-CBA
19	L	303	CLA	C1A-C2A-CAA-CBA
19	L	303	CLA	C2-C1-O2A-CGA
19	L	305	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	1	514	CHL	C3A-C2A-CAA-CBA
20	1	514	CHL	C11-C10-C8-C9
20	2	515	CHL	C1A-C2A-CAA-CBA
20	2	516	CHL	C1A-C2A-CAA-CBA
20	3	314	CHL	C1A-C2A-CAA-CBA
20	3	314	CHL	C3A-C2A-CAA-CBA
20	4	314	CHL	C4C-C3C-CAC-CBC
20	4	316	CHL	C3A-C2A-CAA-CBA
20	4	316	CHL	C4C-C3C-CAC-CBC
21	1	517	LHG	O1-C1-C2-C3
21	1	517	LHG	O2-C2-C3-O3
21	1	517	LHG	C3-O3-P-O4
21	1	520	LHG	O1-C1-C2-O2
21	1	520	LHG	O1-C1-C2-C3
21	1	520	LHG	C3-O3-P-O6
21	1	520	LHG	O9-C7-O7-C5
21	1	520	LHG	C8-C7-O7-C5
21	2	517	LHG	C4-O6-P-O3
21	A	845	LHG	O2-C2-C3-O3
21	A	845	LHG	C4-O6-P-O3
21	A	845	LHG	C4-O6-P-O5
21	A	845	LHG	O6-C4-C5-O7
21	A	853	LHG	C3-O3-P-O6
21	A	853	LHG	C4-O6-P-O3
21	A	853	LHG	C4-O6-P-O4
21	B	842	LHG	O1-C1-C2-C3
21	B	842	LHG	C4-O6-P-O3
21	B	842	LHG	C4-O6-P-O4
21	B	842	LHG	C4-O6-P-O5
21	B	842	LHG	C8-C7-O7-C5
21	B	843	LHG	O1-C1-C2-C3
21	B	843	LHG	C1-C2-C3-O3
21	B	843	LHG	C3-O3-P-O4
21	B	843	LHG	C3-O3-P-O6
21	B	843	LHG	C8-C7-O7-C5
22	2	518	LMG	O9-C10-O7-C8
22	2	518	LMG	C11-C10-O7-C8
22	2	519	LMG	C2-C1-O1-C7
22	2	519	LMG	O6-C1-O1-C7
22	2	522	LMG	C2-C1-O1-C7
22	2	522	LMG	O6-C1-O1-C7
22	4	322	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
22	4	322	LMG	C11-C10-O7-C8
22	A	847	LMG	C11-C10-O7-C8
22	B	844	LMG	O9-C10-O7-C8
22	B	845	LMG	O9-C10-O7-C8
22	B	845	LMG	C11-C10-O7-C8
22	F	304	LMG	O9-C10-O7-C8
22	F	304	LMG	O10-C28-O8-C9
22	G	206	LMG	O6-C1-O1-C7
22	G	210	LMG	C11-C10-O7-C8
22	J	1103	LMG	C11-C10-O7-C8
22	J	1104	LMG	C11-C10-O7-C8
23	2	502	XAT	O4-C6-C7-C8
23	2	502	XAT	C7-C8-C9-C10
23	2	502	XAT	C7-C8-C9-C19
24	2	523	LMT	O5'-C1'-O1'-C1
24	G	208	LMT	C2-C1-O1'-C1'
24	J	1107	LMT	O5'-C1'-O1'-C1
26	B	801	DGD	O6D-C1D-O3G-C3G
26	B	801	DGD	O6E-C1E-O5D-C6D
26	B	854	DGD	C2B-C1B-O2G-C2G
26	B	854	DGD	O1B-C1B-O2G-C2G
26	G	207	DGD	O6E-C1E-O5D-C6D
26	J	1106	DGD	O6E-C1E-O5D-C6D
27	A	801	CL0	CHA-CBD-CGD-O1D
27	A	801	CL0	CHA-CBD-CGD-O2D
29	A	844	PQN	C14-C13-C15-C16
30	F	301	ZEX	C25-C26-C27-C28
19	1	511	CLA	O1D-CGD-O2D-CED
19	3	311	CLA	O1D-CGD-O2D-CED
19	B	834	CLA	O1D-CGD-O2D-CED
21	B	842	LHG	O9-C7-O7-C5
19	J	1105	CLA	C4C-C3C-CAC-CBC
19	1	506	CLA	O1D-CGD-O2D-CED
19	1	509	CLA	O1D-CGD-O2D-CED
19	1	515	CLA	O1D-CGD-O2D-CED
19	2	509	CLA	O1D-CGD-O2D-CED
19	3	305	CLA	O1D-CGD-O2D-CED
19	3	307	CLA	O1D-CGD-O2D-CED
19	3	308	CLA	O1D-CGD-O2D-CED
19	A	828	CLA	O1D-CGD-O2D-CED
19	B	804	CLA	O1D-CGD-O2D-CED
19	1	506	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	1	509	CLA	CBD-CGD-O2D-CED
19	1	511	CLA	CBD-CGD-O2D-CED
19	1	513	CLA	CBD-CGD-O2D-CED
19	1	515	CLA	CBD-CGD-O2D-CED
19	2	505	CLA	CBD-CGD-O2D-CED
19	2	506	CLA	CBD-CGD-O2D-CED
19	2	509	CLA	CBD-CGD-O2D-CED
19	2	510	CLA	CBD-CGD-O2D-CED
19	3	306	CLA	CBD-CGD-O2D-CED
19	3	311	CLA	CBD-CGD-O2D-CED
19	3	312	CLA	CBD-CGD-O2D-CED
19	3	316	CLA	CBD-CGD-O2D-CED
19	4	304	CLA	CBD-CGD-O2D-CED
19	4	305	CLA	CBD-CGD-O2D-CED
19	4	310	CLA	CBD-CGD-O2D-CED
19	4	315	CLA	CBD-CGD-O2D-CED
19	A	807	CLA	CBD-CGD-O2D-CED
19	A	811	CLA	CBD-CGD-O2D-CED
19	A	815	CLA	CBD-CGD-O2D-CED
19	A	816	CLA	CBD-CGD-O2D-CED
19	A	818	CLA	CBD-CGD-O2D-CED
19	A	820	CLA	CBD-CGD-O2D-CED
19	A	822	CLA	CBD-CGD-O2D-CED
19	A	828	CLA	CBD-CGD-O2D-CED
19	A	831	CLA	CBD-CGD-O2D-CED
19	A	832	CLA	CBD-CGD-O2D-CED
19	B	816	CLA	CBD-CGD-O2D-CED
19	B	822	CLA	CBD-CGD-O2D-CED
19	B	827	CLA	CBD-CGD-O2D-CED
19	G	203	CLA	CBD-CGD-O2D-CED
19	H	1000	CLA	CBD-CGD-O2D-CED
19	J	1101	CLA	CBD-CGD-O2D-CED
19	J	1102	CLA	CBD-CGD-O2D-CED
19	K	1002	CLA	CBD-CGD-O2D-CED
19	L	301	CLA	CBD-CGD-O2D-CED
19	1	509	CLA	O1A-CGA-O2A-C1
19	2	510	CLA	O1A-CGA-O2A-C1
19	3	307	CLA	O1A-CGA-O2A-C1
19	4	306	CLA	O1A-CGA-O2A-C1
19	A	824	CLA	O1A-CGA-O2A-C1
19	L	301	CLA	O1A-CGA-O2A-C1
21	1	520	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
22	G	210	LMG	O10-C28-O8-C9
19	1	505	CLA	O1A-CGA-O2A-C1
19	1	510	CLA	O1A-CGA-O2A-C1
19	1	511	CLA	O1A-CGA-O2A-C1
19	A	816	CLA	O1A-CGA-O2A-C1
19	G	203	CLA	O1A-CGA-O2A-C1
19	J	1105	CLA	C2C-C3C-CAC-CBC
19	3	310	CLA	O1D-CGD-O2D-CED
19	A	806	CLA	O1D-CGD-O2D-CED
24	B	846	LMT	O5B-C1B-O1B-C4'
19	1	511	CLA	CBA-CGA-O2A-C1
19	3	317	CLA	CBA-CGA-O2A-C1
19	A	816	CLA	CBA-CGA-O2A-C1
24	G	209	LMT	C4B-C5B-C6B-O6B
26	B	801	DGD	C2G-C1G-O1G-C1A
19	1	513	CLA	O1D-CGD-O2D-CED
19	3	306	CLA	O1D-CGD-O2D-CED
19	3	312	CLA	O1D-CGD-O2D-CED
19	A	816	CLA	O1D-CGD-O2D-CED
19	A	822	CLA	O1D-CGD-O2D-CED
19	B	822	CLA	O1D-CGD-O2D-CED
19	1	509	CLA	CBA-CGA-O2A-C1
19	2	506	CLA	CBA-CGA-O2A-C1
19	2	510	CLA	CBA-CGA-O2A-C1
19	3	307	CLA	CBA-CGA-O2A-C1
19	3	309	CLA	CBA-CGA-O2A-C1
19	4	305	CLA	CBA-CGA-O2A-C1
19	4	306	CLA	CBA-CGA-O2A-C1
19	A	824	CLA	CBA-CGA-O2A-C1
19	B	830	CLA	CBA-CGA-O2A-C1
21	1	520	LHG	C24-C23-O8-C6
19	A	834	CLA	CBD-CGD-O2D-CED
19	G	202	CLA	CBD-CGD-O2D-CED
19	2	506	CLA	O1A-CGA-O2A-C1
19	3	306	CLA	O1A-CGA-O2A-C1
19	3	309	CLA	O1A-CGA-O2A-C1
19	3	315	CLA	O1A-CGA-O2A-C1
19	4	305	CLA	O1A-CGA-O2A-C1
19	4	310	CLA	O1A-CGA-O2A-C1
19	4	315	CLA	O1A-CGA-O2A-C1
19	A	831	CLA	O1A-CGA-O2A-C1
19	A	855	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B	818	CLA	O1A-CGA-O2A-C1
19	B	822	CLA	O1A-CGA-O2A-C1
19	B	825	CLA	O1A-CGA-O2A-C1
19	B	830	CLA	O1A-CGA-O2A-C1
19	F	303	CLA	O1A-CGA-O2A-C1
19	G	202	CLA	O1A-CGA-O2A-C1
19	L	303	CLA	O1A-CGA-O2A-C1
22	1	518	LMG	O10-C28-O8-C9
22	4	322	LMG	O10-C28-O8-C9
19	B	834	CLA	C5-C6-C7-C8
19	A	817	CLA	O1D-CGD-O2D-CED
19	A	818	CLA	O1D-CGD-O2D-CED
19	A	840	CLA	O1D-CGD-O2D-CED
19	B	807	CLA	O1D-CGD-O2D-CED
19	B	810	CLA	O1D-CGD-O2D-CED
19	B	812	CLA	O1D-CGD-O2D-CED
19	B	827	CLA	O1D-CGD-O2D-CED
19	G	203	CLA	O1D-CGD-O2D-CED
19	H	1000	CLA	O1D-CGD-O2D-CED
19	K	1001	CLA	O1D-CGD-O2D-CED
24	B	846	LMT	C2B-C1B-O1B-C4'
19	4	306	CLA	O1D-CGD-O2D-CED
19	4	308	CLA	O1D-CGD-O2D-CED
19	A	809	CLA	O1D-CGD-O2D-CED
19	A	823	CLA	O1D-CGD-O2D-CED
19	A	842	CLA	O1D-CGD-O2D-CED
19	B	811	CLA	O1D-CGD-O2D-CED
19	B	839	CLA	O1D-CGD-O2D-CED
19	1	504	CLA	CBD-CGD-O2D-CED
19	1	507	CLA	CBD-CGD-O2D-CED
19	3	309	CLA	CBD-CGD-O2D-CED
19	A	804	CLA	CBD-CGD-O2D-CED
19	G	204	CLA	CBD-CGD-O2D-CED
19	L	305	CLA	CBD-CGD-O2D-CED
22	G	206	LMG	O10-C28-O8-C9
22	1	518	LMG	O9-C10-O7-C8
22	4	322	LMG	O9-C10-O7-C8
22	A	847	LMG	O9-C10-O7-C8
22	J	1103	LMG	O9-C10-O7-C8
22	J	1104	LMG	O9-C10-O7-C8
24	G	209	LMT	C4'-C5'-C6'-O6'
19	1	508	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
19	2	504	CLA	C3-C5-C6-C7
19	2	508	CLA	C3-C5-C6-C7
19	3	305	CLA	C3-C5-C6-C7
19	3	309	CLA	C3-C5-C6-C7
19	A	804	CLA	C3-C5-C6-C7
19	A	806	CLA	C3-C5-C6-C7
19	A	812	CLA	C3-C5-C6-C7
19	A	814	CLA	C3-C5-C6-C7
19	A	818	CLA	C3-C5-C6-C7
19	A	827	CLA	C3-C5-C6-C7
19	A	831	CLA	C3-C5-C6-C7
19	B	808	CLA	C3-C5-C6-C7
19	B	811	CLA	C3-C5-C6-C7
19	B	823	CLA	C3-C5-C6-C7
19	1	510	CLA	O1D-CGD-O2D-CED
19	B	819	CLA	O1D-CGD-O2D-CED
19	3	306	CLA	CBA-CGA-O2A-C1
19	3	315	CLA	CBA-CGA-O2A-C1
19	4	310	CLA	CBA-CGA-O2A-C1
19	4	312	CLA	CBA-CGA-O2A-C1
19	A	823	CLA	CBA-CGA-O2A-C1
19	A	831	CLA	CBA-CGA-O2A-C1
19	A	855	CLA	CBA-CGA-O2A-C1
19	B	815	CLA	CBA-CGA-O2A-C1
19	B	818	CLA	CBA-CGA-O2A-C1
19	B	825	CLA	CBA-CGA-O2A-C1
19	F	303	CLA	CBA-CGA-O2A-C1
19	L	301	CLA	CBA-CGA-O2A-C1
19	L	303	CLA	CBA-CGA-O2A-C1
22	1	518	LMG	C29-C28-O8-C9
22	2	519	LMG	C29-C28-O8-C9
22	4	322	LMG	C29-C28-O8-C9
22	A	847	LMG	C29-C28-O8-C9
22	F	304	LMG	C29-C28-O8-C9
22	G	210	LMG	C29-C28-O8-C9
19	1	508	CLA	CBD-CGD-O2D-CED
19	2	511	CLA	CBD-CGD-O2D-CED
19	3	313	CLA	CBD-CGD-O2D-CED
19	3	317	CLA	CBD-CGD-O2D-CED
19	4	307	CLA	CBD-CGD-O2D-CED
19	4	311	CLA	CBD-CGD-O2D-CED
19	A	805	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A	814	CLA	CBD-CGD-O2D-CED
19	A	819	CLA	CBD-CGD-O2D-CED
19	A	833	CLA	CBD-CGD-O2D-CED
19	A	836	CLA	CBD-CGD-O2D-CED
19	A	855	CLA	CBD-CGD-O2D-CED
19	B	806	CLA	CBD-CGD-O2D-CED
19	B	813	CLA	CBD-CGD-O2D-CED
19	B	814	CLA	CBD-CGD-O2D-CED
19	B	818	CLA	CBD-CGD-O2D-CED
19	B	835	CLA	CBD-CGD-O2D-CED
19	B	838	CLA	CBD-CGD-O2D-CED
19	F	303	CLA	CBD-CGD-O2D-CED
19	J	1105	CLA	CBD-CGD-O2D-CED
22	1	518	LMG	C11-C10-O7-C8
22	B	844	LMG	C11-C10-O7-C8
22	F	304	LMG	C11-C10-O7-C8
19	1	505	CLA	O1D-CGD-O2D-CED
19	1	516	CLA	O1D-CGD-O2D-CED
19	2	506	CLA	O1D-CGD-O2D-CED
19	3	315	CLA	O1D-CGD-O2D-CED
19	3	316	CLA	O1D-CGD-O2D-CED
19	A	820	CLA	O1D-CGD-O2D-CED
19	A	828	CLA	O1A-CGA-O2A-C1
19	B	809	CLA	O1D-CGD-O2D-CED
19	3	307	CLA	C4-C3-C5-C6
19	4	306	CLA	C4-C3-C5-C6
19	A	802	CLA	C4-C3-C5-C6
19	A	808	CLA	C4-C3-C5-C6
19	A	809	CLA	C4-C3-C5-C6
19	A	818	CLA	C4-C3-C5-C6
19	A	838	CLA	C4-C3-C5-C6
19	B	824	CLA	C4-C3-C5-C6
19	B	828	CLA	C4-C3-C5-C6
19	B	832	CLA	C4-C3-C5-C6
19	B	839	CLA	C4-C3-C5-C6
19	G	201	CLA	C4-C3-C5-C6
20	2	526	CHL	C4-C3-C5-C6
20	4	316	CHL	C4-C3-C5-C6
19	3	307	CLA	C2-C3-C5-C6
19	4	306	CLA	C2-C3-C5-C6
19	A	802	CLA	C2-C3-C5-C6
19	A	808	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	A	809	CLA	C2-C3-C5-C6
19	A	818	CLA	C2-C3-C5-C6
19	A	824	CLA	C2-C3-C5-C6
19	A	840	CLA	C2-C3-C5-C6
19	B	832	CLA	C2-C3-C5-C6
19	B	834	CLA	C2-C3-C5-C6
19	G	201	CLA	C2-C3-C5-C6
20	4	316	CHL	C2-C3-C5-C6
29	A	844	PQN	C12-C13-C15-C16
19	4	315	CLA	O1D-CGD-O2D-CED
19	A	815	CLA	O1D-CGD-O2D-CED
19	2	510	CLA	C3-C5-C6-C7
19	A	805	CLA	C3-C5-C6-C7
19	A	823	CLA	C3-C5-C6-C7
19	B	810	CLA	C3-C5-C6-C7
19	B	829	CLA	C3-C5-C6-C7
19	B	835	CLA	C3-C5-C6-C7
19	2	514	CLA	CBA-CGA-O2A-C1
19	4	308	CLA	CBA-CGA-O2A-C1
19	4	315	CLA	CBA-CGA-O2A-C1
19	4	318	CLA	CBA-CGA-O2A-C1
19	A	806	CLA	CBA-CGA-O2A-C1
19	B	808	CLA	CBA-CGA-O2A-C1
19	B	810	CLA	CBA-CGA-O2A-C1
19	B	812	CLA	CBA-CGA-O2A-C1
19	B	822	CLA	CBA-CGA-O2A-C1
19	B	832	CLA	CBA-CGA-O2A-C1
19	B	834	CLA	CBA-CGA-O2A-C1
19	G	202	CLA	CBA-CGA-O2A-C1
19	L	305	CLA	CBA-CGA-O2A-C1
22	G	206	LMG	C29-C28-O8-C9
26	G	207	DGD	C2A-C1A-O1G-C1G
22	G	206	LMG	C35-C36-C37-C38
26	B	801	DGD	O6D-C5D-C6D-O5D
24	G	209	LMT	O5'-C5'-C6'-O6'
17	1	502	LUT	C29-C30-C31-C32
18	3	303	BCR	C9-C10-C11-C12
18	A	848	BCR	C13-C14-C15-C16
18	B	852	BCR	C19-C20-C21-C22
19	2	514	CLA	O1A-CGA-O2A-C1
19	3	313	CLA	O1A-CGA-O2A-C1
19	4	312	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	4	318	CLA	O1A-CGA-O2A-C1
19	A	823	CLA	O1A-CGA-O2A-C1
19	B	808	CLA	O1A-CGA-O2A-C1
19	B	810	CLA	O1A-CGA-O2A-C1
19	B	812	CLA	O1A-CGA-O2A-C1
19	G	204	CLA	O1A-CGA-O2A-C1
19	J	1105	CLA	O1A-CGA-O2A-C1
22	2	519	LMG	O10-C28-O8-C9
22	A	847	LMG	O10-C28-O8-C9
26	G	207	DGD	O1A-C1A-O1G-C1G
21	B	843	LHG	O9-C7-O7-C5
22	G	210	LMG	O9-C10-O7-C8
19	3	317	CLA	O1A-CGA-O2A-C1
22	G	206	LMG	C17-C18-C19-C20
26	B	854	DGD	C8A-C9A-CAA-CBA
19	2	510	CLA	O1D-CGD-O2D-CED
19	4	305	CLA	O1D-CGD-O2D-CED
19	B	809	CLA	C3-C5-C6-C7
19	A	810	CLA	CBD-CGD-O2D-CED
19	A	812	CLA	CBD-CGD-O2D-CED
19	A	830	CLA	CBD-CGD-O2D-CED
19	B	805	CLA	CBD-CGD-O2D-CED
19	B	833	CLA	CBD-CGD-O2D-CED
22	A	847	LMG	C17-C18-C19-C20
24	A	846	LMT	C2B-C1B-O1B-C4'
21	B	843	LHG	O2-C2-C3-O3
19	B	816	CLA	O1D-CGD-O2D-CED
19	L	301	CLA	O1D-CGD-O2D-CED
19	A	810	CLA	CBA-CGA-O2A-C1
19	A	818	CLA	CBA-CGA-O2A-C1
19	A	828	CLA	CBA-CGA-O2A-C1
19	B	823	CLA	CBA-CGA-O2A-C1
19	J	1105	CLA	CBA-CGA-O2A-C1
22	B	844	LMG	C29-C28-O8-C9
22	B	845	LMG	C29-C28-O8-C9
26	J	1106	DGD	C2A-C1A-O1G-C1G
24	G	208	LMT	O5B-C5B-C6B-O6B
19	4	308	CLA	O1A-CGA-O2A-C1
19	B	815	CLA	O1A-CGA-O2A-C1
19	B	832	CLA	O1A-CGA-O2A-C1
19	B	834	CLA	O1A-CGA-O2A-C1
19	L	305	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	844	LMG	O10-C28-O8-C9
24	J	1107	LMT	C4B-C5B-C6B-O6B
19	J	1102	CLA	O1D-CGD-O2D-CED
22	2	519	LMG	O6-C5-C6-O5
24	B	846	LMT	O5B-C5B-C6B-O6B
26	B	801	DGD	O6E-C5E-C6E-O5E
24	2	523	LMT	C4B-C5B-C6B-O6B
24	A	846	LMT	C4B-C5B-C6B-O6B
19	A	802	CLA	CBD-CGD-O2D-CED
19	A	808	CLA	CBD-CGD-O2D-CED
21	1	517	LHG	C8-C7-O7-C5
22	F	305	LMG	C11-C10-O7-C8
22	G	206	LMG	C11-C10-O7-C8
26	G	207	DGD	C2B-C1B-O2G-C2G
19	4	304	CLA	O1D-CGD-O2D-CED
19	A	807	CLA	O1D-CGD-O2D-CED
19	A	831	CLA	O1D-CGD-O2D-CED
19	K	1002	CLA	O1D-CGD-O2D-CED
19	2	508	CLA	CBD-CGD-O2D-CED
19	B	817	CLA	CBD-CGD-O2D-CED
19	B	840	CLA	CBD-CGD-O2D-CED
24	G	209	LMT	O5B-C5B-C6B-O6B
24	J	1107	LMT	O5B-C5B-C6B-O6B
19	2	505	CLA	O1D-CGD-O2D-CED
19	4	310	CLA	O1D-CGD-O2D-CED
19	A	811	CLA	O1D-CGD-O2D-CED
19	A	832	CLA	O1D-CGD-O2D-CED
19	3	313	CLA	CBA-CGA-O2A-C1
19	G	204	CLA	CBA-CGA-O2A-C1
19	1	508	CLA	C4-C3-C5-C6
19	3	308	CLA	C4-C3-C5-C6
19	A	811	CLA	C4-C3-C5-C6
19	A	826	CLA	C4-C3-C5-C6
19	A	834	CLA	C4-C3-C5-C6
19	B	808	CLA	C4-C3-C5-C6
19	F	303	CLA	C4-C3-C5-C6
19	1	508	CLA	C2-C3-C5-C6
19	3	308	CLA	C2-C3-C5-C6
19	A	811	CLA	C2-C3-C5-C6
19	A	834	CLA	C2-C3-C5-C6
20	2	526	CHL	C2-C3-C5-C6
19	A	806	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A	810	CLA	O1A-CGA-O2A-C1
19	B	823	CLA	O1A-CGA-O2A-C1
26	J	1106	DGD	O1A-C1A-O1G-C1G
19	3	305	CLA	C2C-C3C-CAC-CBC
24	A	846	LMT	O5B-C5B-C6B-O6B
19	2	507	CLA	CBD-CGD-O2D-CED
19	B	830	CLA	CBD-CGD-O2D-CED
21	B	843	LHG	C2-C3-O3-P
19	3	306	CLA	C3-C5-C6-C7
19	A	835	CLA	C2A-CAA-CBA-CGA
24	A	846	LMT	O5B-C1B-O1B-C4'
19	G	204	CLA	O1D-CGD-O2D-CED
24	A	846	LMT	O5'-C5'-C6'-O6'
24	B	846	LMT	C4B-C5B-C6B-O6B
19	A	834	CLA	O1D-CGD-O2D-CED
19	G	202	CLA	O1D-CGD-O2D-CED
19	2	511	CLA	CBA-CGA-O2A-C1
19	A	814	CLA	CBA-CGA-O2A-C1
19	A	835	CLA	CBA-CGA-O2A-C1
19	2	504	CLA	CBD-CGD-O2D-CED
19	4	318	CLA	CBD-CGD-O2D-CED
19	A	803	CLA	CBD-CGD-O2D-CED
19	A	829	CLA	CBD-CGD-O2D-CED
19	A	839	CLA	CBD-CGD-O2D-CED
19	B	821	CLA	CBD-CGD-O2D-CED
19	B	836	CLA	CBD-CGD-O2D-CED
19	G	201	CLA	CBD-CGD-O2D-CED
19	2	511	CLA	O1A-CGA-O2A-C1
19	A	818	CLA	O1A-CGA-O2A-C1
19	A	835	CLA	O1A-CGA-O2A-C1
22	B	845	LMG	O10-C28-O8-C9
22	G	206	LMG	O6-C5-C6-O5
24	2	523	LMT	O5B-C5B-C6B-O6B
19	1	507	CLA	O1D-CGD-O2D-CED
19	4	311	CLA	O1D-CGD-O2D-CED
26	B	801	DGD	C4E-C5E-C6E-O5E
19	A	827	CLA	CBD-CGD-O2D-CED
19	A	841	CLA	CBD-CGD-O2D-CED
19	L	304	CLA	CBD-CGD-O2D-CED
19	F	303	CLA	C3-C5-C6-C7
24	G	209	LMT	C5'-C4'-O1B-C1B
19	1	504	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	1	501	LUT	C29-C30-C31-C32
18	L	307	BCR	C13-C14-C15-C16
22	G	206	LMG	O9-C10-O7-C8
26	G	207	DGD	O1B-C1B-O2G-C2G
21	2	517	LHG	C1-C2-C3-O3
19	A	804	CLA	O1D-CGD-O2D-CED
19	J	1101	CLA	O1D-CGD-O2D-CED
19	2	505	CLA	CBA-CGA-O2A-C1
19	2	507	CLA	CBA-CGA-O2A-C1
19	3	308	CLA	CBA-CGA-O2A-C1
19	3	310	CLA	CBA-CGA-O2A-C1
19	4	309	CLA	CBA-CGA-O2A-C1
19	A	802	CLA	CBA-CGA-O2A-C1
19	A	807	CLA	CBA-CGA-O2A-C1
19	A	809	CLA	CBA-CGA-O2A-C1
19	A	817	CLA	CBA-CGA-O2A-C1
19	A	820	CLA	CBA-CGA-O2A-C1
19	A	822	CLA	CBA-CGA-O2A-C1
19	A	826	CLA	CBA-CGA-O2A-C1
19	A	836	CLA	CBA-CGA-O2A-C1
19	A	842	CLA	CBA-CGA-O2A-C1
19	B	806	CLA	CBA-CGA-O2A-C1
19	B	829	CLA	CBA-CGA-O2A-C1
19	B	837	CLA	CBA-CGA-O2A-C1
19	B	840	CLA	CBA-CGA-O2A-C1
19	K	1002	CLA	CBA-CGA-O2A-C1
26	4	319	DGD	C2A-C1A-O1G-C1G
19	B	831	CLA	CBD-CGD-O2D-CED
21	1	520	LHG	C13-C14-C15-C16
19	3	309	CLA	O1D-CGD-O2D-CED
19	3	313	CLA	O1D-CGD-O2D-CED
19	3	317	CLA	O1D-CGD-O2D-CED
19	A	805	CLA	O1D-CGD-O2D-CED
19	A	819	CLA	O1D-CGD-O2D-CED
19	A	833	CLA	O1D-CGD-O2D-CED
19	A	855	CLA	O1D-CGD-O2D-CED
19	L	305	CLA	O1D-CGD-O2D-CED
19	A	817	CLA	C4-C3-C5-C6
19	B	819	CLA	C4-C3-C5-C6
19	H	1000	CLA	C4-C3-C5-C6
19	K	1002	CLA	C4-C3-C5-C6
19	A	817	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	A	838	CLA	C2-C3-C5-C6
19	A	855	CLA	C2-C3-C5-C6
19	B	808	CLA	C2-C3-C5-C6
19	B	824	CLA	C2-C3-C5-C6
19	B	828	CLA	C2-C3-C5-C6
19	B	839	CLA	C2-C3-C5-C6
19	F	303	CLA	C2-C3-C5-C6
19	H	1000	CLA	C2-C3-C5-C6
19	K	1002	CLA	C2-C3-C5-C6
19	A	835	CLA	C3-C5-C6-C7
19	B	832	CLA	CBD-CGD-O2D-CED
19	L	303	CLA	CBD-CGD-O2D-CED
19	1	504	CLA	C11-C10-C8-C9
19	1	507	CLA	C14-C13-C15-C16
19	1	508	CLA	C14-C13-C15-C16
19	3	313	CLA	C11-C10-C8-C9
19	4	315	CLA	C14-C13-C15-C16
19	4	318	CLA	C14-C13-C15-C16
19	A	802	CLA	C11-C10-C8-C9
19	A	804	CLA	C11-C10-C8-C9
19	A	805	CLA	C14-C13-C15-C16
19	A	809	CLA	C6-C7-C8-C9
19	A	814	CLA	C14-C13-C15-C16
19	A	817	CLA	C14-C13-C15-C16
19	A	828	CLA	C14-C13-C15-C16
19	A	832	CLA	C11-C12-C13-C14
19	B	804	CLA	C14-C13-C15-C16
19	B	810	CLA	C14-C13-C15-C16
19	B	811	CLA	C11-C10-C8-C9
19	B	812	CLA	C11-C10-C8-C9
19	B	818	CLA	C11-C10-C8-C9
19	B	818	CLA	C11-C12-C13-C14
19	B	820	CLA	C11-C12-C13-C14
19	B	820	CLA	C14-C13-C15-C16
19	B	825	CLA	C6-C7-C8-C9
19	B	825	CLA	C14-C13-C15-C16
19	B	829	CLA	C11-C12-C13-C14
19	B	831	CLA	C11-C10-C8-C9
19	B	839	CLA	C11-C10-C8-C9
19	F	303	CLA	C11-C12-C13-C14
22	G	206	LMG	C4-C5-C6-O5
24	G	208	LMT	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
19	1	508	CLA	O1D-CGD-O2D-CED
19	F	303	CLA	O1D-CGD-O2D-CED
24	J	1107	LMT	C2'-C1'-O1'-C1
26	4	319	DGD	C2A-C3A-C4A-C5A
19	3	316	CLA	CBA-CGA-O2A-C1
21	2	517	LHG	O2-C2-C3-O3
19	2	511	CLA	O1D-CGD-O2D-CED
19	B	813	CLA	O1D-CGD-O2D-CED
19	3	308	CLA	O1A-CGA-O2A-C1
22	2	519	LMG	C4-C5-C6-O5
17	1	502	LUT	C31-C32-C33-C40
17	2	501	LUT	C31-C32-C33-C40
17	J	1109	LUT	C27-C28-C29-C39
18	3	303	BCR	C11-C12-C13-C35
18	3	303	BCR	C37-C22-C23-C24
18	3	304	BCR	C37-C22-C23-C24
18	4	301	BCR	C11-C12-C13-C35
18	4	301	BCR	C36-C18-C19-C20
18	A	849	BCR	C36-C18-C19-C20
18	A	851	BCR	C36-C18-C19-C20
18	A	852	BCR	C7-C8-C9-C34
18	A	856	BCR	C37-C22-C23-C24
18	B	850	BCR	C36-C18-C19-C20
18	B	851	BCR	C7-C8-C9-C34
18	B	852	BCR	C11-C12-C13-C35
18	B	853	BCR	C37-C22-C23-C24
18	B	856	BCR	C7-C8-C9-C34
18	I	101	BCR	C36-C18-C19-C20
18	I	102	BCR	C7-C8-C9-C34
18	I	102	BCR	C36-C18-C19-C20
18	K	1005	BCR	C37-C22-C23-C24
18	L	307	BCR	C11-C12-C13-C35
18	3	304	BCR	C21-C22-C23-C24
18	4	301	BCR	C11-C12-C13-C14
18	A	856	BCR	C21-C22-C23-C24
18	B	851	BCR	C7-C8-C9-C10
18	B	852	BCR	C11-C12-C13-C14
18	K	1005	BCR	C21-C22-C23-C24
19	2	506	CLA	C2A-CAA-CBA-CGA
19	A	808	CLA	C2A-CAA-CBA-CGA
19	B	818	CLA	C2A-CAA-CBA-CGA
19	B	839	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	A	847	LMG	C10-C11-C12-C13
19	2	505	CLA	O1A-CGA-O2A-C1
19	A	802	CLA	O1A-CGA-O2A-C1
19	A	820	CLA	O1A-CGA-O2A-C1
19	A	826	CLA	O1A-CGA-O2A-C1
19	A	842	CLA	O1A-CGA-O2A-C1
19	B	806	CLA	O1A-CGA-O2A-C1
19	B	829	CLA	O1A-CGA-O2A-C1
19	B	840	CLA	O1A-CGA-O2A-C1
19	B	832	CLA	C3-C5-C6-C7
19	L	304	CLA	C3-C5-C6-C7
22	F	305	LMG	O9-C10-O7-C8
22	2	519	LMG	C11-C10-O7-C8
19	A	821	CLA	CBA-CGA-O2A-C1
19	A	807	CLA	C8-C10-C11-C12
19	B	812	CLA	C10-C11-C12-C13
19	1	508	CLA	C2-C1-O2A-CGA
19	1	513	CLA	C2-C1-O2A-CGA
19	2	509	CLA	C2-C1-O2A-CGA
19	2	511	CLA	C2-C1-O2A-CGA
19	3	315	CLA	C2-C1-O2A-CGA
19	4	309	CLA	C2-C1-O2A-CGA
19	A	803	CLA	C2-C1-O2A-CGA
19	A	805	CLA	C2-C1-O2A-CGA
19	A	809	CLA	C2-C1-O2A-CGA
19	A	814	CLA	C2-C1-O2A-CGA
19	A	822	CLA	C2-C1-O2A-CGA
19	A	823	CLA	C2-C1-O2A-CGA
19	A	835	CLA	C2-C1-O2A-CGA
19	A	838	CLA	C2-C1-O2A-CGA
19	B	811	CLA	C2-C1-O2A-CGA
19	B	823	CLA	C2-C1-O2A-CGA
19	B	832	CLA	C2-C1-O2A-CGA
19	B	838	CLA	C2-C1-O2A-CGA
19	L	305	CLA	C2-C1-O2A-CGA
19	2	507	CLA	O1A-CGA-O2A-C1
19	4	307	CLA	O1D-CGD-O2D-CED
19	B	806	CLA	O1D-CGD-O2D-CED
19	B	814	CLA	O1D-CGD-O2D-CED
19	B	818	CLA	O1D-CGD-O2D-CED
19	J	1105	CLA	O1D-CGD-O2D-CED
24	G	208	LMT	C3'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
19	1	507	CLA	C15-C16-C17-C18
19	4	307	CLA	C10-C11-C12-C13
19	4	310	CLA	C8-C10-C11-C12
19	A	831	CLA	C15-C16-C17-C18
19	B	804	CLA	C13-C15-C16-C17
19	B	806	CLA	C15-C16-C17-C18
19	B	828	CLA	C15-C16-C17-C18
19	B	830	CLA	C15-C16-C17-C18
21	1	517	LHG	O1-C1-C2-O2
21	A	845	LHG	O1-C1-C2-O2
19	1	516	CLA	C3-C5-C6-C7
19	4	306	CLA	C3-C5-C6-C7
19	B	815	CLA	C3-C5-C6-C7
19	B	822	CLA	C3-C5-C6-C7
19	K	1002	CLA	C3-C5-C6-C7
19	3	310	CLA	O1A-CGA-O2A-C1
19	A	807	CLA	O1A-CGA-O2A-C1
19	B	805	CLA	C15-C16-C17-C18
19	A	821	CLA	CBD-CGD-O2D-CED
19	A	826	CLA	CBD-CGD-O2D-CED
19	B	820	CLA	CBD-CGD-O2D-CED
22	2	518	LMG	O6-C5-C6-O5
19	A	806	CLA	C12-C13-C15-C16
19	A	824	CLA	C12-C13-C15-C16
19	A	855	CLA	C4-C3-C5-C6
26	B	854	DGD	O6E-C5E-C6E-O5E
22	4	322	LMG	C14-C15-C16-C17
19	4	308	CLA	C8-C10-C11-C12
22	B	844	LMG	C10-C11-C12-C13
18	2	503	BCR	C19-C20-C21-C22
18	4	301	BCR	C13-C14-C15-C16
18	4	301	BCR	C19-C20-C21-C22
22	4	322	LMG	C29-C30-C31-C32
19	B	838	CLA	O1D-CGD-O2D-CED
19	A	828	CLA	C3-C5-C6-C7
19	A	824	CLA	C13-C15-C16-C17
19	A	830	CLA	C5-C6-C7-C8
19	B	825	CLA	C5-C6-C7-C8
19	B	832	CLA	C5-C6-C7-C8
19	B	839	CLA	C5-C6-C7-C8
19	J	1101	CLA	C8-C10-C11-C12
19	A	814	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	A	853	LHG	C7-C8-C9-C10
22	J	1104	LMG	C28-C29-C30-C31
19	A	817	CLA	O1A-CGA-O2A-C1
19	A	822	CLA	O1A-CGA-O2A-C1
19	B	837	CLA	O1A-CGA-O2A-C1
26	4	319	DGD	O1A-C1A-O1G-C1G
19	1	507	CLA	CBA-CGA-O2A-C1
19	1	504	CLA	C8-C10-C11-C12
19	2	506	CLA	C13-C15-C16-C17
19	2	510	CLA	C5-C6-C7-C8
19	3	308	CLA	C5-C6-C7-C8
19	A	804	CLA	C13-C15-C16-C17
19	A	804	CLA	C15-C16-C17-C18
19	A	806	CLA	C8-C10-C11-C12
19	A	819	CLA	C10-C11-C12-C13
19	A	821	CLA	C10-C11-C12-C13
19	A	828	CLA	C15-C16-C17-C18
19	A	838	CLA	C13-C15-C16-C17
19	A	855	CLA	C8-C10-C11-C12
19	A	855	CLA	C10-C11-C12-C13
19	B	819	CLA	C8-C10-C11-C12
19	B	825	CLA	C15-C16-C17-C18
19	G	201	CLA	C13-C15-C16-C17
19	G	202	CLA	C5-C6-C7-C8
29	A	844	PQN	C18-C20-C21-C22
24	G	208	LMT	O5'-C5'-C6'-O6'
19	1	516	CLA	C2A-CAA-CBA-CGA
19	2	511	CLA	C2A-CAA-CBA-CGA
19	3	310	CLA	C2A-CAA-CBA-CGA
19	3	313	CLA	C2A-CAA-CBA-CGA
19	3	316	CLA	C2A-CAA-CBA-CGA
19	A	821	CLA	C2A-CAA-CBA-CGA
19	B	828	CLA	C2A-CAA-CBA-CGA
19	K	1001	CLA	C2A-CAA-CBA-CGA
20	1	512	CHL	C2A-CAA-CBA-CGA
20	2	512	CHL	C2A-CAA-CBA-CGA
20	3	314	CHL	C2A-CAA-CBA-CGA
18	B	849	BCR	C10-C11-C12-C13
18	B	852	BCR	C10-C11-C12-C13
18	K	1005	BCR	C10-C11-C12-C13
19	4	304	CLA	C8-C10-C11-C12
19	A	806	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	A	817	CLA	C5-C6-C7-C8
19	A	822	CLA	C8-C10-C11-C12
19	A	829	CLA	C15-C16-C17-C18
19	A	837	CLA	C5-C6-C7-C8
19	A	854	CLA	C5-C6-C7-C8
19	B	807	CLA	C8-C10-C11-C12
19	B	808	CLA	C8-C10-C11-C12
19	B	808	CLA	C15-C16-C17-C18
19	B	811	CLA	C5-C6-C7-C8
19	B	825	CLA	C13-C15-C16-C17
19	F	303	CLA	C8-C10-C11-C12
21	B	843	LHG	C23-C24-C25-C26
26	B	801	DGD	C1A-C2A-C3A-C4A
26	G	207	DGD	C1B-C2B-C3B-C4B
19	A	836	CLA	O1D-CGD-O2D-CED
19	4	309	CLA	O1A-CGA-O2A-C1
19	A	814	CLA	O1A-CGA-O2A-C1
19	A	836	CLA	O1A-CGA-O2A-C1
19	G	204	CLA	C3-C5-C6-C7
24	B	846	LMT	O5'-C1'-O1'-C1
24	B	847	LMT	O5'-C1'-O1'-C1
24	G	209	LMT	O5'-C1'-O1'-C1
19	1	516	CLA	C5-C6-C7-C8
19	2	506	CLA	C15-C16-C17-C18
19	3	308	CLA	C8-C10-C11-C12
19	3	308	CLA	C13-C15-C16-C17
19	4	306	CLA	C8-C10-C11-C12
19	4	306	CLA	C10-C11-C12-C13
19	4	307	CLA	C8-C10-C11-C12
19	4	318	CLA	C8-C10-C11-C12
19	A	809	CLA	C10-C11-C12-C13
19	A	809	CLA	C13-C15-C16-C17
19	B	805	CLA	C13-C15-C16-C17
19	B	811	CLA	C8-C10-C11-C12
19	B	812	CLA	C8-C10-C11-C12
19	B	818	CLA	C15-C16-C17-C18
19	B	820	CLA	C13-C15-C16-C17
19	B	824	CLA	C15-C16-C17-C18
19	B	831	CLA	C5-C6-C7-C8
19	B	831	CLA	C8-C10-C11-C12
19	B	836	CLA	C15-C16-C17-C18
19	B	838	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	F	303	CLA	C5-C6-C7-C8
21	1	520	LHG	O2-C2-C3-O3
24	G	208	LMT	O1'-C1-C2-C3
19	B	805	CLA	O1D-CGD-O2D-CED
19	A	809	CLA	O1A-CGA-O2A-C1
19	K	1002	CLA	O1A-CGA-O2A-C1
21	1	520	LHG	C23-C24-C25-C26
19	4	304	CLA	C10-C11-C12-C13
19	4	306	CLA	C5-C6-C7-C8
19	A	835	CLA	C5-C6-C7-C8
19	B	830	CLA	C8-C10-C11-C12
21	1	517	LHG	O9-C7-O7-C5
22	2	519	LMG	O9-C10-O7-C8
19	A	802	CLA	O1D-CGD-O2D-CED
24	B	855	LMT	O1'-C1-C2-C3
19	B	807	CLA	C3-C5-C6-C7
19	4	308	CLA	C5-C6-C7-C8
19	4	315	CLA	C13-C15-C16-C17
19	A	808	CLA	C5-C6-C7-C8
19	A	828	CLA	C10-C11-C12-C13
19	A	833	CLA	C5-C6-C7-C8
19	A	840	CLA	C8-C10-C11-C12
19	B	814	CLA	C5-C6-C7-C8
19	A	826	CLA	C2-C3-C5-C6
21	A	845	LHG	C23-C24-C25-C26
22	F	304	LMG	C34-C35-C36-C37
24	G	208	LMT	C5'-C4'-O1B-C1B
19	A	812	CLA	O1D-CGD-O2D-CED
19	A	830	CLA	O1D-CGD-O2D-CED
19	B	835	CLA	O1D-CGD-O2D-CED
19	B	840	CLA	O1D-CGD-O2D-CED
24	3	318	LMT	O5'-C5'-C6'-O6'
19	3	307	CLA	C5-C6-C7-C8
19	A	805	CLA	C13-C15-C16-C17
19	A	819	CLA	C5-C6-C7-C8
19	A	833	CLA	C15-C16-C17-C18
19	A	839	CLA	C15-C16-C17-C18
19	A	854	CLA	C13-C15-C16-C17
19	A	855	CLA	C13-C15-C16-C17
19	B	818	CLA	C8-C10-C11-C12
19	B	828	CLA	C5-C6-C7-C8
19	B	833	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	J	1106	DGD	CDA-CEA-CFA-CGA
19	A	821	CLA	O1A-CGA-O2A-C1
19	A	825	CLA	C15-C16-C17-C18
19	A	833	CLA	C8-C10-C11-C12
19	B	836	CLA	C3-C5-C6-C7
19	B	803	CLA	CBD-CGD-O2D-CED
17	J	1109	LUT	C29-C30-C31-C32
18	J	1108	BCR	C19-C20-C21-C22
19	A	817	CLA	C10-C11-C12-C13
19	A	817	CLA	C13-C15-C16-C17
21	1	517	LHG	C1-C2-C3-O3
21	1	520	LHG	C1-C2-C3-O3
21	A	845	LHG	C1-C2-C3-O3
19	3	307	CLA	C2A-CAA-CBA-CGA
19	B	833	CLA	O1D-CGD-O2D-CED
19	2	508	CLA	CBA-CGA-O2A-C1
19	3	305	CLA	CBA-CGA-O2A-C1
19	B	835	CLA	CBA-CGA-O2A-C1
19	3	305	CLA	C4C-C3C-CAC-CBC
19	2	506	CLA	C5-C6-C7-C8
19	A	811	CLA	C10-C11-C12-C13
19	A	811	CLA	C13-C15-C16-C17
19	A	813	CLA	C13-C15-C16-C17
19	A	814	CLA	C8-C10-C11-C12
19	A	838	CLA	C10-C11-C12-C13
19	B	806	CLA	C13-C15-C16-C17
19	B	829	CLA	C10-C11-C12-C13
19	B	833	CLA	C8-C10-C11-C12
19	B	839	CLA	C15-C16-C17-C18
19	F	303	CLA	C13-C15-C16-C17
19	L	301	CLA	C5-C6-C7-C8
19	A	810	CLA	O1D-CGD-O2D-CED
19	2	508	CLA	O1D-CGD-O2D-CED
19	A	808	CLA	O1D-CGD-O2D-CED
19	1	504	CLA	C13-C15-C16-C17
19	2	507	CLA	C15-C16-C17-C18
19	4	310	CLA	C5-C6-C7-C8
19	A	832	CLA	C13-C15-C16-C17
19	A	833	CLA	C13-C15-C16-C17
19	A	854	CLA	C8-C10-C11-C12
19	B	815	CLA	C15-C16-C17-C18
19	B	819	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	B	846	LMT	O5'-C5'-C6'-O6'
24	3	318	LMT	C4'-C5'-C6'-O6'
19	1	513	CLA	C15-C16-C17-C18
19	A	831	CLA	C5-C6-C7-C8
19	A	840	CLA	C15-C16-C17-C18
19	B	822	CLA	C15-C16-C17-C18
19	B	825	CLA	C8-C10-C11-C12
19	F	302	CLA	C13-C15-C16-C17
19	G	204	CLA	C13-C15-C16-C17
19	2	507	CLA	C4-C3-C5-C6
19	A	834	CLA	C13-C15-C16-C17
19	B	822	CLA	C5-C6-C7-C8
19	3	308	CLA	C11-C12-C13-C14
22	J	1103	LMG	C11-C12-C13-C14
22	4	322	LMG	C2-C1-O1-C7
22	B	845	LMG	C2-C1-O1-C7
22	J	1104	LMG	C2-C1-O1-C7
24	B	846	LMT	C2'-C1'-O1'-C1
24	B	847	LMT	C2'-C1'-O1'-C1
24	G	209	LMT	C2'-C1'-O1'-C1
26	4	319	DGD	C2D-C1D-O3G-C3G
26	B	801	DGD	C2D-C1D-O3G-C3G
19	B	817	CLA	O1D-CGD-O2D-CED
19	A	823	CLA	C11-C12-C13-C15
19	B	811	CLA	C16-C17-C18-C19
19	L	304	CLA	C11-C12-C13-C15
19	A	806	CLA	C15-C16-C17-C18
19	B	820	CLA	C10-C11-C12-C13
18	G	205	BCR	C11-C10-C9-C34
24	J	1107	LMT	O5'-C5'-C6'-O6'
19	B	816	CLA	C5-C6-C7-C8
18	3	304	BCR	C11-C12-C13-C35
18	A	856	BCR	C7-C8-C9-C34
18	B	856	BCR	C11-C12-C13-C35
18	G	205	BCR	C11-C12-C13-C35
18	I	102	BCR	C37-C22-C23-C24
18	K	1005	BCR	C11-C12-C13-C35
17	1	502	LUT	C31-C32-C33-C34
18	3	303	BCR	C11-C12-C13-C14
18	3	304	BCR	C11-C12-C13-C14
18	B	856	BCR	C11-C12-C13-C14
18	I	102	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
18	K	1005	BCR	C11-C12-C13-C14
18	L	307	BCR	C11-C12-C13-C14
19	2	508	CLA	O1A-CGA-O2A-C1
19	4	309	CLA	C2A-CAA-CBA-CGA
19	A	816	CLA	C2A-CAA-CBA-CGA
19	A	842	CLA	C2A-CAA-CBA-CGA
19	B	805	CLA	C2A-CAA-CBA-CGA
19	G	202	CLA	C2A-CAA-CBA-CGA
20	2	516	CHL	C2A-CAA-CBA-CGA
21	2	517	LHG	O1-C1-C2-C3
21	A	845	LHG	O1-C1-C2-C3
19	2	507	CLA	O1D-CGD-O2D-CED
19	A	828	CLA	O2A-C1-C2-C3
18	I	102	BCR	C13-C14-C15-C16
18	L	307	BCR	C15-C16-C17-C18
19	1	508	CLA	C16-C17-C18-C19
19	4	307	CLA	C11-C12-C13-C14
19	4	310	CLA	C11-C12-C13-C14
19	A	826	CLA	C6-C7-C8-C9
19	A	838	CLA	C16-C17-C18-C19
19	A	855	CLA	C16-C17-C18-C19
19	B	815	CLA	C16-C17-C18-C20
24	4	320	LMT	O1'-C1-C2-C3
19	A	829	CLA	O1D-CGD-O2D-CED
19	1	507	CLA	O1A-CGA-O2A-C1
19	3	305	CLA	O1A-CGA-O2A-C1
19	A	819	CLA	C3-C5-C6-C7
19	A	854	CLA	C3-C5-C6-C7
20	1	521	CHL	C2C-C3C-CAC-CBC
18	G	205	BCR	C11-C10-C9-C8
22	B	845	LMG	O6-C1-O1-C7
22	J	1104	LMG	O6-C1-O1-C7
26	4	319	DGD	O6D-C1D-O3G-C3G
26	B	801	DGD	C2B-C1B-O2G-C2G
26	B	801	DGD	C4D-C5D-C6D-O5D
22	4	322	LMG	O6-C5-C6-O5
19	A	814	CLA	C13-C15-C16-C17
19	3	305	CLA	C2-C1-O2A-CGA
19	3	310	CLA	C2-C1-O2A-CGA
19	3	312	CLA	C2-C1-O2A-CGA
19	4	305	CLA	C2-C1-O2A-CGA
19	A	818	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
19	A	824	CLA	C2-C1-O2A-CGA
19	A	825	CLA	C2-C1-O2A-CGA
19	A	826	CLA	C2-C1-O2A-CGA
19	A	828	CLA	C2-C1-O2A-CGA
19	A	833	CLA	C2-C1-O2A-CGA
19	A	834	CLA	C2-C1-O2A-CGA
19	B	807	CLA	C2-C1-O2A-CGA
19	B	817	CLA	C2-C1-O2A-CGA
19	B	839	CLA	C2-C1-O2A-CGA
20	4	314	CHL	C2-C1-O2A-CGA
19	2	510	CLA	C11-C12-C13-C14
19	3	307	CLA	C6-C7-C8-C9
19	4	307	CLA	C11-C12-C13-C15
19	B	811	CLA	C16-C17-C18-C20
19	B	815	CLA	C16-C17-C18-C19
19	B	824	CLA	C16-C17-C18-C20
19	B	825	CLA	C16-C17-C18-C20
19	B	834	CLA	C6-C7-C8-C9
19	F	302	CLA	C16-C17-C18-C19
19	G	202	CLA	C6-C7-C8-C9
20	4	316	CHL	C11-C12-C13-C15
19	B	835	CLA	O1A-CGA-O2A-C1
19	A	804	CLA	C8-C10-C11-C12
19	B	814	CLA	C15-C16-C17-C18
19	A	839	CLA	O1D-CGD-O2D-CED
22	G	206	LMG	C15-C16-C17-C18
21	1	517	LHG	C9-C10-C11-C12
26	B	854	DGD	C3A-C4A-C5A-C6A
19	B	818	CLA	C10-C11-C12-C13
21	1	517	LHG	C11-C10-C9-C8
19	A	829	CLA	CBA-CGA-O2A-C1
19	A	854	CLA	CBA-CGA-O2A-C1
22	B	844	LMG	C11-C12-C13-C14
26	B	801	DGD	O1B-C1B-O2G-C2G
21	B	842	LHG	O1-C1-C2-O2
21	B	843	LHG	O1-C1-C2-O2
24	3	318	LMT	C2-C1-O1'-C1'
24	A	846	LMT	C2-C1-O1'-C1'
24	B	846	LMT	C7-C8-C9-C10
19	A	803	CLA	O1D-CGD-O2D-CED
19	B	830	CLA	O1D-CGD-O2D-CED
19	4	312	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	A	832	CLA	C4B-C3B-CAB-CBB
19	B	808	CLA	C4B-C3B-CAB-CBB
19	B	823	CLA	C4B-C3B-CAB-CBB
19	F	303	CLA	C4B-C3B-CAB-CBB
24	G	209	LMT	C3'-C4'-O1B-C1B
19	1	508	CLA	C16-C17-C18-C20
19	2	510	CLA	C11-C12-C13-C15
19	3	305	CLA	C6-C7-C8-C10
19	A	814	CLA	C16-C17-C18-C19
19	A	822	CLA	C11-C12-C13-C14
19	A	822	CLA	C11-C12-C13-C15
19	A	823	CLA	C11-C12-C13-C14
19	A	826	CLA	C6-C7-C8-C10
19	A	840	CLA	C16-C17-C18-C20
19	A	854	CLA	C16-C17-C18-C19
19	A	855	CLA	C16-C17-C18-C20
19	B	807	CLA	C16-C17-C18-C20
19	B	812	CLA	C11-C12-C13-C14
19	B	812	CLA	C11-C12-C13-C15
19	B	824	CLA	C16-C17-C18-C19
19	B	825	CLA	C16-C17-C18-C19
19	B	834	CLA	C6-C7-C8-C10
19	B	840	CLA	C16-C17-C18-C20
19	F	302	CLA	C16-C17-C18-C20
19	L	304	CLA	C11-C12-C13-C14
19	4	311	CLA	C2A-CAA-CBA-CGA
19	A	818	CLA	C2A-CAA-CBA-CGA
20	4	316	CHL	C2A-CAA-CBA-CGA
19	4	306	CLA	C13-C15-C16-C17
19	4	318	CLA	C13-C15-C16-C17
19	A	832	CLA	C5-C6-C7-C8
19	B	809	CLA	C10-C11-C12-C13
19	H	1000	CLA	C10-C11-C12-C13
19	4	307	CLA	C11-C10-C8-C7
19	A	819	CLA	C6-C7-C8-C10
29	B	841	PQN	C17-C18-C20-C21
21	B	843	LHG	C7-C8-C9-C10
19	3	305	CLA	C5-C6-C7-C8
19	K	1002	CLA	C5-C6-C7-C8
21	1	517	LHG	C25-C26-C27-C28
21	1	517	LHG	C28-C29-C30-C31
29	A	844	PQN	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	1	506	CLA	C3A-C2A-CAA-CBA
19	3	309	CLA	C3A-C2A-CAA-CBA
19	3	316	CLA	C3A-C2A-CAA-CBA
19	3	317	CLA	C3A-C2A-CAA-CBA
19	4	308	CLA	C3A-C2A-CAA-CBA
19	A	805	CLA	C3A-C2A-CAA-CBA
19	A	806	CLA	C3A-C2A-CAA-CBA
19	A	815	CLA	C3A-C2A-CAA-CBA
19	B	814	CLA	C3A-C2A-CAA-CBA
19	B	824	CLA	C3A-C2A-CAA-CBA
19	B	835	CLA	C3A-C2A-CAA-CBA
19	G	201	CLA	C3A-C2A-CAA-CBA
19	G	203	CLA	C3A-C2A-CAA-CBA
19	J	1101	CLA	C3A-C2A-CAA-CBA
19	J	1105	CLA	C3A-C2A-CAA-CBA
19	K	1001	CLA	C3A-C2A-CAA-CBA
19	K	1002	CLA	C3A-C2A-CAA-CBA
20	2	515	CHL	C3A-C2A-CAA-CBA
20	2	516	CHL	C3A-C2A-CAA-CBA
22	2	519	LMG	C14-C15-C16-C17
19	B	819	CLA	C2-C3-C5-C6
22	2	524	LMG	O6-C5-C6-O5
19	1	507	CLA	C13-C15-C16-C17
19	A	808	CLA	C8-C10-C11-C12
19	2	504	CLA	O1D-CGD-O2D-CED
19	B	821	CLA	O1D-CGD-O2D-CED
21	1	517	LHG	C34-C35-C36-C37
18	A	848	BCR	C15-C16-C17-C18
18	B	850	BCR	C13-C14-C15-C16
19	A	814	CLA	C16-C17-C18-C20
19	A	829	CLA	C16-C17-C18-C19
19	A	829	CLA	C16-C17-C18-C20
19	A	840	CLA	C16-C17-C18-C19
19	A	854	CLA	C16-C17-C18-C20
19	B	840	CLA	C16-C17-C18-C19
19	F	303	CLA	C16-C17-C18-C19
19	F	303	CLA	C16-C17-C18-C20
22	G	210	LMG	O6-C5-C6-O5
19	B	833	CLA	O1A-CGA-O2A-C1
21	A	853	LHG	C28-C29-C30-C31
19	3	306	CLA	C2C-C3C-CAC-CBC
29	B	841	PQN	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
19	4	309	CLA	CBD-CGD-O2D-CED
21	B	843	LHG	C24-C25-C26-C27
19	F	302	CLA	CBA-CGA-O2A-C1
21	A	853	LHG	C13-C14-C15-C16
26	J	1106	DGD	CCA-CDA-CEA-CFA
22	B	845	LMG	C10-C11-C12-C13
22	G	206	LMG	C28-C29-C30-C31
21	1	520	LHG	C14-C15-C16-C17
21	A	845	LHG	C9-C10-C11-C12
21	A	853	LHG	C29-C30-C31-C32
21	A	853	LHG	C34-C35-C36-C37
22	F	305	LMG	C32-C33-C34-C35
24	G	208	LMT	C4-C5-C6-C7
19	L	304	CLA	O1D-CGD-O2D-CED
19	3	307	CLA	C6-C7-C8-C10
17	1	501	LUT	C1-C6-C7-C8
17	1	501	LUT	C5-C6-C7-C8
18	2	503	BCR	C1-C6-C7-C8
18	2	503	BCR	C5-C6-C7-C8
18	3	304	BCR	C23-C24-C25-C26
18	3	304	BCR	C23-C24-C25-C30
18	4	301	BCR	C1-C6-C7-C8
18	4	301	BCR	C5-C6-C7-C8
18	B	853	BCR	C1-C6-C7-C8
18	I	102	BCR	C23-C24-C25-C30
18	J	1108	BCR	C1-C6-C7-C8
18	J	1108	BCR	C5-C6-C7-C8
18	L	302	BCR	C23-C24-C25-C26
18	L	302	BCR	C23-C24-C25-C30
19	4	312	CLA	C2B-C3B-CAB-CBB
19	B	808	CLA	C2B-C3B-CAB-CBB
19	F	303	CLA	C2B-C3B-CAB-CBB
19	2	514	CLA	CBD-CGD-O2D-CED
19	B	807	CLA	C5-C6-C7-C8
19	B	840	CLA	C8-C10-C11-C12
19	3	313	CLA	C3-C5-C6-C7
22	1	518	LMG	C11-C12-C13-C14
19	A	827	CLA	O1D-CGD-O2D-CED
21	2	517	LHG	C9-C10-C11-C12
19	3	308	CLA	C2A-CAA-CBA-CGA
19	4	306	CLA	C2A-CAA-CBA-CGA
22	1	518	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
26	B	854	DGD	C6A-C7A-C8A-C9A
19	A	829	CLA	O1A-CGA-O2A-C1
19	A	854	CLA	O1A-CGA-O2A-C1
21	1	517	LHG	C14-C15-C16-C17
19	B	822	CLA	C4-C3-C5-C6
19	B	840	CLA	C4-C3-C5-C6
26	B	854	DGD	C2A-C3A-C4A-C5A
18	A	848	BCR	C10-C11-C12-C13
18	B	856	BCR	C10-C11-C12-C13
18	L	307	BCR	C10-C11-C12-C13
19	A	809	CLA	C5-C6-C7-C8
19	B	822	CLA	C2-C3-C5-C6
19	G	202	CLA	C6-C7-C8-C10
21	1	520	LHG	C16-C17-C18-C19
19	A	825	CLA	CBA-CGA-O2A-C1
19	A	830	CLA	CBA-CGA-O2A-C1
19	A	817	CLA	C11-C10-C8-C9
19	B	822	CLA	C11-C10-C8-C9
19	A	832	CLA	C15-C16-C17-C18
19	B	839	CLA	C10-C11-C12-C13
19	3	316	CLA	O1A-CGA-O2A-C1
19	B	836	CLA	O1D-CGD-O2D-CED
21	A	845	LHG	C13-C14-C15-C16
26	4	319	DGD	C3B-C4B-C5B-C6B
22	B	845	LMG	O6-C5-C6-O5
24	3	318	LMT	O5B-C5B-C6B-O6B
19	4	318	CLA	O1D-CGD-O2D-CED
19	1	504	CLA	C15-C16-C17-C18
19	B	826	CLA	C15-C16-C17-C18
19	G	201	CLA	C5-C6-C7-C8
19	B	821	CLA	CBA-CGA-O2A-C1
24	2	523	LMT	C2-C3-C4-C5
26	B	854	DGD	C4B-C5B-C6B-C7B
18	3	304	BCR	C19-C20-C21-C22
18	L	306	BCR	C19-C20-C21-C22
19	4	310	CLA	C11-C12-C13-C15
21	2	517	LHG	C8-C7-O7-C5
22	F	305	LMG	C28-C29-C30-C31
19	1	513	CLA	C5-C6-C7-C8
19	4	315	CLA	C10-C11-C12-C13
19	A	821	CLA	C8-C10-C11-C12
19	A	827	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	A	844	PQN	C25-C26-C27-C28
24	B	847	LMT	C4-C5-C6-C7
19	2	514	CLA	C5-C6-C7-C8
19	B	808	CLA	C5-C6-C7-C8
18	A	849	BCR	C37-C22-C23-C24
21	A	853	LHG	C25-C26-C27-C28
18	A	849	BCR	C21-C22-C23-C24
18	I	102	BCR	C7-C8-C9-C10
21	1	517	LHG	C35-C36-C37-C38
22	1	518	LMG	C8-C7-O1-C1
26	B	801	DGD	C2G-C3G-O3G-C1D
22	B	844	LMG	C4-C5-C6-O5
21	1	517	LHG	C11-C12-C13-C14
19	B	821	CLA	C2A-CAA-CBA-CGA
19	G	204	CLA	C2A-CAA-CBA-CGA
19	1	506	CLA	C6-C7-C8-C9
19	1	506	CLA	C6-C7-C8-C10
19	A	838	CLA	C16-C17-C18-C20
19	B	828	CLA	CBD-CGD-O2D-CED
19	4	304	CLA	C4-C3-C5-C6
19	A	833	CLA	C4-C3-C5-C6
19	2	507	CLA	C2-C3-C5-C6
21	1	520	LHG	C11-C12-C13-C14
19	F	302	CLA	O1A-CGA-O2A-C1
19	A	832	CLA	C10-C11-C12-C13
19	K	1002	CLA	C8-C10-C11-C12
19	G	201	CLA	O1D-CGD-O2D-CED
19	4	307	CLA	CBA-CGA-O2A-C1
22	F	305	LMG	C10-C11-C12-C13
22	A	847	LMG	O6-C5-C6-O5
26	B	854	DGD	C2G-C1G-O1G-C1A
26	4	319	DGD	C2B-C1B-O2G-C2G
19	4	308	CLA	C10-C11-C12-C13
19	B	840	CLA	C10-C11-C12-C13
21	B	843	LHG	C34-C35-C36-C37
19	3	313	CLA	C8-C10-C11-C12
19	A	824	CLA	C5-C6-C7-C8
19	B	829	CLA	C8-C10-C11-C12
19	J	1101	CLA	C15-C16-C17-C18
19	A	841	CLA	O1D-CGD-O2D-CED
24	B	847	LMT	O5B-C5B-C6B-O6B
24	B	855	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
22	G	206	LMG	O1-C7-C8-O7
19	A	825	CLA	O1A-CGA-O2A-C1
21	1	517	LHG	C29-C30-C31-C32
21	1	520	LHG	C18-C19-C20-C21
26	4	319	DGD	C5A-C6A-C7A-C8A
21	A	845	LHG	C11-C12-C13-C14
21	A	853	LHG	C33-C34-C35-C36
22	4	322	LMG	C11-C12-C13-C14
19	1	509	CLA	C2-C1-O2A-CGA
19	2	510	CLA	C2-C1-O2A-CGA
19	A	820	CLA	C2-C1-O2A-CGA
19	J	1101	CLA	C2-C1-O2A-CGA
24	2	523	LMT	O5'-C5'-C6'-O6'
24	4	320	LMT	O5B-C5B-C6B-O6B
19	A	817	CLA	C16-C17-C18-C20
19	B	819	CLA	C15-C16-C17-C18
21	1	520	LHG	C12-C13-C14-C15
22	2	519	LMG	C12-C13-C14-C15
22	A	847	LMG	C18-C19-C20-C21
19	B	832	CLA	O1D-CGD-O2D-CED
19	L	303	CLA	O1D-CGD-O2D-CED
19	1	508	CLA	C15-C16-C17-C18
19	A	805	CLA	C10-C11-C12-C13
19	A	827	CLA	C10-C11-C12-C13
24	2	523	LMT	C1-C2-C3-C4
22	B	845	LMG	C12-C13-C14-C15
20	1	514	CHL	C11-C12-C13-C15
22	B	844	LMG	O6-C5-C6-O5
19	A	821	CLA	O1D-CGD-O2D-CED
19	B	831	CLA	O1D-CGD-O2D-CED
20	1	521	CHL	C3-C5-C6-C7
21	A	845	LHG	C16-C17-C18-C19
24	4	320	LMT	C9-C10-C11-C12
19	1	504	CLA	C1A-C2A-CAA-CBA
19	2	504	CLA	C1A-C2A-CAA-CBA
19	2	507	CLA	C1A-C2A-CAA-CBA
19	3	307	CLA	C1A-C2A-CAA-CBA
19	3	308	CLA	C1A-C2A-CAA-CBA
19	3	309	CLA	C1A-C2A-CAA-CBA
19	3	316	CLA	C1A-C2A-CAA-CBA
19	3	317	CLA	C1A-C2A-CAA-CBA
19	4	304	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	4	308	CLA	C1A-C2A-CAA-CBA
19	A	805	CLA	C1A-C2A-CAA-CBA
19	A	806	CLA	C1A-C2A-CAA-CBA
19	A	808	CLA	C1A-C2A-CAA-CBA
19	A	809	CLA	C1A-C2A-CAA-CBA
19	A	814	CLA	C1A-C2A-CAA-CBA
19	A	818	CLA	C1A-C2A-CAA-CBA
19	A	822	CLA	C1A-C2A-CAA-CBA
19	A	834	CLA	C1A-C2A-CAA-CBA
19	A	838	CLA	C1A-C2A-CAA-CBA
19	B	806	CLA	C1A-C2A-CAA-CBA
19	B	817	CLA	C1A-C2A-CAA-CBA
19	B	821	CLA	C1A-C2A-CAA-CBA
19	B	823	CLA	C1A-C2A-CAA-CBA
19	B	824	CLA	C1A-C2A-CAA-CBA
19	B	829	CLA	C1A-C2A-CAA-CBA
19	B	835	CLA	C1A-C2A-CAA-CBA
19	B	837	CLA	C1A-C2A-CAA-CBA
19	G	203	CLA	C1A-C2A-CAA-CBA
19	G	204	CLA	C1A-C2A-CAA-CBA
19	J	1101	CLA	C1A-C2A-CAA-CBA
19	A	830	CLA	O1A-CGA-O2A-C1
21	A	845	LHG	C15-C16-C17-C18
24	G	209	LMT	C4-C5-C6-C7
19	A	839	CLA	C8-C10-C11-C12
21	A	845	LHG	O6-C4-C5-C6
21	2	517	LHG	O9-C7-O7-C5
19	1	516	CLA	C6-C7-C8-C10
19	2	510	CLA	C11-C10-C8-C7
19	4	306	CLA	C12-C13-C15-C16
19	A	813	CLA	C11-C10-C8-C7
19	A	828	CLA	C11-C10-C8-C7
19	A	831	CLA	C6-C7-C8-C10
19	A	834	CLA	C11-C12-C13-C15
19	A	842	CLA	C6-C7-C8-C10
19	B	805	CLA	C11-C10-C8-C7
19	B	818	CLA	C11-C12-C13-C15
19	B	819	CLA	C6-C7-C8-C10
19	B	819	CLA	C11-C10-C8-C7
19	B	822	CLA	C12-C13-C15-C16
19	B	825	CLA	C6-C7-C8-C10
19	B	827	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	B	827	CLA	C12-C13-C15-C16
19	B	828	CLA	C12-C13-C15-C16
19	B	833	CLA	C6-C7-C8-C10
19	B	839	CLA	C6-C7-C8-C10
19	B	839	CLA	C11-C10-C8-C7
19	B	839	CLA	C11-C12-C13-C15
19	F	303	CLA	C11-C10-C8-C7
19	G	201	CLA	C6-C7-C8-C10
19	G	204	CLA	C12-C13-C15-C16
29	B	841	PQN	C21-C22-C23-C25
19	A	808	CLA	C16-C17-C18-C19
19	B	840	CLA	C5-C6-C7-C8
22	G	206	LMG	C16-C17-C18-C19
19	3	313	CLA	C4-C3-C5-C6
19	A	807	CLA	C4-C3-C5-C6
19	3	313	CLA	C2-C3-C5-C6
21	B	843	LHG	C11-C12-C13-C14
19	A	808	CLA	C3-C5-C6-C7
19	B	820	CLA	O1D-CGD-O2D-CED
19	B	837	CLA	C2A-CAA-CBA-CGA
19	L	305	CLA	C2A-CAA-CBA-CGA
19	1	508	CLA	C6-C7-C8-C9
19	4	307	CLA	C11-C10-C8-C9
19	A	803	CLA	C14-C13-C15-C16
19	A	804	CLA	C11-C12-C13-C14
19	A	811	CLA	C6-C7-C8-C9
19	A	813	CLA	C11-C10-C8-C9
19	A	829	CLA	C11-C12-C13-C14
19	A	834	CLA	C6-C7-C8-C9
19	A	854	CLA	C14-C13-C15-C16
19	B	807	CLA	C11-C12-C13-C14
19	B	808	CLA	C11-C12-C13-C14
19	B	819	CLA	C6-C7-C8-C9
19	B	822	CLA	C14-C13-C15-C16
19	B	827	CLA	C11-C10-C8-C9
19	B	827	CLA	C14-C13-C15-C16
19	B	839	CLA	C11-C12-C13-C14
19	2	509	CLA	CBA-CGA-O2A-C1
19	A	838	CLA	CBA-CGA-O2A-C1
19	B	831	CLA	CBA-CGA-O2A-C1
21	2	517	LHG	C7-C8-C9-C10
21	1	517	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
21	B	843	LHG	C4-C5-C6-O8
22	F	305	LMG	C7-C8-C9-O8
22	G	206	LMG	O1-C7-C8-C9
26	B	801	DGD	O1G-C1G-C2G-C3G
19	B	803	CLA	O1D-CGD-O2D-CED
19	B	823	CLA	C5-C6-C7-C8
26	B	854	DGD	C2A-C1A-O1G-C1G
21	A	853	LHG	C11-C12-C13-C14
18	J	1108	BCR	C11-C10-C9-C34
19	B	803	CLA	C8-C10-C11-C12
22	F	304	LMG	C28-C29-C30-C31
19	B	806	CLA	C4-C3-C5-C6
19	A	807	CLA	C2-C3-C5-C6
19	B	806	CLA	C2-C3-C5-C6
19	B	824	CLA	C10-C11-C12-C13
19	B	827	CLA	C8-C10-C11-C12
19	G	204	CLA	C10-C11-C12-C13
29	A	844	PQN	C15-C16-C17-C18
17	3	302	LUT	C7-C8-C9-C19
18	1	503	BCR	C37-C22-C23-C24
26	4	319	DGD	O1B-C1B-O2G-C2G
19	A	809	CLA	C16-C17-C18-C20
26	B	854	DGD	C7A-C8A-C9A-CAA
18	1	503	BCR	C21-C22-C23-C24
19	B	814	CLA	C8-C10-C11-C12
19	A	802	CLA	C10-C11-C12-C13
19	4	307	CLA	O1A-CGA-O2A-C1
19	A	826	CLA	O1D-CGD-O2D-CED
19	G	201	CLA	CBA-CGA-O2A-C1
22	J	1104	LMG	C33-C34-C35-C36
20	4	314	CHL	C2C-C3C-CAC-CBC
22	2	522	LMG	C4-C5-C6-O5
19	B	822	CLA	O2A-C1-C2-C3
21	A	853	LHG	C12-C13-C14-C15
18	2	503	BCR	C10-C11-C12-C13
19	4	315	CLA	C15-C16-C17-C18
19	A	817	CLA	C16-C17-C18-C19
19	A	821	CLA	C13-C15-C16-C17
19	A	807	CLA	C5-C6-C7-C8
19	A	840	CLA	CBA-CGA-O2A-C1
19	B	805	CLA	CBA-CGA-O2A-C1
19	B	814	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B	820	CLA	CBA-CGA-O2A-C1
27	A	801	CL0	CBA-CGA-O2A-C1
19	B	829	CLA	C4-C3-C5-C6
20	1	521	CHL	C2-C3-C5-C6
26	B	854	DGD	C4E-C5E-C6E-O5E
21	A	853	LHG	O7-C5-C6-O8
26	B	801	DGD	O1G-C1G-C2G-O2G
26	B	801	DGD	O2G-C2G-C3G-O3G
22	J	1104	LMG	C29-C28-O8-C9
22	F	305	LMG	C33-C34-C35-C36
19	A	811	CLA	C2A-CAA-CBA-CGA
19	A	829	CLA	C2A-CAA-CBA-CGA
19	4	310	CLA	C3-C5-C6-C7
19	G	201	CLA	C3-C5-C6-C7
27	A	801	CL0	C3-C5-C6-C7
26	4	319	DGD	C4A-C5A-C6A-C7A
21	B	843	LHG	C35-C36-C37-C38
19	G	202	CLA	C2-C1-O2A-CGA
19	A	808	CLA	C16-C17-C18-C20
19	B	819	CLA	C16-C17-C18-C20
19	A	838	CLA	O1A-CGA-O2A-C1
26	B	854	DGD	O1A-C1A-O1G-C1G
19	4	309	CLA	O1D-CGD-O2D-CED
19	A	805	CLA	CBA-CGA-O2A-C1
19	A	812	CLA	CBA-CGA-O2A-C1
19	A	837	CLA	CBA-CGA-O2A-C1
19	J	1101	CLA	CBA-CGA-O2A-C1
19	B	810	CLA	C5-C6-C7-C8
19	A	818	CLA	C11-C10-C8-C9
19	B	829	CLA	C13-C15-C16-C17
21	2	517	LHG	O1-C1-C2-O2
24	2	523	LMT	C2-C1-O1'-C1'
24	B	846	LMT	C2-C1-O1'-C1'
19	2	510	CLA	C11-C10-C8-C9
19	4	306	CLA	C14-C13-C15-C16
19	A	806	CLA	C14-C13-C15-C16
19	A	809	CLA	C14-C13-C15-C16
19	A	833	CLA	C6-C7-C8-C9
19	A	834	CLA	C11-C12-C13-C14
19	A	842	CLA	C6-C7-C8-C9
19	A	842	CLA	C11-C10-C8-C9
19	A	855	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	B	805	CLA	C11-C10-C8-C9
19	B	806	CLA	C14-C13-C15-C16
19	B	810	CLA	C11-C12-C13-C14
19	B	828	CLA	C14-C13-C15-C16
19	B	830	CLA	C11-C12-C13-C14
19	B	839	CLA	C6-C7-C8-C9
19	F	302	CLA	C14-C13-C15-C16
19	F	303	CLA	C11-C10-C8-C9
19	G	201	CLA	C6-C7-C8-C9
19	G	201	CLA	C11-C10-C8-C9
19	G	204	CLA	C14-C13-C15-C16
19	H	1000	CLA	C6-C7-C8-C9
19	A	805	CLA	C8-C10-C11-C12
21	1	517	LHG	C2-C3-O3-P
19	1	511	CLA	C4B-C3B-CAB-CBB
19	1	516	CLA	C4B-C3B-CAB-CBB
19	3	310	CLA	C4B-C3B-CAB-CBB
19	A	810	CLA	C4B-C3B-CAB-CBB
19	G	204	CLA	C4B-C3B-CAB-CBB
19	K	1002	CLA	C4B-C3B-CAB-CBB
21	A	845	LHG	C11-C10-C9-C8
19	4	315	CLA	C16-C17-C18-C19
26	B	801	DGD	C2E-C1E-O5D-C6D
26	J	1106	DGD	C2E-C1E-O5D-C6D
19	A	840	CLA	C5-C6-C7-C8
21	B	843	LHG	C33-C34-C35-C36
26	B	854	DGD	C4A-C5A-C6A-C7A
21	1	520	LHG	O6-C4-C5-C6
19	1	508	CLA	C6-C7-C8-C10
19	3	308	CLA	C6-C7-C8-C10
19	3	313	CLA	C6-C7-C8-C10
19	4	304	CLA	C6-C7-C8-C10
19	4	318	CLA	C12-C13-C15-C16
19	A	802	CLA	C11-C12-C13-C15
19	A	804	CLA	C6-C7-C8-C10
19	A	804	CLA	C11-C10-C8-C7
19	A	804	CLA	C11-C12-C13-C15
19	A	809	CLA	C12-C13-C15-C16
19	A	811	CLA	C6-C7-C8-C10
19	A	821	CLA	C11-C10-C8-C7
19	A	828	CLA	C6-C7-C8-C10
19	A	829	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	A	833	CLA	C6-C7-C8-C10
19	A	834	CLA	C6-C7-C8-C10
19	A	854	CLA	C11-C12-C13-C15
19	A	854	CLA	C12-C13-C15-C16
19	B	804	CLA	C11-C10-C8-C7
19	B	804	CLA	C12-C13-C15-C16
19	B	806	CLA	C12-C13-C15-C16
19	B	807	CLA	C6-C7-C8-C10
19	B	807	CLA	C11-C12-C13-C15
19	B	808	CLA	C6-C7-C8-C10
19	B	808	CLA	C11-C10-C8-C7
19	B	808	CLA	C11-C12-C13-C15
19	B	810	CLA	C11-C12-C13-C15
19	B	829	CLA	C11-C12-C13-C15
19	B	830	CLA	C11-C10-C8-C7
19	B	830	CLA	C11-C12-C13-C15
19	F	302	CLA	C12-C13-C15-C16
19	H	1000	CLA	C6-C7-C8-C10
19	K	1002	CLA	C11-C10-C8-C7
20	1	514	CHL	C11-C10-C8-C7
19	4	310	CLA	C10-C11-C12-C13
19	G	204	CLA	C8-C10-C11-C12
19	B	831	CLA	O1A-CGA-O2A-C1
26	B	854	DGD	C1B-C2B-C3B-C4B
21	A	853	LHG	C35-C36-C37-C38
19	A	807	CLA	C10-C11-C12-C13
24	A	846	LMT	C4'-C5'-C6'-O6'
19	2	511	CLA	C3A-C2A-CAA-CBA
19	3	312	CLA	C3A-C2A-CAA-CBA
19	3	315	CLA	C3A-C2A-CAA-CBA
19	4	318	CLA	C3A-C2A-CAA-CBA
19	A	806	CLA	C4-C3-C5-C6
19	A	821	CLA	C3A-C2A-CAA-CBA
19	A	828	CLA	C3A-C2A-CAA-CBA
19	B	817	CLA	C3A-C2A-CAA-CBA
19	L	303	CLA	C3A-C2A-CAA-CBA
19	L	304	CLA	C3A-C2A-CAA-CBA
20	1	521	CHL	C4-C3-C5-C6
19	A	833	CLA	C2-C3-C5-C6
22	B	845	LMG	C11-C12-C13-C14
19	G	201	CLA	O1A-CGA-O2A-C1
27	A	801	CL0	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	3	308	CLA	C10-C11-C12-C13
21	B	843	LHG	C9-C10-C11-C12
21	A	845	LHG	C26-C27-C28-C29
18	1	503	BCR	C19-C20-C21-C22
23	2	502	XAT	C27-C28-C29-C39
19	A	836	CLA	C4-C3-C5-C6
19	2	509	CLA	O1A-CGA-O2A-C1
19	J	1101	CLA	O1A-CGA-O2A-C1
21	B	843	LHG	C30-C31-C32-C33
18	I	102	BCR	C17-C18-C19-C20
21	A	853	LHG	C8-C7-O7-C5
21	A	845	LHG	C4-C5-C6-O8
22	B	844	LMG	C7-C8-C9-O8
26	B	801	DGD	C1G-C2G-C3G-O3G
21	A	845	LHG	C7-C8-C9-C10
19	A	812	CLA	C6-C7-C8-C10
19	A	839	CLA	C16-C17-C18-C19
19	3	306	CLA	C4C-C3C-CAC-CBC
21	2	517	LHG	C26-C27-C28-C29
26	B	854	DGD	CCB-CDB-CEB-CFB
20	4	316	CHL	C1A-C2A-CAA-CBA
19	A	805	CLA	O1A-CGA-O2A-C1
19	A	855	CLA	C5-C6-C7-C8
19	A	807	CLA	C11-C12-C13-C14
19	A	809	CLA	C16-C17-C18-C19
19	A	812	CLA	C6-C7-C8-C9
20	4	316	CHL	C11-C12-C13-C14
21	1	520	LHG	O6-C4-C5-O7
21	B	842	LHG	C24-C23-O8-C6
17	2	501	LUT	C1-C6-C7-C8
17	3	301	LUT	C1-C6-C7-C8
18	A	848	BCR	C1-C6-C7-C8
18	A	849	BCR	C23-C24-C25-C30
18	A	851	BCR	C23-C24-C25-C30
18	B	851	BCR	C1-C6-C7-C8
18	L	306	BCR	C1-C6-C7-C8
18	L	306	BCR	C23-C24-C25-C30
19	1	511	CLA	C2B-C3B-CAB-CBB
19	A	855	CLA	C15-C16-C17-C18
22	2	522	LMG	O6-C5-C6-O5
26	J	1106	DGD	C2B-C3B-C4B-C5B
19	A	802	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	B	811	CLA	C10-C11-C12-C13
19	B	828	CLA	C8-C10-C11-C12
29	B	841	PQN	C23-C25-C26-C27
24	G	209	LMT	C1-C2-C3-C4
19	B	807	CLA	C16-C17-C18-C19
29	B	841	PQN	C26-C27-C28-C30
22	B	844	LMG	O7-C8-C9-O8
22	B	845	LMG	O1-C7-C8-O7
26	4	319	DGD	O1G-C1G-C2G-O2G
24	B	847	LMT	C3-C4-C5-C6
21	1	520	LHG	C26-C27-C28-C29
21	A	853	LHG	C27-C28-C29-C30
19	B	814	CLA	O1A-CGA-O2A-C1
20	1	514	CHL	C4-C3-C5-C6
18	B	851	BCR	C10-C11-C12-C13
19	H	1000	CLA	C5-C6-C7-C8
19	3	305	CLA	C6-C7-C8-C9
21	B	843	LHG	C24-C23-O8-C6
19	3	313	CLA	C6-C7-C8-C9
19	A	804	CLA	C6-C7-C8-C9
19	B	812	CLA	C6-C7-C8-C9
19	B	833	CLA	C6-C7-C8-C9
19	L	304	CLA	C6-C7-C8-C9
19	G	204	CLA	C16-C17-C18-C20
19	A	817	CLA	C3-C5-C6-C7
22	A	847	LMG	C2-C1-O1-C7
19	A	837	CLA	O1A-CGA-O2A-C1
18	1	503	BCR	C17-C18-C19-C20
19	A	813	CLA	C15-C16-C17-C18
19	1	513	CLA	C8-C10-C11-C12
18	F	306	BCR	C13-C14-C15-C16
20	1	514	CHL	C2-C3-C5-C6
21	1	517	LHG	C30-C31-C32-C33
19	A	840	CLA	O1A-CGA-O2A-C1
19	B	828	CLA	O1D-CGD-O2D-CED
22	J	1104	LMG	O10-C28-O8-C9
19	A	833	CLA	C3-C5-C6-C7
19	1	513	CLA	CBA-CGA-O2A-C1
19	A	804	CLA	CBA-CGA-O2A-C1
19	B	838	CLA	CBA-CGA-O2A-C1
21	A	853	LHG	O6-C4-C5-C6
21	B	842	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
19	A	823	CLA	C5-C6-C7-C8
19	A	829	CLA	C10-C11-C12-C13
18	3	304	BCR	C7-C8-C9-C34
19	A	806	CLA	C11-C12-C13-C15
19	A	807	CLA	C6-C7-C8-C10
19	A	809	CLA	C6-C7-C8-C10
19	A	819	CLA	C11-C12-C13-C15
19	B	812	CLA	C6-C7-C8-C10
19	B	817	CLA	C6-C7-C8-C10
19	B	822	CLA	C11-C12-C13-C15
19	B	825	CLA	C11-C12-C13-C15
19	B	825	CLA	C12-C13-C15-C16
19	F	302	CLA	C5-C6-C7-C8
18	G	205	BCR	C11-C12-C13-C14
19	B	836	CLA	CBA-CGA-O2A-C1
19	A	804	CLA	O1A-CGA-O2A-C1
19	B	805	CLA	O1A-CGA-O2A-C1
19	B	820	CLA	O1A-CGA-O2A-C1
22	G	206	LMG	C8-C7-O1-C1
26	J	1106	DGD	C5D-C6D-O5D-C1E
21	A	853	LHG	C23-C24-C25-C26
19	A	822	CLA	C5-C6-C7-C8
19	A	855	CLA	C2A-CAA-CBA-CGA
19	B	808	CLA	C2A-CAA-CBA-CGA
19	A	805	CLA	C4-C3-C5-C6
19	A	812	CLA	O1A-CGA-O2A-C1
19	B	840	CLA	C2-C3-C5-C6
22	A	847	LMG	C31-C32-C33-C34
22	J	1104	LMG	C9-C8-O7-C10
22	1	518	LMG	O7-C10-C11-C12
19	A	829	CLA	C5-C6-C7-C8
18	3	303	BCR	C19-C20-C21-C22
18	A	848	BCR	C19-C20-C21-C22
18	B	850	BCR	C9-C10-C11-C12
18	I	101	BCR	C19-C20-C21-C22
19	4	315	CLA	C16-C17-C18-C20
19	A	807	CLA	C11-C12-C13-C15
19	A	828	CLA	C16-C17-C18-C20
19	A	805	CLA	C15-C16-C17-C18
26	4	319	DGD	C2B-C3B-C4B-C5B
24	J	1107	LMT	C5'-C4'-O1B-C1B
19	4	315	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	A	839	CLA	C16-C17-C18-C20
19	B	819	CLA	C16-C17-C18-C19
19	2	514	CLA	O1D-CGD-O2D-CED
21	A	853	LHG	C24-C25-C26-C27
19	B	836	CLA	O1A-CGA-O2A-C1
24	G	209	LMT	C2B-C1B-O1B-C4'
19	2	510	CLA	C10-C11-C12-C13
19	B	811	CLA	C15-C16-C17-C18
19	A	825	CLA	C4-C3-C5-C6
19	A	803	CLA	C2A-CAA-CBA-CGA
19	B	831	CLA	C2A-CAA-CBA-CGA
24	G	208	LMT	C4'-C5'-C6'-O6'
22	A	847	LMG	O1-C7-C8-O7
19	A	805	CLA	C11-C12-C13-C14
19	A	819	CLA	C11-C12-C13-C14
19	A	825	CLA	C11-C12-C13-C14
19	A	854	CLA	C11-C12-C13-C14
19	B	817	CLA	C6-C7-C8-C9
19	B	818	CLA	C14-C13-C15-C16
19	B	822	CLA	C6-C7-C8-C9
24	B	846	LMT	C3-C4-C5-C6
26	4	319	DGD	C7A-C8A-C9A-CAA
21	A	845	LHG	C14-C15-C16-C17
24	B	847	LMT	C2-C3-C4-C5
22	F	304	LMG	C15-C16-C17-C18
19	L	304	CLA	C10-C11-C12-C13
19	B	804	CLA	C8-C10-C11-C12
19	1	516	CLA	C2-C1-O2A-CGA
19	B	833	CLA	C2-C1-O2A-CGA
19	F	303	CLA	C2-C1-O2A-CGA
19	L	301	CLA	C2-C1-O2A-CGA
19	A	833	CLA	CBA-CGA-O2A-C1
19	A	827	CLA	C16-C17-C18-C20
29	B	841	PQN	C26-C27-C28-C29
19	A	834	CLA	C10-C11-C12-C13
19	A	823	CLA	C4-C3-C5-C6
19	B	815	CLA	C4-C3-C5-C6
21	A	853	LHG	O9-C7-O7-C5
19	B	825	CLA	C10-C11-C12-C13
19	A	825	CLA	C16-C17-C18-C19
19	B	818	CLA	C16-C17-C18-C20
19	B	823	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
21	A	853	LHG	C17-C18-C19-C20
19	1	513	CLA	O1A-CGA-O2A-C1
21	B	843	LHG	O10-C23-O8-C6
21	B	843	LHG	C26-C27-C28-C29
21	2	517	LHG	C28-C29-C30-C31
19	B	828	CLA	C13-C15-C16-C17
22	4	322	LMG	C13-C14-C15-C16
19	3	313	CLA	C11-C12-C13-C15
19	A	811	CLA	C16-C17-C18-C20
19	B	818	CLA	C16-C17-C18-C19
19	B	821	CLA	O1A-CGA-O2A-C1
19	3	308	CLA	C3-C5-C6-C7
18	B	852	BCR	C36-C18-C19-C20
21	B	843	LHG	C28-C29-C30-C31
19	1	509	CLA	C1A-C2A-CAA-CBA
19	1	511	CLA	C1A-C2A-CAA-CBA
19	3	305	CLA	C4B-C3B-CAB-CBB
19	3	311	CLA	C4B-C3B-CAB-CBB
19	4	318	CLA	C1A-C2A-CAA-CBA
19	A	804	CLA	C4B-C3B-CAB-CBB
19	A	820	CLA	C4B-C3B-CAB-CBB
19	A	823	CLA	C1A-C2A-CAA-CBA
19	A	824	CLA	C1A-C2A-CAA-CBA
19	A	841	CLA	C4B-C3B-CAB-CBB
19	B	805	CLA	C4B-C3B-CAB-CBB
19	B	813	CLA	C1A-C2A-CAA-CBA
19	B	814	CLA	C1A-C2A-CAA-CBA
19	B	818	CLA	C4B-C3B-CAB-CBB
19	B	819	CLA	C1A-C2A-CAA-CBA
19	B	820	CLA	C4B-C3B-CAB-CBB
19	B	821	CLA	C4B-C3B-CAB-CBB
19	B	838	CLA	C4B-C3B-CAB-CBB
19	F	302	CLA	C1A-C2A-CAA-CBA
19	A	825	CLA	C10-C11-C12-C13
19	J	1101	CLA	C2C-C3C-CAC-CBC
19	B	838	CLA	O1A-CGA-O2A-C1
19	1	510	CLA	C2C-C3C-CAC-CBC
22	2	519	LMG	C13-C14-C15-C16
19	A	836	CLA	C2-C3-C5-C6
19	1	513	CLA	C11-C12-C13-C15
19	4	308	CLA	C11-C10-C8-C7
19	4	315	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	A	802	CLA	C11-C10-C8-C7
19	A	805	CLA	C11-C10-C8-C7
19	A	813	CLA	C6-C7-C8-C10
19	A	830	CLA	C11-C10-C8-C7
19	A	839	CLA	C11-C12-C13-C15
19	A	841	CLA	C11-C10-C8-C7
19	B	818	CLA	C11-C10-C8-C7
19	B	820	CLA	C12-C13-C15-C16
19	B	827	CLA	C6-C7-C8-C10
19	B	831	CLA	C6-C7-C8-C10
19	J	1101	CLA	C11-C12-C13-C15
29	B	841	PQN	C16-C17-C18-C20
29	B	841	PQN	C22-C23-C25-C26
19	2	504	CLA	C11-C12-C13-C14
19	A	806	CLA	C16-C17-C18-C19
19	B	823	CLA	C6-C7-C8-C10
22	G	206	LMG	C29-C30-C31-C32
19	A	833	CLA	O1A-CGA-O2A-C1
19	B	811	CLA	C13-C15-C16-C17
19	L	305	CLA	C3A-C2A-CAA-CBA
19	B	820	CLA	C16-C17-C18-C19
19	B	820	CLA	C16-C17-C18-C20
21	A	853	LHG	O6-C4-C5-O7
21	B	842	LHG	O6-C4-C5-O7
19	1	513	CLA	C11-C12-C13-C14
19	A	802	CLA	C11-C12-C13-C14
19	A	807	CLA	C6-C7-C8-C9
19	B	822	CLA	C11-C12-C13-C14
19	B	827	CLA	C6-C7-C8-C9
29	B	841	PQN	C21-C22-C23-C24
24	J	1107	LMT	C2-C1-O1'-C1'
18	B	802	BCR	C9-C10-C11-C12
18	F	306	BCR	C19-C20-C21-C22
19	B	805	CLA	C5-C6-C7-C8
19	B	840	CLA	C15-C16-C17-C18
19	4	304	CLA	C3-C5-C6-C7
24	2	523	LMT	C3-C4-C5-C6
19	A	827	CLA	C8-C10-C11-C12
21	1	517	LHG	O7-C5-C6-O8
21	A	845	LHG	O7-C5-C6-O8
21	B	843	LHG	O7-C5-C6-O8
22	1	518	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
22	2	519	LMG	O7-C8-C9-O8
22	F	305	LMG	O7-C8-C9-O8
19	A	802	CLA	C5-C6-C7-C8
19	B	812	CLA	C5-C6-C7-C8
19	B	827	CLA	C10-C11-C12-C13
22	1	518	LMG	C7-C8-C9-O8
22	2	519	LMG	C7-C8-C9-O8
22	B	845	LMG	O1-C7-C8-C9
27	A	801	CL0	CAA-CBA-CGA-O2A
19	4	304	CLA	C2-C3-C5-C6
19	A	823	CLA	C2-C3-C5-C6
22	B	844	LMG	C12-C13-C14-C15
19	3	311	CLA	CAD-CBD-CGD-O2D
19	4	312	CLA	CAD-CBD-CGD-O2D
19	B	814	CLA	CAD-CBD-CGD-O2D
19	B	835	CLA	CAD-CBD-CGD-O2D
19	3	309	CLA	C6-C7-C8-C9
20	1	514	CHL	C11-C12-C13-C14
19	A	820	CLA	C2A-CAA-CBA-CGA
19	1	508	CLA	C5-C6-C7-C8
17	4	302	LUT	C29-C30-C31-C32
18	2	503	BCR	C15-C16-C17-C18
18	A	851	BCR	C9-C10-C11-C12
18	A	852	BCR	C19-C20-C21-C22
18	B	849	BCR	C19-C20-C21-C22
18	B	852	BCR	C13-C14-C15-C16
19	3	311	CLA	CAD-CBD-CGD-O1D
19	4	307	CLA	CHA-CBD-CGD-O1D
19	4	312	CLA	CAD-CBD-CGD-O1D
19	A	816	CLA	CHA-CBD-CGD-O1D
19	A	816	CLA	CHA-CBD-CGD-O2D
19	B	814	CLA	CAD-CBD-CGD-O1D
19	B	835	CLA	CAD-CBD-CGD-O1D
19	J	1105	CLA	CAD-CBD-CGD-O1D
21	1	517	LHG	C3-O3-P-O6
21	1	517	LHG	C4-O6-P-O5
21	1	520	LHG	C3-O3-P-O4
21	1	520	LHG	C3-O3-P-O5
21	2	517	LHG	C4-O6-P-O5
21	A	845	LHG	C3-O3-P-O5
21	A	845	LHG	C4-O6-P-O4
21	A	853	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
21	A	853	LHG	C4-O6-P-O5
21	B	843	LHG	C3-O3-P-O5
19	A	838	CLA	C5-C6-C7-C8
19	A	810	CLA	C2B-C3B-CAB-CBB
19	A	832	CLA	C2B-C3B-CAB-CBB
19	A	841	CLA	C2B-C3B-CAB-CBB
19	B	805	CLA	C2B-C3B-CAB-CBB
19	B	818	CLA	C2B-C3B-CAB-CBB
19	B	823	CLA	C2B-C3B-CAB-CBB
19	B	838	CLA	C2B-C3B-CAB-CBB
22	2	518	LMG	O7-C10-C11-C12
19	A	805	CLA	C2-C3-C5-C6
18	A	849	BCR	C11-C12-C13-C35
23	2	502	XAT	C27-C28-C29-C30
21	A	845	LHG	C17-C18-C19-C20
22	1	518	LMG	C10-C11-C12-C13
19	A	818	CLA	C11-C10-C8-C7
22	2	519	LMG	C7-C8-O7-C10
22	2	519	LMG	C9-C8-O7-C10
22	4	322	LMG	C9-C8-O7-C10
22	G	210	LMG	C9-C8-O7-C10
26	B	801	DGD	C1G-C2G-O2G-C1B
18	2	503	BCR	C18-C19-C20-C21
18	B	851	BCR	C18-C19-C20-C21
18	K	1005	BCR	C18-C19-C20-C21
19	G	201	CLA	C15-C16-C17-C18
19	A	825	CLA	C2-C3-C5-C6
19	B	829	CLA	C2-C3-C5-C6
18	A	856	BCR	C13-C14-C15-C16
19	A	806	CLA	C16-C17-C18-C20
19	B	835	CLA	C6-C7-C8-C9
19	G	204	CLA	C16-C17-C18-C19
24	2	523	LMT	O1'-C1-C2-C3
19	1	513	CLA	C11-C10-C8-C9
19	3	308	CLA	C6-C7-C8-C9
19	A	804	CLA	C14-C13-C15-C16
19	A	805	CLA	C11-C10-C8-C9
19	A	806	CLA	C11-C12-C13-C14
19	A	819	CLA	C6-C7-C8-C9
19	A	824	CLA	C14-C13-C15-C16
19	A	830	CLA	C11-C10-C8-C9
19	A	838	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	A	839	CLA	C14-C13-C15-C16
19	A	855	CLA	C11-C12-C13-C14
19	B	804	CLA	C11-C10-C8-C9
19	B	815	CLA	C11-C10-C8-C9
19	B	824	CLA	C11-C12-C13-C14
19	B	825	CLA	C11-C12-C13-C14
19	B	830	CLA	C11-C10-C8-C9
19	G	204	CLA	C11-C12-C13-C14
19	K	1002	CLA	C11-C10-C8-C9
20	2	526	CHL	C11-C12-C13-C14
19	1	513	CLA	C11-C10-C8-C7
19	A	802	CLA	C6-C7-C8-C10
19	A	805	CLA	C11-C12-C13-C15
19	A	840	CLA	C6-C7-C8-C10
19	B	831	CLA	C11-C10-C8-C7
19	K	1002	CLA	C6-C7-C8-C10
18	A	852	BCR	C11-C10-C9-C8
18	J	1108	BCR	C11-C10-C9-C8
19	J	1101	CLA	C4C-C3C-CAC-CBC
22	G	210	LMG	C2-C1-O1-C7
19	3	309	CLA	C6-C7-C8-C10
21	1	517	LHG	C13-C14-C15-C16
24	G	209	LMT	O5B-C1B-O1B-C4'
22	4	322	LMG	C4-C5-C6-O5
19	A	831	CLA	C13-C15-C16-C17
18	I	102	BCR	C19-C20-C21-C22
22	2	519	LMG	O7-C10-C11-C12
19	A	832	CLA	C8-C10-C11-C12
20	1	514	CHL	C5-C6-C7-C8
19	A	831	CLA	C2-C1-O2A-CGA
19	B	830	CLA	C2-C1-O2A-CGA
19	B	825	CLA	C4-C3-C5-C6
19	A	828	CLA	C16-C17-C18-C19
21	2	517	LHG	O8-C23-C24-C25
21	A	853	LHG	C4-C5-C6-O8
24	4	320	LMT	C1-C2-C3-C4
19	B	823	CLA	CAA-CBA-CGA-O2A
19	B	808	CLA	C13-C15-C16-C17
17	3	302	LUT	C7-C8-C9-C10
22	2	518	LMG	O9-C10-C11-C12
19	1	513	CLA	C10-C11-C12-C13
19	1	507	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	2	509	CLA	C2A-CAA-CBA-CGA
19	A	807	CLA	C2A-CAA-CBA-CGA
19	A	824	CLA	C2A-CAA-CBA-CGA
19	B	814	CLA	C2A-CAA-CBA-CGA
19	B	827	CLA	C4-C3-C5-C6
19	G	202	CLA	C4-C3-C5-C6
19	G	201	CLA	C16-C17-C18-C20
21	A	853	LHG	C10-C11-C12-C13
19	A	840	CLA	C6-C7-C8-C9
19	A	841	CLA	C11-C10-C8-C9
19	J	1101	CLA	C11-C12-C13-C14
29	B	841	PQN	C16-C17-C18-C19
29	B	841	PQN	C24-C23-C25-C26
19	1	506	CLA	C4B-C3B-CAB-CBB
19	A	823	CLA	C4B-C3B-CAB-CBB
19	A	826	CLA	C4B-C3B-CAB-CBB
19	1	515	CLA	CAA-CBA-CGA-O2A
19	B	833	CLA	C3-C5-C6-C7
19	A	803	CLA	C10-C11-C12-C13
26	J	1106	DGD	C6A-C7A-C8A-C9A
19	1	507	CLA	C16-C17-C18-C20
19	B	833	CLA	C11-C12-C13-C14
19	A	814	CLA	C10-C11-C12-C13
19	G	204	CLA	C15-C16-C17-C18
19	1	513	CLA	C4-C3-C5-C6
19	B	814	CLA	C4-C3-C5-C6
19	B	815	CLA	C2-C3-C5-C6
19	B	825	CLA	C2-C3-C5-C6
18	A	856	BCR	C19-C20-C21-C22
19	A	827	CLA	C16-C17-C18-C19
19	A	805	CLA	C6-C7-C8-C10
19	A	821	CLA	C12-C13-C15-C16
19	B	807	CLA	C12-C13-C15-C16
19	B	810	CLA	C12-C13-C15-C16
19	B	814	CLA	C11-C12-C13-C15
19	B	824	CLA	C11-C12-C13-C15
19	A	813	CLA	C3-C5-C6-C7
24	B	855	LMT	C3-C4-C5-C6
19	A	811	CLA	C16-C17-C18-C19
19	B	835	CLA	C6-C7-C8-C10
26	J	1106	DGD	C3B-C4B-C5B-C6B
19	A	804	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	A	819	CLA	C4-C3-C5-C6
19	A	830	CLA	C3A-C2A-CAA-CBA
19	B	819	CLA	C3A-C2A-CAA-CBA
19	B	820	CLA	C4-C3-C5-C6
19	B	826	CLA	C3A-C2A-CAA-CBA
27	A	801	CL0	C3A-C2A-CAA-CBA
19	B	840	CLA	CAA-CBA-CGA-O2A
18	3	304	BCR	C16-C17-C18-C36
18	A	850	BCR	C16-C17-C18-C36
18	A	852	BCR	C11-C10-C9-C34
18	A	852	BCR	C16-C17-C18-C36
18	B	802	BCR	C16-C17-C18-C36
18	B	849	BCR	C35-C13-C14-C15
18	B	849	BCR	C16-C17-C18-C36
18	B	850	BCR	C11-C10-C9-C34
18	B	851	BCR	C11-C10-C9-C34
18	F	306	BCR	C16-C17-C18-C36
18	G	205	BCR	C16-C17-C18-C36
18	I	101	BCR	C35-C13-C14-C15
18	L	302	BCR	C16-C17-C18-C36
18	L	302	BCR	C20-C21-C22-C37
19	B	803	CLA	C5-C6-C7-C8
19	2	507	CLA	C2-C1-O2A-CGA
19	4	308	CLA	C2-C1-O2A-CGA
19	A	811	CLA	C2-C1-O2A-CGA
19	B	828	CLA	C2-C1-O2A-CGA
19	1	508	CLA	C13-C15-C16-C17
18	A	848	BCR	C36-C18-C19-C20
18	G	205	BCR	C36-C18-C19-C20
21	2	517	LHG	C2-C3-O3-P
19	1	515	CLA	CAA-CBA-CGA-O1A
21	1	517	LHG	C32-C33-C34-C35
19	K	1001	CLA	CAA-CBA-CGA-O1A
19	2	506	CLA	C16-C17-C18-C19
19	A	834	CLA	C2A-CAA-CBA-CGA
26	B	854	DGD	O1G-C1G-C2G-C3G
26	B	854	DGD	O6D-C5D-C6D-O5D
19	K	1001	CLA	CAA-CBA-CGA-O2A
19	1	516	CLA	O1A-CGA-O2A-C1
19	A	805	CLA	C6-C7-C8-C9
19	A	808	CLA	C6-C7-C8-C9
19	A	808	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
19	A	813	CLA	C6-C7-C8-C9
19	A	822	CLA	C11-C10-C8-C9
19	A	827	CLA	C11-C10-C8-C9
19	A	833	CLA	C14-C13-C15-C16
19	A	834	CLA	C11-C10-C8-C9
19	A	854	CLA	C6-C7-C8-C9
19	B	805	CLA	C14-C13-C15-C16
19	B	811	CLA	C6-C7-C8-C9
19	B	811	CLA	C11-C12-C13-C14
19	B	824	CLA	C11-C10-C8-C9
19	B	828	CLA	C11-C12-C13-C14
19	B	829	CLA	C6-C7-C8-C9
29	A	844	PQN	C21-C22-C23-C24
22	F	305	LMG	C7-C8-O7-C10
26	4	319	DGD	C3G-C2G-O2G-C1B
26	B	801	DGD	C3G-C2G-O2G-C1B
26	G	207	DGD	C1G-C2G-O2G-C1B
26	J	1106	DGD	C1G-C2G-O2G-C1B
20	1	512	CHL	C1A-C2A-CAA-CBA
21	B	843	LHG	C29-C30-C31-C32
26	J	1106	DGD	C1B-C2B-C3B-C4B
19	1	507	CLA	C16-C17-C18-C19
19	B	814	CLA	C13-C15-C16-C17
19	1	513	CLA	C2-C3-C5-C6
19	B	827	CLA	C2-C3-C5-C6
22	G	206	LMG	C13-C14-C15-C16
18	3	304	BCR	C16-C17-C18-C19
18	A	850	BCR	C16-C17-C18-C19
18	A	852	BCR	C16-C17-C18-C19
18	B	802	BCR	C16-C17-C18-C19
18	B	849	BCR	C12-C13-C14-C15
18	B	849	BCR	C16-C17-C18-C19
18	B	850	BCR	C11-C10-C9-C8
18	F	306	BCR	C16-C17-C18-C19
18	G	205	BCR	C16-C17-C18-C19
18	I	101	BCR	C12-C13-C14-C15
18	L	302	BCR	C16-C17-C18-C19
18	L	302	BCR	C20-C21-C22-C23
19	3	315	CLA	C1A-C2A-CAA-CBA
19	A	828	CLA	C1A-C2A-CAA-CBA
19	B	826	CLA	C1A-C2A-CAA-CBA
19	K	1001	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	L	304	CLA	C1A-C2A-CAA-CBA
19	A	835	CLA	C6-C7-C8-C10
19	B	820	CLA	C15-C16-C17-C18
17	2	501	LUT	C5-C6-C7-C8
17	3	301	LUT	C5-C6-C7-C8
17	3	302	LUT	C1-C6-C7-C8
18	A	848	BCR	C5-C6-C7-C8
18	A	849	BCR	C23-C24-C25-C26
18	A	851	BCR	C1-C6-C7-C8
18	A	851	BCR	C23-C24-C25-C26
18	B	850	BCR	C1-C6-C7-C8
18	B	851	BCR	C5-C6-C7-C8
18	B	851	BCR	C23-C24-C25-C30
18	B	852	BCR	C23-C24-C25-C30
18	B	853	BCR	C5-C6-C7-C8
18	K	1005	BCR	C1-C6-C7-C8
18	L	306	BCR	C5-C6-C7-C8
19	3	305	CLA	C2B-C3B-CAB-CBB
19	3	310	CLA	C2B-C3B-CAB-CBB
19	3	311	CLA	C2B-C3B-CAB-CBB
19	A	804	CLA	C2B-C3B-CAB-CBB
19	A	816	CLA	C2B-C3B-CAB-CBB
19	A	820	CLA	C2B-C3B-CAB-CBB
19	A	823	CLA	C2B-C3B-CAB-CBB
19	A	826	CLA	C2B-C3B-CAB-CBB
19	A	834	CLA	C2B-C3B-CAB-CBB
19	B	820	CLA	C2B-C3B-CAB-CBB
19	B	821	CLA	C2B-C3B-CAB-CBB
20	2	515	CHL	CAA-CBA-CGA-O2A
22	A	847	LMG	C15-C16-C17-C18
19	4	306	CLA	C16-C17-C18-C20
19	B	828	CLA	C16-C17-C18-C19
19	B	809	CLA	C4-C3-C5-C6
19	A	819	CLA	C2-C3-C5-C6
19	B	814	CLA	C2-C3-C5-C6
19	A	834	CLA	C15-C16-C17-C18
22	A	847	LMG	C14-C15-C16-C17
19	1	507	CLA	C11-C12-C13-C15
19	1	508	CLA	C12-C13-C15-C16
19	A	806	CLA	C6-C7-C8-C10
19	A	814	CLA	C12-C13-C15-C16
19	A	819	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	A	824	CLA	C11-C12-C13-C15
19	A	834	CLA	C12-C13-C15-C16
19	A	854	CLA	C6-C7-C8-C10
19	B	803	CLA	C11-C12-C13-C15
19	B	829	CLA	C6-C7-C8-C10
19	B	829	CLA	C11-C10-C8-C7
19	B	840	CLA	C11-C12-C13-C15
19	F	303	CLA	C11-C12-C13-C15
20	2	526	CHL	C6-C7-C8-C10
19	A	805	CLA	C5-C6-C7-C8
19	A	812	CLA	C4-C3-C5-C6
19	A	822	CLA	C4-C3-C5-C6
19	B	816	CLA	C4-C3-C5-C6
19	A	830	CLA	C10-C11-C12-C13
19	A	837	CLA	O1D-CGD-O2D-CED
19	A	802	CLA	C15-C16-C17-C18
19	B	831	CLA	C11-C12-C13-C14
24	2	523	LMT	C11-C10-C9-C8
20	2	515	CHL	CAA-CBA-CGA-O1A
19	A	831	CLA	C11-C12-C13-C14
19	A	833	CLA	C11-C12-C13-C14
19	A	832	CLA	C16-C17-C18-C19
19	A	828	CLA	C4-C3-C5-C6
19	A	829	CLA	C4-C3-C5-C6
19	A	832	CLA	C4-C3-C5-C6
19	F	303	CLA	C10-C11-C12-C13
19	A	806	CLA	C2-C3-C5-C6
20	2	516	CHL	C2-C3-C5-C6
19	B	824	CLA	C5-C6-C7-C8
19	2	506	CLA	C16-C17-C18-C20
19	B	816	CLA	CBA-CGA-O2A-C1
26	4	319	DGD	O1G-C1A-C2A-C3A
19	4	307	CLA	C2A-CAA-CBA-CGA
19	A	854	CLA	C2A-CAA-CBA-CGA
26	G	207	DGD	C3A-C4A-C5A-C6A
19	B	808	CLA	C16-C17-C18-C20
19	A	830	CLA	C15-C16-C17-C18
19	4	307	CLA	C4-C3-C5-C6
19	A	813	CLA	C4-C3-C5-C6
19	4	311	CLA	CAA-CBA-CGA-O2A
19	A	829	CLA	CAA-CBA-CGA-O2A
19	B	803	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
19	B	810	CLA	C8-C10-C11-C12
19	2	505	CLA	C4B-C3B-CAB-CBB
19	4	305	CLA	C4B-C3B-CAB-CBB
19	A	816	CLA	C4B-C3B-CAB-CBB
19	A	834	CLA	C4B-C3B-CAB-CBB
19	B	816	CLA	O1A-CGA-O2A-C1
22	G	210	LMG	C4-C5-C6-O5
19	1	516	CLA	CBA-CGA-O2A-C1
19	3	308	CLA	CAA-CBA-CGA-O2A
26	J	1106	DGD	C7A-C8A-C9A-CAA
19	A	837	CLA	CBD-CGD-O2D-CED
22	2	518	LMG	C4-C5-C6-O5
20	1	521	CHL	CHA-CBD-CGD-O1D
20	1	521	CHL	CHA-CBD-CGD-O2D
20	2	512	CHL	CHA-CBD-CGD-O2D
20	4	313	CHL	CHA-CBD-CGD-O1D
20	4	313	CHL	CHA-CBD-CGD-O2D
19	2	506	CLA	C8-C10-C11-C12
19	B	819	CLA	CAA-CBA-CGA-O2A
26	4	319	DGD	O2G-C2G-C3G-O3G
19	B	826	CLA	C8-C10-C11-C12
19	A	829	CLA	C2-C3-C5-C6
19	B	809	CLA	C2-C3-C5-C6
22	G	210	LMG	O6-C1-O1-C7
21	B	842	LHG	O10-C23-O8-C6
26	B	801	DGD	C3A-C4A-C5A-C6A
20	2	513	CHL	C2-C1-O2A-CGA
19	2	508	CLA	C5-C6-C7-C8
21	1	520	LHG	C25-C26-C27-C28
19	1	504	CLA	C6-C7-C8-C9
19	1	508	CLA	C11-C10-C8-C9
19	1	513	CLA	C6-C7-C8-C9
19	4	315	CLA	C11-C12-C13-C14
19	A	808	CLA	C11-C12-C13-C14
19	A	825	CLA	C11-C10-C8-C9
19	A	829	CLA	C14-C13-C15-C16
19	A	840	CLA	C11-C10-C8-C9
20	2	526	CHL	C5-C6-C7-C8
22	2	519	LMG	C8-C7-O1-C1
22	4	322	LMG	C8-C7-O1-C1
19	2	504	CLA	C2A-CAA-CBA-CGA
19	A	830	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
19	2	507	CLA	C5-C6-C7-C8
19	1	508	CLA	C3A-C2A-CAA-CBA
19	2	514	CLA	C3A-C2A-CAA-CBA
19	A	829	CLA	C3A-C2A-CAA-CBA
26	B	801	DGD	O1G-C1A-C2A-C3A
19	B	840	CLA	C3-C5-C6-C7
19	B	816	CLA	C6-C7-C8-C9
19	3	313	CLA	CAA-CBA-CGA-O2A
20	2	526	CHL	O2A-C1-C2-C3
22	F	305	LMG	C9-C8-O7-C10
26	G	207	DGD	C3G-C2G-O2G-C1B
26	G	207	DGD	O6D-C5D-C6D-O5D
24	B	846	LMT	C1-C2-C3-C4
18	B	851	BCR	C11-C10-C9-C8
19	A	827	CLA	CBA-CGA-O2A-C1
26	4	319	DGD	C1G-C2G-C3G-O3G
22	F	304	LMG	C12-C13-C14-C15
19	A	830	CLA	C4-C3-C5-C6
19	B	830	CLA	C4-C3-C5-C6
19	B	838	CLA	C2A-CAA-CBA-CGA
19	A	828	CLA	CAA-CBA-CGA-O2A
19	G	202	CLA	C2-C3-C5-C6
17	3	302	LUT	C29-C30-C31-C32
17	J	1109	LUT	C33-C34-C35-C15
19	A	835	CLA	C6-C7-C8-C9
19	B	808	CLA	C16-C17-C18-C19
19	2	504	CLA	C10-C11-C12-C13
19	B	819	CLA	CBA-CGA-O2A-C1
21	A	845	LHG	C19-C20-C21-C22
19	A	802	CLA	C6-C7-C8-C9
19	B	804	CLA	C11-C12-C13-C14
19	B	815	CLA	C11-C12-C13-C14
19	K	1002	CLA	C6-C7-C8-C9
20	2	526	CHL	C6-C7-C8-C9
29	B	841	PQN	C19-C18-C20-C21
18	3	304	BCR	C7-C8-C9-C10
19	B	836	CLA	C5-C6-C7-C8
21	A	853	LHG	O8-C23-C24-C25
19	2	507	CLA	C16-C17-C18-C19
19	4	308	CLA	C11-C12-C13-C15
19	4	315	CLA	C12-C13-C15-C16
19	A	805	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	A	806	CLA	C11-C10-C8-C7
19	A	808	CLA	C11-C12-C13-C15
19	A	817	CLA	C12-C13-C15-C16
19	A	825	CLA	C11-C10-C8-C7
19	A	829	CLA	C12-C13-C15-C16
19	A	831	CLA	C11-C12-C13-C15
19	A	832	CLA	C11-C12-C13-C15
19	A	833	CLA	C11-C12-C13-C15
19	A	840	CLA	C11-C10-C8-C7
19	B	805	CLA	C6-C7-C8-C10
19	B	812	CLA	C11-C10-C8-C7
19	B	827	CLA	C11-C12-C13-C15
20	2	526	CHL	C12-C13-C15-C16
20	2	516	CHL	C3-C5-C6-C7
17	1	502	LUT	C1-C6-C7-C8
17	3	302	LUT	C5-C6-C7-C8
18	A	851	BCR	C5-C6-C7-C8
18	B	850	BCR	C5-C6-C7-C8
18	B	851	BCR	C23-C24-C25-C26
18	B	852	BCR	C23-C24-C25-C26
18	F	306	BCR	C23-C24-C25-C26
18	F	306	BCR	C23-C24-C25-C30
18	G	205	BCR	C23-C24-C25-C30
18	K	1005	BCR	C5-C6-C7-C8
19	1	516	CLA	C2B-C3B-CAB-CBB
19	3	309	CLA	C2B-C3B-CAB-CBB
19	G	204	CLA	C2B-C3B-CAB-CBB
19	K	1002	CLA	C2B-C3B-CAB-CBB
19	L	303	CLA	C2B-C3B-CAB-CBB
22	G	210	LMG	O8-C28-C29-C30
19	A	812	CLA	C2-C1-O2A-CGA
19	B	825	CLA	C2-C1-O2A-CGA
19	B	829	CLA	C2-C1-O2A-CGA
21	B	843	LHG	C13-C14-C15-C16
19	1	508	CLA	C10-C11-C12-C13
19	A	824	CLA	C15-C16-C17-C18
19	F	302	CLA	C4-C3-C5-C6
20	2	516	CHL	C4-C3-C5-C6
19	F	302	CLA	C3-C5-C6-C7
19	A	804	CLA	C2-C3-C5-C6
19	F	302	CLA	C2-C3-C5-C6
20	4	314	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	A	827	CLA	CAA-CBA-CGA-O2A
19	B	831	CLA	C11-C12-C13-C15
22	J	1104	LMG	C32-C33-C34-C35
19	B	823	CLA	C4-C3-C5-C6
19	G	201	CLA	CAA-CBA-CGA-O2A
20	1	512	CHL	CAA-CBA-CGA-O2A
19	B	820	CLA	C2-C3-C5-C6
22	F	304	LMG	C36-C37-C38-C39
19	A	827	CLA	O1A-CGA-O2A-C1
19	A	822	CLA	CAA-CBA-CGA-O2A
19	A	808	CLA	C15-C16-C17-C18
19	1	507	CLA	C11-C12-C13-C14
19	A	806	CLA	C6-C7-C8-C9
19	A	817	CLA	C11-C12-C13-C14
19	A	824	CLA	C11-C12-C13-C14
19	A	828	CLA	C11-C10-C8-C9
19	A	834	CLA	C14-C13-C15-C16
19	B	809	CLA	C14-C13-C15-C16
21	A	853	LHG	C31-C32-C33-C34
19	1	508	CLA	C1A-C2A-CAA-CBA
19	1	515	CLA	C4B-C3B-CAB-CBB
19	2	506	CLA	C1A-C2A-CAA-CBA
19	3	309	CLA	C4B-C3B-CAB-CBB
19	3	312	CLA	C4B-C3B-CAB-CBB
19	4	307	CLA	C1A-C2A-CAA-CBA
19	4	310	CLA	C4B-C3B-CAB-CBB
19	4	311	CLA	C4B-C3B-CAB-CBB
19	A	811	CLA	C4B-C3B-CAB-CBB
19	A	821	CLA	C1A-C2A-CAA-CBA
19	B	820	CLA	C1A-C2A-CAA-CBA
19	B	839	CLA	C4B-C3B-CAB-CBB
19	L	303	CLA	C4B-C3B-CAB-CBB
21	A	853	LHG	C30-C31-C32-C33
19	2	509	CLA	CAA-CBA-CGA-O2A
19	B	836	CLA	CAA-CBA-CGA-O2A
17	1	502	LUT	C7-C8-C9-C10
18	A	848	BCR	C17-C18-C19-C20
18	A	849	BCR	C11-C12-C13-C14
18	A	856	BCR	C7-C8-C9-C10
18	B	852	BCR	C17-C18-C19-C20
18	B	853	BCR	C17-C18-C19-C20
18	G	205	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
18	J	1108	BCR	C17-C18-C19-C20
18	B	851	BCR	C9-C10-C11-C12
18	B	856	BCR	C9-C10-C11-C12
18	B	856	BCR	C19-C20-C21-C22
19	3	305	CLA	C2A-CAA-CBA-CGA
19	B	819	CLA	C10-C11-C12-C13
19	3	316	CLA	CAA-CBA-CGA-O2A
19	A	814	CLA	CAA-CBA-CGA-O2A
19	B	834	CLA	CAA-CBA-CGA-O2A
19	B	839	CLA	CAA-CBA-CGA-O2A
22	1	518	LMG	O9-C10-C11-C12
19	A	821	CLA	C5-C6-C7-C8
19	1	504	CLA	C2-C1-O2A-CGA
19	A	804	CLA	C2-C1-O2A-CGA
19	A	829	CLA	C2-C1-O2A-CGA
19	A	836	CLA	C2-C1-O2A-CGA
19	B	831	CLA	C2-C1-O2A-CGA
19	1	507	CLA	C12-C13-C15-C16
19	1	513	CLA	C6-C7-C8-C10
19	B	803	CLA	C13-C15-C16-C17
19	B	822	CLA	C16-C17-C18-C19
19	A	807	CLA	CAA-CBA-CGA-O2A
19	K	1002	CLA	CAA-CBA-CGA-O2A
19	B	804	CLA	C15-C16-C17-C18
24	G	209	LMT	C5-C6-C7-C8
18	A	851	BCR	C19-C20-C21-C22
19	A	819	CLA	C2A-CAA-CBA-CGA
19	A	813	CLA	C16-C17-C18-C19
24	J	1107	LMT	C3'-C4'-O1B-C1B
19	B	805	CLA	C10-C11-C12-C13
26	J	1106	DGD	C7B-C8B-C9B-CAB
19	1	508	CLA	CAA-CBA-CGA-O2A
19	B	838	CLA	CAA-CBA-CGA-O2A
19	A	827	CLA	CAA-CBA-CGA-O1A
19	A	818	CLA	CAA-CBA-CGA-O2A
21	1	517	LHG	O8-C23-C24-C25
21	A	845	LHG	O7-C7-C8-C9
22	A	847	LMG	C12-C13-C14-C15
22	A	847	LMG	C32-C33-C34-C35
22	B	844	LMG	C28-C29-C30-C31
19	4	308	CLA	C11-C10-C8-C9
19	A	839	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	B	803	CLA	C11-C12-C13-C14
19	B	805	CLA	C11-C12-C13-C14
19	B	819	CLA	C11-C10-C8-C9
19	B	829	CLA	C11-C10-C8-C9
19	B	831	CLA	C6-C7-C8-C9
19	B	838	CLA	C6-C7-C8-C9
19	B	840	CLA	C11-C12-C13-C14
19	B	826	CLA	O1A-CGA-O2A-C1
19	B	828	CLA	C16-C17-C18-C20
17	1	501	LUT	C21-C26-C27-C28
17	3	301	LUT	C21-C26-C27-C28
17	3	302	LUT	C21-C26-C27-C28
23	2	502	XAT	C1-C6-C7-C8
24	A	846	LMT	C2-C3-C4-C5
19	A	822	CLA	CAA-CBA-CGA-O1A
19	G	201	CLA	CAA-CBA-CGA-O1A
19	A	815	CLA	CAA-CBA-CGA-O2A
19	A	807	CLA	CAA-CBA-CGA-O1A
19	K	1002	CLA	CAA-CBA-CGA-O1A
19	B	820	CLA	C8-C10-C11-C12
22	B	844	LMG	C8-C7-O1-C1
19	A	814	CLA	CAA-CBA-CGA-O1A
21	A	853	LHG	O10-C23-C24-C25
19	A	837	CLA	CAA-CBA-CGA-O2A
19	A	839	CLA	C2A-CAA-CBA-CGA
21	B	842	LHG	C4-C5-C6-O8
22	A	847	LMG	O1-C7-C8-C9
19	B	834	CLA	CAA-CBA-CGA-O1A
27	A	801	CL0	CAA-CBA-CGA-O1A
19	A	803	CLA	C4-C3-C5-C6
22	1	519	LMG	O6-C5-C6-O5
19	A	825	CLA	C5-C6-C7-C8
19	A	827	CLA	C13-C15-C16-C17
19	B	828	CLA	C10-C11-C12-C13
19	B	806	CLA	CAA-CBA-CGA-O2A
21	1	520	LHG	O8-C23-C24-C25
19	2	509	CLA	CAA-CBA-CGA-O1A
19	1	511	CLA	CAD-CBD-CGD-O2D
19	4	305	CLA	CAD-CBD-CGD-O2D
19	A	816	CLA	CAD-CBD-CGD-O2D
22	J	1103	LMG	O7-C10-C11-C12
19	4	315	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
19	B	838	CLA	CAA-CBA-CGA-O1A
19	B	839	CLA	CAA-CBA-CGA-O1A
27	A	801	CL0	C1A-C2A-CAA-CBA
19	A	825	CLA	C16-C17-C18-C20
26	B	854	DGD	C9A-CAA-CBA-CCA
19	3	316	CLA	CAA-CBA-CGA-O1A
20	4	316	CHL	C10-C11-C12-C13
19	2	504	CLA	CAA-CBA-CGA-O2A
19	4	309	CLA	CAA-CBA-CGA-O2A
19	4	306	CLA	C16-C17-C18-C19
21	1	517	LHG	O10-C23-C24-C25
19	1	511	CLA	CAA-CBA-CGA-O2A
19	A	824	CLA	CAA-CBA-CGA-O2A
19	B	811	CLA	CAA-CBA-CGA-O2A
22	F	304	LMG	O7-C10-C11-C12
22	J	1104	LMG	O7-C10-C11-C12
19	A	811	CLA	C5-C6-C7-C8
19	B	836	CLA	CAA-CBA-CGA-O1A
19	4	315	CLA	C2C-C3C-CAC-CBC

There are no ring outliers.

229 monomers are involved in 878 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	810	CLA	3	0
19	A	808	CLA	6	0
23	4	303	XAT	9	0
19	3	316	CLA	4	0
22	G	206	LMG	5	0
18	A	849	BCR	1	0
19	A	830	CLA	8	0
18	B	849	BCR	1	0
19	B	825	CLA	9	0
19	A	839	CLA	6	0
19	3	308	CLA	12	0
19	B	839	CLA	6	0
17	2	501	LUT	7	0
22	F	305	LMG	2	0
19	B	830	CLA	10	0
19	A	828	CLA	8	0
19	4	304	CLA	6	0
19	B	835	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	4	309	CLA	9	0
22	G	210	LMG	1	0
19	K	1002	CLA	1	0
19	K	1003	CLA	1	0
19	A	836	CLA	3	0
18	A	856	BCR	3	0
18	B	802	BCR	4	0
18	B	852	BCR	4	0
19	B	804	CLA	4	0
22	J	1104	LMG	2	0
29	B	841	PQN	8	0
19	A	816	CLA	1	0
19	A	842	CLA	8	0
19	2	507	CLA	4	0
19	A	806	CLA	6	0
19	B	806	CLA	7	0
19	F	302	CLA	4	0
19	A	821	CLA	9	0
19	B	821	CLA	1	0
20	1	512	CHL	4	0
22	2	518	LMG	2	0
19	2	506	CLA	6	0
19	B	828	CLA	2	0
19	H	1000	CLA	2	0
18	G	205	BCR	3	0
19	3	309	CLA	2	0
19	A	814	CLA	2	0
19	B	838	CLA	9	0
19	G	203	CLA	3	0
19	4	308	CLA	3	0
18	I	102	BCR	5	0
19	B	824	CLA	3	0
21	1	520	LHG	11	0
19	G	202	CLA	3	0
21	A	853	LHG	3	0
19	A	827	CLA	8	0
19	1	511	CLA	1	0
19	A	819	CLA	7	0
19	2	509	CLA	1	0
22	F	304	LMG	8	0
22	2	519	LMG	7	0
22	4	322	LMG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	820	CLA	2	0
19	A	840	CLA	3	0
19	B	840	CLA	14	0
19	B	818	CLA	5	0
20	1	521	CHL	7	0
19	A	829	CLA	4	0
19	B	829	CLA	10	0
19	2	508	CLA	5	0
19	A	813	CLA	8	0
19	A	835	CLA	2	0
19	1	508	CLA	13	0
19	A	825	CLA	8	0
18	B	851	BCR	4	0
19	3	306	CLA	9	0
22	B	845	LMG	2	0
19	J	1102	CLA	5	0
20	2	526	CHL	10	0
22	A	847	LMG	4	0
19	A	822	CLA	4	0
24	A	846	LMT	3	0
19	B	827	CLA	2	0
19	4	307	CLA	7	0
24	B	847	LMT	2	0
19	1	507	CLA	5	0
19	B	826	CLA	6	0
21	A	845	LHG	6	0
19	3	313	CLA	3	0
17	J	1109	LUT	8	0
19	3	310	CLA	7	0
19	3	317	CLA	3	0
19	B	832	CLA	7	0
19	4	310	CLA	5	0
20	4	313	CHL	1	0
22	2	524	LMG	1	0
19	3	307	CLA	5	0
19	4	311	CLA	4	0
18	L	306	BCR	2	0
19	A	823	CLA	3	0
19	B	813	CLA	1	0
26	G	207	DGD	1	0
28	C	102	SF4	2	0
18	J	1108	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1	516	CLA	4	0
19	2	514	CLA	3	0
19	B	836	CLA	5	0
21	B	843	LHG	6	0
19	G	204	CLA	13	0
30	F	301	ZEX	5	0
19	B	810	CLA	3	0
24	G	208	LMT	4	0
18	1	503	BCR	4	0
18	A	850	BCR	5	0
18	A	851	BCR	4	0
19	4	305	CLA	4	0
19	L	303	CLA	2	0
19	G	201	CLA	6	0
24	B	846	LMT	3	0
18	L	302	BCR	3	0
19	A	817	CLA	3	0
19	A	854	CLA	8	0
19	1	515	CLA	4	0
17	4	302	LUT	3	0
19	B	834	CLA	7	0
18	B	856	BCR	6	0
19	L	304	CLA	3	0
19	A	812	CLA	6	0
19	B	817	CLA	3	0
19	L	305	CLA	1	0
18	A	848	BCR	1	0
18	3	304	BCR	4	0
19	4	315	CLA	3	0
19	A	833	CLA	7	0
20	2	515	CHL	4	0
21	1	517	LHG	7	0
19	A	841	CLA	8	0
19	B	823	CLA	9	0
19	2	505	CLA	1	0
19	A	818	CLA	8	0
19	A	809	CLA	9	0
18	B	850	BCR	2	0
19	3	315	CLA	4	0
19	A	826	CLA	3	0
17	1	501	LUT	6	0
18	I	101	BCR	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	4	317	CHL	5	0
18	L	307	BCR	1	0
19	4	306	CLA	5	0
19	A	838	CLA	4	0
17	1	502	LUT	5	0
29	A	844	PQN	3	0
26	B	801	DGD	5	0
19	B	819	CLA	12	0
19	A	834	CLA	6	0
19	B	837	CLA	6	0
18	2	503	BCR	11	0
19	B	833	CLA	6	0
26	4	319	DGD	6	0
19	A	804	CLA	5	0
26	B	854	DGD	9	0
19	B	807	CLA	3	0
19	A	831	CLA	4	0
19	B	831	CLA	1	0
19	B	822	CLA	5	0
19	J	1101	CLA	11	0
19	4	312	CLA	2	0
19	4	318	CLA	10	0
19	A	803	CLA	5	0
18	A	852	BCR	6	0
18	B	853	BCR	6	0
20	1	514	CHL	9	0
19	A	824	CLA	12	0
19	K	1001	CLA	6	0
19	L	301	CLA	2	0
22	B	844	LMG	4	0
19	B	816	CLA	4	0
19	B	811	CLA	5	0
19	F	303	CLA	6	0
19	A	805	CLA	10	0
26	J	1106	DGD	6	0
19	2	504	CLA	6	0
19	1	505	CLA	3	0
19	1	509	CLA	3	0
19	A	855	CLA	8	0
23	2	502	XAT	4	0
19	B	814	CLA	4	0
22	J	1103	LMG	1	0

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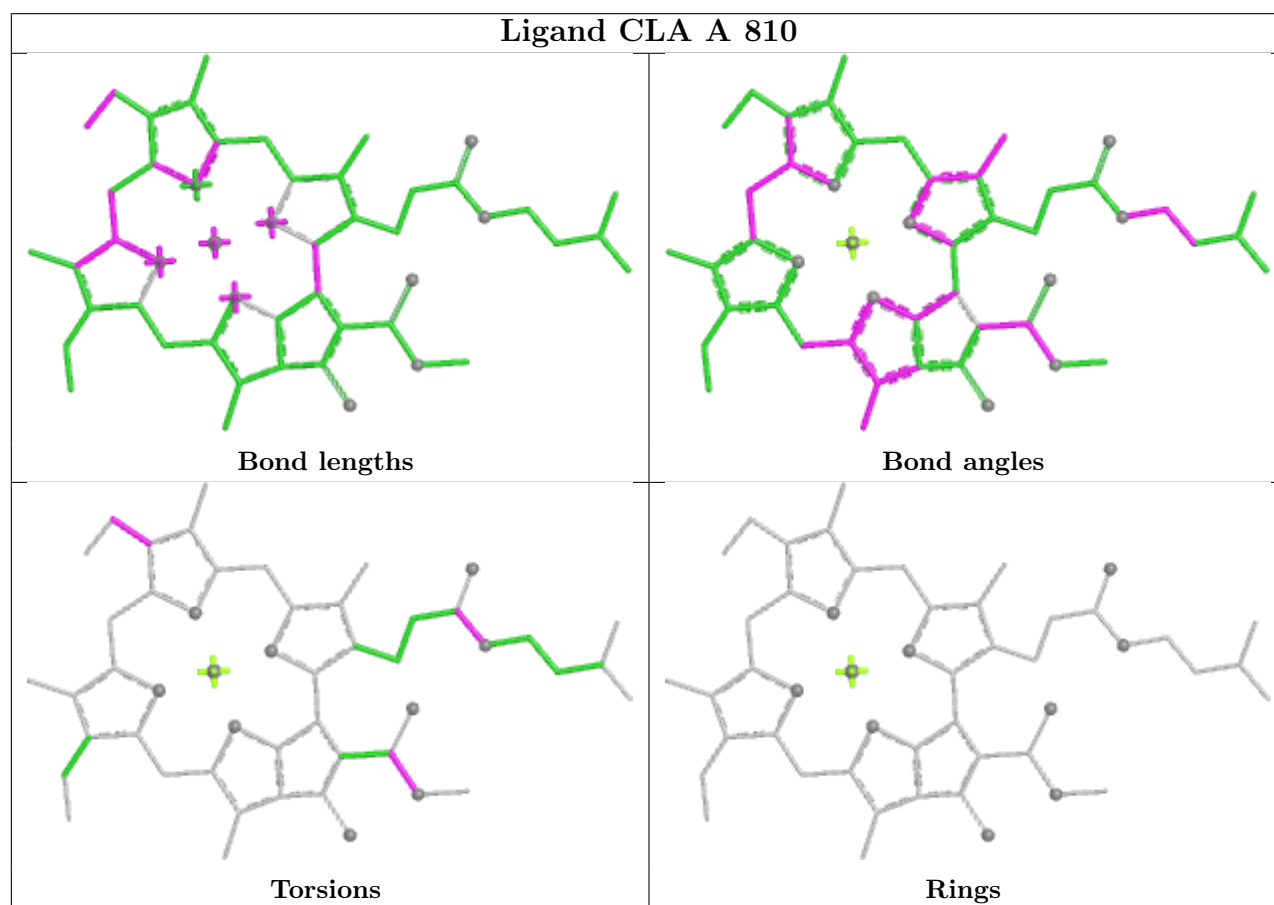
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	815	CLA	1	0
24	G	209	LMT	1	0
19	1	513	CLA	2	0
19	B	815	CLA	4	0
24	B	855	LMT	3	0
19	A	832	CLA	6	0
19	3	305	CLA	18	0
28	A	843	SF4	1	0
19	B	805	CLA	7	0
19	1	510	CLA	8	0
19	J	1105	CLA	7	0
19	B	812	CLA	6	0
17	3	301	LUT	11	0
19	B	803	CLA	5	0
17	3	302	LUT	9	0
19	B	808	CLA	6	0
20	4	314	CHL	6	0
21	2	517	LHG	9	0
19	B	820	CLA	5	0
18	F	306	BCR	1	0
19	A	807	CLA	4	0
20	2	513	CHL	7	0
18	4	301	BCR	9	0
19	A	811	CLA	10	0
24	4	320	LMT	2	0
19	2	511	CLA	4	0
19	A	802	CLA	11	0
20	4	316	CHL	8	0
24	3	318	LMT	2	0
19	1	504	CLA	10	0
19	2	510	CLA	4	0
19	A	837	CLA	5	0
27	A	801	CL0	6	0
24	J	1107	LMT	1	0
18	3	303	BCR	8	0
19	B	809	CLA	5	0
20	2	512	CHL	8	0
20	2	516	CHL	3	0
20	3	314	CHL	9	0
19	K	1004	CLA	2	0
21	B	842	LHG	2	0
18	K	1005	BCR	7	0

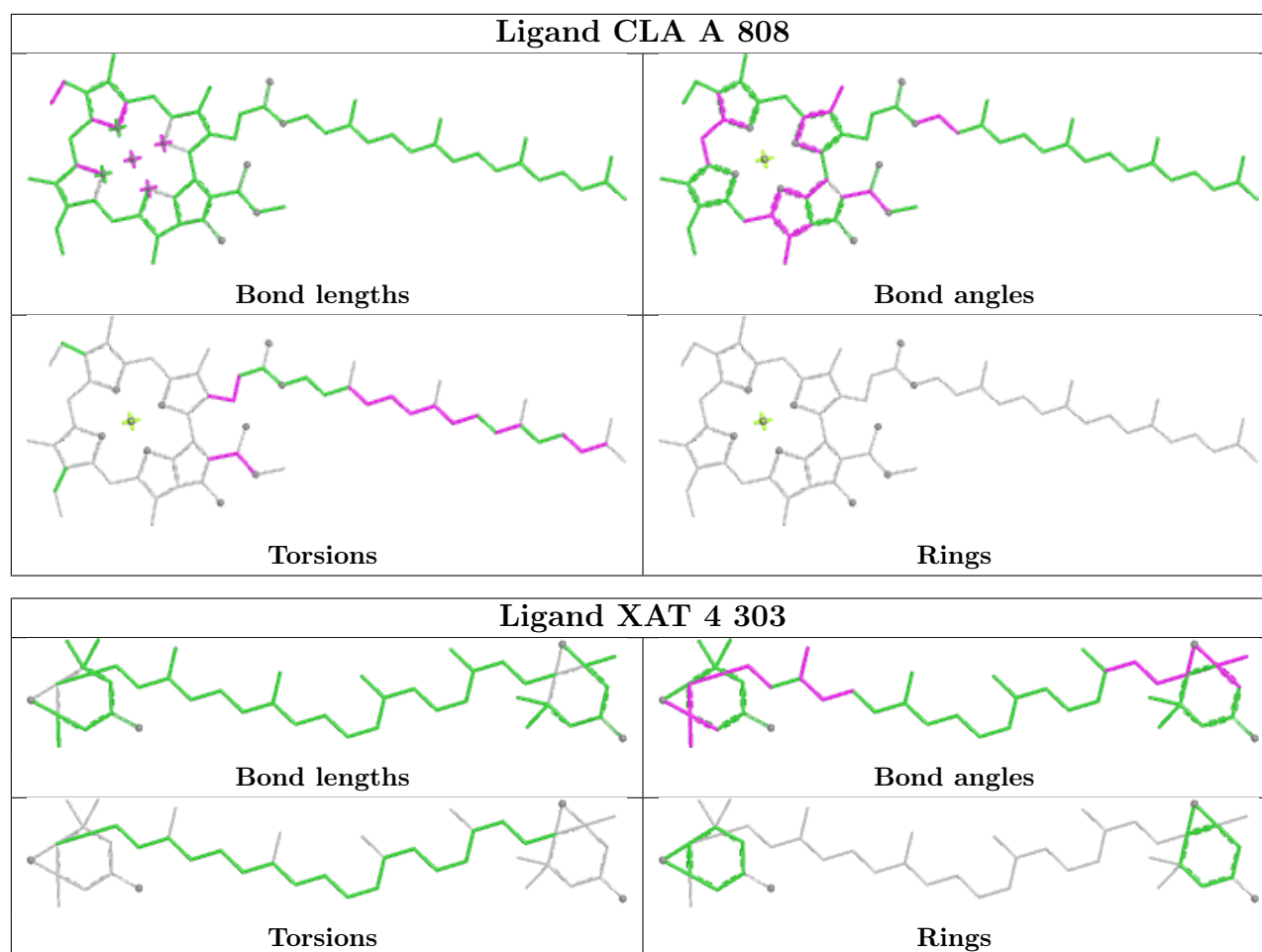
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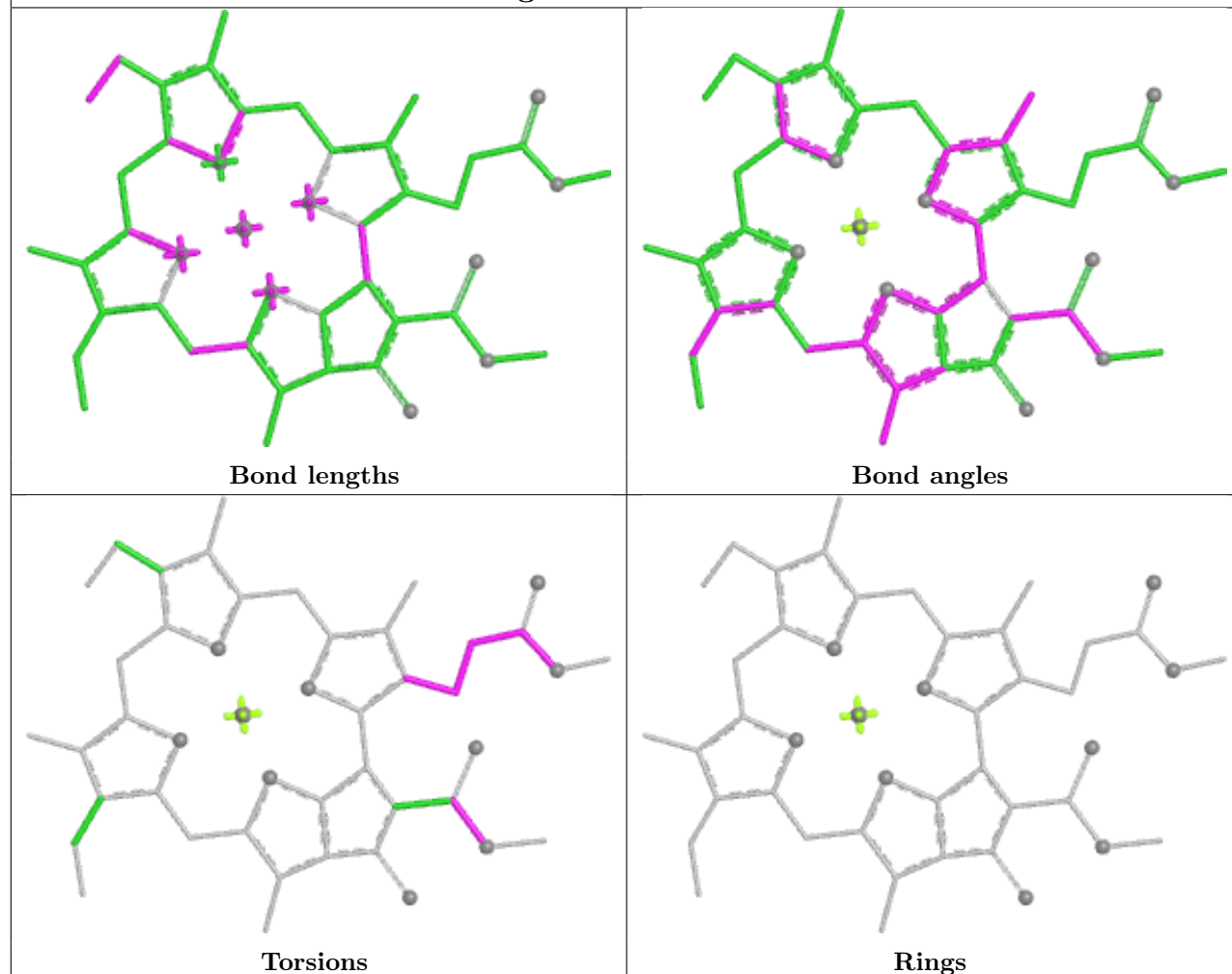
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1	518	LMG	4	0

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



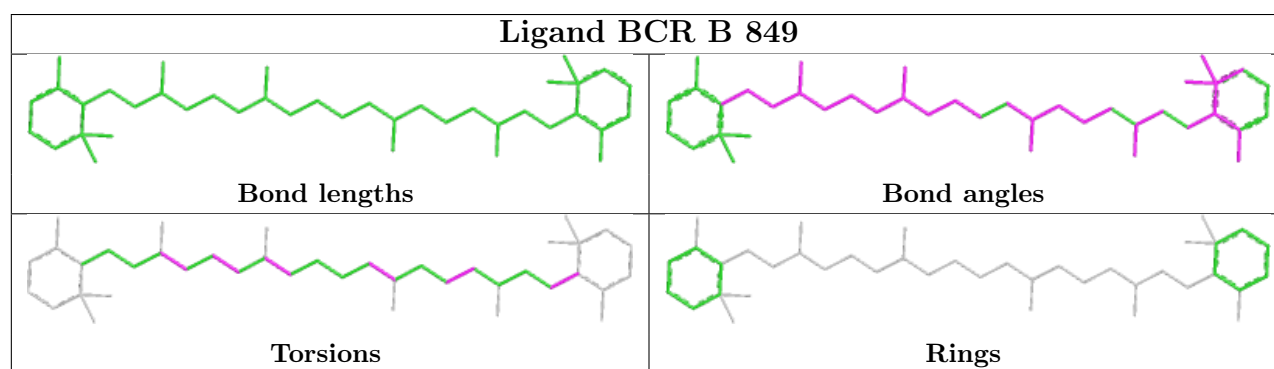
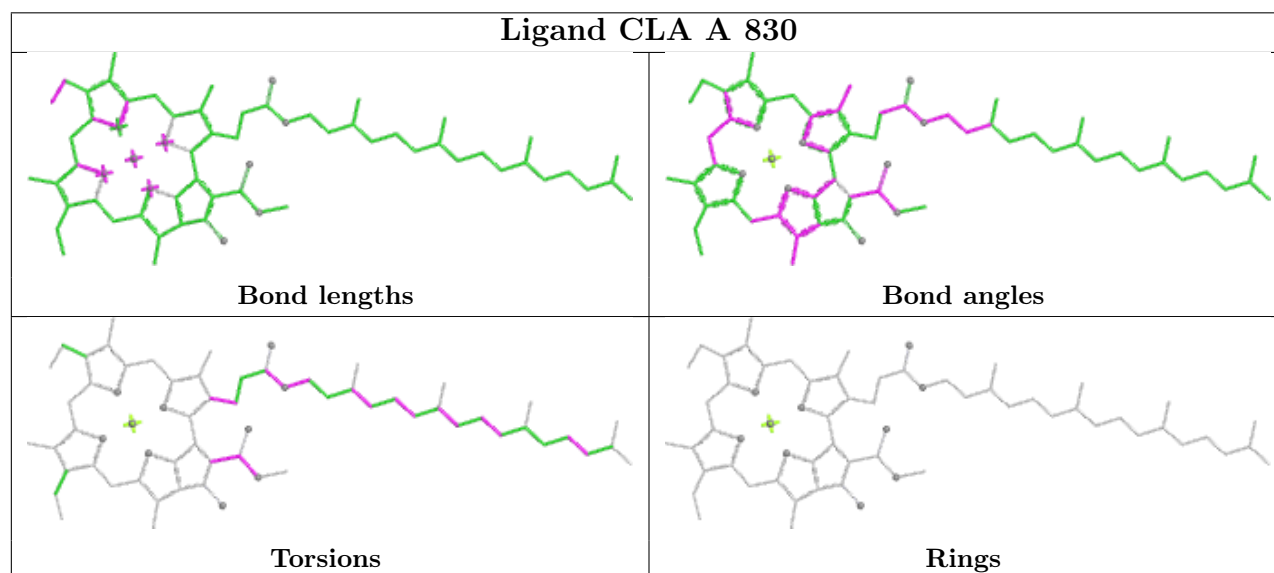
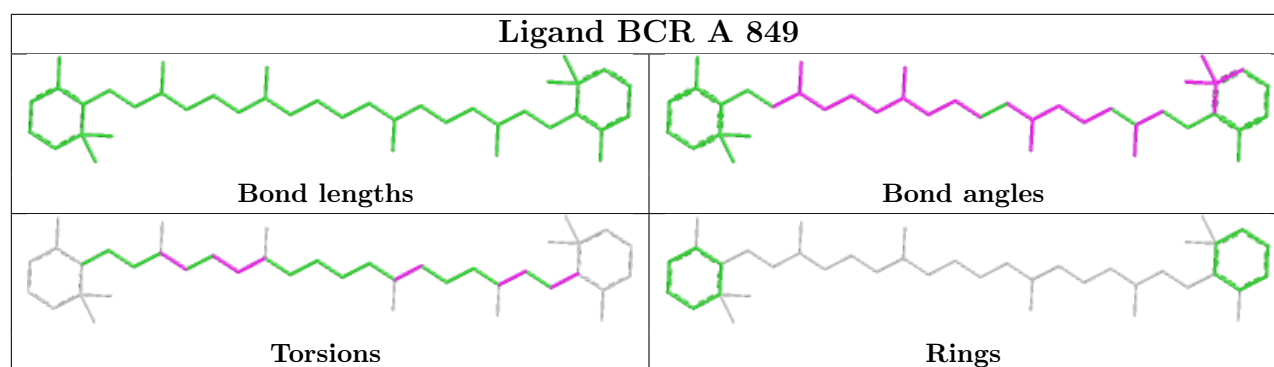


Ligand CLA 3 316

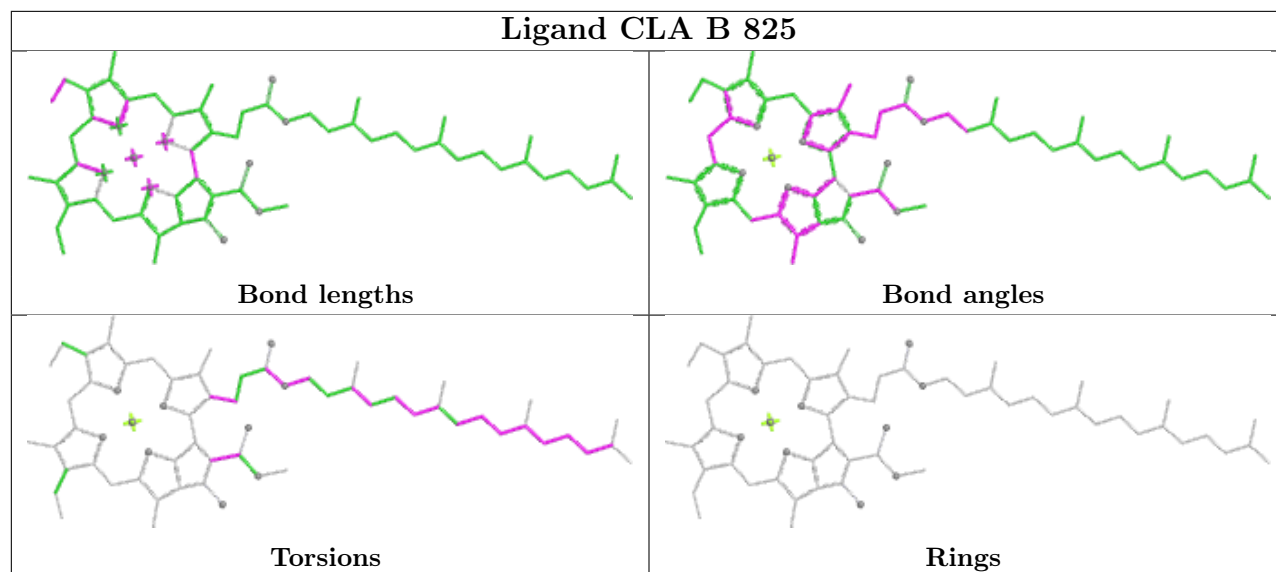


Ligand LMG G 206

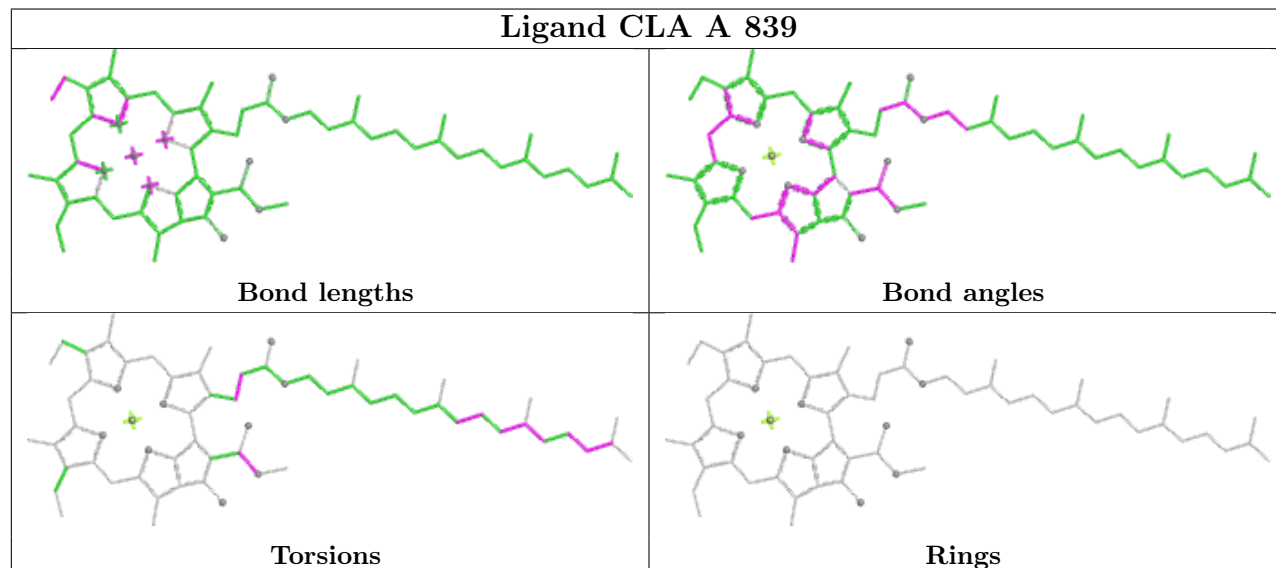




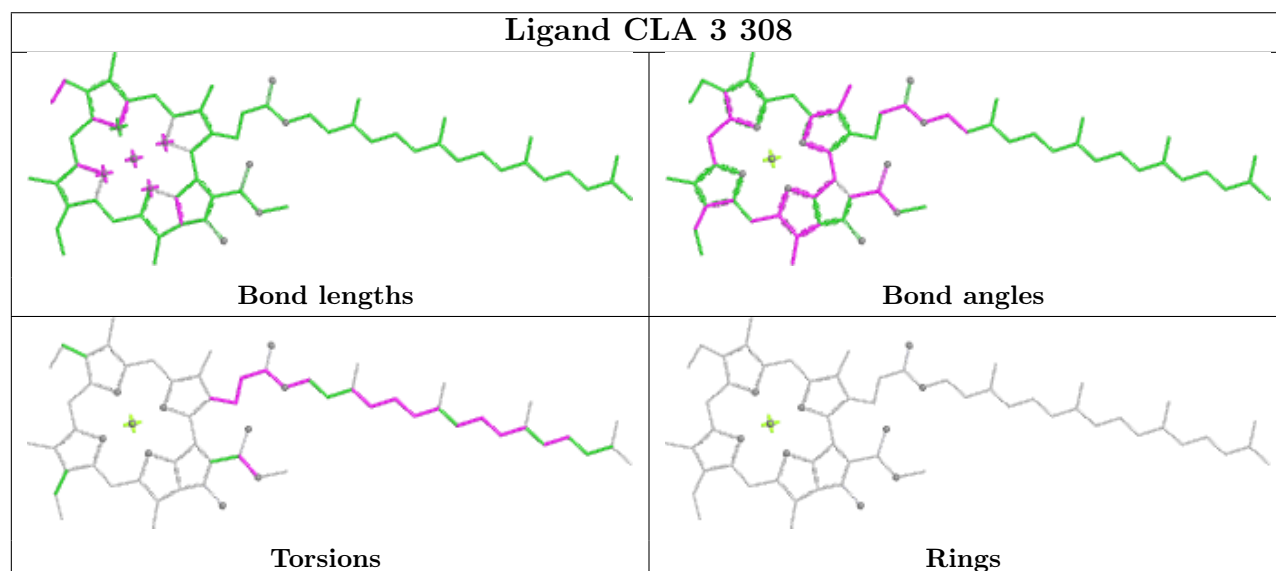
Ligand CLA B 825

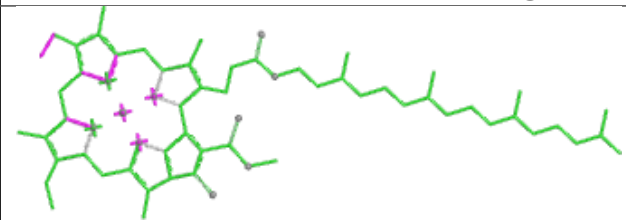
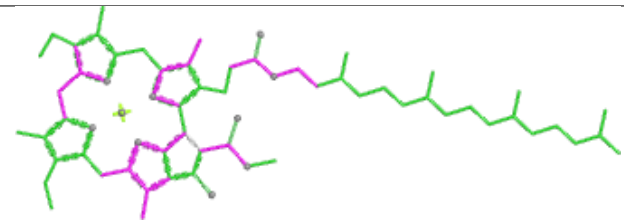
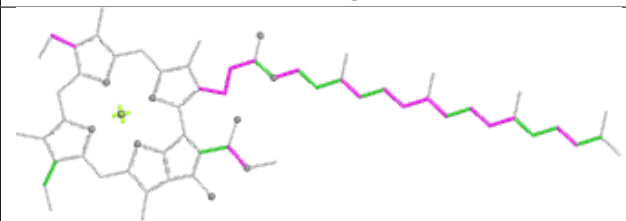
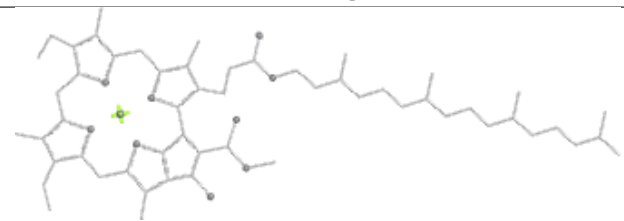


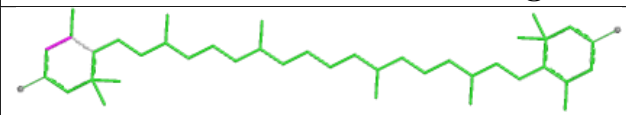
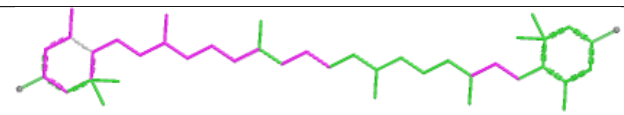
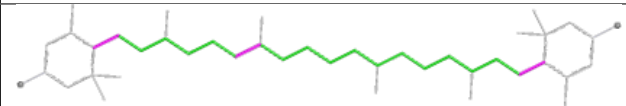
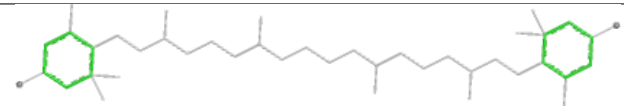
Ligand CLA A 839

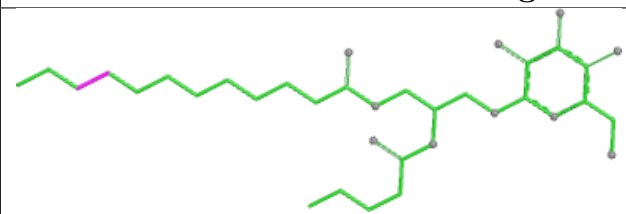
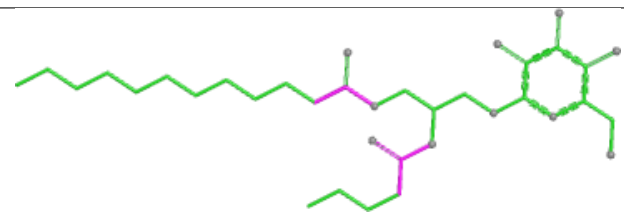
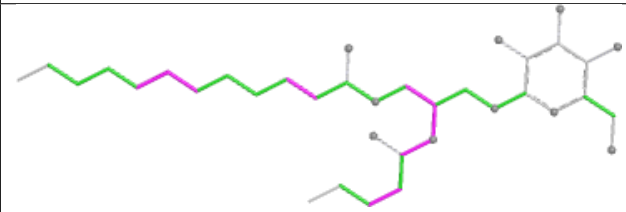
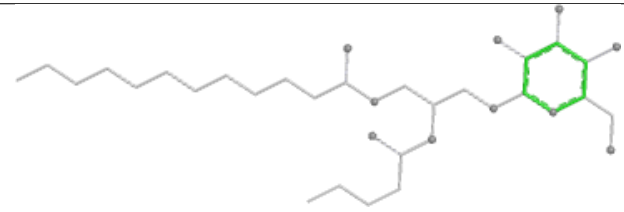


Ligand CLA 3 308

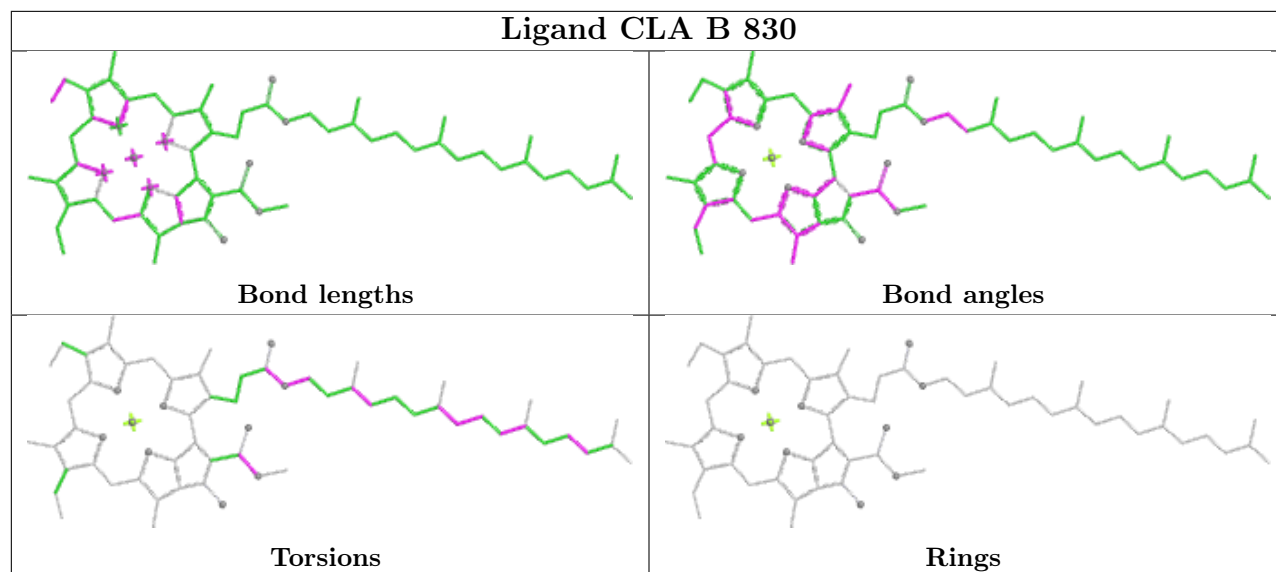


Ligand CLA B 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

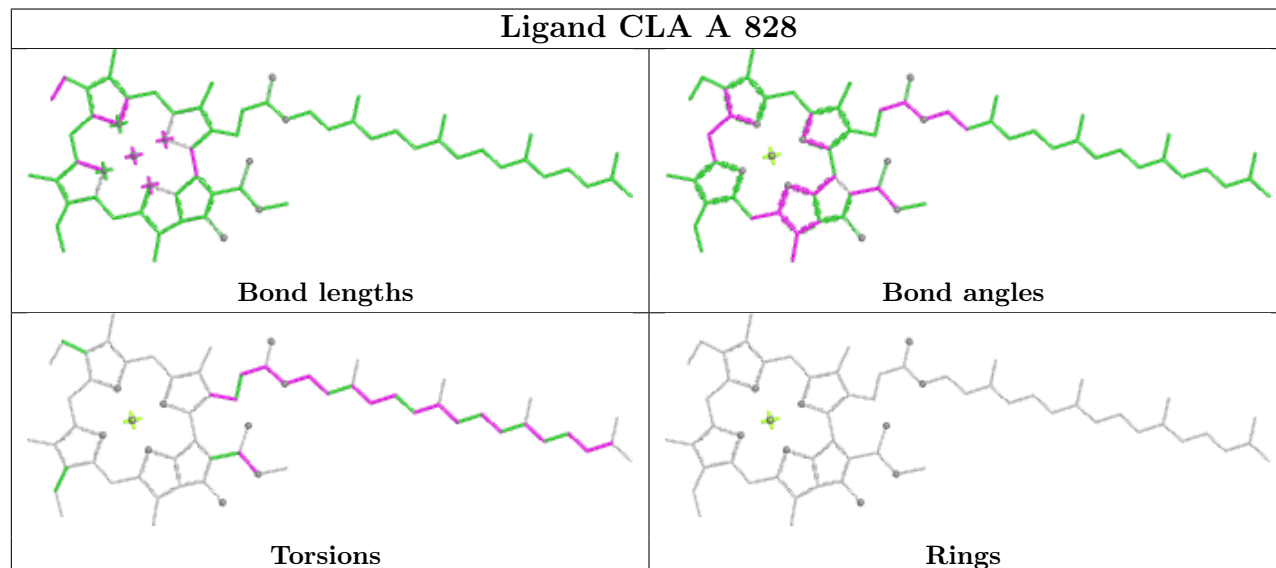
Ligand LUT 2 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG F 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

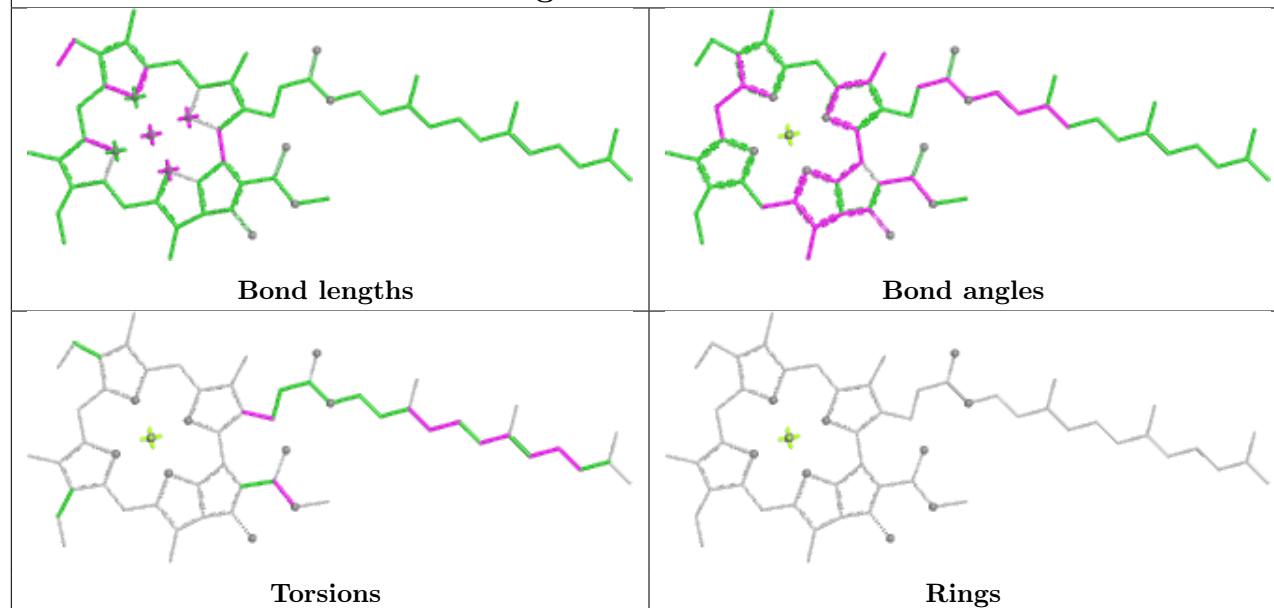
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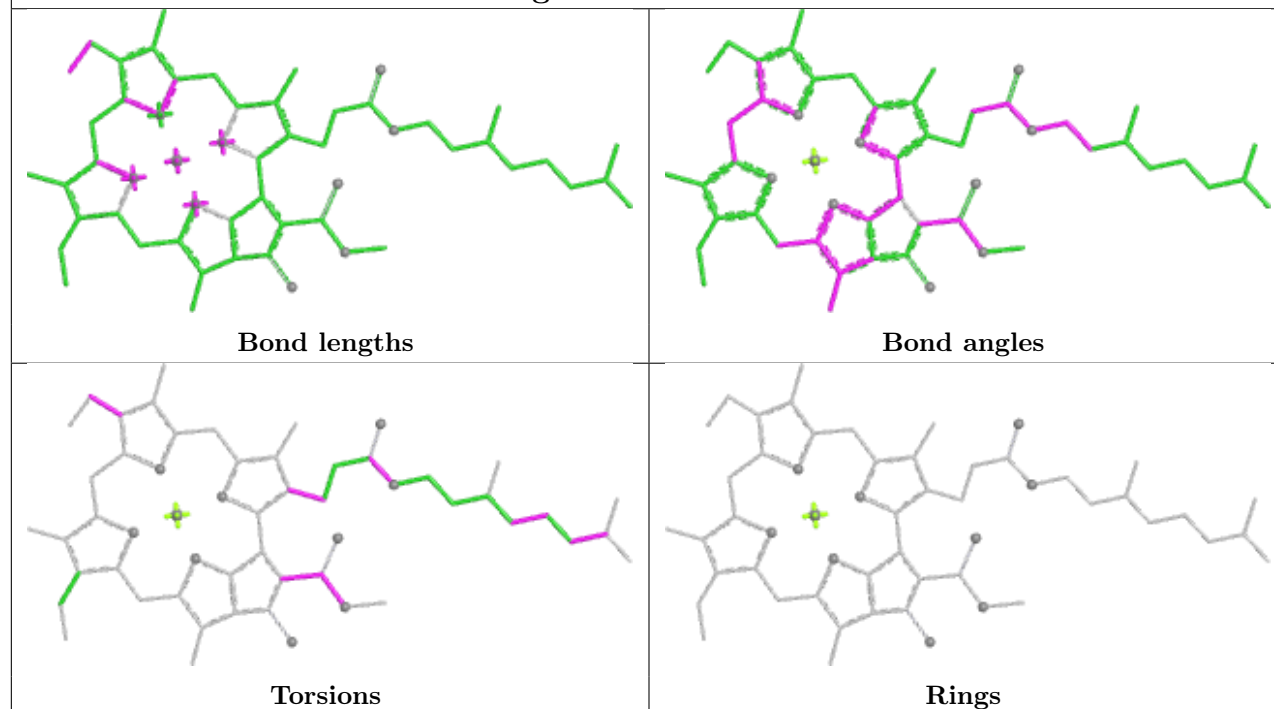
Ligand CLA A 828



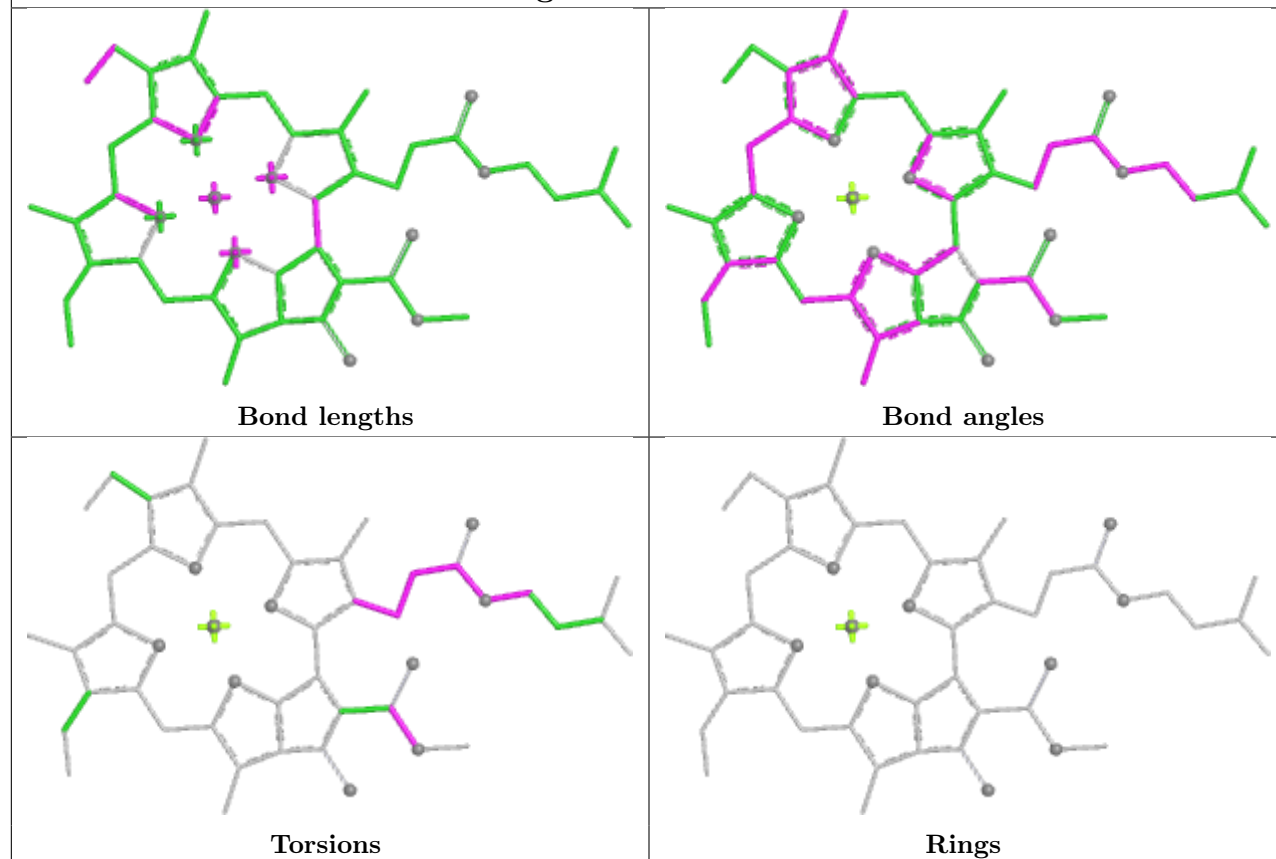
Ligand CLA 4 304



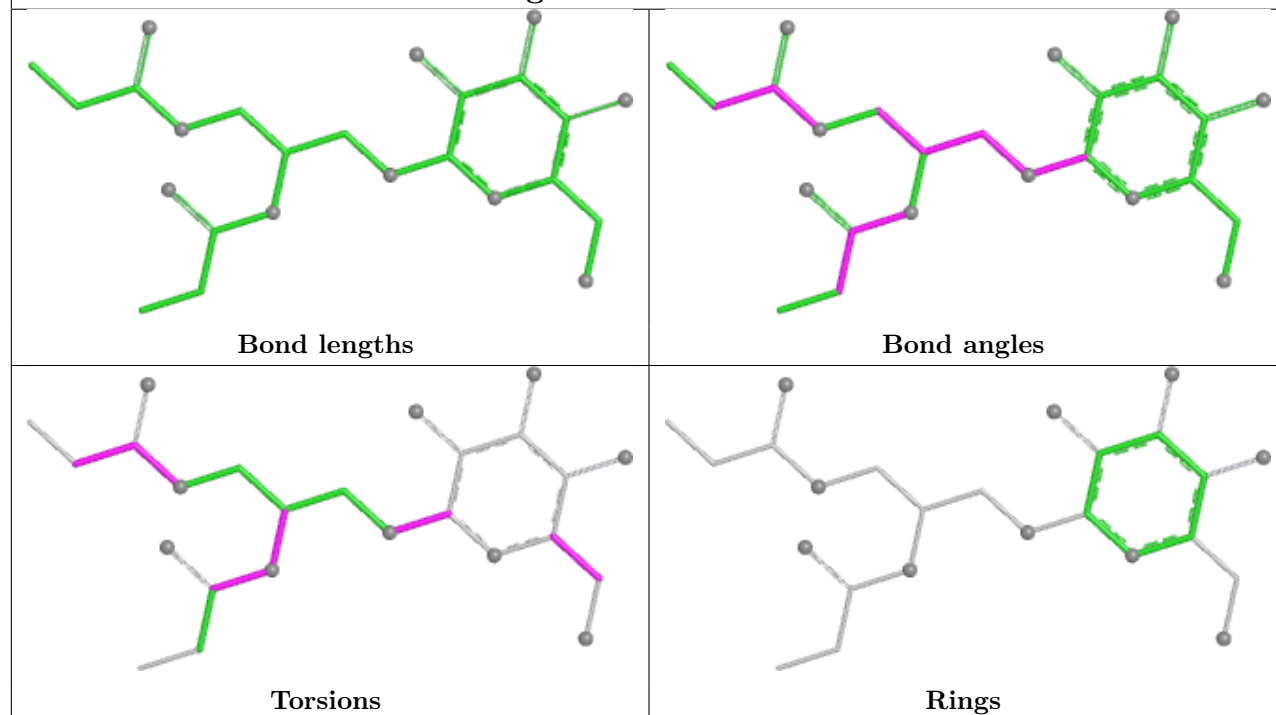
Ligand CLA B 835

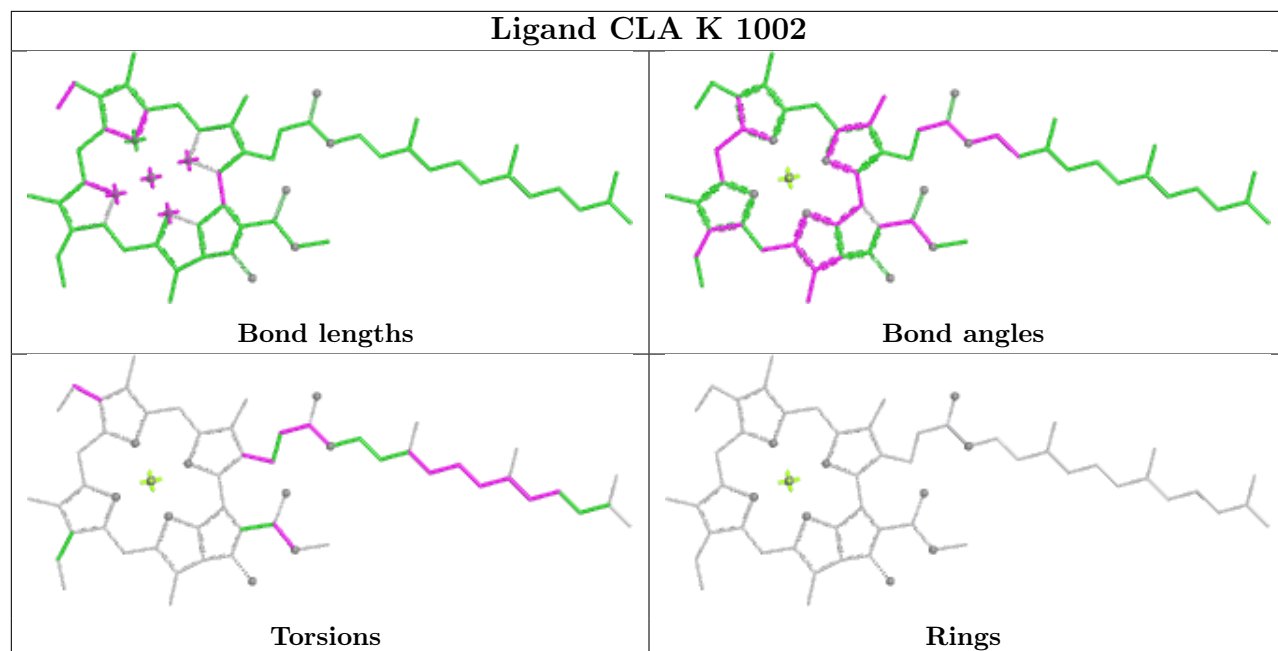


Ligand CLA 4 309

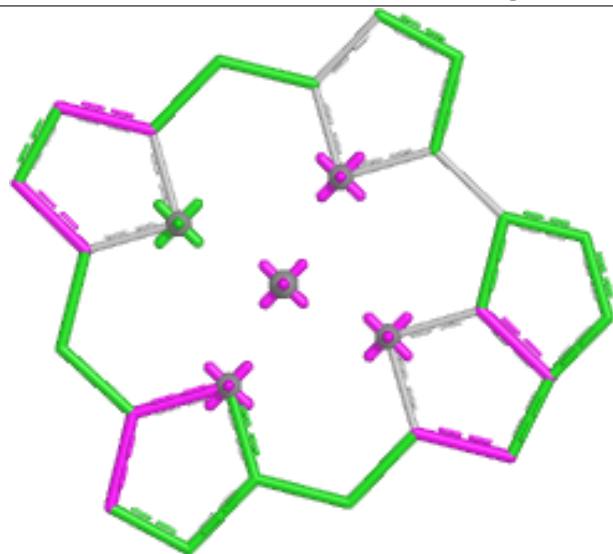


Ligand LMG G 210

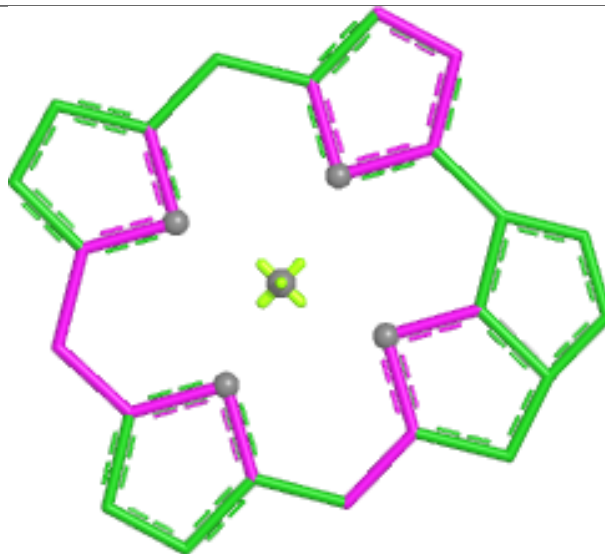




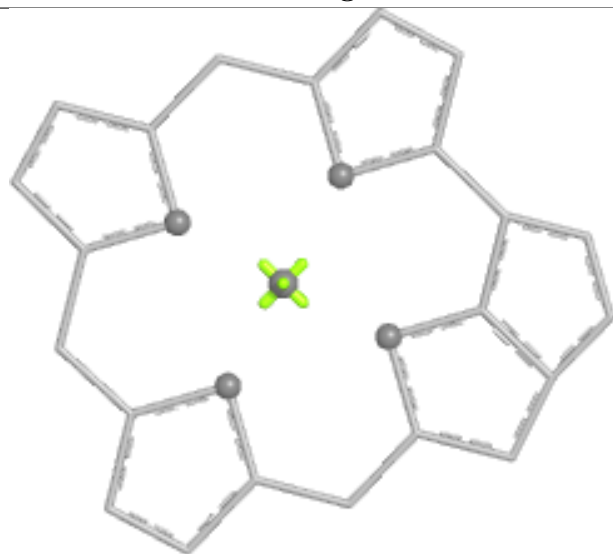
Ligand CLA K 1003



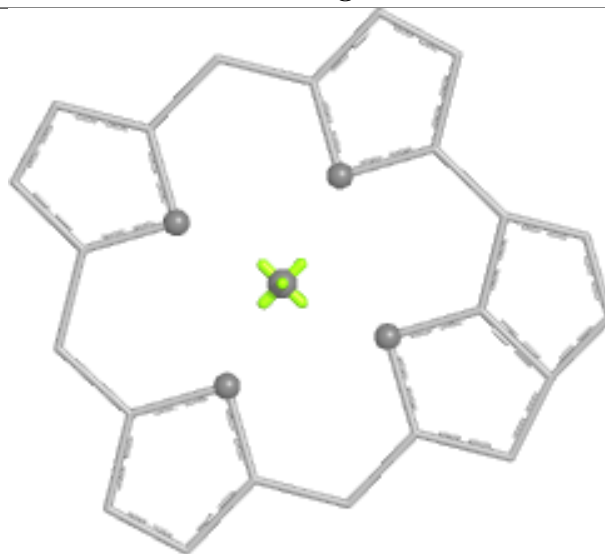
Bond lengths



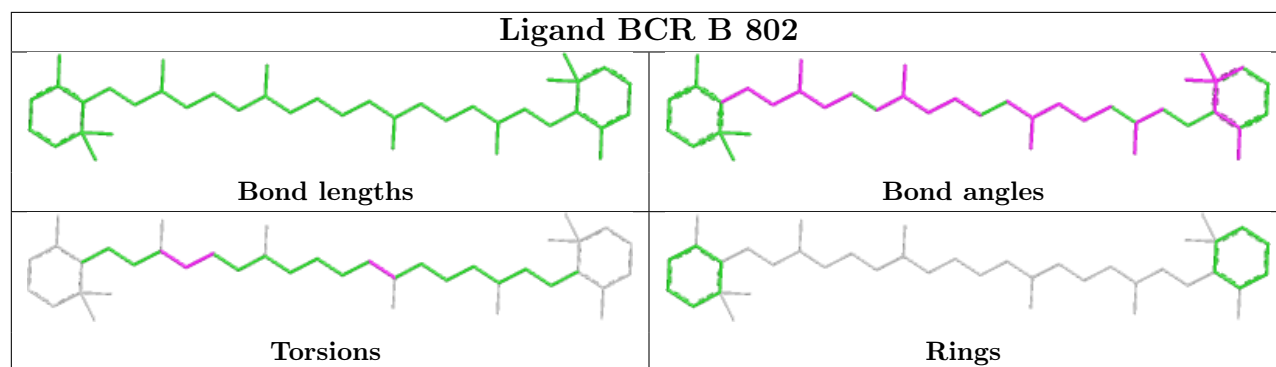
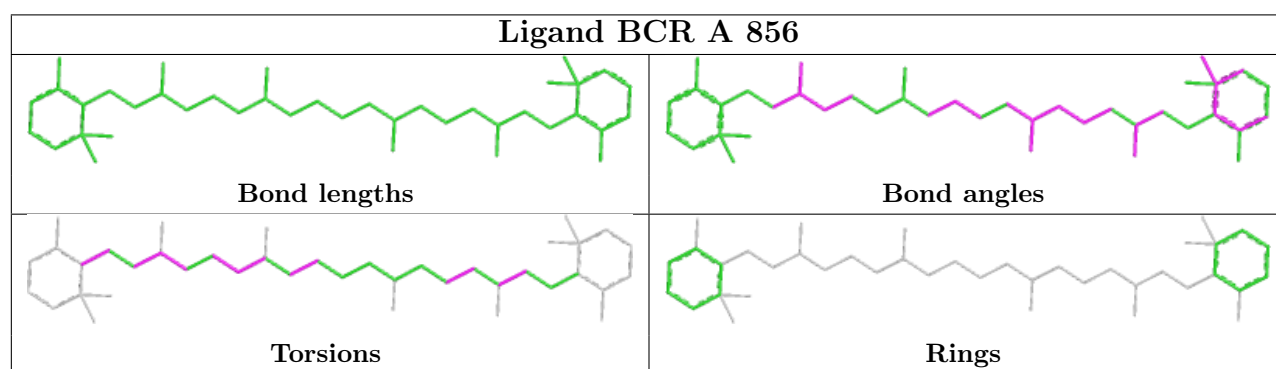
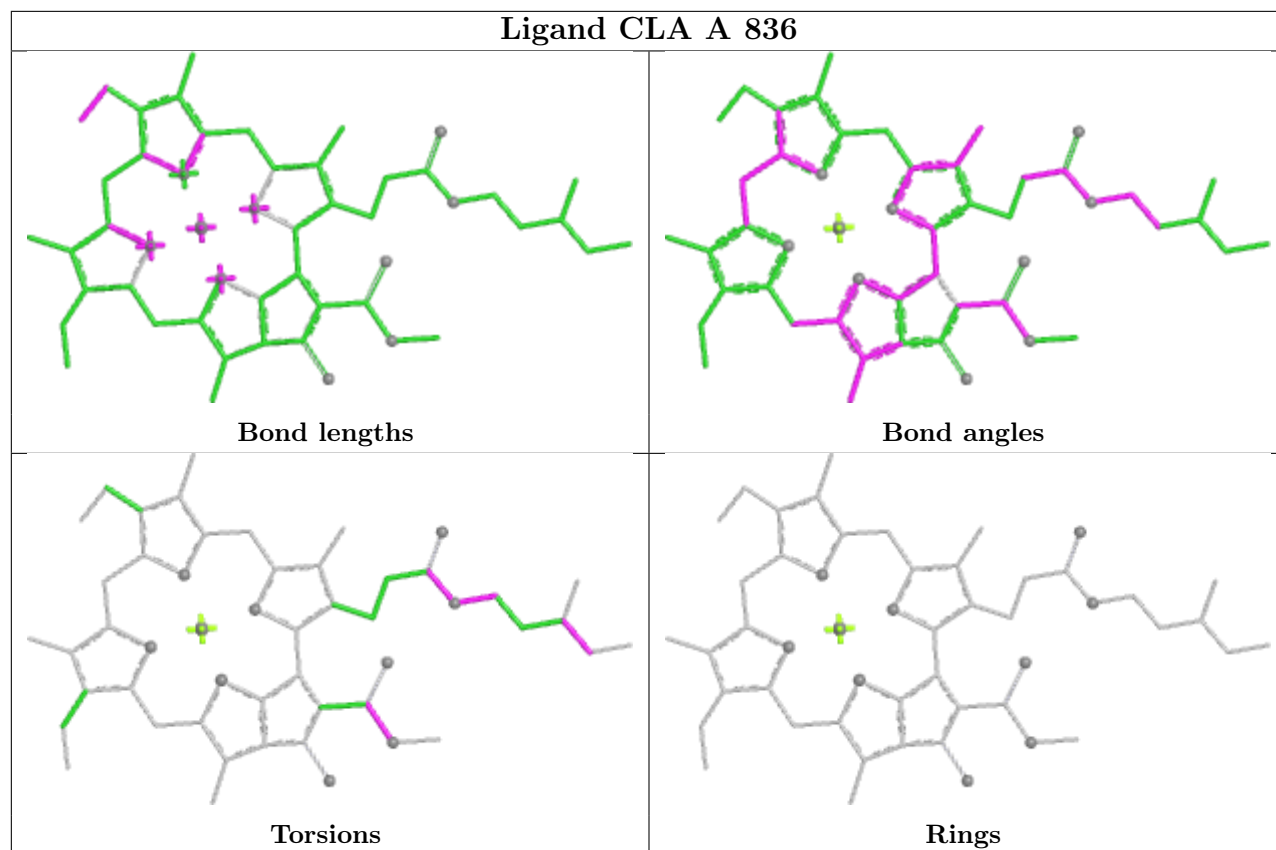
Bond angles

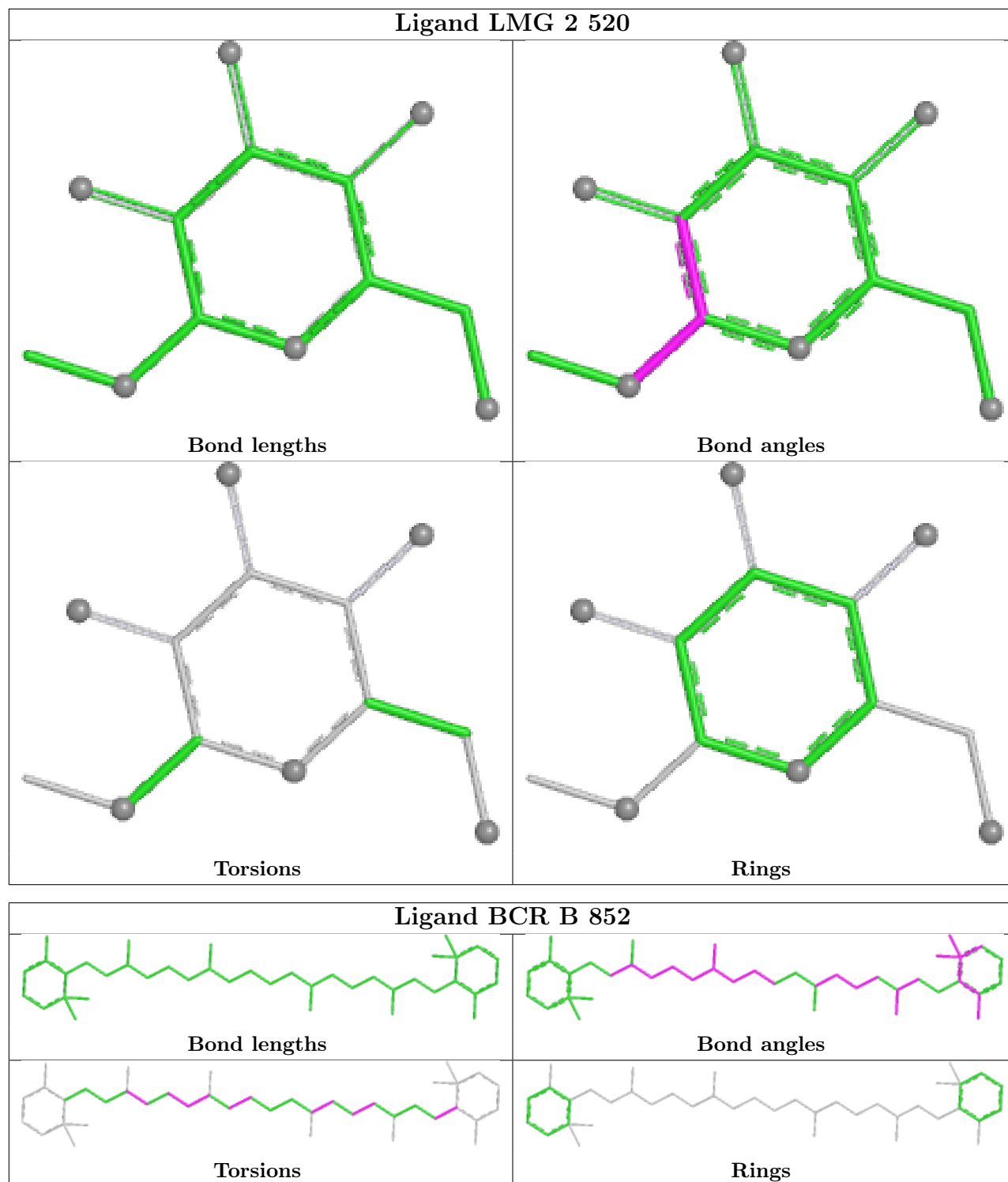


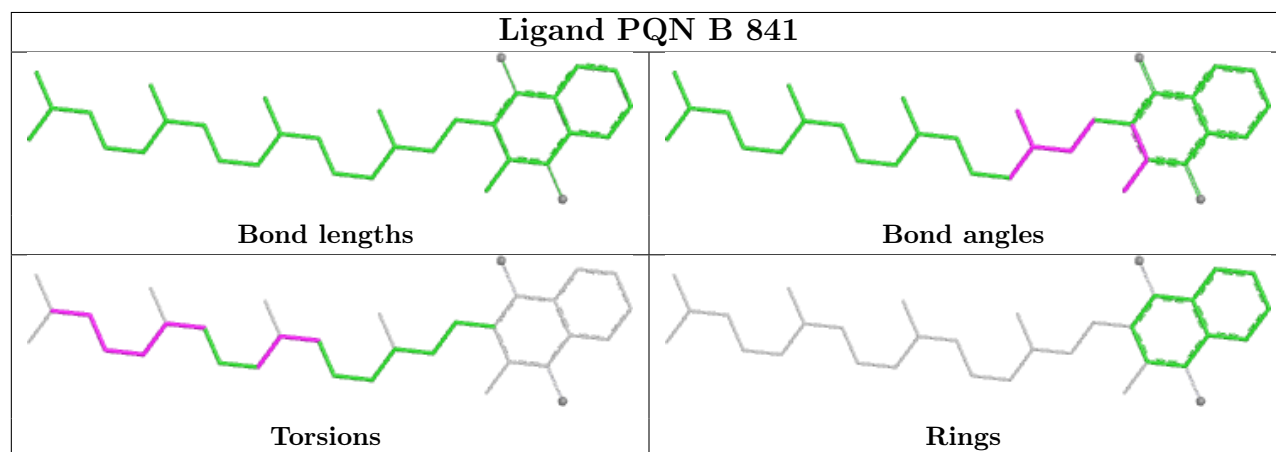
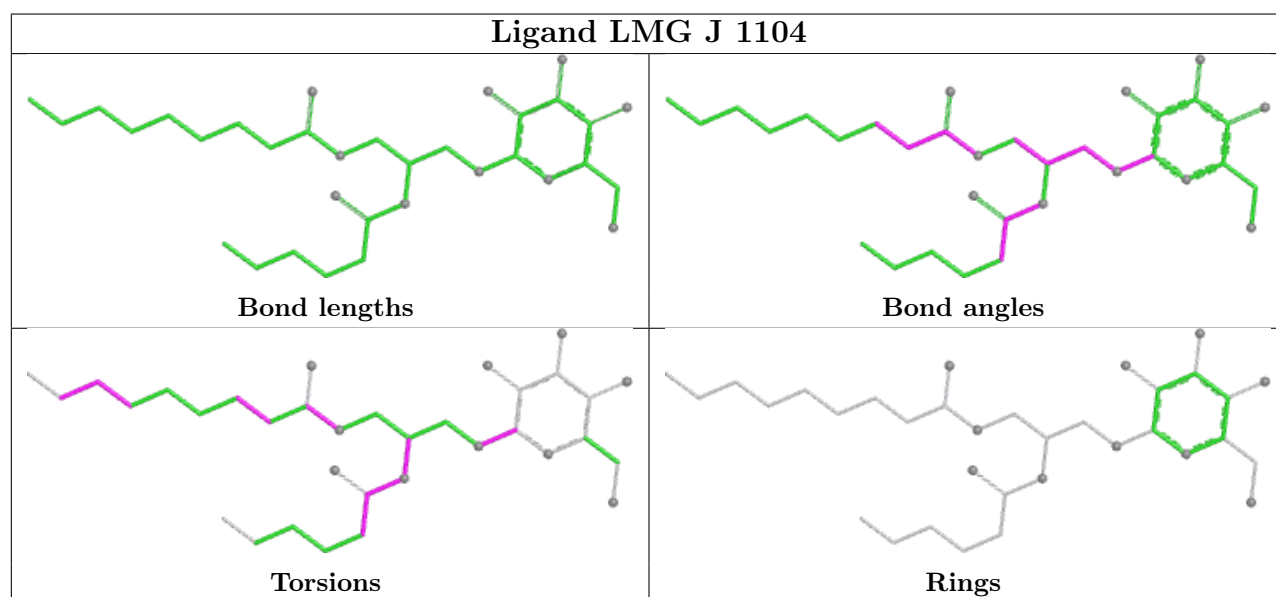
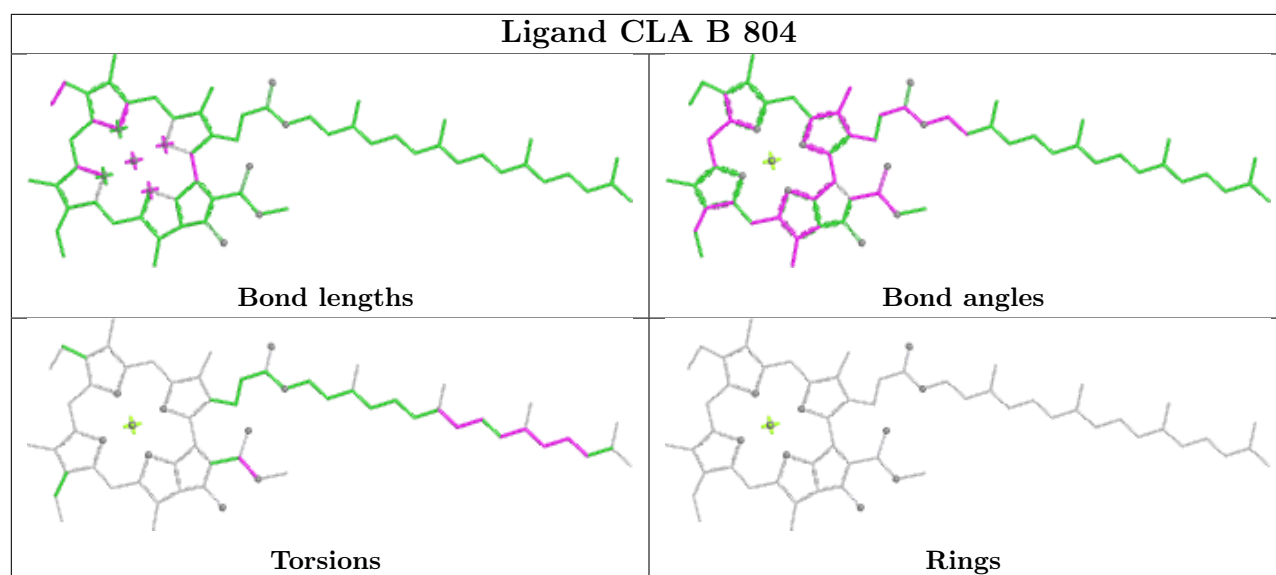
Torsions



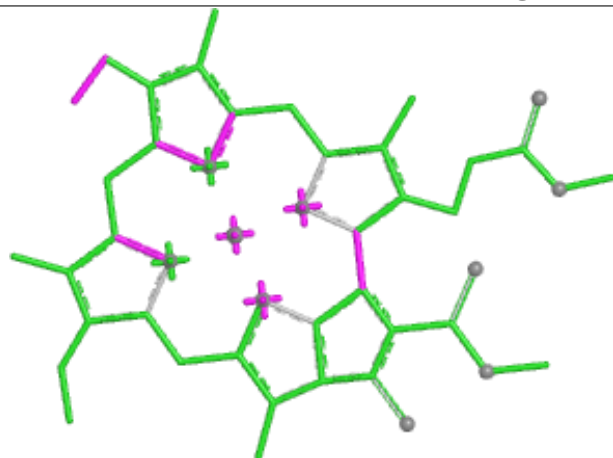
Rings



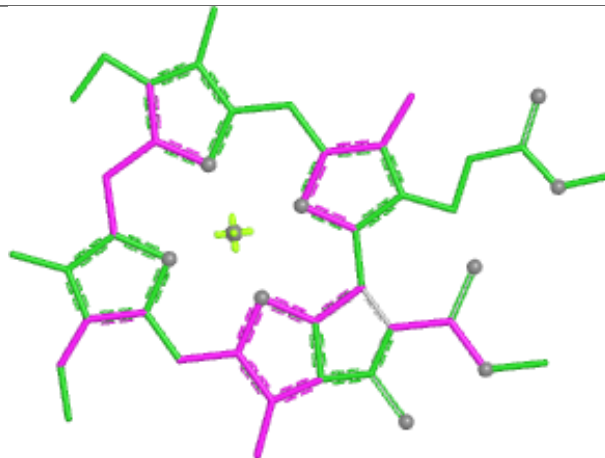




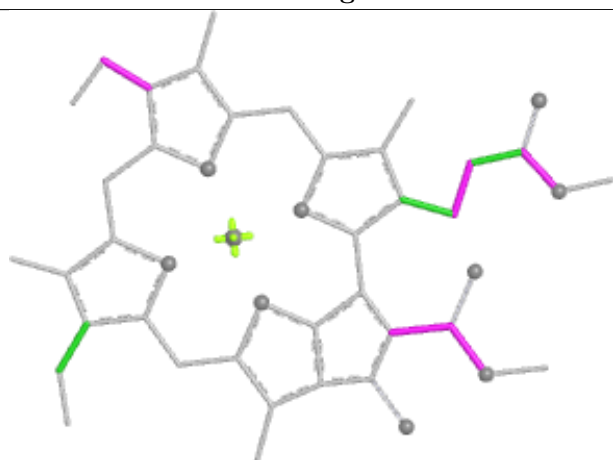
Ligand CLA A 816



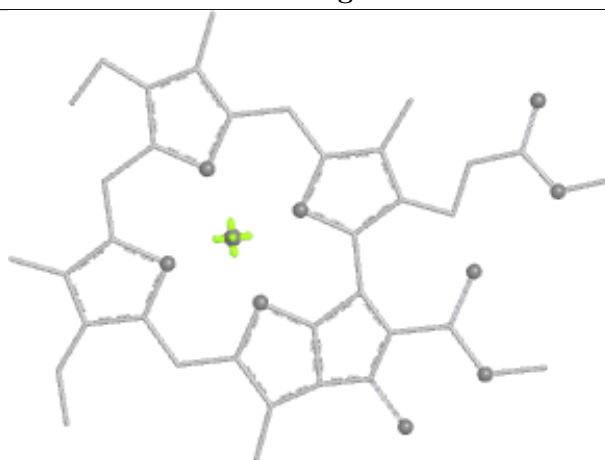
Bond lengths



Bond angles

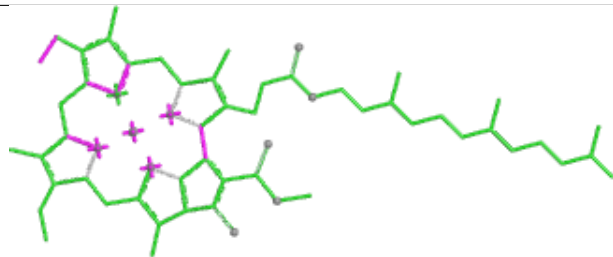


Torsions

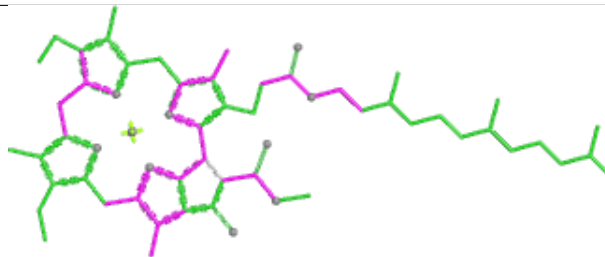


Rings

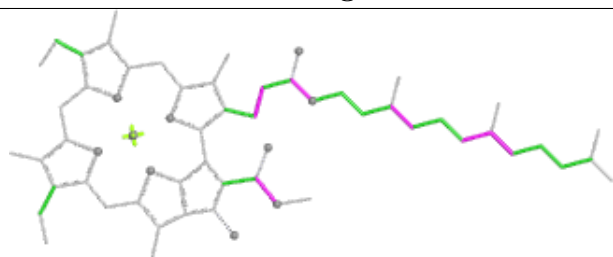
Ligand CLA A 842



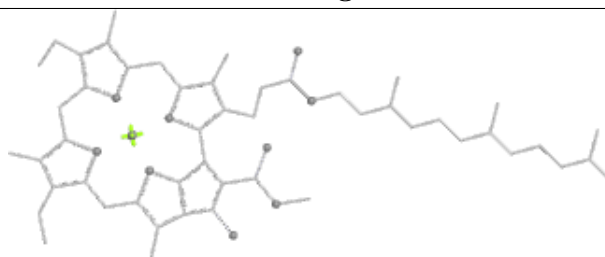
Bond lengths



Bond angles

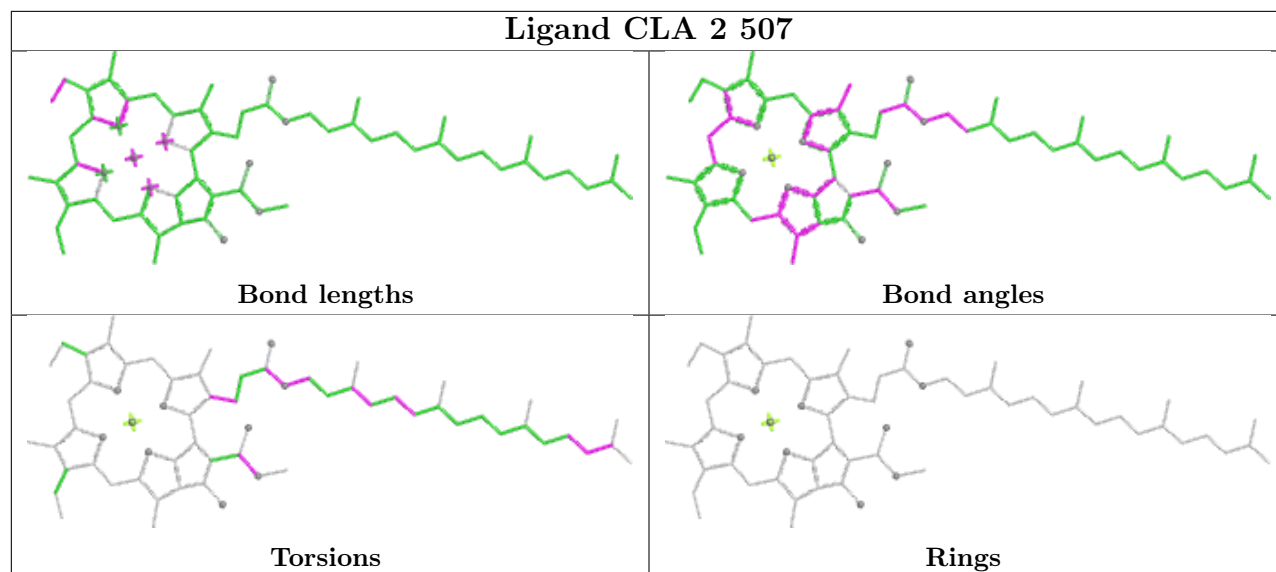


Torsions

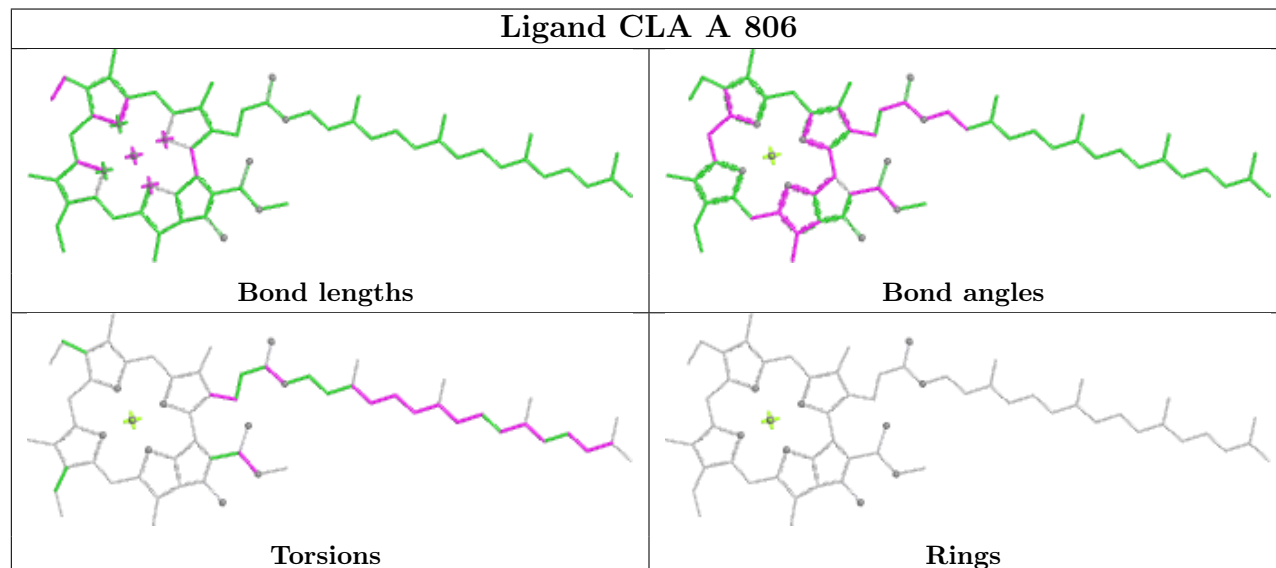


Rings

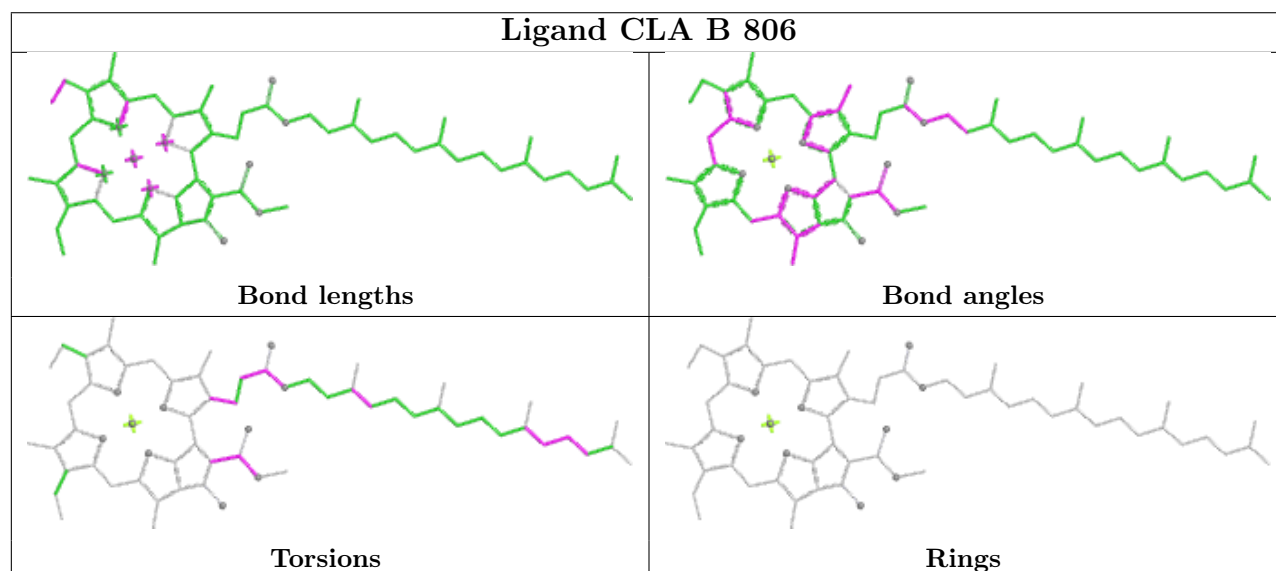
Ligand CLA 2 507



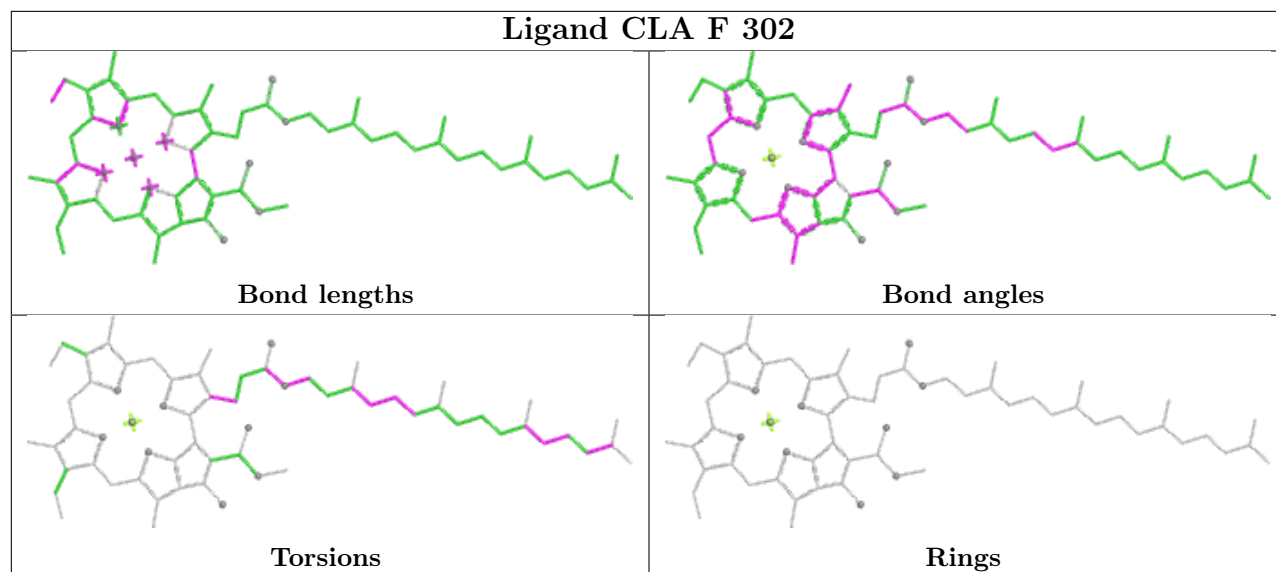
Ligand CLA A 806



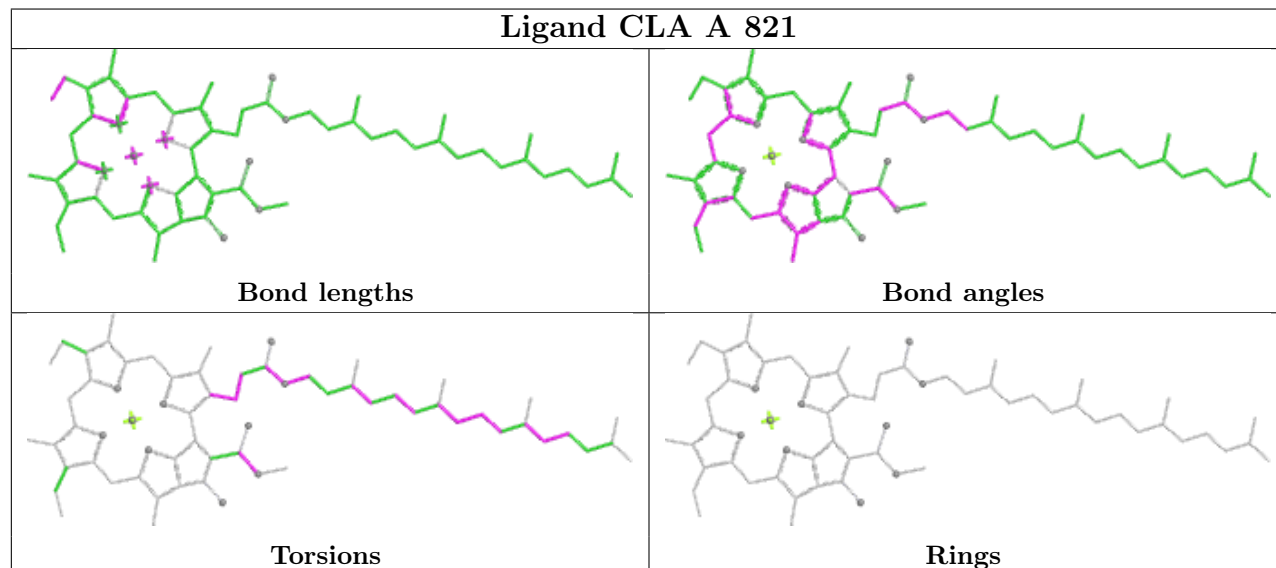
Ligand CLA B 806



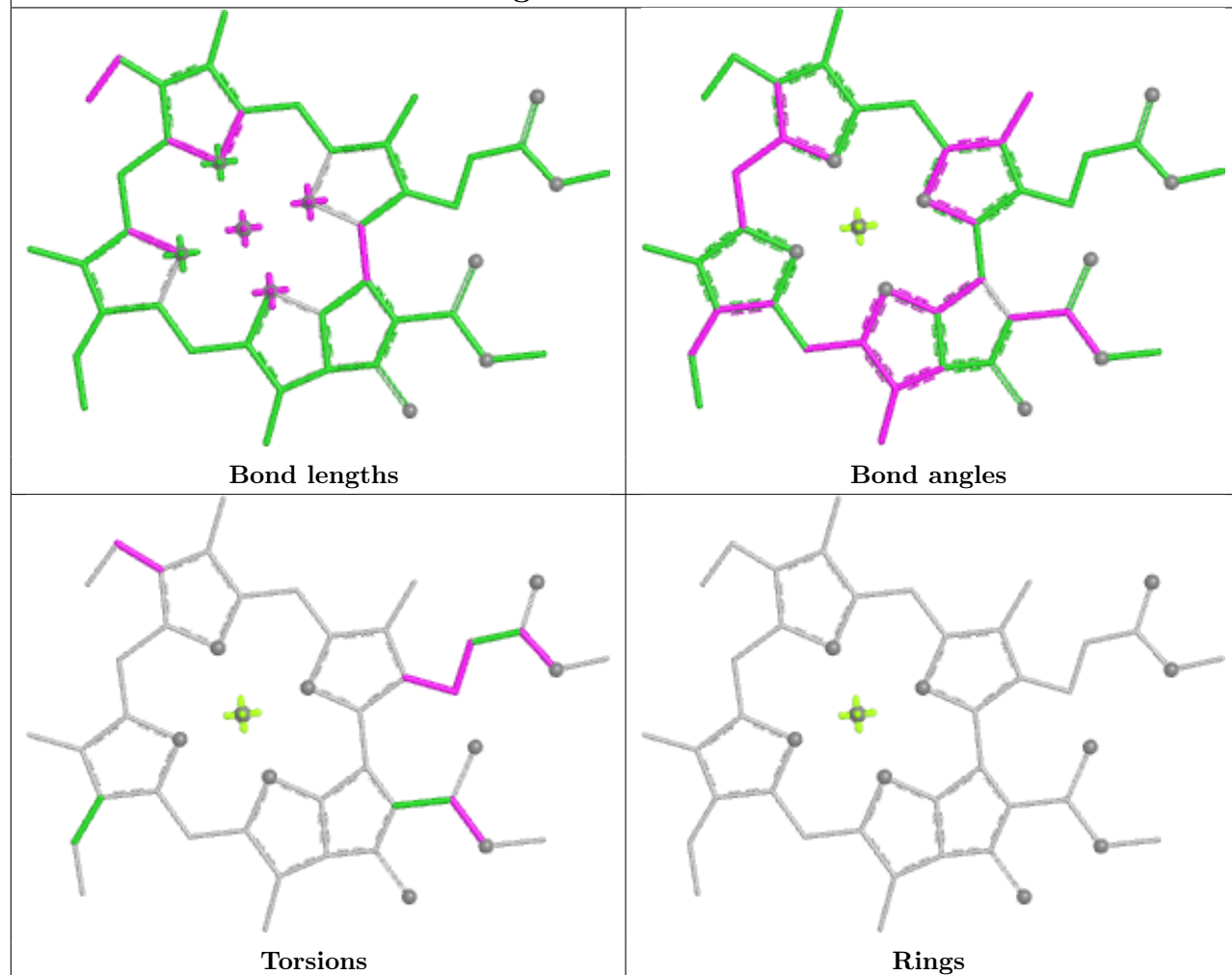
Ligand CLA F 302



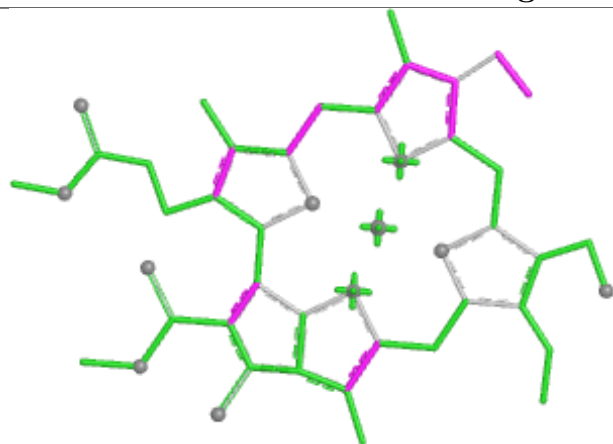
Ligand CLA A 821



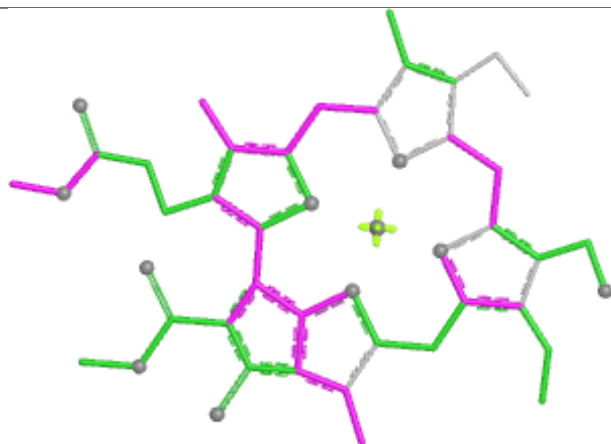
Ligand CLA B 821



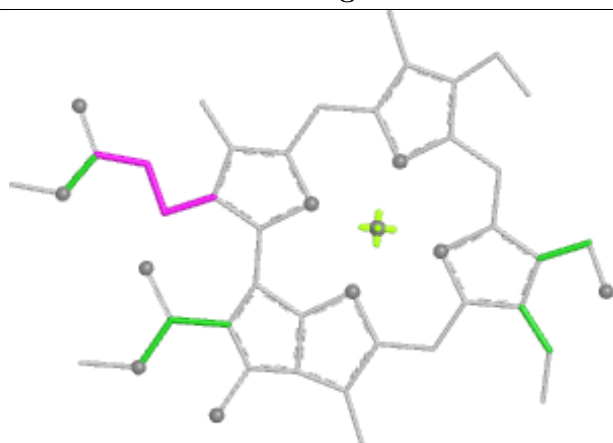
Ligand CHL 1 512



Bond lengths



Bond angles

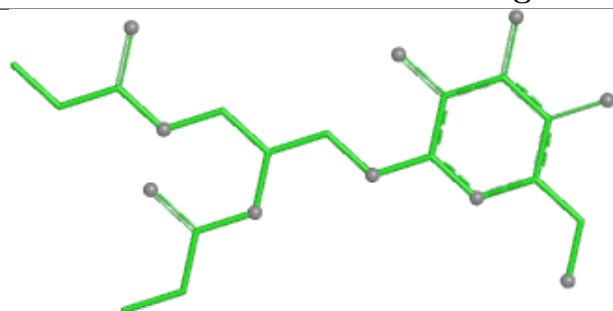


Torsions

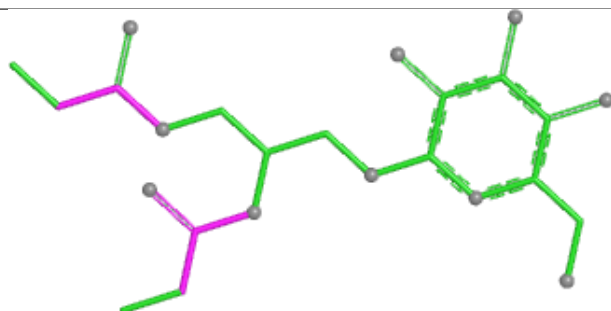


Rings

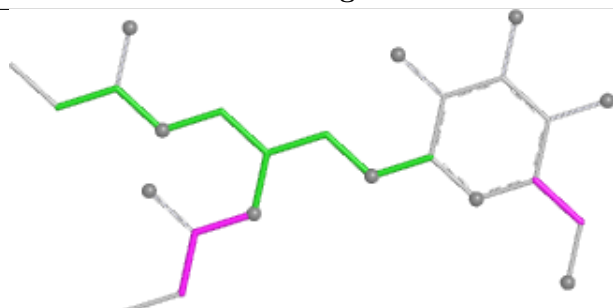
Ligand LMG 2 518



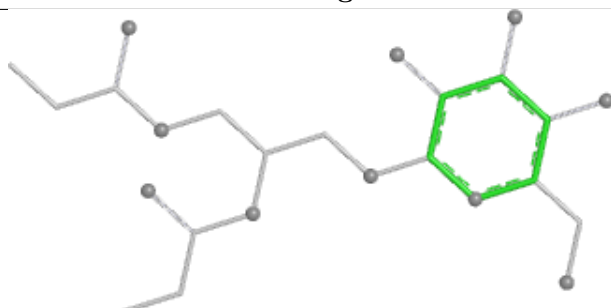
Bond lengths



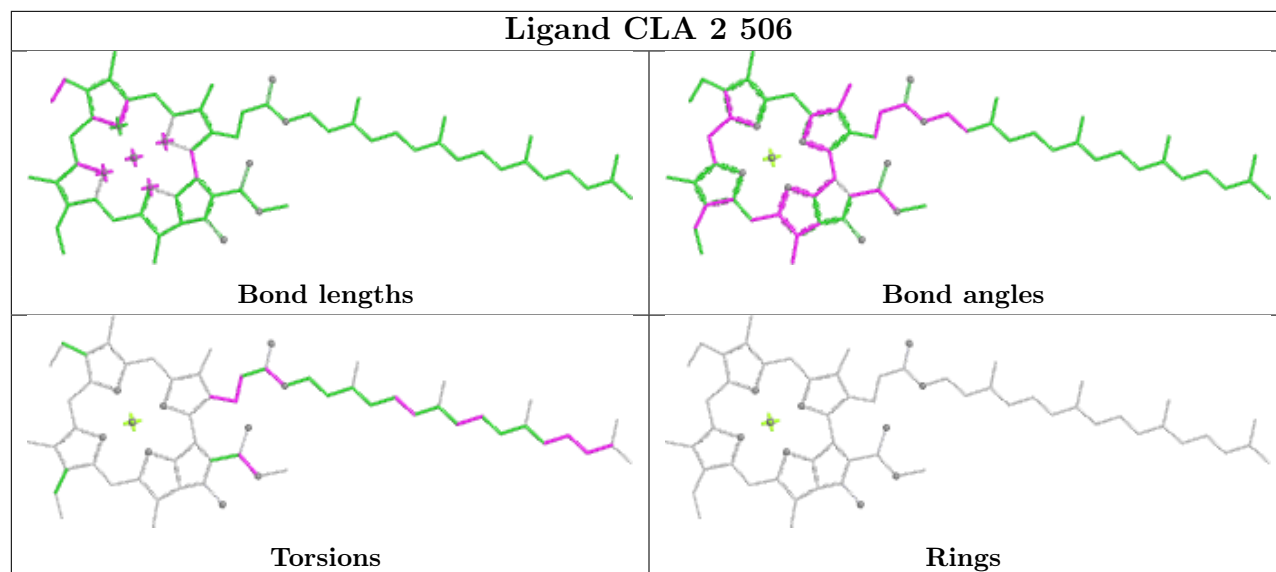
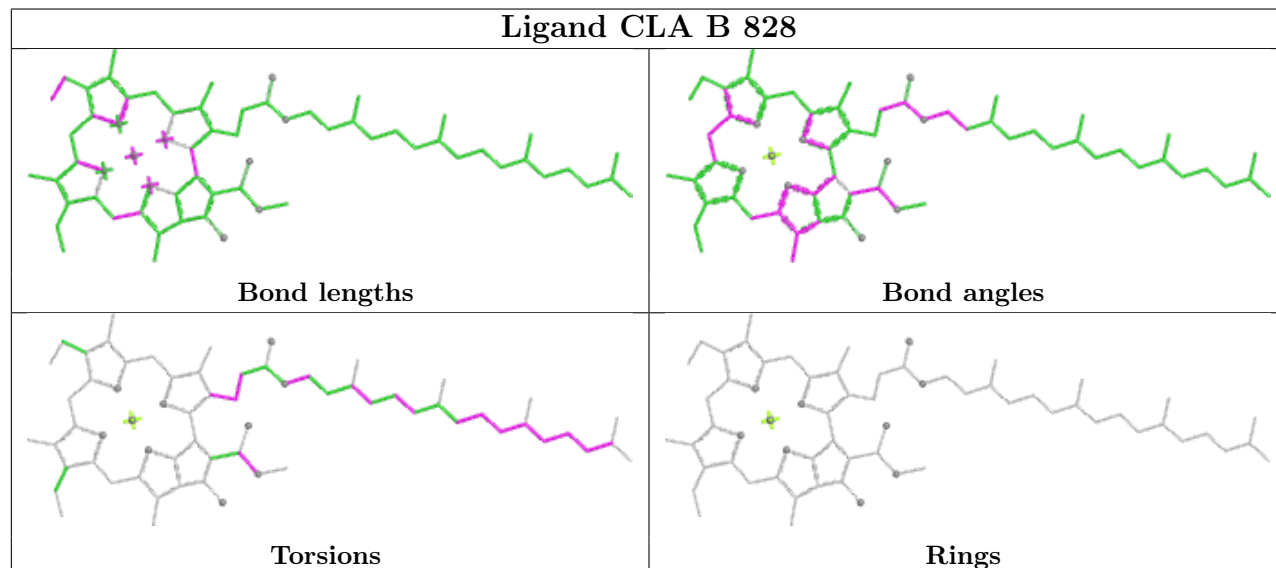
Bond angles

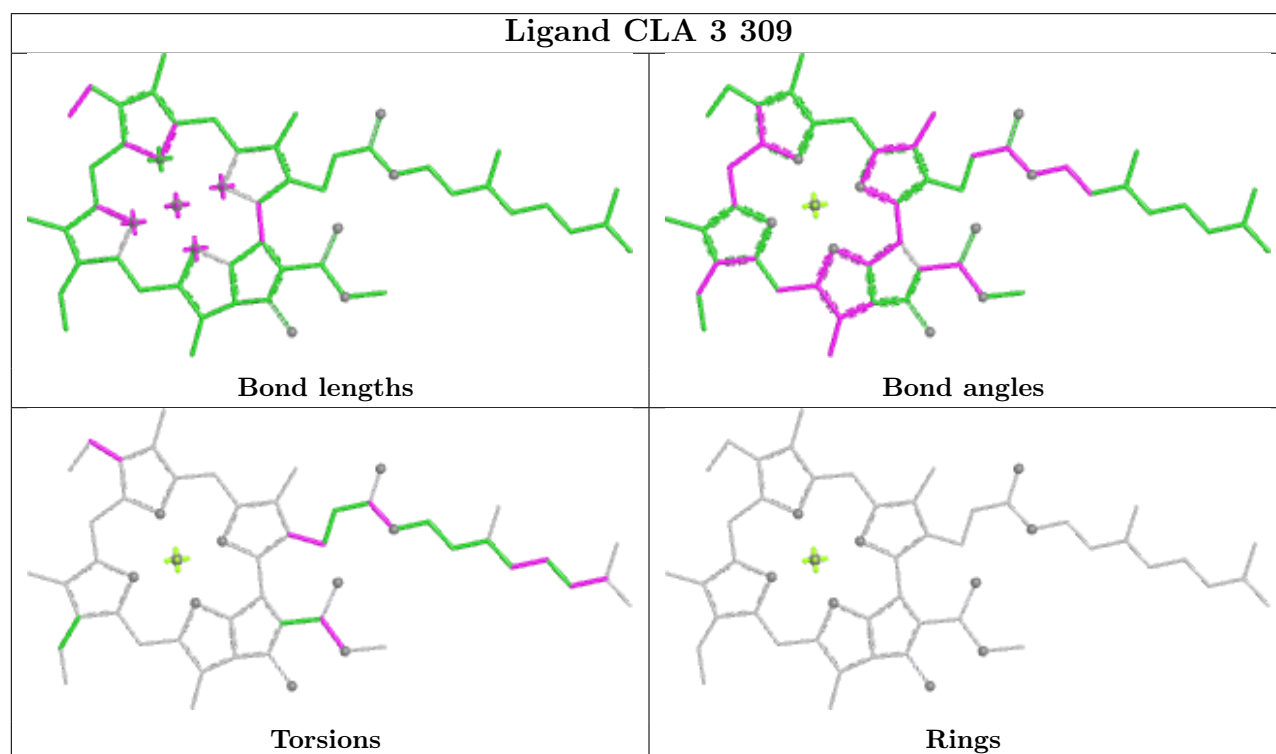
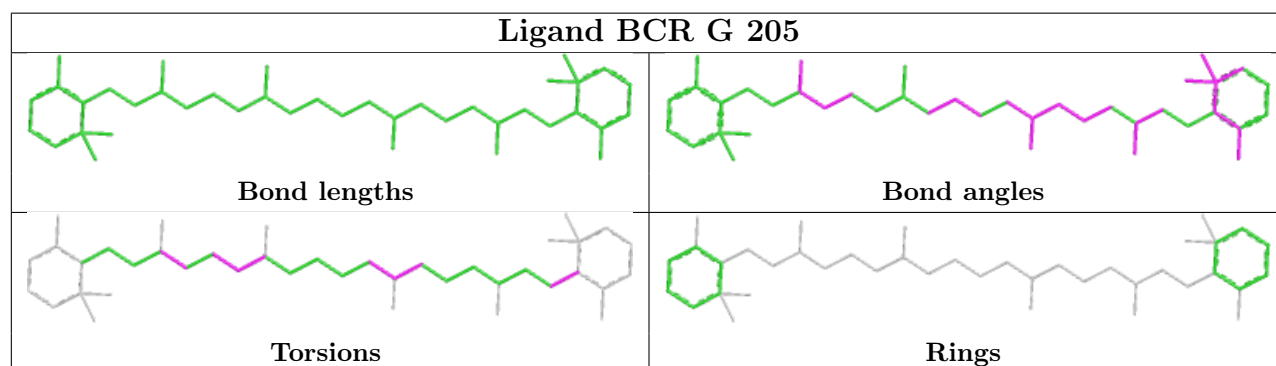
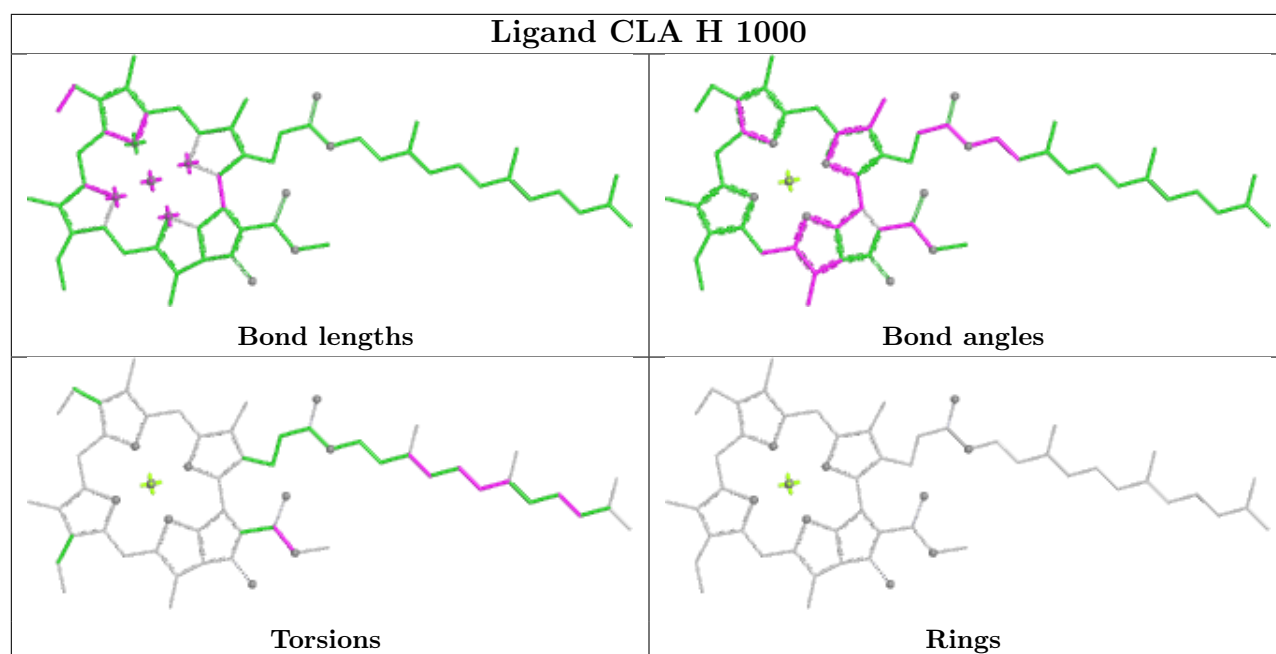


Torsions

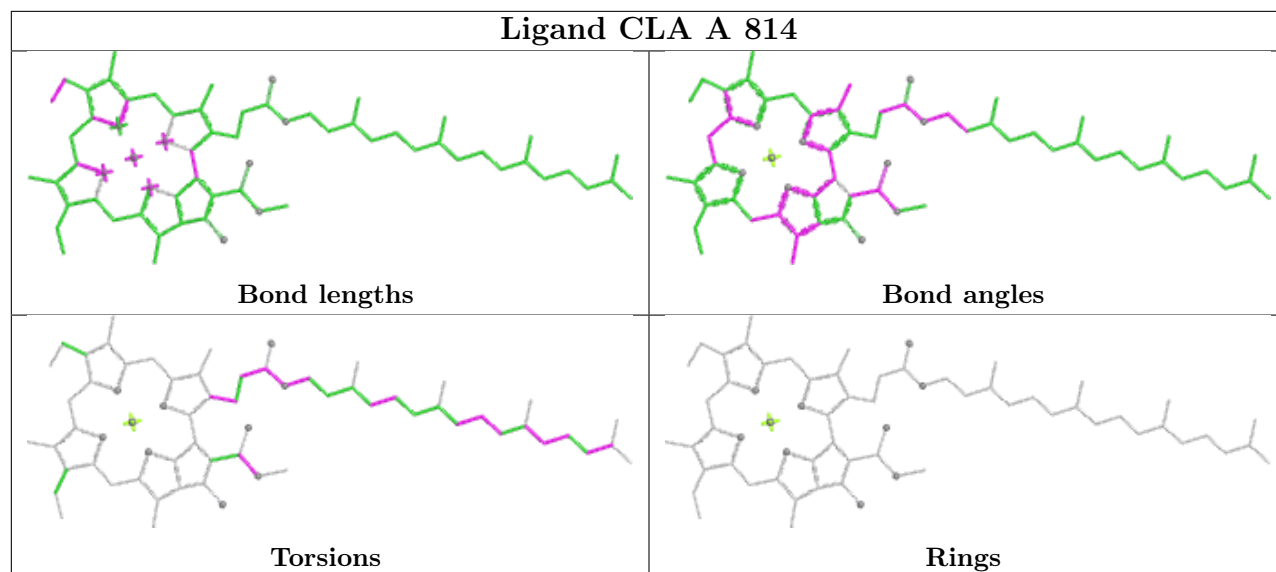


Rings

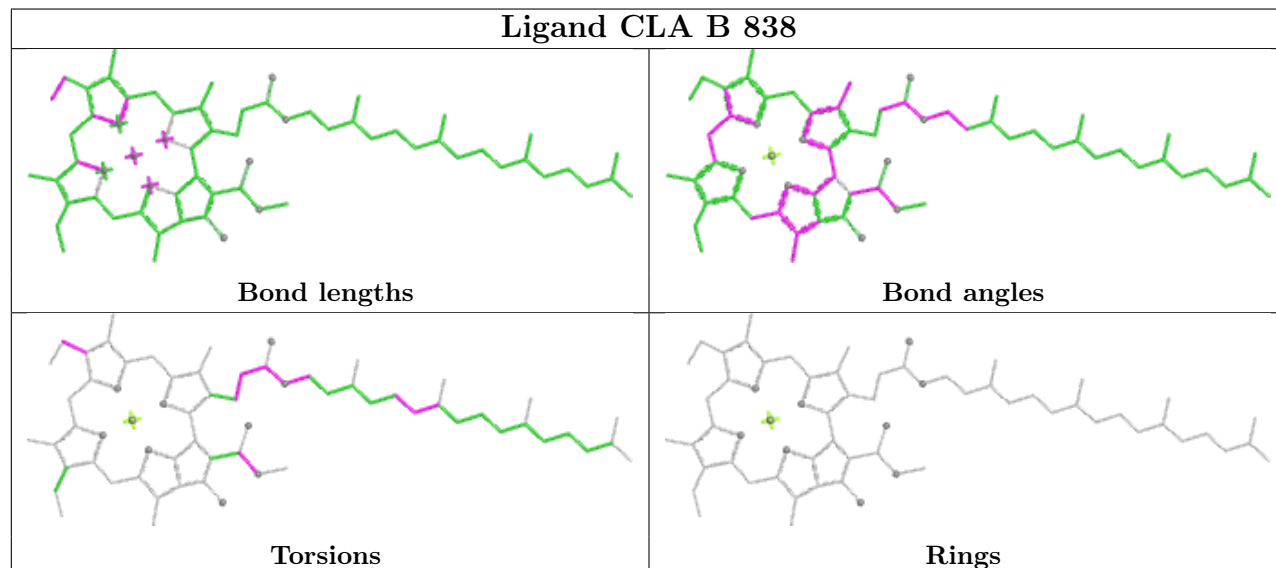
Ligand CLA 2 506**Ligand CLA B 828**



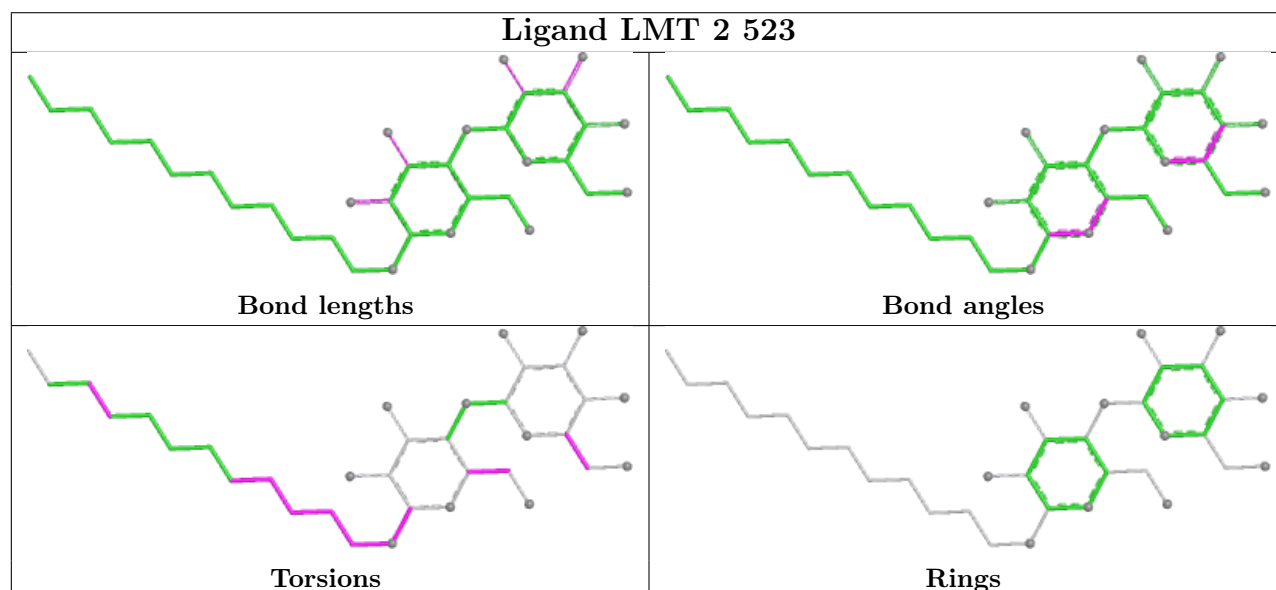
Ligand CLA A 814



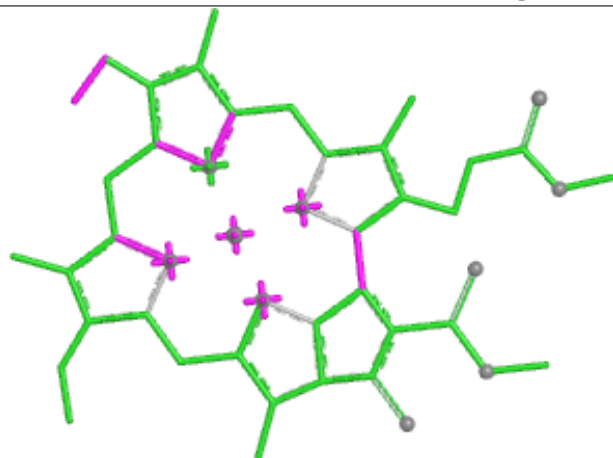
Ligand CLA B 838



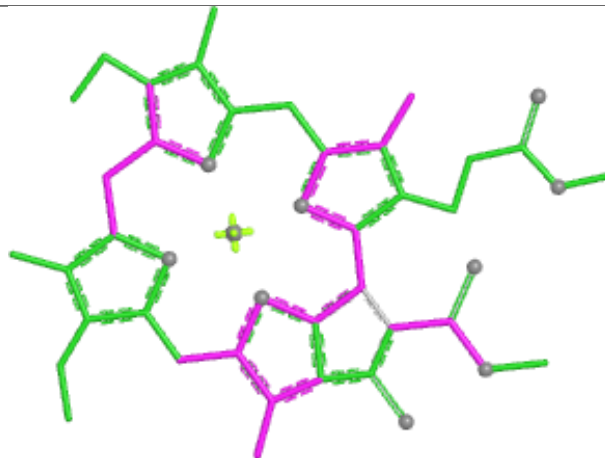
Ligand LMT 2 523



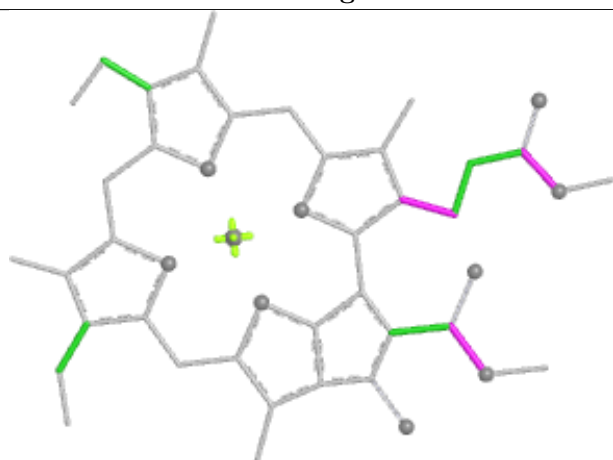
Ligand CLA G 203



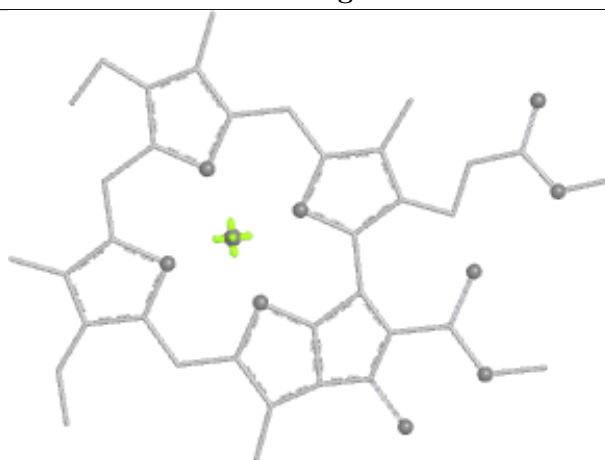
Bond lengths



Bond angles

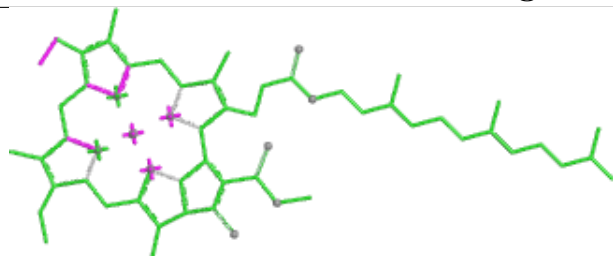


Torsions

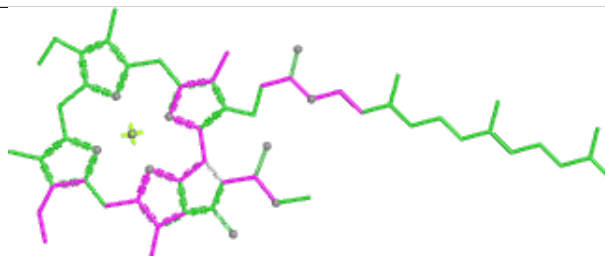


Rings

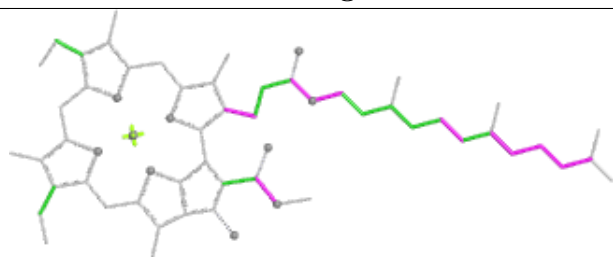
Ligand CLA 4 308



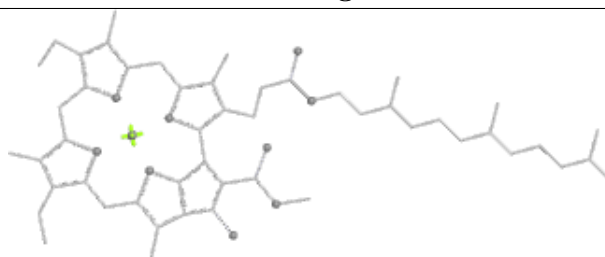
Bond lengths



Bond angles

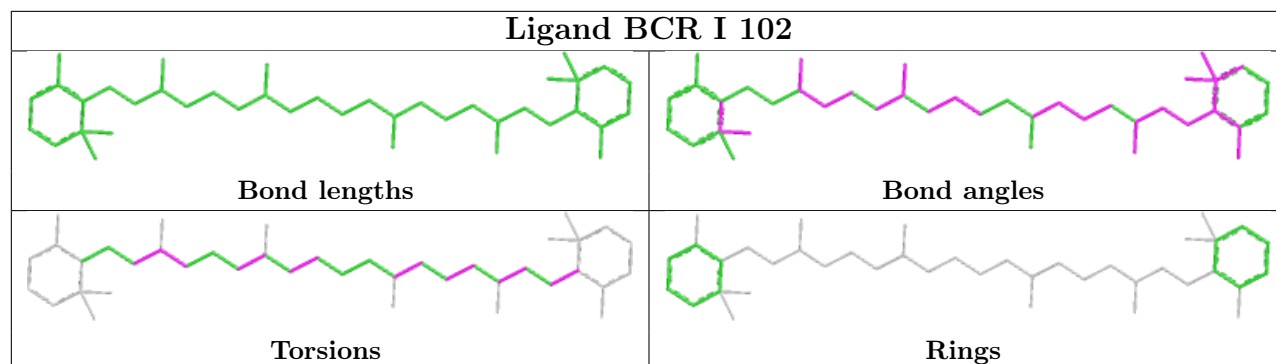


Torsions

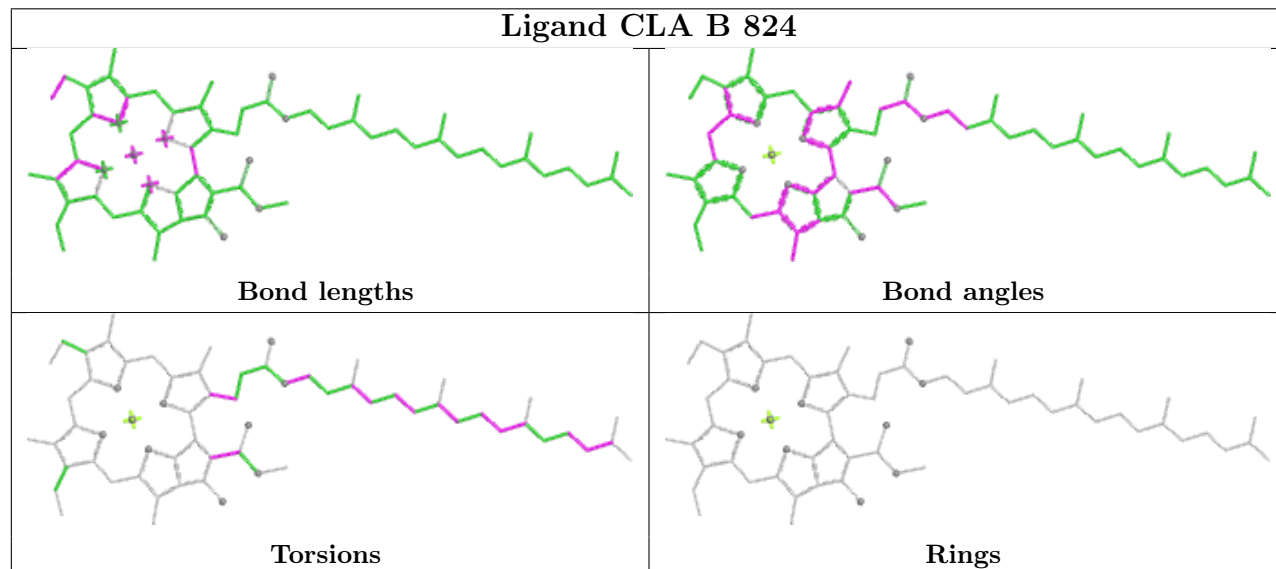


Rings

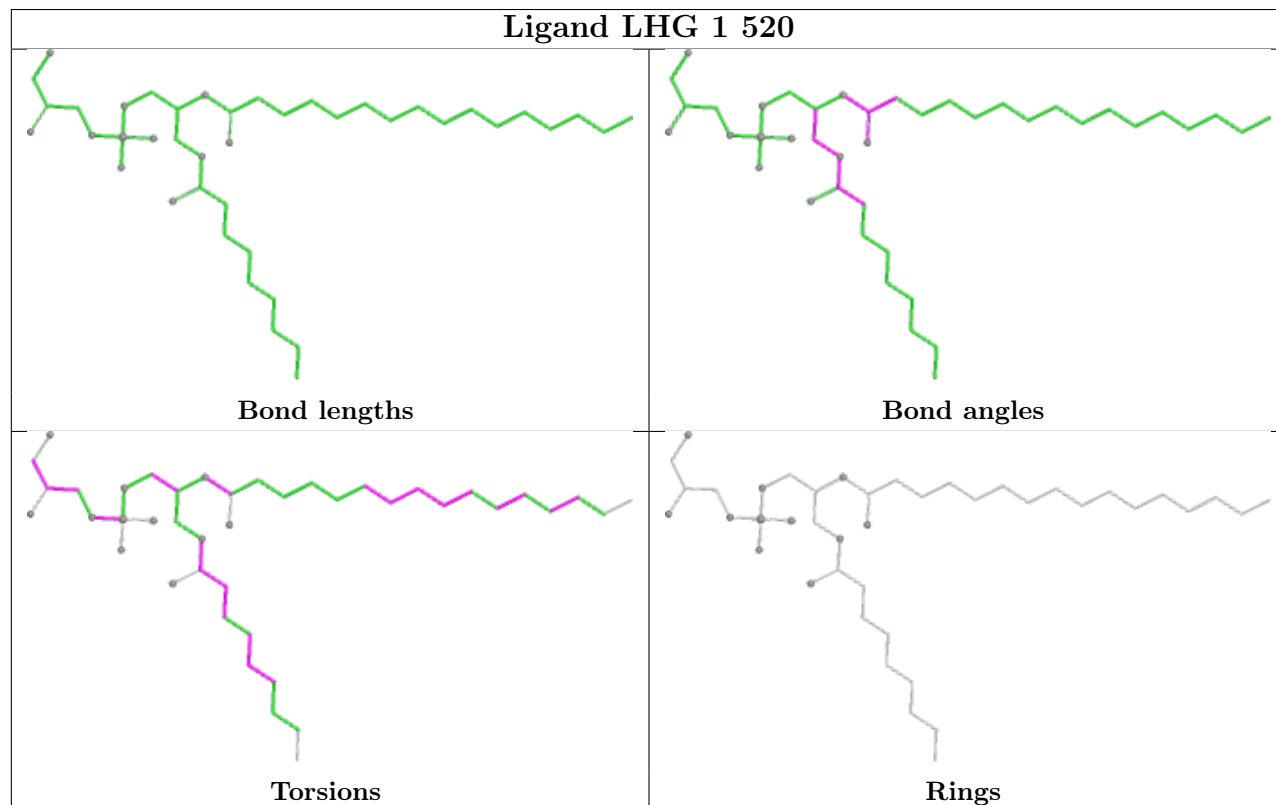
Ligand BCR I 102

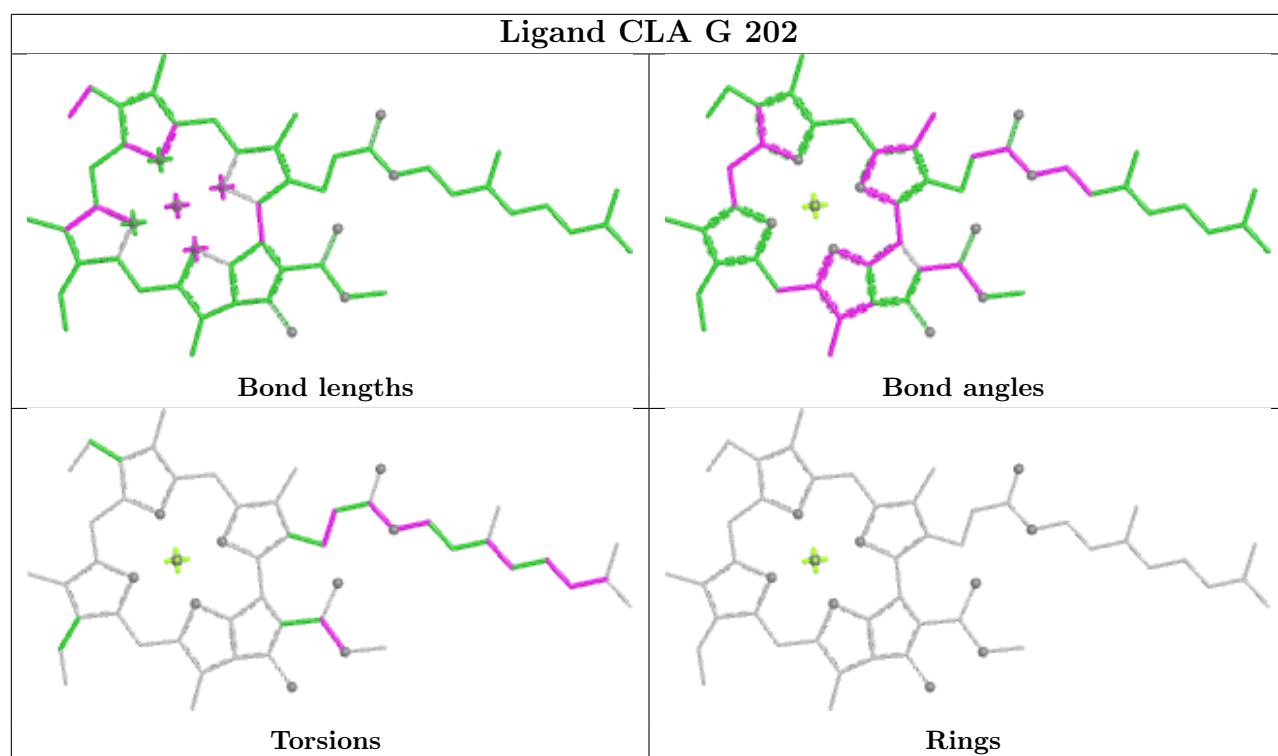


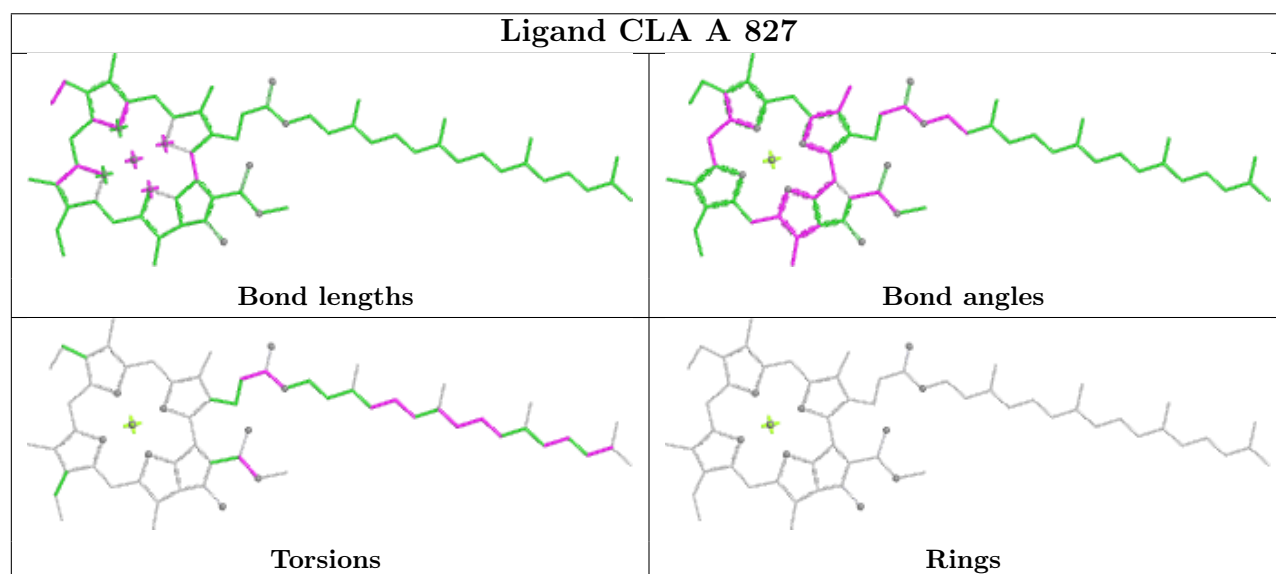
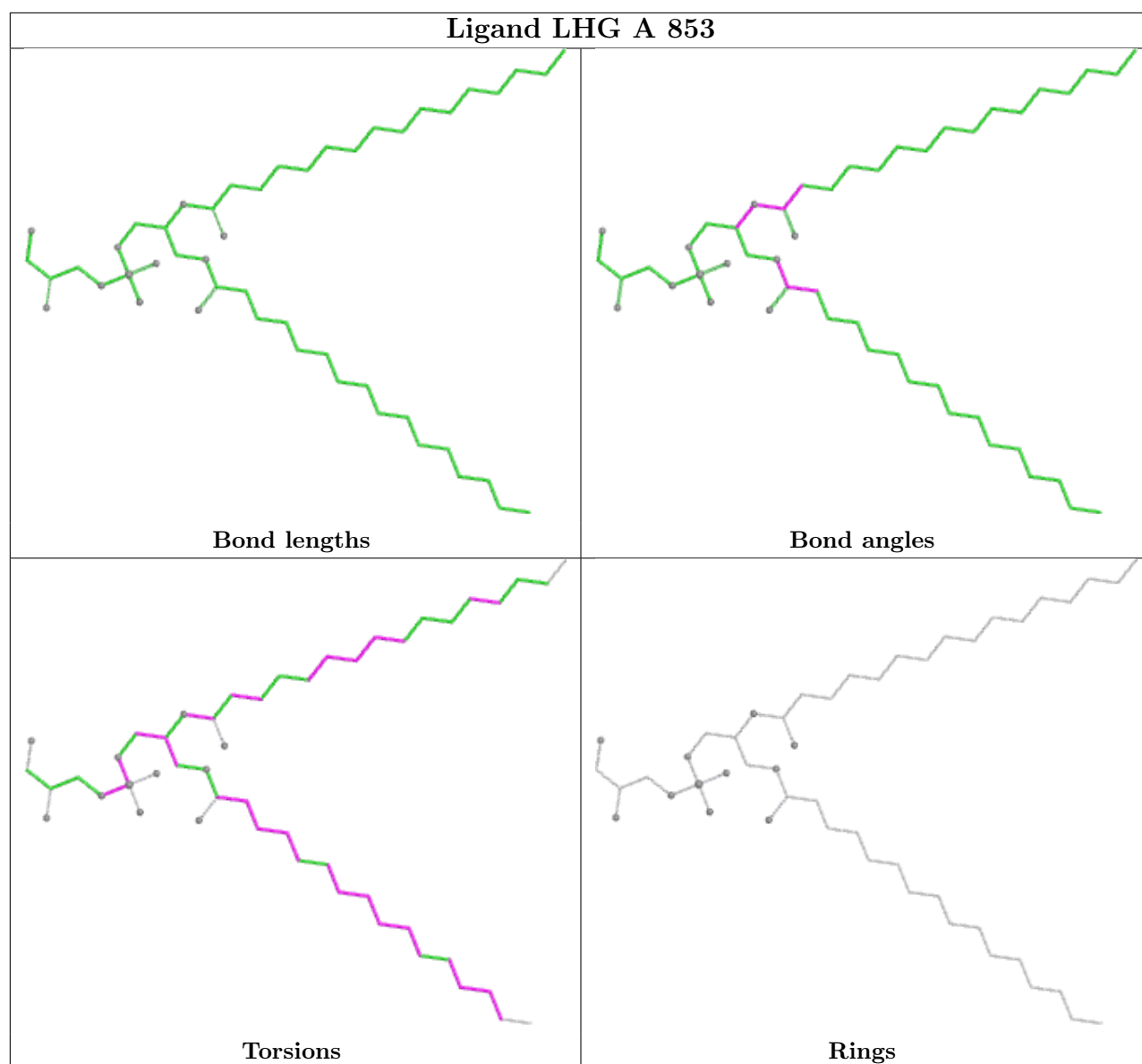
Ligand CLA B 824

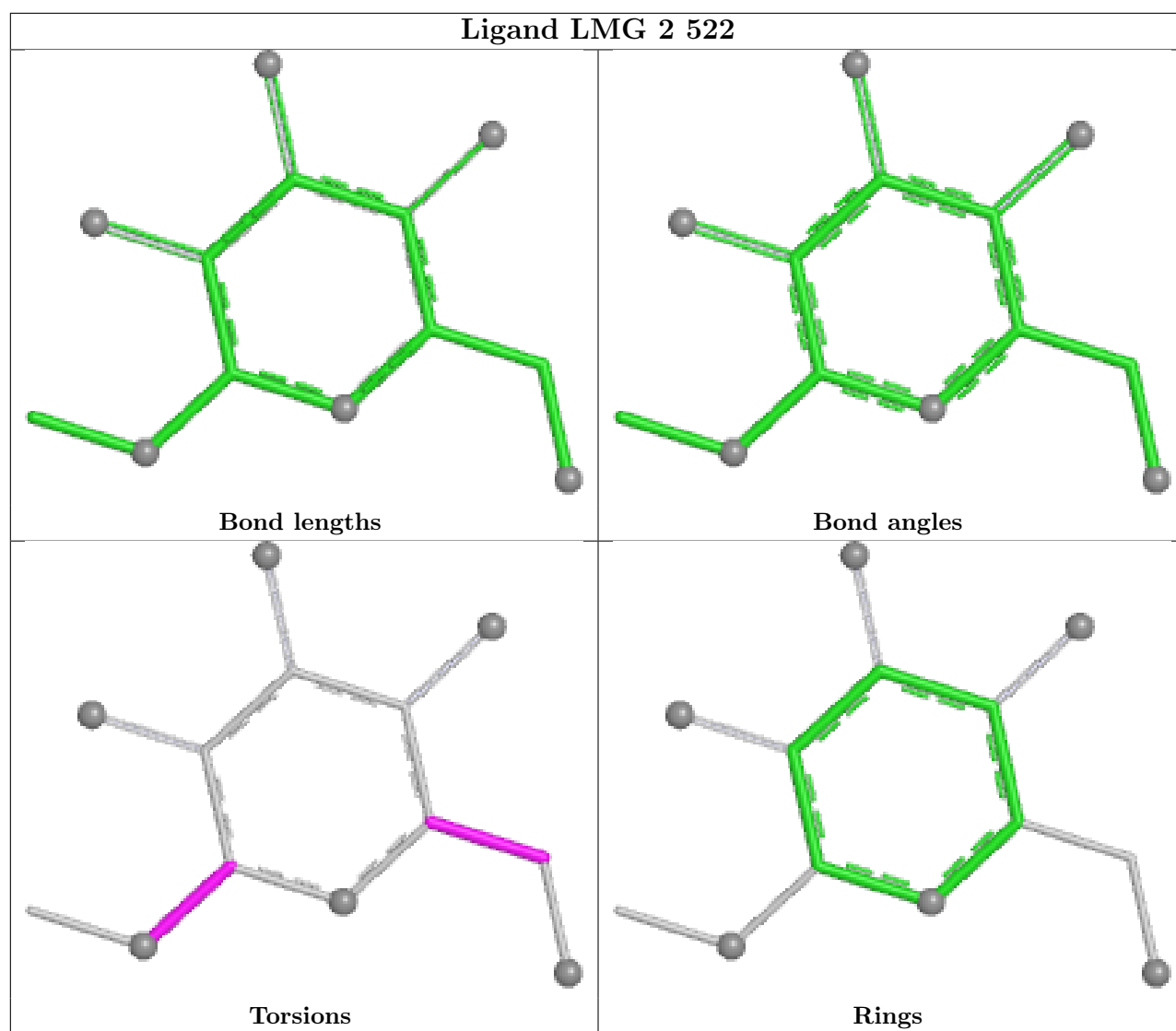


Ligand LHG 1 520

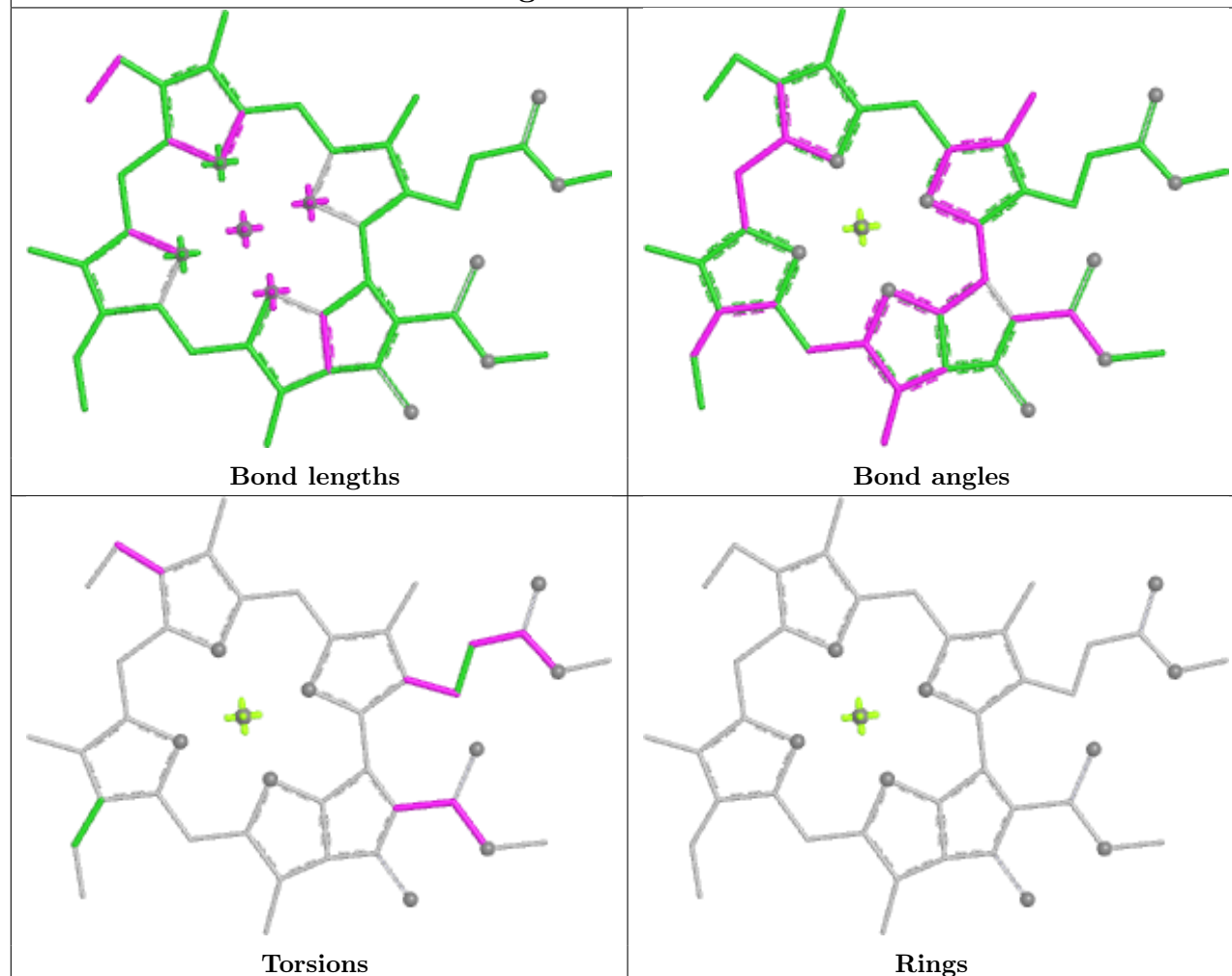




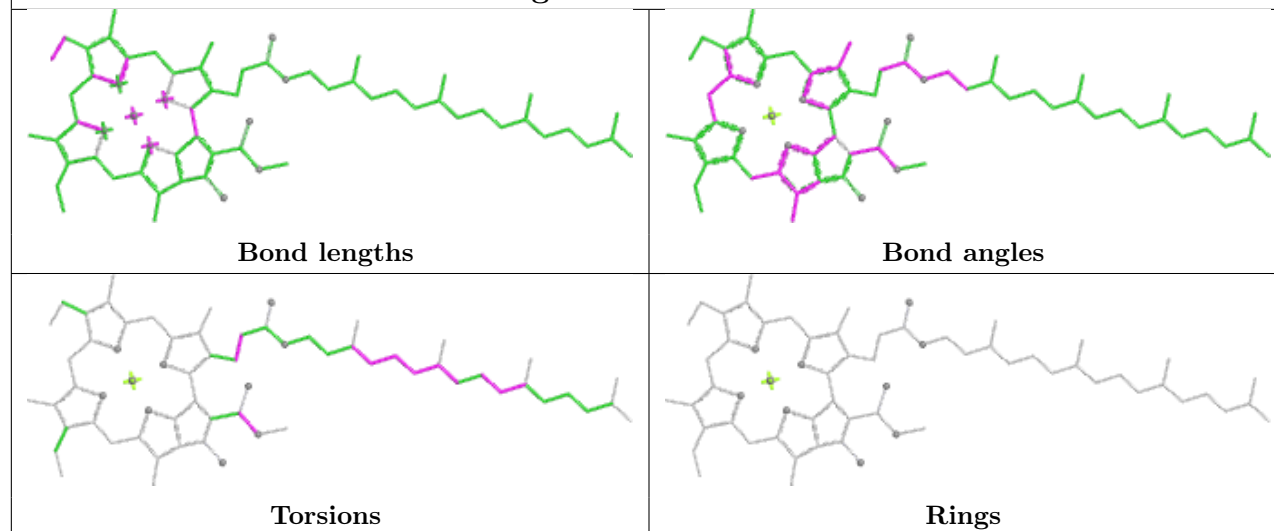




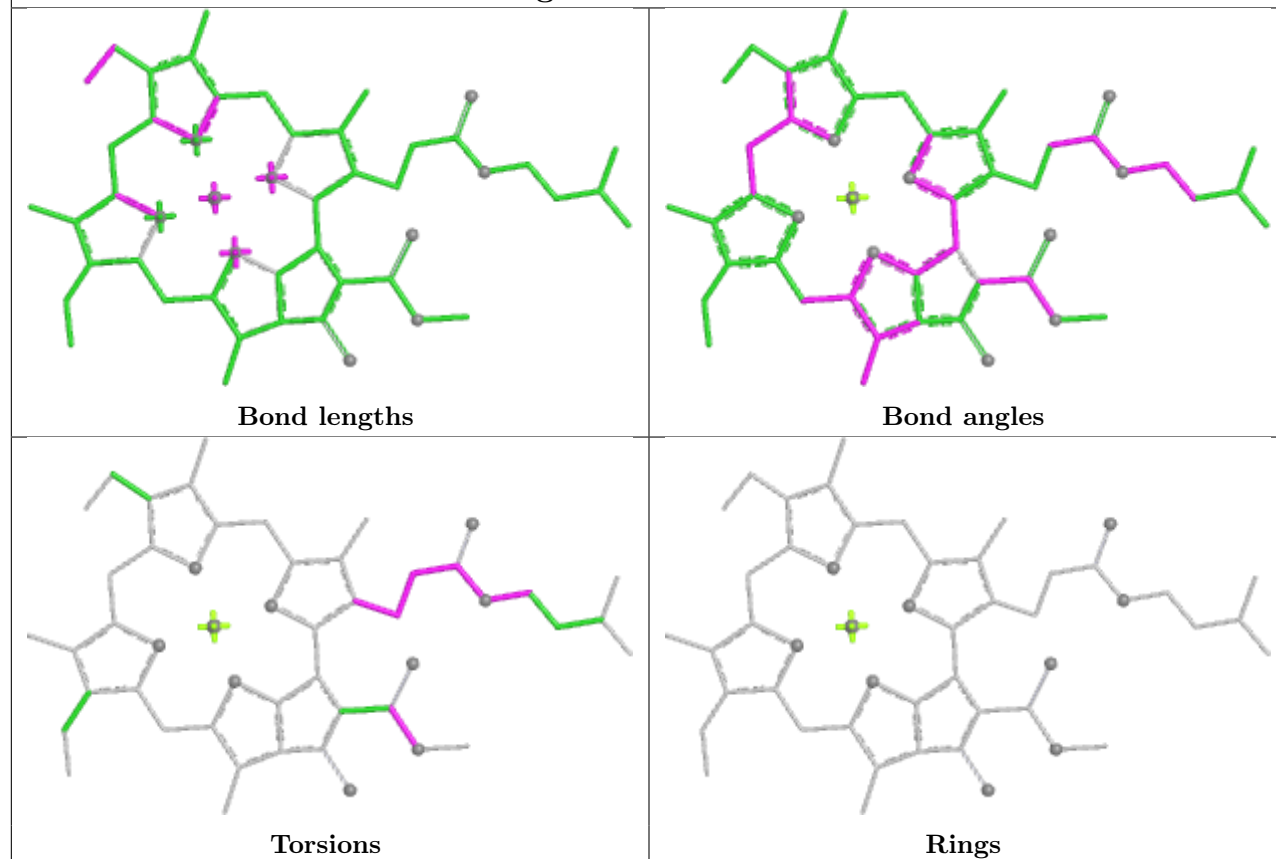
Ligand CLA 1 511



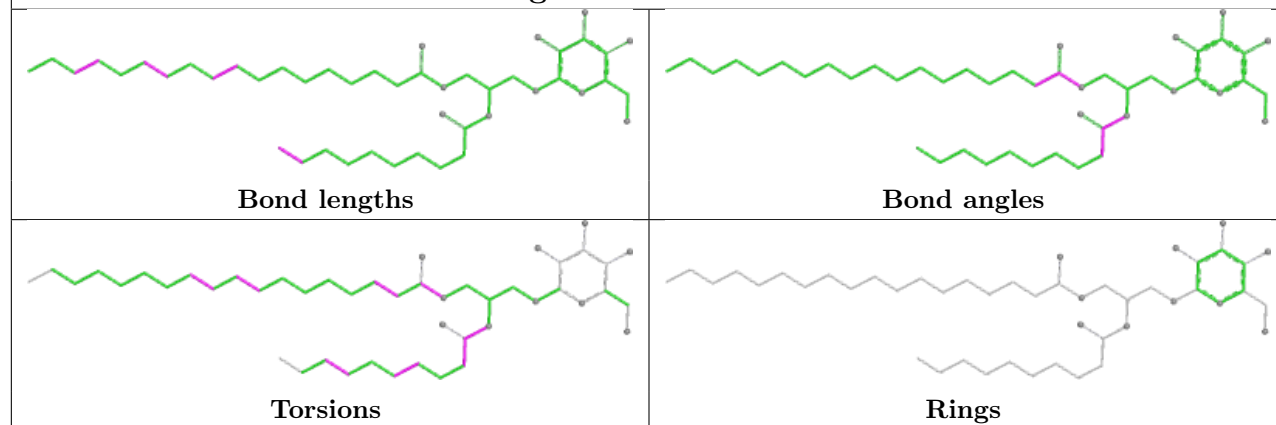
Ligand CLA A 819

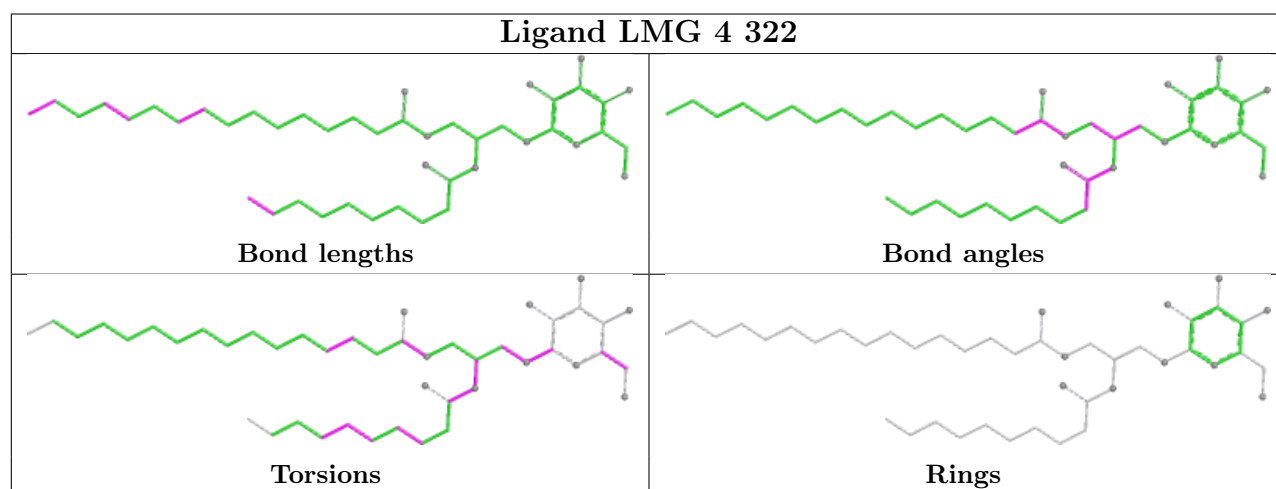
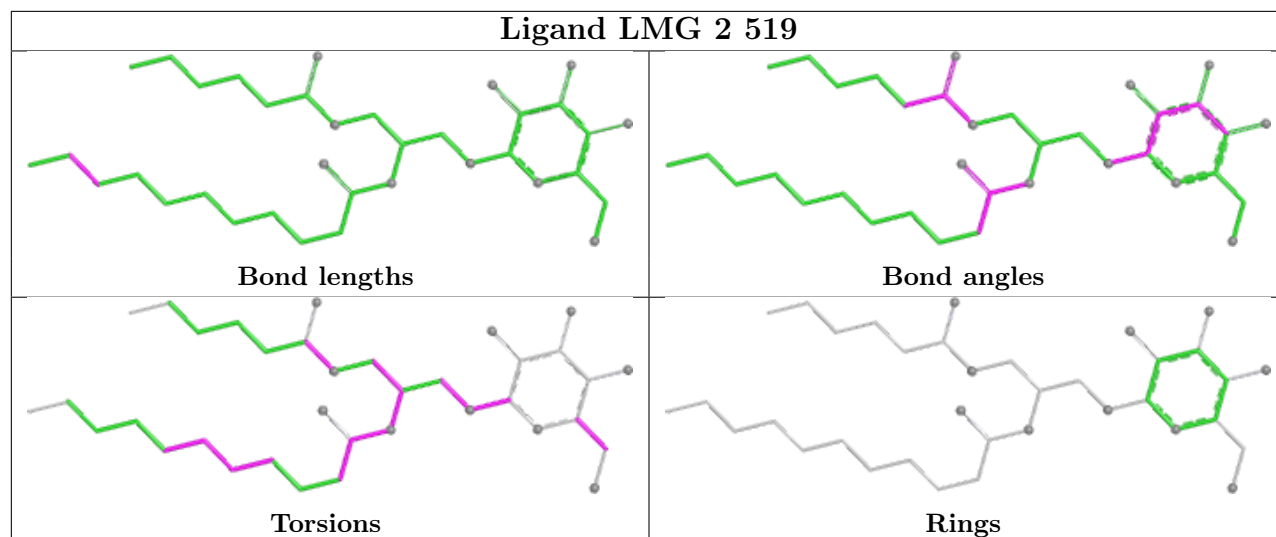


Ligand CLA 2 509

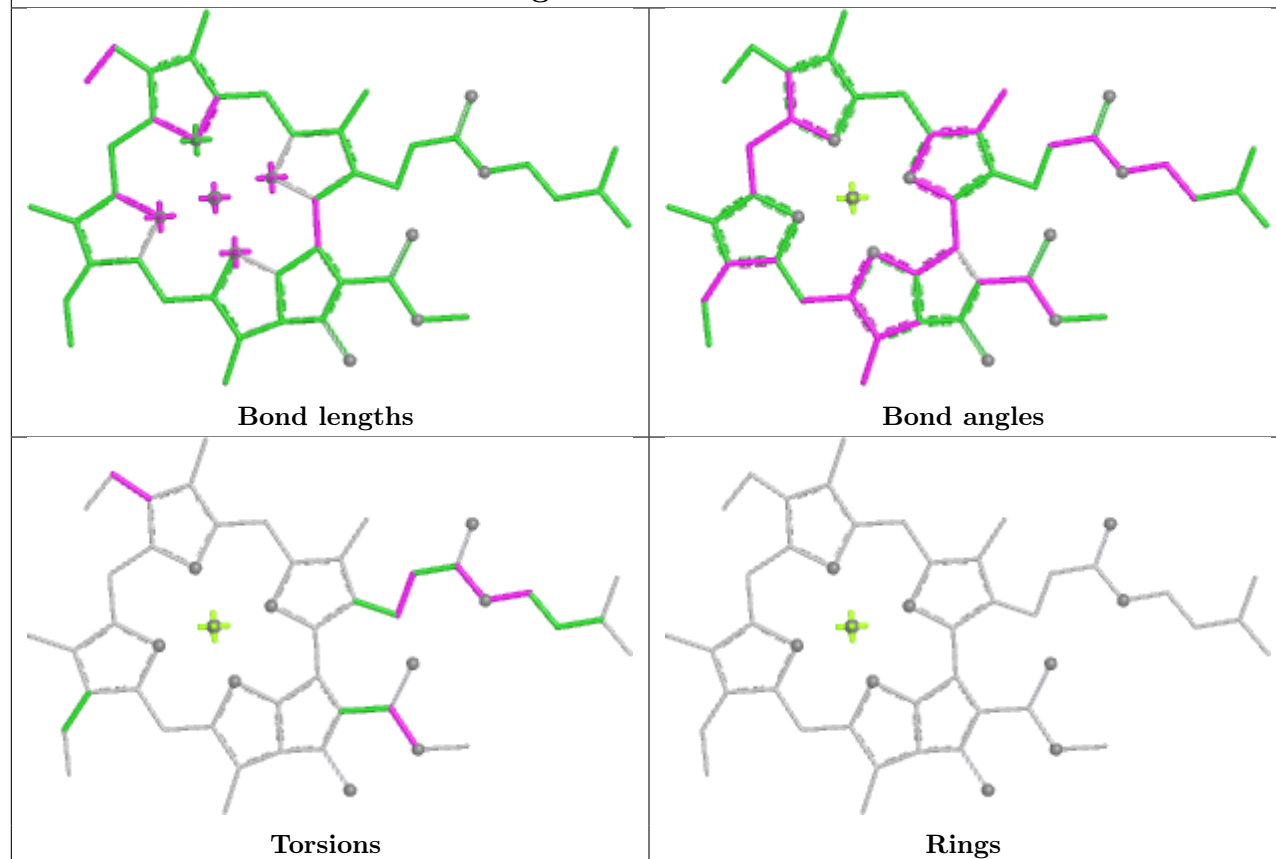


Ligand LMG F 304

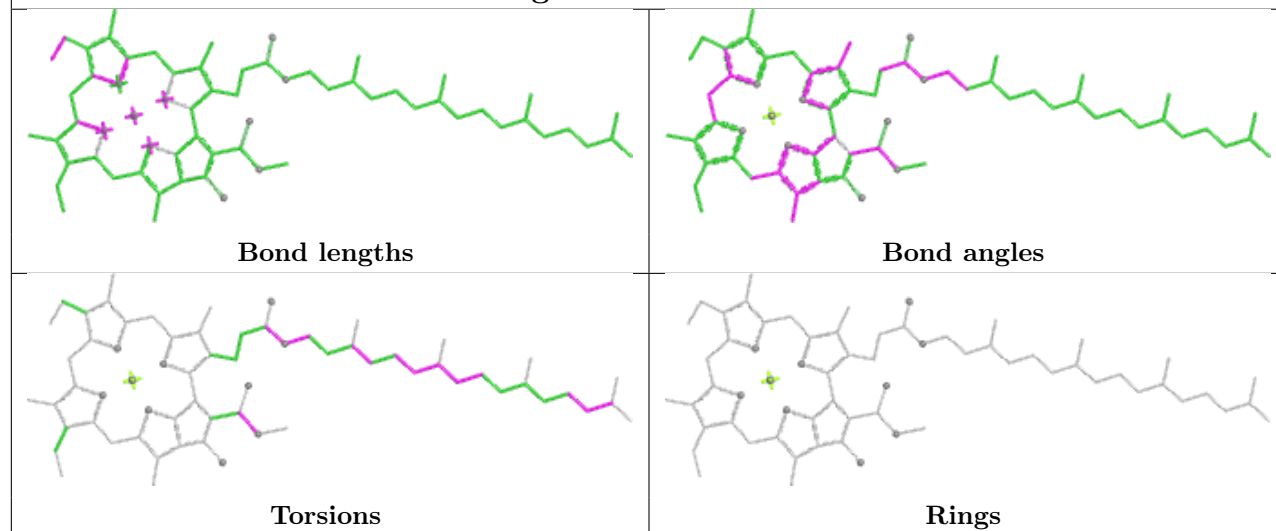




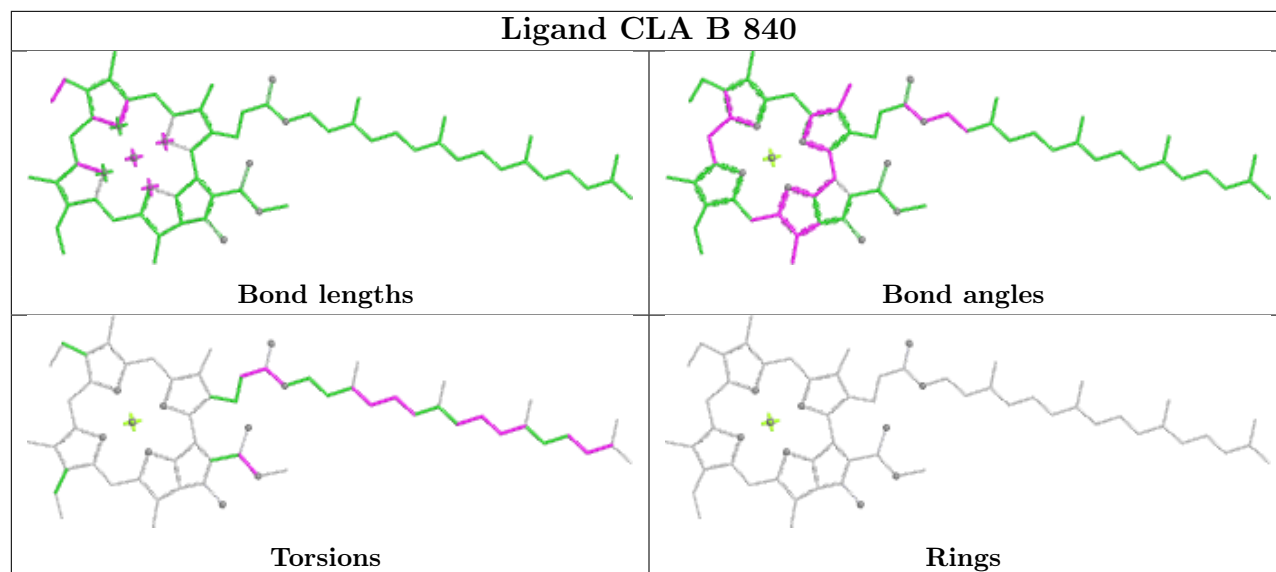
Ligand CLA A 820



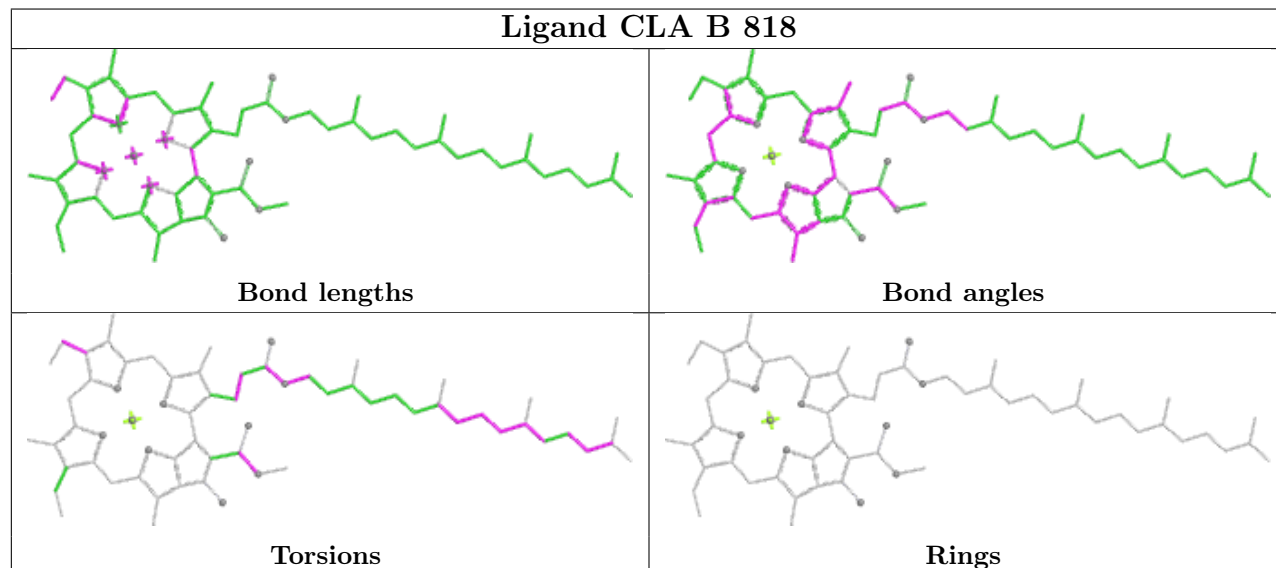
Ligand CLA A 840



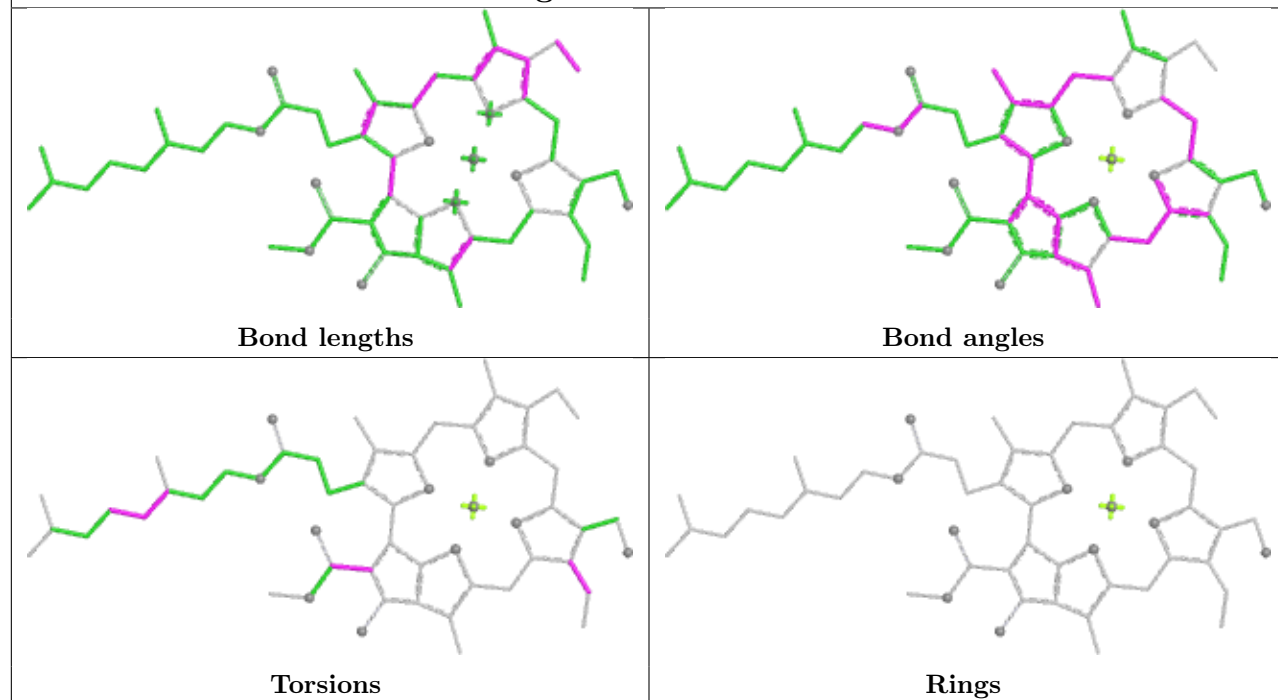
Ligand CLA B 840



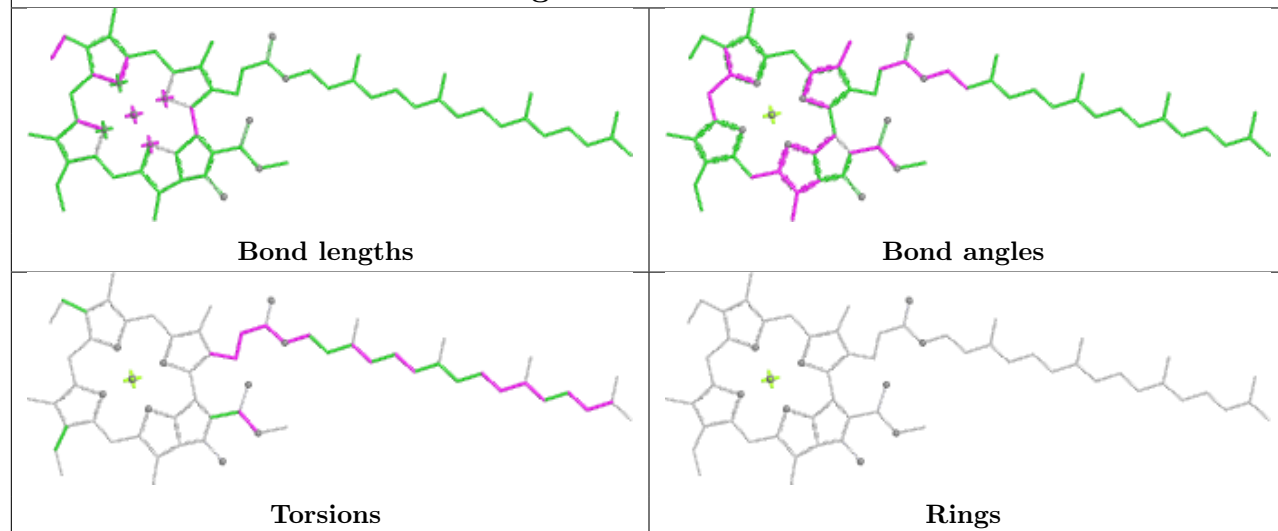
Ligand CLA B 818



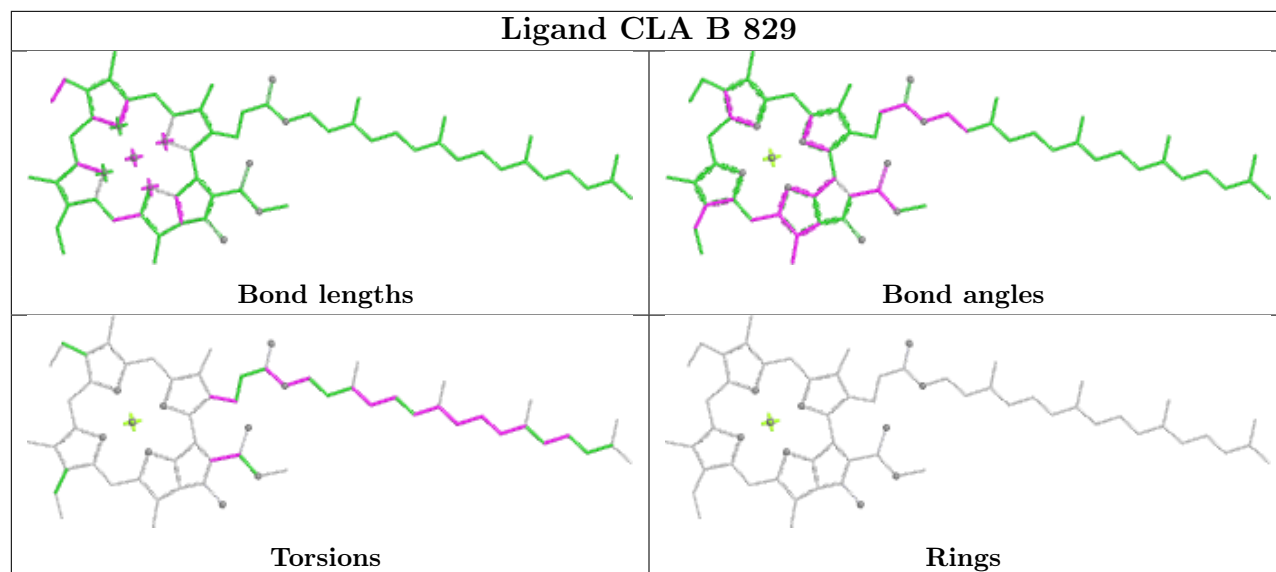
Ligand CHL 1 521



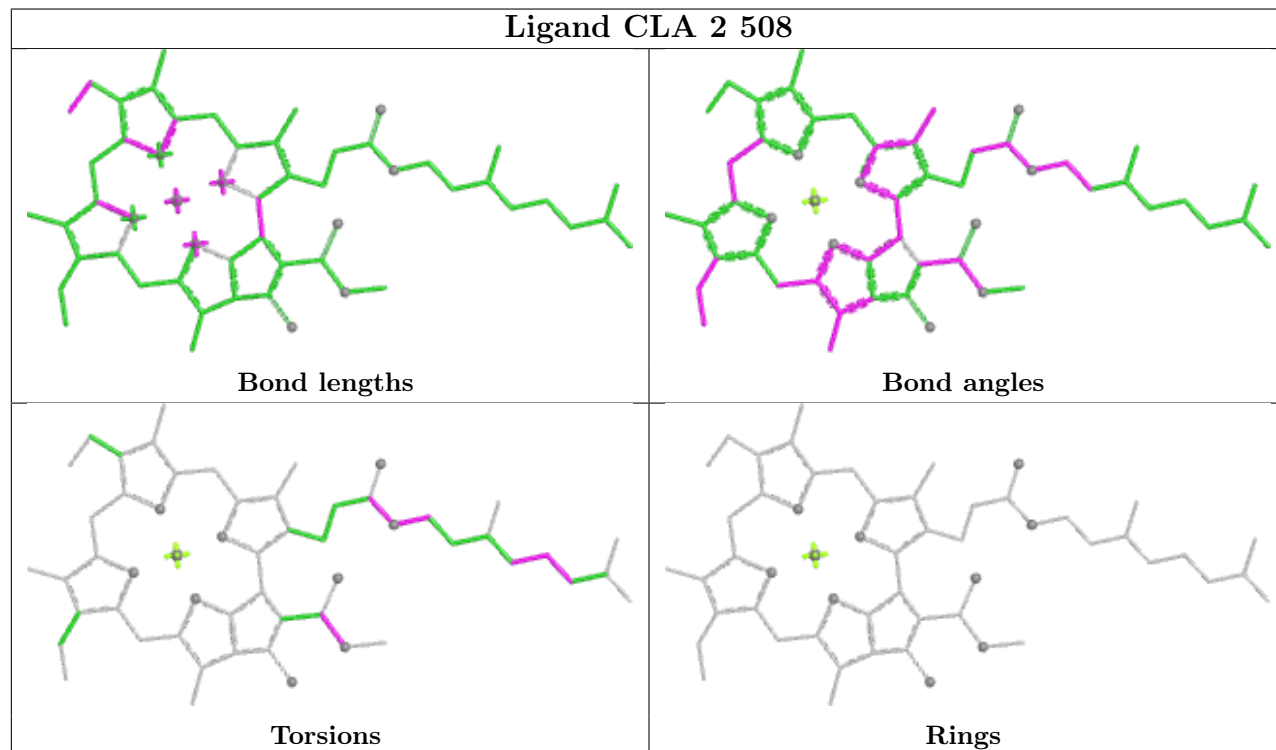
Ligand CLA A 829



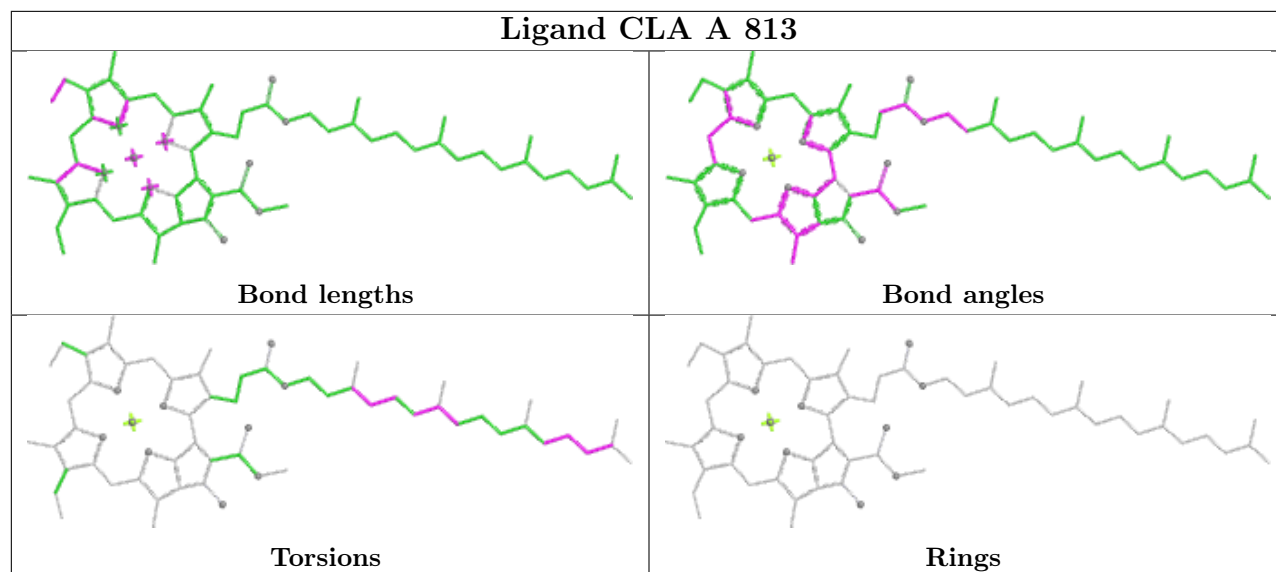
Ligand CLA B 829



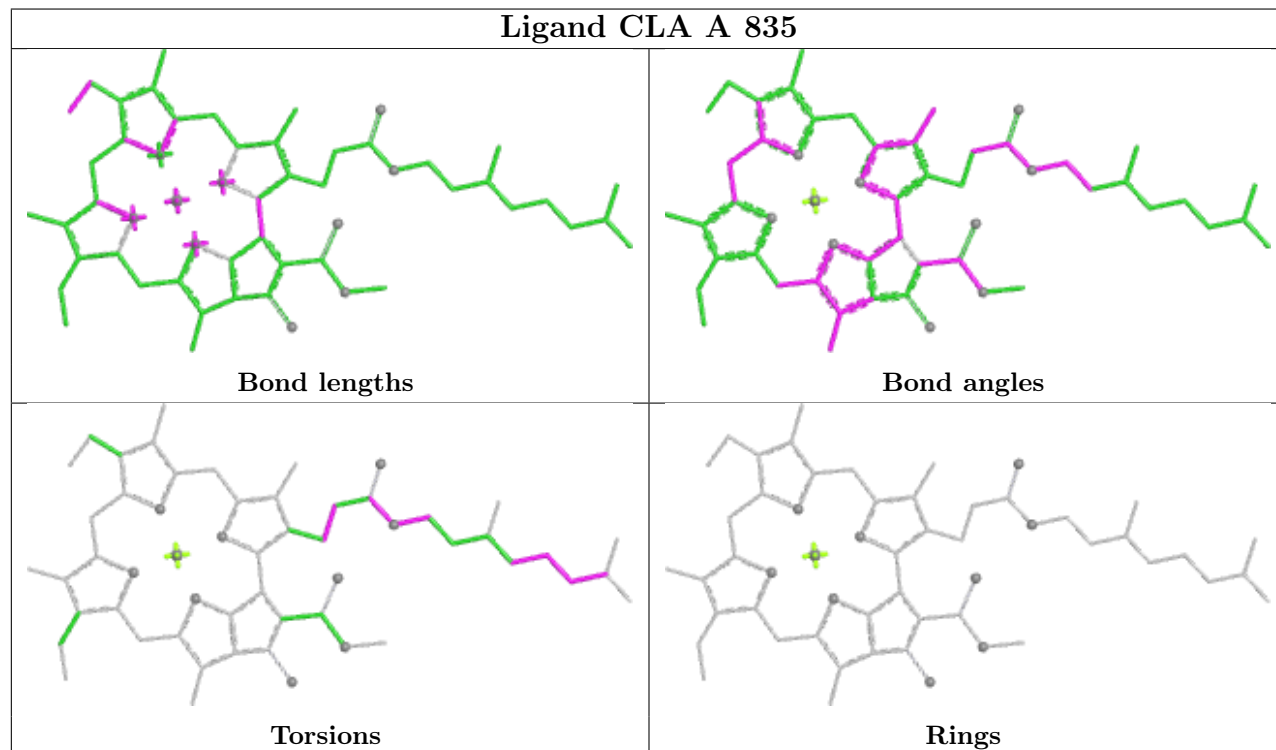
Ligand CLA 2 508



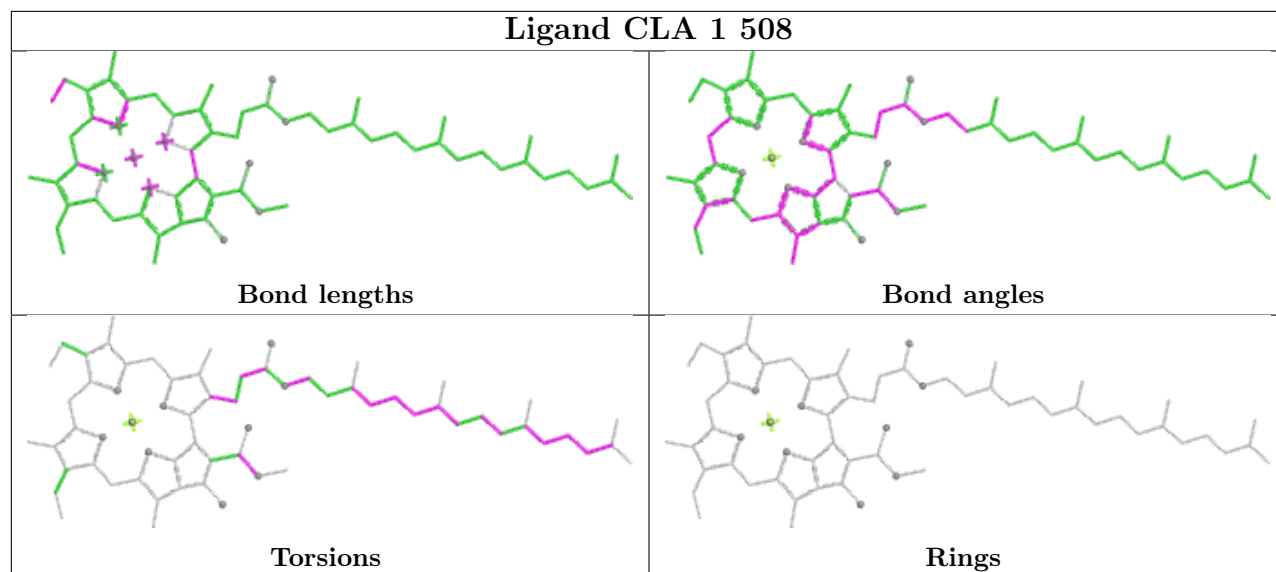
Ligand CLA A 813



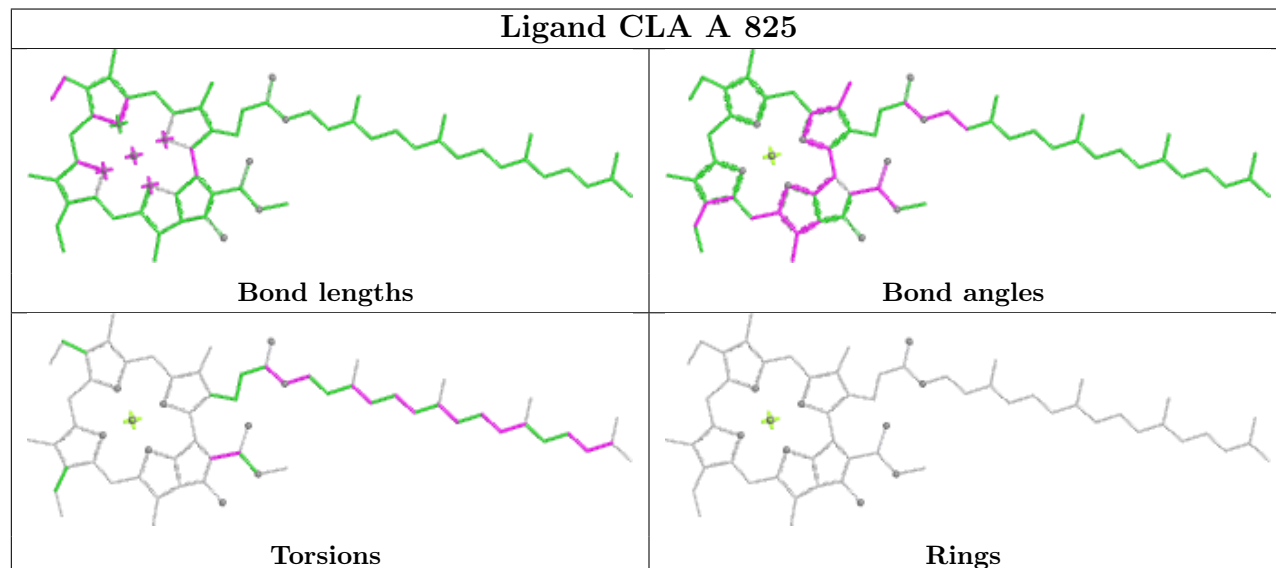
Ligand CLA A 835



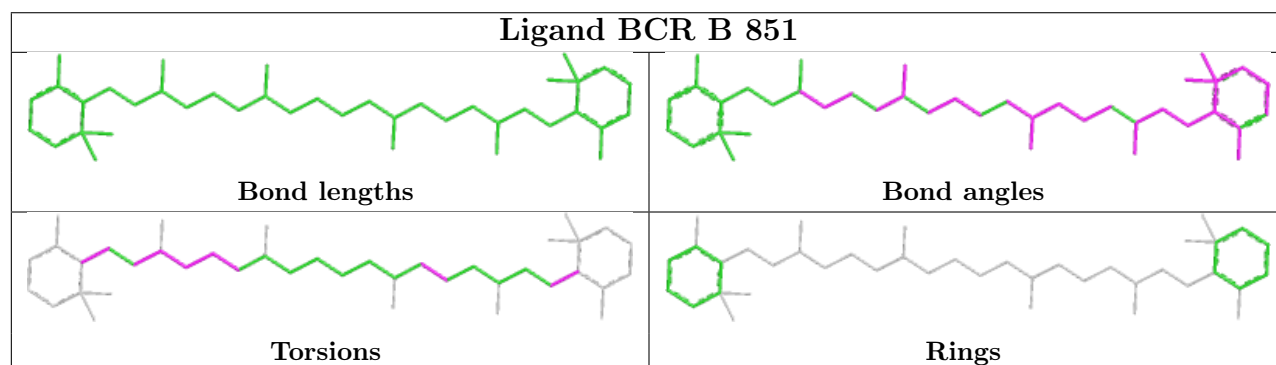
Ligand CLA 1 508



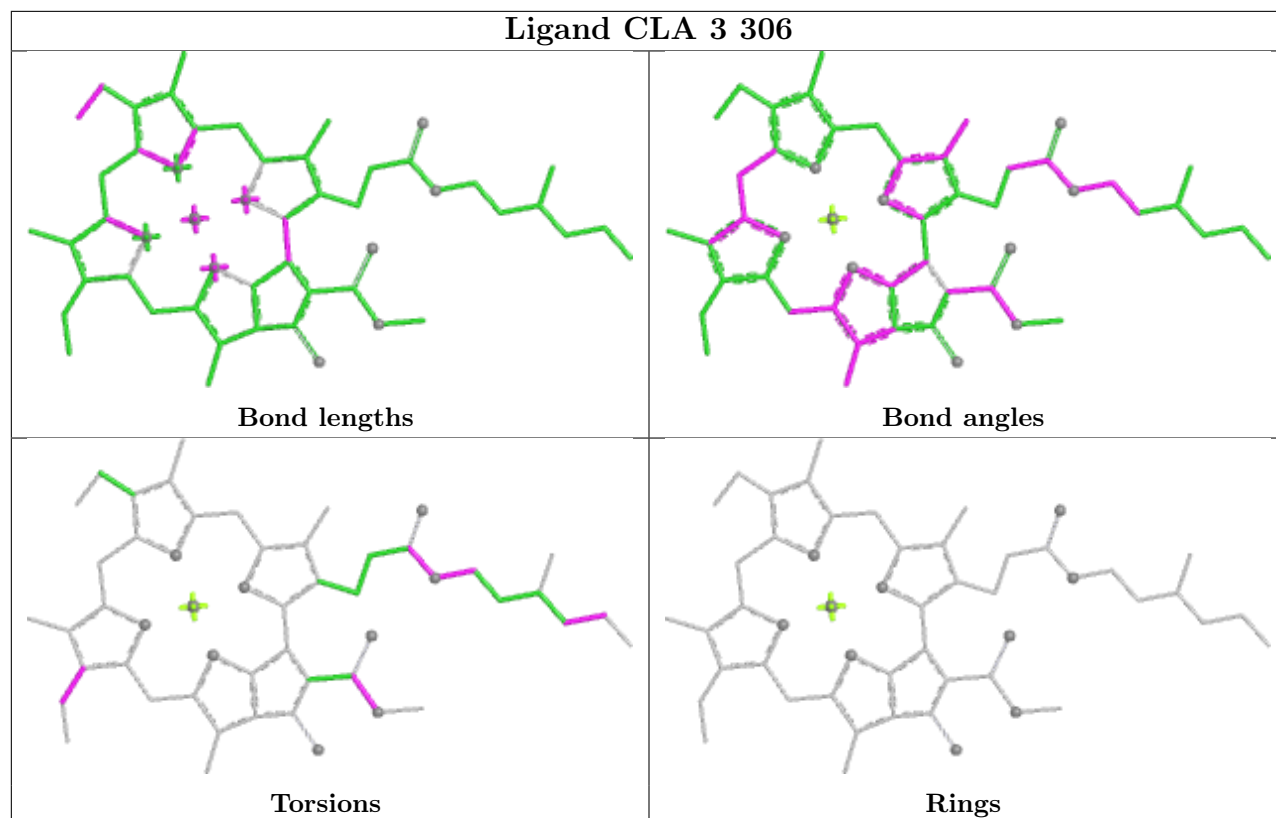
Ligand CLA A 825



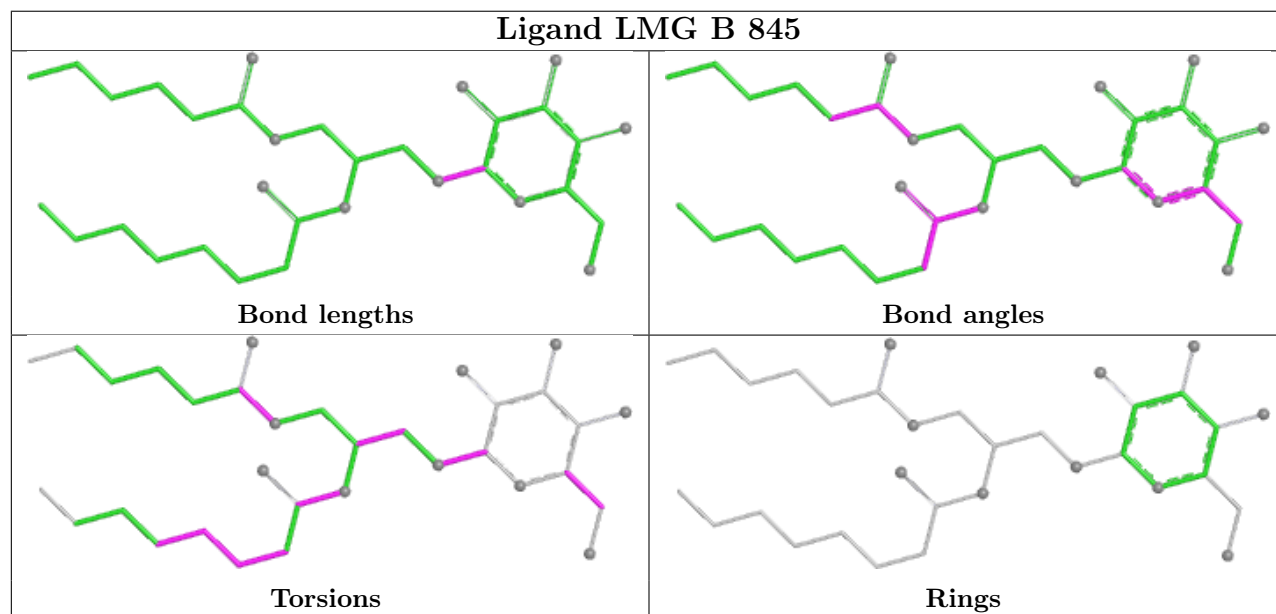
Ligand BCR B 851

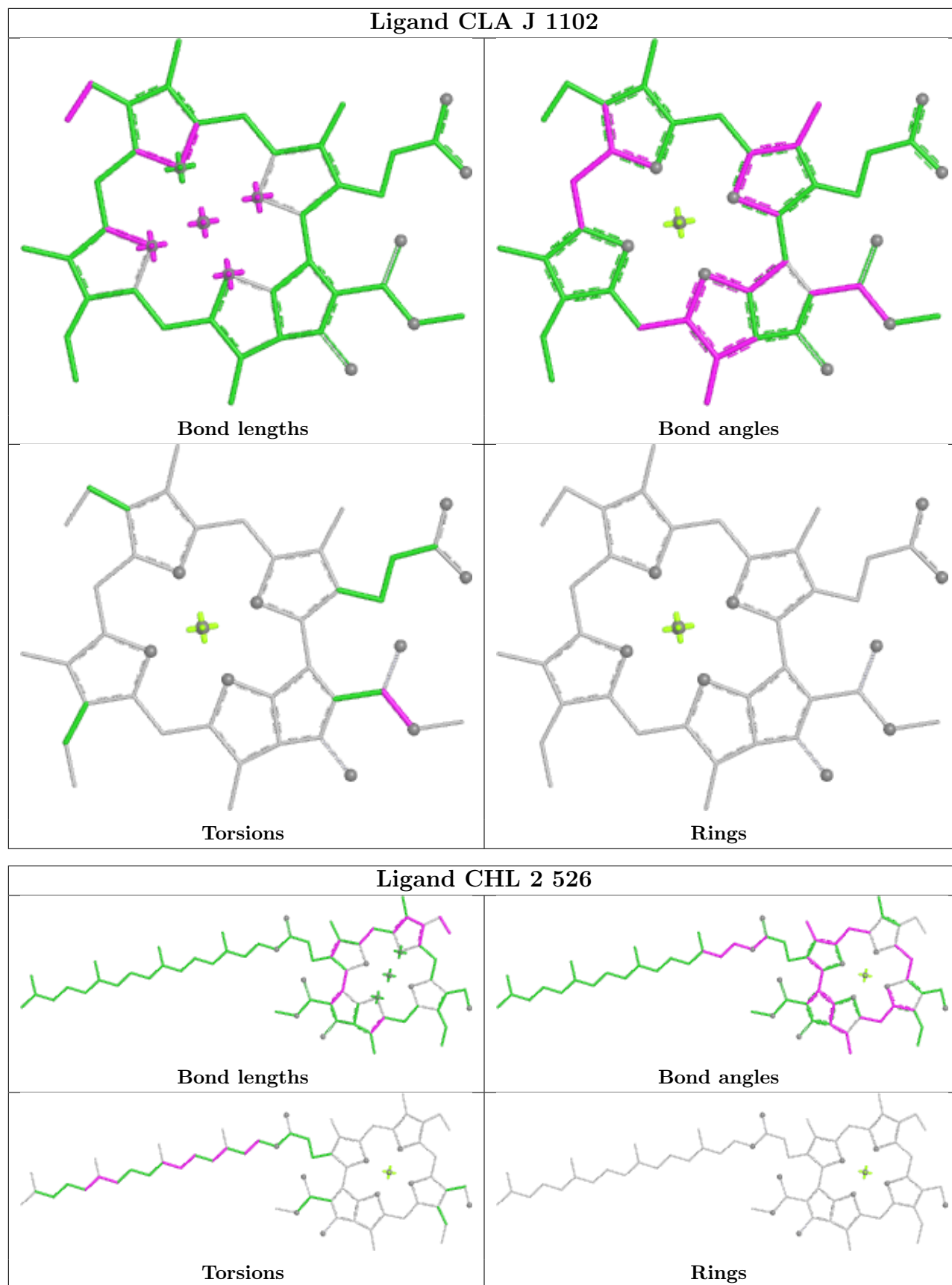


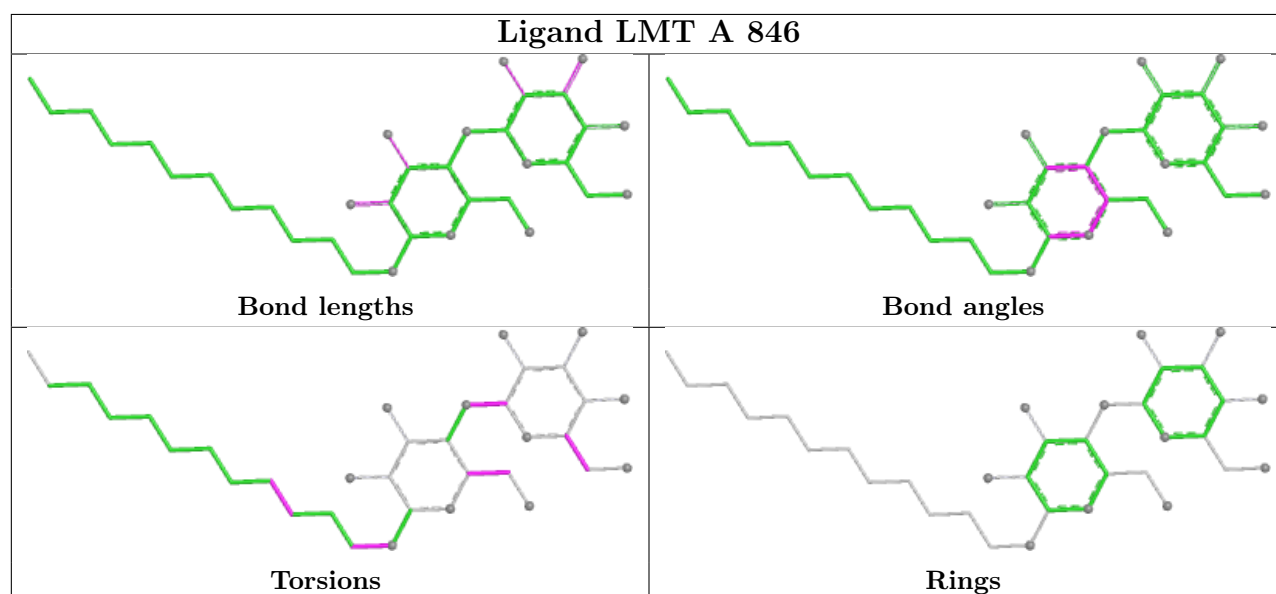
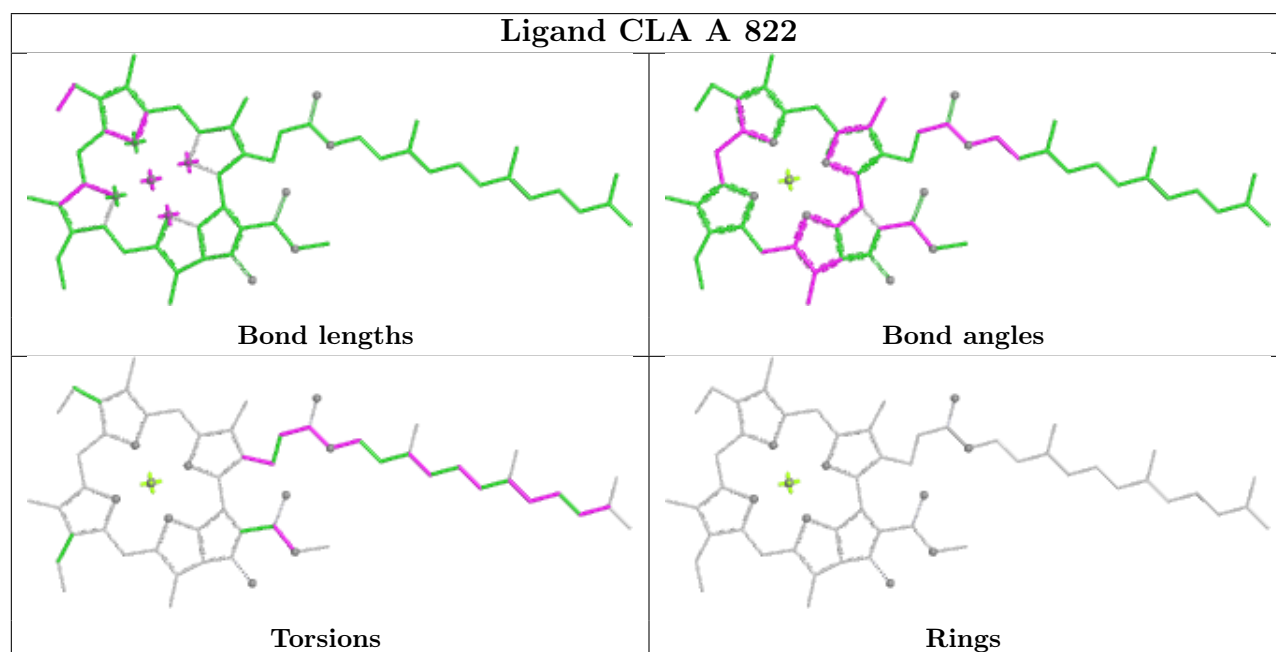
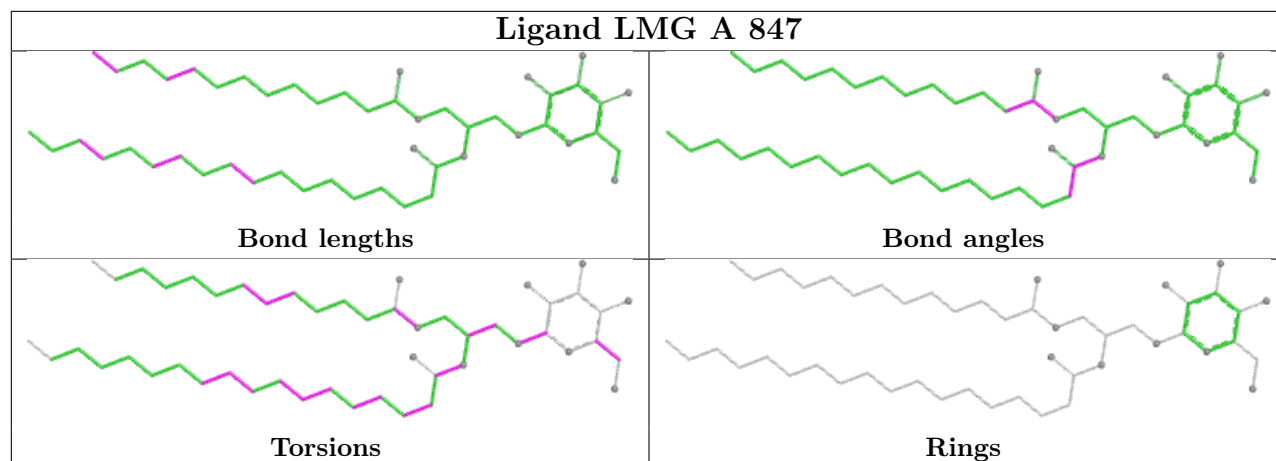
Ligand CLA 3 306



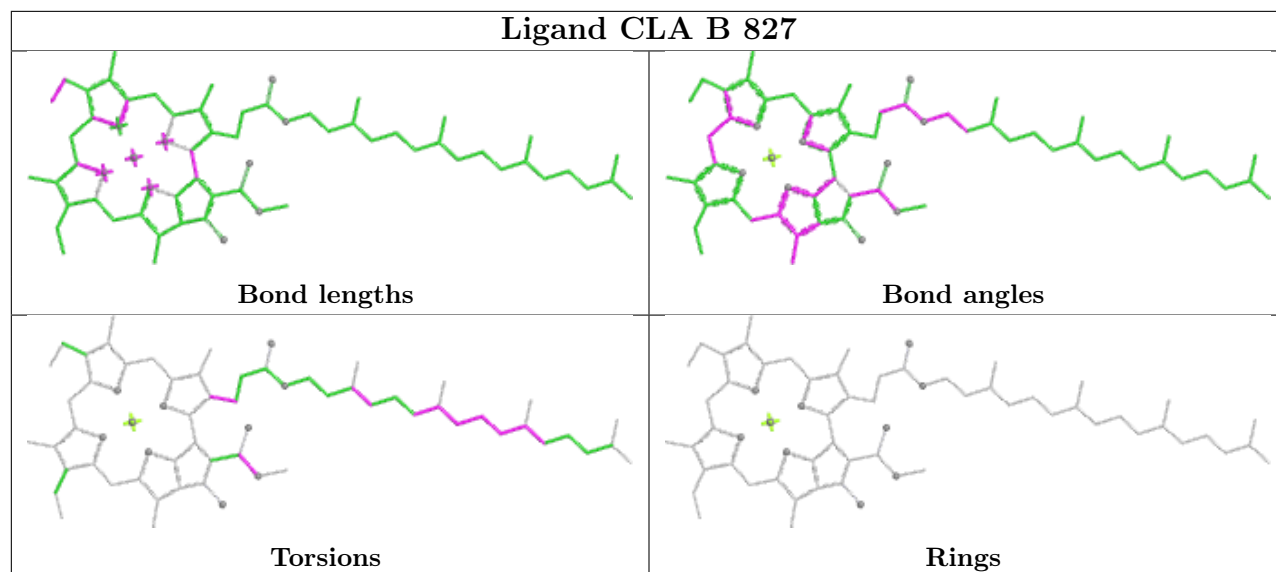
Ligand LMG B 845



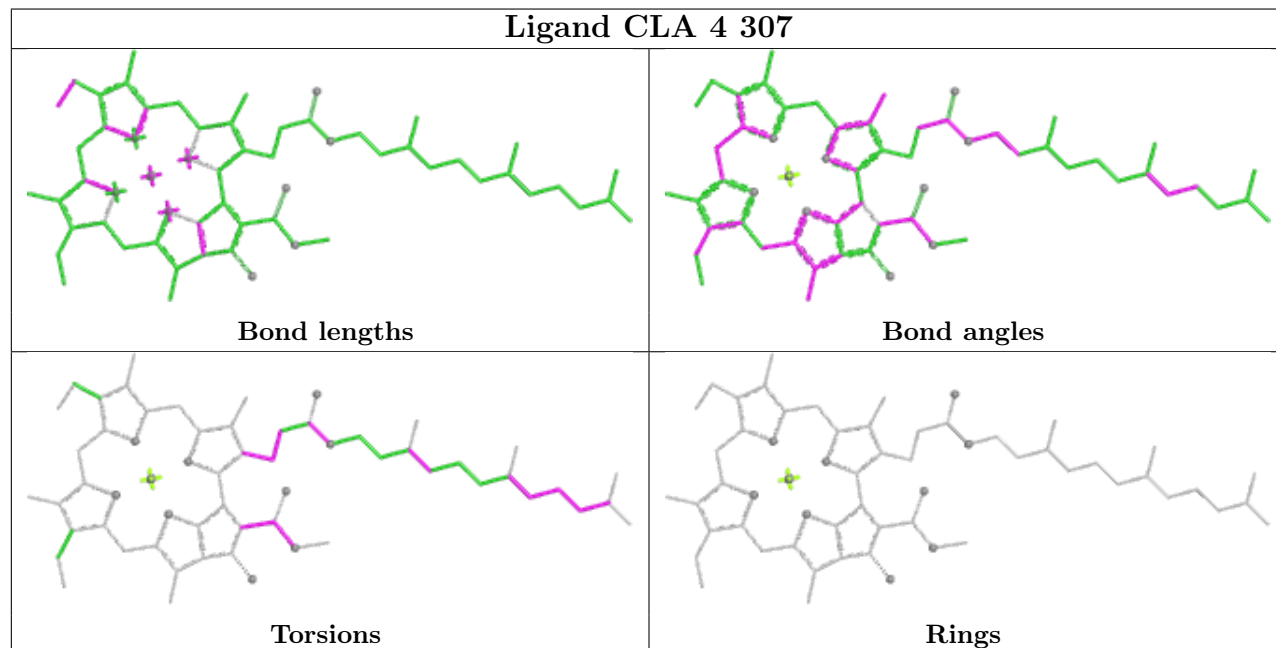


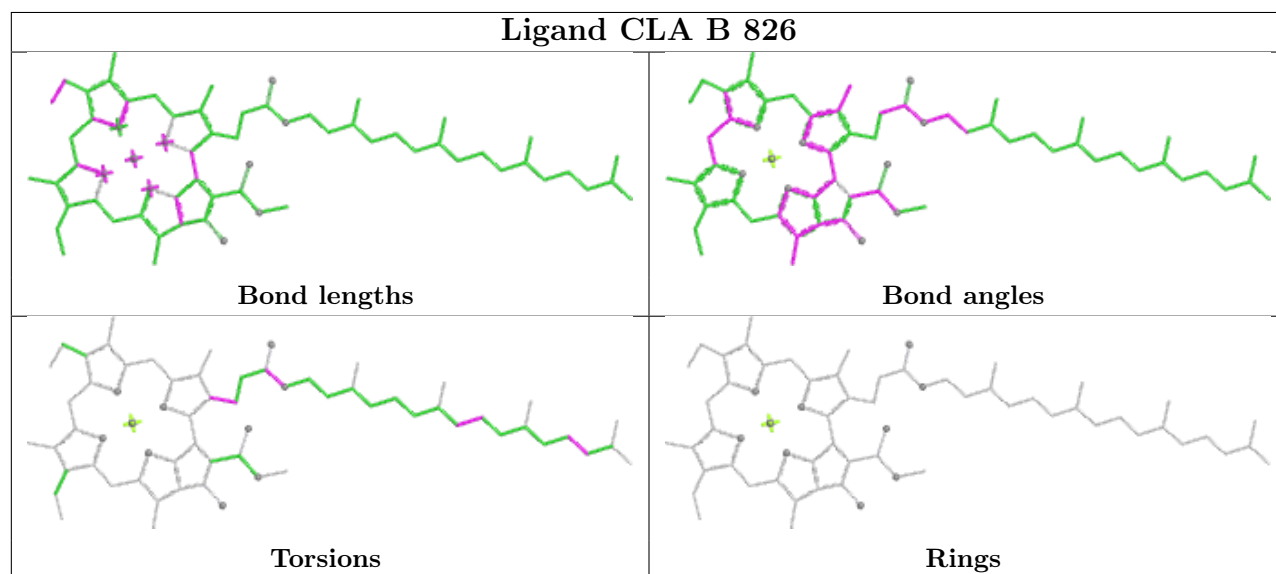
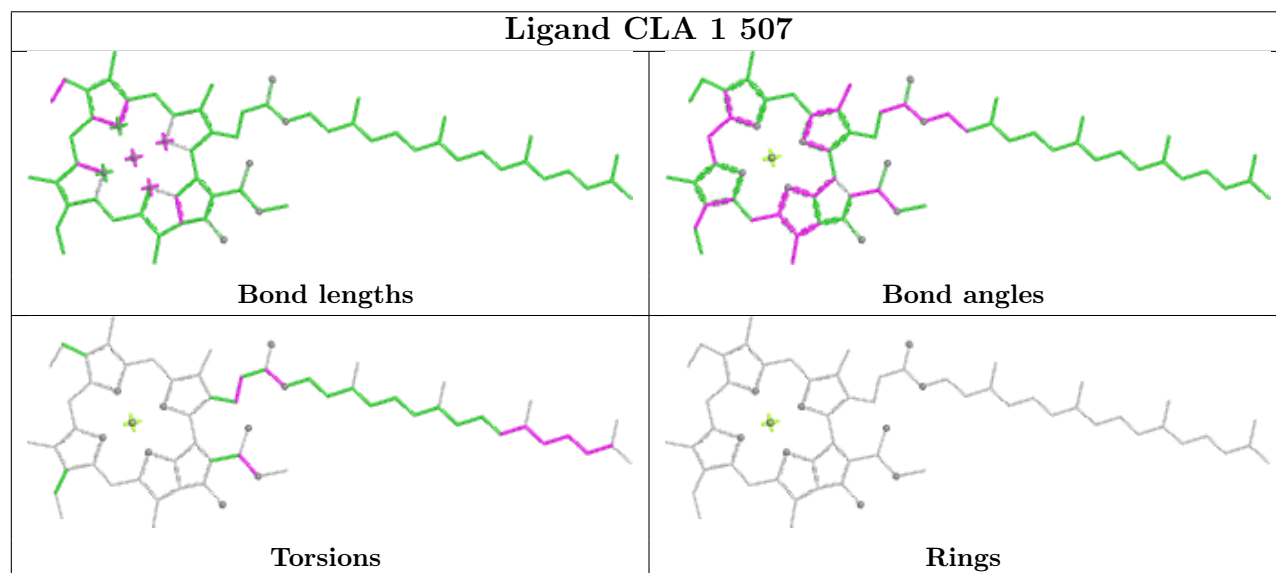
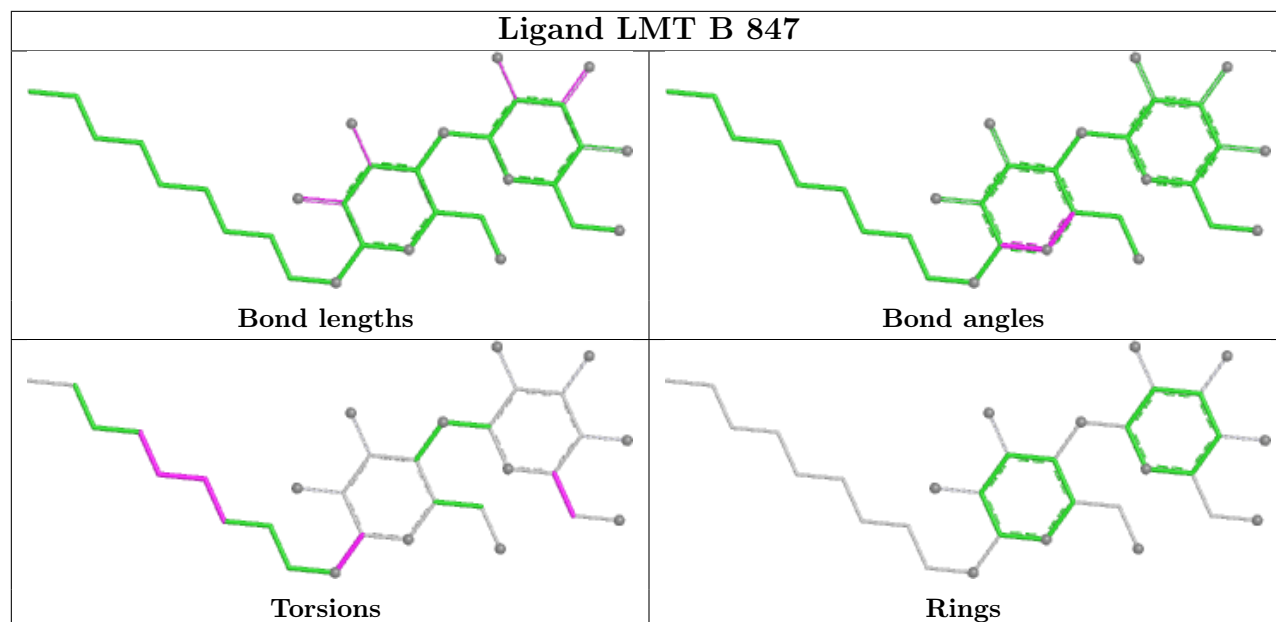


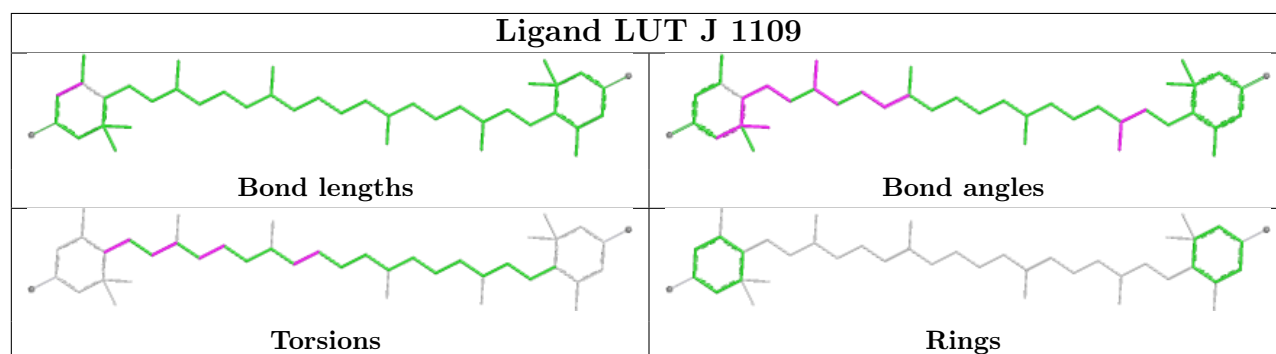
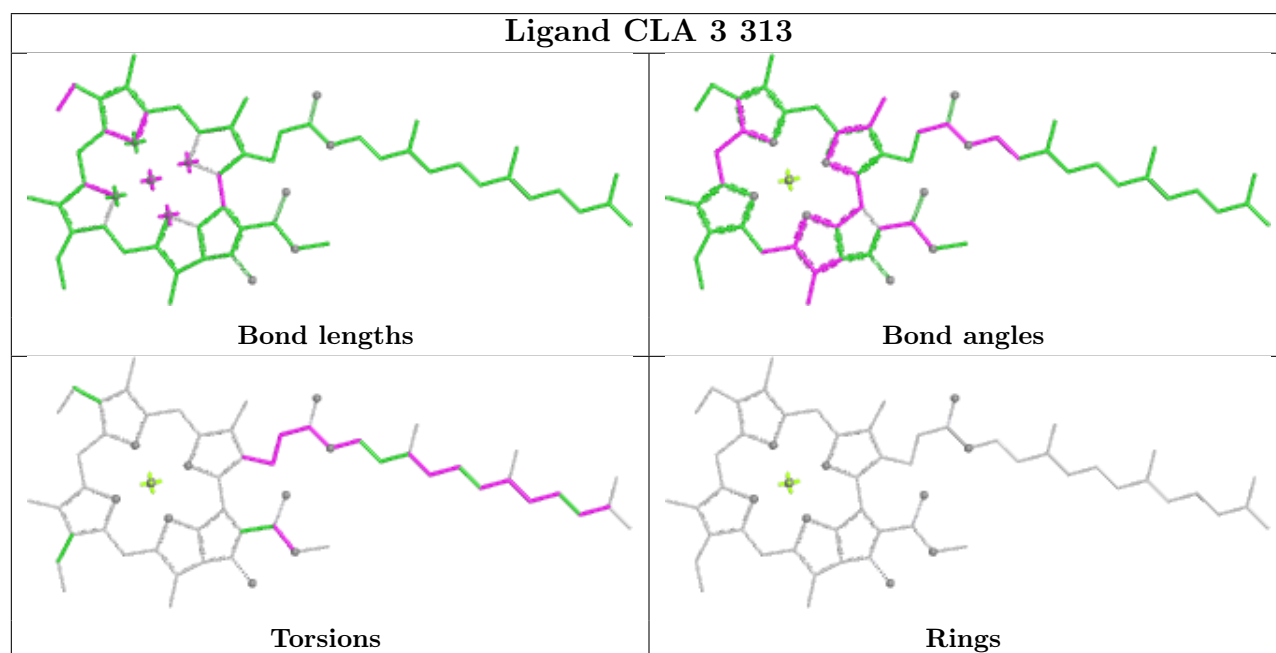
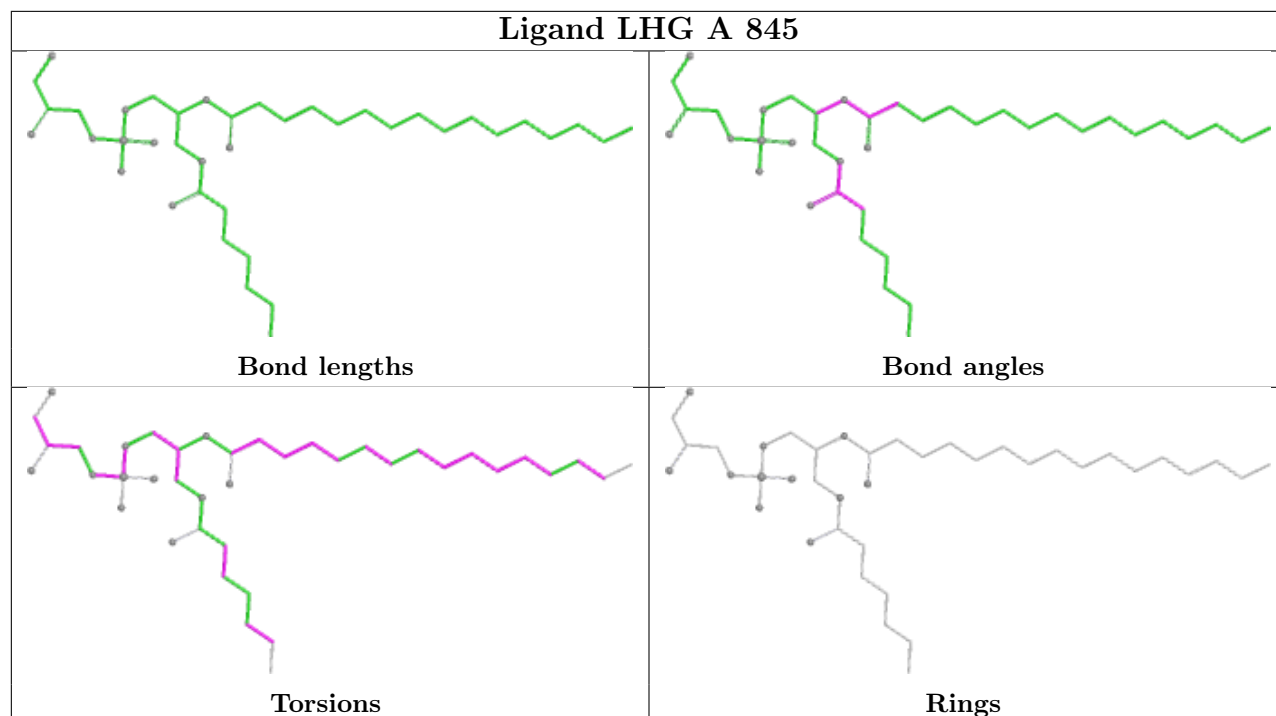
Ligand CLA B 827



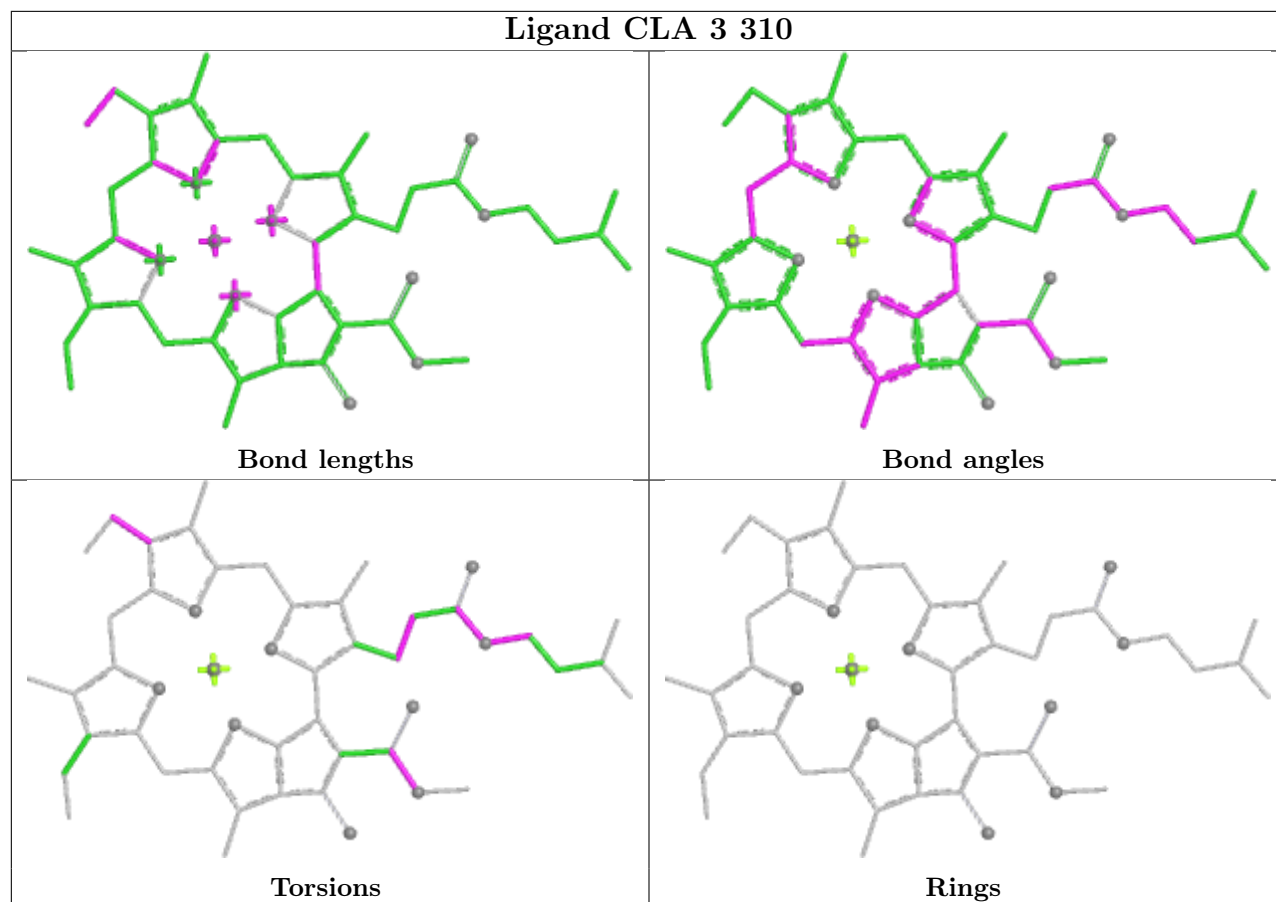
Ligand CLA 4 307



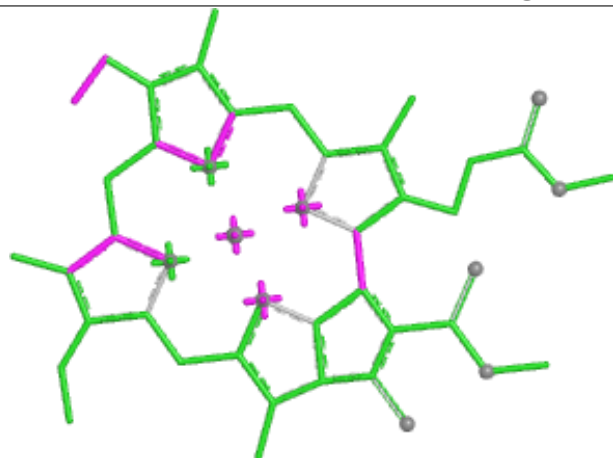




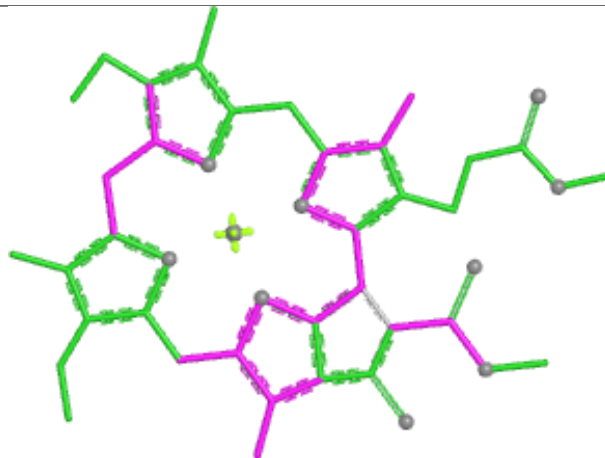
Ligand CLA 3 310



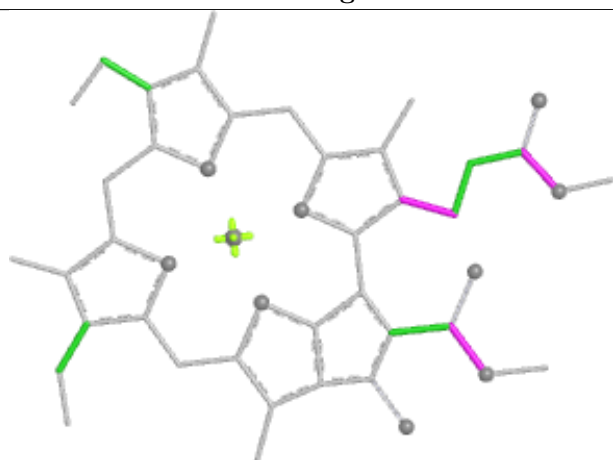
Ligand CLA 3 317



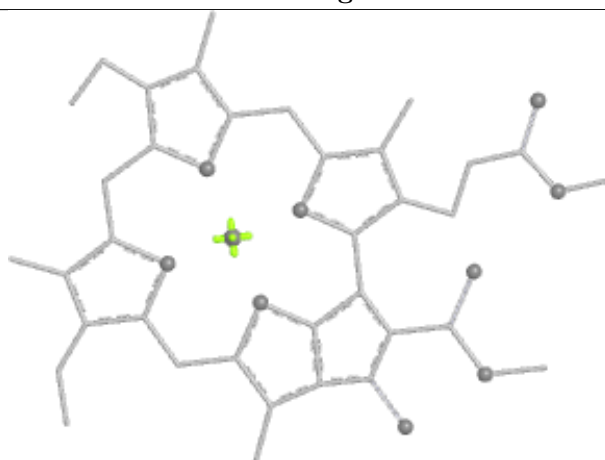
Bond lengths



Bond angles

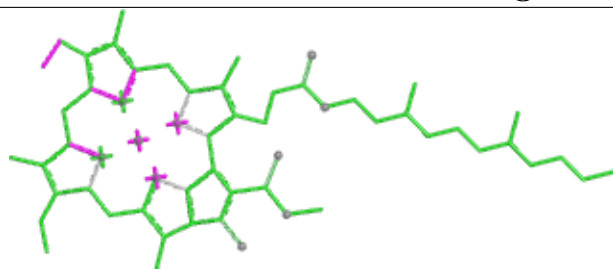


Torsions

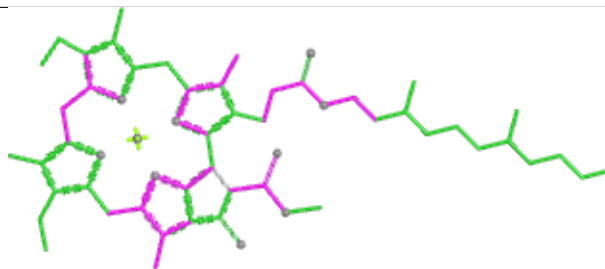


Rings

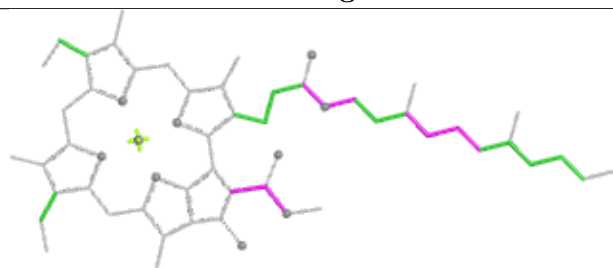
Ligand CLA B 832



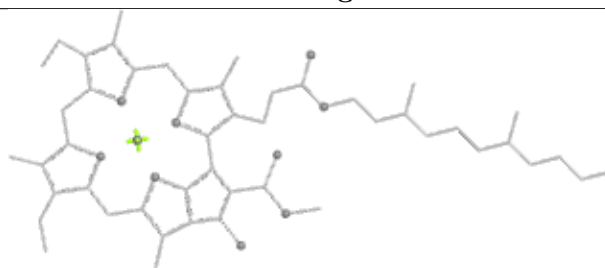
Bond lengths



Bond angles

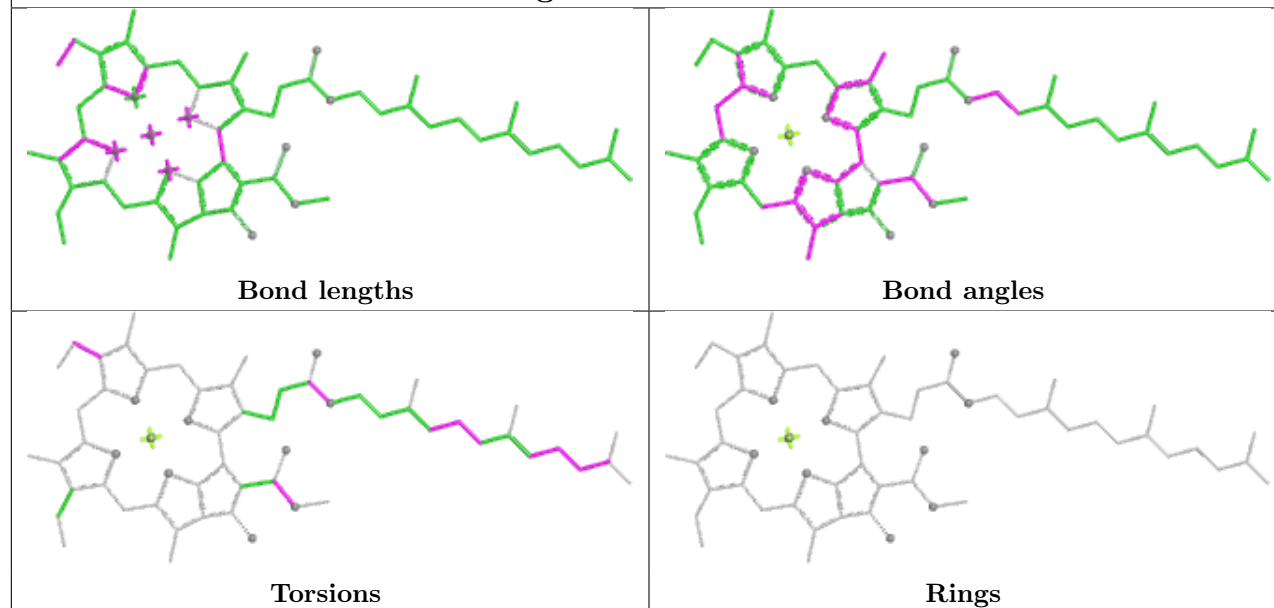


Torsions

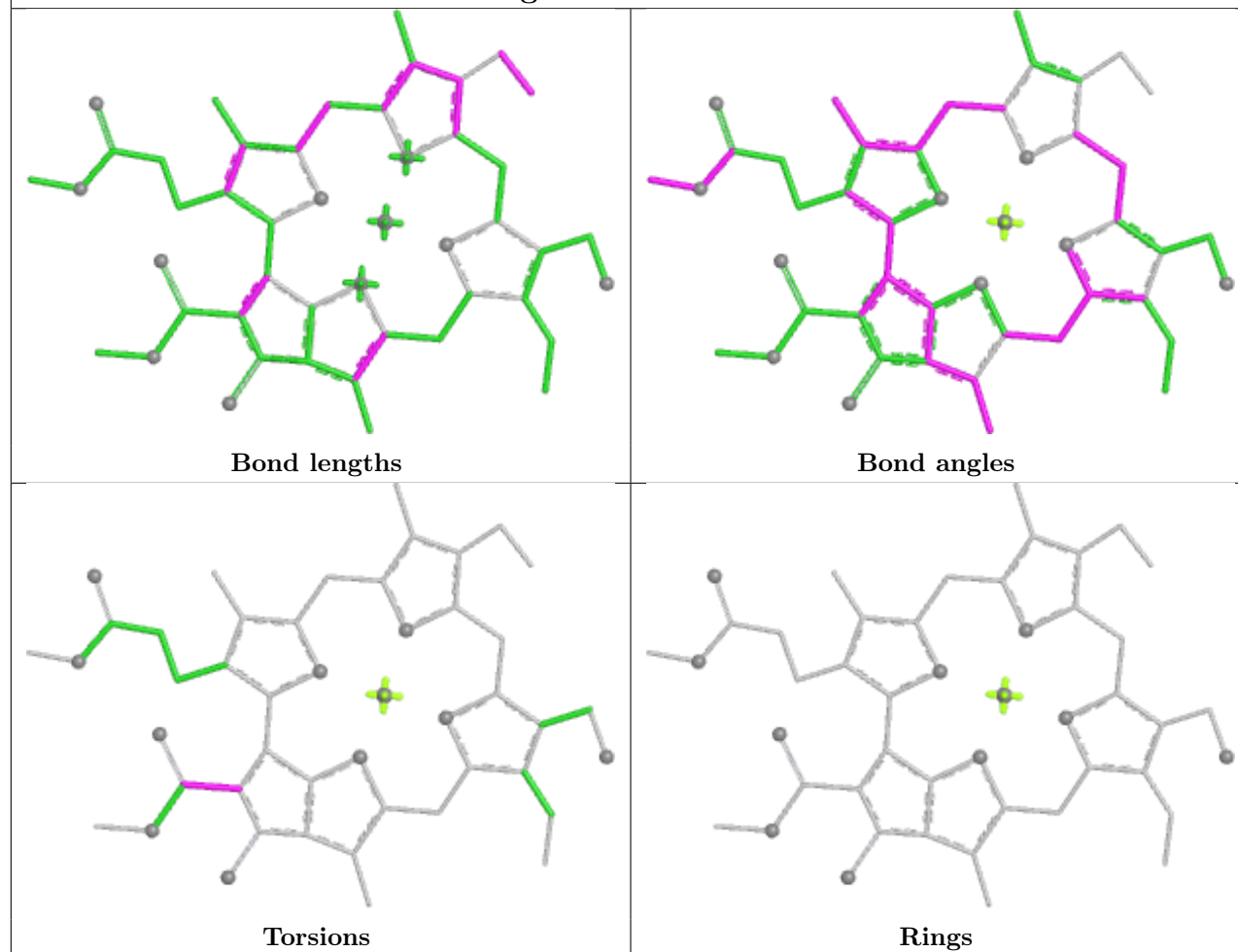


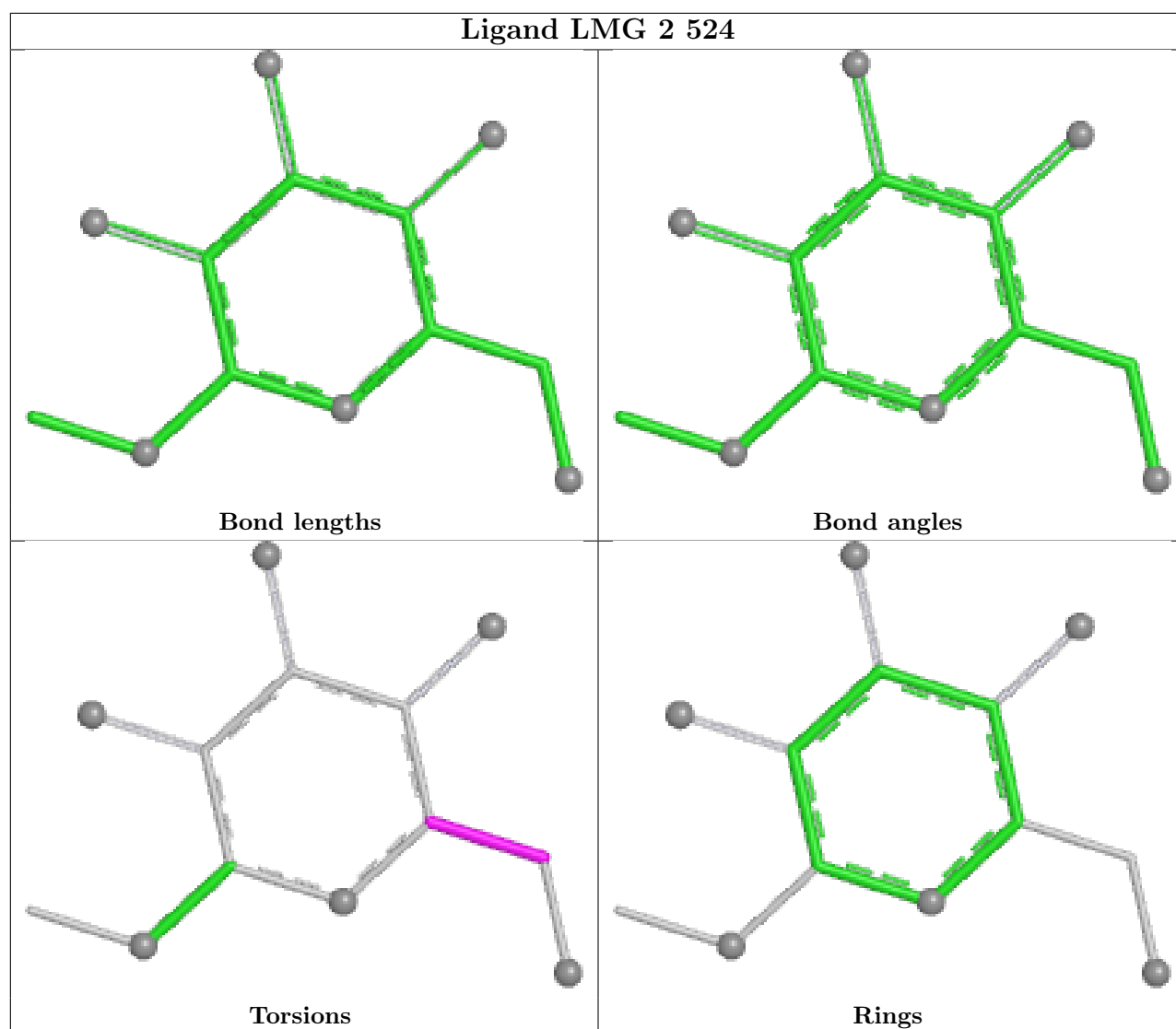
Rings

Ligand CLA 4 310

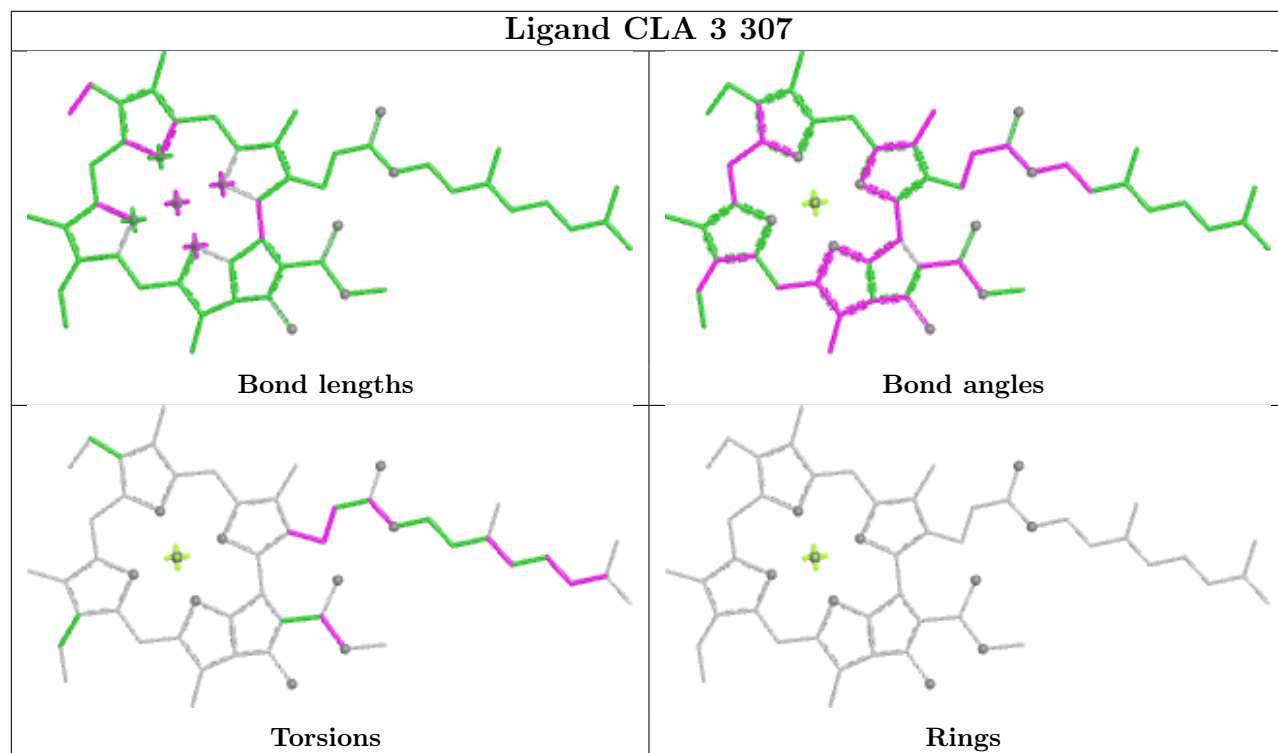


Ligand CHL 4 313

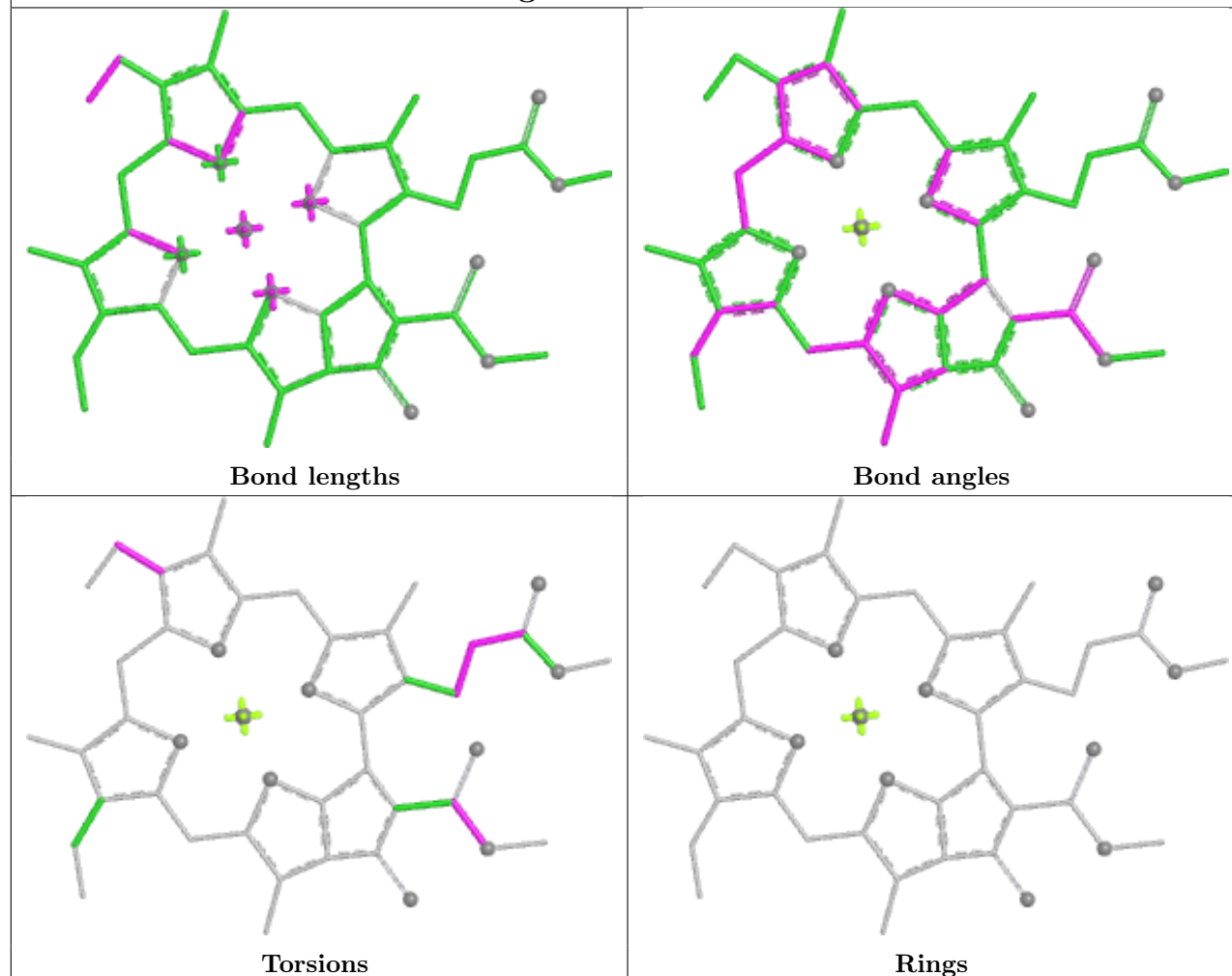




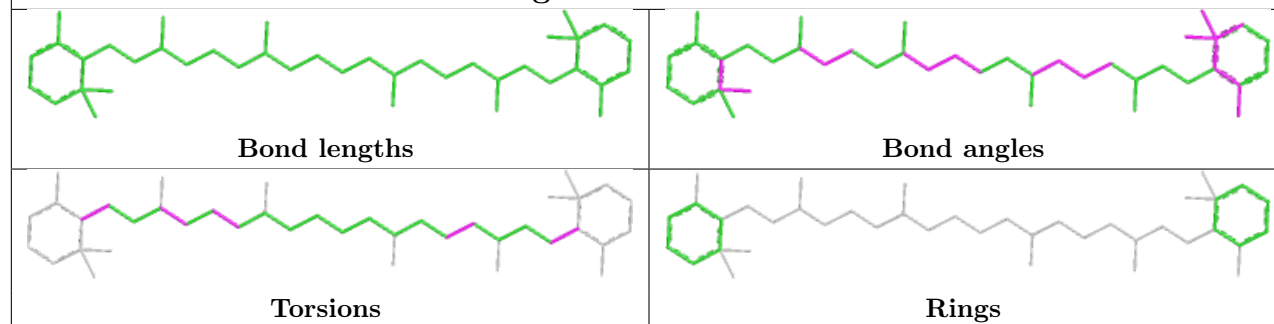
Ligand CLA 3 307



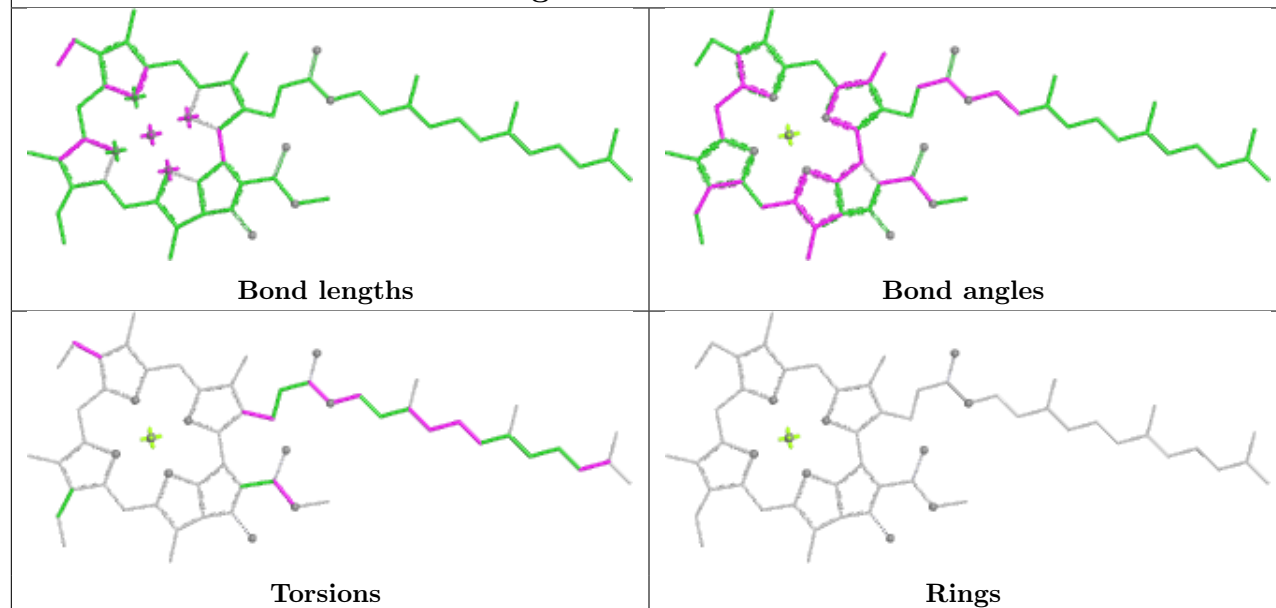
Ligand CLA 4 311



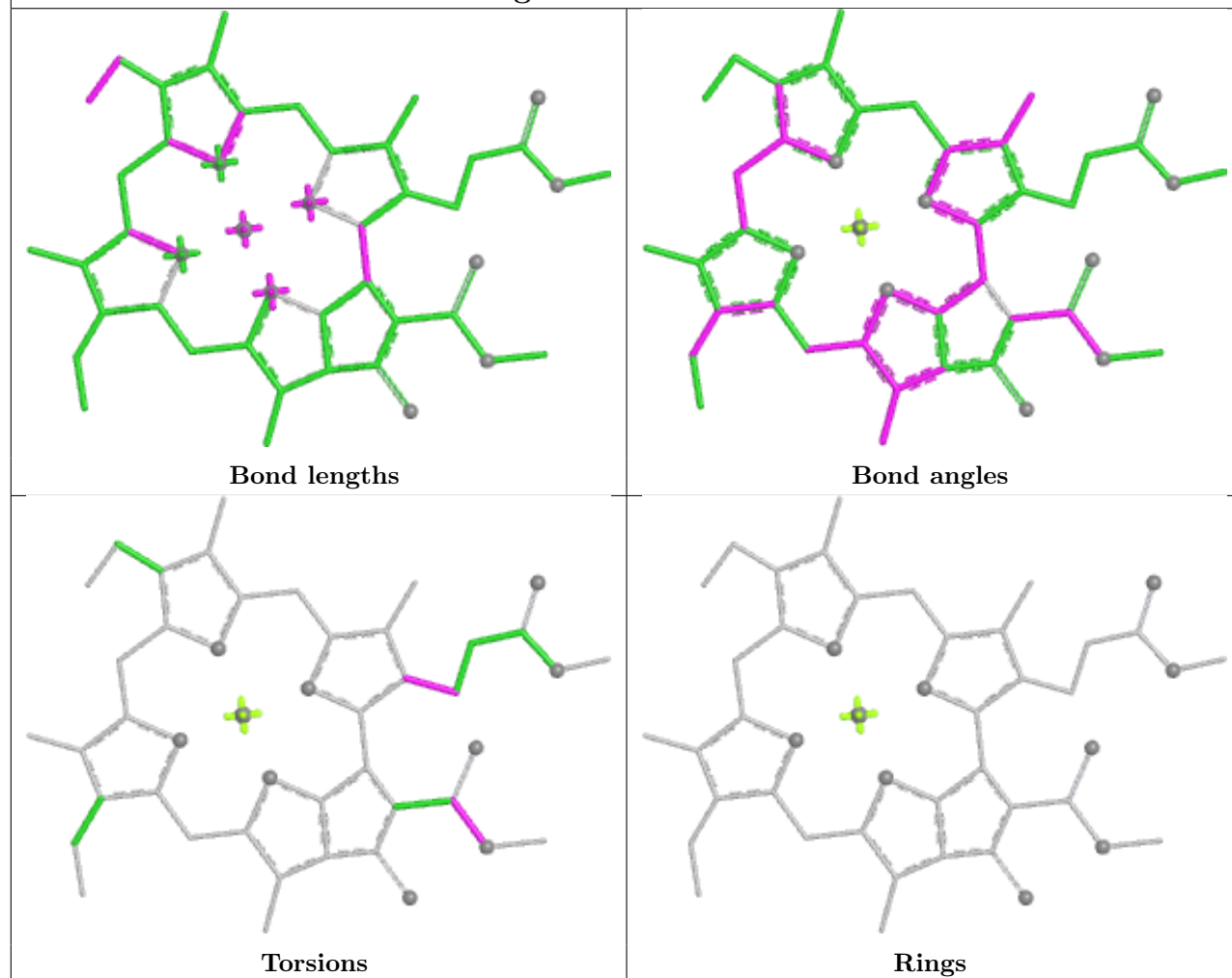
Ligand BCR L 306

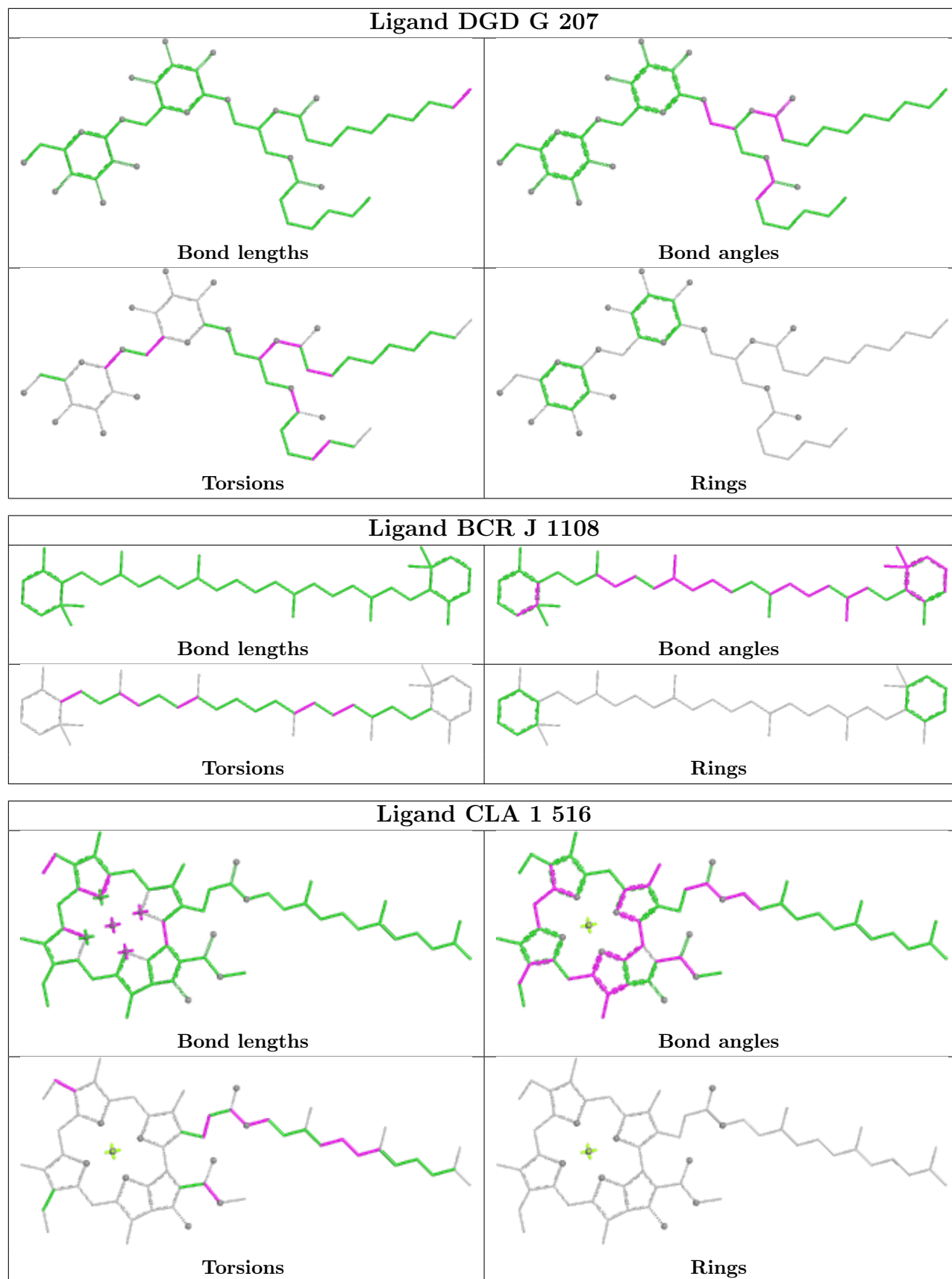


Ligand CLA A 823

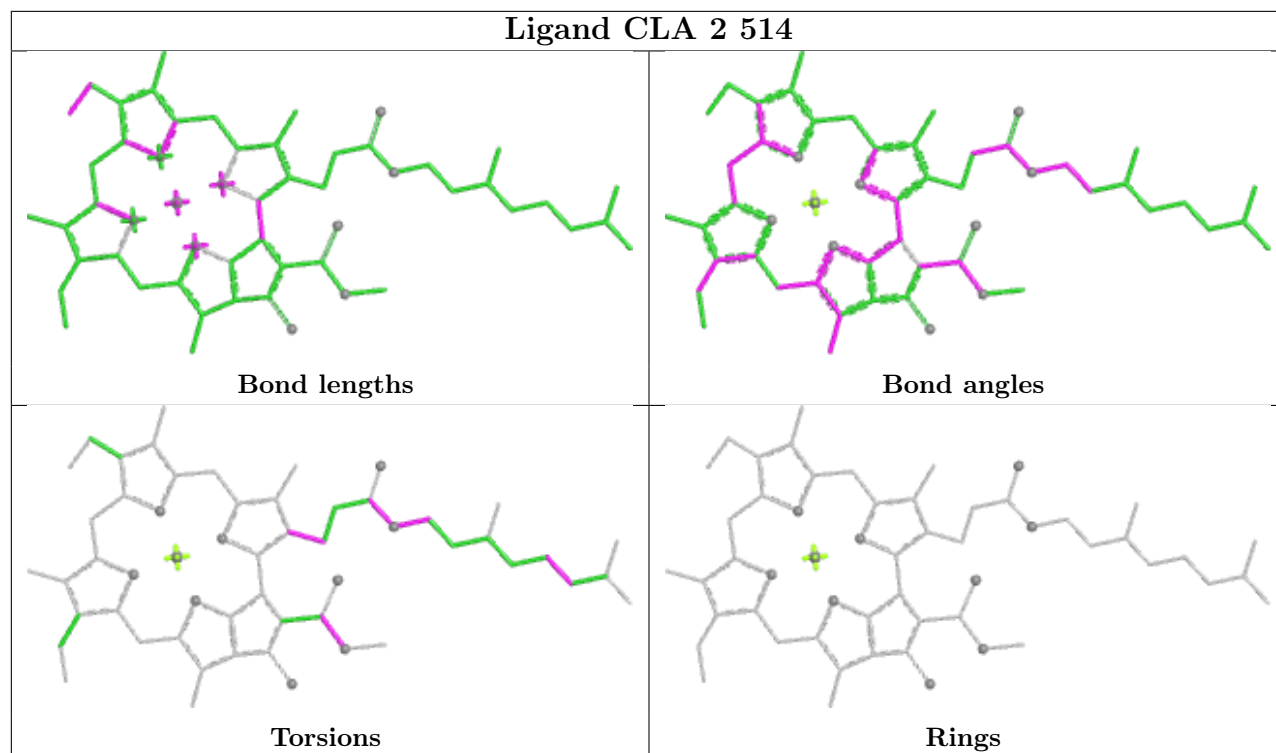


Ligand CLA B 813

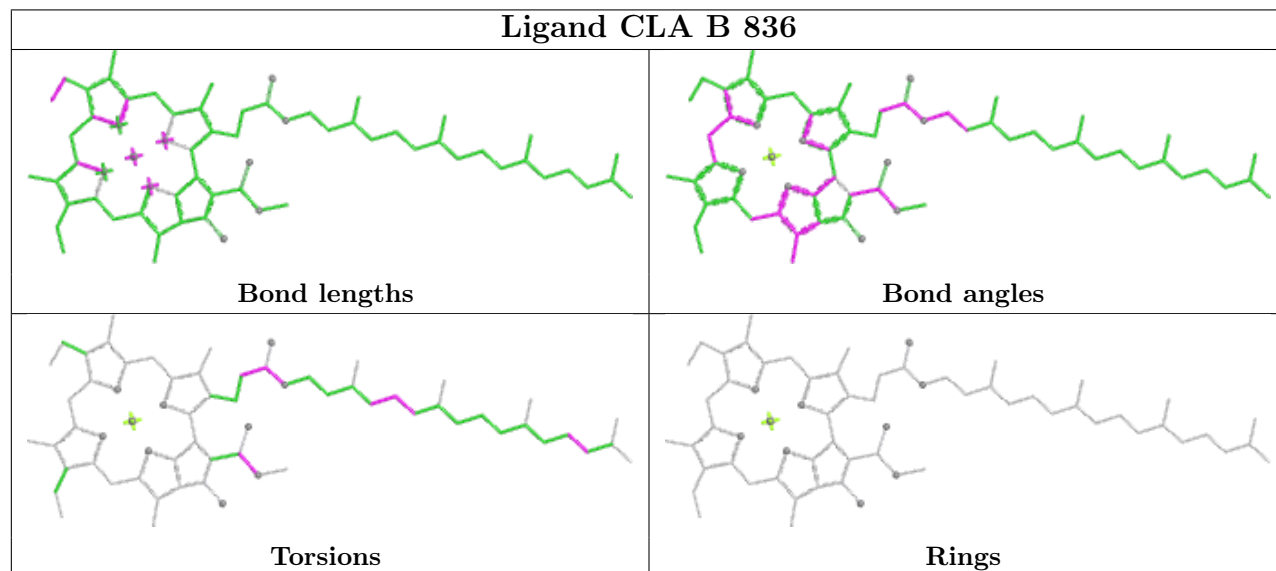


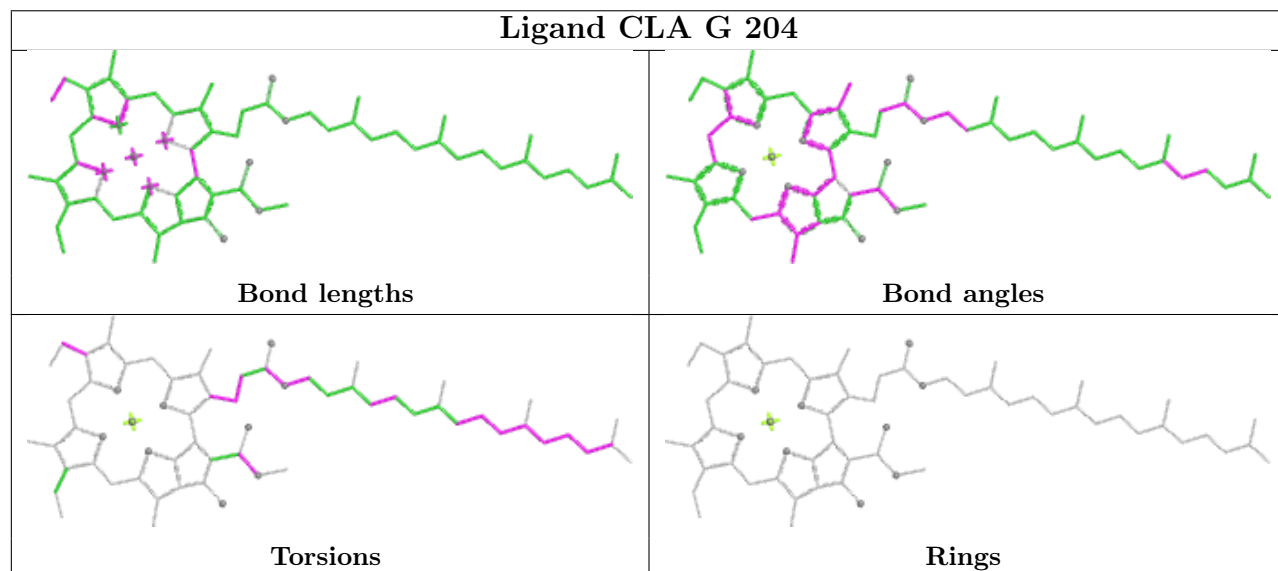
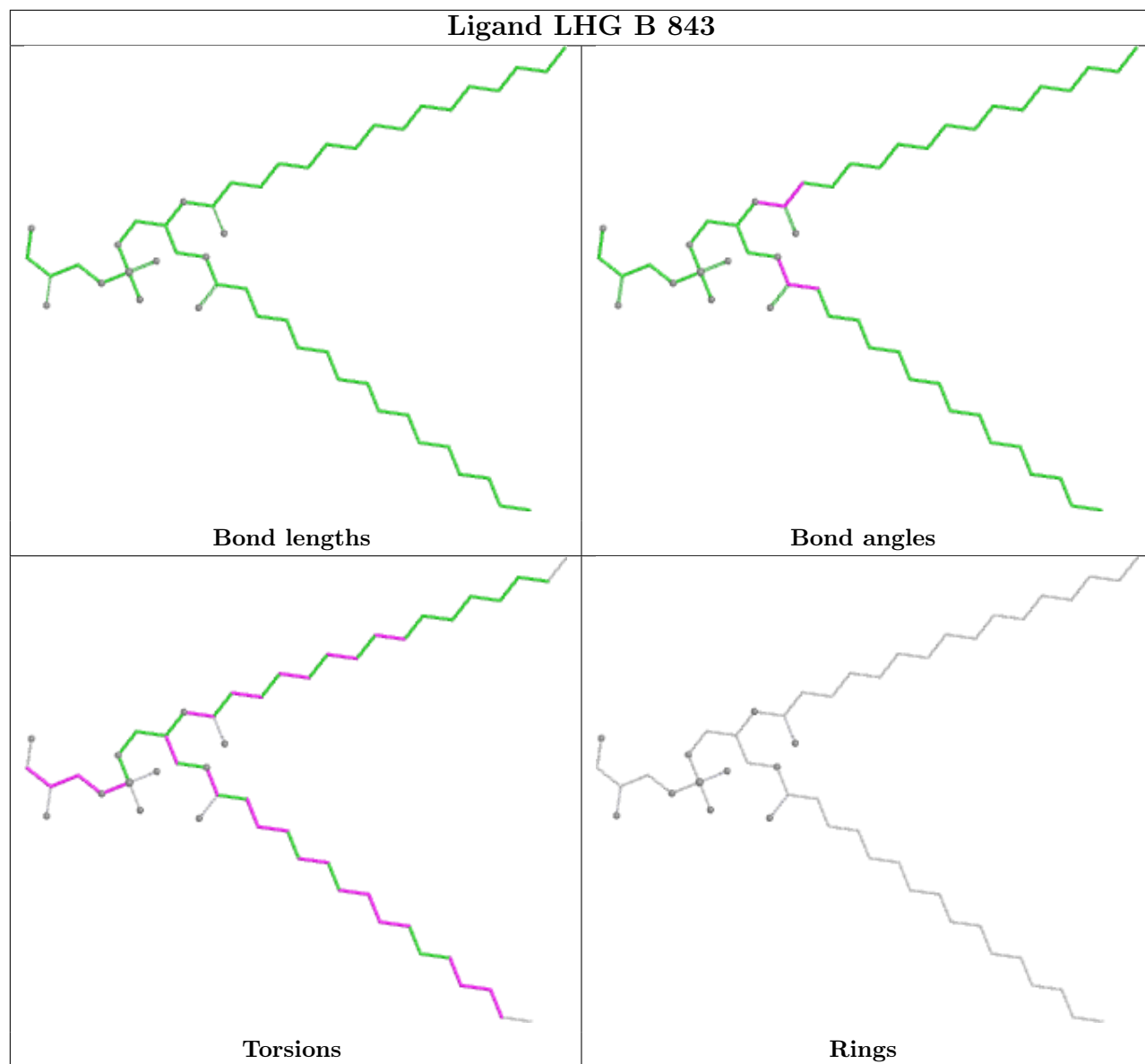


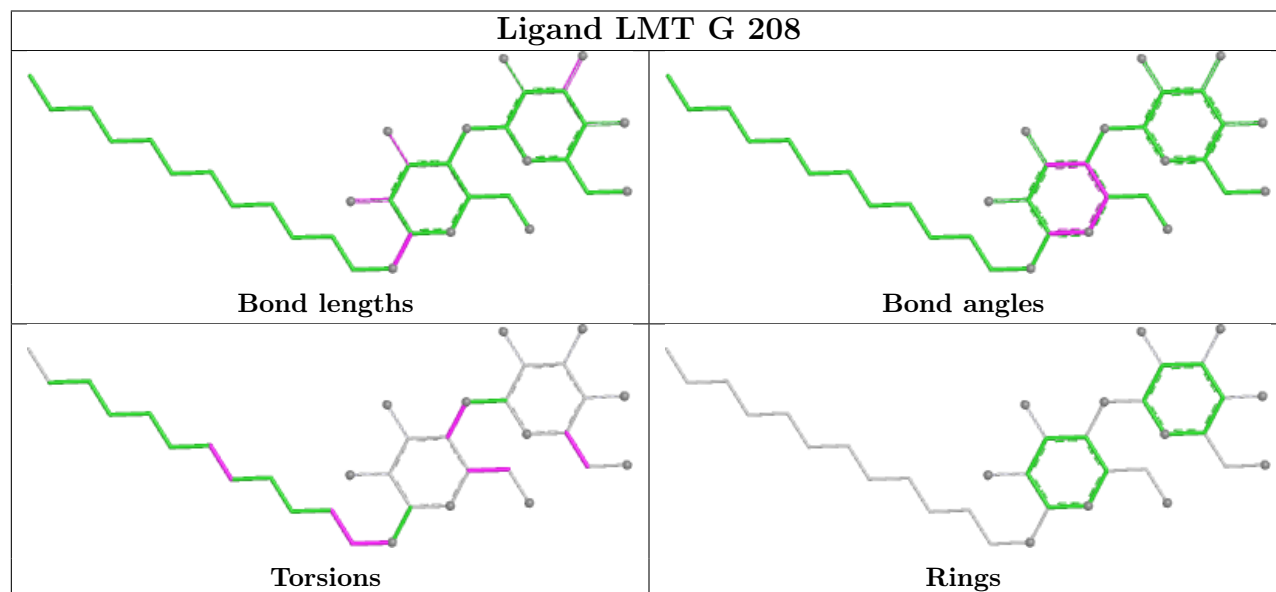
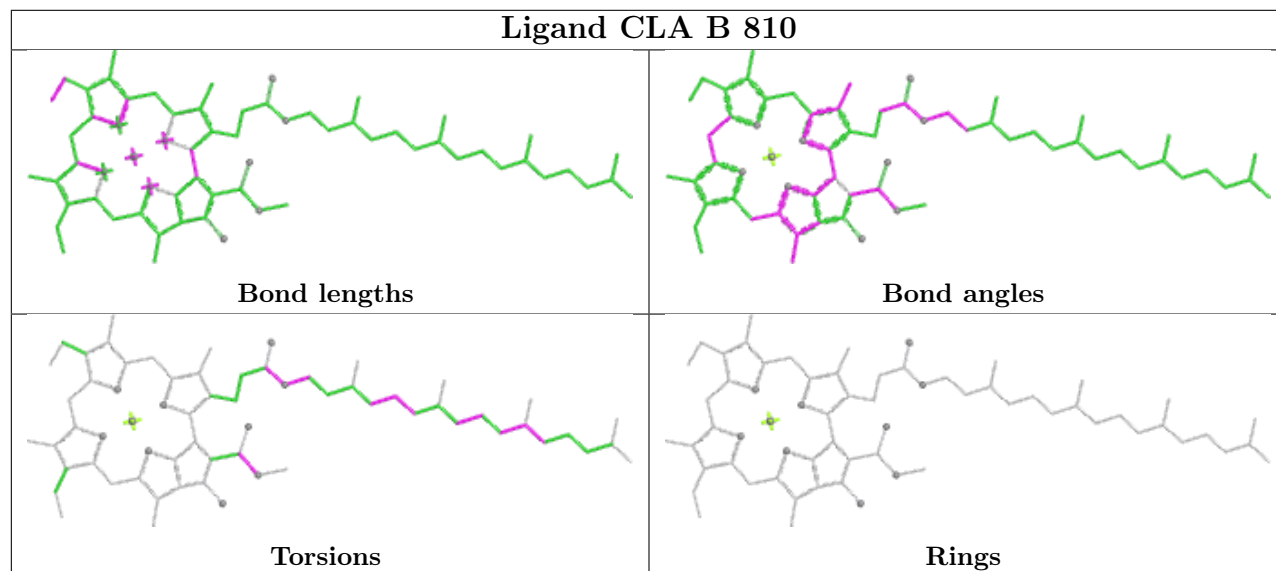
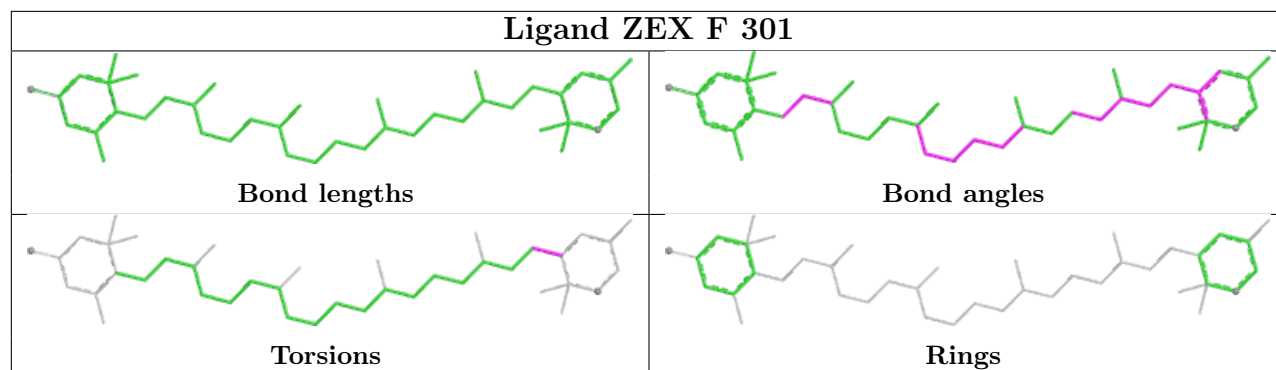
Ligand CLA 2 514

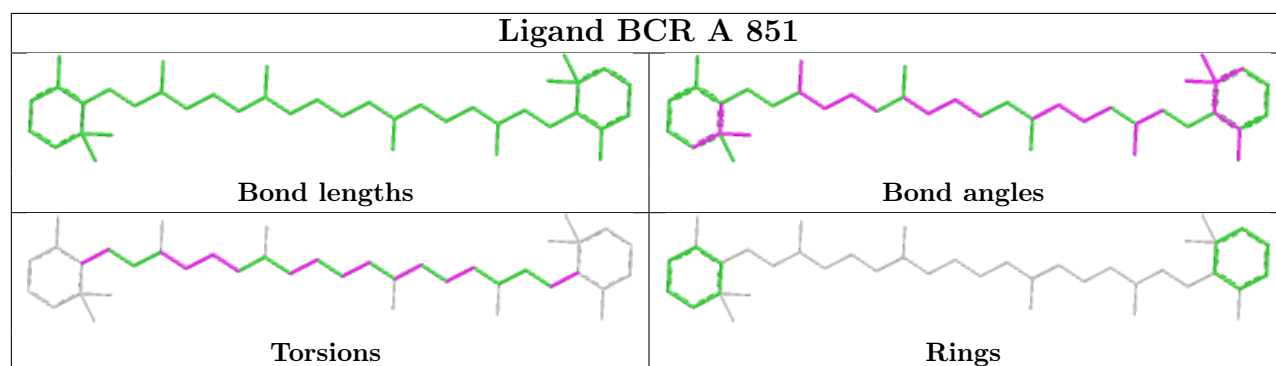
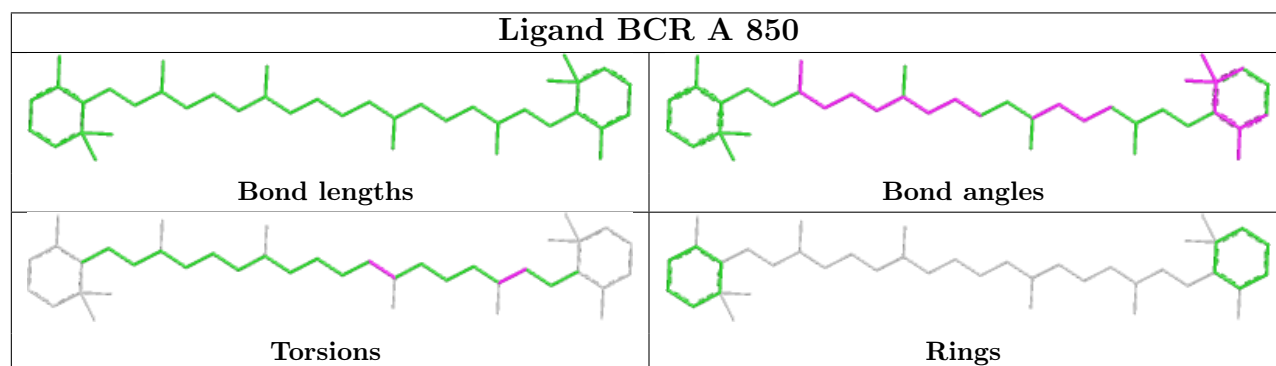
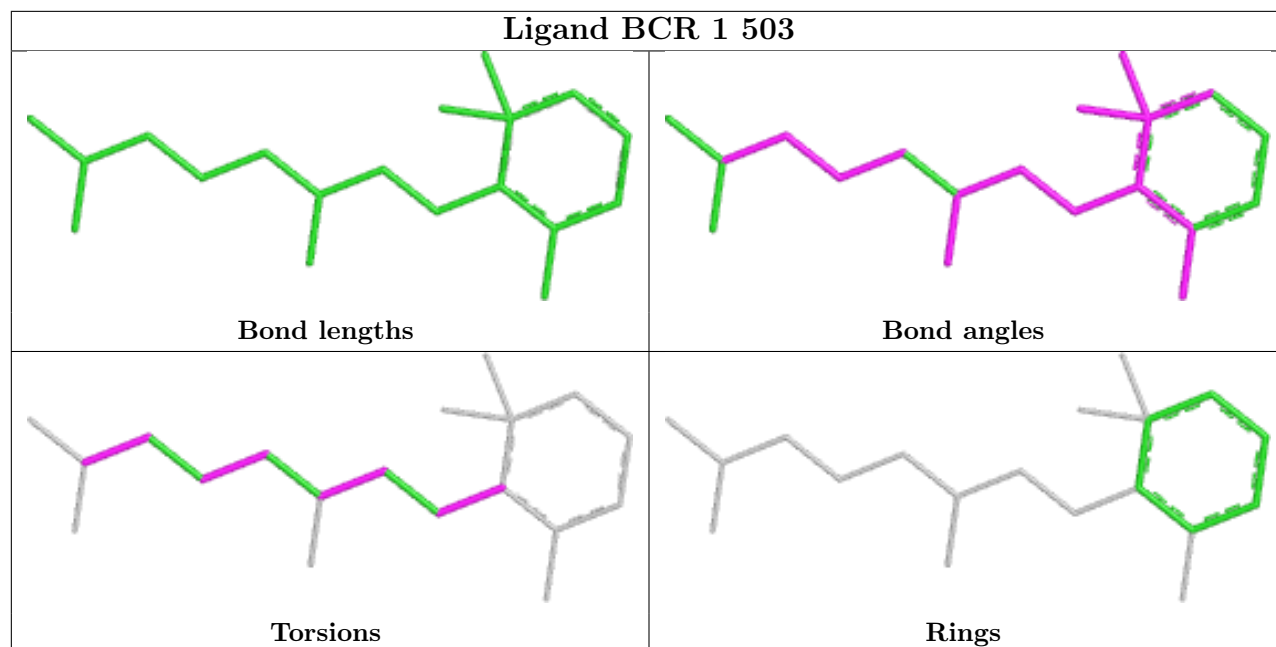


Ligand CLA B 836

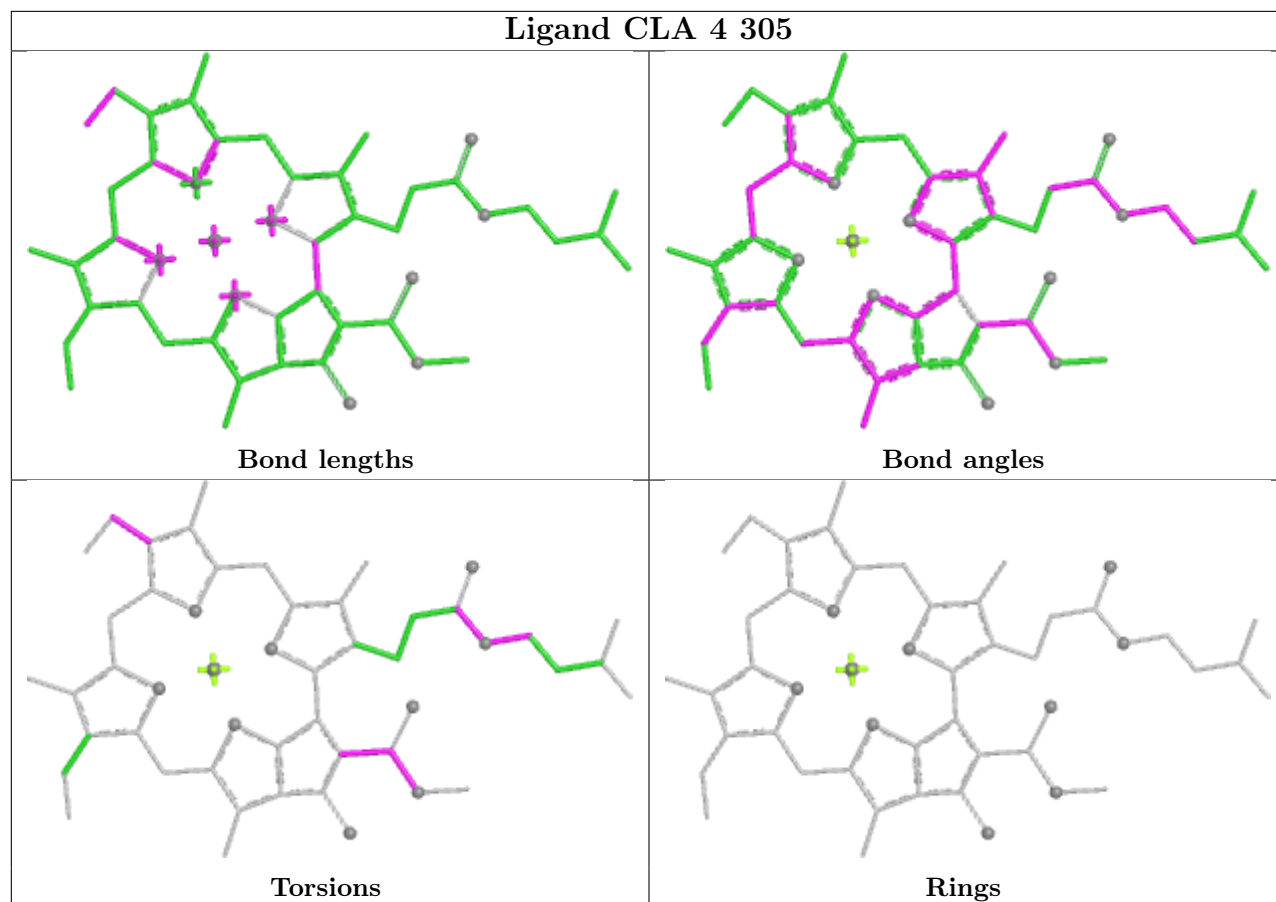




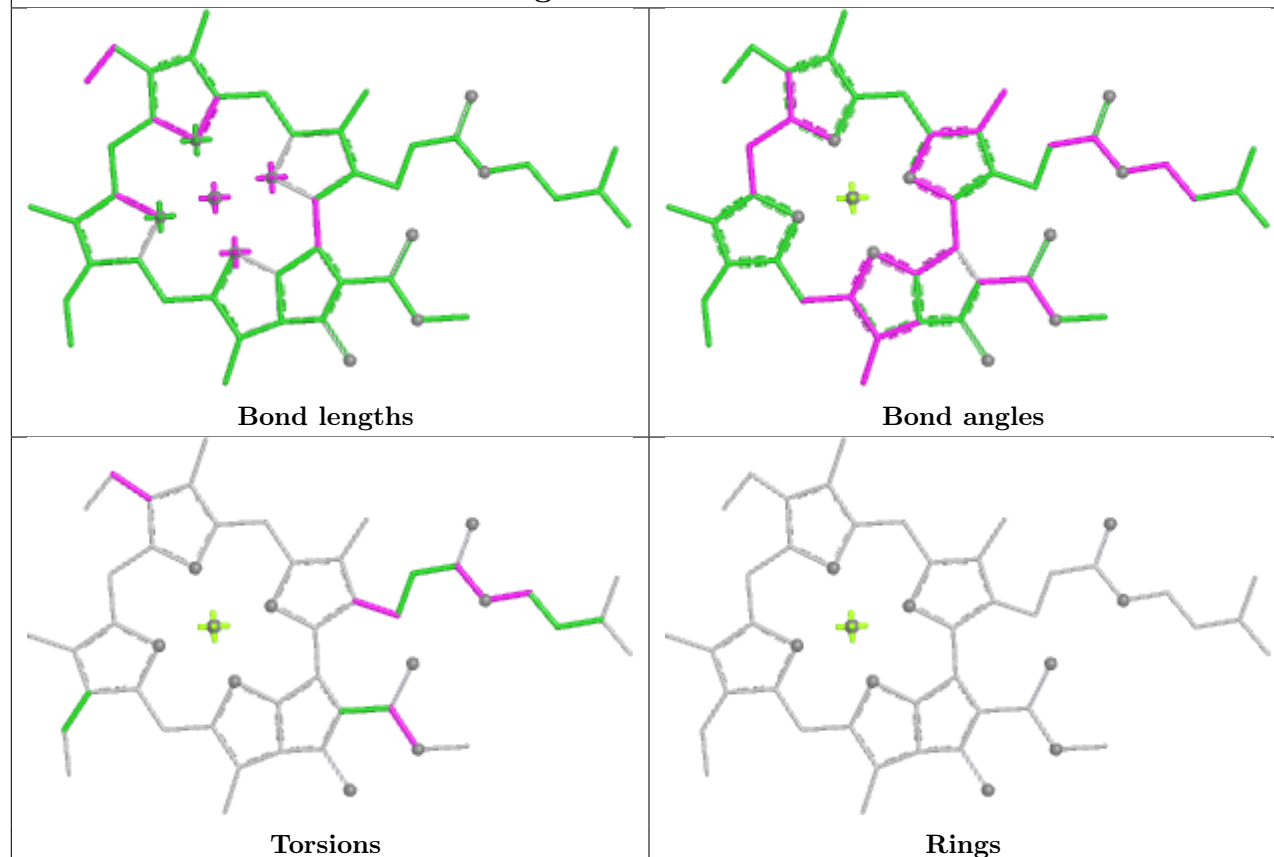




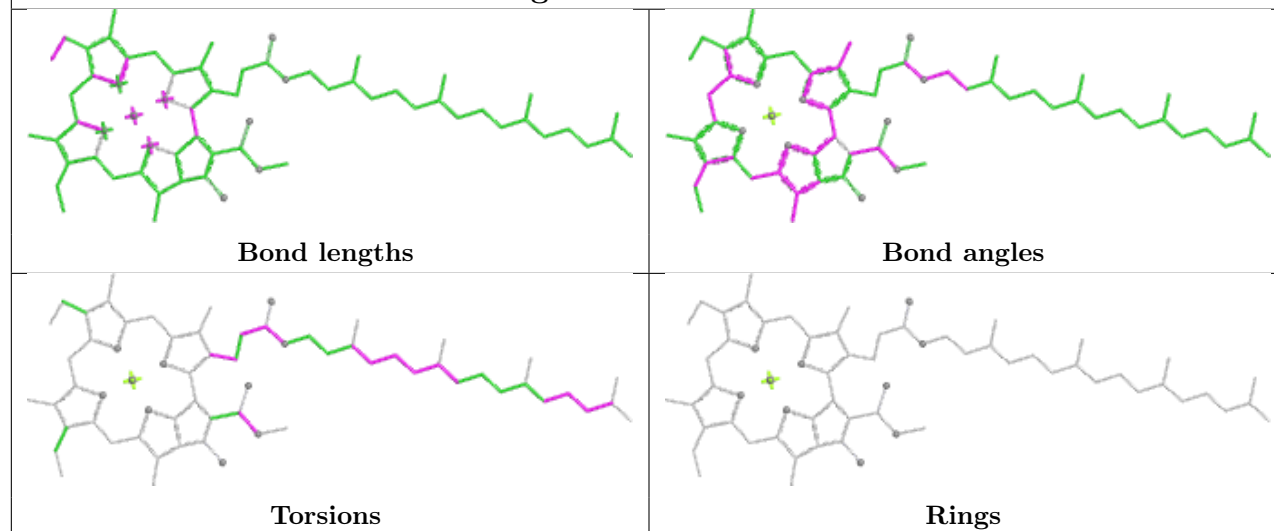
Ligand CLA 4 305

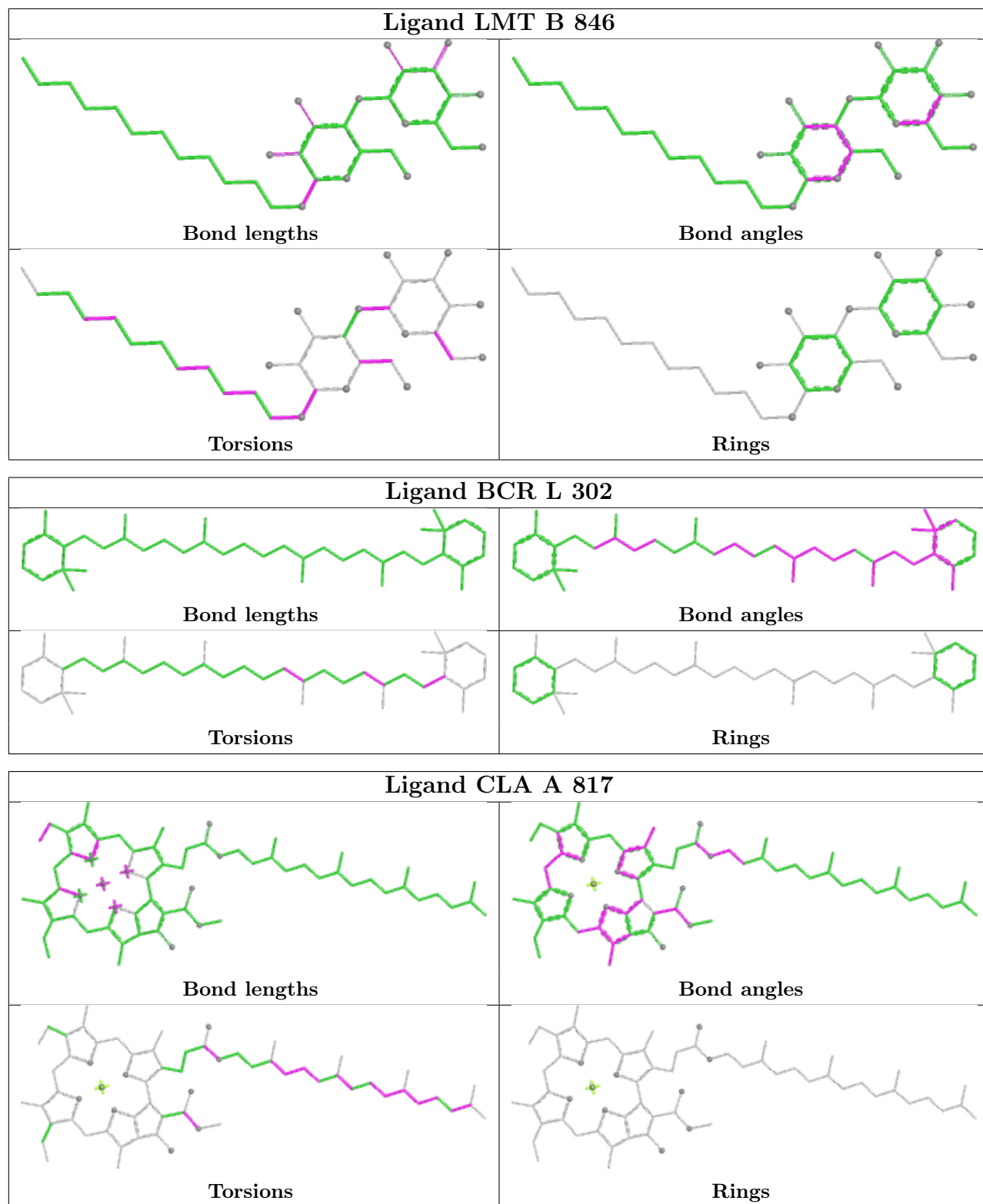


Ligand CLA L 303

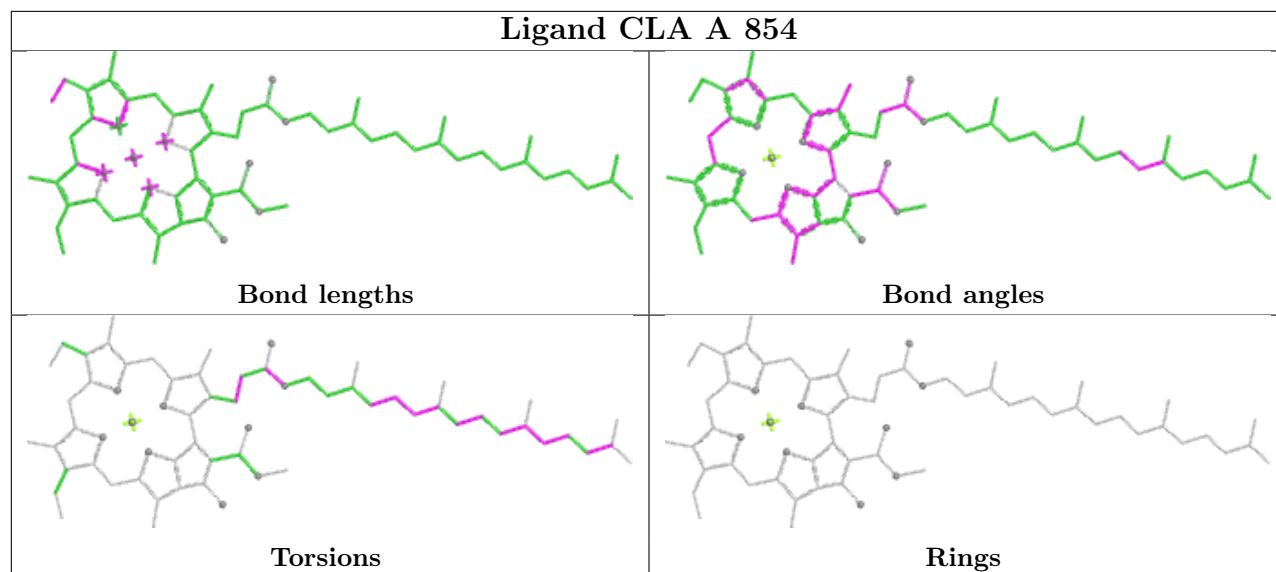


Ligand CLA G 201

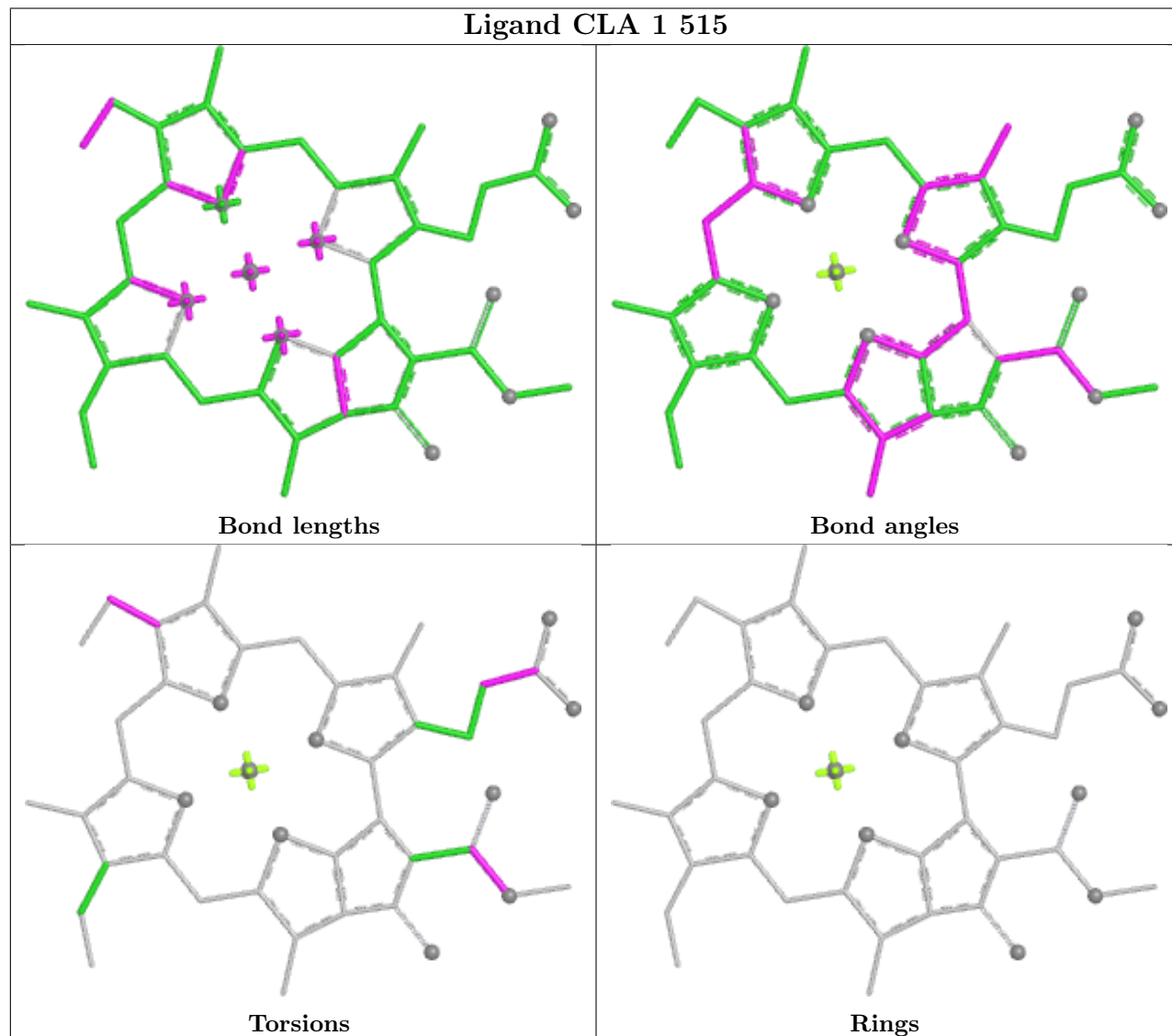




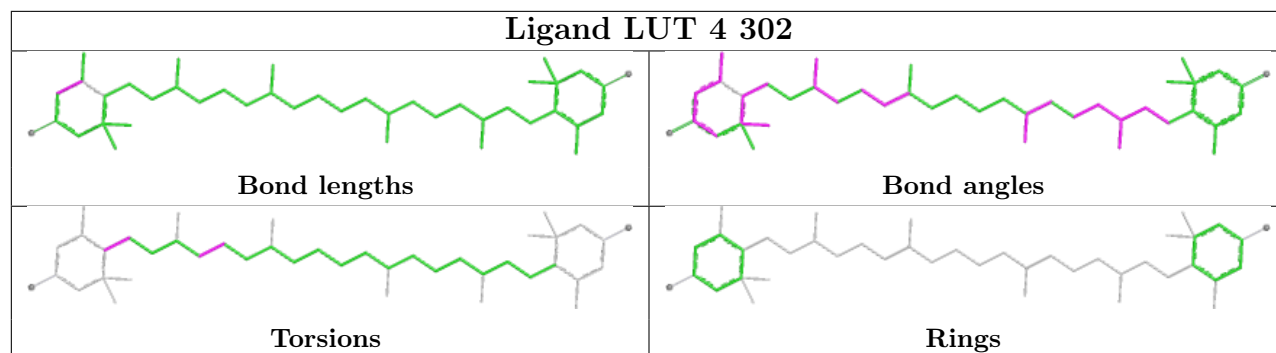
Ligand CLA A 854



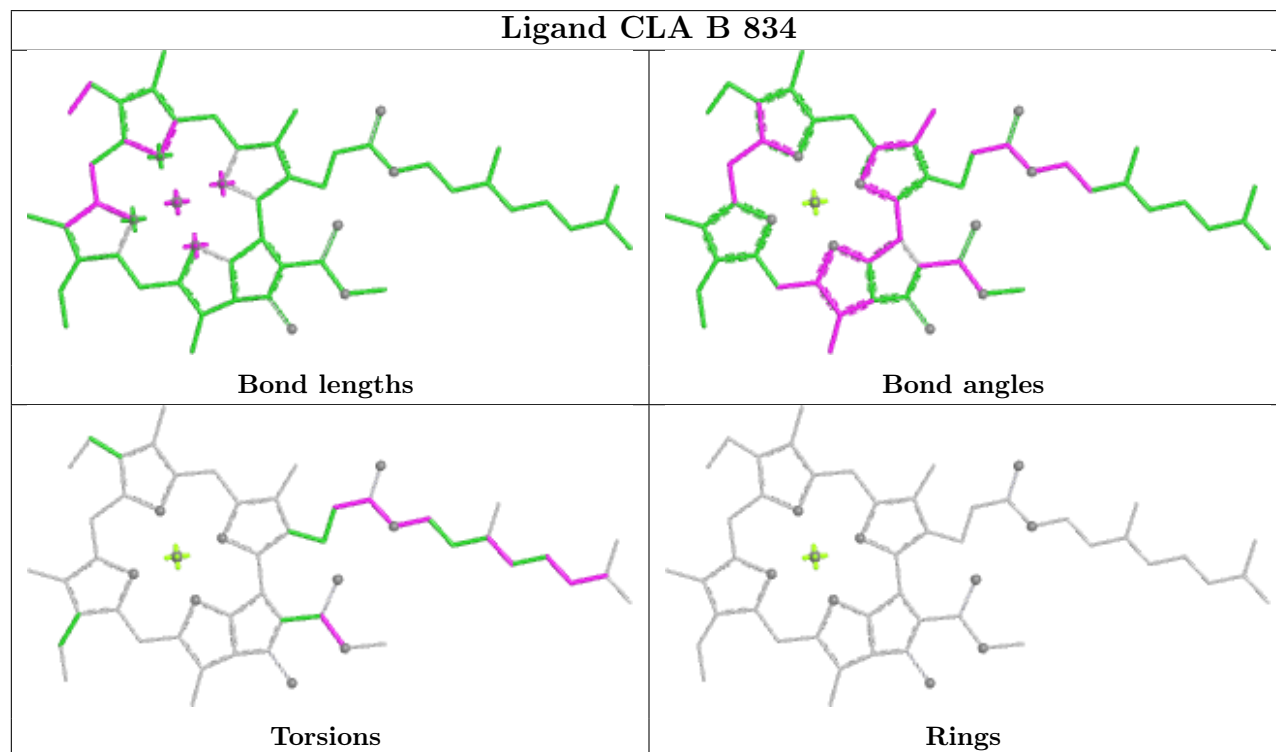
Ligand CLA 1 515



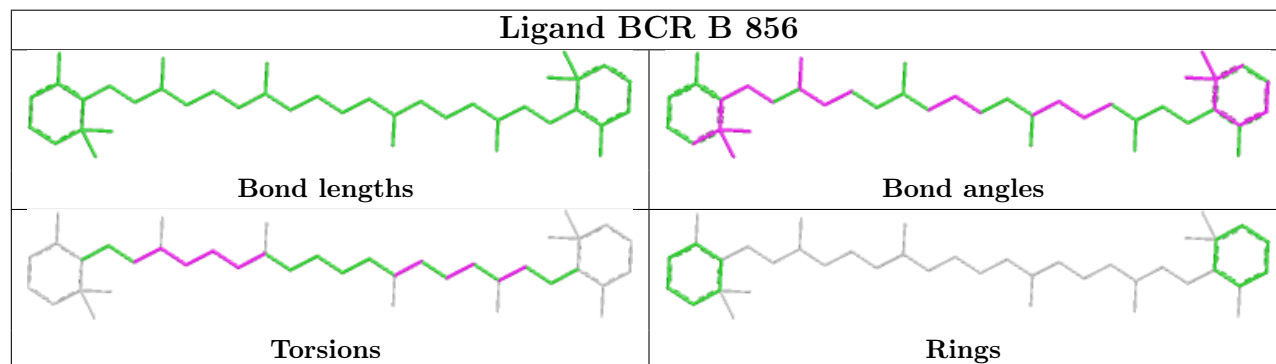
Ligand LUT 4 302



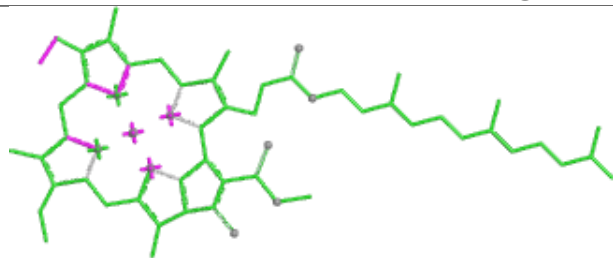
Ligand CLA B 834



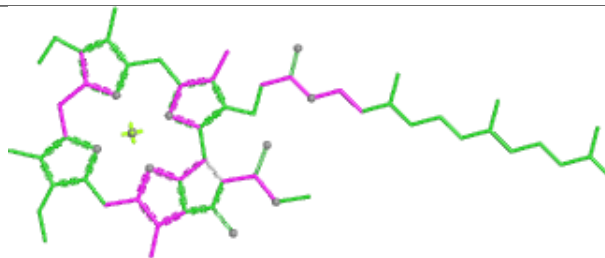
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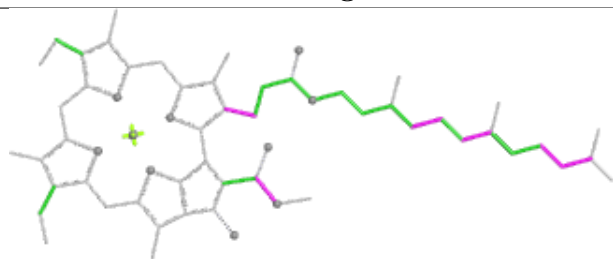
Ligand CLA L 304



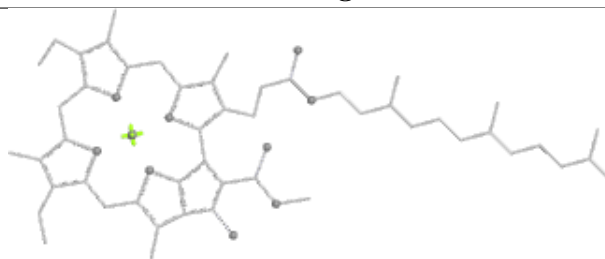
Bond lengths



Bond angles

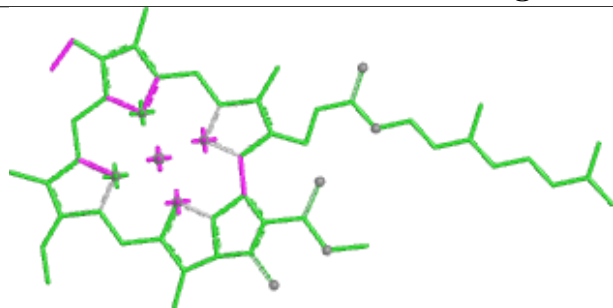


Torsions

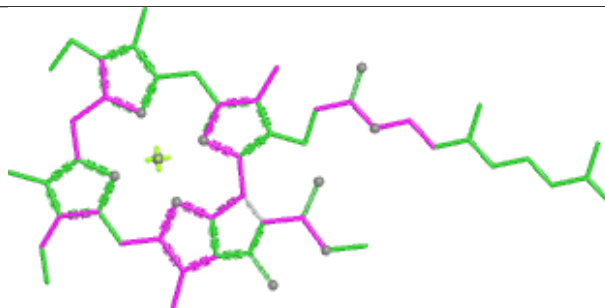


Rings

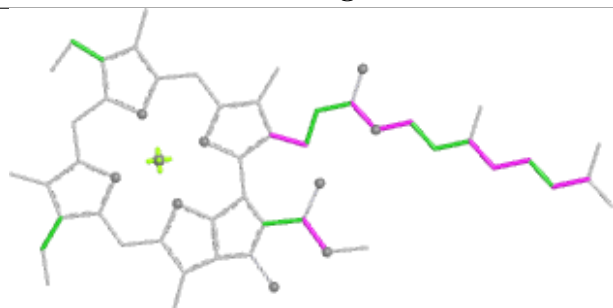
Ligand CLA A 812



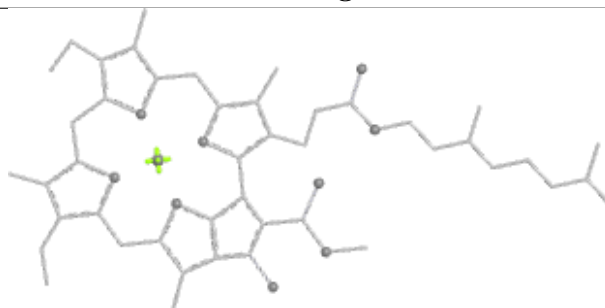
Bond lengths



Bond angles

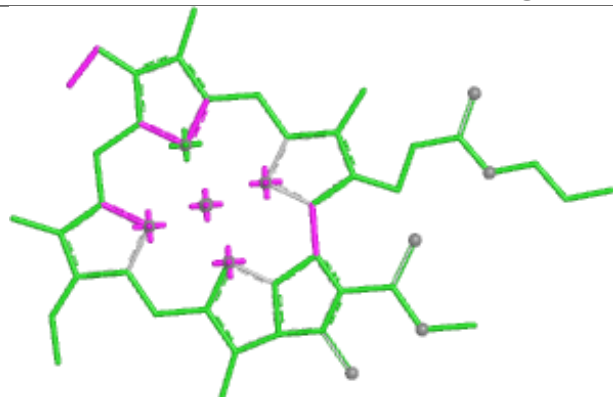


Torsions

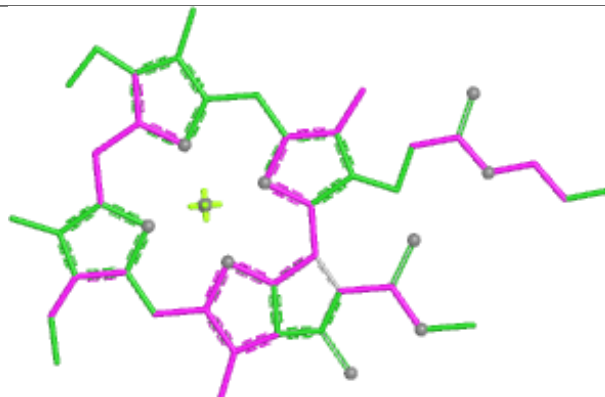


Rings

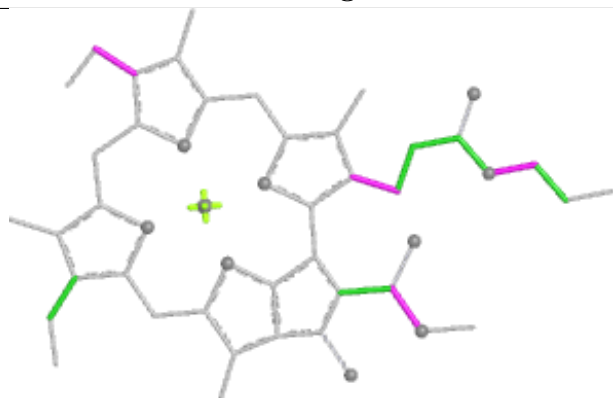
Ligand CLA 3 312



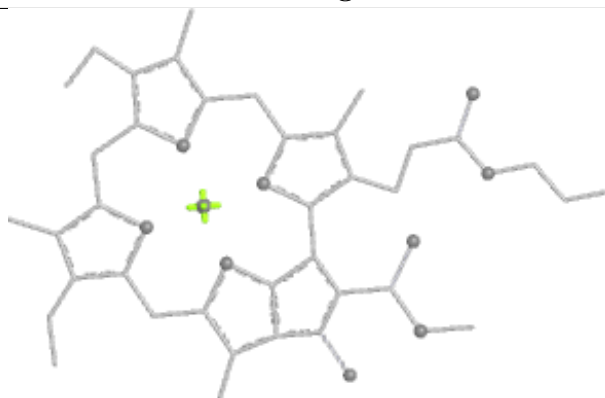
Bond lengths



Bond angles

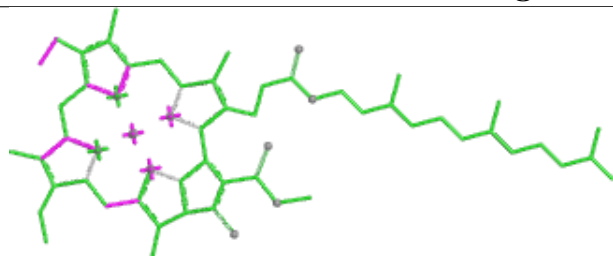


Torsions

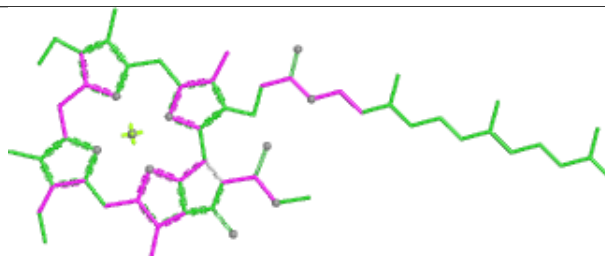


Rings

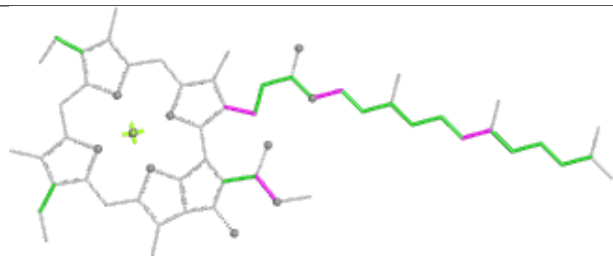
Ligand CLA B 817



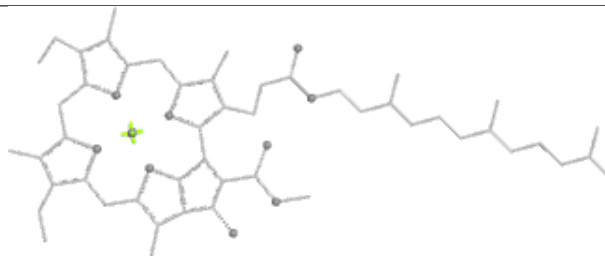
Bond lengths



Bond angles

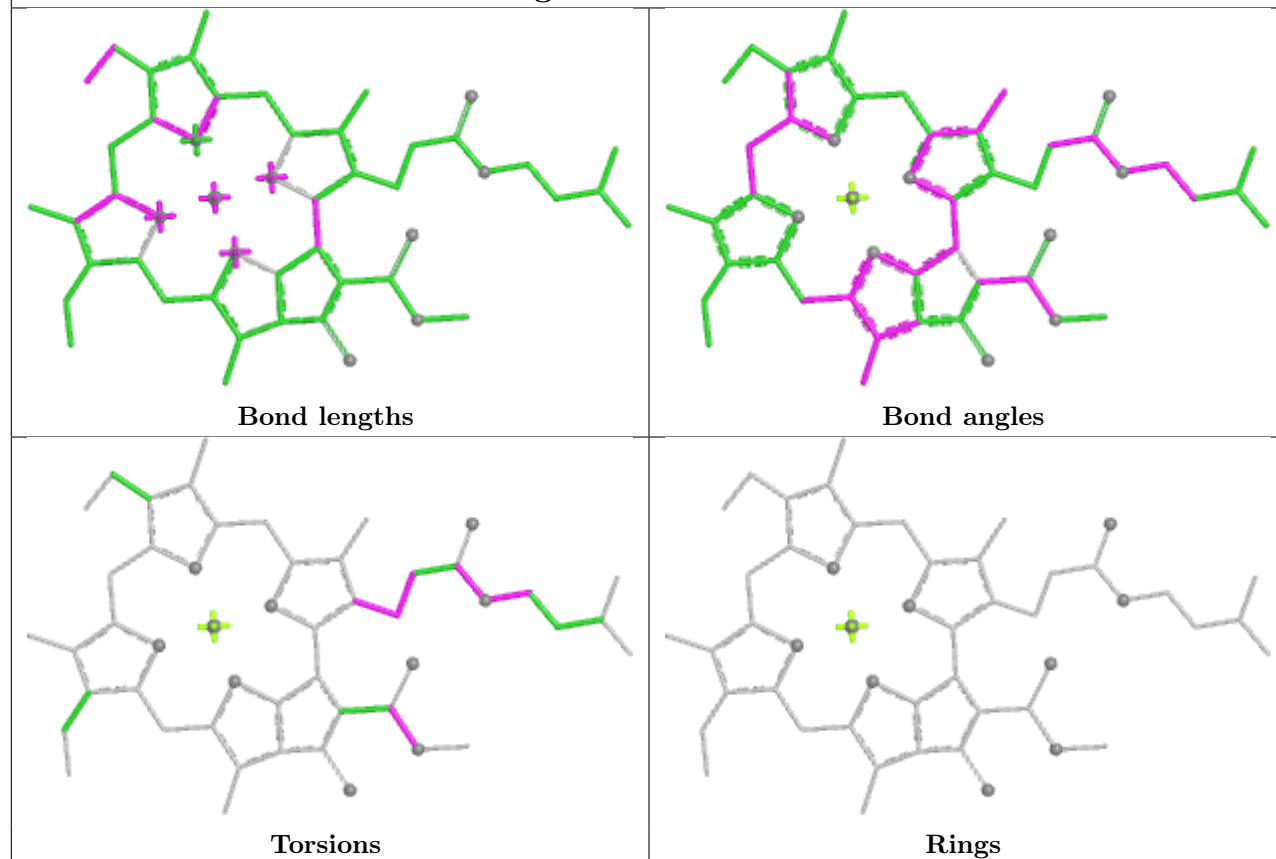


Torsions

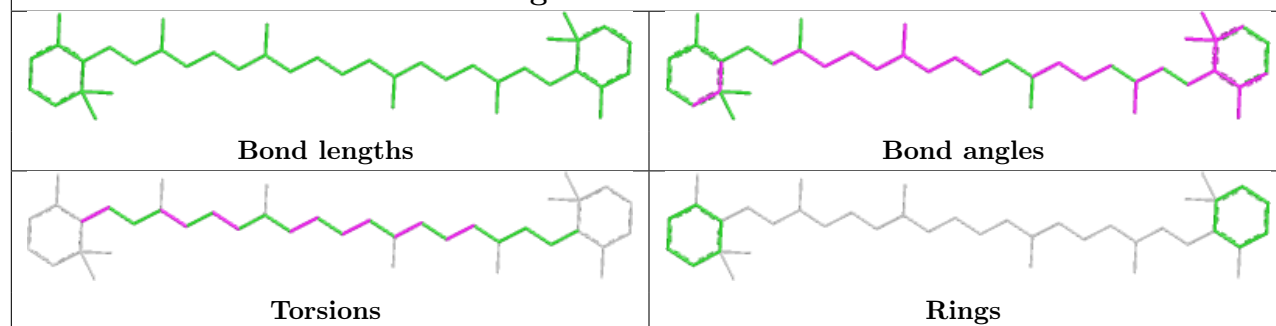


Rings

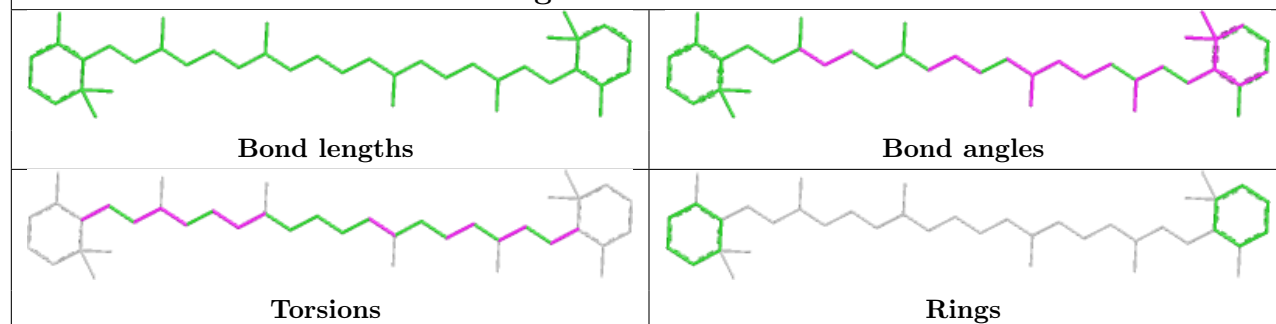
Ligand CLA L 305

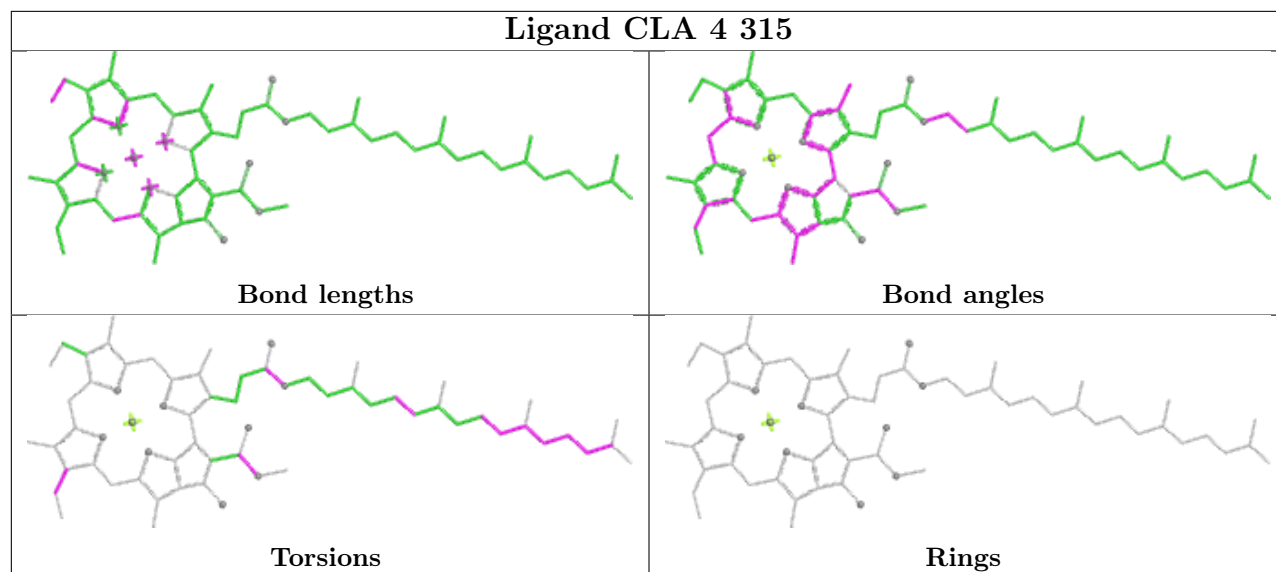
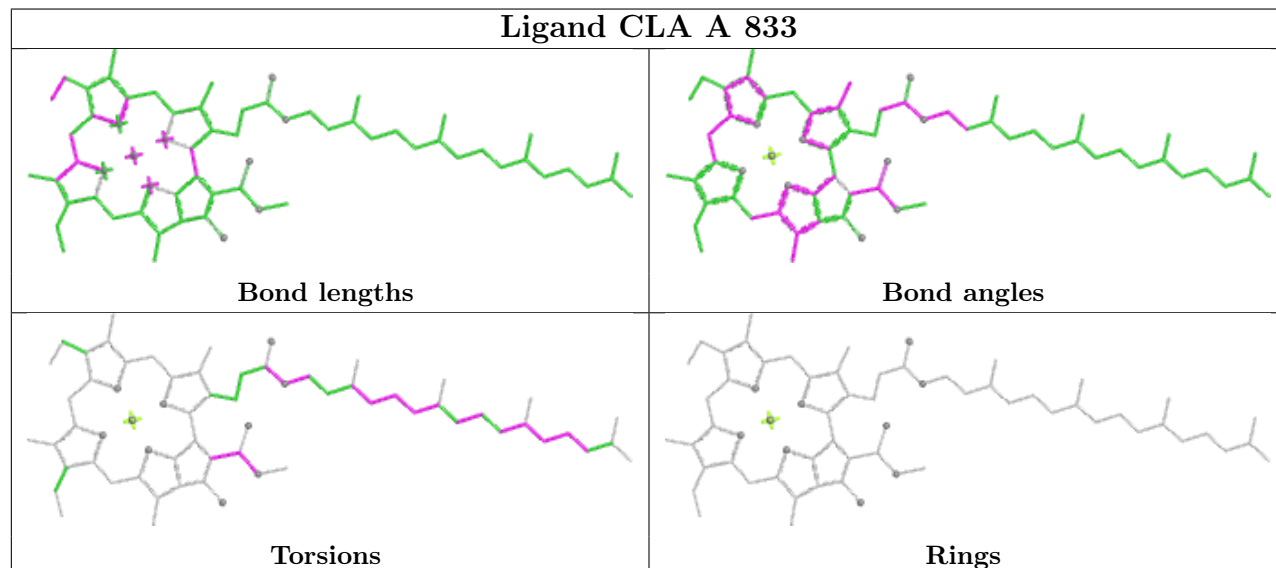


Ligand BCR A 848

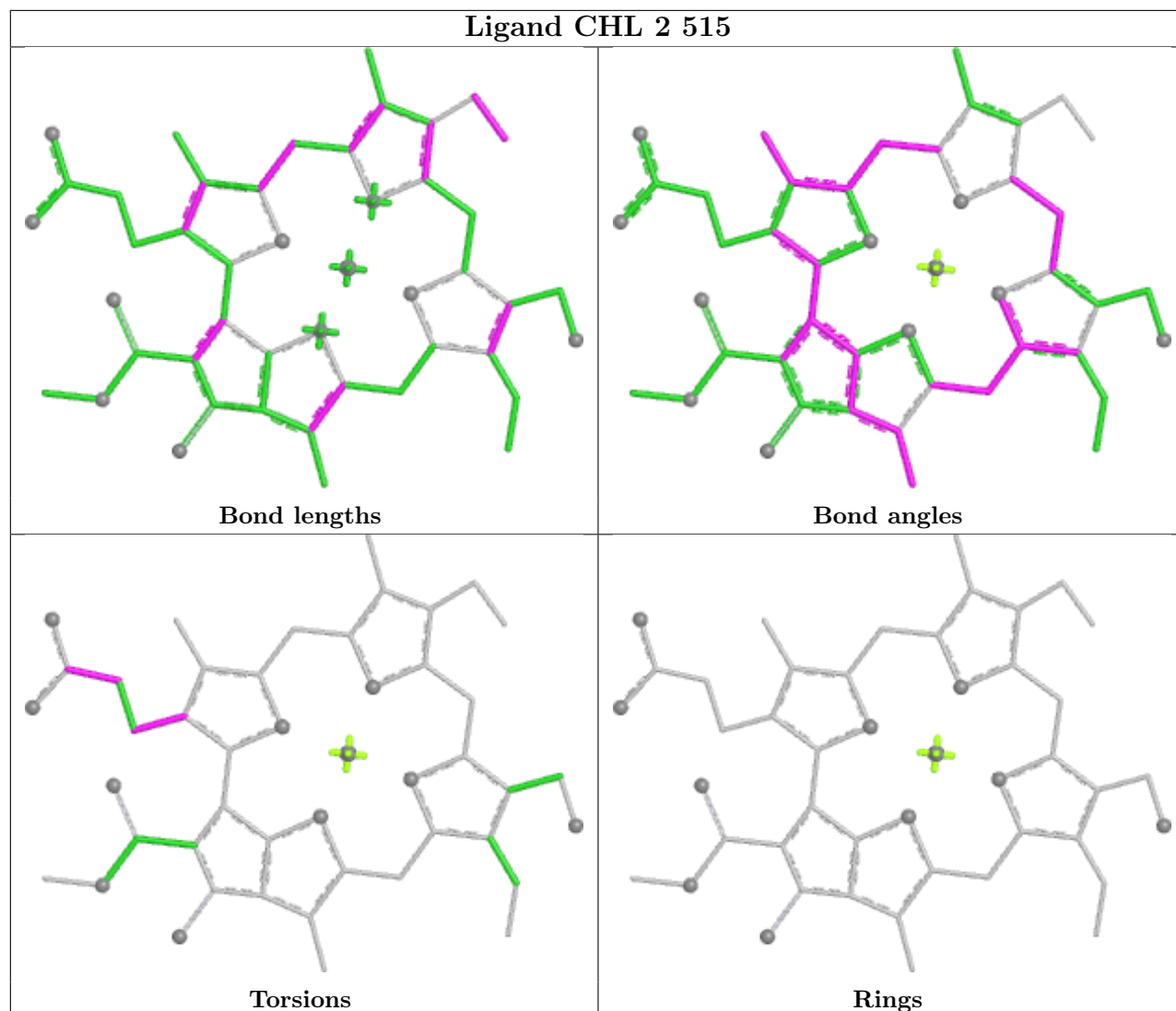


Ligand BCR 3 304

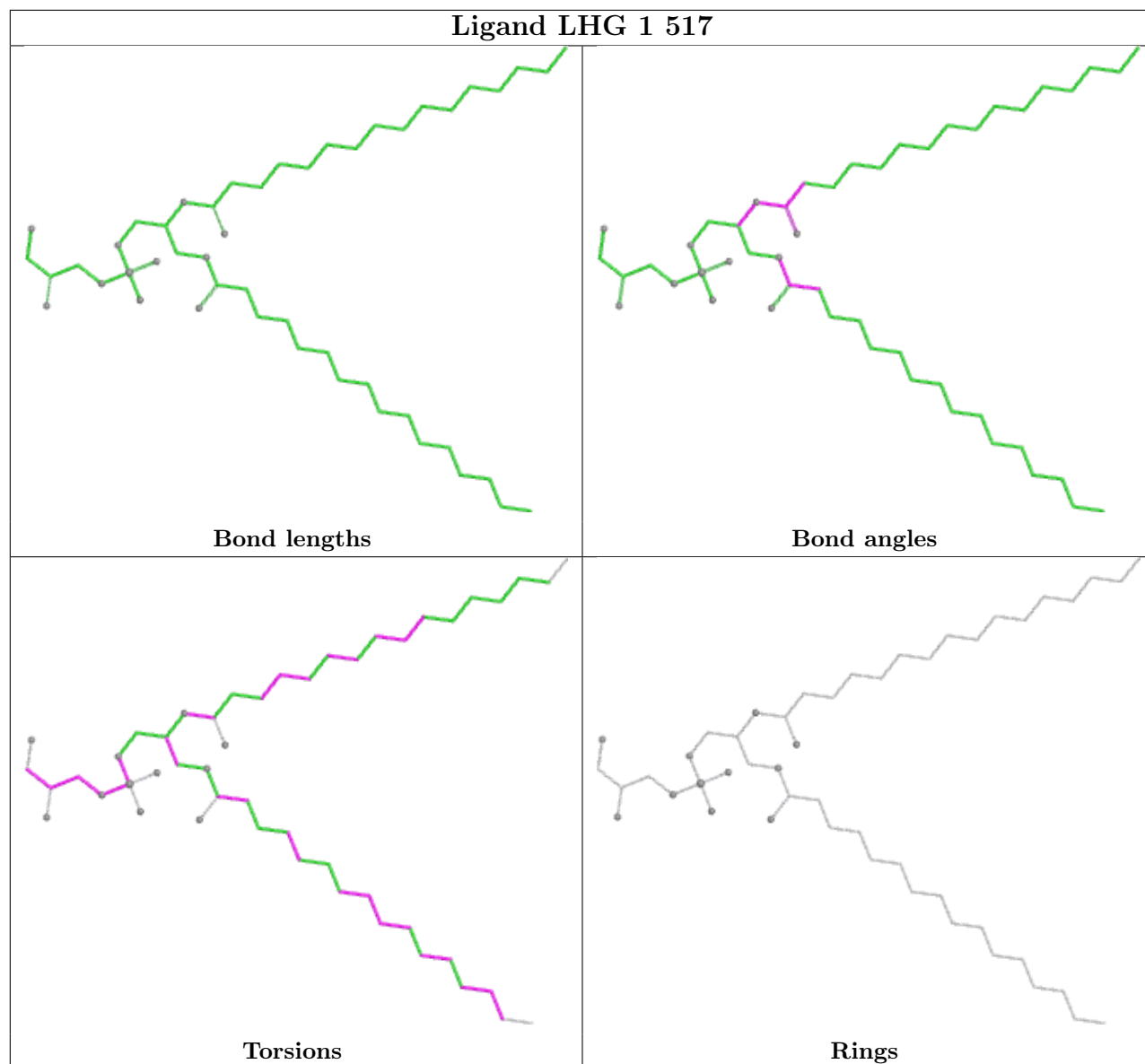


Ligand CLA 4 315**Ligand CLA A 833**

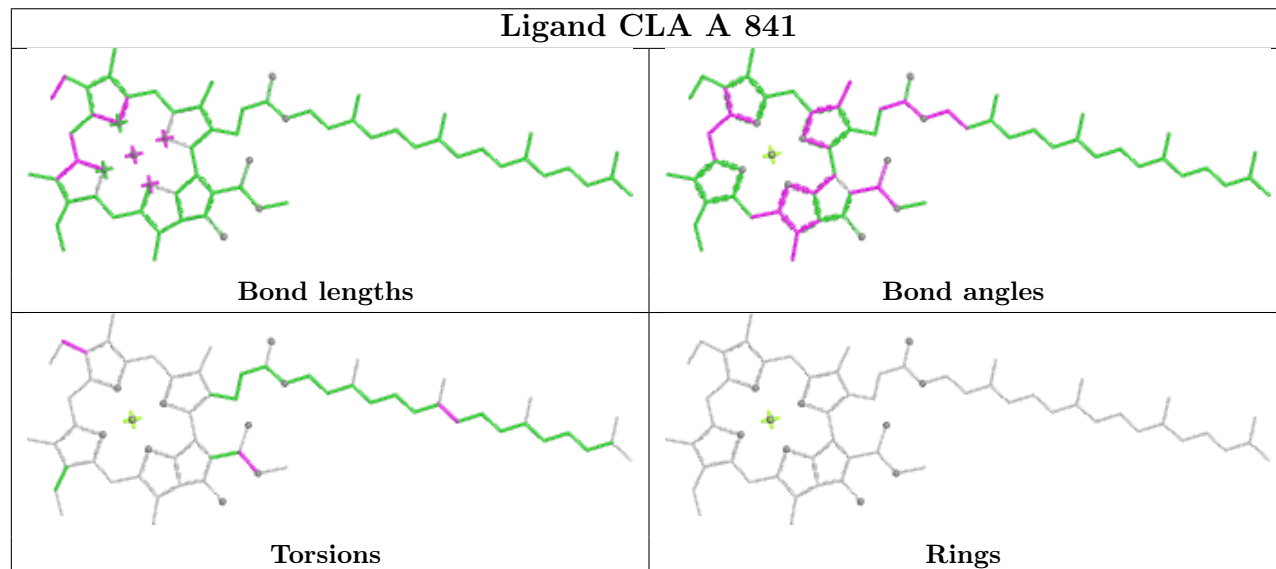
Ligand CHL 2 515



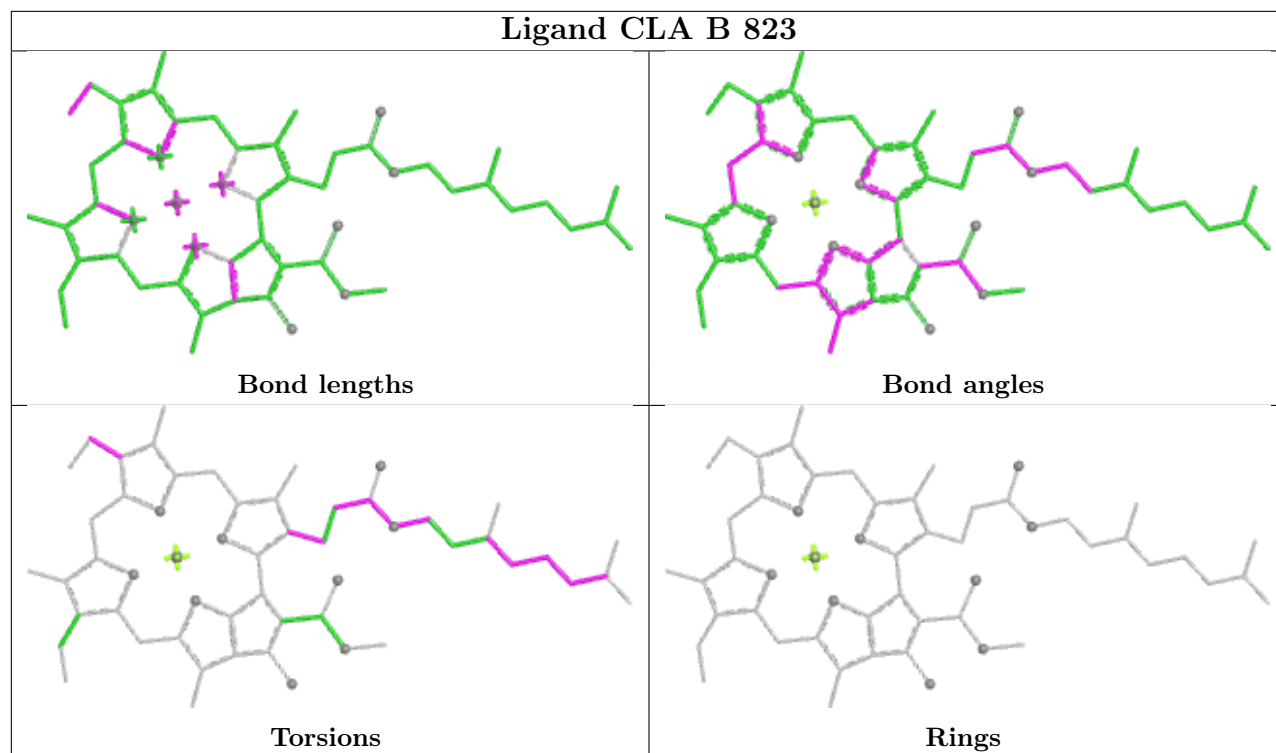
Ligand LHG 1 517



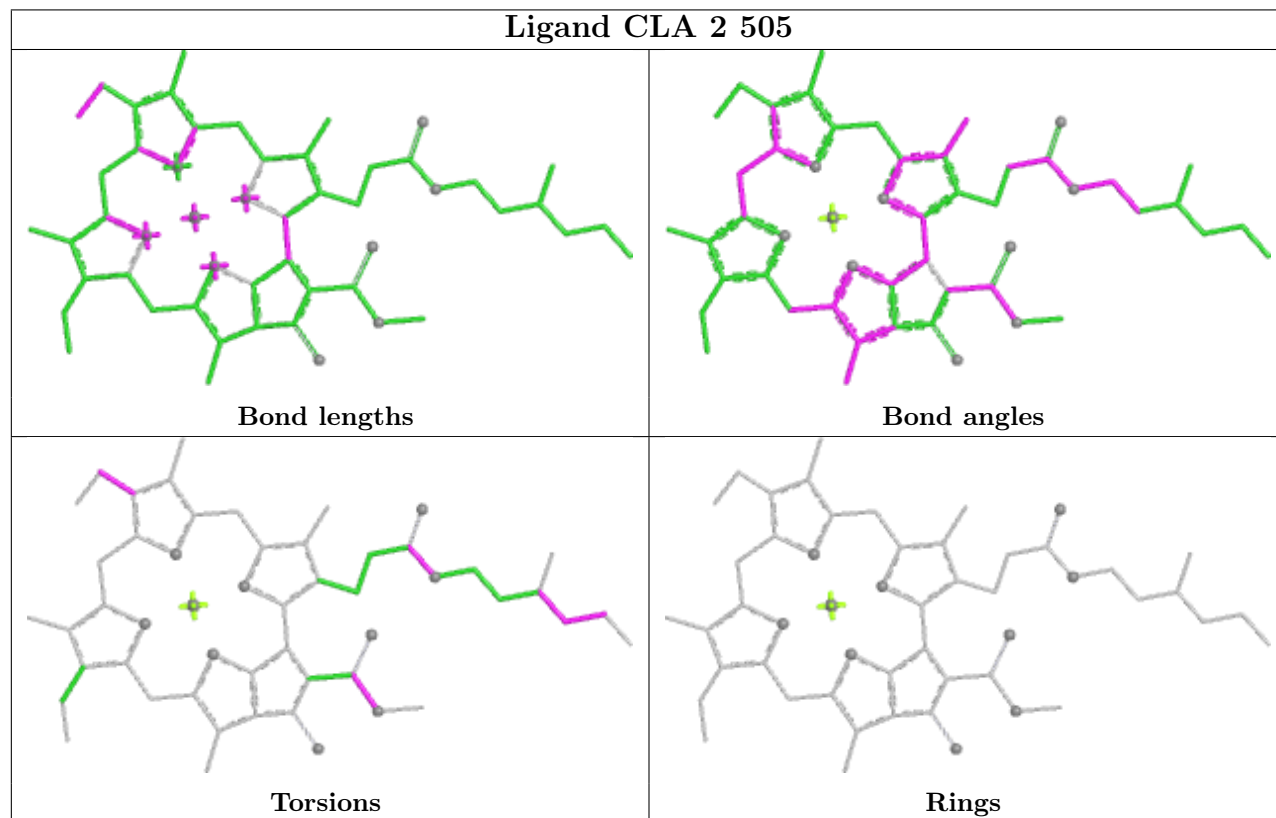
Ligand CLA A 841

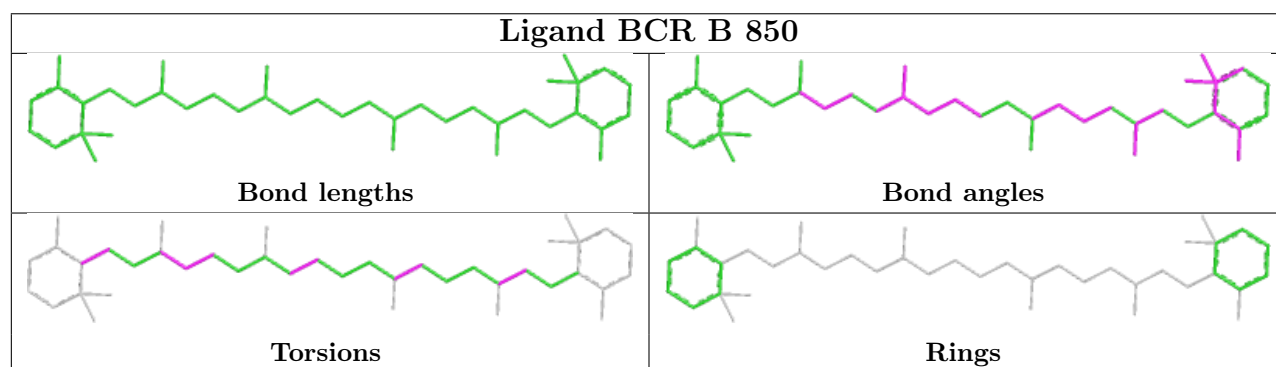
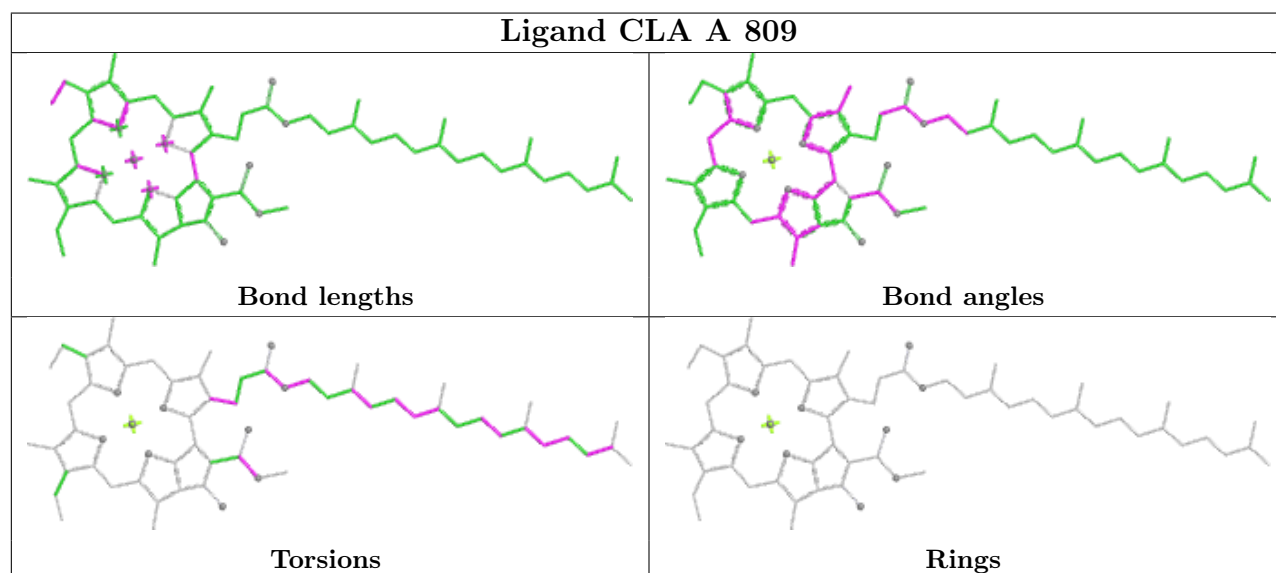
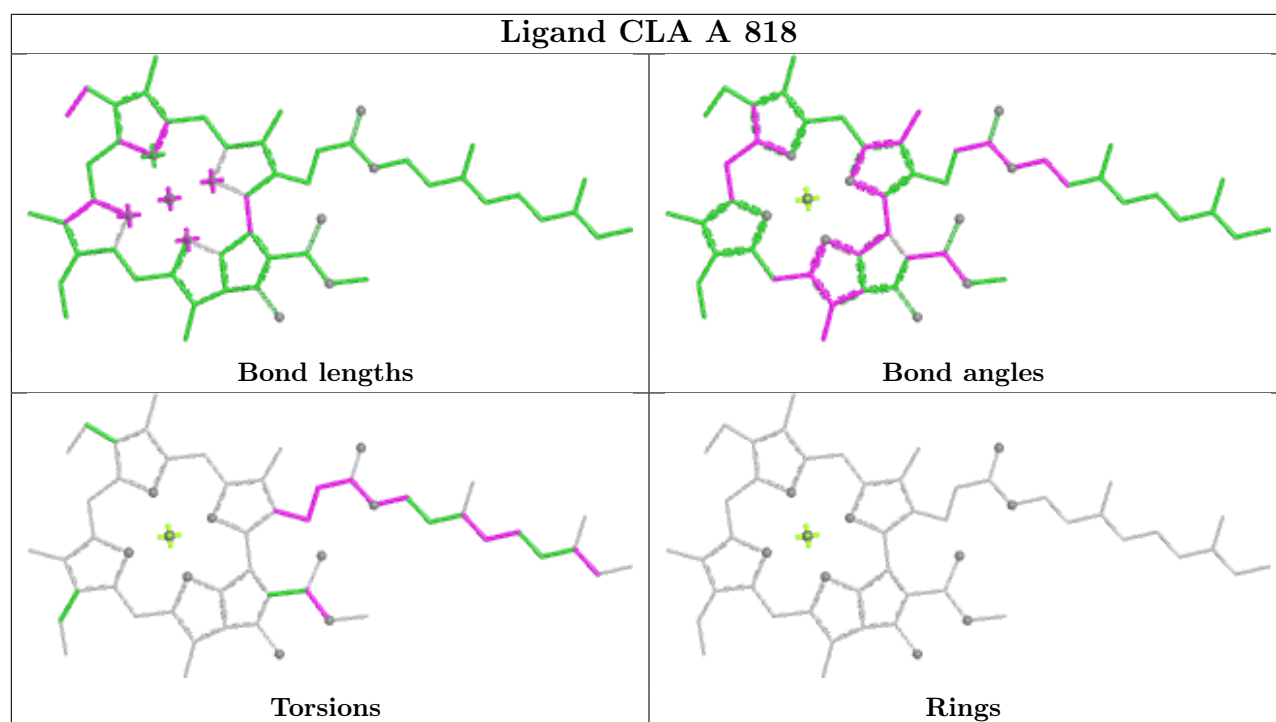


Ligand CLA B 823

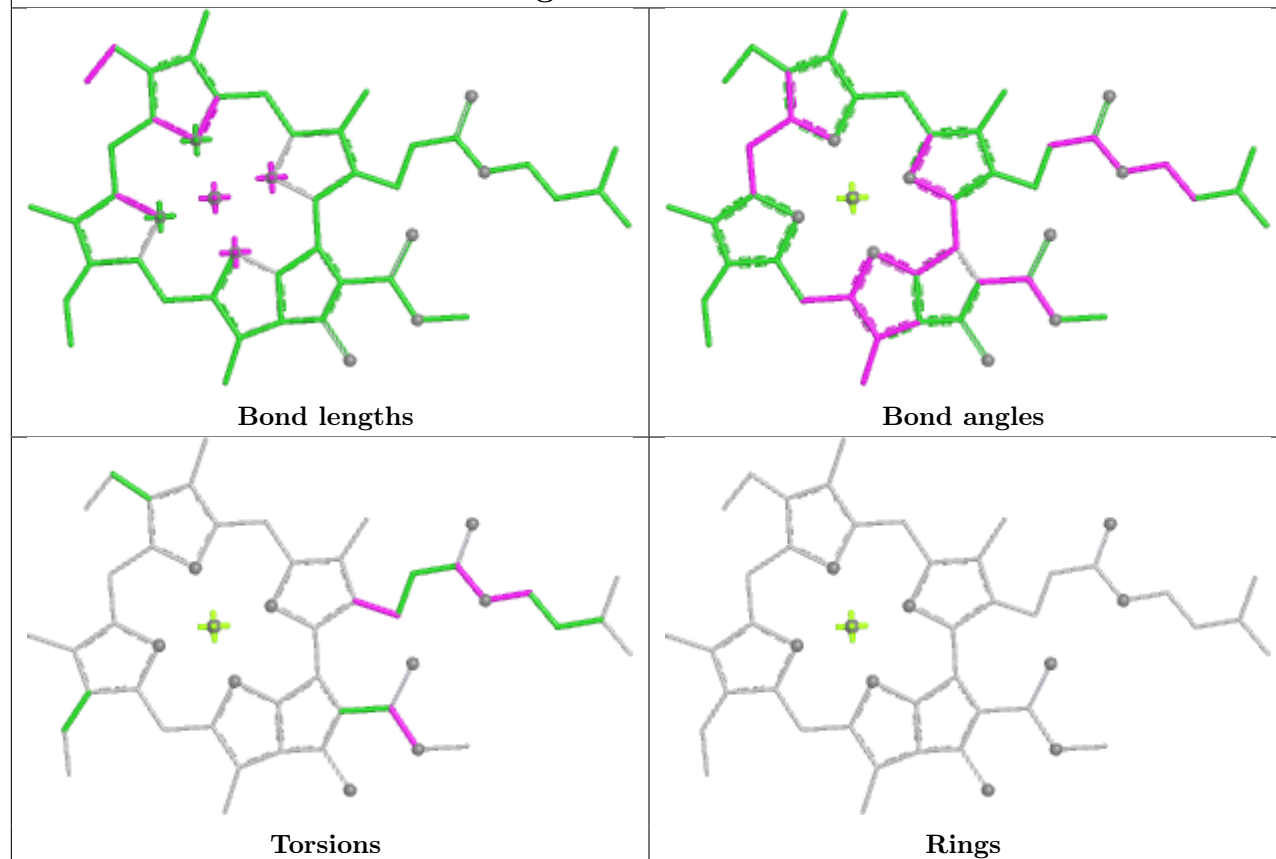


Ligand CLA 2 505

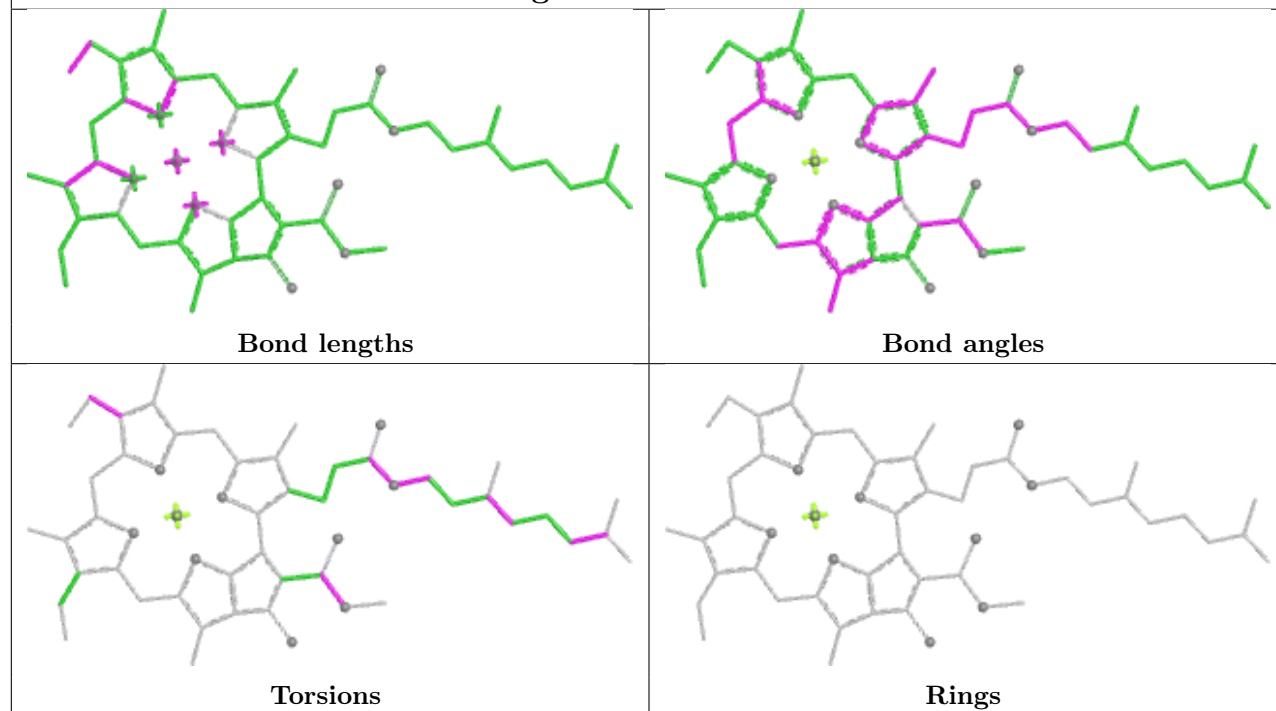


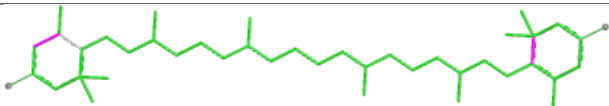
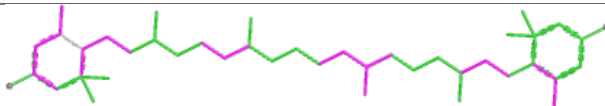
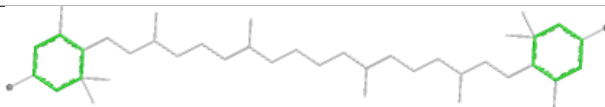


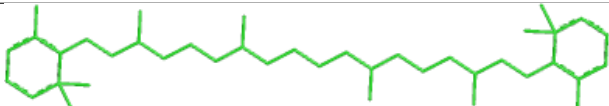
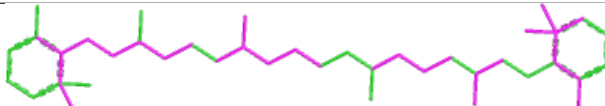
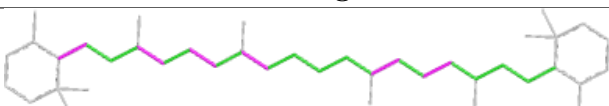
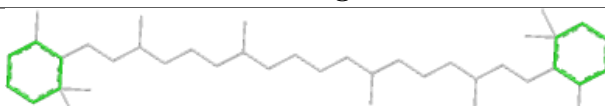
Ligand CLA 3 315



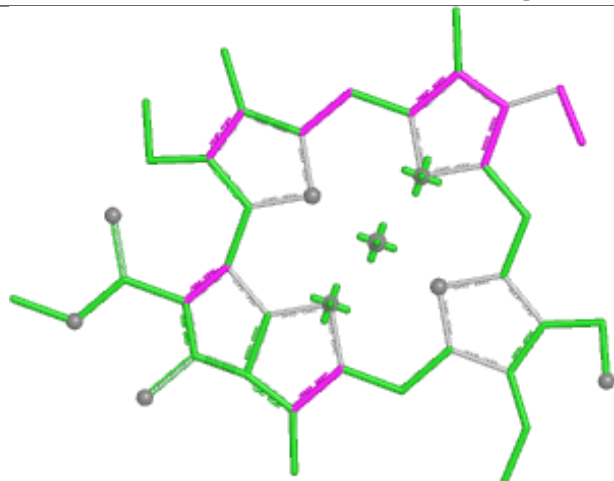
Ligand CLA A 826



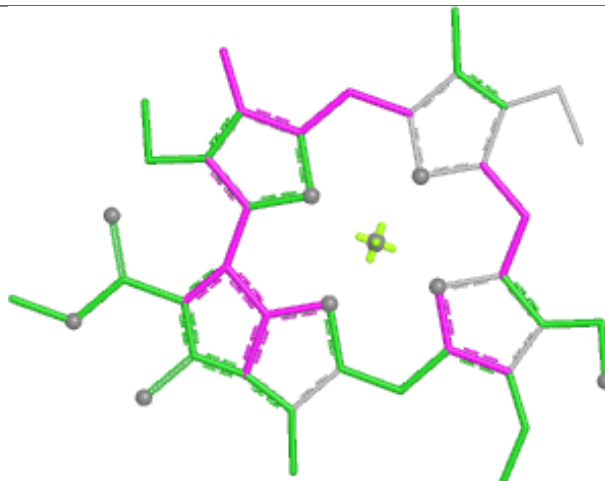
Ligand LUT 1 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

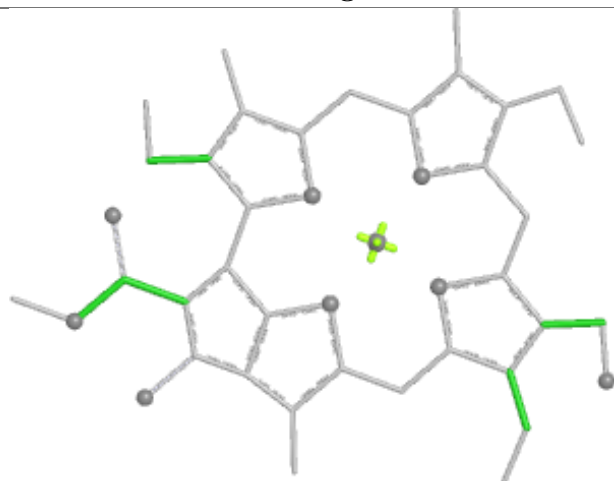
Ligand CHL 4 317



Bond lengths



Bond angles

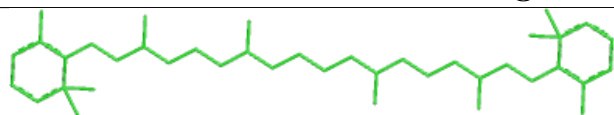


Torsions

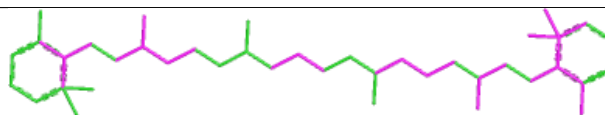


Rings

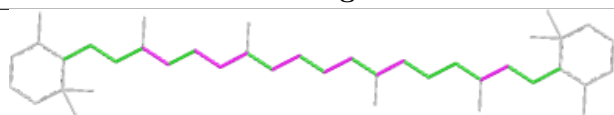
Ligand BCR L 307



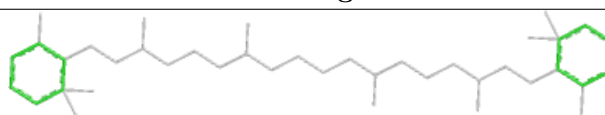
Bond lengths



Bond angles

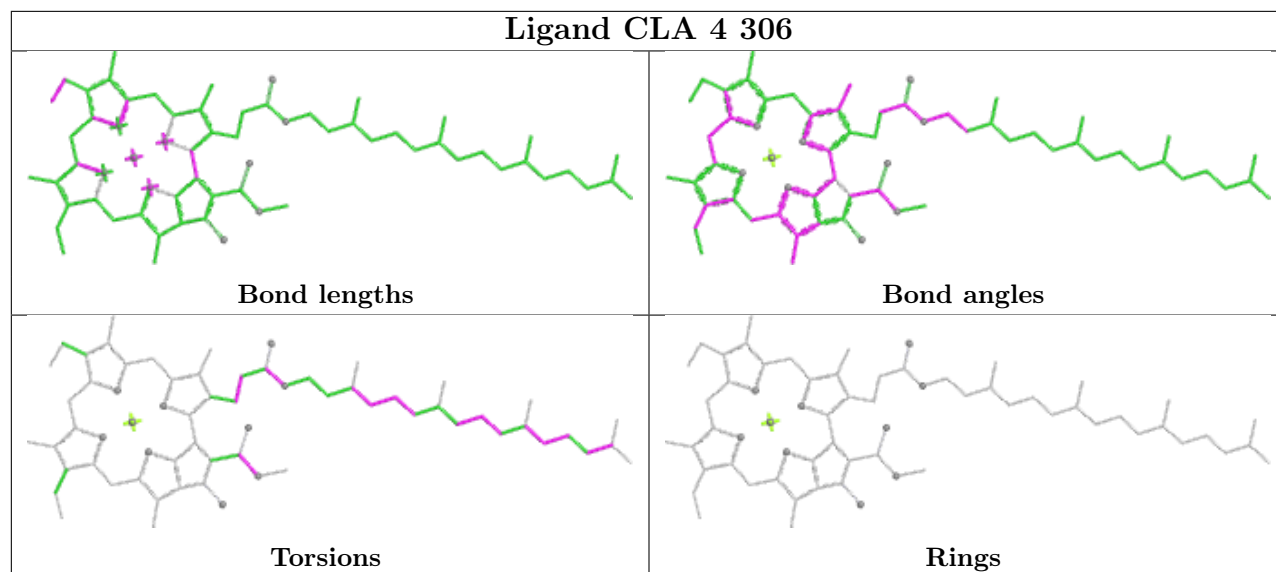


Torsions

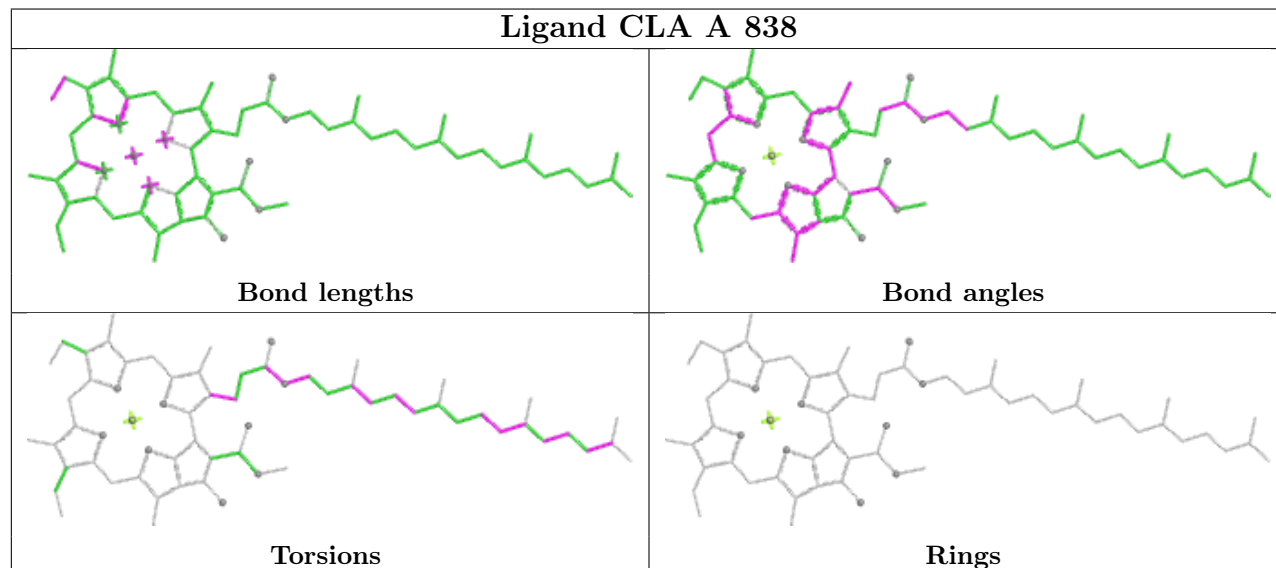


Rings

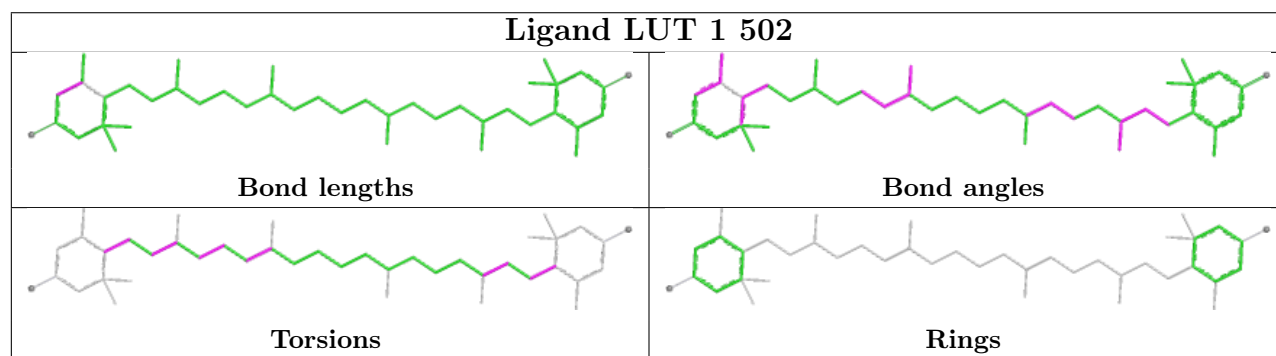
Ligand CLA 4 306

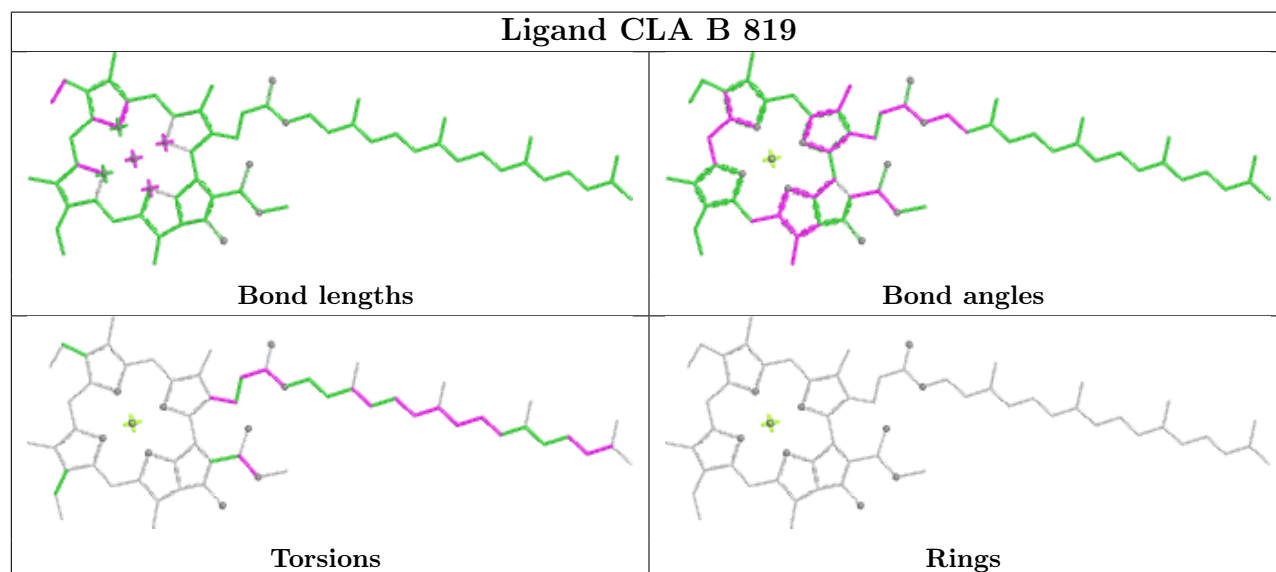
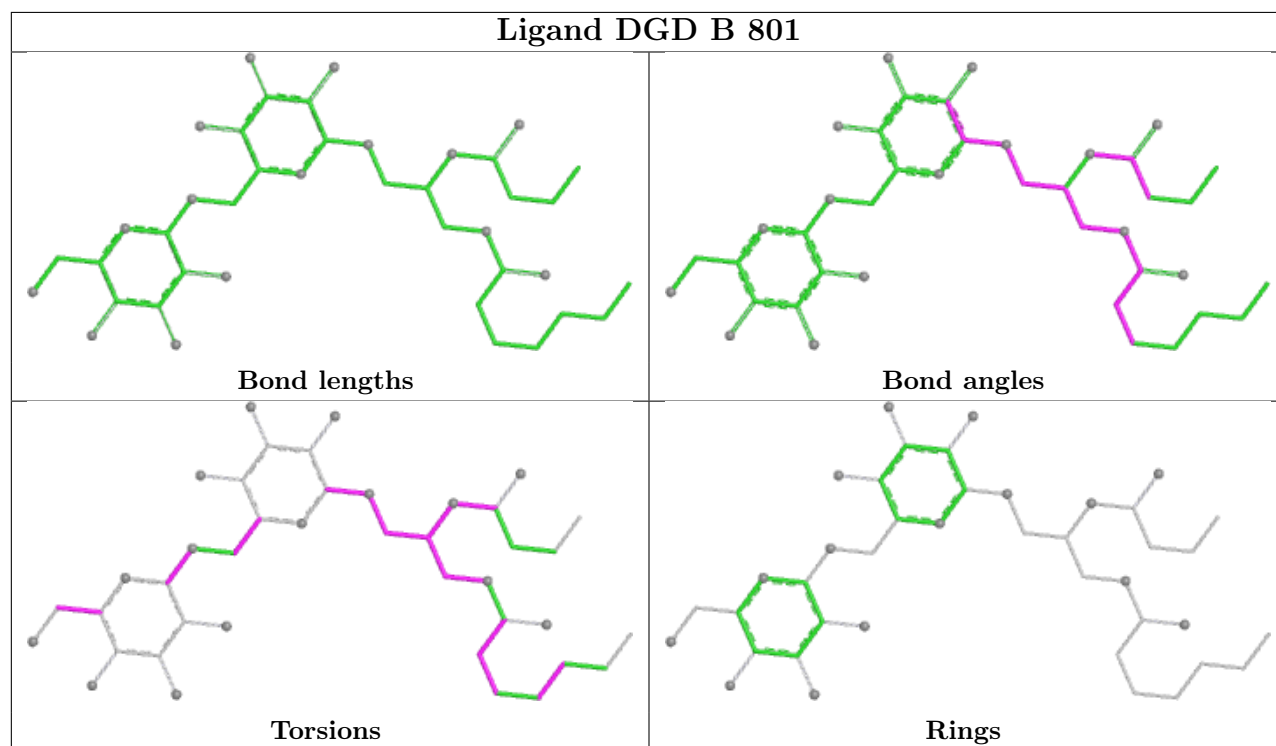
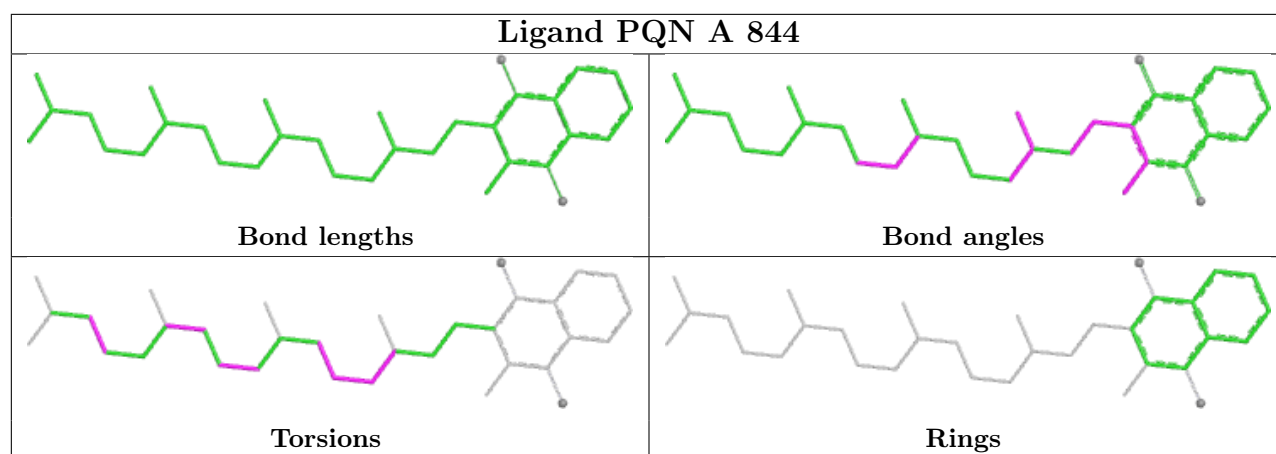


Ligand CLA A 838

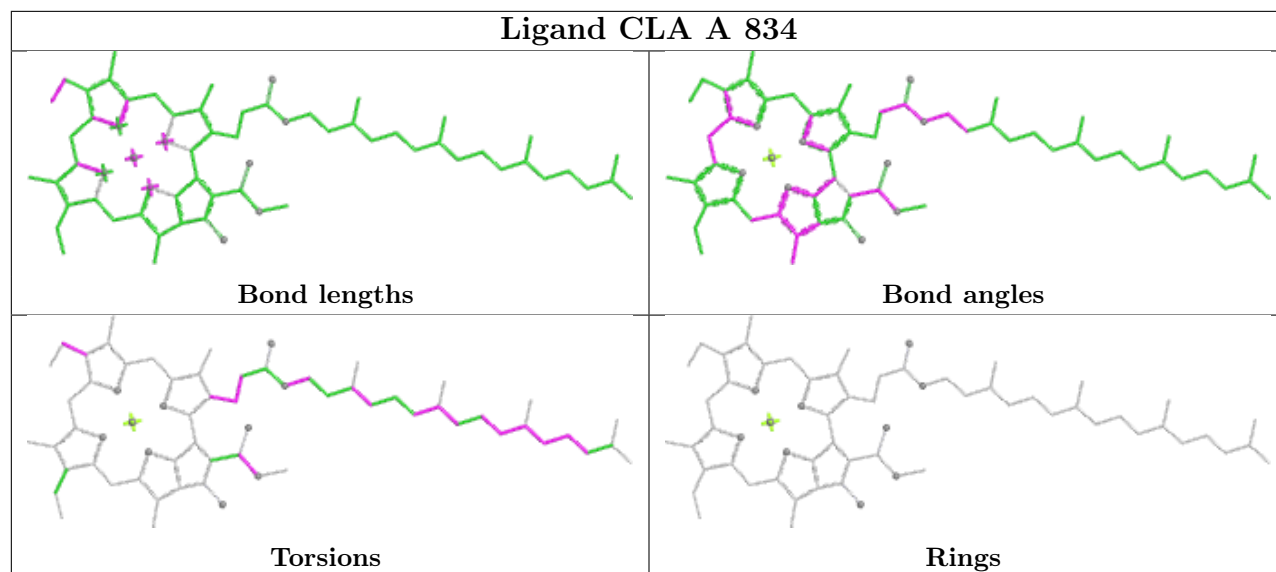


Ligand LUT 1 502

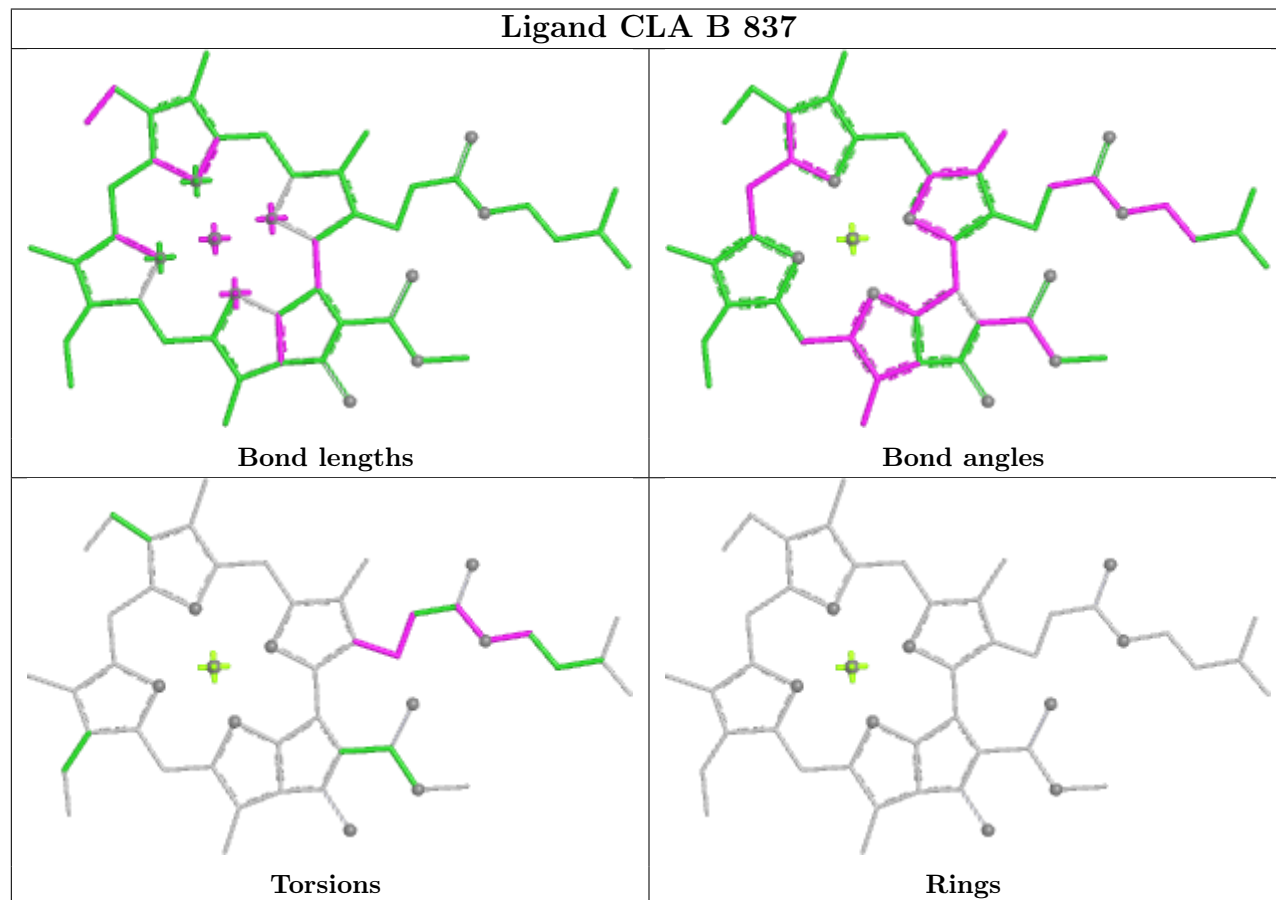




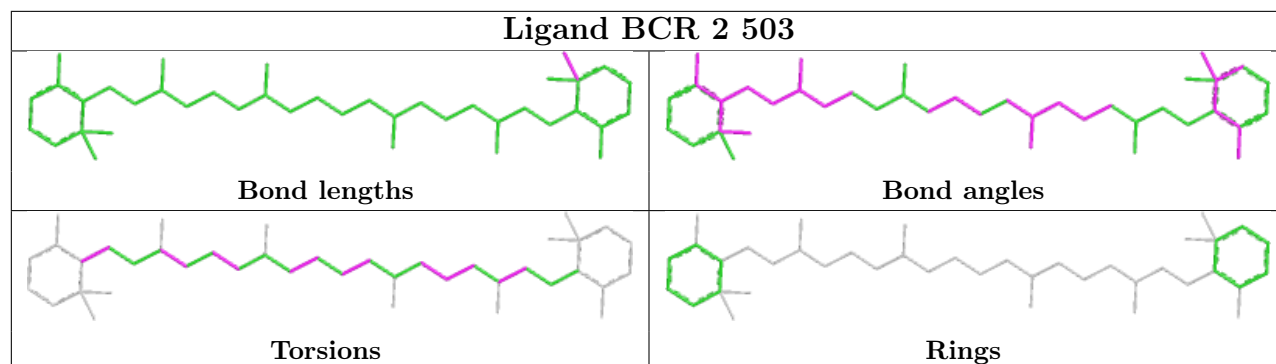
Ligand CLA A 834



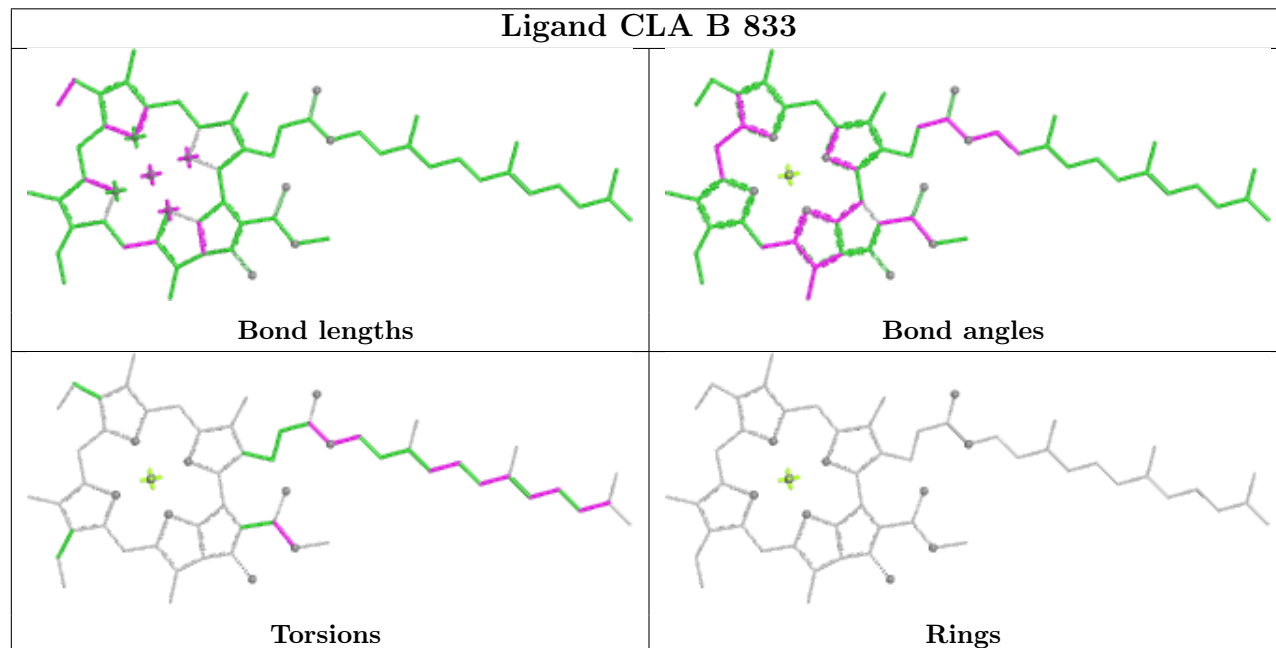
Ligand CLA B 837



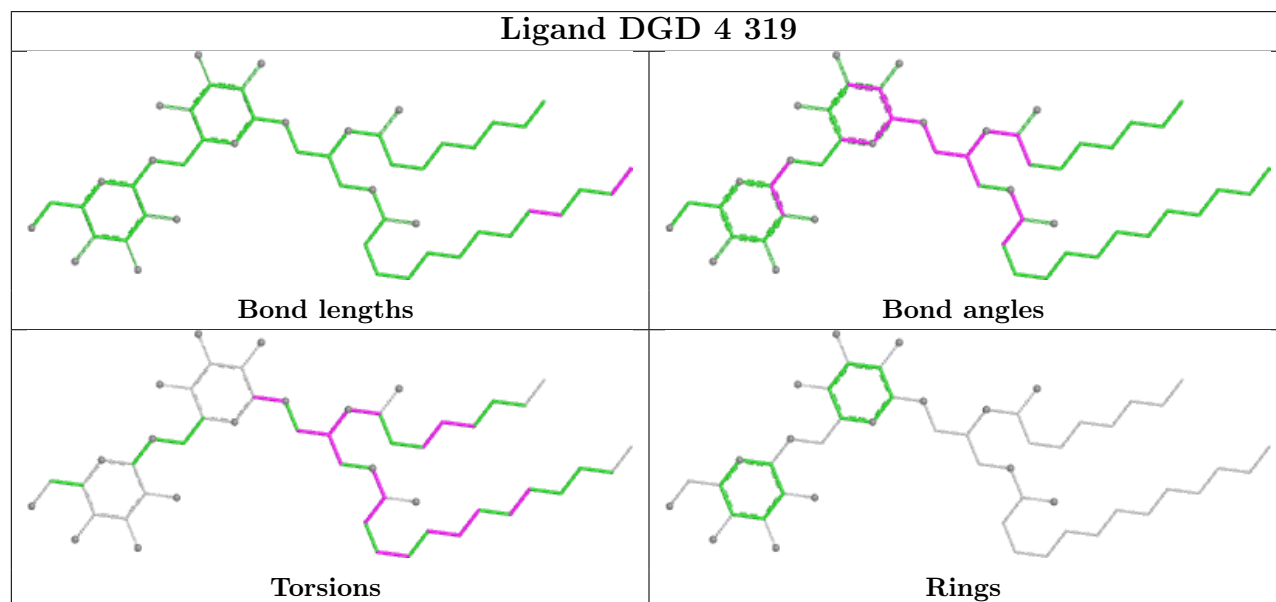
Ligand BCR 2 503



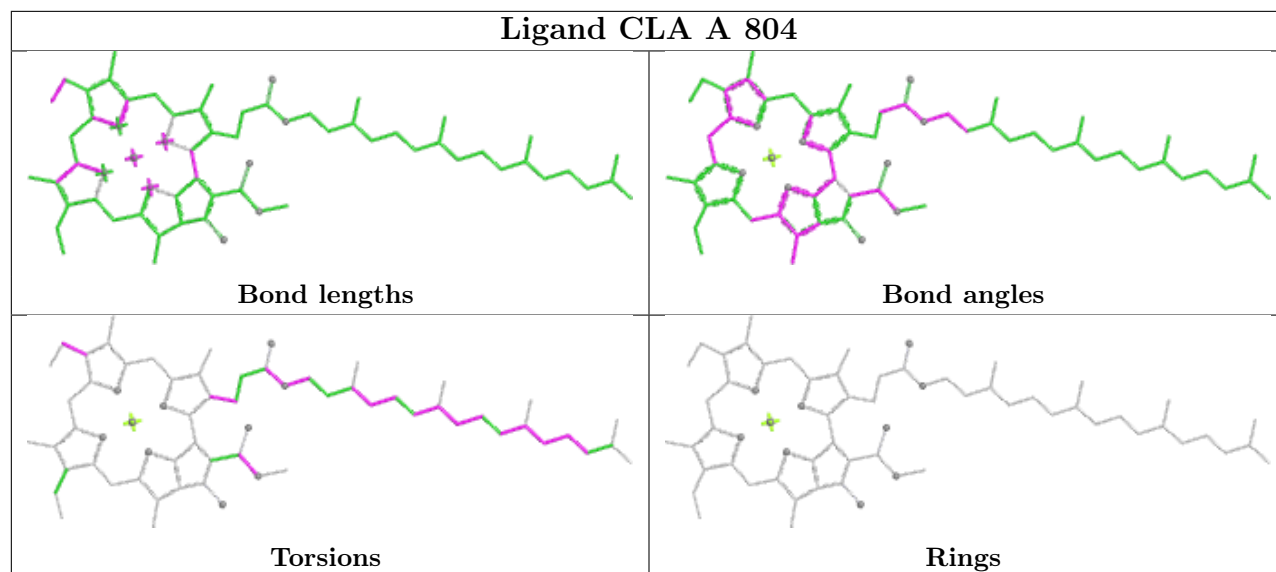
Ligand CLA B 833



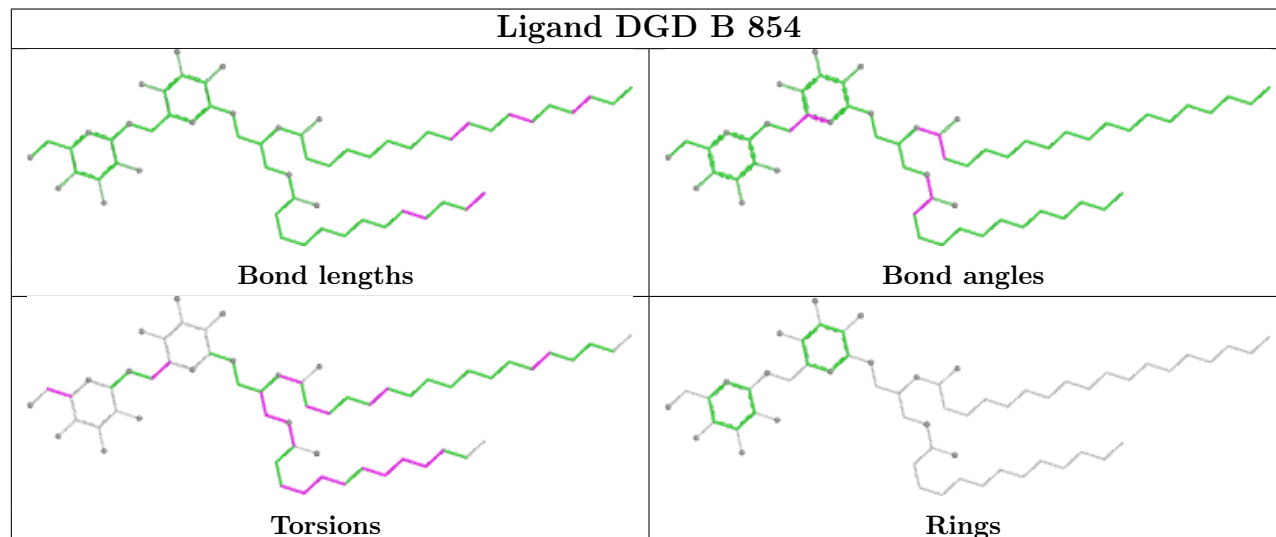
Ligand DGD 4 319



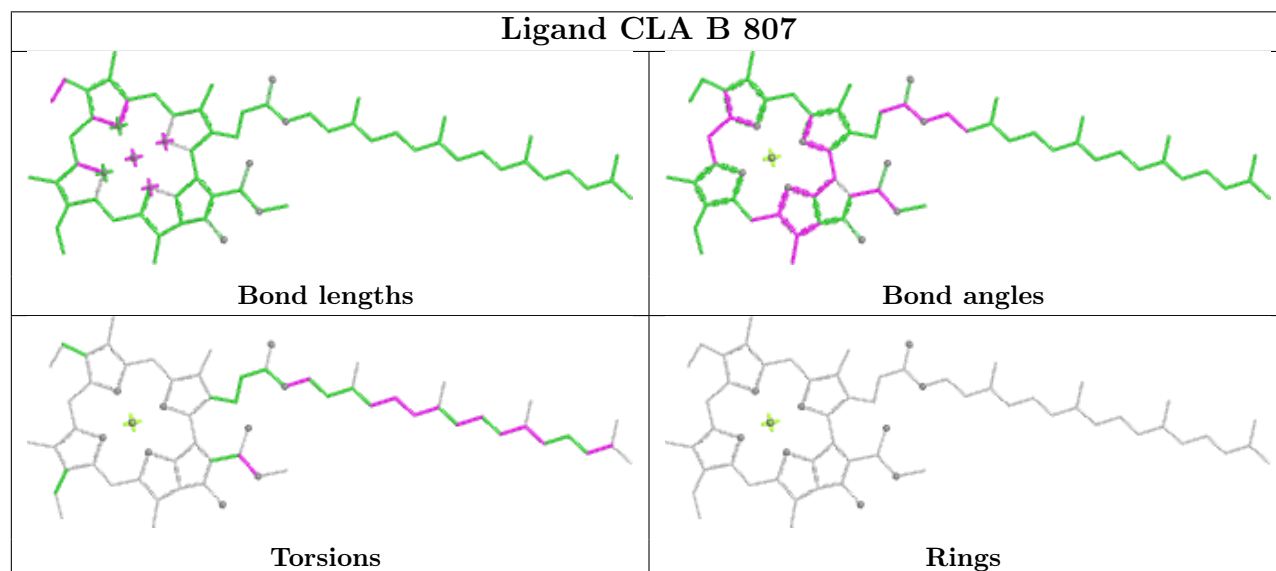
Ligand CLA A 804



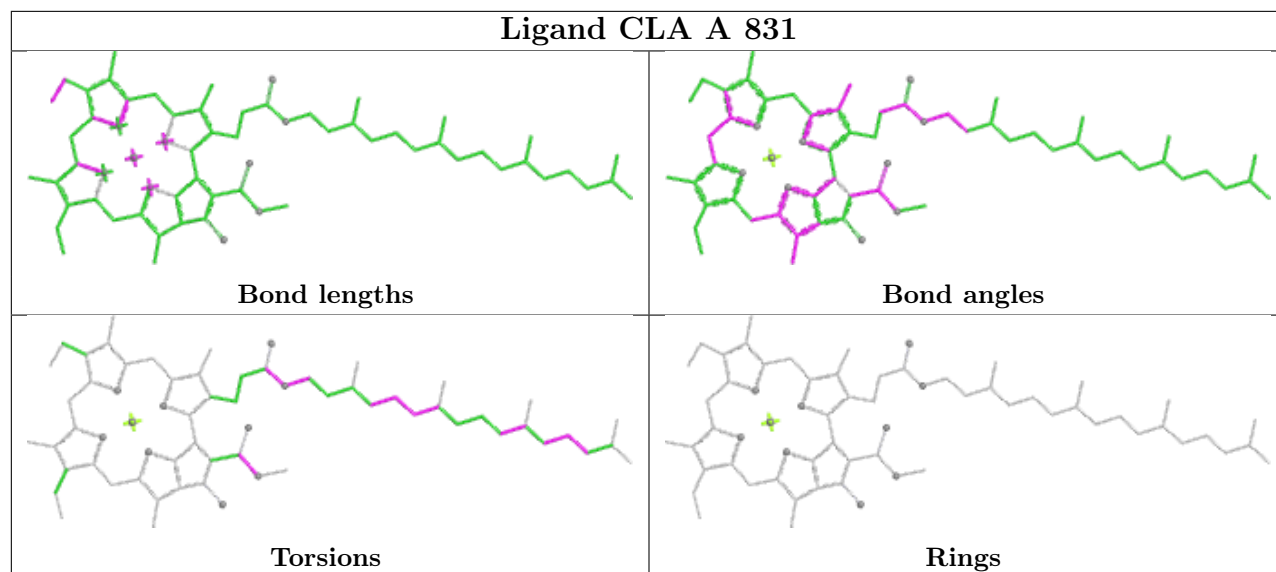
Ligand DGD B 854



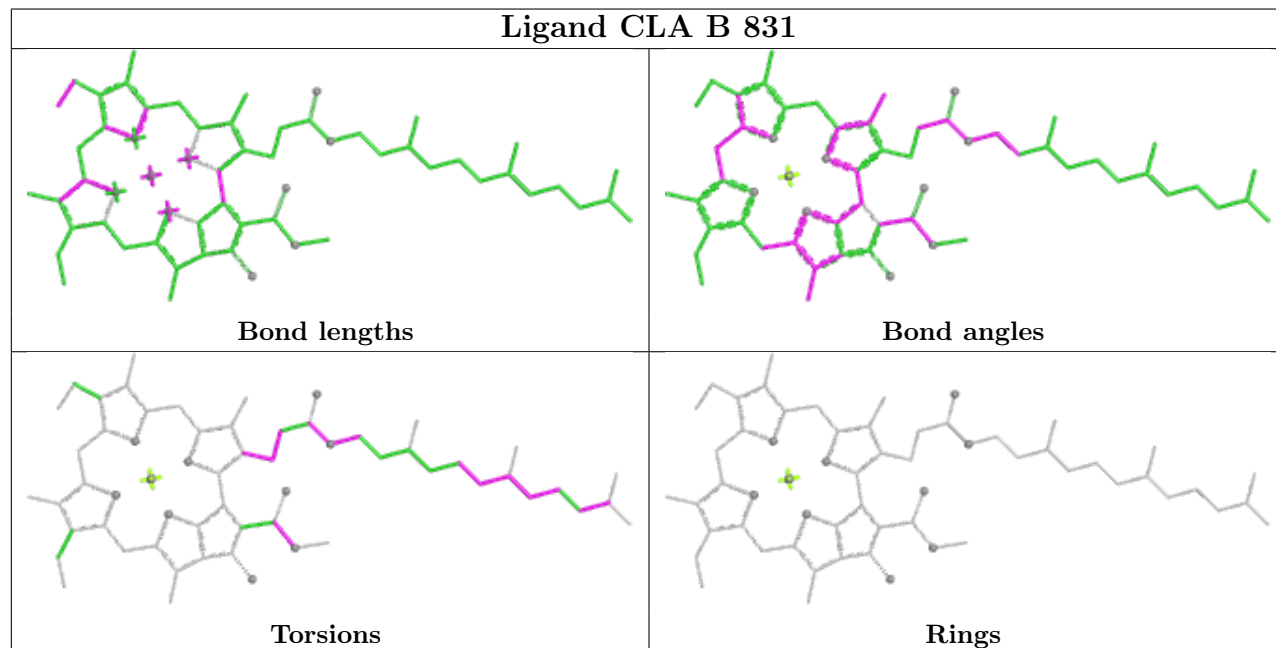
Ligand CLA B 807



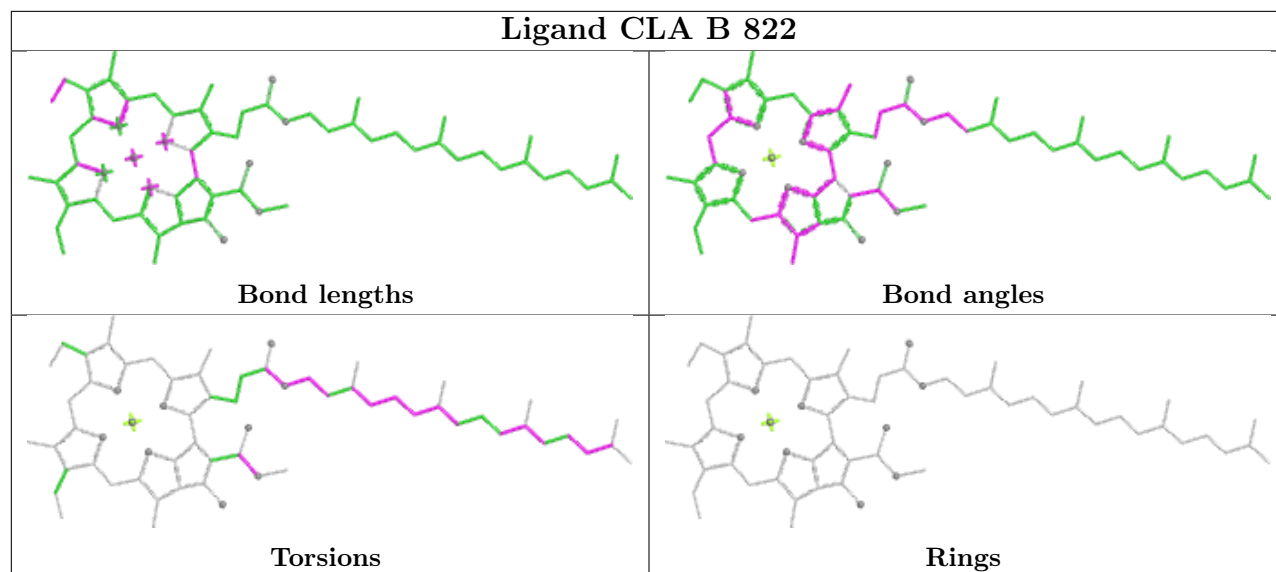
Ligand CLA A 831



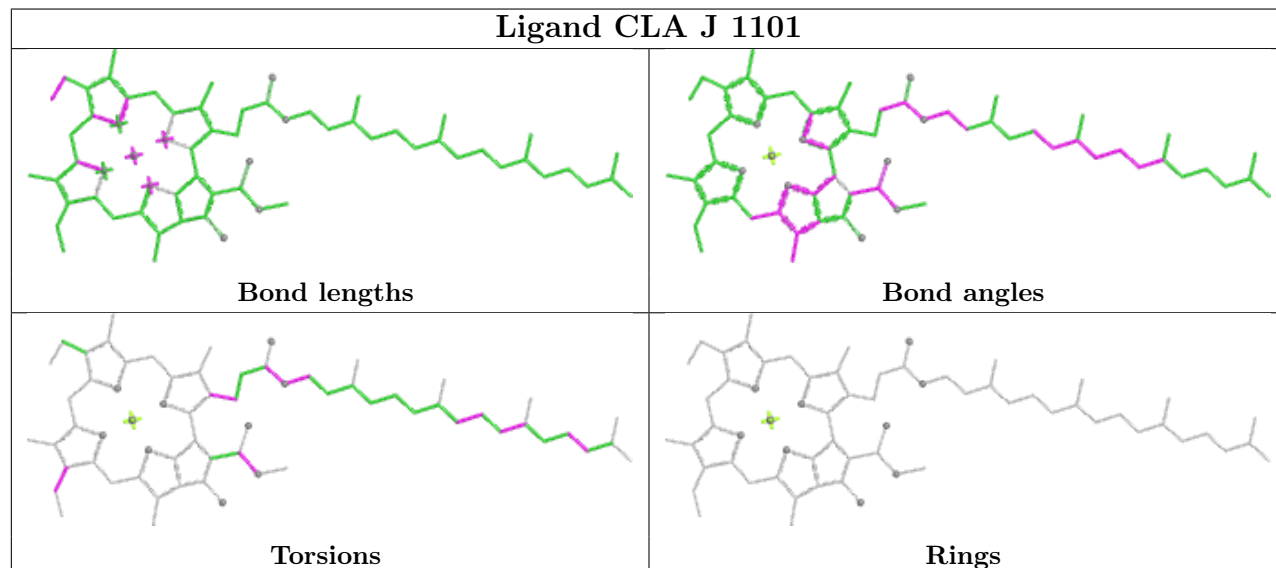
Ligand CLA B 831



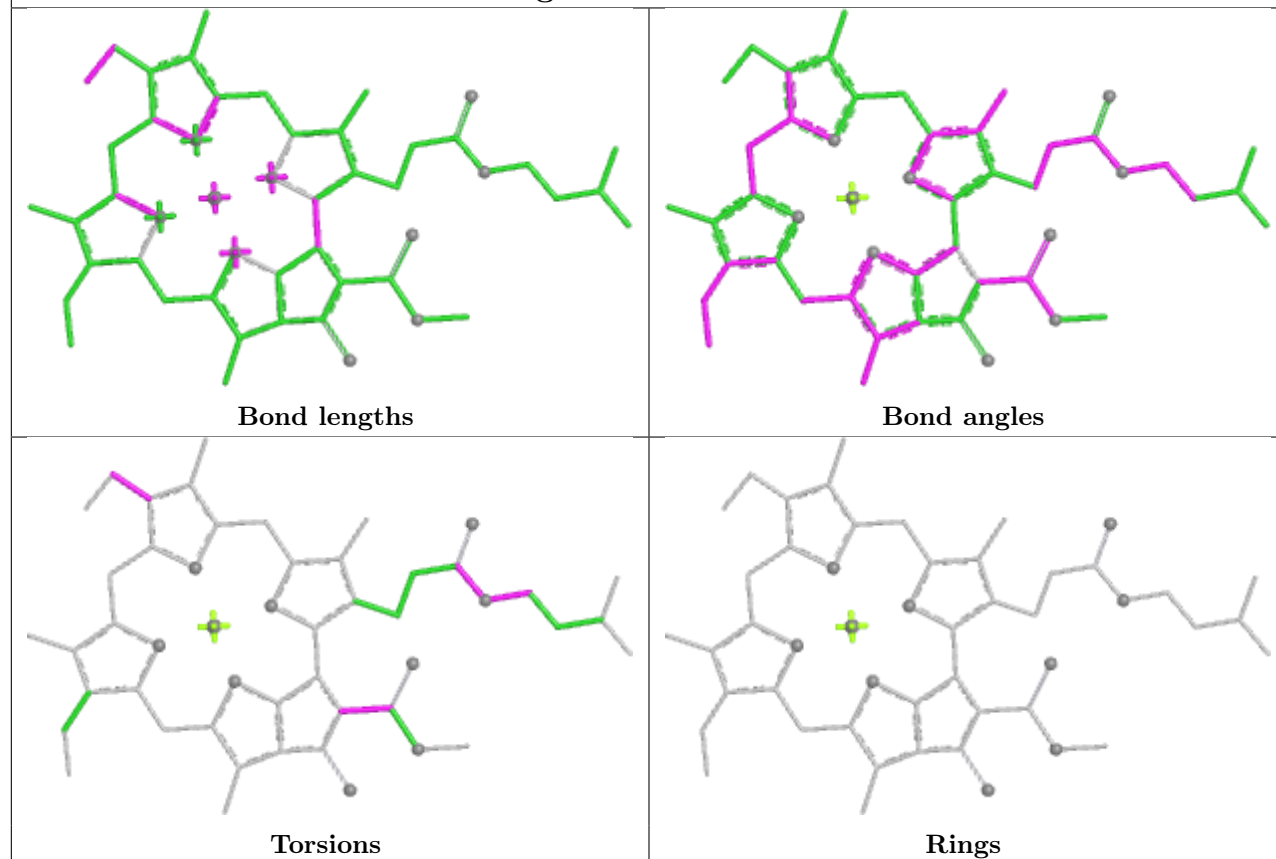
Ligand CLA B 822



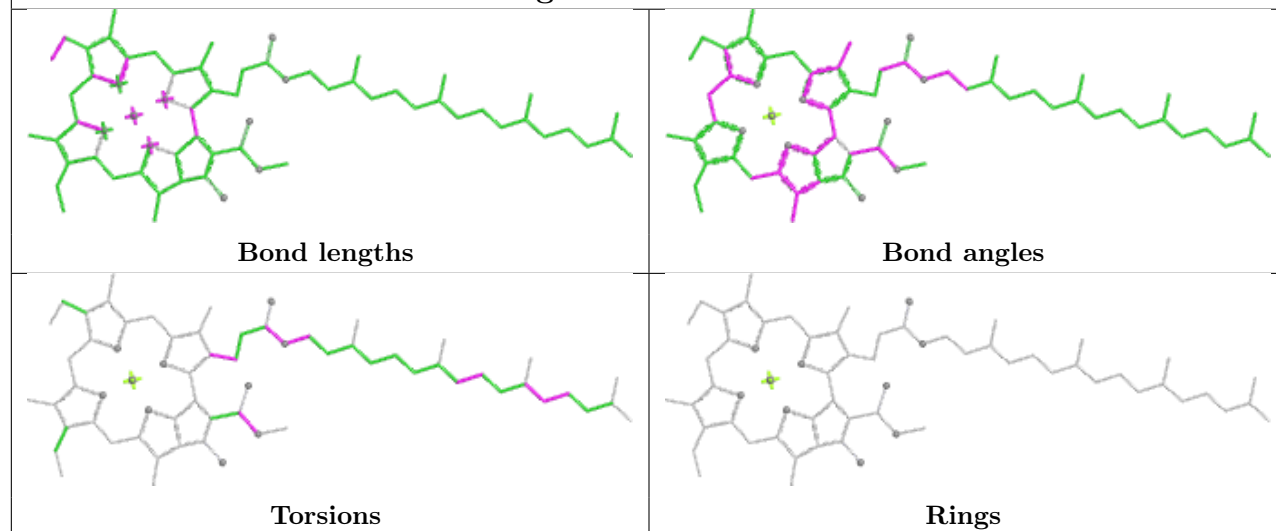
Ligand CLA J 1101

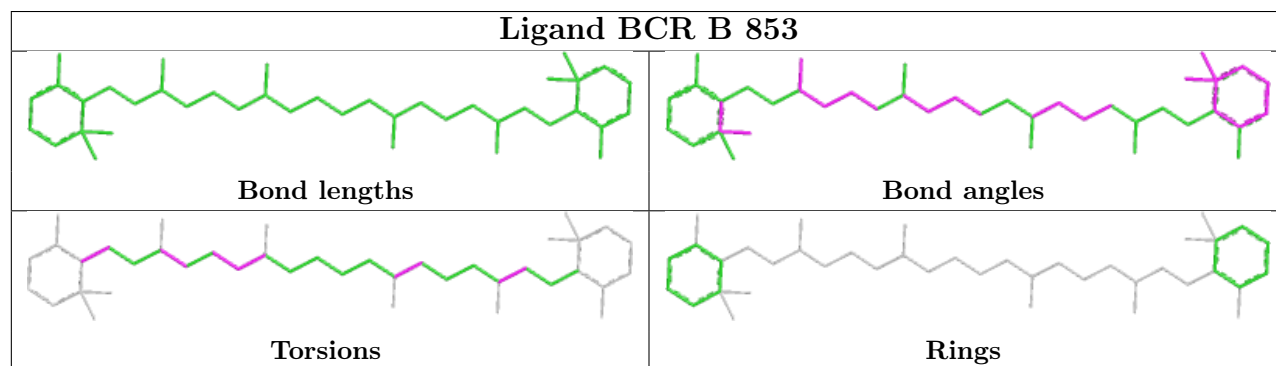
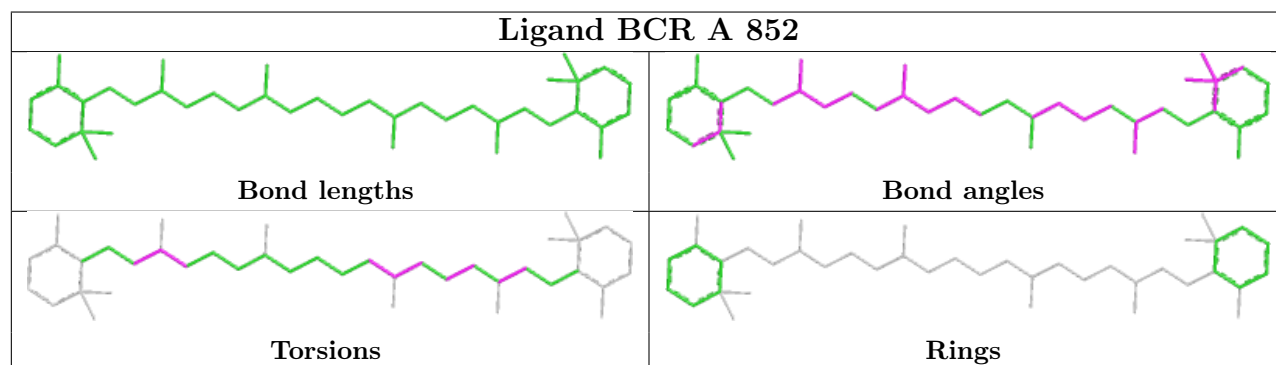
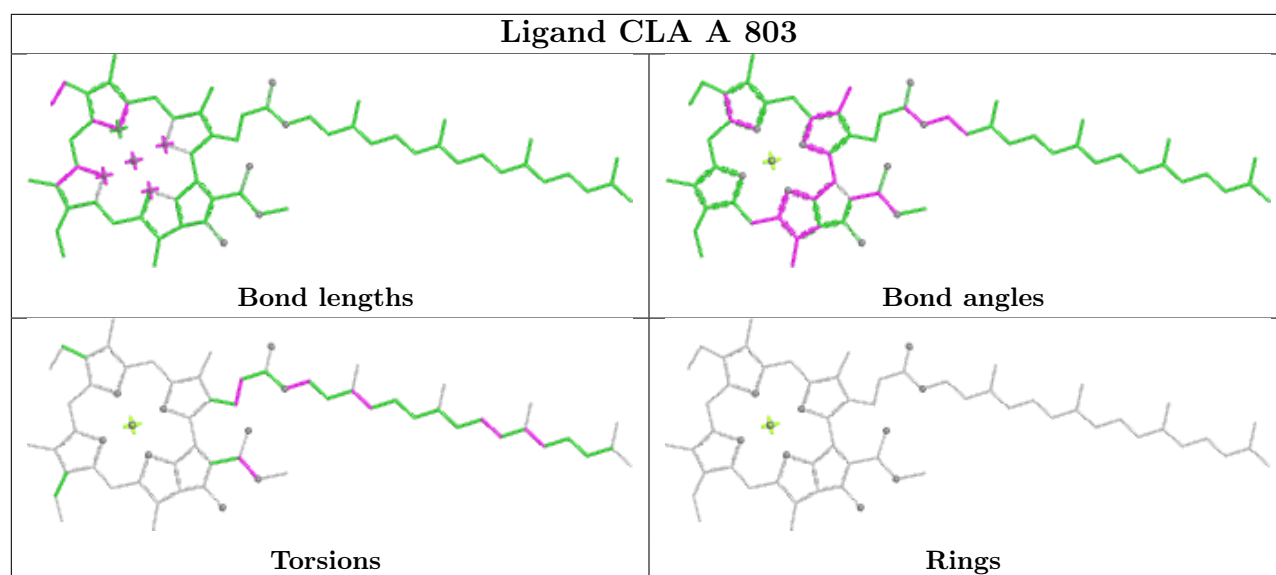


Ligand CLA 4 312

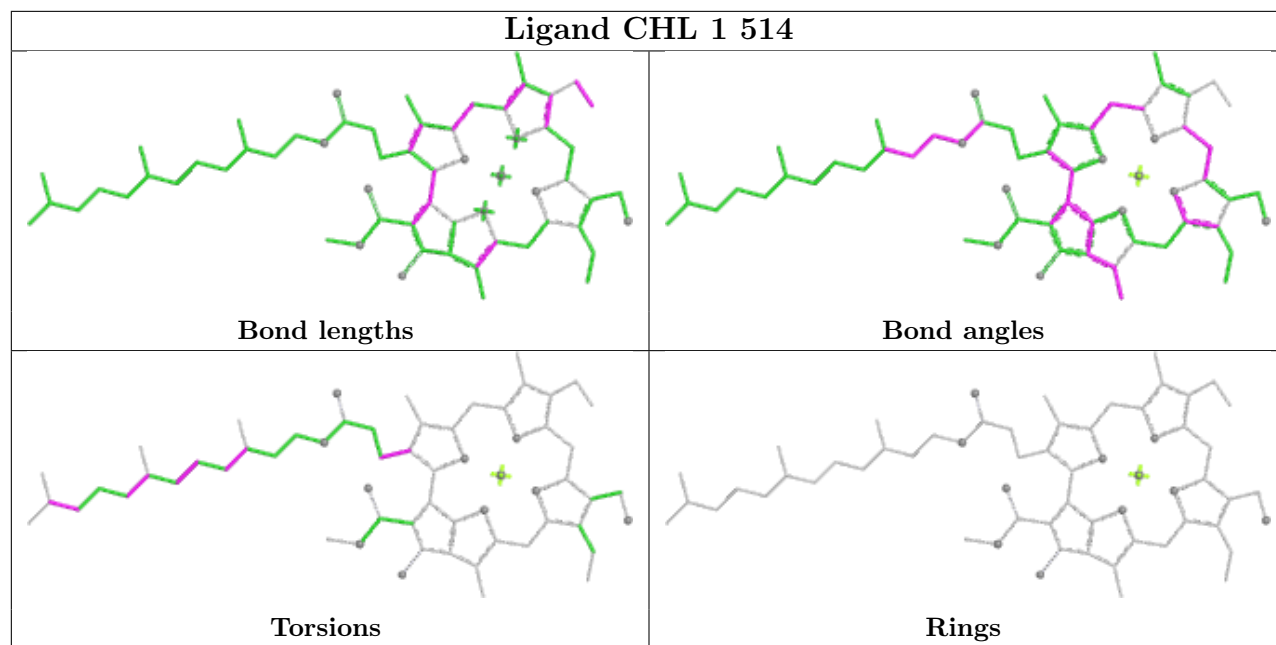


Ligand CLA 4 318

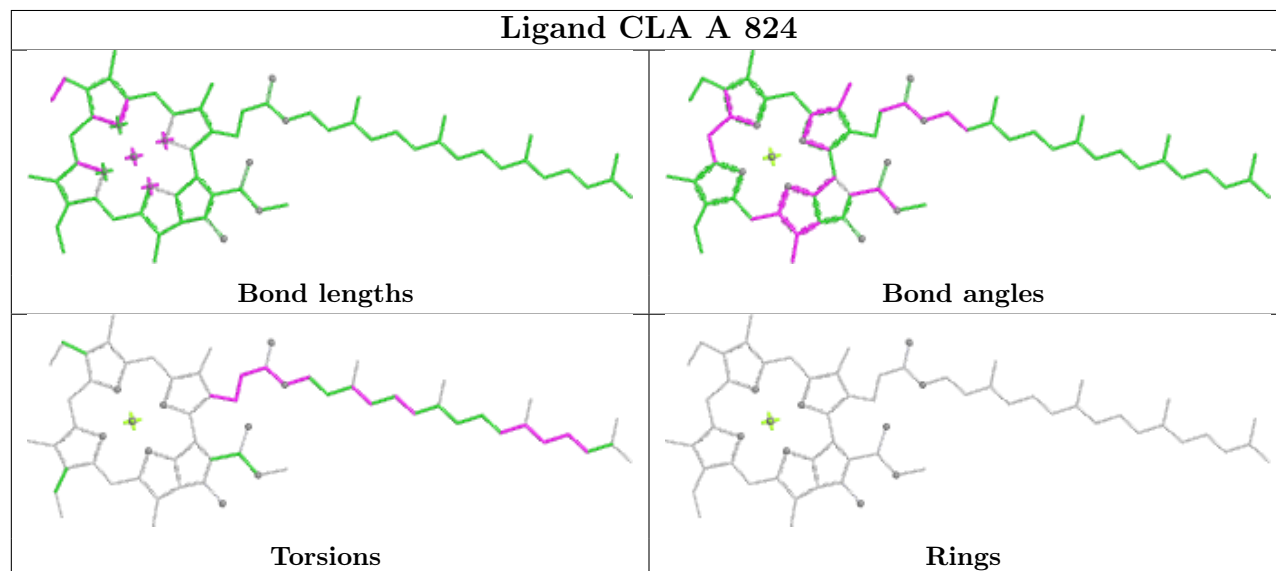




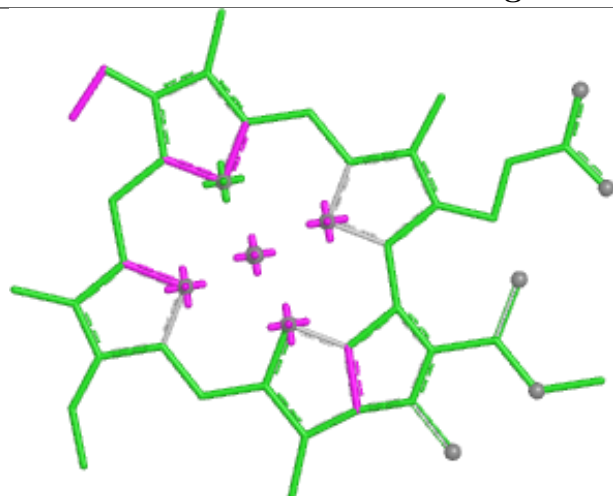
Ligand CHL 1 514



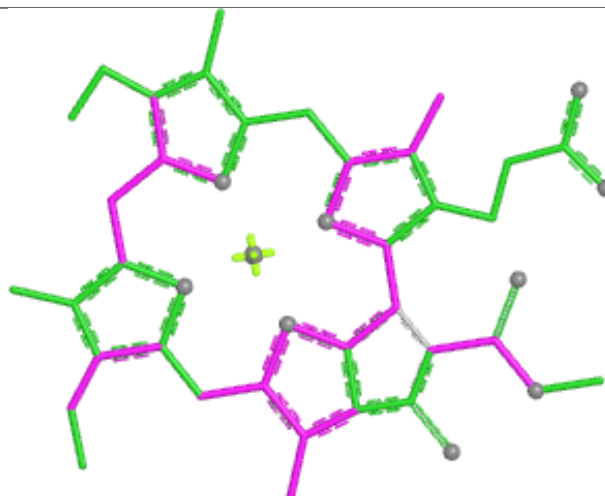
Ligand CLA A 824



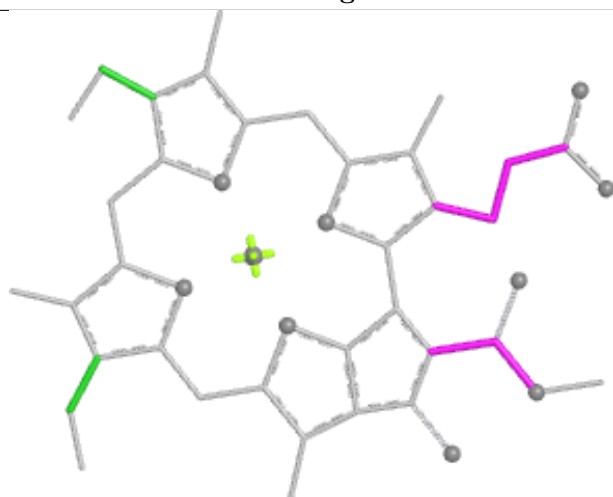
Ligand CLA K 1001



Bond lengths



Bond angles

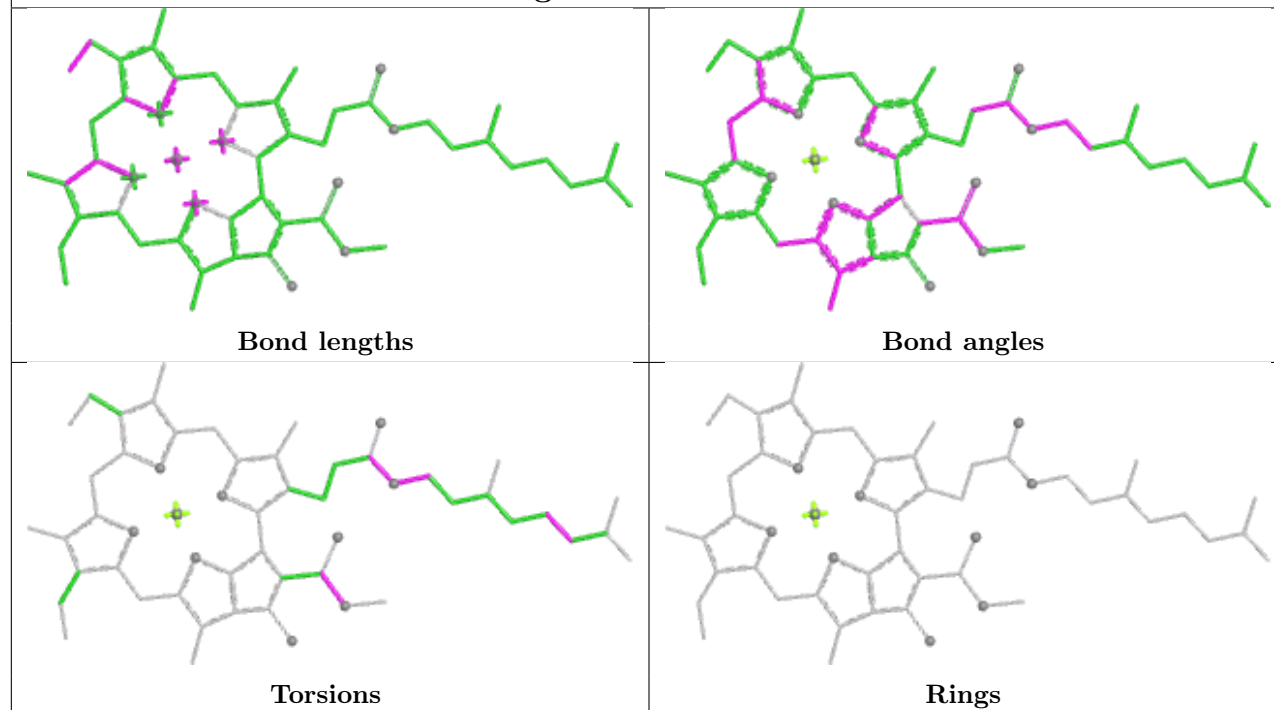


Torsions

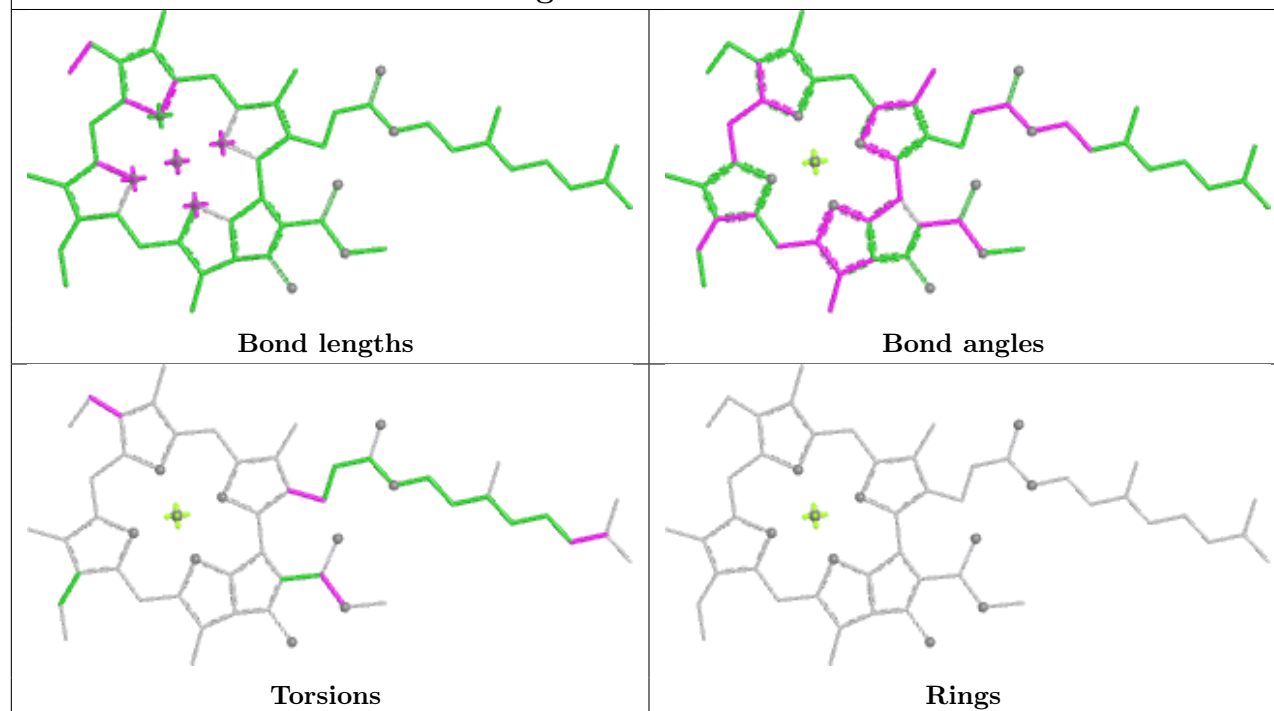


Rings

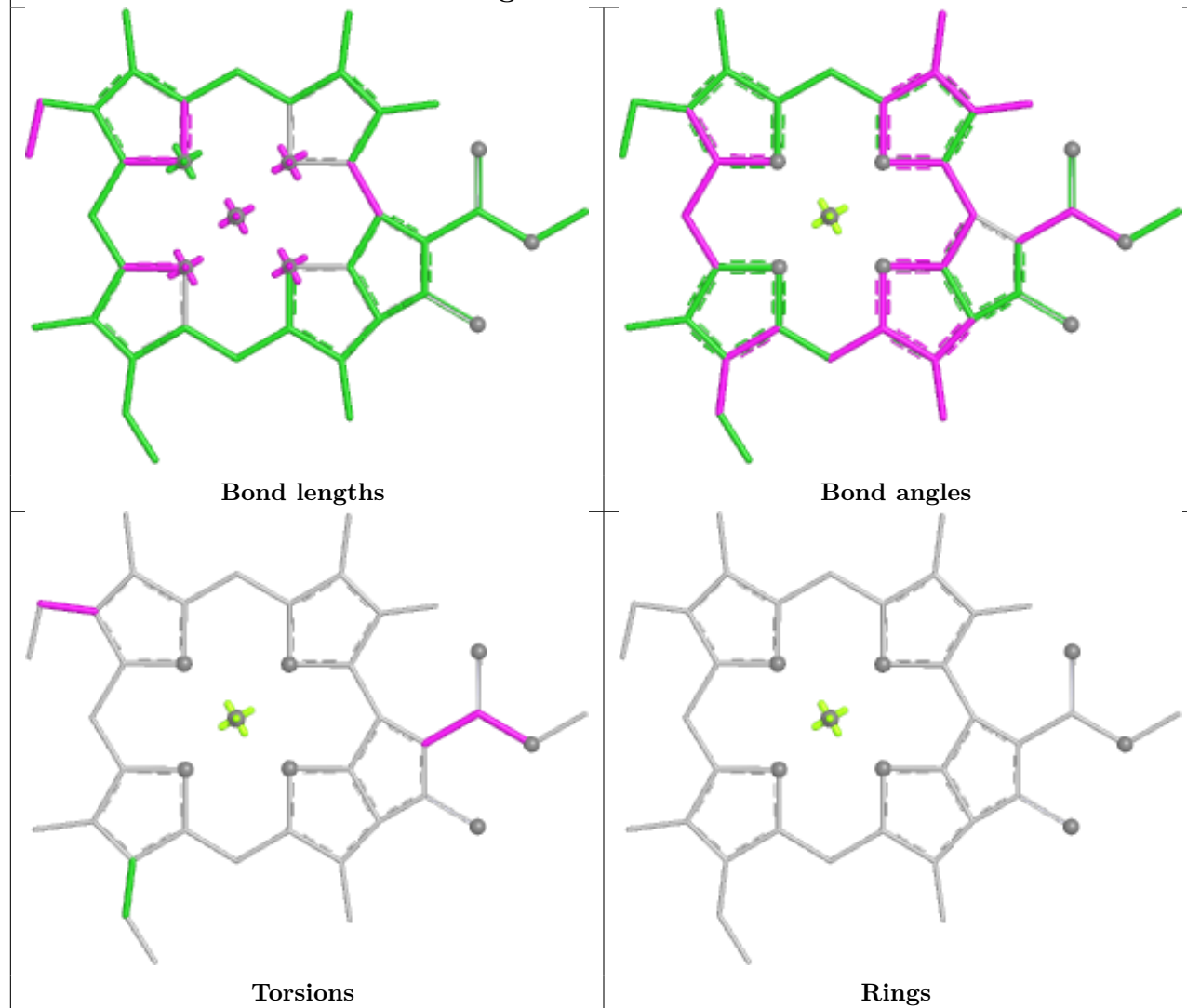
Ligand CLA L 301



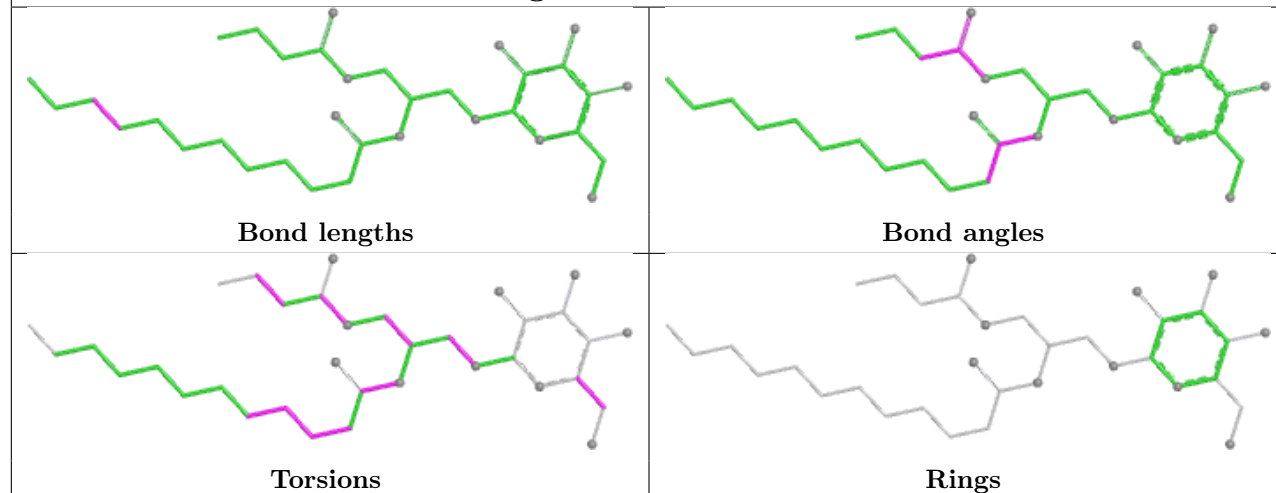
Ligand CLA 1 506

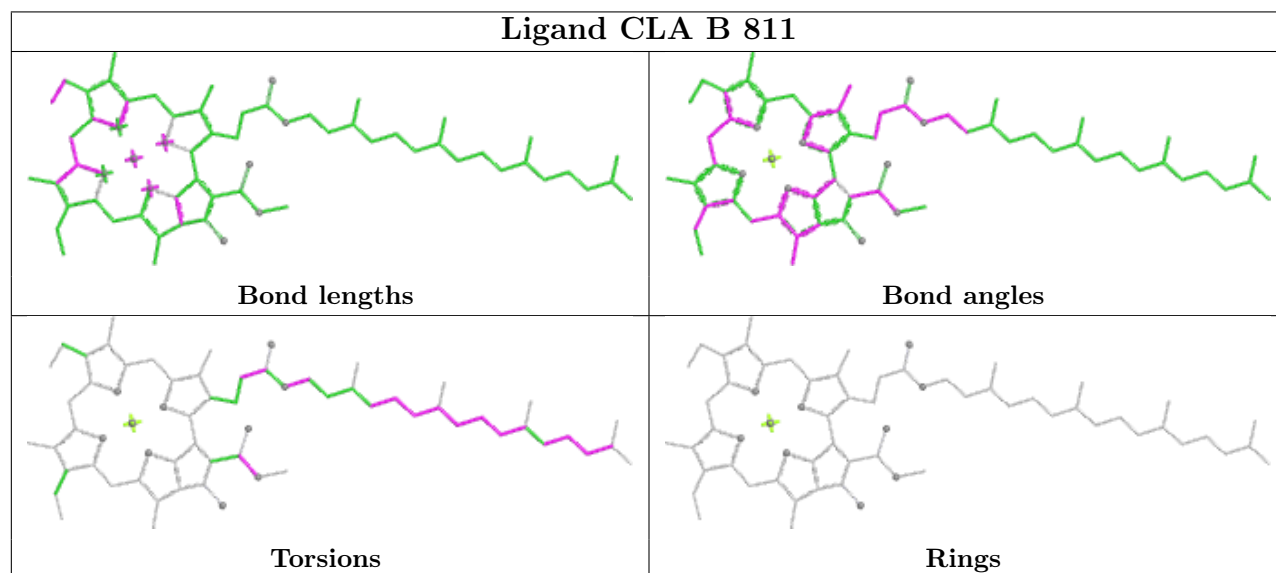
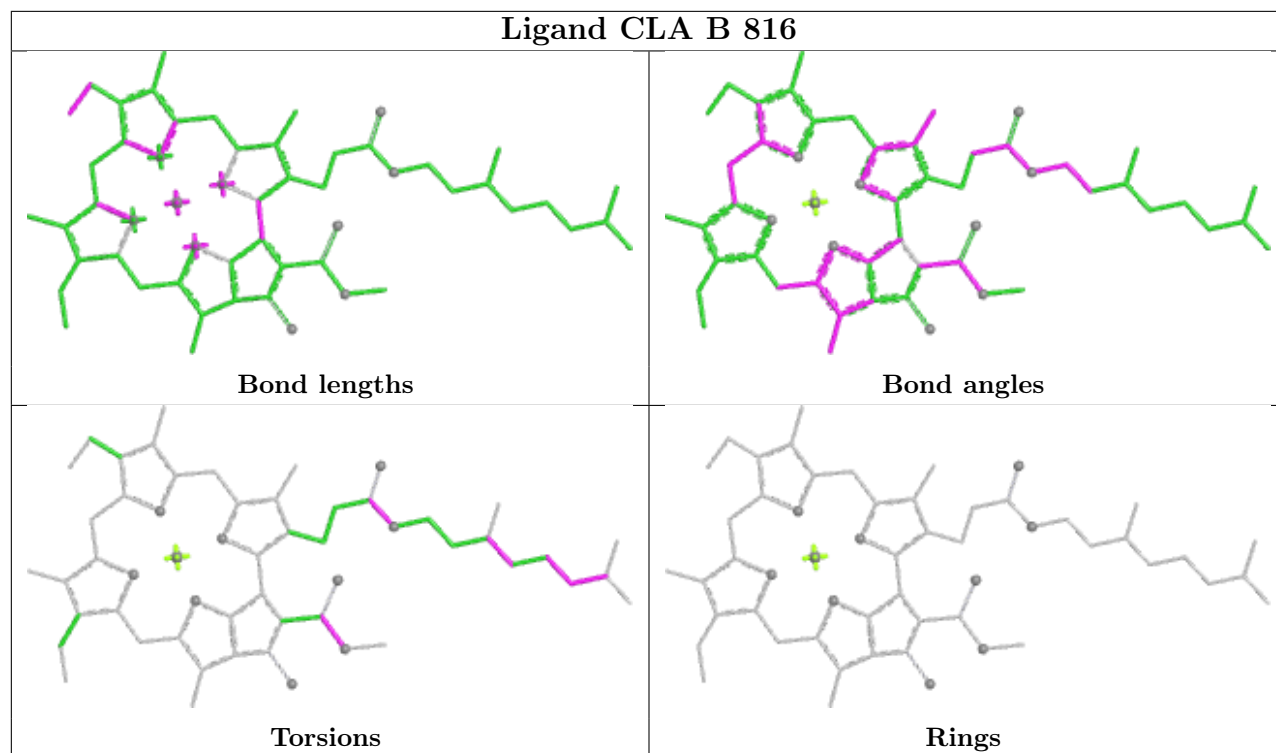


Ligand CLA 3 311

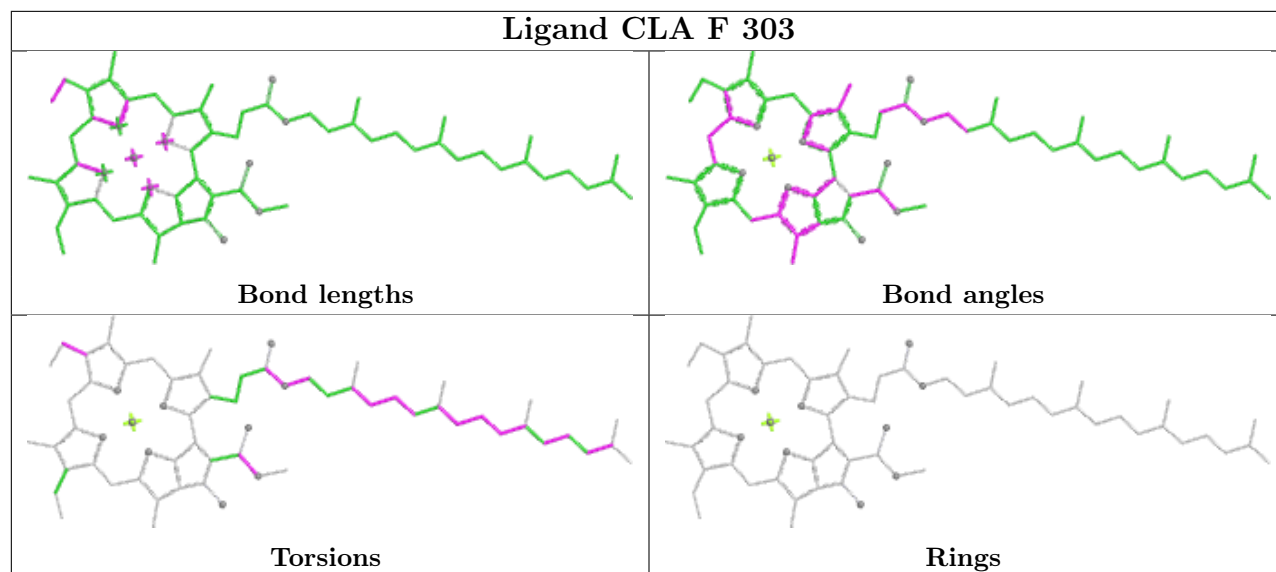


Ligand LMG B 844

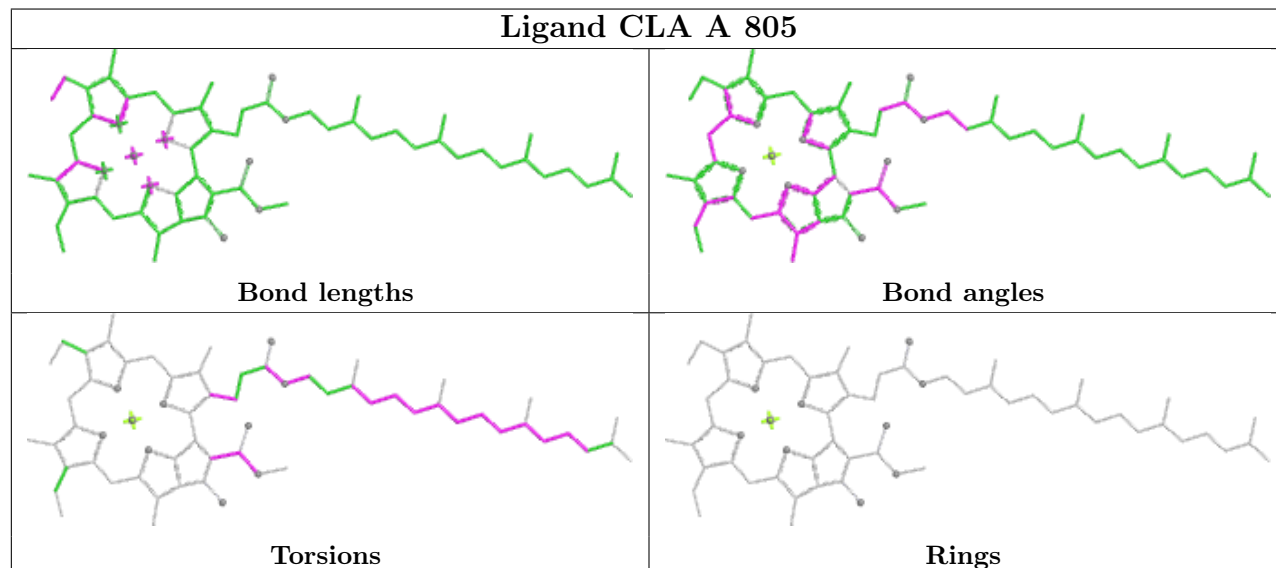




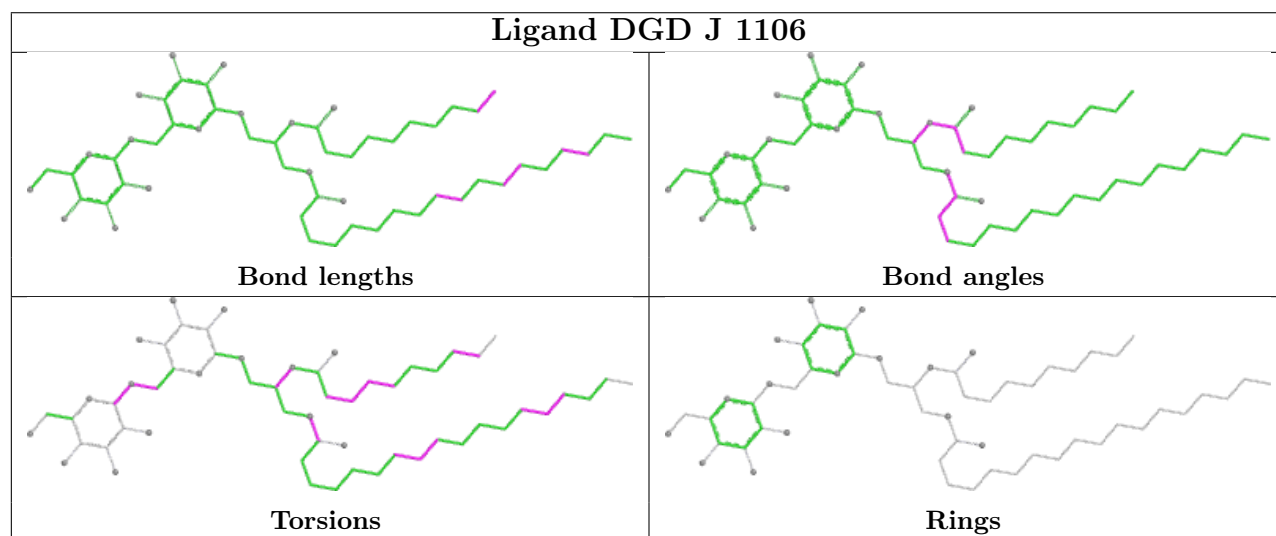
Ligand CLA F 303



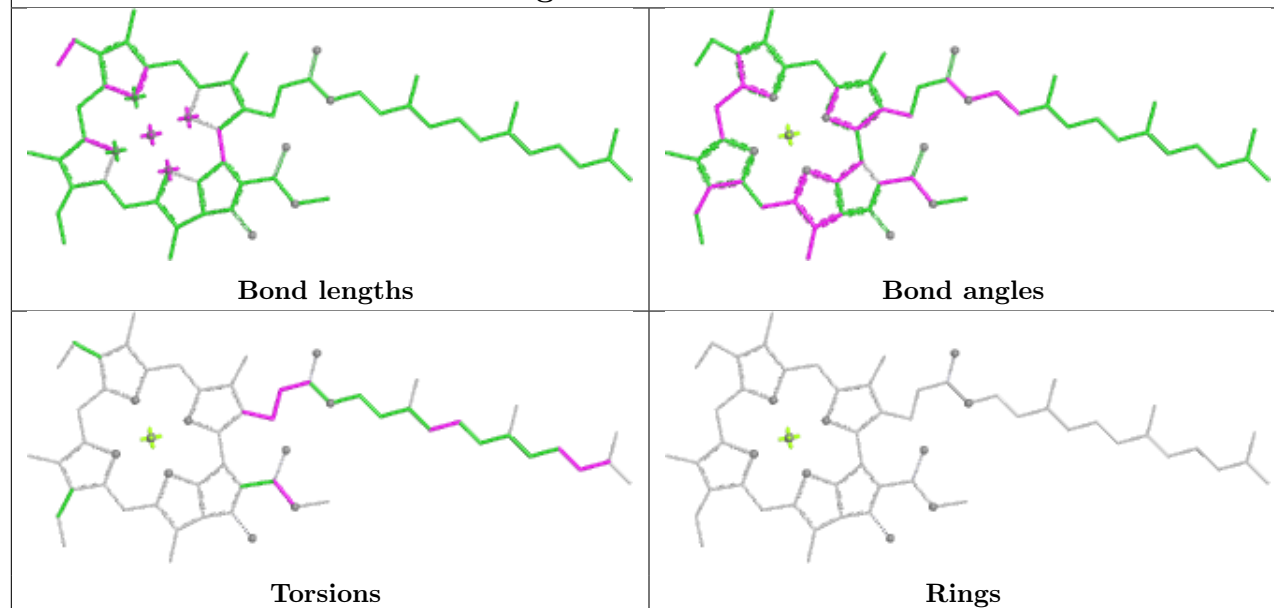
Ligand CLA A 805



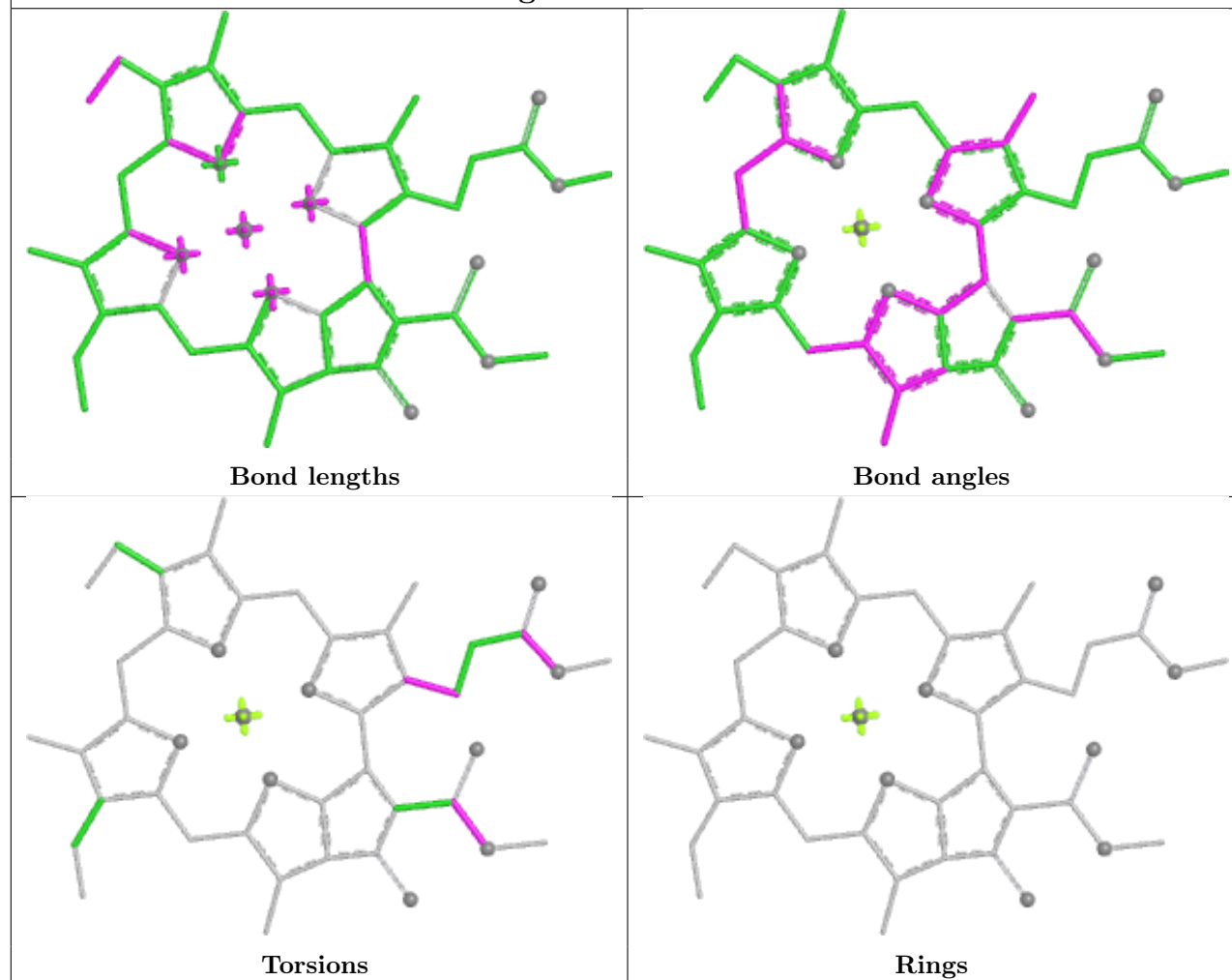
Ligand DGD J 1106



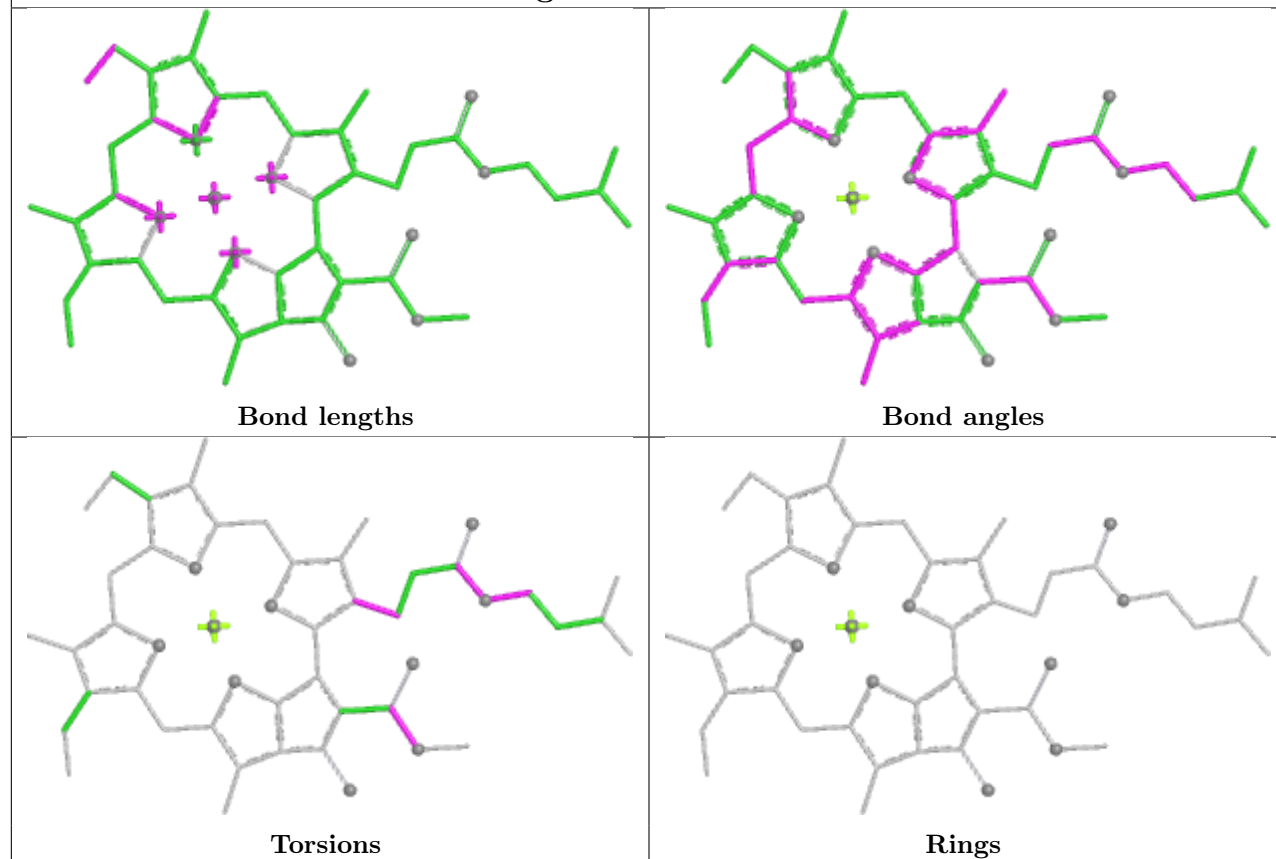
Ligand CLA 2 504



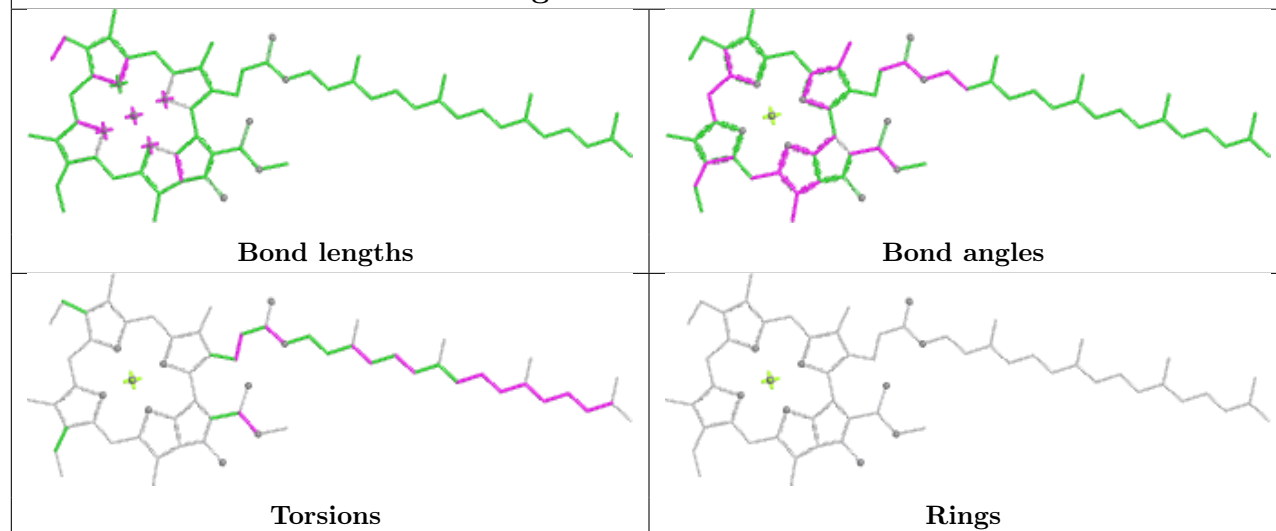
Ligand CLA 1 505



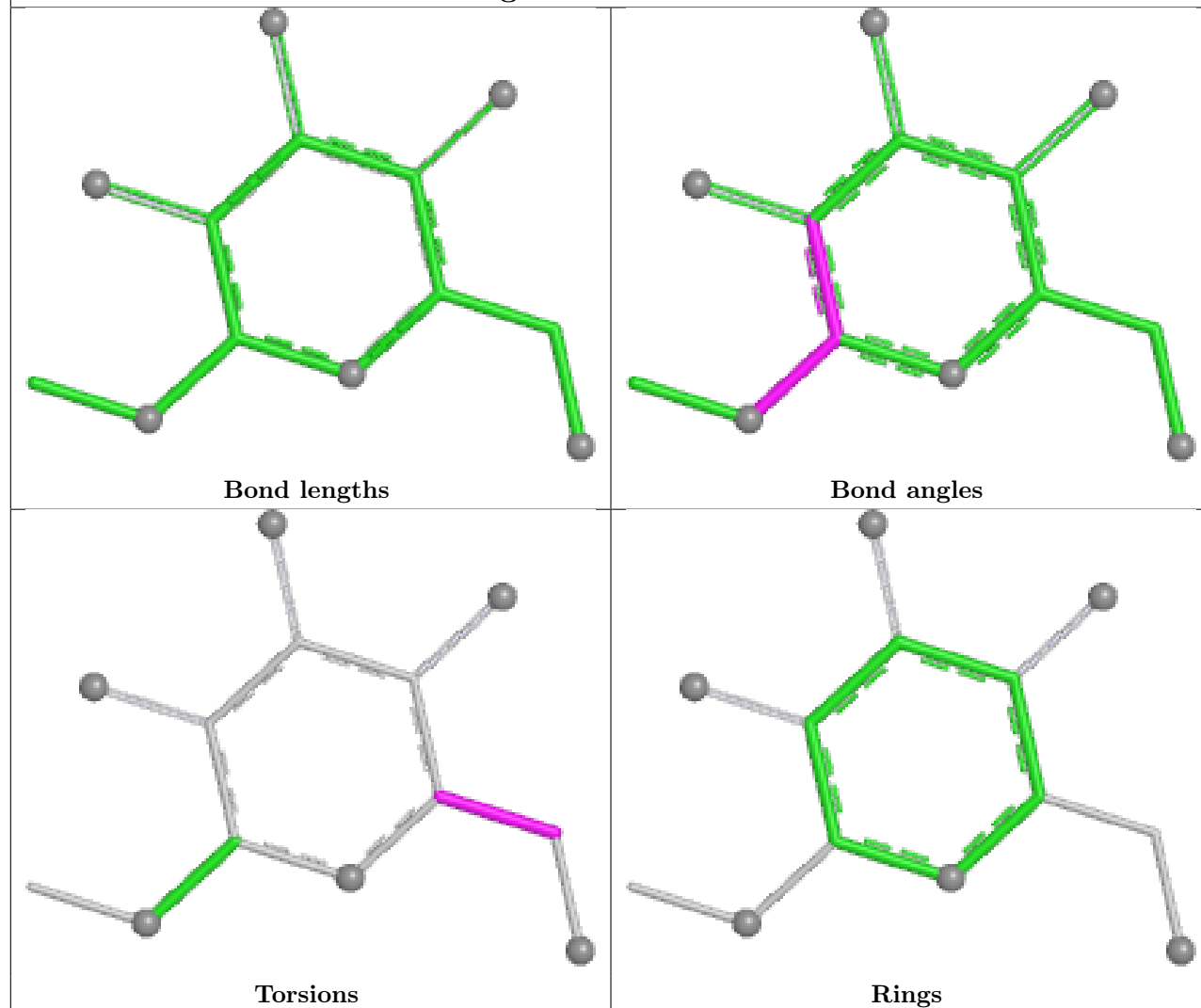
Ligand CLA 1 509



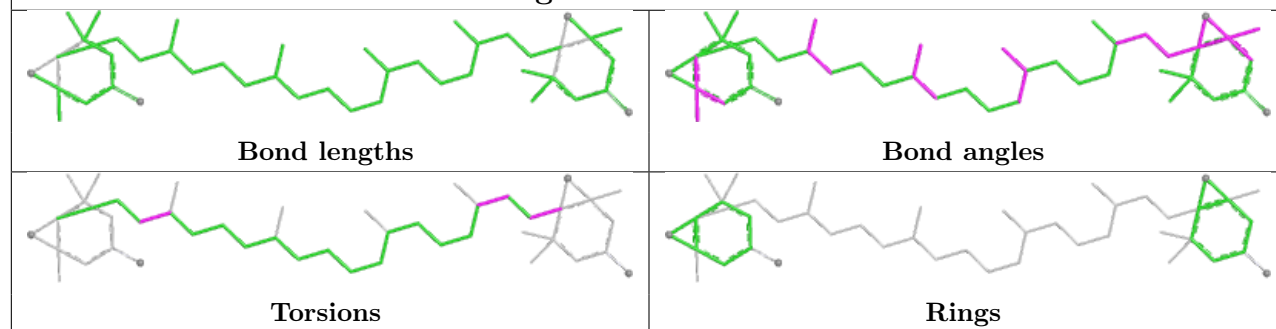
Ligand CLA A 855

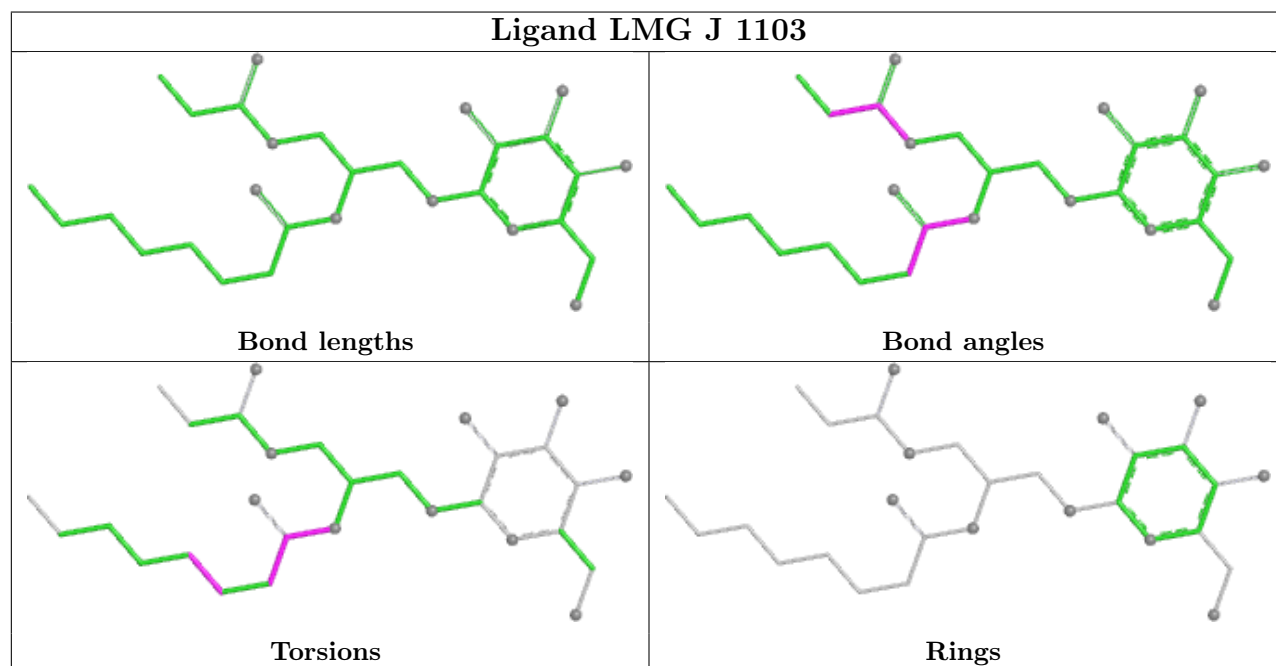
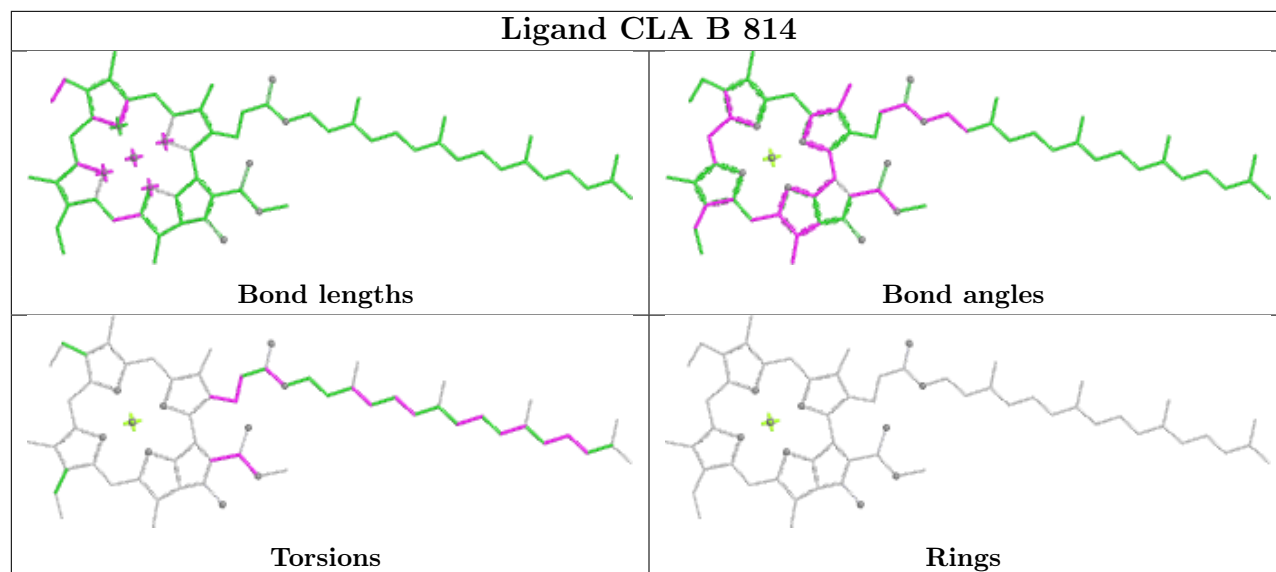


Ligand LMG 1 519

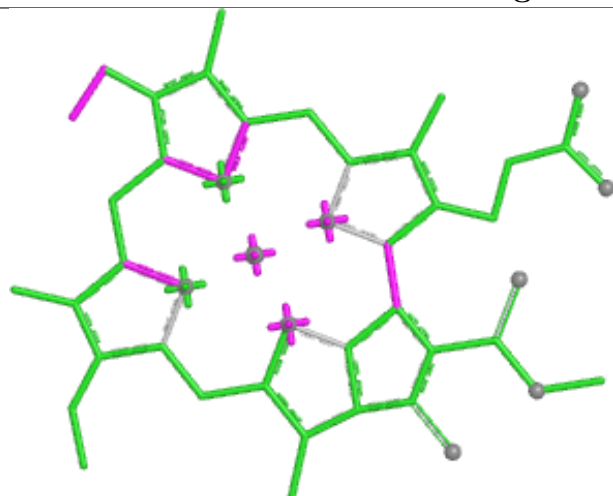


Ligand XAT 2 502

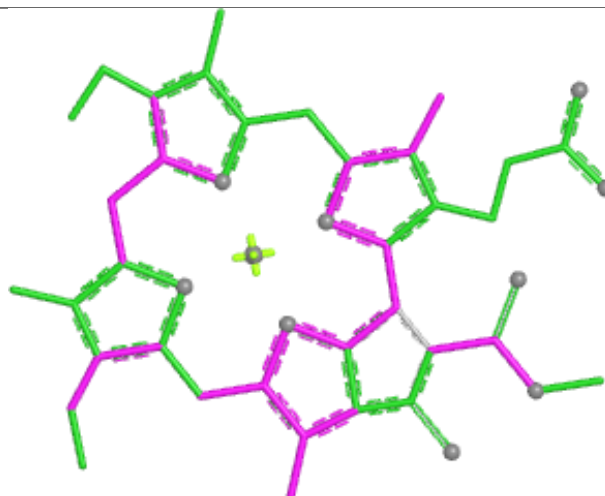




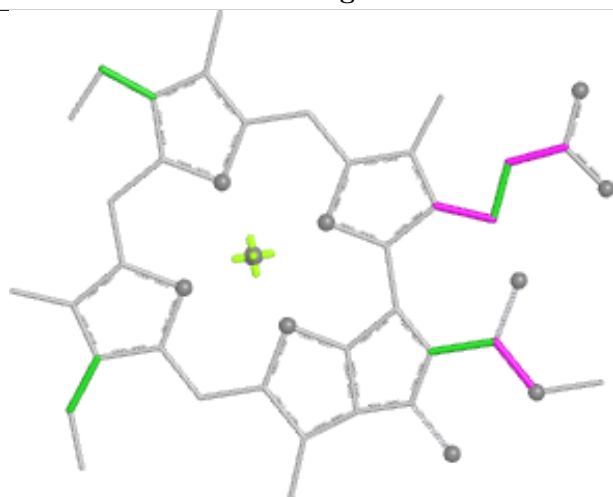
Ligand CLA A 815



Bond lengths



Bond angles

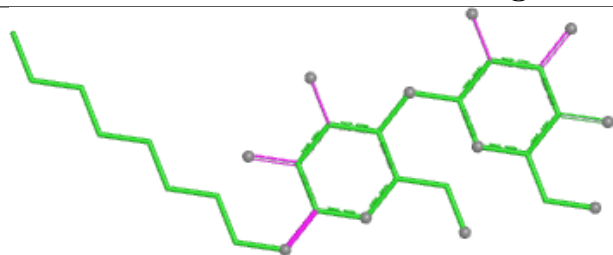


Torsions

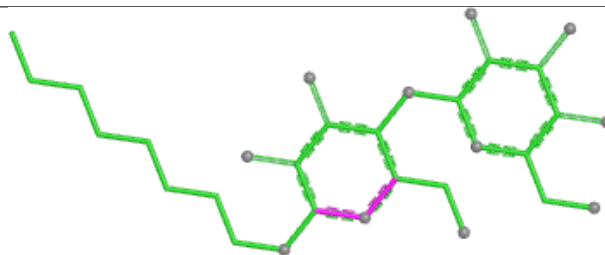


Rings

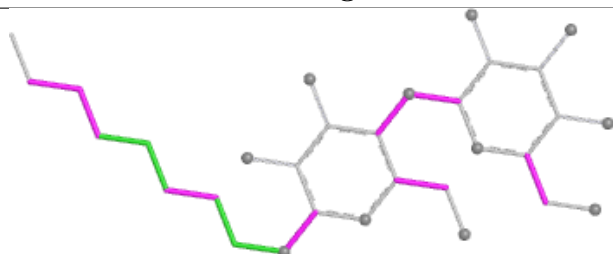
Ligand LMT G 209



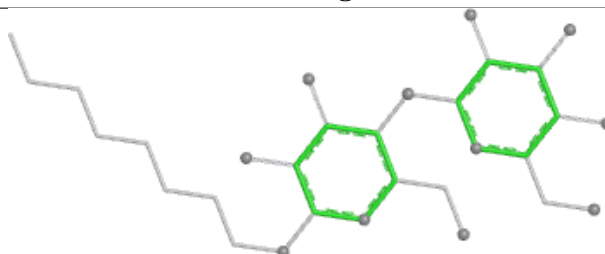
Bond lengths



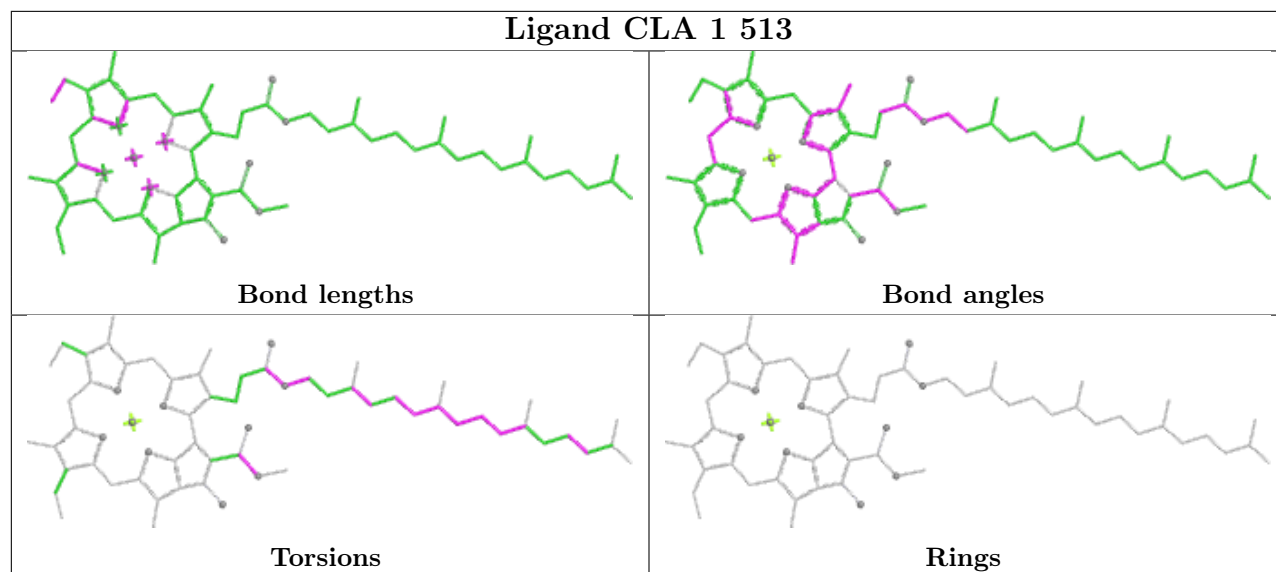
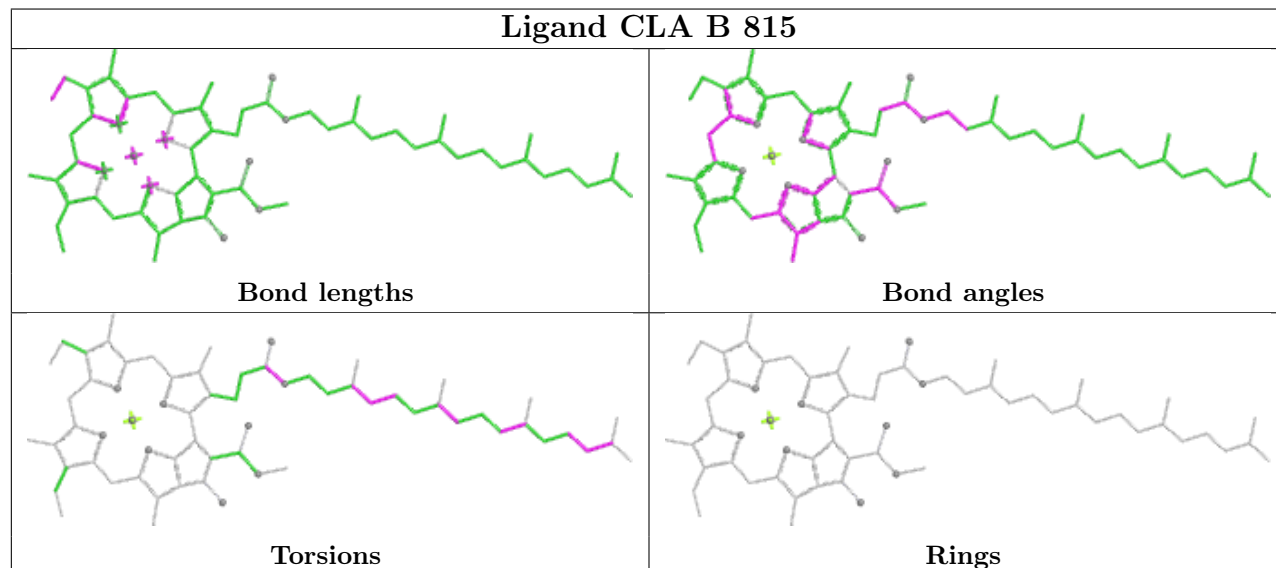
Bond angles

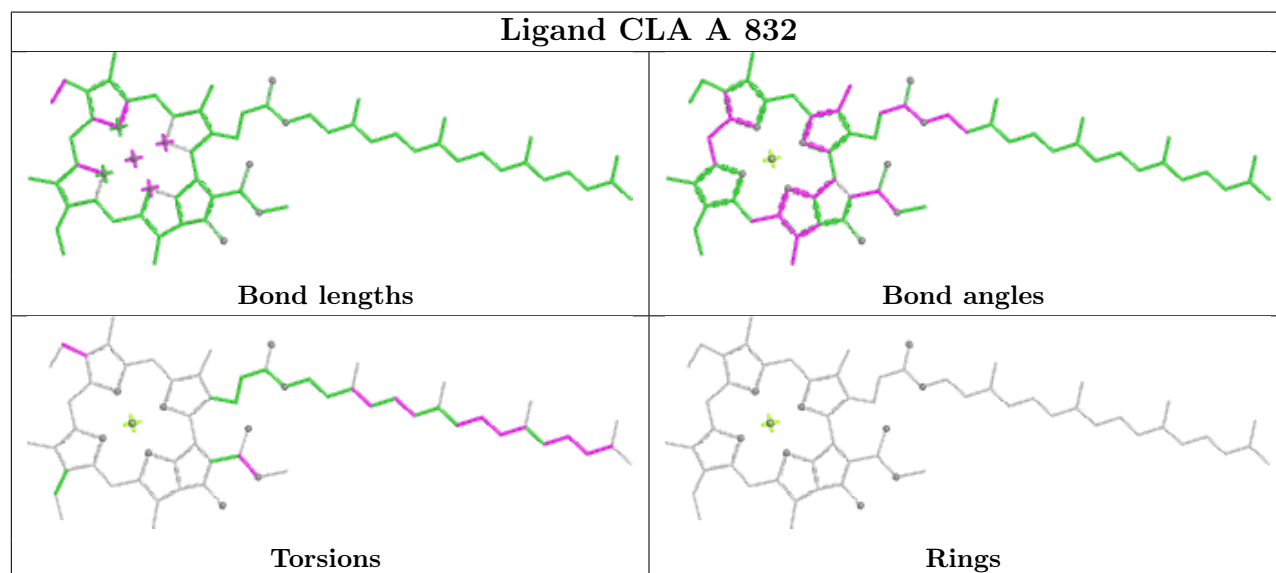
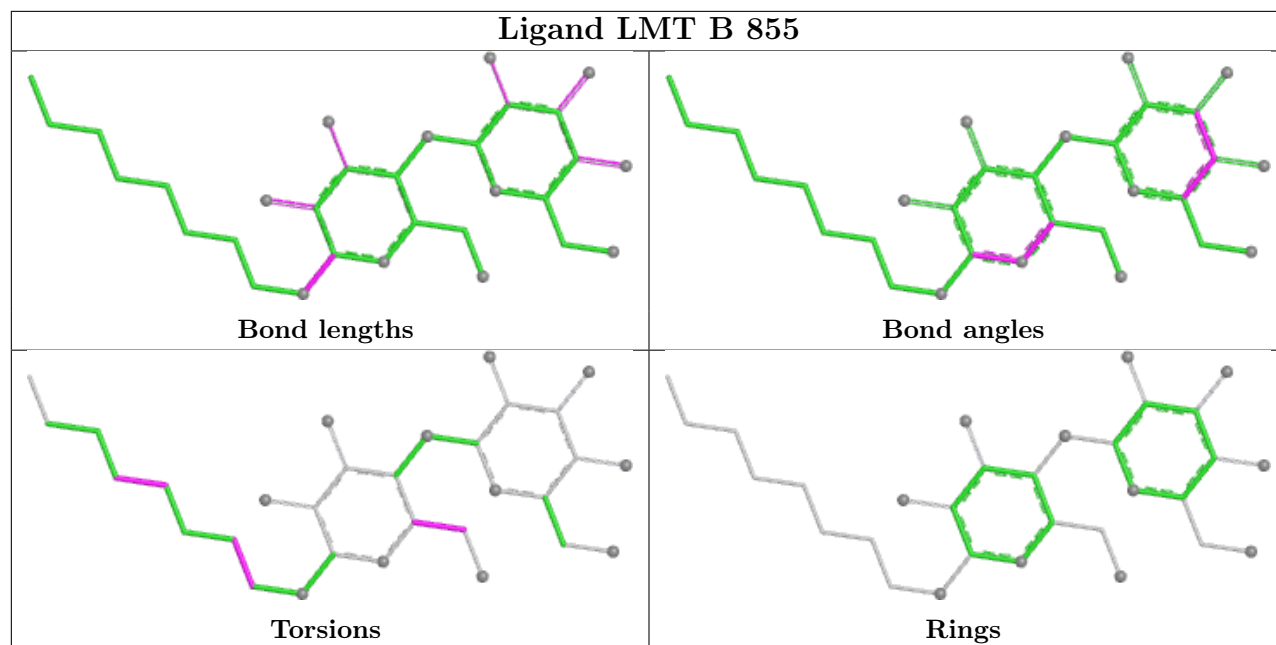


Torsions

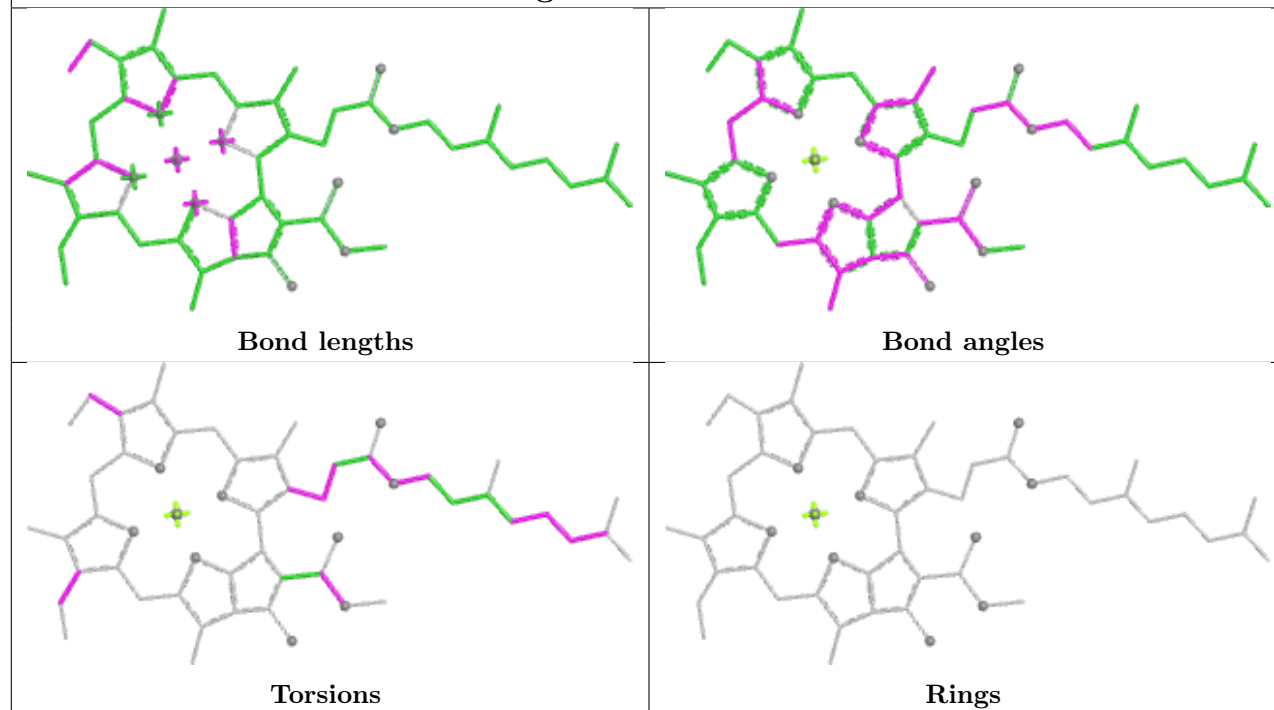


Rings

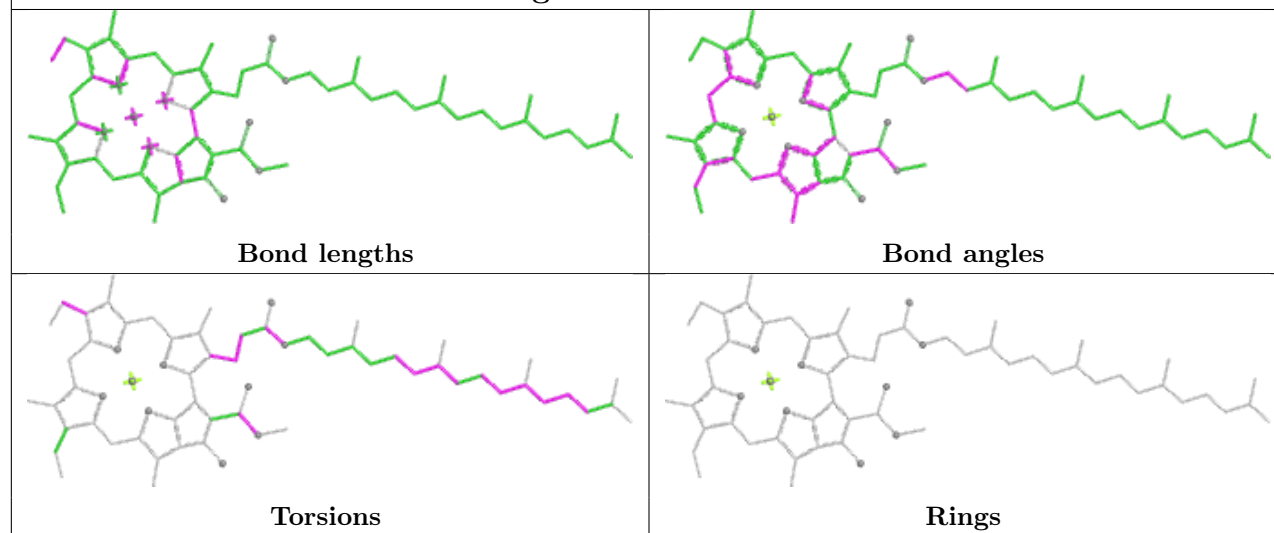
Ligand CLA 1 513**Ligand CLA B 815**



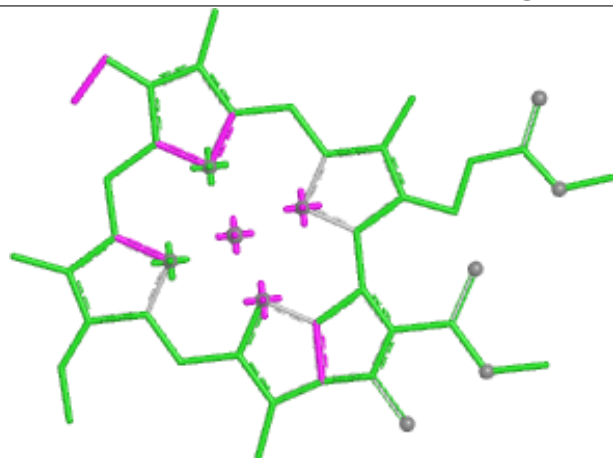
Ligand CLA 3 305



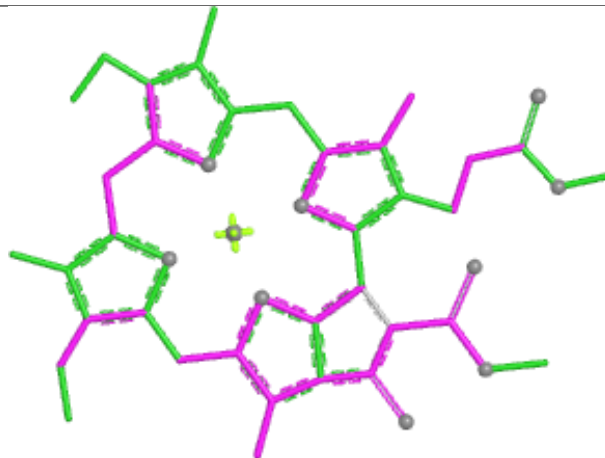
Ligand CLA B 805



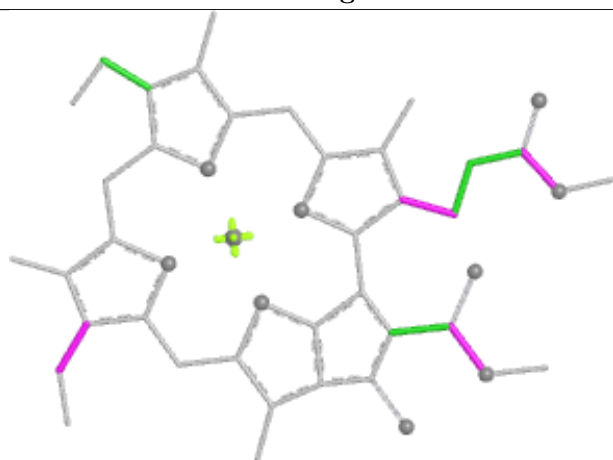
Ligand CLA 1 510



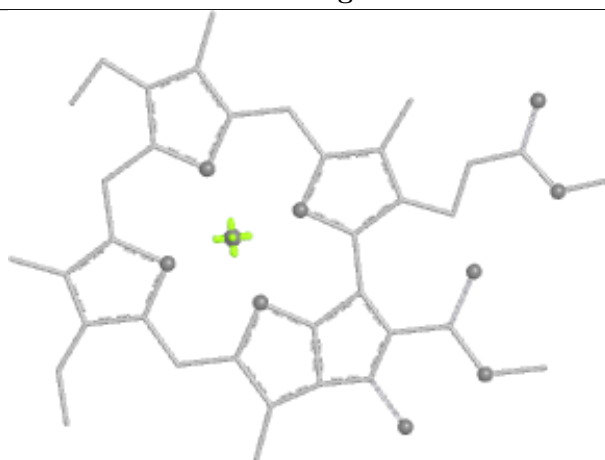
Bond lengths



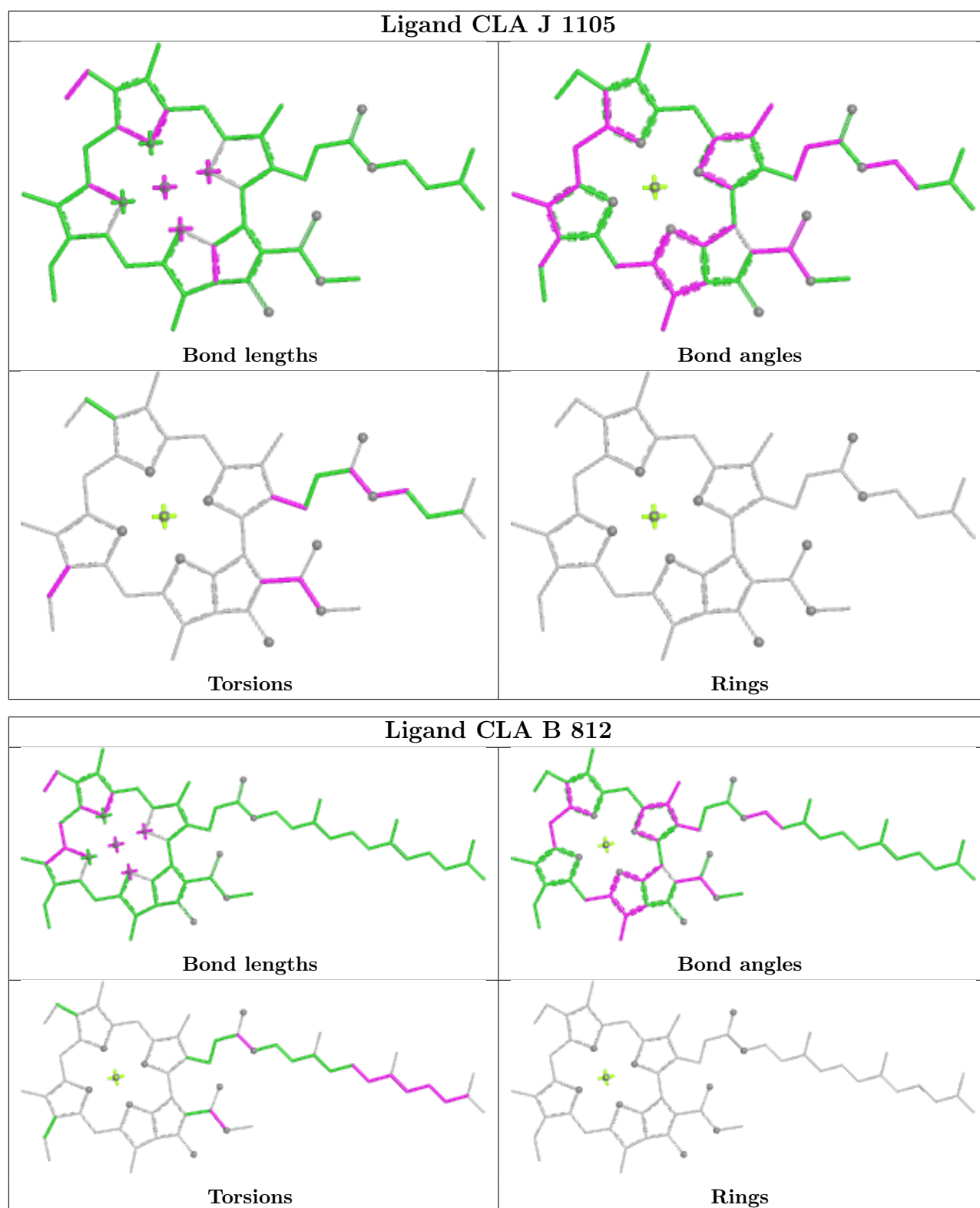
Bond angles



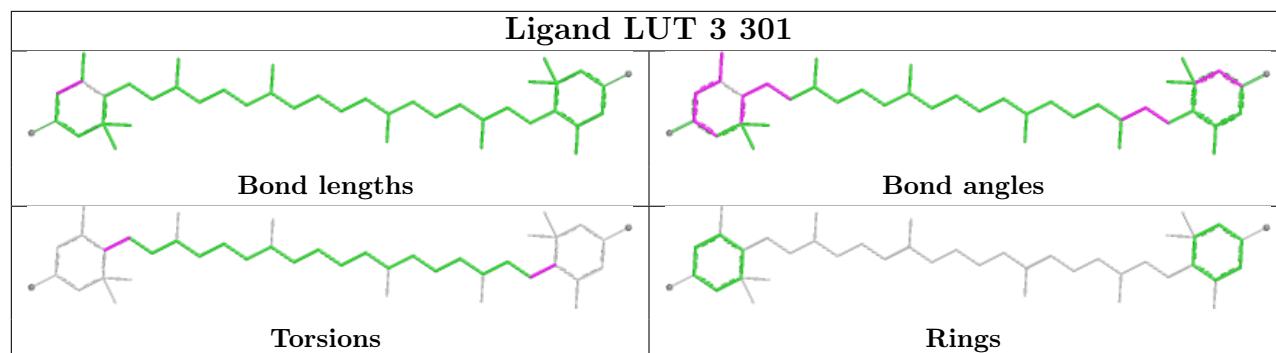
Torsions



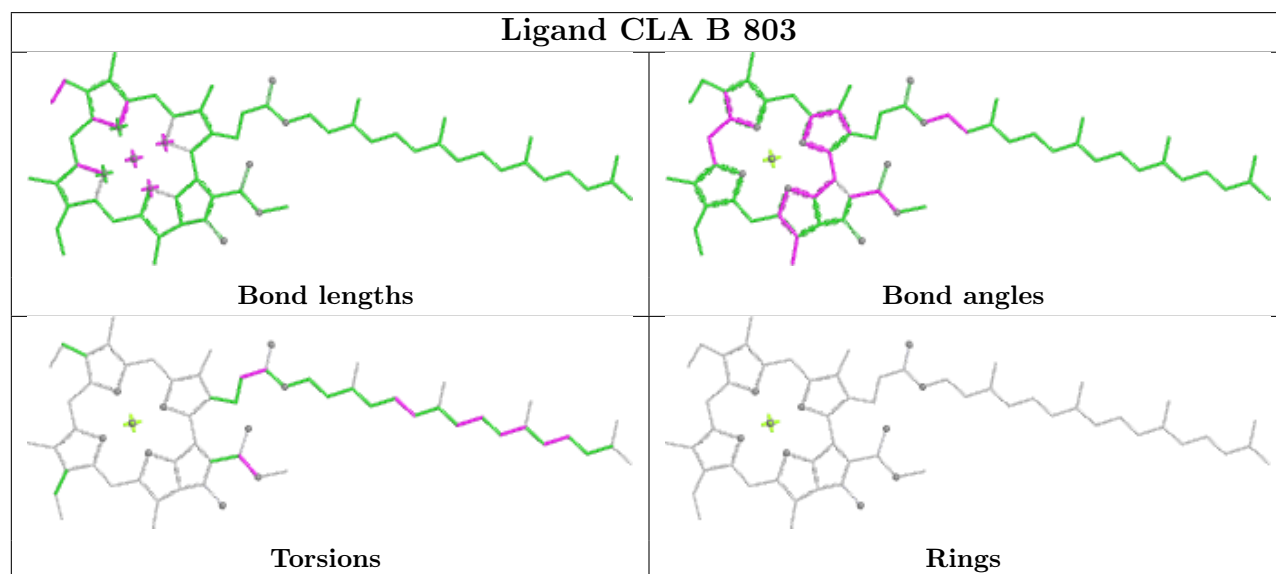
Rings



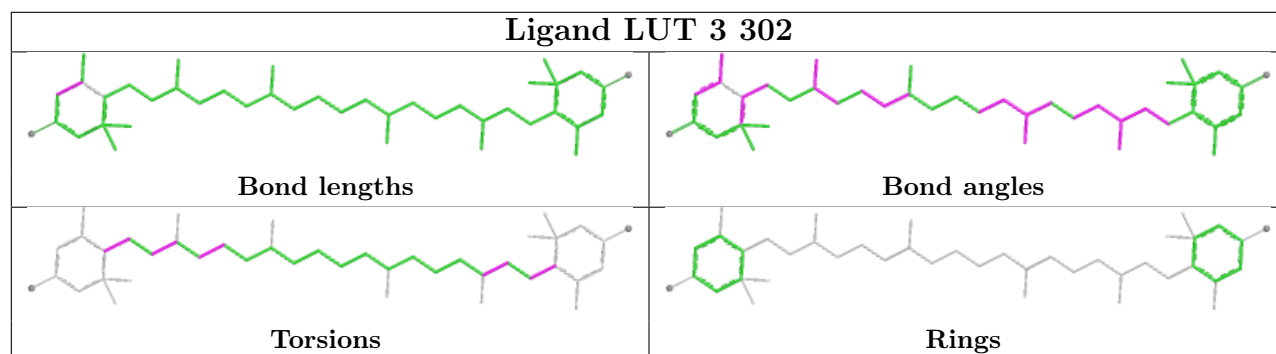
Ligand LUT 3 301



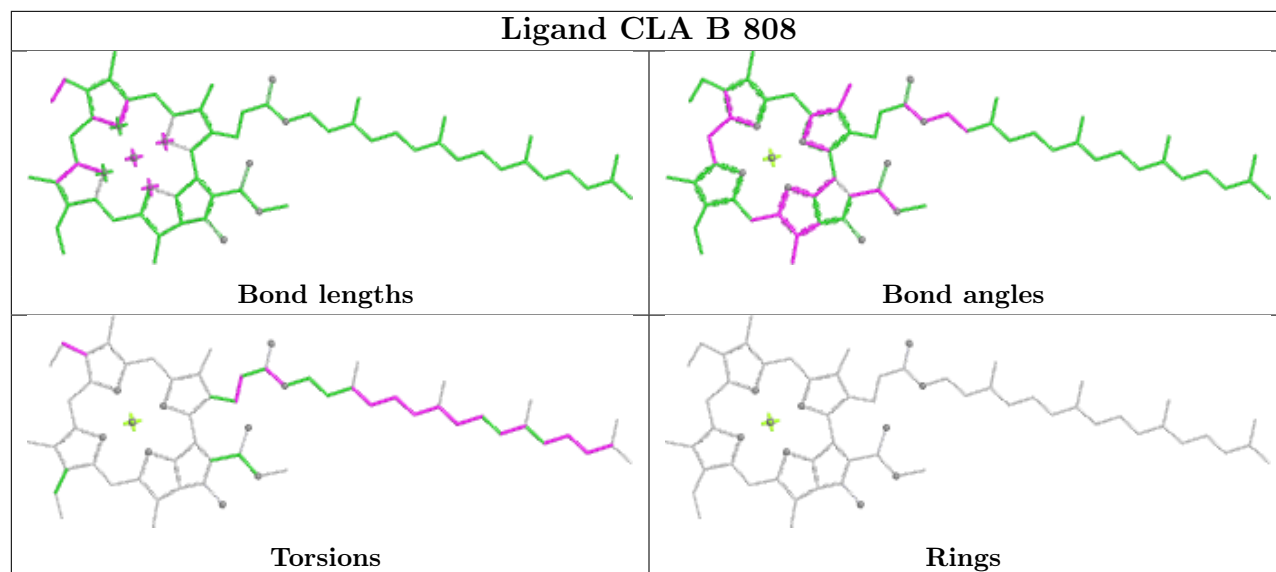
Ligand CLA B 803



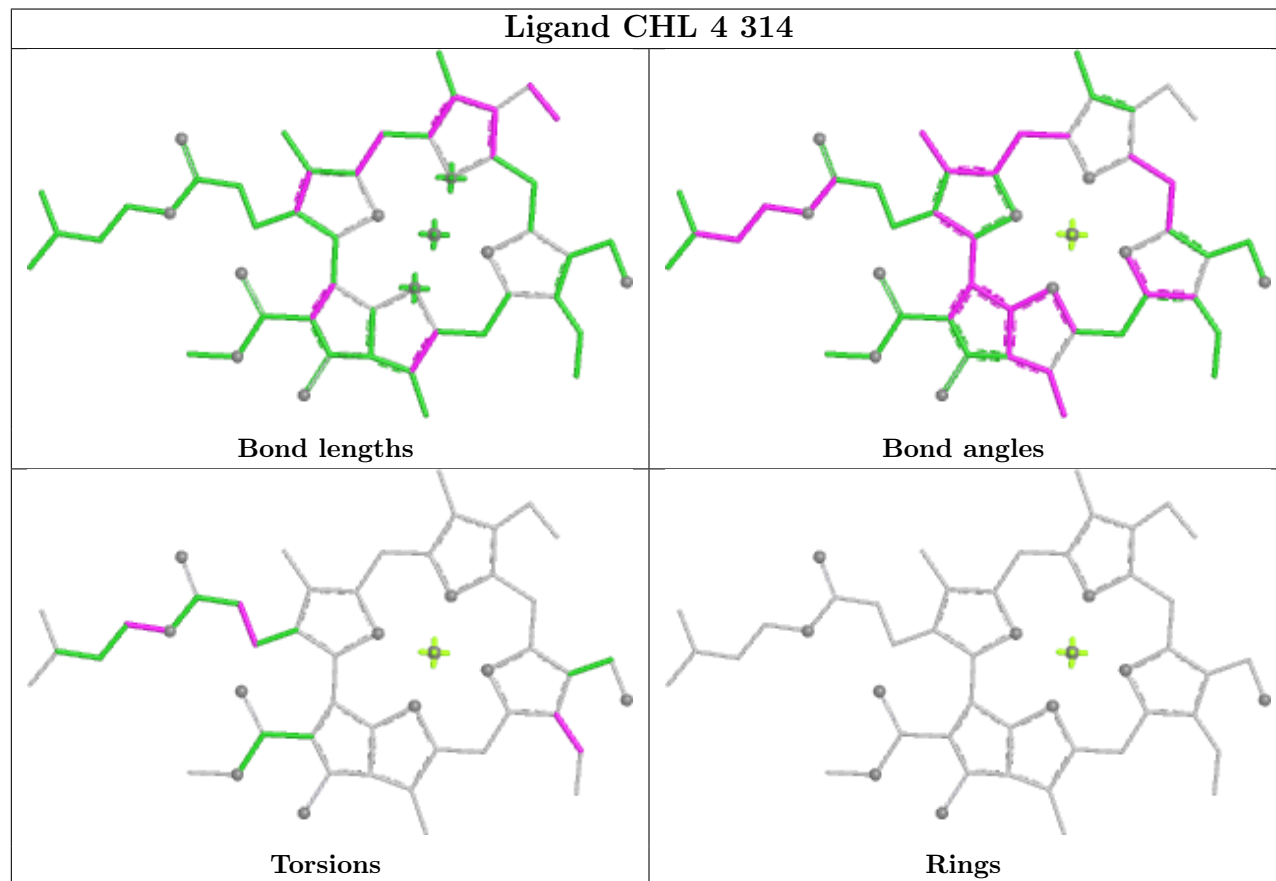
Ligand LUT 3 302



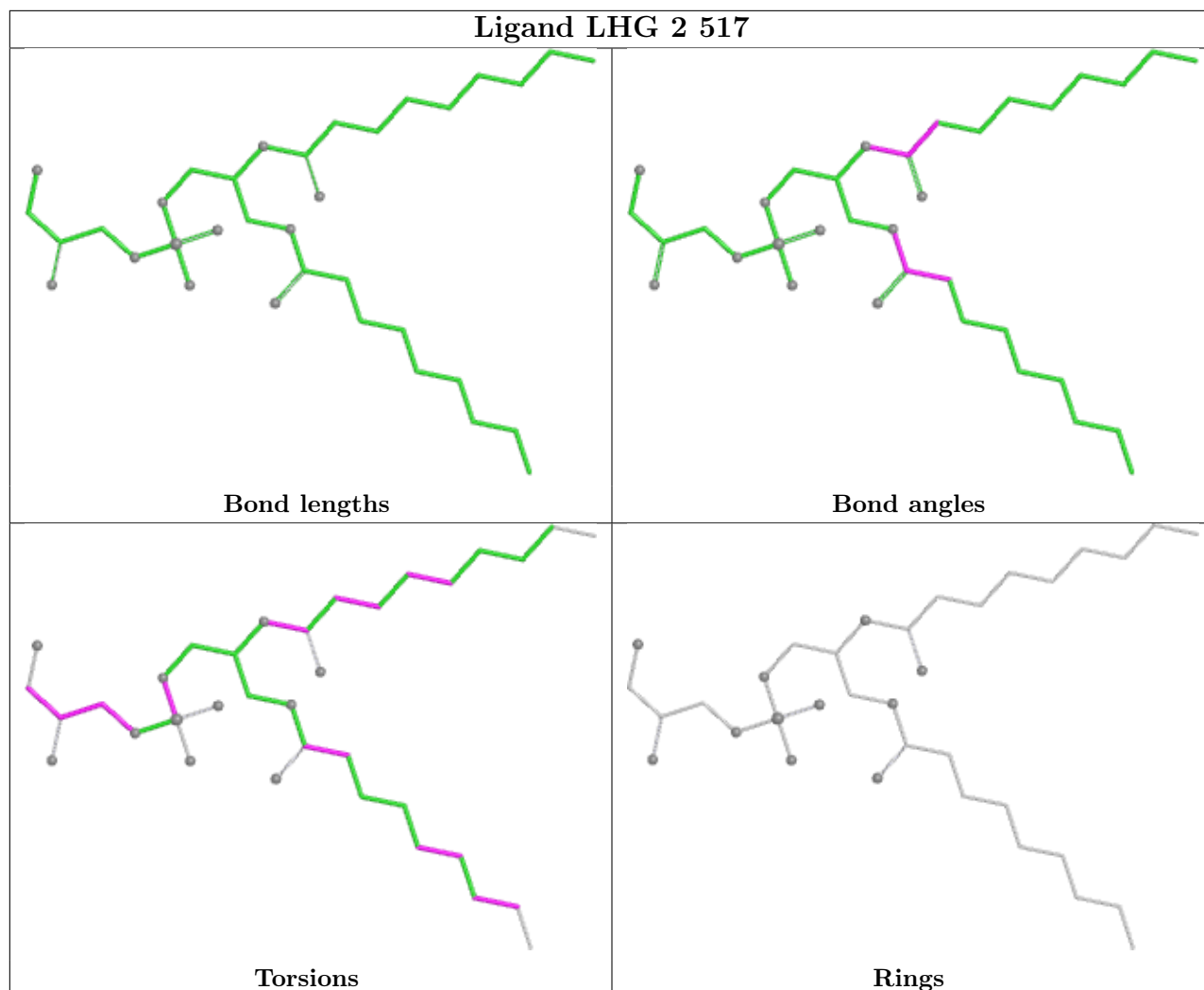
Ligand CLA B 808



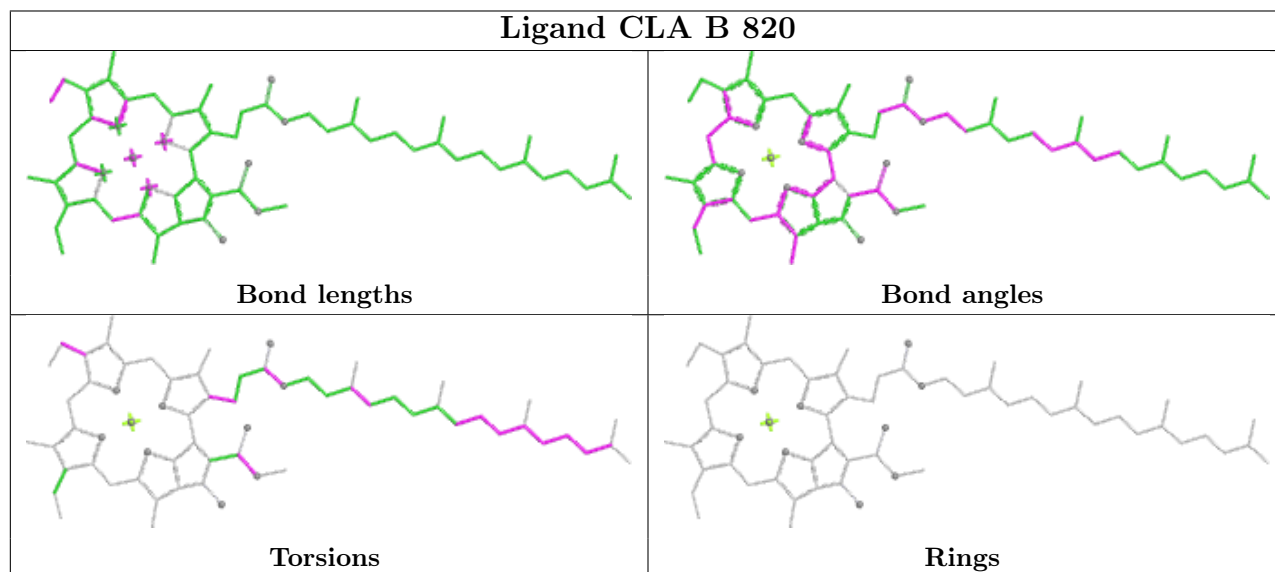
Ligand CHL 4 314



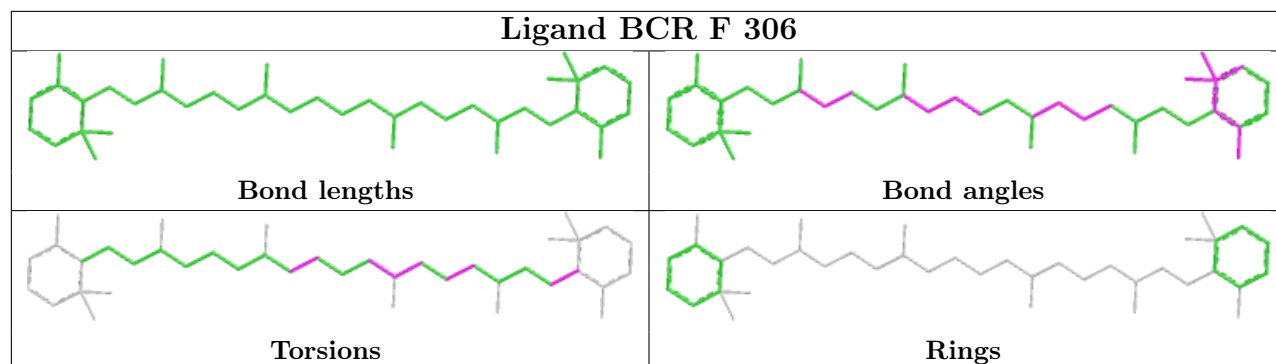
Ligand LHG 2 517



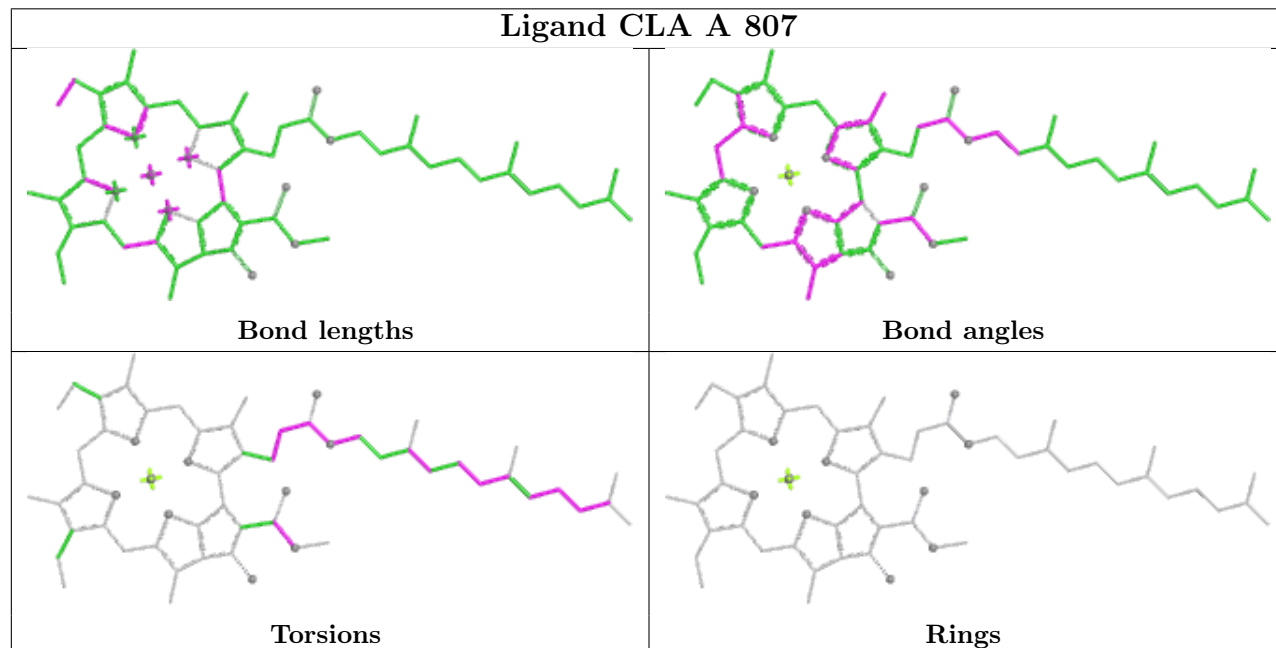
Ligand CLA B 820



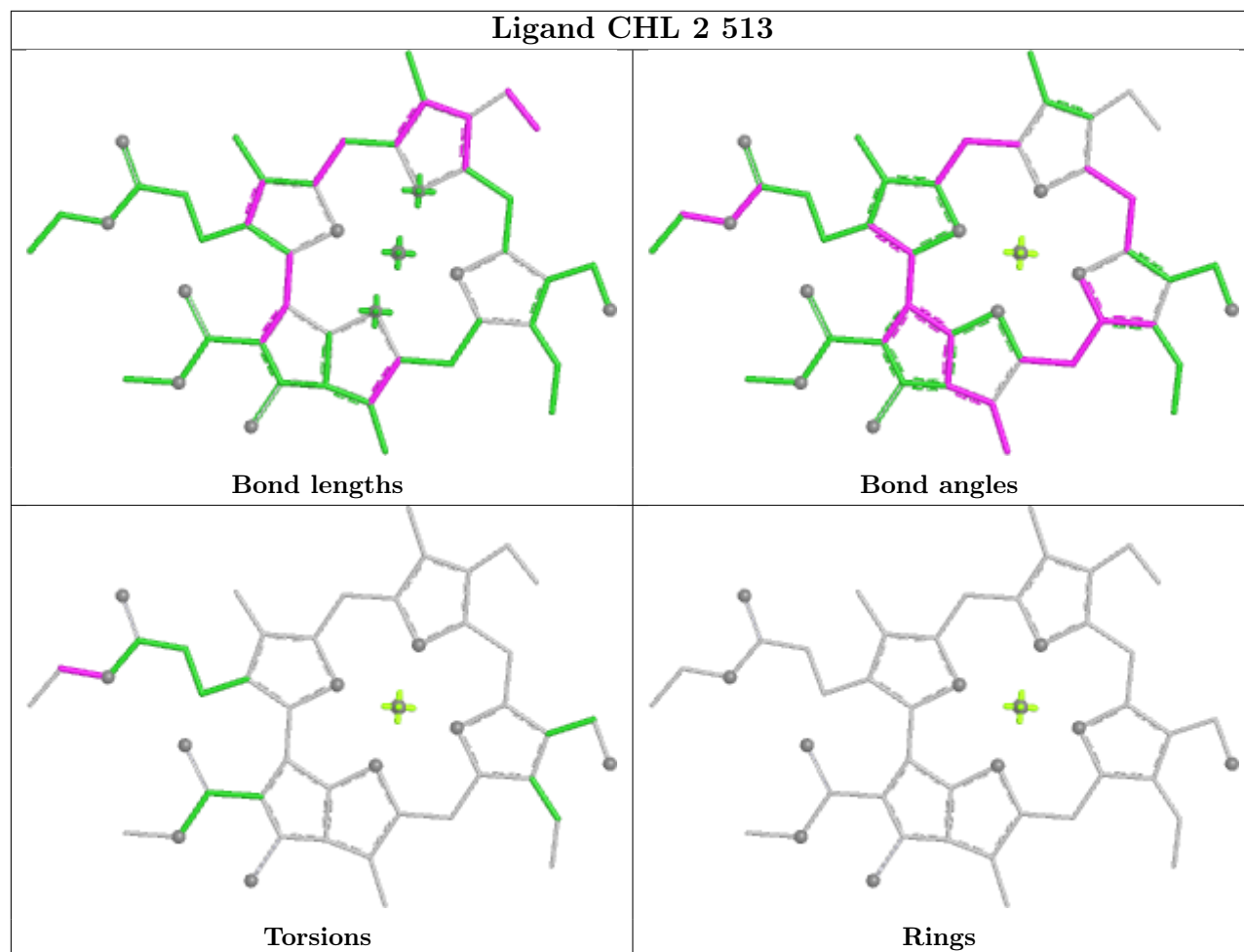
Ligand BCR F 306



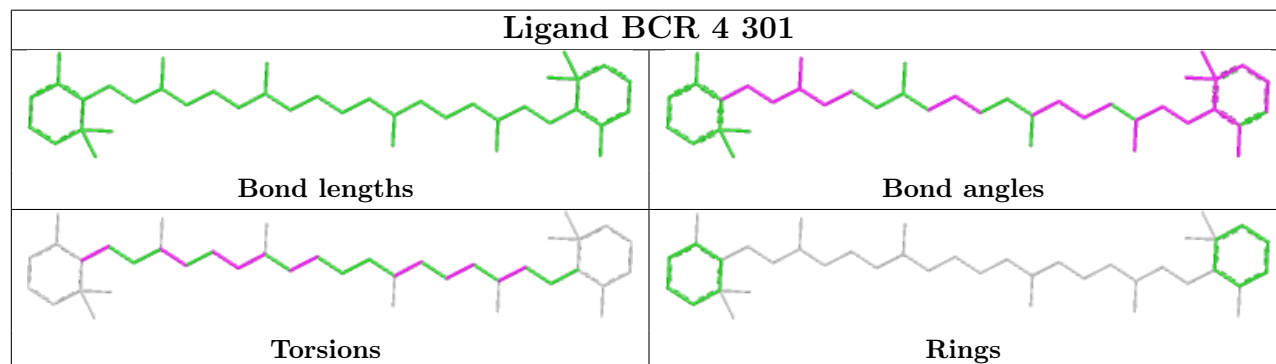
Ligand CLA A 807

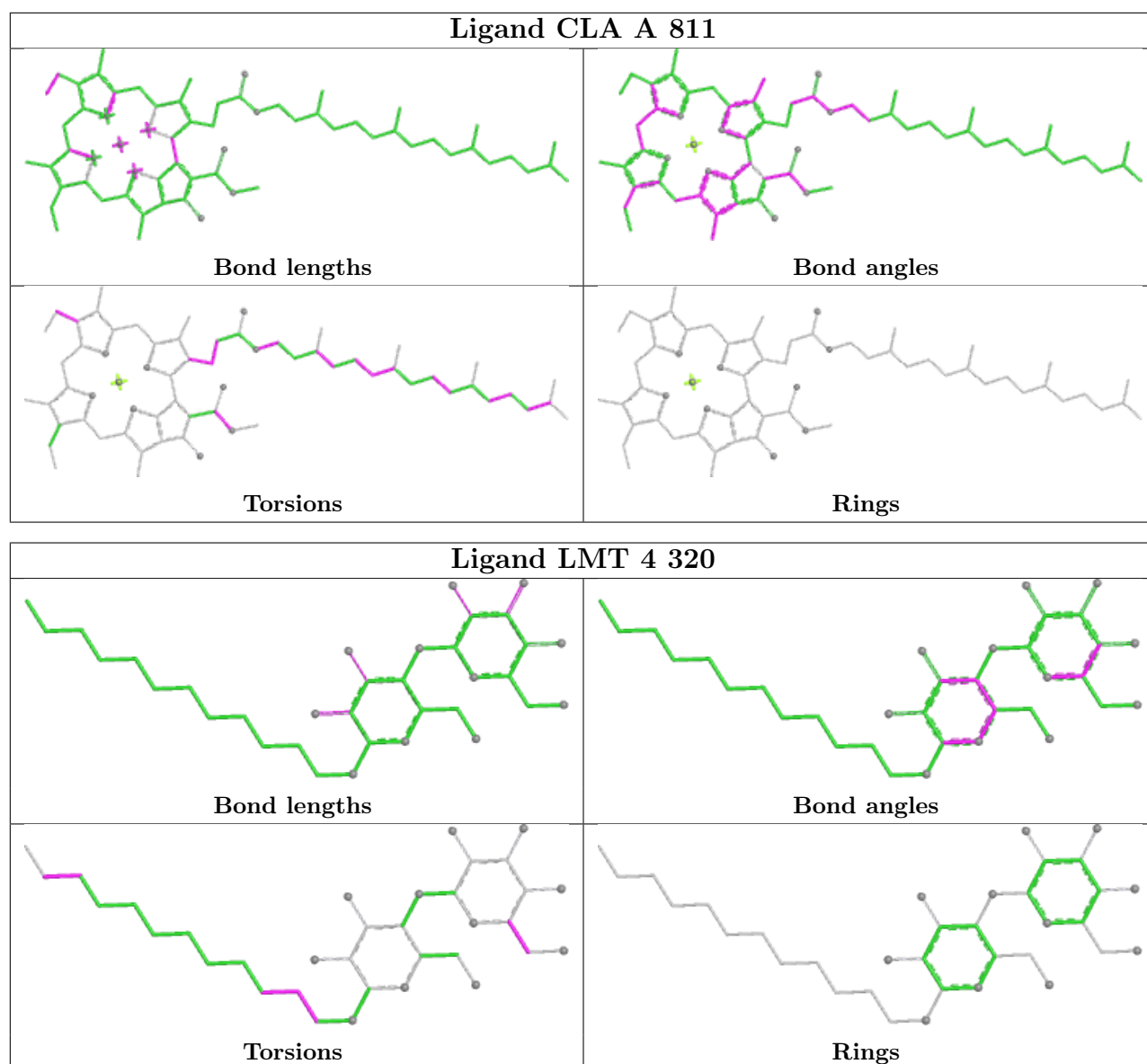


Ligand CHL 2 513

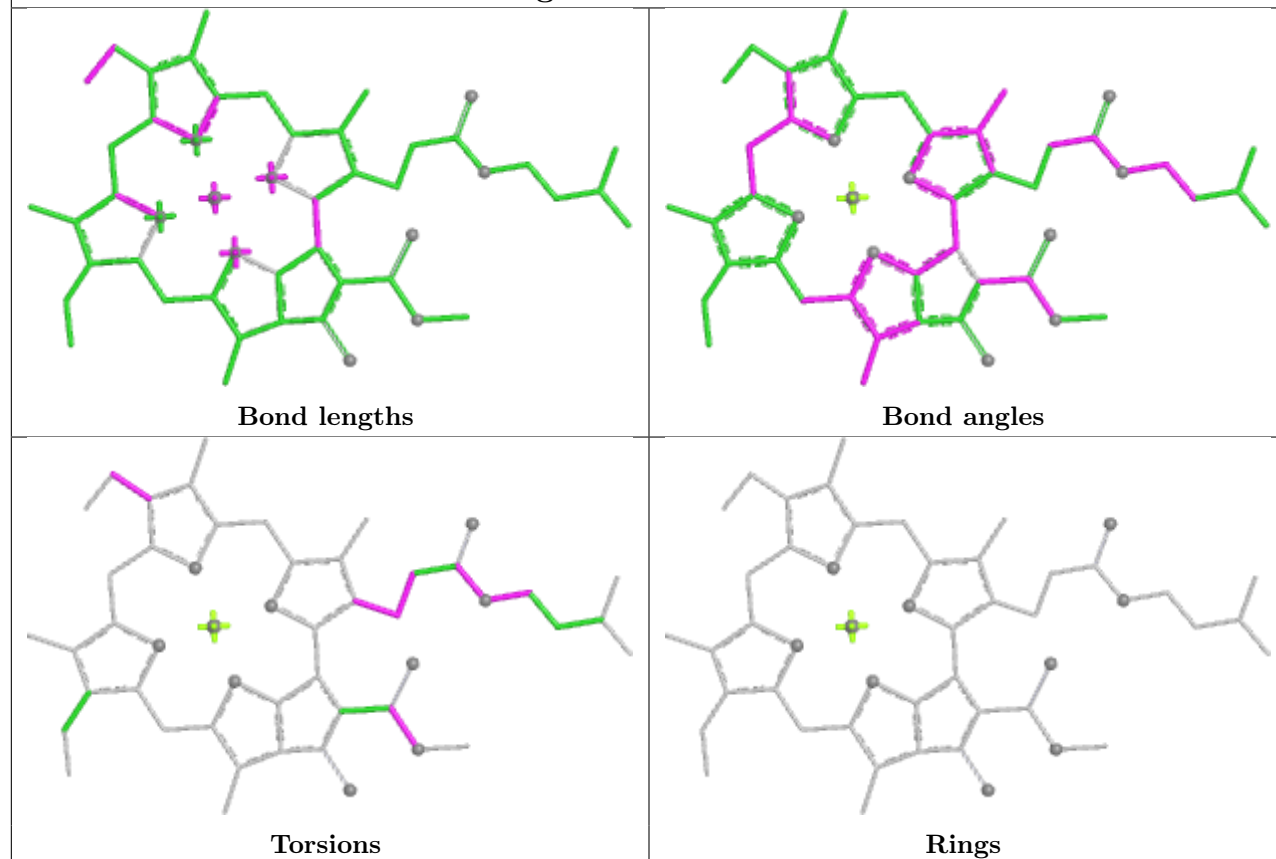


Ligand BCR 4 301

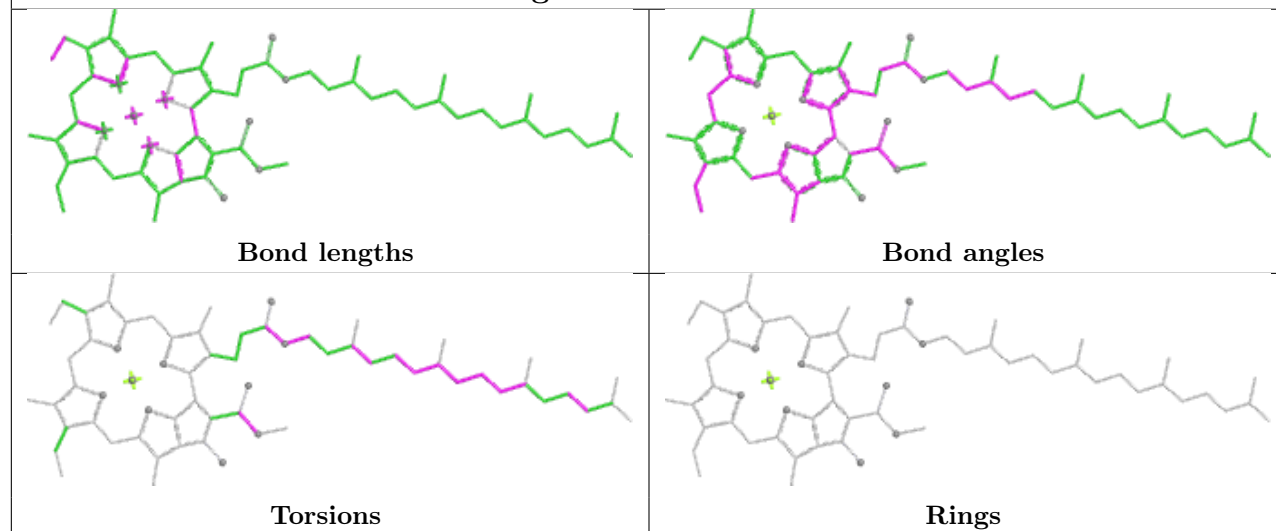




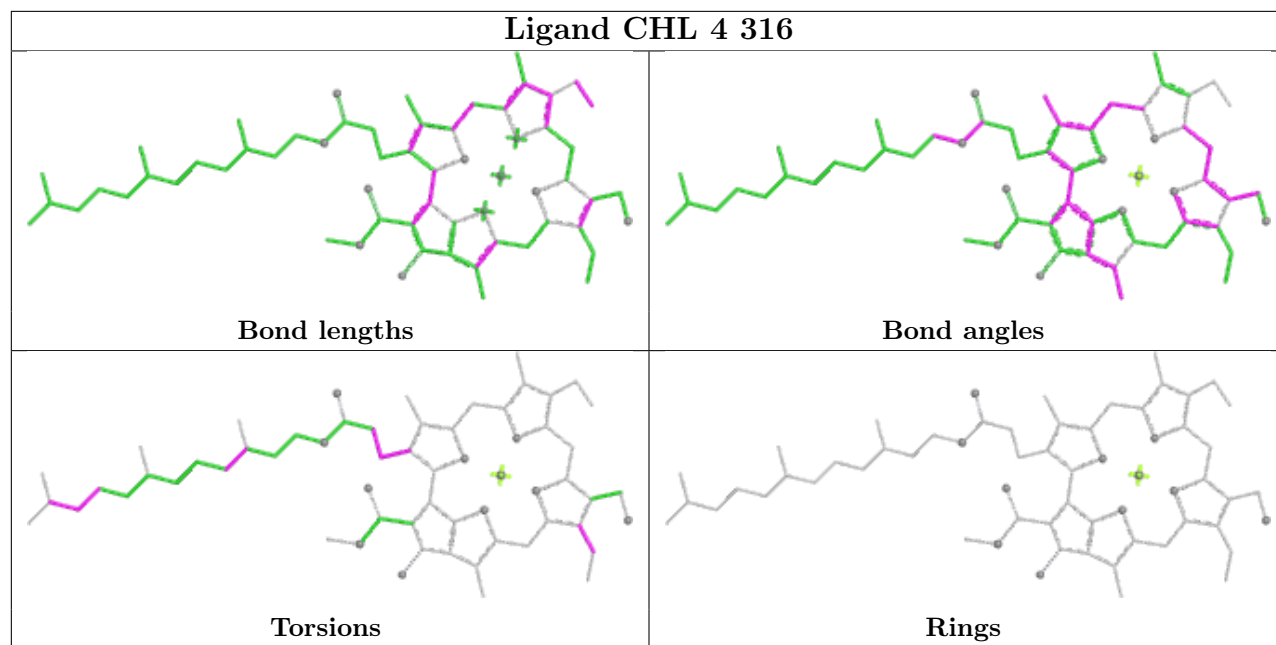
Ligand CLA 2 511



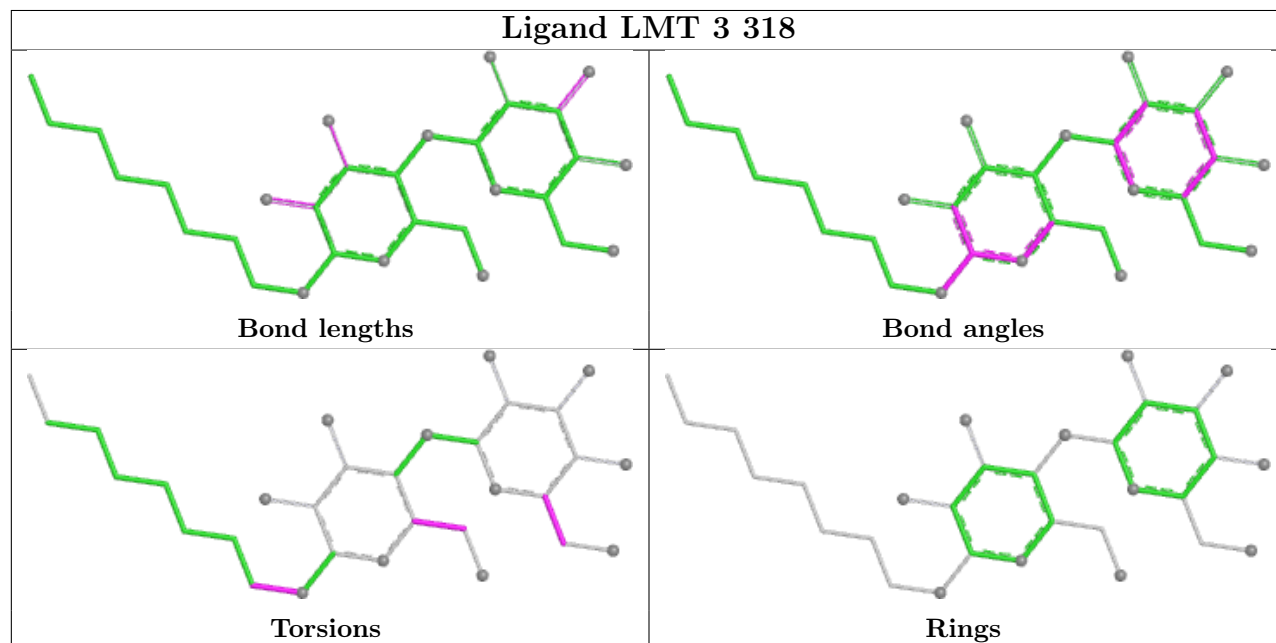
Ligand CLA A 802



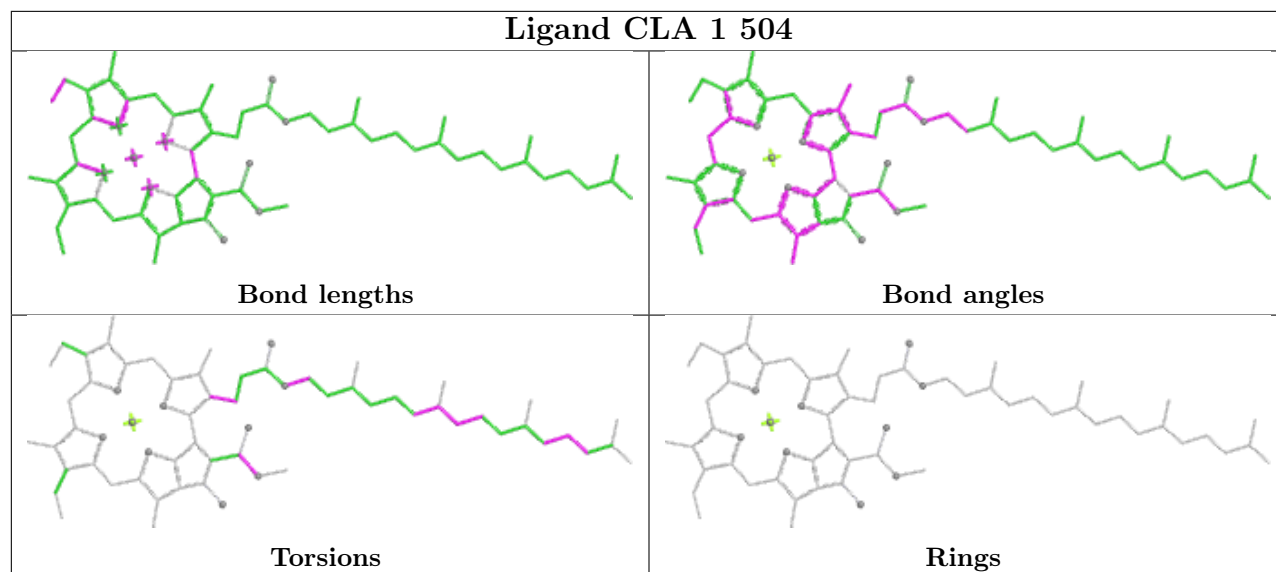
Ligand CHL 4 316



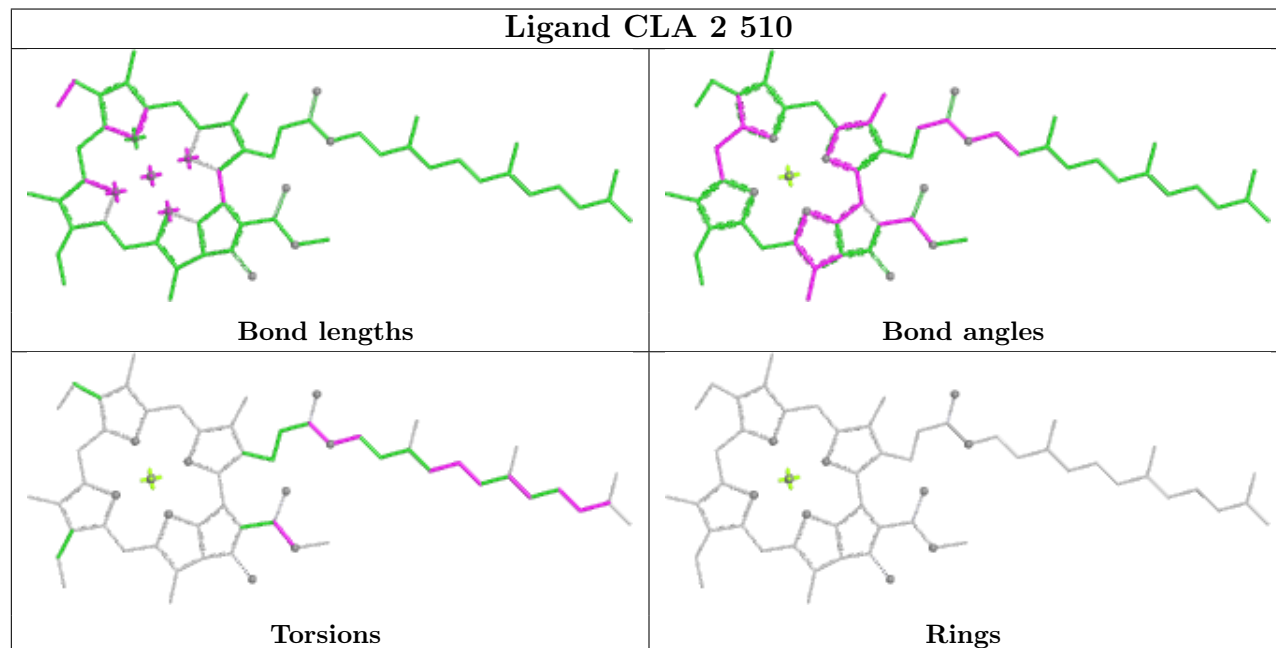
Ligand LMT 3 318

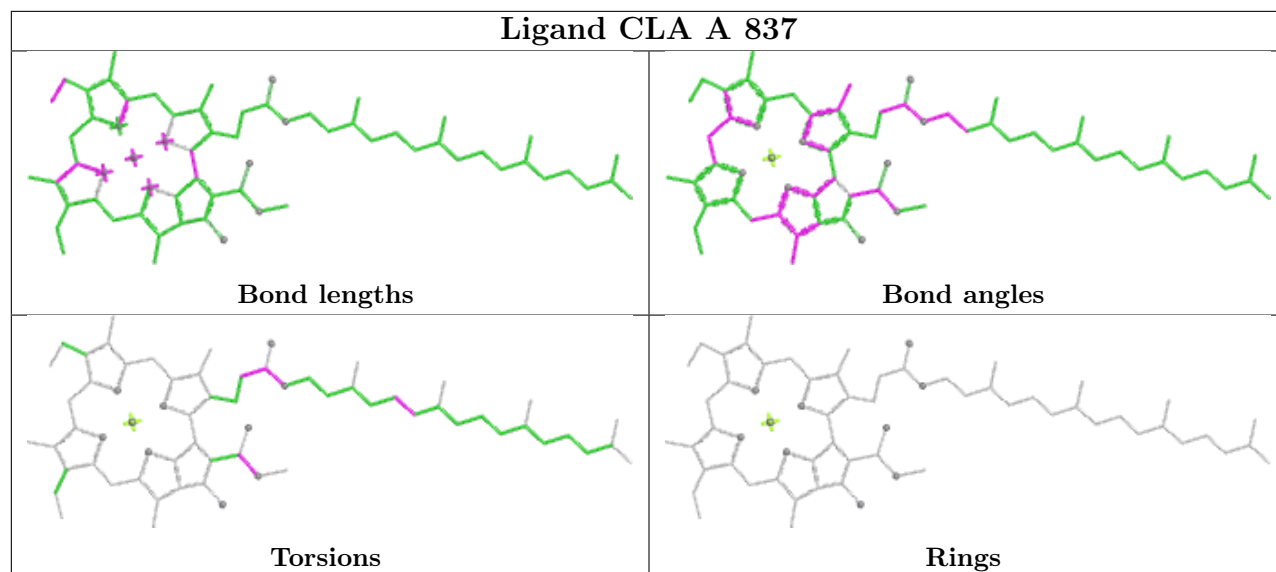
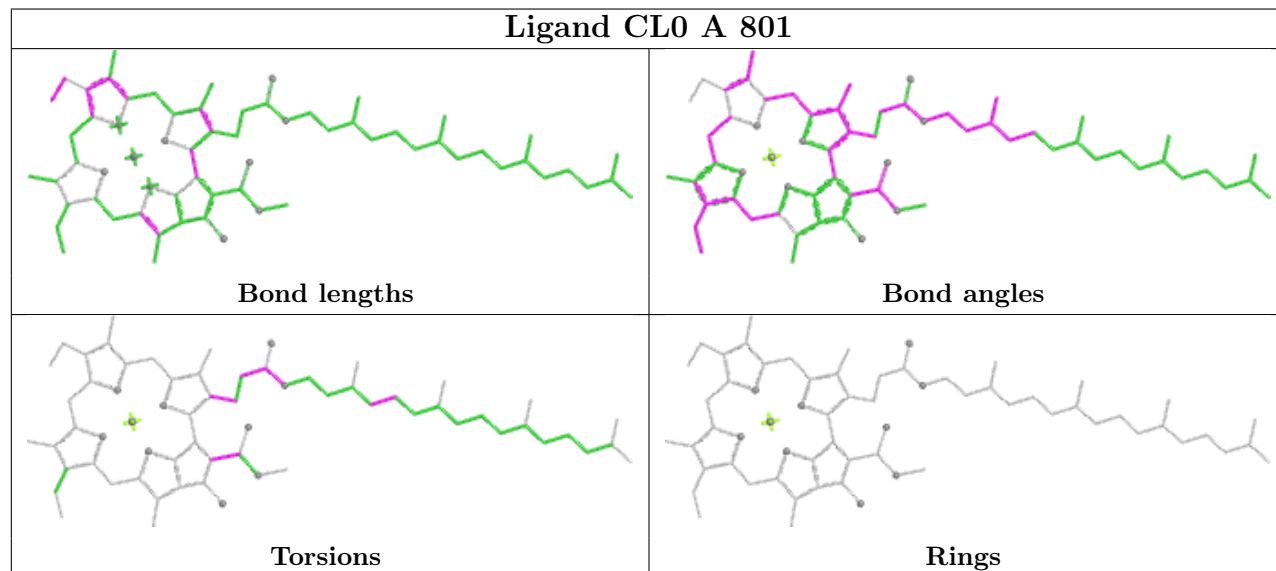


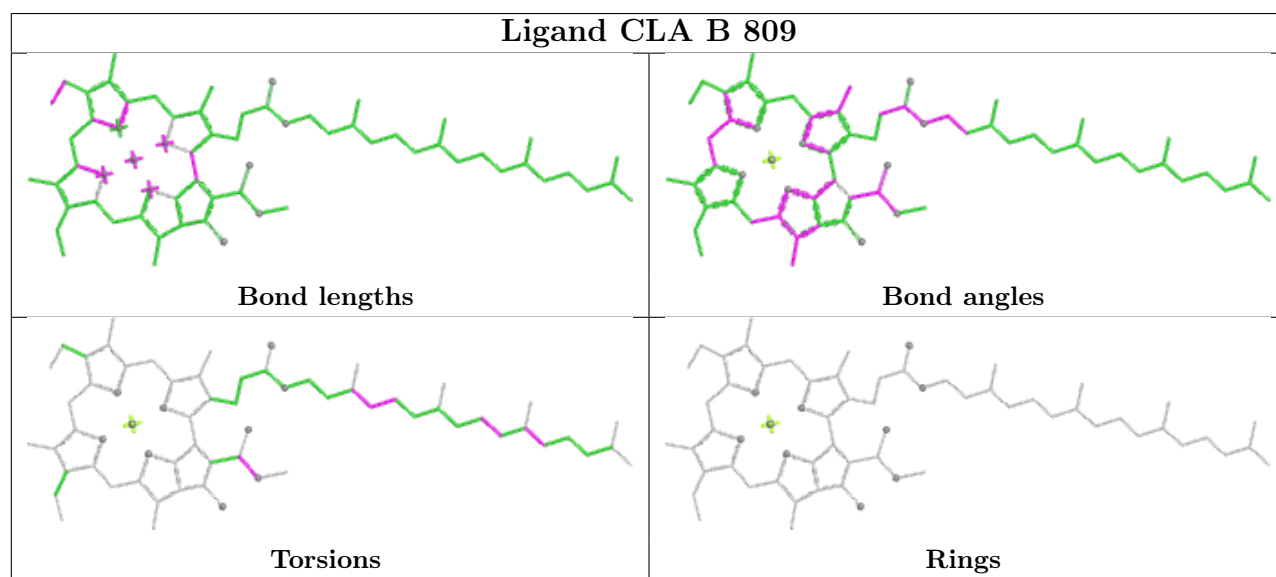
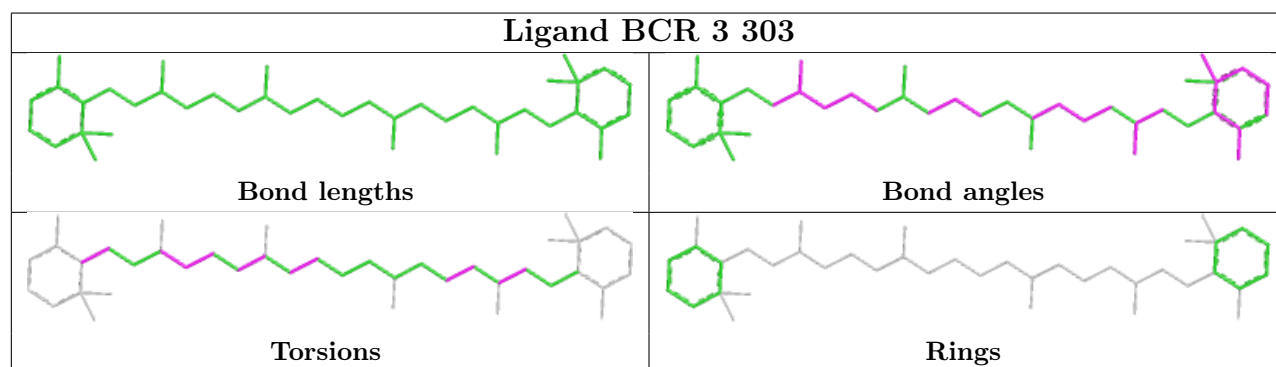
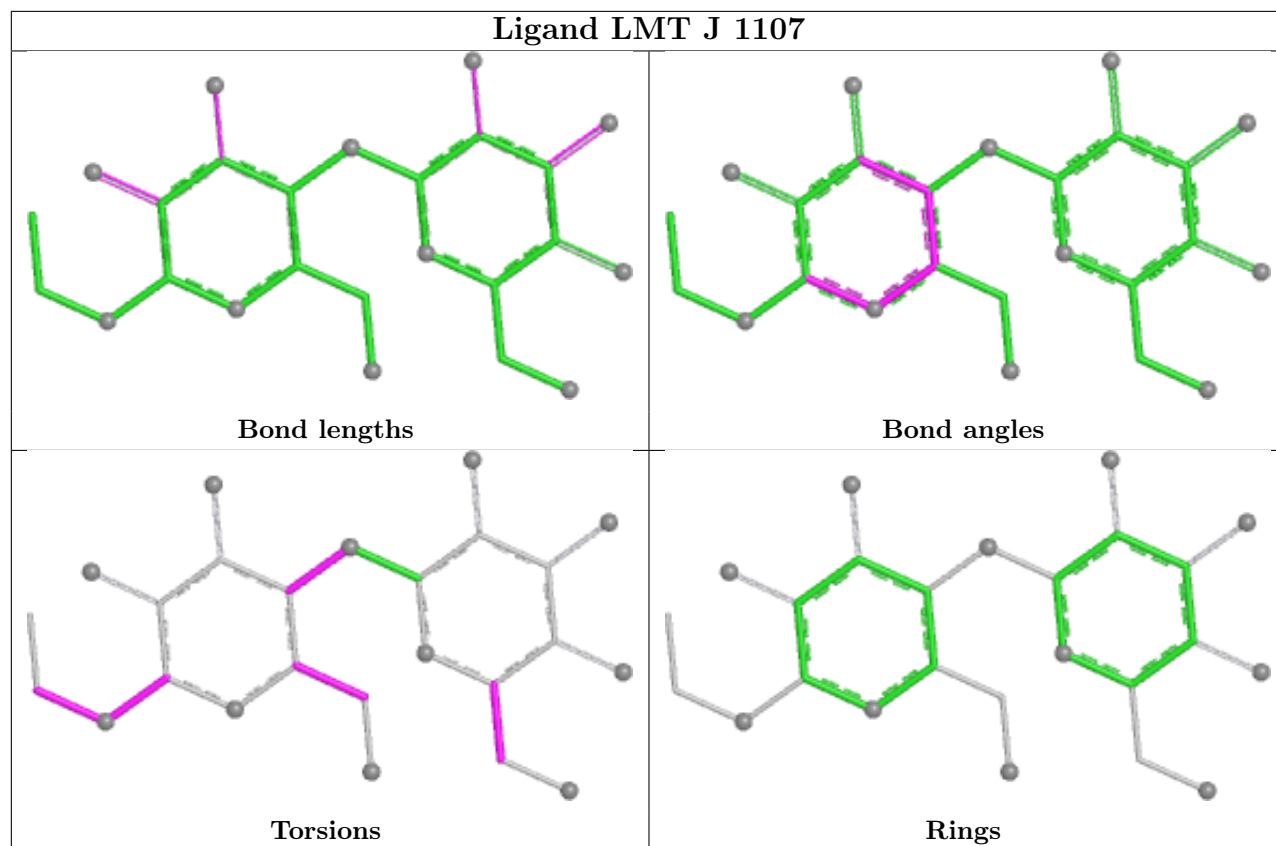
Ligand CLA 1 504



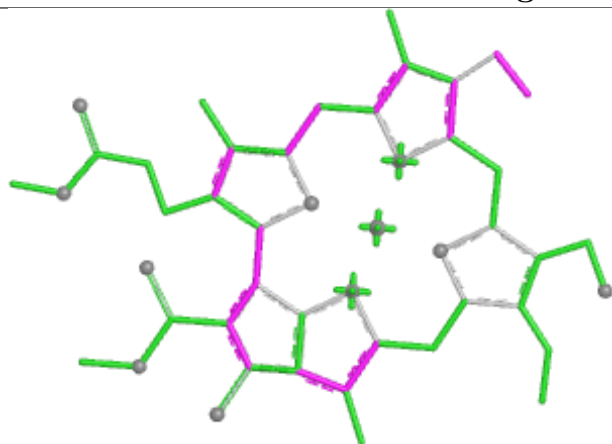
Ligand CLA 2 510



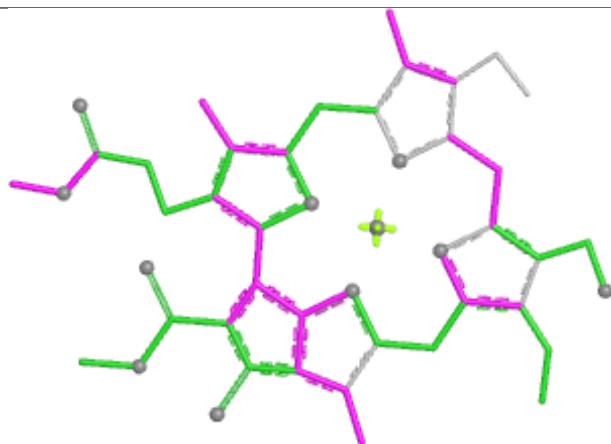
Ligand CLA A 837**Ligand CL0 A 801**



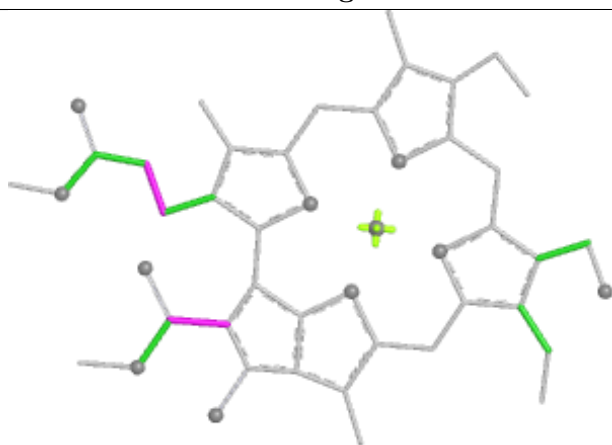
Ligand CHL 2 512



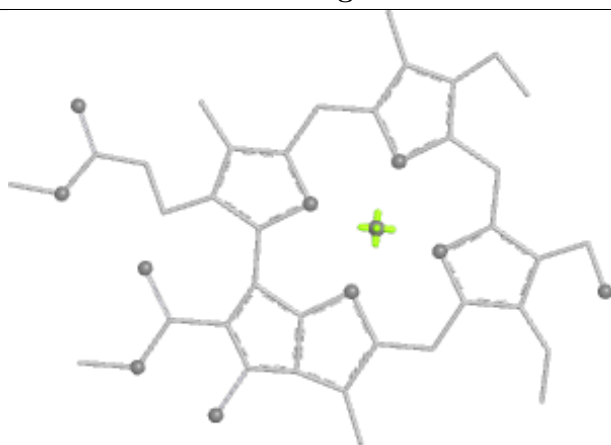
Bond lengths



Bond angles

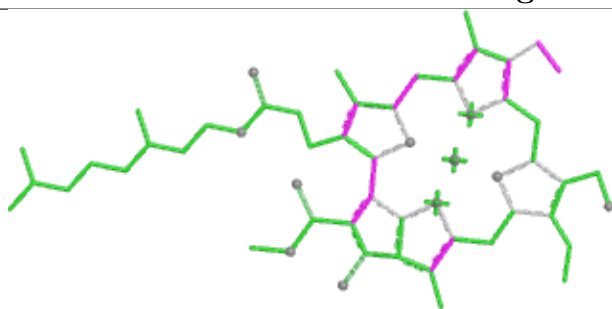


Torsions

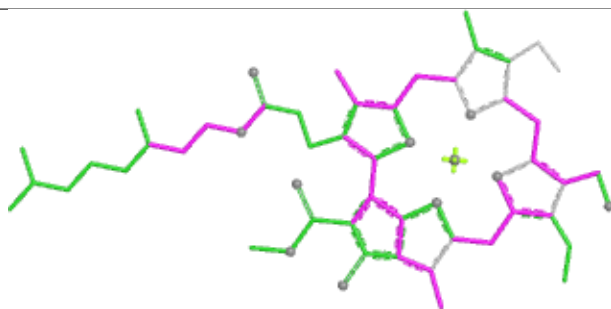


Rings

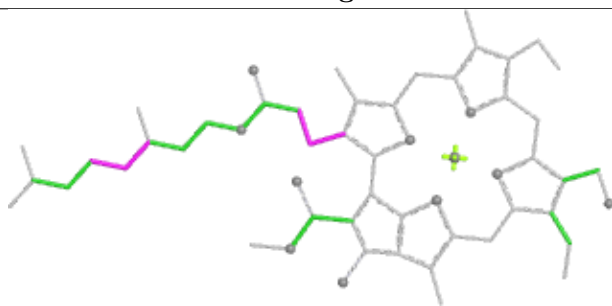
Ligand CHL 2 516



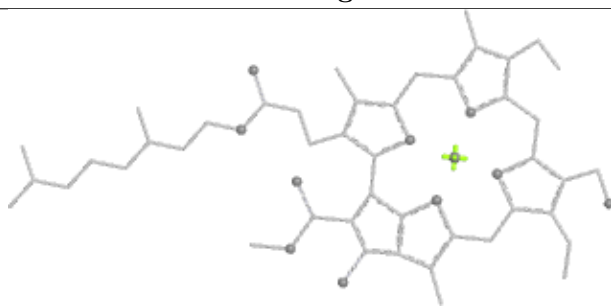
Bond lengths



Bond angles

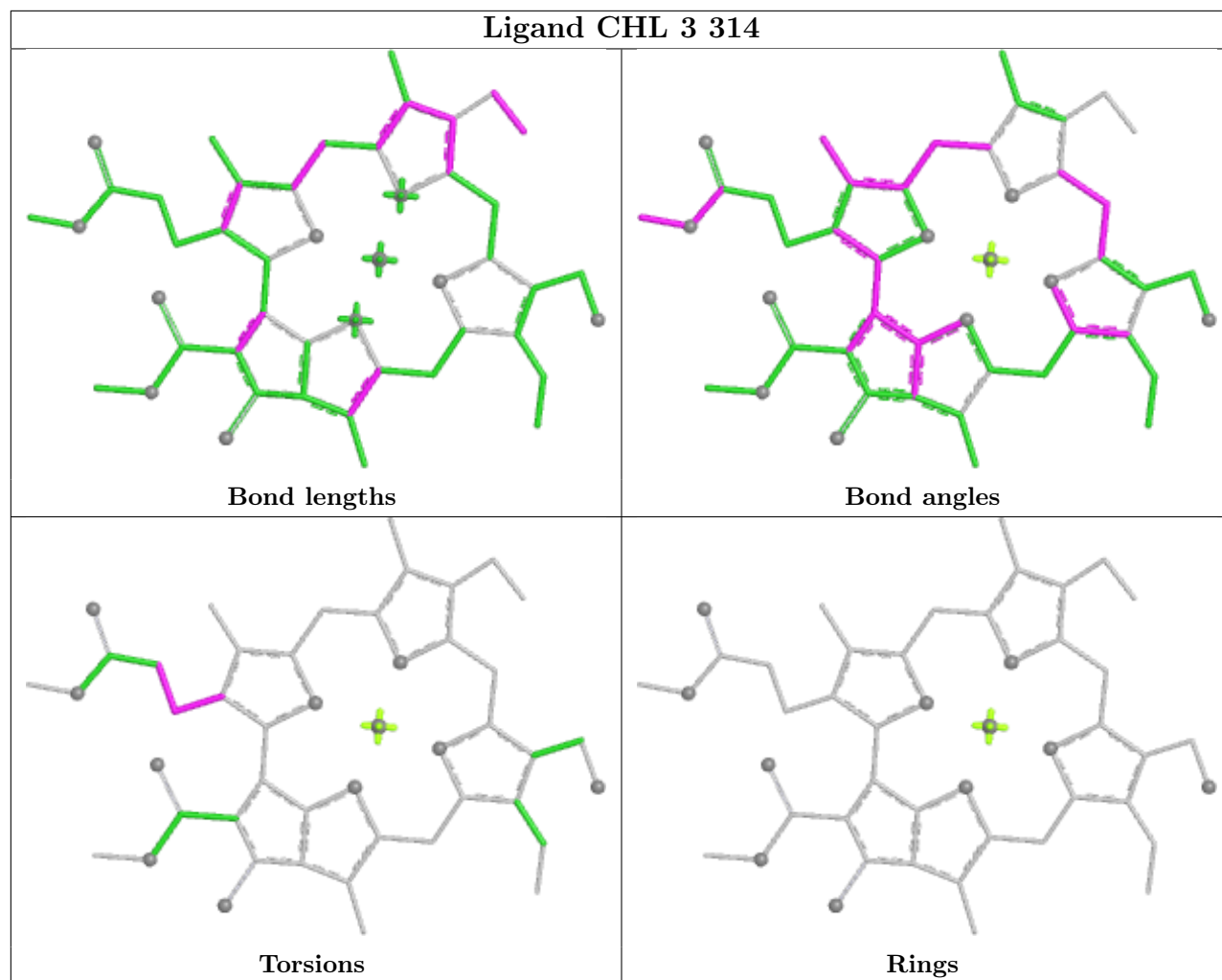


Torsions

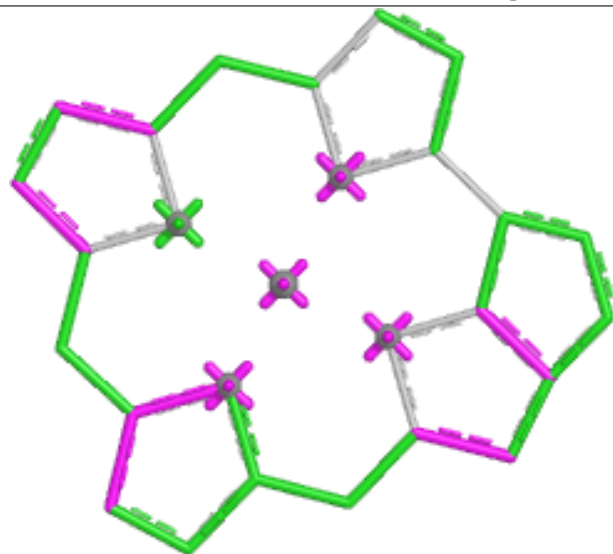


Rings

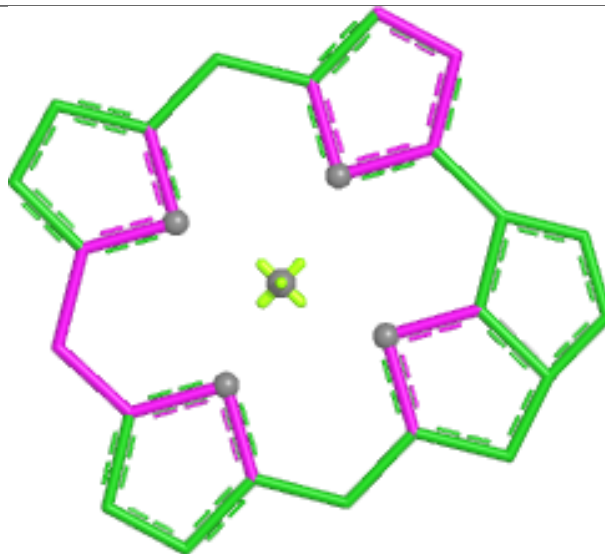
Ligand CHL 3 314



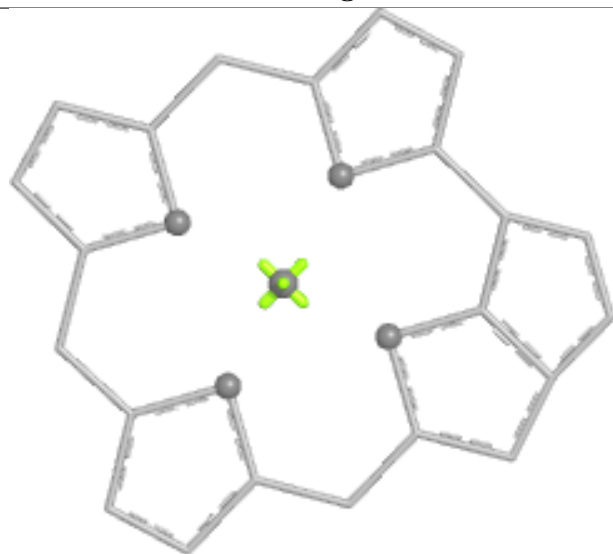
Ligand CLA K 1004



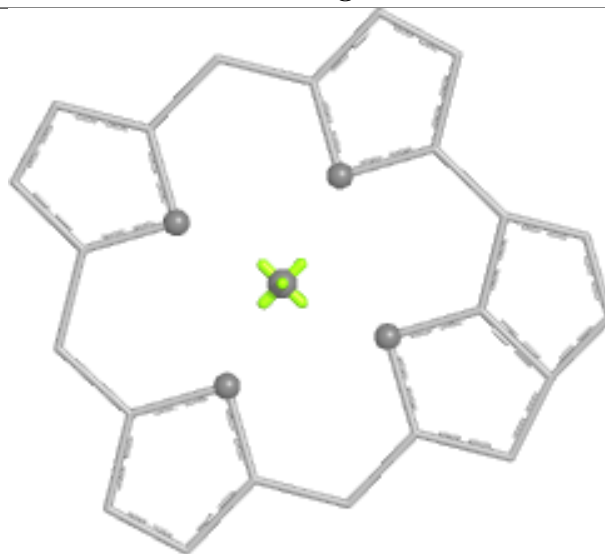
Bond lengths



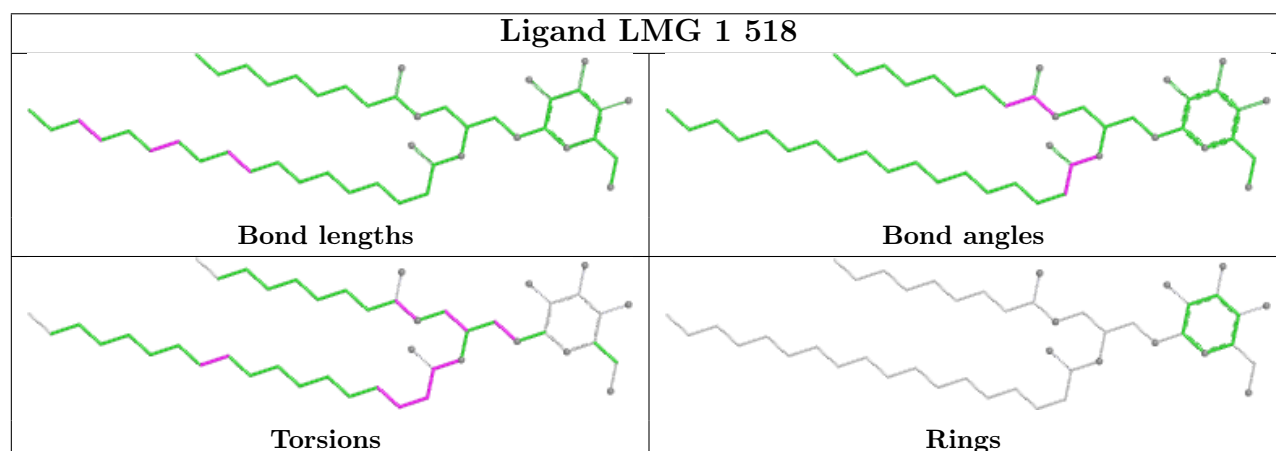
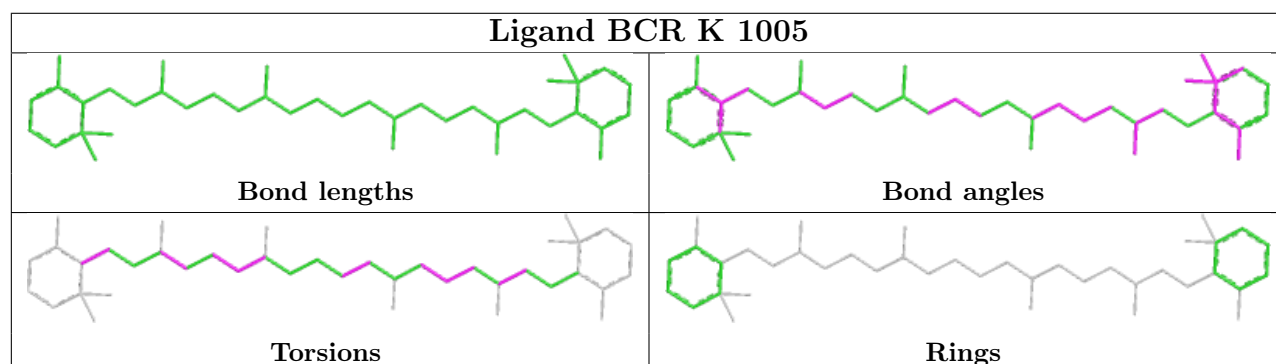
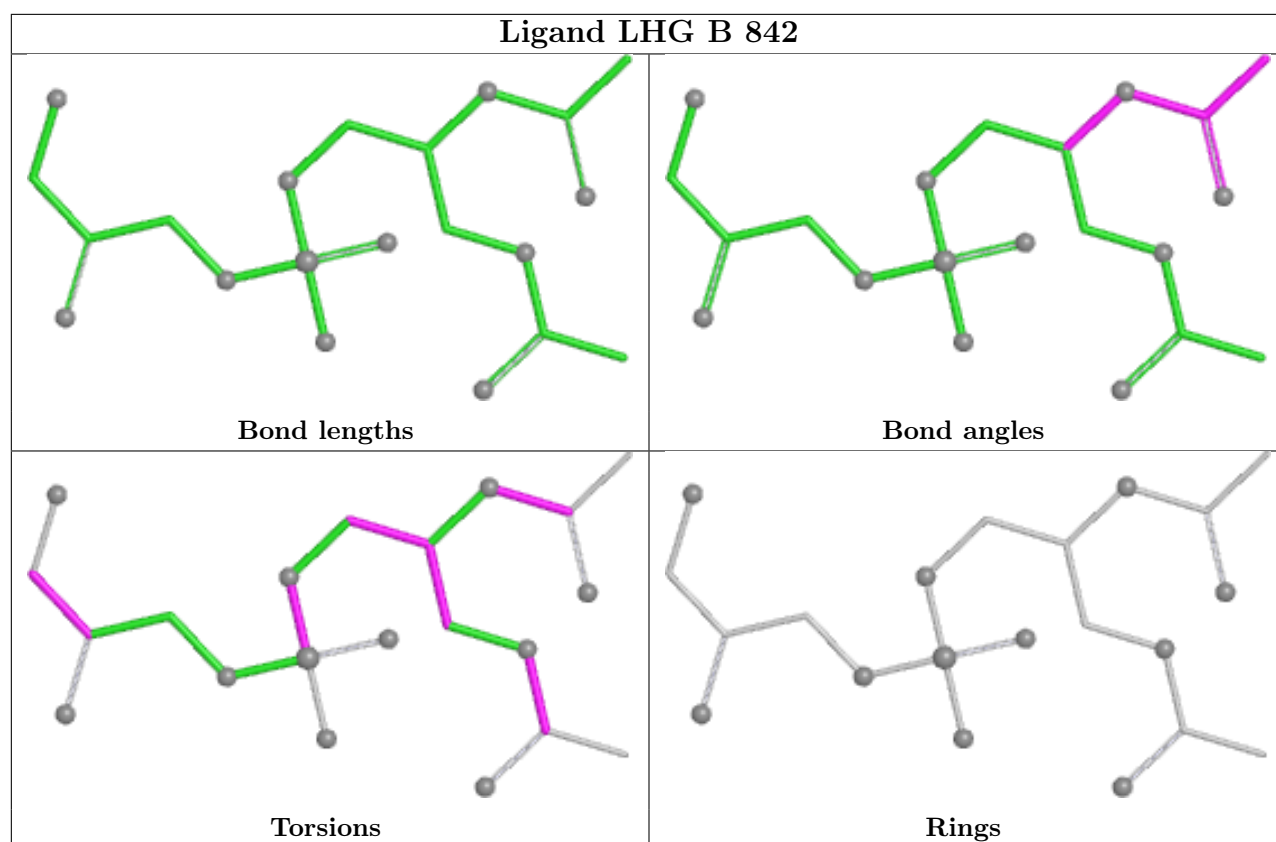
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	193/193 (100%)	1.08	37 (19%) 3 2	86, 127, 178, 218	0
2	2	208/269 (77%)	0.35	11 (5%) 32 26	82, 113, 154, 201	0
3	3	221/275 (80%)	0.86	35 (15%) 5 4	101, 148, 202, 253	0
4	4	198/198 (100%)	0.35	14 (7%) 22 17	73, 107, 149, 196	0
5	A	743/758 (98%)	0.34	45 (6%) 27 22	47, 79, 137, 192	0
6	B	733/734 (99%)	0.29	49 (6%) 24 19	49, 76, 116, 160	0
7	C	80/81 (98%)	0.42	6 (7%) 20 16	55, 66, 89, 121	0
8	D	143/143 (100%)	0.78	18 (12%) 8 6	60, 77, 107, 153	0
9	E	66/66 (100%)	0.36	4 (6%) 27 22	51, 81, 122, 147	0
10	F	154/154 (100%)	0.03	4 (2%) 57 51	54, 76, 116, 168	0
11	G	97/97 (100%)	0.67	11 (11%) 10 8	76, 113, 151, 161	0
12	H	88/88 (100%)	0.66	8 (9%) 15 11	80, 112, 146, 178	0
13	I	30/40 (75%)	0.32	2 (6%) 24 19	76, 99, 136, 138	0
14	J	42/42 (100%)	0.06	2 (4%) 35 30	57, 69, 96, 145	0
15	K	77/80 (96%)	1.21	16 (20%) 2 2	131, 168, 192, 218	0
16	L	157/157 (100%)	0.78	21 (13%) 7 5	77, 105, 151, 209	0
All	All	3230/3375 (95%)	0.47	283 (8%) 15 12	47, 94, 164, 253	0

All (283) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	103	GLY	11.1
1	1	101	GLY	11.0
8	D	196	VAL	9.8
8	D	200	GLU	8.4
3	3	177	ALA	8.3

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Mol	Chain	Res	Type	RSRZ
8	D	208	PRO	8.2
5	A	263	ALA	7.9
11	G	153	LYS	7.8
12	H	53	VAL	7.6
11	G	110	GLU	7.0
8	D	206	LYS	7.0
6	B	294	ASN	7.0
1	1	102	LEU	6.9
9	E	98	ASN	6.6
6	B	70	TRP	6.5
6	B	295	PHE	6.4
8	D	197	SER	6.1
16	L	172	GLN	6.0
16	L	163	SER	6.0
1	1	161	PRO	5.8
1	1	100	LEU	5.7
2	2	58	THR	5.6
6	B	92	TRP	5.4
5	A	264	GLU	5.2
8	D	201	VAL	5.2
7	C	13	GLY	5.1
8	D	211	LEU	5.1
6	B	211	ASN	5.1
3	3	92	PHE	5.1
7	C	35	LYS	5.1
11	G	58	LEU	5.0
11	G	111	TYR	5.0
3	3	173	PHE	5.0
1	1	225	THR	4.9
8	D	207	GLN	4.9
16	L	186	THR	4.8
3	3	96	ARG	4.7
3	3	176	TRP	4.7
15	K	80	ALA	4.7
3	3	269	LEU	4.5
14	J	42	PHE	4.4
6	B	136	TYR	4.3
15	K	47	ILE	4.3
5	A	261	SER	4.3
1	1	226	ILE	4.3
6	B	566	GLY	4.3
5	A	262	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
15	K	90	LEU	4.2
15	K	50	PRO	4.2
12	H	78	TYR	4.1
1	1	98	GLU	4.1
2	2	168	TRP	4.1
9	E	64	PRO	4.0
3	3	127	LEU	4.0
6	B	165	VAL	4.0
5	A	278	ALA	4.0
2	2	206	TRP	3.9
16	L	205	TYR	3.9
3	3	125	VAL	3.9
1	1	99	ALA	3.9
10	F	231	VAL	3.9
1	1	131	LEU	3.9
5	A	277	TYR	3.8
6	B	505	SER	3.8
10	F	227	VAL	3.8
12	H	115	SER	3.8
6	B	552	ASP	3.7
1	1	219	ALA	3.7
9	E	91	VAL	3.7
16	L	115	VAL	3.7
5	A	519	ASP	3.7
15	K	51	THR	3.7
1	1	228	ASN	3.7
1	1	96	VAL	3.7
6	B	293	THR	3.7
3	3	178	LYS	3.6
16	L	171	LYS	3.6
11	G	106	THR	3.6
16	L	173	PRO	3.5
6	B	291	TYR	3.5
16	L	111	VAL	3.5
3	3	192	LYS	3.5
4	4	52	LYS	3.5
4	4	53	LYS	3.5
8	D	205	GLY	3.5
5	A	139	GLY	3.5
3	3	272	LEU	3.5
7	C	34	CYS	3.4
4	4	191	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
11	G	104	GLY	3.4
2	2	59	VAL	3.4
3	3	264	VAL	3.4
5	A	276	LYS	3.4
1	1	229	VAL	3.4
6	B	266	GLN	3.3
12	H	73	ASP	3.3
1	1	218	LEU	3.3
15	K	105	ALA	3.3
3	3	59	PHE	3.2
16	L	125	ILE	3.2
5	A	203	LEU	3.2
3	3	275	HIS	3.2
3	3	174	GLN	3.2
16	L	128	GLN	3.2
6	B	604	GLY	3.2
1	1	227	GLY	3.2
7	C	32	GLY	3.2
3	3	141	VAL	3.2
6	B	487	ASN	3.1
16	L	96	LEU	3.1
1	1	160	TYR	3.1
6	B	296	GLY	3.1
6	B	734	GLY	3.1
8	D	193	GLY	3.1
3	3	149	ASN	3.0
12	H	133	PRO	3.0
5	A	141	ARG	3.0
15	K	125	GLY	3.0
6	B	212	PHE	3.0
8	D	183	GLN	2.9
8	D	195	ASN	2.9
8	D	199	ILE	2.9
1	1	57	GLY	2.9
11	G	115	LEU	2.9
12	H	81	LEU	2.9
5	A	657	LEU	2.8
5	A	180	PHE	2.8
1	1	125	PRO	2.8
5	A	618	TRP	2.8
6	B	491	SER	2.8
16	L	184	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
6	B	554	GLY	2.8
5	A	401	TRP	2.8
13	I	6	SER	2.8
1	1	72	ASN	2.8
16	L	109	LEU	2.8
16	L	162	PRO	2.8
5	A	249	ILE	2.8
8	D	210	ASP	2.8
6	B	259	GLY	2.7
5	A	386	ALA	2.7
9	E	65	PRO	2.7
15	K	53	LEU	2.7
5	A	374	HIS	2.7
8	D	78	ASN	2.7
5	A	259	TYR	2.7
6	B	490	ARG	2.7
13	I	3	ASN	2.7
1	1	153	LYS	2.7
6	B	669	GLY	2.7
5	A	198	ASP	2.7
3	3	98	LEU	2.6
5	A	511	THR	2.6
16	L	116	LYS	2.6
3	3	252	PRO	2.6
15	K	103	THR	2.6
2	2	207	GLY	2.6
4	4	193	ASN	2.6
5	A	396	PHE	2.6
8	D	133	ALA	2.6
1	1	150	SER	2.6
1	1	201	GLN	2.6
5	A	179	LEU	2.6
1	1	144	PHE	2.6
3	3	268	VAL	2.5
4	4	67	THR	2.5
1	1	60	GLY	2.5
4	4	173	LYS	2.5
6	B	89	HIS	2.5
1	1	71	GLU	2.5
3	3	103	VAL	2.5
6	B	66	PHE	2.5
10	F	228	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
5	A	46	LYS	2.5
6	B	87	ILE	2.5
6	B	330	ILE	2.5
2	2	251	PHE	2.5
6	B	292	ARG	2.4
12	H	76	SER	2.4
3	3	87	GLU	2.4
3	3	116	ALA	2.4
5	A	387	THR	2.4
4	4	66	LEU	2.4
15	K	102	ASP	2.4
1	1	59	PHE	2.4
5	A	614	PHE	2.4
6	B	88	ALA	2.4
6	B	61	THR	2.4
3	3	81	LEU	2.4
6	B	300	SER	2.4
2	2	246	PRO	2.4
6	B	298	GLY	2.4
15	K	85	ALA	2.4
5	A	453	LEU	2.3
7	C	15	THR	2.3
1	1	40	ASP	2.3
1	1	162	GLY	2.3
5	A	493	GLN	2.3
6	B	177	HIS	2.3
2	2	208	SER	2.3
15	K	49	SER	2.3
6	B	154	TRP	2.3
6	B	357	ALA	2.3
16	L	209	LEU	2.3
5	A	494	ASN	2.3
6	B	166	SER	2.3
6	B	214	SER	2.3
3	3	86	PRO	2.3
2	2	130	GLY	2.3
3	3	123	GLY	2.3
16	L	130	GLY	2.3
4	4	143	VAL	2.3
4	4	213	LEU	2.3
6	B	244	PHE	2.3
4	4	190	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
5	A	111	ASN	2.3
1	1	232	PRO	2.3
3	3	271	SER	2.3
10	F	230	ASP	2.3
3	3	245	GLY	2.3
3	3	261	ALA	2.2
5	A	546	ALA	2.2
6	B	361	ILE	2.2
5	A	550	HIS	2.2
6	B	551	LYS	2.2
1	1	58	ASP	2.2
6	B	164	SER	2.2
1	1	95	LEU	2.2
6	B	2	ALA	2.2
5	A	107	GLU	2.2
3	3	121	TYR	2.2
3	3	129	PRO	2.2
5	A	260	PRO	2.2
12	H	132	PRO	2.2
4	4	64	GLY	2.2
5	A	373	ALA	2.2
6	B	401	GLU	2.2
6	B	558	PRO	2.2
11	G	151	ASP	2.2
5	A	140	PHE	2.2
5	A	407	ILE	2.2
7	C	36	ALA	2.2
14	J	7	TYR	2.2
2	2	212	GLN	2.2
15	K	122	LYS	2.2
4	4	192	LEU	2.2
5	A	258	LEU	2.2
6	B	565	GLY	2.2
16	L	108	PHE	2.2
1	1	157	LYS	2.1
8	D	209	TYR	2.1
11	G	109	LYS	2.1
11	G	112	VAL	2.1
8	D	194	LYS	2.1
5	A	644	GLN	2.1
15	K	48	GLY	2.1
16	L	201	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
15	K	101	ALA	2.1
5	A	33	GLN	2.1
6	B	229	GLN	2.1
5	A	583	GLY	2.1
5	A	175	ALA	2.1
5	A	610	SER	2.1
3	3	97	TRP	2.1
16	L	170	LYS	2.1
3	3	143	PRO	2.1
2	2	209	ALA	2.0
1	1	97	PRO	2.0
6	B	71	GLN	2.0
1	1	53	GLY	2.0
3	3	93	ILE	2.0
5	A	314	GLY	2.0
6	B	395	ILE	2.0
1	1	69	VAL	2.0
5	A	279	ASP	2.0
3	3	229	LYS	2.0
1	1	56	PRO	2.0
6	B	237	PRO	2.0
16	L	106	HIS	2.0
4	4	120	ILE	2.0
15	K	123	ASN	2.0
4	4	65	TYR	2.0
11	G	150	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	LMG	2	520	13/55	0.39	0.19	101,133,145,149	0
24	LMT	J	1107	25/35	0.39	0.16	174,178,183,184	0
24	LMT	2	523	35/35	0.44	0.23	182,208,216,216	0
19	CLA	K	1004	27/65	0.46	0.18	166,177,185,190	0
26	DGD	B	801	41/66	0.56	0.24	170,200,207,208	0
24	LMT	G	209	31/35	0.58	0.17	136,187,203,205	0
22	LMG	2	521	13/55	0.62	0.24	120,140,149,150	0
22	LMG	2	522	13/55	0.64	0.16	166,181,188,190	0
22	LMG	G	210	25/55	0.64	0.23	145,173,190,195	0
19	CLA	K	1003	27/65	0.65	0.16	189,198,202,205	0
24	LMT	A	846	35/35	0.67	0.17	90,128,143,148	0
22	LMG	B	845	33/55	0.68	0.17	107,163,172,176	0
22	LMG	2	524	13/55	0.68	0.15	143,153,159,162	0
22	LMG	A	847	50/55	0.68	0.18	133,155,181,184	0
24	LMT	3	318	31/35	0.68	0.17	127,164,183,187	0
22	LMG	2	525	13/55	0.70	0.17	100,129,143,143	0
19	CLA	H	1000	60/65	0.70	0.18	124,150,167,178	0
22	LMG	2	519	36/55	0.71	0.16	108,148,158,160	0
22	LMG	4	321	13/55	0.73	0.15	159,168,171,172	0
19	CLA	J	1105	50/65	0.75	0.17	113,150,159,164	0
21	LHG	B	843	49/49	0.76	0.22	104,125,175,186	0
19	CLA	3	312	48/65	0.76	0.15	176,192,204,209	0
21	LHG	1	520	42/49	0.76	0.22	86,136,161,165	0
22	LMG	B	844	35/55	0.76	0.14	59,114,124,125	0
26	DGD	G	207	47/66	0.76	0.22	162,204,212,214	0
19	CLA	K	1002	60/65	0.77	0.16	119,151,162,167	0
19	CLA	3	311	41/65	0.78	0.19	184,202,209,211	0
24	LMT	B	855	31/35	0.78	0.14	117,141,151,154	0
24	LMT	B	846	35/35	0.79	0.14	153,194,203,209	0
22	LMG	J	1104	34/55	0.79	0.14	97,129,137,141	0
22	LMG	F	305	36/55	0.79	0.19	124,141,152,159	0
19	CLA	3	306	52/65	0.80	0.15	152,181,190,195	0
19	CLA	1	513	65/65	0.81	0.21	129,151,169,170	0
24	LMT	B	847	32/35	0.82	0.13	103,134,152,153	0
20	CHL	4	317	43/66	0.82	0.12	116,136,152,161	0
18	BCR	K	1005	40/40	0.82	0.19	145,157,181,184	0
22	LMG	1	519	13/55	0.83	0.13	131,138,144,147	0
22	LMG	G	206	50/55	0.83	0.20	123,149,163,164	0
22	LMG	2	518	25/55	0.83	0.16	110,121,138,142	0
24	LMT	4	320	35/35	0.83	0.15	98,133,152,158	0
19	CLA	3	310	50/65	0.84	0.14	135,159,166,168	0
18	BCR	L	307	40/40	0.84	0.18	126,138,165,167	0
19	CLA	K	1001	45/65	0.85	0.15	148,174,184,185	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	LMT	G	208	35/35	0.85	0.14	101,158,170,173	0
18	BCR	3	304	40/40	0.85	0.23	144,156,180,182	0
19	CLA	1	510	46/65	0.85	0.15	105,140,169,174	0
18	BCR	2	503	40/40	0.85	0.25	134,153,166,170	0
19	CLA	L	303	50/65	0.85	0.13	105,127,146,157	0
20	CHL	4	313	47/66	0.86	0.12	80,110,137,147	0
20	CHL	2	512	47/66	0.86	0.11	101,123,140,175	0
22	LMG	4	322	45/55	0.87	0.20	87,126,133,138	0
21	LHG	1	517	49/49	0.87	0.18	96,108,141,145	0
19	CLA	L	305	50/65	0.87	0.13	88,104,132,135	0
19	CLA	G	204	65/65	0.87	0.16	91,119,134,140	0
19	CLA	A	816	46/65	0.88	0.12	109,126,142,148	0
19	CLA	A	842	60/65	0.88	0.11	94,119,157,159	0
19	CLA	1	509	50/65	0.88	0.13	130,145,153,162	0
19	CLA	1	516	60/65	0.88	0.13	79,105,143,146	0
17	LUT	3	301	42/42	0.88	0.15	146,159,165,171	0
22	LMG	1	518	46/55	0.88	0.17	81,129,140,144	0
19	CLA	3	313	60/65	0.88	0.15	108,137,146,156	0
19	CLA	A	835	55/65	0.89	0.13	107,124,142,152	0
18	BCR	G	205	40/40	0.89	0.17	93,120,154,157	0
20	CHL	2	516	56/66	0.89	0.12	102,129,157,164	0
19	CLA	3	305	55/65	0.89	0.11	154,168,178,185	0
22	LMG	F	304	47/55	0.89	0.11	89,102,119,134	0
18	BCR	3	303	40/40	0.89	0.18	115,133,145,150	0
18	BCR	A	850	40/40	0.89	0.14	61,78,127,129	0
30	ZEX	F	301	42/42	0.89	0.17	84,105,116,122	0
19	CLA	A	823	60/65	0.90	0.12	106,123,152,160	0
19	CLA	1	504	65/65	0.90	0.14	118,136,149,153	0
19	CLA	4	309	50/65	0.90	0.13	109,120,137,143	0
20	CHL	4	316	61/66	0.90	0.14	104,118,136,142	0
19	CLA	B	831	60/65	0.90	0.14	48,59,97,100	0
19	CLA	F	303	65/65	0.90	0.13	63,81,109,121	0
19	CLA	G	201	65/65	0.90	0.14	75,90,116,123	0
22	LMG	J	1103	30/55	0.90	0.11	72,82,102,102	0
25	CA	3	319	1/1	0.90	0.10	118,118,118,118	0
21	LHG	A	845	40/49	0.90	0.14	78,102,116,124	0
19	CLA	G	203	46/65	0.90	0.09	125,139,150,154	0
18	BCR	B	851	40/40	0.90	0.20	84,110,134,137	0
19	CLA	1	515	45/65	0.91	0.13	149,166,184,188	0
19	CLA	B	808	65/65	0.91	0.13	73,91,117,121	0
17	LUT	J	1109	42/42	0.91	0.12	62,88,104,109	0
18	BCR	I	102	40/40	0.91	0.18	70,86,109,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	LUT	1	502	42/42	0.91	0.19	79,114,132,135	0
19	CLA	A	817	65/65	0.91	0.15	104,135,150,154	0
19	CLA	1	511	46/65	0.91	0.16	99,129,147,160	0
26	DGD	4	319	51/66	0.91	0.16	97,112,143,149	0
19	CLA	A	831	65/65	0.91	0.13	66,93,128,132	0
26	DGD	B	854	61/66	0.91	0.16	53,79,99,120	0
20	CHL	3	314	47/66	0.91	0.11	134,140,156,163	0
17	LUT	3	302	42/42	0.91	0.18	120,141,154,161	0
19	CLA	A	838	65/65	0.92	0.14	63,80,126,130	0
18	BCR	A	856	40/40	0.92	0.20	137,144,158,161	0
20	CHL	1	512	47/66	0.92	0.11	108,140,147,152	0
20	CHL	1	514	61/66	0.92	0.13	114,131,139,162	0
19	CLA	B	805	65/65	0.92	0.12	80,93,126,135	0
19	CLA	1	505	46/65	0.92	0.11	111,135,149,157	0
19	CLA	B	816	55/65	0.92	0.12	92,110,131,141	0
17	LUT	4	302	42/42	0.92	0.14	90,106,118,128	0
18	BCR	L	306	40/40	0.92	0.13	99,119,127,132	0
28	SF4	C	102	8/8	0.92	0.16	67,106,137,151	0
18	BCR	A	851	40/40	0.92	0.17	63,90,106,108	0
19	CLA	4	310	60/65	0.93	0.13	104,115,132,138	0
19	CLA	4	318	65/65	0.93	0.14	87,106,128,131	0
19	CLA	A	804	65/65	0.93	0.13	49,65,110,119	0
19	CLA	A	813	65/65	0.93	0.14	67,89,108,109	0
19	CLA	A	814	65/65	0.93	0.13	89,113,129,135	0
18	BCR	B	852	40/40	0.93	0.13	50,66,83,89	0
19	CLA	2	509	50/65	0.93	0.11	99,120,140,143	0
19	CLA	2	510	60/65	0.93	0.12	108,128,143,151	0
19	CLA	2	511	50/65	0.93	0.12	112,133,142,146	0
20	CHL	2	526	66/66	0.93	0.14	97,120,138,144	0
19	CLA	2	514	55/65	0.93	0.12	81,94,116,121	0
23	XAT	2	502	44/44	0.93	0.15	82,99,114,118	0
23	XAT	4	303	44/44	0.93	0.12	72,92,116,128	0
19	CLA	A	836	51/65	0.93	0.12	66,82,95,110	0
18	BCR	B	853	40/40	0.93	0.13	50,64,74,78	0
18	BCR	F	306	40/40	0.93	0.10	48,64,72,77	0
19	CLA	3	307	55/65	0.93	0.13	154,177,191,198	0
19	CLA	3	309	55/65	0.93	0.13	97,123,131,135	0
21	LHG	2	517	35/49	0.93	0.15	116,124,130,132	0
17	LUT	2	501	42/42	0.93	0.16	108,118,128,134	0
19	CLA	B	822	65/65	0.93	0.14	70,89,119,127	0
18	BCR	B	849	40/40	0.93	0.17	90,98,109,114	0
19	CLA	B	840	65/65	0.93	0.11	52,80,91,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	BCR	J	1108	40/40	0.93	0.13	52,64,79,82	0
18	BCR	B	850	40/40	0.93	0.18	69,89,130,131	0
19	CLA	3	315	50/65	0.93	0.12	109,125,133,147	0
19	CLA	3	316	46/65	0.93	0.10	142,149,159,163	0
19	CLA	3	317	46/65	0.93	0.12	91,105,132,138	0
26	DGD	J	1106	58/66	0.93	0.11	52,80,117,120	0
19	CLA	4	305	50/65	0.93	0.12	107,126,138,142	0
18	BCR	A	848	40/40	0.93	0.17	75,105,142,143	0
19	CLA	A	821	65/65	0.94	0.12	60,86,95,101	0
19	CLA	A	822	60/65	0.94	0.11	94,114,155,161	0
18	BCR	I	101	40/40	0.94	0.13	72,86,105,107	0
19	CLA	A	827	65/65	0.94	0.13	69,87,107,114	0
18	BCR	1	503	19/40	0.94	0.13	121,134,143,146	0
19	CLA	A	832	65/65	0.94	0.13	62,81,91,98	0
19	CLA	A	834	65/65	0.94	0.11	79,98,117,132	0
18	BCR	A	849	40/40	0.94	0.17	69,91,119,124	0
19	CLA	4	311	46/65	0.94	0.10	109,121,132,139	0
20	CHL	1	521	56/66	0.94	0.13	100,112,123,126	0
19	CLA	4	315	65/65	0.94	0.13	74,96,118,123	0
17	LUT	1	501	42/42	0.94	0.13	105,125,144,146	0
19	CLA	1	507	65/65	0.94	0.12	77,101,114,120	0
19	CLA	A	807	60/65	0.94	0.10	67,88,115,118	0
19	CLA	B	815	65/65	0.94	0.13	84,97,119,123	0
19	CLA	A	811	65/65	0.94	0.10	56,73,87,108	0
19	CLA	B	817	60/65	0.94	0.12	87,97,110,129	0
19	CLA	B	821	46/65	0.94	0.10	86,100,118,122	0
19	CLA	A	812	55/65	0.94	0.13	80,104,117,123	0
19	CLA	B	825	65/65	0.94	0.11	48,64,93,98	0
19	CLA	B	827	65/65	0.94	0.15	54,77,98,103	0
19	CLA	B	830	65/65	0.94	0.11	50,63,97,110	0
19	CLA	1	508	65/65	0.94	0.13	89,115,123,137	0
19	CLA	B	833	60/65	0.94	0.10	59,75,106,107	0
19	CLA	B	839	65/65	0.94	0.13	54,70,104,119	0
19	CLA	2	504	60/65	0.94	0.11	99,111,133,136	0
19	CLA	A	815	45/65	0.94	0.11	108,124,153,163	0
19	CLA	3	308	65/65	0.94	0.14	118,129,139,143	0
19	CLA	4	304	60/65	0.94	0.12	99,113,137,139	0
27	CL0	A	801	65/65	0.94	0.11	48,59,71,80	0
19	CLA	A	818	56/65	0.94	0.12	79,107,125,133	0
19	CLA	A	820	50/65	0.94	0.13	88,110,136,137	0
19	CLA	4	306	65/65	0.95	0.12	74,105,121,130	0
19	CLA	B	834	55/65	0.95	0.09	66,88,118,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	CLA	B	835	55/65	0.95	0.11	54,68,96,100	0
19	CLA	B	836	65/65	0.95	0.09	48,61,68,73	0
19	CLA	A	833	65/65	0.95	0.11	67,85,101,113	0
19	CLA	4	308	60/65	0.95	0.11	64,85,96,102	0
19	CLA	1	506	55/65	0.95	0.12	89,115,132,141	0
18	BCR	L	302	40/40	0.95	0.12	77,84,97,97	0
19	CLA	G	202	55/65	0.95	0.09	109,131,152,153	0
19	CLA	A	837	65/65	0.95	0.11	69,88,110,121	0
18	BCR	4	301	40/40	0.95	0.14	105,124,131,136	0
18	BCR	B	856	40/40	0.95	0.11	42,57,69,76	0
19	CLA	J	1102	45/65	0.95	0.09	52,65,80,89	0
19	CLA	A	854	65/65	0.95	0.12	44,57,76,89	0
19	CLA	A	855	65/65	0.95	0.11	63,77,98,107	0
19	CLA	B	803	65/65	0.95	0.11	46,59,68,71	0
19	CLA	B	804	65/65	0.95	0.10	48,62,82,85	0
19	CLA	2	505	52/65	0.95	0.11	116,134,141,144	0
19	CLA	L	301	55/65	0.95	0.11	74,85,116,125	0
19	CLA	B	807	65/65	0.95	0.10	54,72,82,95	0
19	CLA	L	304	60/65	0.95	0.10	79,93,113,122	0
19	CLA	2	508	55/65	0.95	0.10	74,87,111,116	0
19	CLA	B	810	65/65	0.95	0.11	70,84,102,108	0
19	CLA	B	811	65/65	0.95	0.11	71,95,111,114	0
19	CLA	B	812	60/65	0.95	0.10	79,100,117,126	0
19	CLA	A	805	65/65	0.95	0.11	54,71,89,93	0
20	CHL	2	513	48/66	0.95	0.11	91,105,114,141	0
20	CHL	2	515	46/66	0.95	0.09	113,121,131,142	0
18	BCR	B	802	40/40	0.95	0.13	57,71,85,94	0
19	CLA	A	809	65/65	0.95	0.11	51,65,99,102	0
19	CLA	B	818	65/65	0.95	0.12	66,82,104,109	0
19	CLA	A	824	65/65	0.95	0.12	67,85,106,124	0
20	CHL	4	314	51/66	0.95	0.13	89,114,129,133	0
19	CLA	A	826	55/65	0.95	0.11	59,71,96,109	0
19	CLA	A	810	50/65	0.95	0.11	78,96,106,121	0
19	CLA	A	828	65/65	0.95	0.12	53,67,78,88	0
19	CLA	B	828	65/65	0.95	0.12	60,71,91,103	0
19	CLA	B	829	65/65	0.95	0.12	50,67,92,100	0
19	CLA	A	829	65/65	0.95	0.12	60,75,86,95	0
28	SF4	A	843	8/8	0.95	0.14	45,78,104,173	0
21	LHG	B	842	21/49	0.95	0.09	69,92,102,116	0
18	BCR	A	852	40/40	0.95	0.12	45,55,71,75	0
19	CLA	A	825	65/65	0.96	0.11	64,79,85,89	0
19	CLA	A	803	65/65	0.96	0.10	49,64,79,83	0

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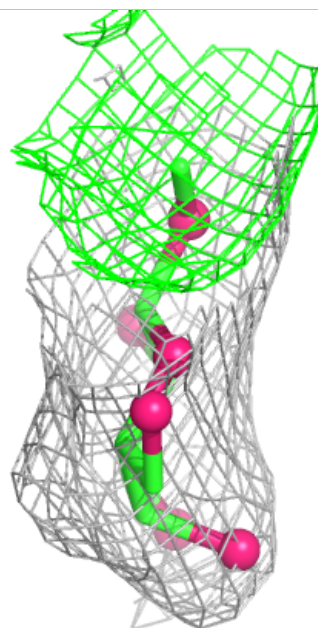
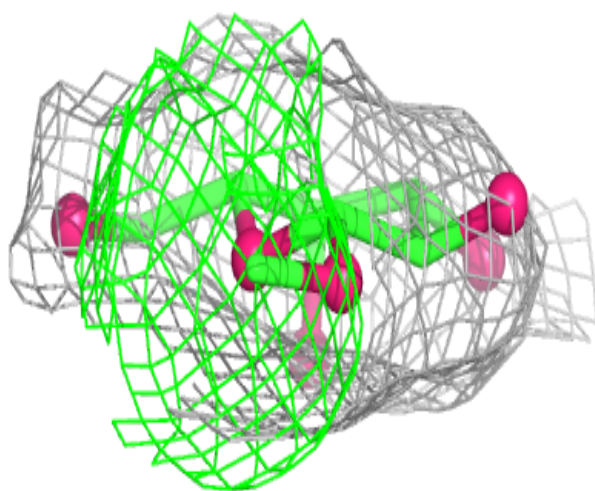
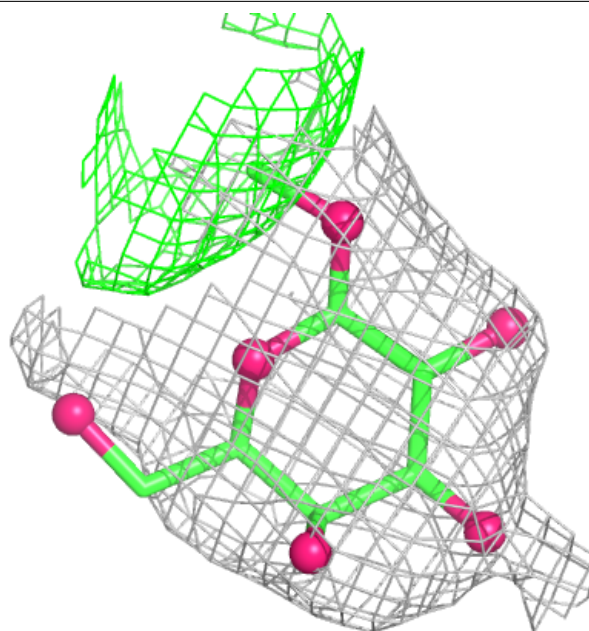
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	CLA	B	809	65/65	0.96	0.11	66,82,95,126	0
21	LHG	A	853	49/49	0.96	0.10	49,60,72,79	0
19	CLA	2	506	65/65	0.96	0.11	88,121,139,150	0
19	CLA	A	819	65/65	0.96	0.13	77,88,99,104	0
19	CLA	B	832	58/65	0.96	0.08	48,60,76,78	0
19	CLA	A	840	65/65	0.96	0.10	43,58,88,96	0
19	CLA	B	813	46/65	0.96	0.08	84,95,120,135	0
19	CLA	4	312	50/65	0.96	0.10	79,91,116,121	0
19	CLA	A	830	65/65	0.96	0.10	46,58,72,78	0
19	CLA	B	837	50/65	0.96	0.10	48,58,81,100	0
19	CLA	B	838	65/65	0.96	0.10	58,75,94,115	0
19	CLA	A	806	65/65	0.96	0.10	52,61,79,86	0
19	CLA	2	507	65/65	0.96	0.10	78,91,100,102	0
19	CLA	F	302	65/65	0.96	0.10	45,60,75,80	0
19	CLA	B	820	65/65	0.96	0.12	61,78,98,105	0
19	CLA	A	808	65/65	0.96	0.10	54,65,82,91	0
19	CLA	4	307	60/65	0.96	0.10	73,86,97,99	0
19	CLA	B	823	55/65	0.96	0.09	54,74,98,105	0
19	CLA	B	824	65/65	0.96	0.10	59,69,90,93	0
19	CLA	B	806	65/65	0.96	0.12	58,72,82,99	0
19	CLA	J	1101	65/65	0.96	0.09	48,64,87,101	0
29	PQN	B	841	33/33	0.96	0.10	49,64,82,85	0
19	CLA	B	826	65/65	0.96	0.10	52,69,80,84	0
19	CLA	A	839	65/65	0.97	0.08	44,53,62,70	0
25	CA	B	848	1/1	0.97	0.09	83,83,83,83	0
19	CLA	A	802	65/65	0.97	0.09	42,50,63,75	0
19	CLA	B	814	65/65	0.97	0.10	71,80,87,92	0
29	PQN	A	844	33/33	0.97	0.09	42,54,68,74	0
19	CLA	B	819	65/65	0.97	0.10	69,76,96,101	0
19	CLA	A	841	65/65	0.97	0.09	44,57,65,67	0
28	SF4	C	101	8/8	0.99	0.10	53,58,74,74	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

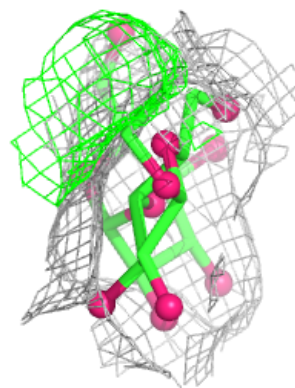
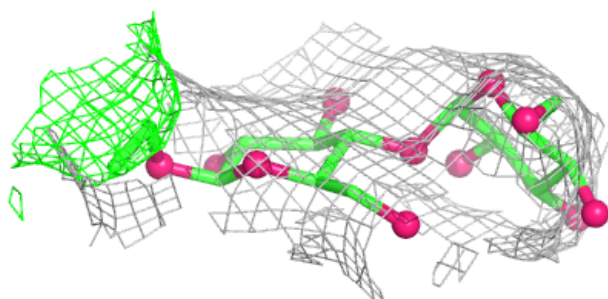
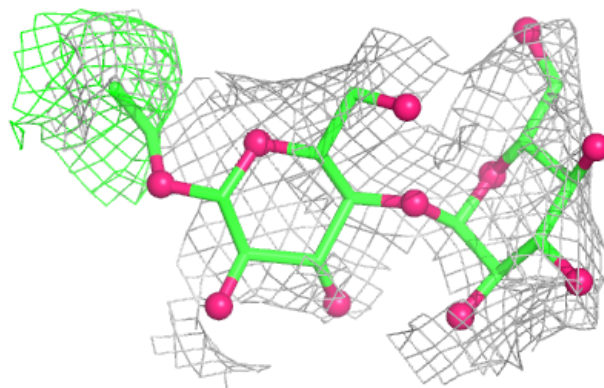
Electron density around LMG 2 520:

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

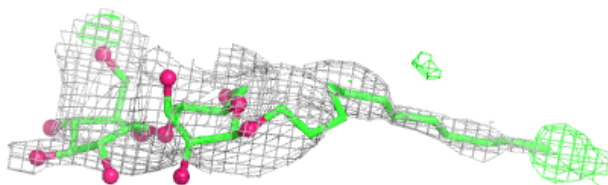


Electron density around LMT J 1107:

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

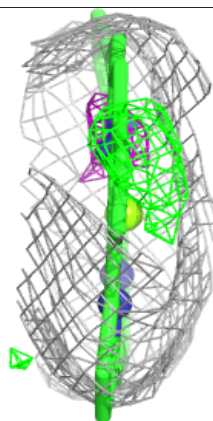
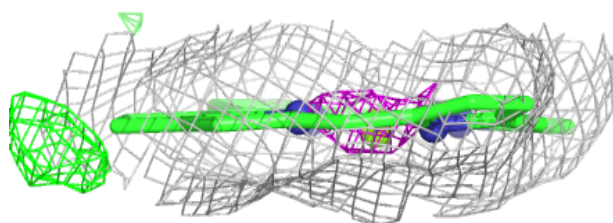
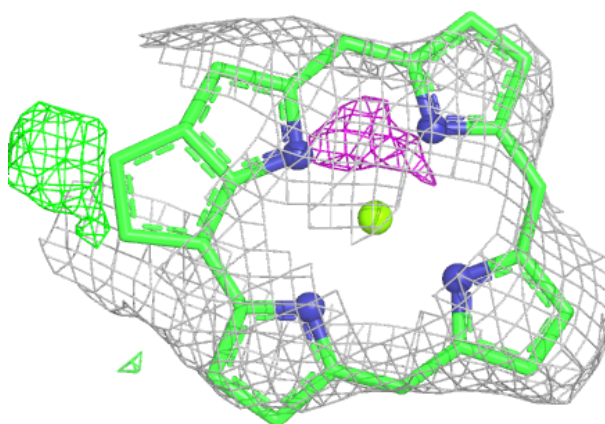
**Electron density around LMT 2 523:**

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

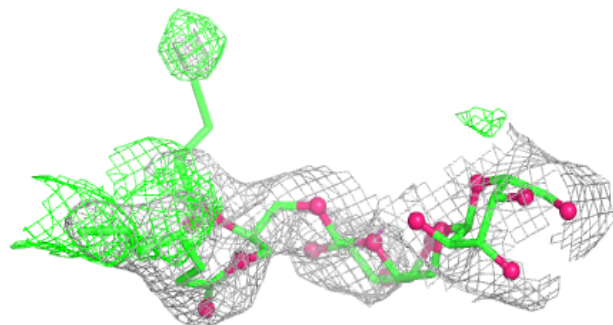
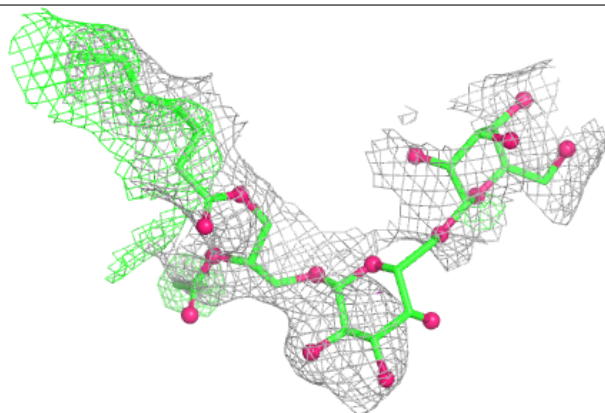


Electron density around CLA K 1004:

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

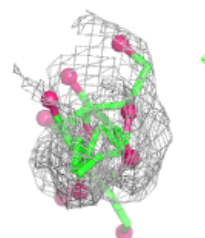
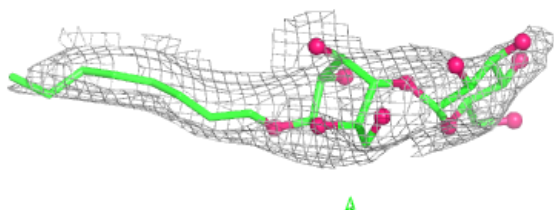
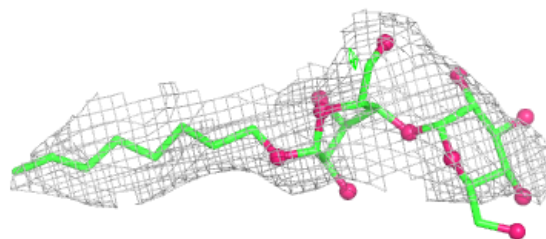
**Electron density around DGD B 801:**

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



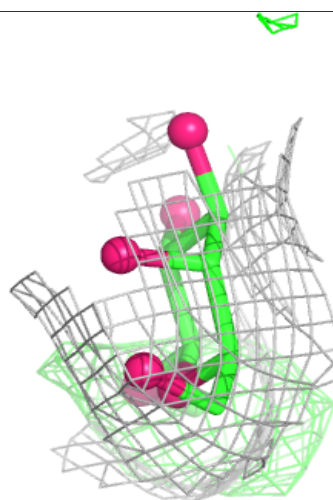
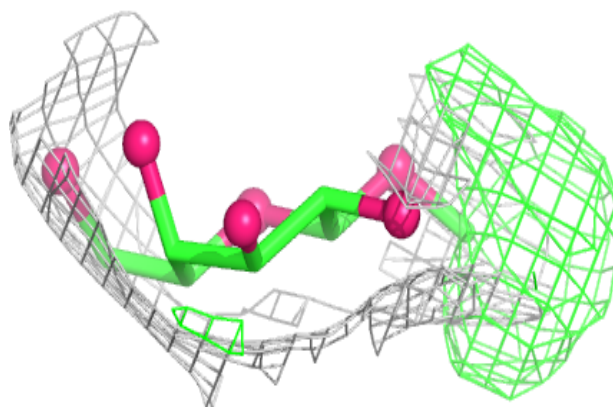
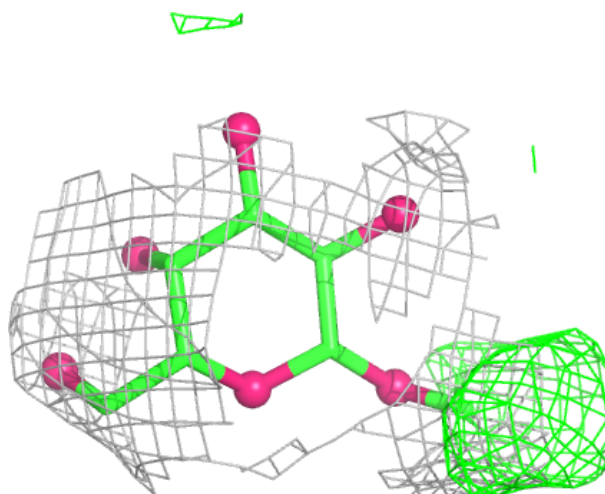
Electron density around LMT G 209:

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



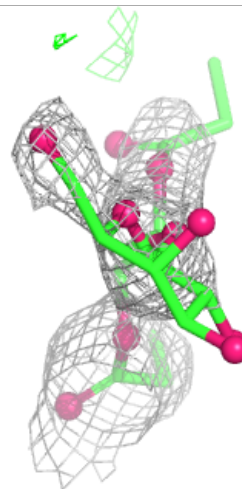
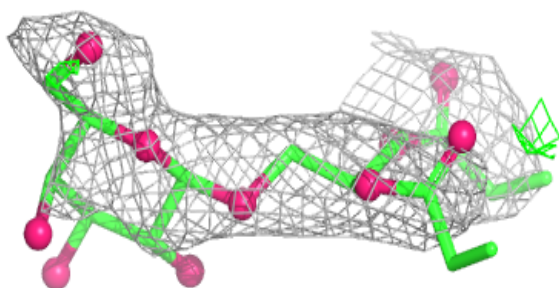
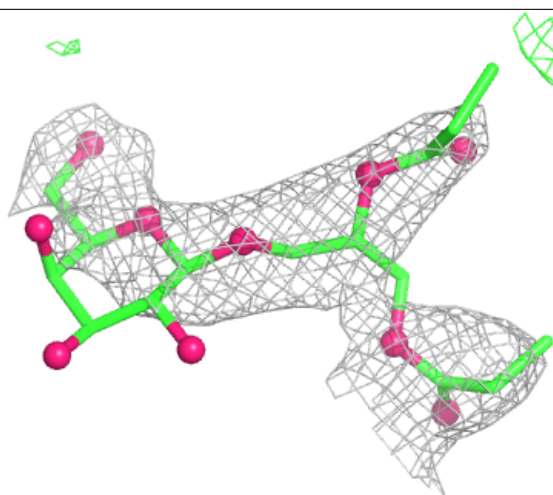
Electron density around LMG 2 522:

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



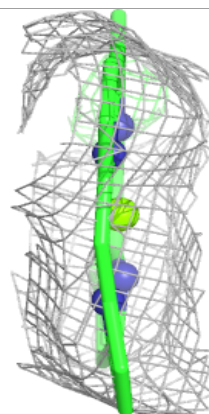
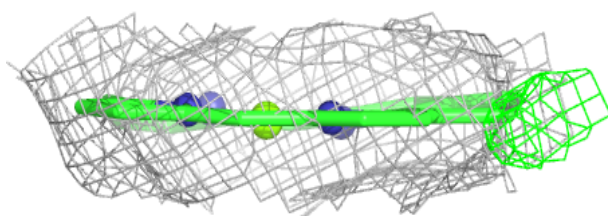
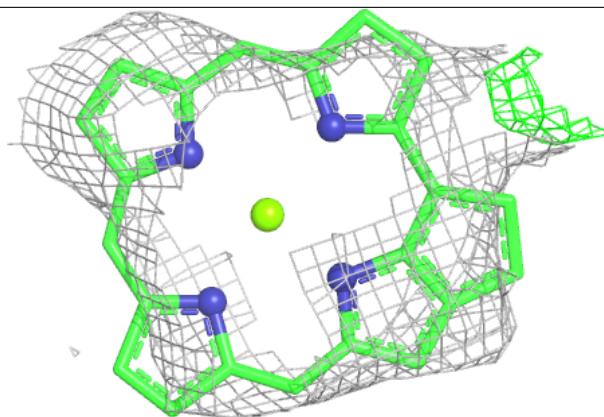
Electron density around LMG G 210:

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

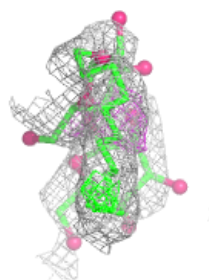
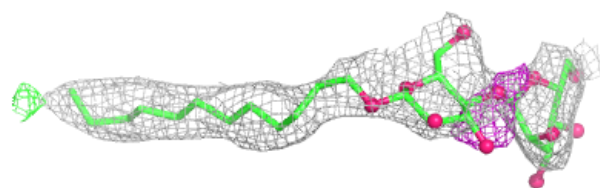
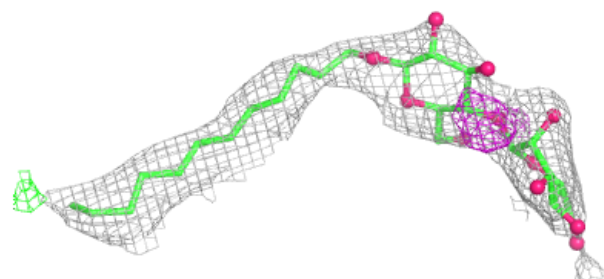


Electron density around CLA K 1003:

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

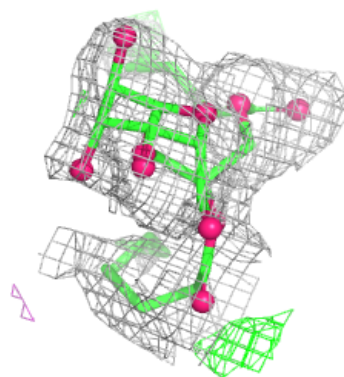
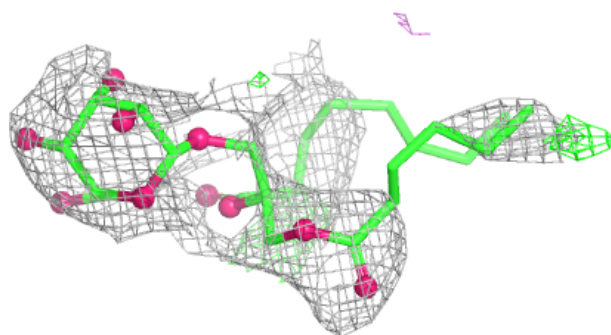
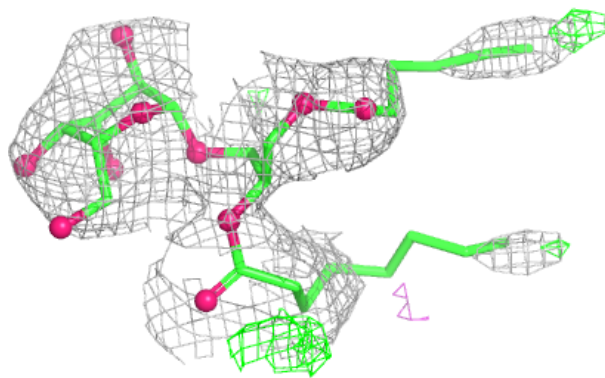
**Electron density around LMT A 846:**

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



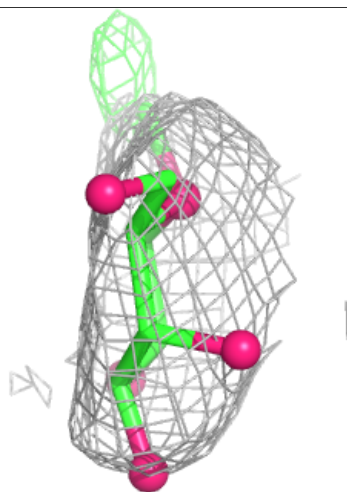
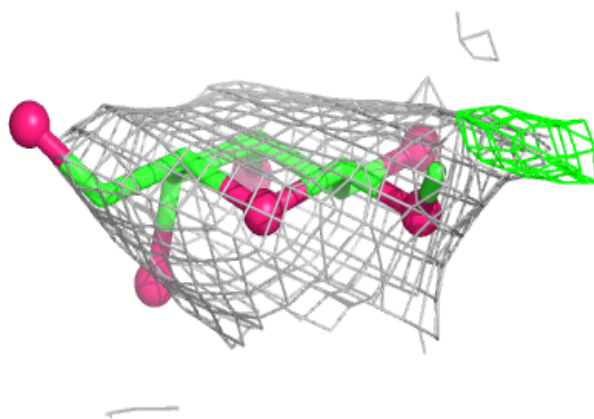
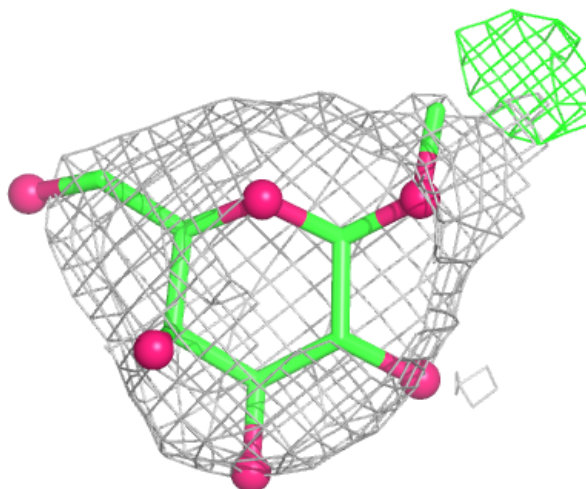
Electron density around LMG B 845:

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



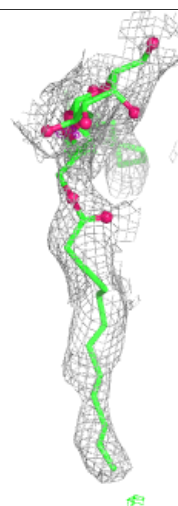
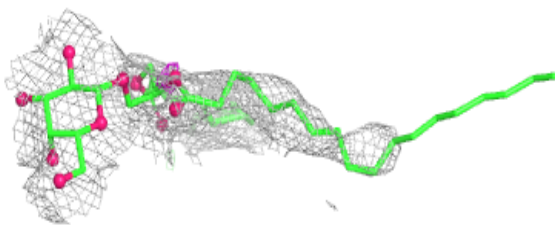
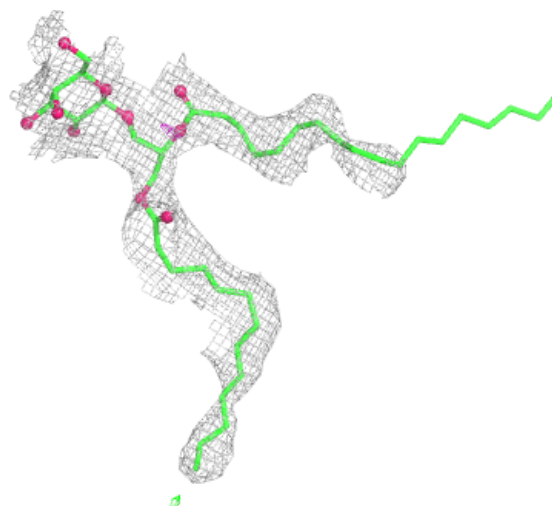
Electron density around LMG 2 524:

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



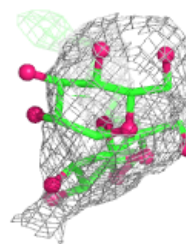
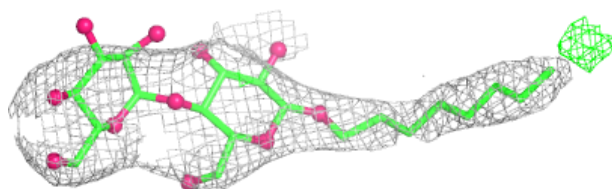
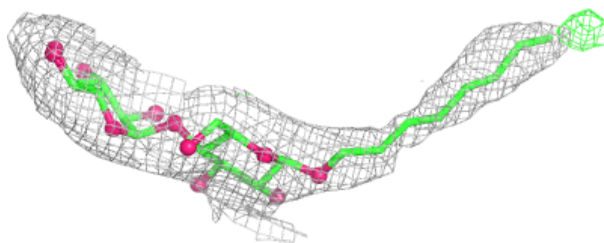
Electron density around LMG A 847:

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

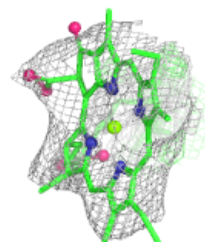
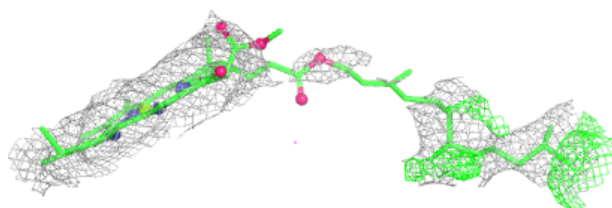
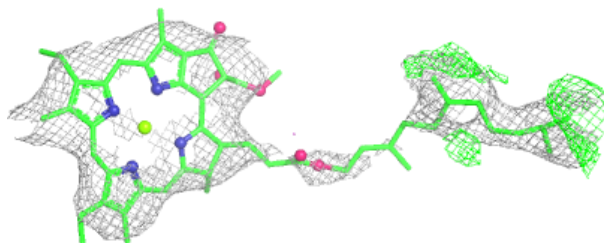


Electron density around LMT 3 318:

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

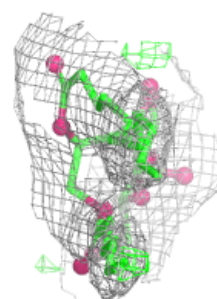
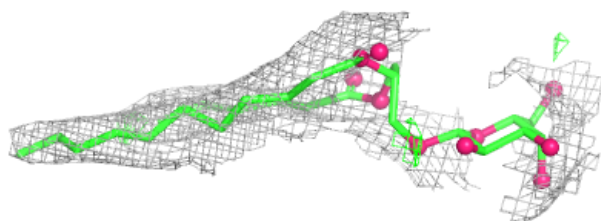
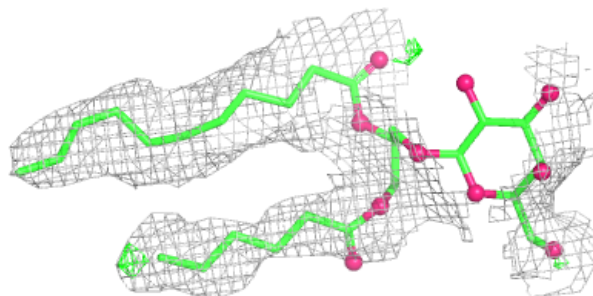
**Electron density around CLA H 1000:**

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



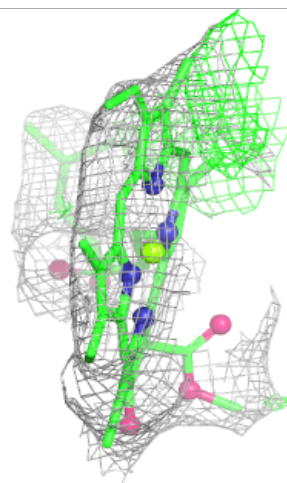
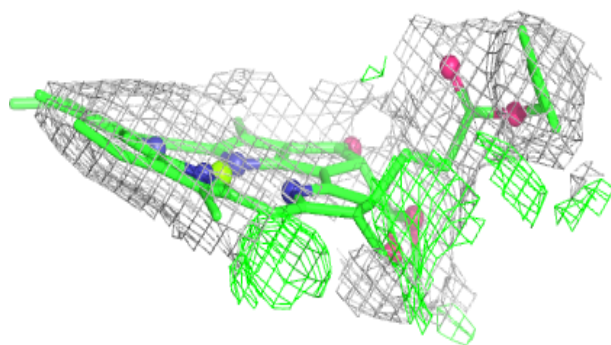
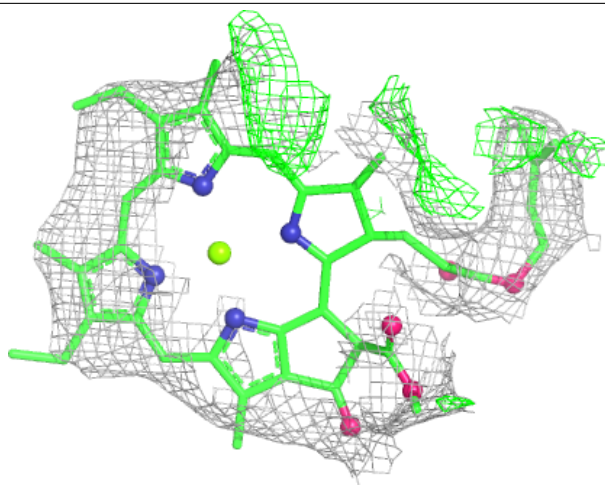
Electron density around LMG 2 519:

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



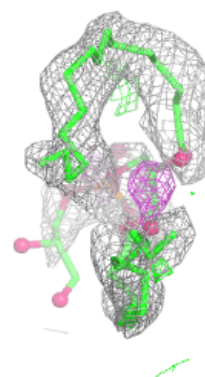
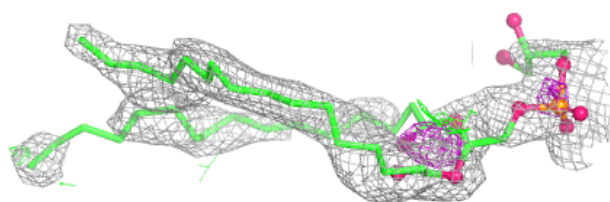
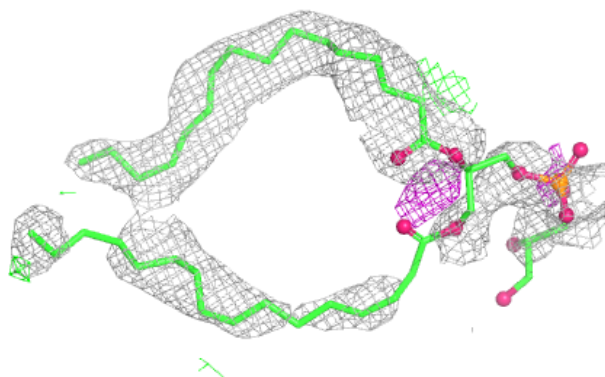
Electron density around CLA J 1105:

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



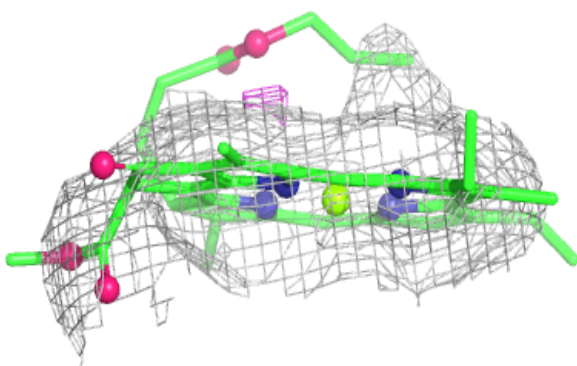
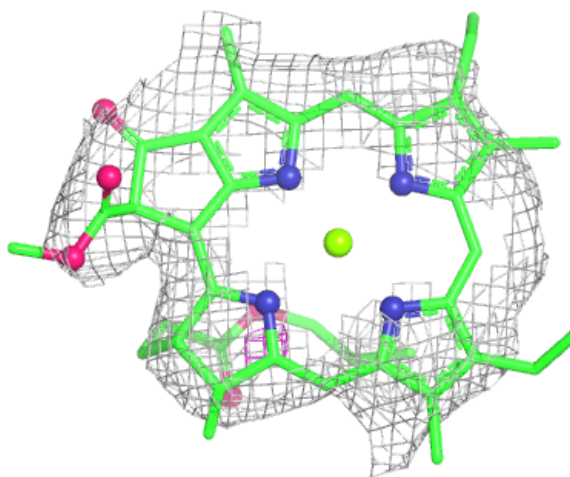
Electron density around LHG B 843:

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



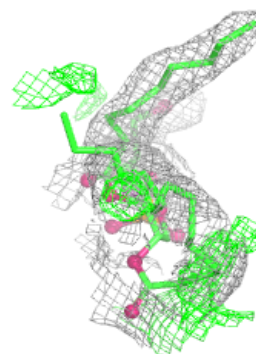
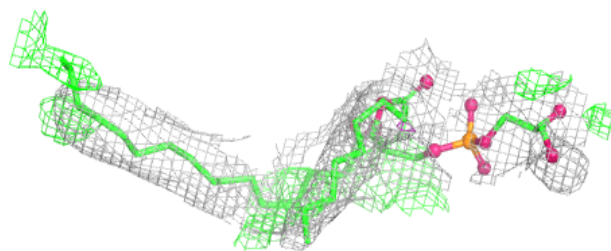
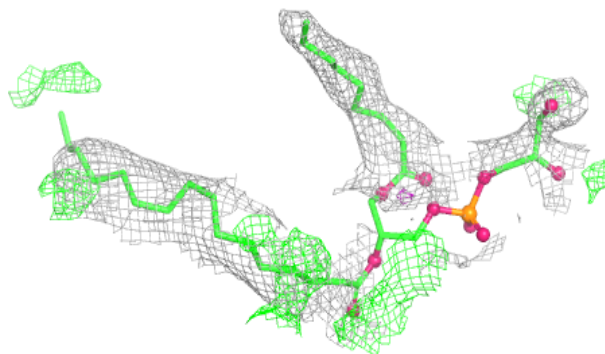
Electron density around CLA 3 312:

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

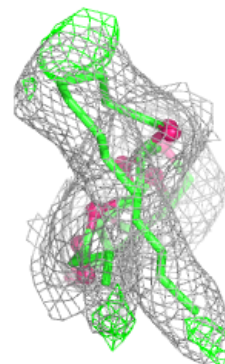
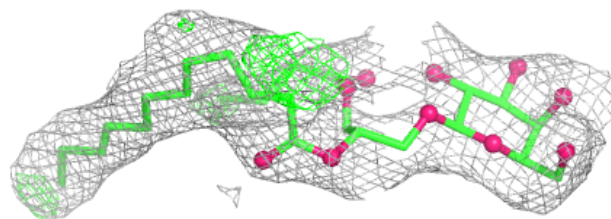
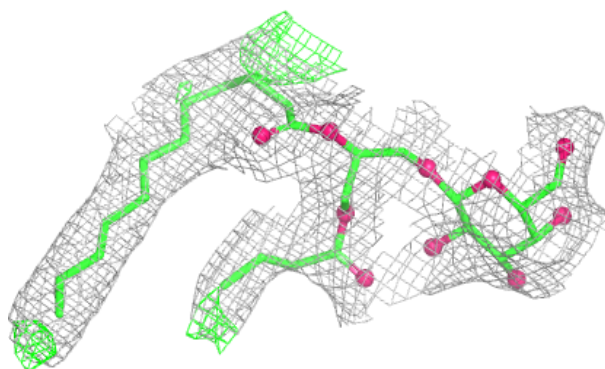


Electron density around LHG 1 520:

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

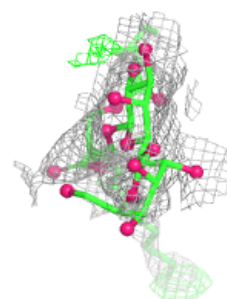
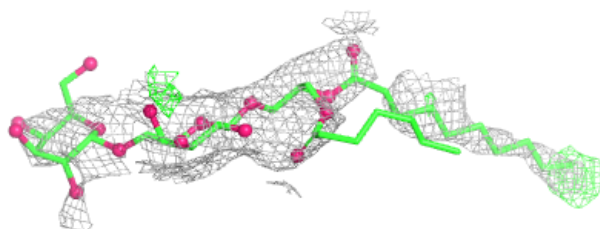
**Electron density around LMG B 844:**

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

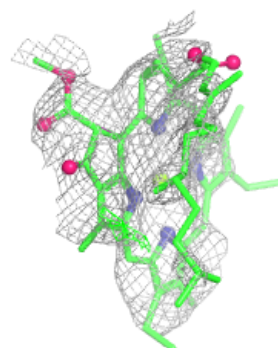
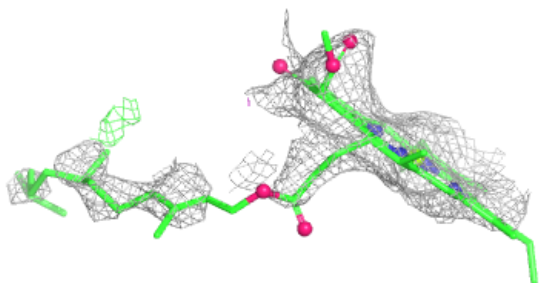
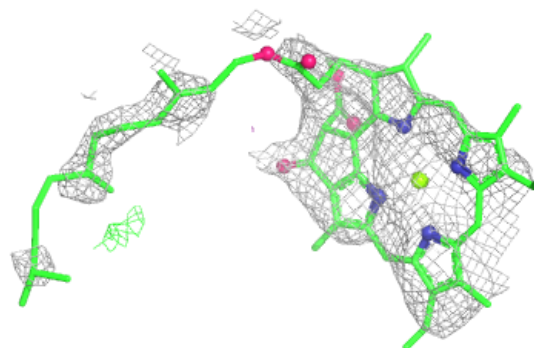


Electron density around DGD G 207:

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

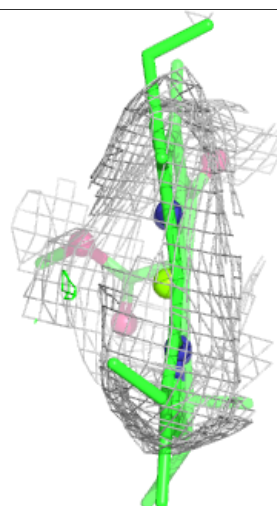
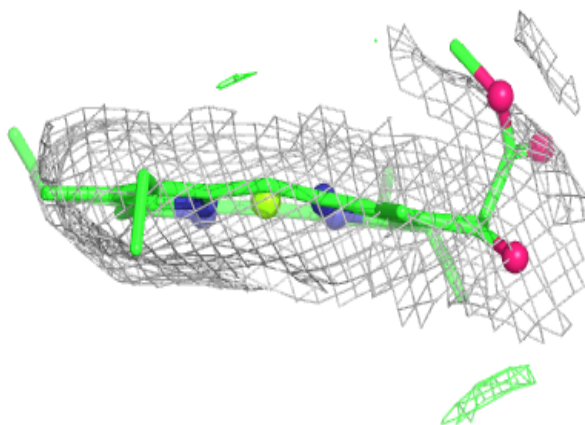
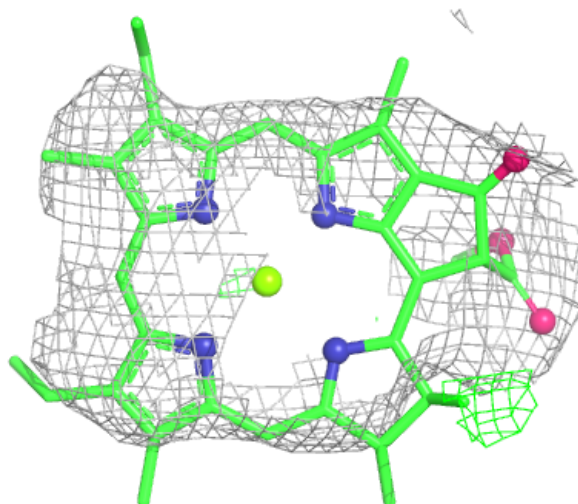
**Electron density around CLA K 1002:**

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



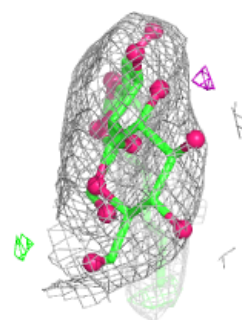
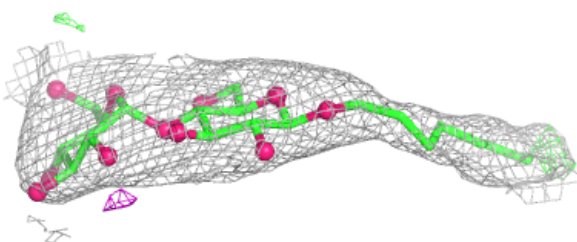
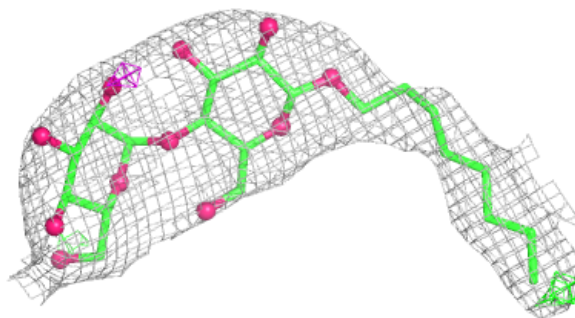
Electron density around CLA 3 311:

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

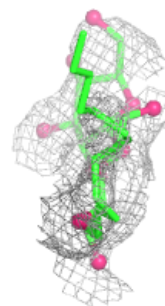
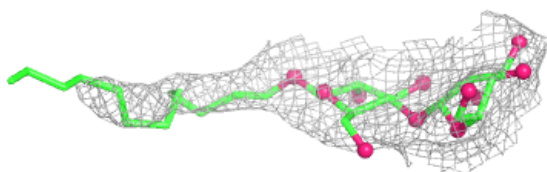
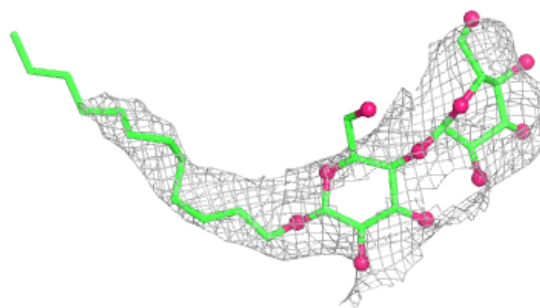


Electron density around LMT B 855:

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

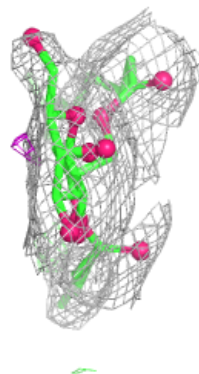
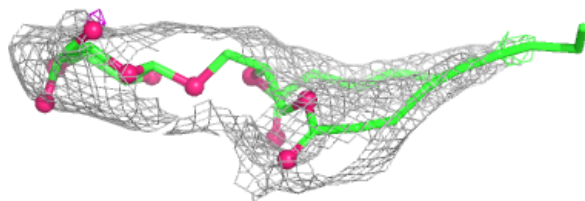
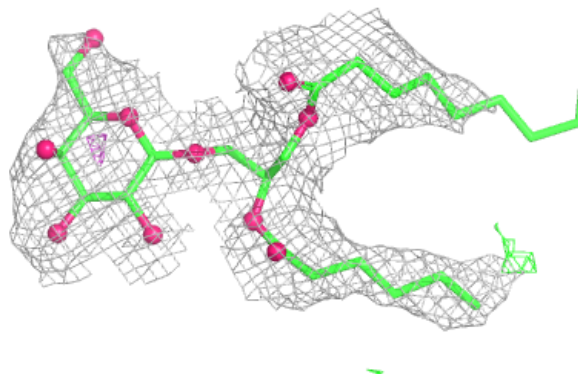
**Electron density around LMT B 846:**

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

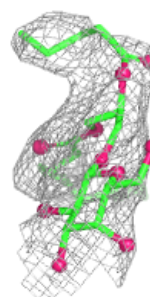
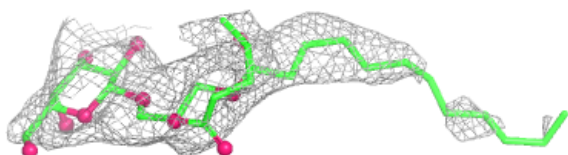


Electron density around LMG J 1104:

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

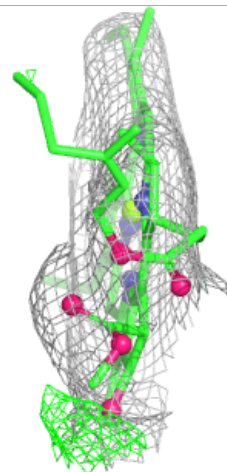
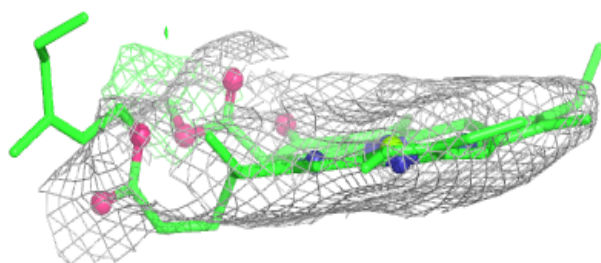
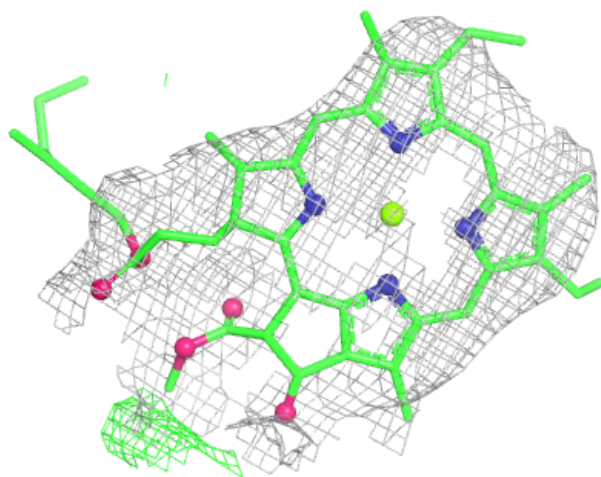
**Electron density around LMG F 305:**

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



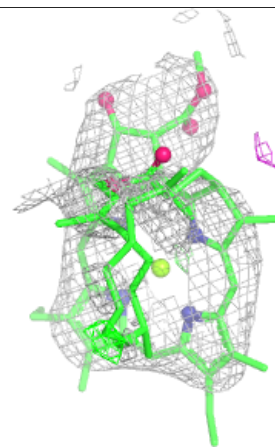
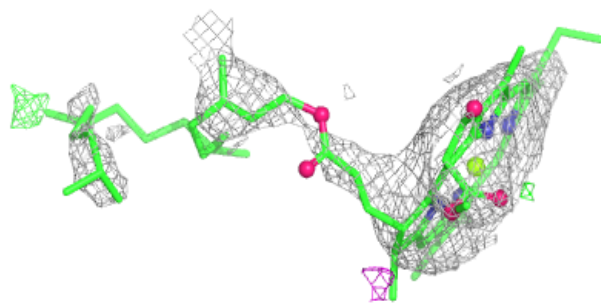
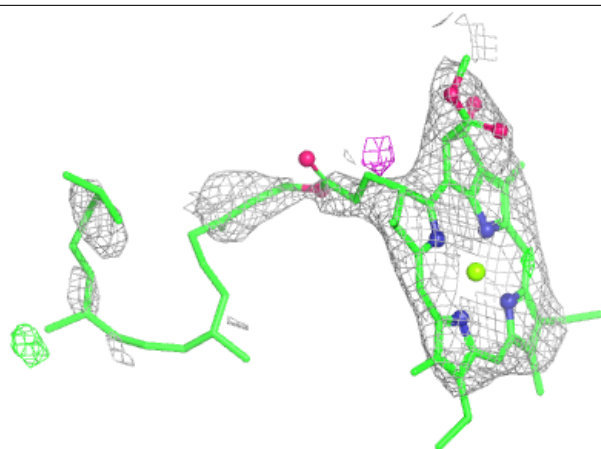
Electron density around CLA 3 306:

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



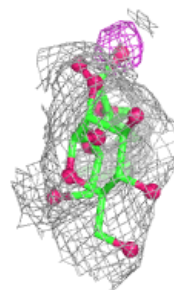
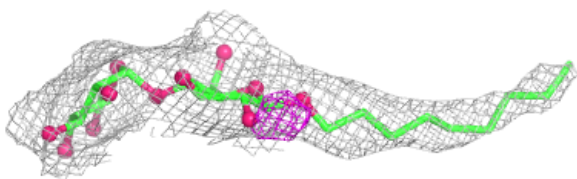
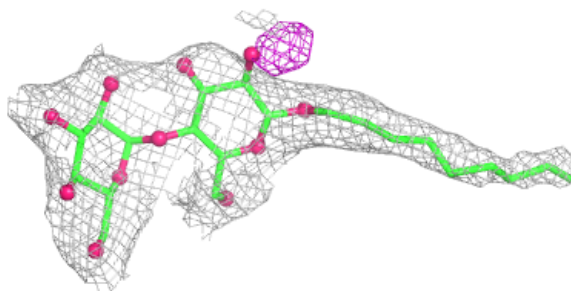
Electron density around CLA 1 513:

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



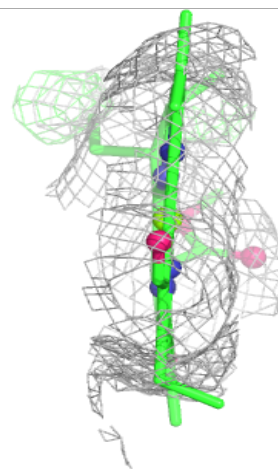
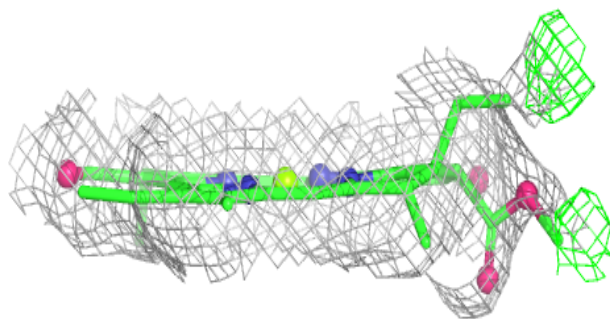
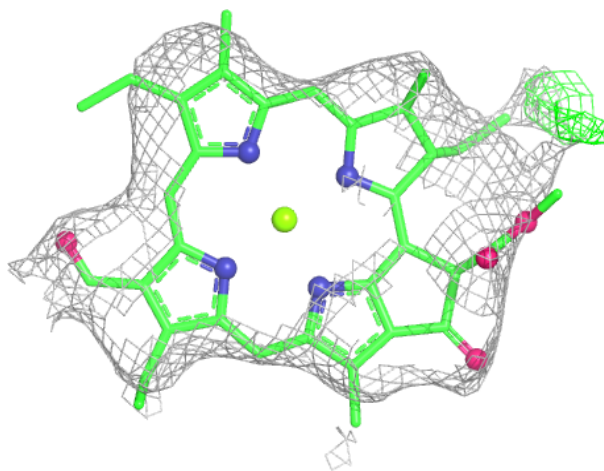
Electron density around LMT B 847:

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



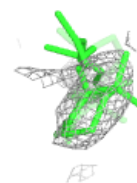
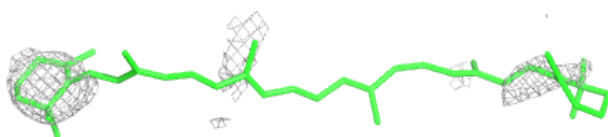
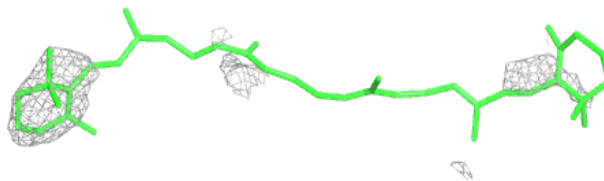
Electron density around CHL 4 317:

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



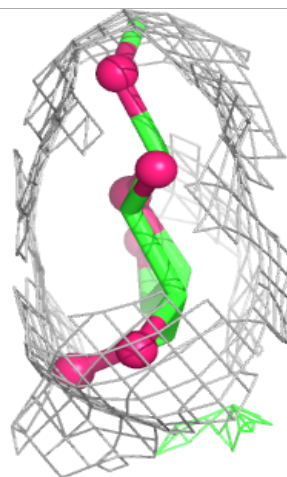
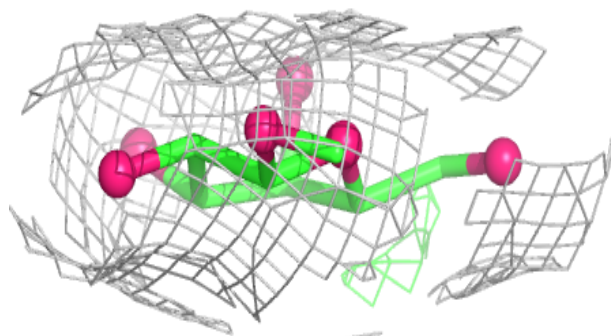
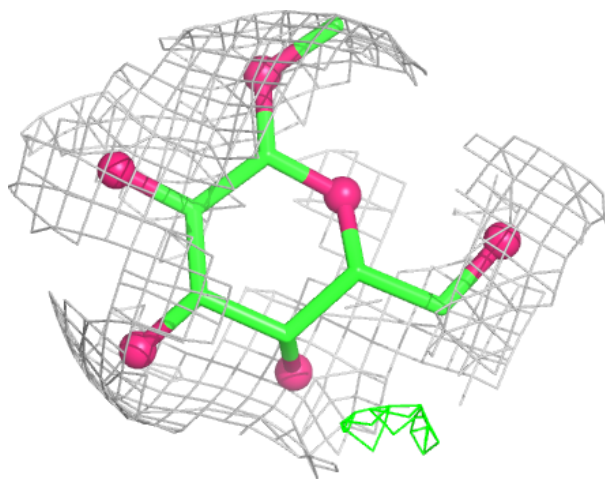
Electron density around BCR K 1005:

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



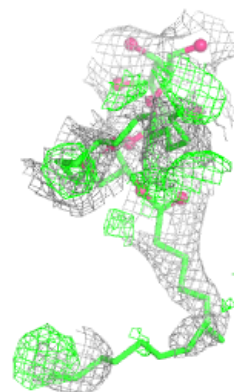
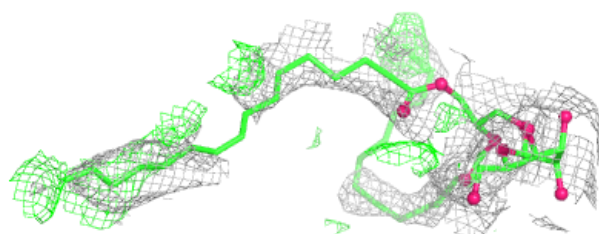
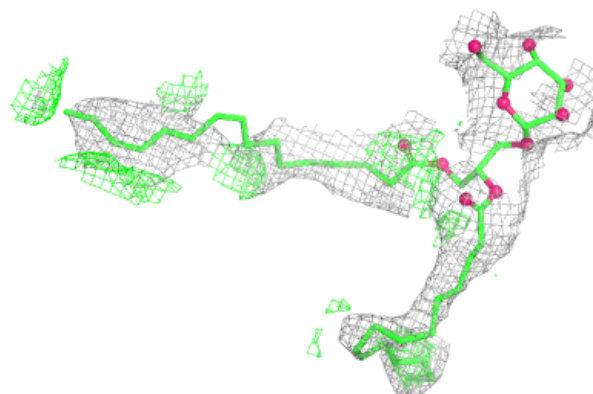
Electron density around LMG 1 519:

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

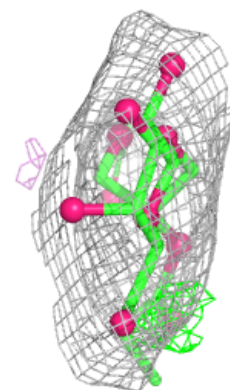
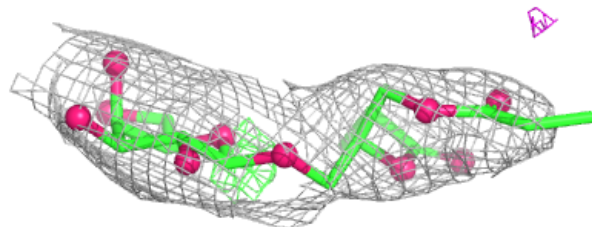
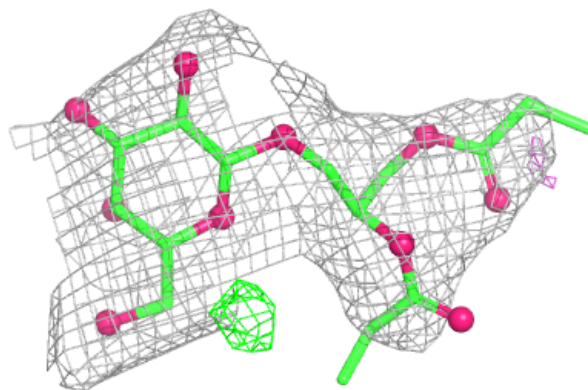


Electron density around LMG G 206:

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

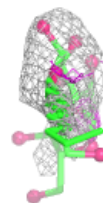
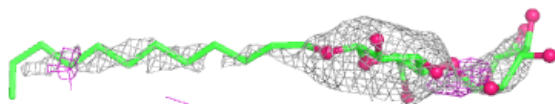
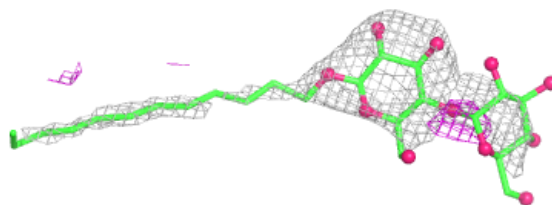
**Electron density around LMG 2 518:**

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



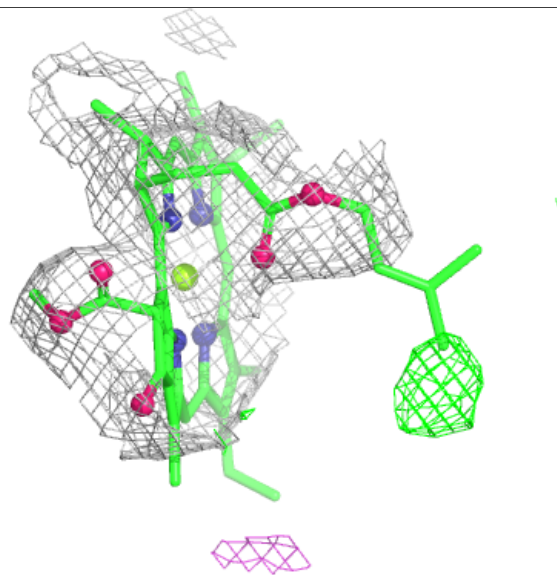
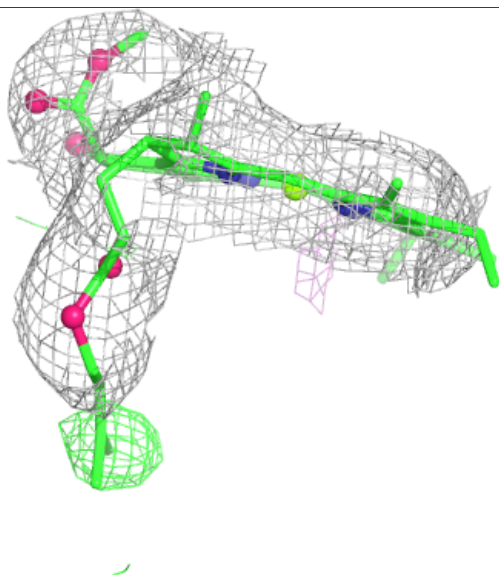
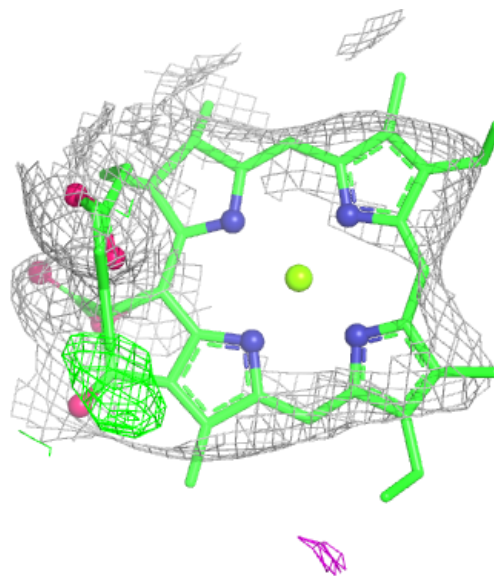
Electron density around LMT 4 320:

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



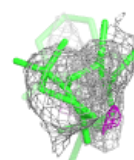
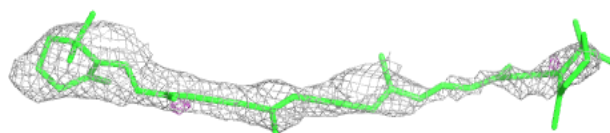
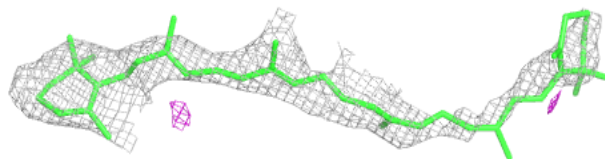
Electron density around CLA 3 310:

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



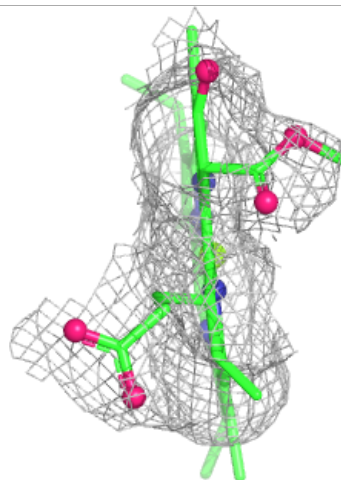
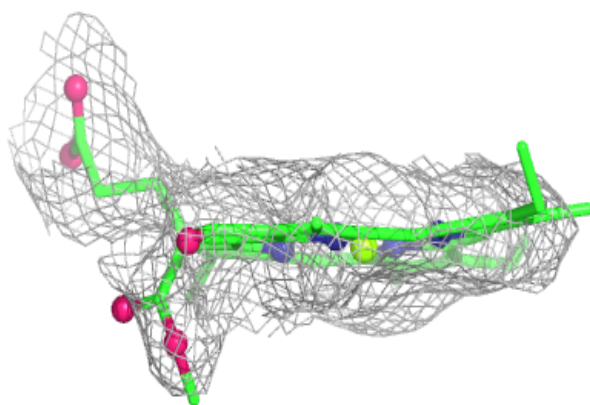
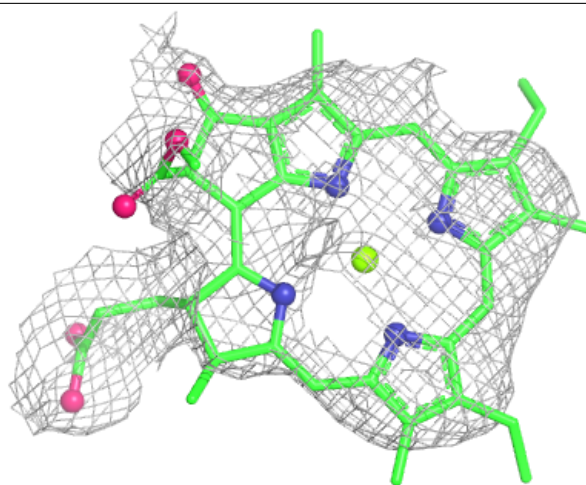
Electron density around BCR L 307:

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



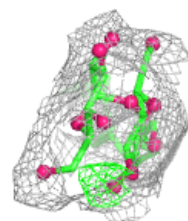
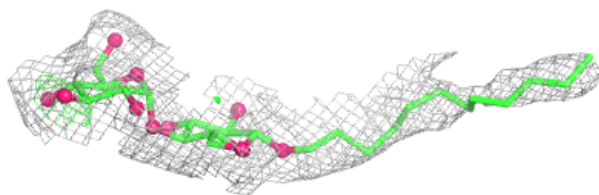
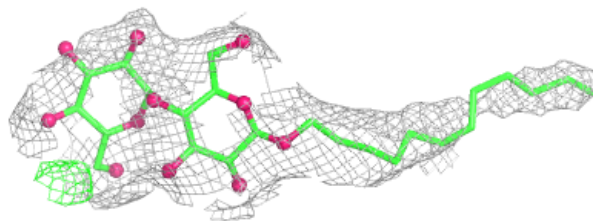
Electron density around CLA K 1001:

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

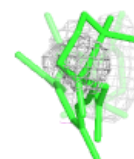
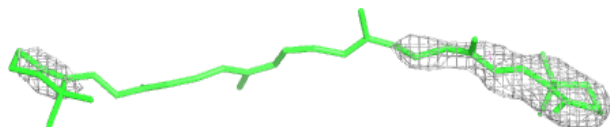
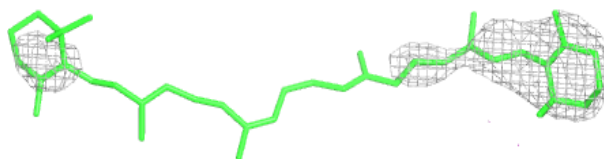


Electron density around LMT G 208:

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

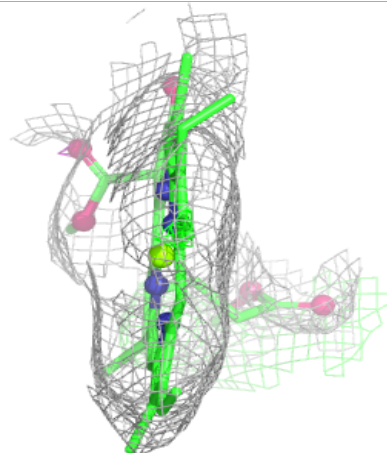
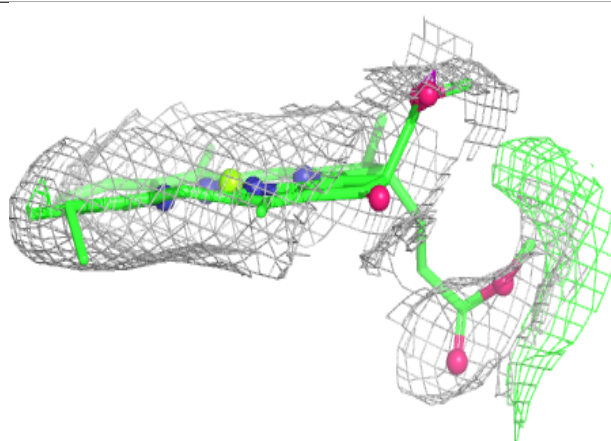
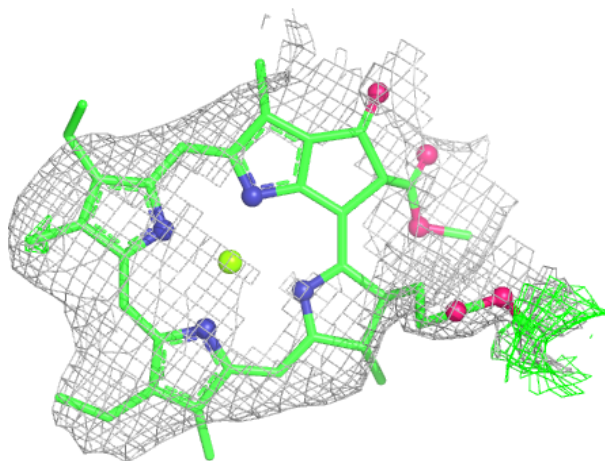
**Electron density around BCR 3 304:**

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



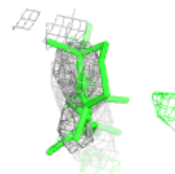
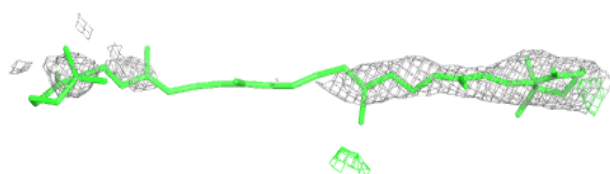
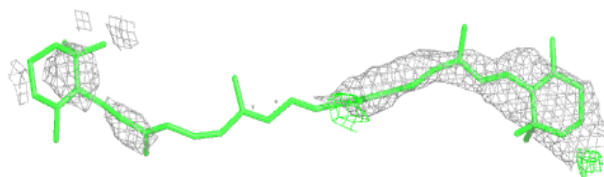
Electron density around CLA 1 510:

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

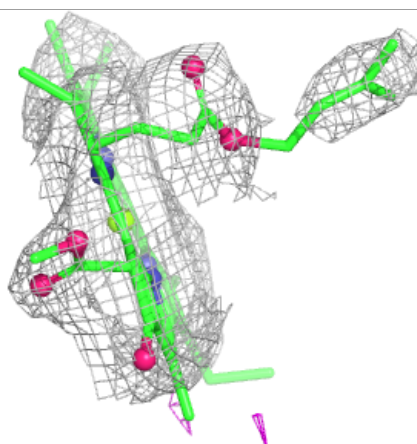
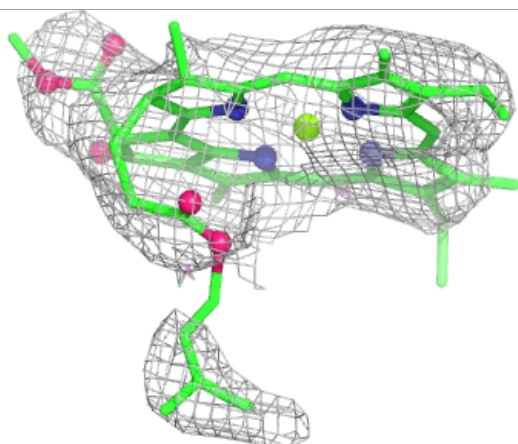
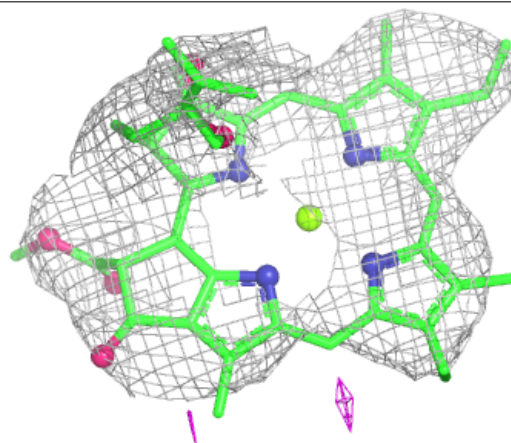


Electron density around BCR 2 503:

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

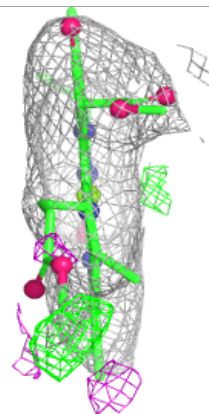
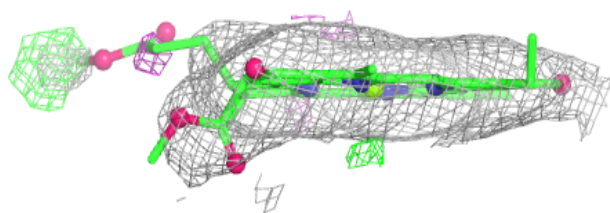
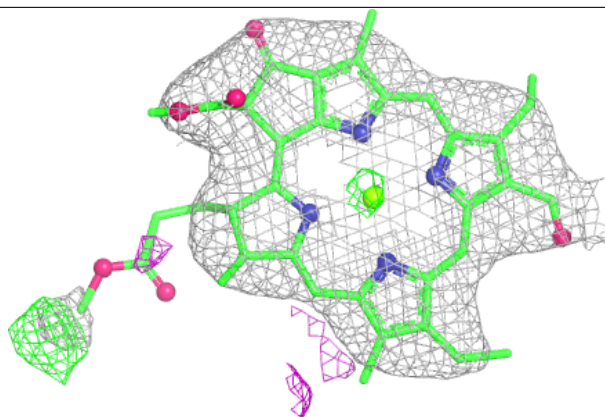
**Electron density around CLA L 303:**

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

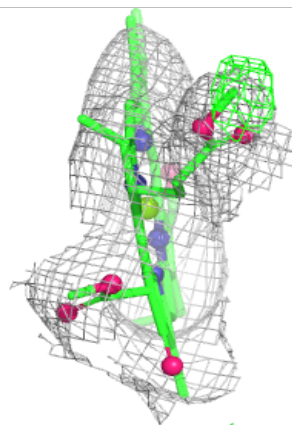
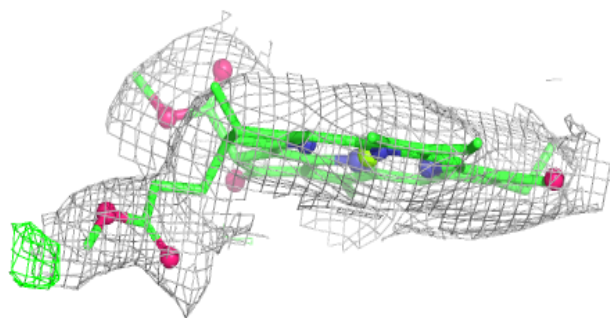
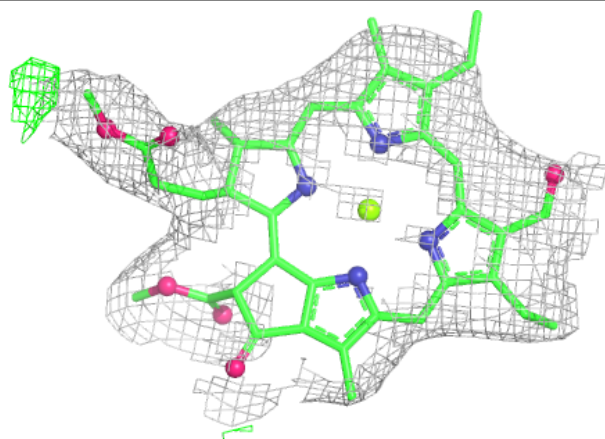


Electron density around CHL 4 313:

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

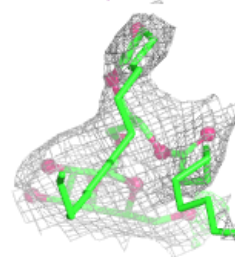
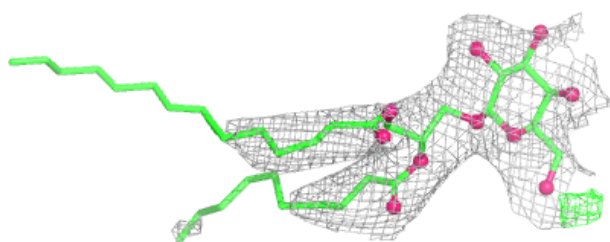
**Electron density around CHL 2 512:**

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

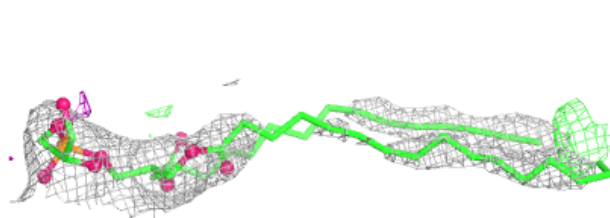
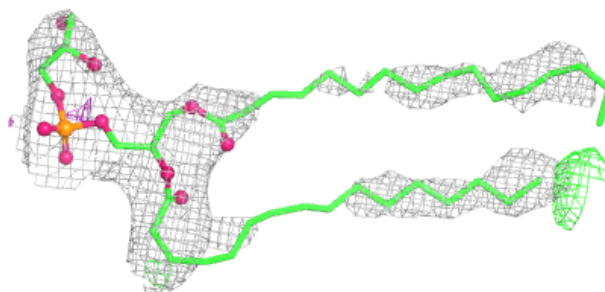


Electron density around LMG 4 322:

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

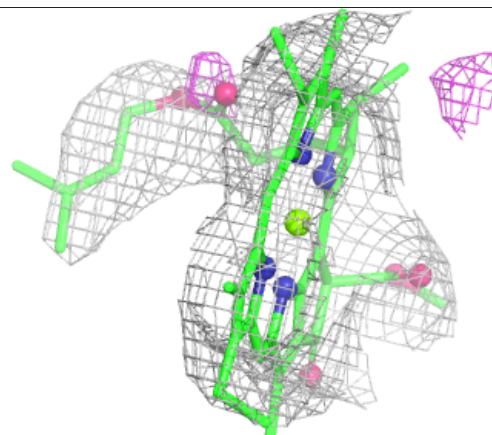
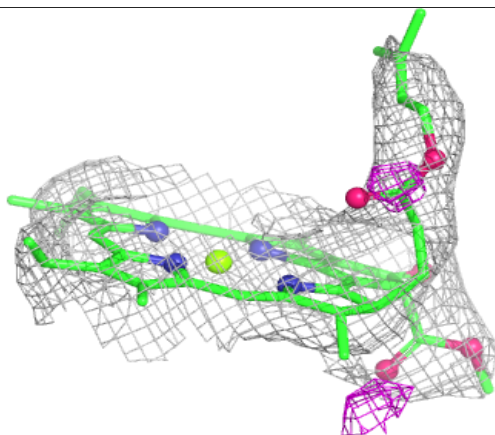
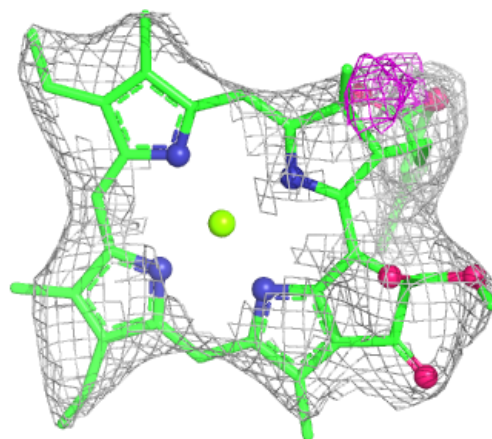
**Electron density around LHG 1 517:**

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

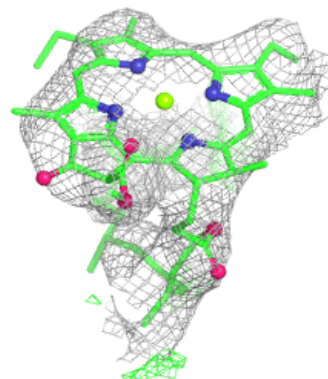
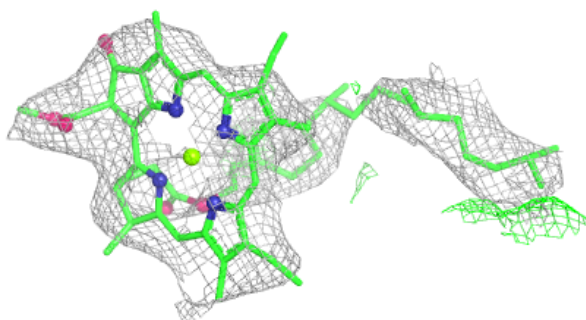
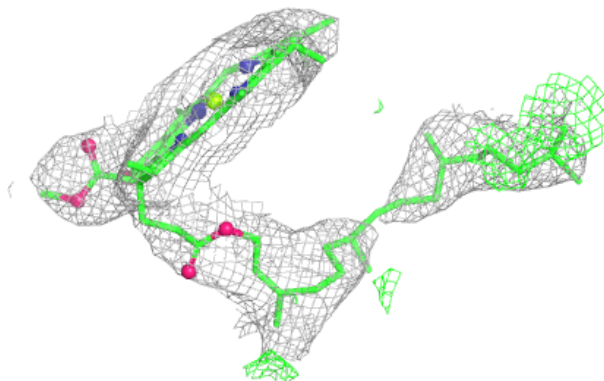


Electron density around CLA L 305:

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

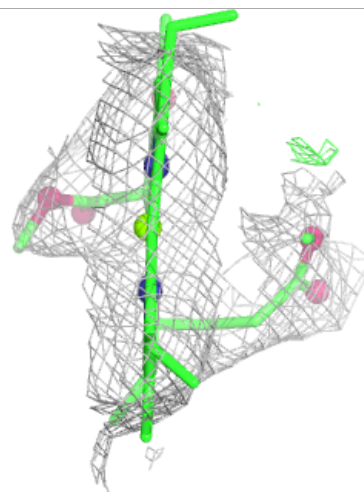
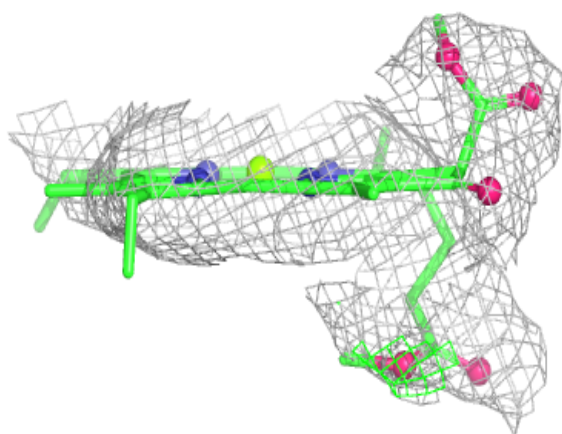
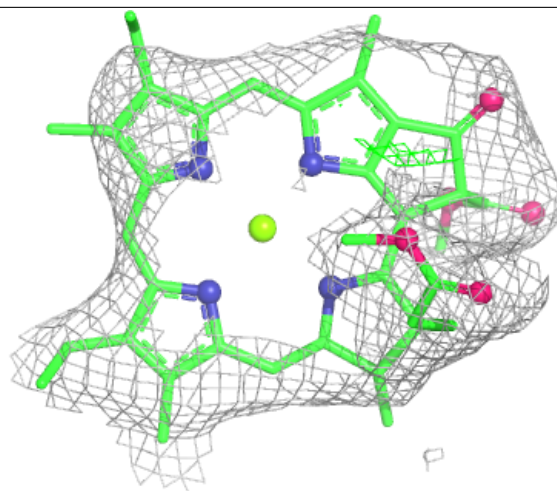
**Electron density around CLA G 204:**

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



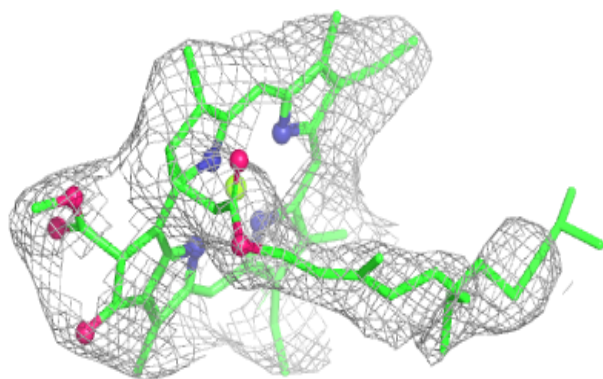
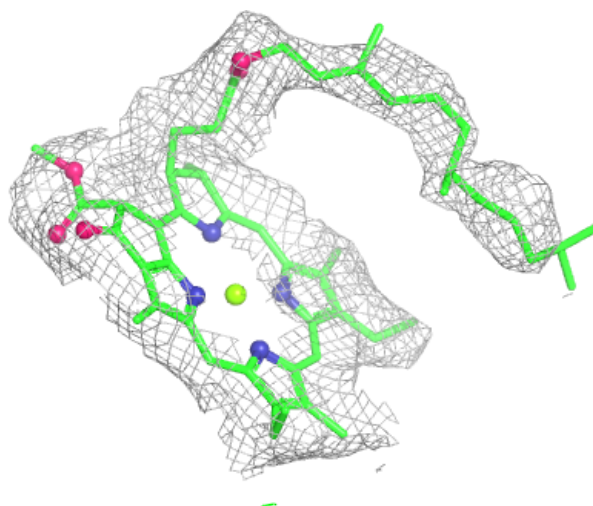
Electron density around CLA A 816:

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



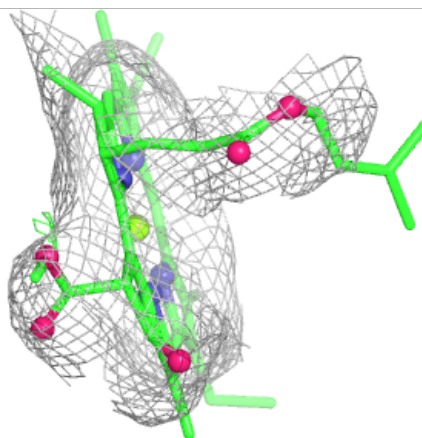
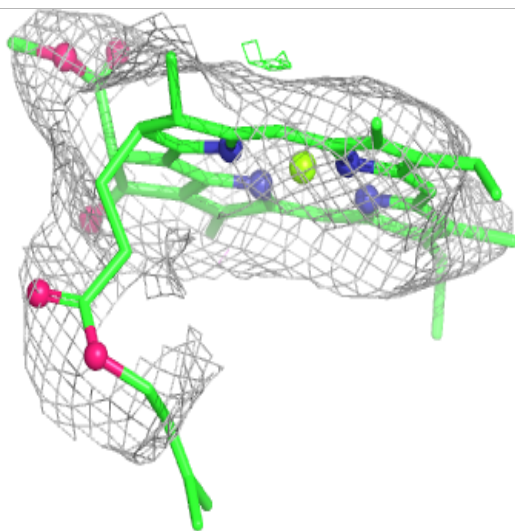
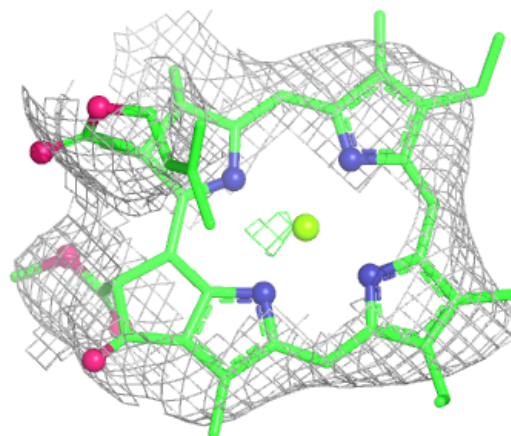
Electron density around CLA A 842:

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



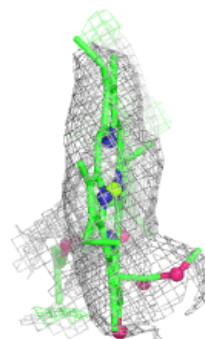
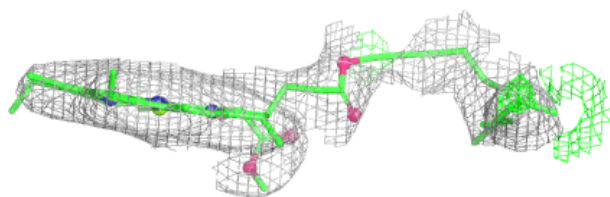
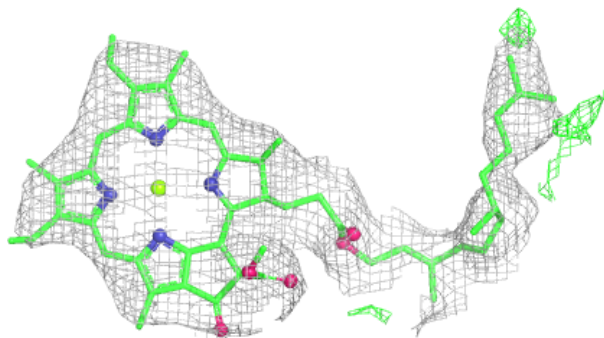
Electron density around CLA 1 509:

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

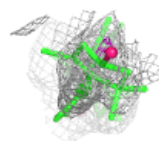
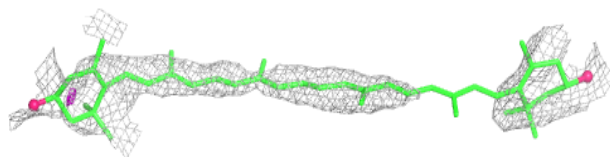
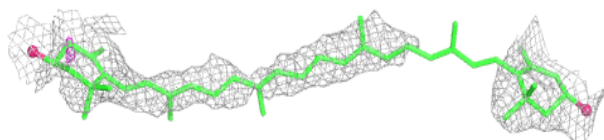


Electron density around CLA 1 516:

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

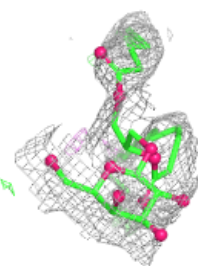
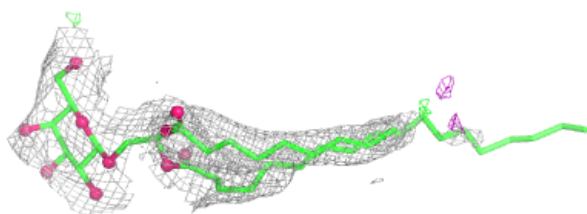
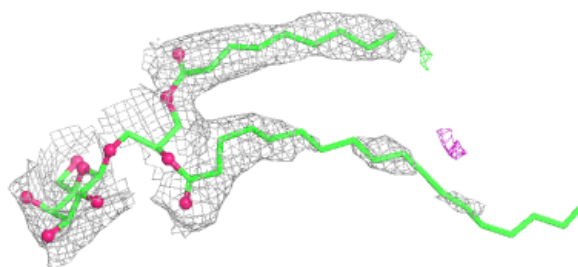
**Electron density around LUT 3 301:**

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



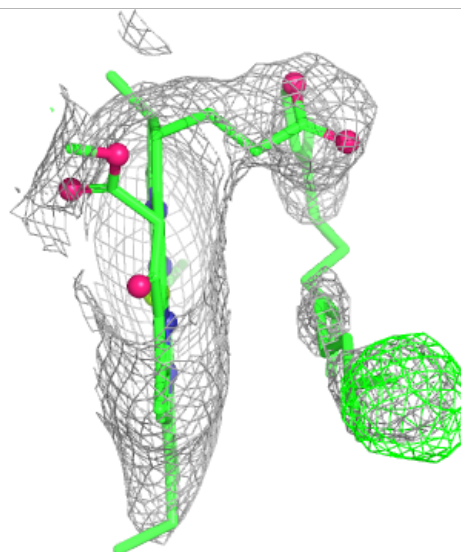
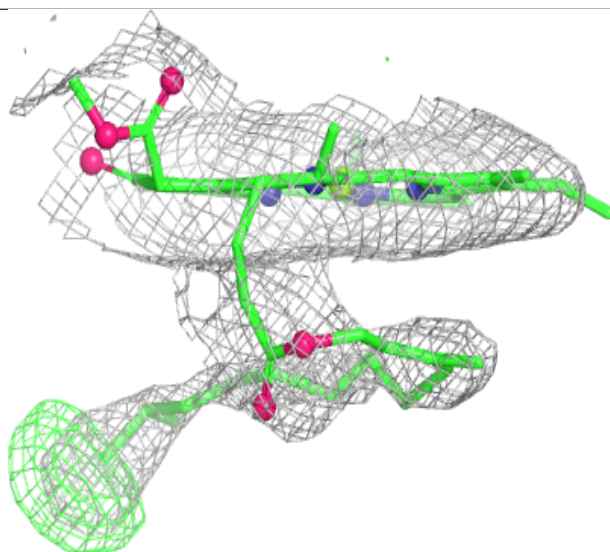
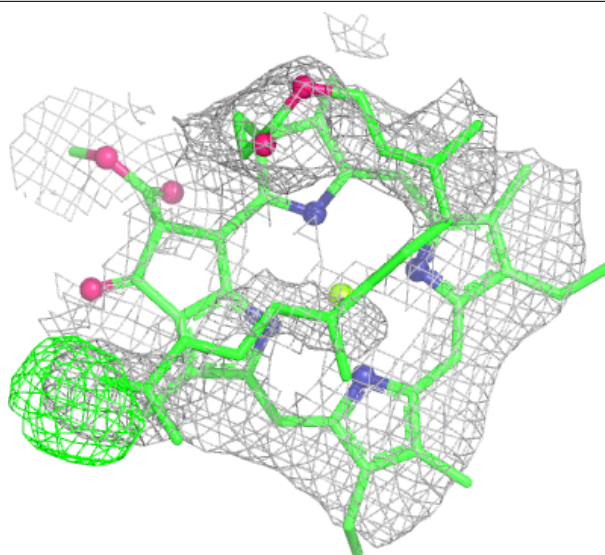
Electron density around LMG 1 518:

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



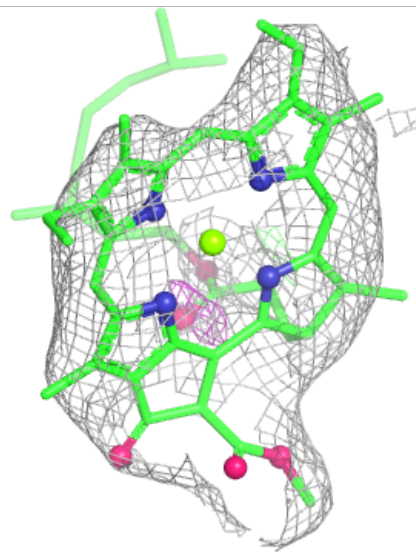
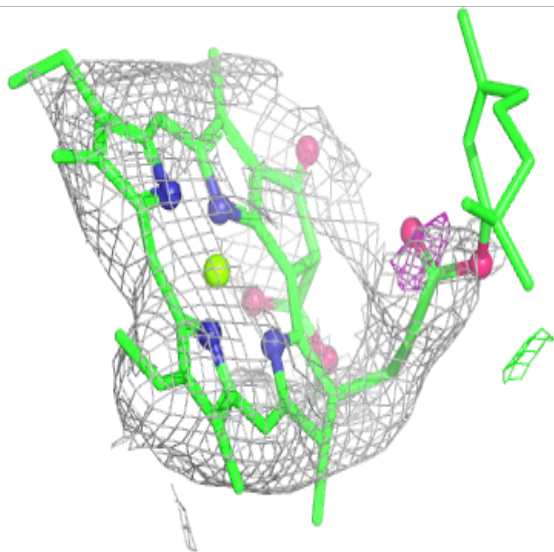
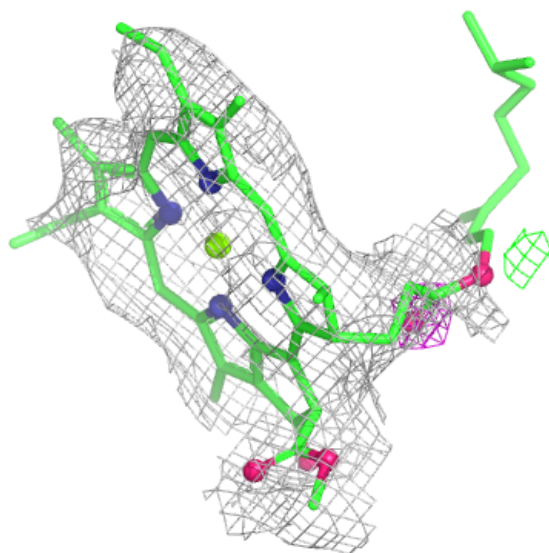
Electron density around CLA 3 313:

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



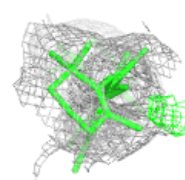
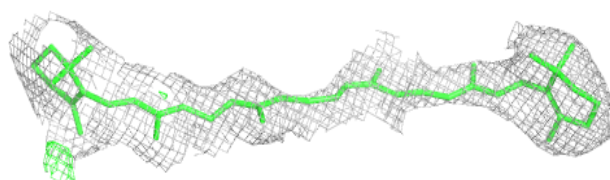
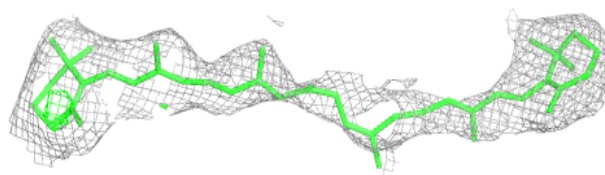
Electron density around CLA A 835:

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

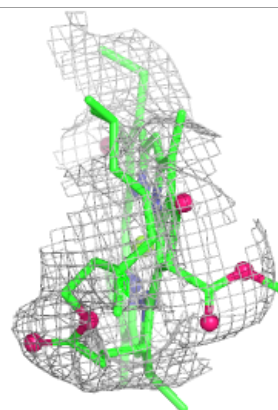
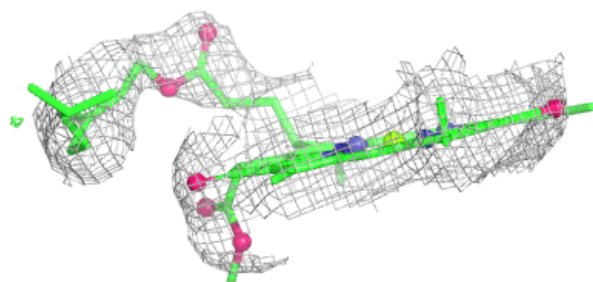
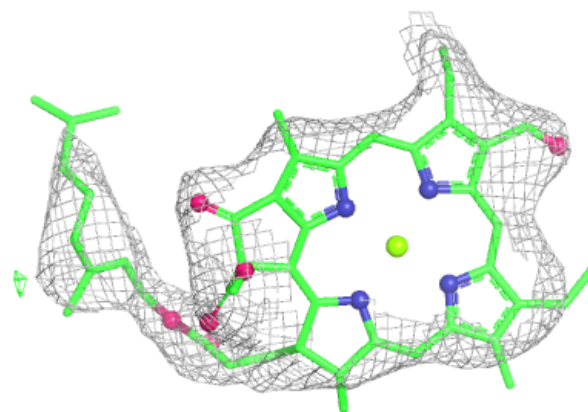


Electron density around BCR G 205:

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

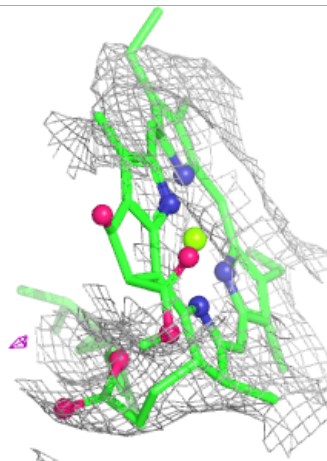
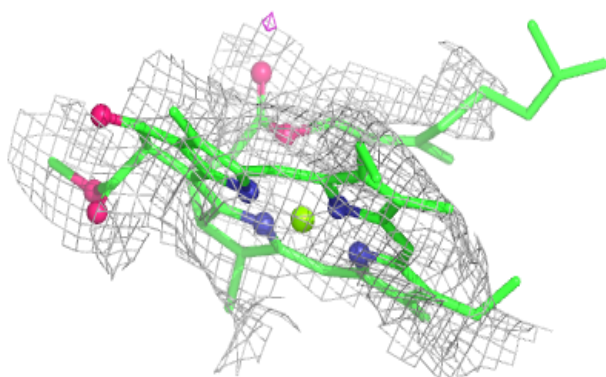
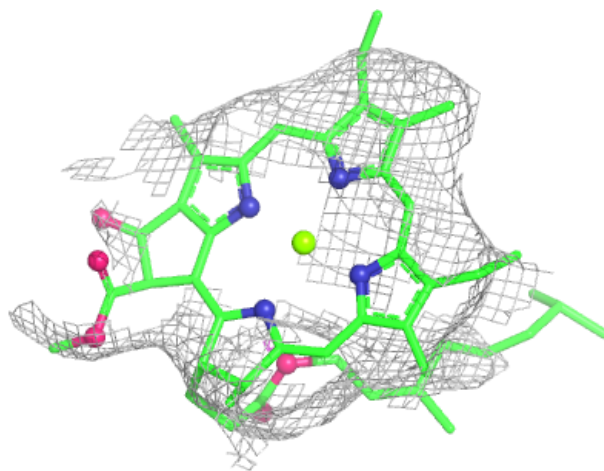
**Electron density around CHL 2 516:**

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



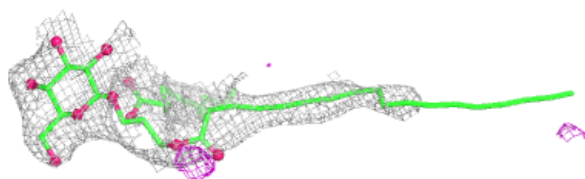
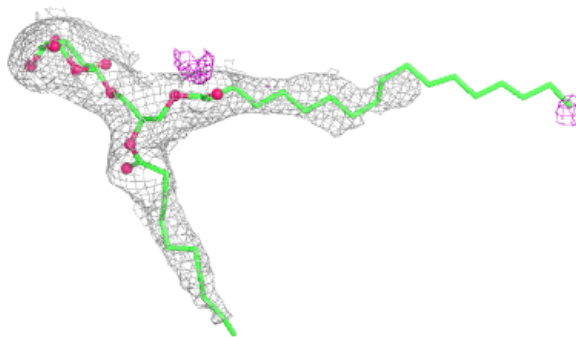
Electron density around CLA 3 305:

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

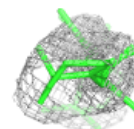
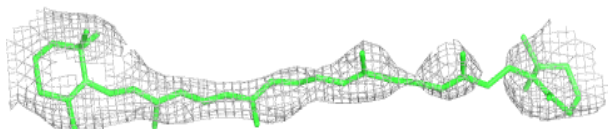
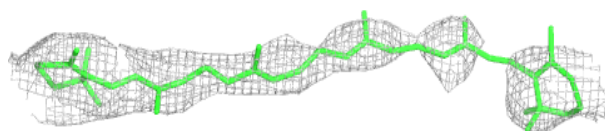


Electron density around LMG F 304:

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

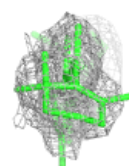
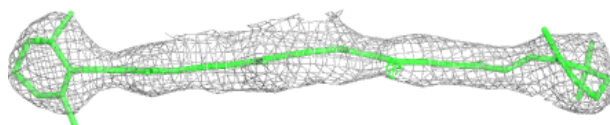
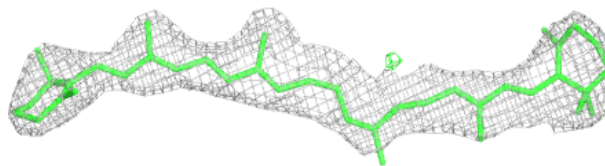
**Electron density around BCR 3 303:**

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

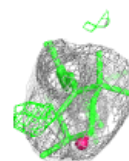
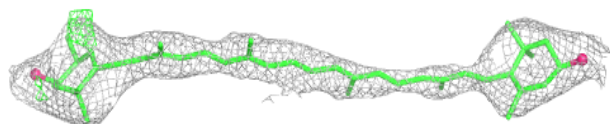
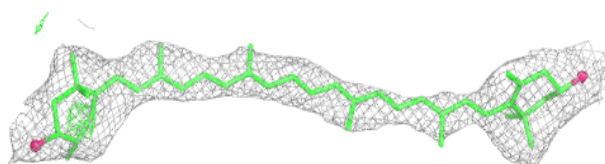


Electron density around BCR A 850:

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

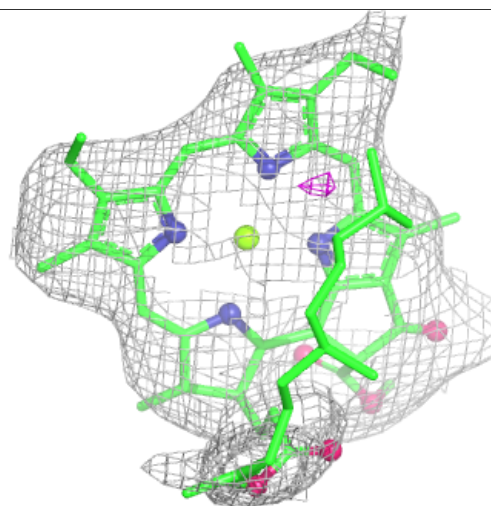
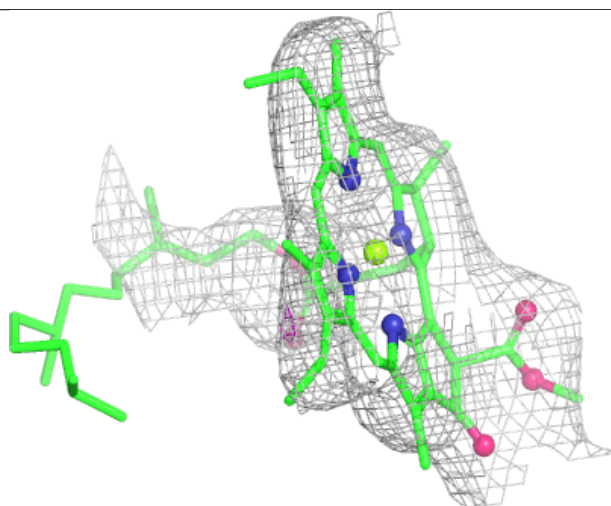
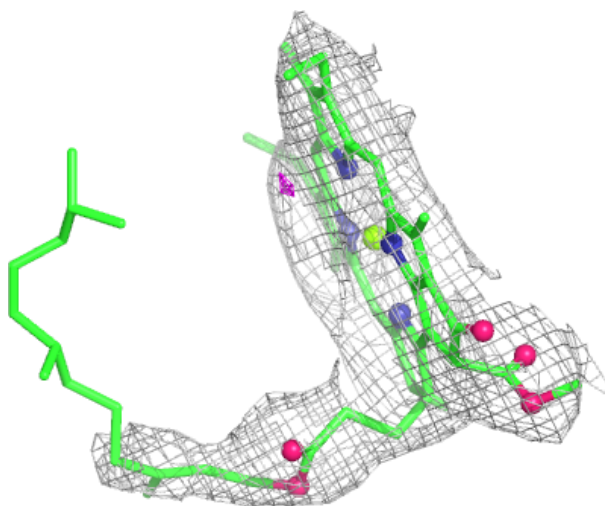
**Electron density around ZEX F 301:**

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



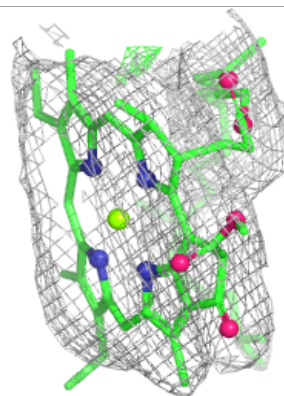
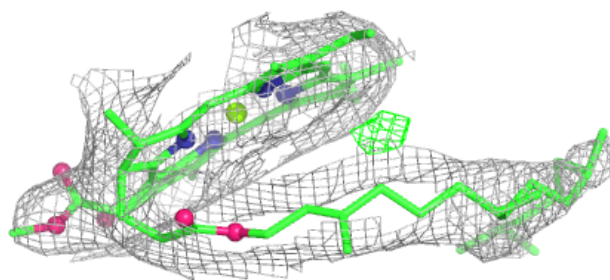
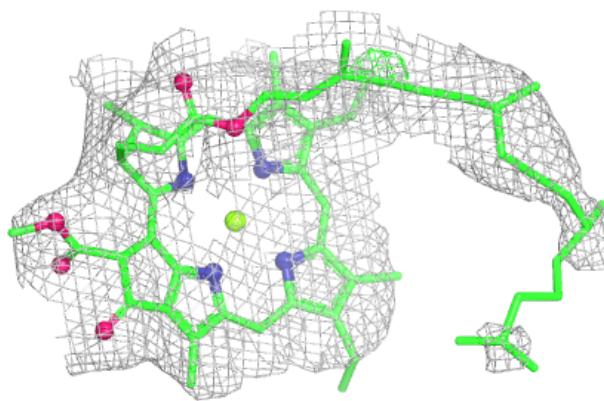
Electron density around CLA A 823:

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



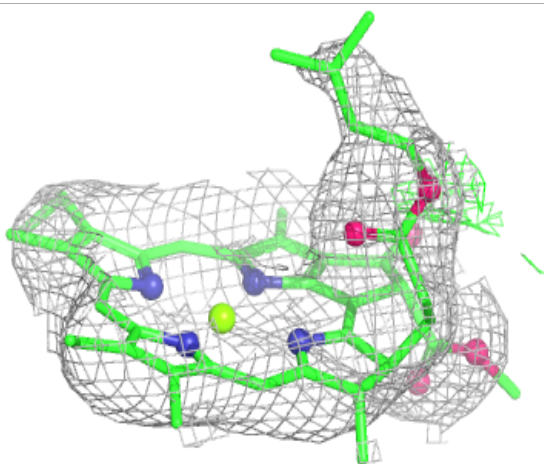
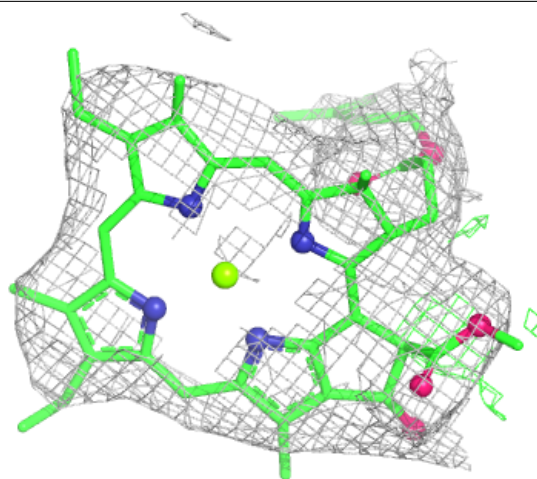
Electron density around CLA 1 504:

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



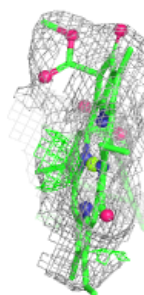
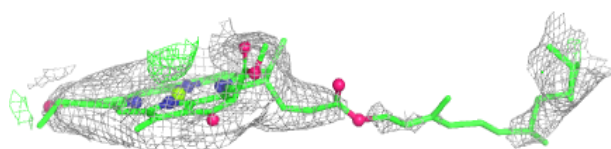
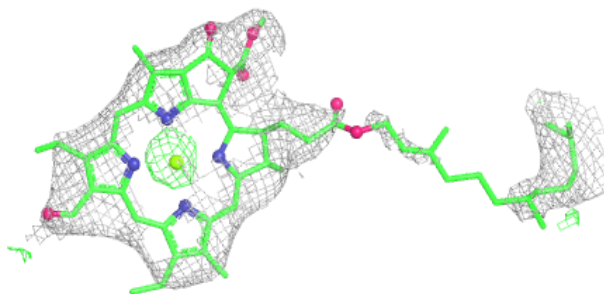
Electron density around CLA 4 309:

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

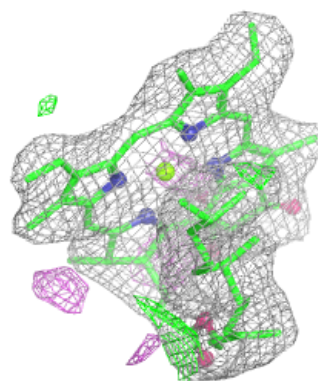
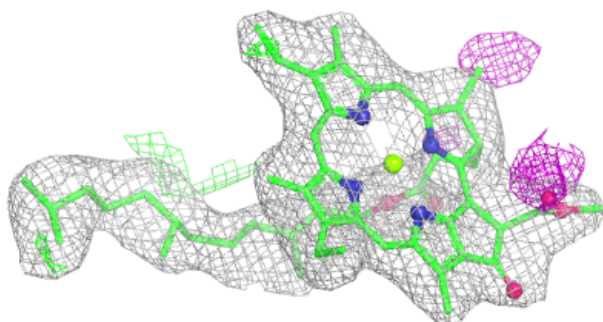
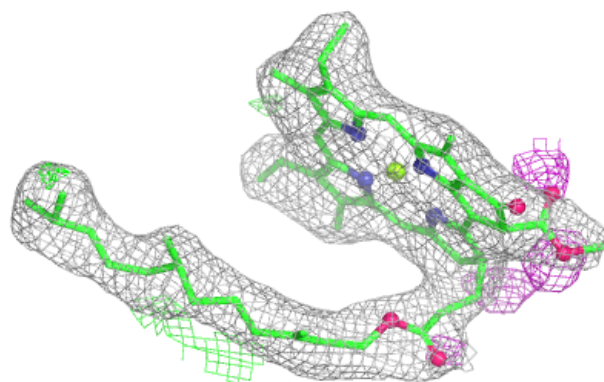


Electron density around CHL 4 316:

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

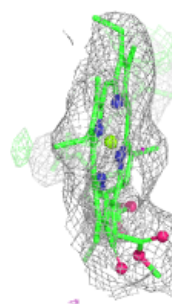
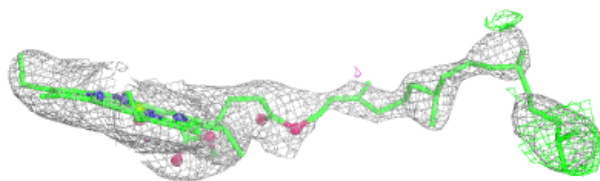
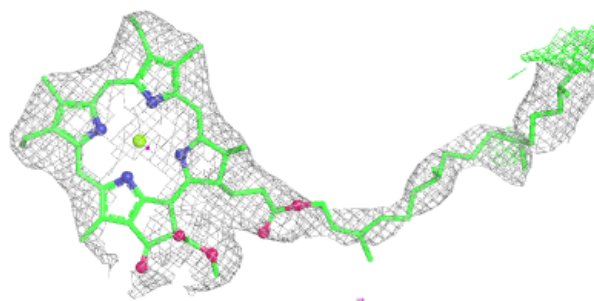
**Electron density around CLA B 831:**

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

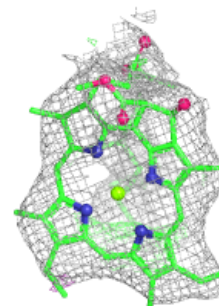
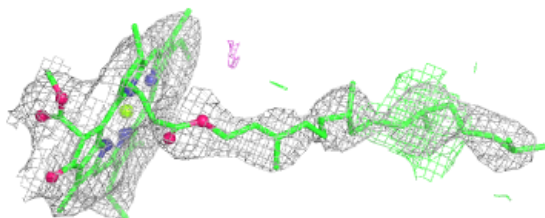
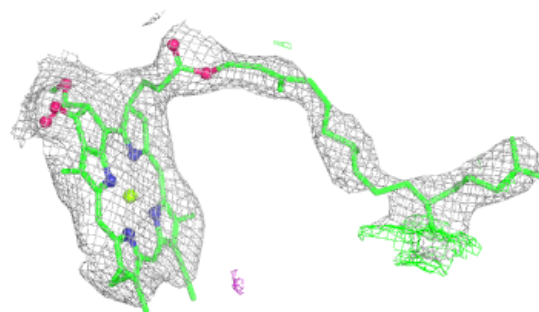


Electron density around CLA F 303:

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

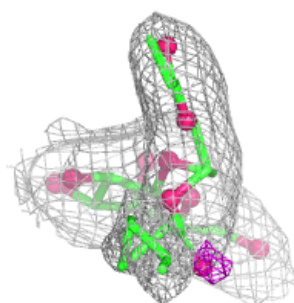
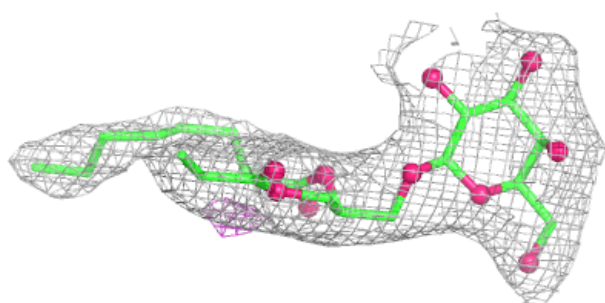
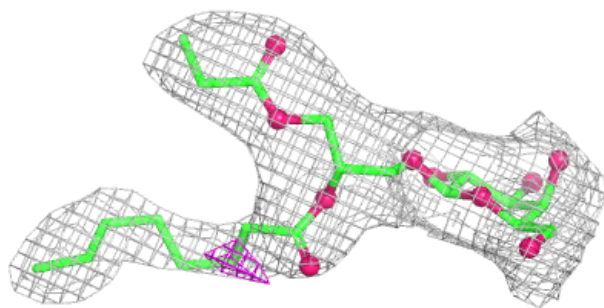
**Electron density around CLA G 201:**

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

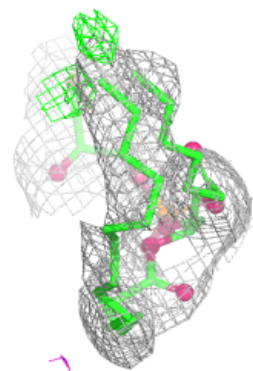
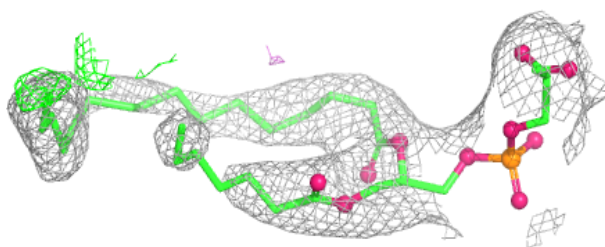
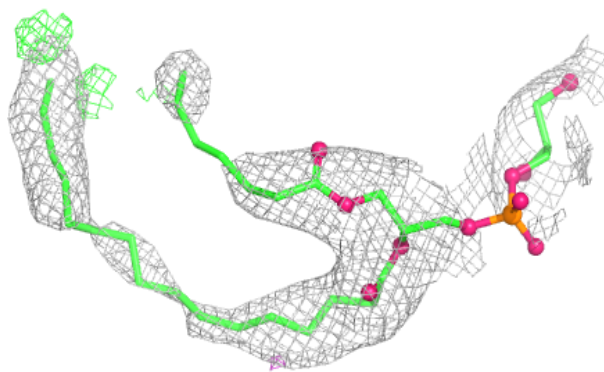


Electron density around LMG J 1103:

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

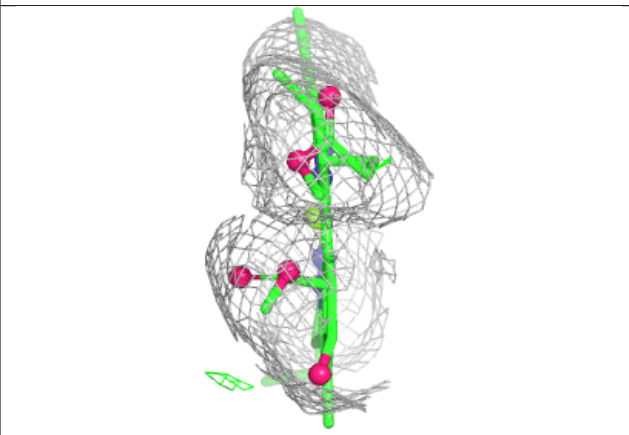
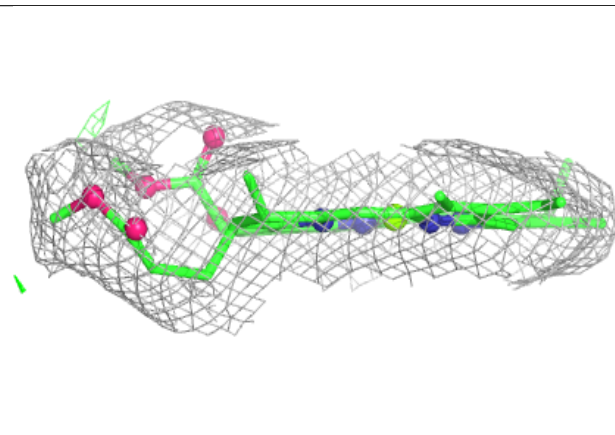
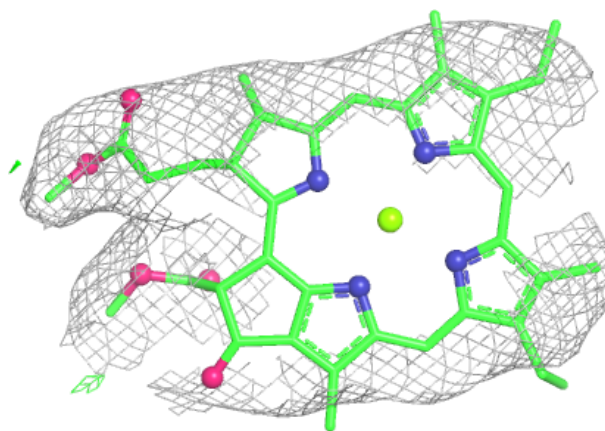
**Electron density around LHG A 845:**

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

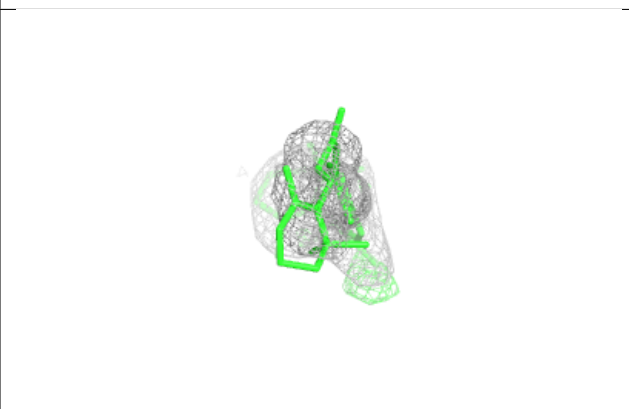
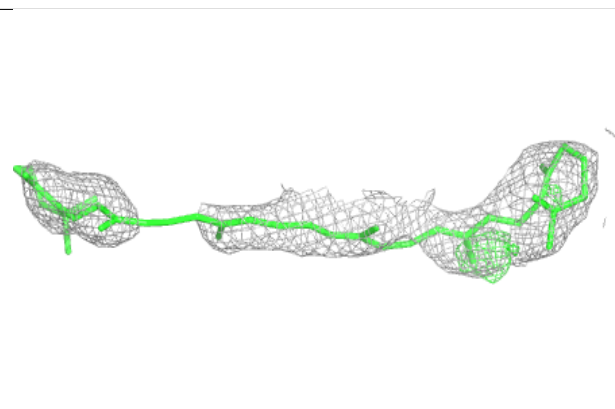
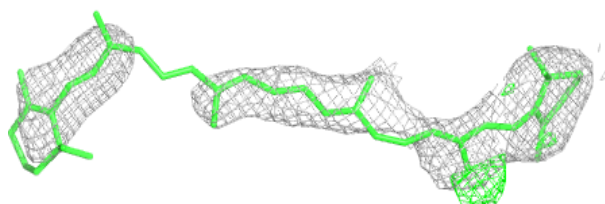


Electron density around CLA G 203:

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

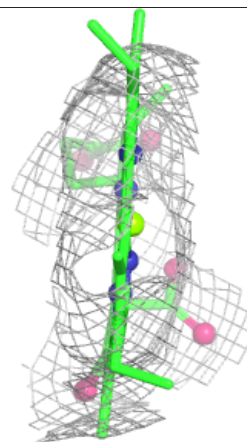
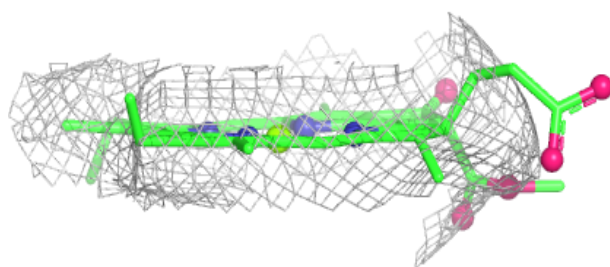
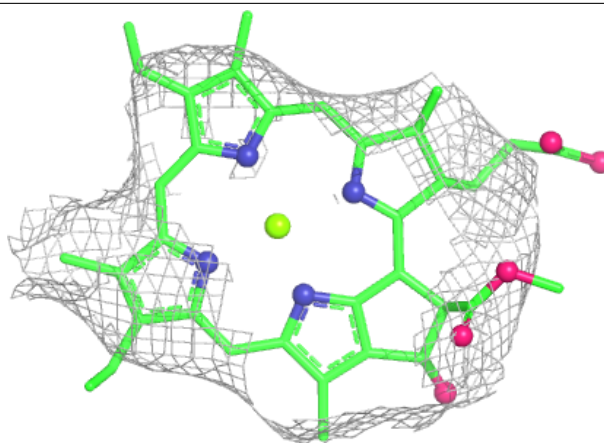
**Electron density around BCR B 851:**

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

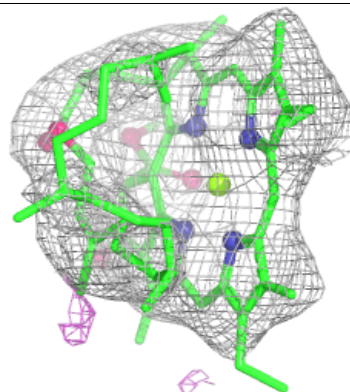
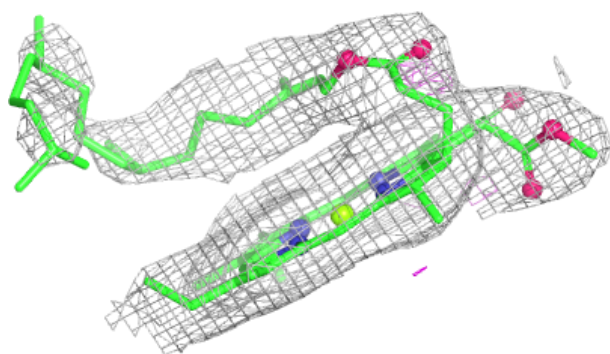
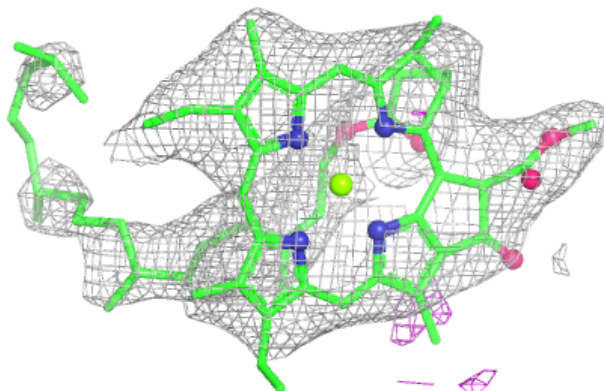


Electron density around CLA 1 515:

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

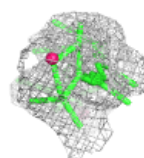
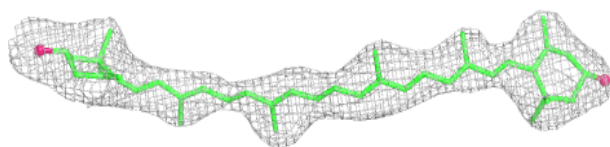
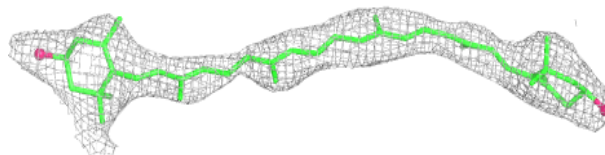
**Electron density around CLA B 808:**

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

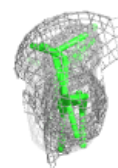
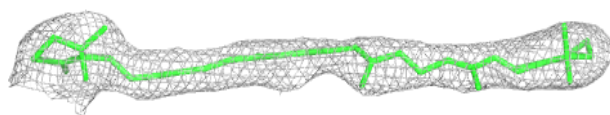
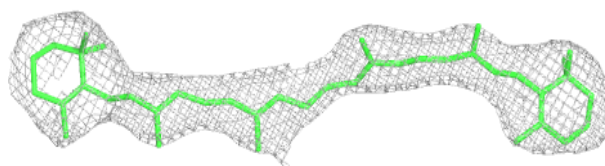


Electron density around LUT J 1109:

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

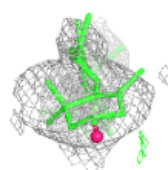
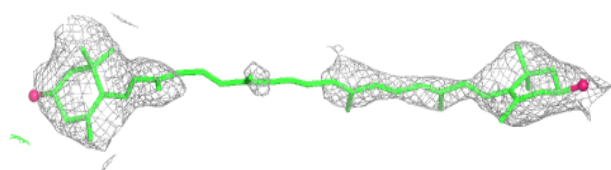
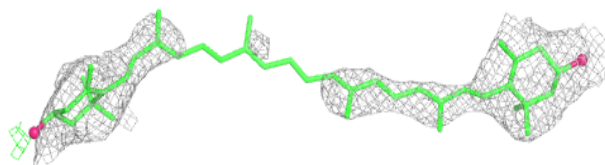
**Electron density around BCR I 102:**

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

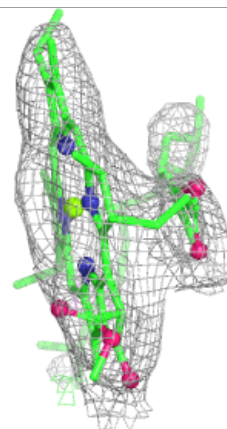
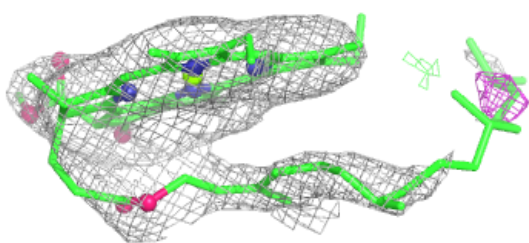
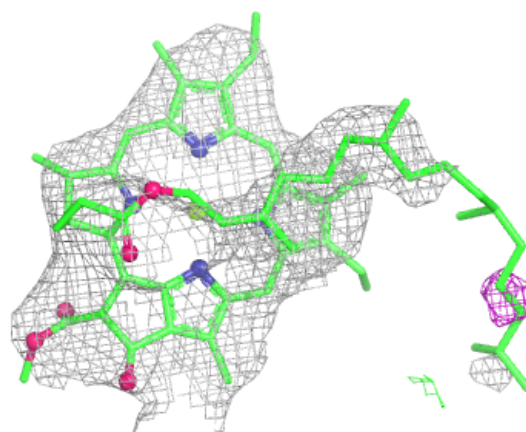


Electron density around LUT 1 502:

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

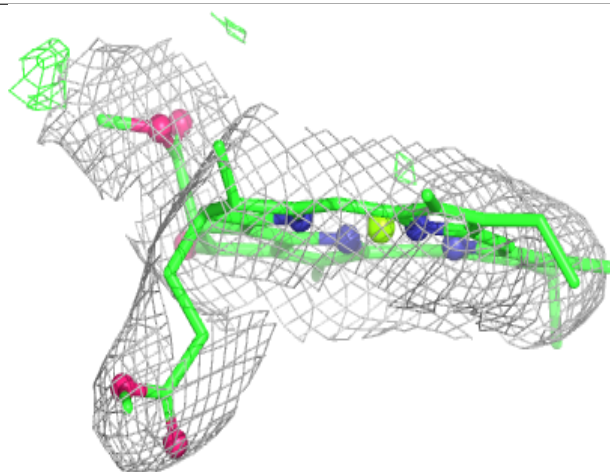
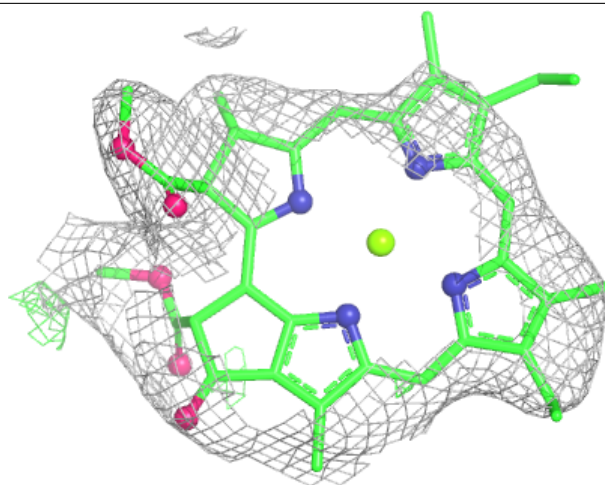
**Electron density around CLA A 817:**

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



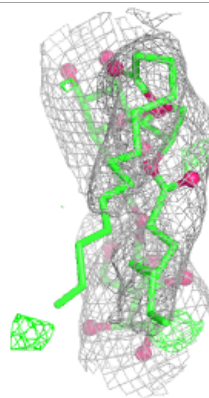
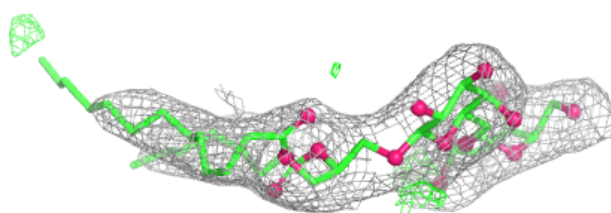
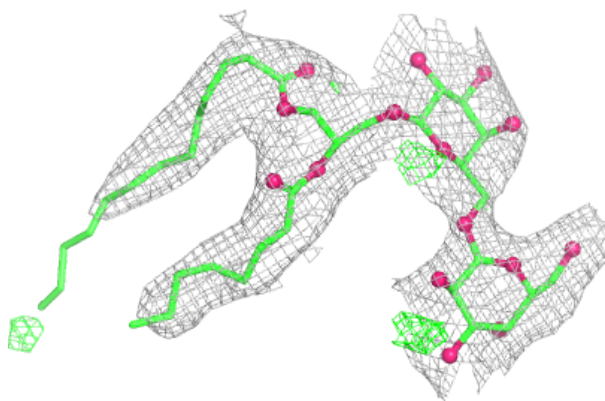
Electron density around CLA 1 511:

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

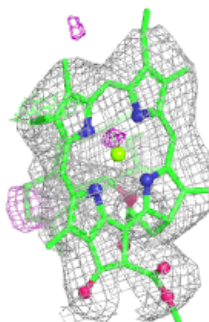
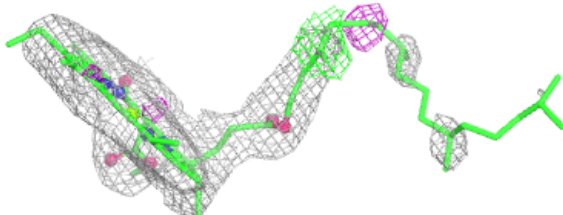
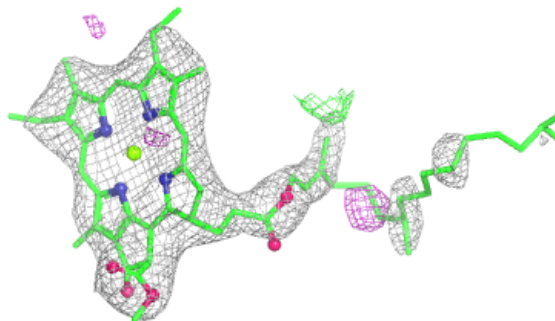


Electron density around DGD 4 319:

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

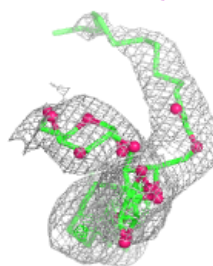
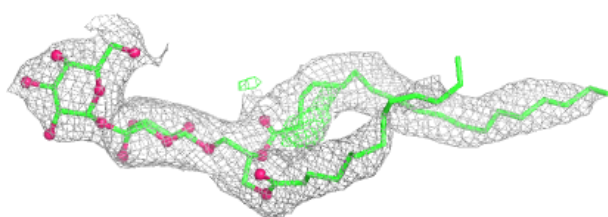
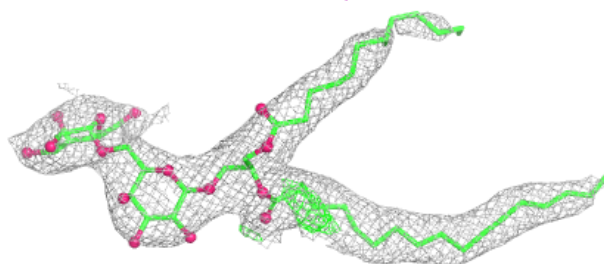
**Electron density around CLA A 831:**

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

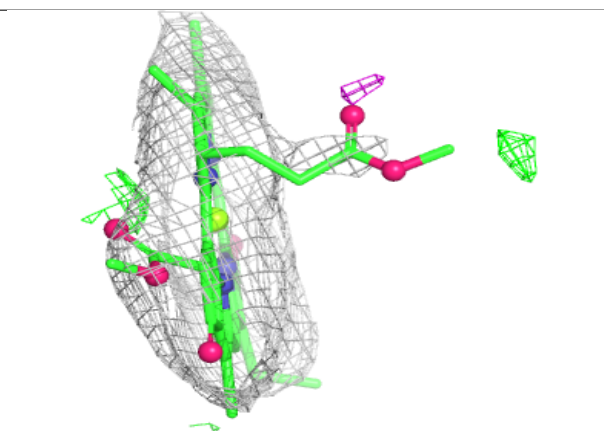
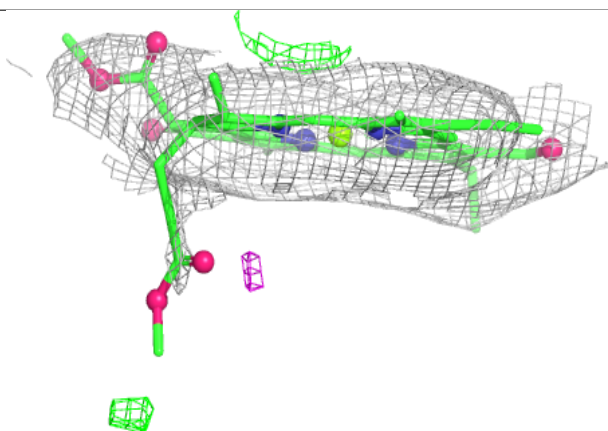
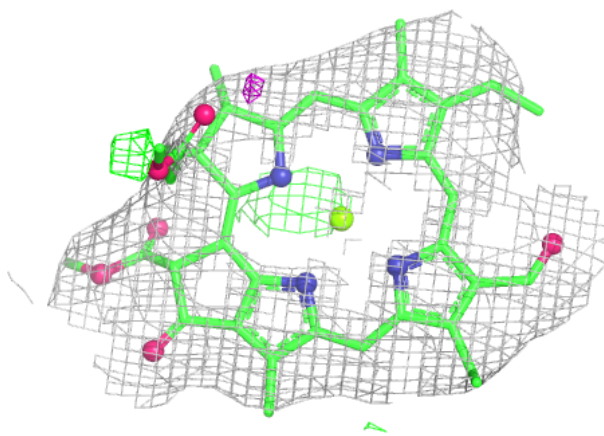


Electron density around DGD B 854:

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

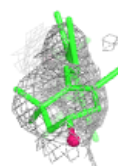
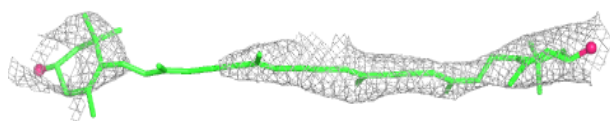
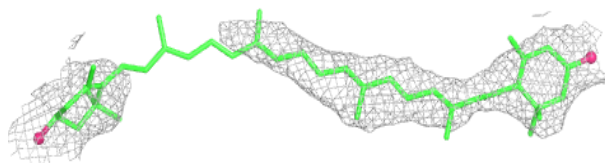
**Electron density around CHL 3 314:**

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



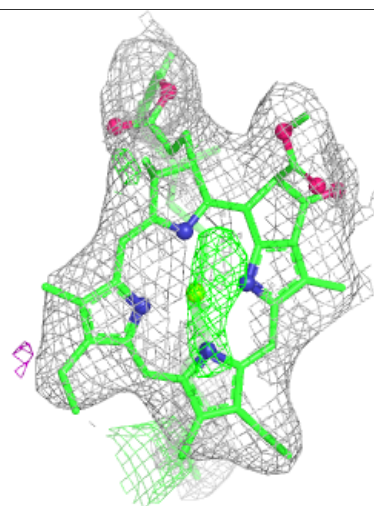
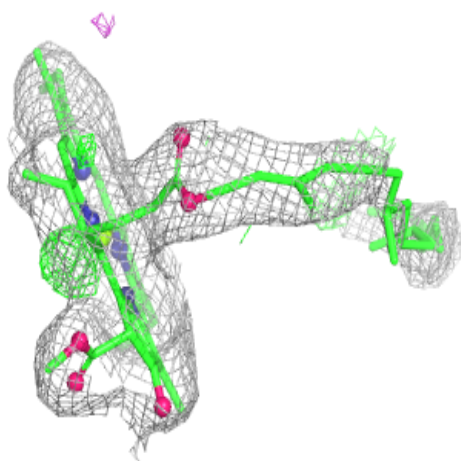
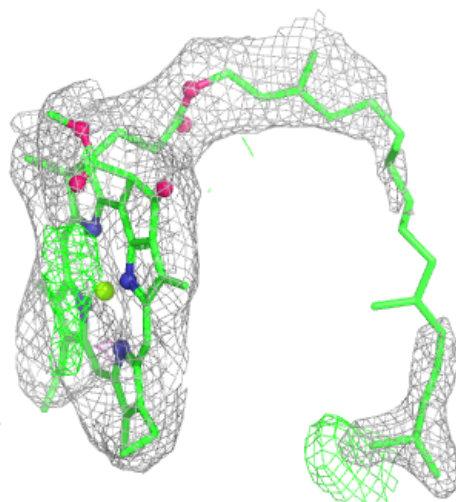
Electron density around LUT 3 302:

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



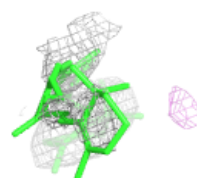
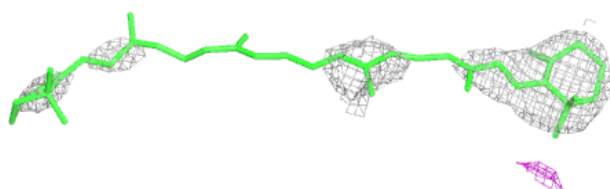
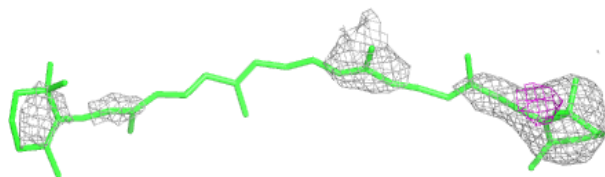
Electron density around CLA A 838:

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

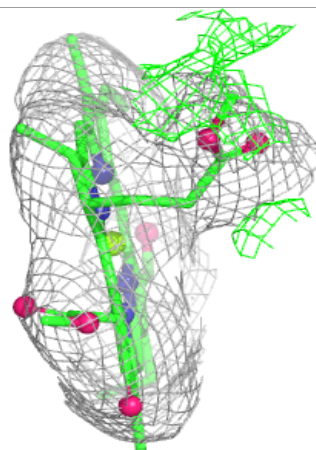
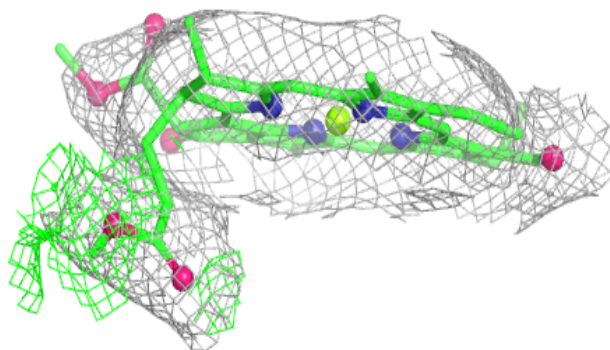
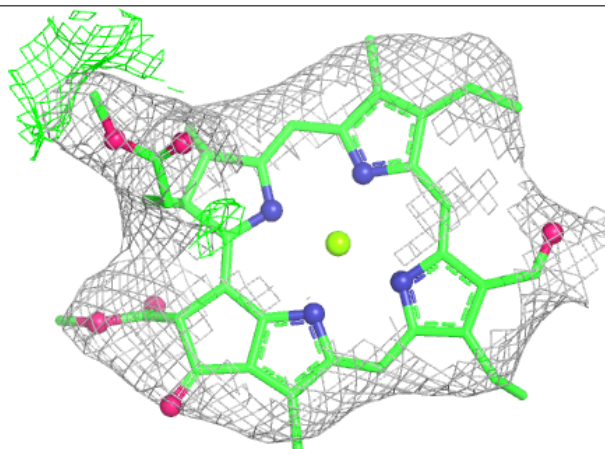


Electron density around BCR A 856:

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

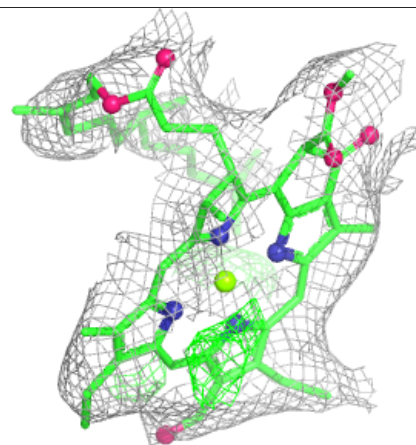
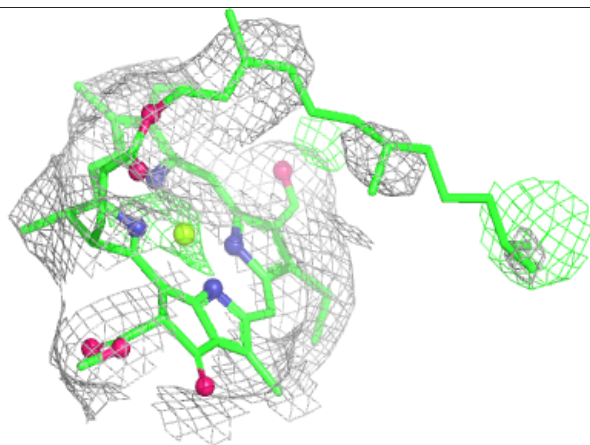
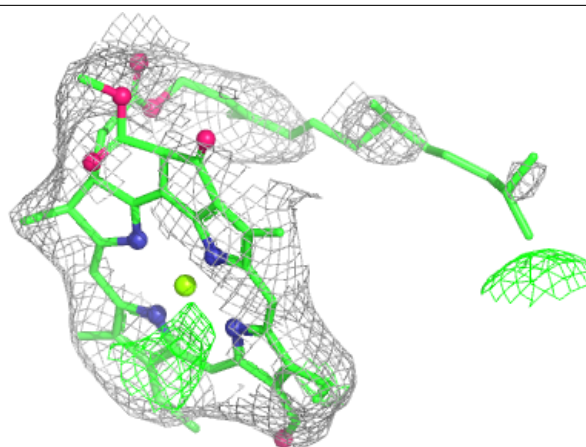
**Electron density around CHL 1 512:**

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



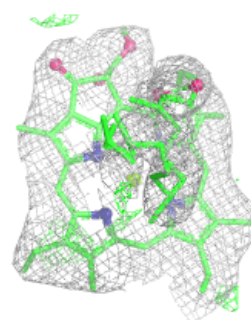
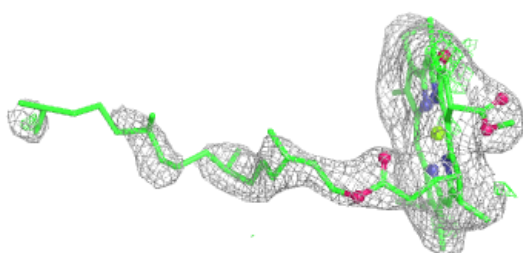
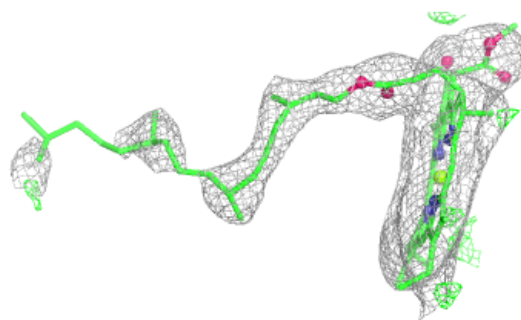
Electron density around CHL 1 514:

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



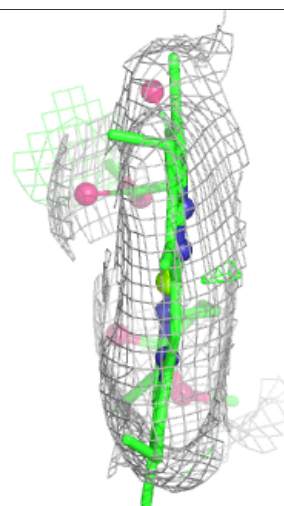
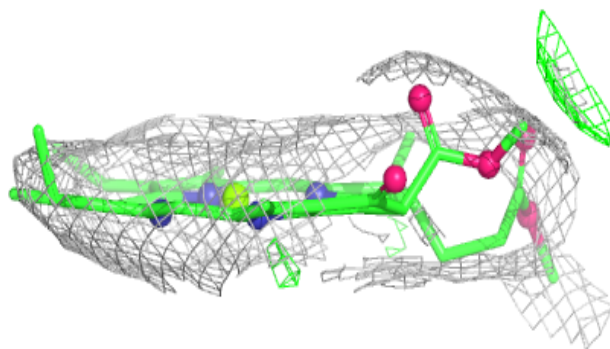
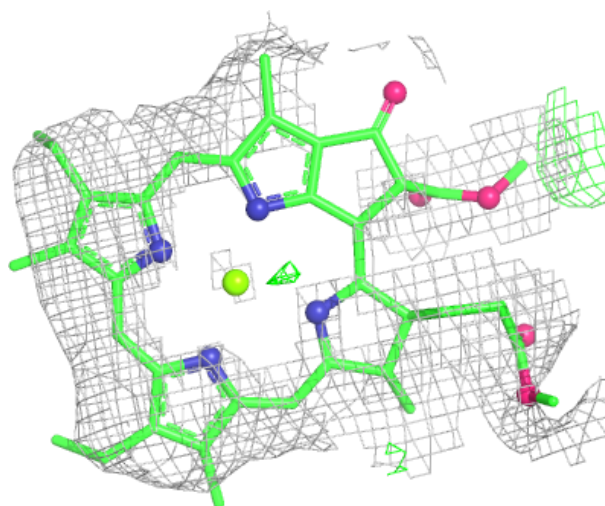
Electron density around CLA B 805:

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



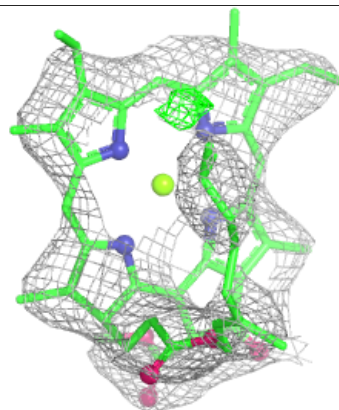
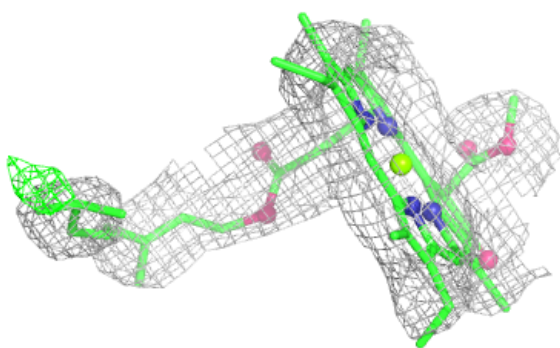
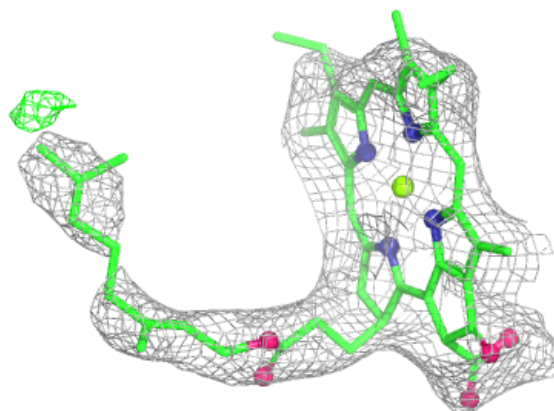
Electron density around CLA 1 505:

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

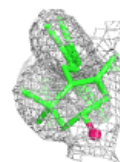
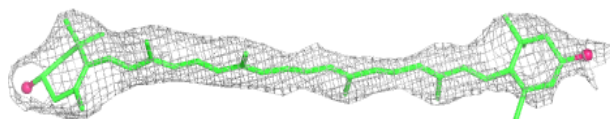
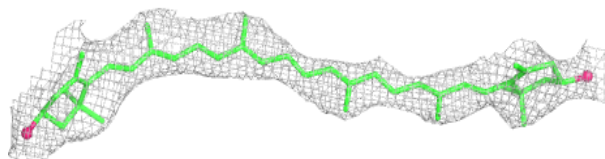


Electron density around CLA B 816:

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

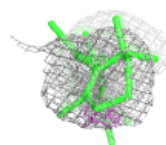
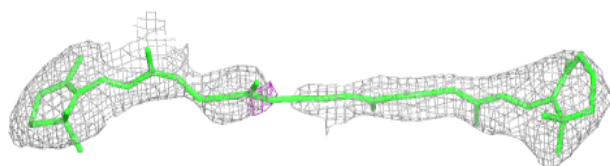
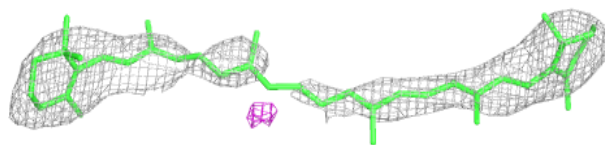
**Electron density around LUT 4 302:**

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

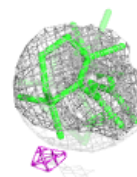
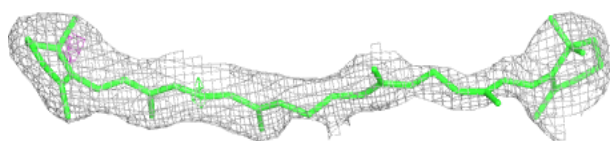
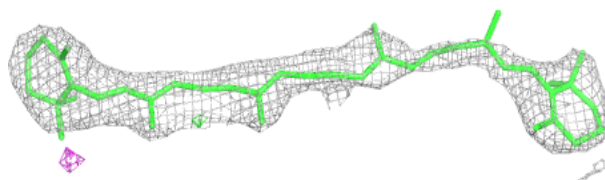


Electron density around BCR L 306:

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

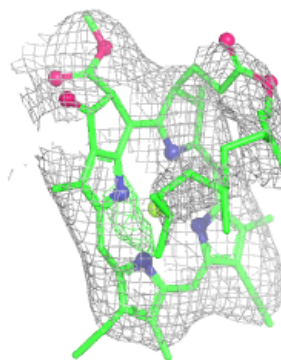
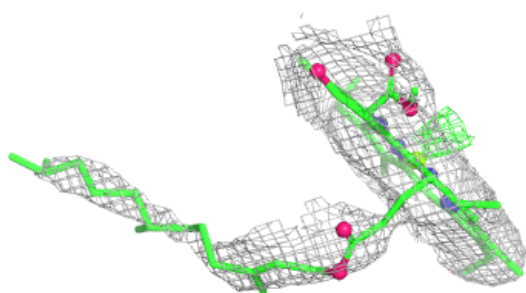
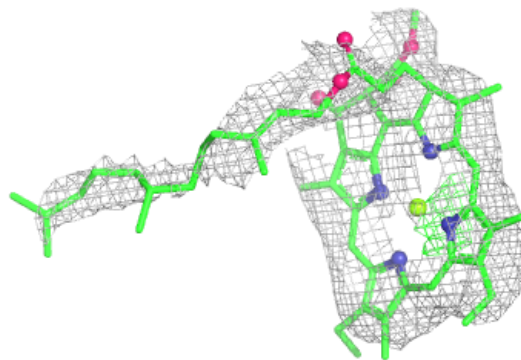
**Electron density around BCR A 851:**

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

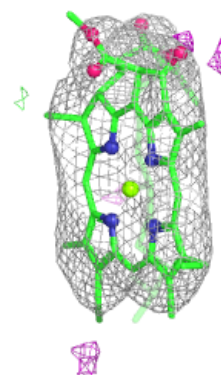
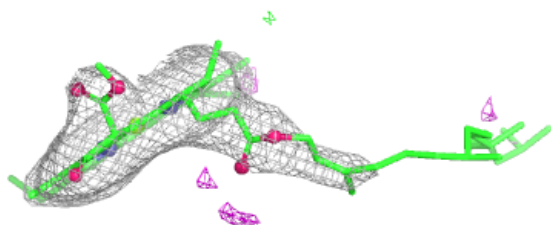
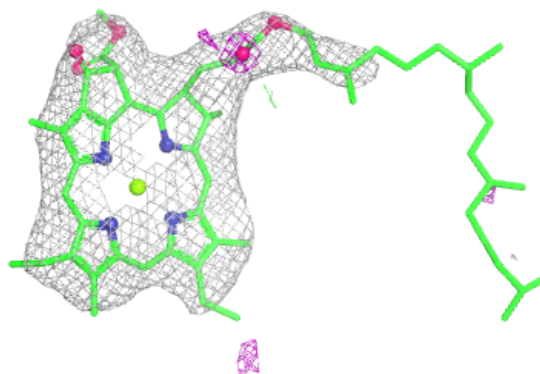


Electron density around CLA 4 310:

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

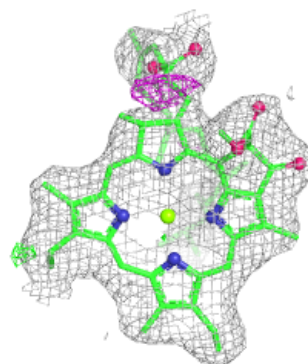
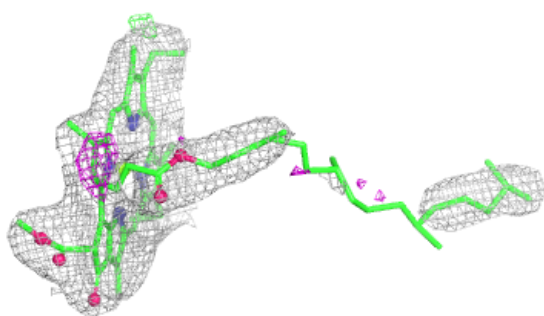
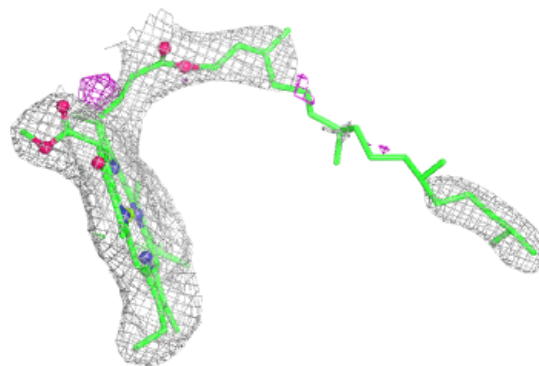
**Electron density around CLA 4 318:**

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



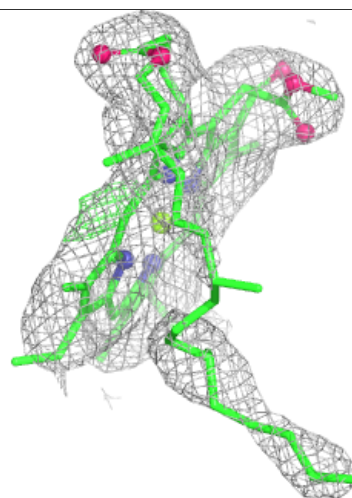
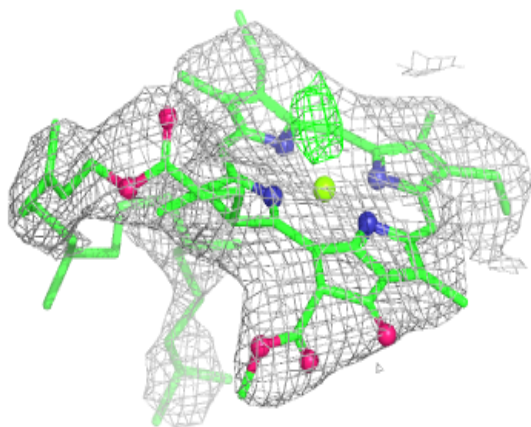
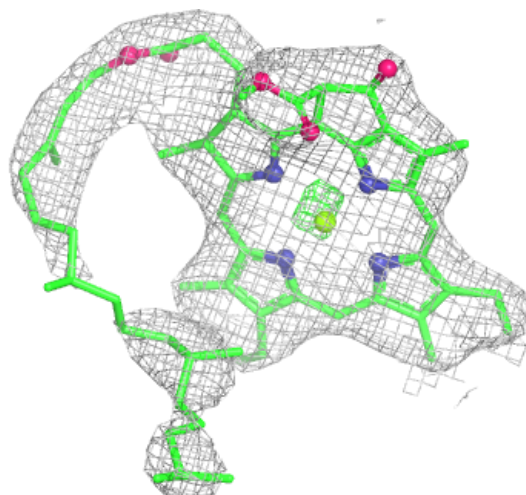
Electron density around CLA A 804:

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



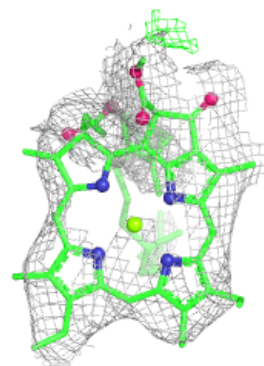
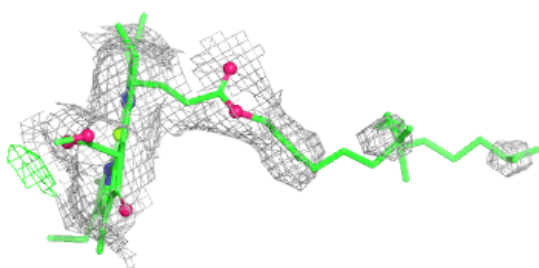
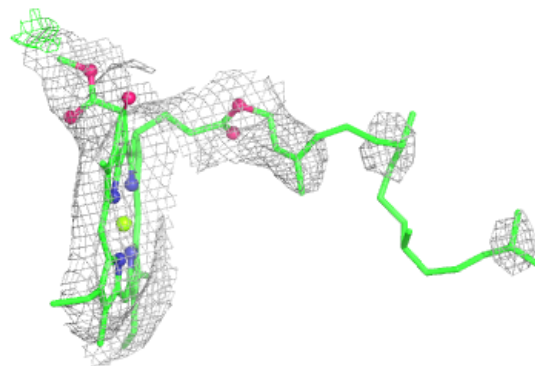
Electron density around CLA A 813:

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

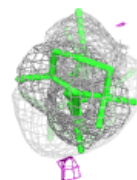
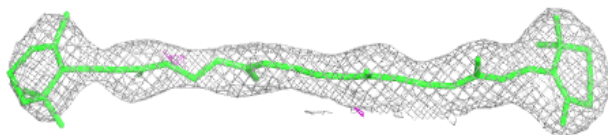
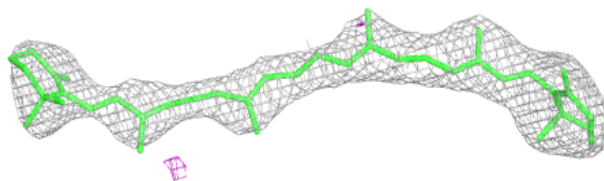


Electron density around CLA A 814:

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

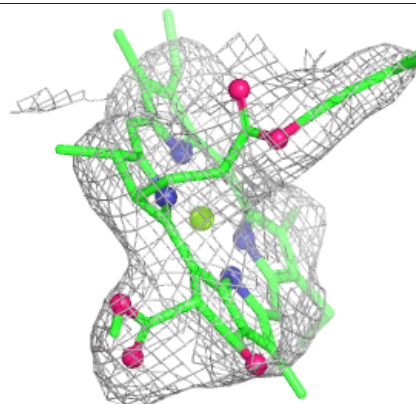
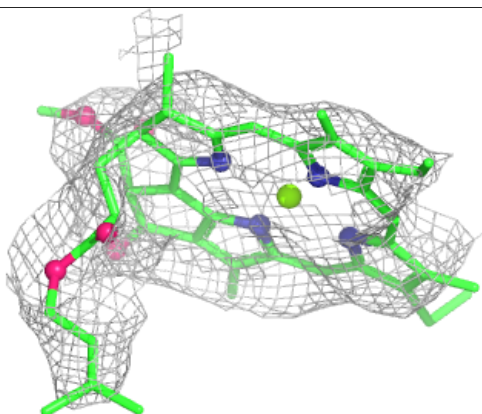
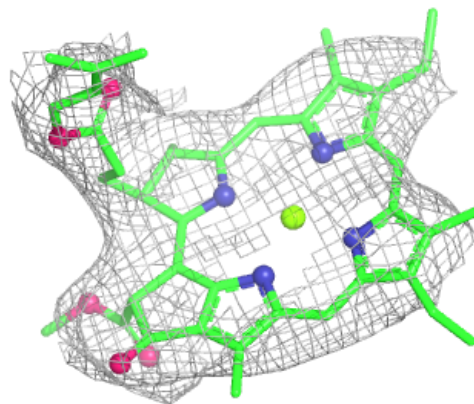
**Electron density around BCR B 852:**

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

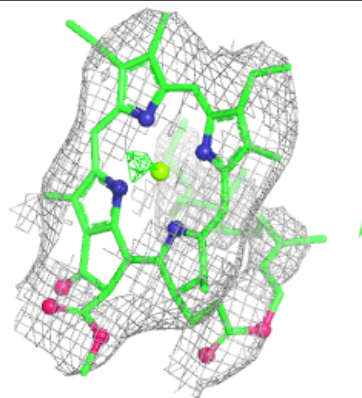
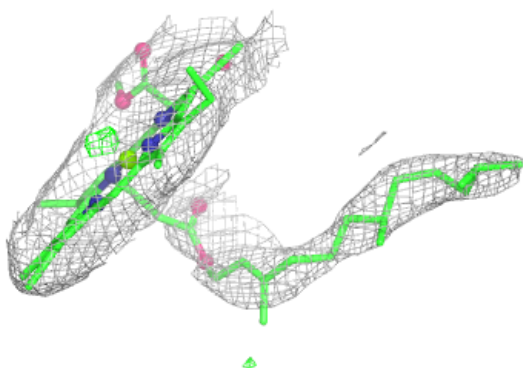
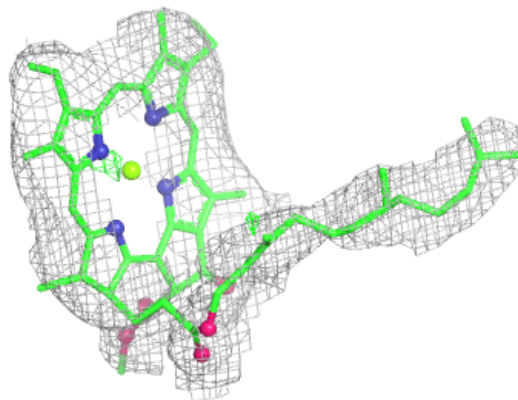


Electron density around CLA 2 509:

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

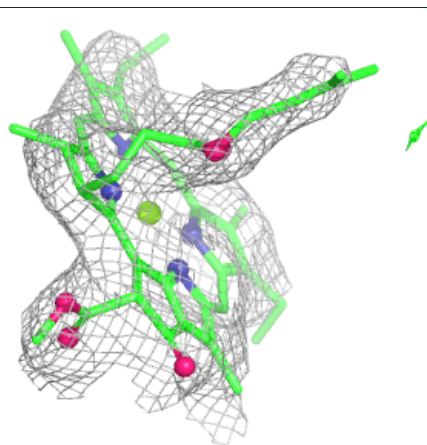
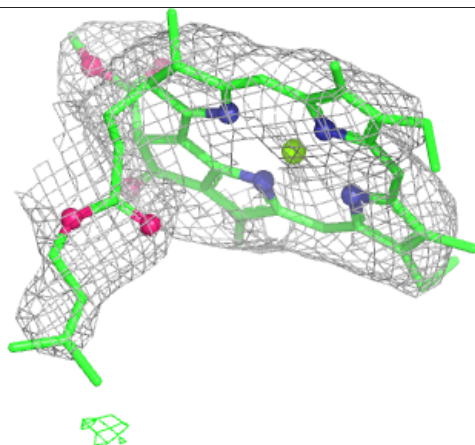
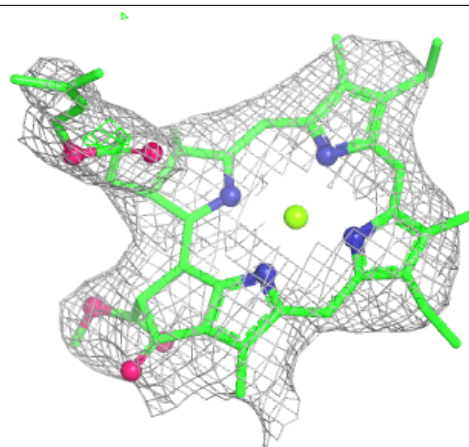
**Electron density around CLA 2 510:**

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



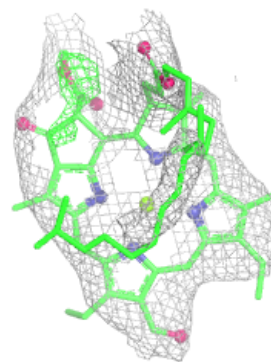
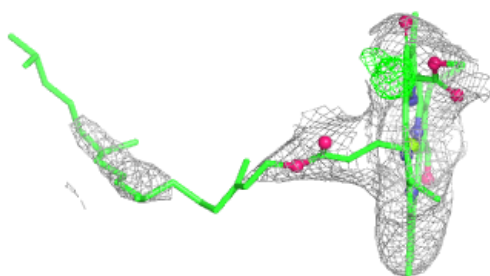
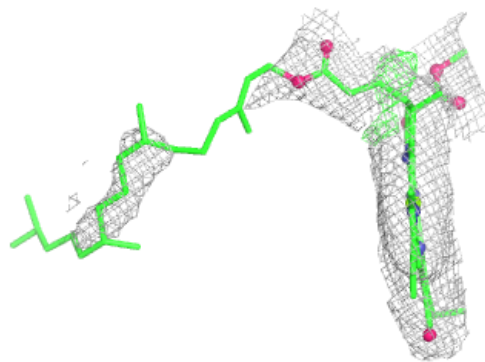
Electron density around CLA 2 511:

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



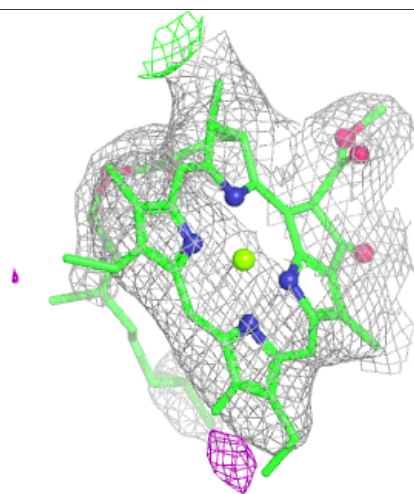
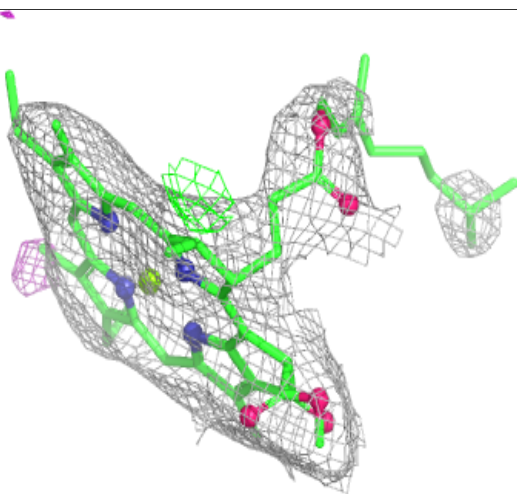
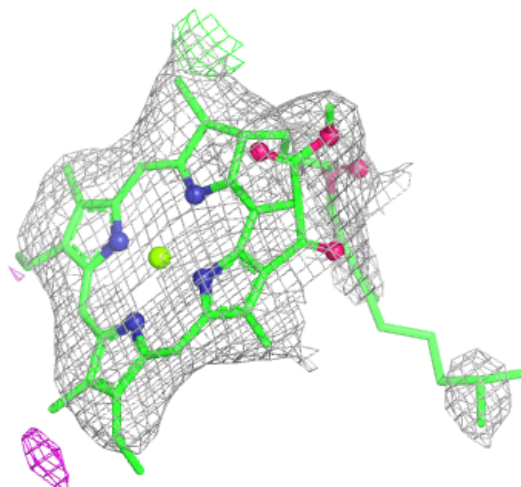
Electron density around CHL 2 526:

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



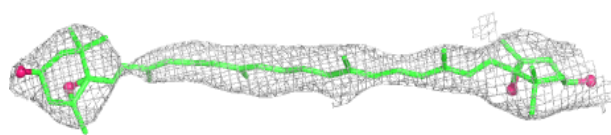
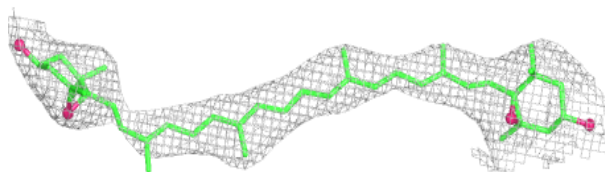
Electron density around CLA 2 514:

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

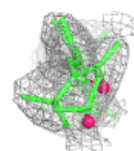
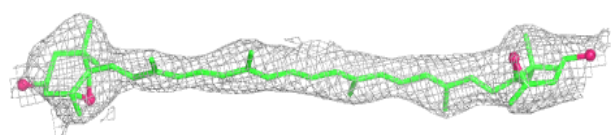
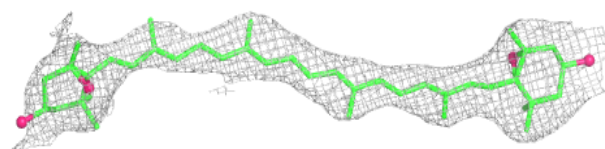


Electron density around XAT 2 502:

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

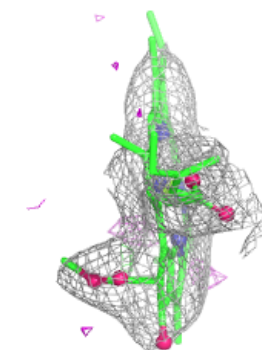
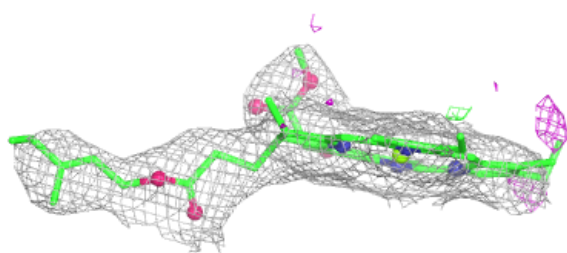
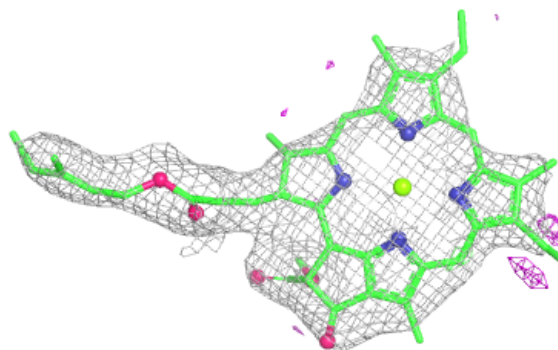
**Electron density around XAT 4 303:**

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

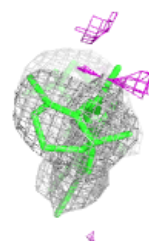
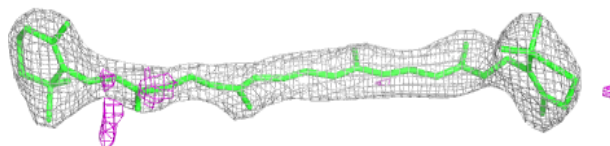
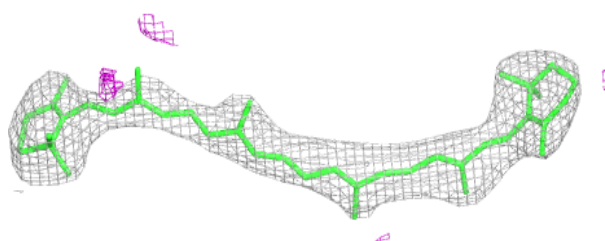


Electron density around CLA A 836:

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

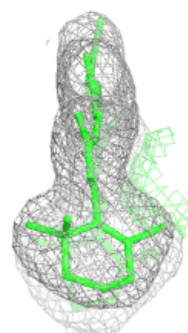
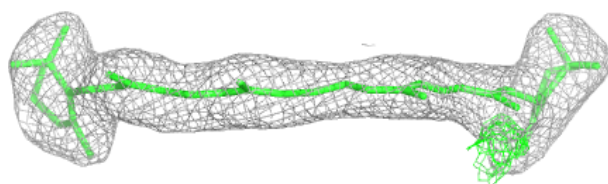
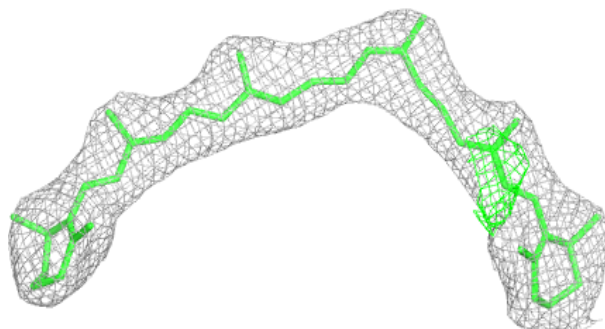
**Electron density around BCR B 853:**

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

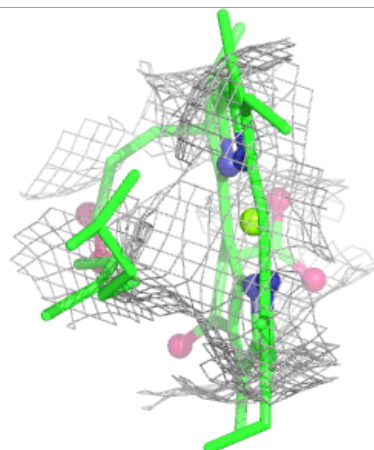
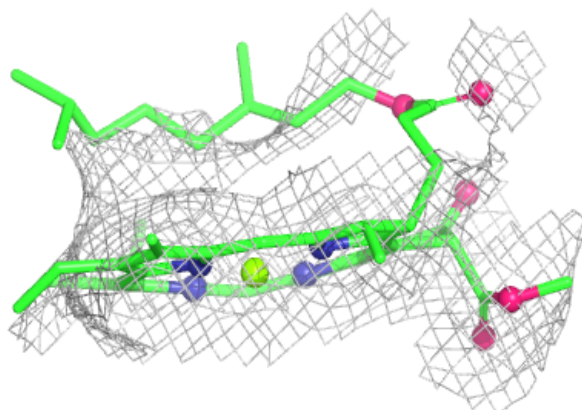
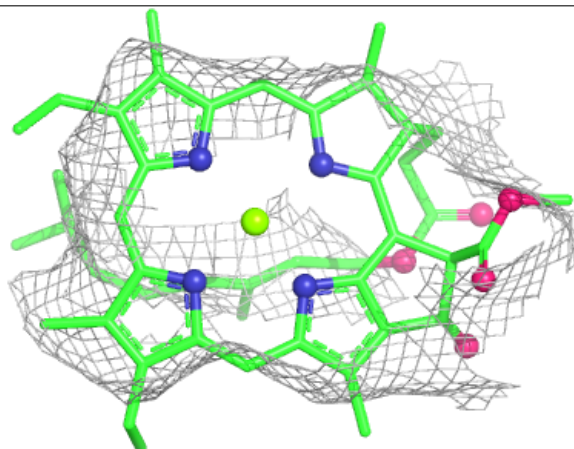


Electron density around BCR F 306:

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

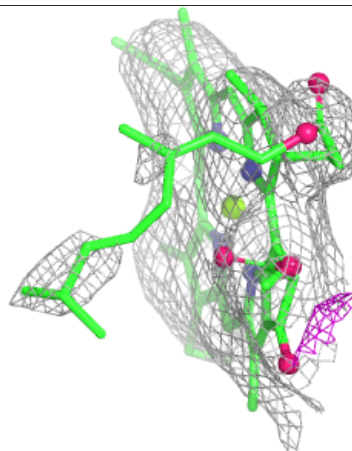
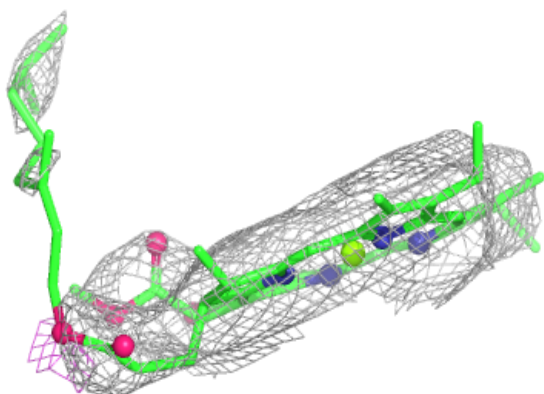
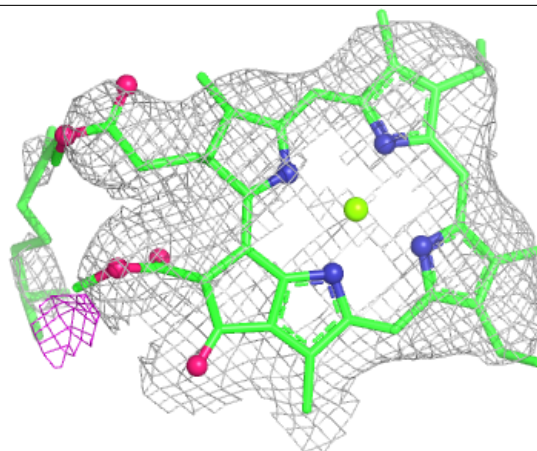
**Electron density around CLA 3 307:**

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



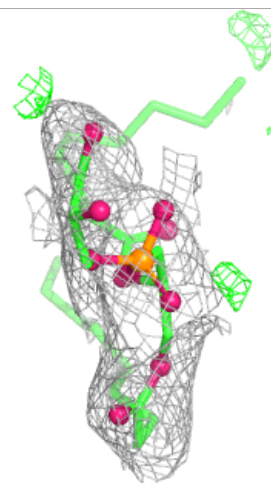
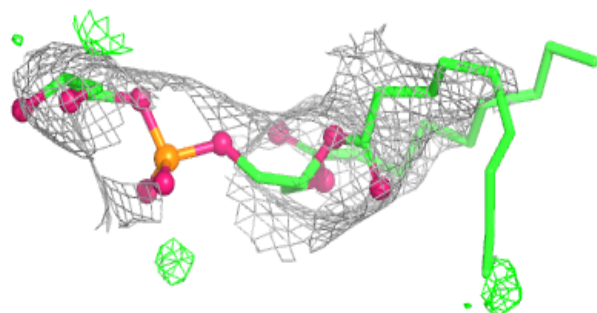
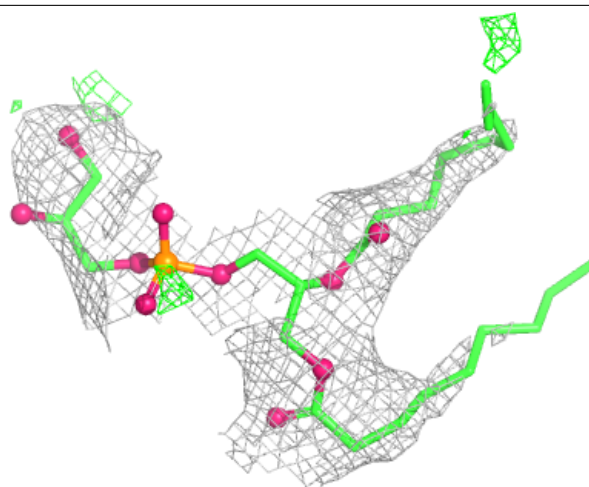
Electron density around CLA 3 309:

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



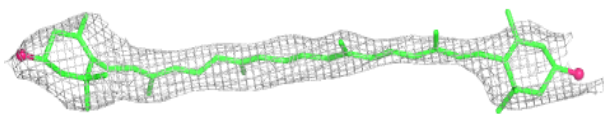
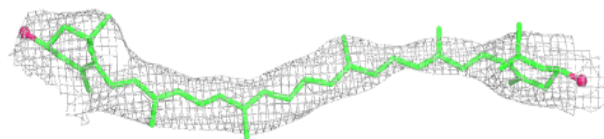
Electron density around LHG 2 517:

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

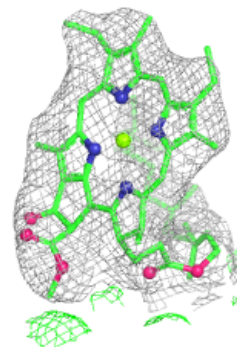
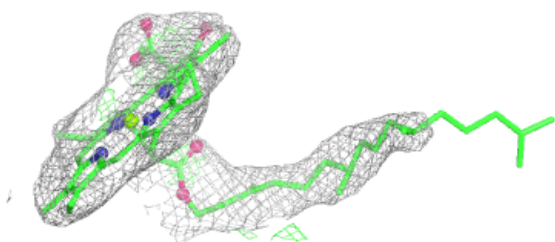
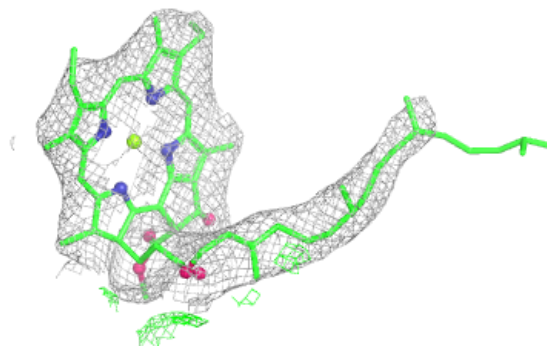


Electron density around LUT 2 501:

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

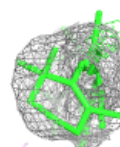
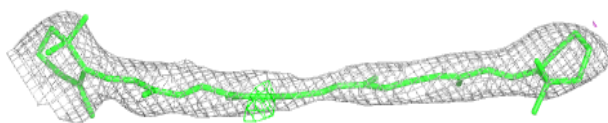
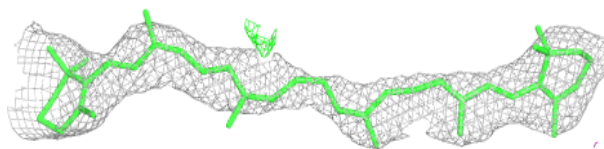
**Electron density around CLA B 822:**

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

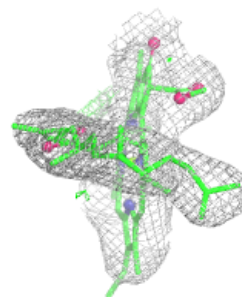
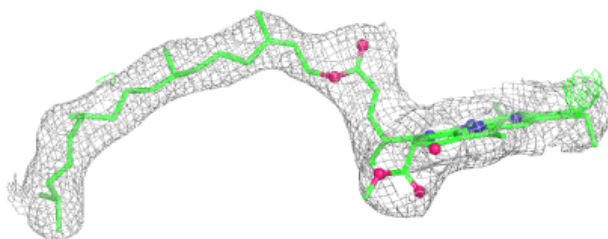
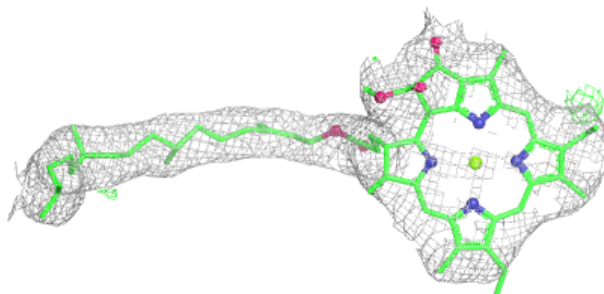


Electron density around BCR B 849:

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

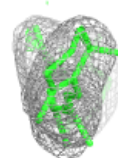
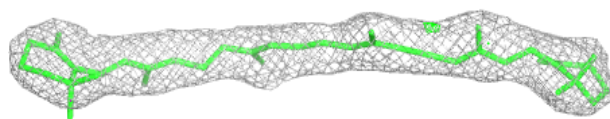
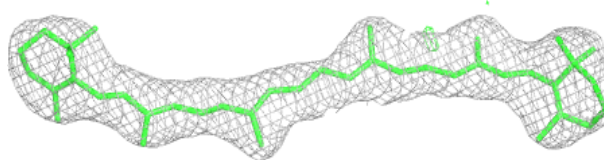
**Electron density around CLA B 840:**

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

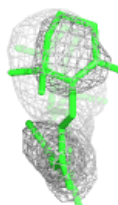
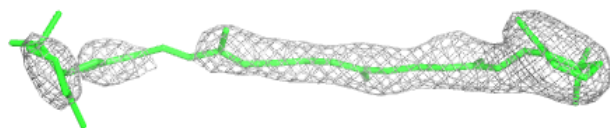
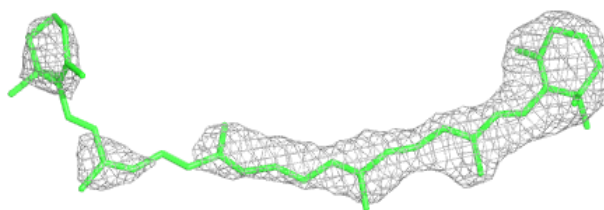


Electron density around BCR J 1108:

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

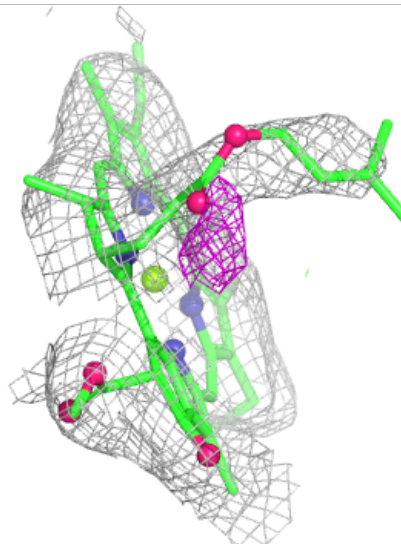
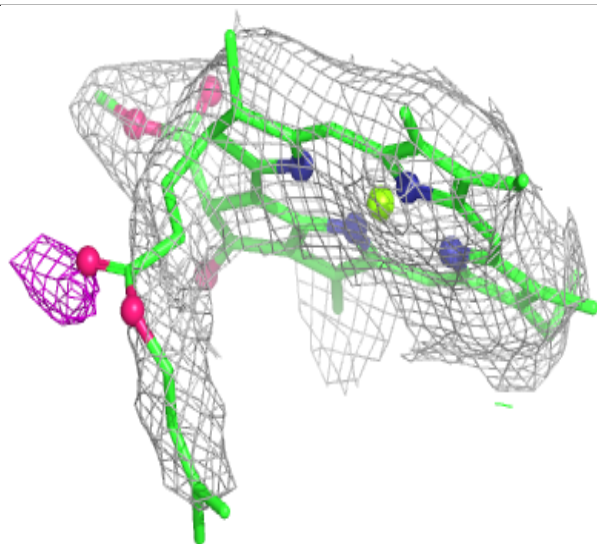
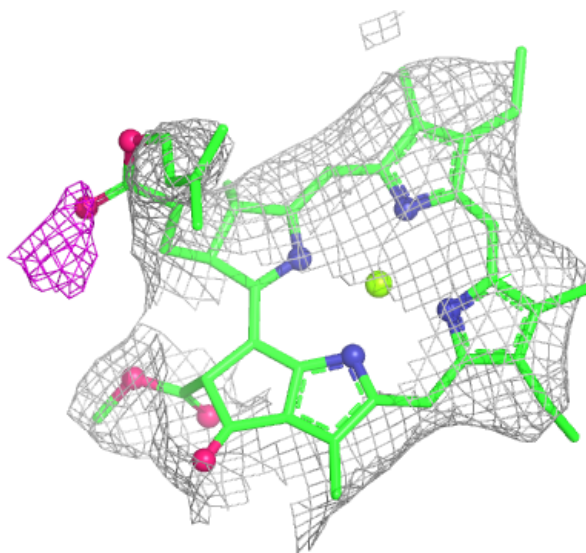
**Electron density around BCR B 850:**

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



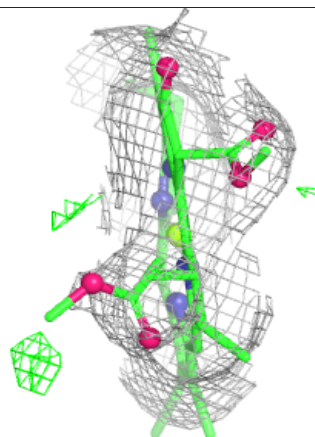
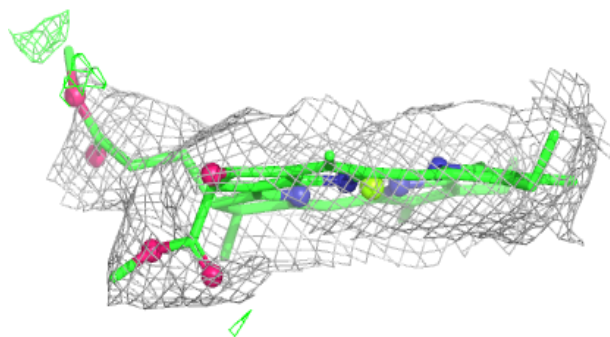
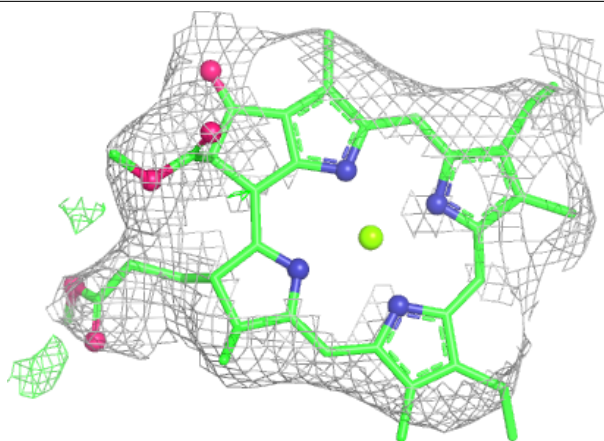
Electron density around CLA 3 315:

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



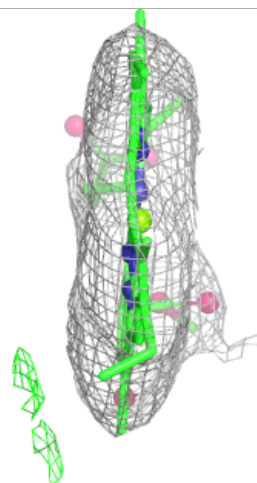
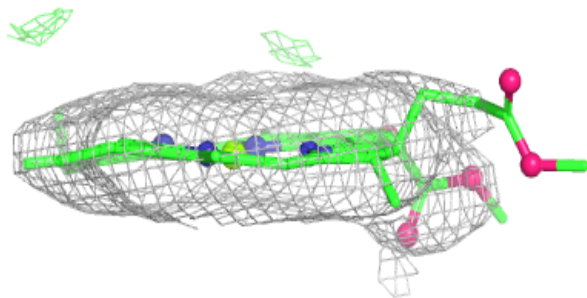
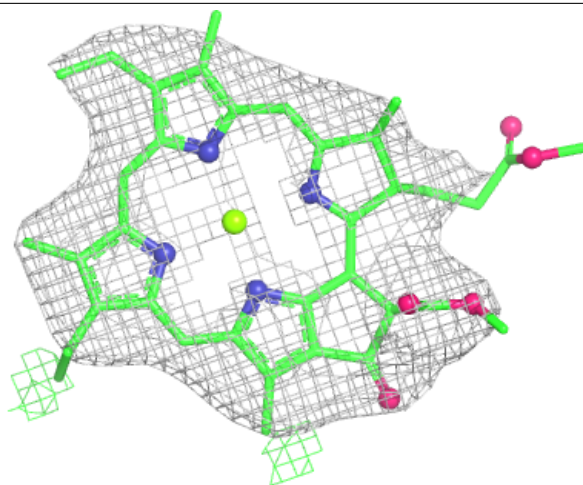
Electron density around CLA 3 316:

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



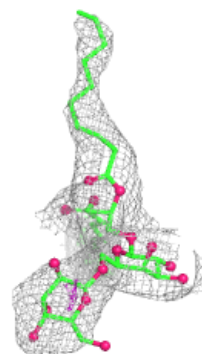
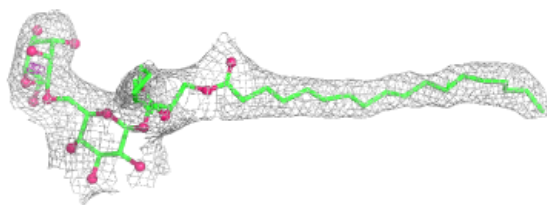
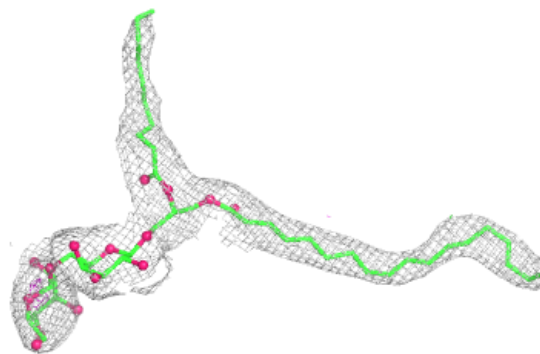
Electron density around CLA 3 317:

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



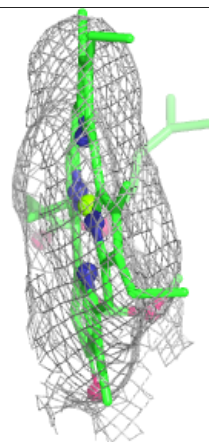
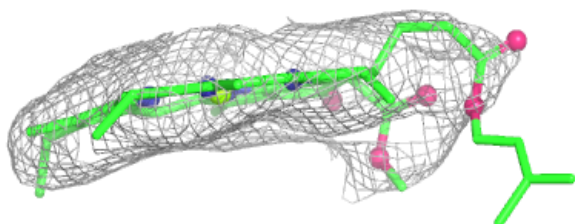
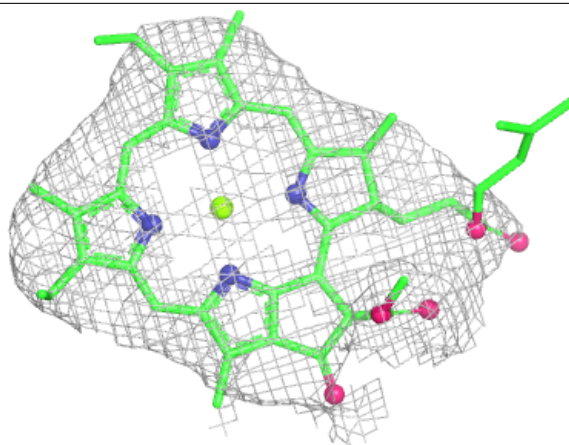
Electron density around DGD J 1106:

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

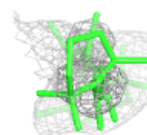
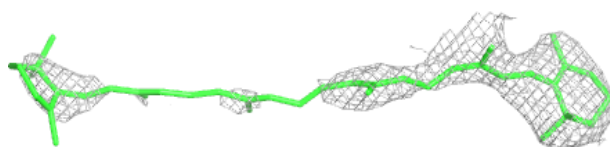
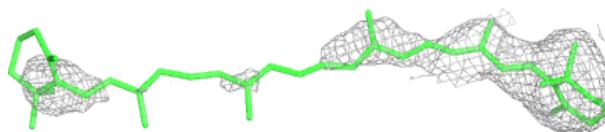


Electron density around CLA 4 305:

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

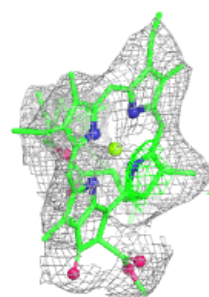
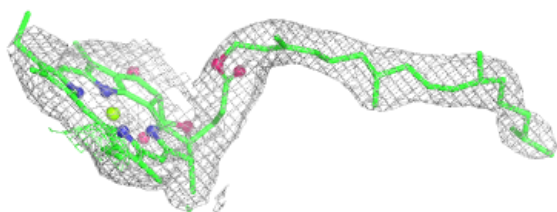
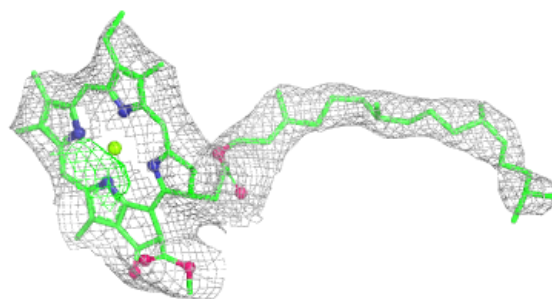
**Electron density around BCR A 848:**

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

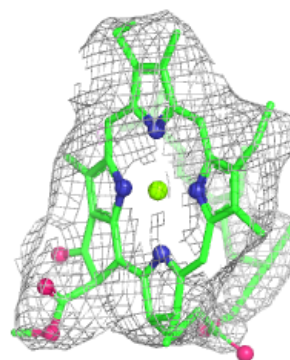
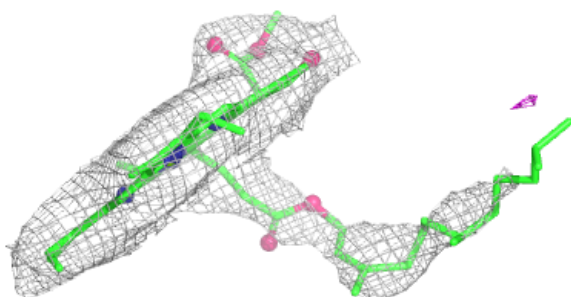
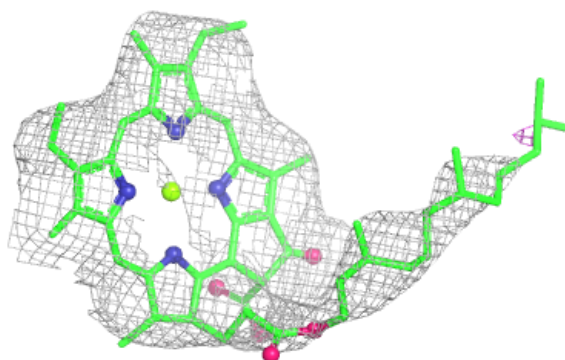


Electron density around CLA A 821:

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

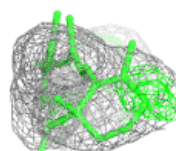
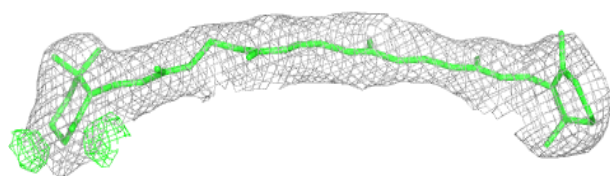
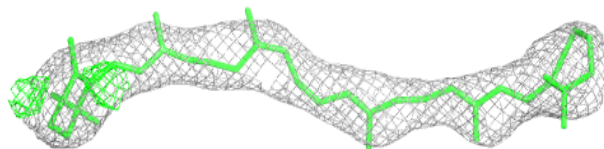
**Electron density around CLA A 822:**

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

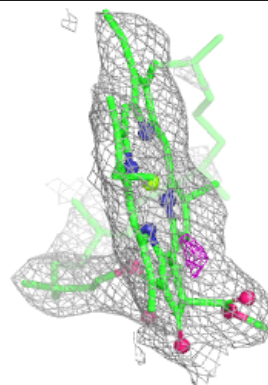
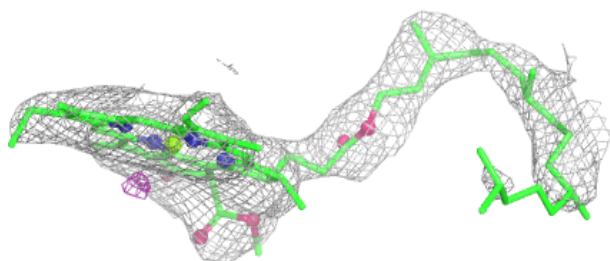
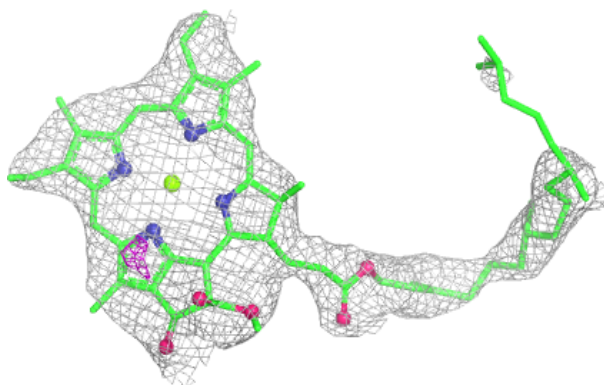


Electron density around BCR I 101:

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

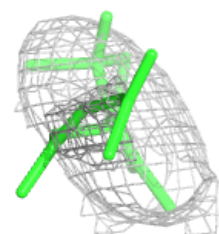
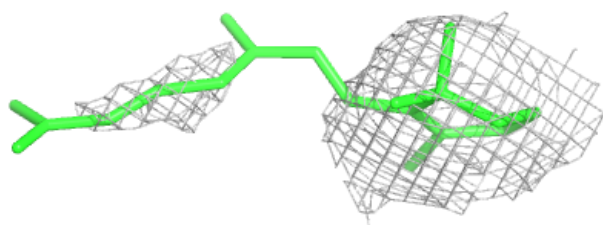
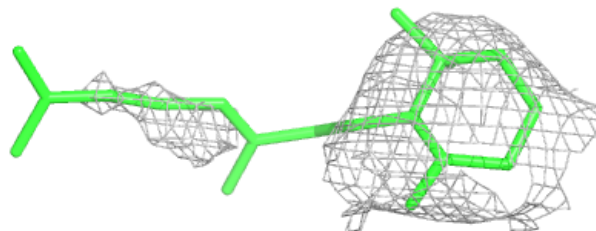
**Electron density around CLA A 827:**

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

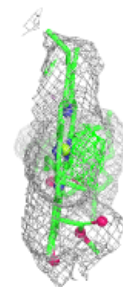
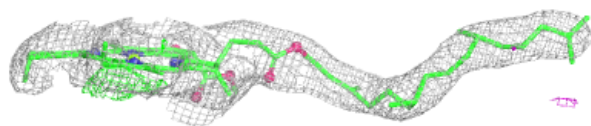
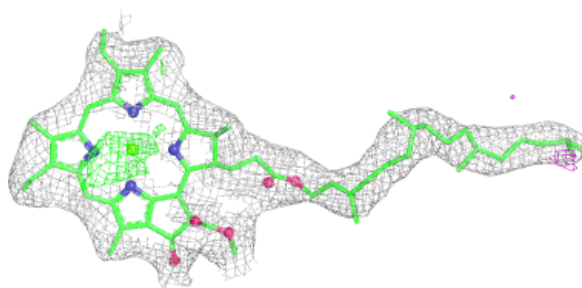


Electron density around BCR 1 503:

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

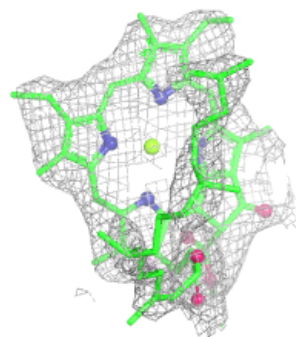
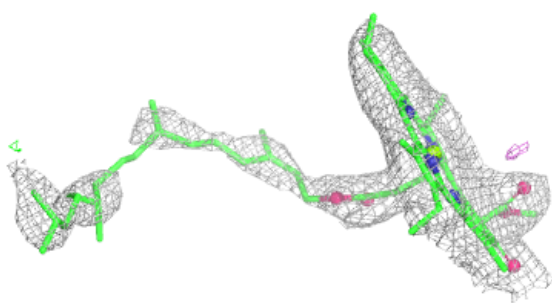
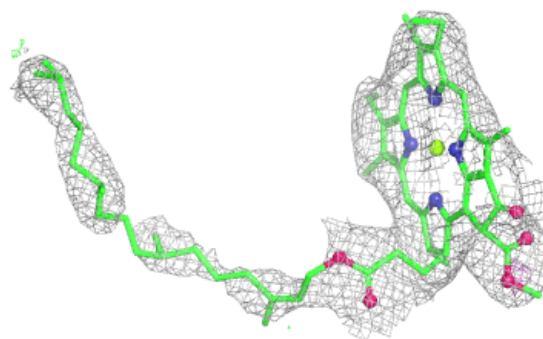
**Electron density around CLA A 832:**

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

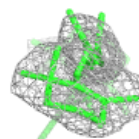
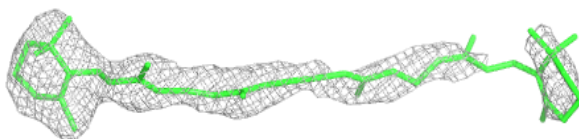
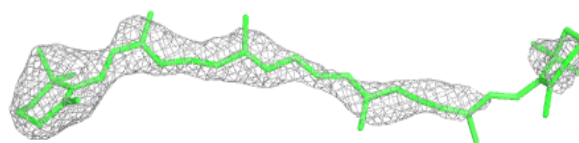


Electron density around CLA A 834:

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

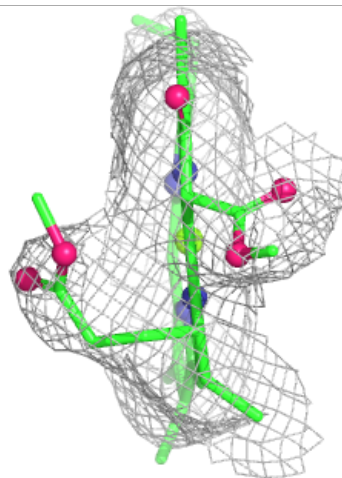
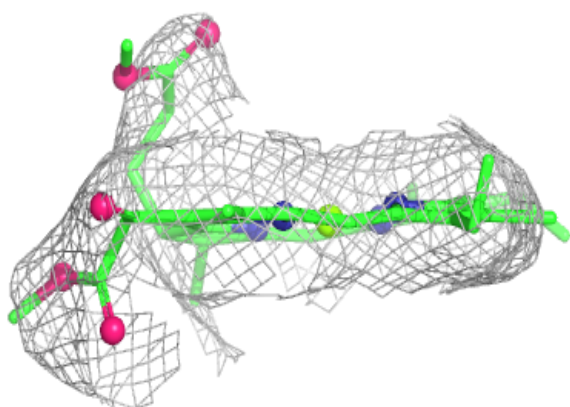
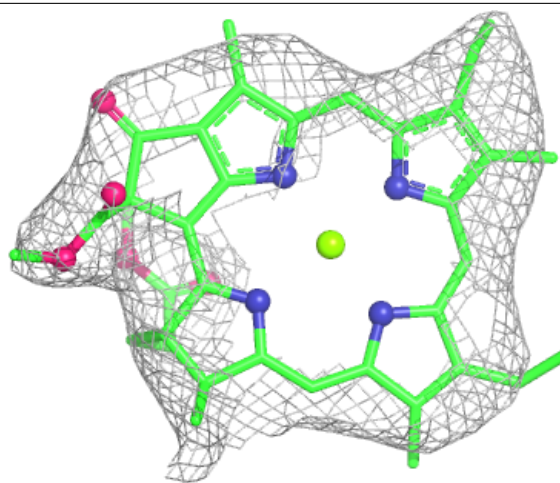
**Electron density around BCR A 849:**

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



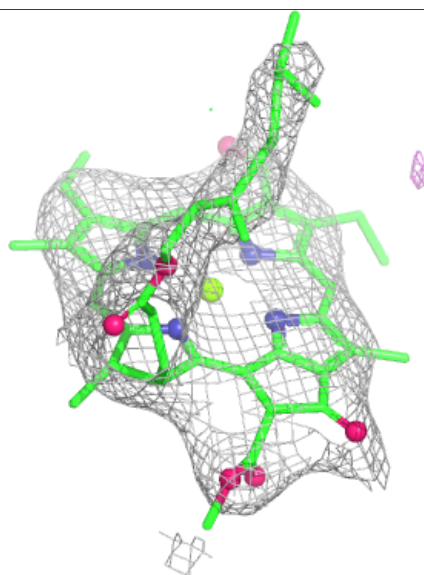
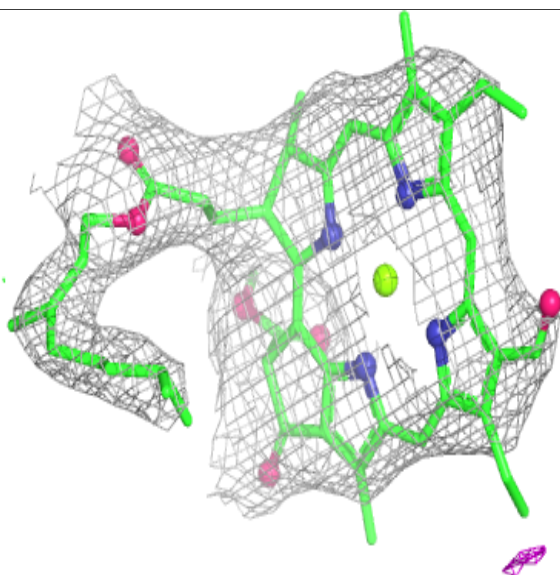
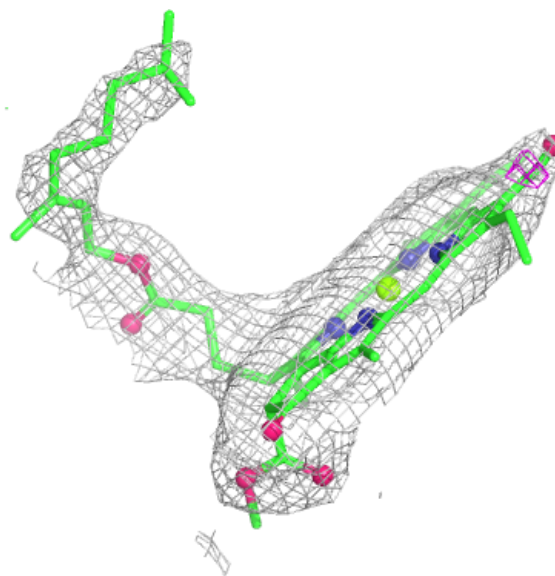
Electron density around CLA 4 311:

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



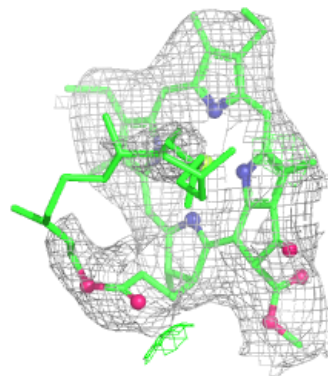
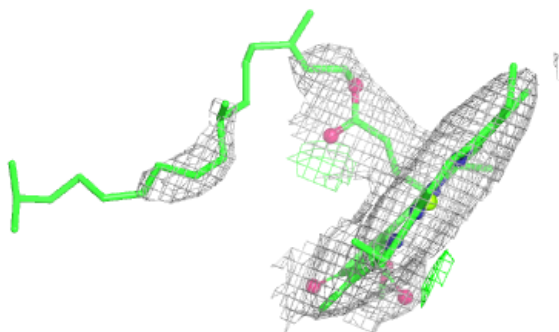
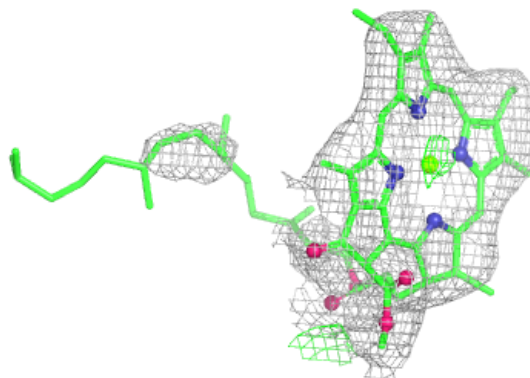
Electron density around CHL 1 521:

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

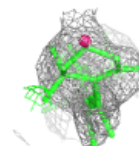
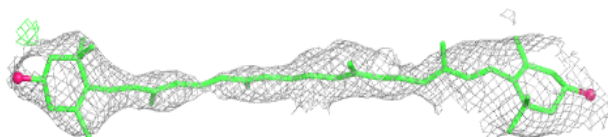
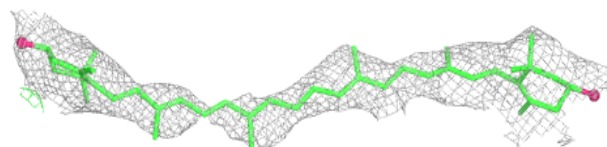


Electron density around CLA 4 315:

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

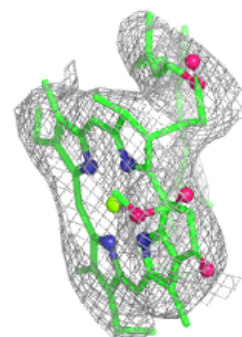
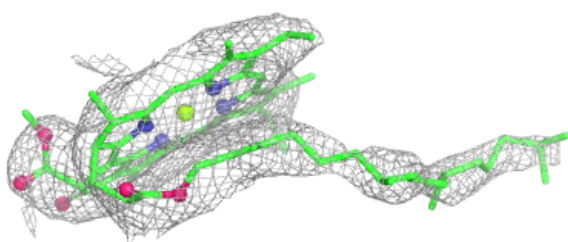
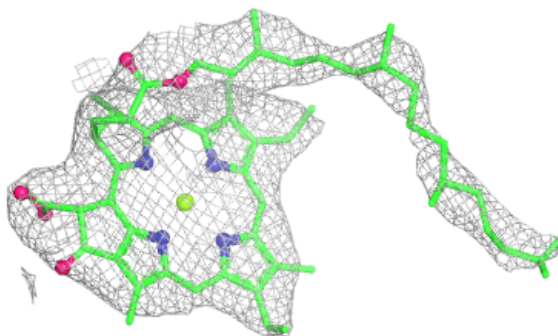
**Electron density around LUT 1 501:**

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

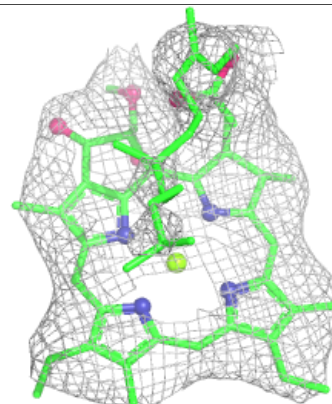
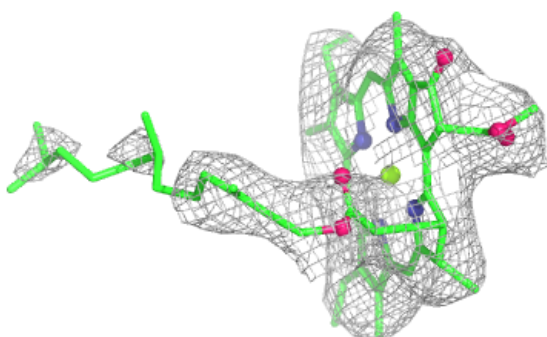
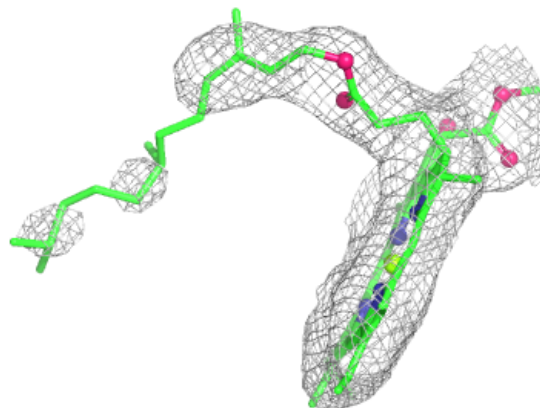


Electron density around CLA 1 507:

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

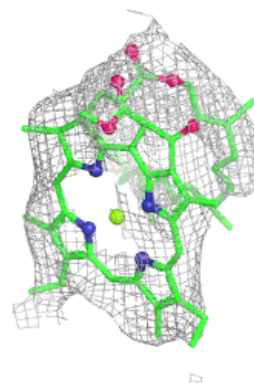
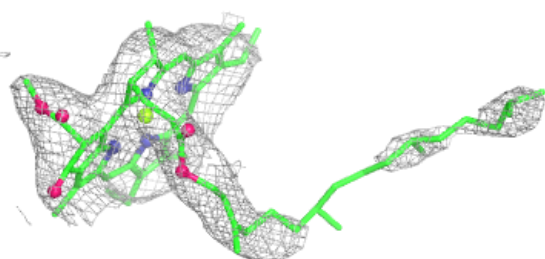
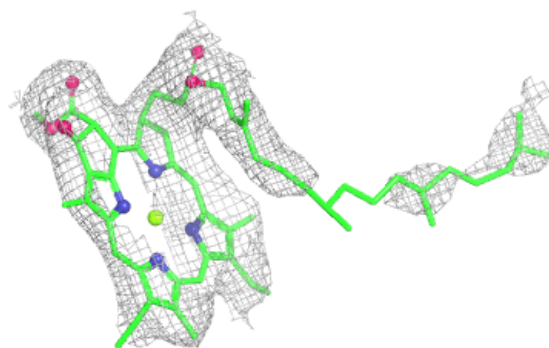
**Electron density around CLA A 807:**

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

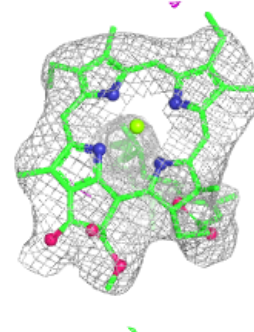
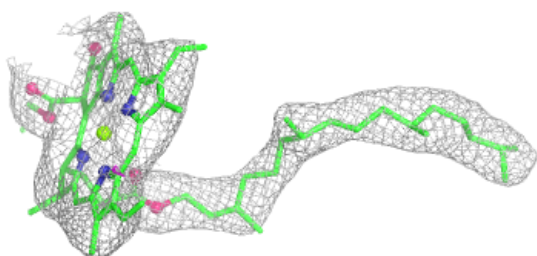
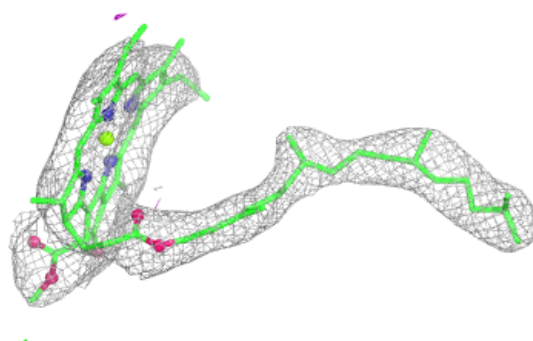


Electron density around CLA B 815:

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

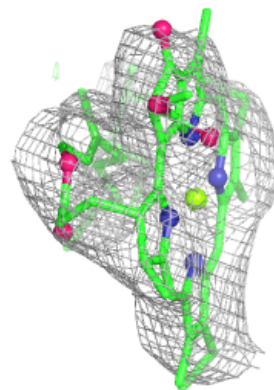
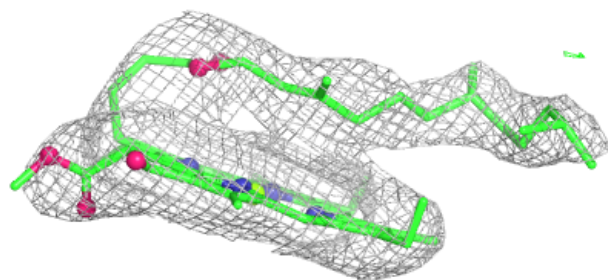
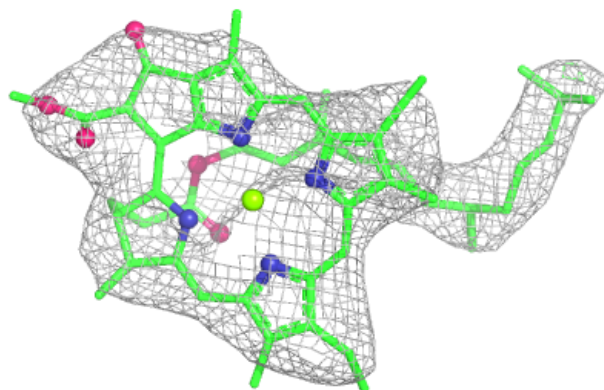
**Electron density around CLA A 811:**

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



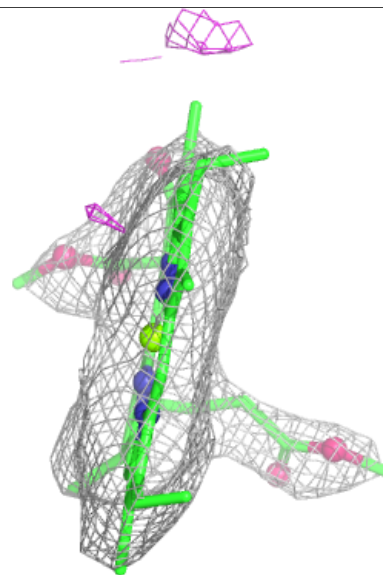
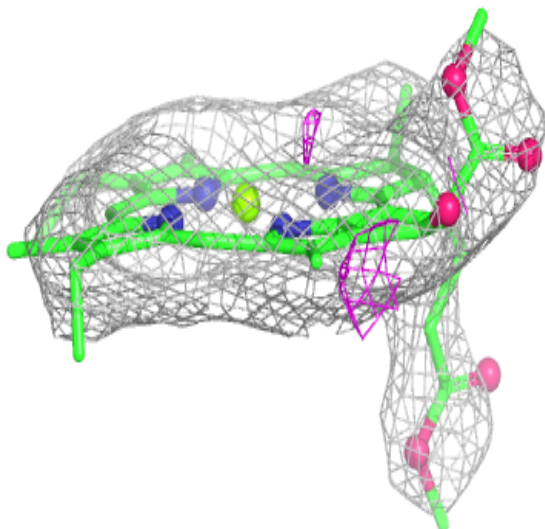
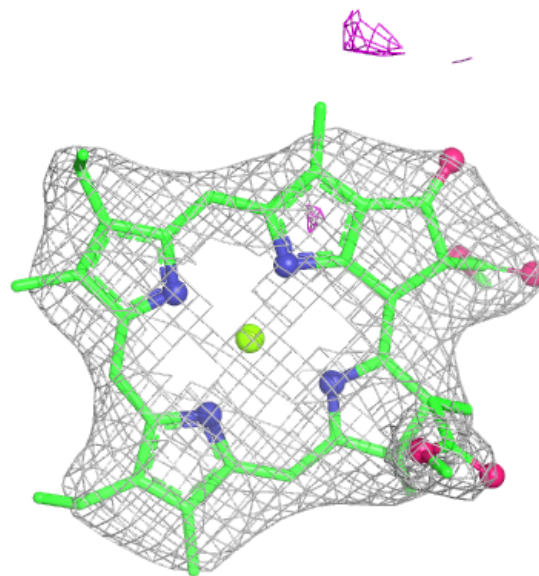
Electron density around CLA B 817:

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



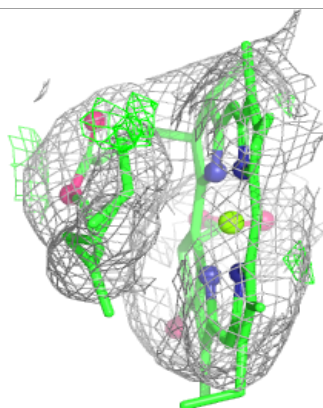
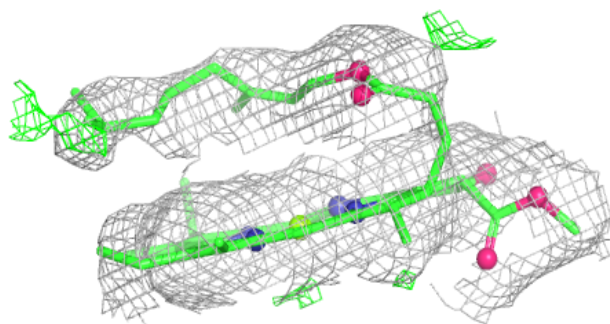
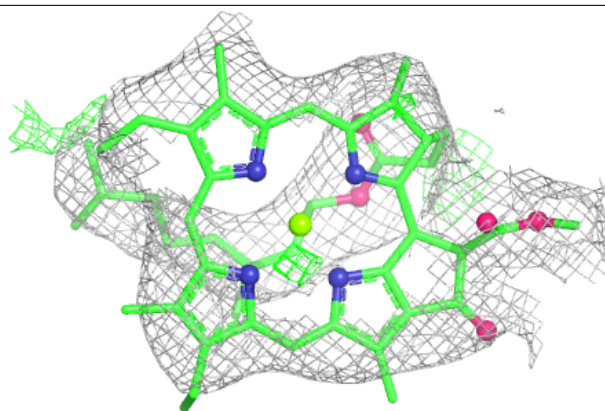
Electron density around CLA B 821:

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

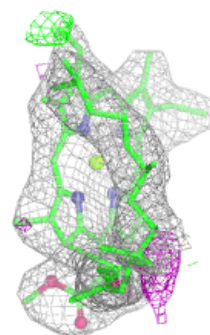
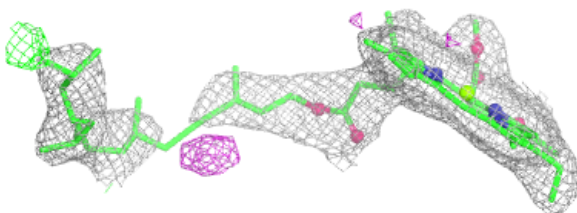
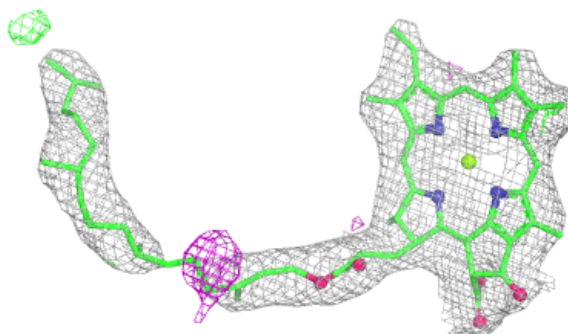


Electron density around CLA A 812:

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

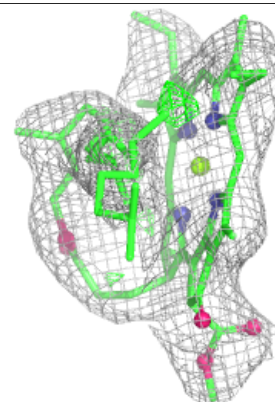
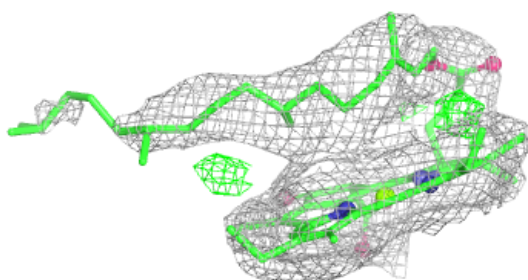
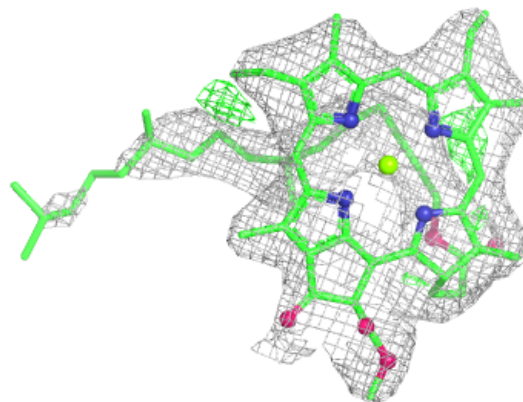
**Electron density around CLA B 825:**

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



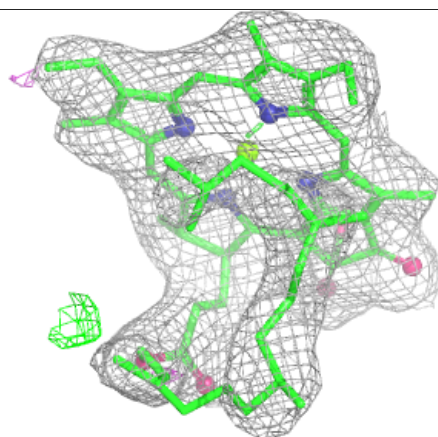
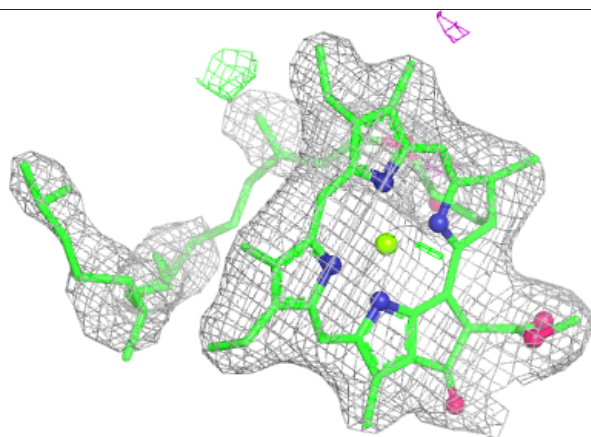
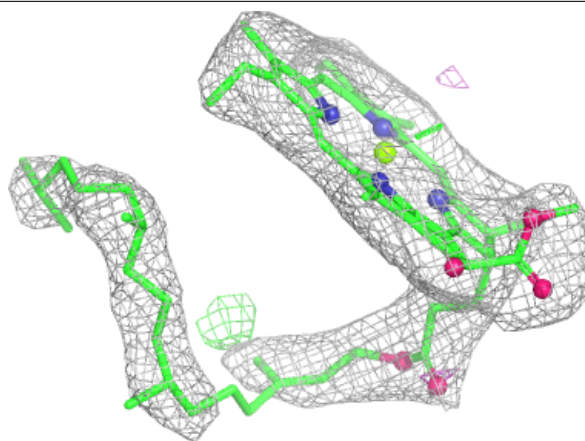
Electron density around CLA B 827:

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



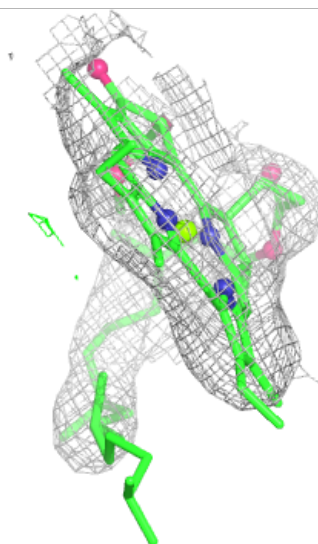
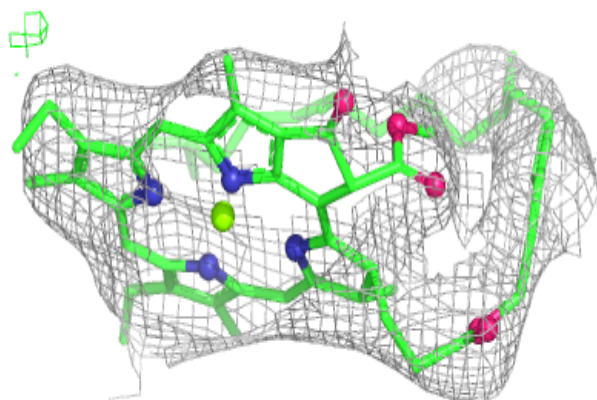
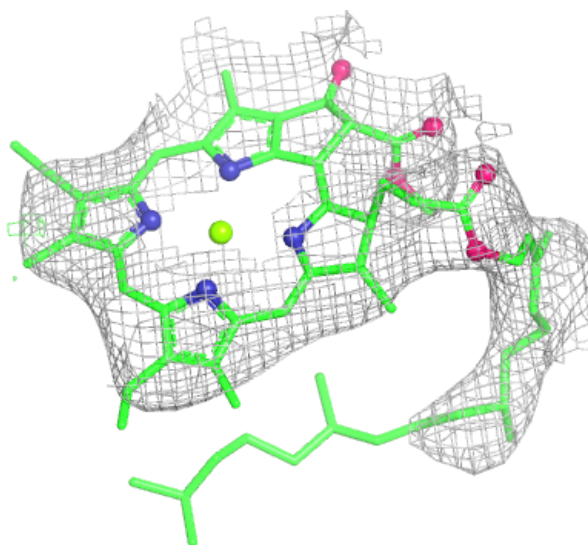
Electron density around CLA B 830:

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



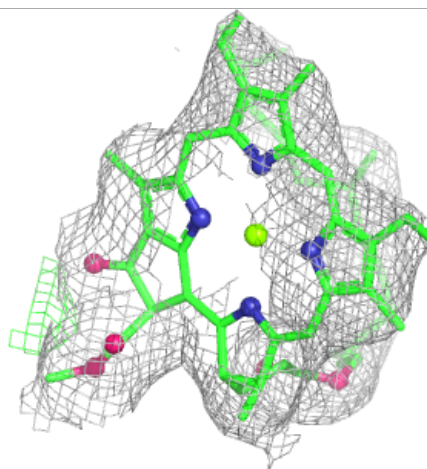
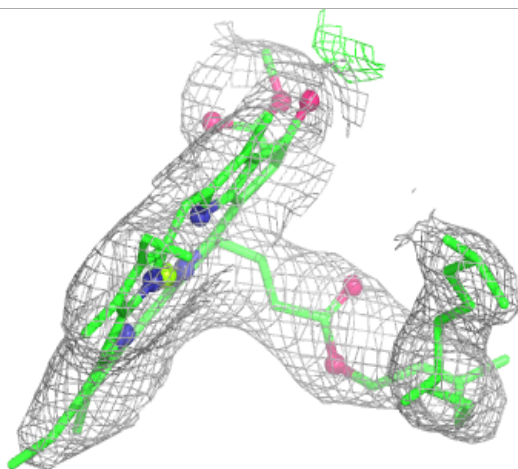
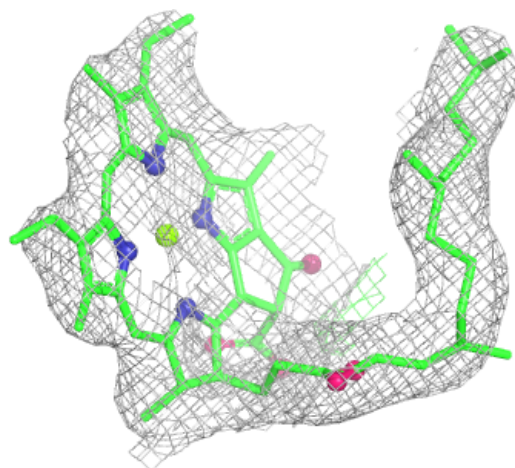
Electron density around CLA 1 508:

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



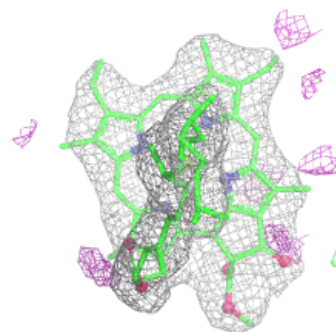
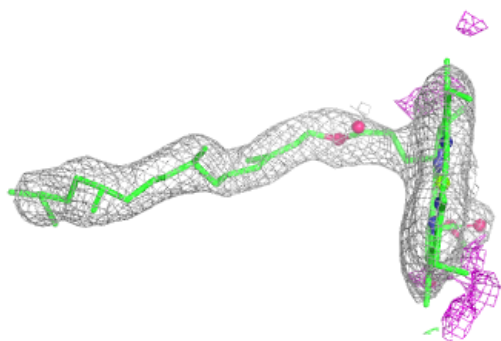
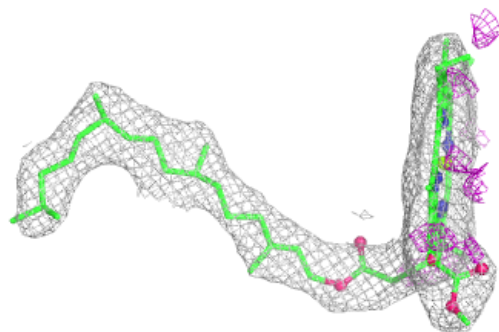
Electron density around CLA B 833:

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

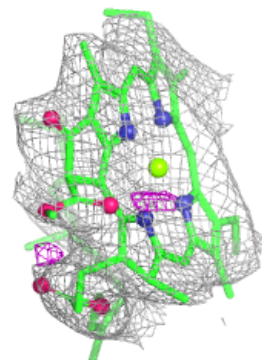
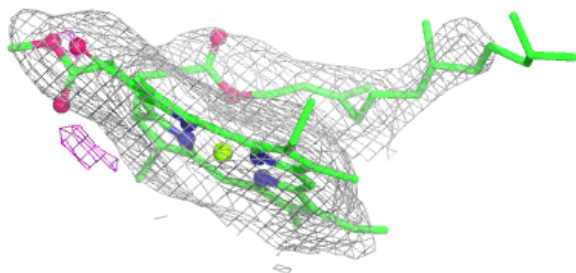
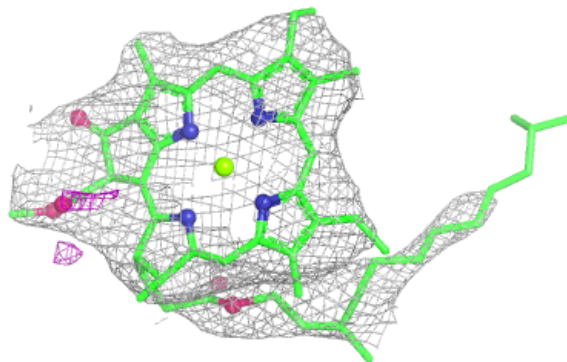


Electron density around CLA B 839:

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

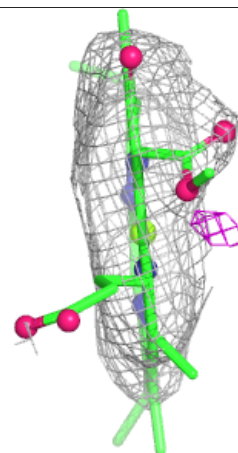
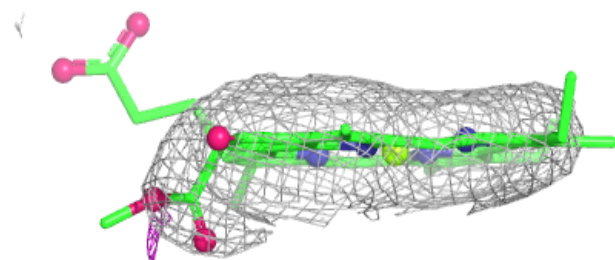
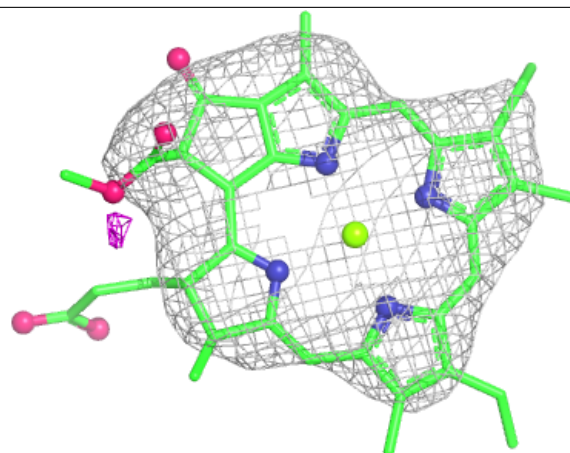
**Electron density around CLA 2 504:**

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



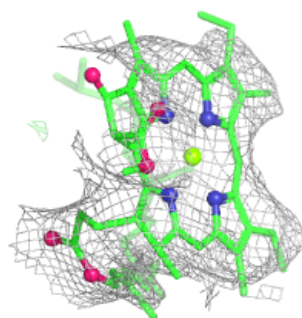
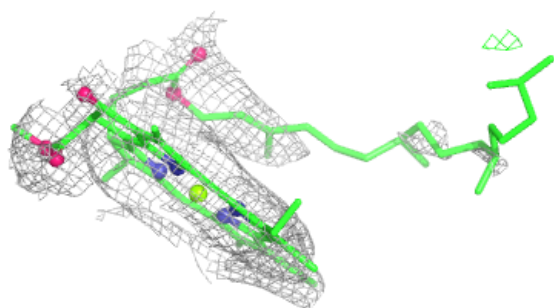
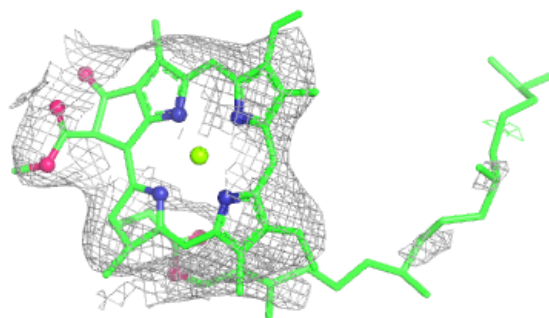
Electron density around CLA A 815:

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

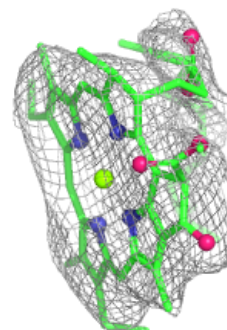
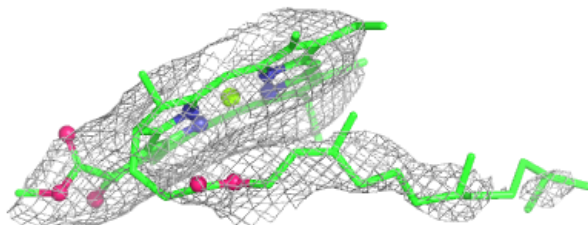
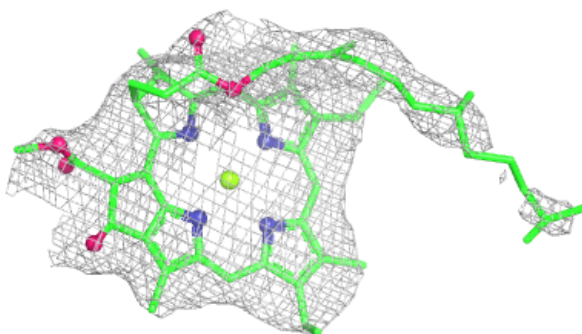


Electron density around CLA 3 308:

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

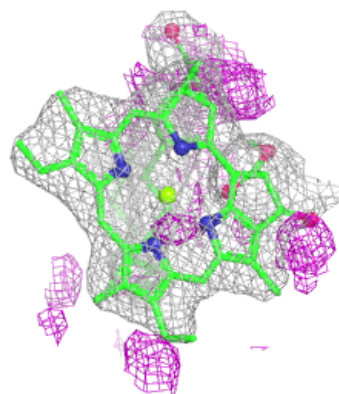
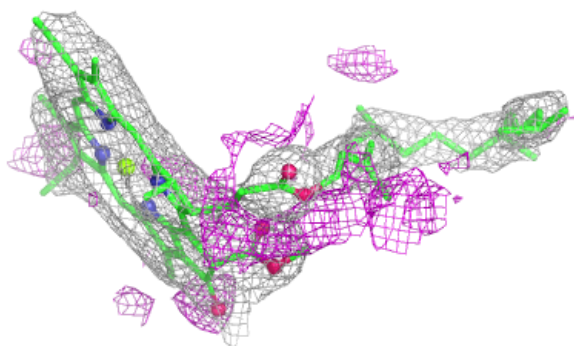
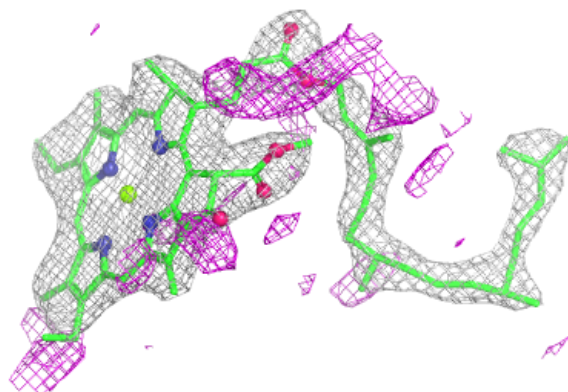
**Electron density around CLA 4 304:**

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

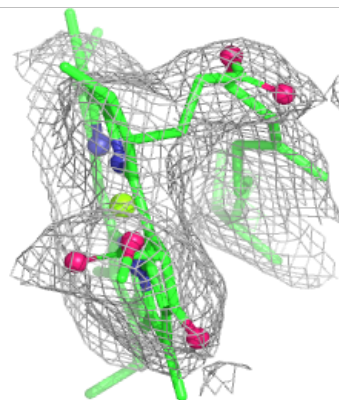
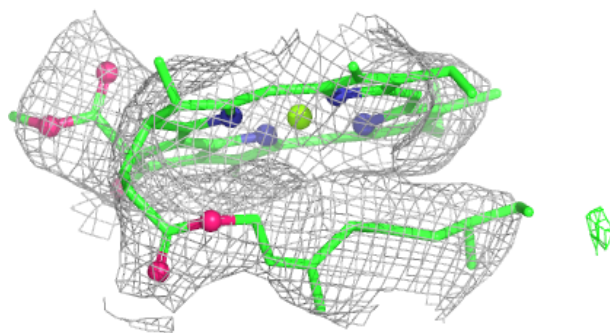
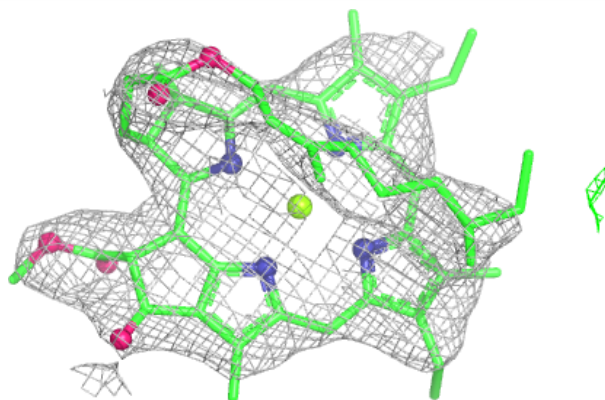


Electron density around CL0 A 801:

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

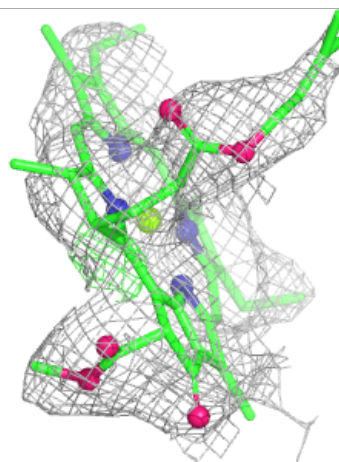
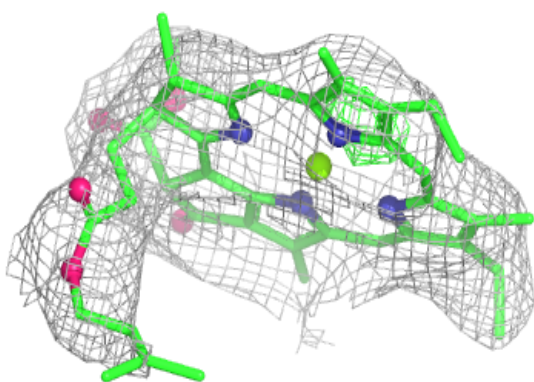
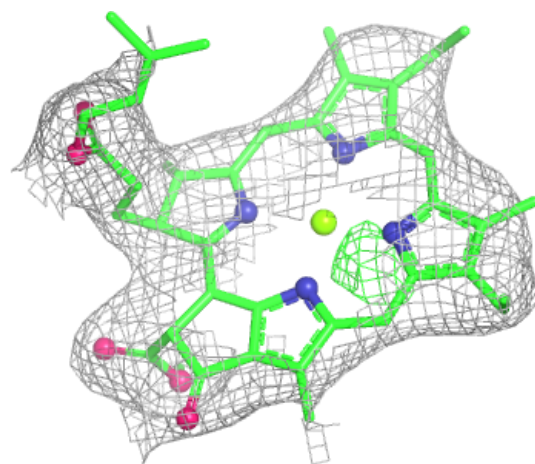
**Electron density around CLA A 818:**

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



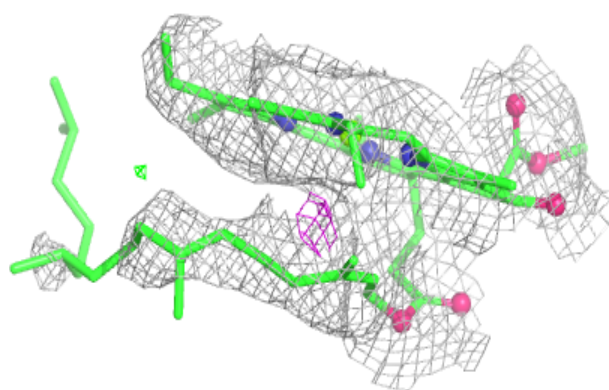
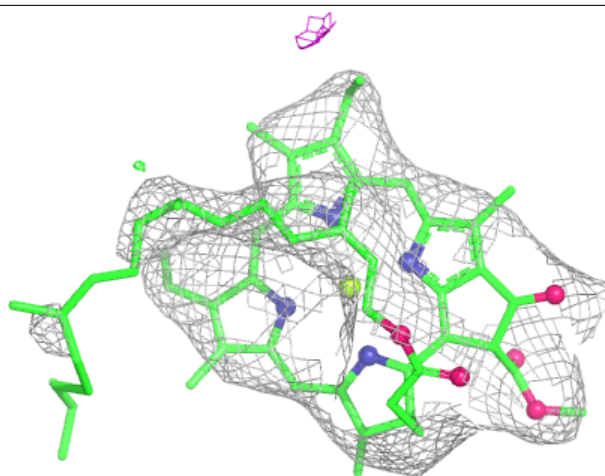
Electron density around CLA A 820:

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



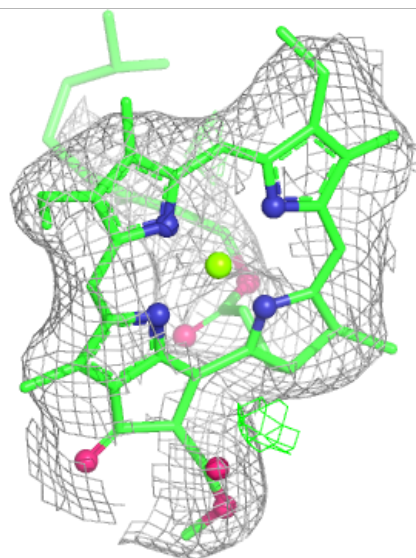
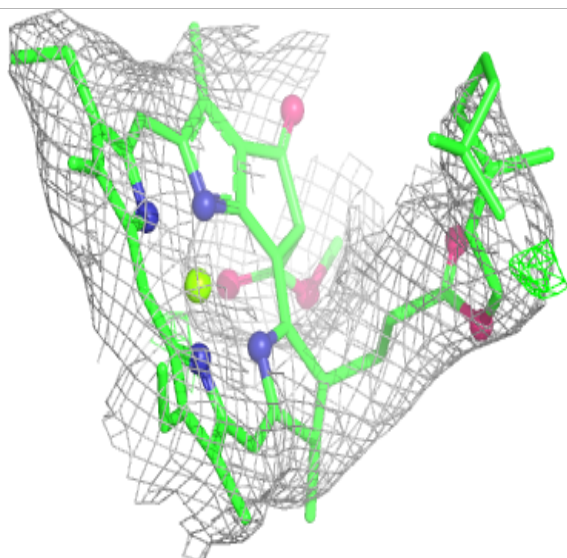
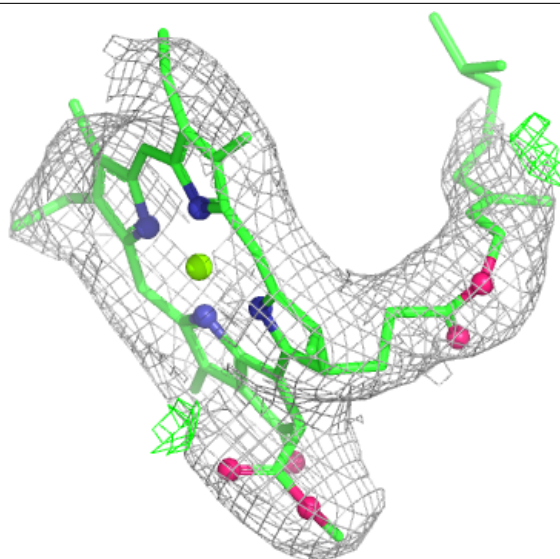
Electron density around CLA 4 306:

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



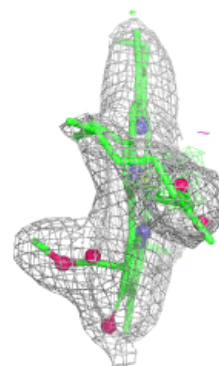
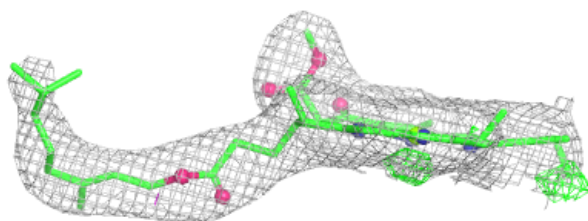
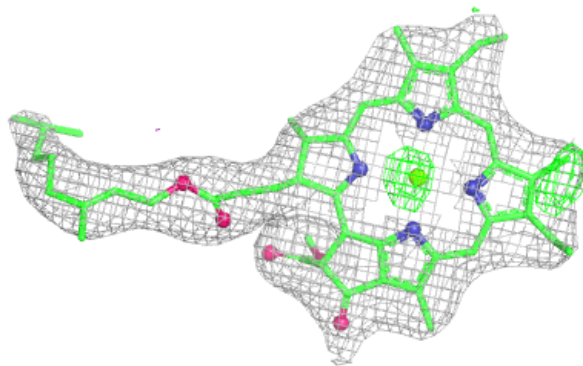
Electron density around CLA B 834:

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

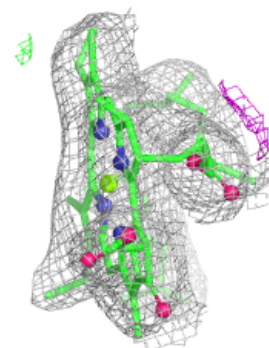
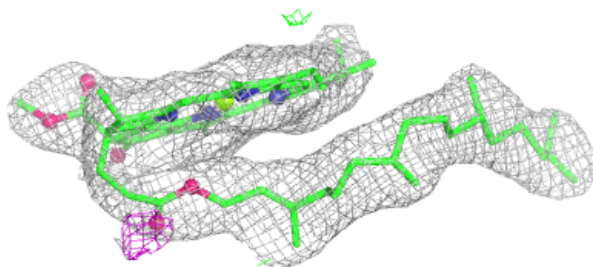
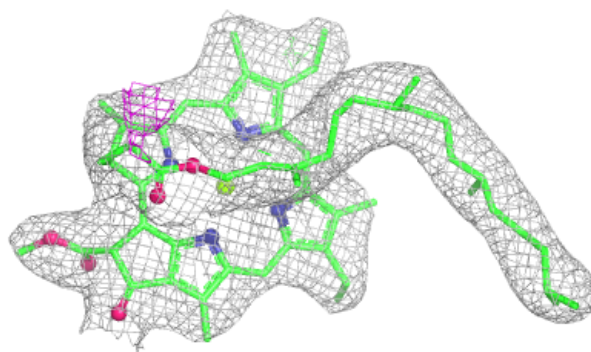


Electron density around CLA B 835:

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

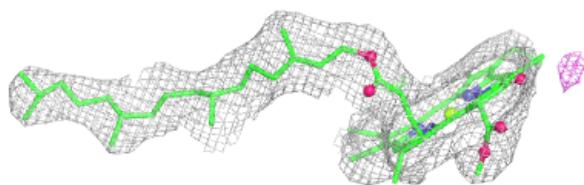
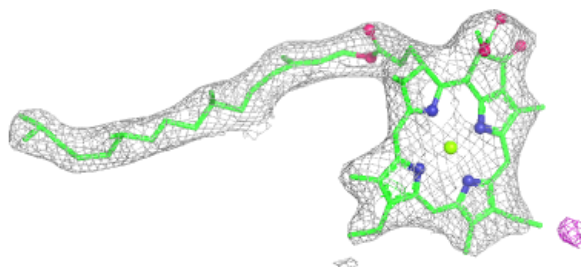
**Electron density around CLA B 836:**

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



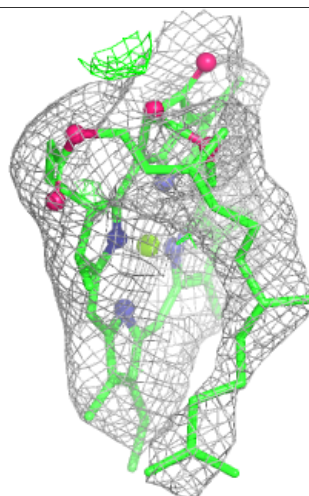
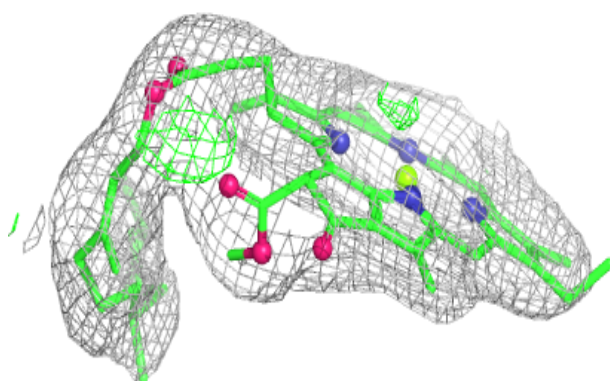
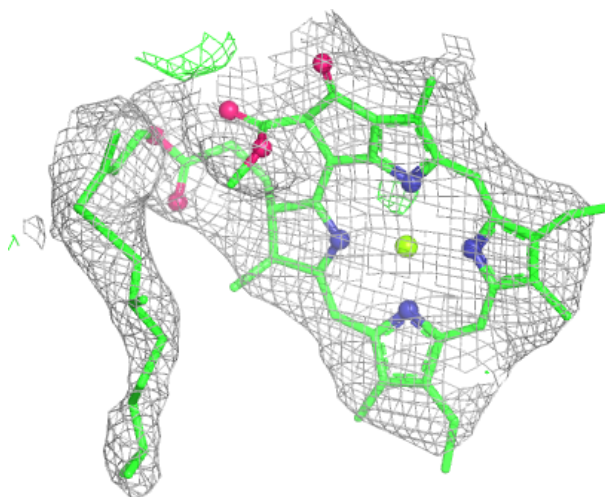
Electron density around CLA A 833:

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



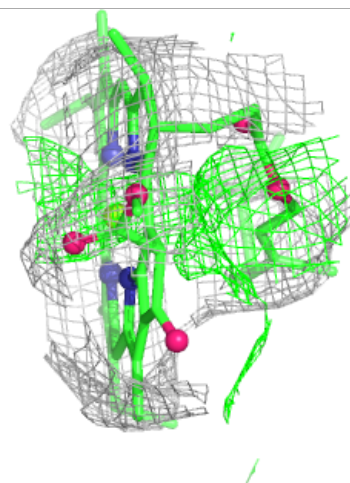
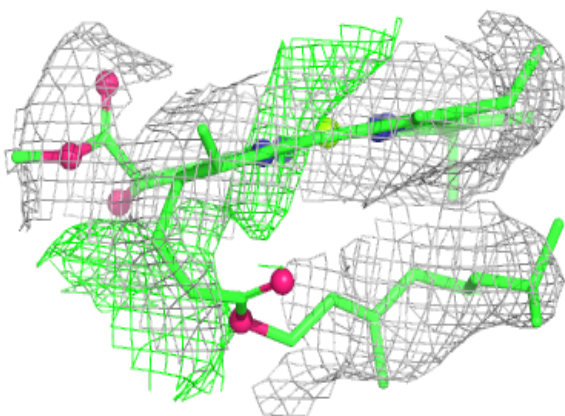
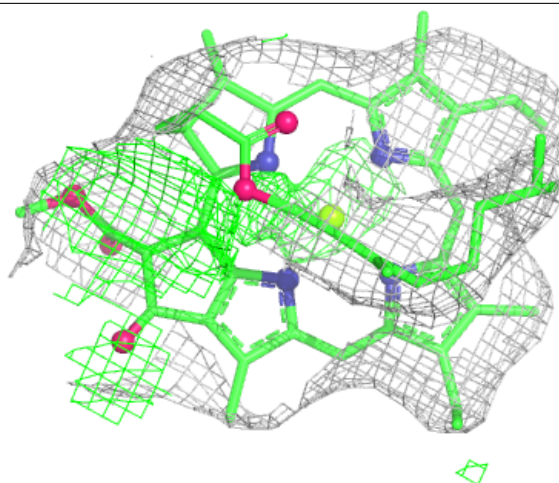
Electron density around CLA 4 308:

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



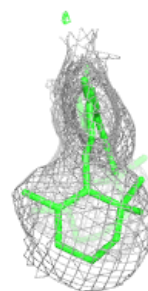
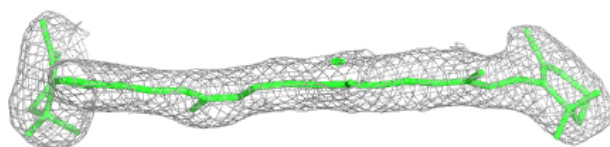
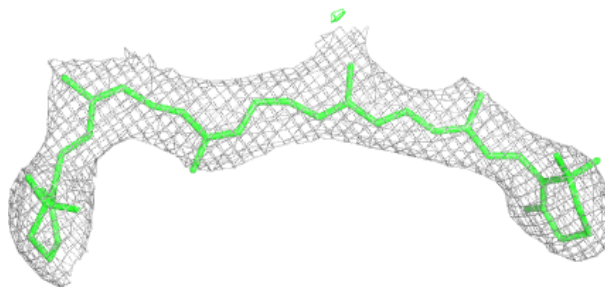
Electron density around CLA 1 506:

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

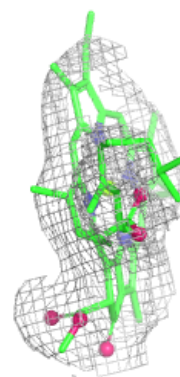
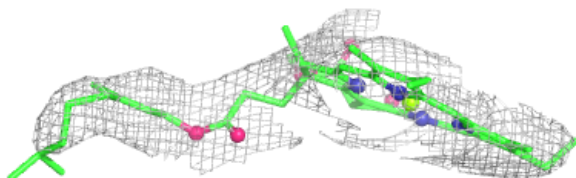
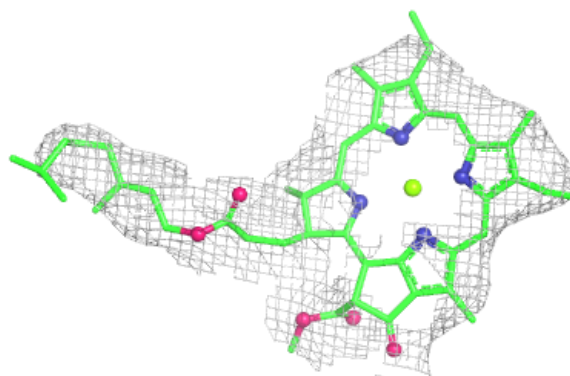


Electron density around BCR L 302:

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

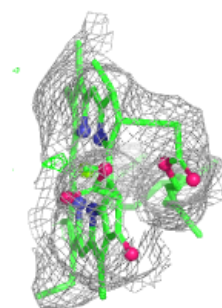
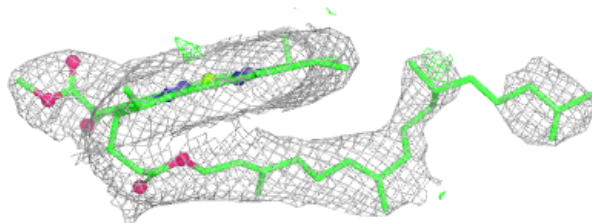
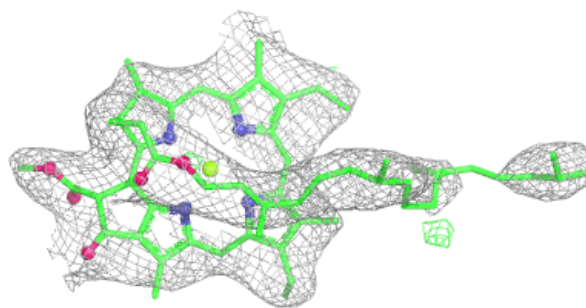
**Electron density around CLA G 202:**

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

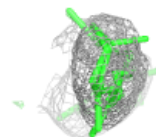
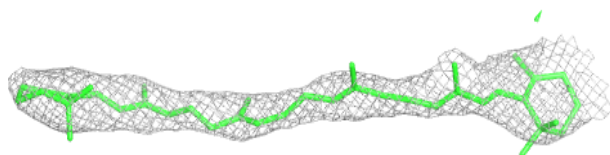
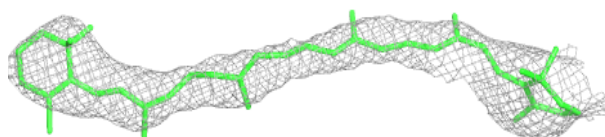


Electron density around CLA A 837:

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

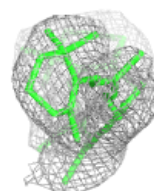
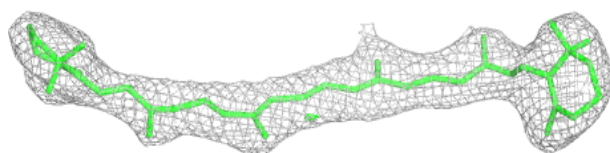
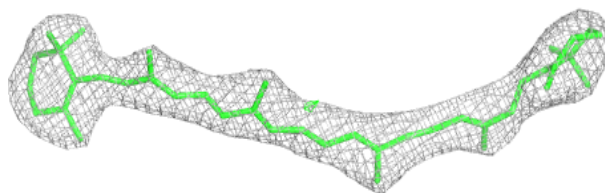
**Electron density around BCR 4 301:**

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

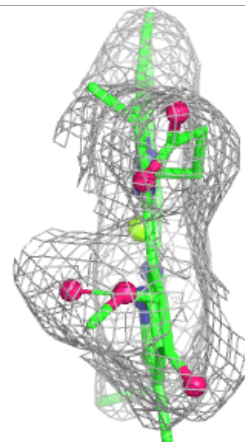
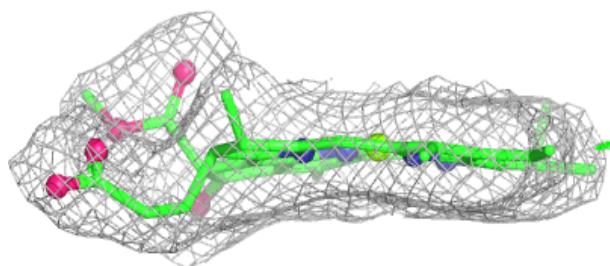
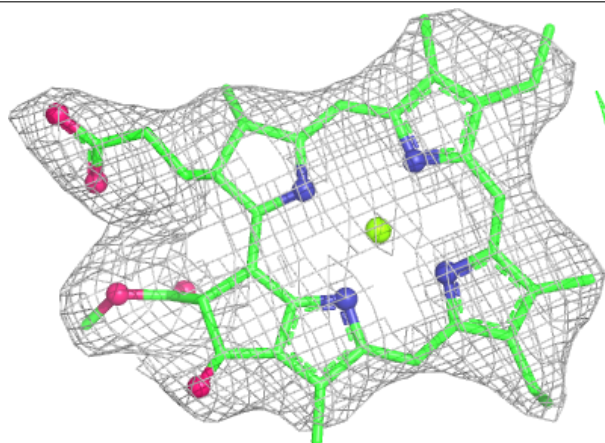


Electron density around BCR B 856:

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

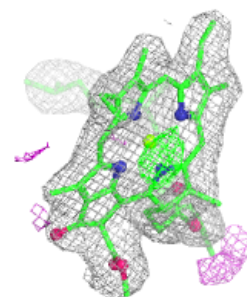
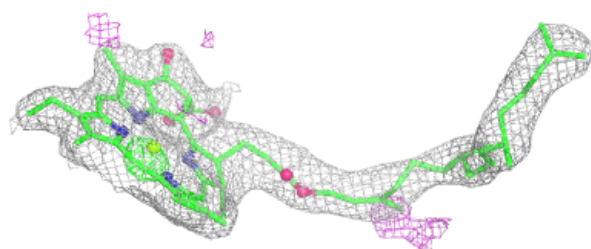
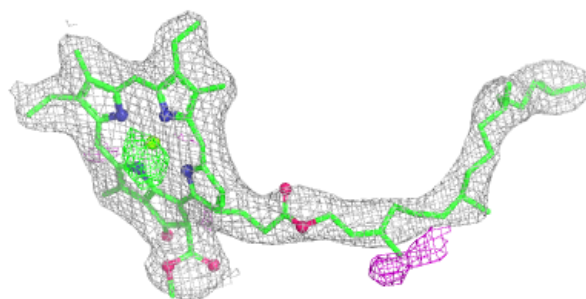
**Electron density around CLA J 1102:**

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



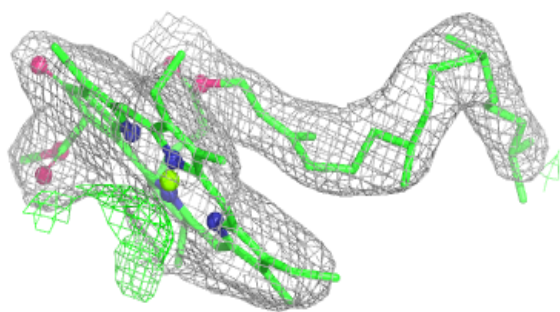
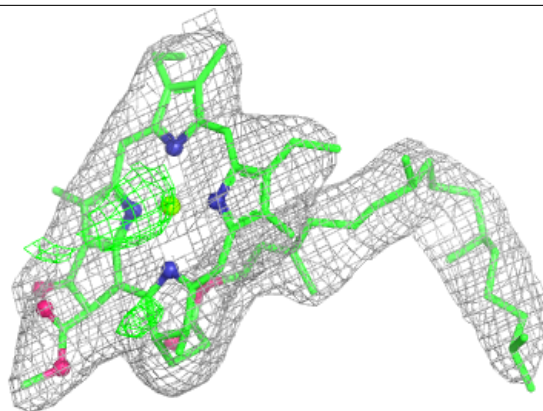
Electron density around CLA A 854:

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



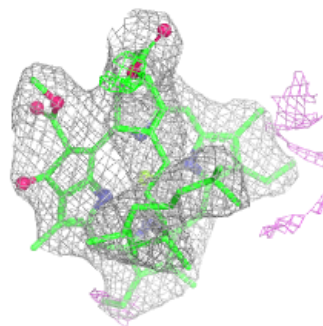
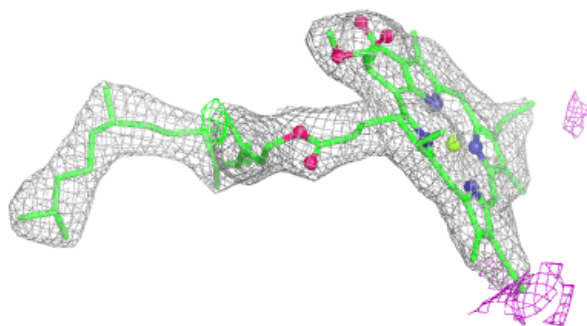
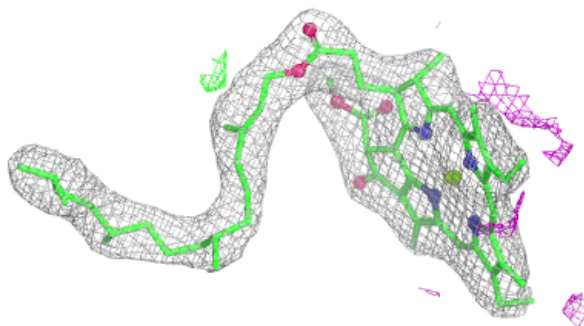
Electron density around CLA A 855:

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

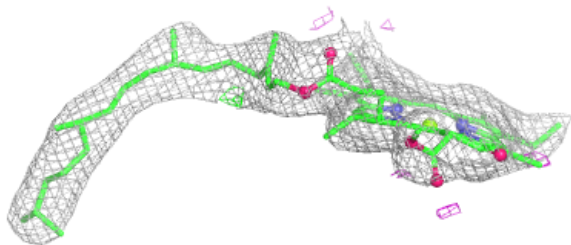
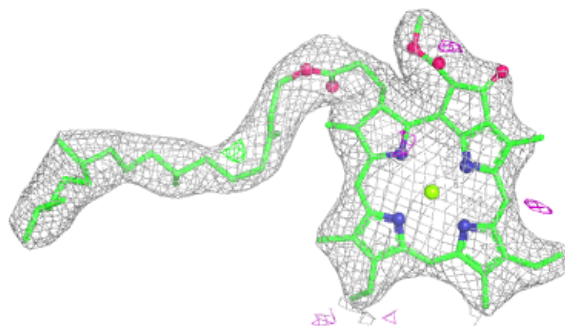


Electron density around CLA B 803:

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

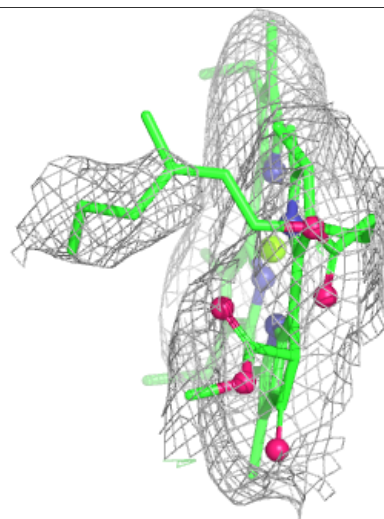
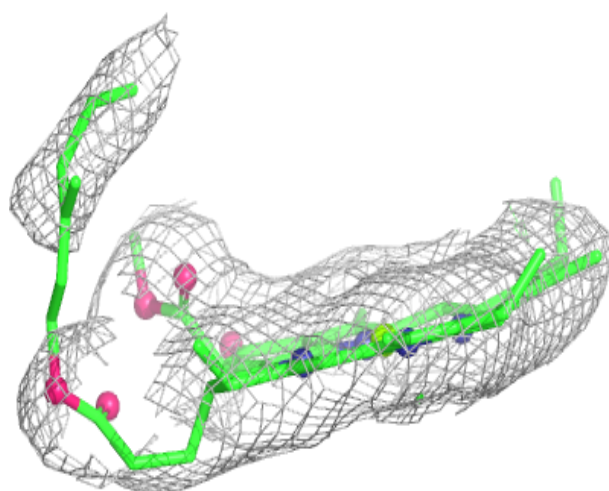
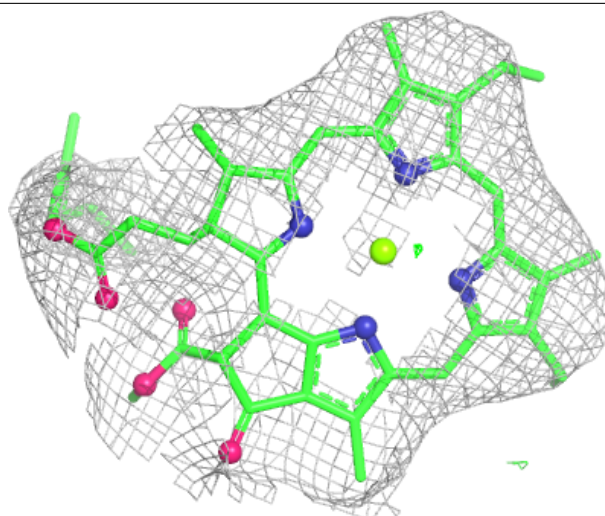
**Electron density around CLA B 804:**

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



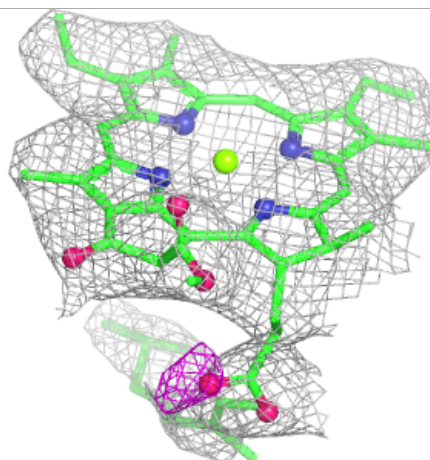
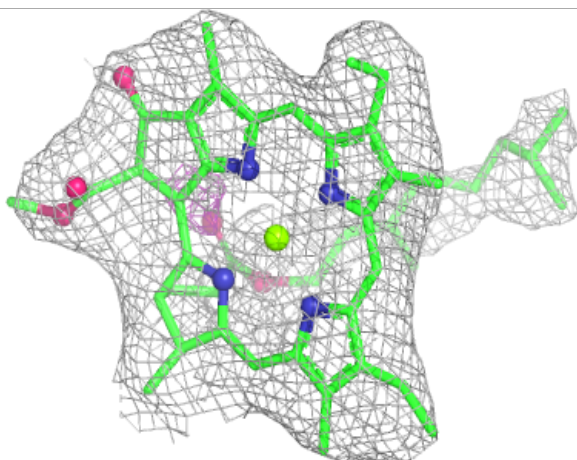
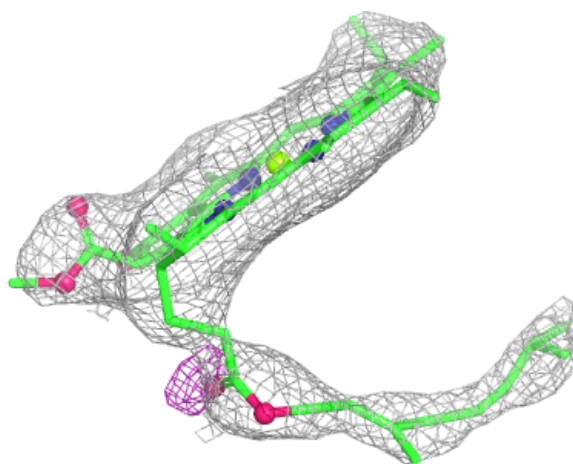
Electron density around CLA 2 505:

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



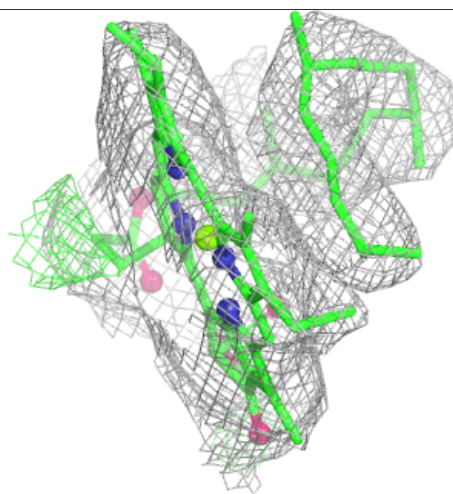
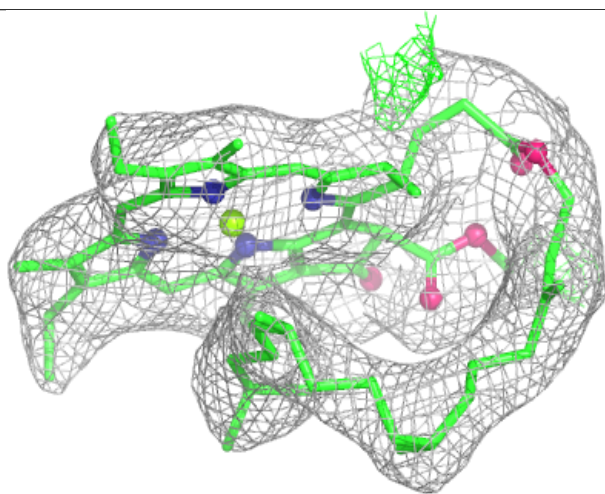
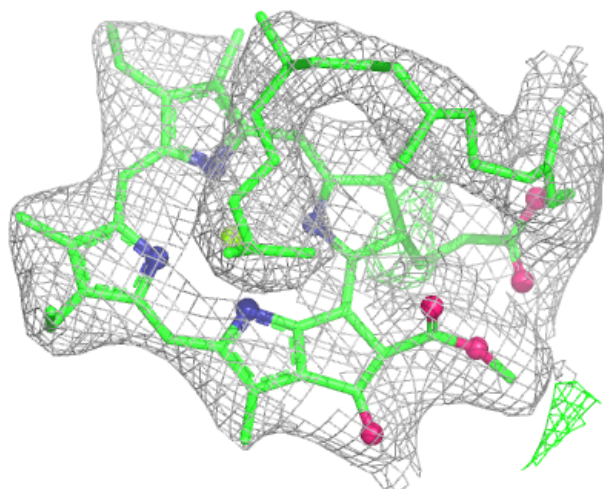
Electron density around CLA L 301:

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



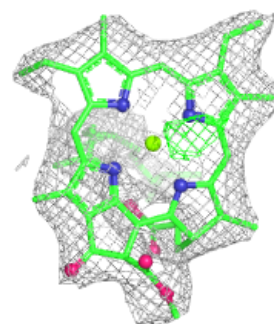
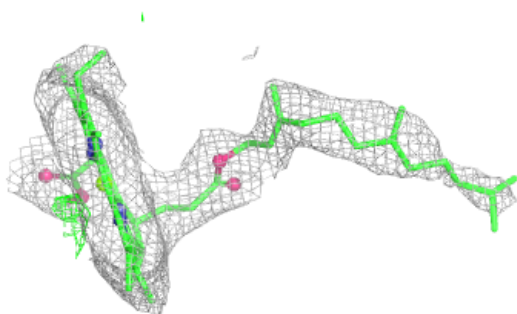
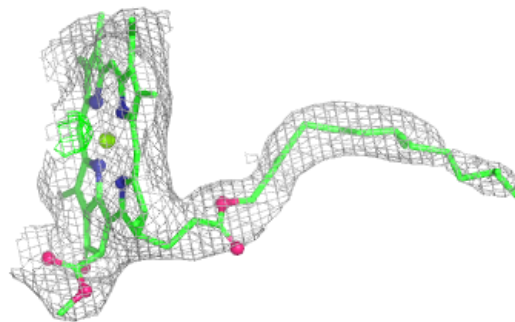
Electron density around CLA B 807:

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



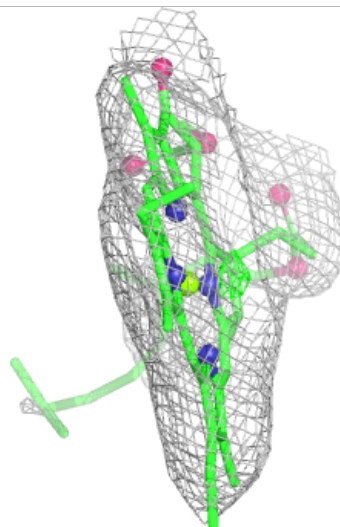
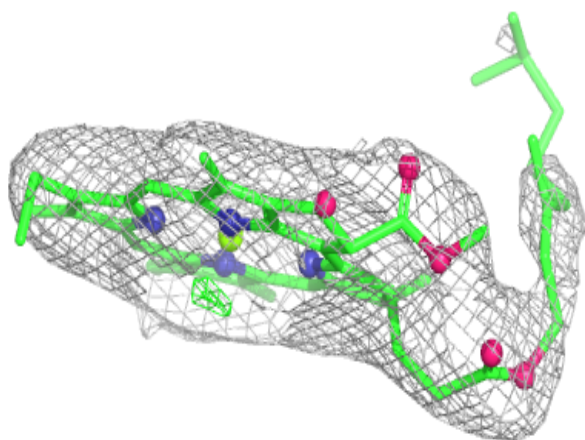
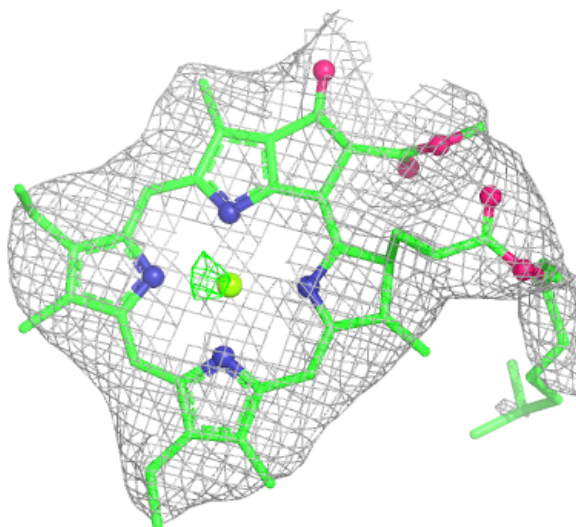
Electron density around CLA L 304:

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



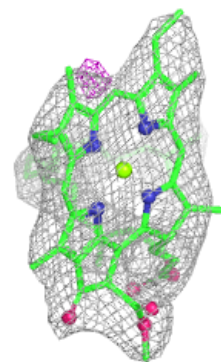
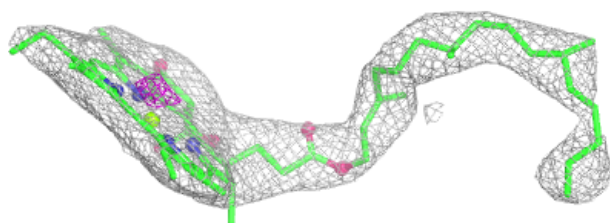
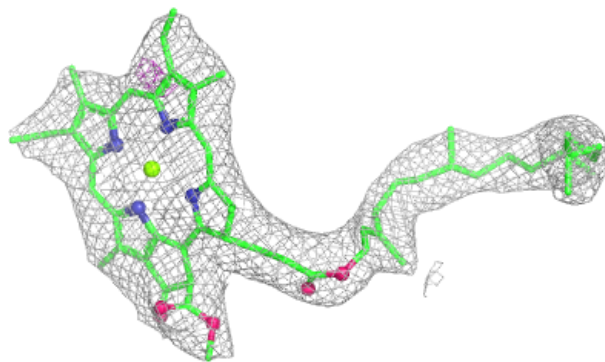
Electron density around CLA 2 508:

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



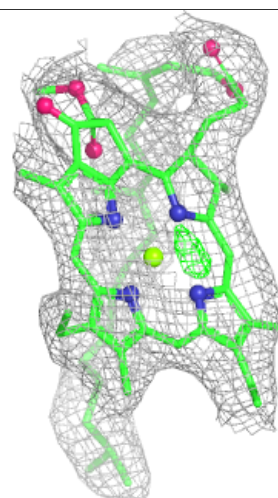
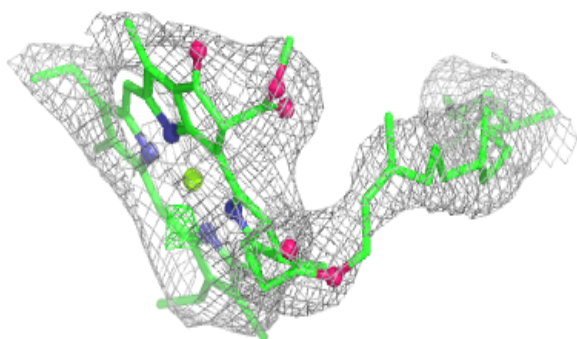
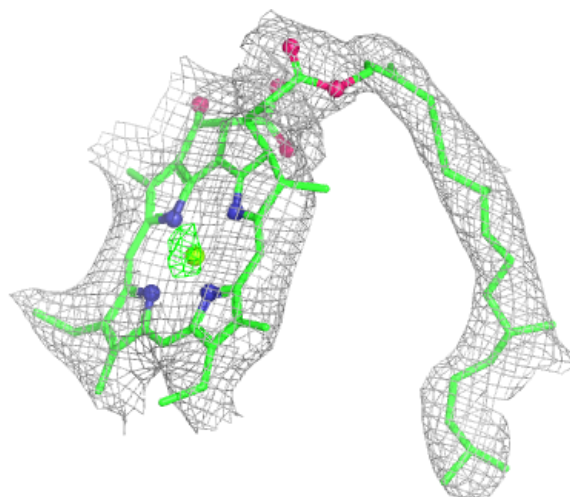
Electron density around CLA B 810:

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



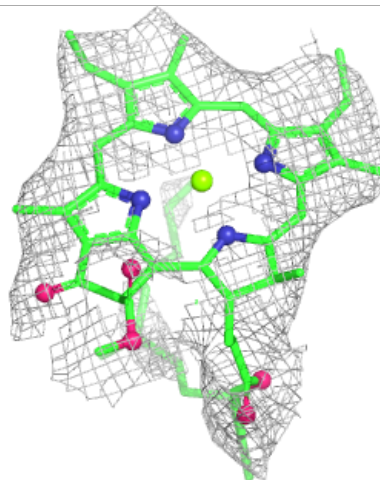
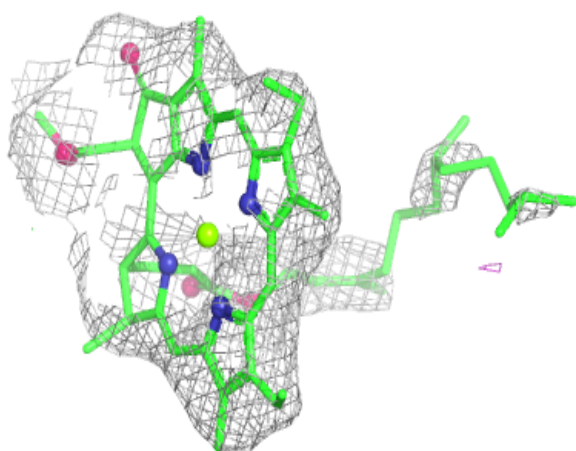
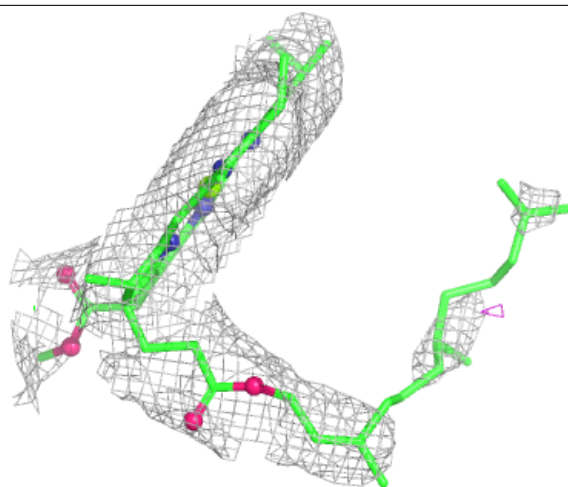
Electron density around CLA B 811:

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



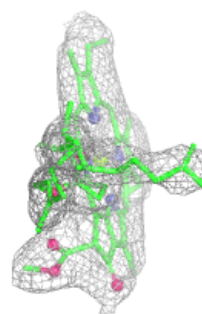
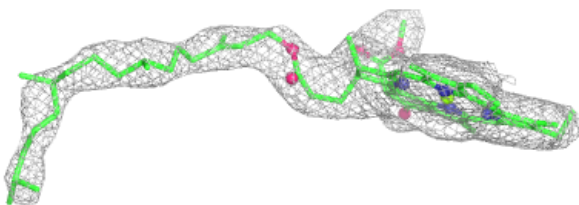
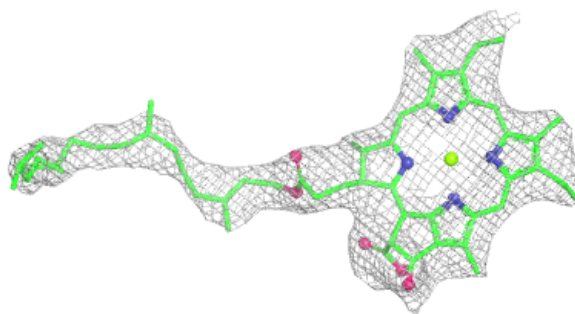
Electron density around CLA B 812:

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



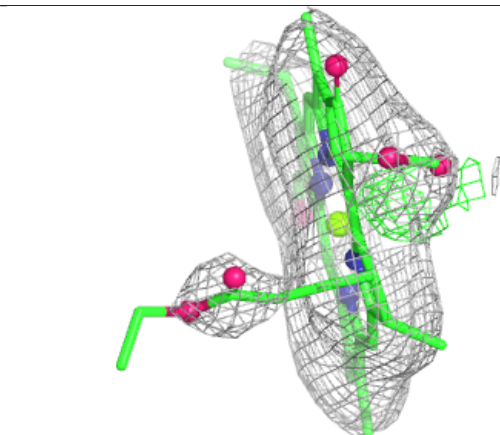
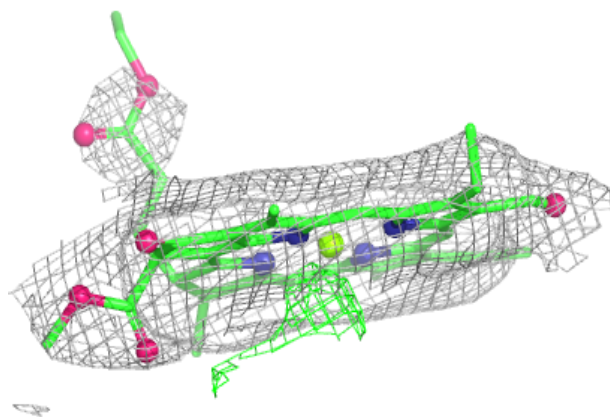
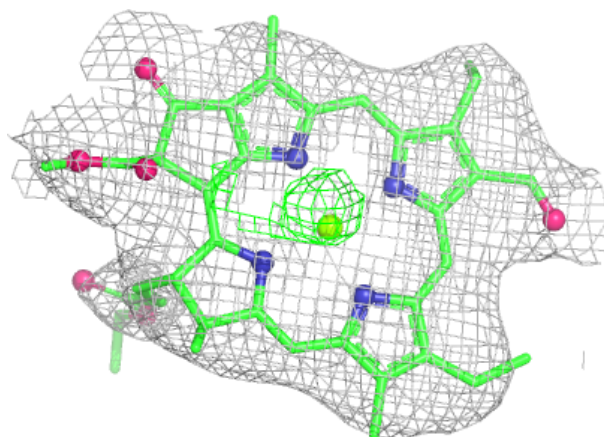
Electron density around CLA A 805:

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

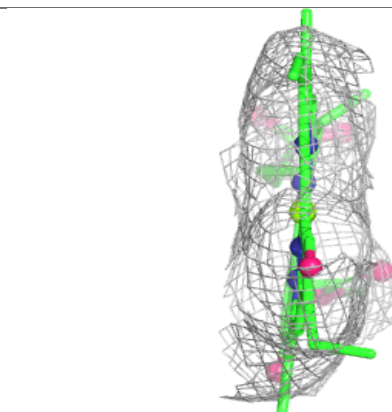
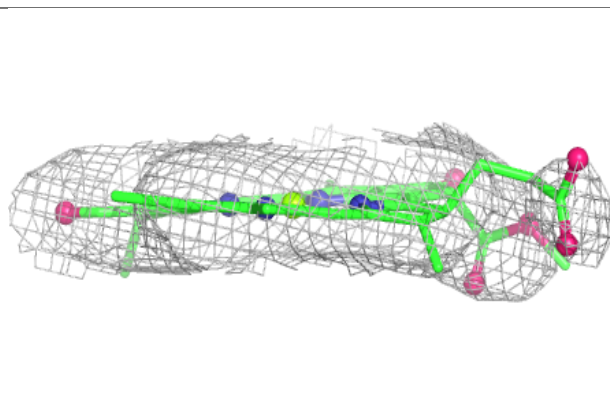
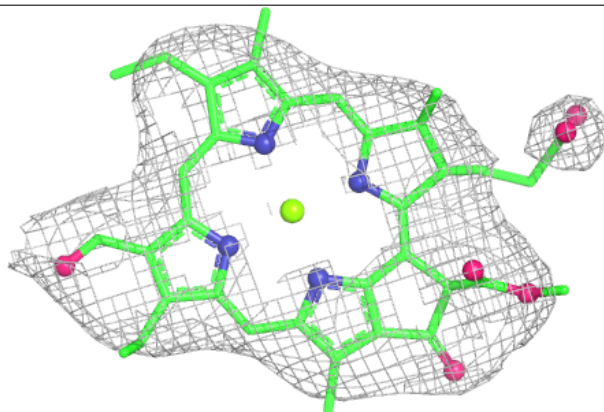


Electron density around CHL 2 513:

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

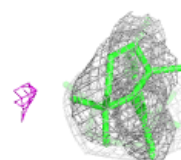
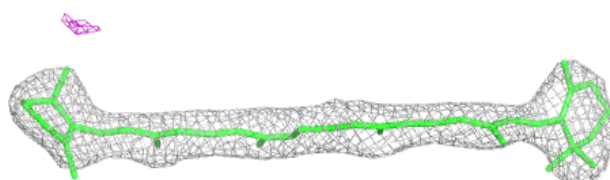
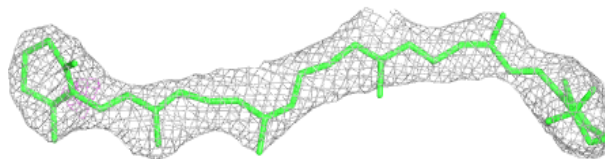
**Electron density around CHL 2 515:**

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

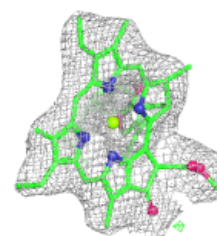
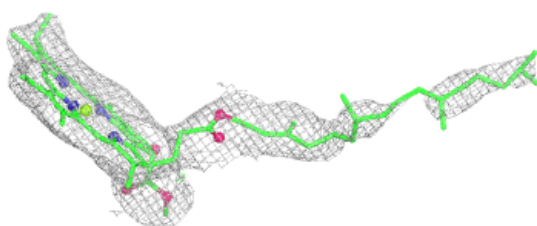
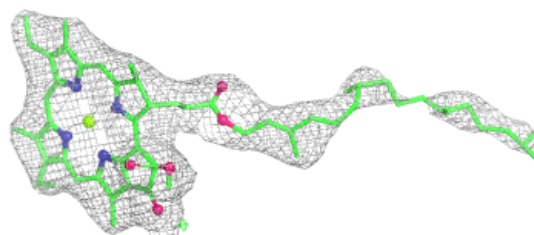


Electron density around BCR B 802:

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

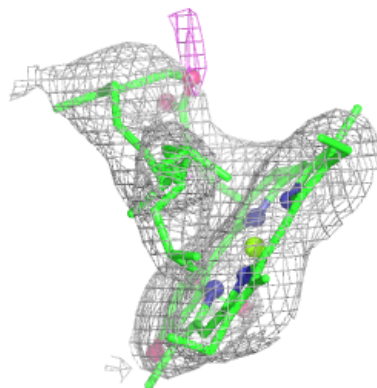
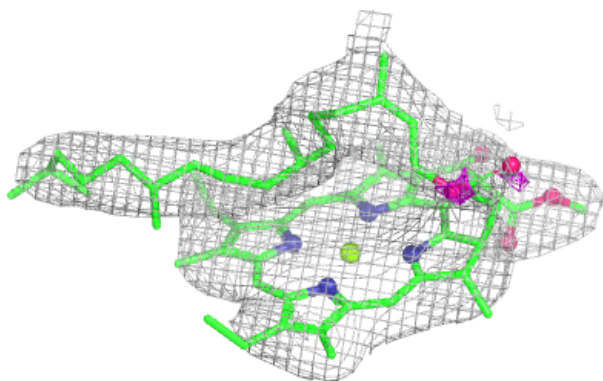
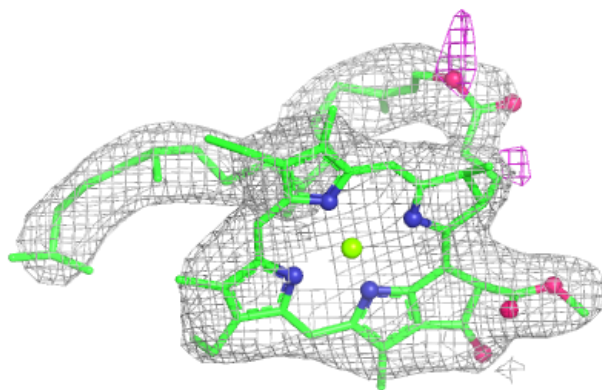
**Electron density around CLA A 809:**

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

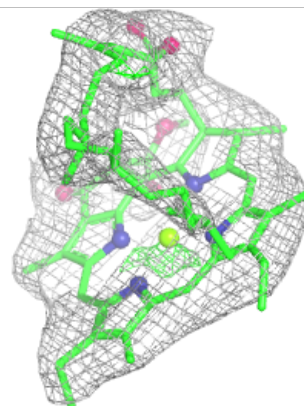
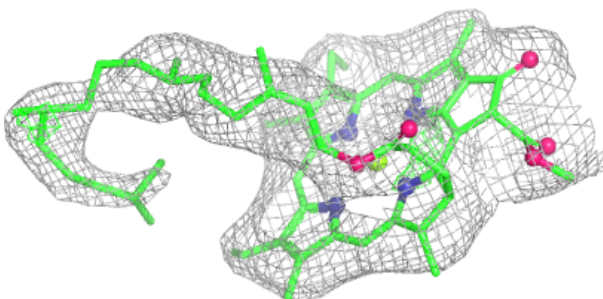
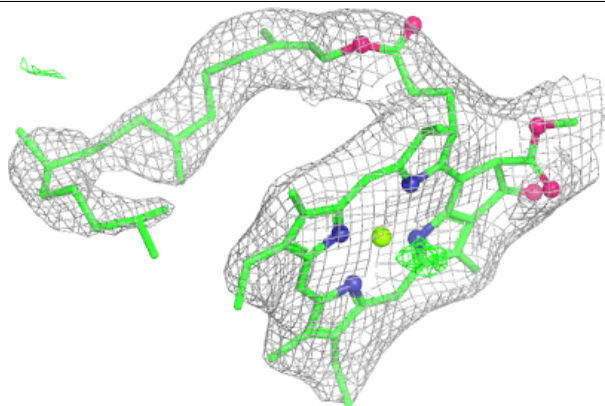


Electron density around CLA B 818:

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

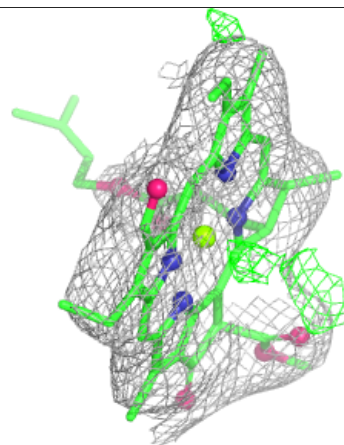
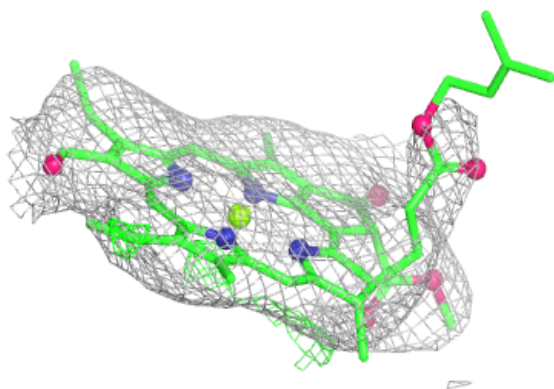
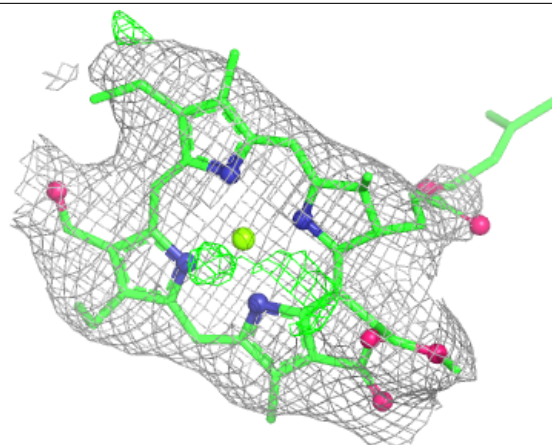
**Electron density around CLA A 824:**

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



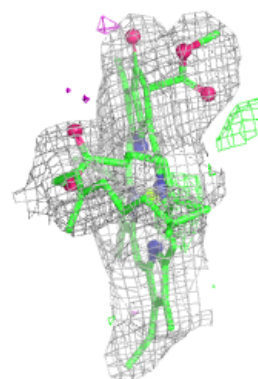
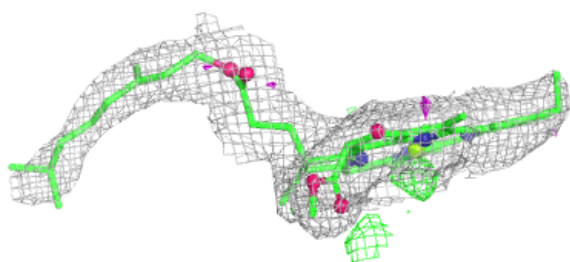
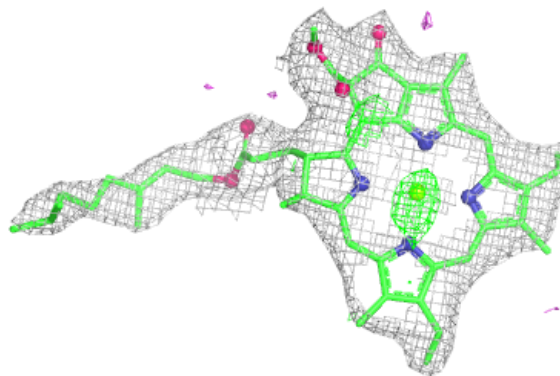
Electron density around CHL 4 314:

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

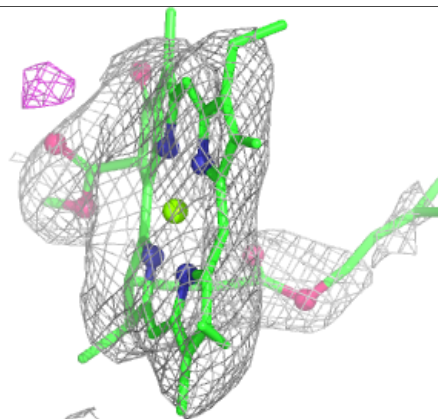
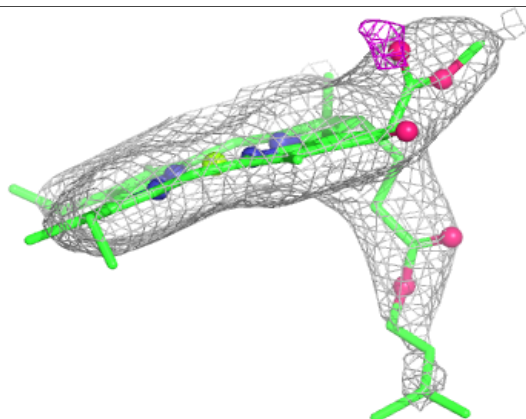
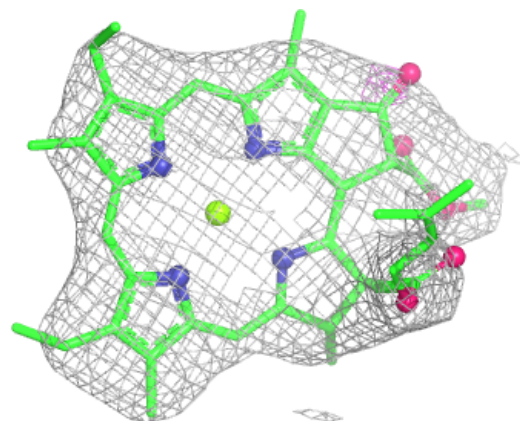


Electron density around CLA A 826:

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

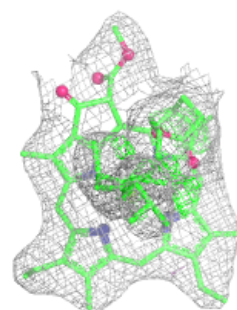
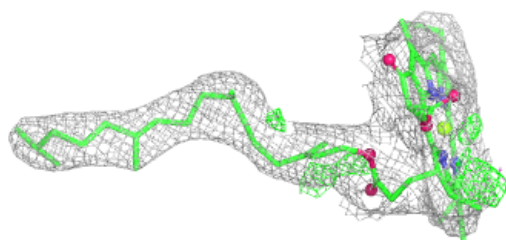
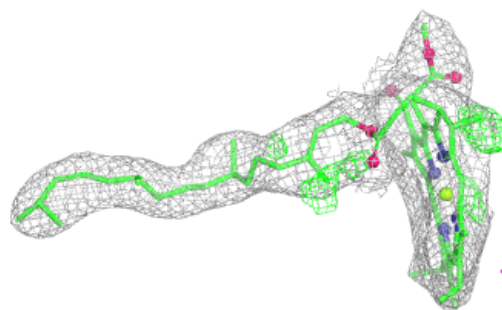
**Electron density around CLA A 810:**

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

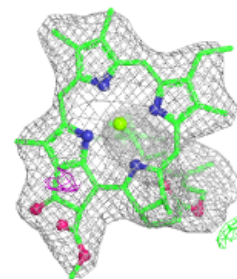
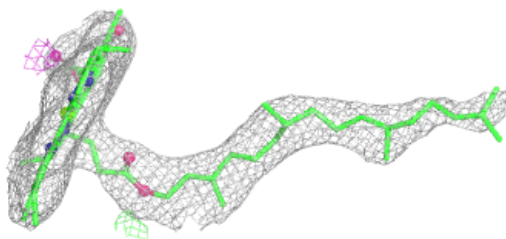
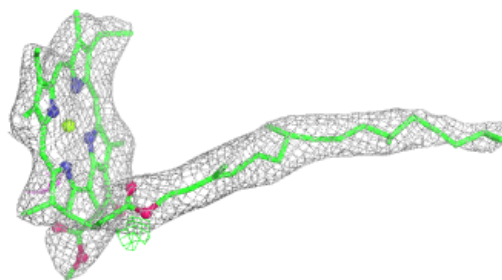


Electron density around CLA A 828:

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

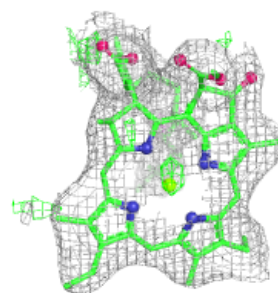
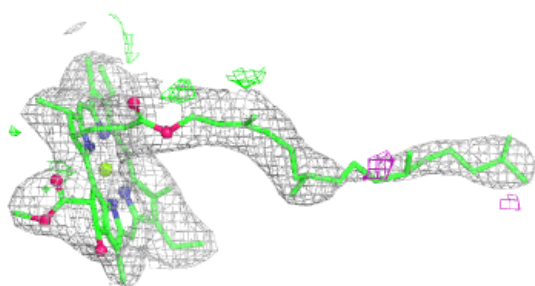
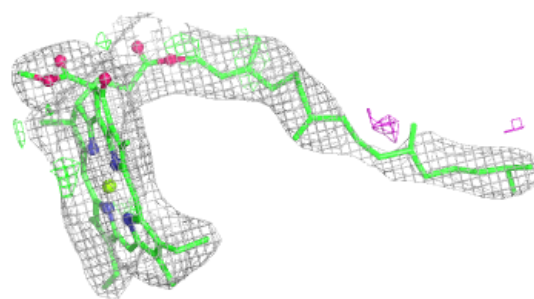
**Electron density around CLA B 828:**

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

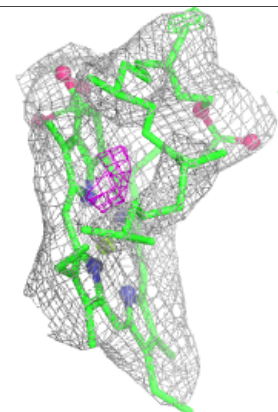
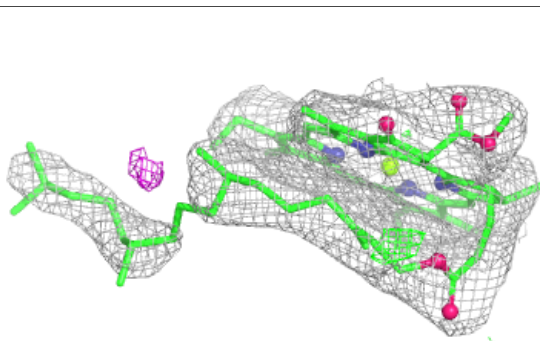
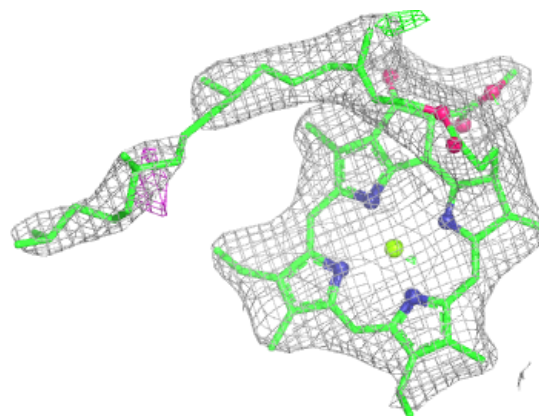


Electron density around CLA B 829:

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

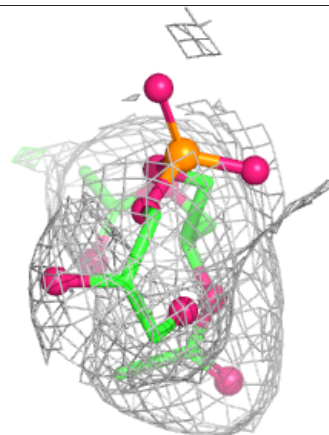
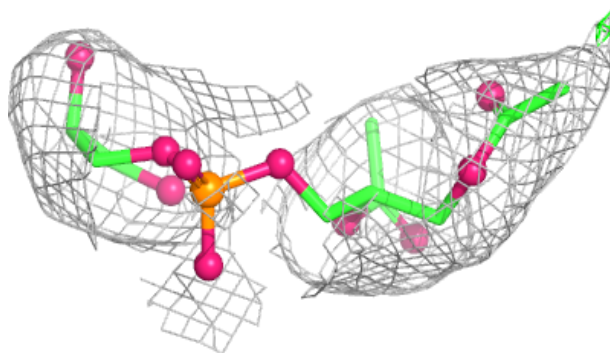
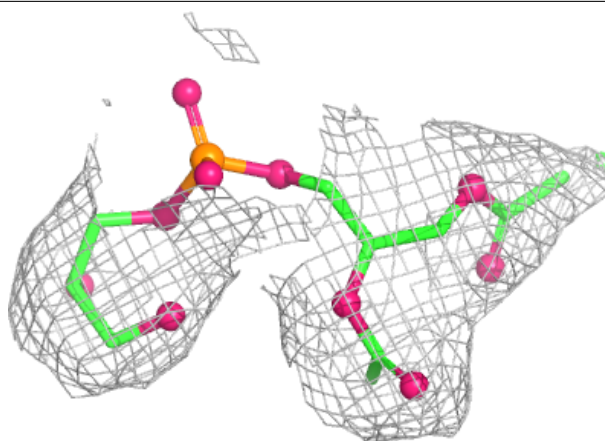
**Electron density around CLA A 829:**

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

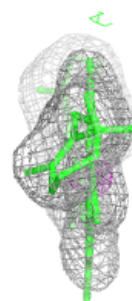
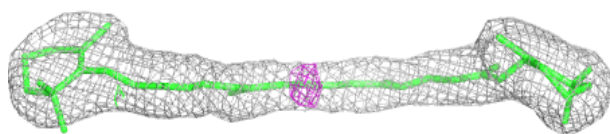
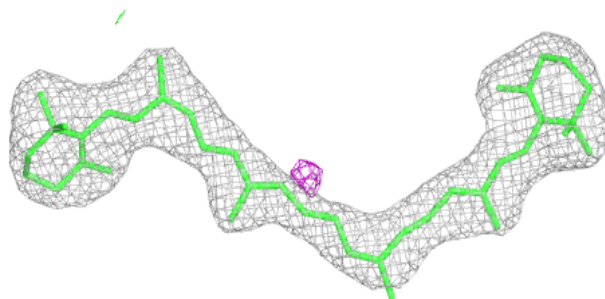


Electron density around LHG B 842:

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

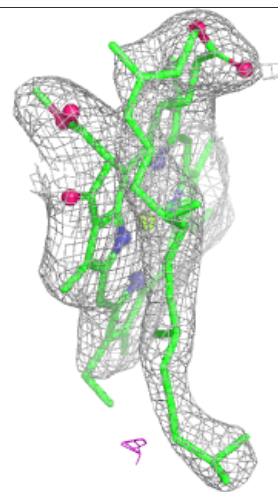
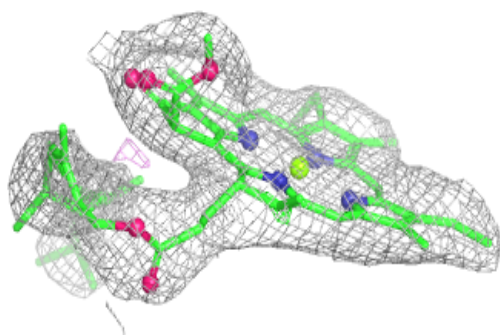
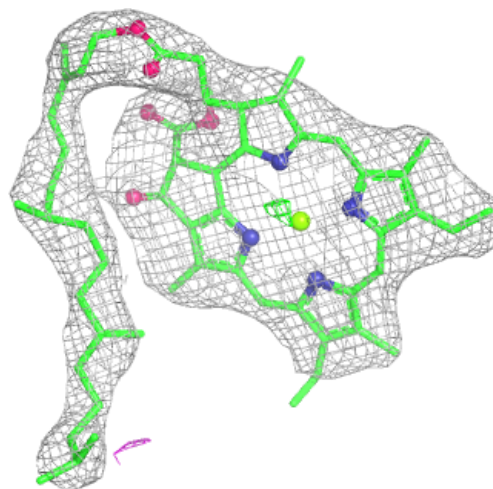
**Electron density around BCR A 852:**

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



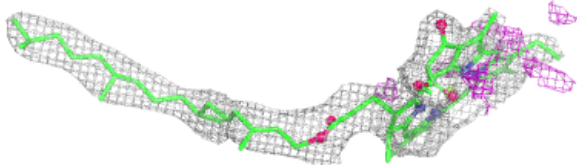
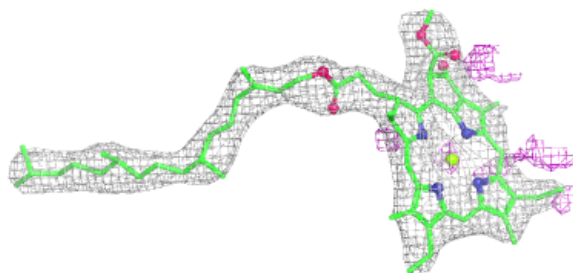
Electron density around CLA A 825:

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



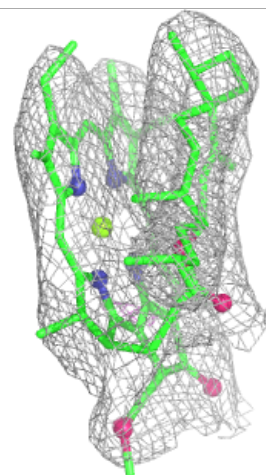
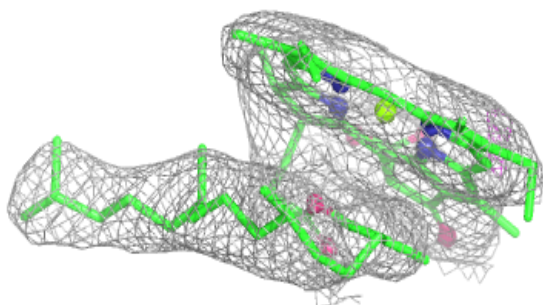
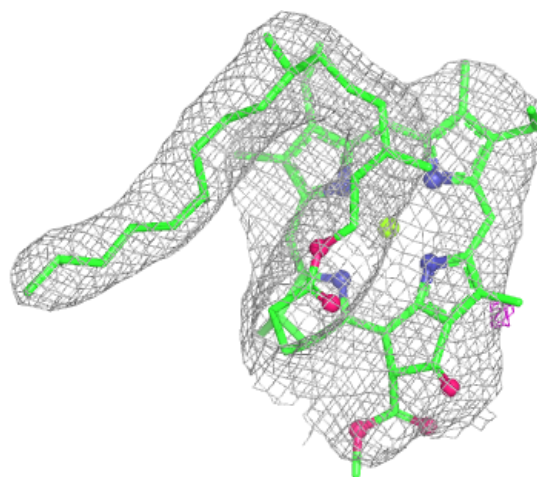
Electron density around CLA A 803:

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



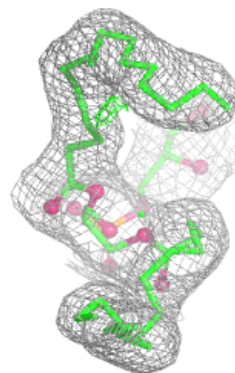
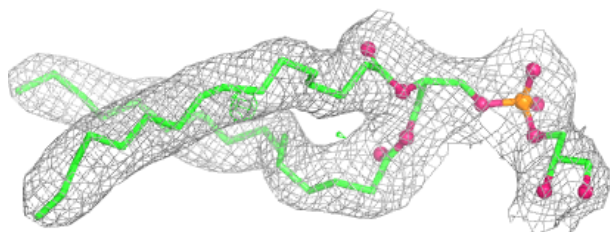
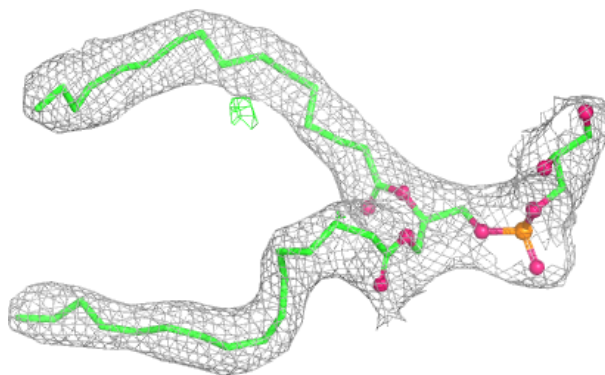
Electron density around CLA B 809:

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

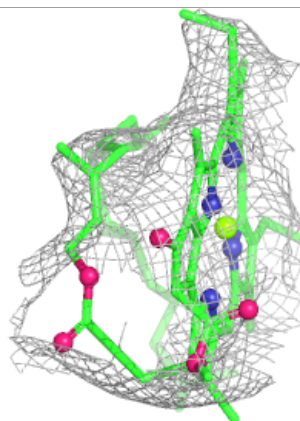
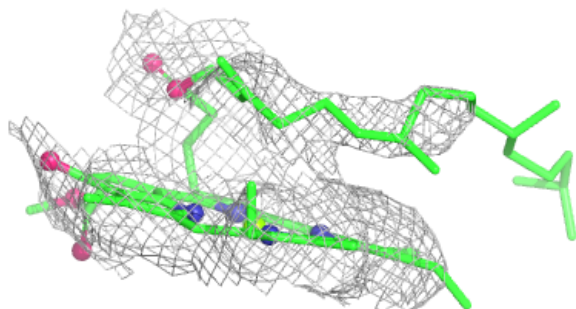
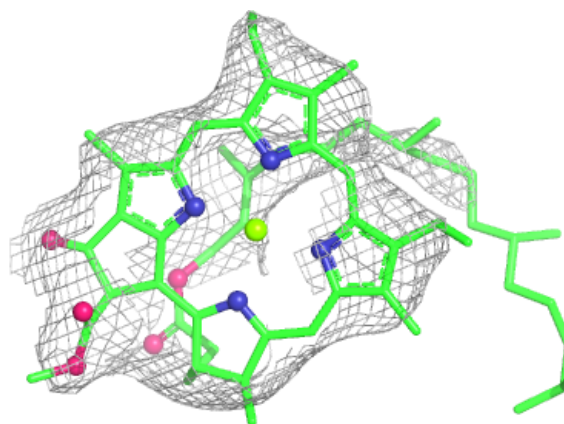


Electron density around LHG A 853:

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

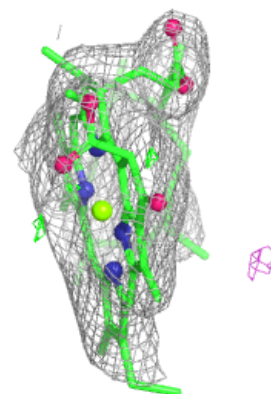
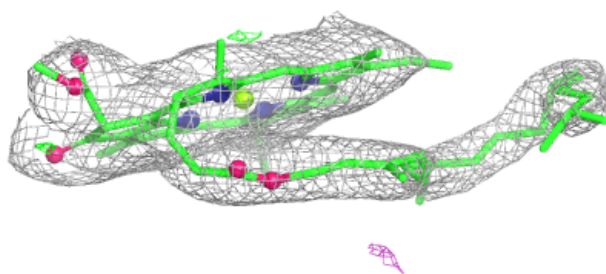
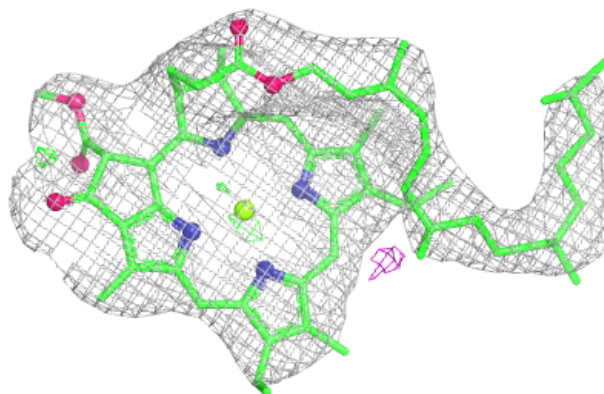
**Electron density around CLA 2 506:**

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

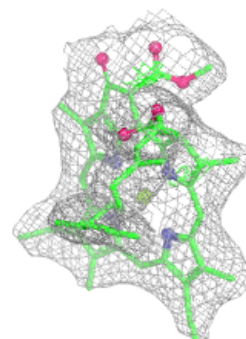
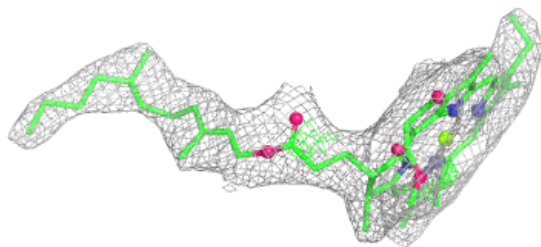
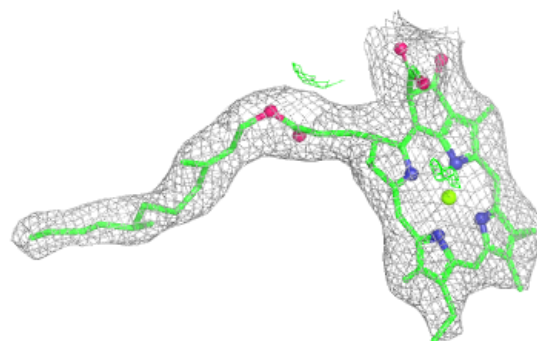


Electron density around CLA A 819:

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

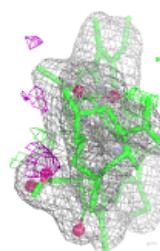
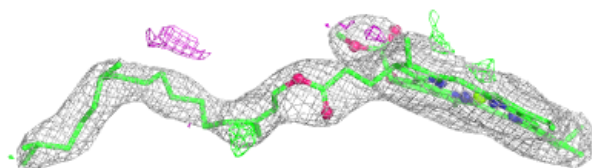
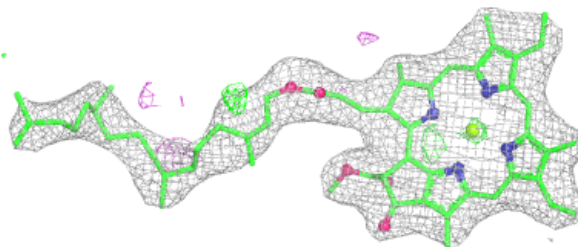
**Electron density around CLA B 832:**

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

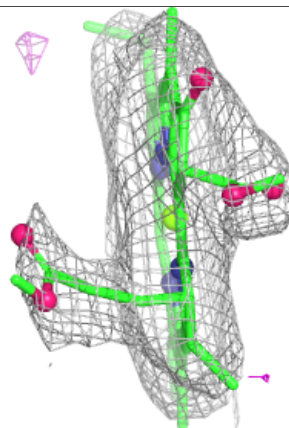
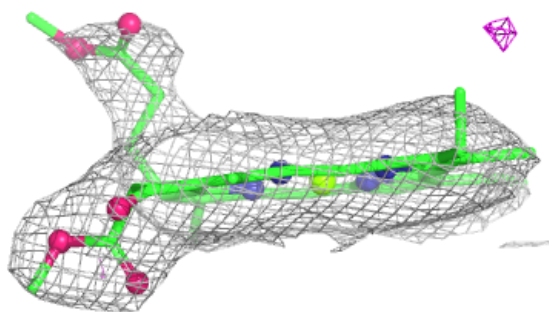
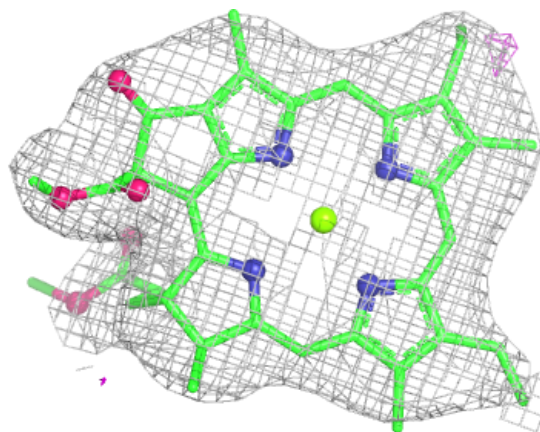


Electron density around CLA A 840:

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

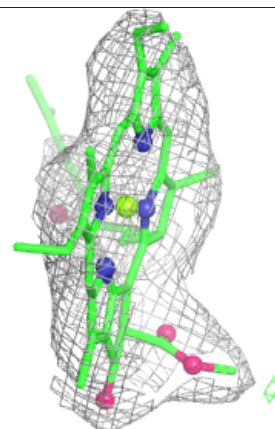
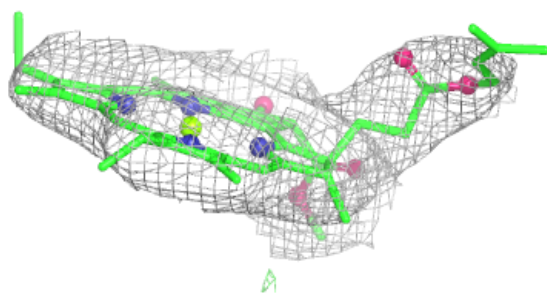
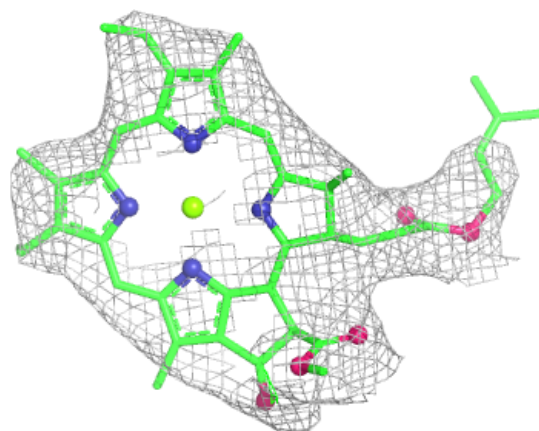
**Electron density around CLA B 813:**

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

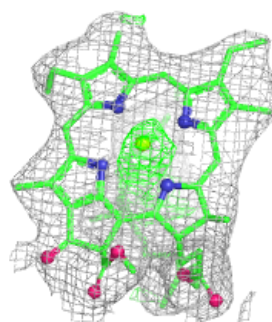
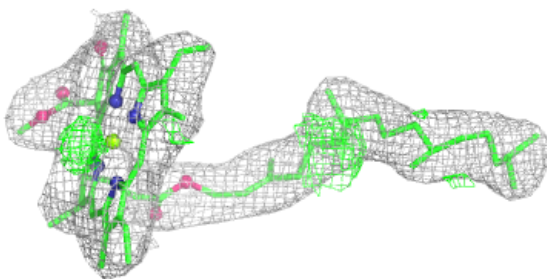
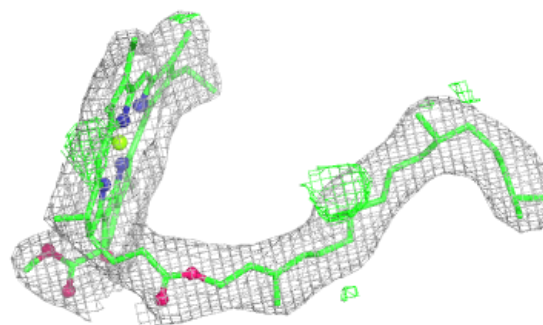


Electron density around CLA 4 312:

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

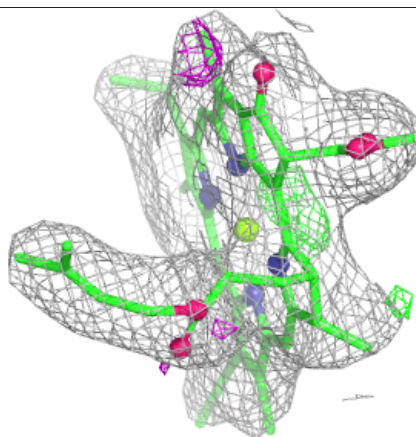
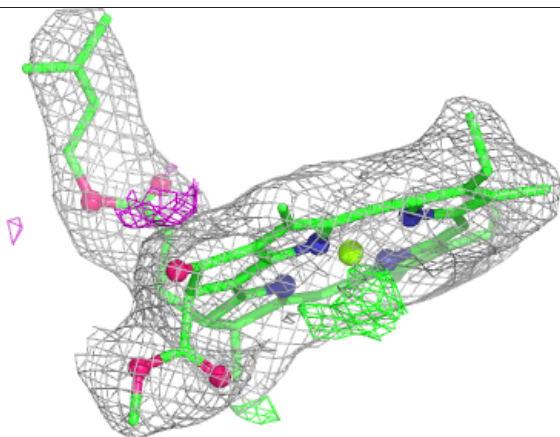
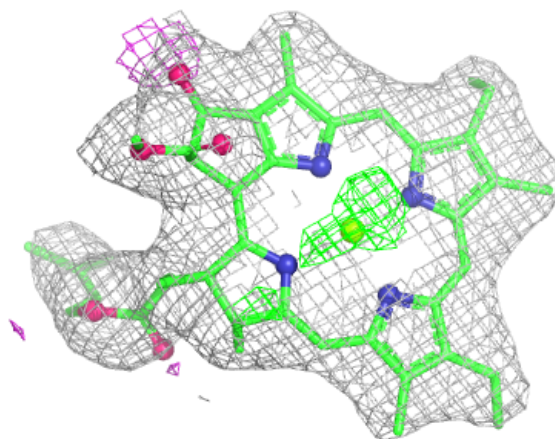
**Electron density around CLA A 830:**

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



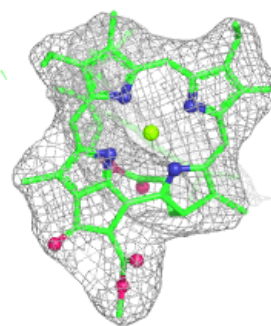
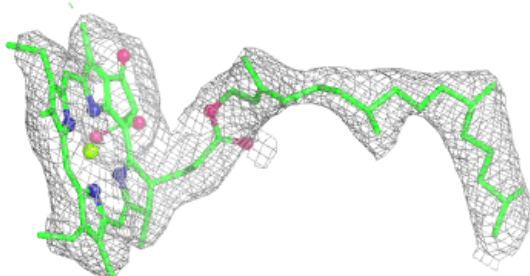
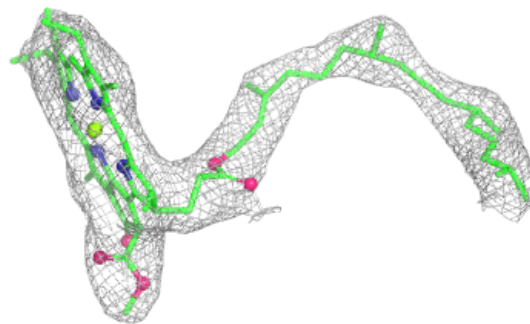
Electron density around CLA B 837:

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



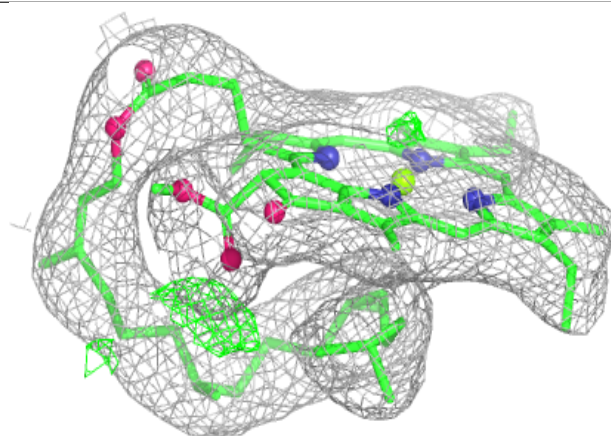
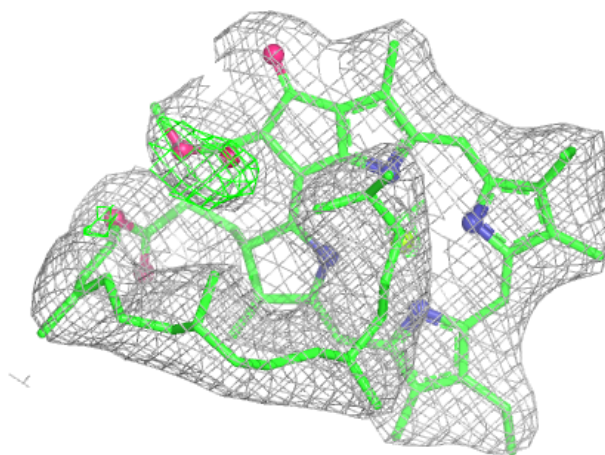
Electron density around CLA B 838:

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



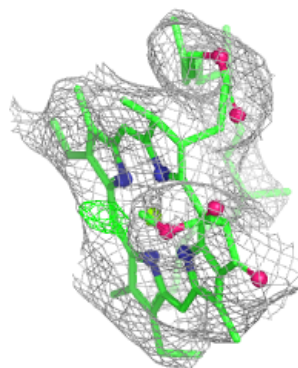
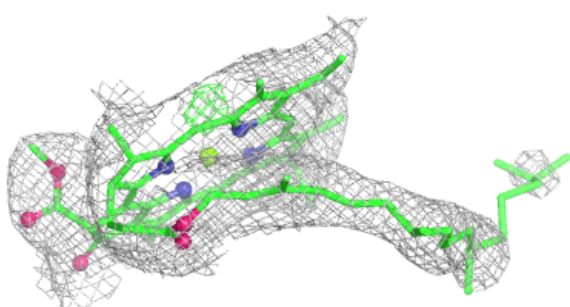
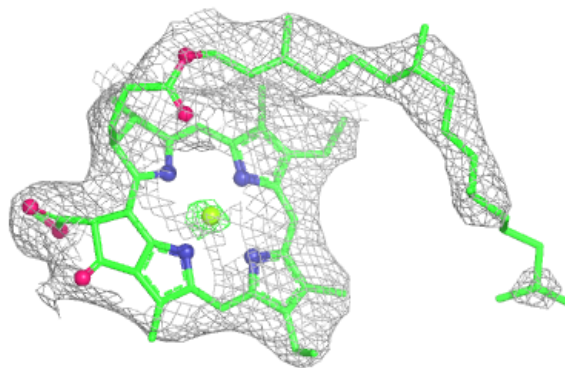
Electron density around CLA A 806:

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

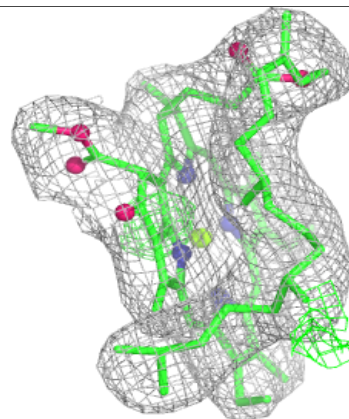
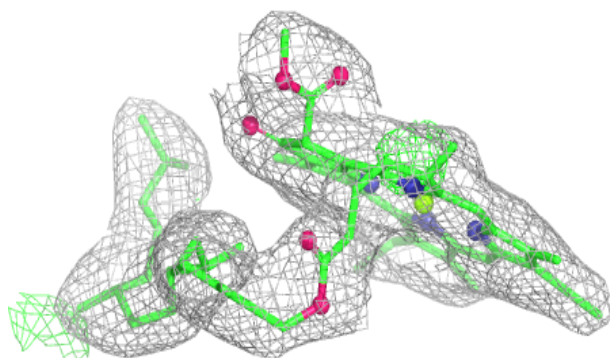
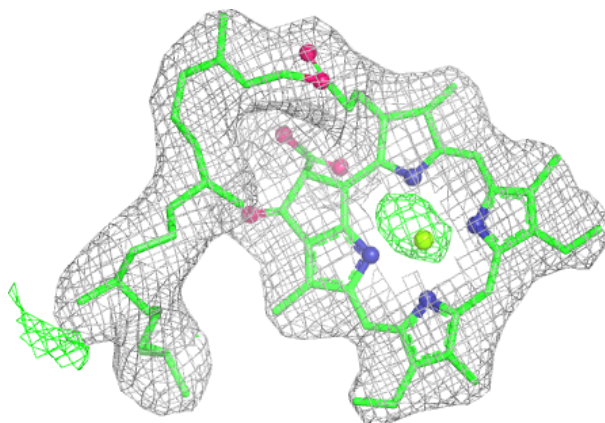


Electron density around CLA 2 507:

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

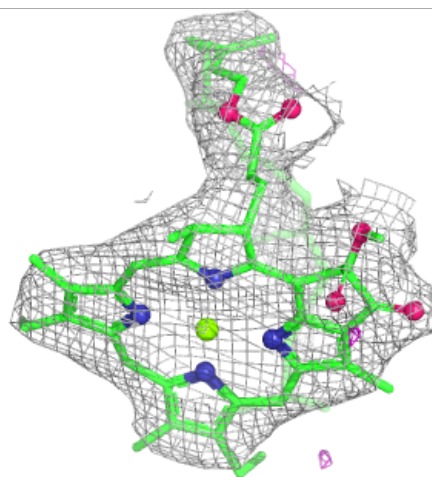
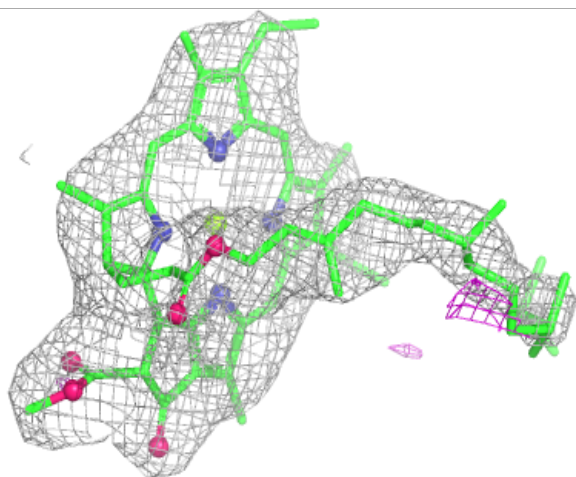
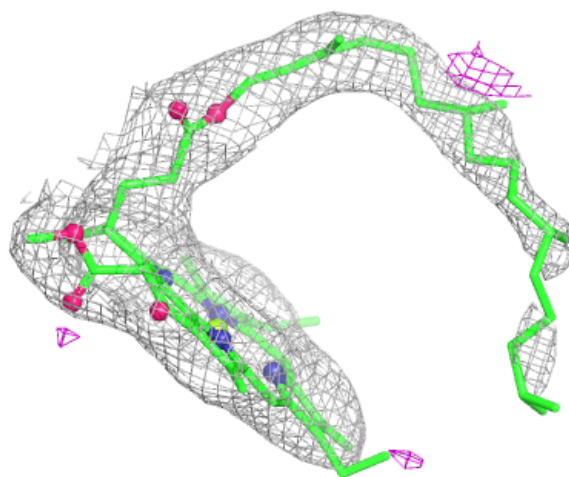
**Electron density around CLA F 302:**

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



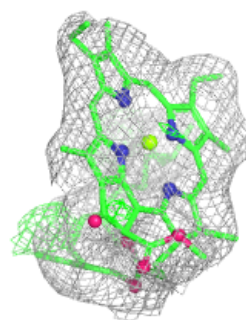
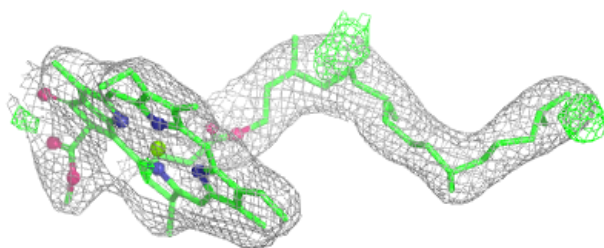
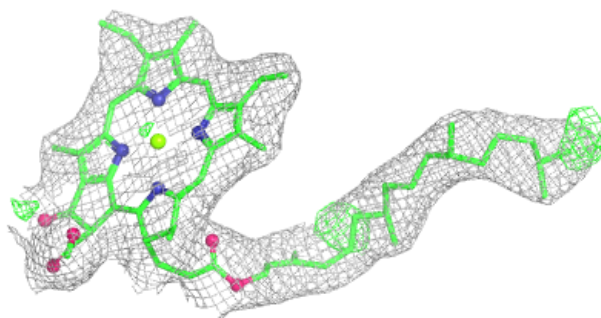
Electron density around CLA B 820:

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

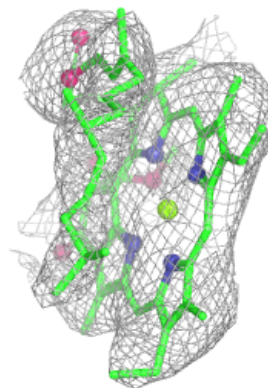
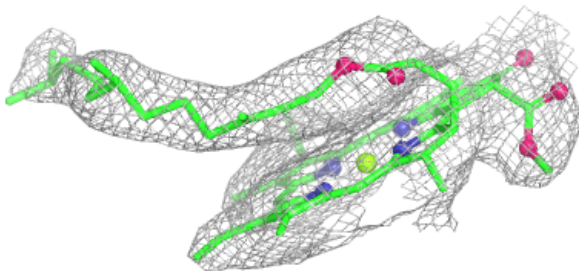
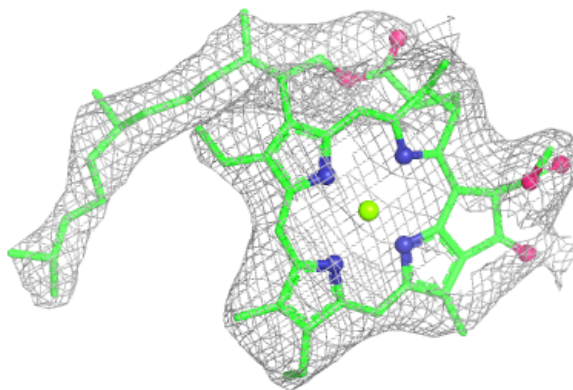


Electron density around CLA A 808:

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

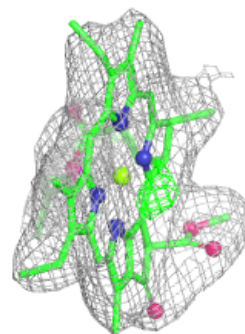
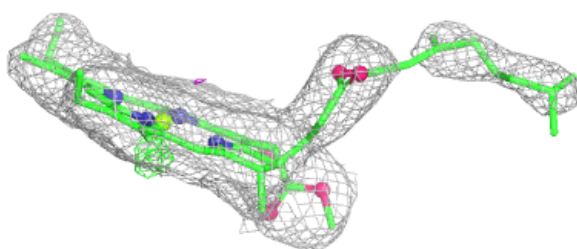
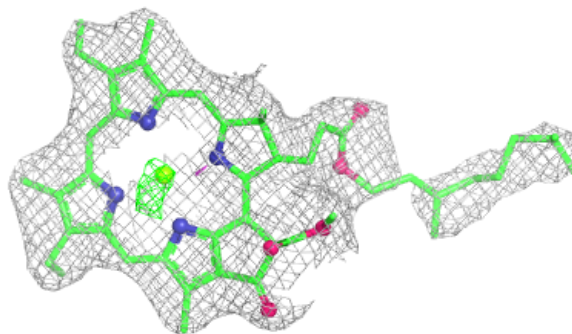
**Electron density around CLA 4 307:**

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

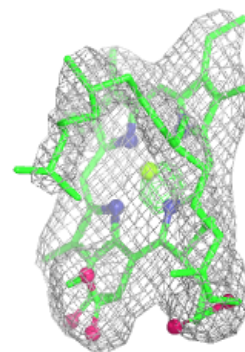
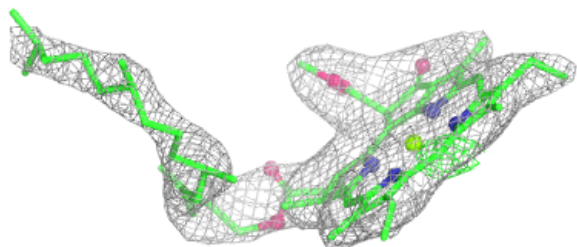
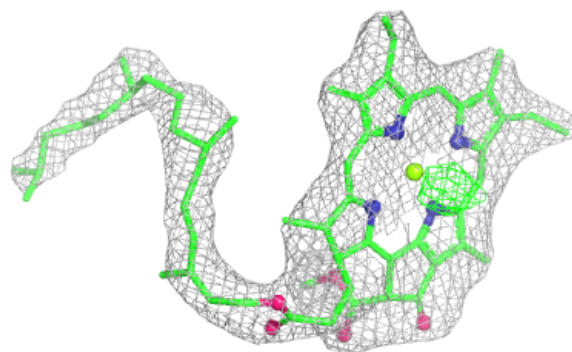


Electron density around CLA B 823:

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

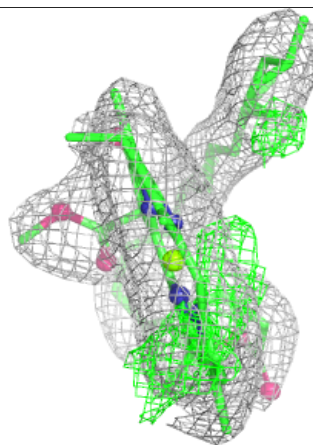
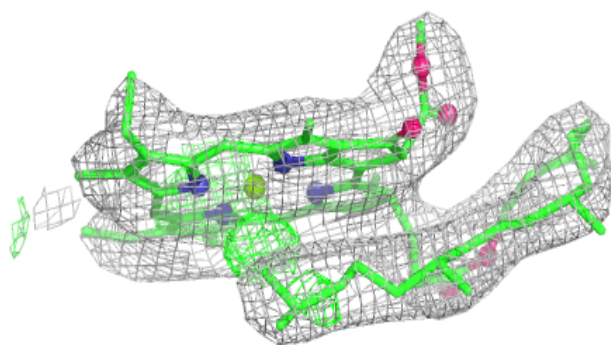
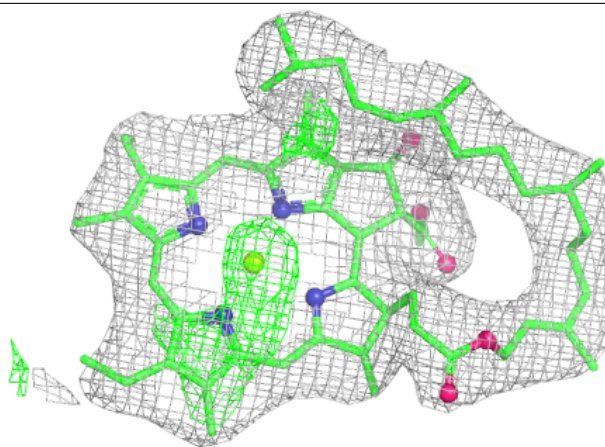
**Electron density around CLA B 824:**

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

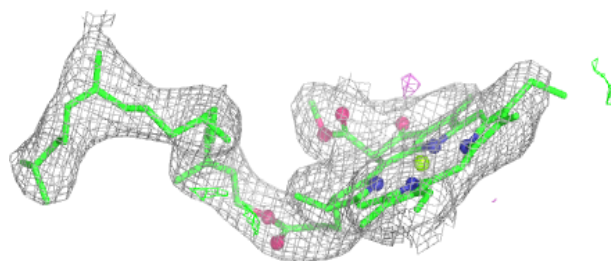
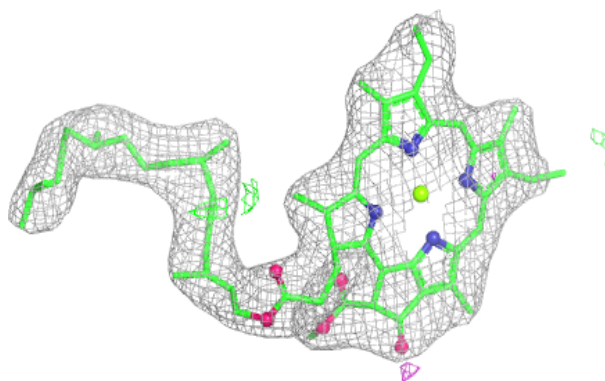


Electron density around CLA B 806:

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

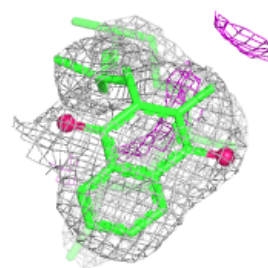
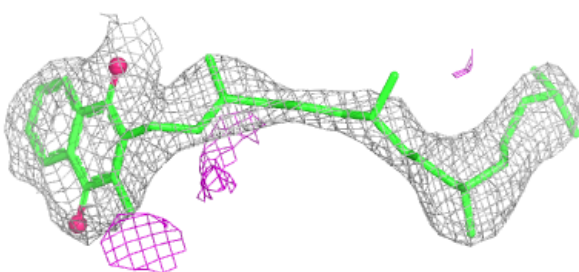
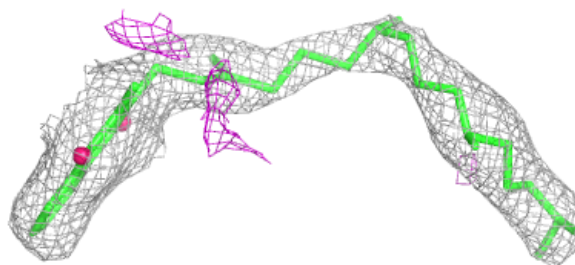
**Electron density around CLA J 1101:**

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

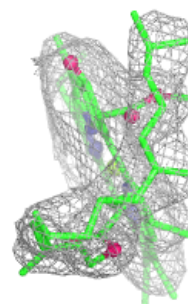
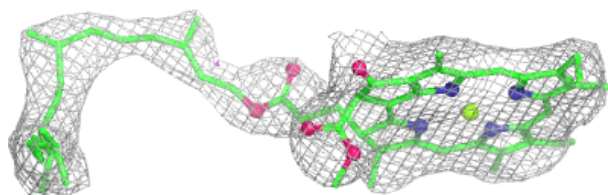
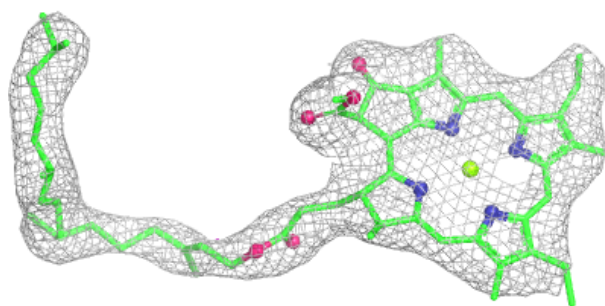


Electron density around PQN B 841:

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

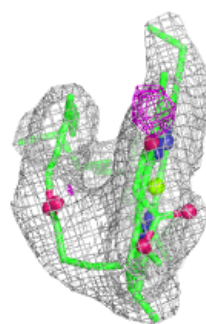
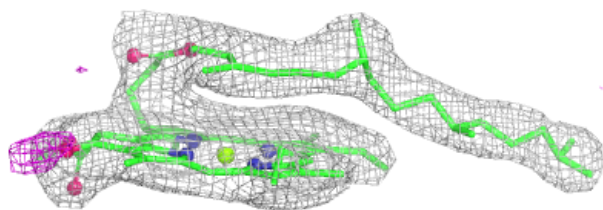
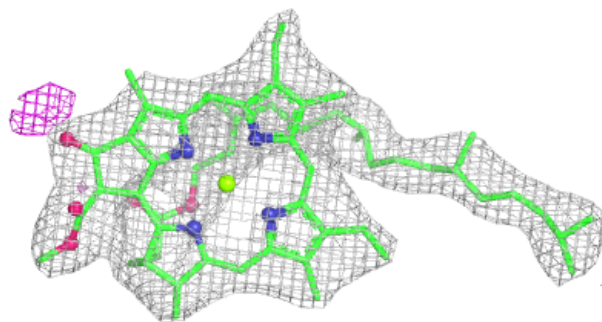
**Electron density around CLA B 826:**

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

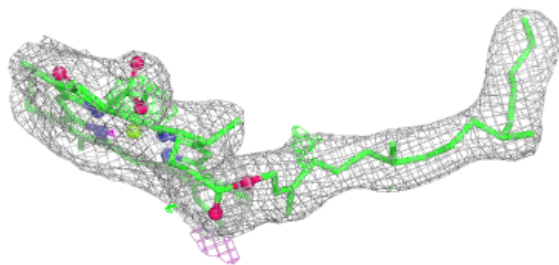
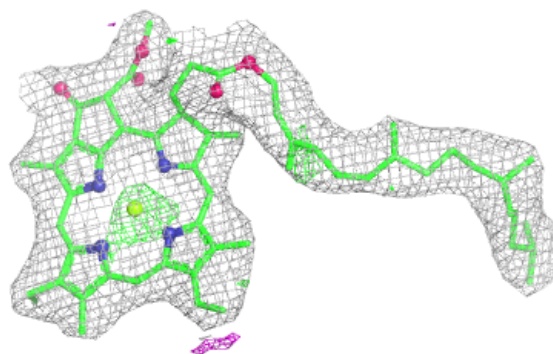


Electron density around CLA A 839:

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

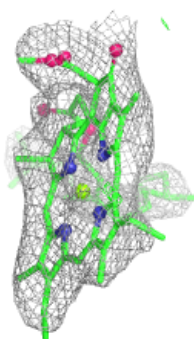
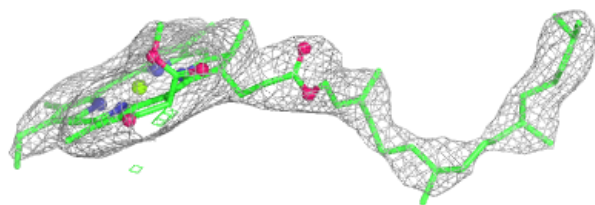
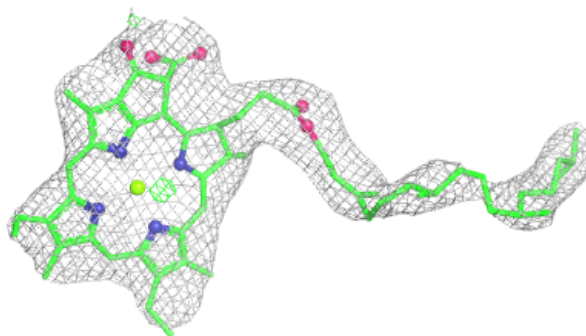
**Electron density around CLA A 802:**

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

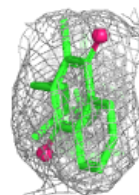
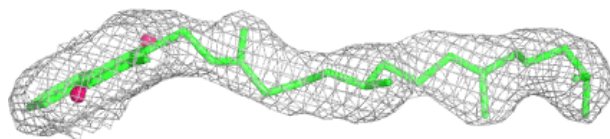
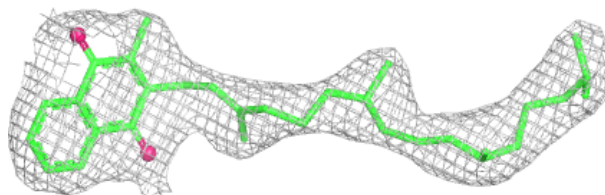


Electron density around CLA B 814:

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

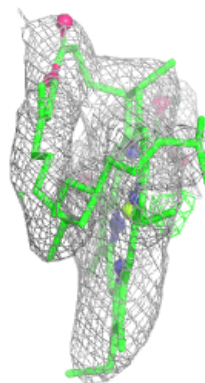
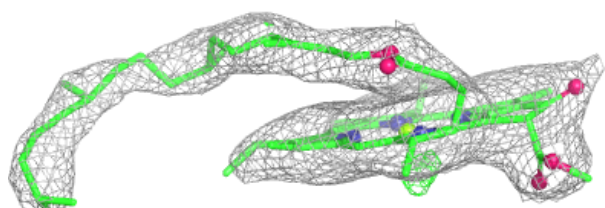
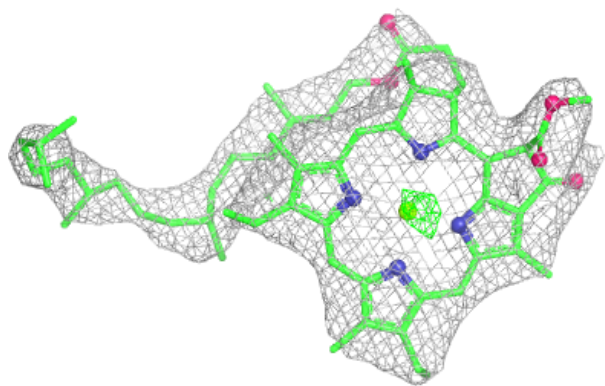
**Electron density around PQN A 844:**

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

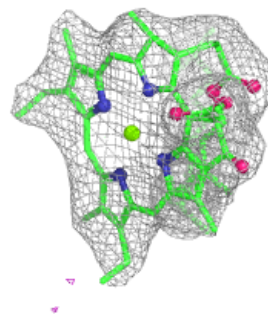
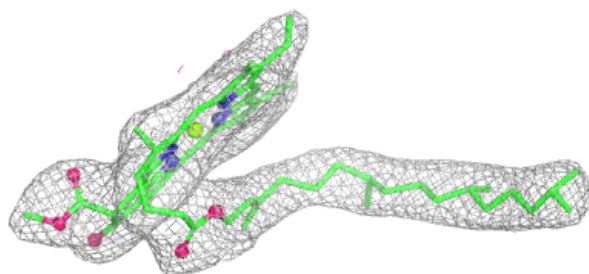
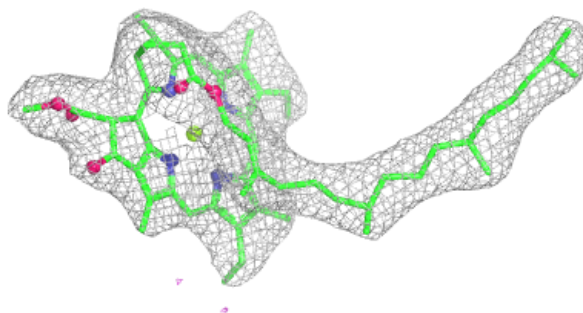


Electron density around CLA B 819:

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

**Electron density around CLA A 841:**

$2mF_o-DF_c$ (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.