



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2024 – 08:42 am BST

PDB ID : 5L8R
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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

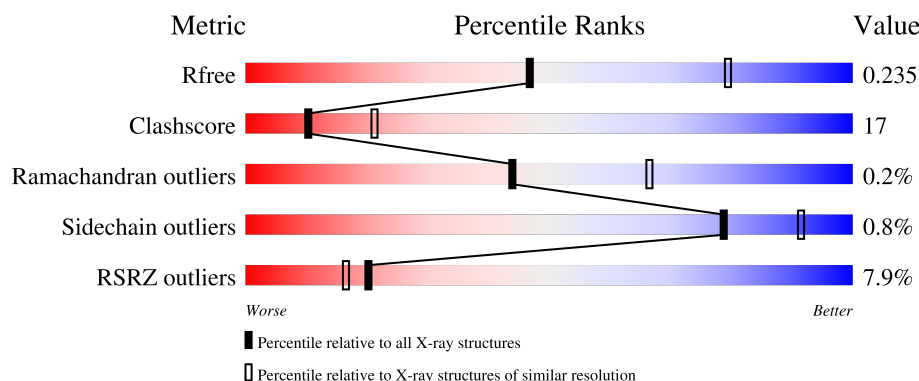
1 Overall quality at a glance

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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (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	<div> <div>17%</div> <div> <div></div> <div>70%</div> <div>29%</div> <div>.</div> </div> </div>
2	2	269	<div> <div>4%</div> <div> <div></div> <div>56%</div> <div>22%</div> <div>23%</div> </div> </div>
3	3	275	<div> <div>11%</div> <div> <div></div> <div>60%</div> <div>20%</div> <div>20%</div> </div> </div>
4	4	198	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>26%</div> </div> </div>
5	A	758	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>.</div> </div> </div>

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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

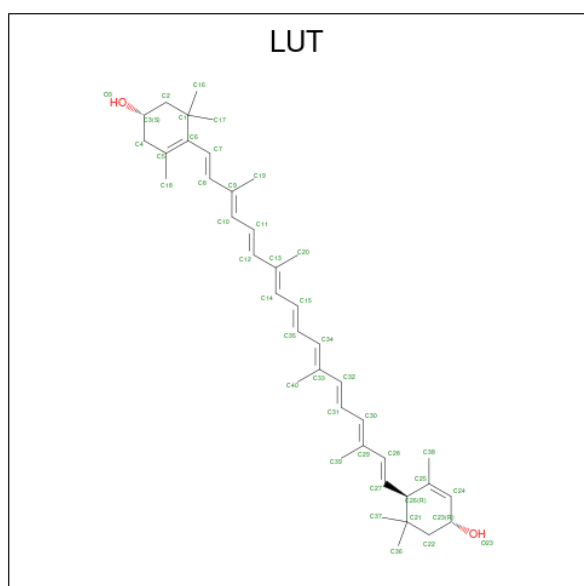
- Molecule 16 is a protein called Putative uncharacterized protein.

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 (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



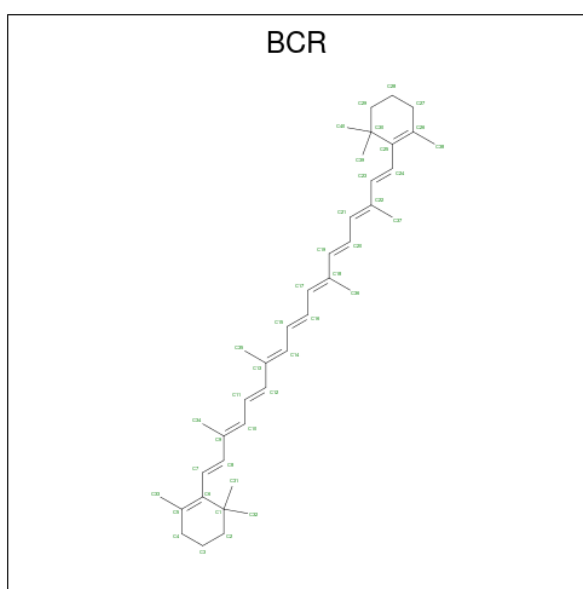
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	1	1	Total	C	O	0	0
			42	40	2		
17	1	1	Total	C	O	0	0
			42	40	2		
17	2	1	Total	C	O	0	0
			42	40	2		

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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 (three-letter code: BCR) (formula: $C_{40}H_{56}$).



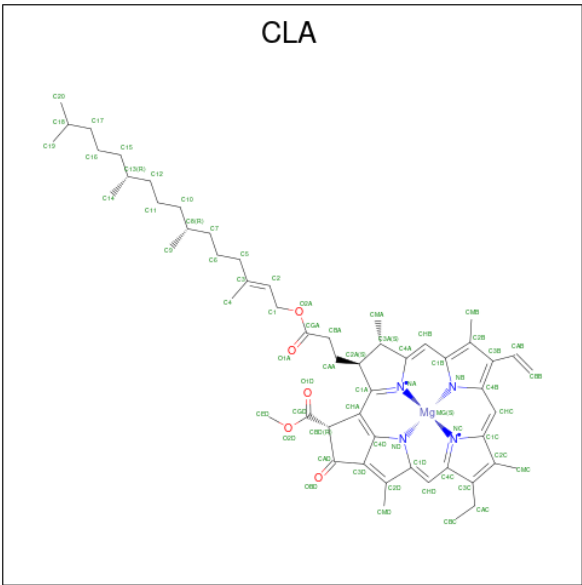
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	1	1	Total	C	0	0
			19	19		
18	2	1	Total	C	0	0
			40	40		
18	3	1	Total	C	0	0
			40	40		
18	3	1	Total	C	0	0
			40	40		
18	4	1	Total	C	0	0
			40	40		
18	A	1	Total	C	0	0
			40	40		
18	A	1	Total	C	0	0
			40	40		

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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 (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	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
			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
			46	36	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
			55	45	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
			58	48	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
			55	45	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

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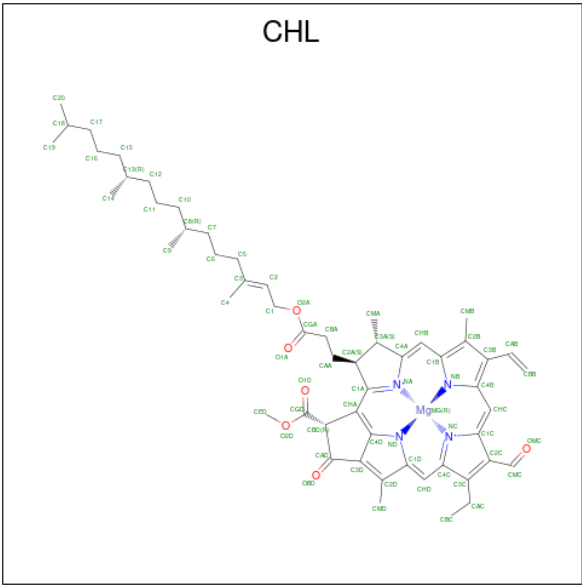
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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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 (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



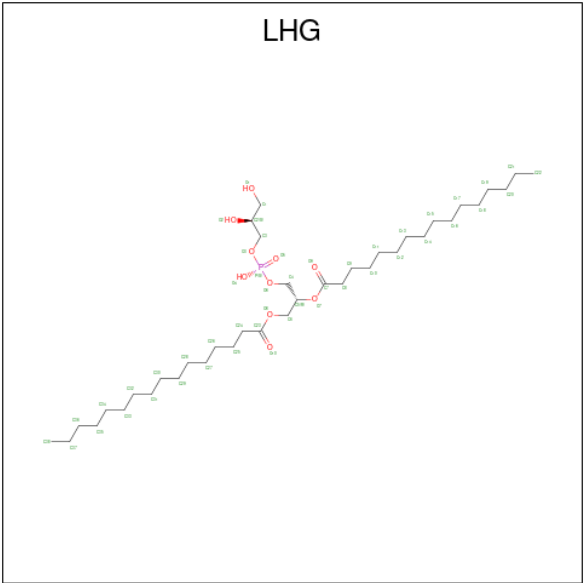
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	1	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
20	1	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
20	1	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
20	2	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
20	2	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
20	2	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
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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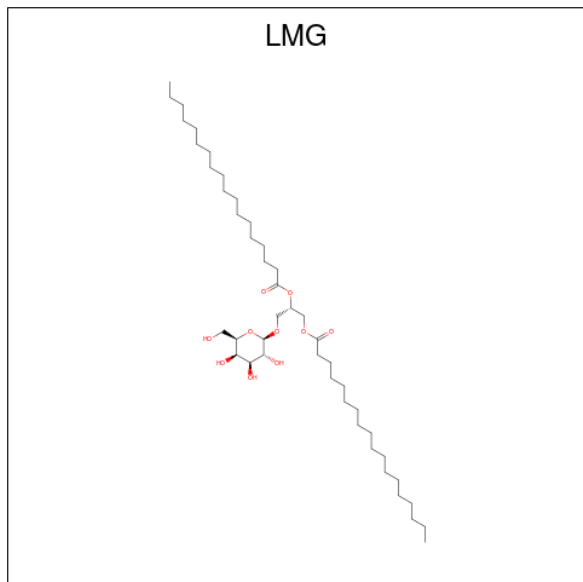
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	4	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
20	4	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
20	4	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
20	4	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		

- Molecule 21 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: 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 (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



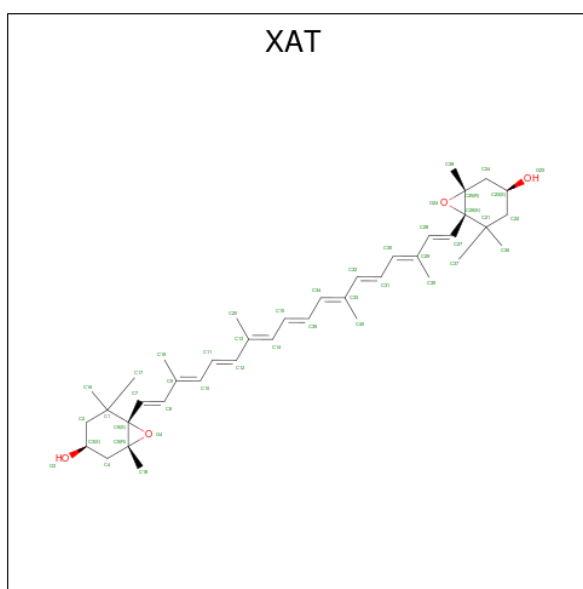
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	1	1	Total	C	O	0	0
			46	36	10		
22	1	1	Total	C	O	0	0
			13	7	6		
22	2	1	Total	C	O	0	0
			25	15	10		
22	2	1	Total	C	O	0	0
			36	26	10		
22	2	1	Total	C	O	0	0
			13	7	6		
22	2	1	Total	C	O	0	0
			13	7	6		
22	2	1	Total	C	O	0	0
			13	7	6		
22	2	1	Total	C	O	0	0
			13	7	6		
22	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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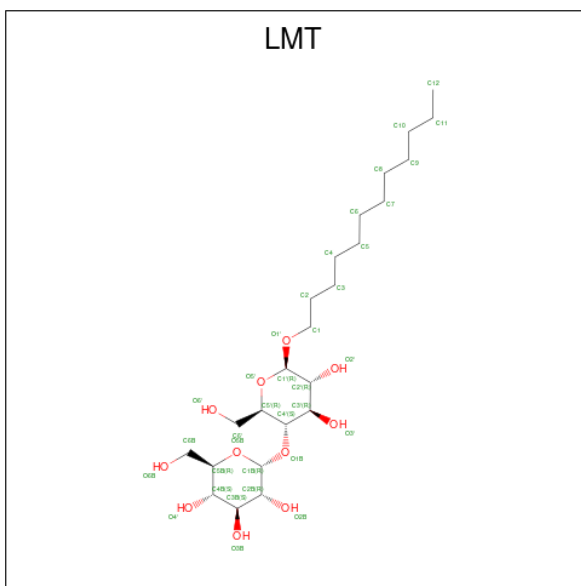
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			35	25	10		
22	B	1	Total	C	O	0	0
			33	23	10		
22	F	1	Total	C	O	0	0
			47	37	10		
22	F	1	Total	C	O	0	0
			36	26	10		
22	G	1	Total	C	O	0	0
			50	40	10		
22	G	1	Total	C	O	0	0
			25	15	10		
22	J	1	Total	C	O	0	0
			30	20	10		
22	J	1	Total	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 (three-letter code: 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 (three-letter code: LMT) (formula:

$\text{C}_{24}\text{H}_{46}\text{O}_{11}$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	2	1	Total 35	C 24	O 11	0	0
24	3	1	Total 31	C 20	O 11	0	0
24	4	1	Total 35	C 24	O 11	0	0
24	A	1	Total 35	C 24	O 11	0	0
24	B	1	Total 35	C 24	O 11	0	0
24	B	1	Total 32	C 21	O 11	0	0
24	B	1	Total 31	C 20	O 11	0	0
24	G	1	Total 35	C 24	O 11	0	0
24	G	1	Total 31	C 20	O 11	0	0
24	J	1	Total 25	C 14	O 11	0	0

- Molecule 25 is CALCIUM ION (three-letter code: CA) (formula: Ca).

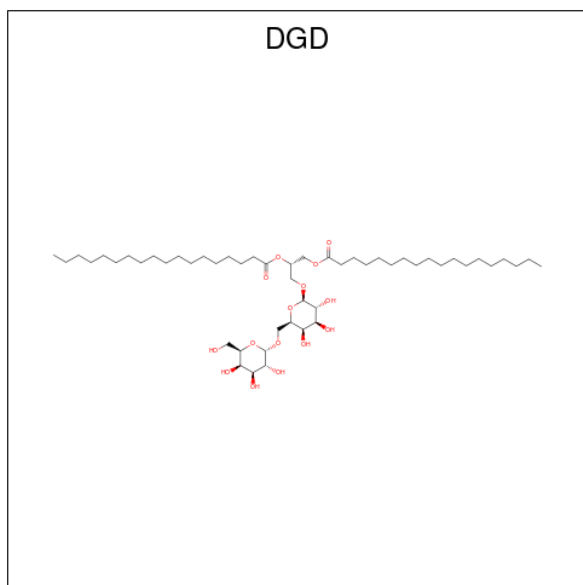
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	3	1	Total	Ca	0	0
			1	1		

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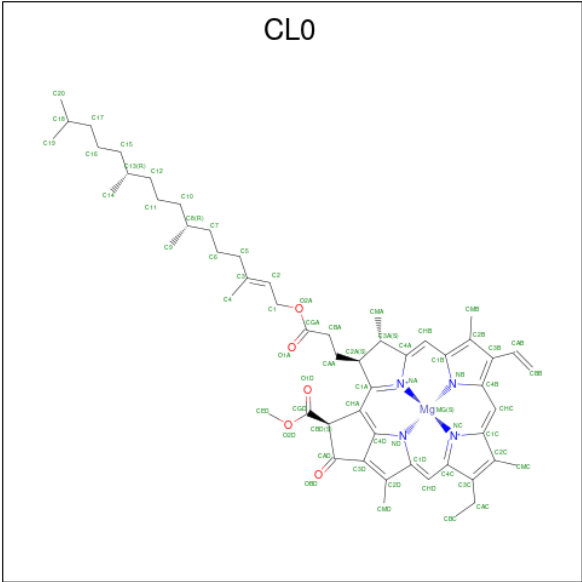
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	B	1	Total	Ca	0	0
			1	1		

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGD) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



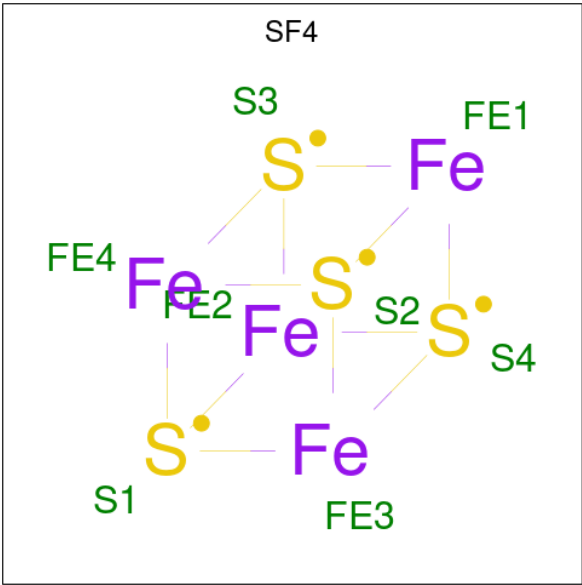
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	4	1	Total	C	O	0	0
			51	36	15		
26	B	1	Total	C	O	0	0
			41	26	15		
26	B	1	Total	C	O	0	0
			61	46	15		
26	G	1	Total	C	O	0	0
			47	32	15		
26	J	1	Total	C	O	0	0
			58	43	15		

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



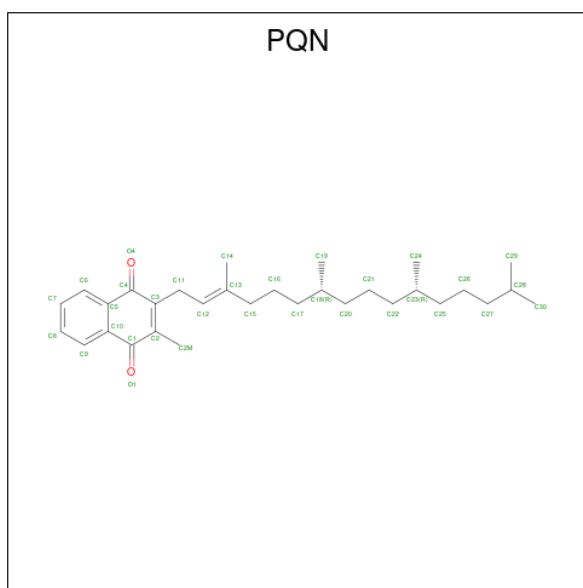
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 28 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



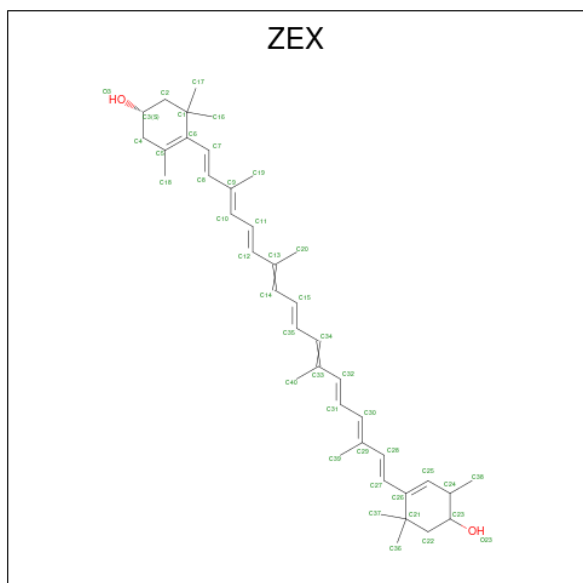
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	Fe	S	0	0
			8	4	4		
28	C	1	Total	Fe	S	0	0
			8	4	4		
28	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 29 is PHYLLOQUINONE (three-letter code: 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 (three-letter code: 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		

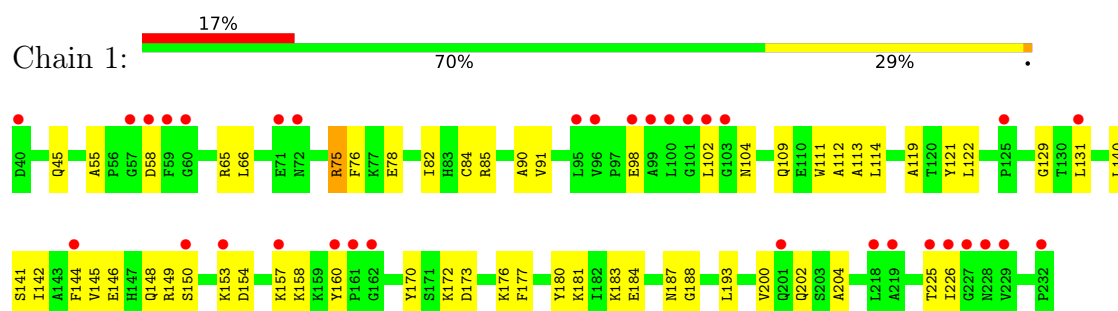
- Molecule 31 is water.

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			

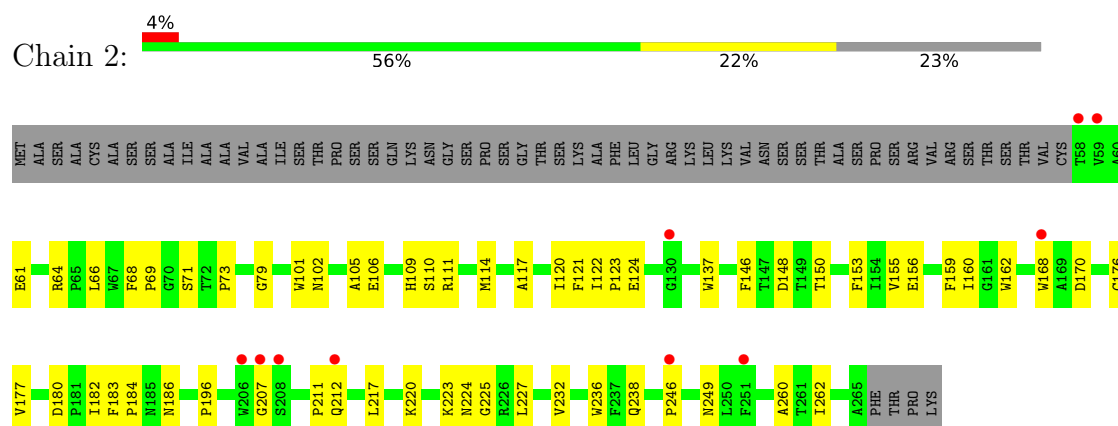
3 Residue-property plots [i](#)

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

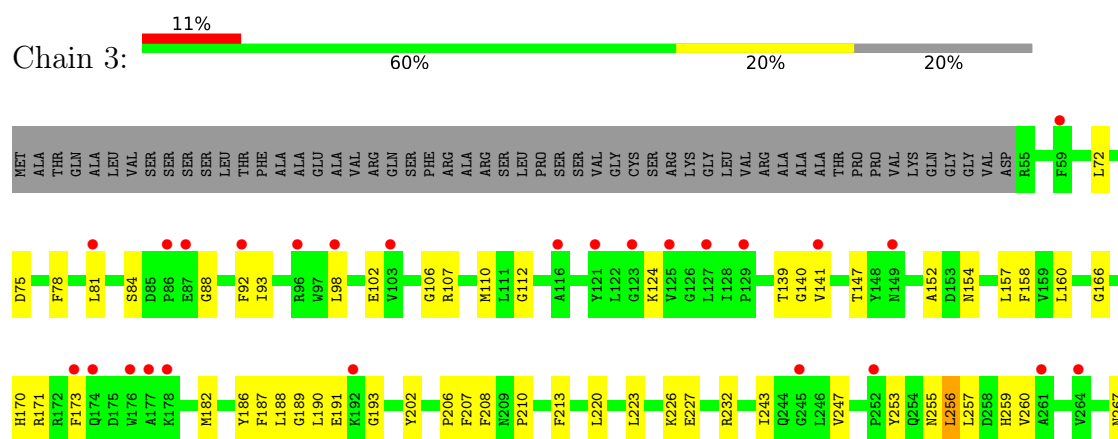
- Molecule 1: Lhca1



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

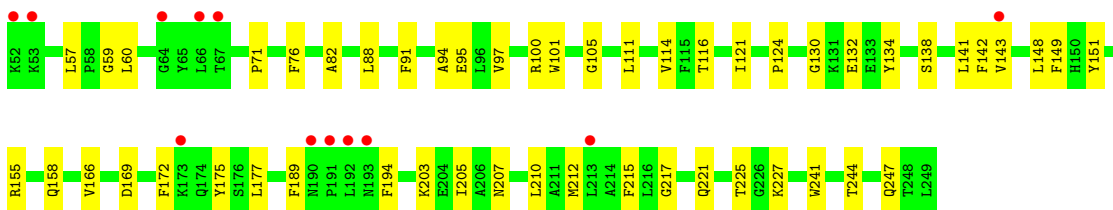
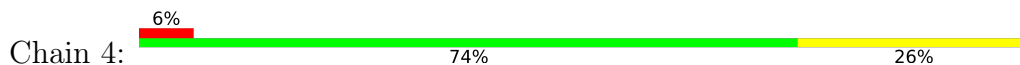


- Molecule 3: Chlorophyll a-b binding protein 3, chloroplastic

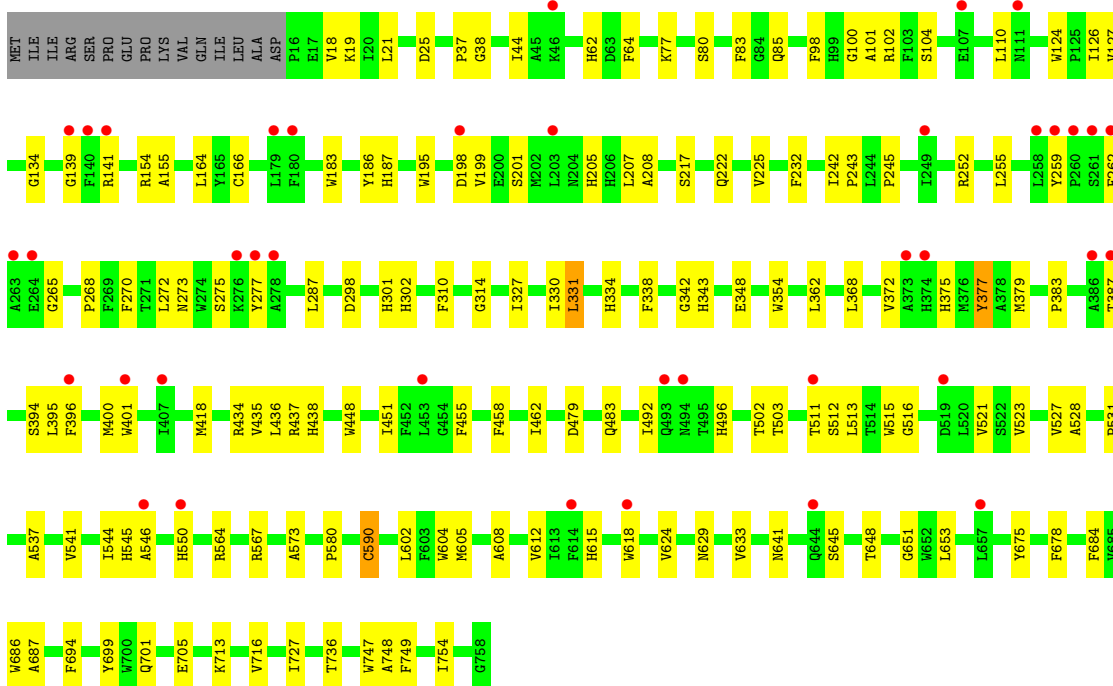
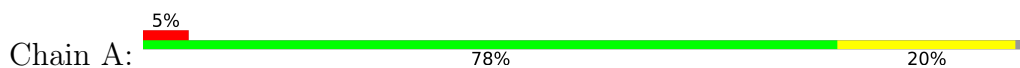




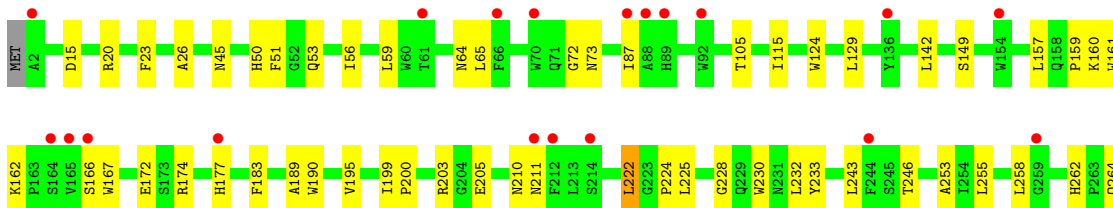
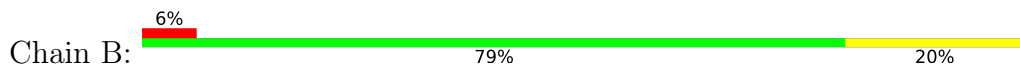
- Molecule 4: Chlorophyll a-b binding protein P4, chloroplastic

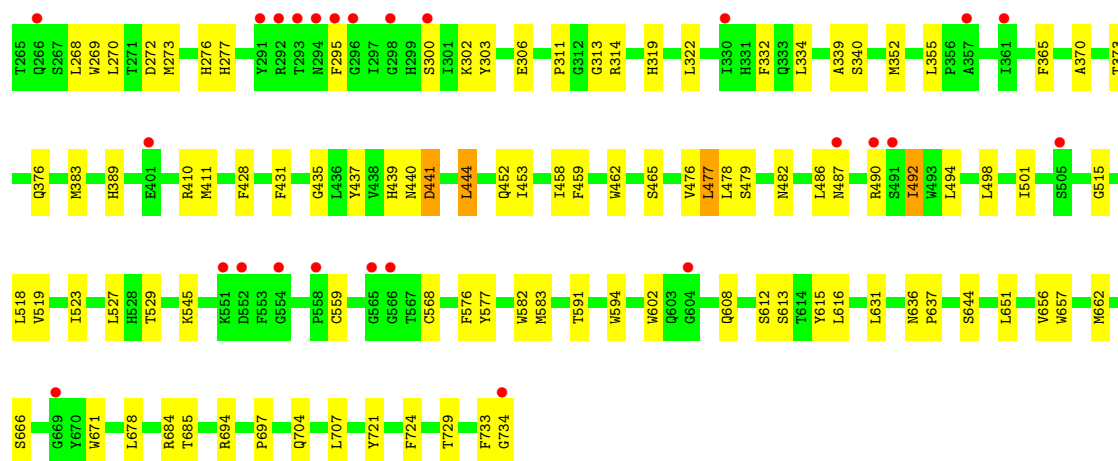


- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

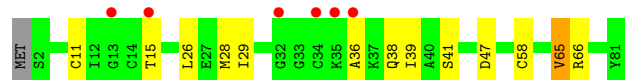
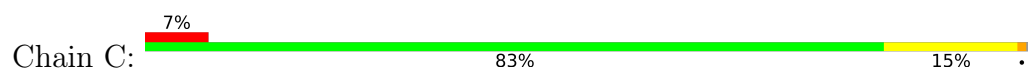


- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

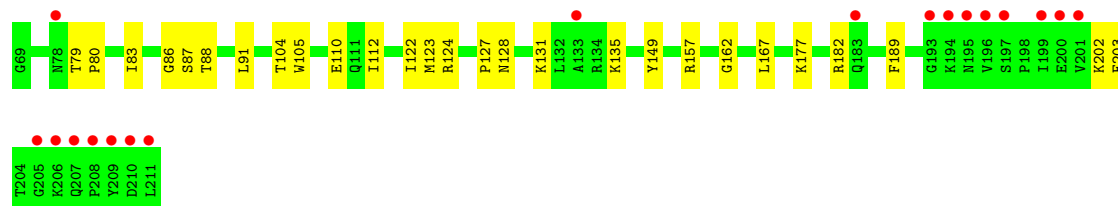
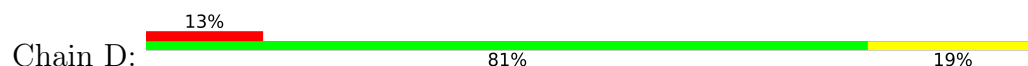




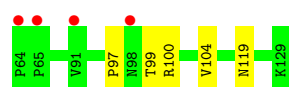
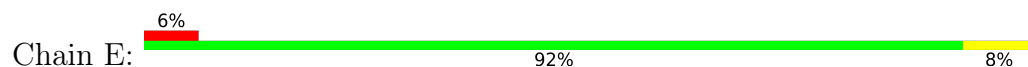
• Molecule 7: Photosystem I iron-sulfur center



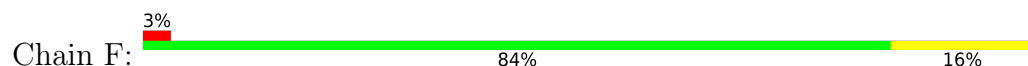
• Molecule 8: Psad



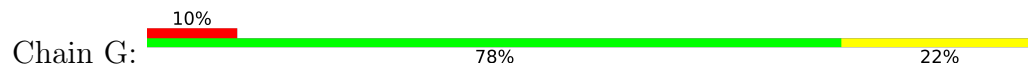
• Molecule 9: Putative uncharacterized protein

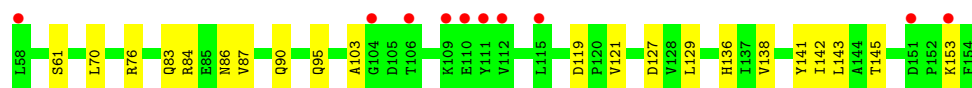


• Molecule 10: Photosystem I reaction center subunit III

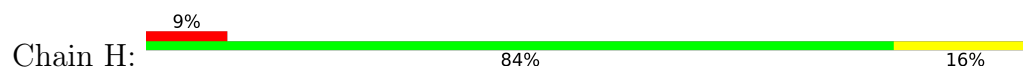


• Molecule 11: PsaG





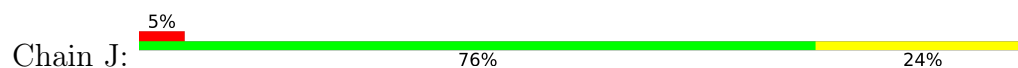
- Molecule 12: Photosystem I reaction center subunit VI



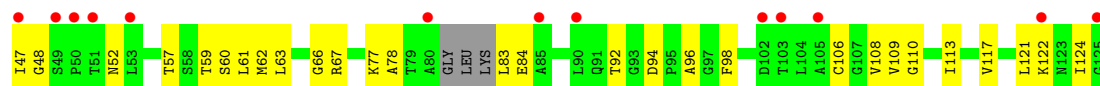
- Molecule 13: Photosystem I reaction center subunit VIII



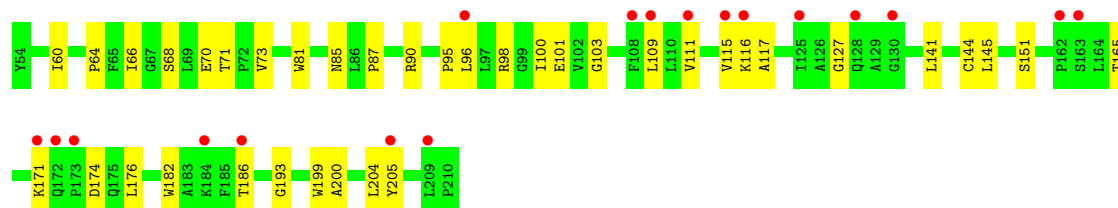
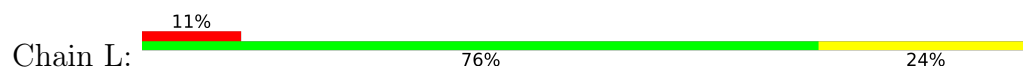
- Molecule 14: Photosystem I reaction center subunit IX



- 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 0.212 , 0.235	Depositor DCC
R_{free} test set	4924 reflections (1.98%)	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: LMG, ZEX, DGD, PQN, CHL, LHG, SF4, LMT, CL0, CA, LUT, XAT, CLA, BCR

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	0.27	0/1558	0.40	0/2125
2	2	0.28	0/1679	0.44	0/2302
3	3	0.28	0/1753	0.43	0/2382
4	4	0.30	0/1608	0.41	0/2191
5	A	0.28	0/6057	0.44	0/8264
6	B	0.28	0/6069	0.44	0/8286
7	C	0.32	0/625	0.51	0/846
8	D	0.29	0/1163	0.48	0/1572
9	E	0.26	0/540	0.45	0/734
10	F	0.28	0/1241	0.43	0/1679
11	G	0.26	0/776	0.42	0/1054
12	H	0.27	0/693	0.44	0/942
13	I	0.27	0/238	0.41	0/324
14	J	0.39	0/349	0.48	0/476
15	K	0.25	0/520	0.45	0/707
16	L	0.27	0/1207	0.45	0/1651
All	All	0.28	0/26076	0.44	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	60	0
2	2	1620	0	1557	55	0
3	3	1699	0	1648	62	0
4	4	1559	0	1527	49	0
5	A	5858	0	5719	148	0
6	B	5857	0	5653	140	0
7	C	612	0	592	8	0
8	D	1132	0	1141	19	0
9	E	528	0	528	3	0
10	F	1213	0	1241	19	0
11	G	757	0	743	20	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	26	0
16	L	1174	0	1183	35	0
17	1	84	0	110	12	0
17	2	42	0	55	8	0
17	3	84	0	110	19	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	13	0
18	3	80	0	109	11	0
18	4	40	0	55	9	0
18	A	240	0	329	21	0
18	B	280	0	384	28	0
18	F	40	0	55	1	0
18	G	40	0	55	3	0
18	I	80	0	110	12	0
18	J	40	0	55	4	0
18	K	40	0	55	7	0
18	L	120	0	165	8	0
19	1	608	0	563	58	0
19	2	512	0	479	38	0
19	3	623	0	526	63	0
19	4	631	0	599	61	0
19	A	2653	0	2772	246	0
19	B	2350	0	2461	202	0
19	F	130	0	144	12	0
19	G	231	0	225	24	0
19	H	60	0	59	4	0
19	J	160	0	143	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	K	159	0	96	13	0
19	L	215	0	185	11	0
20	1	164	0	134	24	0
20	2	263	0	210	31	0
20	3	47	0	30	9	0
20	4	202	0	150	21	0
21	1	91	0	131	17	0
21	2	35	0	40	9	0
21	A	89	0	127	10	0
21	B	70	0	86	8	0
22	1	59	0	76	3	0
22	2	126	0	117	9	0
22	4	58	0	71	4	0
22	A	50	0	73	3	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	10	0
24	2	35	0	46	0	0
24	3	31	0	34	1	0
24	4	35	0	45	3	0
24	A	35	0	46	3	0
24	B	98	0	114	9	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	8	0
28	A	8	0	0	1	0
28	C	16	0	0	2	0
29	A	33	0	46	4	0
29	B	33	0	46	8	0
30	F	42	0	56	6	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	1261	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 17.

All (1261) 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:B:823:CLA:HAB	19:B:830:CLA:HMD2	1.50	0.93
18:2:503:BCR:H17C	20:2:513:CHL:HMB3	1.55	0.88
19:J:1105:CLA:HHC	19:J:1105:CLA:HBB1	1.55	0.86
19:B:823:CLA:HMA1	19:B:840:CLA:HED2	1.59	0.85
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:394:SER:HB3	19:A:828:CLA:HMA1	1.60	0.82
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
19:B:805:CLA:HMA2	21:B:843:LHG:H262	1.66	0.78
19:A:824:CLA:HMA1	19:A:842:CLA:HAB	1.66	0.78
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
3:3:208:PHE:HB3	19:3:305:CLA:HMD1	1.66	0.77
4:4:134:TYR:HE1	19:4:309:CLA:HAA2	1.48	0.77
19:3:305:CLA:H71	19:3:306:CLA:HMA1	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:511:CLA:HBA1	3:3:160:LEU:HD13	1.67	0.76
20:2:512:CHL:HBB1	20:2:512:CHL:HMB1	1.66	0.76
19:4:309:CLA:HMA2	20:4:316:CHL:HBC2	1.68	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
19:G:204:CLA:HMC2	22:G:206:LMG:H361	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
6:B:477:LEU:HD13	19:B:833:CLA:HMD3	1.68	0.75
3:3:107:ARG:HB3	19:3:305:CLA:HBC3	1.69	0.74
3:3:139:THR:HG23	19:3:310:CLA:HED3	1.69	0.74
19:B:832:CLA:H91	19:J:1102:CLA:HMA1	1.70	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
19:A:835:CLA:HMB1	18:A:851:BCR:HC31	1.70	0.73
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
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
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
21:1:517:LHG:H223	19:4:318:CLA:HMA2	1.72	0.71
18:A:856:BCR:H353	18:K:1005:BCR:H323	1.71	0.71
19:4:307:CLA:HMB1	19:4:307:CLA:HBB1	1.73	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:A:831:CLA:HMA2	16:L:71:THR:HG21	1.72	0.70
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:168:TRP:CE3	19:2:514:CLA:HMA2	2.27	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
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
18:3:303:BCR:H351	20:3:314:CHL:HMB1	1.74	0.69
1:1:153:LYS:HD3	1:1:158:LYS:HD2	1.74	0.69
19:1:516:CLA:HBA2	30:F:301:ZEX:H41	1.75	0.69
19:A:802:CLA:HBB1	19:A:802:CLA:HMB1	1.75	0.69
19:4:307:CLA:H71	19:4:308:CLA:HMA1	1.72	0.69
5:A:604:TRP:CH2	19:A:803:CLA:HAB	2.28	0.69
19:J:1102:CLA:HBB1	19:J:1102:CLA:HMB1	1.75	0.69
11:G:61:SER:HB3	19:G:202:CLA:HED2	1.75	0.68
19:2:506:CLA:HMA1	19:2:511:CLA:HBC3	1.73	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
19:J:1101:CLA:HBB1	19:J:1101:CLA:HMB1	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
14:J:32:PHE:CZ	19:J:1105:CLA:HMA3	2.29	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:G:203:CLA:HMB1	19:G:203:CLA:HBB1	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
19:B:813:CLA:HMB1	19:B:813:CLA:HBB1	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:A:807:CLA:HBB1	19:A:807:CLA:HMB1	1.77	0.66
6:B:523:ILE:HG21	19:B:835:CLA:HAB	1.77	0.66
19:3:308:CLA:HMB1	19:3:308:CLA:HBB1	1.78	0.66
19:A:840:CLA:HMB1	19:A:840:CLA:HBB1	1.77	0.66
5:A:567:ARG:NH2	8:D:88:THR:O	2.29	0.65
19:B:831:CLA:HMB1	19:B:831:CLA:HBB1	1.76	0.65
10:F:207:VAL:HB	19:J:1102:CLA:HED2	1.79	0.65
19:4:308:CLA:HMB1	19:4:308:CLA:HBB1	1.79	0.65
24:B:847:LMT:H11	22:F:304:LMG:H301	1.78	0.65
19:A:825:CLA:HBB1	19:A:825:CLA:HMB1	1.76	0.65
19:2:507:CLA:HBB1	19:2:507:CLA:HMB1	1.78	0.65
19:2:510:CLA:HMB1	19:2:510:CLA:HBB1	1.79	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: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
19:2:508:CLA:HBB1	19:2:508:CLA:HMB1	1.79	0.65
19:A:806:CLA:H152	19:A:829:CLA:HBB2	1.78	0.65
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
19:F:302:CLA:HBB1	19:F:302:CLA:HMB1	1.78	0.64
5:A:208:ALA:HB2	5:A:314:GLY:HA3	1.80	0.64
19:A:830:CLA:HMB1	19:A:830:CLA:HBB1	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: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
19:2:504:CLA:H41	19:2:505:CLA:HMA2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:2:223:LYS:NZ	21:2:517:LHG:O5	2.17	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
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
16:L:109:LEU:O	31:L:401:HOH:O	2.16	0.62
18:A:852:BCR:H24C	19:B:832:CLA:HMC2	1.80	0.62
19:B:823:CLA:HBB1	19:B:830:CLA:H13	1.82	0.62
19:A:854:CLA:HBB1	19:A:854:CLA:HMB1	1.82	0.62
29:B:841:PQN:H28	18:I:102:BCR:H343	1.81	0.62
19:1:504:CLA:HBB1	19:1:504:CLA:HMB1	1.82	0.61
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
5:A:379:MET:HE3	19:A:827:CLA:HHC	1.82	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: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
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:824:CLA:H151	19:A:831:CLA:HMC2	1.82	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
19:4:307:CLA:H91	19:4:308:CLA:H142	1.83	0.61
19:A:818:CLA:H101	19:A:818:CLA:HMC2	1.81	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
16:L:116:LYS:HD3	19:L:305:CLA:HMB2	1.82	0.61
3:3:92:PHE:HB3	19:3:309:CLA:H11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:3:308:CLA:HMB2	19:3:308:CLA:H43	1.82	0.60
6:B:662:MET:HE2	29:B:841:PQN:H2M3	1.83	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
5:A:458:PHE:HE1	19:A:803:CLA:HMA1	1.66	0.60
19:3:310:CLA:HBA1	19:3:316:CLA:C1D	2.32	0.60
19:B:825:CLA:HMB1	19:B:825:CLA:HBB1	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
19:2:509:CLA:HMB1	19:2:509:CLA:HBB1	1.84	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:A:804:CLA:HMA2	19:A:811:CLA:HMD2	1.84	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
6:B:370:ALA:HB1	19:B:827:CLA:HMA1	1.84	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
20:2:513:CHL:HHC	20:2:513:CHL:HBB1	1.83	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
6:B:167:TRP:CZ2	19:B:812:CLA:HMA1	2.37	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
6:B:373:THR:HG23	6:B:591:THR:HG21	1.84	0.59
19:A:824:CLA:HBB1	19:A:831:CLA:HMD2	1.83	0.58
6:B:51:PHE:HE1	19:B:812:CLA:HBB1	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:A:808:CLA:HBB1	19:A:808:CLA:HMB1	1.85	0.58
19:B:830:CLA:H92	19:B:840:CLA:HMA2	1.85	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
3:3:220:LEU:HD12	19:3:305:CLA:HMA2	1.85	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
27:A:801:CL0:H15	27:A:801:CL0:H11	1.85	0.58
19:A:839:CLA:H92	18:B:856:BCR:H16C	1.84	0.58
12:H:55:PHE:HA	12:H:63:THR:HG23	1.85	0.58
27:A:801:CL0:H13	19:A:854:CLA:OBD	2.04	0.58
6:B:465:SER:O	6:B:479:SER:HB2	2.03	0.58
19:B:815:CLA:HMA2	18:B:851:BCR:H393	1.86	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
1:1:84:CYS:HB3	1:1:188:GLY:HA3	1.86	0.57
5:A:77:LYS:NZ	19:A:811:CLA:OBD	2.35	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
19:3:315:CLA:HMB1	19:3:315:CLA:HBB1	1.87	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
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: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
19:B:810:CLA:HMB1	19:B:810:CLA:HBB1	1.87	0.56
5:A:195:TRP:CZ2	19:A:810:CLA:HMA1	2.40	0.56
6:B:59:LEU:HG	19:B:808:CLA:HBB2	1.88	0.56
15:K:117:VAL:HG23	19:K:1002:CLA:HMC3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:64:PHE:CD2	19:A:805:CLA:HMC2	2.41	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
5:A:310:PHE:CE1	19:A:821:CLA:HAB	2.32	0.56
20:2:526:CHL:HMB2	19:3:317:CLA:HED2	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
18:B:802:BCR:H362	19:B:804:CLA:H122	1.87	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
19:B:835:CLA:HMB2	19:B:837:CLA:HED1	1.88	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
20:1:521:CHL:HBC3	20:1:521:CHL:HHH	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
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
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
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
19:3:308:CLA:H92	19:3:309:CLA:HMA1	1.89	0.54
19:4:318:CLA:H101	30:F:301:ZEX:H163	1.89	0.54
19:A:836:CLA:HBB1	19:A:836:CLA:HMB1	1.87	0.54
19:A:854:CLA:HAB	6:B:582:TRP:CH2	2.42	0.54
19:J:1105:CLA:HBC2	19:J:1105:CLA:HMC1	1.89	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
5:A:85:GLN:HG2	19:A:805:CLA:HMA1	1.90	0.54
19:A:834:CLA:HBA2	19:A:835:CLA:HMB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
19:B:833:CLA:HBA2	19:B:834:CLA:HMB3	1.88	0.54
1:1:109:GLN:HG2	19:1:515:CLA:HMC1	1.90	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
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
5:A:205:HIS:CG	19:A:813:CLA:HMC2	2.42	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:B:823:CLA:CMA	19:B:840:CLA:HED2	2.34	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
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
17:3:301:LUT:C32	19:3:305:CLA:HMC2	2.39	0.53
1:1:180:TYR:HA	1:1:183:LYS:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:510:CLA:H2A	19:1:510:CLA:O2D	2.08	0.53
6:B:545:LYS:NZ	31:B:907:HOH:O	2.37	0.53
6:B:657:TRP:CE3	19:B:803:CLA:HMA1	2.44	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:A:809:CLA:HBB1	19:A:809:CLA:HMB1	1.90	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
19:B:825:CLA:HMA1	18:B:853:BCR:H14C	1.90	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
19:A:821:CLA:HMA2	19:A:825:CLA:C1C	2.39	0.52
19:B:829:CLA:HBB1	19:B:829:CLA:HMB1	1.92	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: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
6:B:272:ASP:HB3	19:B:818:CLA:HMA1	1.91	0.52
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:B:820:CLA:HMB2	19:B:824:CLA:HMA3	1.92	0.52
19:1:516:CLA:C4D	22:F:304:LMG:H121	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:155:ALA:HB2	5:A:383:PRO:HD2	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
19:A:855:CLA:HMA2	18:L:302:BCR:H401	1.92	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
2:2:217:LEU:HB3	19:2:504:CLA:HMA1	1.92	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
19:1:507:CLA:HMD2	20:1:521:CHL:CBB	2.40	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
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
5:A:379:MET:HE1	5:A:511:THR:HG22	1.92	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:A:826:CLA:H2	19:A:836:CLA:HMA2	1.92	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
18:2:503:BCR:H372	20:2:513:CHL:HMA2	1.93	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
19:A:808:CLA:H192	19:J:1101:CLA:HMA2	1.93	0.50
1:1:146:GLU:HG2	20:1:514:CHL:NB	2.26	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
19:A:821:CLA:HMB2	19:A:825:CLA:HMA3	1.93	0.50
6:B:195:VAL:HA	6:B:199:ILE:HD12	1.93	0.50
19:3:313:CLA:HMD1	19:3:316:CLA:HAB	1.92	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
19:B:830:CLA:HMB1	19:B:830:CLA:HBB1	1.92	0.50
11:G:76:ARG:HG2	19:G:203:CLA:CAB	2.42	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
6:B:383:MET:HE1	18:B:853:BCR:H361	1.94	0.50
4:4:101:TRP:CE2	20:4:314:CHL:HED3	2.47	0.50
5:A:252:ARG:HH22	5:A:265:GLY:HA2	1.75	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
17:4:302:LUT:H371	19:4:304:CLA:H51	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
3:3:223:LEU:C	19:3:305:CLA:HMA1	2.33	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
19:1:516:CLA:HMA1	30:F:301:ZEX:H8	1.94	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:A:830:CLA:H122	19:A:841:CLA:HMA2	1.95	0.49
19:B:834:CLA:O1A	19:G:204:CLA:HHB	2.12	0.49
15:K:124:ILE:HD11	19:K:1002:CLA:HMA1	1.94	0.49
1:1:202:GLN:HG3	26:B:801:DGD:HA32	1.94	0.49
2:2:236:TRP:CZ3	20:2:512:CHL:HMA1	2.47	0.49
20:2:512:CHL:HAB	20:2:515:CHL:HBB2	1.93	0.49
19:4:309:CLA:HBA1	20:4:316:CHL:HMD2	1.93	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
19:2:509:CLA:HMA2	20:2:515:CHL:HAC2	1.93	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
5:A:615:HIS:HD2	19:A:836:CLA:HMC2	1.77	0.49
21:A:845:LHG:H261	18:A:850:BCR:H373	1.94	0.49
4:4:210:LEU:HA	26:4:319:DGD:HA31	1.94	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
19:4:306:CLA:H18	19:4:306:CLA:HMB1	1.95	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
19:3:310:CLA:HMB2	19:3:316:CLA:C4B	2.42	0.49
19:A:833:CLA:HMA2	16:L:117:ALA:HB1	1.95	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:205:HIS:ND1	19:A:813:CLA:HMC2	2.28	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:401:TRP:HB3	19:A:828:CLA:HMC3	1.94	0.48
5:A:521:VAL:HG12	5:A:528:ALA:HB3	1.95	0.48
19:A:826:CLA:O1A	19:A:836:CLA:HMA1	2.13	0.48
19:B:818:CLA:HMC2	19:B:818:CLA:H143	1.96	0.48
1:1:170:TYR:CE2	17:1:501:LUT:H221	2.49	0.48
5:A:546:ALA:HB1	19:A:837:CLA:HMB3	1.95	0.48
27:A:801:CL0:H13	19:A:854:CLA:CAD	2.42	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
19:L:304:CLA:HMB1	19:L:304:CLA:HBB1	1.94	0.48
3:3:193:GLY:HA3	3:3:207:PHE:CD2	2.49	0.48
19:A:802:CLA:H71	19:A:841:CLA:HMC3	1.94	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
19:A:802:CLA:HMA2	19:A:802:CLA:H12	1.95	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
17:1:502:LUT:H363	19:1:515:CLA:HMC2	1.96	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
21:A:853:LHG:H161	19:J:1101:CLA:HMB2	1.94	0.48
6:B:411:MET:HE3	19:B:830:CLA:HMD3	1.94	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
18:2:503:BCR:H333	19:4:310:CLA:HMC3	1.96	0.48
17:3:301:LUT:H162	19:3:307:CLA:HMB3	1.96	0.48
19:A:821:CLA:HMB1	19:A:821:CLA:HBB1	1.96	0.48
6:B:142:LEU:HD11	18:B:851:BCR:H402	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:A:808:CLA:H203	19:J:1101:CLA:HMA1	1.95	0.48
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
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
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
19:2:507: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
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
4:4:149:PHE:CG	19:4:315:CLA:HMC3	2.49	0.47
19:4:306:CLA:C4C	19:4:306:CLA:H42	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
16:L:103:GLY:O	16:L:193:GLY:HA2	2.15	0.47
1:1:180:TYR:C	19:1:504:CLA:HMA1	2.34	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
19:3:305:CLA:HBC2	19:3:305:CLA:HMC1	1.97	0.47
5:A:302:HIS:HB2	19:A:818:CLA:CHB	2.45	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:842:CLA:H61	19:A:842:CLA:H41	1.71	0.47
19:B:803:CLA:HMB1	19:B:803:CLA:HBB1	1.96	0.47
7:C:15:THR:HG22	7:C:28:MET:HG3	1.97	0.47
7:C:47:ASP:OD2	8:D:135:LYS:NZ	2.37	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
5:A:686:TRP:CE3	27:A:801:CL0:H4	2.49	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
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:819:CLA:HBB1	19:A:819:CLA:HMB1	1.96	0.46
19:A:822:CLA:HHC	19:A:822:CLA:HBB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:1:507:CLA:HMD2	20:1:521:CHL:HBB1	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
5:A:301:HIS:CD2	19:A:818:CLA:HMB1	2.50	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:808:CLA:HMA1	19:B:809:CLA:CHB	2.45	0.46
19:B:828:CLA:H3A	19:B:828:CLA:HBA2	1.37	0.46
5:A:100:GLY:O	5:A:104:SER:HB2	2.15	0.46
5:A:195:TRP:CE2	19:A:810:CLA:HMA1	2.51	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:H:1000:CLA:HMB2	19:L:303:CLA:HAA1	1.96	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
17:3:301:LUT:C31	19:3:305:CLA:HMC2	2.45	0.46
5:A:268:PRO:HB3	5:A:273:ASN:HB2	1.96	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
19:A:832:CLA:HMC2	19:L:305:CLA:HBB2	1.96	0.46
6:B:172:GLU:OE1	6:B:172:GLU:N	2.46	0.46
6:B:656:VAL:HG22	19:B:839:CLA:HMB3	1.96	0.46
6:B:662:MET:HE2	29:B:841:PQN:C2M	2.45	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
19:1:508:CLA:HBA1	19:1:508:CLA:H3A	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:310:CLA:HMA2	19:3:316:CLA:CBC	2.45	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: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
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
4:4:91:PHE:C	19:4:307:CLA:HMA1	2.37	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
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
19:A:854:CLA:HMA1	19:B:803:CLA:H202	1.97	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
14:J:32:PHE:CE2	19:J:1105:CLA:HMA3	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:A:713:LYS:HB3	19:B:831:CLA:HMA2	1.98	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
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
19:A:806:CLA:H192	19:A:806:CLA:H162	1.67	0.45
19:A:824:CLA:HMA1	19:A:842:CLA:CAB	2.43	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
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:842:CLA:CHB	21:A:845:LHG:HC62	2.47	0.45
6:B:174:ARG:HE	19:B:824:CLA:HMD1	1.82	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:H:1000:CLA:HMB3	18:L:307:BCR:H372	1.99	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
19:1:508:CLA:H12	19:B:840:CLA:HMC3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
19:B:820:CLA:HMC2	19:B:824:CLA:H161	1.99	0.45
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:806:CLA:HBB1	19:A:806:CLA:HMB1	1.98	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:827:CLA:O1D	19:B:828:CLA:HMA1	2.17	0.45
19:B:830:CLA:HMB2	19:B:831:CLA:C2D	2.47	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
18:2:503:BCR:C33	19:4:310:CLA:HMC3	2.47	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:828:CLA:O1D	19:A:829:CLA:HMA1	2.17	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
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
6:B:311:PRO:C	6:B:313:GLY:H	2.21	0.44
19:B:817:CLA:H3A	19:B:817:CLA:HBA2	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
22:2:519:LMG:C10	19:J:1105:CLA:H11	2.47	0.44
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
14:J:34:PRO:O	26:J:1106:DGD:O2D	2.28	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
20:4:313:CHL:HMD2	24:4:320:LMT:H12	2.00	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:53:GLN:HG2	19:B:806:CLA:HMA1	1.99	0.44
6:B:268:LEU:HD13	19:B:818:CLA:HMA2	1.99	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
15:K:113:ILE:HA	19:K:1002:CLA:HMC1	1.99	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
6:B:59:LEU:HD21	19:B:808:CLA:H111	2.00	0.44
19:B:815:CLA:HMB1	19:B:815:CLA:HBB1	1.99	0.44
19:B:832:CLA:HMA2	26:J:1106:DGD:HA42	1.99	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
20:1:512:CHL:C2C	19:1:515:CLA:HMC3	2.47	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
17:2:501:LUT:H31	19:2:505:CLA:HMC2	2.00	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
19:A:842:CLA:HMC3	21:A:845:LHG:O1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:828:CLA:HBB1	19:B:828:CLA:HMB1	2.00	0.43
1:1:112:ALA:HB3	20:1:512:CHL:HMD3	1.99	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:418:MET:HE1	5:A:436:LEU:HD11	2.00	0.43
5:A:675:TYR:O	5:A:748:ALA:HB1	2.18	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
19:3:307: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
23:4:303:XAT:C32	19:4:308:CLA:HMB2	2.48	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
5:A:749:PHE:CD2	27:A:801:CL0:H25	2.53	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
19:A:826:CLA:HMB3	18:A:851:BCR:H19C	2.01	0.43
6:B:410:ARG:HD3	19:B:830:CLA:OBD	2.18	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
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
5:A:298:ASP:HB3	19:A:818:CLA:HMA1	2.01	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
19:4:309:CLA:HMA2	20:4:316:CHL:CBC	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:832:CLA:HMA1	18:I:101:BCR:HC32	2.00	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
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
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:807:CLA:HBA1	19:B:829:CLA:HMB2	2.01	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
22:2:519:LMG:HC8	22:2:519:LMG:HC1	1.87	0.43
19:3:315:CLA:HMB2	19:3:317:CLA:C4B	2.49	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:270:LEU:HD23	6:B:273:MET:HE3	2.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:820:CLA:HMA2	19:B:824:CLA:C1C	2.49	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
1:1:76:PHE:C	19:1:507:CLA:HMA1	2.39	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
9:E:97:PRO:C	9:E:99:THR:H	2.22	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
6:B:159:PRO:C	6:B:161:TRP:H	2.23	0.42
19:B:816:CLA:H61	19:B:816:CLA:H92	1.81	0.42
19:B:826:CLA:H93	19:B:826:CLA:H111	1.74	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
18:2:503:BCR:H322	19:4:312:CLA:HMD2	2.01	0.42
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
4:4:97:VAL:HG12	19:4:315:CLA:HMD3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:805:CLA:H3A	19:B:805:CLA:HBA2	1.50	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
2:2:238: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
4:4:203:LYS:O	4:4:207:ASN:ND2	2.38	0.42
5:A:272:LEU:HD13	19:K:1001:CLA:HMD2	2.01	0.42
5:A:699:TYR:CZ	19:A:802:CLA:HMD1	2.55	0.42
19:A:818:CLA:O1D	19:A:819:CLA:HMA1	2.19	0.42
19:A:818:CLA:H71	19:A:835:CLA:HMA2	2.00	0.42
19:A:821:CLA:HBA1	19:A:825:CLA:CAB	2.50	0.42
19:B:806:CLA:H3A	19:B:806:CLA:HBA1	1.47	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:645:SER:O	5:A:651:GLY:HA3	2.20	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:177:HIS:CG	19:B:814:CLA:HMC2	2.54	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
19:B:829:CLA:H141	19:B:829:CLA:H161	1.65	0.42
18:B:849:BCR:H24C	19:G:201:CLA:HMD2	2.00	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
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
20:2:512:CHL:HMB1	20:2:512:CHL:CBB	2.43	0.42
5:A:183:TRP:HB2	19:A:811:CLA:HMC3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:831:CLA:HMB1	19:A:831:CLA:HBB1	2.02	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
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
20:1:512:CHL:C1C	19:1:515:CLA:HMC3	2.50	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: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
12:H:73:ASP:HB2	16:L:171:LYS:HE2	2.01	0.41
19:2:506:CLA:H161	19:2:506:CLA:H192	1.69	0.41
3:3:189:GLY:C	3:3:191:GLU:H	2.24	0.41
19:A:824:CLA:H191	19:A:824:CLA:HAB	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:822:CLA:HMB3	19:B:840:CLA:C1D	2.50	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
19:A:855:CLA:HMD3	6:B:678:LEU:HD13	2.02	0.41
6:B:115:ILE:O	19:B:809:CLA:HMD3	2.20	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
13:I:14:LEU:C	13:I:17:PRO:HD2	2.41	0.41
21:2:517:LHG:H122	21:2:517:LHG:HC92	1.76	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:685:THR:OG1	19:L:301:CLA:HMA1	2.19	0.41
19:B:808:CLA:H91	19:B:808:CLA:H112	1.70	0.41
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
29:A:844:PQN:H111	29:A:844:PQN:H2M1	1.88	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
6:B:411:MET:HE1	19:B:830:CLA:C1D	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:F:301:ZEX:H31	30:F:301:ZEX:H401	1.85	0.41
1:1:78:GLU:CD	1:1:158:LYS:HE3	2.41	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
19:4:307:CLA:HMD2	19:4:312:CLA:HBB1	2.03	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
17:2:501:LUT:C31	19:2:505:CLA:HMC2	2.51	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: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
6:B:594:TRP:HB2	19:B:835:CLA:HMC1	2.02	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
2:2:102:ASN:C	19:2:507:CLA:HMA1	2.41	0.41
2:2:120:ILE:HG22	2:2:121:PHE:CD1	2.56	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
3:3:166:GLY:C	3:3:170:HIS:HD1	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:3:173:PHE:CD1	19:3:315:CLA:HMA2	2.55	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
5:A:716:VAL:HG21	19:A:839:CLA:HMB3	2.02	0.41
19:A:827:CLA:CAB	19:A:834:CLA:HMA2	2.51	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:CBC	20:1:514:CHL:HAC1	2.52	0.40
19:1:508:CLA:HBD	20:1:514:CHL:HBD	2.03	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:502:THR:OG1	5:A:503:THR:N	2.51	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
19:A:824:CLA:HHB	19:A:842:CLA:HAB	2.02	0.40
19:B:809:CLA:H111	19:B:809:CLA:H142	1.87	0.40
19:B:820:CLA:HMD3	19:G:201:CLA:HMC3	2.03	0.40
19:F:303:CLA:ND	22:F:304:LMG:H302	2.36	0.40
19:J:1101:CLA:H162	19:J:1101:CLA:H122	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:4:175:TYR:CD2	20:4:317:CHL:HAA2	2.55	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:295:PHE:HE2	19:B:813:CLA:HMA1	1.86	0.40
6:B:300:SER:H	11:G:90:GLN:HE21	1.68	0.40
6:B:411:MET:HE2	6:B:411:MET:CA	2.51	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
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
19:A:839:CLA:HMA2	19:B:831:CLA:HMB3	2.03	0.40
22:A:847:LMG:H352	22:A:847:LMG:H321	1.68	0.40
19:B:814:CLA:C14	19:B:819:CLA:H2	2.50	0.40
19:B:833:CLA:HMB1	19:B:833:CLA:HBB1	2.02	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
19:4:307:CLA:HMD2	19:4:312:CLA:CBB	2.52	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
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
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
24:B:847:LMT:H51	19:F:303:CLA:HMC3	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	191/193 (99%)	184 (96%)	6 (3%)	1 (0%)	25	47
2	2	206/269 (77%)	196 (95%)	9 (4%)	1 (0%)	25	47
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	71
6	B	731/734 (100%)	710 (97%)	18 (2%)	3 (0%)	30	52
7	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
8	D	141/143 (99%)	135 (96%)	6 (4%)	0	100	100
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	44	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%)	65	84
2	2	167/216 (77%)	167 (100%)	0	100	100
3	3	169/213 (79%)	168 (99%)	1 (1%)	84	94
4	4	164/164 (100%)	164 (100%)	0	100	100
5	A	604/618 (98%)	599 (99%)	5 (1%)	79	91
6	B	598/599 (100%)	589 (98%)	9 (2%)	60	81
7	C	69/70 (99%)	67 (97%)	2 (3%)	37	64
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%)	80 (98%)	2 (2%)	44	70
12	H	71/71 (100%)	71 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	124 (100%)	0	100	100
All	All	2624/2751 (95%)	2603 (99%)	21 (1%)	79	91

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	75	ARG
1	1	114	LEU
3	3	256	LEU
5	A	331	LEU
5	A	377	TYR
5	A	590	CYS
5	A	605	MET
5	A	618	TRP
6	B	157	LEU
6	B	332	PHE
6	B	441	ASP
6	B	444	LEU
6	B	477	LEU
6	B	482	ASN
6	B	568	CYS
6	B	577	TYR
6	B	583	MET
7	C	65	VAL
7	C	66	ARG
11	G	83	GLN
11	G	121	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	109	HIS
2	2	249	ASN
3	3	267	ASN
4	4	74	ASN
5	A	222	GLN
5	A	273	ASN

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Mol	Chain	Res	Type
5	A	301	HIS
5	A	303	HIS
5	A	445	HIS
5	A	496	HIS
5	A	545	HIS
5	A	550	HIS
5	A	615	HIS
5	A	721	GLN
6	B	196	HIS
6	B	231	ASN
6	B	350	GLN
6	B	452	GLN
6	B	467	HIS
8	D	168	HIS
9	E	119	ASN
10	F	154	GLN
10	F	193	GLN
11	G	95	GLN
12	H	130	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
18	BCR	A	851	-	41,41,41	0.66	0	56,56,56	3.23	14 (25%)
19	CLA	4	306	-	65,73,73	1.34	7 (10%)	76,113,113	1.83	15 (19%)
19	CLA	A	810	-	50,58,73	1.52	8 (16%)	58,95,113	2.07	11 (18%)
18	BCR	A	849	-	41,41,41	0.63	0	56,56,56	3.28	16 (28%)
19	CLA	B	812	-	60,68,73	1.40	7 (11%)	70,107,113	1.78	11 (15%)
18	BCR	A	856	-	41,41,41	0.67	0	56,56,56	3.27	15 (26%)
18	BCR	4	301	-	41,41,41	0.65	0	56,56,56	3.34	15 (26%)
18	BCR	L	307	-	41,41,41	0.69	0	56,56,56	3.34	11 (19%)
19	CLA	B	815	-	65,73,73	1.31	5 (7%)	76,113,113	1.87	12 (15%)
29	PQN	B	841	-	34,34,34	0.37	0	42,45,45	1.14	3 (7%)
19	CLA	A	812	-	55,63,73	1.46	7 (12%)	64,101,113	1.94	14 (21%)
30	ZEX	F	301	-	42,43,43	0.73	0	55,60,60	1.76	11 (20%)
23	XAT	4	303	-	39,47,47	0.64	0	54,74,74	2.45	13 (24%)
19	CLA	B	806	-	65,73,73	1.32	6 (9%)	76,113,113	1.80	12 (15%)
19	CLA	3	312	-	48,56,73	1.56	8 (16%)	55,92,113	2.10	13 (23%)
19	CLA	B	817	-	60,68,73	1.40	8 (13%)	70,107,113	1.93	13 (18%)
18	BCR	L	302	-	41,41,41	0.84	0	56,56,56	3.17	15 (26%)
24	LMT	B	846	-	36,36,36	1.14	6 (16%)	47,47,47	1.04	3 (6%)
19	CLA	F	302	-	65,73,73	1.34	7 (10%)	76,113,113	1.84	15 (19%)
19	CLA	1	516	1	60,68,73	1.40	7 (11%)	70,107,113	1.89	14 (20%)
19	CLA	A	806	5	65,73,73	1.31	6 (9%)	76,113,113	1.83	13 (17%)
19	CLA	A	817	-	65,73,73	1.33	6 (9%)	76,113,113	1.74	11 (14%)
17	LUT	4	302	-	42,43,43	2.46	1 (2%)	51,60,60	1.92	12 (23%)
19	CLA	K	1003	-	29,35,73	2.60	10 (34%)	28,60,113	2.31	8 (28%)
27	CL0	A	801	-	65,73,73	1.64	9 (13%)	76,113,113	2.16	16 (21%)
19	CLA	2	504	2	60,68,73	1.36	6 (10%)	70,107,113	2.00	14 (20%)
19	CLA	J	1105	-	50,58,73	1.50	6 (12%)	58,95,113	2.30	18 (31%)
28	SF4	A	843	6,5	0,12,12	-	-	-	-	-
22	LMG	G	210	-	25,25,55	0.54	0	33,33,63	1.29	4 (12%)
24	LMT	B	855	-	32,32,36	1.25	6 (18%)	43,43,47	0.97	2 (4%)
19	CLA	A	840	31	65,73,73	1.28	6 (9%)	76,113,113	1.85	14 (18%)
22	LMG	J	1104	-	34,34,55	0.46	0	42,42,63	1.23	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	LHG	1	520	-	41,41,48	0.45	0	44,47,54	1.15	4 (9%)
19	CLA	A	821	-	65,73,73	1.31	5 (7%)	76,113,113	1.73	15 (19%)
19	CLA	B	825	31	65,73,73	1.30	6 (9%)	76,113,113	1.93	17 (22%)
24	LMT	J	1107	-	26,26,36	1.34	5 (19%)	37,37,47	1.08	2 (5%)
22	LMG	2	518	-	25,25,55	0.59	0	33,33,63	1.13	3 (9%)
22	LMG	G	206	-	50,50,55	1.05	4 (8%)	58,58,63	1.07	3 (5%)
19	CLA	B	826	-	65,73,73	1.34	8 (12%)	76,113,113	1.82	13 (17%)
19	CLA	3	306	-	52,60,73	1.50	7 (13%)	60,97,113	1.99	13 (21%)
19	CLA	L	301	-	55,63,73	1.45	7 (12%)	64,101,113	1.99	14 (21%)
19	CLA	3	308	-	65,73,73	1.32	6 (9%)	76,113,113	1.90	16 (21%)
20	CHL	4	317	4	43,51,74	1.07	4 (9%)	45,86,114	1.72	12 (26%)
23	XAT	2	502	-	39,47,47	0.62	0	54,74,74	1.72	11 (20%)
19	CLA	G	202	-	55,63,73	1.46	8 (14%)	64,101,113	1.95	14 (21%)
19	CLA	A	829	-	65,73,73	1.30	8 (12%)	76,113,113	1.82	13 (17%)
19	CLA	A	807	-	60,68,73	1.40	6 (10%)	70,107,113	1.89	13 (18%)
19	CLA	A	828	-	65,73,73	1.31	7 (10%)	76,113,113	1.90	11 (14%)
19	CLA	A	802	-	65,73,73	1.29	7 (10%)	76,113,113	1.86	18 (23%)
19	CLA	A	855	-	65,73,73	1.30	8 (12%)	76,113,113	1.84	13 (17%)
22	LMG	F	304	-	47,47,55	0.97	4 (8%)	55,55,63	1.09	2 (3%)
19	CLA	B	820	31	65,73,73	1.35	8 (12%)	76,113,113	1.70	12 (15%)
19	CLA	4	318	-	65,73,73	1.29	6 (9%)	76,113,113	1.86	13 (17%)
20	CHL	2	516	2	56,64,74	0.91	3 (5%)	61,102,114	1.34	10 (16%)
20	CHL	1	514	1	61,69,74	0.86	2 (3%)	67,108,114	1.36	11 (16%)
19	CLA	B	808	-	65,73,73	1.35	7 (10%)	76,113,113	1.75	12 (15%)
19	CLA	L	305	31	50,58,73	1.54	9 (18%)	58,95,113	1.98	13 (22%)
18	BCR	2	503	-	41,41,41	0.86	0	56,56,56	3.25	14 (25%)
19	CLA	B	803	-	65,73,73	1.30	5 (7%)	76,113,113	1.78	10 (13%)
17	LUT	J	1109	-	42,43,43	2.28	1 (2%)	51,60,60	1.94	9 (17%)
19	CLA	A	826	31	55,63,73	1.44	7 (12%)	64,101,113	1.95	13 (20%)
19	CLA	3	307	-	55,63,73	1.45	7 (12%)	64,101,113	2.05	16 (25%)
19	CLA	4	309	-	50,58,73	1.48	7 (14%)	58,95,113	2.11	13 (22%)
18	BCR	B	850	-	41,41,41	0.66	0	56,56,56	3.01	11 (19%)
19	CLA	G	203	11	46,54,73	1.57	7 (15%)	53,90,113	2.02	12 (22%)
17	LUT	3	301	-	42,43,43	2.41	1 (2%)	51,60,60	1.68	7 (13%)
18	BCR	F	306	-	41,41,41	0.65	0	56,56,56	3.05	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	835	5	55,63,73	1.47	8 (14%)	64,101,113	1.93	14 (21%)
26	DGD	4	319	-	52,52,67	0.73	2 (3%)	66,66,81	1.44	9 (13%)
20	CHL	2	515	-	46,54,74	1.00	2 (4%)	49,90,114	1.38	10 (20%)
20	CHL	4	314	31	51,59,74	1.09	4 (7%)	55,96,114	1.90	14 (25%)
19	CLA	2	510	21	60,68,73	1.38	7 (11%)	70,107,113	1.90	14 (20%)
19	CLA	4	307	4	60,68,73	1.36	6 (10%)	70,107,113	1.96	16 (22%)
18	BCR	B	802	-	41,41,41	0.68	0	56,56,56	4.02	18 (32%)
19	CLA	B	816	-	55,63,73	1.45	8 (14%)	64,101,113	1.96	11 (17%)
18	BCR	G	205	-	41,41,41	0.73	0	56,56,56	3.09	11 (19%)
19	CLA	1	510	-	46,54,73	1.62	7 (15%)	53,90,113	2.34	14 (26%)
19	CLA	B	810	6	65,73,73	1.31	6 (9%)	76,113,113	1.85	13 (17%)
19	CLA	L	303	16	50,58,73	1.50	7 (14%)	58,95,113	2.04	12 (20%)
20	CHL	2	513	-	48,56,74	1.05	4 (8%)	51,92,114	1.35	8 (15%)
19	CLA	2	506	-	65,73,73	1.33	8 (12%)	76,113,113	1.92	14 (18%)
19	CLA	4	315	4	65,73,73	1.33	7 (10%)	76,113,113	1.83	14 (18%)
19	CLA	B	837	-	50,58,73	1.49	8 (16%)	58,95,113	1.98	14 (24%)
17	LUT	2	501	-	42,43,43	2.35	1 (2%)	51,60,60	1.78	9 (17%)
18	BCR	A	848	-	41,41,41	0.63	0	56,56,56	3.27	18 (32%)
19	CLA	1	505	1	46,54,73	1.58	8 (17%)	53,90,113	2.02	11 (20%)
19	CLA	1	509	-	50,58,73	1.50	7 (14%)	58,95,113	2.05	16 (27%)
19	CLA	3	310	31	50,58,73	1.50	7 (14%)	58,95,113	2.23	11 (18%)
19	CLA	1	506	-	55,63,73	1.43	8 (14%)	64,101,113	1.99	12 (18%)
19	CLA	3	313	3	60,68,73	1.37	6 (10%)	70,107,113	1.89	14 (20%)
19	CLA	A	825	31	65,73,73	1.36	8 (12%)	76,113,113	1.92	17 (22%)
19	CLA	A	841	-	65,73,73	1.35	7 (10%)	76,113,113	1.76	12 (15%)
22	LMG	4	322	-	45,45,55	0.93	3 (6%)	53,53,63	1.08	4 (7%)
22	LMG	B	845	-	33,33,55	0.57	1 (3%)	41,41,63	1.24	5 (12%)
19	CLA	4	308	4	60,68,73	1.35	5 (8%)	70,107,113	2.04	15 (21%)
24	LMT	3	318	-	32,32,36	1.17	5 (15%)	43,43,47	1.19	5 (11%)
19	CLA	1	504	1	65,73,73	1.32	6 (9%)	76,113,113	1.88	16 (21%)
19	CLA	3	311	-	41,49,73	1.68	8 (19%)	47,84,113	2.10	13 (27%)
19	CLA	A	854	31	65,73,73	1.29	6 (9%)	76,113,113	1.88	16 (21%)
19	CLA	L	304	-	60,68,73	1.35	5 (8%)	70,107,113	1.94	13 (18%)
19	CLA	B	813	-	46,54,73	1.57	6 (13%)	53,90,113	2.08	14 (26%)
19	CLA	A	815	-	45,53,73	1.61	8 (17%)	52,89,113	1.99	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	1	511	-	46,54,73	1.58	6 (13%)	53,90,113	1.98	11 (20%)
26	DGD	J	1106	-	59,59,67	0.92	4 (6%)	73,73,81	1.06	5 (6%)
19	CLA	A	808	5	65,73,73	1.30	5 (7%)	76,113,113	1.90	12 (15%)
24	LMT	A	846	-	36,36,36	1.14	5 (13%)	47,47,47	1.13	2 (4%)
18	BCR	1	503	-	19,19,41	0.66	0	26,26,56	3.15	7 (26%)
19	CLA	A	836	-	51,59,73	1.49	6 (11%)	59,96,113	2.05	15 (25%)
20	CHL	3	314	-	47,55,74	1.03	4 (8%)	50,91,114	1.67	12 (24%)
18	BCR	L	306	-	41,41,41	0.67	0	56,56,56	3.01	13 (23%)
19	CLA	4	311	-	46,54,73	1.57	6 (13%)	53,90,113	2.03	10 (18%)
21	LHG	1	517	-	48,48,48	0.41	0	51,54,54	1.09	4 (7%)
19	CLA	A	824	-	65,73,73	1.33	7 (10%)	76,113,113	1.75	12 (15%)
19	CLA	A	813	-	65,73,73	1.29	7 (10%)	76,113,113	1.88	14 (18%)
19	CLA	2	507	2	65,73,73	1.32	5 (7%)	76,113,113	1.92	14 (18%)
19	CLA	3	315	3	50,58,73	1.49	5 (10%)	58,95,113	2.08	13 (22%)
20	CHL	2	512	-	47,55,74	1.14	3 (6%)	50,91,114	1.83	13 (26%)
19	CLA	4	305	4	50,58,73	1.56	8 (16%)	58,95,113	2.08	16 (27%)
18	BCR	K	1005	-	41,41,41	0.67	0	56,56,56	3.18	13 (23%)
22	LMG	4	321	-	13,13,55	0.57	0	18,18,63	0.68	0
19	CLA	F	303	10	65,73,73	1.32	6 (9%)	76,113,113	1.80	12 (15%)
19	CLA	A	837	-	65,73,73	1.34	8 (12%)	76,113,113	1.77	12 (15%)
26	DGD	B	801	-	42,42,67	0.61	0	56,56,81	1.16	6 (10%)
19	CLA	B	809	-	65,73,73	1.34	8 (12%)	76,113,113	1.75	12 (15%)
19	CLA	B	807	6	65,73,73	1.32	6 (9%)	76,113,113	1.82	12 (15%)
24	LMT	4	320	-	36,36,36	1.15	4 (11%)	47,47,47	0.95	3 (6%)
19	CLA	K	1002	-	60,68,73	1.40	8 (13%)	70,107,113	1.90	14 (20%)
22	LMG	2	524	-	13,13,55	0.56	0	18,18,63	0.81	0
19	CLA	B	824	31	65,73,73	1.32	7 (10%)	76,113,113	1.97	14 (18%)
19	CLA	H	1000	-	60,68,73	1.39	8 (13%)	70,107,113	1.90	14 (20%)
24	LMT	G	209	-	32,32,36	1.23	6 (18%)	43,43,47	0.97	1 (2%)
19	CLA	2	505	2	52,60,73	1.50	9 (17%)	60,97,113	2.02	13 (21%)
19	CLA	1	508	-	65,73,73	1.33	8 (12%)	76,113,113	1.87	15 (19%)
18	BCR	3	303	-	41,41,41	0.65	0	56,56,56	3.22	12 (21%)
19	CLA	B	839	-	65,73,73	1.34	6 (9%)	76,113,113	1.79	12 (15%)
19	CLA	G	204	31	65,73,73	1.31	9 (13%)	76,113,113	1.86	13 (17%)
19	CLA	4	312	4	50,58,73	1.52	7 (14%)	58,95,113	2.03	15 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LMG	2	519	-	36,36,55	0.66	1 (2%)	44,44,63	1.24	7 (15%)
19	CLA	J	1102	31	45,53,73	1.54	6 (13%)	52,89,113	2.10	11 (21%)
22	LMG	B	844	-	35,35,55	0.74	1 (2%)	43,43,63	1.08	3 (6%)
19	CLA	A	833	-	65,73,73	1.32	7 (10%)	76,113,113	1.83	15 (19%)
19	CLA	B	830	-	65,73,73	1.32	9 (13%)	76,113,113	1.82	14 (18%)
19	CLA	A	820	-	50,58,73	1.53	8 (16%)	58,95,113	2.01	12 (20%)
22	LMG	A	847	-	50,50,55	1.03	5 (10%)	58,58,63	0.98	2 (3%)
19	CLA	2	514	2	55,63,73	1.44	7 (12%)	64,101,113	1.96	12 (18%)
17	LUT	3	302	-	42,43,43	2.31	1 (2%)	51,60,60	1.61	13 (25%)
18	BCR	B	852	-	41,41,41	0.61	0	56,56,56	2.95	14 (25%)
21	LHG	A	853	-	48,48,48	0.40	0	51,54,54	1.04	3 (5%)
19	CLA	A	803	31	65,73,73	1.31	7 (10%)	76,113,113	1.87	13 (17%)
29	PQN	A	844	-	34,34,34	0.39	0	42,45,45	1.25	5 (11%)
18	BCR	3	304	-	41,41,41	0.69	0	56,56,56	3.40	14 (25%)
20	CHL	1	512	-	47,55,74	0.98	3 (6%)	50,91,114	1.57	12 (24%)
19	CLA	3	317	-	46,54,73	1.60	8 (17%)	53,90,113	1.97	11 (20%)
22	LMG	1	519	-	13,13,55	0.56	0	18,18,63	0.89	1 (5%)
22	LMG	J	1103	-	30,30,55	0.51	0	38,38,63	1.08	2 (5%)
18	BCR	A	850	-	41,41,41	0.64	0	56,56,56	3.20	14 (25%)
19	CLA	A	839	-	65,73,73	1.32	6 (9%)	76,113,113	1.73	11 (14%)
18	BCR	B	851	-	41,41,41	0.66	0	56,56,56	2.67	15 (26%)
19	CLA	B	821	-	46,54,73	1.59	7 (15%)	53,90,113	2.02	11 (20%)
26	DGD	G	207	-	48,48,67	0.59	1 (2%)	62,62,81	1.07	3 (4%)
17	LUT	1	501	-	42,43,43	2.39	1 (2%)	51,60,60	1.69	10 (19%)
22	LMG	1	518	-	46,46,55	0.92	3 (6%)	54,54,63	1.04	2 (3%)
19	CLA	A	814	-	65,73,73	1.33	8 (12%)	76,113,113	1.89	16 (21%)
19	CLA	B	827	-	65,73,73	1.30	8 (12%)	76,113,113	1.86	13 (17%)
19	CLA	B	828	-	65,73,73	1.29	7 (10%)	76,113,113	1.82	11 (14%)
19	CLA	B	834	31	55,63,73	1.46	7 (12%)	64,101,113	1.87	13 (20%)
19	CLA	B	840	21	65,73,73	1.32	6 (9%)	76,113,113	1.81	12 (15%)
18	BCR	B	856	-	41,41,41	0.66	0	56,56,56	3.05	13 (23%)
19	CLA	A	816	-	46,54,73	1.58	7 (15%)	53,90,113	2.04	11 (20%)
28	SF4	C	101	7	0,12,12	-	-	-	-	-
28	SF4	C	102	7	0,12,12	-	-	-	-	-
21	LHG	B	842	19	20,20,48	0.59	0	23,26,54	1.55	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	819	-	65,73,73	1.30	6 (9%)	76,113,113	1.86	14 (18%)
19	CLA	B	838	31	65,73,73	1.34	7 (10%)	76,113,113	1.81	13 (17%)
24	LMT	B	847	-	33,33,36	1.22	5 (15%)	44,44,47	0.96	1 (2%)
19	CLA	A	811	-	65,73,73	1.32	7 (10%)	76,113,113	1.85	13 (17%)
19	CLA	3	316	-	46,54,73	1.58	9 (19%)	53,90,113	2.07	13 (24%)
19	CLA	4	310	-	60,68,73	1.40	9 (15%)	70,107,113	1.85	11 (15%)
18	BCR	I	101	-	41,41,41	0.73	0	56,56,56	3.50	16 (28%)
19	CLA	B	831	-	60,68,73	1.37	7 (11%)	70,107,113	1.83	13 (18%)
19	CLA	B	818	-	65,73,73	1.35	9 (13%)	76,113,113	1.76	14 (18%)
19	CLA	K	1004	-	29,35,73	2.60	10 (34%)	28,60,113	2.18	7 (25%)
19	CLA	G	201	-	65,73,73	1.34	7 (10%)	76,113,113	1.88	15 (19%)
19	CLA	A	823	-	60,68,73	1.41	8 (13%)	70,107,113	1.83	13 (18%)
19	CLA	A	805	-	65,73,73	1.34	7 (10%)	76,113,113	1.80	10 (13%)
19	CLA	A	838	-	65,73,73	1.34	7 (10%)	76,113,113	1.79	13 (17%)
19	CLA	A	832	-	65,73,73	1.34	6 (9%)	76,113,113	1.77	11 (14%)
20	CHL	1	521	1	56,64,74	0.96	4 (7%)	61,102,114	1.28	8 (13%)
19	CLA	A	831	-	65,73,73	1.33	5 (7%)	76,113,113	1.83	15 (19%)
21	LHG	B	843	-	48,48,48	0.40	0	51,54,54	1.01	2 (3%)
18	BCR	A	852	-	41,41,41	0.63	0	56,56,56	2.90	14 (25%)
19	CLA	1	515	-	45,53,73	1.62	9 (20%)	52,89,113	1.88	10 (19%)
19	CLA	A	819	-	65,73,73	1.31	6 (9%)	76,113,113	1.81	14 (18%)
22	LMG	2	520	-	13,13,55	0.59	0	18,18,63	0.87	1 (5%)
18	BCR	J	1108	-	41,41,41	0.60	0	56,56,56	2.87	15 (26%)
19	CLA	J	1101	-	65,73,73	1.31	6 (9%)	76,113,113	1.96	18 (23%)
21	LHG	A	845	19	39,39,48	0.42	0	42,45,54	1.25	4 (9%)
19	CLA	A	818	-	56,64,73	1.44	9 (16%)	65,102,113	1.92	13 (20%)
19	CLA	B	823	-	55,63,73	1.45	8 (14%)	64,101,113	1.93	10 (15%)
22	LMG	F	305	-	36,36,55	0.72	1 (2%)	44,44,63	1.10	2 (4%)
19	CLA	A	809	5	65,73,73	1.30	6 (9%)	76,113,113	1.87	15 (19%)
17	LUT	1	502	-	42,43,43	2.37	1 (2%)	51,60,60	1.81	9 (17%)
19	CLA	A	827	-	65,73,73	1.33	7 (10%)	76,113,113	1.84	14 (18%)
19	CLA	1	513	-	65,73,73	1.31	7 (10%)	76,113,113	1.84	14 (18%)
19	CLA	B	805	-	65,73,73	1.33	7 (10%)	76,113,113	1.78	11 (14%)
18	BCR	B	849	-	41,41,41	0.79	0	56,56,56	3.73	20 (35%)
19	CLA	A	804	-	65,73,73	1.31	8 (12%)	76,113,113	1.84	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	829	-	65,73,73	1.35	7 (10%)	76,113,113	1.80	14 (18%)
19	CLA	B	811	-	65,73,73	1.36	8 (12%)	76,113,113	1.82	13 (17%)
19	CLA	2	511	-	50,58,73	1.52	7 (14%)	58,95,113	2.07	13 (22%)
20	CHL	4	316	-	61,69,74	0.98	4 (6%)	67,108,114	1.42	11 (16%)
24	LMT	2	523	-	36,36,36	1.13	5 (13%)	47,47,47	1.00	2 (4%)
19	CLA	4	304	4	60,68,73	1.38	6 (10%)	70,107,113	2.11	18 (25%)
19	CLA	A	822	-	60,68,73	1.41	7 (11%)	70,107,113	1.86	13 (18%)
19	CLA	B	832	-	58,66,73	1.38	6 (10%)	67,104,113	1.98	15 (22%)
21	LHG	2	517	19	34,34,48	0.46	0	37,40,54	1.07	2 (5%)
19	CLA	2	508	-	55,63,73	1.39	6 (10%)	64,101,113	2.06	16 (25%)
22	LMG	2	522	-	13,13,55	0.58	0	18,18,63	0.63	0
19	CLA	1	507	1	65,73,73	1.32	7 (10%)	76,113,113	1.87	13 (17%)
20	CHL	4	313	-	47,55,74	1.02	4 (8%)	50,91,114	1.48	11 (22%)
19	CLA	B	835	-	55,63,73	1.44	7 (12%)	64,101,113	1.88	11 (17%)
18	BCR	B	853	-	41,41,41	0.63	0	56,56,56	3.06	13 (23%)
19	CLA	2	509	-	50,58,73	1.49	5 (10%)	58,95,113	1.99	13 (22%)
24	LMT	G	208	-	36,36,36	1.15	5 (13%)	47,47,47	0.98	2 (4%)
26	DGD	B	854	-	62,62,67	0.97	5 (8%)	76,76,81	1.00	3 (3%)
19	CLA	A	830	-	65,73,73	1.31	7 (10%)	76,113,113	1.85	15 (19%)
19	CLA	A	834	-	65,73,73	1.31	6 (9%)	76,113,113	1.80	12 (15%)
19	CLA	3	309	-	55,63,73	1.48	8 (14%)	64,101,113	1.98	15 (23%)
19	CLA	B	814	-	65,73,73	1.33	8 (12%)	76,113,113	1.82	13 (17%)
19	CLA	B	804	-	65,73,73	1.34	6 (9%)	76,113,113	1.94	15 (19%)
22	LMG	2	521	-	13,13,55	0.59	0	18,18,63	0.75	0
19	CLA	K	1001	-	45,53,73	1.59	7 (15%)	52,89,113	2.11	13 (25%)
19	CLA	A	842	21	60,68,73	1.36	7 (11%)	70,107,113	1.94	13 (18%)
22	LMG	2	525	-	13,13,55	0.62	0	18,18,63	0.70	0
18	BCR	I	102	-	41,41,41	0.65	0	56,56,56	3.13	13 (23%)
19	CLA	B	822	-	65,73,73	1.35	8 (12%)	76,113,113	1.81	13 (17%)
20	CHL	2	526	2	66,74,74	0.86	3 (4%)	73,114,114	1.24	11 (15%)
19	CLA	3	305	-	55,63,73	1.46	8 (14%)	64,101,113	2.07	14 (21%)
19	CLA	B	833	-	60,68,73	1.36	7 (11%)	70,107,113	1.86	12 (17%)
19	CLA	B	836	-	65,73,73	1.32	6 (9%)	76,113,113	1.76	12 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
 '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	A	851	-	-	12/29/63/63	0/2/2/2
19	CLA	4	306	-	1/1/15/20	16/37/115/115	-
19	CLA	A	810	-	1/1/12/20	6/19/97/115	-
18	BCR	A	849	-	-	11/29/63/63	0/2/2/2
19	CLA	B	812	-	1/1/14/20	13/31/109/115	-
18	BCR	A	856	-	-	13/29/63/63	0/2/2/2
18	BCR	4	301	-	-	13/29/63/63	0/2/2/2
19	CLA	B	815	-	1/1/15/20	10/37/115/115	-
18	BCR	L	307	-	-	11/29/63/63	0/2/2/2
29	PQN	B	841	-	-	12/23/43/43	0/2/2/2
19	CLA	A	812	-	-	11/25/103/115	-
30	ZEX	F	301	-	-	3/29/67/67	0/2/2/2
23	XAT	4	303	-	2/2/12/26	0/31/93/93	0/4/4/4
19	CLA	B	806	-	1/1/15/20	18/37/115/115	-
19	CLA	3	312	-	1/1/11/20	7/17/95/115	-
19	CLA	B	817	-	1/1/14/20	8/31/109/115	-
18	BCR	L	302	-	-	6/29/63/63	0/2/2/2
24	LMT	B	846	-	-	11/21/61/61	0/2/2/2
19	CLA	F	302	-	1/1/15/20	13/37/115/115	-
19	CLA	1	516	1	1/1/14/20	11/31/109/115	-
19	CLA	A	806	5	1/1/15/20	21/37/115/115	-
19	CLA	A	817	-	1/1/15/20	17/37/115/115	-
17	LUT	4	302	-	-	3/29/67/67	0/2/2/2
19	CLA	K	1003	-	1/1/5/20	-	-
27	CL0	A	801	-	3/3/20/25	7/37/135/135	-
19	CLA	2	504	2	1/1/14/20	9/31/109/115	-
19	CLA	J	1105	-	1/1/12/20	10/19/97/115	-
28	SF4	A	843	6,5	-	-	0/6/5/5
22	LMG	G	210	-	-	10/20/40/70	0/1/1/1
24	LMT	B	855	-	-	4/17/57/61	0/2/2/2
19	CLA	A	840	31	1/1/15/20	16/37/115/115	-
22	LMG	J	1104	-	-	12/29/49/70	0/1/1/1
21	LHG	1	520	-	-	26/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	821	-	1/1/15/20	17/37/115/115	-
19	CLA	B	825	31	1/1/15/20	22/37/115/115	-
24	LMT	J	1107	-	-	7/11/51/61	0/2/2/2
22	LMG	2	518	-	-	6/20/40/70	0/1/1/1
22	LMG	G	206	-	-	18/45/65/70	0/1/1/1
19	CLA	B	826	-	1/1/15/20	6/37/115/115	-
19	CLA	3	306	-	1/1/12/20	8/22/100/115	-
19	CLA	L	301	-	1/1/13/20	8/25/103/115	-
19	CLA	3	308	-	1/1/15/20	22/37/115/115	-
20	CHL	4	317	4	3/3/15/26	2/12/110/137	-
23	XAT	2	502	-	-	5/31/93/93	0/4/4/4
19	CLA	G	202	-	-	13/25/103/115	-
19	CLA	A	829	-	1/1/15/20	19/37/115/115	-
19	CLA	A	807	-	1/1/14/20	17/31/109/115	-
19	CLA	A	828	-	1/1/15/20	22/37/115/115	-
19	CLA	A	802	-	1/1/15/20	19/37/115/115	-
19	CLA	A	855	-	1/1/15/20	19/37/115/115	-
22	LMG	F	304	-	-	11/42/62/70	0/1/1/1
19	CLA	B	820	31	1/1/15/20	16/37/115/115	-
19	CLA	4	318	-	1/1/15/20	13/37/115/115	-
20	CHL	2	516	2	4/4/18/26	7/27/125/137	-
20	CHL	1	514	1	4/4/19/26	11/33/131/137	-
19	CLA	B	808	-	1/1/15/20	19/37/115/115	-
19	CLA	L	305	31	1/1/12/20	10/19/97/115	-
19	CLA	B	803	-	1/1/15/20	8/37/115/115	-
18	BCR	2	503	-	-	11/29/63/63	0/2/2/2
17	LUT	J	1109	-	1/1/12/27	6/29/67/67	0/2/2/2
19	CLA	A	826	31	1/1/13/20	9/25/103/115	-
19	CLA	3	307	-	1/1/13/20	13/25/103/115	-
19	CLA	4	309	-	1/1/12/20	12/19/97/115	-
18	BCR	B	850	-	-	10/29/63/63	0/2/2/2
19	CLA	G	203	11	1/1/11/20	6/15/93/115	-
19	CLA	A	835	5	1/1/13/20	10/25/103/115	-
17	LUT	3	301	-	-	3/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	F	306	-	-	8/29/63/63	0/2/2/2
26	DGD	4	319	-	-	17/40/80/95	0/2/2/2
20	CHL	2	515	-	3/3/16/26	4/15/113/137	-
20	CHL	4	314	31	3/3/17/26	4/21/119/137	-
19	CLA	2	510	21	1/1/14/20	15/31/109/115	-
19	CLA	4	307	4	1/1/14/20	13/31/109/115	-
18	BCR	B	802	-	-	5/29/63/63	0/2/2/2
19	CLA	B	816	-	1/1/13/20	8/25/103/115	-
19	CLA	1	510	-	1/1/11/20	7/15/93/115	-
19	CLA	B	810	6	1/1/15/20	12/37/115/115	-
19	CLA	L	303	16	1/1/12/20	7/19/97/115	-
18	BCR	G	205	-	-	11/29/63/63	0/2/2/2
20	CHL	2	513	-	3/3/16/26	1/18/116/137	-
19	CLA	2	506	-	1/1/15/20	14/37/115/115	-
19	CLA	4	315	4	1/1/15/20	15/37/115/115	-
19	CLA	B	837	-	1/1/12/20	5/19/97/115	-
17	LUT	2	501	-	1/1/12/27	5/29/67/67	0/2/2/2
19	CLA	1	509	-	1/1/12/20	8/19/97/115	-
19	CLA	3	310	31	1/1/12/20	6/19/97/115	-
19	CLA	A	841	-	1/1/15/20	4/37/115/115	-
19	CLA	3	313	3	1/1/14/20	16/31/109/115	-
19	CLA	1	506	-	1/1/13/20	8/25/103/115	-
18	BCR	A	848	-	-	10/29/63/63	0/2/2/2
19	CLA	A	825	31	1/1/15/20	14/37/115/115	-
19	CLA	1	505	1	-	6/15/93/115	-
22	LMG	4	322	-	-	13/40/60/70	0/1/1/1
22	LMG	B	845	-	-	13/28/48/70	0/1/1/1
19	CLA	4	308	4	-	13/31/109/115	-
24	LMT	3	318	-	-	4/17/57/61	0/2/2/2
19	CLA	1	504	1	1/1/15/20	14/37/115/115	-
19	CLA	3	311	-	1/1/10/20	5/8/86/115	-
19	CLA	A	854	31	1/1/15/20	16/37/115/115	-
19	CLA	L	304	-	1/1/14/20	12/31/109/115	-
19	CLA	B	813	-	1/1/11/20	3/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	815	-	1/1/11/20	7/13/91/115	-
19	CLA	1	511	-	1/1/11/20	7/15/93/115	-
26	DGD	J	1106	-	-	14/47/87/95	0/2/2/2
19	CLA	A	808	5	1/1/15/20	19/37/115/115	-
24	LMT	A	846	-	-	8/21/61/61	0/2/2/2
18	BCR	1	503	-	-	7/11/28/63	0/1/1/2
19	CLA	A	836	-	-	9/21/99/115	-
20	CHL	3	314	-	3/3/16/26	4/17/115/137	-
19	CLA	4	311	-	1/1/11/20	6/15/93/115	-
18	BCR	L	306	-	-	8/29/63/63	0/2/2/2
21	LHG	1	517	-	-	28/53/53/53	-
19	CLA	A	824	-	1/1/15/20	18/37/115/115	-
19	CLA	A	813	-	1/1/15/20	11/37/115/115	-
19	CLA	2	507	2	1/1/15/20	13/37/115/115	-
19	CLA	3	315	3	1/1/12/20	7/19/97/115	-
20	CHL	2	512	-	3/3/16/26	2/17/115/137	-
19	CLA	4	305	4	1/1/12/20	6/19/97/115	-
18	BCR	K	1005	-	-	12/29/63/63	0/2/2/2
22	LMG	4	321	-	-	0/4/24/70	0/1/1/1
19	CLA	F	303	10	-	18/37/115/115	-
19	CLA	A	837	-	1/1/15/20	9/37/115/115	-
26	DGD	B	801	-	-	21/30/70/95	0/2/2/2
19	CLA	B	809	-	1/1/15/20	10/37/115/115	-
19	CLA	B	807	6	1/1/15/20	13/37/115/115	-
24	LMT	4	320	-	-	4/21/61/61	0/2/2/2
19	CLA	K	1002	-	1/1/14/20	19/31/109/115	-
22	LMG	2	524	-	-	1/4/24/70	0/1/1/1
19	CLA	B	824	31	1/1/15/20	15/37/115/115	-
19	CLA	H	1000	-	1/1/14/20	10/31/109/115	-
24	LMT	G	209	-	-	13/17/57/61	0/2/2/2
19	CLA	2	505	2	1/1/12/20	7/22/100/115	-
19	CLA	1	508	-	-	22/37/115/115	-
18	BCR	3	303	-	-	12/29/63/63	0/2/2/2
19	CLA	B	839	-	1/1/15/20	19/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	G	204	31	1/1/15/20	18/37/115/115	-
19	CLA	4	312	4	-	6/19/97/115	-
22	LMG	2	519	-	-	17/31/51/70	0/1/1/1
19	CLA	J	1102	31	1/1/11/20	2/13/91/115	-
22	LMG	B	844	-	-	11/30/50/70	0/1/1/1
19	CLA	A	833	-	1/1/15/20	20/37/115/115	-
19	CLA	B	830	-	-	13/37/115/115	-
19	CLA	A	820	-	1/1/12/20	8/19/97/115	-
22	LMG	A	847	-	-	15/45/65/70	0/1/1/1
19	CLA	2	514	2	1/1/13/20	7/25/103/115	-
17	LUT	3	302	-	1/1/12/27	8/29/67/67	0/2/2/2
18	BCR	B	852	-	-	11/29/63/63	0/2/2/2
21	LHG	A	853	-	-	30/53/53/53	-
19	CLA	A	803	31	1/1/15/20	8/37/115/115	-
29	PQN	A	844	-	-	7/23/43/43	0/2/2/2
18	BCR	3	304	-	-	16/29/63/63	0/2/2/2
20	CHL	1	512	-	3/3/16/26	3/17/115/137	-
19	CLA	3	317	-	1/1/11/20	6/15/93/115	-
22	LMG	1	519	-	-	1/4/24/70	0/1/1/1
22	LMG	J	1103	-	-	4/25/45/70	0/1/1/1
19	CLA	A	839	-	1/1/15/20	14/37/115/115	-
18	BCR	A	850	-	-	5/29/63/63	0/2/2/2
18	BCR	B	851	-	-	11/29/63/63	0/2/2/2
19	CLA	B	821	-	1/1/11/20	7/15/93/115	-
26	DGD	G	207	-	-	10/36/76/95	0/2/2/2
17	LUT	1	501	-	-	3/29/67/67	0/2/2/2
22	LMG	1	518	-	-	12/41/61/70	0/1/1/1
19	CLA	A	814	-	1/1/15/20	16/37/115/115	-
19	CLA	B	827	-	1/1/15/20	19/37/115/115	-
19	CLA	B	828	-	1/1/15/20	18/37/115/115	-
19	CLA	B	834	31	1/1/13/20	12/25/103/115	-
19	CLA	B	840	21	-	18/37/115/115	-
18	BCR	B	856	-	-	13/29/63/63	0/2/2/2
19	CLA	A	816	-	1/1/11/20	6/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SF4	C	101	7	-	-	0/6/5/5
28	SF4	C	102	7	-	-	0/6/5/5
21	LHG	B	842	19	-	12/23/23/53	-
19	CLA	B	819	-	1/1/15/20	18/37/115/115	-
19	CLA	B	838	31	1/1/15/20	11/37/115/115	-
24	LMT	B	847	-	-	6/18/58/61	0/2/2/2
19	CLA	A	811	-	1/1/15/20	16/37/115/115	-
19	CLA	3	316	-	1/1/11/20	11/15/93/115	-
19	CLA	4	310	-	1/1/14/20	12/31/109/115	-
18	BCR	I	101	-	-	11/29/63/63	0/2/2/2
19	CLA	B	831	-	1/1/14/20	17/31/109/115	-
19	CLA	B	818	-	1/1/15/20	16/37/115/115	-
19	CLA	K	1004	-	1/1/5/20	-	-
19	CLA	G	201	-	1/1/15/20	20/37/115/115	-
19	CLA	A	823	-	1/1/14/20	13/31/109/115	-
19	CLA	A	805	-	1/1/15/20	28/37/115/115	-
19	CLA	A	838	-	1/1/15/20	14/37/115/115	-
19	CLA	A	832	-	1/1/15/20	11/37/115/115	-
20	CHL	1	521	1	4/4/18/26	7/27/125/137	-
19	CLA	A	831	-	1/1/15/20	13/37/115/115	-
21	LHG	B	843	-	-	28/53/53/53	-
19	CLA	1	515	-	1/1/11/20	6/13/91/115	-
19	CLA	A	819	-	1/1/15/20	16/37/115/115	-
18	BCR	A	852	-	-	12/29/63/63	0/2/2/2
22	LMG	2	520	-	-	0/4/24/70	0/1/1/1
18	BCR	J	1108	-	-	9/29/63/63	0/2/2/2
19	CLA	J	1101	-	1/1/15/20	13/37/115/115	-
21	LHG	A	845	19	-	27/44/44/53	-
19	CLA	A	818	-	1/1/13/20	15/27/105/115	-
19	CLA	B	823	-	1/1/13/20	13/25/103/115	-
22	LMG	F	305	-	-	10/31/51/70	0/1/1/1
19	CLA	A	809	5	1/1/15/20	17/37/115/115	-
17	LUT	1	502	-	1/1/12/27	9/29/67/67	0/2/2/2
19	CLA	A	827	-	1/1/15/20	16/37/115/115	-
19	CLA	1	513	-	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	805	-	1/1/15/20	19/37/115/115	-
18	BCR	B	849	-	-	10/29/63/63	0/2/2/2
19	CLA	A	804	-	1/1/15/20	22/37/115/115	-
19	CLA	B	829	-	1/1/15/20	20/37/115/115	-
19	CLA	B	811	-	1/1/15/20	17/37/115/115	-
19	CLA	2	511	-	1/1/12/20	10/19/97/115	-
20	CHL	4	316	-	4/4/19/26	8/33/131/137	-
24	LMT	2	523	-	-	10/21/61/61	0/2/2/2
19	CLA	4	304	4	1/1/14/20	10/31/109/115	-
19	CLA	A	822	-	1/1/14/20	14/31/109/115	-
19	CLA	B	832	-	1/1/13/20	11/29/107/115	-
21	LHG	2	517	19	-	15/39/39/53	-
19	CLA	2	508	-	1/1/13/20	7/25/103/115	-
22	LMG	2	522	-	-	4/4/24/70	0/1/1/1
19	CLA	1	507	1	1/1/15/20	14/37/115/115	-
20	CHL	4	313	-	3/3/16/26	0/17/115/137	-
19	CLA	B	835	-	-	10/25/103/115	-
19	CLA	2	509	-	1/1/12/20	11/19/97/115	-
18	BCR	B	853	-	-	10/29/63/63	0/2/2/2
24	LMT	G	208	-	-	9/21/61/61	0/2/2/2
26	DGD	B	854	-	-	19/50/90/95	0/2/2/2
19	CLA	A	830	-	1/1/15/20	16/37/115/115	-
19	CLA	A	834	-	-	17/37/115/115	-
19	CLA	3	309	-	-	9/25/103/115	-
19	CLA	B	814	-	1/1/15/20	18/37/115/115	-
19	CLA	B	804	-	1/1/15/20	13/37/115/115	-
22	LMG	2	521	-	-	0/4/24/70	0/1/1/1
19	CLA	K	1001	-	1/1/11/20	10/13/91/115	-
19	CLA	A	842	21	1/1/14/20	13/31/109/115	-
22	LMG	2	525	-	-	0/4/24/70	0/1/1/1
19	CLA	B	822	-	1/1/15/20	20/37/115/115	-
20	CHL	2	526	2	4/4/20/26	10/39/137/137	-
18	BCR	I	102	-	-	14/29/63/63	0/2/2/2
19	CLA	3	305	-	1/1/13/20	16/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	833	-	1/1/14/20	10/31/109/115	-
19	CLA	B	836	-	1/1/15/20	11/37/115/115	-

All (1144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	302	LUT	C24-C25	14.95	1.51	1.33
17	3	301	LUT	C24-C25	14.77	1.51	1.33
17	1	501	LUT	C24-C25	14.56	1.51	1.33
17	1	502	LUT	C24-C25	14.52	1.51	1.33
17	2	501	LUT	C24-C25	14.34	1.51	1.33
17	3	302	LUT	C24-C25	14.18	1.50	1.33
17	J	1109	LUT	C24-C25	13.94	1.50	1.33
19	K	1004	CLA	CHB-C4A	8.25	1.41	1.34
19	K	1003	CLA	CHB-C4A	8.16	1.41	1.34
27	A	801	CL0	MG-NA	7.48	2.24	2.06
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
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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
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
19	A	802	CLA	MG-NA	5.86	2.20	2.06
27	A	801	CL0	C3B-C2B	5.58	1.48	1.40
19	1	510	CLA	MG-ND	-4.32	1.97	2.05
20	4	314	CHL	C3B-C2B	-3.94	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
19	J	1105	CLA	C1C-NC	-3.81	1.32	1.37
19	B	804	CLA	MG-ND	-3.81	1.98	2.05
19	A	820	CLA	MG-ND	-3.80	1.98	2.05
19	A	825	CLA	MG-ND	-3.78	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	824	CLA	MG-ND	-3.73	1.98	2.05
19	3	311	CLA	MG-ND	-3.73	1.98	2.05
19	A	827	CLA	MG-ND	-3.72	1.98	2.05
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
19	J	1101	CLA	MG-ND	-3.70	1.98	2.05
19	4	304	CLA	MG-ND	-3.69	1.98	2.05
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
19	4	305	CLA	MG-ND	-3.68	1.98	2.05
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
19	A	835	CLA	MG-ND	-3.67	1.98	2.05
19	B	822	CLA	MG-ND	-3.67	1.98	2.05
19	B	814	CLA	MG-ND	-3.66	1.98	2.05
19	A	807	CLA	MG-ND	-3.65	1.98	2.05
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
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
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
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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
19	3	315	CLA	MG-ND	-3.58	1.98	2.05
19	1	504	CLA	MG-ND	-3.58	1.98	2.05
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	K	1003	CLA	C3B-C4B	3.57	1.46	1.39
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
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
19	4	308	CLA	MG-ND	-3.55	1.98	2.05
19	K	1004	CLA	C3B-C4B	3.55	1.46	1.39
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	1	510	CLA	C1C-NC	-3.53	1.32	1.37
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
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	513	CHL	C3B-C2B	-3.49	1.35	1.40
19	3	306	CLA	C1C-NC	-3.49	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
19	A	824	CLA	MG-ND	-3.48	1.98	2.05
19	A	805	CLA	MG-ND	-3.48	1.98	2.05
20	2	516	CHL	C4B-NB	3.48	1.38	1.35
19	1	513	CLA	MG-ND	-3.48	1.98	2.05
27	A	801	CL0	C1D-ND	-3.47	1.33	1.37
19	B	817	CLA	MG-ND	-3.47	1.98	2.05
19	K	1003	CLA	MG-ND	-3.47	1.98	2.05
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
19	G	202	CLA	MG-ND	-3.45	1.98	2.05
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
19	3	313	CLA	MG-ND	-3.43	1.99	2.05
19	J	1105	CLA	CBB-CAB	3.43	1.52	1.29
19	B	815	CLA	MG-ND	-3.41	1.99	2.05
20	1	521	CHL	C4B-NB	3.40	1.38	1.35
19	A	810	CLA	MG-ND	-3.40	1.99	2.05
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	F	302	CLA	CBB-CAB	3.39	1.51	1.29
19	2	510	CLA	CBB-CAB	3.38	1.51	1.29
19	4	306	CLA	CBB-CAB	3.38	1.51	1.29
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	B	810	CLA	CBB-CAB	3.38	1.51	1.29
19	G	201	CLA	MG-ND	-3.37	1.99	2.05
19	A	806	CLA	CBB-CAB	3.37	1.51	1.29
19	4	307	CLA	CBB-CAB	3.37	1.51	1.29
20	2	515	CHL	CBB-CAB	3.37	1.51	1.29
19	1	516	CLA	CBB-CAB	3.37	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	509	CLA	CBB-CAB	3.37	1.51	1.29
19	B	836	CLA	MG-ND	-3.37	1.99	2.05
19	4	311	CLA	CBB-CAB	3.37	1.51	1.29
19	A	826	CLA	CBB-CAB	3.37	1.51	1.29
19	3	315	CLA	CBB-CAB	3.37	1.51	1.29
20	2	512	CHL	C3A-C2A	-3.37	1.45	1.54
19	B	807	CLA	CBB-CAB	3.37	1.51	1.29
19	3	307	CLA	CBB-CAB	3.37	1.51	1.29
19	3	312	CLA	CBB-CAB	3.37	1.51	1.29
19	G	203	CLA	CBB-CAB	3.37	1.51	1.29
19	1	509	CLA	CBB-CAB	3.36	1.51	1.29
19	L	303	CLA	MG-ND	-3.36	1.99	2.05
19	K	1001	CLA	CBB-CAB	3.36	1.51	1.29
19	A	820	CLA	CBB-CAB	3.36	1.51	1.29
19	L	303	CLA	CBB-CAB	3.36	1.51	1.29
19	A	825	CLA	CBB-CAB	3.36	1.51	1.29
19	3	306	CLA	CBB-CAB	3.36	1.51	1.29
19	J	1102	CLA	CBB-CAB	3.36	1.51	1.29
19	A	819	CLA	CBB-CAB	3.36	1.51	1.29
19	B	826	CLA	CBB-CAB	3.36	1.51	1.29
19	3	316	CLA	CBB-CAB	3.36	1.51	1.29
19	A	808	CLA	CBB-CAB	3.36	1.51	1.29
19	B	813	CLA	CBB-CAB	3.36	1.51	1.29
19	4	305	CLA	CBB-CAB	3.36	1.51	1.29
27	A	801	CL0	CBB-CAB	3.36	1.51	1.29
19	A	835	CLA	CBB-CAB	3.36	1.51	1.29
19	A	833	CLA	CBB-CAB	3.36	1.51	1.29
19	F	302	CLA	MG-ND	-3.36	1.99	2.05
19	3	311	CLA	CBB-CAB	3.36	1.51	1.29
19	J	1102	CLA	MG-ND	-3.35	1.99	2.05
19	1	513	CLA	CBB-CAB	3.35	1.51	1.29
19	1	515	CLA	CBB-CAB	3.35	1.51	1.29
19	4	308	CLA	CBB-CAB	3.35	1.51	1.29
19	B	815	CLA	C1C-NC	-3.35	1.32	1.37
19	B	812	CLA	MG-ND	-3.35	1.99	2.05
19	1	510	CLA	CBB-CAB	3.35	1.51	1.29
19	L	305	CLA	CBB-CAB	3.35	1.51	1.29
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	3	313	CLA	CBB-CAB	3.35	1.51	1.29
19	B	836	CLA	CBB-CAB	3.35	1.51	1.29
19	H	1000	CLA	CBB-CAB	3.35	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	K	1002	CLA	CBB-CAB	3.35	1.51	1.29
19	1	508	CLA	CBB-CAB	3.35	1.51	1.29
19	A	815	CLA	CBB-CAB	3.35	1.51	1.29
19	4	307	CLA	MG-ND	-3.35	1.99	2.05
19	A	834	CLA	MG-ND	-3.35	1.99	2.05
19	B	817	CLA	CBB-CAB	3.35	1.51	1.29
19	2	507	CLA	CBB-CAB	3.35	1.51	1.29
19	2	505	CLA	CBB-CAB	3.35	1.51	1.29
19	4	309	CLA	CBB-CAB	3.35	1.51	1.29
19	G	201	CLA	CBB-CAB	3.35	1.51	1.29
19	A	830	CLA	CBB-CAB	3.35	1.51	1.29
19	B	819	CLA	CBB-CAB	3.35	1.51	1.29
19	A	811	CLA	MG-ND	-3.35	1.99	2.05
19	A	807	CLA	CBB-CAB	3.35	1.51	1.29
19	B	815	CLA	CBB-CAB	3.35	1.51	1.29
19	4	304	CLA	CBB-CAB	3.34	1.51	1.29
19	A	813	CLA	CBB-CAB	3.34	1.51	1.29
19	G	202	CLA	CBB-CAB	3.34	1.51	1.29
26	J	1106	DGD	CAA-C9A	-3.34	1.32	1.51
19	A	836	CLA	CBB-CAB	3.34	1.51	1.29
19	2	504	CLA	CBB-CAB	3.34	1.51	1.29
19	3	309	CLA	CBB-CAB	3.34	1.51	1.29
19	A	818	CLA	CBB-CAB	3.34	1.51	1.29
19	B	832	CLA	MG-ND	-3.34	1.99	2.05
19	1	505	CLA	CBB-CAB	3.34	1.51	1.29
19	B	840	CLA	CBB-CAB	3.34	1.51	1.29
19	A	811	CLA	CBB-CAB	3.34	1.51	1.29
19	A	842	CLA	CBB-CAB	3.34	1.51	1.29
19	1	511	CLA	CBB-CAB	3.34	1.51	1.29
19	A	812	CLA	CBB-CAB	3.34	1.51	1.29
19	A	816	CLA	CBB-CAB	3.34	1.51	1.29
19	2	506	CLA	CBB-CAB	3.34	1.51	1.29
19	B	839	CLA	CBB-CAB	3.34	1.51	1.29
19	2	508	CLA	CBB-CAB	3.34	1.51	1.29
19	L	301	CLA	CBB-CAB	3.34	1.51	1.29
19	A	814	CLA	CBB-CAB	3.34	1.51	1.29
19	A	831	CLA	CBB-CAB	3.34	1.51	1.29
19	3	308	CLA	CBB-CAB	3.34	1.51	1.29
19	2	514	CLA	CBB-CAB	3.34	1.51	1.29
19	B	820	CLA	CBB-CAB	3.34	1.51	1.29
19	B	832	CLA	CBB-CAB	3.34	1.51	1.29
19	4	310	CLA	CBB-CAB	3.34	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	838	CLA	CBB-CAB	3.34	1.51	1.29
19	L	304	CLA	CBB-CAB	3.34	1.51	1.29
19	1	504	CLA	CBB-CAB	3.34	1.51	1.29
20	1	514	CHL	CBB-CAB	3.34	1.51	1.29
19	1	507	CLA	CBB-CAB	3.33	1.51	1.29
19	B	821	CLA	CBB-CAB	3.33	1.51	1.29
19	B	825	CLA	CBB-CAB	3.33	1.51	1.29
19	B	822	CLA	CBB-CAB	3.33	1.51	1.29
19	B	816	CLA	CBB-CAB	3.33	1.51	1.29
19	B	824	CLA	CBB-CAB	3.33	1.51	1.29
19	4	315	CLA	CBB-CAB	3.33	1.51	1.29
19	B	830	CLA	CBB-CAB	3.33	1.51	1.29
19	B	833	CLA	CBB-CAB	3.33	1.51	1.29
19	B	818	CLA	CBB-CAB	3.33	1.51	1.29
19	B	827	CLA	CBB-CAB	3.33	1.51	1.29
19	B	831	CLA	CBB-CAB	3.33	1.51	1.29
20	1	512	CHL	C4B-NB	3.33	1.38	1.35
19	A	824	CLA	CBB-CAB	3.33	1.51	1.29
19	4	318	CLA	CBB-CAB	3.33	1.51	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	A	822	CLA	CBB-CAB	3.33	1.51	1.29
19	A	841	CLA	CBB-CAB	3.33	1.51	1.29
19	B	809	CLA	CBB-CAB	3.32	1.51	1.29
19	F	303	CLA	CBB-CAB	3.32	1.51	1.29
19	1	506	CLA	CBB-CAB	3.32	1.51	1.29
19	A	855	CLA	CBB-CAB	3.32	1.51	1.29
19	A	839	CLA	CBB-CAB	3.32	1.51	1.29
19	B	811	CLA	CBB-CAB	3.32	1.51	1.29
19	A	829	CLA	CBB-CAB	3.32	1.51	1.29
19	A	803	CLA	CBB-CAB	3.32	1.51	1.29
19	A	823	CLA	CBB-CAB	3.31	1.51	1.29
19	2	508	CLA	MG-ND	-3.31	1.99	2.05
19	A	817	CLA	CBB-CAB	3.31	1.51	1.29
19	2	511	CLA	CBB-CAB	3.31	1.51	1.29
26	B	854	DGD	CAB-C9B	-3.31	1.33	1.51
19	B	834	CLA	CBB-CAB	3.31	1.51	1.29
19	F	303	CLA	MG-ND	-3.31	1.99	2.05
19	B	829	CLA	CBB-CAB	3.31	1.51	1.29
19	3	307	CLA	MG-ND	-3.31	1.99	2.05
19	A	810	CLA	CBB-CAB	3.31	1.51	1.29
19	G	204	CLA	CBB-CAB	3.31	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	821	CLA	CBB-CAB	3.31	1.51	1.29
20	2	526	CHL	CBB-CAB	3.31	1.51	1.29
19	A	828	CLA	CBB-CAB	3.31	1.51	1.29
19	A	829	CLA	MG-ND	-3.31	1.99	2.05
19	G	201	CLA	C1C-NC	-3.31	1.32	1.37
19	A	827	CLA	CBB-CAB	3.30	1.51	1.29
19	J	1101	CLA	CBB-CAB	3.30	1.51	1.29
19	B	804	CLA	CBB-CAB	3.30	1.51	1.29
19	A	838	CLA	CBB-CAB	3.30	1.51	1.29
19	A	832	CLA	CBB-CAB	3.30	1.51	1.29
19	B	814	CLA	CBB-CAB	3.30	1.51	1.29
19	A	809	CLA	CBB-CAB	3.30	1.51	1.29
19	4	306	CLA	C1C-NC	-3.30	1.32	1.37
19	A	854	CLA	CBB-CAB	3.30	1.51	1.29
19	A	802	CLA	CBB-CAB	3.30	1.51	1.29
19	3	310	CLA	CBB-CAB	3.30	1.51	1.29
19	B	837	CLA	CBB-CAB	3.30	1.51	1.29
19	B	803	CLA	CBB-CAB	3.30	1.51	1.29
19	K	1004	CLA	MG-ND	-3.30	1.99	2.05
19	B	808	CLA	CBB-CAB	3.29	1.51	1.29
19	A	837	CLA	CBB-CAB	3.29	1.51	1.29
19	B	812	CLA	CBB-CAB	3.29	1.51	1.29
19	B	805	CLA	CBB-CAB	3.29	1.51	1.29
26	J	1106	DGD	CDA-CCA	-3.29	1.33	1.51
19	A	840	CLA	CBB-CAB	3.29	1.51	1.29
20	4	313	CHL	C4B-NB	3.29	1.38	1.35
20	2	515	CHL	C4B-NB	3.28	1.38	1.35
19	B	805	CLA	MG-ND	-3.28	1.99	2.05
19	B	835	CLA	CBB-CAB	3.28	1.51	1.29
20	4	317	CHL	CBB-CAB	3.28	1.51	1.29
26	4	319	DGD	CAA-C9A	-3.28	1.33	1.51
19	4	312	CLA	CBB-CAB	3.28	1.51	1.29
20	4	317	CHL	C4B-NB	3.28	1.38	1.35
22	F	304	LMG	C40-C39	-3.27	1.33	1.51
19	B	823	CLA	CBB-CAB	3.27	1.51	1.29
19	B	838	CLA	MG-ND	-3.27	1.99	2.05
19	B	806	CLA	CBB-CAB	3.27	1.51	1.29
20	4	313	CHL	CBB-CAB	3.27	1.51	1.29
22	F	304	LMG	C43-C42	-3.27	1.33	1.51
20	2	516	CHL	CBB-CAB	3.27	1.51	1.29
19	A	834	CLA	CBB-CAB	3.26	1.50	1.29
19	A	855	CLA	MG-ND	-3.26	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	828	CLA	CBB-CAB	3.26	1.50	1.29
19	B	821	CLA	C1C-NC	-3.26	1.32	1.37
22	4	322	LMG	C40-C39	-3.26	1.33	1.51
19	3	310	CLA	C1C-NC	-3.25	1.32	1.37
19	3	305	CLA	C1C-NC	-3.25	1.33	1.37
22	1	518	LMG	C19-C18	-3.25	1.33	1.51
19	A	804	CLA	CBB-CAB	3.24	1.50	1.29
20	2	526	CHL	C4B-NB	3.24	1.38	1.35
22	G	206	LMG	C40-C39	-3.24	1.33	1.51
20	1	512	CHL	CBB-CAB	3.24	1.50	1.29
22	A	847	LMG	C19-C18	-3.24	1.33	1.51
22	F	304	LMG	C37-C36	-3.24	1.33	1.51
22	A	847	LMG	C25-C24	-3.24	1.33	1.51
19	3	305	CLA	CBB-CAB	3.24	1.50	1.29
20	2	513	CHL	C4B-NB	3.24	1.38	1.35
19	3	317	CLA	CBB-CAB	3.23	1.50	1.29
19	4	311	CLA	C1C-NC	-3.23	1.33	1.37
19	A	841	CLA	MG-ND	-3.23	1.99	2.05
26	J	1106	DGD	CGA-CFA	-3.23	1.33	1.51
19	B	831	CLA	C1C-NC	-3.23	1.33	1.37
20	4	316	CHL	C4B-NB	3.23	1.38	1.35
22	4	322	LMG	C37-C36	-3.22	1.33	1.51
22	A	847	LMG	C22-C21	-3.22	1.33	1.51
20	4	316	CHL	C3B-C2B	-3.22	1.35	1.40
22	G	206	LMG	C37-C36	-3.22	1.33	1.51
19	A	807	CLA	C1C-NC	-3.22	1.33	1.37
26	B	854	DGD	CGB-CFB	-3.21	1.33	1.51
19	B	832	CLA	C1C-NC	-3.21	1.33	1.37
22	F	305	LMG	C37-C36	-3.21	1.33	1.51
19	A	805	CLA	C1C-NC	-3.21	1.33	1.37
22	1	518	LMG	C22-C21	-3.21	1.33	1.51
19	4	309	CLA	MG-ND	-3.21	1.99	2.05
22	A	847	LMG	C37-C36	-3.21	1.33	1.51
19	3	316	CLA	C1C-NC	-3.21	1.33	1.37
19	G	202	CLA	C1C-NC	-3.20	1.33	1.37
26	B	854	DGD	CAA-C9A	-3.20	1.33	1.51
19	L	304	CLA	MG-ND	-3.20	1.99	2.05
19	A	826	CLA	C1C-NC	-3.20	1.33	1.37
19	B	839	CLA	MG-ND	-3.20	1.99	2.05
19	A	841	CLA	CHC-C1C	3.20	1.43	1.35
22	G	206	LMG	C22-C21	-3.19	1.33	1.51
19	A	838	CLA	C1C-NC	-3.19	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	805	CLA	CBB-CAB	3.19	1.50	1.29
22	1	518	LMG	C25-C24	-3.19	1.33	1.51
19	K	1004	CLA	C4D-C3D	-3.18	1.40	1.46
26	B	854	DGD	CDB-CCB	-3.18	1.33	1.51
19	4	315	CLA	C1C-NC	-3.18	1.33	1.37
19	L	303	CLA	C1C-NC	-3.18	1.33	1.37
22	G	206	LMG	C19-C18	-3.18	1.33	1.51
19	B	822	CLA	C1C-NC	-3.17	1.33	1.37
19	A	828	CLA	C1C-NC	-3.17	1.33	1.37
19	4	308	CLA	C1C-NC	-3.16	1.33	1.37
22	B	844	LMG	C19-C18	-3.16	1.33	1.51
20	1	521	CHL	CBB-CAB	3.16	1.50	1.29
20	4	316	CHL	CBB-CAB	3.16	1.50	1.29
19	A	831	CLA	C1C-NC	-3.15	1.33	1.37
19	4	318	CLA	C1C-NC	-3.15	1.33	1.37
19	3	311	CLA	C1C-NC	-3.15	1.33	1.37
19	B	840	CLA	C1C-NC	-3.14	1.33	1.37
19	A	841	CLA	C1C-NC	-3.13	1.33	1.37
19	4	307	CLA	C1C-NC	-3.13	1.33	1.37
19	A	813	CLA	C1C-NC	-3.13	1.33	1.37
19	B	828	CLA	MG-ND	-3.12	1.99	2.05
19	H	1000	CLA	C1C-NC	-3.12	1.33	1.37
19	K	1003	CLA	C4D-C3D	-3.12	1.40	1.46
19	1	508	CLA	C1C-NC	-3.12	1.33	1.37
19	2	510	CLA	C1C-NC	-3.12	1.33	1.37
19	4	304	CLA	C1C-NC	-3.12	1.33	1.37
19	3	313	CLA	C1C-NC	-3.12	1.33	1.37
19	A	808	CLA	C1C-NC	-3.12	1.33	1.37
19	2	504	CLA	C1C-NC	-3.11	1.33	1.37
19	A	822	CLA	C1C-NC	-3.11	1.33	1.37
19	A	832	CLA	C1C-NC	-3.11	1.33	1.37
19	A	855	CLA	C1C-NC	-3.11	1.33	1.37
19	B	803	CLA	C1C-NC	-3.10	1.33	1.37
19	B	805	CLA	C1C-NC	-3.10	1.33	1.37
19	B	810	CLA	C1C-NC	-3.10	1.33	1.37
19	A	823	CLA	C1C-NC	-3.10	1.33	1.37
19	A	816	CLA	C1C-NC	-3.09	1.33	1.37
19	B	820	CLA	C1C-NC	-3.09	1.33	1.37
19	2	511	CLA	C1C-NC	-3.09	1.33	1.37
19	A	812	CLA	C1C-NC	-3.09	1.33	1.37
20	1	514	CHL	C4B-NB	3.09	1.38	1.35
19	2	514	CLA	C1C-NC	-3.08	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	K	1001	CLA	C1C-NC	-3.08	1.33	1.37
19	B	839	CLA	C1C-NC	-3.07	1.33	1.37
19	B	826	CLA	C1C-NC	-3.06	1.33	1.37
19	3	308	CLA	C1C-NC	-3.06	1.33	1.37
19	A	854	CLA	C1C-NC	-3.06	1.33	1.37
19	B	828	CLA	C1C-NC	-3.06	1.33	1.37
19	A	837	CLA	C1C-NC	-3.06	1.33	1.37
19	4	305	CLA	C1C-NC	-3.05	1.33	1.37
19	A	811	CLA	C1C-NC	-3.05	1.33	1.37
19	A	821	CLA	C1C-NC	-3.05	1.33	1.37
19	A	839	CLA	C1C-NC	-3.05	1.33	1.37
19	2	509	CLA	C1C-NC	-3.05	1.33	1.37
19	B	807	CLA	C1C-NC	-3.05	1.33	1.37
20	3	314	CHL	CBB-CAB	3.05	1.49	1.29
19	B	813	CLA	C1C-NC	-3.04	1.33	1.37
19	A	827	CLA	C1C-NC	-3.04	1.33	1.37
19	A	814	CLA	C1C-NC	-3.04	1.33	1.37
19	4	309	CLA	C1C-NC	-3.04	1.33	1.37
19	2	507	CLA	C1C-NC	-3.04	1.33	1.37
19	B	823	CLA	C1C-NC	-3.04	1.33	1.37
19	4	312	CLA	C1C-NC	-3.04	1.33	1.37
19	B	834	CLA	CHC-C1C	3.03	1.42	1.35
19	B	835	CLA	C1C-NC	-3.03	1.33	1.37
20	3	314	CHL	C4B-NB	3.03	1.37	1.35
19	B	812	CLA	C1C-NC	-3.03	1.33	1.37
19	B	816	CLA	C1C-NC	-3.03	1.33	1.37
19	1	505	CLA	C1C-NC	-3.02	1.33	1.37
19	B	808	CLA	C1C-NC	-3.02	1.33	1.37
19	G	204	CLA	C1C-NC	-3.02	1.33	1.37
19	1	507	CLA	C1C-NC	-3.02	1.33	1.37
19	B	811	CLA	C1C-NC	-3.02	1.33	1.37
19	1	515	CLA	C1C-NC	-3.02	1.33	1.37
20	2	513	CHL	CBB-CAB	3.01	1.49	1.29
19	B	827	CLA	C1C-NC	-3.01	1.33	1.37
19	J	1102	CLA	C1C-NC	-3.01	1.33	1.37
19	A	809	CLA	C1C-NC	-3.01	1.33	1.37
19	B	804	CLA	C1C-NC	-3.01	1.33	1.37
19	1	504	CLA	C1C-NC	-3.01	1.33	1.37
19	B	806	CLA	C1C-NC	-3.01	1.33	1.37
19	A	810	CLA	C1C-NC	-3.00	1.33	1.37
19	A	817	CLA	C1C-NC	-3.00	1.33	1.37
19	B	809	CLA	C1C-NC	-2.99	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	817	CLA	C1C-NC	-2.99	1.33	1.37
19	A	824	CLA	C1C-NC	-2.99	1.33	1.37
19	2	506	CLA	C1C-NC	-2.99	1.33	1.37
19	B	814	CLA	C1C-NC	-2.99	1.33	1.37
19	1	516	CLA	C1C-NC	-2.99	1.33	1.37
19	G	203	CLA	C1C-NC	-2.99	1.33	1.37
19	B	833	CLA	C1C-NC	-2.99	1.33	1.37
19	L	304	CLA	C1C-NC	-2.98	1.33	1.37
19	3	307	CLA	C1C-NC	-2.98	1.33	1.37
19	2	505	CLA	C1C-NC	-2.98	1.33	1.37
20	3	314	CHL	C3B-C2B	-2.98	1.36	1.40
19	A	810	CLA	CHC-C1C	2.98	1.42	1.35
19	3	315	CLA	C1C-NC	-2.98	1.33	1.37
19	B	836	CLA	C1C-NC	-2.98	1.33	1.37
19	A	834	CLA	C1C-NC	-2.97	1.33	1.37
19	A	833	CLA	CHC-C1C	2.97	1.42	1.35
19	K	1002	CLA	C1C-NC	-2.97	1.33	1.37
19	B	819	CLA	C1C-NC	-2.96	1.33	1.37
19	B	829	CLA	C1C-NC	-2.96	1.33	1.37
19	A	835	CLA	C1C-NC	-2.96	1.33	1.37
19	K	1003	CLA	C2B-C1B	2.96	1.45	1.39
19	1	509	CLA	C1C-NC	-2.96	1.33	1.37
19	A	820	CLA	C1C-NC	-2.96	1.33	1.37
20	4	314	CHL	C4B-NB	2.96	1.37	1.35
19	L	301	CLA	C1C-NC	-2.95	1.33	1.37
19	B	812	CLA	CHC-C1C	2.94	1.42	1.35
20	4	314	CHL	CBB-CAB	2.94	1.48	1.29
19	A	815	CLA	C1C-NC	-2.94	1.33	1.37
19	B	811	CLA	CHC-C1C	2.94	1.42	1.35
19	2	508	CLA	C1C-NC	-2.94	1.33	1.37
19	B	825	CLA	C1C-NC	-2.94	1.33	1.37
19	1	511	CLA	C1C-NC	-2.94	1.33	1.37
19	B	839	CLA	C3B-C2B	-2.93	1.36	1.40
19	A	840	CLA	C1C-NC	-2.93	1.33	1.37
19	3	309	CLA	C1C-NC	-2.93	1.33	1.37
19	3	312	CLA	C1C-NC	-2.93	1.33	1.37
19	B	818	CLA	C1C-NC	-2.93	1.33	1.37
19	A	805	CLA	C3B-C2B	-2.93	1.36	1.40
19	B	838	CLA	C1C-NC	-2.93	1.33	1.37
19	A	806	CLA	C1C-NC	-2.92	1.33	1.37
19	F	303	CLA	C1C-NC	-2.92	1.33	1.37
19	A	836	CLA	C1C-NC	-2.92	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	802	CLA	C1C-NC	-2.92	1.33	1.37
19	3	317	CLA	C1C-NC	-2.92	1.33	1.37
19	B	834	CLA	C1C-NC	-2.92	1.33	1.37
19	A	802	CLA	CHC-C1C	2.91	1.42	1.35
19	A	819	CLA	C1C-NC	-2.91	1.33	1.37
19	A	842	CLA	C1C-NC	-2.91	1.33	1.37
19	1	513	CLA	C1C-NC	-2.91	1.33	1.37
19	A	833	CLA	C1C-NC	-2.91	1.33	1.37
19	K	1004	CLA	C2B-C1B	2.91	1.45	1.39
19	F	302	CLA	C1C-NC	-2.91	1.33	1.37
19	J	1101	CLA	C1C-NC	-2.91	1.33	1.37
19	A	805	CLA	CHC-C1C	2.90	1.42	1.35
19	4	310	CLA	C1C-NC	-2.90	1.33	1.37
19	A	830	CLA	C1C-NC	-2.89	1.33	1.37
19	A	804	CLA	CHC-C1C	2.89	1.42	1.35
19	1	506	CLA	C1C-NC	-2.89	1.33	1.37
20	2	512	CHL	CBB-CAB	2.89	1.48	1.29
19	B	817	CLA	CHC-C1C	2.89	1.42	1.35
19	A	829	CLA	C1C-NC	-2.88	1.33	1.37
19	L	305	CLA	C1C-NC	-2.88	1.33	1.37
19	A	826	CLA	CHC-C1C	2.88	1.42	1.35
19	B	836	CLA	CHC-C1C	2.87	1.42	1.35
19	F	302	CLA	CHC-C1C	2.86	1.42	1.35
19	A	837	CLA	CHC-C1C	2.86	1.42	1.35
19	B	832	CLA	CHC-C1C	2.86	1.42	1.35
19	A	806	CLA	CHC-C1C	2.85	1.42	1.35
19	A	818	CLA	C1C-NC	-2.85	1.33	1.37
19	B	824	CLA	C1C-NC	-2.85	1.33	1.37
19	L	301	CLA	CHC-C1C	2.84	1.42	1.35
19	A	818	CLA	CHC-C1C	2.84	1.42	1.35
19	B	838	CLA	CHC-C1C	2.83	1.42	1.35
19	B	808	CLA	CHC-C1C	2.83	1.42	1.35
19	4	310	CLA	CHC-C1C	2.82	1.42	1.35
19	L	305	CLA	CHC-C1C	2.82	1.42	1.35
19	A	829	CLA	CHC-C1C	2.82	1.42	1.35
19	A	803	CLA	CHC-C1C	2.81	1.42	1.35
19	A	823	CLA	CHC-C1C	2.81	1.42	1.35
19	1	515	CLA	CHC-C1C	2.81	1.42	1.35
19	3	305	CLA	CHC-C1C	2.81	1.42	1.35
19	A	854	CLA	CHC-C1C	2.80	1.42	1.35
19	B	805	CLA	CHC-C1C	2.80	1.42	1.35
19	A	822	CLA	CHC-C1C	2.80	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	809	CLA	CHC-C1C	2.79	1.42	1.35
19	B	833	CLA	CHC-C1C	2.79	1.42	1.35
19	A	825	CLA	C1C-NC	-2.79	1.33	1.37
19	A	827	CLA	CHC-C1C	2.79	1.42	1.35
19	L	304	CLA	CHC-C1C	2.79	1.42	1.35
19	A	839	CLA	CHC-C1C	2.78	1.42	1.35
19	B	830	CLA	C1C-NC	-2.78	1.33	1.37
19	A	831	CLA	CHC-C1C	2.78	1.42	1.35
19	B	819	CLA	CHC-C1C	2.78	1.42	1.35
19	B	825	CLA	CHC-C1C	2.78	1.42	1.35
19	A	803	CLA	C1C-NC	-2.77	1.33	1.37
19	B	837	CLA	C1C-NC	-2.77	1.33	1.37
19	B	830	CLA	CHC-C1C	2.77	1.42	1.35
19	3	306	CLA	C3B-C2B	-2.77	1.36	1.40
19	A	804	CLA	C1C-NC	-2.77	1.33	1.37
19	A	813	CLA	CHC-C1C	2.76	1.42	1.35
19	B	823	CLA	CHC-C1C	2.76	1.42	1.35
19	3	317	CLA	C3B-C2B	-2.76	1.36	1.40
19	A	821	CLA	CHC-C1C	2.76	1.42	1.35
19	A	842	CLA	CHC-C1C	2.76	1.42	1.35
19	B	835	CLA	CHC-C1C	2.76	1.42	1.35
19	B	831	CLA	CHC-C1C	2.76	1.42	1.35
19	1	511	CLA	CHC-C1C	2.76	1.42	1.35
24	B	855	LMT	O3'-C3'	-2.75	1.36	1.43
19	G	204	CLA	CHC-C1C	2.75	1.42	1.35
19	B	824	CLA	CHC-C1C	2.75	1.42	1.35
19	4	307	CLA	CHC-C1C	2.74	1.42	1.35
19	K	1001	CLA	CHC-C1C	2.74	1.42	1.35
19	4	304	CLA	CHC-C1C	2.74	1.42	1.35
19	B	840	CLA	CHC-C1C	2.74	1.42	1.35
19	B	822	CLA	C3B-C2B	-2.74	1.36	1.40
19	A	815	CLA	CHC-C1C	2.74	1.42	1.35
19	G	202	CLA	CHC-C1C	2.74	1.42	1.35
19	B	821	CLA	CHC-C1C	2.73	1.42	1.35
19	B	803	CLA	CHC-C1C	2.73	1.42	1.35
19	B	828	CLA	CHC-C1C	2.73	1.42	1.35
19	A	838	CLA	C3B-C2B	-2.73	1.36	1.40
24	4	320	LMT	O3'-C3'	-2.73	1.36	1.43
19	2	509	CLA	CHC-C1C	2.73	1.42	1.35
19	B	812	CLA	C3B-C2B	-2.73	1.36	1.40
19	A	817	CLA	CHC-C1C	2.73	1.42	1.35
19	2	504	CLA	CHC-C1C	2.72	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	808	CLA	CHC-C1C	2.72	1.41	1.35
27	A	801	CL0	MG-NC	2.72	2.12	2.06
19	4	312	CLA	C3B-C2B	-2.72	1.36	1.40
19	A	807	CLA	CHC-C1C	2.72	1.41	1.35
19	B	820	CLA	CHC-C1C	2.71	1.41	1.35
19	3	310	CLA	C3B-C2B	-2.71	1.36	1.40
19	B	806	CLA	C3B-C2B	-2.71	1.36	1.40
19	3	305	CLA	C3B-C2B	-2.71	1.36	1.40
19	G	201	CLA	C3B-C2B	-2.71	1.36	1.40
19	4	312	CLA	CHC-C1C	2.71	1.41	1.35
19	B	807	CLA	CHC-C1C	2.71	1.41	1.35
19	1	513	CLA	CHC-C1C	2.71	1.41	1.35
19	3	315	CLA	CHC-C1C	2.71	1.41	1.35
19	1	516	CLA	CHC-C1C	2.70	1.41	1.35
19	3	317	CLA	CHC-C1C	2.70	1.41	1.35
19	A	824	CLA	CHC-C1C	2.70	1.41	1.35
19	B	820	CLA	C3B-C2B	-2.70	1.36	1.40
19	A	838	CLA	CHC-C1C	2.70	1.41	1.35
19	J	1102	CLA	CHC-C1C	2.70	1.41	1.35
19	1	504	CLA	CHC-C1C	2.70	1.41	1.35
19	3	308	CLA	CHC-C1C	2.70	1.41	1.35
19	G	203	CLA	CHC-C1C	2.69	1.41	1.35
19	A	840	CLA	CHC-C1C	2.69	1.41	1.35
19	B	816	CLA	CHC-C1C	2.69	1.41	1.35
19	B	818	CLA	CHC-C1C	2.69	1.41	1.35
19	1	507	CLA	CHC-C1C	2.69	1.41	1.35
19	K	1002	CLA	CHC-C1C	2.69	1.41	1.35
19	2	507	CLA	CHC-C1C	2.69	1.41	1.35
19	A	819	CLA	CHC-C1C	2.68	1.41	1.35
19	A	811	CLA	CHC-C1C	2.68	1.41	1.35
19	A	812	CLA	CHC-C1C	2.67	1.41	1.35
19	A	834	CLA	CHC-C1C	2.67	1.41	1.35
19	A	836	CLA	CHC-C1C	2.67	1.41	1.35
19	A	832	CLA	CHC-C1C	2.67	1.41	1.35
19	B	821	CLA	C3B-C2B	-2.67	1.36	1.40
19	2	506	CLA	CHC-C1C	2.67	1.41	1.35
24	B	846	LMT	O3'-C3'	-2.67	1.36	1.43
27	A	801	CL0	CHC-C1C	2.67	1.41	1.35
20	4	314	CHL	C3A-C2A	-2.66	1.47	1.54
19	3	311	CLA	CHC-C1C	2.65	1.41	1.35
19	B	822	CLA	CHC-C1C	2.65	1.41	1.35
19	J	1101	CLA	CHC-C1C	2.65	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	509	CLA	CHC-C1C	2.65	1.41	1.35
27	A	801	CL0	C1C-NC	-2.65	1.33	1.37
19	4	306	CLA	CHC-C1C	2.65	1.41	1.35
19	2	510	CLA	CHC-C1C	2.64	1.41	1.35
19	A	811	CLA	C3B-C2B	-2.64	1.36	1.40
19	A	812	CLA	C3B-C2B	-2.64	1.36	1.40
19	4	315	CLA	CHC-C1C	2.64	1.41	1.35
19	A	824	CLA	C3B-C2B	-2.64	1.36	1.40
19	B	839	CLA	CHC-C1C	2.64	1.41	1.35
19	2	511	CLA	CHC-C1C	2.63	1.41	1.35
24	G	208	LMT	O3'-C3'	-2.63	1.36	1.43
19	B	835	CLA	C3B-C2B	-2.63	1.36	1.40
24	B	847	LMT	O3'-C3'	-2.63	1.36	1.43
19	3	313	CLA	CHC-C1C	2.63	1.41	1.35
19	A	830	CLA	CHC-C1C	2.63	1.41	1.35
19	B	837	CLA	CHC-C1C	2.62	1.41	1.35
19	3	307	CLA	C3B-C2B	-2.62	1.36	1.40
19	2	505	CLA	CHC-C1C	2.62	1.41	1.35
19	B	813	CLA	CHC-C1C	2.62	1.41	1.35
19	2	514	CLA	CHC-C1C	2.62	1.41	1.35
19	A	816	CLA	C3B-C2B	-2.62	1.36	1.40
19	B	834	CLA	C3B-C2B	-2.62	1.36	1.40
19	3	307	CLA	CHC-C1C	2.61	1.41	1.35
19	F	303	CLA	CHC-C1C	2.61	1.41	1.35
24	3	318	LMT	O3'-C3'	-2.61	1.36	1.43
19	B	818	CLA	C3B-C2B	-2.60	1.36	1.40
19	A	855	CLA	CHC-C1C	2.60	1.41	1.35
19	4	309	CLA	CHC-C1C	2.60	1.41	1.35
19	1	505	CLA	CHC-C1C	2.60	1.41	1.35
19	4	305	CLA	CHC-C1C	2.60	1.41	1.35
19	4	305	CLA	C3B-C2B	-2.59	1.36	1.40
27	A	801	CL0	C4C-C3C	2.59	1.49	1.45
19	A	834	CLA	C3B-C2B	-2.59	1.36	1.40
19	B	811	CLA	C3B-C2B	-2.59	1.36	1.40
19	A	835	CLA	CHC-C1C	2.59	1.41	1.35
19	A	828	CLA	CHC-C1C	2.58	1.41	1.35
19	H	1000	CLA	CHC-C1C	2.58	1.41	1.35
19	A	825	CLA	CHC-C1C	2.58	1.41	1.35
19	B	806	CLA	CHC-C1C	2.58	1.41	1.35
19	1	506	CLA	CHC-C1C	2.58	1.41	1.35
19	3	312	CLA	CHC-C1C	2.58	1.41	1.35
19	4	318	CLA	CHC-C1C	2.58	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	814	CLA	CHC-C1C	2.57	1.41	1.35
19	1	506	CLA	C3B-C2B	-2.57	1.36	1.40
19	B	826	CLA	CHC-C1C	2.57	1.41	1.35
19	2	511	CLA	C3B-C2B	-2.57	1.36	1.40
19	4	311	CLA	CHC-C1C	2.57	1.41	1.35
19	F	303	CLA	C3B-C2B	-2.56	1.36	1.40
19	B	804	CLA	CHC-C1C	2.56	1.41	1.35
19	B	829	CLA	CHC-C1C	2.56	1.41	1.35
19	G	201	CLA	CHC-C1C	2.56	1.41	1.35
19	B	815	CLA	CHC-C1C	2.55	1.41	1.35
19	3	316	CLA	CHC-C1C	2.55	1.41	1.35
19	B	827	CLA	CHC-C1C	2.54	1.41	1.35
19	B	805	CLA	C3B-C2B	-2.54	1.36	1.40
22	2	519	LMG	C19-C18	-2.54	1.33	1.51
19	A	823	CLA	C3B-C2B	-2.53	1.36	1.40
24	G	209	LMT	O3'-C3'	-2.53	1.37	1.43
24	A	846	LMT	O3'-C3'	-2.53	1.37	1.43
19	B	809	CLA	C3B-C2B	-2.53	1.36	1.40
19	A	837	CLA	C3B-C2B	-2.52	1.36	1.40
19	B	814	CLA	CHC-C1C	2.52	1.41	1.35
19	3	309	CLA	CHC-C1C	2.52	1.41	1.35
19	1	508	CLA	CHC-C1C	2.52	1.41	1.35
19	1	505	CLA	C3B-C2B	-2.52	1.36	1.40
19	2	505	CLA	C3B-C2B	-2.51	1.36	1.40
19	A	809	CLA	CHC-C1C	2.51	1.41	1.35
20	1	521	CHL	C3B-C2B	-2.51	1.36	1.40
19	2	508	CLA	CHC-C1C	2.50	1.41	1.35
24	J	1107	LMT	O3'-C3'	-2.50	1.37	1.43
19	A	820	CLA	CHC-C1C	2.50	1.41	1.35
24	B	847	LMT	O2'-C2'	-2.50	1.37	1.43
19	3	310	CLA	CHC-C1C	2.50	1.41	1.35
19	A	835	CLA	C3B-C2B	-2.49	1.36	1.40
19	A	841	CLA	C3B-C2B	-2.49	1.36	1.40
19	K	1004	CLA	C2D-C1D	2.49	1.47	1.42
19	4	310	CLA	C3B-C2B	-2.48	1.36	1.40
19	A	820	CLA	C3B-C2B	-2.48	1.36	1.40
19	A	822	CLA	C3B-C2B	-2.48	1.36	1.40
19	B	808	CLA	C3B-C2B	-2.47	1.36	1.40
19	B	810	CLA	CHC-C1C	2.47	1.41	1.35
20	2	512	CHL	C4B-NB	2.47	1.37	1.35
20	4	313	CHL	C3B-C2B	-2.47	1.36	1.40
19	K	1003	CLA	C2D-C1D	2.46	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	811	CLA	C1C-C2C	2.46	1.49	1.44
19	A	832	CLA	C3B-C2B	-2.45	1.37	1.40
19	1	511	CLA	C3B-C2B	-2.45	1.37	1.40
19	3	312	CLA	C3B-C2B	-2.45	1.37	1.40
19	A	804	CLA	C3B-C2B	-2.45	1.37	1.40
19	L	303	CLA	CHC-C1C	2.45	1.41	1.35
19	1	510	CLA	CHC-C1C	2.42	1.41	1.35
19	A	816	CLA	CHC-C1C	2.42	1.41	1.35
19	A	810	CLA	C3B-C2B	-2.41	1.37	1.40
24	2	523	LMT	O3'-C3'	-2.41	1.37	1.43
24	B	855	LMT	O2B-C2B	-2.41	1.37	1.43
19	K	1003	CLA	C1C-NC	-2.41	1.33	1.38
19	3	311	CLA	C3B-C2B	-2.40	1.37	1.40
20	4	317	CHL	C3B-C2B	-2.40	1.37	1.40
19	4	311	CLA	C3B-C2B	-2.40	1.37	1.40
19	3	309	CLA	C3B-C2B	-2.40	1.37	1.40
24	A	846	LMT	O3B-C3B	-2.39	1.37	1.43
19	G	204	CLA	C3B-C2B	-2.39	1.37	1.40
19	B	819	CLA	C3B-C2B	-2.39	1.37	1.40
19	3	306	CLA	CHC-C1C	2.39	1.41	1.35
19	B	823	CLA	C3B-C2B	-2.38	1.37	1.40
19	K	1004	CLA	C1C-NC	-2.38	1.33	1.38
19	1	515	CLA	C3B-C2B	-2.38	1.37	1.40
27	A	801	CL0	C1D-C2D	2.37	1.50	1.45
24	J	1107	LMT	O2B-C2B	-2.37	1.37	1.43
19	B	838	CLA	C3B-C2B	-2.36	1.37	1.40
19	L	305	CLA	C3B-C2B	-2.34	1.37	1.40
19	J	1105	CLA	CHC-C1C	2.34	1.41	1.35
24	3	318	LMT	O2'-C2'	-2.33	1.37	1.43
20	4	313	CHL	CHC-C1C	2.33	1.40	1.35
19	A	825	CLA	MG-NC	2.33	2.11	2.06
24	B	855	LMT	O4'-C4B	-2.32	1.37	1.43
19	4	308	CLA	CHC-C1C	2.32	1.40	1.35
24	B	855	LMT	O2'-C2'	-2.32	1.37	1.43
19	B	817	CLA	C3B-C2B	-2.32	1.37	1.40
24	B	846	LMT	O3B-C3B	-2.31	1.37	1.43
19	1	510	CLA	C3B-C2B	-2.31	1.37	1.40
19	K	1003	CLA	C2C-C1C	2.31	1.48	1.43
19	K	1002	CLA	C3B-C2B	-2.29	1.37	1.40
20	2	526	CHL	C3B-C2B	-2.28	1.37	1.40
24	B	855	LMT	O3B-C3B	-2.28	1.37	1.43
19	B	830	CLA	CHD-C1D	2.27	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	303	CLA	C3B-C2B	-2.27	1.37	1.40
24	G	208	LMT	O3B-C3B	-2.27	1.37	1.43
24	2	523	LMT	O2B-C2B	-2.26	1.37	1.43
19	F	302	CLA	C1C-C2C	2.25	1.48	1.44
19	B	816	CLA	C3B-C2B	-2.24	1.37	1.40
19	A	836	CLA	MG-NC	2.24	2.11	2.06
24	G	209	LMT	O3B-C3B	-2.24	1.37	1.43
24	B	846	LMT	O2B-C2B	-2.24	1.37	1.43
19	B	812	CLA	C1C-C2C	2.24	1.48	1.44
19	H	1000	CLA	C3B-C2B	-2.24	1.37	1.40
24	B	847	LMT	O2B-C2B	-2.24	1.37	1.43
24	4	320	LMT	O2'-C2'	-2.23	1.37	1.43
19	K	1004	CLA	C2C-C1C	2.23	1.48	1.43
24	B	846	LMT	O2'-C2'	-2.23	1.37	1.43
24	B	847	LMT	O3B-C3B	-2.23	1.37	1.43
20	1	512	CHL	C3B-C2B	-2.22	1.37	1.40
19	B	804	CLA	C1A-CHA	2.22	1.52	1.43
24	J	1107	LMT	O3B-C3B	-2.22	1.37	1.43
24	G	209	LMT	O2B-C2B	-2.22	1.37	1.43
24	4	320	LMT	O2B-C2B	-2.22	1.37	1.43
19	A	833	CLA	C1C-C2C	2.22	1.48	1.44
24	G	209	LMT	O2'-C2'	-2.21	1.37	1.43
19	A	817	CLA	C3B-C2B	-2.21	1.37	1.40
24	4	320	LMT	O3B-C3B	-2.21	1.37	1.43
20	2	516	CHL	CHC-C1C	2.21	1.40	1.35
24	A	846	LMT	O2B-C2B	-2.21	1.37	1.43
19	3	309	CLA	MG-NC	2.20	2.11	2.06
19	4	310	CLA	C1C-C2C	2.20	1.48	1.44
24	2	523	LMT	O3B-C3B	-2.19	1.37	1.43
20	4	316	CHL	C2C-C3C	2.19	1.41	1.36
19	B	834	CLA	C1C-C2C	2.19	1.48	1.44
19	A	805	CLA	C1C-C2C	2.19	1.48	1.44
19	2	506	CLA	C1A-CHA	2.18	1.52	1.43
19	3	310	CLA	C1A-CHA	2.18	1.52	1.43
24	J	1107	LMT	O2'-C2'	-2.18	1.37	1.43
19	A	810	CLA	C1C-C2C	2.18	1.48	1.44
19	4	304	CLA	C1A-CHA	2.18	1.52	1.43
19	H	1000	CLA	C1A-CHA	2.17	1.52	1.43
19	1	510	CLA	C3D-C4D	-2.17	1.39	1.44
24	G	208	LMT	O2'-C2'	-2.17	1.37	1.43
19	3	317	CLA	C1C-C2C	2.17	1.48	1.44
19	3	309	CLA	C1A-CHA	2.17	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	318	LMT	O3B-C3B	-2.17	1.37	1.43
19	B	826	CLA	MG-NC	2.17	2.11	2.06
19	4	306	CLA	C3B-C2B	-2.17	1.37	1.40
19	1	513	CLA	C3B-C2B	-2.16	1.37	1.40
19	3	316	CLA	C3B-C2B	-2.16	1.37	1.40
19	1	505	CLA	C1A-CHA	2.16	1.52	1.43
19	2	510	CLA	C1A-CHA	2.15	1.52	1.43
19	B	837	CLA	C3D-C4D	-2.15	1.39	1.44
19	L	301	CLA	C1C-C2C	2.15	1.48	1.44
19	B	814	CLA	C3B-C2B	-2.15	1.37	1.40
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	840	CLA	C3B-C2B	-2.14	1.37	1.40
19	A	818	CLA	C1C-C2C	2.14	1.48	1.44
24	G	208	LMT	O1'-C1'	-2.14	1.36	1.40
19	3	305	CLA	C1C-C2C	2.14	1.48	1.44
19	A	818	CLA	MG-NC	2.14	2.11	2.06
19	4	309	CLA	C3B-C2B	-2.14	1.37	1.40
19	A	828	CLA	C3B-C2B	-2.14	1.37	1.40
19	B	807	CLA	C3B-C2B	-2.14	1.37	1.40
19	1	508	CLA	C1A-CHA	2.14	1.52	1.43
19	A	827	CLA	C1C-C2C	2.14	1.48	1.44
19	A	841	CLA	C1C-C2C	2.13	1.48	1.44
19	L	305	CLA	MG-NC	2.13	2.11	2.06
19	A	839	CLA	C3B-C2B	-2.13	1.37	1.40
19	3	312	CLA	C1A-CHA	2.13	1.52	1.43
19	A	823	CLA	C1C-C2C	2.13	1.48	1.44
19	L	305	CLA	C1C-C2C	2.13	1.48	1.44
19	B	824	CLA	C1C-C2C	2.13	1.48	1.44
24	A	846	LMT	O2'-C2'	-2.13	1.38	1.43
19	1	516	CLA	C1A-CHA	2.13	1.51	1.43
19	B	831	CLA	C1C-C2C	2.13	1.48	1.44
19	K	1003	CLA	MG-NC	2.13	2.11	2.06
24	2	523	LMT	O2'-C2'	-2.13	1.38	1.43
19	B	826	CLA	C3D-C4D	-2.13	1.39	1.44
19	A	825	CLA	C1A-CHA	2.12	1.51	1.43
19	A	820	CLA	C1A-CHA	2.12	1.51	1.43
19	2	508	CLA	C1A-CHA	2.12	1.51	1.43
19	3	313	CLA	C1A-CHA	2.12	1.51	1.43
19	B	824	CLA	C1A-CHA	2.12	1.51	1.43
20	3	314	CHL	CHC-C1C	2.12	1.40	1.35
19	K	1002	CLA	MG-NC	2.11	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	K	1004	CLA	MG-NC	2.11	2.11	2.06
19	B	836	CLA	C3B-C2B	-2.11	1.37	1.40
19	4	305	CLA	C1A-CHA	2.11	1.51	1.43
19	1	516	CLA	C3B-C2B	-2.11	1.37	1.40
19	2	504	CLA	C1A-CHA	2.11	1.51	1.43
19	B	808	CLA	C1C-C2C	2.11	1.48	1.44
19	B	811	CLA	C3D-C4D	-2.11	1.39	1.44
19	B	816	CLA	C1A-CHA	2.11	1.51	1.43
19	A	814	CLA	C3B-C2B	-2.11	1.37	1.40
19	1	507	CLA	C3B-C2B	-2.11	1.37	1.40
19	2	506	CLA	MG-NC	2.11	2.11	2.06
19	A	815	CLA	C3B-C2B	-2.11	1.37	1.40
19	3	312	CLA	MG-NC	2.10	2.11	2.06
19	A	830	CLA	C3B-C2B	-2.10	1.37	1.40
19	A	837	CLA	C1C-C2C	2.10	1.48	1.44
19	A	826	CLA	C3B-C2B	-2.10	1.37	1.40
19	B	814	CLA	MG-NC	2.10	2.11	2.06
19	A	804	CLA	C1C-C2C	2.10	1.48	1.44
19	A	818	CLA	C1A-CHA	2.10	1.51	1.43
19	A	811	CLA	C1A-CHA	2.10	1.51	1.43
19	L	303	CLA	C1A-CHA	2.10	1.51	1.43
24	G	208	LMT	O2B-C2B	-2.10	1.38	1.43
19	B	817	CLA	C1C-C2C	2.10	1.48	1.44
24	G	209	LMT	O1'-C1'	-2.10	1.36	1.40
19	2	505	CLA	C1A-CHA	2.10	1.51	1.43
19	A	826	CLA	C1C-C2C	2.10	1.48	1.44
19	A	812	CLA	C1A-CHA	2.10	1.51	1.43
20	1	521	CHL	CHC-C1C	2.10	1.40	1.35
19	A	855	CLA	C3B-C2B	-2.10	1.37	1.40
24	G	209	LMT	O4'-C4B	-2.10	1.38	1.43
19	4	310	CLA	C1A-CHA	2.09	1.51	1.43
19	1	515	CLA	MG-NC	2.09	2.11	2.06
22	B	845	LMG	O1-C1	2.09	1.43	1.40
24	A	846	LMT	O4'-C4B	-2.09	1.38	1.43
24	2	523	LMT	O4'-C4B	-2.09	1.38	1.43
19	B	833	CLA	C3D-C4D	-2.09	1.39	1.44
19	G	201	CLA	C1A-CHA	2.09	1.51	1.43
19	B	829	CLA	CHD-C1D	2.09	1.42	1.38
19	H	1000	CLA	MG-NC	2.08	2.11	2.06
19	A	823	CLA	C1A-CHA	2.08	1.51	1.43
19	1	507	CLA	C3D-C4D	-2.08	1.39	1.44
19	B	828	CLA	CHD-C1D	2.08	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	820	CLA	MG-NC	2.08	2.11	2.06
19	B	821	CLA	C1A-CHA	2.08	1.51	1.43
19	K	1002	CLA	C1A-CHA	2.08	1.51	1.43
19	A	813	CLA	C1C-C2C	2.08	1.48	1.44
19	A	818	CLA	C3B-C2B	-2.08	1.37	1.40
19	A	822	CLA	C1C-C2C	2.08	1.48	1.44
19	G	202	CLA	C1C-C2C	2.08	1.48	1.44
19	J	1105	CLA	C3D-C4D	-2.08	1.39	1.44
19	2	505	CLA	MG-NC	2.08	2.11	2.06
24	3	318	LMT	O4'-C4B	-2.08	1.38	1.43
19	B	814	CLA	CHD-C1D	2.08	1.42	1.38
19	B	813	CLA	C1A-CHA	2.08	1.51	1.43
19	A	803	CLA	C1C-C2C	2.08	1.48	1.44
19	G	202	CLA	C1A-CHA	2.08	1.51	1.43
19	G	202	CLA	C3B-C2B	-2.07	1.37	1.40
19	A	815	CLA	C1A-CHA	2.07	1.51	1.43
19	B	822	CLA	C1A-CHA	2.07	1.51	1.43
19	G	203	CLA	C1A-CHA	2.07	1.51	1.43
19	A	803	CLA	MG-NC	2.07	2.11	2.06
19	3	311	CLA	MG-NC	2.07	2.11	2.06
19	2	506	CLA	C3B-C2B	-2.07	1.37	1.40
19	1	504	CLA	C1A-CHA	2.07	1.51	1.43
19	L	301	CLA	C3B-C2B	-2.07	1.37	1.40
19	3	316	CLA	CHD-C1D	2.07	1.42	1.38
19	B	818	CLA	C1A-CHA	2.06	1.51	1.43
19	A	802	CLA	C1A-CHA	2.06	1.51	1.43
19	B	829	CLA	C3B-C2B	-2.06	1.37	1.40
19	A	816	CLA	C1A-CHA	2.06	1.51	1.43
19	A	837	CLA	MG-NC	2.06	2.11	2.06
19	G	204	CLA	MG-NC	2.06	2.11	2.06
19	B	823	CLA	C3D-C4D	-2.06	1.39	1.44
19	B	825	CLA	C1A-CHA	2.06	1.51	1.43
19	A	814	CLA	MG-NC	2.06	2.11	2.06
19	A	814	CLA	C1A-CHA	2.06	1.51	1.43
19	A	835	CLA	C1A-CHA	2.06	1.51	1.43
19	1	509	CLA	C3B-C2B	-2.05	1.37	1.40
19	B	832	CLA	C3B-C2B	-2.05	1.37	1.40
19	A	838	CLA	C1C-C2C	2.05	1.48	1.44
19	B	810	CLA	C1A-CHA	2.05	1.51	1.43
19	B	828	CLA	C1A-CHA	2.05	1.51	1.43
24	J	1107	LMT	O4'-C4B	-2.05	1.38	1.43
20	2	513	CHL	CHC-C1C	2.05	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	846	LMT	O4'-C4B	-2.05	1.38	1.43
19	4	315	CLA	CHD-C1D	2.04	1.42	1.38
19	B	820	CLA	CHD-C1D	2.04	1.42	1.38
19	B	830	CLA	MG-NC	2.04	2.11	2.06
19	A	813	CLA	C3B-C2B	-2.04	1.37	1.40
19	B	817	CLA	CHD-C1D	2.04	1.42	1.38
19	A	827	CLA	C1A-CHA	2.04	1.51	1.43
19	2	511	CLA	C1A-CHA	2.04	1.51	1.43
19	3	316	CLA	C1A-CHA	2.04	1.51	1.43
19	1	508	CLA	C3B-C2B	-2.04	1.37	1.40
19	2	514	CLA	C3B-C2B	-2.04	1.37	1.40
19	G	204	CLA	C1C-C2C	2.04	1.48	1.44
19	L	305	CLA	C1A-CHA	2.04	1.51	1.43
19	K	1001	CLA	MG-NC	2.04	2.11	2.06
19	A	855	CLA	C3D-C4D	-2.04	1.39	1.44
19	1	513	CLA	C1C-C2C	2.04	1.48	1.44
19	A	833	CLA	C1A-CHA	2.04	1.51	1.43
19	A	819	CLA	C1A-CHA	2.04	1.51	1.43
20	4	317	CHL	CHC-C1C	2.04	1.40	1.35
19	3	316	CLA	MG-NC	2.04	2.11	2.06
19	4	318	CLA	C1A-CHA	2.04	1.51	1.43
19	B	830	CLA	C1C-C2C	2.03	1.48	1.44
19	A	807	CLA	CHD-C1D	2.03	1.42	1.38
19	A	829	CLA	C3B-C2B	-2.03	1.37	1.40
19	G	203	CLA	MG-NC	2.03	2.11	2.06
19	2	510	CLA	MG-NC	2.03	2.11	2.06
19	3	305	CLA	C3D-C4D	-2.03	1.39	1.44
19	4	315	CLA	C3B-C2B	-2.03	1.37	1.40
19	A	842	CLA	C1A-CHA	2.03	1.51	1.43
19	A	824	CLA	C1C-C2C	2.03	1.48	1.44
19	4	305	CLA	MG-NC	2.03	2.11	2.06
19	B	833	CLA	CHD-C1D	2.03	1.42	1.38
19	1	515	CLA	C1C-C2C	2.03	1.48	1.44
19	3	317	CLA	C1A-CHA	2.03	1.51	1.43
19	A	854	CLA	MG-NC	2.02	2.11	2.06
19	2	514	CLA	C1A-CHA	2.02	1.51	1.43
19	B	818	CLA	MG-NC	2.02	2.11	2.06
19	B	830	CLA	C3D-C4D	-2.02	1.39	1.44
19	4	306	CLA	C1A-CHA	2.02	1.51	1.43
19	4	309	CLA	C1A-CHA	2.02	1.51	1.43
19	A	804	CLA	C1A-CHA	2.02	1.51	1.43
19	A	855	CLA	MG-NC	2.02	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	318	LMT	O2B-C2B	-2.02	1.38	1.43
19	B	827	CLA	C1A-CHA	2.02	1.51	1.43
19	A	840	CLA	MG-NC	2.02	2.11	2.06
19	A	828	CLA	C1A-CHA	2.02	1.51	1.43
19	3	311	CLA	C1A-CHA	2.02	1.51	1.43
19	1	509	CLA	MG-NC	2.02	2.11	2.06
19	B	827	CLA	C3B-C2B	-2.02	1.37	1.40
24	B	846	LMT	O1'-C1'	-2.02	1.36	1.40
19	B	831	CLA	C1A-CHA	2.02	1.51	1.43
19	B	837	CLA	C3B-C2B	-2.02	1.37	1.40
19	J	1101	CLA	C3B-C2B	-2.02	1.37	1.40
26	B	854	DGD	CDA-CCA	-2.02	1.33	1.49
19	B	835	CLA	MG-NC	2.02	2.11	2.06
19	B	809	CLA	MG-NC	2.01	2.11	2.06
19	1	505	CLA	MG-NC	2.01	2.11	2.06
19	A	829	CLA	C1C-C2C	2.01	1.48	1.44
19	B	820	CLA	C1C-C2C	2.01	1.48	1.44
22	4	322	LMG	C19-C18	-2.01	1.33	1.49
19	K	1001	CLA	C3D-C4D	-2.01	1.39	1.44
19	A	810	CLA	MG-NC	2.01	2.11	2.06
19	A	806	CLA	C1A-CHA	2.01	1.51	1.43
19	B	838	CLA	C1C-C2C	2.01	1.48	1.44
19	4	307	CLA	C3D-C4D	-2.01	1.39	1.44
19	4	310	CLA	MG-NC	2.01	2.11	2.06
19	A	825	CLA	C1C-C2C	2.01	1.48	1.44
19	B	822	CLA	C1C-C2C	2.01	1.48	1.44
19	B	826	CLA	C1A-CHA	2.01	1.51	1.43
19	A	829	CLA	C1A-CHA	2.01	1.51	1.43
19	B	818	CLA	CHD-C1D	2.01	1.42	1.38
19	1	506	CLA	C1C-C2C	2.01	1.48	1.44
19	A	802	CLA	C3D-C4D	-2.01	1.39	1.44
19	1	508	CLA	CHD-C1D	2.01	1.42	1.38
26	G	207	DGD	CAB-C9B	-2.01	1.33	1.49
26	J	1106	DGD	CAB-C9B	-2.01	1.33	1.49
19	B	837	CLA	C1A-CHA	2.01	1.51	1.43
19	A	815	CLA	C1C-C2C	2.01	1.48	1.44
19	3	307	CLA	C1A-CHA	2.01	1.51	1.43
19	B	816	CLA	C1C-C2C	2.01	1.48	1.44
24	B	847	LMT	O4'-C4B	-2.01	1.38	1.43
24	B	855	LMT	O1'-C1'	-2.01	1.36	1.40
19	B	823	CLA	C1C-C2C	2.01	1.48	1.44
19	B	805	CLA	C1A-CHA	2.01	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	F	302	CLA	MG-NC	2.01	2.11	2.06
19	3	306	CLA	C1A-CHA	2.00	1.51	1.43
19	A	842	CLA	MG-NC	2.00	2.11	2.06
19	4	312	CLA	C1A-CHA	2.00	1.51	1.43
19	J	1102	CLA	MG-NC	2.00	2.11	2.06
19	B	827	CLA	MG-NC	2.00	2.11	2.06
19	G	204	CLA	C1A-CHA	2.00	1.51	1.43
19	2	505	CLA	C1C-C2C	2.00	1.48	1.44
26	4	319	DGD	CDA-CCA	-2.00	1.33	1.49
22	A	847	LMG	C40-C39	-2.00	1.33	1.49
19	A	809	CLA	C1A-CHA	2.00	1.51	1.43
19	3	308	CLA	MG-NC	2.00	2.11	2.06
19	1	515	CLA	C3D-C4D	-2.00	1.39	1.44
19	B	809	CLA	CHD-C1D	2.00	1.42	1.38
22	F	304	LMG	C19-C18	-2.00	1.33	1.49
19	A	830	CLA	MG-NC	2.00	2.11	2.06

All (2633) 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	123.47
18	I	101	BCR	C16-C15-C14	15.15	154.50	123.47
18	B	849	BCR	C21-C20-C19	14.35	168.01	123.22
18	3	304	BCR	C16-C15-C14	13.99	152.13	123.47
18	3	304	BCR	C21-C20-C19	13.99	166.87	123.22
18	3	303	BCR	C16-C15-C14	13.92	152.00	123.47
18	2	503	BCR	C16-C15-C14	13.71	151.55	123.47
18	A	856	BCR	C21-C20-C19	13.56	165.52	123.22
18	A	850	BCR	C16-C15-C14	13.51	151.15	123.47
18	A	849	BCR	C11-C10-C9	13.42	146.47	127.31
18	L	302	BCR	C16-C15-C14	13.36	150.85	123.47
18	G	205	BCR	C16-C15-C14	13.36	150.85	123.47
18	4	301	BCR	C16-C15-C14	13.20	150.51	123.47
18	A	850	BCR	C21-C20-C19	13.13	164.19	123.22
18	B	802	BCR	C11-C10-C9	13.00	145.86	127.31
18	L	307	BCR	C16-C15-C14	12.90	149.89	123.47
18	A	856	BCR	C16-C15-C14	12.84	149.78	123.47
18	K	1005	BCR	C16-C15-C14	12.80	149.70	123.47
18	A	849	BCR	C21-C20-C19	12.73	162.95	123.22
18	I	102	BCR	C16-C15-C14	12.41	148.90	123.47
18	L	307	BCR	C11-C10-C9	12.34	144.92	127.31
18	A	848	BCR	C11-C10-C9	12.13	144.62	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	849	BCR	C11-C10-C9	12.06	144.52	127.31
18	2	503	BCR	C11-C10-C9	11.98	144.41	127.31
18	K	1005	BCR	C11-C10-C9	11.98	144.41	127.31
18	L	302	BCR	C21-C20-C19	11.90	160.37	123.22
18	G	205	BCR	C21-C20-C19	11.86	160.23	123.22
18	A	851	BCR	C16-C15-C14	11.81	147.66	123.47
18	A	851	BCR	C11-C10-C9	11.79	144.13	127.31
18	A	848	BCR	C21-C20-C19	11.76	159.91	123.22
18	F	306	BCR	C16-C15-C14	11.69	147.42	123.47
18	B	850	BCR	C16-C15-C14	11.69	147.42	123.47
18	B	853	BCR	C11-C10-C9	11.68	143.98	127.31
18	B	802	BCR	C21-C20-C19	11.67	159.62	123.22
18	L	307	BCR	C21-C20-C19	11.51	159.15	123.22
18	4	301	BCR	C11-C10-C9	11.50	143.73	127.31
18	A	848	BCR	C16-C15-C14	11.42	146.86	123.47
18	I	101	BCR	C11-C10-C9	11.40	143.57	127.31
19	3	310	CLA	C4A-NA-C1A	11.39	111.83	106.71
18	B	851	BCR	C16-C15-C14	11.35	146.73	123.47
18	I	102	BCR	C21-C20-C19	11.21	158.19	123.22
18	B	853	BCR	C16-C15-C14	11.16	146.34	123.47
18	4	301	BCR	C21-C20-C19	11.16	158.05	123.22
23	4	303	XAT	O4-C5-C18	-10.98	101.90	115.06
18	3	303	BCR	C11-C10-C9	10.88	142.83	127.31
18	J	1108	BCR	C21-C20-C19	10.88	157.16	123.22
27	A	801	CL0	C4A-NA-C1A	10.86	111.59	106.71
18	F	306	BCR	C21-C20-C19	10.83	157.00	123.22
18	K	1005	BCR	C21-C20-C19	10.72	156.69	123.22
18	L	306	BCR	C21-C20-C19	10.69	156.57	123.22
18	B	856	BCR	C16-C15-C14	10.62	145.23	123.47
18	L	306	BCR	C11-C10-C9	10.60	142.44	127.31
18	B	856	BCR	C21-C20-C19	10.59	156.27	123.22
18	A	856	BCR	C11-C10-C9	10.56	142.38	127.31
18	A	851	BCR	C21-C20-C19	10.55	156.15	123.22
18	B	856	BCR	C11-C10-C9	10.45	142.22	127.31
19	A	828	CLA	C4A-NA-C1A	10.40	111.38	106.71
18	I	101	BCR	C21-C20-C19	10.39	155.65	123.22
18	A	849	BCR	C16-C15-C14	10.39	144.75	123.47
19	2	504	CLA	C4A-NA-C1A	10.35	111.36	106.71
18	A	852	BCR	C16-C15-C14	10.34	144.66	123.47
18	3	304	BCR	C11-C10-C9	10.30	142.01	127.31
18	B	852	BCR	C11-C10-C9	10.28	141.98	127.31
18	2	503	BCR	C21-C20-C19	10.25	155.21	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	306	BCR	C16-C15-C14	10.23	144.42	123.47
18	B	850	BCR	C21-C20-C19	10.21	155.09	123.22
18	B	852	BCR	C16-C15-C14	10.19	144.35	123.47
18	I	102	BCR	C11-C10-C9	10.18	141.84	127.31
18	1	503	BCR	C21-C20-C19	10.16	154.92	123.22
18	F	306	BCR	C11-C10-C9	10.08	141.69	127.31
19	B	803	CLA	C4A-NA-C1A	10.07	111.23	106.71
18	3	303	BCR	C21-C20-C19	9.93	154.22	123.22
18	A	852	BCR	C21-C20-C19	9.89	154.09	123.22
18	B	850	BCR	C11-C10-C9	9.78	141.26	127.31
19	B	804	CLA	C4A-NA-C1A	9.77	111.10	106.71
19	3	305	CLA	C4A-NA-C1A	9.72	111.08	106.71
19	4	318	CLA	C4A-NA-C1A	9.71	111.07	106.71
19	4	304	CLA	C4A-NA-C1A	9.69	111.06	106.71
18	J	1108	BCR	C16-C15-C14	9.65	143.25	123.47
19	2	508	CLA	C4A-NA-C1A	9.64	111.04	106.71
18	B	852	BCR	C20-C19-C18	9.60	153.39	126.42
19	A	803	CLA	C4A-NA-C1A	9.58	111.01	106.71
19	B	810	CLA	C4A-NA-C1A	9.57	111.01	106.71
19	2	506	CLA	C4A-NA-C1A	9.55	111.00	106.71
19	A	840	CLA	C4A-NA-C1A	9.54	110.99	106.71
19	B	824	CLA	C4A-NA-C1A	9.52	110.99	106.71
18	B	849	BCR	C16-C15-C14	9.51	142.96	123.47
18	B	851	BCR	C11-C10-C9	9.51	140.88	127.31
19	3	312	CLA	C4A-NA-C1A	9.51	110.98	106.71
19	3	315	CLA	C4A-NA-C1A	9.51	110.98	106.71
19	A	808	CLA	C4A-NA-C1A	9.50	110.97	106.71
19	H	1000	CLA	C4A-NA-C1A	9.48	110.97	106.71
19	4	309	CLA	C4A-NA-C1A	9.48	110.97	106.71
19	G	201	CLA	C4A-NA-C1A	9.44	110.95	106.71
19	A	802	CLA	C4A-NA-C1A	9.43	110.94	106.71
18	A	852	BCR	C20-C19-C18	9.42	152.88	126.42
19	A	810	CLA	C4A-NA-C1A	9.41	110.94	106.71
19	A	854	CLA	C4A-NA-C1A	9.40	110.93	106.71
19	J	1105	CLA	C4A-NA-C1A	9.40	110.93	106.71
18	B	853	BCR	C20-C19-C18	9.40	152.82	126.42
19	A	804	CLA	C4A-NA-C1A	9.40	110.93	106.71
19	B	806	CLA	C4A-NA-C1A	9.38	110.92	106.71
19	B	815	CLA	C4A-NA-C1A	9.38	110.92	106.71
19	B	825	CLA	C4A-NA-C1A	9.38	110.92	106.71
19	L	303	CLA	C4A-NA-C1A	9.37	110.92	106.71
19	2	514	CLA	C4A-NA-C1A	9.37	110.92	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	827	CLA	C4A-NA-C1A	9.37	110.92	106.71
18	B	852	BCR	C21-C20-C19	9.37	152.45	123.22
19	A	811	CLA	C4A-NA-C1A	9.36	110.92	106.71
17	J	1109	LUT	C21-C26-C27	9.34	124.51	112.70
19	4	315	CLA	C4A-NA-C1A	9.34	110.91	106.71
19	B	828	CLA	C4A-NA-C1A	9.34	110.91	106.71
19	J	1102	CLA	C4A-NA-C1A	9.34	110.90	106.71
18	I	101	BCR	C20-C19-C18	9.31	152.58	126.42
18	1	503	BCR	C20-C19-C18	9.30	152.53	126.42
19	2	510	CLA	C4A-NA-C1A	9.29	110.88	106.71
18	F	306	BCR	C20-C19-C18	9.26	152.43	126.42
19	A	820	CLA	C4A-NA-C1A	9.25	110.87	106.71
19	3	306	CLA	C4A-NA-C1A	9.24	110.86	106.71
19	4	311	CLA	C4A-NA-C1A	9.22	110.85	106.71
18	3	303	BCR	C20-C19-C18	9.20	152.25	126.42
19	A	842	CLA	C4A-NA-C1A	9.18	110.83	106.71
19	1	504	CLA	C4A-NA-C1A	9.17	110.83	106.71
19	4	308	CLA	C4A-NA-C1A	9.16	110.82	106.71
19	A	829	CLA	C4A-NA-C1A	9.15	110.82	106.71
19	2	511	CLA	C4A-NA-C1A	9.12	110.81	106.71
19	A	816	CLA	C4A-NA-C1A	9.12	110.81	106.71
19	3	316	CLA	C4A-NA-C1A	9.11	110.80	106.71
19	A	806	CLA	C4A-NA-C1A	9.11	110.80	106.71
19	B	822	CLA	C4A-NA-C1A	9.10	110.80	106.71
19	B	816	CLA	C4A-NA-C1A	9.08	110.79	106.71
19	1	505	CLA	C4A-NA-C1A	9.07	110.78	106.71
19	1	516	CLA	C4A-NA-C1A	9.06	110.78	106.71
19	1	506	CLA	C4A-NA-C1A	9.06	110.78	106.71
19	B	821	CLA	C4A-NA-C1A	9.06	110.78	106.71
18	J	1108	BCR	C11-C10-C9	9.03	140.20	127.31
19	A	841	CLA	C4A-NA-C1A	8.99	110.75	106.71
18	B	856	BCR	C20-C19-C18	8.97	151.60	126.42
19	3	313	CLA	C4A-NA-C1A	8.96	110.74	106.71
18	G	205	BCR	C11-C10-C9	8.93	140.06	127.31
19	A	825	CLA	C4A-NA-C1A	8.93	110.72	106.71
19	B	805	CLA	C4A-NA-C1A	8.93	110.72	106.71
19	A	813	CLA	C4A-NA-C1A	8.93	110.72	106.71
19	A	827	CLA	C4A-NA-C1A	8.92	110.72	106.71
19	A	809	CLA	C4A-NA-C1A	8.91	110.71	106.71
19	G	204	CLA	C4A-NA-C1A	8.90	110.71	106.71
19	K	1003	CLA	C4A-NA-C1A	8.89	110.70	106.71
18	A	852	BCR	C11-C10-C9	8.87	139.97	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	839	CLA	C4A-NA-C1A	8.87	110.69	106.71
18	L	302	BCR	C11-C10-C9	8.86	139.96	127.31
19	2	507	CLA	C4A-NA-C1A	8.83	110.68	106.71
19	1	508	CLA	C4A-NA-C1A	8.83	110.67	106.71
19	B	832	CLA	C4A-NA-C1A	8.83	110.67	106.71
18	A	851	BCR	C20-C19-C18	8.79	151.11	126.42
19	A	807	CLA	C4A-NA-C1A	8.78	110.65	106.71
19	L	305	CLA	C4A-NA-C1A	8.78	110.65	106.71
18	B	850	BCR	C20-C19-C18	8.77	151.05	126.42
19	K	1001	CLA	C4A-NA-C1A	8.77	110.65	106.71
19	B	814	CLA	C4A-NA-C1A	8.76	110.65	106.71
18	B	853	BCR	C21-C20-C19	8.76	150.57	123.22
19	B	840	CLA	C4A-NA-C1A	8.76	110.64	106.71
19	1	507	CLA	C4A-NA-C1A	8.75	110.64	106.71
19	J	1101	CLA	C4A-NA-C1A	8.75	110.64	106.71
19	A	812	CLA	C4A-NA-C1A	8.73	110.63	106.71
19	A	834	CLA	C4A-NA-C1A	8.72	110.63	106.71
19	A	832	CLA	C4A-NA-C1A	8.72	110.63	106.71
19	K	1002	CLA	C4A-NA-C1A	8.72	110.63	106.71
19	L	304	CLA	C4A-NA-C1A	8.72	110.63	106.71
19	B	807	CLA	C4A-NA-C1A	8.71	110.62	106.71
19	A	837	CLA	C4A-NA-C1A	8.71	110.62	106.71
19	G	203	CLA	C4A-NA-C1A	8.71	110.62	106.71
19	B	813	CLA	C4A-NA-C1A	8.69	110.61	106.71
19	F	302	CLA	C4A-NA-C1A	8.69	110.61	106.71
19	A	818	CLA	C4A-NA-C1A	8.68	110.61	106.71
19	F	303	CLA	C4A-NA-C1A	8.65	110.60	106.71
18	I	102	BCR	C20-C19-C18	8.65	150.71	126.42
18	L	306	BCR	C20-C19-C18	8.65	150.70	126.42
19	A	814	CLA	C4A-NA-C1A	8.63	110.59	106.71
19	A	831	CLA	C4A-NA-C1A	8.63	110.59	106.71
19	B	826	CLA	C4A-NA-C1A	8.62	110.58	106.71
19	G	202	CLA	C4A-NA-C1A	8.61	110.58	106.71
19	1	513	CLA	C4A-NA-C1A	8.60	110.57	106.71
19	B	833	CLA	C4A-NA-C1A	8.60	110.57	106.71
19	3	311	CLA	C4A-NA-C1A	8.59	110.57	106.71
19	A	815	CLA	C4A-NA-C1A	8.59	110.57	106.71
19	B	836	CLA	C4A-NA-C1A	8.58	110.56	106.71
19	A	855	CLA	C4A-NA-C1A	8.57	110.56	106.71
19	A	824	CLA	C4A-NA-C1A	8.56	110.56	106.71
19	A	838	CLA	C4A-NA-C1A	8.56	110.55	106.71
19	A	826	CLA	C4A-NA-C1A	8.55	110.55	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	831	CLA	C4A-NA-C1A	8.55	110.55	106.71
19	3	317	CLA	C4A-NA-C1A	8.55	110.55	106.71
19	B	823	CLA	C4A-NA-C1A	8.54	110.55	106.71
19	A	819	CLA	C4A-NA-C1A	8.54	110.54	106.71
19	4	305	CLA	C4A-NA-C1A	8.53	110.54	106.71
19	1	509	CLA	C4A-NA-C1A	8.52	110.54	106.71
19	A	836	CLA	C4A-NA-C1A	8.52	110.54	106.71
19	3	307	CLA	C4A-NA-C1A	8.51	110.53	106.71
19	3	309	CLA	C4A-NA-C1A	8.51	110.53	106.71
19	K	1004	CLA	C4A-NA-C1A	8.51	110.53	106.71
19	2	509	CLA	C4A-NA-C1A	8.50	110.53	106.71
19	B	809	CLA	C4A-NA-C1A	8.48	110.52	106.71
19	4	306	CLA	C4A-NA-C1A	8.48	110.52	106.71
19	2	505	CLA	C4A-NA-C1A	8.47	110.51	106.71
19	B	818	CLA	C4A-NA-C1A	8.47	110.51	106.71
19	A	835	CLA	C4A-NA-C1A	8.44	110.50	106.71
19	4	312	CLA	C4A-NA-C1A	8.42	110.49	106.71
19	A	817	CLA	C4A-NA-C1A	8.41	110.49	106.71
18	4	301	BCR	C20-C19-C18	8.39	149.98	126.42
19	4	310	CLA	C4A-NA-C1A	8.37	110.47	106.71
19	A	822	CLA	C4A-NA-C1A	8.37	110.47	106.71
19	A	830	CLA	C4A-NA-C1A	8.36	110.46	106.71
19	1	511	CLA	C4A-NA-C1A	8.34	110.45	106.71
19	A	821	CLA	C4A-NA-C1A	8.34	110.45	106.71
19	A	823	CLA	C4A-NA-C1A	8.33	110.45	106.71
19	B	839	CLA	C4A-NA-C1A	8.33	110.45	106.71
19	3	308	CLA	C4A-NA-C1A	8.30	110.44	106.71
19	B	834	CLA	C4A-NA-C1A	8.28	110.43	106.71
18	J	1108	BCR	C20-C19-C18	8.27	149.65	126.42
19	A	805	CLA	C4A-NA-C1A	8.27	110.42	106.71
19	4	307	CLA	C4A-NA-C1A	8.24	110.41	106.71
19	B	817	CLA	C4A-NA-C1A	8.24	110.41	106.71
19	B	837	CLA	C4A-NA-C1A	8.23	110.41	106.71
18	A	850	BCR	C11-C10-C9	8.19	139.00	127.31
19	B	820	CLA	C4A-NA-C1A	8.17	110.38	106.71
19	L	301	CLA	C4A-NA-C1A	8.16	110.37	106.71
19	B	808	CLA	C4A-NA-C1A	8.15	110.37	106.71
18	L	307	BCR	C20-C19-C18	8.14	149.29	126.42
19	B	835	CLA	C4A-NA-C1A	8.14	110.37	106.71
19	A	833	CLA	C4A-NA-C1A	8.13	110.36	106.71
18	B	849	BCR	C15-C14-C13	8.03	138.77	127.31
19	B	812	CLA	C4A-NA-C1A	8.02	110.31	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	819	CLA	C4A-NA-C1A	8.01	110.31	106.71
19	1	510	CLA	C4A-NA-C1A	7.96	110.28	106.71
19	1	515	CLA	C4A-NA-C1A	7.94	110.28	106.71
19	B	838	CLA	C4A-NA-C1A	7.93	110.27	106.71
23	4	303	XAT	C18-C5-C4	7.84	123.10	114.28
19	B	829	CLA	C4A-NA-C1A	7.84	110.23	106.71
19	B	830	CLA	C4A-NA-C1A	7.82	110.22	106.71
19	B	811	CLA	C4A-NA-C1A	7.59	110.12	106.71
18	B	802	BCR	C15-C14-C13	-7.54	116.55	127.31
18	A	848	BCR	C20-C19-C18	7.50	147.49	126.42
19	1	510	CLA	O2D-CGD-CBD	7.23	124.11	111.27
17	1	502	LUT	C21-C26-C27	7.15	121.73	112.70
18	K	1005	BCR	C20-C19-C18	7.07	146.28	126.42
18	B	849	BCR	C12-C13-C14	6.94	129.59	118.94
18	A	850	BCR	C20-C19-C18	6.89	145.77	126.42
19	1	510	CLA	O2D-CGD-O1D	-6.77	110.60	123.84
18	G	205	BCR	C20-C19-C18	6.77	145.43	126.42
18	B	851	BCR	C21-C20-C19	6.72	144.20	123.22
18	L	302	BCR	C20-C19-C18	6.70	145.23	126.42
19	4	304	CLA	O2A-C1-C2	6.60	125.97	108.64
26	4	319	DGD	C3G-O3G-C1D	-6.56	100.92	113.74
19	1	507	CLA	CMD-C2D-C1D	6.48	136.13	124.71
18	2	503	BCR	C20-C19-C18	6.44	144.50	126.42
20	4	314	CHL	C4D-CHA-C1A	6.36	128.99	121.25
19	4	308	CLA	O2A-C1-C2	6.34	125.31	108.64
18	A	849	BCR	C20-C19-C18	6.33	144.20	126.42
17	2	501	LUT	C21-C26-C25	6.23	122.57	111.42
19	K	1001	CLA	CMD-C2D-C1D	6.22	135.68	124.71
18	B	802	BCR	C20-C19-C18	6.16	143.71	126.42
17	1	501	LUT	C21-C26-C25	6.13	122.40	111.42
19	B	811	CLA	CMD-C2D-C1D	6.10	135.47	124.71
19	L	301	CLA	O2A-C1-C2	6.09	124.64	108.64
27	A	801	CL0	CMD-C2D-C1D	6.08	135.43	124.71
18	A	856	BCR	C20-C19-C18	6.06	143.44	126.42
19	4	307	CLA	CMD-C2D-C1D	5.99	135.27	124.71
17	3	301	LUT	C21-C26-C25	5.99	122.15	111.42
19	B	817	CLA	O2A-C1-C2	5.97	124.34	108.64
19	A	809	CLA	O2A-C1-C2	5.93	124.21	108.64
19	A	810	CLA	CMD-C2D-C1D	5.89	135.09	124.71
19	2	507	CLA	CMD-C2D-C1D	5.88	135.07	124.71
19	A	805	CLA	CMD-C2D-C1D	5.86	135.05	124.71
19	J	1102	CLA	CMD-C2D-C1D	5.86	135.03	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	J	1105	CLA	CMD-C2D-C1D	5.85	135.03	124.71
19	4	304	CLA	CMD-C2D-C1D	5.85	135.02	124.71
19	A	822	CLA	CMD-C2D-C1D	5.84	135.01	124.71
18	3	304	BCR	C20-C19-C18	5.84	142.81	126.42
19	B	833	CLA	CMD-C2D-C1D	5.83	135.00	124.71
19	B	838	CLA	CMD-C2D-C1D	5.81	134.96	124.71
19	A	808	CLA	CMD-C2D-C1D	5.81	134.94	124.71
19	2	507	CLA	O2A-C1-C2	5.81	123.89	108.64
19	1	506	CLA	O2A-C1-C2	5.80	123.88	108.64
18	B	849	BCR	C19-C18-C17	5.78	127.80	118.94
19	B	823	CLA	CMD-C2D-C1D	5.77	134.88	124.71
19	3	307	CLA	O2A-C1-C2	5.77	123.79	108.64
19	B	819	CLA	O2A-C1-C2	5.76	123.77	108.64
19	G	202	CLA	CMD-C2D-C1D	5.76	134.86	124.71
19	A	827	CLA	CMD-C2D-C1D	5.72	134.80	124.71
19	B	813	CLA	CMD-C2D-C1D	5.71	134.78	124.71
19	4	305	CLA	O2A-C1-C2	5.71	123.65	108.64
19	1	515	CLA	CMD-C2D-C1D	5.71	134.77	124.71
19	3	306	CLA	CMD-C2D-C1D	5.70	134.76	124.71
19	1	513	CLA	CMD-C2D-C1D	5.70	134.76	124.71
19	B	817	CLA	CMD-C2D-C1D	5.70	134.75	124.71
19	3	310	CLA	CMD-C2D-C1D	5.69	134.73	124.71
19	2	505	CLA	CMD-C2D-C1D	5.68	134.73	124.71
19	A	807	CLA	CMD-C2D-C1D	5.67	134.71	124.71
19	J	1105	CLA	CMA-C3A-C4A	5.67	127.01	111.77
19	3	309	CLA	CMD-C2D-C1D	5.66	134.68	124.71
19	G	203	CLA	CMD-C2D-C1D	5.65	134.68	124.71
19	1	511	CLA	CMD-C2D-C1D	5.65	134.67	124.71
19	A	804	CLA	CMD-C2D-C1D	5.65	134.66	124.71
19	3	307	CLA	CMD-C2D-C1D	5.65	134.66	124.71
19	B	808	CLA	CMD-C2D-C1D	5.64	134.66	124.71
19	B	838	CLA	O2A-C1-C2	5.64	123.47	108.64
19	A	816	CLA	CMD-C2D-C1D	5.64	134.66	124.71
19	B	819	CLA	CMD-C2D-C1D	5.64	134.65	124.71
19	B	814	CLA	CMD-C2D-C1D	5.63	134.64	124.71
19	J	1101	CLA	CMD-C2D-C1D	5.63	134.64	124.71
19	2	504	CLA	CMD-C2D-C1D	5.63	134.63	124.71
19	A	825	CLA	CMD-C2D-C1D	5.63	134.63	124.71
19	3	308	CLA	O2A-C1-C2	5.62	123.42	108.64
19	B	830	CLA	CMD-C2D-C1D	5.61	134.60	124.71
19	B	812	CLA	CMD-C2D-C1D	5.61	134.60	124.71
19	F	303	CLA	CMD-C2D-C1D	5.60	134.59	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	508	CLA	CMD-C2D-C1D	5.60	134.58	124.71
19	B	821	CLA	CMD-C2D-C1D	5.60	134.58	124.71
19	B	805	CLA	CMD-C2D-C1D	5.60	134.58	124.71
19	B	825	CLA	CMD-C2D-C1D	5.60	134.57	124.71
19	K	1002	CLA	CMD-C2D-C1D	5.59	134.56	124.71
19	A	838	CLA	CMD-C2D-C1D	5.59	134.56	124.71
19	3	311	CLA	CMD-C2D-C1D	5.58	134.55	124.71
19	4	305	CLA	CMD-C2D-C1D	5.58	134.54	124.71
19	A	842	CLA	CMD-C2D-C1D	5.57	134.54	124.71
19	A	835	CLA	CMD-C2D-C1D	5.57	134.53	124.71
19	A	814	CLA	CMD-C2D-C1D	5.56	134.52	124.71
19	B	839	CLA	CMD-C2D-C1D	5.56	134.51	124.71
18	B	849	BCR	C36-C18-C19	-5.56	109.32	118.08
19	G	204	CLA	CMD-C2D-C1D	5.56	134.51	124.71
19	4	312	CLA	CMD-C2D-C1D	5.56	134.50	124.71
19	1	516	CLA	CMD-C2D-C1D	5.55	134.50	124.71
19	H	1000	CLA	CMD-C2D-C1D	5.55	134.49	124.71
19	B	840	CLA	CMD-C2D-C1D	5.54	134.49	124.71
19	3	316	CLA	CMD-C2D-C1D	5.54	134.48	124.71
19	4	315	CLA	CMD-C2D-C1D	5.54	134.48	124.71
19	B	806	CLA	CMD-C2D-C1D	5.54	134.47	124.71
19	B	834	CLA	CMD-C2D-C1D	5.52	134.44	124.71
19	1	509	CLA	CMD-C2D-C1D	5.51	134.43	124.71
19	A	855	CLA	O2A-C1-C2	5.50	123.09	108.64
19	B	811	CLA	O2A-C1-C2	5.49	123.06	108.64
19	L	303	CLA	CMD-C2D-C1D	5.49	134.38	124.71
19	L	301	CLA	CMD-C2D-C1D	5.49	134.38	124.71
19	A	813	CLA	CMD-C2D-C1D	5.49	134.38	124.71
19	4	318	CLA	CMD-C2D-C1D	5.47	134.36	124.71
17	4	302	LUT	C21-C26-C27	5.47	119.62	112.70
19	A	832	CLA	CMD-C2D-C1D	5.47	134.36	124.71
19	B	818	CLA	CMD-C2D-C1D	5.47	134.35	124.71
19	3	313	CLA	CMD-C2D-C1D	5.47	134.35	124.71
19	A	819	CLA	CMD-C2D-C1D	5.47	134.35	124.71
19	G	201	CLA	CMD-C2D-C1D	5.47	134.35	124.71
19	B	824	CLA	CMD-C2D-C1D	5.46	134.33	124.71
19	B	836	CLA	CMD-C2D-C1D	5.45	134.32	124.71
19	1	508	CLA	O2A-C1-C2	5.45	122.95	108.64
19	3	312	CLA	CMD-C2D-C1D	5.45	134.31	124.71
19	4	309	CLA	CMD-C2D-C1D	5.44	134.31	124.71
20	4	314	CHL	C1B-CHB-C4A	-5.44	119.34	130.12
19	A	831	CLA	CMD-C2D-C1D	5.44	134.29	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	505	CLA	CMD-C2D-C1D	5.43	134.29	124.71
19	4	306	CLA	CMD-C2D-C1D	5.43	134.28	124.71
19	B	809	CLA	CMD-C2D-C1D	5.43	134.28	124.71
19	2	509	CLA	CMD-C2D-C1D	5.42	134.27	124.71
19	3	317	CLA	CMD-C2D-C1D	5.42	134.26	124.71
19	A	830	CLA	CMD-C2D-C1D	5.42	134.26	124.71
23	2	502	XAT	C18-C5-C4	5.42	120.37	114.28
19	A	836	CLA	CMD-C2D-C1D	5.41	134.25	124.71
19	B	807	CLA	O2A-C1-C2	5.41	122.86	108.64
19	A	815	CLA	CMD-C2D-C1D	5.41	134.25	124.71
19	B	807	CLA	CMD-C2D-C1D	5.41	134.25	124.71
19	B	837	CLA	CMD-C2D-C1D	5.39	134.22	124.71
19	B	837	CLA	O2A-C1-C2	5.39	122.81	108.64
19	1	509	CLA	O2A-C1-C2	5.39	122.80	108.64
19	3	308	CLA	CMD-C2D-C1D	5.39	134.21	124.71
19	B	835	CLA	CMD-C2D-C1D	5.39	134.21	124.71
19	A	834	CLA	O2A-C1-C2	5.38	122.78	108.64
19	1	504	CLA	CMD-C2D-C1D	5.38	134.19	124.71
19	L	305	CLA	CMD-C2D-C1D	5.37	134.18	124.71
19	1	508	CLA	CMD-C2D-C1D	5.37	134.18	124.71
19	A	824	CLA	CMD-C2D-C1D	5.37	134.17	124.71
19	B	810	CLA	O2A-C1-C2	5.37	122.74	108.64
19	A	833	CLA	CMD-C2D-C1D	5.36	134.16	124.71
19	L	304	CLA	CMD-C2D-C1D	5.35	134.14	124.71
19	B	827	CLA	CMD-C2D-C1D	5.35	134.14	124.71
19	4	308	CLA	CMD-C2D-C1D	5.34	134.13	124.71
19	A	829	CLA	CMD-C2D-C1D	5.34	134.12	124.71
17	4	302	LUT	C21-C26-C25	5.34	120.98	111.42
19	3	309	CLA	O2A-C1-C2	5.33	122.65	108.64
19	A	837	CLA	CMD-C2D-C1D	5.33	134.11	124.71
19	B	804	CLA	O2A-C1-C2	5.33	122.63	108.64
19	A	812	CLA	CMD-C2D-C1D	5.32	134.10	124.71
19	B	808	CLA	O2A-C1-C2	5.32	122.62	108.64
27	A	801	CL0	O2D-CGD-CBD	5.32	120.72	111.27
19	2	511	CLA	CMD-C2D-C1D	5.32	134.09	124.71
19	B	815	CLA	CMD-C2D-C1D	5.30	134.05	124.71
19	J	1101	CLA	O2A-C1-C2	5.29	122.53	108.64
19	A	834	CLA	CMD-C2D-C1D	5.28	134.02	124.71
19	B	826	CLA	CMD-C2D-C1D	5.28	134.02	124.71
19	A	821	CLA	CMD-C2D-C1D	5.28	134.01	124.71
19	4	310	CLA	CMD-C2D-C1D	5.27	134.00	124.71
23	4	303	XAT	C38-C25-C24	5.27	120.20	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	855	CLA	CMD-C2D-C1D	5.26	133.99	124.71
19	B	828	CLA	CMD-C2D-C1D	5.26	133.99	124.71
19	A	823	CLA	CMD-C2D-C1D	5.25	133.97	124.71
19	A	811	CLA	CMD-C2D-C1D	5.25	133.96	124.71
19	A	840	CLA	CMD-C2D-C1D	5.25	133.96	124.71
19	L	304	CLA	O2A-C1-C2	5.24	122.40	108.64
19	A	818	CLA	CMD-C2D-C1D	5.24	133.94	124.71
19	A	835	CLA	O2A-C1-C2	5.24	122.39	108.64
19	A	807	CLA	O2A-C1-C2	5.23	122.37	108.64
19	2	510	CLA	CMD-C2D-C1D	5.22	133.91	124.71
19	B	822	CLA	CMD-C2D-C1D	5.20	133.88	124.71
19	A	817	CLA	CMD-C2D-C1D	5.20	133.87	124.71
19	B	839	CLA	O2A-C1-C2	5.18	122.25	108.64
19	B	826	CLA	O2A-C1-C2	5.18	122.24	108.64
19	B	832	CLA	CMD-C2D-C1D	5.17	133.82	124.71
19	B	832	CLA	O2D-CGD-CBD	5.16	120.44	111.27
18	B	849	BCR	C35-C13-C14	-5.16	115.69	122.92
19	A	806	CLA	O2A-C1-C2	5.15	122.17	108.64
19	A	828	CLA	O2A-C1-C2	5.15	122.17	108.64
19	B	831	CLA	CMD-C2D-C1D	5.15	133.78	124.71
19	B	824	CLA	O2A-C1-C2	5.15	122.16	108.64
19	3	315	CLA	O2A-C1-C2	5.15	122.16	108.64
19	3	315	CLA	CMD-C2D-C1D	5.14	133.77	124.71
19	A	820	CLA	CMD-C2D-C1D	5.13	133.75	124.71
19	4	311	CLA	CMD-C2D-C1D	5.12	133.74	124.71
20	4	314	CHL	CHD-C1D-ND	-5.12	119.75	124.45
19	2	510	CLA	O2A-C1-C2	5.12	122.08	108.64
19	B	816	CLA	O2A-C1-C2	5.11	122.08	108.64
19	A	831	CLA	O2A-C1-C2	5.11	122.07	108.64
19	B	823	CLA	O2A-C1-C2	5.10	122.04	108.64
19	A	806	CLA	CMD-C2D-C1D	5.10	133.70	124.71
19	A	826	CLA	CMD-C2D-C1D	5.10	133.70	124.71
30	F	301	ZEX	C28-C27-C26	-5.10	118.38	127.09
19	A	817	CLA	O2A-C1-C2	5.09	122.02	108.64
19	H	1000	CLA	O2A-C1-C2	5.09	122.02	108.64
19	2	511	CLA	O2A-C1-C2	5.09	122.02	108.64
19	1	506	CLA	CMD-C2D-C1D	5.08	133.66	124.71
20	4	316	CHL	CHD-C1D-ND	-5.07	119.80	124.45
20	2	512	CHL	C4D-CHA-C1A	5.06	127.41	121.25
19	A	804	CLA	O2A-C1-C2	5.06	121.94	108.64
19	2	506	CLA	CMD-C2D-C1D	5.05	133.61	124.71
19	A	827	CLA	O2A-C1-C2	5.04	121.89	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	812	CLA	O2A-C1-C2	5.04	121.88	108.64
19	3	305	CLA	CMD-C2D-C1D	5.03	133.58	124.71
21	B	842	LHG	O7-C7-C8	5.02	120.33	111.09
19	B	829	CLA	CMD-C2D-C1D	5.02	133.57	124.71
19	A	818	CLA	O2A-C1-C2	5.02	121.83	108.64
19	4	310	CLA	O2A-C1-C2	5.02	121.83	108.64
19	A	811	CLA	O2A-C1-C2	5.00	121.77	108.64
19	A	824	CLA	O2A-C1-C2	4.99	121.74	108.64
19	1	507	CLA	O2A-C1-C2	4.98	121.73	108.64
20	2	512	CHL	C1B-CHB-C4A	-4.98	120.26	130.12
19	B	816	CLA	CMD-C2D-C1D	4.96	133.46	124.71
19	A	826	CLA	O2A-C1-C2	4.96	121.67	108.64
19	B	820	CLA	CMD-C2D-C1D	4.95	133.44	124.71
19	4	307	CLA	O2A-C1-C2	4.95	121.64	108.64
19	4	306	CLA	O2A-C1-C2	4.95	121.64	108.64
19	A	832	CLA	O2A-C1-C2	4.94	121.62	108.64
19	2	514	CLA	CMD-C2D-C1D	4.94	133.42	124.71
19	A	828	CLA	CMD-C2D-C1D	4.94	133.42	124.71
19	B	815	CLA	O2A-C1-C2	4.93	121.60	108.64
19	A	825	CLA	O2A-C1-C2	4.92	121.58	108.64
19	3	305	CLA	O2D-CGD-CBD	4.92	120.01	111.27
19	A	814	CLA	O2D-CGD-CBD	4.90	119.97	111.27
17	3	301	LUT	C21-C26-C27	4.88	118.88	112.70
19	1	504	CLA	O2A-C1-C2	4.87	121.43	108.64
19	A	805	CLA	O2A-C1-C2	4.87	121.42	108.64
19	F	302	CLA	CMD-C2D-C1D	4.86	133.28	124.71
19	2	508	CLA	O2A-C1-C2	4.86	121.41	108.64
19	A	836	CLA	O2A-C1-C2	4.86	121.41	108.64
19	B	805	CLA	O2A-C1-C2	4.84	121.36	108.64
19	2	506	CLA	O2A-C1-C2	4.84	121.35	108.64
19	A	809	CLA	CMD-C2D-C1D	4.83	133.23	124.71
19	3	305	CLA	O2A-C1-C2	4.82	121.30	108.64
19	B	810	CLA	CMD-C2D-C1D	4.82	133.20	124.71
19	2	505	CLA	O2A-C1-C2	4.80	121.25	108.64
19	K	1002	CLA	O2A-C1-C2	4.78	121.20	108.64
19	A	842	CLA	O2A-C1-C2	4.78	121.20	108.64
19	A	838	CLA	O2A-C1-C2	4.78	121.20	108.64
19	2	509	CLA	O2A-C1-C2	4.77	121.17	108.64
19	B	830	CLA	O2A-C1-C2	4.77	121.17	108.64
19	B	804	CLA	CMD-C2D-C1D	4.76	133.10	124.71
19	B	835	CLA	O2A-C1-C2	4.76	121.13	108.64
19	A	854	CLA	CMD-C2D-C1D	4.75	133.08	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	516	CLA	O2A-C1-C2	4.74	121.09	108.64
23	2	502	XAT	C38-C25-C24	4.74	119.61	114.28
20	4	317	CHL	CHD-C1D-ND	-4.74	120.10	124.45
19	B	814	CLA	O2A-C1-C2	4.73	121.07	108.64
19	B	828	CLA	O2A-C1-C2	4.72	121.05	108.64
19	G	202	CLA	O2A-C1-C2	4.72	121.05	108.64
19	A	814	CLA	O2A-C1-C2	4.72	121.04	108.64
19	A	810	CLA	O2A-C1-C2	4.71	121.03	108.64
21	1	520	LHG	O7-C7-C8	4.71	121.66	111.50
19	A	841	CLA	CMD-C2D-C1D	4.71	133.02	124.71
17	1	502	LUT	C21-C26-C25	4.71	119.86	111.42
19	A	822	CLA	O2A-C1-C2	4.71	121.01	108.64
19	B	812	CLA	O2A-C1-C2	4.70	120.98	108.64
19	F	303	CLA	O2A-C1-C2	4.69	120.96	108.64
19	2	514	CLA	O2A-C1-C2	4.67	120.92	108.64
19	A	819	CLA	O2A-C1-C2	4.67	120.92	108.64
19	A	808	CLA	O2A-C1-C2	4.66	120.89	108.64
19	A	803	CLA	O2A-C1-C2	4.65	120.87	108.64
30	F	301	ZEX	C15-C14-C13	-4.61	120.74	127.31
19	A	833	CLA	O2A-C1-C2	4.60	120.73	108.64
19	A	825	CLA	O2D-CGD-CBD	4.60	119.44	111.27
19	A	839	CLA	CMD-C2D-C1D	4.60	132.81	124.71
21	A	845	LHG	O7-C7-C8	4.59	121.39	111.50
19	A	830	CLA	O2D-CGD-CBD	4.59	119.42	111.27
19	A	833	CLA	O2D-CGD-CBD	4.58	119.41	111.27
19	A	820	CLA	O2A-C1-C2	4.57	120.66	108.64
19	B	803	CLA	CMD-C2D-C1D	4.57	132.77	124.71
19	4	315	CLA	O2A-C1-C2	4.57	120.64	108.64
18	I	101	BCR	C1-C6-C5	-4.57	116.18	122.61
20	3	314	CHL	CHD-C1D-ND	-4.56	120.26	124.45
18	1	503	BCR	C38-C26-C25	-4.56	119.41	124.53
22	B	845	LMG	O7-C10-C11	4.54	121.28	111.50
19	B	822	CLA	O2A-C1-C2	4.54	120.56	108.64
19	B	829	CLA	O2D-CGD-CBD	4.53	119.33	111.27
19	B	827	CLA	O2A-C1-C2	4.53	120.55	108.64
19	B	831	CLA	O2A-C1-C2	4.52	120.53	108.64
19	A	830	CLA	O2A-C1-C2	4.52	120.50	108.64
19	A	813	CLA	O2D-CGD-CBD	4.52	119.29	111.27
19	2	504	CLA	O2A-C1-C2	4.50	120.47	108.64
22	F	304	LMG	O7-C10-C11	4.47	121.13	111.50
17	2	501	LUT	C21-C26-C27	4.46	118.34	112.70
17	3	302	LUT	C21-C26-C27	4.46	118.34	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	G	207	DGD	O2G-C1B-C2B	4.46	121.11	111.50
19	1	513	CLA	O2A-C1-C2	4.46	120.34	108.64
23	4	303	XAT	O4-C5-C4	-4.45	110.04	113.38
22	G	206	LMG	O7-C10-C11	4.45	121.09	111.50
19	A	823	CLA	O2A-C1-C2	4.45	120.33	108.64
19	4	309	CLA	CMB-C2B-C1B	-4.45	121.63	128.46
19	B	815	CLA	O2D-CGD-CBD	4.42	119.11	111.27
19	B	833	CLA	O2A-C1-C2	4.39	120.19	108.64
30	F	301	ZEX	C7-C8-C9	-4.39	119.60	126.23
19	B	840	CLA	O2A-C1-C2	4.37	120.11	108.64
19	A	803	CLA	CMD-C2D-C1D	4.35	132.37	124.71
19	B	836	CLA	O2A-C1-C2	4.33	120.01	108.64
19	A	829	CLA	O2A-C1-C2	4.33	120.01	108.64
19	3	310	CLA	O2A-C1-C2	4.32	119.98	108.64
19	A	839	CLA	O2A-C1-C2	4.30	119.94	108.64
19	3	313	CLA	O2A-C1-C2	4.29	119.91	108.64
27	A	801	CL0	CHD-C1D-ND	-4.28	120.52	124.45
19	B	804	CLA	O2D-CGD-CBD	4.27	118.85	111.27
19	B	829	CLA	O2A-C1-C2	4.26	119.84	108.64
19	A	808	CLA	O2D-CGD-CBD	4.26	118.84	111.27
19	B	832	CLA	O2A-C1-C2	4.25	119.81	108.64
19	J	1101	CLA	CHD-C1D-ND	-4.24	120.56	124.45
19	A	837	CLA	O2A-C1-C2	4.23	119.75	108.64
19	J	1101	CLA	O2D-CGD-CBD	4.23	118.78	111.27
20	1	512	CHL	CHD-C1D-ND	-4.22	120.57	124.45
19	F	302	CLA	O2A-C1-C2	4.21	119.69	108.64
19	A	802	CLA	CMD-C2D-C1D	4.20	132.11	124.71
19	B	824	CLA	O2D-CGD-CBD	4.19	118.72	111.27
18	B	802	BCR	C35-C13-C14	-4.18	117.06	122.92
19	A	804	CLA	O2D-CGD-CBD	4.18	118.69	111.27
19	B	809	CLA	O2A-C1-C2	4.17	119.61	108.64
19	B	830	CLA	O2D-CGD-CBD	4.17	118.68	111.27
20	3	314	CHL	C4D-CHA-C1A	4.17	126.33	121.25
22	F	305	LMG	O7-C10-C11	4.16	120.47	111.50
27	A	801	CL0	O2A-C1-C2	4.16	119.56	108.64
19	2	507	CLA	O2D-CGD-CBD	4.15	118.64	111.27
19	B	820	CLA	O2A-C1-C2	4.14	119.51	108.64
20	2	526	CHL	CHD-C1D-ND	-4.13	120.66	124.45
19	2	511	CLA	O2D-CGD-CBD	4.13	118.60	111.27
19	L	303	CLA	O2A-C1-C2	4.12	119.46	108.64
19	1	504	CLA	O2D-CGD-CBD	4.12	118.59	111.27
19	4	318	CLA	O2A-C1-C2	4.10	119.42	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	1104	LMG	O7-C10-C11	4.10	120.34	111.50
18	B	849	BCR	C20-C19-C18	4.10	137.93	126.42
19	L	305	CLA	O2A-C1-C2	4.09	119.40	108.64
19	4	307	CLA	O2D-CGD-CBD	4.09	118.53	111.27
19	A	840	CLA	O2A-C1-C2	4.08	119.36	108.64
19	A	841	CLA	O2A-C1-C2	4.07	119.34	108.64
19	A	854	CLA	O2D-CGD-CBD	4.07	118.50	111.27
23	4	303	XAT	C7-C8-C9	-4.06	119.22	125.53
19	B	837	CLA	CHD-C1D-ND	-4.06	120.72	124.45
19	4	312	CLA	O2D-CGD-CBD	4.05	118.47	111.27
20	1	512	CHL	C4D-CHA-C1A	4.05	126.18	121.25
22	1	518	LMG	O7-C10-C11	4.04	120.21	111.50
19	3	308	CLA	O2D-CGD-CBD	4.04	118.45	111.27
30	F	301	ZEX	C31-C30-C29	-4.04	121.54	127.31
19	L	301	CLA	O2D-CGD-CBD	4.04	118.45	111.27
22	2	519	LMG	O7-C10-C11	4.04	120.20	111.50
18	3	304	BCR	C39-C30-C25	-4.02	103.78	110.30
18	A	852	BCR	C15-C14-C13	4.01	133.04	127.31
19	B	825	CLA	O2D-CGD-CBD	4.01	118.40	111.27
19	B	833	CLA	CHD-C1D-ND	-4.00	120.77	124.45
19	4	309	CLA	O2A-C1-C2	4.00	119.15	108.64
20	1	514	CHL	CHD-C1D-ND	-4.00	120.78	124.45
20	2	512	CHL	CMA-C3A-C4A	3.99	122.49	111.77
20	2	513	CHL	CHD-C1D-ND	-3.98	120.80	124.45
17	4	302	LUT	C22-C23-C24	-3.98	107.21	111.74
20	1	514	CHL	C3C-C4C-NC	-3.98	106.11	110.57
17	J	1109	LUT	C21-C26-C25	3.98	118.54	111.42
20	4	313	CHL	CHD-C1D-ND	-3.96	120.81	124.45
19	A	821	CLA	O2A-C1-C2	3.95	119.01	108.64
19	B	806	CLA	CHD-C1D-ND	-3.95	120.83	124.45
19	B	829	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
19	A	803	CLA	C2D-C1D-ND	3.93	113.00	110.10
19	B	818	CLA	O2D-CGD-CBD	3.93	118.25	111.27
18	B	849	BCR	C11-C12-C13	-3.93	115.38	126.42
20	4	317	CHL	C3C-C4C-NC	-3.93	106.17	110.57
19	B	819	CLA	CHD-C1D-ND	-3.92	120.85	124.45
19	B	807	CLA	CHD-C1D-ND	-3.92	120.85	124.45
18	L	306	BCR	C15-C14-C13	3.91	132.90	127.31
21	1	517	LHG	O7-C7-C8	3.91	119.93	111.50
21	B	843	LHG	O7-C7-C8	3.91	119.92	111.50
20	4	317	CHL	C4D-CHA-C1A	3.90	126.00	121.25
17	2	501	LUT	C7-C8-C9	-3.90	120.34	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	851	BCR	C38-C26-C25	-3.90	120.15	124.53
19	B	803	CLA	O2A-C1-C2	3.90	118.88	108.64
19	B	821	CLA	O2D-CGD-CBD	3.90	118.19	111.27
18	4	301	BCR	C38-C26-C25	-3.89	120.16	124.53
20	1	521	CHL	CHD-C1D-ND	-3.89	120.88	124.45
26	B	801	DGD	O2G-C1B-C2B	3.88	119.87	111.50
19	A	809	CLA	O2D-CGD-CBD	3.88	118.16	111.27
19	A	832	CLA	CHD-C1D-ND	-3.87	120.89	124.45
19	4	308	CLA	O2D-CGD-CBD	3.86	118.13	111.27
20	2	512	CHL	CHD-C1D-ND	-3.86	120.91	124.45
20	2	526	CHL	C3C-C4C-NC	-3.86	106.25	110.57
19	B	834	CLA	O2A-C1-C2	3.85	118.76	108.64
17	3	302	LUT	C21-C26-C25	3.84	118.30	111.42
20	4	316	CHL	C4D-CHA-C1A	3.84	125.92	121.25
19	1	510	CLA	CMD-C2D-C1D	3.84	131.47	124.71
19	A	814	CLA	CHD-C1D-ND	-3.82	120.94	124.45
20	2	516	CHL	CHD-C1D-ND	-3.82	120.94	124.45
19	A	802	CLA	C1-C2-C3	3.81	132.63	126.04
19	B	806	CLA	O2D-CGD-CBD	3.81	118.04	111.27
19	A	813	CLA	O2A-C1-C2	3.81	118.64	108.64
19	3	316	CLA	CHD-C1D-ND	-3.81	120.95	124.45
19	G	204	CLA	CHD-C1D-ND	-3.81	120.95	124.45
23	2	502	XAT	C18-C5-C6	-3.81	115.88	122.26
19	B	818	CLA	O2A-C1-C2	3.80	118.63	108.64
19	B	817	CLA	O2D-CGD-CBD	3.80	118.02	111.27
19	G	204	CLA	C2D-C1D-ND	3.80	112.90	110.10
19	4	311	CLA	CHD-C1D-ND	-3.80	120.97	124.45
19	B	813	CLA	O2D-CGD-CBD	3.80	118.01	111.27
19	A	813	CLA	CHD-C1D-ND	-3.79	120.97	124.45
19	A	822	CLA	CHD-C1D-ND	-3.79	120.97	124.45
19	B	836	CLA	CHD-C1D-ND	-3.79	120.97	124.45
19	A	805	CLA	O2D-CGD-CBD	3.78	117.99	111.27
21	2	517	LHG	O7-C7-C8	3.78	119.64	111.50
19	A	819	CLA	CHD-C1D-ND	-3.77	120.99	124.45
17	2	501	LUT	C22-C23-C24	-3.77	107.45	111.74
19	L	301	CLA	CHD-C1D-ND	-3.77	120.99	124.45
29	A	844	PQN	C14-C13-C15	3.77	121.61	115.27
17	4	302	LUT	C37-C21-C26	3.76	115.25	109.55
20	3	314	CHL	C3C-C4C-NC	-3.76	106.35	110.57
19	A	831	CLA	O2D-CGD-CBD	3.76	117.95	111.27
18	L	302	BCR	C40-C30-C25	-3.76	104.20	110.30
19	G	204	CLA	O2D-CGD-CBD	3.76	117.95	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	835	CLA	CHD-C1D-ND	-3.76	121.00	124.45
19	1	511	CLA	CHD-C1D-ND	-3.76	121.00	124.45
19	3	317	CLA	CHD-C1D-ND	-3.76	121.00	124.45
19	B	820	CLA	O2D-CGD-CBD	3.76	117.94	111.27
19	G	201	CLA	O2D-CGD-CBD	3.76	117.94	111.27
20	4	316	CHL	C1-O2A-CGA	3.76	126.30	116.44
19	3	309	CLA	O2D-CGD-CBD	3.75	117.94	111.27
19	B	825	CLA	O2A-C1-C2	3.75	118.50	108.64
19	2	506	CLA	O2D-CGD-CBD	3.75	117.93	111.27
19	3	313	CLA	O2D-CGD-CBD	3.75	117.92	111.27
19	B	823	CLA	CHD-C1D-ND	-3.75	121.01	124.45
19	A	826	CLA	O2D-CGD-CBD	3.74	117.92	111.27
20	2	515	CHL	CHD-C1D-ND	-3.74	121.02	124.45
17	1	501	LUT	C21-C26-C27	3.74	117.43	112.70
19	B	805	CLA	O2D-CGD-CBD	3.74	117.91	111.27
19	F	302	CLA	O2D-CGD-CBD	3.74	117.91	111.27
19	3	316	CLA	O2D-CGD-CBD	3.73	117.90	111.27
20	2	512	CHL	C1D-CHD-C4C	-3.73	118.02	126.06
19	B	809	CLA	O2D-CGD-CBD	3.72	117.89	111.27
19	3	312	CLA	O2A-C1-C2	3.71	122.04	109.49
19	L	304	CLA	C1D-ND-C4D	-3.71	103.70	106.33
19	4	312	CLA	CHD-C1D-ND	-3.71	121.05	124.45
19	B	816	CLA	O2D-CGD-CBD	3.70	117.84	111.27
18	B	802	BCR	C19-C18-C17	3.70	124.61	118.94
19	A	810	CLA	O2D-CGD-CBD	3.70	117.84	111.27
19	3	312	CLA	CHD-C1D-ND	-3.69	121.06	124.45
19	G	201	CLA	CHD-C1D-ND	-3.68	121.07	124.45
19	A	841	CLA	C2D-C1D-ND	3.68	112.82	110.10
19	F	302	CLA	C2D-C1D-ND	3.68	112.82	110.10
19	2	504	CLA	CHD-C1D-ND	-3.67	121.08	124.45
19	2	514	CLA	O2D-CGD-CBD	3.67	117.79	111.27
27	A	801	CL0	C1-C2-C3	-3.66	119.71	126.04
19	A	830	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
19	4	318	CLA	O2D-CGD-CBD	3.66	117.77	111.27
19	1	511	CLA	O2D-CGD-CBD	3.65	117.76	111.27
19	A	823	CLA	CHD-C1D-ND	-3.65	121.10	124.45
21	A	853	LHG	O7-C7-C8	3.65	119.37	111.50
19	2	505	CLA	CHD-C1D-ND	-3.65	121.10	124.45
22	B	844	LMG	O7-C10-C11	3.65	119.36	111.50
19	3	308	CLA	CHD-C1D-ND	-3.65	121.10	124.45
19	4	310	CLA	C2D-C1D-ND	3.64	112.79	110.10
17	1	501	LUT	C22-C23-C24	-3.64	107.60	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	512	CHL	C1B-CHB-C4A	-3.64	122.92	130.12
19	B	839	CLA	CHD-C1D-ND	-3.63	121.12	124.45
19	B	827	CLA	CHD-C1D-ND	-3.62	121.12	124.45
19	B	812	CLA	CHD-C1D-ND	-3.62	121.12	124.45
19	F	303	CLA	C1D-ND-C4D	-3.62	103.76	106.33
19	L	304	CLA	C2D-C1D-ND	3.62	112.77	110.10
19	3	307	CLA	C1D-ND-C4D	-3.62	103.77	106.33
19	B	814	CLA	CHD-C1D-ND	-3.62	121.13	124.45
19	G	203	CLA	O2D-CGD-CBD	3.61	117.69	111.27
22	J	1103	LMG	O7-C10-C11	3.61	119.27	111.50
19	3	307	CLA	C2D-C1D-ND	3.60	112.76	110.10
20	1	521	CHL	C3C-C4C-NC	-3.60	106.53	110.57
19	A	834	CLA	O2D-CGD-CBD	3.60	117.66	111.27
19	A	828	CLA	O2D-CGD-CBD	3.59	117.65	111.27
26	J	1106	DGD	O2G-C1B-C2B	3.59	119.24	111.50
22	A	847	LMG	O7-C10-C11	3.59	119.23	111.50
19	B	826	CLA	O2D-CGD-CBD	3.58	117.64	111.27
29	B	841	PQN	C11-C12-C13	-3.58	120.83	126.79
19	B	832	CLA	C2D-C1D-ND	3.58	112.74	110.10
19	4	311	CLA	O2D-CGD-CBD	3.58	117.63	111.27
19	A	825	CLA	CHD-C1D-ND	-3.57	121.17	124.45
19	4	305	CLA	O2D-CGD-CBD	3.57	117.62	111.27
19	A	840	CLA	O2D-CGD-CBD	3.57	117.60	111.27
19	A	829	CLA	O2D-CGD-CBD	3.56	117.60	111.27
19	B	828	CLA	CHD-C1D-ND	-3.56	121.18	124.45
18	4	301	BCR	C30-C25-C24	3.56	125.85	115.78
18	A	851	BCR	C40-C30-C25	-3.56	104.53	110.30
17	4	302	LUT	C7-C8-C9	-3.56	120.86	126.23
19	B	824	CLA	CHD-C1D-ND	-3.55	121.19	124.45
19	3	308	CLA	CMA-C3A-C4A	3.55	121.32	111.77
19	A	842	CLA	CHD-C1D-ND	-3.55	121.19	124.45
19	1	505	CLA	O2D-CGD-CBD	3.55	117.57	111.27
22	G	210	LMG	O7-C10-C11	3.55	120.69	110.80
19	J	1105	CLA	O2A-C1-C2	3.54	117.95	108.64
19	A	836	CLA	O2D-CGD-CBD	3.54	117.57	111.27
19	B	811	CLA	O2D-CGD-CBD	3.54	117.57	111.27
19	A	810	CLA	CHD-C1D-ND	-3.54	121.20	124.45
18	J	1108	BCR	C15-C14-C13	3.54	132.36	127.31
19	K	1001	CLA	CHD-C1D-ND	-3.54	121.20	124.45
19	3	306	CLA	O2A-C1-C2	3.53	117.92	108.64
19	A	805	CLA	CHD-C1D-ND	-3.53	121.21	124.45
19	L	304	CLA	O2D-CGD-CBD	3.53	117.54	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	507	CLA	CHD-C1D-ND	-3.53	121.21	124.45
19	3	306	CLA	CHD-C1D-ND	-3.53	121.21	124.45
26	B	801	DGD	O3G-C1D-C2D	3.53	113.81	108.30
19	G	202	CLA	CHD-C1D-ND	-3.53	121.21	124.45
19	K	1002	CLA	CHD-C1D-ND	-3.53	121.21	124.45
19	4	306	CLA	O2D-CGD-CBD	3.52	117.53	111.27
18	B	851	BCR	C20-C19-C18	3.52	136.31	126.42
22	2	518	LMG	O7-C10-C11	3.52	120.60	110.80
19	A	815	CLA	CHD-C1D-ND	-3.51	121.22	124.45
19	F	303	CLA	CHD-C1D-ND	-3.51	121.23	124.45
19	L	305	CLA	O2D-CGD-CBD	3.51	117.50	111.27
19	A	803	CLA	O2D-CGD-CBD	3.50	117.49	111.27
18	B	802	BCR	C12-C13-C14	3.50	124.31	118.94
19	A	806	CLA	CHD-C1D-ND	-3.50	121.24	124.45
19	A	841	CLA	O2D-CGD-CBD	3.50	117.49	111.27
18	B	802	BCR	C34-C9-C10	-3.50	118.02	122.92
19	B	833	CLA	O2D-CGD-CBD	3.50	117.48	111.27
19	B	817	CLA	CHD-C1D-ND	-3.50	121.24	124.45
19	A	836	CLA	CHD-C1D-ND	-3.49	121.25	124.45
20	1	512	CHL	CMA-C3A-C4A	3.49	121.15	111.77
19	1	507	CLA	O2D-CGD-CBD	3.49	117.47	111.27
20	2	516	CHL	C3C-C4C-NC	-3.49	106.66	110.57
19	L	303	CLA	O2D-CGD-CBD	3.49	117.46	111.27
17	3	301	LUT	C22-C23-C24	-3.48	107.78	111.74
19	3	317	CLA	O2D-CGD-CBD	3.47	117.44	111.27
19	A	803	CLA	CHD-C1D-ND	-3.47	121.26	124.45
19	3	312	CLA	O2D-CGD-CBD	3.47	117.44	111.27
18	2	503	BCR	C40-C30-C25	-3.47	104.67	110.30
19	3	310	CLA	CHD-C1D-ND	-3.47	121.27	124.45
19	4	318	CLA	CHD-C1D-ND	-3.47	121.27	124.45
19	4	307	CLA	CHD-C1D-ND	-3.47	121.27	124.45
19	B	814	CLA	O2D-CGD-CBD	3.47	117.43	111.27
19	B	808	CLA	CHD-C1D-ND	-3.47	121.27	124.45
19	A	838	CLA	O2D-CGD-CBD	3.47	117.43	111.27
21	1	517	LHG	C5-O7-C7	-3.46	109.26	117.79
19	J	1102	CLA	C2D-C1D-ND	3.46	112.66	110.10
19	K	1001	CLA	O2D-CGD-CBD	3.46	117.42	111.27
19	B	808	CLA	O2D-CGD-CBD	3.46	117.41	111.27
19	4	308	CLA	C2D-C1D-ND	3.46	112.65	110.10
19	J	1102	CLA	C1D-ND-C4D	-3.45	103.89	106.33
18	3	304	BCR	C30-C25-C24	3.45	125.53	115.78
19	J	1105	CLA	O2D-CGD-CBD	3.44	117.38	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	833	CLA	CHD-C1D-ND	-3.44	121.29	124.45
18	L	302	BCR	C19-C18-C17	3.44	124.22	118.94
17	1	502	LUT	C7-C8-C9	-3.44	121.04	126.23
19	2	505	CLA	O2D-CGD-CBD	3.43	117.37	111.27
19	J	1105	CLA	CAC-C3C-C2C	3.43	133.40	127.53
19	B	838	CLA	CHD-C1D-ND	-3.43	121.30	124.45
19	4	305	CLA	CHD-C1D-ND	-3.43	121.30	124.45
19	4	315	CLA	CHD-C1D-ND	-3.43	121.31	124.45
19	4	304	CLA	O2D-CGD-CBD	3.43	117.36	111.27
18	B	856	BCR	C2-C1-C6	3.42	115.75	110.48
19	A	818	CLA	CHD-C1D-ND	-3.42	121.31	124.45
19	L	303	CLA	CHD-C1D-ND	-3.42	121.31	124.45
19	2	504	CLA	O2D-CGD-CBD	3.41	117.33	111.27
19	G	202	CLA	O2D-CGD-CBD	3.41	117.32	111.27
19	B	819	CLA	O2D-CGD-CBD	3.41	117.32	111.27
19	1	509	CLA	O2D-CGD-CBD	3.41	117.32	111.27
19	4	306	CLA	CHD-C1D-ND	-3.41	121.32	124.45
22	G	210	LMG	O8-C28-C29	3.40	120.30	111.38
19	L	304	CLA	CHD-C1D-ND	-3.40	121.33	124.45
19	A	838	CLA	CHD-C1D-ND	-3.40	121.33	124.45
19	A	816	CLA	O2D-CGD-CBD	3.40	117.30	111.27
19	4	312	CLA	CAA-CBA-CGA	-3.40	103.33	113.25
19	A	807	CLA	O2D-CGD-CBD	3.40	117.30	111.27
19	A	831	CLA	CHD-C1D-ND	-3.39	121.34	124.45
19	B	831	CLA	C2D-C1D-ND	3.39	112.60	110.10
18	A	849	BCR	C15-C14-C13	3.39	132.15	127.31
19	A	841	CLA	CHD-C1D-ND	-3.39	121.34	124.45
19	B	838	CLA	C2D-C1D-ND	3.39	112.60	110.10
18	B	802	BCR	C36-C18-C19	-3.39	112.74	118.08
20	3	314	CHL	C1B-CHB-C4A	-3.39	123.41	130.12
19	G	203	CLA	CHD-C1D-ND	-3.38	121.34	124.45
19	A	813	CLA	C2D-C1D-ND	3.38	112.60	110.10
19	A	832	CLA	O2D-CGD-CBD	3.38	117.28	111.27
18	3	304	BCR	C30-C25-C26	-3.38	117.85	122.61
19	A	821	CLA	O2D-CGD-CBD	3.38	117.27	111.27
20	4	313	CHL	C3C-C4C-NC	-3.38	106.78	110.57
19	1	504	CLA	CHD-C1D-ND	-3.38	121.35	124.45
19	A	820	CLA	O2D-CGD-CBD	3.37	117.26	111.27
19	A	823	CLA	O2D-CGD-CBD	3.37	117.26	111.27
19	1	513	CLA	CHD-C1D-ND	-3.37	121.36	124.45
18	I	101	BCR	C40-C30-C25	-3.37	104.83	110.30
26	B	854	DGD	O2G-C1B-C2B	3.36	118.75	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	503	BCR	C8-C7-C6	3.36	136.65	127.20
22	4	322	LMG	O7-C10-C11	3.36	118.75	111.50
19	J	1102	CLA	CHD-C1D-ND	-3.36	121.37	124.45
19	B	835	CLA	CHD-C1D-ND	-3.36	121.37	124.45
22	2	518	LMG	O8-C28-C29	3.36	120.19	111.38
19	B	806	CLA	O2A-C1-C2	3.36	117.46	108.64
19	A	811	CLA	O2D-CGD-CBD	3.36	117.23	111.27
19	A	854	CLA	C2D-C1D-ND	3.35	112.58	110.10
19	A	817	CLA	O2D-CGD-CBD	3.35	117.22	111.27
20	4	314	CHL	CHD-C4C-C3C	3.35	129.76	124.84
19	4	315	CLA	O2D-CGD-CBD	3.35	117.22	111.27
19	B	832	CLA	C1D-ND-C4D	-3.35	103.96	106.33
19	B	819	CLA	O2A-CGA-CBA	3.35	122.41	111.91
19	B	839	CLA	O2D-CGD-CBD	3.34	117.21	111.27
19	1	506	CLA	C2D-C1D-ND	3.34	112.56	110.10
19	B	822	CLA	O2D-CGD-CBD	3.34	117.20	111.27
19	B	836	CLA	O2D-CGD-CBD	3.33	117.19	111.27
20	4	317	CHL	C1B-CHB-C4A	-3.33	123.53	130.12
19	B	838	CLA	C1D-ND-C4D	-3.33	103.97	106.33
19	A	804	CLA	CHD-C1D-ND	-3.32	121.40	124.45
20	2	513	CHL	C3C-C4C-NC	-3.32	106.85	110.57
19	4	312	CLA	O2A-C1-C2	3.32	117.36	108.64
19	A	828	CLA	CHD-C1D-ND	-3.32	121.40	124.45
19	A	829	CLA	CHD-C1D-ND	-3.32	121.41	124.45
19	2	510	CLA	O2D-CGD-CBD	3.32	117.16	111.27
19	A	837	CLA	O2D-CGD-CBD	3.32	117.16	111.27
19	A	821	CLA	CHD-C1D-ND	-3.32	121.41	124.45
19	4	318	CLA	C2D-C1D-ND	3.32	112.55	110.10
19	A	830	CLA	CHD-C1D-ND	-3.32	121.41	124.45
19	A	802	CLA	CHD-C1D-ND	-3.31	121.41	124.45
19	4	309	CLA	CAA-CBA-CGA	-3.31	103.57	113.25
19	4	309	CLA	CHD-C1D-ND	-3.31	121.41	124.45
19	A	819	CLA	O2D-CGD-CBD	3.31	117.14	111.27
19	A	802	CLA	O2D-CGD-CBD	3.31	117.14	111.27
19	B	834	CLA	C2D-C1D-ND	3.31	112.54	110.10
18	B	850	BCR	C40-C30-C25	-3.31	104.94	110.30
19	A	826	CLA	CHD-C1D-ND	-3.30	121.42	124.45
18	3	303	BCR	C38-C26-C25	-3.30	120.82	124.53
19	B	840	CLA	CHD-C1D-ND	-3.30	121.42	124.45
19	B	835	CLA	O2D-CGD-CBD	3.30	117.13	111.27
19	2	509	CLA	O2D-CGD-CBD	3.30	117.13	111.27
19	1	513	CLA	C2D-C1D-ND	3.30	112.53	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	309	CLA	O2D-CGD-CBD	3.30	117.13	111.27
19	B	835	CLA	C2D-C1D-ND	3.29	112.53	110.10
19	3	311	CLA	O2D-CGD-CBD	3.29	117.12	111.27
19	2	507	CLA	CHD-C1D-ND	-3.29	121.43	124.45
18	B	851	BCR	C38-C26-C25	-3.29	120.83	124.53
19	2	506	CLA	CMA-C3A-C4A	3.29	120.62	111.77
19	H	1000	CLA	CHD-C1D-ND	-3.29	121.43	124.45
19	3	305	CLA	O1D-CGD-CBD	-3.29	117.75	124.48
19	B	825	CLA	C2D-C1D-ND	3.29	112.53	110.10
19	3	307	CLA	CHD-C1D-ND	-3.29	121.43	124.45
19	3	308	CLA	O2A-CGA-CBA	3.29	122.22	111.91
26	4	319	DGD	O2G-C1B-C2B	3.29	118.58	111.50
19	A	826	CLA	C1D-ND-C4D	-3.28	104.00	106.33
29	B	841	PQN	C14-C13-C15	3.28	120.79	115.27
19	2	508	CLA	C2D-C1D-ND	3.28	112.52	110.10
19	3	309	CLA	CHD-C1D-ND	-3.28	121.44	124.45
19	A	841	CLA	C1D-ND-C4D	-3.28	104.01	106.33
19	A	812	CLA	O2D-CGD-CBD	3.27	117.08	111.27
20	1	514	CHL	C1-C2-C3	-3.27	120.39	126.04
19	3	315	CLA	O2D-CGD-CBD	3.27	117.07	111.27
19	1	513	CLA	O2D-CGD-CBD	3.26	117.07	111.27
19	F	303	CLA	C2D-C1D-ND	3.26	112.51	110.10
18	L	302	BCR	C36-C18-C19	-3.26	112.94	118.08
20	2	515	CHL	C3C-C4C-NC	-3.26	106.92	110.57
18	G	205	BCR	C19-C18-C17	3.26	123.94	118.94
20	4	314	CHL	C3C-C4C-NC	-3.26	106.92	110.57
19	B	823	CLA	C1D-ND-C4D	-3.25	104.02	106.33
19	F	302	CLA	CHD-C1D-ND	-3.25	121.46	124.45
19	3	306	CLA	O2D-CGD-CBD	3.25	117.05	111.27
20	4	314	CHL	C1D-CHD-C4C	-3.25	119.05	126.06
19	1	516	CLA	O2D-CGD-CBD	3.25	117.04	111.27
19	2	509	CLA	CHD-C1D-ND	-3.25	121.47	124.45
19	G	204	CLA	O2A-C1-C2	3.25	117.17	108.64
19	A	855	CLA	CHD-C1D-ND	-3.24	121.47	124.45
19	A	808	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
18	A	848	BCR	C40-C30-C25	-3.24	105.04	110.30
17	4	302	LUT	C38-C25-C24	-3.24	116.62	123.56
20	4	314	CHL	CMA-C3A-C4A	3.24	120.48	111.77
19	B	813	CLA	CHD-C1D-ND	-3.24	121.48	124.45
19	B	820	CLA	CHD-C1D-ND	-3.24	121.48	124.45
19	B	837	CLA	O2D-CGD-CBD	3.24	117.02	111.27
18	F	306	BCR	C40-C30-C25	-3.24	105.05	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	805	CLA	CHD-C1D-ND	-3.23	121.48	124.45
19	B	825	CLA	CHD-C1D-ND	-3.23	121.49	124.45
20	4	313	CHL	CMA-C3A-C4A	3.23	120.45	111.77
19	4	304	CLA	CHD-C1D-ND	-3.22	121.50	124.45
19	B	827	CLA	O2D-CGD-CBD	3.22	116.99	111.27
19	A	834	CLA	CHD-C1D-ND	-3.22	121.50	124.45
19	B	807	CLA	O2D-CGD-CBD	3.22	116.99	111.27
19	1	515	CLA	O2D-CGD-CBD	3.22	116.98	111.27
19	L	305	CLA	CHD-C1D-ND	-3.21	121.50	124.45
18	K	1005	BCR	C40-C30-C25	-3.21	105.09	110.30
19	A	837	CLA	C2D-C1D-ND	3.21	112.47	110.10
18	A	848	BCR	C15-C14-C13	3.21	131.89	127.31
19	K	1003	CLA	C1C-NC-C4C	-3.20	105.27	106.71
19	B	827	CLA	O2A-CGA-CBA	3.20	121.94	111.91
18	B	853	BCR	C39-C30-C25	-3.19	105.13	110.30
19	B	839	CLA	C2D-C1D-ND	3.19	112.45	110.10
19	A	818	CLA	O2D-CGD-CBD	3.19	116.93	111.27
19	B	831	CLA	O2D-CGD-CBD	3.18	116.92	111.27
19	A	820	CLA	CHD-C1D-ND	-3.18	121.53	124.45
18	B	853	BCR	C15-C14-C13	3.18	131.85	127.31
20	4	317	CHL	CMA-C3A-C4A	3.18	120.31	111.77
19	K	1002	CLA	O2D-CGD-CBD	3.18	116.91	111.27
19	H	1000	CLA	O2D-CGD-CBD	3.17	116.90	111.27
19	A	837	CLA	CHD-C1D-ND	-3.17	121.54	124.45
19	A	842	CLA	O2D-CGD-CBD	3.16	116.89	111.27
19	A	808	CLA	C2D-C1D-ND	3.16	112.44	110.10
19	4	310	CLA	C1D-ND-C4D	-3.16	104.09	106.33
19	G	204	CLA	C1D-ND-C4D	-3.16	104.09	106.33
19	A	812	CLA	CHD-C1D-ND	-3.16	121.55	124.45
19	G	201	CLA	O2A-C1-C2	3.16	116.94	108.64
18	A	850	BCR	C40-C30-C25	-3.16	105.18	110.30
19	A	817	CLA	CHD-C1D-ND	-3.16	121.55	124.45
19	B	811	CLA	CHD-C1D-ND	-3.16	121.55	124.45
19	B	821	CLA	CHD-C1D-ND	-3.15	121.56	124.45
19	1	516	CLA	CHD-C1D-ND	-3.15	121.56	124.45
19	A	842	CLA	C2D-C1D-ND	3.15	112.43	110.10
19	B	838	CLA	O2D-CGD-CBD	3.15	116.86	111.27
19	B	827	CLA	C2D-C1D-ND	3.15	112.42	110.10
19	3	313	CLA	CHD-C1D-ND	-3.14	121.56	124.45
19	B	828	CLA	O2D-CGD-CBD	3.14	116.85	111.27
18	B	802	BCR	C8-C9-C10	3.14	123.76	118.94
18	B	852	BCR	C40-C30-C25	-3.14	105.21	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	316	CHL	C1B-CHB-C4A	-3.14	123.90	130.12
19	2	508	CLA	CHD-C1D-ND	-3.13	121.57	124.45
20	1	514	CHL	C2C-C3C-C4C	3.13	108.72	106.49
19	B	834	CLA	O2D-CGD-CBD	3.13	116.83	111.27
19	A	855	CLA	C2D-C1D-ND	3.13	112.41	110.10
18	G	205	BCR	C36-C18-C19	-3.13	113.15	118.08
19	B	810	CLA	O2D-CGD-CBD	3.13	116.82	111.27
18	A	851	BCR	C2-C1-C6	3.13	115.29	110.48
19	B	840	CLA	C2D-C1D-ND	3.12	112.41	110.10
19	2	511	CLA	CHD-C1D-ND	-3.12	121.58	124.45
19	B	834	CLA	CHD-C1D-ND	-3.12	121.58	124.45
19	A	835	CLA	O2D-CGD-CBD	3.12	116.81	111.27
19	K	1003	CLA	CHD-C1D-ND	-3.12	121.50	124.52
19	B	830	CLA	CHD-C1D-ND	-3.11	121.59	124.45
19	K	1002	CLA	CMA-C3A-C4A	3.11	120.14	111.77
18	L	302	BCR	C38-C26-C25	-3.11	121.03	124.53
19	A	854	CLA	CHD-C1D-ND	-3.11	121.60	124.45
17	3	302	LUT	C15-C14-C13	3.10	131.74	127.31
18	L	307	BCR	C40-C30-C25	-3.10	105.27	110.30
20	4	316	CHL	CMA-C3A-C4A	3.10	120.11	111.77
19	G	201	CLA	CMA-C3A-C4A	3.10	120.11	111.77
18	A	856	BCR	C40-C30-C25	-3.10	105.27	110.30
19	A	855	CLA	C1D-ND-C4D	-3.10	104.13	106.33
19	A	822	CLA	O2D-CGD-CBD	3.10	116.77	111.27
19	A	839	CLA	CHD-C1D-ND	-3.09	121.61	124.45
19	B	829	CLA	CHD-C1D-ND	-3.09	121.61	124.45
20	2	512	CHL	C3A-C2A-C1A	3.09	105.97	101.34
18	B	851	BCR	C19-C18-C17	3.09	123.68	118.94
19	A	815	CLA	CMA-C3A-C4A	3.09	120.07	111.77
19	3	315	CLA	C2D-C1D-ND	3.09	112.38	110.10
19	A	829	CLA	C2D-C1D-ND	3.08	112.38	110.10
19	A	816	CLA	CMA-C3A-C4A	3.08	120.06	111.77
21	A	845	LHG	C5-O7-C7	-3.08	110.21	117.79
19	3	311	CLA	CMA-C3A-C4A	3.08	120.05	111.77
18	2	503	BCR	C38-C26-C25	-3.08	121.07	124.53
18	L	307	BCR	C38-C26-C25	-3.08	121.07	124.53
19	1	506	CLA	O2A-CGA-CBA	3.08	121.56	111.91
19	2	505	CLA	C2D-C1D-ND	3.08	112.37	110.10
19	A	824	CLA	C2D-C1D-ND	3.08	112.37	110.10
19	G	201	CLA	C2D-C1D-ND	3.07	112.37	110.10
19	3	305	CLA	CHD-C1D-ND	-3.07	121.63	124.45
19	2	508	CLA	C1D-ND-C4D	-3.07	104.15	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	507	CLA	CMA-C3A-C4A	3.07	120.02	111.77
17	1	502	LUT	C22-C23-C24	-3.07	108.25	111.74
18	B	856	BCR	C27-C26-C25	-3.07	118.28	122.73
19	4	308	CLA	CHD-C1D-ND	-3.07	121.64	124.45
19	A	816	CLA	CHD-C1D-ND	-3.07	121.64	124.45
21	B	842	LHG	C5-O7-C7	-3.07	112.18	117.90
19	4	311	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
19	2	506	CLA	C2D-C1D-ND	3.06	112.36	110.10
21	A	845	LHG	O8-C23-C24	3.06	121.51	111.91
19	4	308	CLA	C1D-ND-C4D	-3.06	104.16	106.33
19	2	514	CLA	CHD-C1D-ND	-3.06	121.64	124.45
19	B	825	CLA	C1D-ND-C4D	-3.05	104.17	106.33
19	A	827	CLA	O2D-CGD-CBD	3.05	116.69	111.27
19	1	509	CLA	CHD-C1D-ND	-3.05	121.65	124.45
19	B	815	CLA	CHD-C1D-ND	-3.05	121.65	124.45
19	B	816	CLA	CHD-C1D-ND	-3.05	121.65	124.45
19	1	505	CLA	C2D-C1D-ND	3.05	112.35	110.10
19	A	802	CLA	C2D-C1D-ND	3.05	112.35	110.10
19	1	505	CLA	CHD-C1D-ND	-3.05	121.65	124.45
19	1	508	CLA	O2D-CGD-CBD	3.05	116.68	111.27
23	2	502	XAT	C38-C25-C26	-3.05	117.16	122.26
19	A	833	CLA	C2D-C1D-ND	3.04	112.34	110.10
20	3	314	CHL	CMA-C3A-C4A	3.03	119.91	111.77
19	B	816	CLA	C2D-C1D-ND	3.03	112.34	110.10
19	B	804	CLA	CHD-C1D-ND	-3.03	121.67	124.45
19	B	823	CLA	O2D-CGD-CBD	3.03	116.64	111.27
19	B	812	CLA	C2D-C1D-ND	3.02	112.33	110.10
19	A	808	CLA	CHD-C1D-ND	-3.02	121.68	124.45
19	2	508	CLA	CBC-CAC-C3C	-3.02	104.10	112.43
18	L	307	BCR	C1-C6-C5	-3.02	118.36	122.61
18	L	306	BCR	C40-C30-C25	-3.02	105.41	110.30
19	A	809	CLA	C2D-C1D-ND	3.02	112.33	110.10
19	A	855	CLA	O2D-CGD-CBD	3.02	116.63	111.27
19	J	1105	CLA	C2D-C1D-ND	3.02	112.33	110.10
19	3	307	CLA	CMA-C3A-C4A	3.01	119.88	111.77
18	B	849	BCR	C38-C26-C25	-3.01	121.14	124.53
26	4	319	DGD	C3G-C2G-C1G	-3.01	104.66	111.79
19	A	807	CLA	CHD-C1D-ND	-3.01	121.69	124.45
19	2	504	CLA	C2D-C1D-ND	3.01	112.32	110.10
19	3	310	CLA	C2D-C1D-ND	3.01	112.32	110.10
19	B	824	CLA	CMA-C3A-C4A	3.01	119.86	111.77
19	1	513	CLA	CMA-C3A-C4A	3.01	119.86	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	501	LUT	C38-C25-C24	-3.01	117.12	123.56
19	2	508	CLA	O2D-CGD-CBD	3.01	116.61	111.27
19	A	828	CLA	C2D-C1D-ND	3.01	112.32	110.10
19	A	837	CLA	C1D-ND-C4D	-3.01	104.20	106.33
19	B	839	CLA	C1D-ND-C4D	-3.01	104.20	106.33
19	1	513	CLA	C1D-ND-C4D	-3.00	104.20	106.33
18	F	306	BCR	C38-C26-C25	-3.00	121.16	124.53
19	3	311	CLA	CHD-C1D-ND	-3.00	121.69	124.45
19	L	303	CLA	CMA-C3A-C4A	3.00	119.84	111.77
19	3	307	CLA	O2D-CGD-CBD	3.00	116.59	111.27
19	B	831	CLA	CHD-C1D-ND	-2.99	121.70	124.45
19	G	201	CLA	C1D-ND-C4D	-2.99	104.21	106.33
19	A	811	CLA	CHD-C1D-ND	-2.99	121.71	124.45
17	2	501	LUT	C38-C25-C24	-2.99	117.17	123.56
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	506	CLA	O2D-CGD-CBD	2.98	116.57	111.27
27	A	801	CL0	O2D-CGD-O1D	-2.98	118.00	123.84
18	I	102	BCR	C39-C30-C25	-2.98	105.46	110.30
19	3	305	CLA	C2D-C1D-ND	2.98	112.30	110.10
19	A	834	CLA	C1D-ND-C4D	-2.98	104.22	106.33
19	1	516	CLA	C2D-C1D-ND	2.98	112.30	110.10
19	3	310	CLA	O2D-CGD-CBD	2.98	116.56	111.27
19	G	202	CLA	C2D-C1D-ND	2.97	112.30	110.10
18	A	852	BCR	C39-C30-C25	-2.97	105.48	110.30
19	1	508	CLA	CHD-C1D-ND	-2.97	121.72	124.45
22	B	844	LMG	O8-C28-C29	2.97	121.23	111.91
19	F	302	CLA	C1D-ND-C4D	-2.97	104.22	106.33
19	A	827	CLA	C2D-C1D-ND	2.97	112.29	110.10
19	B	832	CLA	CHD-C1D-ND	-2.97	121.73	124.45
30	F	301	ZEX	C15-C35-C34	-2.97	117.40	123.47
19	3	305	CLA	C1D-ND-C4D	-2.97	104.23	106.33
19	A	813	CLA	C1D-ND-C4D	-2.97	104.23	106.33
23	2	502	XAT	C20-C13-C14	-2.96	118.77	122.92
18	B	849	BCR	C34-C9-C10	-2.96	118.77	122.92
19	K	1001	CLA	CMA-C3A-C4A	2.96	119.74	111.77
24	A	846	LMT	C1'-O5'-C5'	-2.96	107.87	113.69
19	A	818	CLA	C2D-C1D-ND	2.96	112.29	110.10
19	B	824	CLA	C2D-C1D-ND	2.96	112.29	110.10
18	B	851	BCR	C30-C25-C26	-2.96	118.45	122.61
19	B	810	CLA	C2D-C1D-ND	2.96	112.28	110.10
18	B	849	BCR	C30-C25-C26	-2.96	118.45	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	510	CLA	C2D-C1D-ND	2.96	112.28	110.10
20	4	313	CHL	C4D-CHA-C1A	2.95	124.84	121.25
20	2	516	CHL	CMA-C3A-C4A	2.95	119.71	111.77
19	A	824	CLA	CHD-C1D-ND	-2.95	121.74	124.45
18	B	802	BCR	C38-C26-C25	-2.95	121.21	124.53
19	J	1102	CLA	O2D-CGD-CBD	2.95	116.51	111.27
19	4	310	CLA	CMA-C3A-C4A	2.95	119.70	111.77
24	2	523	LMT	C1'-O5'-C5'	-2.95	107.90	113.69
19	B	813	CLA	CMA-C3A-C4A	2.95	119.69	111.77
19	B	834	CLA	C1D-ND-C4D	-2.95	104.24	106.33
20	2	516	CHL	C1-O2A-CGA	2.95	124.17	116.44
19	3	312	CLA	CMA-C3A-C4A	2.94	119.69	111.77
19	1	507	CLA	CMD-C2D-C3D	-2.94	120.84	127.61
19	A	819	CLA	CMA-C3A-C4A	2.94	119.69	111.77
19	B	835	CLA	C1D-ND-C4D	-2.94	104.24	106.33
19	A	836	CLA	CMA-C3A-C4A	2.94	119.68	111.77
19	B	826	CLA	C2D-C1D-ND	2.94	112.27	110.10
19	B	828	CLA	C1D-ND-C4D	-2.94	104.25	106.33
19	A	838	CLA	C2D-C1D-ND	2.94	112.27	110.10
20	1	512	CHL	C3C-C4C-NC	-2.94	107.28	110.57
18	B	856	BCR	C34-C9-C10	-2.94	118.81	122.92
19	A	823	CLA	C2D-C1D-ND	2.93	112.27	110.10
19	4	310	CLA	O2D-CGD-CBD	2.93	116.48	111.27
19	B	819	CLA	C1D-ND-C4D	-2.93	104.25	106.33
19	A	802	CLA	CMB-C2B-C3B	2.93	130.16	124.68
19	3	315	CLA	CHD-C1D-ND	-2.93	121.76	124.45
20	3	314	CHL	C2C-C3C-C4C	2.93	108.58	106.49
18	I	102	BCR	C40-C30-C25	-2.93	105.55	110.30
19	3	309	CLA	CMA-C3A-C4A	2.93	119.64	111.77
19	L	305	CLA	C2D-C1D-ND	2.92	112.26	110.10
19	4	310	CLA	CHD-C1D-ND	-2.92	121.77	124.45
19	A	827	CLA	CHD-C1D-ND	-2.92	121.77	124.45
19	A	826	CLA	C2D-C1D-ND	2.92	112.26	110.10
19	A	835	CLA	CMA-C3A-C4A	2.92	119.62	111.77
19	A	834	CLA	C2D-C1D-ND	2.92	112.25	110.10
20	2	516	CHL	C1-C2-C3	-2.92	121.00	126.04
19	A	823	CLA	CMA-C3A-C4A	2.92	119.61	111.77
19	B	812	CLA	O2D-CGD-CBD	2.92	116.45	111.27
20	2	526	CHL	C2C-C3C-C4C	2.91	108.56	106.49
19	3	317	CLA	C2D-C1D-ND	2.90	112.24	110.10
19	A	822	CLA	C2D-C1D-ND	2.90	112.24	110.10
19	F	303	CLA	O2D-CGD-CBD	2.90	116.43	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	816	CLA	CMA-C3A-C4A	2.90	119.58	111.77
22	B	845	LMG	O8-C28-C29	2.90	121.02	111.91
22	J	1103	LMG	O8-C28-C29	2.90	118.99	111.38
18	B	849	BCR	C8-C9-C10	2.90	123.39	118.94
17	3	301	LUT	C38-C25-C24	-2.89	117.36	123.56
20	1	514	CHL	C1B-CHB-C4A	-2.89	124.39	130.12
19	B	830	CLA	C1D-ND-C4D	-2.89	104.28	106.33
18	I	101	BCR	C38-C26-C25	-2.89	121.28	124.53
21	B	843	LHG	O8-C23-C24	2.89	120.98	111.91
18	B	851	BCR	C36-C18-C19	-2.88	113.53	118.08
19	3	311	CLA	C2D-C1D-ND	2.88	112.23	110.10
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
17	3	301	LUT	C7-C8-C9	-2.88	121.89	126.23
19	4	312	CLA	CMA-C3A-C4A	2.88	119.50	111.77
18	B	853	BCR	C34-C9-C10	-2.88	118.89	122.92
19	B	818	CLA	CHD-C1D-ND	-2.88	121.81	124.45
18	I	101	BCR	C1-C6-C7	2.88	123.91	115.78
19	B	828	CLA	C2D-C1D-ND	2.87	112.22	110.10
19	K	1001	CLA	C2D-C1D-ND	2.87	112.22	110.10
18	B	849	BCR	C30-C25-C24	2.87	123.90	115.78
20	4	317	CHL	C2C-C3C-C4C	2.87	108.54	106.49
24	J	1107	LMT	C3'-C4'-C5'	-2.87	104.34	110.93
19	J	1102	CLA	CMB-C2B-C1B	-2.87	124.05	128.46
18	B	851	BCR	C40-C30-C39	-2.87	99.72	108.53
18	1	503	BCR	C40-C30-C25	-2.87	105.65	110.30
22	F	305	LMG	O8-C28-C29	2.87	120.91	111.91
19	A	815	CLA	O2D-CGD-CBD	2.87	116.36	111.27
19	3	306	CLA	O2A-CGA-CBA	2.87	120.90	111.91
19	B	824	CLA	C1-O2A-CGA	2.87	123.96	116.44
19	1	510	CLA	CAA-CBA-CGA	-2.86	104.88	113.25
19	L	303	CLA	C1D-ND-C4D	-2.86	104.30	106.33
26	B	854	DGD	O1G-C1A-C2A	2.86	120.89	111.91
18	4	301	BCR	C24-C25-C26	-2.86	114.54	121.46
19	4	306	CLA	CMB-C2B-C1B	-2.86	124.07	128.46
19	A	809	CLA	CHD-C1D-ND	-2.86	121.83	124.45
20	2	512	CHL	C3C-C4C-NC	-2.86	107.37	110.57
19	4	306	CLA	C2D-C1D-ND	2.86	112.21	110.10
19	B	812	CLA	CMA-C3A-C4A	2.85	119.44	111.77
19	2	506	CLA	O2A-CGA-CBA	2.85	120.86	111.91
18	I	102	BCR	C38-C26-C25	-2.85	121.33	124.53
19	4	304	CLA	O2A-CGA-CBA	2.85	120.86	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	817	CLA	O2A-CGA-CBA	2.85	120.85	111.91
19	1	504	CLA	CMA-C3A-C4A	2.85	119.43	111.77
19	4	304	CLA	C2D-C1D-ND	2.85	112.20	110.10
19	B	807	CLA	C2D-C1D-ND	2.85	112.20	110.10
19	A	842	CLA	C1D-ND-C4D	-2.85	104.31	106.33
19	A	825	CLA	CAC-C3C-C4C	2.85	128.50	124.81
19	B	819	CLA	C2D-C1D-ND	2.84	112.20	110.10
19	A	803	CLA	C1D-ND-C4D	-2.84	104.31	106.33
19	A	806	CLA	C2D-C1D-ND	2.84	112.20	110.10
19	A	817	CLA	C2D-C1D-ND	2.84	112.20	110.10
19	A	824	CLA	O2D-CGD-CBD	2.84	116.32	111.27
19	B	827	CLA	C1D-ND-C4D	-2.84	104.32	106.33
19	G	204	CLA	CMA-C3A-C4A	2.84	119.39	111.77
19	A	840	CLA	C2D-C1D-ND	2.83	112.19	110.10
19	B	822	CLA	CMA-C3A-C4A	2.83	119.39	111.77
18	B	852	BCR	C15-C14-C13	2.83	131.35	127.31
19	B	810	CLA	CHD-C1D-ND	-2.83	121.85	124.45
19	K	1004	CLA	C3B-C4B-NB	-2.83	107.62	110.11
18	K	1005	BCR	C1-C6-C5	-2.83	118.63	122.61
19	1	506	CLA	C1D-ND-C4D	-2.83	104.33	106.33
19	B	840	CLA	C1D-ND-C4D	-2.83	104.33	106.33
24	3	318	LMT	C3B-C4B-C5B	-2.83	105.19	110.24
18	I	101	BCR	C35-C13-C14	-2.83	118.96	122.92
20	1	521	CHL	C2C-C3C-C4C	2.83	108.50	106.49
19	F	302	CLA	CMB-C2B-C3B	2.83	129.96	124.68
19	B	836	CLA	C2D-C1D-ND	2.83	112.19	110.10
18	3	303	BCR	C40-C30-C25	-2.82	105.72	110.30
20	1	514	CHL	CHD-C4C-C3C	2.82	128.99	124.84
19	B	826	CLA	OBD-CAD-C3D	-2.82	121.73	128.52
20	2	515	CHL	CMA-C3A-C4A	2.82	119.35	111.77
19	1	505	CLA	CMA-C3A-C4A	2.82	119.34	111.77
19	1	509	CLA	C2D-C1D-ND	2.82	112.18	110.10
19	L	301	CLA	C2D-C1D-ND	2.82	112.18	110.10
18	B	856	BCR	C40-C30-C25	-2.82	105.73	110.30
19	K	1003	CLA	C3B-C4B-NB	-2.81	107.64	110.11
18	A	850	BCR	C34-C9-C10	-2.81	118.98	122.92
19	4	309	CLA	C2D-C1D-ND	2.81	112.18	110.10
19	J	1105	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
19	4	307	CLA	O2A-CGA-CBA	2.81	120.71	111.91
17	3	302	LUT	C7-C8-C9	-2.81	122.00	126.23
17	1	501	LUT	C7-C8-C9	-2.80	122.00	126.23
19	A	811	CLA	C2D-C1D-ND	2.80	112.17	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	825	CLA	CMA-C3A-C4A	2.80	119.30	111.77
19	4	309	CLA	C1D-ND-C4D	-2.80	104.34	106.33
18	A	850	BCR	C39-C30-C25	-2.80	105.76	110.30
19	B	830	CLA	CMB-C2B-C3B	2.80	129.91	124.68
19	3	315	CLA	C1D-ND-C4D	-2.80	104.35	106.33
22	F	304	LMG	O8-C28-C29	2.80	120.69	111.91
18	B	850	BCR	C15-C14-C13	2.80	131.30	127.31
19	4	307	CLA	CMB-C2B-C1B	-2.80	124.17	128.46
20	2	512	CHL	CHD-C4C-C3C	2.79	128.94	124.84
19	J	1105	CLA	CHD-C1D-ND	-2.79	121.89	124.45
19	A	822	CLA	CMA-C3A-C4A	2.79	119.27	111.77
19	4	318	CLA	C1D-ND-C4D	-2.79	104.36	106.33
19	1	506	CLA	CHD-C1D-ND	-2.78	121.90	124.45
18	A	856	BCR	C34-C9-C10	-2.78	119.03	122.92
19	1	504	CLA	C2D-C1D-ND	2.78	112.15	110.10
19	B	808	CLA	C2D-C1D-ND	2.78	112.15	110.10
19	B	812	CLA	C1D-ND-C4D	-2.78	104.36	106.33
18	4	301	BCR	C23-C24-C25	2.78	135.01	127.20
18	A	851	BCR	C15-C14-C13	2.78	131.28	127.31
24	A	846	LMT	C3'-C4'-C5'	-2.78	104.56	110.93
19	A	821	CLA	CMB-C2B-C3B	2.78	129.88	124.68
19	A	839	CLA	C2D-C1D-ND	2.78	112.15	110.10
24	J	1107	LMT	C1'-O5'-C5'	-2.77	108.25	113.69
19	G	202	CLA	C1D-ND-C4D	-2.77	104.37	106.33
19	4	305	CLA	O2A-CGA-CBA	2.77	120.60	111.91
19	A	830	CLA	C2D-C1D-ND	2.77	112.14	110.10
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	809	CLA	CHD-C1D-ND	-2.77	121.91	124.45
20	4	314	CHL	C1-C2-C3	-2.76	122.28	126.75
20	1	521	CHL	CMA-C3A-C4A	2.76	119.20	111.77
19	1	510	CLA	CMA-C3A-C4A	2.76	119.20	111.77
19	J	1105	CLA	C1D-ND-C4D	-2.76	104.37	106.33
18	A	856	BCR	C30-C25-C26	-2.76	118.72	122.61
18	A	850	BCR	C15-C14-C13	-2.76	123.37	127.31
18	B	852	BCR	C35-C13-C12	2.76	122.43	118.08
18	L	307	BCR	C34-C9-C10	-2.76	119.06	122.92
19	1	505	CLA	C1D-ND-C4D	-2.76	104.38	106.33
27	A	801	CL0	CMB-C2B-C3B	2.76	129.84	124.68
23	2	502	XAT	C39-C29-C30	-2.75	119.06	122.92
19	A	840	CLA	CHD-C1D-ND	-2.75	121.92	124.45
19	2	506	CLA	CHD-C1D-ND	-2.75	121.92	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	317	CHL	CHD-C4C-C3C	2.75	128.88	124.84
18	I	102	BCR	C34-C9-C10	-2.75	119.07	122.92
19	A	810	CLA	C2D-C1D-ND	2.75	112.13	110.10
19	2	507	CLA	C2D-C1D-ND	2.75	112.13	110.10
19	A	836	CLA	C1D-ND-C4D	-2.75	104.38	106.33
19	A	855	CLA	CMA-C3A-C4A	2.75	119.16	111.77
19	L	301	CLA	O2A-CGA-CBA	2.75	120.53	111.91
19	A	837	CLA	CMA-C3A-C4A	2.75	119.15	111.77
19	A	855	CLA	CAC-C3C-C4C	2.75	128.37	124.81
19	4	307	CLA	C1D-ND-C4D	-2.74	104.39	106.33
19	B	824	CLA	CMB-C2B-C3B	2.74	129.81	124.68
19	A	854	CLA	C1D-ND-C4D	-2.74	104.39	106.33
18	B	851	BCR	C23-C24-C25	-2.74	119.50	127.20
20	4	316	CHL	C3C-C4C-NC	-2.74	107.50	110.57
19	B	809	CLA	C1D-ND-C4D	-2.73	104.39	106.33
19	L	305	CLA	CMA-C3A-C4A	2.73	119.12	111.77
19	A	807	CLA	CMA-C3A-C4A	2.73	119.11	111.77
19	A	816	CLA	C2D-C1D-ND	2.73	112.11	110.10
19	B	811	CLA	CMD-C2D-C3D	-2.73	121.34	127.61
19	2	511	CLA	C2D-C1D-ND	2.73	112.11	110.10
19	A	806	CLA	O2A-CGA-CBA	2.73	120.46	111.91
19	B	803	CLA	O2D-CGD-CBD	2.72	116.11	111.27
20	2	512	CHL	CHC-C1C-NC	2.72	128.34	124.20
19	B	817	CLA	C1D-ND-C4D	-2.72	104.40	106.33
19	1	509	CLA	C1D-ND-C4D	-2.72	104.40	106.33
19	A	815	CLA	C2D-C1D-ND	2.72	112.11	110.10
20	2	526	CHL	CMA-C3A-C4A	2.72	119.08	111.77
19	2	508	CLA	CMA-C3A-C4A	2.72	119.08	111.77
19	B	811	CLA	C1D-ND-C4D	-2.72	104.41	106.33
19	A	825	CLA	CMB-C2B-C3B	2.72	129.76	124.68
19	B	804	CLA	C2D-C1D-ND	2.71	112.10	110.10
19	A	811	CLA	CMA-C3A-C4A	2.71	119.05	111.77
19	B	822	CLA	C2D-C1D-ND	2.71	112.10	110.10
19	J	1101	CLA	CMB-C2B-C1B	-2.71	124.30	128.46
19	B	808	CLA	CMA-C3A-C4A	2.71	119.05	111.77
18	A	849	BCR	C40-C30-C25	-2.71	105.91	110.30
19	4	315	CLA	C2D-C1D-ND	2.71	112.10	110.10
19	A	840	CLA	C1D-ND-C4D	-2.71	104.41	106.33
27	A	801	CL0	O2A-CGA-CBA	2.70	120.39	111.91
19	A	812	CLA	C2D-C1D-ND	2.70	112.10	110.10
19	A	829	CLA	C1D-ND-C4D	-2.70	104.41	106.33
20	2	516	CHL	C2C-C3C-C4C	2.70	108.42	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	822	CLA	C1D-ND-C4D	-2.70	104.42	106.33
20	2	526	CHL	C1-O2A-CGA	2.70	123.53	116.44
19	1	510	CLA	CAC-C3C-C4C	2.70	128.31	124.81
19	B	804	CLA	CAC-C3C-C4C	2.70	128.31	124.81
19	A	836	CLA	C2D-C1D-ND	2.70	112.09	110.10
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
24	B	846	LMT	C3'-C4'-C5'	-2.69	104.75	110.93
18	G	205	BCR	C38-C26-C25	-2.69	121.50	124.53
27	A	801	CL0	C2D-C1D-ND	2.69	112.09	110.10
19	B	822	CLA	CHD-C1D-ND	-2.69	121.98	124.45
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
22	2	519	LMG	O8-C28-C29	2.69	120.34	111.91
19	1	508	CLA	CAC-C3C-C4C	2.69	128.29	124.81
19	J	1101	CLA	CMB-C2B-C3B	2.69	129.70	124.68
19	1	510	CLA	CHD-C1D-ND	-2.68	121.99	124.45
19	A	839	CLA	O2D-CGD-CBD	2.68	116.04	111.27
18	A	849	BCR	C35-C13-C12	2.68	122.31	118.08
19	A	806	CLA	CAA-C2A-C3A	-2.68	105.43	112.78
19	A	820	CLA	C2D-C1D-ND	2.68	112.08	110.10
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
19	A	835	CLA	C2D-C1D-ND	2.68	112.08	110.10
19	2	511	CLA	CMA-C3A-C4A	2.68	118.97	111.77
18	A	848	BCR	C35-C13-C12	2.68	122.29	118.08
24	3	318	LMT	O1'-C1'-C2'	2.67	112.48	108.30
19	1	515	CLA	CHD-C1D-ND	-2.67	122.00	124.45
19	L	303	CLA	C2D-C1D-ND	2.67	112.07	110.10
19	4	304	CLA	OBD-CAD-C3D	-2.67	122.09	128.52
18	A	849	BCR	C34-C9-C10	-2.67	119.18	122.92
19	B	826	CLA	CHA-C4D-ND	2.67	138.09	132.50
19	4	305	CLA	CMA-C3A-C4A	2.67	118.95	111.77
26	J	1106	DGD	O1G-C1A-C2A	2.67	120.28	111.91
19	2	509	CLA	C1D-ND-C4D	-2.67	104.44	106.33
19	A	824	CLA	C1D-ND-C4D	-2.67	104.44	106.33
17	1	502	LUT	C38-C25-C24	-2.67	117.85	123.56
17	4	302	LUT	C31-C32-C33	-2.67	118.92	126.42
30	F	301	ZEX	C27-C26-C25	-2.67	118.53	122.84
30	F	301	ZEX	C27-C28-C29	-2.67	122.21	126.23
19	K	1002	CLA	O2A-CGA-CBA	2.66	120.26	111.91
19	1	507	CLA	C1D-ND-C4D	-2.66	104.44	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	G	203	CLA	CMB-C2B-C3B	2.66	129.65	124.68
19	A	809	CLA	C1-O2A-CGA	2.66	123.42	116.44
19	B	804	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
17	1	501	LUT	C31-C32-C33	-2.66	118.95	126.42
19	A	831	CLA	C2D-C1D-ND	2.66	112.06	110.10
18	A	856	BCR	C27-C26-C25	-2.66	118.87	122.73
17	3	302	LUT	C11-C10-C9	2.66	131.10	127.31
19	3	313	CLA	O2A-CGA-CBA	2.66	120.24	111.91
19	A	818	CLA	CMA-C3A-C4A	2.66	118.91	111.77
18	3	303	BCR	C34-C9-C10	-2.65	119.21	122.92
19	4	307	CLA	CMB-C2B-C3B	2.65	129.64	124.68
17	3	302	LUT	C38-C25-C24	-2.65	117.89	123.56
19	2	509	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
19	B	819	CLA	CAA-C2A-C1A	-2.65	103.30	111.97
18	4	301	BCR	C34-C9-C10	-2.65	119.22	122.92
19	B	823	CLA	C2D-C1D-ND	2.64	112.05	110.10
19	3	315	CLA	CMB-C2B-C3B	2.64	129.62	124.68
18	A	849	BCR	C39-C30-C25	-2.64	106.01	110.30
17	4	302	LUT	C39-C29-C30	-2.64	119.22	122.92
19	1	516	CLA	C1D-ND-C4D	-2.64	104.46	106.33
19	B	825	CLA	CMB-C2B-C1B	-2.64	124.41	128.46
23	2	502	XAT	O24-C25-C24	2.64	115.36	113.38
19	K	1002	CLA	C2D-C1D-ND	2.64	112.05	110.10
18	I	101	BCR	C31-C1-C6	-2.64	106.02	110.30
19	A	810	CLA	C1D-ND-C4D	-2.64	104.46	106.33
19	B	829	CLA	CAC-C3C-C4C	2.64	128.23	124.81
29	A	844	PQN	C2M-C2-C3	-2.64	120.10	124.40
19	B	825	CLA	CMB-C2B-C3B	2.63	129.61	124.68
24	G	209	LMT	C1'-O5'-C5'	-2.63	108.52	113.69
19	A	805	CLA	C1D-ND-C4D	-2.63	104.46	106.33
19	A	842	CLA	CMA-C3A-C4A	2.63	118.85	111.77
19	2	504	CLA	C1D-ND-C4D	-2.63	104.47	106.33
19	B	831	CLA	C1D-ND-C4D	-2.63	104.47	106.33
19	A	810	CLA	CMA-C3A-C4A	2.63	118.85	111.77
19	B	831	CLA	CMB-C2B-C3B	2.63	129.60	124.68
19	A	840	CLA	CMB-C2B-C3B	2.63	129.60	124.68
22	J	1104	LMG	C7-O1-C1	-2.63	108.60	113.74
27	A	801	CL0	CMD-C2D-C3D	-2.63	121.56	127.61
19	A	854	CLA	O2A-CGA-O1A	-2.63	116.96	123.59
18	B	856	BCR	C39-C30-C25	-2.63	106.04	110.30
19	G	202	CLA	CMA-C3A-C4A	2.63	118.83	111.77
19	3	313	CLA	C2D-C1D-ND	2.63	112.04	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	H	1000	CLA	C2D-C1D-ND	2.63	112.04	110.10
18	G	205	BCR	C39-C30-C25	-2.62	106.04	110.30
19	B	836	CLA	C1D-ND-C4D	-2.62	104.47	106.33
19	A	802	CLA	CMB-C2B-C1B	-2.62	124.43	128.46
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	B	809	CLA	CMA-C3A-C4A	2.62	118.81	111.77
23	4	303	XAT	O24-C25-C38	-2.62	111.92	115.06
17	3	302	LUT	C39-C29-C30	-2.62	119.25	122.92
18	3	303	BCR	C29-C28-C27	2.62	117.23	111.38
19	A	831	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
19	4	306	CLA	CMA-C3A-C4A	2.61	118.80	111.77
19	2	509	CLA	CMB-C2B-C3B	2.61	129.57	124.68
19	A	833	CLA	C1D-ND-C4D	-2.61	104.48	106.33
18	4	301	BCR	C39-C30-C25	-2.61	106.06	110.30
19	3	317	CLA	CMA-C3A-C4A	2.61	118.80	111.77
20	4	316	CHL	CHC-C1C-NC	2.61	128.17	124.20
19	A	817	CLA	CMA-C3A-C4A	2.61	118.79	111.77
17	1	502	LUT	C31-C32-C33	-2.61	119.08	126.42
19	A	854	CLA	O2A-CGA-CBA	2.61	120.10	111.91
19	B	823	CLA	CMD-C2D-C3D	-2.61	121.61	127.61
19	J	1105	CLA	CMB-C2B-C1B	-2.61	124.45	128.46
19	B	813	CLA	C2D-C1D-ND	2.61	112.03	110.10
19	A	821	CLA	CMB-C2B-C1B	-2.61	124.46	128.46
19	2	507	CLA	C1D-ND-C4D	-2.61	104.48	106.33
19	A	838	CLA	CMA-C3A-C4A	2.61	118.78	111.77
19	1	504	CLA	CMB-C2B-C3B	2.61	129.55	124.68
19	A	819	CLA	C2D-C1D-ND	2.61	112.02	110.10
19	B	813	CLA	CMB-C2B-C3B	2.60	129.55	124.68
19	A	814	CLA	C2D-C1D-ND	2.60	112.02	110.10
18	B	851	BCR	C35-C13-C12	2.60	122.18	118.08
19	4	307	CLA	C2D-C1D-ND	2.60	112.02	110.10
19	3	309	CLA	CHA-C4D-ND	2.60	137.93	132.50
18	A	848	BCR	C8-C9-C10	2.60	122.93	118.94
18	A	849	BCR	C19-C18-C17	2.60	122.93	118.94
19	B	838	CLA	CMA-C3A-C4A	2.60	118.75	111.77
19	K	1004	CLA	C1C-NC-C4C	-2.60	105.54	106.71
19	4	311	CLA	C2D-C1D-ND	2.59	112.02	110.10
20	2	513	CHL	C2C-C3C-C4C	2.59	108.34	106.49
19	B	803	CLA	CHD-C1D-ND	-2.59	122.07	124.45
19	1	507	CLA	O2A-CGA-CBA	2.59	120.03	111.91
27	A	801	CL0	C6-C5-C3	-2.59	106.67	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	304	CLA	CHA-C4D-ND	2.59	137.91	132.50
19	4	305	CLA	CHA-C4D-ND	2.59	137.91	132.50
23	2	502	XAT	C40-C33-C34	-2.59	119.30	122.92
19	A	804	CLA	C2D-C1D-ND	2.59	112.01	110.10
19	A	836	CLA	CMB-C2B-C3B	2.58	129.51	124.68
19	4	315	CLA	C1D-ND-C4D	-2.58	104.50	106.33
18	2	503	BCR	C32-C1-C6	-2.58	106.11	110.30
19	A	806	CLA	O2D-CGD-CBD	2.58	115.86	111.27
19	B	829	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
19	B	840	CLA	CMA-C3A-C4A	2.58	118.71	111.77
24	G	208	LMT	C3'-C4'-C5'	-2.58	105.01	110.93
19	L	305	CLA	C1D-ND-C4D	-2.58	104.50	106.33
19	G	204	CLA	C3D-C2D-C1D	-2.58	102.31	105.83
19	J	1101	CLA	C2D-C1D-ND	2.58	112.00	110.10
18	B	802	BCR	C40-C30-C25	-2.58	106.12	110.30
19	B	829	CLA	O2A-CGA-CBA	2.58	119.99	111.91
26	G	207	DGD	O1G-C1A-C2A	2.57	119.99	111.91
19	2	510	CLA	CMB-C2B-C3B	2.57	129.49	124.68
23	4	303	XAT	C39-C29-C30	-2.57	119.32	122.92
23	4	303	XAT	C31-C30-C29	-2.57	123.64	127.31
18	A	848	BCR	C12-C13-C14	-2.57	115.00	118.94
20	4	317	CHL	CHC-C1C-NC	2.56	128.09	124.20
19	1	510	CLA	OBD-CAD-C3D	-2.56	122.35	128.52
19	3	309	CLA	C2D-C1D-ND	2.56	111.99	110.10
19	3	313	CLA	CMA-C3A-C4A	2.56	118.66	111.77
19	B	815	CLA	O2A-CGA-CBA	2.56	119.94	111.91
18	A	848	BCR	C38-C26-C25	-2.56	121.66	124.53
19	A	855	CLA	O2A-CGA-CBA	2.55	119.92	111.91
24	B	846	LMT	C1'-O5'-C5'	-2.55	108.67	113.69
26	4	319	DGD	O1G-C1A-C2A	2.55	119.92	111.91
19	B	833	CLA	CMD-C2D-C3D	-2.55	121.74	127.61
19	B	817	CLA	C2D-C1D-ND	2.55	111.98	110.10
19	2	505	CLA	O2A-CGA-CBA	2.55	119.91	111.91
19	1	507	CLA	CMA-C3A-C4A	2.55	118.62	111.77
19	A	819	CLA	CMB-C2B-C3B	2.55	129.44	124.68
19	B	805	CLA	C2D-C1D-ND	2.55	111.98	110.10
19	A	807	CLA	O2A-CGA-CBA	2.55	119.90	111.91
19	4	304	CLA	CMA-C3A-C4A	2.55	118.62	111.77
19	B	836	CLA	CMB-C2B-C3B	2.55	129.44	124.68
19	A	842	CLA	O2A-CGA-CBA	2.55	119.90	111.91
19	A	805	CLA	CMD-C2D-C3D	-2.54	121.76	127.61
19	B	814	CLA	CAC-C3C-C4C	2.54	128.11	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	J	1109	LUT	C39-C29-C30	-2.54	119.36	122.92
19	K	1001	CLA	CMD-C2D-C3D	-2.54	121.77	127.61
20	1	521	CHL	CHB-C4A-NA	2.54	128.02	124.51
22	1	518	LMG	O8-C28-C29	2.54	119.87	111.91
19	B	803	CLA	C2D-C1D-ND	2.54	111.97	110.10
19	A	812	CLA	C1D-ND-C4D	-2.54	104.53	106.33
26	4	319	DGD	O3G-C1D-C2D	2.54	112.26	108.30
19	A	854	CLA	CMB-C2B-C3B	2.54	129.42	124.68
19	1	507	CLA	CHA-C4D-ND	2.54	137.80	132.50
19	A	827	CLA	C1D-ND-C4D	-2.54	104.53	106.33
19	A	838	CLA	C1D-ND-C4D	-2.54	104.53	106.33
19	A	816	CLA	C1D-ND-C4D	-2.53	104.53	106.33
19	3	312	CLA	C2D-C1D-ND	2.53	111.97	110.10
19	A	819	CLA	C1D-ND-C4D	-2.53	104.54	106.33
19	B	837	CLA	C2D-C1D-ND	2.53	111.97	110.10
19	B	816	CLA	C1D-ND-C4D	-2.53	104.54	106.33
19	2	510	CLA	CHA-C4D-ND	2.53	137.79	132.50
19	1	515	CLA	CHA-C4D-ND	2.53	137.78	132.50
19	2	506	CLA	CAA-CBA-CGA	-2.53	105.87	113.25
18	B	850	BCR	C35-C13-C12	2.53	122.06	118.08
19	B	818	CLA	CAC-C3C-C4C	2.52	128.09	124.81
19	A	808	CLA	CHA-C4D-ND	2.52	137.78	132.50
19	1	515	CLA	CMD-C2D-C3D	-2.52	121.81	127.61
19	B	821	CLA	C2D-C1D-ND	2.52	111.96	110.10
19	4	307	CLA	CMD-C2D-C3D	-2.52	121.81	127.61
19	A	830	CLA	CHA-C4D-ND	2.52	137.77	132.50
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
19	B	819	CLA	CMA-C3A-C4A	2.52	118.54	111.77
19	K	1004	CLA	CHD-C1D-ND	-2.52	122.08	124.52
19	3	310	CLA	C1D-ND-C4D	-2.52	104.55	106.33
19	1	515	CLA	CMA-C3A-C4A	2.52	118.54	111.77
19	A	821	CLA	C2D-C1D-ND	2.52	111.96	110.10
19	3	308	CLA	CMB-C2B-C3B	2.51	129.38	124.68
19	A	823	CLA	C1D-ND-C4D	-2.51	104.55	106.33
19	4	304	CLA	CMB-C2B-C3B	2.51	129.38	124.68
19	4	308	CLA	CHA-C4D-ND	2.51	137.75	132.50
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
19	F	302	CLA	O2A-CGA-CBA	2.51	119.78	111.91
19	3	309	CLA	CAC-C3C-C4C	2.51	128.06	124.81
18	B	852	BCR	C12-C13-C14	-2.51	115.09	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	826	CLA	CMA-C3A-C4A	2.51	118.51	111.77
19	B	809	CLA	O2A-CGA-CBA	2.51	119.77	111.91
19	F	302	CLA	CMB-C2B-C1B	-2.50	124.61	128.46
19	A	809	CLA	CMA-C3A-C4A	2.50	118.50	111.77
18	B	852	BCR	C38-C26-C25	-2.50	121.72	124.53
19	B	818	CLA	CMA-C3A-C4A	2.50	118.50	111.77
19	3	306	CLA	C2D-C1D-ND	2.50	111.95	110.10
20	2	515	CHL	C4D-CHA-C1A	2.50	124.29	121.25
19	B	830	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
19	2	509	CLA	C2D-C1D-ND	2.50	111.95	110.10
19	B	808	CLA	C1D-ND-C4D	-2.50	104.56	106.33
19	A	830	CLA	CMB-C2B-C3B	2.50	129.35	124.68
19	B	824	CLA	CHA-C4D-ND	2.50	137.73	132.50
20	2	513	CHL	C4D-CHA-C1A	2.50	124.29	121.25
19	2	505	CLA	CHA-C4D-ND	2.50	137.72	132.50
19	B	807	CLA	C1D-ND-C4D	-2.50	104.56	106.33
19	A	805	CLA	C2D-C1D-ND	2.50	111.94	110.10
19	B	818	CLA	C2D-C1D-ND	2.50	111.94	110.10
19	A	827	CLA	CHA-C4D-ND	2.49	137.72	132.50
20	2	526	CHL	CHB-C4A-NA	2.49	127.96	124.51
19	K	1001	CLA	C1D-ND-C4D	-2.49	104.56	106.33
19	G	202	CLA	CHA-C4D-ND	2.49	137.71	132.50
19	3	308	CLA	C2D-C1D-ND	2.49	111.94	110.10
19	B	826	CLA	C3D-C2D-C1D	-2.49	102.43	105.83
20	4	313	CHL	C2C-C3C-C4C	2.49	108.27	106.49
18	A	856	BCR	C8-C9-C10	2.49	122.76	118.94
19	B	811	CLA	CHA-C4D-ND	2.49	137.71	132.50
18	B	852	BCR	C39-C30-C25	-2.49	106.26	110.30
19	F	303	CLA	CMA-C3A-C4A	2.49	118.47	111.77
19	B	833	CLA	CMB-C2B-C1B	-2.49	124.64	128.46
19	A	811	CLA	C1D-ND-C4D	-2.49	104.57	106.33
20	1	514	CHL	C4D-CHA-C1A	2.49	124.28	121.25
24	B	847	LMT	C1'-O5'-C5'	-2.49	108.81	113.69
17	J	1109	LUT	C37-C21-C22	-2.49	104.73	109.44
19	A	833	CLA	CMB-C2B-C3B	2.48	129.33	124.68
18	B	852	BCR	C37-C22-C23	2.48	121.99	118.08
19	2	507	CLA	CMB-C2B-C3B	2.48	129.32	124.68
19	B	810	CLA	O2A-CGA-CBA	2.48	119.70	111.91
19	A	831	CLA	CMB-C2B-C3B	2.48	129.32	124.68
19	1	508	CLA	CHA-C4D-ND	2.48	137.69	132.50
19	4	306	CLA	C1D-ND-C4D	-2.48	104.57	106.33
19	K	1001	CLA	CHA-C4D-ND	2.48	137.68	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	835	CLA	O2A-CGA-CBA	2.48	119.68	111.91
19	1	509	CLA	O2A-CGA-CBA	2.48	119.68	111.91
19	H	1000	CLA	CHA-C4D-ND	2.48	137.68	132.50
19	A	802	CLA	O2A-C1-C2	2.48	115.14	108.64
19	B	814	CLA	CHA-C4D-ND	2.48	137.68	132.50
19	B	829	CLA	CHA-C4D-ND	2.47	137.68	132.50
19	2	514	CLA	C2D-C1D-ND	2.47	111.93	110.10
19	4	308	CLA	C3D-C2D-C1D	-2.47	102.46	105.83
19	A	825	CLA	CHA-C4D-ND	2.47	137.67	132.50
18	K	1005	BCR	C40-C30-C29	2.47	118.79	108.91
19	B	806	CLA	C1-O2A-CGA	2.47	122.93	116.44
19	A	817	CLA	C1D-ND-C4D	-2.47	104.58	106.33
18	B	849	BCR	C40-C30-C29	2.47	118.77	108.91
19	A	807	CLA	C2D-C1D-ND	2.46	111.92	110.10
18	B	802	BCR	C40-C30-C29	2.46	118.75	108.91
19	A	820	CLA	CHA-C4D-ND	2.46	137.65	132.50
19	A	811	CLA	O2A-CGA-CBA	2.46	119.63	111.91
19	A	854	CLA	CMA-C3A-C4A	2.46	118.38	111.77
19	A	804	CLA	C1D-ND-C4D	-2.46	104.59	106.33
19	B	821	CLA	CHA-C4D-ND	2.46	137.64	132.50
22	A	847	LMG	O8-C28-C29	2.46	119.62	111.91
18	A	849	BCR	C40-C30-C29	2.46	118.74	108.91
19	1	504	CLA	CMB-C2B-C1B	-2.46	124.69	128.46
19	2	507	CLA	CMD-C2D-C3D	-2.46	121.96	127.61
19	A	825	CLA	C2D-C1D-ND	2.46	111.92	110.10
18	G	205	BCR	C40-C30-C29	2.46	118.73	108.91
18	A	852	BCR	C40-C30-C29	2.46	118.73	108.91
19	B	826	CLA	O2A-CGA-CBA	2.46	119.61	111.91
19	2	505	CLA	C1D-ND-C4D	-2.45	104.59	106.33
19	3	313	CLA	C1D-ND-C4D	-2.45	104.59	106.33
19	1	505	CLA	CHA-C4D-ND	2.45	137.63	132.50
18	3	303	BCR	C40-C30-C29	2.45	118.72	108.91
20	3	314	CHL	CHC-C1C-NC	2.45	127.93	124.20
19	B	809	CLA	C2D-C1D-ND	2.45	111.91	110.10
18	F	306	BCR	C40-C30-C29	2.45	118.72	108.91
18	L	306	BCR	C40-C30-C29	2.45	118.72	108.91
18	I	101	BCR	C8-C9-C10	2.45	122.70	118.94
18	I	101	BCR	C40-C30-C29	2.45	118.72	108.91
18	B	852	BCR	C40-C30-C29	2.45	118.72	108.91
19	A	826	CLA	O2A-CGA-CBA	2.45	119.60	111.91
19	B	805	CLA	C1D-ND-C4D	-2.45	104.59	106.33
19	1	510	CLA	C2D-C1D-ND	2.45	111.91	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	805	CLA	CHA-C4D-ND	2.45	137.62	132.50
19	G	203	CLA	CHA-C4D-ND	2.45	137.62	132.50
18	A	856	BCR	C40-C30-C29	2.45	118.70	108.91
19	4	310	CLA	CHA-C4D-ND	2.45	137.62	132.50
18	A	848	BCR	C40-C30-C29	2.45	118.70	108.91
20	2	513	CHL	C1B-CHB-C4A	-2.45	125.27	130.12
18	A	851	BCR	C40-C30-C29	2.45	118.69	108.91
18	L	302	BCR	C40-C30-C29	2.45	118.69	108.91
18	B	853	BCR	C40-C30-C29	2.45	118.69	108.91
30	F	301	ZEX	C35-C34-C33	-2.45	123.82	127.31
19	2	507	CLA	CHA-C4D-ND	2.45	137.62	132.50
19	F	302	CLA	CMA-C3A-C4A	2.45	118.34	111.77
20	4	314	CHL	C3A-C2A-C1A	2.44	105.00	101.34
20	4	314	CHL	CHC-C1C-NC	2.44	127.91	124.20
19	B	833	CLA	CMB-C2B-C3B	2.44	129.25	124.68
18	L	307	BCR	C40-C30-C29	2.44	118.68	108.91
18	B	850	BCR	C40-C30-C29	2.44	118.68	108.91
18	B	851	BCR	C40-C30-C29	2.44	118.67	108.91
19	A	809	CLA	CMB-C2B-C3B	2.44	129.25	124.68
19	A	832	CLA	CMA-C3A-C4A	2.44	118.33	111.77
19	2	514	CLA	CAC-C3C-C4C	2.44	127.98	124.81
18	2	503	BCR	C34-C9-C10	-2.44	119.50	122.92
19	A	839	CLA	CMB-C2B-C3B	2.44	129.24	124.68
20	2	513	CHL	CMA-C3A-C4A	2.44	118.33	111.77
19	B	804	CLA	CHA-C4D-ND	2.44	137.60	132.50
19	K	1003	CLA	C2B-C3B-C4B	2.44	108.38	106.29
19	2	514	CLA	O2A-CGA-CBA	2.44	119.56	111.91
19	1	510	CLA	CMB-C2B-C1B	-2.44	124.72	128.46
18	1	503	BCR	C40-C30-C29	2.44	118.66	108.91
19	4	307	CLA	CHA-C4D-ND	2.44	137.60	132.50
19	A	831	CLA	CHA-C4D-ND	2.44	137.60	132.50
17	4	302	LUT	C19-C9-C8	2.44	121.92	118.08
18	3	304	BCR	C40-C30-C29	2.44	118.65	108.91
18	A	850	BCR	C40-C30-C29	2.44	118.65	108.91
19	1	511	CLA	CAC-C3C-C4C	2.44	127.97	124.81
19	A	841	CLA	CMA-C3A-C4A	2.44	118.32	111.77
20	1	521	CHL	C1-O2A-CGA	2.44	122.83	116.44
19	2	508	CLA	CMB-C2B-C3B	2.44	129.23	124.68
19	B	834	CLA	O2A-CGA-CBA	2.43	119.55	111.91
19	B	820	CLA	CHA-C4D-ND	2.43	137.59	132.50
29	B	841	PQN	C2M-C2-C3	-2.43	120.43	124.40
19	B	809	CLA	CHA-C4D-ND	2.43	137.59	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	514	CHL	CMA-C3A-C4A	2.43	118.31	111.77
18	J	1108	BCR	C40-C30-C29	2.43	118.64	108.91
19	A	832	CLA	O2A-CGA-CBA	2.43	119.54	111.91
18	J	1108	BCR	C12-C13-C14	-2.43	115.21	118.94
19	2	505	CLA	C3D-C2D-C1D	-2.43	102.51	105.83
19	A	822	CLA	CHA-C4D-ND	2.43	137.58	132.50
19	L	301	CLA	CHA-C4D-ND	2.43	137.58	132.50
18	I	102	BCR	C40-C30-C29	2.43	118.62	108.91
19	1	516	CLA	CHA-C4D-ND	2.43	137.58	132.50
18	4	301	BCR	C40-C30-C29	2.43	118.62	108.91
19	1	508	CLA	C2D-C1D-ND	2.43	111.89	110.10
19	B	836	CLA	O2A-CGA-CBA	2.43	119.52	111.91
18	A	849	BCR	C8-C9-C10	2.43	122.66	118.94
19	B	813	CLA	CMB-C2B-C1B	-2.43	124.73	128.46
19	1	508	CLA	C1D-ND-C4D	-2.42	104.61	106.33
19	B	815	CLA	C1D-ND-C4D	-2.42	104.61	106.33
19	A	810	CLA	CMD-C2D-C3D	-2.42	122.04	127.61
19	A	802	CLA	CAA-C2A-C1A	-2.42	104.03	111.97
20	3	314	CHL	CHD-C4C-C3C	2.42	128.40	124.84
19	B	835	CLA	C3D-C2D-C1D	-2.42	102.53	105.83
18	A	851	BCR	C34-C9-C10	-2.42	119.53	122.92
19	B	818	CLA	CHA-C4D-ND	2.42	137.56	132.50
19	B	815	CLA	C2D-C1D-ND	2.42	111.89	110.10
19	1	504	CLA	CHA-C4D-ND	2.42	137.56	132.50
19	3	311	CLA	CHA-C4D-ND	2.42	137.56	132.50
18	A	851	BCR	C32-C1-C6	-2.42	106.38	110.30
19	A	832	CLA	C2D-C1D-ND	2.42	111.89	110.10
18	B	856	BCR	C40-C30-C29	2.42	118.58	108.91
19	4	308	CLA	CMA-C3A-C4A	2.42	118.27	111.77
17	J	1109	LUT	C31-C32-C33	-2.42	119.62	126.42
27	A	801	CL0	CHA-C4D-ND	2.42	137.56	132.50
18	A	849	BCR	C36-C18-C19	-2.42	114.27	118.08
19	B	831	CLA	CMB-C2B-C1B	-2.42	124.75	128.46
19	B	826	CLA	CMA-C3A-C4A	2.42	118.27	111.77
19	B	813	CLA	CHA-C4D-ND	2.42	137.55	132.50
19	J	1101	CLA	CHA-C4D-ND	2.42	137.55	132.50
19	3	316	CLA	C2D-C1D-ND	2.42	111.88	110.10
19	F	302	CLA	C6-C7-C8	-2.42	108.11	115.92
18	A	850	BCR	C38-C26-C27	2.41	118.25	113.62
19	A	810	CLA	CHA-C4D-ND	2.41	137.55	132.50
19	B	817	CLA	CMD-C2D-C3D	-2.41	122.06	127.61
19	L	304	CLA	CMB-C2B-C3B	2.41	129.19	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	301	CLA	C1D-ND-C4D	-2.41	104.62	106.33
19	B	825	CLA	CHA-C4D-ND	2.41	137.54	132.50
19	1	504	CLA	C1D-ND-C4D	-2.41	104.62	106.33
19	A	811	CLA	CHA-C4D-ND	2.41	137.54	132.50
30	F	301	ZEX	C2-C3-C4	-2.41	107.01	110.30
19	2	514	CLA	CMB-C2B-C3B	2.41	129.19	124.68
18	A	848	BCR	C38-C26-C27	2.41	118.24	113.62
19	B	804	CLA	C3D-C2D-C1D	-2.41	102.55	105.83
19	A	806	CLA	C1D-ND-C4D	-2.41	104.62	106.33
18	A	856	BCR	C19-C18-C17	2.41	122.63	118.94
19	A	854	CLA	O2A-C1-C2	2.41	114.96	108.64
19	2	504	CLA	CHA-C4D-ND	2.41	137.53	132.50
19	A	818	CLA	CMB-C2B-C3B	2.40	129.18	124.68
19	J	1105	CLA	CHA-C4D-ND	2.40	137.53	132.50
19	A	840	CLA	CHA-C4D-ND	2.40	137.53	132.50
19	A	808	CLA	C1D-ND-C4D	-2.40	104.63	106.33
19	K	1002	CLA	C1D-ND-C4D	-2.40	104.63	106.33
18	G	205	BCR	C34-C9-C10	-2.40	119.56	122.92
19	A	808	CLA	C3D-C2D-C1D	-2.40	102.55	105.83
19	B	807	CLA	CHA-C4D-ND	2.40	137.52	132.50
19	B	823	CLA	O2A-CGA-CBA	2.40	119.44	111.91
19	K	1001	CLA	C3D-C2D-C1D	-2.40	102.56	105.83
19	2	514	CLA	CHA-C4D-ND	2.40	137.52	132.50
19	B	803	CLA	CHA-C4D-ND	2.40	137.52	132.50
19	B	826	CLA	CHA-C1A-NA	-2.40	120.91	126.40
19	B	811	CLA	CMA-C3A-C4A	2.40	118.22	111.77
18	B	802	BCR	C39-C30-C25	-2.40	106.41	110.30
19	B	821	CLA	CMA-C3A-C4A	2.40	118.21	111.77
18	L	306	BCR	C38-C26-C25	-2.40	121.84	124.53
19	A	807	CLA	CHA-C4D-ND	2.40	137.51	132.50
19	B	822	CLA	CHA-C4D-ND	2.40	137.51	132.50
19	A	828	CLA	C1D-ND-C4D	-2.40	104.63	106.33
19	A	854	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
19	A	854	CLA	CHA-C1A-NA	-2.40	120.91	126.40
19	A	829	CLA	CMA-C3A-C4A	2.39	118.21	111.77
19	4	304	CLA	C3D-C2D-C1D	-2.39	102.57	105.83
18	A	848	BCR	C10-C11-C12	-2.39	115.75	123.22
19	B	820	CLA	CAC-C3C-C4C	2.39	127.91	124.81
19	4	312	CLA	CHA-C4D-ND	2.39	137.49	132.50
19	A	840	CLA	CMB-C2B-C1B	-2.39	124.80	128.46
19	3	308	CLA	C1D-ND-C4D	-2.39	104.64	106.33
19	B	825	CLA	C1-O2A-CGA	2.39	122.70	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	507	CLA	C2D-C1D-ND	2.39	111.86	110.10
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
18	B	852	BCR	C34-C9-C10	-2.39	119.58	122.92
19	A	818	CLA	O2A-CGA-CBA	2.38	119.39	111.91
19	B	830	CLA	C2D-C1D-ND	2.38	111.86	110.10
19	B	814	CLA	O2A-CGA-CBA	2.38	119.39	111.91
19	4	318	CLA	O2A-CGA-CBA	2.38	119.39	111.91
19	L	305	CLA	CHA-C4D-ND	2.38	137.48	132.50
19	H	1000	CLA	CMA-C3A-C4A	2.38	118.17	111.77
19	B	811	CLA	C2D-C1D-ND	2.38	111.86	110.10
19	A	820	CLA	CAC-C3C-C4C	2.38	127.90	124.81
19	B	811	CLA	CAC-C3C-C4C	2.38	127.90	124.81
19	B	837	CLA	CHA-C4D-ND	2.38	137.48	132.50
19	A	812	CLA	CHA-C4D-ND	2.38	137.47	132.50
19	B	839	CLA	CMA-C3A-C4A	2.38	118.17	111.77
19	4	312	CLA	C2D-C1D-ND	2.38	111.86	110.10
19	4	304	CLA	C1-C2-C3	2.38	130.15	126.04
19	B	808	CLA	CHA-C4D-ND	2.38	137.47	132.50
19	3	307	CLA	O2A-CGA-CBA	2.38	119.36	111.91
20	4	313	CHL	C1-O2A-CGA	2.38	123.94	116.11
19	1	509	CLA	CHA-C4D-ND	2.37	137.47	132.50
18	L	307	BCR	C8-C9-C10	2.37	122.58	118.94
19	A	803	CLA	CMA-C3A-C4A	2.37	118.15	111.77
19	B	806	CLA	C1D-ND-C4D	-2.37	104.65	106.33
19	2	510	CLA	CHD-C1D-ND	-2.37	122.27	124.45
19	A	822	CLA	CMD-C2D-C3D	-2.37	122.16	127.61
18	I	101	BCR	C12-C13-C14	2.37	122.58	118.94
19	3	307	CLA	C3D-C2D-C1D	-2.37	102.59	105.83
19	3	306	CLA	C1D-ND-C4D	-2.37	104.65	106.33
17	3	302	LUT	C31-C32-C33	-2.37	119.75	126.42
19	3	311	CLA	C3D-C2D-C1D	-2.37	102.59	105.83
19	B	840	CLA	CMB-C2B-C3B	2.37	129.11	124.68
18	2	503	BCR	C40-C30-C29	2.37	118.39	108.91
19	A	803	CLA	CMB-C2B-C3B	2.37	129.11	124.68
19	L	301	CLA	CMB-C2B-C3B	2.37	129.11	124.68
21	1	517	LHG	O8-C23-C24	2.37	119.34	111.91
17	J	1109	LUT	C40-C33-C34	-2.37	119.61	122.92
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	J	1101	CLA	C6-C7-C8	-2.37	108.27	115.92
18	2	503	BCR	C33-C5-C6	-2.37	121.87	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	838	CLA	O2A-CGA-CBA	2.37	119.33	111.91
19	B	835	CLA	CHA-C4D-ND	2.37	137.45	132.50
21	1	520	LHG	O8-C23-C24	2.37	119.33	111.91
19	A	831	CLA	CMA-C3A-C4A	2.37	118.13	111.77
19	B	821	CLA	C1D-ND-C4D	-2.36	104.66	106.33
19	B	823	CLA	CHA-C4D-ND	2.36	137.44	132.50
19	B	831	CLA	C3D-C2D-C1D	-2.36	102.61	105.83
23	4	303	XAT	C20-C13-C14	-2.36	119.61	122.92
19	B	830	CLA	CMA-C3A-C4A	2.36	118.12	111.77
19	2	506	CLA	CAC-C3C-C4C	2.36	127.87	124.81
19	B	806	CLA	C2D-C1D-ND	2.36	111.84	110.10
19	A	833	CLA	CHA-C4D-ND	2.36	137.44	132.50
26	B	801	DGD	C3A-C2A-C1A	-2.36	105.03	113.62
19	3	305	CLA	O2A-CGA-CBA	2.36	119.31	111.91
19	3	315	CLA	O2A-CGA-CBA	2.36	119.31	111.91
19	4	305	CLA	C2D-C1D-ND	2.36	111.84	110.10
19	A	827	CLA	C3D-C2D-C1D	-2.36	102.61	105.83
19	A	802	CLA	CHA-C4D-ND	2.36	137.43	132.50
18	A	851	BCR	C37-C22-C23	2.36	121.79	118.08
22	G	210	LMG	C9-C8-C7	-2.36	106.21	111.79
19	3	307	CLA	CHA-C4D-ND	2.36	137.43	132.50
19	A	813	CLA	C3D-C2D-C1D	-2.36	102.61	105.83
18	K	1005	BCR	C38-C26-C25	-2.36	121.88	124.53
19	A	831	CLA	CMB-C2B-C1B	-2.36	124.84	128.46
19	A	842	CLA	CHA-C4D-ND	2.36	137.43	132.50
18	L	307	BCR	C39-C30-C25	-2.36	106.48	110.30
19	3	315	CLA	CHA-C4D-ND	2.35	137.43	132.50
19	A	807	CLA	CMD-C2D-C3D	-2.35	122.20	127.61
20	4	314	CHL	C1-O2A-CGA	2.35	122.62	116.44
19	A	832	CLA	CHA-C4D-ND	2.35	137.42	132.50
23	2	502	XAT	O4-C5-C18	-2.35	112.24	115.06
19	B	825	CLA	O2A-CGA-CBA	2.35	119.28	111.91
19	3	306	CLA	CMD-C2D-C3D	-2.35	122.21	127.61
19	4	306	CLA	CAC-C3C-C4C	2.35	127.86	124.81
19	A	829	CLA	O2A-CGA-CBA	2.35	119.28	111.91
19	A	821	CLA	CHA-C4D-ND	2.35	137.41	132.50
19	3	305	CLA	CMA-C3A-C4A	2.35	118.08	111.77
19	B	813	CLA	C1D-ND-C4D	-2.35	104.67	106.33
19	K	1004	CLA	C4D-ND-C1D	-2.35	104.67	106.33
19	B	830	CLA	CMD-C2D-C3D	-2.35	122.22	127.61
18	B	851	BCR	C29-C28-C27	2.35	116.62	111.38
19	A	836	CLA	CHA-C4D-ND	2.35	137.41	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	511	CLA	CMD-C2D-C3D	-2.35	122.22	127.61
19	3	305	CLA	CHA-C4D-ND	2.35	137.41	132.50
19	A	830	CLA	C1D-ND-C4D	-2.35	104.67	106.33
19	B	824	CLA	C3D-C2D-C1D	-2.34	102.63	105.83
19	A	813	CLA	CMB-C2B-C3B	2.34	129.06	124.68
18	2	503	BCR	C8-C9-C10	2.34	122.54	118.94
19	B	805	CLA	CHA-C4D-ND	2.34	137.40	132.50
19	A	826	CLA	CAA-C2A-C1A	-2.34	104.30	111.97
19	2	510	CLA	O2A-CGA-CBA	2.34	119.26	111.91
19	A	804	CLA	CMD-C2D-C3D	-2.34	122.23	127.61
17	3	302	LUT	C2-C3-C4	-2.34	107.10	110.30
19	4	312	CLA	O2A-CGA-CBA	2.34	119.25	111.91
19	3	306	CLA	C2C-C1C-NC	2.34	112.17	109.97
19	J	1105	CLA	CMC-C2C-C1C	-2.34	121.47	125.04
19	B	806	CLA	CMD-C2D-C3D	-2.34	122.23	127.61
19	A	816	CLA	CHA-C4D-ND	2.34	137.39	132.50
19	B	806	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
19	A	835	CLA	CHA-C4D-ND	2.34	137.39	132.50
19	B	804	CLA	CMB-C2B-C3B	2.34	129.05	124.68
18	3	304	BCR	C19-C18-C17	2.34	122.53	118.94
19	B	822	CLA	C1D-ND-C4D	-2.34	104.67	106.33
19	A	839	CLA	O2A-CGA-CBA	2.34	119.24	111.91
19	4	310	CLA	C3D-C2D-C1D	-2.34	102.64	105.83
21	A	853	LHG	C5-O7-C7	-2.34	112.04	117.79
18	J	1108	BCR	C2-C1-C6	2.34	114.08	110.48
19	2	506	CLA	CHA-C4D-ND	2.34	137.38	132.50
23	4	303	XAT	C38-C25-C26	-2.34	118.35	122.26
26	4	319	DGD	C2G-O2G-C1B	2.34	123.54	117.79
19	1	510	CLA	CHA-C4D-ND	2.33	137.38	132.50
19	4	315	CLA	CMA-C3A-C4A	2.33	118.04	111.77
20	2	512	CHL	CMB-C2B-C1B	-2.33	124.88	128.46
19	K	1004	CLA	C2B-C3B-C4B	2.33	108.28	106.29
21	A	853	LHG	O8-C23-C24	2.33	119.23	111.91
18	J	1108	BCR	C35-C13-C12	2.33	121.75	118.08
18	J	1108	BCR	C37-C22-C23	2.33	121.75	118.08
18	B	850	BCR	C39-C30-C25	-2.33	106.52	110.30
19	4	315	CLA	CHA-C4D-ND	2.33	137.38	132.50
19	A	815	CLA	CHA-C4D-ND	2.33	137.38	132.50
19	B	814	CLA	C2D-C1D-ND	2.33	111.82	110.10
19	B	832	CLA	O1D-CGD-CBD	-2.33	119.71	124.48
17	3	302	LUT	C22-C23-C24	-2.33	109.09	111.74
19	2	511	CLA	CHA-C4D-ND	2.33	137.37	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	318	CLA	C3D-C2D-C1D	-2.33	102.65	105.83
19	B	813	CLA	CAC-C3C-C4C	2.33	127.83	124.81
19	B	828	CLA	CMB-C2B-C3B	2.33	129.03	124.68
19	A	834	CLA	CHA-C4D-ND	2.33	137.37	132.50
19	2	511	CLA	C1D-ND-C4D	-2.33	104.68	106.33
19	3	312	CLA	CHA-C4D-ND	2.33	137.37	132.50
19	B	834	CLA	C3D-C2D-C1D	-2.33	102.65	105.83
19	B	811	CLA	CAA-CBA-CGA	-2.33	106.45	113.25
22	G	206	LMG	O8-C28-C29	2.33	119.21	111.91
19	3	317	CLA	CHA-C4D-ND	2.33	137.37	132.50
19	G	203	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
19	B	817	CLA	CHA-C4D-ND	2.32	137.36	132.50
19	4	312	CLA	C1D-ND-C4D	-2.32	104.68	106.33
19	2	508	CLA	C3D-C2D-C1D	-2.32	102.66	105.83
19	J	1105	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
19	B	803	CLA	C1D-ND-C4D	-2.32	104.69	106.33
19	A	838	CLA	CHA-C4D-ND	2.32	137.35	132.50
19	B	833	CLA	CHA-C4D-ND	2.32	137.35	132.50
20	2	516	CHL	CHB-C4A-NA	2.32	127.72	124.51
19	3	313	CLA	CMB-C2B-C3B	2.32	129.02	124.68
19	B	838	CLA	CMD-C2D-C3D	-2.32	122.28	127.61
19	3	306	CLA	CMA-C3A-C4A	2.32	118.00	111.77
19	A	809	CLA	C1D-ND-C4D	-2.32	104.69	106.33
19	A	824	CLA	CHA-C4D-ND	2.32	137.35	132.50
19	J	1102	CLA	CMD-C2D-C3D	-2.32	122.28	127.61
18	J	1108	BCR	C34-C9-C10	-2.32	119.68	122.92
19	2	510	CLA	C1D-ND-C4D	-2.32	104.69	106.33
24	4	320	LMT	C3'-C4'-C5'	-2.32	105.61	110.93
18	K	1005	BCR	C34-C9-C10	-2.32	119.68	122.92
19	4	306	CLA	CHA-C4D-ND	2.32	137.34	132.50
18	A	852	BCR	C2-C1-C6	2.32	114.05	110.48
19	B	838	CLA	CHA-C4D-ND	2.32	137.34	132.50
19	B	806	CLA	CMA-C3A-C4A	2.31	118.00	111.77
19	A	815	CLA	CMB-C2B-C3B	2.31	129.01	124.68
20	2	515	CHL	CHB-C4A-NA	2.31	127.71	124.51
19	K	1002	CLA	CAC-C3C-C4C	2.31	127.81	124.81
19	3	317	CLA	C1D-ND-C4D	-2.31	104.69	106.33
19	A	804	CLA	CHA-C4D-ND	2.31	137.34	132.50
19	A	836	CLA	O2A-CGA-CBA	2.31	119.16	111.91
19	B	837	CLA	O2A-CGA-CBA	2.31	119.16	111.91
19	K	1001	CLA	CAC-C3C-C4C	2.31	127.81	124.81
19	A	803	CLA	C1-O2A-CGA	2.31	122.51	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	511	CLA	CHA-C4D-ND	2.31	137.33	132.50
19	B	815	CLA	CHA-C4D-ND	2.31	137.33	132.50
19	3	307	CLA	CAC-C3C-C4C	2.31	127.81	124.81
18	K	1005	BCR	C30-C25-C26	-2.31	119.36	122.61
19	A	818	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
18	L	306	BCR	C30-C25-C26	-2.31	119.36	122.61
19	2	511	CLA	O2A-CGA-CBA	2.31	119.15	111.91
19	A	830	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
19	A	830	CLA	O2A-CGA-CBA	2.31	119.15	111.91
20	4	313	CHL	CHB-C4A-NA	2.31	127.70	124.51
19	A	806	CLA	CMB-C2B-C3B	2.31	128.99	124.68
19	3	313	CLA	CHA-C4D-ND	2.31	137.32	132.50
19	J	1102	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
19	3	316	CLA	CHA-C4D-ND	2.31	137.32	132.50
24	3	318	LMT	O5B-C1B-C2B	2.30	115.23	110.35
19	L	301	CLA	C1-O2A-CGA	2.30	122.49	116.44
19	A	833	CLA	O2A-CGA-CBA	2.30	119.14	111.91
19	A	811	CLA	CAC-C3C-C4C	2.30	127.80	124.81
18	3	303	BCR	C10-C11-C12	-2.30	116.03	123.22
17	2	501	LUT	C15-C35-C34	-2.30	118.75	123.47
19	4	312	CLA	CMD-C2D-C3D	-2.30	122.31	127.61
19	1	513	CLA	CHA-C4D-ND	2.30	137.31	132.50
19	B	813	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
19	A	829	CLA	CMB-C2B-C3B	2.30	128.98	124.68
19	1	511	CLA	C2D-C1D-ND	2.30	111.80	110.10
26	4	319	DGD	O5D-C1E-C2E	2.30	111.89	108.30
21	2	517	LHG	O8-C23-C24	2.30	119.12	111.91
19	B	828	CLA	O2A-CGA-CBA	2.30	119.12	111.91
19	A	813	CLA	CHA-C4D-ND	2.30	137.31	132.50
19	B	816	CLA	O2A-CGA-CBA	2.30	119.12	111.91
19	1	506	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
19	A	802	CLA	O2A-CGA-CBA	2.30	119.12	111.91
19	2	509	CLA	CHA-C4D-ND	2.30	137.31	132.50
19	G	201	CLA	CHA-C1A-NA	-2.30	121.14	126.40
19	K	1002	CLA	CHA-C4D-ND	2.30	137.30	132.50
19	J	1105	CLA	C3D-C2D-C1D	-2.30	102.70	105.83
19	2	508	CLA	CHA-C4D-ND	2.30	137.30	132.50
20	4	314	CHL	CHD-C1D-C2D	2.30	130.29	125.48
18	B	851	BCR	C30-C25-C24	2.29	122.27	115.78
19	2	506	CLA	C3D-C2D-C1D	-2.29	102.70	105.83
19	B	831	CLA	CHA-C4D-ND	2.29	137.30	132.50
19	1	513	CLA	O2A-CGA-CBA	2.29	119.11	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	316	CLA	CMA-C3A-C4A	2.29	117.94	111.77
19	B	809	CLA	CMD-C2D-C3D	-2.29	122.34	127.61
18	J	1108	BCR	C40-C30-C25	-2.29	106.58	110.30
19	A	813	CLA	CHA-C1A-NA	-2.29	121.15	126.40
19	1	508	CLA	CMB-C2B-C3B	2.29	128.97	124.68
19	4	305	CLA	CHA-C1A-NA	-2.29	121.15	126.40
19	4	318	CLA	CHA-C4D-ND	2.29	137.29	132.50
30	F	301	ZEX	C23-C24-C25	2.29	112.59	109.33
18	A	848	BCR	C39-C30-C25	-2.29	106.58	110.30
19	4	306	CLA	O2A-CGA-CBA	2.29	119.09	111.91
19	A	817	CLA	CHA-C4D-ND	2.29	137.29	132.50
19	3	309	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
18	B	802	BCR	C37-C22-C23	2.29	121.68	118.08
19	1	510	CLA	CGD-CBD-CAD	2.28	118.14	110.73
20	1	512	CHL	C4A-NA-C1A	2.28	107.73	106.71
19	A	818	CLA	CHA-C4D-ND	2.28	137.28	132.50
19	B	821	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
18	L	302	BCR	C8-C9-C10	2.28	122.44	118.94
18	J	1108	BCR	C30-C25-C26	-2.28	119.40	122.61
19	4	304	CLA	C5-C3-C2	2.28	125.73	121.12
19	K	1002	CLA	CHA-C1A-NA	-2.28	121.17	126.40
19	G	202	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
19	B	810	CLA	CHA-C4D-ND	2.28	137.27	132.50
19	4	312	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
26	B	801	DGD	C1G-O1G-C1A	2.28	125.57	117.12
19	2	506	CLA	C1D-ND-C4D	-2.28	104.72	106.33
19	J	1102	CLA	CHA-C4D-ND	2.28	137.27	132.50
19	3	311	CLA	CHA-C1A-NA	-2.28	121.18	126.40
19	A	823	CLA	CHA-C4D-ND	2.28	137.27	132.50
30	F	301	ZEX	C19-C9-C10	-2.28	119.73	122.92
19	B	804	CLA	O2A-CGA-CBA	2.28	119.05	111.91
19	3	309	CLA	C1D-ND-C4D	-2.28	104.72	106.33
19	B	836	CLA	CHA-C4D-ND	2.28	137.26	132.50
17	3	302	LUT	C40-C33-C34	-2.28	119.73	122.92
19	A	802	CLA	C5-C3-C2	2.28	125.72	121.12
19	A	822	CLA	O2A-CGA-CBA	2.27	119.05	111.91
22	1	519	LMG	O1-C1-C2	2.27	110.81	108.15
18	A	851	BCR	C39-C30-C25	-2.27	106.61	110.30
19	L	303	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
19	1	509	CLA	CMA-C3A-C4A	2.27	117.88	111.77
19	3	311	CLA	C1D-ND-C4D	-2.27	104.72	106.33
19	G	202	CLA	O2A-CGA-CBA	2.27	119.03	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	818	CLA	CHA-C1A-NA	-2.27	121.20	126.40
19	2	510	CLA	C3D-C2D-C1D	-2.27	102.73	105.83
19	A	829	CLA	CHA-C4D-ND	2.27	137.24	132.50
19	A	838	CLA	C3D-C2D-C1D	-2.27	102.74	105.83
19	1	508	CLA	C1-O2A-CGA	2.27	122.39	116.44
19	A	807	CLA	C1D-ND-C4D	-2.27	104.72	106.33
19	K	1003	CLA	C4D-ND-C1D	-2.27	104.72	106.33
19	G	203	CLA	C2D-C1D-ND	2.27	111.77	110.10
19	4	308	CLA	CMB-C2B-C1B	-2.27	124.98	128.46
18	I	102	BCR	C32-C1-C6	-2.27	106.62	110.30
19	3	315	CLA	CMB-C2B-C1B	-2.26	124.98	128.46
19	A	837	CLA	CHA-C4D-ND	2.26	137.24	132.50
19	B	805	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
19	4	308	CLA	CHA-C1A-NA	-2.26	121.22	126.40
18	B	802	BCR	C30-C25-C26	-2.26	119.43	122.61
20	4	313	CHL	C1B-CHB-C4A	-2.26	125.64	130.12
19	A	809	CLA	CHA-C1A-NA	-2.26	121.22	126.40
24	4	320	LMT	O5B-C5B-C4B	2.26	113.80	109.69
19	1	506	CLA	CHA-C4D-ND	2.26	137.23	132.50
19	B	837	CLA	CMB-C2B-C3B	2.26	128.91	124.68
19	1	506	CLA	CAC-C3C-C4C	2.26	127.74	124.81
19	L	304	CLA	CMB-C2B-C1B	-2.26	124.99	128.46
19	A	828	CLA	O2A-CGA-CBA	2.26	119.00	111.91
19	2	509	CLA	O2A-CGA-CBA	2.26	119.00	111.91
19	B	816	CLA	CHA-C4D-ND	2.26	137.22	132.50
19	4	304	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
18	B	850	BCR	C38-C26-C25	-2.26	121.99	124.53
19	B	830	CLA	CAC-C3C-C4C	2.26	127.74	124.81
19	3	306	CLA	CHA-C4D-ND	2.26	137.22	132.50
19	A	825	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
19	A	816	CLA	CAC-C3C-C4C	2.26	127.74	124.81
19	B	840	CLA	CHA-C1A-NA	-2.26	121.23	126.40
23	2	502	XAT	C7-C8-C9	-2.26	122.03	125.53
18	K	1005	BCR	C37-C22-C23	2.26	121.63	118.08
19	F	303	CLA	CMD-C2D-C3D	-2.26	122.43	127.61
19	G	202	CLA	CMD-C2D-C3D	-2.26	122.43	127.61
19	3	310	CLA	CHA-C4D-ND	2.25	137.22	132.50
19	A	820	CLA	O2A-CGA-CBA	2.25	118.98	111.91
19	1	511	CLA	C1D-ND-C4D	-2.25	104.73	106.33
19	J	1105	CLA	CMC-C2C-C3C	2.25	132.23	126.12
19	4	311	CLA	CAC-C3C-C4C	2.25	127.73	124.81
19	B	815	CLA	CMB-C2B-C3B	2.25	128.89	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	801	CL0	C2A-C3A-C4A	2.25	105.51	101.87
19	B	808	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
19	A	814	CLA	CHA-C4D-ND	2.25	137.21	132.50
17	4	302	LUT	C40-C33-C34	-2.25	119.77	122.92
18	L	306	BCR	C39-C30-C25	-2.25	106.65	110.30
19	3	312	CLA	CAC-C3C-C4C	2.25	127.73	124.81
19	A	842	CLA	C3D-C2D-C1D	-2.25	102.76	105.83
19	F	302	CLA	CHA-C4D-ND	2.25	137.21	132.50
19	A	842	CLA	CMB-C2B-C3B	2.25	128.89	124.68
20	2	513	CHL	CHB-C4A-NA	2.25	127.62	124.51
19	B	838	CLA	C3D-C2D-C1D	-2.25	102.76	105.83
19	B	829	CLA	CMB-C2B-C3B	2.25	128.88	124.68
19	B	814	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
19	A	802	CLA	C3D-C2D-C1D	-2.25	102.76	105.83
22	B	845	LMG	O6-C5-C6	2.25	112.02	106.44
26	B	801	DGD	O1G-C1G-C2G	2.25	114.97	108.43
19	B	812	CLA	CHA-C4D-ND	2.24	137.19	132.50
19	A	826	CLA	CAA-CBA-CGA	-2.24	106.69	113.25
19	A	814	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
18	K	1005	BCR	C39-C30-C25	-2.24	106.66	110.30
19	3	317	CLA	C3D-C2D-C1D	-2.24	102.77	105.83
19	L	304	CLA	C3D-C2D-C1D	-2.24	102.77	105.83
18	4	301	BCR	C29-C28-C27	2.24	116.39	111.38
19	B	828	CLA	CHA-C4D-ND	2.24	137.19	132.50
19	A	816	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
19	A	854	CLA	C3D-C2D-C1D	-2.24	102.78	105.83
20	4	317	CHL	C3A-C2A-C1A	2.24	104.69	101.34
21	1	520	LHG	O7-C7-O9	-2.24	118.30	123.70
19	A	806	CLA	CHA-C4D-ND	2.24	137.18	132.50
19	A	809	CLA	C3D-C2D-C1D	-2.24	102.78	105.83
24	4	320	LMT	C1'-O5'-C5'	-2.24	109.30	113.69
19	G	204	CLA	O2A-CGA-CBA	2.24	118.92	111.91
19	F	303	CLA	CHA-C4D-ND	2.24	137.18	132.50
19	1	504	CLA	CAA-C2A-C3A	-2.24	106.66	112.78
18	L	306	BCR	C34-C9-C10	-2.24	119.79	122.92
19	2	504	CLA	C3D-C2D-C1D	-2.23	102.78	105.83
19	G	201	CLA	CAC-C3C-C4C	2.23	127.71	124.81
19	4	309	CLA	CHA-C4D-ND	2.23	137.17	132.50
19	A	825	CLA	CMB-C2B-C1B	-2.23	125.03	128.46
19	G	201	CLA	C3D-C2D-C1D	-2.23	102.78	105.83
19	4	305	CLA	C1-O2A-CGA	2.23	122.30	116.44
19	3	310	CLA	CMD-C2D-C3D	-2.23	122.48	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	819	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
18	B	853	BCR	C27-C26-C25	-2.23	119.49	122.73
19	J	1101	CLA	O2A-CGA-CBA	2.23	118.91	111.91
19	L	305	CLA	CHA-C1A-NA	-2.23	121.29	126.40
19	3	316	CLA	CAC-C3C-C4C	2.23	127.70	124.81
19	3	310	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
19	3	307	CLA	OBD-CAD-C3D	-2.23	123.16	128.52
19	4	311	CLA	CHA-C4D-ND	2.23	137.16	132.50
19	B	809	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
18	B	849	BCR	C37-C22-C23	2.23	121.59	118.08
18	1	503	BCR	C39-C30-C25	-2.23	106.69	110.30
18	A	856	BCR	C35-C13-C14	-2.23	119.80	122.92
19	A	812	CLA	CHA-C1A-NA	-2.23	121.30	126.40
19	2	509	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
22	4	322	LMG	C9-C8-C7	-2.23	106.52	111.79
20	2	512	CHL	CMB-C2B-C3B	2.23	128.84	124.68
26	4	319	DGD	C1D-C2D-C3D	-2.23	105.36	110.00
19	3	316	CLA	C2C-C1C-NC	2.22	112.06	109.97
19	2	504	CLA	CAC-C3C-C4C	2.22	127.70	124.81
19	3	316	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
19	G	203	CLA	CMB-C2B-C1B	-2.22	125.05	128.46
19	A	808	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
20	1	512	CHL	C1-O2A-CGA	2.22	123.43	116.11
18	A	852	BCR	C34-C9-C8	2.22	121.58	118.08
19	A	831	CLA	C1D-ND-C4D	-2.22	104.76	106.33
19	4	308	CLA	CAC-C3C-C4C	2.22	127.69	124.81
19	A	809	CLA	CHA-C4D-ND	2.22	137.14	132.50
19	B	818	CLA	O2A-CGA-CBA	2.22	118.88	111.91
19	B	839	CLA	CHA-C4D-ND	2.22	137.14	132.50
19	L	303	CLA	CHA-C4D-ND	2.22	137.14	132.50
20	2	526	CHL	CHD-C4C-C3C	2.22	128.10	124.84
19	A	831	CLA	O2A-CGA-CBA	2.22	118.87	111.91
19	B	830	CLA	CHA-C4D-ND	2.22	137.14	132.50
18	L	302	BCR	C23-C24-C25	2.22	133.43	127.20
19	B	807	CLA	C3D-C2D-C1D	-2.22	102.81	105.83
19	A	821	CLA	C1D-ND-C4D	-2.22	104.76	106.33
19	2	507	CLA	O2A-CGA-CBA	2.22	118.86	111.91
18	A	850	BCR	C11-C12-C13	-2.22	120.19	126.42
19	B	817	CLA	CAC-C3C-C4C	2.21	127.68	124.81
19	B	839	CLA	O2A-CGA-CBA	2.21	118.86	111.91
19	3	308	CLA	CAC-C3C-C4C	2.21	127.68	124.81
18	3	304	BCR	C27-C26-C25	-2.21	119.52	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	812	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
19	B	839	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
19	A	825	CLA	C1-O2A-CGA	2.21	122.25	116.44
19	A	832	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
19	3	309	CLA	O2A-CGA-CBA	2.21	118.84	111.91
19	A	836	CLA	CMB-C2B-C1B	-2.21	125.07	128.46
19	3	308	CLA	CHA-C4D-ND	2.21	137.12	132.50
22	J	1104	LMG	C30-C29-C28	-2.21	105.58	113.62
18	A	848	BCR	C30-C25-C24	2.21	122.03	115.78
19	4	309	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
19	A	835	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
19	1	515	CLA	CHA-C1A-NA	-2.21	121.34	126.40
19	A	819	CLA	CMB-C2B-C1B	-2.21	125.07	128.46
19	A	814	CLA	CMB-C2B-C3B	2.21	128.81	124.68
19	A	803	CLA	CHA-C4D-ND	2.21	137.12	132.50
19	A	819	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
19	J	1101	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
20	2	512	CHL	CHA-C4D-ND	2.21	137.11	132.50
19	B	826	CLA	CHD-C1D-ND	-2.21	122.43	124.45
19	4	304	CLA	CHA-C1A-NA	-2.21	121.35	126.40
19	J	1101	CLA	C3D-C2D-C1D	-2.20	102.82	105.83
18	2	503	BCR	C19-C18-C17	2.20	122.32	118.94
18	A	850	BCR	C27-C26-C25	-2.20	119.53	122.73
19	4	312	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
19	4	315	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
19	B	824	CLA	CMB-C2B-C1B	-2.20	125.08	128.46
20	2	516	CHL	C4D-CHA-C1A	2.20	123.93	121.25
19	A	803	CLA	CHA-C1A-NA	-2.20	121.36	126.40
19	1	507	CLA	CAC-C3C-C4C	2.20	127.67	124.81
19	K	1002	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
19	A	809	CLA	O2A-CGA-CBA	2.20	118.82	111.91
19	A	819	CLA	O2A-CGA-CBA	2.20	118.82	111.91
19	A	839	CLA	C1D-ND-C4D	-2.20	104.77	106.33
20	1	512	CHL	CHD-C4C-C3C	2.20	128.08	124.84
19	1	508	CLA	CHA-C1A-NA	-2.20	121.36	126.40
19	B	811	CLA	C1-O2A-CGA	2.20	122.22	116.44
19	1	516	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
19	A	839	CLA	CHA-C4D-ND	2.20	137.10	132.50
19	2	510	CLA	CMA-C3A-C4A	2.20	117.68	111.77
22	G	210	LMG	C7-O1-C1	-2.20	109.44	113.74
19	A	830	CLA	CMA-C3A-C4A	2.20	117.68	111.77
19	J	1101	CLA	O2D-CGD-O1D	-2.20	119.54	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	J	1106	DGD	C3A-C2A-C1A	-2.20	105.63	113.62
19	A	822	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
18	I	101	BCR	C34-C9-C10	-2.20	119.85	122.92
19	L	305	CLA	O2A-CGA-CBA	2.20	118.80	111.91
19	B	825	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
19	B	831	CLA	O2A-CGA-CBA	2.19	118.79	111.91
18	A	849	BCR	C12-C13-C14	-2.19	115.57	118.94
19	F	302	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
17	1	501	LUT	C15-C14-C13	2.19	130.44	127.31
19	B	825	CLA	CAA-CBA-CGA	-2.19	106.84	113.25
19	1	505	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
19	A	807	CLA	CMB-C2B-C1B	-2.19	125.10	128.46
19	J	1102	CLA	CMA-C3A-C4A	2.19	117.66	111.77
19	1	509	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
19	L	304	CLA	O2A-CGA-CBA	2.19	118.78	111.91
19	2	504	CLA	C1-O2A-CGA	2.19	122.19	116.44
19	B	804	CLA	CHA-C1A-NA	-2.19	121.38	126.40
19	A	819	CLA	CHA-C4D-ND	2.19	137.08	132.50
18	B	853	BCR	C32-C1-C6	-2.19	106.75	110.30
18	3	303	BCR	C37-C22-C23	2.19	121.53	118.08
18	3	304	BCR	C36-C18-C19	-2.19	114.63	118.08
19	B	834	CLA	CHA-C4D-ND	2.19	137.08	132.50
19	3	309	CLA	CHA-C1A-NA	-2.19	121.38	126.40
19	B	810	CLA	CMB-C2B-C1B	-2.19	125.10	128.46
19	1	516	CLA	O2A-CGA-CBA	2.19	118.78	111.91
23	4	303	XAT	C40-C33-C34	-2.19	119.86	122.92
18	A	856	BCR	C36-C18-C19	-2.19	114.63	118.08
19	A	802	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
19	K	1004	CLA	C3A-C2A-C1A	-2.19	101.69	104.74
19	A	814	CLA	C3D-C2D-C1D	-2.19	102.85	105.83
18	3	303	BCR	C8-C9-C10	2.19	122.30	118.94
19	B	833	CLA	O2A-CGA-CBA	2.19	118.77	111.91
19	2	504	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
19	B	810	CLA	C1D-ND-C4D	-2.18	104.78	106.33
19	A	837	CLA	O2A-CGA-CBA	2.18	118.76	111.91
19	H	1000	CLA	C3D-C2D-C1D	-2.18	102.85	105.83
19	A	827	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
19	B	825	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
19	A	815	CLA	C3D-C2D-C1D	-2.18	102.85	105.83
19	B	812	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
19	4	304	CLA	C1D-ND-C4D	-2.18	104.78	106.33
19	B	814	CLA	CHA-C1A-NA	-2.18	121.40	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	856	BCR	C31-C1-C6	-2.18	106.76	110.30
19	A	855	CLA	CHA-C4D-ND	2.18	137.06	132.50
19	4	308	CLA	C1-O2A-CGA	2.18	122.17	116.44
19	B	806	CLA	CHA-C4D-ND	2.18	137.06	132.50
19	4	305	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
22	2	519	LMG	C1-C2-C3	-2.18	105.45	110.00
19	1	511	CLA	CMA-C3A-C4A	2.18	117.63	111.77
19	3	307	CLA	CHA-C1A-NA	-2.18	121.41	126.40
19	A	833	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
19	A	827	CLA	CMB-C2B-C3B	2.18	128.76	124.68
19	B	830	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
17	3	301	LUT	C1-C2-C3	-2.18	108.72	113.64
19	1	515	CLA	C1D-ND-C4D	-2.18	104.79	106.33
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	G	204	CLA	CHA-C1A-NA	-2.18	121.42	126.40
19	A	823	CLA	O2A-CGA-CBA	2.17	118.73	111.91
18	B	856	BCR	C32-C1-C6	-2.17	106.77	110.30
19	B	829	CLA	C2C-C1C-NC	2.17	112.01	109.97
19	1	505	CLA	CHA-C1A-NA	-2.17	121.42	126.40
19	A	826	CLA	CHA-C4D-ND	2.17	137.04	132.50
19	A	828	CLA	CHA-C4D-ND	2.17	137.04	132.50
20	3	314	CHL	C1-O2A-CGA	2.17	123.27	116.11
19	B	815	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
18	A	852	BCR	C35-C13-C12	2.17	121.50	118.08
19	B	819	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
19	B	820	CLA	C2D-C1D-ND	2.17	111.70	110.10
19	1	504	CLA	CAC-C3C-C4C	2.17	127.63	124.81
19	B	827	CLA	CHA-C4D-ND	2.17	137.04	132.50
19	4	311	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
19	1	508	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
19	B	820	CLA	C6-C7-C8	-2.17	108.91	115.92
19	B	832	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
19	1	509	CLA	CAC-C3C-C4C	2.17	127.62	124.81
19	A	854	CLA	C11-C12-C13	-2.17	108.91	115.92
19	B	817	CLA	CMA-C3A-C4A	2.17	117.60	111.77
19	4	318	CLA	CMA-C3A-C4A	2.17	117.60	111.77
24	3	318	LMT	O5'-C1'-C2'	-2.17	105.76	110.35
19	A	814	CLA	C1D-ND-C4D	-2.17	104.80	106.33
19	A	824	CLA	C3D-C2D-C1D	-2.17	102.88	105.83
22	4	322	LMG	O8-C28-C29	2.17	118.70	111.91
19	A	835	CLA	O2A-CGA-CBA	2.17	118.70	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	838	CLA	O2A-CGA-CBA	2.17	118.70	111.91
19	A	810	CLA	C3D-C2D-C1D	-2.17	102.88	105.83
20	1	512	CHL	C1D-CHD-C4C	-2.17	121.39	126.06
19	4	305	CLA	CAC-C3C-C4C	2.16	127.62	124.81
19	J	1105	CLA	CMB-C2B-C3B	2.16	128.73	124.68
21	1	517	LHG	O7-C7-O9	-2.16	118.47	123.70
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	A	814	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
20	2	516	CHL	CMB-C2B-C1B	-2.16	125.14	128.46
19	A	841	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
19	3	311	CLA	CAC-C3C-C4C	2.16	127.61	124.81
19	1	513	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
19	3	309	CLA	C2C-C1C-NC	2.16	112.00	109.97
19	4	305	CLA	C2C-C1C-NC	2.16	112.00	109.97
19	A	816	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
21	1	520	LHG	O8-C6-C5	2.16	114.72	108.43
18	B	849	BCR	C8-C7-C6	2.16	133.27	127.20
20	2	526	CHL	C1-C2-C3	-2.16	122.31	126.04
19	A	835	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
20	2	515	CHL	CHD-C4C-C3C	2.16	128.01	124.84
19	J	1101	CLA	C11-C12-C13	-2.16	108.94	115.92
19	A	814	CLA	CHA-C1A-NA	-2.16	121.46	126.40
26	G	207	DGD	O3G-C3G-C2G	-2.16	105.69	110.90
19	B	835	CLA	CHA-C1A-NA	-2.16	121.46	126.40
19	A	841	CLA	CHA-C4D-ND	2.16	137.01	132.50
19	A	813	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
17	J	1109	LUT	C20-C13-C14	-2.16	119.90	122.92
18	L	302	BCR	C35-C13-C14	-2.16	119.90	122.92
19	K	1002	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
19	B	833	CLA	C2D-C1D-ND	2.15	111.69	110.10
19	H	1000	CLA	CMD-C2D-C3D	-2.15	122.66	127.61
19	A	821	CLA	O2A-CGA-CBA	2.15	118.67	111.91
18	A	852	BCR	C37-C22-C23	2.15	121.47	118.08
19	A	815	CLA	C1D-ND-C4D	-2.15	104.81	106.33
19	A	837	CLA	C3D-C2D-C1D	-2.15	102.89	105.83
19	4	306	CLA	CHA-C1A-NA	-2.15	121.47	126.40
19	B	813	CLA	C3D-C2D-C1D	-2.15	102.89	105.83
19	3	313	CLA	CHA-C1A-NA	-2.15	121.47	126.40
19	1	508	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
20	1	514	CHL	C1-O2A-CGA	2.15	122.08	116.44
19	3	312	CLA	C1D-ND-C4D	-2.15	104.81	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	507	CLA	CMB-C2B-C1B	-2.15	125.16	128.46
19	B	833	CLA	C1D-ND-C4D	-2.15	104.81	106.33
18	L	302	BCR	C30-C25-C26	-2.15	119.59	122.61
19	1	516	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
19	B	825	CLA	CAA-C2A-C1A	-2.15	104.94	111.97
19	3	313	CLA	CMD-C2D-C3D	-2.15	122.68	127.61
19	A	823	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
19	B	807	CLA	O2A-CGA-CBA	2.15	118.64	111.91
19	G	204	CLA	C16-C15-C13	-2.14	108.99	115.92
19	B	817	CLA	CMB-C2B-C3B	2.14	128.69	124.68
17	1	502	LUT	C11-C12-C13	-2.14	120.39	126.42
19	B	822	CLA	CAA-CBA-CGA	-2.14	106.99	113.25
18	A	852	BCR	C40-C30-C25	-2.14	106.82	110.30
19	B	808	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
18	G	205	BCR	C37-C22-C23	2.14	121.45	118.08
19	A	835	CLA	C2C-C1C-NC	2.14	111.98	109.97
19	B	836	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
18	A	856	BCR	C38-C26-C27	2.14	117.73	113.62
18	L	306	BCR	C38-C26-C27	2.14	117.73	113.62
19	A	841	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
19	1	511	CLA	CHA-C1A-NA	-2.14	121.49	126.40
19	B	819	CLA	CHA-C4D-ND	2.14	136.98	132.50
19	A	817	CLA	C1-O2A-CGA	2.14	122.06	116.44
19	A	836	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
17	4	302	LUT	C11-C10-C9	2.14	130.36	127.31
19	B	827	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
19	B	815	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
19	K	1003	CLA	C3A-C2A-C1A	-2.14	101.76	104.74
19	B	810	CLA	CHA-C1A-NA	-2.14	121.50	126.40
19	4	307	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
19	B	820	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
19	B	837	CLA	CHA-C1A-NA	-2.14	121.50	126.40
19	B	821	CLA	CAC-C3C-C4C	2.14	127.58	124.81
19	3	312	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
20	3	314	CHL	CMB-C2B-C1B	-2.14	125.18	128.46
19	2	504	CLA	CMB-C2B-C3B	2.14	128.68	124.68
19	2	514	CLA	CHA-C1A-NA	-2.14	121.51	126.40
19	B	813	CLA	CHA-C1A-NA	-2.14	121.51	126.40
19	B	814	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
19	G	204	CLA	CHA-C4D-ND	2.13	136.97	132.50
19	A	842	CLA	CMD-C2D-C3D	-2.13	122.70	127.61
18	A	851	BCR	C10-C11-C12	-2.13	116.56	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	G	203	CLA	CHA-C1A-NA	-2.13	121.51	126.40
19	H	1000	CLA	CHA-C1A-NA	-2.13	121.51	126.40
18	4	301	BCR	C30-C25-C26	-2.13	119.61	122.61
19	1	509	CLA	CMB-C2B-C3B	2.13	128.67	124.68
19	A	838	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
18	B	849	BCR	C35-C13-C12	-2.13	114.72	118.08
24	B	846	LMT	O5B-C5B-C4B	2.13	113.57	109.69
19	3	308	CLA	CMB-C2B-C1B	-2.13	125.19	128.46
19	A	823	CLA	CAC-C3C-C4C	2.13	127.58	124.81
19	3	317	CLA	CHA-C1A-NA	-2.13	121.52	126.40
19	4	318	CLA	CMB-C2B-C3B	2.13	128.67	124.68
19	B	810	CLA	CMA-C3A-C4A	2.13	117.50	111.77
19	B	818	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
19	A	815	CLA	CHA-C1A-NA	-2.13	121.52	126.40
19	A	829	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
19	K	1001	CLA	CHA-C1A-NA	-2.13	121.52	126.40
22	B	844	LMG	O8-C28-O10	-2.13	118.22	123.59
19	4	311	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
19	A	824	CLA	O2A-CGA-CBA	2.13	118.59	111.91
19	A	838	CLA	CHA-C1A-NA	-2.13	121.53	126.40
19	B	832	CLA	O2A-CGA-CBA	2.13	118.58	111.91
18	L	306	BCR	C32-C1-C6	-2.13	106.85	110.30
17	2	501	LUT	C31-C32-C33	-2.13	120.44	126.42
19	B	832	CLA	CAA-CBA-CGA	-2.13	107.04	113.25
19	B	840	CLA	CHA-C4D-ND	2.12	136.94	132.50
18	I	101	BCR	C8-C7-C6	2.12	133.17	127.20
19	B	831	CLA	CMA-C3A-C4A	2.12	117.48	111.77
19	B	834	CLA	CHA-C1A-NA	-2.12	121.53	126.40
18	1	503	BCR	C37-C22-C23	2.12	121.42	118.08
19	2	510	CLA	CHA-C1A-NA	-2.12	121.53	126.40
22	4	322	LMG	O7-C10-O9	-2.12	118.57	123.70
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
20	1	512	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
19	A	832	CLA	C1D-ND-C4D	-2.12	104.83	106.33
18	A	848	BCR	C37-C22-C23	2.12	121.42	118.08
19	L	301	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
19	1	513	CLA	CHA-C1A-NA	-2.12	121.54	126.40
19	B	837	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
18	B	856	BCR	C28-C27-C26	-2.12	110.29	114.08
20	4	317	CHL	C1D-CHD-C4C	-2.12	121.48	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	824	CLA	CHA-C1A-NA	-2.12	121.55	126.40
18	I	102	BCR	C37-C22-C23	2.12	121.42	118.08
19	H	1000	CLA	C1D-ND-C4D	-2.12	104.83	106.33
18	J	1108	BCR	C39-C30-C25	-2.12	106.86	110.30
29	A	844	PQN	C21-C20-C18	-2.12	109.07	115.92
17	1	501	LUT	C18-C5-C6	-2.12	122.15	124.53
19	3	307	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
19	2	508	CLA	C1-O2A-CGA	2.12	122.00	116.44
19	2	508	CLA	CMB-C2B-C1B	-2.12	125.21	128.46
19	A	830	CLA	CMD-C2D-C3D	-2.12	122.75	127.61
19	B	803	CLA	C2A-C3A-C4A	2.12	105.29	101.87
19	A	836	CLA	CHA-C1A-NA	-2.12	121.55	126.40
20	4	313	CHL	CHD-C4C-C3C	2.12	127.95	124.84
19	A	835	CLA	CHA-C1A-NA	-2.12	121.55	126.40
22	2	519	LMG	O8-C28-O10	-2.12	118.25	123.59
19	G	202	CLA	CHA-C1A-NA	-2.11	121.56	126.40
19	A	809	CLA	CMB-C2B-C1B	-2.11	125.21	128.46
19	3	308	CLA	CHA-C1A-NA	-2.11	121.56	126.40
19	A	802	CLA	CHA-C1A-NA	-2.11	121.56	126.40
24	2	523	LMT	O5B-C5B-C4B	2.11	113.53	109.69
19	2	510	CLA	CMB-C2B-C1B	-2.11	125.22	128.46
20	2	515	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
19	A	825	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
19	A	831	CLA	CMD-C2D-C3D	-2.11	122.75	127.61
19	1	515	CLA	C2D-C1D-ND	2.11	111.66	110.10
19	2	508	CLA	CMD-C2D-C3D	-2.11	122.75	127.61
19	F	303	CLA	O2A-CGA-CBA	2.11	118.53	111.91
19	2	505	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
19	1	509	CLA	CHA-C1A-NA	-2.11	121.56	126.40
19	B	826	CLA	CMB-C2B-C3B	2.11	128.62	124.68
17	2	501	LUT	C31-C30-C29	2.11	130.32	127.31
19	A	831	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
20	4	313	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
19	B	818	CLA	C1D-ND-C4D	-2.11	104.84	106.33
20	3	314	CHL	C1D-CHD-C4C	-2.11	121.51	126.06
19	A	819	CLA	C1-O2A-CGA	2.11	121.97	116.44
19	1	516	CLA	CHA-C1A-NA	-2.11	121.57	126.40
19	1	504	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
19	A	854	CLA	CHA-C4D-ND	2.11	136.90	132.50
26	J	1106	DGD	C2G-O2G-C1B	2.11	122.97	117.79
18	B	852	BCR	C8-C9-C10	2.10	122.17	118.94
20	4	316	CHL	CHD-C1D-C2D	2.10	129.89	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	834	CLA	C1-O2A-CGA	2.10	121.96	116.44
19	A	814	CLA	O2A-CGA-CBA	2.10	118.51	111.91
19	L	304	CLA	CHA-C4D-ND	2.10	136.90	132.50
19	2	511	CLA	CHA-C1A-NA	-2.10	121.58	126.40
21	A	845	LHG	O8-C23-O10	-2.10	118.28	123.59
20	1	512	CHL	C2C-C3C-C4C	2.10	107.99	106.49
19	3	305	CLA	OBD-CAD-C3D	-2.10	123.46	128.52
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	B	816	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
19	4	312	CLA	CAC-C3C-C4C	2.10	127.53	124.81
19	3	310	CLA	CHA-C1A-NA	-2.10	121.59	126.40
18	4	301	BCR	C8-C9-C10	2.10	122.16	118.94
19	G	201	CLA	CHA-C4D-ND	2.10	136.89	132.50
24	G	208	LMT	C1'-O5'-C5'	-2.10	109.57	113.69
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	1	516	CLA	CAC-C3C-C4C	2.10	127.53	124.81
17	3	302	LUT	C19-C9-C8	2.10	121.38	118.08
18	A	849	BCR	C37-C22-C23	2.10	121.38	118.08
20	1	512	CHL	C3A-C2A-C1A	2.10	104.48	101.34
20	4	317	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
19	H	1000	CLA	O2A-CGA-CBA	2.10	118.48	111.91
19	4	310	CLA	CHA-C1A-NA	-2.10	121.60	126.40
19	3	313	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
20	2	516	CHL	C1B-CHB-C4A	-2.09	125.97	130.12
19	2	507	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
20	2	526	CHL	C4D-CHA-C1A	2.09	123.80	121.25
20	4	314	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
19	1	509	CLA	C1-O2A-CGA	2.09	121.94	116.44
19	B	822	CLA	O2A-CGA-CBA	2.09	118.48	111.91
20	4	316	CHL	C4A-NA-C1A	2.09	107.65	106.71
19	4	315	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
19	A	825	CLA	C2C-C1C-NC	2.09	111.93	109.97
19	3	308	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
20	2	526	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
22	J	1104	LMG	C9-C8-C7	-2.09	106.84	111.79
19	B	832	CLA	CHA-C4D-ND	2.09	136.87	132.50
20	4	316	CHL	CHD-C4C-C3C	2.09	127.91	124.84
19	A	825	CLA	CHA-C1A-NA	-2.09	121.61	126.40
19	A	827	CLA	CHA-C1A-NA	-2.09	121.61	126.40
19	3	308	CLA	CMD-C2D-C3D	-2.09	122.81	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	827	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
17	1	502	LUT	C40-C33-C34	-2.09	120.00	122.92
19	B	803	CLA	CHA-C1A-NA	-2.09	121.62	126.40
19	A	812	CLA	CAC-C3C-C4C	2.09	127.52	124.81
18	A	850	BCR	C35-C13-C14	-2.09	120.00	122.92
20	2	526	CHL	C1B-CHB-C4A	-2.09	125.98	130.12
19	K	1001	CLA	CMB-C2B-C3B	2.09	128.58	124.68
19	B	828	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
19	A	827	CLA	O2A-CGA-CBA	2.08	118.45	111.91
19	F	303	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
20	1	514	CHL	CMB-C2B-C1B	-2.08	125.26	128.46
18	F	306	BCR	C39-C30-C25	-2.08	106.92	110.30
18	I	101	BCR	C39-C30-C25	-2.08	106.92	110.30
19	A	817	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
19	A	802	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
18	L	302	BCR	C39-C30-C25	-2.08	106.92	110.30
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	2	506	CLA	CHA-C1A-NA	-2.08	121.63	126.40
22	B	845	LMG	C1-O6-C5	2.08	117.77	113.69
19	3	312	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
19	J	1101	CLA	C11-C10-C8	-2.08	109.19	115.92
19	1	513	CLA	CMB-C2B-C3B	2.08	128.57	124.68
21	B	842	LHG	O7-C7-O9	-2.08	118.83	122.96
19	B	820	CLA	C11-C10-C8	-2.08	109.20	115.92
19	A	820	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
18	B	853	BCR	C29-C28-C27	-2.08	106.73	111.38
20	1	521	CHL	CMB-C2B-C1B	-2.08	125.27	128.46
19	4	308	CLA	O2A-CGA-CBA	2.08	118.43	111.91
19	1	509	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
27	A	801	CL0	C4-C3-C5	2.08	118.76	115.27
19	B	805	CLA	CAC-C3C-C4C	2.08	127.50	124.81
19	1	510	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
19	B	819	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
19	A	802	CLA	CBC-CAC-C3C	-2.07	106.71	112.43
19	B	837	CLA	CMD-C2D-C3D	-2.07	122.84	127.61
20	1	514	CHL	CHC-C1C-NC	2.07	127.35	124.20
20	4	317	CHL	CHD-C1D-C2D	2.07	129.83	125.48
26	B	801	DGD	O3G-C3G-C2G	2.07	115.90	110.90
19	2	505	CLA	CHA-C1A-NA	-2.07	121.65	126.40
18	A	856	BCR	C37-C22-C23	2.07	121.34	118.08
18	4	301	BCR	C37-C22-C23	2.07	121.34	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	824	CLA	O2A-CGA-CBA	2.07	118.41	111.91
19	G	202	CLA	CMB-C2B-C3B	2.07	128.55	124.68
19	J	1101	CLA	C1-O2A-CGA	2.07	121.87	116.44
19	A	855	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
19	B	820	CLA	CHA-C1A-NA	-2.07	121.66	126.40
19	3	305	CLA	CHA-C1A-NA	-2.07	121.66	126.40
19	3	311	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
19	1	504	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
19	A	840	CLA	O2A-CGA-CBA	2.07	118.40	111.91
22	2	520	LMG	O1-C1-C2	2.07	110.57	108.15
27	A	801	CL0	C3D-C2D-C1D	-2.07	103.01	105.83
19	3	316	CLA	C1D-ND-C4D	-2.07	104.87	106.33
20	4	316	CHL	CMB-C2B-C1B	-2.07	125.29	128.46
19	4	306	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
19	2	504	CLA	CAA-C2A-C1A	-2.07	105.21	111.97
17	4	302	LUT	C20-C13-C12	2.07	121.33	118.08
22	2	519	LMG	O1-C1-C2	2.06	111.53	108.30
19	2	509	CLA	CHA-C1A-NA	-2.06	121.67	126.40
19	A	826	CLA	CMD-C2D-C3D	-2.06	122.86	127.61
18	K	1005	BCR	C38-C26-C27	2.06	117.58	113.62
22	B	845	LMG	O7-C10-O9	-2.06	118.72	123.70
19	G	201	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
19	1	505	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
18	A	849	BCR	C10-C11-C12	-2.06	116.78	123.22
19	4	315	CLA	CMB-C2B-C3B	2.06	128.54	124.68
18	A	850	BCR	C38-C26-C25	-2.06	122.21	124.53
19	A	806	CLA	CHA-C1A-NA	-2.06	121.68	126.40
19	3	316	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
19	B	805	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
17	2	501	LUT	C39-C29-C28	2.06	121.32	118.08
18	A	852	BCR	C8-C9-C10	-2.06	115.78	118.94
19	A	812	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
19	A	833	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
19	3	305	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
20	2	512	CHL	C1-O2A-CGA	2.06	122.89	116.11
19	A	828	CLA	C1-O2A-CGA	2.06	121.84	116.44
19	J	1101	CLA	C1D-ND-C4D	-2.06	104.87	106.33
19	3	315	CLA	CHA-C1A-NA	-2.06	121.69	126.40
19	A	812	CLA	C3D-C2D-C1D	-2.06	103.03	105.83
19	3	316	CLA	CHA-C1A-NA	-2.06	121.69	126.40
19	G	201	CLA	C1-O2A-CGA	2.05	121.83	116.44
17	J	1109	LUT	C38-C25-C24	-2.05	119.16	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	821	CLA	CMD-C2D-C3D	-2.05	122.89	127.61
19	3	306	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
19	1	507	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
19	4	307	CLA	C11-C10-C8	-2.05	109.29	115.92
20	3	314	CHL	CHD-C1D-C2D	2.05	129.78	125.48
18	2	503	BCR	C36-C18-C19	-2.05	114.84	118.08
19	A	804	CLA	O2A-CGA-CBA	2.05	118.34	111.91
19	A	815	CLA	CMD-C2D-C3D	-2.05	122.90	127.61
19	3	311	CLA	CAA-C2A-C3A	-2.05	111.31	116.10
19	A	833	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
19	A	841	CLA	C1-O2A-CGA	2.05	121.82	116.44
18	I	102	BCR	C23-C24-C25	2.05	132.96	127.20
19	A	811	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
26	B	854	DGD	O6D-C5D-C6D	2.05	110.80	106.67
19	4	315	CLA	CHA-C1A-NA	-2.05	121.71	126.40
20	2	515	CHL	C4A-NA-C1A	2.05	107.63	106.71
18	A	852	BCR	C12-C13-C14	-2.05	115.80	118.94
19	3	312	CLA	CHA-C1A-NA	-2.05	121.71	126.40
19	A	804	CLA	CHA-C1A-NA	-2.05	121.71	126.40
19	A	822	CLA	CHA-C1A-NA	-2.05	121.71	126.40
18	L	302	BCR	C34-C9-C10	-2.05	120.06	122.92
19	B	829	CLA	C2D-C1D-ND	2.05	111.61	110.10
19	4	307	CLA	CAC-C3C-C4C	2.05	127.46	124.81
19	A	818	CLA	CHA-C1A-NA	-2.04	121.72	126.40
19	B	834	CLA	CMD-C2D-C3D	-2.04	122.91	127.61
19	B	832	CLA	O2D-CGD-O1D	-2.04	119.84	123.84
19	4	309	CLA	CAC-C3C-C4C	2.04	127.46	124.81
22	G	206	LMG	O7-C10-O9	-2.04	118.76	123.70
19	B	832	CLA	CMA-C3A-C4A	2.04	117.27	111.77
19	A	812	CLA	O2A-CGA-CBA	2.04	118.32	111.91
22	2	518	LMG	O7-C10-O9	-2.04	118.76	123.70
20	2	513	CHL	CMB-C2B-C1B	-2.04	125.32	128.46
19	B	840	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
18	B	853	BCR	C10-C11-C12	-2.04	116.84	123.22
18	I	102	BCR	C35-C13-C12	2.04	121.30	118.08
19	A	834	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
19	B	808	CLA	C1-O2A-CGA	2.04	121.80	116.44
19	A	821	CLA	CAC-C3C-C4C	2.04	127.46	124.81
23	2	502	XAT	C6-C7-C8	-2.04	121.68	125.99
24	B	855	LMT	C3B-C4B-C5B	-2.04	106.60	110.24
19	B	837	CLA	C1D-ND-C4D	-2.04	104.89	106.33
19	L	301	CLA	O2D-CGD-O1D	-2.04	119.85	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	504	CLA	CHA-C1A-NA	-2.04	121.73	126.40
24	B	855	LMT	C1'-O5'-C5'	-2.04	109.69	113.69
19	A	834	CLA	O2A-CGA-CBA	2.04	118.30	111.91
19	L	303	CLA	O2A-CGA-CBA	2.04	118.30	111.91
20	4	314	CHL	CHA-C4D-ND	2.04	136.76	132.50
19	G	201	CLA	C4D-CHA-C1A	2.04	123.73	121.25
19	B	822	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
19	A	821	CLA	CHA-C1A-NA	-2.04	121.74	126.40
19	H	1000	CLA	C2C-C1C-NC	2.04	111.88	109.97
19	2	514	CLA	C1D-ND-C4D	-2.04	104.89	106.33
29	A	844	PQN	C11-C12-C13	-2.04	123.40	126.79
19	A	813	CLA	C1-O2A-CGA	2.03	121.78	116.44
19	A	836	CLA	C3D-C2D-C1D	-2.03	103.05	105.83
18	B	853	BCR	C28-C27-C26	-2.03	110.44	114.08
18	B	849	BCR	C40-C30-C25	-2.03	107.00	110.30
20	1	521	CHL	CHD-C4C-C3C	2.03	127.83	124.84
17	3	301	LUT	C40-C33-C34	-2.03	120.08	122.92
19	A	834	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
19	A	820	CLA	CHA-C1A-NA	-2.03	121.74	126.40
19	J	1105	CLA	CAA-CBA-CGA	-2.03	107.32	113.25
19	4	309	CLA	O2A-CGA-CBA	2.03	118.28	111.91
19	L	305	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
18	J	1108	BCR	C29-C28-C27	2.03	115.92	111.38
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
19	B	807	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
18	B	802	BCR	C8-C7-C6	2.03	132.90	127.20
19	A	840	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
19	B	827	CLA	CMD-C2D-C3D	-2.03	122.95	127.61
19	4	315	CLA	CAC-C3C-C4C	2.03	127.44	124.81
19	A	823	CLA	CHA-C1A-NA	-2.03	121.75	126.40
19	A	829	CLA	CMD-C2D-C3D	-2.03	122.95	127.61
19	A	824	CLA	CMD-C2D-C3D	-2.03	122.95	127.61
19	A	839	CLA	O2D-CGD-O1D	-2.03	119.88	123.84
18	A	848	BCR	C34-C9-C10	-2.03	120.09	122.92
19	B	804	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
19	F	302	CLA	CHA-C1A-NA	-2.03	121.76	126.40
20	2	515	CHL	CHC-C1C-NC	2.02	127.28	124.20
19	3	307	CLA	CAA-CBA-CGA	-2.02	107.34	113.25
22	J	1104	LMG	O8-C28-C29	2.02	118.26	111.91
22	2	519	LMG	C4-C3-C2	-2.02	107.29	110.82
23	4	303	XAT	C6-C7-C8	-2.02	121.72	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	814	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
19	A	835	CLA	C1D-ND-C4D	-2.02	104.90	106.33
17	1	502	LUT	C19-C9-C10	-2.02	120.09	122.92
18	B	851	BCR	C37-C22-C23	2.02	121.26	118.08
19	A	805	CLA	O2A-CGA-CBA	2.02	118.25	111.91
19	3	317	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
19	B	829	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
29	A	844	PQN	C2M-C2-C1	2.02	119.62	116.27
22	2	519	LMG	O7-C10-O9	-2.02	118.82	123.70
17	1	501	LUT	C40-C33-C34	-2.02	120.09	122.92
19	3	315	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
17	J	1109	LUT	C28-C29-C30	2.02	122.04	118.94
19	1	508	CLA	CAA-CBA-CGA	-2.02	107.36	113.25
19	B	807	CLA	CHA-C1A-NA	-2.02	121.78	126.40
19	B	837	CLA	CMA-C3A-C4A	2.02	117.19	111.77
19	A	840	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
19	4	304	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
19	A	818	CLA	C1D-ND-C4D	-2.02	104.90	106.33
19	B	827	CLA	CMB-C2B-C3B	2.02	128.45	124.68
18	3	304	BCR	C37-C22-C23	2.02	121.25	118.08
24	3	318	LMT	C1'-O5'-C5'	-2.01	109.73	113.69
19	2	511	CLA	CMD-C2D-C3D	-2.01	122.98	127.61
26	J	1106	DGD	C3E-C4E-C5E	2.01	113.83	110.24
20	4	313	CHL	CHC-C1C-NC	2.01	127.26	124.20
19	4	305	CLA	CMA-C3A-C2A	2.01	121.95	113.83
18	3	304	BCR	C34-C9-C10	-2.01	120.10	122.92
19	4	318	CLA	CMD-C2D-C3D	-2.01	122.98	127.61
19	2	508	CLA	CHA-C1A-NA	-2.01	121.79	126.40
19	A	833	CLA	CMD-C2D-C3D	-2.01	122.99	127.61
18	A	848	BCR	C30-C25-C26	-2.01	119.78	122.61
17	3	302	LUT	C28-C29-C30	2.01	122.03	118.94
19	A	807	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
19	B	832	CLA	CMB-C2B-C3B	2.01	128.44	124.68
19	A	825	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
19	K	1003	CLA	CHA-C1A-NA	-2.01	121.89	126.41
19	B	838	CLA	CHA-C1A-NA	-2.01	121.80	126.40
20	2	515	CHL	C2C-C3C-C4C	2.01	107.92	106.49
19	A	837	CLA	CMD-C2D-C3D	-2.01	123.00	127.61
18	B	850	BCR	C37-C22-C23	2.01	121.24	118.08
19	A	811	CLA	CMD-C2D-C3D	-2.00	123.00	127.61
19	L	303	CLA	CHA-C1A-NA	-2.00	121.81	126.40
19	A	855	CLA	CMD-C2D-C3D	-2.00	123.00	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	304	BCR	C24-C25-C26	-2.00	116.61	121.46
26	4	319	DGD	C1D-O6D-C5D	-2.00	109.75	113.69
19	A	813	CLA	CMD-C2D-C3D	-2.00	123.01	127.61
17	1	501	LUT	C19-C9-C10	-2.00	120.12	122.92
19	A	815	CLA	CAC-C3C-C4C	2.00	127.41	124.81
19	B	822	CLA	CHA-C1A-NA	-2.00	121.82	126.40
19	A	821	CLA	C3D-C2D-C1D	-2.00	103.10	105.83

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
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

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Mol	Chain	Res	Type	Atom
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
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

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Mol	Chain	Res	Type	Atom
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
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

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Mol	Chain	Res	Type	Atom
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	NA
20	1	512	CHL	NC
20	1	512	CHL	ND
20	1	514	CHL	C8
20	1	514	CHL	NA
20	1	514	CHL	NC
20	1	514	CHL	ND
20	1	521	CHL	C8
20	1	521	CHL	NA
20	1	521	CHL	NC
20	1	521	CHL	ND
20	2	512	CHL	NA
20	2	512	CHL	NC
20	2	512	CHL	ND
20	2	513	CHL	NA
20	2	513	CHL	NC
20	2	513	CHL	ND
20	2	515	CHL	NA
20	2	515	CHL	NC
20	2	515	CHL	ND
20	2	516	CHL	C8
20	2	516	CHL	NA
20	2	516	CHL	NC
20	2	516	CHL	ND

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

All (2686) 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	1	502	LUT	C31-C32-C33-C40
17	2	501	LUT	C1-C6-C7-C8
17	2	501	LUT	C21-C26-C27-C28
17	2	501	LUT	C31-C32-C33-C34
17	2	501	LUT	C31-C32-C33-C40
17	3	301	LUT	C1-C6-C7-C8
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

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Mol	Chain	Res	Type	Atoms
17	J	1109	LUT	C27-C28-C29-C30
17	J	1109	LUT	C27-C28-C29-C39
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	C11-C12-C13-C35
18	3	303	BCR	C13-C14-C15-C16
18	3	303	BCR	C21-C22-C23-C24
18	3	303	BCR	C37-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	C36-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
18	A	849	BCR	C17-C18-C19-C20
18	A	849	BCR	C36-C18-C19-C20
18	A	849	BCR	C23-C24-C25-C30
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

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Mol	Chain	Res	Type	Atoms
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	851	BCR	C36-C18-C19-C20
18	A	851	BCR	C23-C24-C25-C30
18	A	852	BCR	C7-C8-C9-C10
18	A	852	BCR	C7-C8-C9-C34
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	C36-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	853	BCR	C37-C22-C23-C24
18	B	856	BCR	C7-C8-C9-C10
18	B	856	BCR	C7-C8-C9-C34
18	B	856	BCR	C11-C10-C9-C8
18	B	856	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
18	B	856	BCR	C17-C18-C19-C20
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	101	BCR	C36-C18-C19-C20
18	I	102	BCR	C7-C8-C9-C34
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	C36-C18-C19-C20
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	C1-C6-C7-C8
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	306	BCR	C23-C24-C25-C30
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

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Mol	Chain	Res	Type	Atoms
19	1	506	CLA	C1A-C2A-CAA-CBA
19	1	509	CLA	CHA-CBD-CGD-O1D
19	1	509	CLA	CHA-CBD-CGD-O2D
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	511	CLA	CAD-CBD-CGD-O2D
19	1	515	CLA	CHA-CBD-CGD-O1D
19	1	515	CLA	CHA-CBD-CGD-O2D
19	1	516	CLA	CBD-CGD-O2D-CED
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	509	CLA	CHA-CBD-CGD-O1D
19	2	509	CLA	CHA-CBD-CGD-O2D
19	2	511	CLA	C1A-C2A-CAA-CBA
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	CHA-CBD-CGD-O1D
19	3	305	CLA	CHA-CBD-CGD-O2D
19	3	305	CLA	CBD-CGD-O2D-CED
19	3	306	CLA	C2-C1-O2A-CGA
19	3	307	CLA	CHA-CBD-CGD-O1D
19	3	307	CLA	CHA-CBD-CGD-O2D
19	3	307	CLA	CBD-CGD-O2D-CED
19	3	307	CLA	C2-C3-C5-C6
19	3	307	CLA	C4-C3-C5-C6
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	312	CLA	CHA-CBD-CGD-O1D
19	3	312	CLA	CHA-CBD-CGD-O2D
19	3	313	CLA	C1A-C2A-CAA-CBA
19	3	313	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
19	3	315	CLA	CBD-CGD-O2D-CED
19	3	316	CLA	CHA-CBD-CGD-O1D
19	3	316	CLA	CHA-CBD-CGD-O2D
19	3	317	CLA	CBA-CGA-O2A-C1
19	4	304	CLA	C6-C7-C8-C9
19	4	306	CLA	CBD-CGD-O2D-CED
19	4	306	CLA	C2-C3-C5-C6
19	4	306	CLA	C4-C3-C5-C6
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	309	CLA	CHA-CBD-CGD-O1D
19	4	309	CLA	CHA-CBD-CGD-O2D
19	4	311	CLA	CHA-CBD-CGD-O1D
19	4	311	CLA	CHA-CBD-CGD-O2D
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	802	CLA	CHA-CBD-CGD-O1D
19	A	802	CLA	CHA-CBD-CGD-O2D
19	A	802	CLA	C2-C3-C5-C6
19	A	802	CLA	C4-C3-C5-C6
19	A	804	CLA	C1A-C2A-CAA-CBA
19	A	804	CLA	C3A-C2A-CAA-CBA
19	A	805	CLA	CHA-CBD-CGD-O1D
19	A	805	CLA	CHA-CBD-CGD-O2D
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
19	A	808	CLA	C2-C3-C5-C6
19	A	808	CLA	C4-C3-C5-C6
19	A	809	CLA	CBD-CGD-O2D-CED
19	A	810	CLA	CHA-CBD-CGD-O1D
19	A	810	CLA	CHA-CBD-CGD-O2D
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

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Mol	Chain	Res	Type	Atoms
19	A	815	CLA	C1A-C2A-CAA-CBA
19	A	815	CLA	CHA-CBD-CGD-O1D
19	A	815	CLA	CHA-CBD-CGD-O2D
19	A	817	CLA	CBD-CGD-O2D-CED
19	A	818	CLA	C3A-C2A-CAA-CBA
19	A	818	CLA	C2-C3-C5-C6
19	A	818	CLA	C4-C3-C5-C6
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	CHA-CBD-CGD-O1D
19	A	824	CLA	CHA-CBD-CGD-O2D
19	A	824	CLA	C2-C3-C5-C6
19	A	824	CLA	C4-C3-C5-C6
19	A	827	CLA	CHA-CBD-CGD-O1D
19	A	827	CLA	CHA-CBD-CGD-O2D
19	A	828	CLA	O2A-C1-C2-C3
19	A	828	CLA	C6-C7-C8-C9
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	835	CLA	CHA-CBD-CGD-O1D
19	A	835	CLA	CHA-CBD-CGD-O2D
19	A	838	CLA	CHA-CBD-CGD-O1D
19	A	838	CLA	CHA-CBD-CGD-O2D
19	A	838	CLA	C4-C3-C5-C6
19	A	839	CLA	CHA-CBD-CGD-O1D
19	A	839	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	C2-C3-C5-C6
19	A	840	CLA	C4-C3-C5-C6
19	A	842	CLA	CHA-CBD-CGD-O1D
19	A	842	CLA	CHA-CBD-CGD-O2D
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	CHA-CBD-CGD-O1D
19	B	804	CLA	CHA-CBD-CGD-O2D
19	B	804	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
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	CHA-CBD-CGD-O1D
19	B	806	CLA	CHA-CBD-CGD-O2D
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
19	B	819	CLA	CBD-CGD-O2D-CED
19	B	822	CLA	C2-C1-O2A-CGA
19	B	822	CLA	CHA-CBD-CGD-O1D
19	B	822	CLA	O2A-C1-C2-C3
19	B	823	CLA	C3A-C2A-CAA-CBA
19	B	824	CLA	C2-C1-O2A-CGA
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	828	CLA	C4-C3-C5-C6
19	B	829	CLA	CHA-CBD-CGD-O1D
19	B	829	CLA	CHA-CBD-CGD-O2D
19	B	829	CLA	CAD-CBD-CGD-O1D
19	B	831	CLA	C1A-C2A-CAA-CBA
19	B	831	CLA	C3A-C2A-CAA-CBA
19	B	832	CLA	C2-C3-C5-C6
19	B	832	CLA	C4-C3-C5-C6
19	B	834	CLA	C2-C1-O2A-CGA
19	B	834	CLA	CBD-CGD-O2D-CED
19	B	834	CLA	C2-C3-C5-C6
19	B	834	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
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	C2A-CAA-CBA-CGA
19	B	839	CLA	CBD-CGD-O2D-CED
19	B	839	CLA	C4-C3-C5-C6
19	B	840	CLA	CHA-CBD-CGD-O1D
19	B	840	CLA	CHA-CBD-CGD-O2D
19	F	302	CLA	C2-C1-O2A-CGA
19	G	201	CLA	C1A-C2A-CAA-CBA
19	G	201	CLA	CHA-CBD-CGD-O1D
19	G	201	CLA	CHA-CBD-CGD-O2D
19	G	201	CLA	C2-C3-C5-C6
19	G	201	CLA	C4-C3-C5-C6
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	CHA-CBD-CGD-O1D
19	K	1001	CLA	CHA-CBD-CGD-O2D
19	K	1001	CLA	CAD-CBD-CGD-O1D
19	K	1001	CLA	CBD-CGD-O2D-CED
19	K	1002	CLA	C1A-C2A-CAA-CBA
19	K	1002	CLA	CHA-CBD-CGD-O1D
19	K	1002	CLA	CHA-CBD-CGD-O2D
19	L	303	CLA	C1A-C2A-CAA-CBA
19	L	303	CLA	C2-C1-O2A-CGA
19	L	304	CLA	CHA-CBD-CGD-O1D
19	L	304	CLA	CHA-CBD-CGD-O2D
19	L	305	CLA	C1A-C2A-CAA-CBA
20	1	514	CHL	C1A-C2A-CAA-CBA
20	1	514	CHL	C3A-C2A-CAA-CBA
20	1	514	CHL	C11-C10-C8-C9
20	2	526	CHL	C4-C3-C5-C6
20	3	314	CHL	C1A-C2A-CAA-CBA
20	3	314	CHL	C3A-C2A-CAA-CBA
20	4	316	CHL	C1A-C2A-CAA-CBA
20	4	316	CHL	C3A-C2A-CAA-CBA
20	4	316	CHL	C2-C3-C5-C6
20	4	316	CHL	C4-C3-C5-C6
21	1	517	LHG	O1-C1-C2-C3
21	1	517	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
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	O9-C7-O7-C5
21	1	520	LHG	C8-C7-O7-C5
21	2	517	LHG	O1-C1-C2-C3
21	A	845	LHG	O2-C2-C3-O3
21	A	845	LHG	C4-O6-P-O5
21	A	845	LHG	O6-C4-C5-O7
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	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	519	LMG	C8-C7-O1-C1
22	2	522	LMG	C2-C1-O1-C7
22	2	522	LMG	O6-C1-O1-C7
22	4	322	LMG	O6-C1-O1-C7
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

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Mol	Chain	Res	Type	Atoms
24	3	318	LMT	C2-C1-O1'-C1'
24	A	846	LMT	C2-C1-O1'-C1'
24	B	846	LMT	C2-C1-O1'-C1'
24	G	208	LMT	C2-C1-O1'-C1'
24	J	1107	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
29	A	844	PQN	C12-C13-C15-C16
29	A	844	PQN	C14-C13-C15-C16
30	F	301	ZEX	C25-C26-C27-C28
21	B	842	LHG	O9-C7-O7-C5
19	1	511	CLA	O1D-CGD-O2D-CED
19	3	311	CLA	O1D-CGD-O2D-CED
19	B	834	CLA	O1D-CGD-O2D-CED
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	504	CLA	CBD-CGD-O2D-CED
19	1	506	CLA	CBD-CGD-O2D-CED
19	1	507	CLA	CBD-CGD-O2D-CED
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	309	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
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	804	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	A	834	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	202	CLA	CBD-CGD-O2D-CED
19	G	203	CLA	CBD-CGD-O2D-CED
19	G	204	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	L	305	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
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

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Mol	Chain	Res	Type	Atoms
19	A	816	CLA	O1A-CGA-O2A-C1
19	G	203	CLA	O1A-CGA-O2A-C1
19	J	1105	CLA	C2C-C3C-CAC-CBC
24	G	209	LMT	C4B-C5B-C6B-O6B
19	1	513	CLA	O1D-CGD-O2D-CED
19	3	306	CLA	O1D-CGD-O2D-CED
19	3	310	CLA	O1D-CGD-O2D-CED
19	3	312	CLA	O1D-CGD-O2D-CED
19	A	806	CLA	O1D-CGD-O2D-CED
19	A	816	CLA	O1D-CGD-O2D-CED
19	A	822	CLA	O1D-CGD-O2D-CED
19	B	810	CLA	O1D-CGD-O2D-CED
19	B	822	CLA	O1D-CGD-O2D-CED
19	B	834	CLA	C5-C6-C7-C8
19	1	511	CLA	CBA-CGA-O2A-C1
19	A	816	CLA	CBA-CGA-O2A-C1
26	B	801	DGD	C2G-C1G-O1G-C1A
24	B	846	LMT	O5B-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	817	CLA	O1D-CGD-O2D-CED
19	A	818	CLA	O1D-CGD-O2D-CED
19	A	823	CLA	O1D-CGD-O2D-CED
19	A	840	CLA	O1D-CGD-O2D-CED
19	B	807	CLA	O1D-CGD-O2D-CED
19	B	811	CLA	O1D-CGD-O2D-CED
19	B	812	CLA	O1D-CGD-O2D-CED
19	B	827	CLA	O1D-CGD-O2D-CED
19	B	839	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
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

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Mol	Chain	Res	Type	Atoms
21	1	520	LHG	C24-C23-O8-C6
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
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
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
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	1	510	CLA	O1D-CGD-O2D-CED
19	A	842	CLA	O1D-CGD-O2D-CED
19	B	819	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	1	505	CLA	O1D-CGD-O2D-CED
19	1	516	CLA	O1D-CGD-O2D-CED
19	3	315	CLA	O1D-CGD-O2D-CED
24	B	846	LMT	C2B-C1B-O1B-C4'
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
19	2	506	CLA	O1D-CGD-O2D-CED
19	3	316	CLA	O1D-CGD-O2D-CED
19	A	820	CLA	O1D-CGD-O2D-CED
19	B	809	CLA	O1D-CGD-O2D-CED
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'
22	G	206	LMG	O10-C28-O8-C9
19	1	508	CLA	C3-C5-C6-C7
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	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

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Mol	Chain	Res	Type	Atoms
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
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	4	315	CLA	O1D-CGD-O2D-CED
19	A	815	CLA	O1D-CGD-O2D-CED
19	A	802	CLA	CBD-CGD-O2D-CED
19	A	808	CLA	CBD-CGD-O2D-CED
19	A	828	CLA	O1A-CGA-O2A-C1
19	A	809	CLA	C4-C3-C5-C6
19	A	826	CLA	C4-C3-C5-C6
19	B	808	CLA	C4-C3-C5-C6
19	B	824	CLA	C4-C3-C5-C6
19	F	303	CLA	C4-C3-C5-C6
19	A	809	CLA	C2-C3-C5-C6
20	2	526	CHL	C2-C3-C5-C6
19	2	508	CLA	CBD-CGD-O2D-CED
19	B	817	CLA	CBD-CGD-O2D-CED
19	B	840	CLA	CBD-CGD-O2D-CED
19	1	516	CLA	C2A-CAA-CBA-CGA
19	2	506	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	A	808	CLA	C2A-CAA-CBA-CGA
19	A	835	CLA	C2A-CAA-CBA-CGA
19	B	828	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
22	A	847	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
22	G	206	LMG	C17-C18-C19-C20
22	G	206	LMG	C35-C36-C37-C38
26	B	854	DGD	C8A-C9A-CAA-CBA
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
24	G	209	LMT	O5'-C5'-C6'-O6'
26	B	801	DGD	O6D-C5D-C6D-O5D
19	2	510	CLA	O1D-CGD-O2D-CED
19	4	305	CLA	O1D-CGD-O2D-CED
19	2	507	CLA	CBD-CGD-O2D-CED
19	B	830	CLA	CBD-CGD-O2D-CED
19	B	816	CLA	O1D-CGD-O2D-CED
19	L	301	CLA	O1D-CGD-O2D-CED
21	B	843	LHG	O9-C7-O7-C5
22	G	210	LMG	O9-C10-O7-C8
19	2	514	CLA	O1A-CGA-O2A-C1
19	3	313	CLA	O1A-CGA-O2A-C1
19	4	312	CLA	O1A-CGA-O2A-C1
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

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Mol	Chain	Res	Type	Atoms
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
19	3	317	CLA	O1A-CGA-O2A-C1
19	J	1102	CLA	O1D-CGD-O2D-CED
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
24	A	846	LMT	O5B-C1B-O1B-C4'
24	A	846	LMT	C2B-C1B-O1B-C4'
24	2	523	LMT	C4B-C5B-C6B-O6B
24	A	846	LMT	C4B-C5B-C6B-O6B
24	J	1107	LMT	C4B-C5B-C6B-O6B
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	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
21	B	843	LHG	O2-C2-C3-O3
19	B	809	CLA	C3-C5-C6-C7
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
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

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Mol	Chain	Res	Type	Atoms
19	L	305	CLA	O1A-CGA-O2A-C1
22	B	844	LMG	O10-C28-O8-C9
22	2	519	LMG	O6-C5-C6-O5
24	B	846	LMT	O5B-C5B-C6B-O6B
24	G	208	LMT	O5B-C5B-C6B-O6B
24	G	209	LMT	O5B-C5B-C6B-O6B
26	B	801	DGD	O6E-C5E-C6E-O5E
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
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	A	827	CLA	CBD-CGD-O2D-CED
19	A	841	CLA	CBD-CGD-O2D-CED
19	B	831	CLA	CBD-CGD-O2D-CED
19	L	304	CLA	CBD-CGD-O2D-CED
24	J	1107	LMT	O5B-C5B-C6B-O6B
21	1	520	LHG	C13-C14-C15-C16
26	4	319	DGD	C2A-C3A-C4A-C5A
24	A	846	LMT	O5'-C5'-C6'-O6'
24	B	846	LMT	C4B-C5B-C6B-O6B
19	G	204	CLA	O1D-CGD-O2D-CED
19	B	832	CLA	CBD-CGD-O2D-CED
19	L	303	CLA	CBD-CGD-O2D-CED
19	3	313	CLA	CBA-CGA-O2A-C1
19	G	204	CLA	CBA-CGA-O2A-C1
19	A	834	CLA	O1D-CGD-O2D-CED
19	G	202	CLA	O1D-CGD-O2D-CED
24	A	846	LMT	O5B-C5B-C6B-O6B
19	3	305	CLA	C2C-C3C-CAC-CBC
21	B	843	LHG	C2-C3-O3-P
19	A	806	CLA	O1A-CGA-O2A-C1
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	306	CLA	C3-C5-C6-C7
19	1	508	CLA	C4-C3-C5-C6
19	3	308	CLA	C4-C3-C5-C6
19	A	811	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	A	817	CLA	C4-C3-C5-C6
19	A	834	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
26	B	801	DGD	C4E-C5E-C6E-O5E
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	817	CLA	C2-C3-C5-C6
19	A	834	CLA	C2-C3-C5-C6
19	A	838	CLA	C2-C3-C5-C6
19	B	828	CLA	C2-C3-C5-C6
19	B	839	CLA	C2-C3-C5-C6
19	H	1000	CLA	C2-C3-C5-C6
19	K	1002	CLA	C2-C3-C5-C6
19	3	307	CLA	C2A-CAA-CBA-CGA
19	B	818	CLA	C2A-CAA-CBA-CGA
19	1	507	CLA	O1D-CGD-O2D-CED
19	4	311	CLA	O1D-CGD-O2D-CED
22	G	206	LMG	O6-C5-C6-O5
24	G	209	LMT	O5'-C1'-O1'-C1
19	1	504	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	A	804	CLA	O1D-CGD-O2D-CED
19	J	1101	CLA	O1D-CGD-O2D-CED
24	2	523	LMT	O5B-C5B-C6B-O6B
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	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
19	1	508	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	2	511	CLA	O1D-CGD-O2D-CED
19	B	813	CLA	O1D-CGD-O2D-CED
19	F	303	CLA	O1D-CGD-O2D-CED
21	2	517	LHG	C1-C2-C3-O3
22	G	206	LMG	O9-C10-O7-C8
26	G	207	DGD	O1B-C1B-O2G-C2G
19	A	835	CLA	C3-C5-C6-C7
19	F	303	CLA	C3-C5-C6-C7
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	A	821	CLA	CBD-CGD-O2D-CED
19	A	826	CLA	CBD-CGD-O2D-CED
19	B	820	CLA	CBD-CGD-O2D-CED
17	1	501	LUT	C29-C30-C31-C32
18	L	307	BCR	C13-C14-C15-C16
22	4	322	LMG	C29-C30-C31-C32
19	A	807	CLA	C8-C10-C11-C12
19	B	812	CLA	C10-C11-C12-C13
24	G	208	LMT	C4B-C5B-C6B-O6B
22	4	322	LMG	C14-C15-C16-C17
24	G	209	LMT	C5'-C4'-O1B-C1B
22	G	206	LMG	C4-C5-C6-O5
19	1	507	CLA	C15-C16-C17-C18
19	4	307	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
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
19	3	316	CLA	CBA-CGA-O2A-C1
21	2	517	LHG	O2-C2-C3-O3
22	A	847	LMG	C10-C11-C12-C13
22	4	322	LMG	C2-C1-O1-C7
24	G	209	LMT	C2'-C1'-O1'-C1
26	B	801	DGD	C2D-C1D-O3G-C3G
19	3	308	CLA	O1A-CGA-O2A-C1
19	A	855	CLA	C4-C3-C5-C6
22	2	519	LMG	C4-C5-C6-O5
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	F	303	CLA	C2-C3-C5-C6
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	308	CLA	C11-C12-C13-C14
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

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Mol	Chain	Res	Type	Atoms
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
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
19	4	308	CLA	C8-C10-C11-C12
19	B	805	CLA	C15-C16-C17-C18
19	A	821	CLA	C2A-CAA-CBA-CGA
19	B	805	CLA	C2A-CAA-CBA-CGA
18	3	304	BCR	C37-C22-C23-C24
18	4	301	BCR	C11-C12-C13-C35
18	A	856	BCR	C7-C8-C9-C34
18	A	856	BCR	C37-C22-C23-C24
18	B	851	BCR	C7-C8-C9-C34
18	B	852	BCR	C11-C12-C13-C35
18	G	205	BCR	C11-C12-C13-C35
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
22	F	305	LMG	O9-C10-O7-C8
22	2	519	LMG	C11-C10-O7-C8
22	J	1104	LMG	C28-C29-C30-C31
26	B	801	DGD	C1A-C2A-C3A-C4A
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

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Mol	Chain	Res	Type	Atoms
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	A	804	CLA	C13-C15-C16-C17
19	A	819	CLA	C10-C11-C12-C13
19	A	821	CLA	C10-C11-C12-C13
19	A	824	CLA	C13-C15-C16-C17
19	A	830	CLA	C5-C6-C7-C8
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	B	832	CLA	C5-C6-C7-C8
22	2	518	LMG	O6-C5-C6-O5
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	B	832	CLA	C3-C5-C6-C7
19	K	1002	CLA	C3-C5-C6-C7
19	L	304	CLA	C3-C5-C6-C7
19	A	821	CLA	CBA-CGA-O2A-C1
19	3	308	CLA	C5-C6-C7-C8
19	A	804	CLA	C15-C16-C17-C18
19	A	806	CLA	C5-C6-C7-C8
19	A	806	CLA	C8-C10-C11-C12
19	A	828	CLA	C15-C16-C17-C18
19	A	829	CLA	C15-C16-C17-C18
19	A	854	CLA	C5-C6-C7-C8
19	B	825	CLA	C5-C6-C7-C8
19	B	839	CLA	C5-C6-C7-C8
19	G	201	CLA	C13-C15-C16-C17
19	G	202	CLA	C5-C6-C7-C8
19	J	1101	CLA	C8-C10-C11-C12
29	A	844	PQN	C18-C20-C21-C22
22	F	304	LMG	C34-C35-C36-C37
22	B	844	LMG	C10-C11-C12-C13
19	B	838	CLA	O1D-CGD-O2D-CED
19	2	507	CLA	O1A-CGA-O2A-C1
26	J	1106	DGD	CDA-CEA-CFA-CGA
19	A	814	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	B	854	DGD	O6E-C5E-C6E-O5E
19	2	506	CLA	C15-C16-C17-C18
19	3	308	CLA	C13-C15-C16-C17
19	4	304	CLA	C8-C10-C11-C12
19	4	306	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	A	822	CLA	C8-C10-C11-C12
19	A	837	CLA	C5-C6-C7-C8
19	B	805	CLA	C13-C15-C16-C17
19	B	808	CLA	C8-C10-C11-C12
19	B	811	CLA	C5-C6-C7-C8
19	B	811	CLA	C8-C10-C11-C12
19	B	820	CLA	C13-C15-C16-C17
19	B	824	CLA	C15-C16-C17-C18
19	B	825	CLA	C13-C15-C16-C17
19	B	831	CLA	C8-C10-C11-C12
19	B	838	CLA	C5-C6-C7-C8
19	F	303	CLA	C5-C6-C7-C8
21	1	517	LHG	O1-C1-C2-O2
21	A	845	LHG	O1-C1-C2-O2
19	3	310	CLA	O1A-CGA-O2A-C1
19	A	807	CLA	O1A-CGA-O2A-C1
21	A	853	LHG	C7-C8-C9-C10
21	B	843	LHG	C23-C24-C25-C26
19	1	516	CLA	C5-C6-C7-C8
19	3	308	CLA	C8-C10-C11-C12
19	4	306	CLA	C10-C11-C12-C13
19	4	307	CLA	C8-C10-C11-C12
19	A	817	CLA	C5-C6-C7-C8
19	B	807	CLA	C8-C10-C11-C12
19	B	808	CLA	C15-C16-C17-C18
19	B	812	CLA	C8-C10-C11-C12
19	B	818	CLA	C15-C16-C17-C18
19	B	831	CLA	C5-C6-C7-C8
19	B	836	CLA	C15-C16-C17-C18
19	F	303	CLA	C8-C10-C11-C12
19	A	836	CLA	O1D-CGD-O2D-CED
19	1	508	CLA	C2-C1-O2A-CGA
19	1	513	CLA	C2-C1-O2A-CGA
19	2	509	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
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	4	304	CLA	C10-C11-C12-C13
19	4	306	CLA	C5-C6-C7-C8
19	A	808	CLA	C5-C6-C7-C8
19	A	833	CLA	C5-C6-C7-C8
19	A	835	CLA	C5-C6-C7-C8
19	A	840	CLA	C8-C10-C11-C12
19	B	830	CLA	C8-C10-C11-C12
19	B	805	CLA	O1D-CGD-O2D-CED
21	1	520	LHG	C23-C24-C25-C26
26	G	207	DGD	C1B-C2B-C3B-C4B
24	G	208	LMT	O5'-C5'-C6'-O6'
24	G	208	LMT	C3'-C4'-O1B-C1B
19	3	307	CLA	C5-C6-C7-C8
19	A	802	CLA	O1D-CGD-O2D-CED
19	A	805	CLA	C6-C7-C8-C10
19	A	806	CLA	C12-C13-C15-C16
19	A	824	CLA	C12-C13-C15-C16
19	B	810	CLA	C12-C13-C15-C16
19	A	828	CLA	C3-C5-C6-C7
19	G	204	CLA	C3-C5-C6-C7
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
18	2	503	BCR	C19-C20-C21-C22
18	4	301	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
18	4	301	BCR	C19-C20-C21-C22
19	B	803	CLA	CBD-CGD-O2D-CED
19	1	507	CLA	CBA-CGA-O2A-C1
19	3	316	CLA	C2A-CAA-CBA-CGA
19	4	309	CLA	C2A-CAA-CBA-CGA
19	K	1001	CLA	C2A-CAA-CBA-CGA
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
19	4	308	CLA	C5-C6-C7-C8
19	4	315	CLA	C13-C15-C16-C17
19	A	828	CLA	C10-C11-C12-C13
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	814	CLA	C5-C6-C7-C8
19	B	818	CLA	C8-C10-C11-C12
19	B	828	CLA	C5-C6-C7-C8
22	J	1103	LMG	C11-C12-C13-C14
24	B	855	LMT	O1'-C1-C2-C3
19	4	309	CLA	O1A-CGA-O2A-C1
19	A	814	CLA	O1A-CGA-O2A-C1
19	A	836	CLA	O1A-CGA-O2A-C1
24	B	846	LMT	O5'-C1'-O1'-C1
24	B	847	LMT	O5'-C1'-O1'-C1
19	A	805	CLA	C13-C15-C16-C17
19	A	819	CLA	C5-C6-C7-C8
19	A	825	CLA	C15-C16-C17-C18
19	A	833	CLA	C8-C10-C11-C12
24	G	208	LMT	O1'-C1-C2-C3
21	A	845	LHG	C23-C24-C25-C26
18	2	503	BCR	C10-C11-C12-C13
18	A	848	BCR	C10-C11-C12-C13
18	B	849	BCR	C10-C11-C12-C13
18	B	852	BCR	C10-C11-C12-C13
18	B	856	BCR	C10-C11-C12-C13
18	K	1005	BCR	C10-C11-C12-C13
18	L	307	BCR	C10-C11-C12-C13
21	1	520	LHG	O2-C2-C3-O3
21	1	517	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
22	2	519	LMG	O9-C10-O7-C8
19	1	513	CLA	C15-C16-C17-C18
19	2	506	CLA	C5-C6-C7-C8
19	A	811	CLA	C10-C11-C12-C13
19	A	813	CLA	C13-C15-C16-C17
19	A	817	CLA	C10-C11-C12-C13
19	A	817	CLA	C13-C15-C16-C17
19	B	822	CLA	C15-C16-C17-C18
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	B	833	CLA	O1D-CGD-O2D-CED
19	A	809	CLA	O1A-CGA-O2A-C1
19	K	1002	CLA	O1A-CGA-O2A-C1
24	3	318	LMT	C4'-C5'-C6'-O6'
19	A	810	CLA	O1D-CGD-O2D-CED
19	2	507	CLA	C15-C16-C17-C18
19	4	310	CLA	C5-C6-C7-C8
19	A	811	CLA	C13-C15-C16-C17
19	A	814	CLA	C8-C10-C11-C12
19	A	832	CLA	C13-C15-C16-C17
19	A	833	CLA	C13-C15-C16-C17
19	A	838	CLA	C10-C11-C12-C13
19	B	806	CLA	C13-C15-C16-C17
19	B	815	CLA	C15-C16-C17-C18
19	B	829	CLA	C10-C11-C12-C13
19	2	508	CLA	O1D-CGD-O2D-CED
19	A	808	CLA	O1D-CGD-O2D-CED
19	A	821	CLA	O1A-CGA-O2A-C1
19	3	305	CLA	C4C-C3C-CAC-CBC
19	1	504	CLA	C13-C15-C16-C17
19	A	831	CLA	C5-C6-C7-C8
19	A	840	CLA	C15-C16-C17-C18
19	A	854	CLA	C8-C10-C11-C12
19	B	819	CLA	C5-C6-C7-C8
19	B	822	CLA	C5-C6-C7-C8
19	B	825	CLA	C8-C10-C11-C12
19	F	302	CLA	C13-C15-C16-C17
19	G	204	CLA	C13-C15-C16-C17
21	1	520	LHG	C3-O3-P-O6
21	2	517	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
21	A	845	LHG	C4-O6-P-O3
21	A	853	LHG	C3-O3-P-O6
21	A	853	LHG	C4-O6-P-O3
24	3	318	LMT	O5'-C5'-C6'-O6'
19	B	807	CLA	C3-C5-C6-C7
19	B	836	CLA	C3-C5-C6-C7
19	B	833	CLA	CBA-CGA-O2A-C1
19	A	806	CLA	C15-C16-C17-C18
19	A	834	CLA	C13-C15-C16-C17
19	B	820	CLA	C10-C11-C12-C13
21	1	517	LHG	C1-C2-C3-O3
21	1	520	LHG	C1-C2-C3-O3
21	A	845	LHG	C1-C2-C3-O3
24	B	846	LMT	O5'-C5'-C6'-O6'
19	2	507	CLA	C4-C3-C5-C6
19	A	826	CLA	C2-C3-C5-C6
19	B	816	CLA	C5-C6-C7-C8
19	B	817	CLA	O1D-CGD-O2D-CED
24	G	208	LMT	C5'-C4'-O1B-C1B
19	4	306	CLA	C2A-CAA-CBA-CGA
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	A	823	CLA	C11-C12-C13-C15
19	B	811	CLA	C16-C17-C18-C19
19	L	304	CLA	C11-C12-C13-C15
19	2	508	CLA	CBA-CGA-O2A-C1
19	3	305	CLA	CBA-CGA-O2A-C1
19	B	835	CLA	CBA-CGA-O2A-C1
17	J	1109	LUT	C29-C30-C31-C32
18	J	1108	BCR	C19-C20-C21-C22
22	G	206	LMG	C15-C16-C17-C18
19	2	507	CLA	O1D-CGD-O2D-CED
18	G	205	BCR	C11-C10-C9-C34
24	J	1107	LMT	O5'-C5'-C6'-O6'
21	1	517	LHG	C11-C10-C9-C8
21	1	517	LHG	C9-C10-C11-C12
26	B	854	DGD	C3A-C4A-C5A-C6A
19	A	829	CLA	O1D-CGD-O2D-CED
19	1	508	CLA	C16-C17-C18-C19
19	4	307	CLA	C11-C12-C13-C14
19	4	310	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
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
22	B	844	LMG	C11-C12-C13-C14
19	B	814	CLA	C15-C16-C17-C18
20	1	521	CHL	C2C-C3C-CAC-CBC
22	4	322	LMG	O6-C5-C6-O5
21	1	517	LHG	C25-C26-C27-C28
21	1	517	LHG	C28-C29-C30-C31
19	B	818	CLA	C10-C11-C12-C13
24	4	320	LMT	O1'-C1-C2-C3
21	B	843	LHG	C7-C8-C9-C10
19	A	839	CLA	O1D-CGD-O2D-CED
18	G	205	BCR	C11-C10-C9-C8
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
26	4	319	DGD	C2D-C1D-O3G-C3G
21	A	853	LHG	C13-C14-C15-C16
21	B	843	LHG	C24-C25-C26-C27
24	B	846	LMT	C7-C8-C9-C10
26	J	1106	DGD	CCA-CDA-CEA-CFA
19	A	814	CLA	C13-C15-C16-C17
19	2	508	CLA	O1A-CGA-O2A-C1
19	2	510	CLA	C11-C12-C13-C14
19	3	307	CLA	C6-C7-C8-C9
19	B	825	CLA	C16-C17-C18-C20
19	G	202	CLA	C6-C7-C8-C9
19	A	803	CLA	O1D-CGD-O2D-CED
19	B	830	CLA	O1D-CGD-O2D-CED
20	1	514	CHL	C4-C3-C5-C6
21	1	520	LHG	C14-C15-C16-C17
21	A	853	LHG	C29-C30-C31-C32
22	2	519	LMG	C14-C15-C16-C17
19	1	504	CLA	C6-C7-C8-C9
19	1	513	CLA	C6-C7-C8-C9
19	A	808	CLA	C11-C12-C13-C14
19	A	817	CLA	C11-C10-C8-C9
19	A	825	CLA	C11-C10-C8-C9
19	A	829	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	A	831	CLA	C11-C12-C13-C14
19	A	833	CLA	C11-C12-C13-C14
19	A	840	CLA	C11-C10-C8-C9
19	B	804	CLA	C11-C12-C13-C14
19	B	822	CLA	C11-C10-C8-C9
21	1	517	LHG	C34-C35-C36-C37
26	B	854	DGD	C6A-C7A-C8A-C9A
19	4	306	CLA	C13-C15-C16-C17
19	A	804	CLA	C8-C10-C11-C12
19	A	832	CLA	C5-C6-C7-C8
19	3	308	CLA	C2A-CAA-CBA-CGA
19	A	816	CLA	C2A-CAA-CBA-CGA
19	A	842	CLA	C2A-CAA-CBA-CGA
19	G	202	CLA	C2A-CAA-CBA-CGA
20	2	516	CHL	C2A-CAA-CBA-CGA
19	1	507	CLA	O1A-CGA-O2A-C1
19	3	305	CLA	O1A-CGA-O2A-C1
17	3	302	LUT	C7-C8-C9-C19
18	3	304	BCR	C11-C12-C13-C35
18	B	856	BCR	C11-C12-C13-C35
18	I	102	BCR	C37-C22-C23-C24
18	K	1005	BCR	C11-C12-C13-C35
26	B	854	DGD	C2A-C3A-C4A-C5A
21	A	845	LHG	O1-C1-C2-C3
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
18	K	1005	BCR	C11-C12-C13-C14
18	L	307	BCR	C11-C12-C13-C14
19	A	819	CLA	C3-C5-C6-C7
19	A	854	CLA	C3-C5-C6-C7
26	B	801	DGD	O1B-C1B-O2G-C2G
19	3	305	CLA	C5-C6-C7-C8
26	B	801	DGD	C2B-C1B-O2G-C2G
21	1	520	LHG	C16-C17-C18-C19
21	A	853	LHG	C28-C29-C30-C31
22	B	845	LMG	C10-C11-C12-C13
22	G	206	LMG	C28-C29-C30-C31
21	A	845	LHG	C13-C14-C15-C16
26	B	854	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
19	4	307	CLA	C11-C12-C13-C15
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	840	CLA	C16-C17-C18-C20
19	A	854	CLA	C16-C17-C18-C19
19	B	811	CLA	C16-C17-C18-C20
19	B	812	CLA	C11-C12-C13-C14
19	B	812	CLA	C11-C12-C13-C15
19	B	815	CLA	C16-C17-C18-C19
19	B	824	CLA	C16-C17-C18-C19
19	B	824	CLA	C16-C17-C18-C20
19	B	834	CLA	C6-C7-C8-C9
19	B	840	CLA	C16-C17-C18-C20
19	F	302	CLA	C16-C17-C18-C19
19	F	302	CLA	C16-C17-C18-C20
20	4	316	CHL	C11-C12-C13-C15
22	B	845	LMG	O6-C1-O1-C7
22	J	1104	LMG	O6-C1-O1-C7
26	4	319	DGD	O6D-C1D-O3G-C3G
19	1	507	CLA	C13-C15-C16-C17
19	4	318	CLA	C13-C15-C16-C17
19	B	809	CLA	C10-C11-C12-C13
19	H	1000	CLA	C10-C11-C12-C13
21	A	845	LHG	C9-C10-C11-C12
21	A	853	LHG	C34-C35-C36-C37
22	1	518	LMG	C11-C12-C13-C14
22	F	305	LMG	C32-C33-C34-C35
24	2	523	LMT	C2-C3-C4-C5
24	G	208	LMT	C4-C5-C6-C7
26	B	801	DGD	C4D-C5D-C6D-O5D
19	4	309	CLA	CBD-CGD-O2D-CED
19	2	504	CLA	O1D-CGD-O2D-CED
19	B	821	CLA	O1D-CGD-O2D-CED
21	1	517	LHG	C11-C12-C13-C14
21	2	517	LHG	C9-C10-C11-C12
19	K	1002	CLA	C5-C6-C7-C8
29	B	841	PQN	C25-C26-C27-C28
19	B	835	CLA	O1A-CGA-O2A-C1
21	1	520	LHG	C11-C12-C13-C14
19	L	304	CLA	O1D-CGD-O2D-CED
19	1	506	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
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
19	A	808	CLA	C8-C10-C11-C12
22	2	524	LMG	O6-C5-C6-O5
18	I	102	BCR	C13-C14-C15-C16
18	L	307	BCR	C15-C16-C17-C18
19	1	508	CLA	C16-C17-C18-C20
19	3	305	CLA	C6-C7-C8-C10
19	A	814	CLA	C16-C17-C18-C20
19	A	823	CLA	C11-C12-C13-C14
19	A	826	CLA	C6-C7-C8-C10
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	A	855	CLA	C16-C17-C18-C20
19	B	807	CLA	C16-C17-C18-C20
19	B	825	CLA	C16-C17-C18-C19
19	B	834	CLA	C6-C7-C8-C10
19	B	840	CLA	C16-C17-C18-C19
19	F	303	CLA	C16-C17-C18-C19
19	F	303	CLA	C16-C17-C18-C20
19	L	304	CLA	C11-C12-C13-C14
22	1	518	LMG	C18-C19-C20-C21
19	A	827	CLA	O1D-CGD-O2D-CED
22	G	210	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
19	2	514	CLA	CBD-CGD-O2D-CED
21	1	517	LHG	C14-C15-C16-C17
29	A	844	PQN	C13-C15-C16-C17
21	1	517	LHG	C29-C30-C31-C32
22	2	519	LMG	C12-C13-C14-C15
19	A	807	CLA	C4-C3-C5-C6
19	B	806	CLA	C4-C3-C5-C6
19	A	829	CLA	CBA-CGA-O2A-C1
19	A	854	CLA	CBA-CGA-O2A-C1
21	1	520	LHG	C12-C13-C14-C15
21	A	845	LHG	C11-C12-C13-C14
21	A	853	LHG	C33-C34-C35-C36
22	4	322	LMG	C11-C12-C13-C14
24	G	209	LMT	C3'-C4'-O1B-C1B
26	4	319	DGD	C5A-C6A-C7A-C8A
19	B	836	CLA	O1D-CGD-O2D-CED
19	G	204	CLA	C2A-CAA-CBA-CGA
21	B	842	LHG	O1-C1-C2-O2
21	B	843	LHG	O1-C1-C2-O2
19	3	306	CLA	C2C-C3C-CAC-CBC
21	1	520	LHG	C18-C19-C20-C21
19	4	318	CLA	O1D-CGD-O2D-CED
19	2	510	CLA	C11-C12-C13-C15
26	4	319	DGD	C3B-C4B-C5B-C6B
19	B	807	CLA	C5-C6-C7-C8
19	B	840	CLA	C8-C10-C11-C12
19	B	833	CLA	O1A-CGA-O2A-C1
19	1	509	CLA	C2-C1-O2A-CGA
19	2	510	CLA	C2-C1-O2A-CGA
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
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

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Mol	Chain	Res	Type	Atoms
19	B	839	CLA	C2-C1-O2A-CGA
19	G	202	CLA	C2-C1-O2A-CGA
19	J	1101	CLA	C2-C1-O2A-CGA
20	4	314	CHL	C2-C1-O2A-CGA
19	A	809	CLA	C5-C6-C7-C8
19	A	832	CLA	C15-C16-C17-C18
19	B	839	CLA	C10-C11-C12-C13
24	B	847	LMT	C4-C5-C6-C7
22	F	305	LMG	C28-C29-C30-C31
19	3	316	CLA	O1A-CGA-O2A-C1
17	1	501	LUT	C1-C6-C7-C8
17	1	501	LUT	C5-C6-C7-C8
17	2	501	LUT	C5-C6-C7-C8
17	3	301	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	A	848	BCR	C1-C6-C7-C8
18	A	848	BCR	C5-C6-C7-C8
18	A	849	BCR	C23-C24-C25-C26
18	A	851	BCR	C23-C24-C25-C26
18	B	851	BCR	C1-C6-C7-C8
18	B	851	BCR	C5-C6-C7-C8
18	B	853	BCR	C1-C6-C7-C8
18	B	853	BCR	C5-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
18	L	306	BCR	C5-C6-C7-C8
19	3	313	CLA	C3-C5-C6-C7
22	B	845	LMG	O6-C5-C6-O5
24	3	318	LMT	O5B-C5B-C6B-O6B
21	A	853	LHG	C25-C26-C27-C28
19	F	302	CLA	CBA-CGA-O2A-C1
19	1	504	CLA	C15-C16-C17-C18
19	1	513	CLA	C5-C6-C7-C8
19	2	514	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	A	821	CLA	C8-C10-C11-C12
19	A	827	CLA	C5-C6-C7-C8
19	B	808	CLA	C5-C6-C7-C8
19	B	826	CLA	C15-C16-C17-C18
19	G	201	CLA	C5-C6-C7-C8
29	A	844	PQN	C25-C26-C27-C28
22	F	305	LMG	C10-C11-C12-C13
24	G	209	LMT	C4-C5-C6-C7
19	A	832	CLA	C10-C11-C12-C13
19	G	201	CLA	O1D-CGD-O2D-CED
19	3	313	CLA	C4-C3-C5-C6
19	B	822	CLA	C4-C3-C5-C6
19	B	840	CLA	C4-C3-C5-C6
19	A	841	CLA	O1D-CGD-O2D-CED
19	1	513	CLA	C6-C7-C8-C10
19	1	513	CLA	C11-C10-C8-C7
19	3	313	CLA	C2-C3-C5-C6
19	4	307	CLA	C11-C10-C8-C7
19	4	315	CLA	C12-C13-C15-C16
19	A	805	CLA	C11-C12-C13-C15
19	A	805	CLA	C12-C13-C15-C16
19	A	807	CLA	C2-C3-C5-C6
19	A	808	CLA	C11-C12-C13-C15
19	A	814	CLA	C12-C13-C15-C16
19	A	817	CLA	C12-C13-C15-C16
19	A	819	CLA	C6-C7-C8-C10
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	C6-C7-C8-C10
19	A	840	CLA	C11-C10-C8-C7
19	A	854	CLA	C6-C7-C8-C10
19	B	806	CLA	C2-C3-C5-C6
19	B	812	CLA	C11-C10-C8-C7
19	B	819	CLA	C2-C3-C5-C6
19	B	824	CLA	C11-C12-C13-C15
19	B	829	CLA	C6-C7-C8-C10
19	B	831	CLA	C11-C10-C8-C7
19	F	303	CLA	C11-C12-C13-C15
20	1	514	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	B	841	PQN	C17-C18-C20-C21
19	B	821	CLA	CBA-CGA-O2A-C1
19	A	829	CLA	O1A-CGA-O2A-C1
19	A	854	CLA	O1A-CGA-O2A-C1
19	4	315	CLA	C10-C11-C12-C13
18	A	848	BCR	C15-C16-C17-C18
18	B	850	BCR	C13-C14-C15-C16
19	B	828	CLA	CBD-CGD-O2D-CED
19	3	307	CLA	C6-C7-C8-C10
19	A	825	CLA	CBA-CGA-O2A-C1
19	A	830	CLA	CBA-CGA-O2A-C1
19	3	313	CLA	C8-C10-C11-C12
19	4	308	CLA	C10-C11-C12-C13
19	B	829	CLA	C8-C10-C11-C12
19	B	840	CLA	C10-C11-C12-C13
21	B	843	LHG	C34-C35-C36-C37
19	B	832	CLA	O1D-CGD-O2D-CED
19	L	303	CLA	O1D-CGD-O2D-CED
19	A	824	CLA	C5-C6-C7-C8
19	J	1101	CLA	C15-C16-C17-C18
21	1	517	LHG	C35-C36-C37-C38
19	1	506	CLA	C6-C7-C8-C9
19	G	202	CLA	C6-C7-C8-C10
19	A	821	CLA	O1D-CGD-O2D-CED
19	B	831	CLA	O1D-CGD-O2D-CED
22	A	847	LMG	C18-C19-C20-C21
21	2	517	LHG	C8-C7-O7-C5
18	B	851	BCR	C10-C11-C12-C13
22	B	844	LMG	C4-C5-C6-O5
19	A	827	CLA	C10-C11-C12-C13
19	K	1002	CLA	C8-C10-C11-C12
21	A	853	LHG	C11-C12-C13-C14
21	2	517	LHG	O9-C7-O7-C5
21	A	845	LHG	C16-C17-C18-C19
26	B	801	DGD	C2E-C1E-O5D-C6D
22	G	206	LMG	O1-C7-C8-O7
19	4	310	CLA	C11-C12-C13-C15
22	B	845	LMG	C12-C13-C14-C15
22	A	847	LMG	O6-C5-C6-O5
24	4	320	LMT	O5B-C5B-C6B-O6B
19	4	304	CLA	C4-C3-C5-C6
19	A	825	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	A	833	CLA	C4-C3-C5-C6
22	F	304	LMG	C28-C29-C30-C31
19	B	822	CLA	C2-C3-C5-C6
20	1	521	CHL	C2-C3-C5-C6
19	1	513	CLA	C11-C10-C8-C9
19	4	307	CLA	C11-C10-C8-C9
19	A	803	CLA	C14-C13-C15-C16
19	A	805	CLA	C6-C7-C8-C9
19	A	805	CLA	C11-C12-C13-C14
19	A	813	CLA	C11-C10-C8-C9
19	A	830	CLA	C11-C10-C8-C9
19	A	840	CLA	C6-C7-C8-C9
19	A	854	CLA	C6-C7-C8-C9
19	B	819	CLA	C6-C7-C8-C9
19	B	822	CLA	C14-C13-C15-C16
19	B	824	CLA	C11-C12-C13-C14
19	B	829	CLA	C6-C7-C8-C9
19	B	833	CLA	C6-C7-C8-C9
19	B	839	CLA	C11-C12-C13-C14
19	B	820	CLA	O1D-CGD-O2D-CED
26	B	854	DGD	C2G-C1G-O1G-C1A
21	A	853	LHG	C12-C13-C14-C15
19	B	821	CLA	C2A-CAA-CBA-CGA
19	L	305	CLA	C2A-CAA-CBA-CGA
24	2	523	LMT	C1-C2-C3-C4
21	A	845	LHG	C15-C16-C17-C18
24	B	847	LMT	O5B-C5B-C6B-O6B
24	B	855	LMT	O5'-C5'-C6'-O6'
19	4	307	CLA	CBA-CGA-O2A-C1
18	A	849	BCR	C37-C22-C23-C24
23	2	502	XAT	C27-C28-C29-C39
19	B	819	CLA	C15-C16-C17-C18
18	A	849	BCR	C21-C22-C23-C24
18	I	102	BCR	C7-C8-C9-C10
19	F	302	CLA	O1A-CGA-O2A-C1
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

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Mol	Chain	Res	Type	Atoms
19	3	317	CLA	C1A-C2A-CAA-CBA
19	4	304	CLA	C1A-C2A-CAA-CBA
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
20	1	512	CHL	C1A-C2A-CAA-CBA
20	2	515	CHL	C1A-C2A-CAA-CBA
20	2	516	CHL	C1A-C2A-CAA-CBA
19	1	506	CLA	C6-C7-C8-C10
19	A	817	CLA	C16-C17-C18-C20
19	A	838	CLA	C16-C17-C18-C20
26	4	319	DGD	C2B-C1B-O2G-C2G
21	B	843	LHG	C11-C12-C13-C14
22	G	206	LMG	C16-C17-C18-C19
18	3	304	BCR	C19-C20-C21-C22
18	L	306	BCR	C19-C20-C21-C22
19	B	803	CLA	O1D-CGD-O2D-CED
19	1	508	CLA	C15-C16-C17-C18
19	A	805	CLA	C10-C11-C12-C13
19	B	840	CLA	C5-C6-C7-C8
21	2	517	LHG	C3-O3-P-O6
21	B	843	LHG	C3-O3-P-O6
24	2	523	LMT	O5'-C5'-C6'-O6'
20	1	521	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
19	A	825	CLA	O1A-CGA-O2A-C1
19	A	839	CLA	C8-C10-C11-C12
21	A	845	LHG	O6-C4-C5-C6
21	2	517	LHG	C7-C8-C9-C10
20	1	514	CHL	C11-C12-C13-C15
24	4	320	LMT	C9-C10-C11-C12
22	B	844	LMG	O6-C5-C6-O5
26	4	319	DGD	O1B-C1B-O2G-C2G
19	2	507	CLA	C2-C3-C5-C6
19	B	823	CLA	C5-C6-C7-C8
19	B	837	CLA	C2A-CAA-CBA-CGA
19	A	808	CLA	C16-C17-C18-C19
19	A	826	CLA	O1D-CGD-O2D-CED
19	A	808	CLA	C3-C5-C6-C7
21	1	517	LHG	C4-C5-C6-O8
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	A	830	CLA	O1A-CGA-O2A-C1
22	1	518	LMG	C8-C7-O1-C1
22	G	206	LMG	C8-C7-O1-C1
26	B	801	DGD	C2G-C3G-O3G-C1D
26	J	1106	DGD	C5D-C6D-O5D-C1E
22	F	305	LMG	C33-C34-C35-C36
29	A	844	PQN	C15-C16-C17-C18
19	A	818	CLA	C11-C10-C8-C9
21	B	843	LHG	C35-C36-C37-C38
26	4	319	DGD	C4A-C5A-C6A-C7A
26	B	854	DGD	C7A-C8A-C9A-CAA
19	A	821	CLA	C13-C15-C16-C17
19	B	803	CLA	C8-C10-C11-C12
19	B	827	CLA	C8-C10-C11-C12
26	B	854	DGD	C1B-C2B-C3B-C4B
22	2	522	LMG	C4-C5-C6-O5
19	B	814	CLA	C8-C10-C11-C12
19	B	824	CLA	C10-C11-C12-C13
19	G	204	CLA	C10-C11-C12-C13
18	J	1108	BCR	C11-C10-C9-C34
20	1	521	CHL	C4-C3-C5-C6
19	2	509	CLA	CBA-CGA-O2A-C1
19	A	838	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B	831	CLA	CBA-CGA-O2A-C1
26	B	854	DGD	C4E-C5E-C6E-O5E
20	4	314	CHL	C2C-C3C-CAC-CBC
20	4	316	CHL	C4C-C3C-CAC-CBC
19	4	309	CLA	O1D-CGD-O2D-CED
19	A	811	CLA	C2A-CAA-CBA-CGA
19	A	802	CLA	C10-C11-C12-C13
19	1	516	CLA	C2-C1-O2A-CGA
19	A	820	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
22	J	1104	LMG	C33-C34-C35-C36
19	B	810	CLA	C5-C6-C7-C8
21	A	845	LHG	C11-C10-C9-C8
26	B	854	DGD	C2A-C1A-O1G-C1G
19	A	809	CLA	C16-C17-C18-C20
19	4	315	CLA	C15-C16-C17-C18
21	B	843	LHG	C33-C34-C35-C36
26	B	854	DGD	C4A-C5A-C6A-C7A
21	A	845	LHG	C7-C8-C9-C10
19	A	805	CLA	C8-C10-C11-C12
22	A	847	LMG	C2-C1-O1-C7
26	J	1106	DGD	C2E-C1E-O5D-C6D
21	A	853	LHG	O7-C5-C6-O8
26	B	801	DGD	O1G-C1G-C2G-O2G
26	B	801	DGD	O2G-C2G-C3G-O3G
19	A	807	CLA	C5-C6-C7-C8
19	A	840	CLA	C5-C6-C7-C8
19	1	504	CLA	C11-C10-C8-C7
19	1	513	CLA	C11-C12-C13-C15
19	1	516	CLA	C6-C7-C8-C10
19	2	510	CLA	C11-C10-C8-C7
19	3	308	CLA	C6-C7-C8-C10
19	4	306	CLA	C12-C13-C15-C16
19	4	318	CLA	C12-C13-C15-C16
19	A	802	CLA	C11-C12-C13-C15
19	A	804	CLA	C11-C10-C8-C7
19	A	813	CLA	C11-C10-C8-C7
19	A	817	CLA	C11-C10-C8-C7
19	A	828	CLA	C11-C10-C8-C7
19	A	830	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
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	804	CLA	C11-C10-C8-C7
19	B	804	CLA	C12-C13-C15-C16
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
19	B	827	CLA	C12-C13-C15-C16
19	B	828	CLA	C12-C13-C15-C16
19	B	830	CLA	C11-C10-C8-C7
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
19	K	1002	CLA	C11-C10-C8-C7
29	B	841	PQN	C21-C22-C23-C25
27	A	801	CL0	C3-C5-C6-C7
19	4	307	CLA	O1A-CGA-O2A-C1
19	1	508	CLA	C6-C7-C8-C9
19	1	513	CLA	C11-C12-C13-C14
19	A	804	CLA	C11-C12-C13-C14
19	A	811	CLA	C6-C7-C8-C9
19	A	829	CLA	C11-C12-C13-C14
19	A	834	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	854	CLA	C14-C13-C15-C16
19	A	855	CLA	C14-C13-C15-C16
19	B	805	CLA	C11-C10-C8-C9
19	B	805	CLA	C11-C12-C13-C14
19	B	806	CLA	C14-C13-C15-C16
19	B	807	CLA	C11-C12-C13-C14
19	B	808	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	B	827	CLA	C11-C10-C8-C9
19	B	827	CLA	C14-C13-C15-C16
19	B	828	CLA	C14-C13-C15-C16
19	B	838	CLA	C6-C7-C8-C9
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
29	B	841	PQN	C21-C22-C23-C24
21	B	843	LHG	C9-C10-C11-C12
19	G	201	CLA	CBA-CGA-O2A-C1
19	4	310	CLA	C10-C11-C12-C13
19	G	204	CLA	C8-C10-C11-C12
19	A	829	CLA	C2A-CAA-CBA-CGA
18	1	503	BCR	C37-C22-C23-C24
18	3	304	BCR	C7-C8-C9-C34
19	A	817	CLA	C16-C17-C18-C19
18	1	503	BCR	C21-C22-C23-C24
18	I	102	BCR	C17-C18-C19-C20
19	4	310	CLA	C3-C5-C6-C7
19	G	201	CLA	C3-C5-C6-C7
19	3	308	CLA	C10-C11-C12-C13
19	A	840	CLA	CBA-CGA-O2A-C1
19	B	805	CLA	CBA-CGA-O2A-C1
19	B	814	CLA	CBA-CGA-O2A-C1
19	B	820	CLA	CBA-CGA-O2A-C1
27	A	801	CL0	CBA-CGA-O2A-C1
21	A	845	LHG	C26-C27-C28-C29
21	A	853	LHG	C35-C36-C37-C38
22	B	845	LMG	C11-C12-C13-C14
19	B	829	CLA	C13-C15-C16-C17
21	1	520	LHG	O6-C4-C5-C6
22	J	1104	LMG	C29-C28-O8-C9
21	2	517	LHG	C26-C27-C28-C29
26	B	854	DGD	CCB-CDB-CEB-CFB
19	B	829	CLA	C4-C3-C5-C6
19	3	306	CLA	C4C-C3C-CAC-CBC
21	B	843	LHG	C30-C31-C32-C33
19	A	838	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	B	854	DGD	O1A-C1A-O1G-C1G
19	A	808	CLA	C16-C17-C18-C20
19	B	819	CLA	C16-C17-C18-C20
19	A	855	CLA	C5-C6-C7-C8
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
21	1	517	LHG	C2-C3-O3-P
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	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
19	A	807	CLA	C10-C11-C12-C13
24	2	523	LMT	C2-C1-O1'-C1'
26	J	1106	DGD	C2B-C3B-C4B-C5B
19	A	855	CLA	C15-C16-C17-C18
21	A	853	LHG	C27-C28-C29-C30
19	A	802	CLA	C8-C10-C11-C12
19	B	811	CLA	C10-C11-C12-C13
19	B	828	CLA	C8-C10-C11-C12
29	B	841	PQN	C23-C25-C26-C27
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	1	520	LHG	C26-C27-C28-C29
24	B	847	LMT	C3-C4-C5-C6
24	A	846	LMT	C4'-C5'-C6'-O6'
24	G	209	LMT	C2B-C1B-O1B-C4'
19	B	831	CLA	O1A-CGA-O2A-C1
19	A	806	CLA	C4-C3-C5-C6
19	4	315	CLA	C16-C17-C18-C19
19	A	812	CLA	C6-C7-C8-C9
20	4	316	CHL	C11-C12-C13-C14
19	A	825	CLA	C2-C3-C5-C6
19	A	833	CLA	C2-C3-C5-C6
21	A	853	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
21	2	517	LHG	O1-C1-C2-O2
21	1	520	LHG	O6-C4-C5-O7
19	G	201	CLA	O1A-CGA-O2A-C1
27	A	801	CL0	O1A-CGA-O2A-C1
21	A	853	LHG	C23-C24-C25-C26
21	B	842	LHG	C24-C23-O8-C6
19	B	807	CLA	C16-C17-C18-C19
19	2	509	CLA	O1A-CGA-O2A-C1
19	J	1101	CLA	O1A-CGA-O2A-C1
22	B	844	LMG	O7-C8-C9-O8
22	B	845	LMG	O1-C7-C8-O7
26	4	319	DGD	O1G-C1G-C2G-O2G
19	B	828	CLA	O1D-CGD-O2D-CED
22	2	522	LMG	O6-C5-C6-O5
19	3	305	CLA	C6-C7-C8-C9
19	A	812	CLA	C6-C7-C8-C10
19	A	839	CLA	C16-C17-C18-C19
24	G	209	LMT	C1-C2-C3-C4
19	A	813	CLA	C15-C16-C17-C18
19	A	811	CLA	C2-C1-O2A-CGA
19	B	829	CLA	C2-C1-O2A-CGA
21	1	517	LHG	C30-C31-C32-C33
19	1	513	CLA	C8-C10-C11-C12
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	825	CLA	C11-C12-C13-C14
19	A	833	CLA	C6-C7-C8-C9
19	B	810	CLA	C11-C12-C13-C14
19	B	818	CLA	C14-C13-C15-C16
19	B	822	CLA	C6-C7-C8-C9
19	B	830	CLA	C11-C12-C13-C14
19	L	304	CLA	C6-C7-C8-C9
19	H	1000	CLA	C5-C6-C7-C8
19	A	836	CLA	C4-C3-C5-C6
19	A	805	CLA	O1A-CGA-O2A-C1
19	A	855	CLA	C2A-CAA-CBA-CGA
19	B	808	CLA	C2A-CAA-CBA-CGA
19	A	807	CLA	C11-C12-C13-C14
17	3	302	LUT	C1-C6-C7-C8
17	3	302	LUT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
18	A	851	BCR	C1-C6-C7-C8
18	A	851	BCR	C5-C6-C7-C8
18	B	850	BCR	C1-C6-C7-C8
18	B	850	BCR	C5-C6-C7-C8
18	B	851	BCR	C23-C24-C25-C26
18	B	851	BCR	C23-C24-C25-C30
18	B	852	BCR	C23-C24-C25-C26
18	B	852	BCR	C23-C24-C25-C30
18	F	306	BCR	C23-C24-C25-C26
18	K	1005	BCR	C1-C6-C7-C8
18	K	1005	BCR	C5-C6-C7-C8
18	B	852	BCR	C36-C18-C19-C20
18	G	205	BCR	C11-C12-C13-C14
19	A	823	CLA	C5-C6-C7-C8
19	A	829	CLA	C10-C11-C12-C13
19	F	302	CLA	C5-C6-C7-C8
22	1	518	LMG	O7-C10-C11-C12
19	4	315	CLA	C16-C17-C18-C20
19	A	809	CLA	C16-C17-C18-C19
19	A	828	CLA	C16-C17-C18-C20
19	A	817	CLA	C3-C5-C6-C7
22	A	847	LMG	C31-C32-C33-C34
19	B	814	CLA	O1A-CGA-O2A-C1
19	A	829	CLA	C5-C6-C7-C8
21	A	853	LHG	O6-C4-C5-C6
21	B	842	LHG	O6-C4-C5-C6
19	2	514	CLA	O1D-CGD-O2D-CED
19	1	504	CLA	C6-C7-C8-C10
19	1	508	CLA	C6-C7-C8-C10
19	3	308	CLA	C11-C12-C13-C15
19	3	313	CLA	C6-C7-C8-C10
19	4	304	CLA	C6-C7-C8-C10
19	A	804	CLA	C6-C7-C8-C10
19	A	804	CLA	C11-C12-C13-C15
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	809	CLA	C12-C13-C15-C16
19	A	811	CLA	C6-C7-C8-C10
19	A	819	CLA	C11-C12-C13-C15
19	A	821	CLA	C11-C10-C8-C7
19	A	828	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	A	829	CLA	C11-C12-C13-C15
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-C12-C13-C15
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	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	B	829	CLA	C11-C12-C13-C15
19	B	830	CLA	C11-C12-C13-C15
19	F	302	CLA	C12-C13-C15-C16
19	H	1000	CLA	C6-C7-C8-C10
20	1	514	CHL	C11-C10-C8-C7
19	A	805	CLA	C15-C16-C17-C18
18	1	503	BCR	C19-C20-C21-C22
19	B	819	CLA	C16-C17-C18-C19
29	B	841	PQN	C26-C27-C28-C30
21	B	843	LHG	C24-C23-O8-C6
21	A	853	LHG	C24-C25-C26-C27
26	4	319	DGD	C2B-C3B-C4B-C5B
19	4	315	CLA	C5-C6-C7-C8
19	A	803	CLA	C2A-CAA-CBA-CGA
19	A	833	CLA	C3-C5-C6-C7
19	A	837	CLA	O1A-CGA-O2A-C1
19	G	204	CLA	C16-C17-C18-C20
19	1	513	CLA	CBA-CGA-O2A-C1
19	A	804	CLA	CBA-CGA-O2A-C1
19	A	818	CLA	C11-C10-C8-C7
19	L	304	CLA	C10-C11-C12-C13
19	1	508	CLA	CAD-CBD-CGD-O2D
19	2	507	CLA	CAD-CBD-CGD-O2D
19	A	804	CLA	CAD-CBD-CGD-O2D
19	A	816	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	B	811	CLA	CAD-CBD-CGD-O2D
19	B	821	CLA	CAD-CBD-CGD-O2D
19	B	829	CLA	CAD-CBD-CGD-O2D
22	J	1104	LMG	C9-C8-O7-C10
21	A	853	LHG	O9-C7-O7-C5
21	A	845	LHG	C14-C15-C16-C17
24	B	847	LMT	C2-C3-C4-C5
19	A	834	CLA	C10-C11-C12-C13
19	B	804	CLA	C8-C10-C11-C12
26	4	319	DGD	C7A-C8A-C9A-CAA
19	A	840	CLA	O1A-CGA-O2A-C1
19	B	836	CLA	CBA-CGA-O2A-C1
19	B	838	CLA	CBA-CGA-O2A-C1
19	A	805	CLA	C4-C3-C5-C6
22	F	304	LMG	C15-C16-C17-C18
19	A	822	CLA	C5-C6-C7-C8
24	B	846	LMT	C3-C4-C5-C6
19	A	804	CLA	O1A-CGA-O2A-C1
19	B	820	CLA	O1A-CGA-O2A-C1
22	J	1104	LMG	O10-C28-O8-C9
21	2	517	LHG	C28-C29-C30-C31
24	G	208	LMT	C4'-C5'-C6'-O6'
19	B	831	CLA	C2A-CAA-CBA-CGA
19	B	823	CLA	C6-C7-C8-C9
29	B	841	PQN	C26-C27-C28-C29
19	2	510	CLA	CHA-CBD-CGD-O1D
19	2	510	CLA	CHA-CBD-CGD-O2D
19	3	308	CLA	CHA-CBD-CGD-O1D
19	3	308	CLA	CHA-CBD-CGD-O2D
19	3	311	CLA	CHA-CBD-CGD-O1D
19	3	311	CLA	CHA-CBD-CGD-O2D
19	4	310	CLA	CHA-CBD-CGD-O1D
19	4	310	CLA	CHA-CBD-CGD-O2D
19	4	312	CLA	CHA-CBD-CGD-O1D
19	4	312	CLA	CHA-CBD-CGD-O2D
19	A	825	CLA	CHA-CBD-CGD-O1D
19	A	825	CLA	CHA-CBD-CGD-O2D
19	A	830	CLA	CHA-CBD-CGD-O1D
19	B	809	CLA	CHA-CBD-CGD-O1D
19	B	809	CLA	CHA-CBD-CGD-O2D
19	B	814	CLA	CHA-CBD-CGD-O1D
19	B	822	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	B	824	CLA	CHA-CBD-CGD-O1D
19	B	832	CLA	CHA-CBD-CGD-O1D
19	B	832	CLA	CHA-CBD-CGD-O2D
20	4	317	CHL	CHA-CBD-CGD-O2D
24	J	1107	LMT	C2-C1-O1'-C1'
19	A	812	CLA	O1A-CGA-O2A-C1
19	B	805	CLA	O1A-CGA-O2A-C1
22	A	847	LMG	O1-C7-C8-O7
19	A	825	CLA	C10-C11-C12-C13
19	B	836	CLA	O1A-CGA-O2A-C1
20	1	521	CHL	C4C-C3C-CAC-CBC
21	A	853	LHG	C17-C18-C19-C20
19	3	313	CLA	C11-C12-C13-C15
19	A	825	CLA	C16-C17-C18-C19
19	B	818	CLA	C16-C17-C18-C19
21	B	843	LHG	C26-C27-C28-C29
19	B	811	CLA	C15-C16-C17-C18
19	B	840	CLA	C2-C3-C5-C6
22	4	322	LMG	C13-C14-C15-C16
19	2	510	CLA	C10-C11-C12-C13
19	3	313	CLA	C6-C7-C8-C9
19	A	804	CLA	C6-C7-C8-C9
19	B	812	CLA	C6-C7-C8-C9
21	B	843	LHG	C28-C29-C30-C31
27	A	801	CL0	CAA-CBA-CGA-O2A
18	A	849	BCR	C11-C12-C13-C35
22	2	519	LMG	C13-C14-C15-C16
19	J	1101	CLA	C2C-C3C-CAC-CBC
23	2	502	XAT	C27-C28-C29-C30
18	1	503	BCR	C17-C18-C19-C20
19	1	509	CLA	C1A-C2A-CAA-CBA
19	1	511	CLA	C1A-C2A-CAA-CBA
19	4	318	CLA	C1A-C2A-CAA-CBA
19	A	823	CLA	C1A-C2A-CAA-CBA
19	A	824	CLA	C1A-C2A-CAA-CBA
19	B	813	CLA	C1A-C2A-CAA-CBA
19	B	814	CLA	C1A-C2A-CAA-CBA
19	B	819	CLA	C1A-C2A-CAA-CBA
19	F	302	CLA	C1A-C2A-CAA-CBA
19	2	504	CLA	C11-C12-C13-C14
19	A	806	CLA	C16-C17-C18-C19
19	A	807	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	B	811	CLA	C13-C15-C16-C17
19	2	507	CLA	C2-C1-O2A-CGA
19	4	308	CLA	C2-C1-O2A-CGA
19	A	831	CLA	C2-C1-O2A-CGA
19	B	828	CLA	C2-C1-O2A-CGA
19	B	830	CLA	C2-C1-O2A-CGA
19	A	833	CLA	CBA-CGA-O2A-C1
24	J	1107	LMT	C5'-C4'-O1B-C1B
18	F	306	BCR	C13-C14-C15-C16
21	1	517	LHG	C3-O3-P-O6
21	1	520	LHG	C4-O6-P-O3
21	B	843	LHG	C4-O6-P-O3
19	1	510	CLA	C2C-C3C-CAC-CBC
19	A	823	CLA	C4-C3-C5-C6
19	B	825	CLA	C10-C11-C12-C13
19	1	513	CLA	O1A-CGA-O2A-C1
21	B	843	LHG	O10-C23-O8-C6
19	B	821	CLA	O1A-CGA-O2A-C1
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	C4-O6-P-O4
21	A	853	LHG	C3-O3-P-O5
21	A	853	LHG	C4-O6-P-O5
21	B	843	LHG	C3-O3-P-O5
19	A	827	CLA	C16-C17-C18-C20
19	A	839	CLA	C16-C17-C18-C20
19	B	820	CLA	C16-C17-C18-C20
22	G	206	LMG	C29-C30-C31-C32
19	B	805	CLA	C5-C6-C7-C8
19	B	828	CLA	C13-C15-C16-C17
22	1	518	LMG	C10-C11-C12-C13
19	3	308	CLA	C3-C5-C6-C7
24	G	209	LMT	O5B-C1B-O1B-C4'
19	A	811	CLA	C16-C17-C18-C20
24	2	523	LMT	C3-C4-C5-C6
19	3	311	CLA	CAD-CBD-CGD-O1D
19	4	312	CLA	CAD-CBD-CGD-O1D
19	A	836	CLA	C2-C3-C5-C6
19	B	814	CLA	CAD-CBD-CGD-O1D
19	B	835	CLA	CAD-CBD-CGD-O1D
19	J	1105	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	B	812	CLA	C5-C6-C7-C8
19	B	827	CLA	C10-C11-C12-C13
19	B	838	CLA	O1A-CGA-O2A-C1
22	B	844	LMG	C12-C13-C14-C15
19	3	309	CLA	C6-C7-C8-C9
19	B	815	CLA	C4-C3-C5-C6
17	3	302	LUT	C25-C26-C27-C28
17	J	1109	LUT	C25-C26-C27-C28
19	4	308	CLA	C11-C10-C8-C7
19	4	315	CLA	C11-C12-C13-C15
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	839	CLA	C11-C12-C13-C15
19	A	841	CLA	C11-C10-C8-C7
19	B	812	CLA	C6-C7-C8-C10
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
19	L	305	CLA	C3A-C2A-CAA-CBA
21	A	853	LHG	O6-C4-C5-O7
21	B	842	LHG	O6-C4-C5-O7
29	B	841	PQN	C16-C17-C18-C20
29	B	841	PQN	C22-C23-C25-C26
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	A	833	CLA	O1A-CGA-O2A-C1
19	A	820	CLA	C2A-CAA-CBA-CGA
19	B	818	CLA	C16-C17-C18-C20
22	1	518	LMG	C7-C8-C9-O8
22	2	519	LMG	C7-C8-C9-O8
22	B	845	LMG	O1-C7-C8-C9
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
22	2	519	LMG	O7-C8-C9-O8
22	F	305	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
19	G	201	CLA	C15-C16-C17-C18
19	4	304	CLA	C3-C5-C6-C7
21	2	517	LHG	C2-C3-O3-P
20	2	516	CHL	C2-C3-C5-C6
19	B	840	CLA	C15-C16-C17-C18
19	A	802	CLA	C11-C12-C13-C14
19	A	804	CLA	C14-C13-C15-C16
19	A	807	CLA	C6-C7-C8-C9
19	A	819	CLA	C6-C7-C8-C9
19	A	819	CLA	C11-C12-C13-C14
19	A	838	CLA	C11-C12-C13-C14
19	A	839	CLA	C14-C13-C15-C16
19	A	854	CLA	C11-C12-C13-C14
19	A	855	CLA	C11-C12-C13-C14
19	B	815	CLA	C11-C10-C8-C9
19	B	817	CLA	C6-C7-C8-C9
19	B	822	CLA	C11-C12-C13-C14
19	B	827	CLA	C6-C7-C8-C9
19	G	204	CLA	C11-C12-C13-C14
20	2	526	CHL	C11-C12-C13-C14
19	B	823	CLA	C6-C7-C8-C10
19	A	827	CLA	C8-C10-C11-C12
19	A	838	CLA	C5-C6-C7-C8
21	A	845	LHG	C17-C18-C19-C20
19	A	802	CLA	C5-C6-C7-C8
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	B	820	CLA	C16-C17-C18-C19
19	J	1101	CLA	C4C-C3C-CAC-CBC
17	3	302	LUT	C7-C8-C9-C10
22	2	519	LMG	O7-C10-C11-C12
19	4	304	CLA	C2-C3-C5-C6
19	A	823	CLA	C2-C3-C5-C6
19	1	508	CLA	C5-C6-C7-C8
21	1	517	LHG	C13-C14-C15-C16
21	2	517	LHG	O8-C23-C24-C25
19	A	832	CLA	C8-C10-C11-C12
20	1	514	CHL	C5-C6-C7-C8
22	2	519	LMG	C7-C8-O7-C10
22	2	519	LMG	C9-C8-O7-C10
22	4	322	LMG	C9-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
22	G	210	LMG	C9-C8-O7-C10
26	B	801	DGD	C1G-C2G-O2G-C1B
19	1	507	CLA	C2A-CAA-CBA-CGA
19	B	814	CLA	C2A-CAA-CBA-CGA
19	A	829	CLA	C2-C1-O2A-CGA
19	A	830	CLA	C2-C1-O2A-CGA
19	B	831	CLA	C2-C1-O2A-CGA
24	2	523	LMT	O1'-C1-C2-C3
20	1	514	CHL	C11-C12-C13-C14
20	4	314	CHL	C4C-C3C-CAC-CBC
19	B	823	CLA	CAA-CBA-CGA-O2A
19	B	808	CLA	C13-C15-C16-C17
17	1	502	LUT	C1-C6-C7-C8
17	1	502	LUT	C5-C6-C7-C8
18	F	306	BCR	C23-C24-C25-C30
18	G	205	BCR	C23-C24-C25-C30
18	L	306	BCR	C23-C24-C25-C26
19	A	805	CLA	C2-C3-C5-C6
19	1	513	CLA	C10-C11-C12-C13
19	B	835	CLA	C6-C7-C8-C9
24	4	320	LMT	C1-C2-C3-C4
22	G	210	LMG	O6-C1-O1-C7
19	2	509	CLA	C2A-CAA-CBA-CGA
19	A	807	CLA	C2A-CAA-CBA-CGA
19	A	824	CLA	C2A-CAA-CBA-CGA
18	A	852	BCR	C11-C10-C9-C8
18	J	1108	BCR	C11-C10-C9-C8
22	G	210	LMG	C2-C1-O1-C7
21	1	517	LHG	C4-O6-P-O3
21	A	845	LHG	C3-O3-P-O6
21	B	842	LHG	C3-O3-P-O6
22	4	322	LMG	C4-C5-C6-O5
19	G	201	CLA	C16-C17-C18-C20
26	J	1106	DGD	C6A-C7A-C8A-C9A
21	A	853	LHG	C4-C5-C6-O8
26	B	854	DGD	O1G-C1G-C2G-C3G
19	A	802	CLA	C6-C7-C8-C10
19	A	803	CLA	C11-C10-C8-C7
19	A	842	CLA	C11-C10-C8-C7
19	B	805	CLA	C11-C12-C13-C15
19	B	829	CLA	C2-C3-C5-C6
19	B	838	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	K	1002	CLA	C6-C7-C8-C10
21	A	853	LHG	C10-C11-C12-C13
19	3	308	CLA	C6-C7-C8-C9
19	A	803	CLA	C11-C10-C8-C9
19	A	805	CLA	C11-C10-C8-C9
19	A	806	CLA	C11-C12-C13-C14
19	A	824	CLA	C14-C13-C15-C16
19	A	841	CLA	C11-C10-C8-C9
19	B	804	CLA	C11-C10-C8-C9
19	B	825	CLA	C11-C12-C13-C14
19	B	830	CLA	C11-C10-C8-C9
19	J	1101	CLA	C11-C12-C13-C14
19	K	1002	CLA	C11-C10-C8-C9
22	2	518	LMG	O7-C10-C11-C12
29	B	841	PQN	C16-C17-C18-C19
29	B	841	PQN	C24-C23-C25-C26
19	A	803	CLA	C10-C11-C12-C13
18	B	802	BCR	C9-C10-C11-C12
18	F	306	BCR	C19-C20-C21-C22
19	1	507	CLA	C16-C17-C18-C20
19	A	806	CLA	C16-C17-C18-C20
19	B	833	CLA	C11-C12-C13-C14
19	G	204	CLA	C16-C17-C18-C19
24	B	855	LMT	C3-C4-C5-C6
19	A	814	CLA	C10-C11-C12-C13
19	A	831	CLA	C13-C15-C16-C17
18	A	848	BCR	C36-C18-C19-C20
18	G	205	BCR	C36-C18-C19-C20
26	J	1106	DGD	C1B-C2B-C3B-C4B
19	F	302	CLA	C2-C3-C5-C6
19	3	309	CLA	C6-C7-C8-C10
19	A	828	CLA	C16-C17-C18-C19
26	J	1106	DGD	C3B-C4B-C5B-C6B
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	B	840	CLA	CAA-CBA-CGA-O2A
19	F	302	CLA	C4-C3-C5-C6
19	G	202	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	2	516	CHL	C4-C3-C5-C6
19	1	508	CLA	C13-C15-C16-C17
21	1	517	LHG	C32-C33-C34-C35
19	A	812	CLA	C2-C1-O2A-CGA
19	B	825	CLA	C2-C1-O2A-CGA
19	G	204	CLA	C15-C16-C17-C18
19	2	506	CLA	C16-C17-C18-C19
19	A	834	CLA	C2A-CAA-CBA-CGA
22	2	518	LMG	O9-C10-C11-C12
22	G	206	LMG	C13-C14-C15-C16
19	A	830	CLA	C3A-C2A-CAA-CBA
19	B	819	CLA	C3A-C2A-CAA-CBA
19	B	826	CLA	C3A-C2A-CAA-CBA
27	A	801	CL0	C3A-C2A-CAA-CBA
19	B	814	CLA	C13-C15-C16-C17
18	A	856	BCR	C13-C14-C15-C16
22	A	847	LMG	C15-C16-C17-C18
19	1	515	CLA	CAA-CBA-CGA-O2A
20	2	515	CHL	CAA-CBA-CGA-O2A
19	B	825	CLA	C4-C3-C5-C6
19	A	808	CLA	C6-C7-C8-C9
19	A	808	CLA	C11-C10-C8-C9
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	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
29	A	844	PQN	C21-C22-C23-C24
19	A	827	CLA	C16-C17-C18-C19
19	B	820	CLA	C15-C16-C17-C18
21	B	843	LHG	C29-C30-C31-C32
17	3	301	LUT	C21-C26-C27-C28
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

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Mol	Chain	Res	Type	Atoms
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
26	B	854	DGD	O6D-C5D-C6D-O5D
19	B	833	CLA	C3-C5-C6-C7
19	K	1001	CLA	CAA-CBA-CGA-O1A
19	1	516	CLA	O1A-CGA-O2A-C1
19	A	837	CLA	O1D-CGD-O2D-CED
19	A	811	CLA	C16-C17-C18-C19
19	B	835	CLA	C6-C7-C8-C10
20	2	526	CHL	O2A-C1-C2-C3
19	1	515	CLA	CAA-CBA-CGA-O1A
19	A	834	CLA	C15-C16-C17-C18
19	B	803	CLA	C5-C6-C7-C8
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
19	A	804	CLA	C4-C3-C5-C6
19	B	820	CLA	C4-C3-C5-C6
19	B	827	CLA	C4-C3-C5-C6
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
19	L	304	CLA	C1A-C2A-CAA-CBA
27	A	801	CL0	C1A-C2A-CAA-CBA
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	819	CLA	C11-C10-C8-C7
19	A	821	CLA	C12-C13-C15-C16
19	A	824	CLA	C11-C12-C13-C15
19	A	834	CLA	C12-C13-C15-C16
19	B	803	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	B	807	CLA	C12-C13-C15-C16
19	B	814	CLA	C11-C12-C13-C15
19	B	829	CLA	C11-C10-C8-C7
19	B	840	CLA	C11-C12-C13-C15
20	2	526	CHL	C6-C7-C8-C10
19	A	813	CLA	C3-C5-C6-C7
18	I	102	BCR	C19-C20-C21-C22
22	A	847	LMG	C14-C15-C16-C17
24	2	523	LMT	C11-C10-C9-C8
19	A	805	CLA	C5-C6-C7-C8
19	4	307	CLA	C2A-CAA-CBA-CGA
19	A	854	CLA	C2A-CAA-CBA-CGA
19	A	802	CLA	C15-C16-C17-C18
19	A	830	CLA	C10-C11-C12-C13
19	1	513	CLA	C4-C3-C5-C6
19	B	814	CLA	C4-C3-C5-C6
19	F	303	CLA	C10-C11-C12-C13
19	B	815	CLA	C2-C3-C5-C6
19	B	824	CLA	C5-C6-C7-C8
19	A	837	CLA	CBD-CGD-O2D-CED
19	A	835	CLA	C6-C7-C8-C10
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	K	1001	CLA	CAA-CBA-CGA-O2A
19	B	816	CLA	CBA-CGA-O2A-C1
18	A	856	BCR	C19-C20-C21-C22
20	2	515	CHL	CAA-CBA-CGA-O1A
19	1	507	CLA	C16-C17-C18-C19
19	4	306	CLA	C16-C17-C18-C20
19	A	832	CLA	C16-C17-C18-C19
19	B	828	CLA	C16-C17-C18-C19
19	A	830	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
19	A	819	CLA	C4-C3-C5-C6
19	B	809	CLA	C4-C3-C5-C6
19	1	504	CLA	C2-C1-O2A-CGA
19	A	804	CLA	C2-C1-O2A-CGA
19	A	836	CLA	C2-C1-O2A-CGA
19	B	825	CLA	C2-C3-C5-C6
26	4	319	DGD	O1G-C1A-C2A-C3A
19	1	508	CLA	C11-C10-C8-C9
19	4	311	CLA	CAA-CBA-CGA-O2A
26	G	207	DGD	C3A-C4A-C5A-C6A
19	2	504	CLA	C2A-CAA-CBA-CGA
19	B	838	CLA	C2A-CAA-CBA-CGA
19	B	808	CLA	C16-C17-C18-C20
19	B	831	CLA	C11-C12-C13-C14
19	1	516	CLA	CBA-CGA-O2A-C1
19	B	816	CLA	O1A-CGA-O2A-C1
17	4	302	LUT	C1-C6-C7-C8
18	3	303	BCR	C23-C24-C25-C30
18	A	852	BCR	C23-C24-C25-C30
18	J	1108	BCR	C23-C24-C25-C30
30	F	301	ZEX	C1-C6-C7-C8
26	J	1106	DGD	C7A-C8A-C9A-CAA
19	3	308	CLA	CAA-CBA-CGA-O2A
19	A	829	CLA	CAA-CBA-CGA-O2A
19	B	803	CLA	CAA-CBA-CGA-O2A
19	B	826	CLA	C8-C10-C11-C12
26	B	801	DGD	C3A-C4A-C5A-C6A
18	3	304	BCR	C7-C8-C9-C10
21	1	520	LHG	C25-C26-C27-C28
19	2	508	CLA	C5-C6-C7-C8
19	B	819	CLA	CAA-CBA-CGA-O2A
19	2	507	CLA	C5-C6-C7-C8
22	2	518	LMG	C4-C5-C6-O5
22	G	210	LMG	C4-C5-C6-O5
20	4	314	CHL	C2A-CAA-CBA-CGA
19	B	840	CLA	C3-C5-C6-C7
21	B	842	LHG	O10-C23-O8-C6
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	1	513	CLA	C2-C3-C5-C6
19	B	827	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	B	810	CLA	C8-C10-C11-C12
26	B	801	DGD	O1G-C1A-C2A-C3A
19	B	816	CLA	C6-C7-C8-C9
20	2	513	CHL	C2-C1-O2A-CGA
26	4	319	DGD	O2G-C2G-C3G-O3G
19	2	506	CLA	C8-C10-C11-C12
19	3	313	CLA	CAA-CBA-CGA-O2A
24	B	846	LMT	C1-C2-C3-C4
19	2	506	CLA	C16-C17-C18-C20
19	A	827	CLA	CBA-CGA-O2A-C1
19	A	813	CLA	C4-C3-C5-C6
19	A	828	CLA	C4-C3-C5-C6
19	A	832	CLA	C4-C3-C5-C6
19	A	806	CLA	C2-C3-C5-C6
19	A	819	CLA	C2-C3-C5-C6
19	B	814	CLA	C2-C3-C5-C6
19	B	819	CLA	CBA-CGA-O2A-C1
21	A	853	LHG	O8-C23-C24-C25
19	1	507	CLA	C11-C12-C13-C14
19	4	315	CLA	C11-C12-C13-C14
19	A	802	CLA	C6-C7-C8-C9
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
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
20	2	526	CHL	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
19	1	507	CLA	CAD-CBD-CGD-O2D
19	2	510	CLA	CAD-CBD-CGD-O2D
19	3	308	CLA	CAD-CBD-CGD-O2D
19	A	823	CLA	CAD-CBD-CGD-O2D
19	B	830	CLA	CAD-CBD-CGD-O2D
20	3	314	CHL	CAD-CBD-CGD-O2D
22	F	305	LMG	C9-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
26	G	207	DGD	C3G-C2G-O2G-C1B
19	2	504	CLA	C10-C11-C12-C13
21	A	845	LHG	C19-C20-C21-C22
22	F	304	LMG	C12-C13-C14-C15
19	4	307	CLA	C4-C3-C5-C6
19	A	829	CLA	C4-C3-C5-C6
19	A	827	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
18	J	1108	BCR	C17-C18-C19-C20
26	4	319	DGD	C1G-C2G-C3G-O3G
26	G	207	DGD	O6D-C5D-C6D-O5D
19	G	201	CLA	CAA-CBA-CGA-O2A
21	B	843	LHG	C13-C14-C15-C16
19	1	508	CLA	C10-C11-C12-C13
19	2	509	CLA	CAA-CBA-CGA-O2A
19	A	824	CLA	C15-C16-C17-C18
19	2	507	CLA	C16-C17-C18-C19
19	4	308	CLA	C11-C12-C13-C15
19	1	504	CLA	CHA-CBD-CGD-O1D
19	1	504	CLA	CHA-CBD-CGD-O2D
19	1	506	CLA	CHA-CBD-CGD-O1D
19	1	506	CLA	CHA-CBD-CGD-O2D
19	1	516	CLA	CHA-CBD-CGD-O2D
19	2	506	CLA	CHA-CBD-CGD-O2D
19	2	511	CLA	CHA-CBD-CGD-O1D
19	2	511	CLA	CHA-CBD-CGD-O2D
19	4	318	CLA	CHA-CBD-CGD-O1D
19	4	318	CLA	CHA-CBD-CGD-O2D
19	A	811	CLA	CHA-CBD-CGD-O1D
19	A	811	CLA	CHA-CBD-CGD-O2D
19	A	813	CLA	CHA-CBD-CGD-O1D
19	A	813	CLA	CHA-CBD-CGD-O2D
19	A	819	CLA	CHA-CBD-CGD-O1D
19	A	819	CLA	CHA-CBD-CGD-O2D
19	A	828	CLA	CHA-CBD-CGD-O2D
19	A	837	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	A	837	CLA	CHA-CBD-CGD-O2D
19	B	805	CLA	CHA-CBD-CGD-O1D
19	B	805	CLA	CHA-CBD-CGD-O2D
19	B	814	CLA	CHA-CBD-CGD-O2D
19	B	816	CLA	CHA-CBD-CGD-O2D
19	B	823	CLA	CHA-CBD-CGD-O1D
19	B	823	CLA	CHA-CBD-CGD-O2D
19	B	824	CLA	CHA-CBD-CGD-O2D
19	B	827	CLA	CHA-CBD-CGD-O1D
19	B	827	CLA	CHA-CBD-CGD-O2D
19	B	836	CLA	CHA-CBD-CGD-O1D
19	B	836	CLA	CHA-CBD-CGD-O2D
19	G	202	CLA	CHA-CBD-CGD-O1D
19	G	202	CLA	CHA-CBD-CGD-O2D
19	H	1000	CLA	CHA-CBD-CGD-O1D
19	H	1000	CLA	CHA-CBD-CGD-O2D
19	L	301	CLA	CHA-CBD-CGD-O1D
19	L	301	CLA	CHA-CBD-CGD-O2D
20	1	521	CHL	CHA-CBD-CGD-O2D
20	2	512	CHL	CHA-CBD-CGD-O1D
20	4	317	CHL	CHA-CBD-CGD-O1D
19	A	822	CLA	CAA-CBA-CGA-O2A
19	B	839	CLA	CAA-CBA-CGA-O2A
18	B	851	BCR	C11-C10-C9-C8
19	A	828	CLA	CAA-CBA-CGA-O2A
22	J	1104	LMG	C32-C33-C34-C35
19	B	836	CLA	C5-C6-C7-C8
19	B	836	CLA	CAA-CBA-CGA-O2A
19	B	834	CLA	CAA-CBA-CGA-O2A
19	A	829	CLA	C2-C3-C5-C6
19	B	809	CLA	C2-C3-C5-C6
19	B	827	CLA	C11-C12-C13-C15
19	A	835	CLA	C6-C7-C8-C9
19	B	808	CLA	C16-C17-C18-C19
19	3	316	CLA	CAA-CBA-CGA-O2A
19	A	814	CLA	CAA-CBA-CGA-O2A
19	4	308	CLA	C11-C10-C8-C9
19	A	839	CLA	C11-C12-C13-C14
19	B	803	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

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Mol	Chain	Res	Type	Atoms
19	B	840	CLA	C11-C12-C13-C14
22	G	210	LMG	O8-C28-C29-C30
17	3	302	LUT	C29-C30-C31-C32
17	J	1109	LUT	C33-C34-C35-C15
21	A	853	LHG	C31-C32-C33-C34
19	A	827	CLA	O1A-CGA-O2A-C1
19	3	305	CLA	C2A-CAA-CBA-CGA
20	1	514	CHL	C2A-CAA-CBA-CGA
21	A	853	LHG	C30-C31-C32-C33
26	J	1106	DGD	C7B-C8B-C9B-CAB
19	A	807	CLA	CAA-CBA-CGA-O2A
19	K	1002	CLA	CAA-CBA-CGA-O2A
22	F	304	LMG	C36-C37-C38-C39
19	B	831	CLA	C11-C12-C13-C15
19	A	830	CLA	C4-C3-C5-C6
19	B	830	CLA	C4-C3-C5-C6
19	1	508	CLA	C1A-C2A-CAA-CBA
19	2	506	CLA	C1A-C2A-CAA-CBA
19	4	307	CLA	C1A-C2A-CAA-CBA
19	A	821	CLA	C1A-C2A-CAA-CBA
19	A	830	CLA	C1A-C2A-CAA-CBA
19	A	836	CLA	C1A-C2A-CAA-CBA
19	B	820	CLA	C1A-C2A-CAA-CBA
20	1	521	CHL	C1A-C2A-CAA-CBA
20	2	526	CHL	C1A-C2A-CAA-CBA
19	A	827	CLA	CAA-CBA-CGA-O1A
20	1	512	CHL	CAA-CBA-CGA-O2A
19	A	855	CLA	C2-C1-O2A-CGA
19	A	807	CLA	CAA-CBA-CGA-O1A
22	1	518	LMG	O9-C10-C11-C12
19	B	838	CLA	CAA-CBA-CGA-O2A
19	A	819	CLA	C2A-CAA-CBA-CGA
24	G	209	LMT	C5-C6-C7-C8
19	A	813	CLA	C16-C17-C18-C19
19	B	822	CLA	C16-C17-C18-C19
19	A	822	CLA	CAA-CBA-CGA-O1A
19	A	808	CLA	C15-C16-C17-C18
19	1	508	CLA	CAA-CBA-CGA-O2A
19	A	818	CLA	CAA-CBA-CGA-O2A
21	1	517	LHG	O8-C23-C24-C25
21	A	845	LHG	O7-C7-C8-C9
19	G	201	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
19	K	1002	CLA	CAA-CBA-CGA-O1A
19	G	202	CLA	C2-C3-C5-C6
19	B	803	CLA	C13-C15-C16-C17
21	1	517	LHG	C3-O3-P-O5
21	1	517	LHG	C4-O6-P-O5
21	A	845	LHG	C3-O3-P-O5
19	A	814	CLA	CAA-CBA-CGA-O1A
18	G	205	BCR	C23-C24-C25-C26
18	I	101	BCR	C23-C24-C25-C30
30	F	301	ZEX	C5-C6-C7-C8
19	B	804	CLA	C15-C16-C17-C18
19	2	509	CLA	CAA-CBA-CGA-O1A
19	B	839	CLA	CAA-CBA-CGA-O1A
22	J	1104	LMG	O7-C10-C11-C12
19	B	819	CLA	C10-C11-C12-C13
21	A	853	LHG	O10-C23-C24-C25
20	2	516	CHL	C3-C5-C6-C7
19	A	821	CLA	C5-C6-C7-C8
19	B	823	CLA	C4-C3-C5-C6
19	A	804	CLA	C2-C3-C5-C6
19	A	815	CLA	CAA-CBA-CGA-O2A
19	1	511	CLA	CAD-CBD-CGD-O1D
19	2	506	CLA	CAD-CBD-CGD-O1D
19	4	305	CLA	CAD-CBD-CGD-O1D
19	A	820	CLA	CAD-CBD-CGD-O1D
19	A	828	CLA	CAD-CBD-CGD-O1D
19	A	831	CLA	CAD-CBD-CGD-O1D
19	A	833	CLA	CAD-CBD-CGD-O1D
19	A	836	CLA	CAD-CBD-CGD-O1D
19	A	854	CLA	CAD-CBD-CGD-O1D
19	A	855	CLA	CAD-CBD-CGD-O1D
19	B	808	CLA	CAD-CBD-CGD-O1D
19	B	827	CLA	CAD-CBD-CGD-O1D
20	2	516	CHL	CAD-CBD-CGD-O1D
19	B	826	CLA	O1A-CGA-O2A-C1
19	B	834	CLA	CAA-CBA-CGA-O1A
19	A	837	CLA	CAA-CBA-CGA-O2A
19	1	504	CLA	C14-C13-C15-C16
19	4	306	CLA	C11-C12-C13-C14
19	A	819	CLA	C11-C10-C8-C9
19	A	839	CLA	C11-C10-C8-C9
19	B	806	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	B	808	CLA	C6-C7-C8-C9
19	B	814	CLA	C11-C12-C13-C14
19	B	817	CLA	C11-C10-C8-C9
19	B	827	CLA	C11-C12-C13-C14
20	2	526	CHL	C14-C13-C15-C16
19	4	315	CLA	C4C-C3C-CAC-CBC
19	F	302	CLA	C3-C5-C6-C7
19	L	304	CLA	CAA-CBA-CGA-O2A
21	1	520	LHG	O8-C23-C24-C25
22	J	1103	LMG	O7-C10-C11-C12
19	B	805	CLA	C10-C11-C12-C13
22	A	847	LMG	C12-C13-C14-C15
19	B	838	CLA	CAA-CBA-CGA-O1A
22	A	847	LMG	C32-C33-C34-C35
19	A	839	CLA	C2A-CAA-CBA-CGA
19	4	309	CLA	CAA-CBA-CGA-O2A
19	A	824	CLA	CAA-CBA-CGA-O2A
19	B	811	CLA	CAA-CBA-CGA-O2A
19	L	305	CLA	CAA-CBA-CGA-O2A
22	B	845	LMG	O7-C10-C11-C12
22	F	304	LMG	O7-C10-C11-C12
19	3	316	CLA	CAA-CBA-CGA-O1A
24	A	846	LMT	C2-C3-C4-C5
19	B	828	CLA	C16-C17-C18-C20
19	B	820	CLA	C8-C10-C11-C12
22	G	206	LMG	C21-C22-C23-C24
26	B	854	DGD	C9A-CAA-CBA-CCA
19	1	507	CLA	C12-C13-C15-C16
19	A	804	CLA	C12-C13-C15-C16
19	A	806	CLA	C11-C10-C8-C7
19	A	839	CLA	C11-C10-C8-C7
19	A	855	CLA	C11-C12-C13-C15
19	B	805	CLA	C6-C7-C8-C10
19	B	820	CLA	C2-C3-C5-C6
20	2	526	CHL	C12-C13-C15-C16
19	B	836	CLA	CAA-CBA-CGA-O1A
21	1	517	LHG	O10-C23-C24-C25
19	2	504	CLA	CAA-CBA-CGA-O2A
19	A	805	CLA	CAA-CBA-CGA-O2A
19	A	820	CLA	CAA-CBA-CGA-O2A
19	B	806	CLA	CAA-CBA-CGA-O2A
19	G	204	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	1	520	LHG	O7-C7-C8-C9
18	A	850	BCR	C17-C18-C19-C20
19	1	508	CLA	CAA-CBA-CGA-O1A
19	A	824	CLA	CAA-CBA-CGA-O1A
19	B	811	CLA	CAA-CBA-CGA-O1A
21	A	845	LHG	O9-C7-C8-C9
18	B	851	BCR	C9-C10-C11-C12
18	B	856	BCR	C9-C10-C11-C12
18	B	856	BCR	C19-C20-C21-C22
24	B	855	LMT	C2-C1-O1'-C1'
19	A	830	CLA	CAA-CBA-CGA-O2A
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	A	818	CLA	CAA-CBA-CGA-O1A
19	L	305	CLA	CAA-CBA-CGA-O1A
27	A	801	CL0	CAA-CBA-CGA-O1A
20	1	514	CHL	C2C-C3C-CAC-CBC
22	J	1104	LMG	C30-C31-C32-C33
22	1	519	LMG	O6-C5-C6-O5
19	B	809	CLA	CAA-CBA-CGA-O2A
19	4	309	CLA	CAA-CBA-CGA-O1A
21	1	520	LHG	O9-C7-C8-C9
19	B	826	CLA	CBA-CGA-O2A-C1
19	A	837	CLA	CAA-CBA-CGA-O1A
22	F	304	LMG	O9-C10-C11-C12
19	B	831	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

228 monomers are involved in 966 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	851	BCR	5	0
19	4	306	CLA	6	0
19	A	810	CLA	5	0
18	A	849	BCR	1	0
19	B	812	CLA	7	0
18	A	856	BCR	3	0
18	4	301	BCR	9	0
18	L	307	BCR	2	0
19	B	815	CLA	6	0
29	B	841	PQN	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	812	CLA	6	0
30	F	301	ZEX	6	0
23	4	303	XAT	10	0
19	B	806	CLA	6	0
19	B	817	CLA	3	0
18	L	302	BCR	4	0
24	B	846	LMT	3	0
19	F	302	CLA	5	0
19	1	516	CLA	5	0
19	A	806	CLA	6	0
19	A	817	CLA	3	0
17	4	302	LUT	3	0
19	K	1003	CLA	1	0
27	A	801	CL0	8	0
19	2	504	CLA	7	0
19	J	1105	CLA	9	0
28	A	843	SF4	1	0
22	G	210	LMG	1	0
24	B	855	LMT	3	0
19	A	840	CLA	4	0
22	J	1104	LMG	2	0
21	1	520	LHG	10	0
19	A	821	CLA	11	0
19	B	825	CLA	10	0
24	J	1107	LMT	1	0
22	2	518	LMG	2	0
22	G	206	LMG	5	0
19	B	826	CLA	5	0
19	3	306	CLA	6	0
19	L	301	CLA	2	0
19	3	308	CLA	14	0
20	4	317	CHL	5	0
23	2	502	XAT	4	0
19	G	202	CLA	3	0
19	A	829	CLA	5	0
19	A	807	CLA	5	0
19	A	828	CLA	9	0
19	A	802	CLA	13	0
19	A	855	CLA	10	0
22	F	304	LMG	8	0
19	B	820	CLA	9	0
19	4	318	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	2	516	CHL	3	0
20	1	514	CHL	9	0
19	B	808	CLA	7	0
19	L	305	CLA	2	0
18	2	503	BCR	13	0
19	B	803	CLA	7	0
17	J	1109	LUT	8	0
19	A	826	CLA	5	0
19	3	307	CLA	6	0
19	4	309	CLA	11	0
18	B	850	BCR	1	0
19	G	203	CLA	2	0
17	3	301	LUT	13	0
18	F	306	BCR	1	0
19	A	835	CLA	4	0
26	4	319	DGD	6	0
20	2	515	CHL	4	0
20	4	314	CHL	6	0
19	2	510	CLA	5	0
19	4	307	CLA	10	0
18	B	802	BCR	4	0
19	B	816	CLA	4	0
18	G	205	BCR	3	0
19	1	510	CLA	8	0
19	B	810	CLA	4	0
19	L	303	CLA	3	0
20	2	513	CHL	6	0
19	2	506	CLA	5	0
19	4	315	CLA	5	0
19	B	837	CLA	5	0
17	2	501	LUT	8	0
18	A	848	BCR	1	0
19	1	505	CLA	1	0
19	1	509	CLA	3	0
19	3	310	CLA	5	0
19	3	313	CLA	4	0
19	A	825	CLA	10	0
19	A	841	CLA	8	0
22	4	322	LMG	4	0
22	B	845	LMG	2	0
19	4	308	CLA	5	0
24	3	318	LMT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1	504	CLA	10	0
19	A	854	CLA	11	0
19	L	304	CLA	4	0
19	B	813	CLA	2	0
19	A	815	CLA	1	0
19	1	511	CLA	1	0
26	J	1106	DGD	6	0
19	A	808	CLA	7	0
24	A	846	LMT	3	0
18	1	503	BCR	4	0
19	A	836	CLA	6	0
20	3	314	CHL	9	0
18	L	306	BCR	2	0
19	4	311	CLA	2	0
21	1	517	LHG	7	0
19	A	824	CLA	15	0
19	A	813	CLA	8	0
19	2	507	CLA	6	0
19	3	315	CLA	6	0
20	2	512	CHL	9	0
19	4	305	CLA	3	0
18	K	1005	BCR	7	0
19	F	303	CLA	7	0
19	A	837	CLA	6	0
26	B	801	DGD	5	0
19	B	809	CLA	7	0
19	B	807	CLA	3	0
24	4	320	LMT	3	0
19	K	1002	CLA	4	0
22	2	524	LMG	1	0
19	B	824	CLA	7	0
19	H	1000	CLA	4	0
24	G	209	LMT	1	0
19	2	505	CLA	4	0
19	1	508	CLA	13	0
18	3	303	BCR	7	0
19	B	839	CLA	5	0
19	G	204	CLA	12	0
19	4	312	CLA	4	0
22	2	519	LMG	6	0
19	J	1102	CLA	5	0
22	B	844	LMG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	833	CLA	7	0
19	B	830	CLA	11	0
19	A	820	CLA	1	0
22	A	847	LMG	3	0
19	2	514	CLA	3	0
17	3	302	LUT	6	0
18	B	852	BCR	4	0
21	A	853	LHG	3	0
19	A	803	CLA	6	0
29	A	844	PQN	4	0
18	3	304	BCR	4	0
20	1	512	CHL	7	0
19	3	317	CLA	5	0
22	J	1103	LMG	1	0
18	A	850	BCR	5	0
19	A	839	CLA	6	0
18	B	851	BCR	5	0
26	G	207	DGD	1	0
17	1	501	LUT	6	0
22	1	518	LMG	3	0
19	A	814	CLA	2	0
19	B	827	CLA	4	0
19	B	828	CLA	4	0
19	B	834	CLA	6	0
19	B	840	CLA	16	0
18	B	856	BCR	6	0
19	A	816	CLA	1	0
28	C	102	SF4	2	0
21	B	842	LHG	2	0
19	B	819	CLA	11	0
19	B	838	CLA	9	0
24	B	847	LMT	3	0
19	A	811	CLA	12	0
19	3	316	CLA	5	0
19	4	310	CLA	7	0
18	I	101	BCR	7	0
19	B	831	CLA	5	0
19	B	818	CLA	7	0
19	K	1004	CLA	2	0
19	G	201	CLA	8	0
19	A	823	CLA	3	0
19	A	805	CLA	10	0

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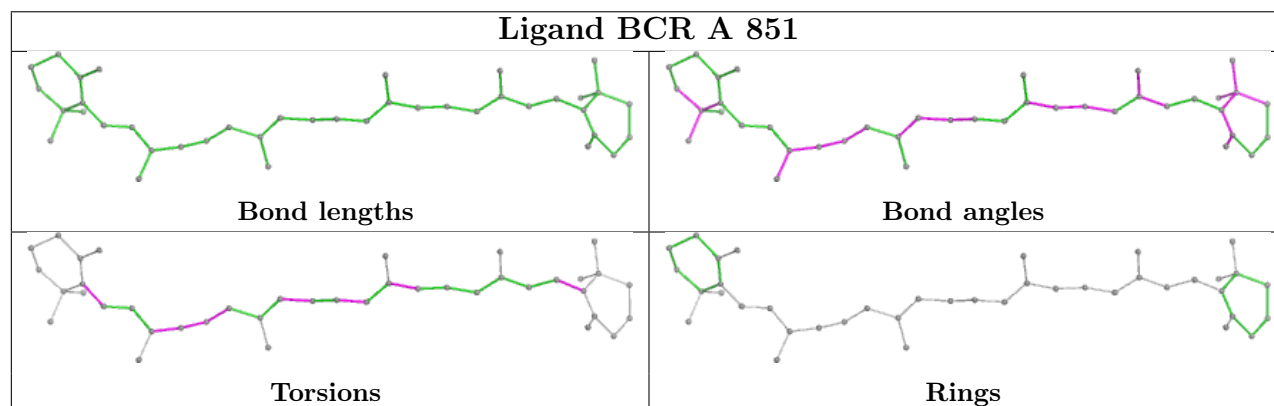
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19	A	832	CLA	8	0
20	1	521	CHL	8	0
19	A	831	CLA	6	0
21	B	843	LHG	6	0
18	A	852	BCR	6	0
19	1	515	CLA	8	0
19	A	819	CLA	8	0
18	J	1108	BCR	4	0
19	J	1101	CLA	13	0
21	A	845	LHG	7	0
19	A	818	CLA	11	0
19	B	823	CLA	8	0
22	F	305	LMG	2	0
19	A	809	CLA	9	0
17	1	502	LUT	6	0
19	A	827	CLA	5	0
19	1	513	CLA	2	0
19	B	805	CLA	7	0
18	B	849	BCR	2	0
19	A	804	CLA	6	0
19	B	829	CLA	9	0
19	B	811	CLA	5	0
19	2	511	CLA	4	0
20	4	316	CHL	10	0
19	4	304	CLA	6	0
19	A	822	CLA	4	0
19	B	832	CLA	7	0
21	2	517	LHG	9	0
19	2	508	CLA	5	0
19	1	507	CLA	8	0
20	4	313	CHL	2	0
19	B	835	CLA	5	0
18	B	853	BCR	6	0
19	2	509	CLA	2	0
24	G	208	LMT	4	0
26	B	854	DGD	9	0
19	A	830	CLA	9	0
19	A	834	CLA	6	0
19	3	309	CLA	3	0
19	B	814	CLA	5	0
19	B	804	CLA	4	0

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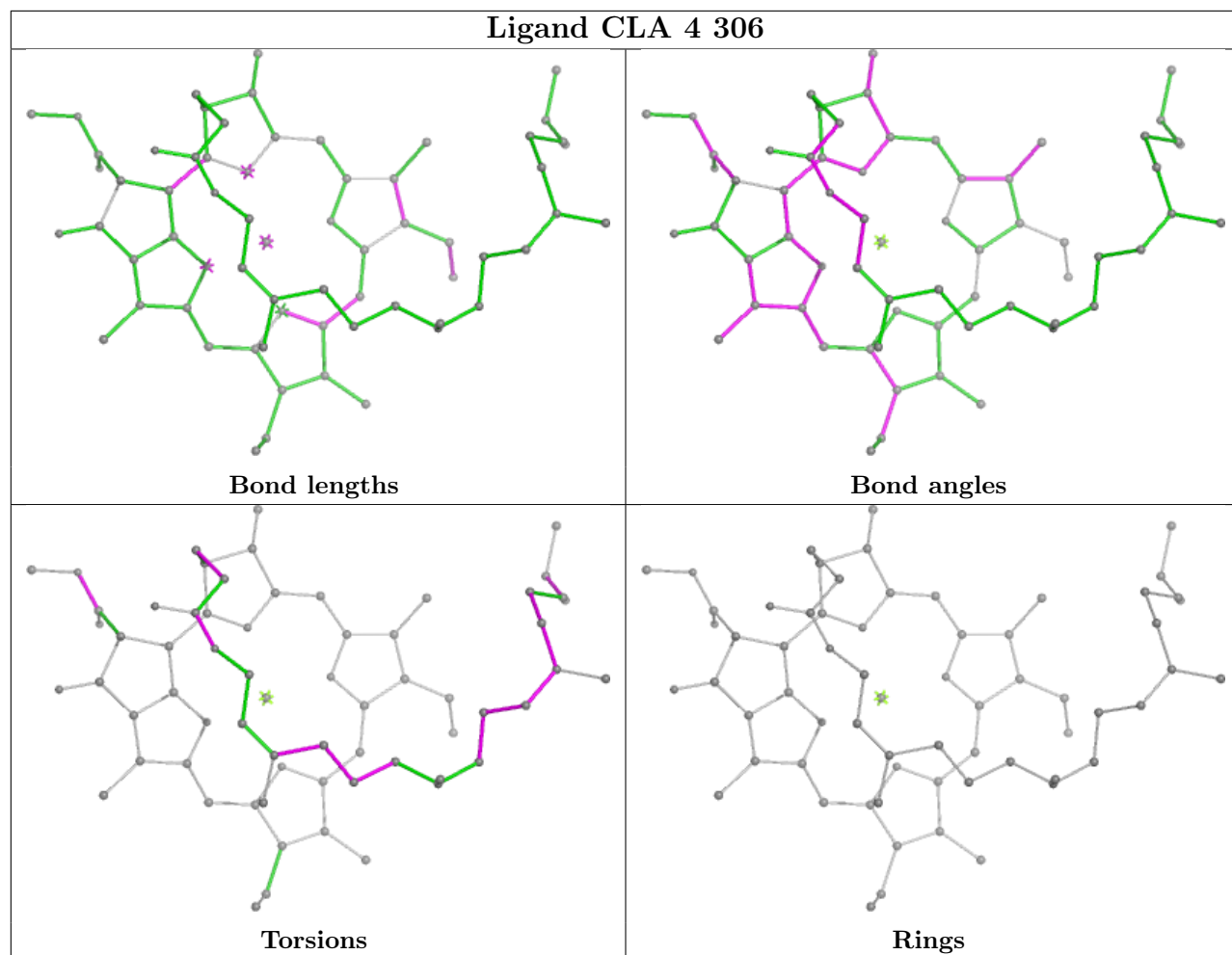
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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19	A	842	CLA	9	0
18	I	102	BCR	5	0
19	B	822	CLA	6	0
20	2	526	CHL	11	0
19	3	305	CLA	20	0
19	B	833	CLA	7	0
19	B	836	CLA	4	0

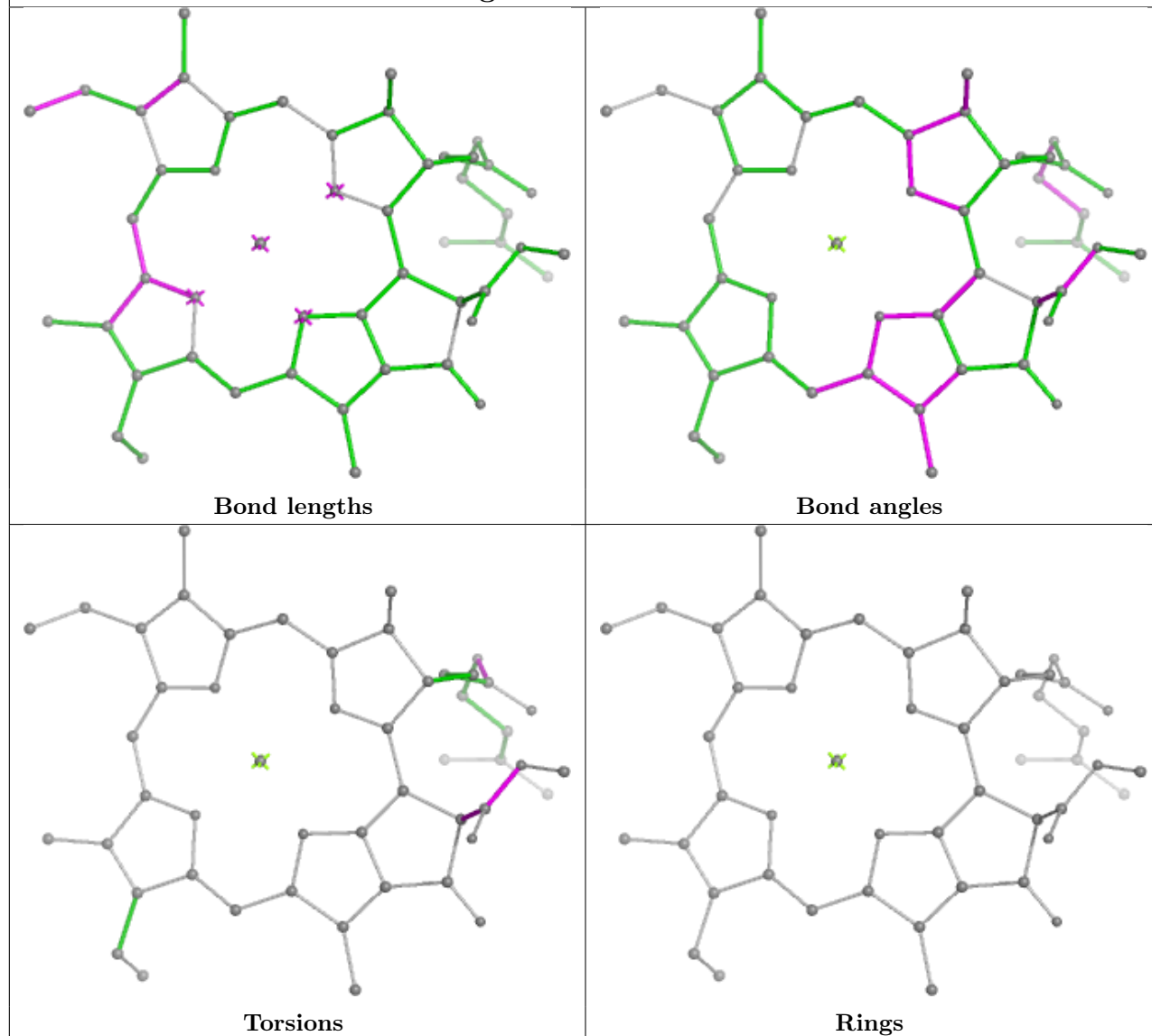
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



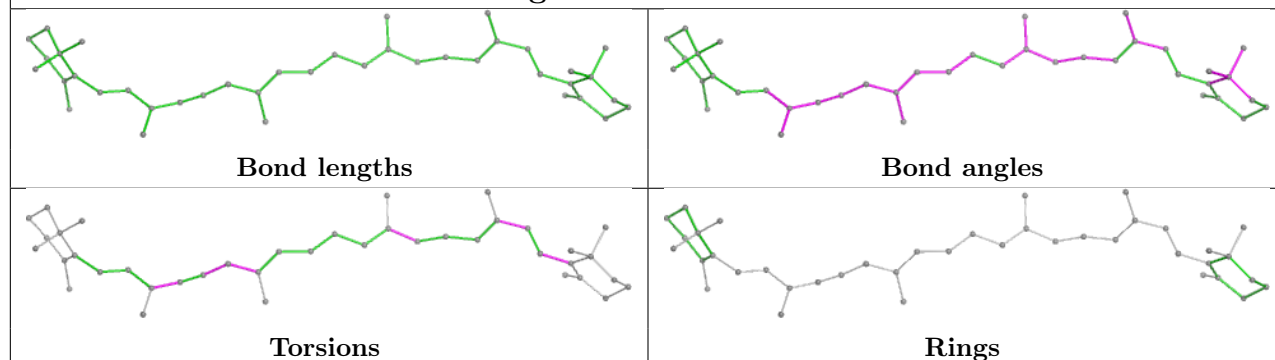
Ligand CLA 4 306



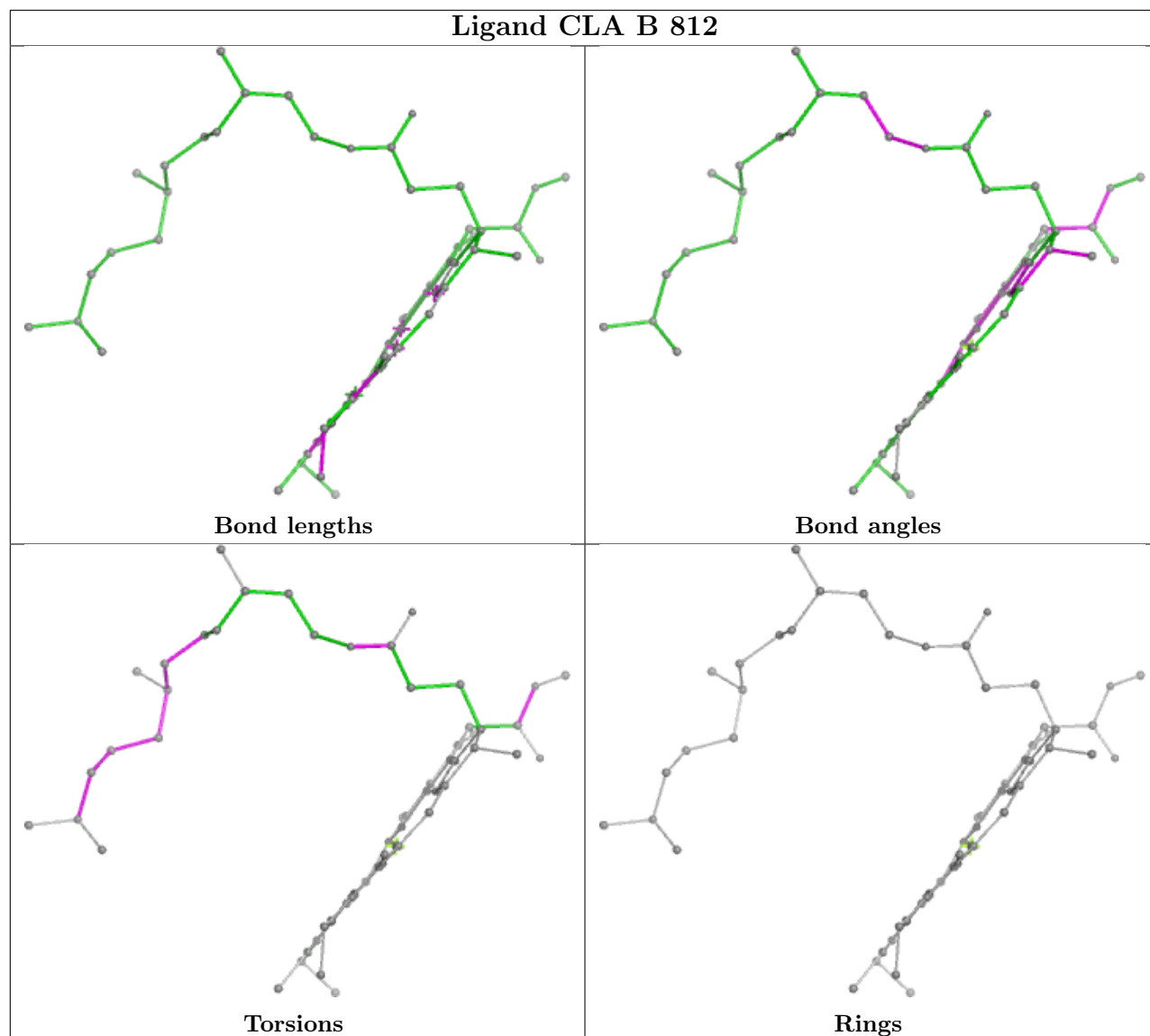
Ligand CLA A 810



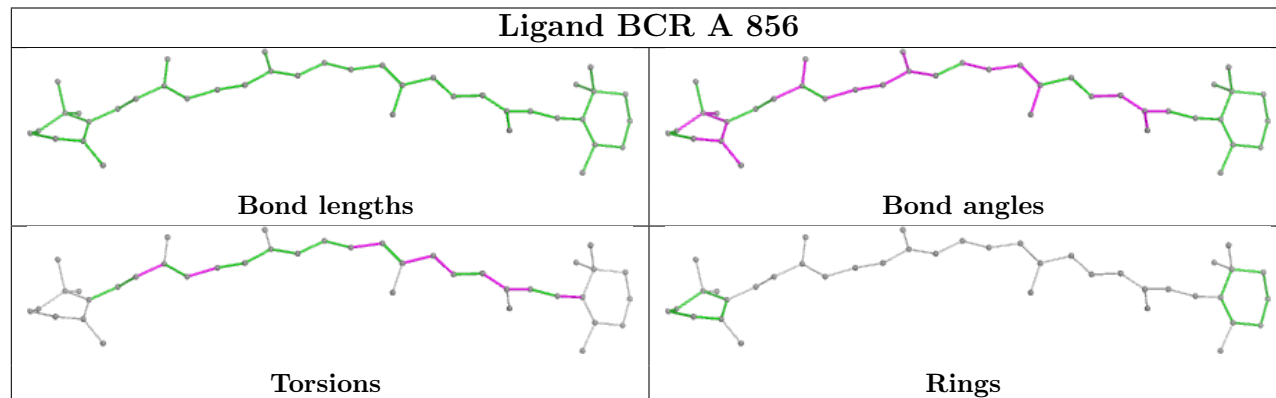
Ligand BCR A 849

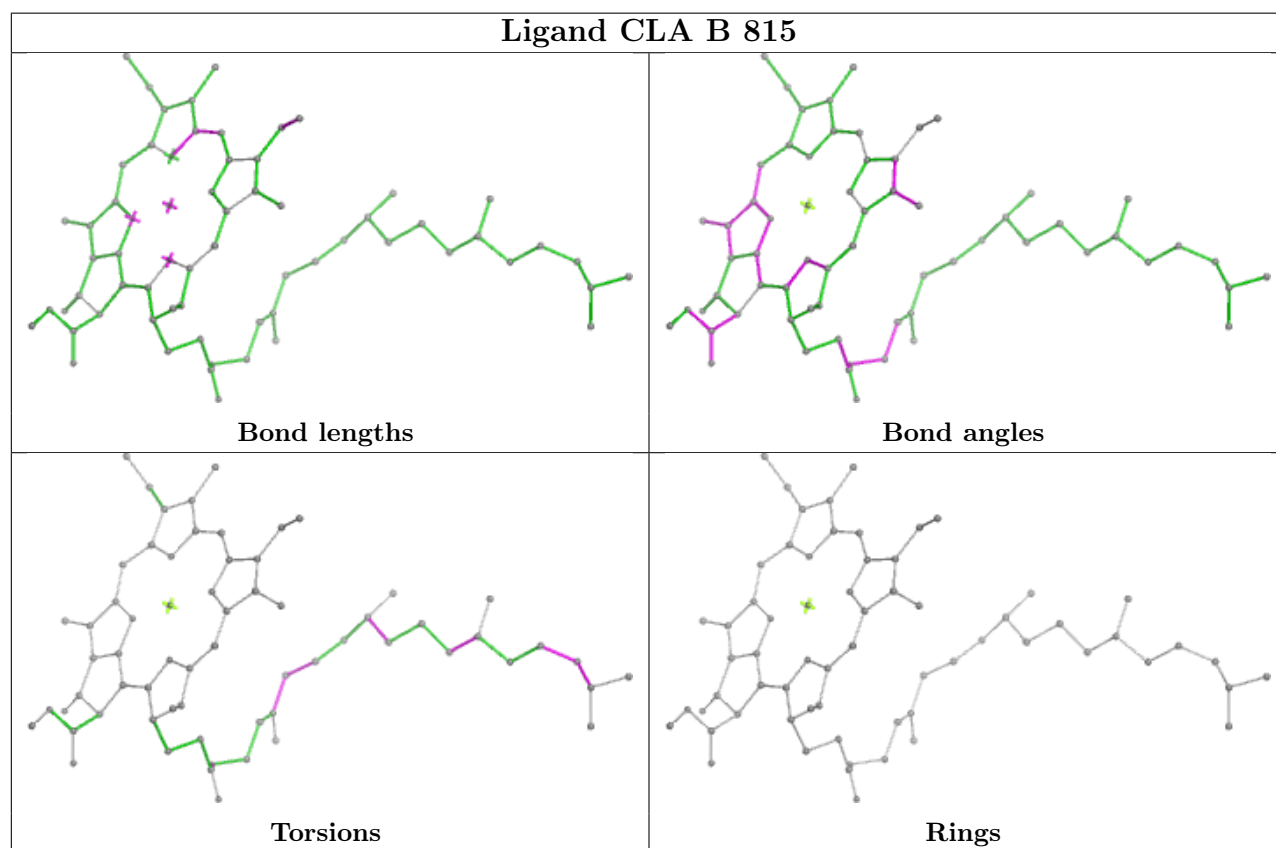
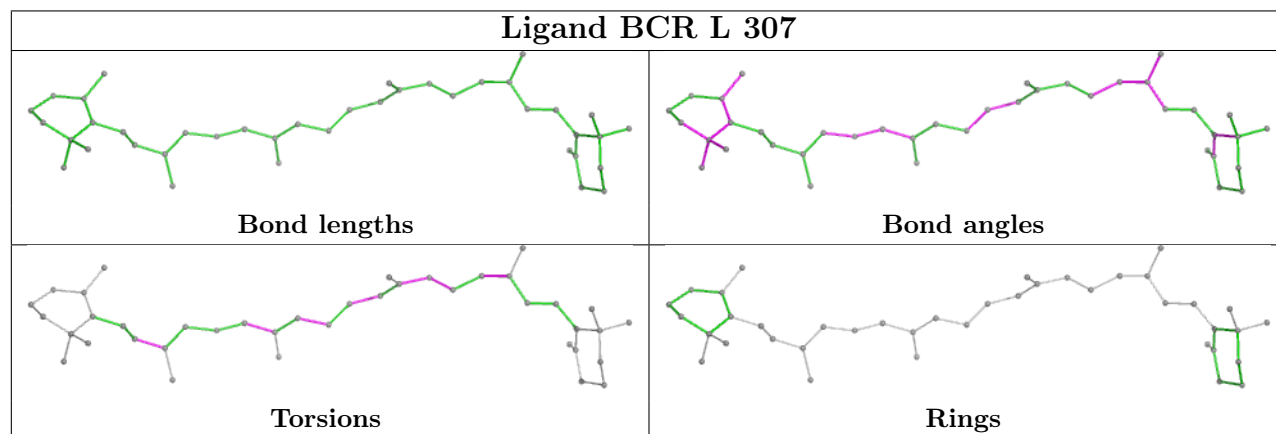
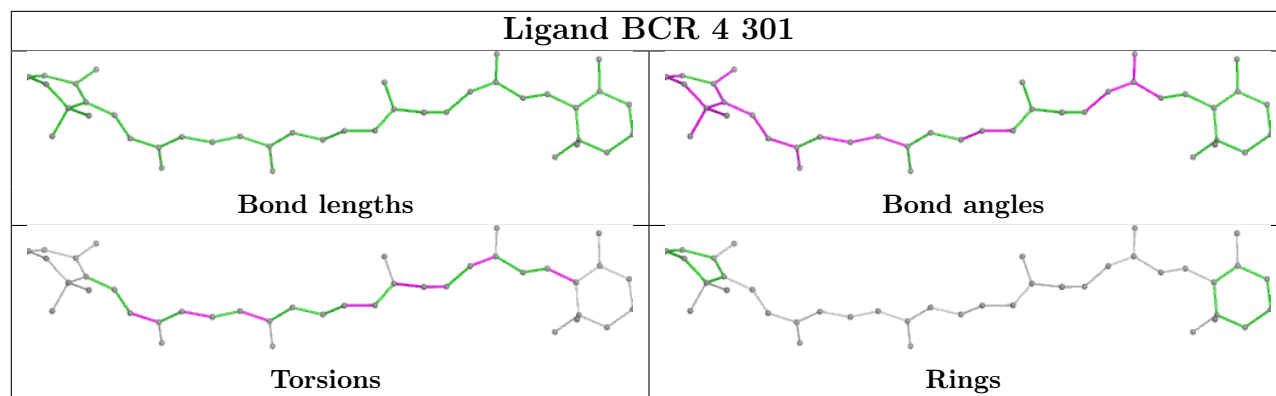


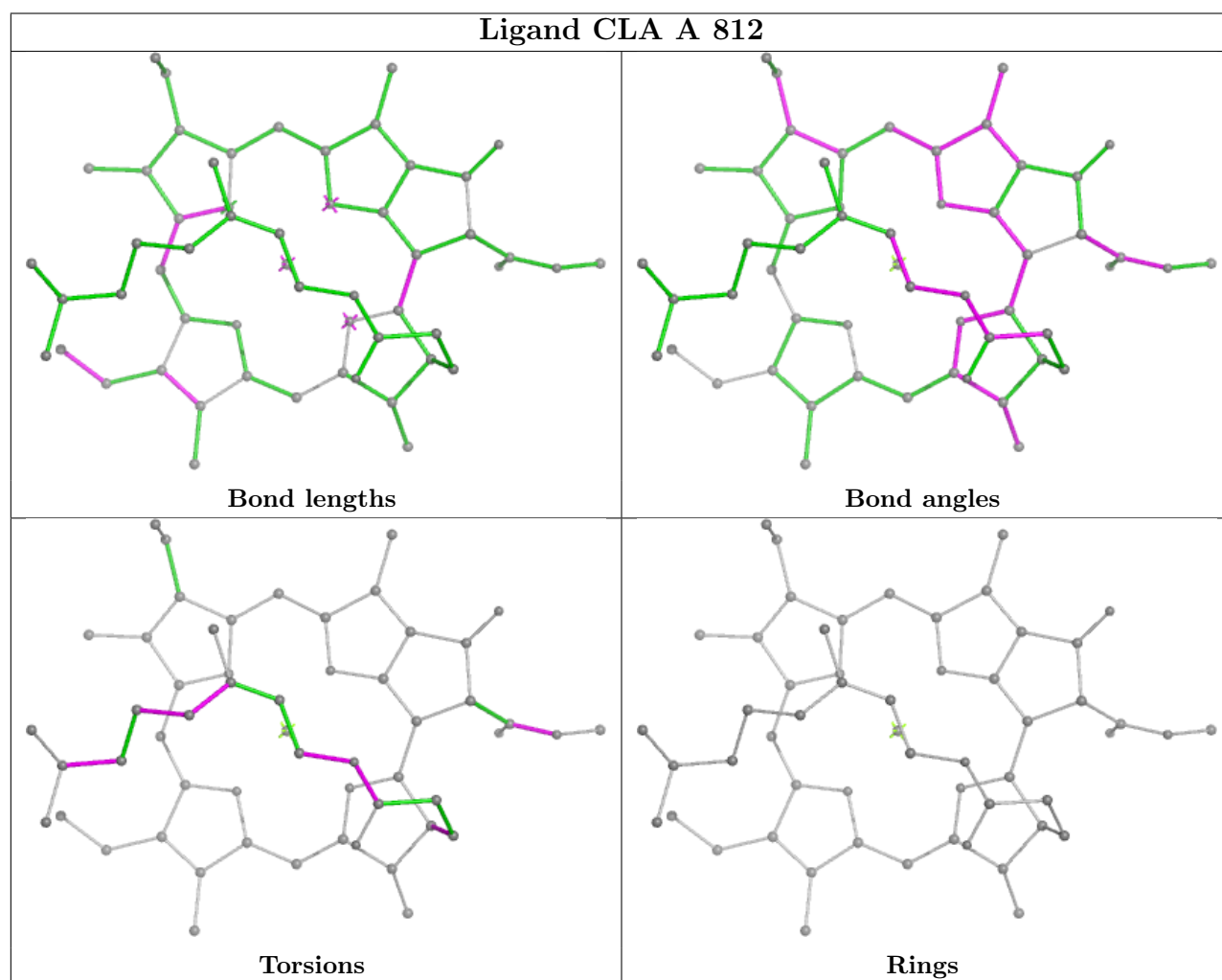
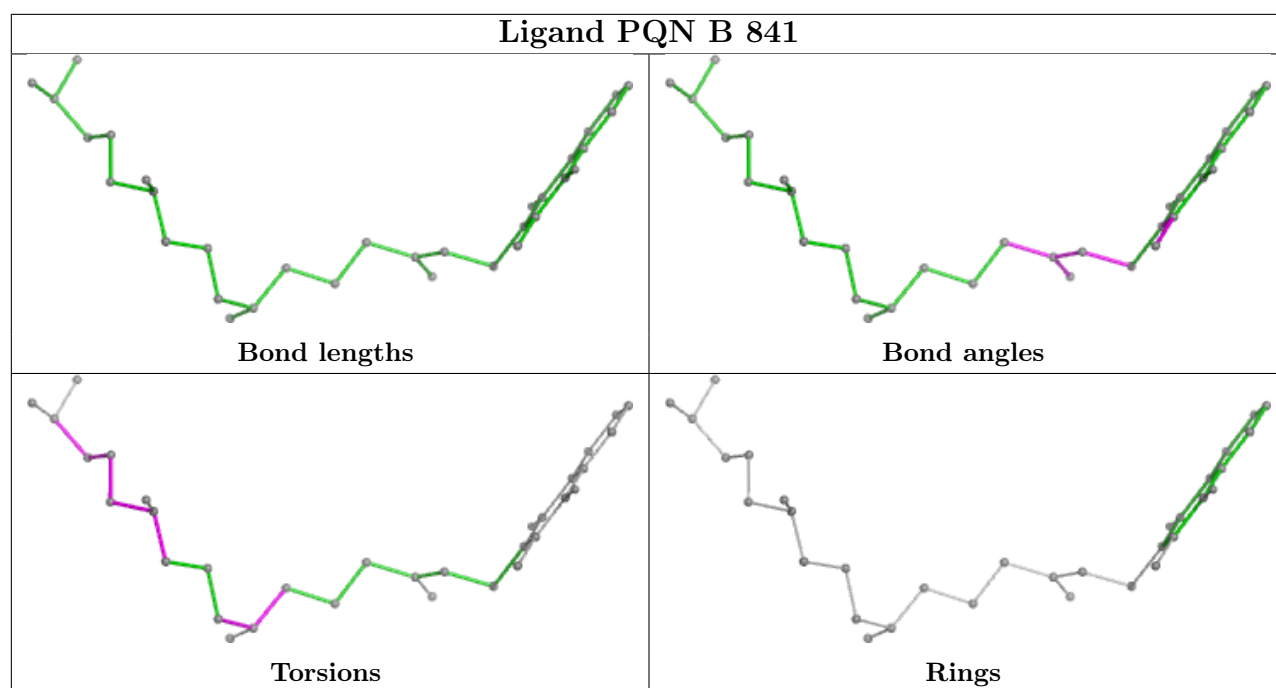
Ligand CLA B 812

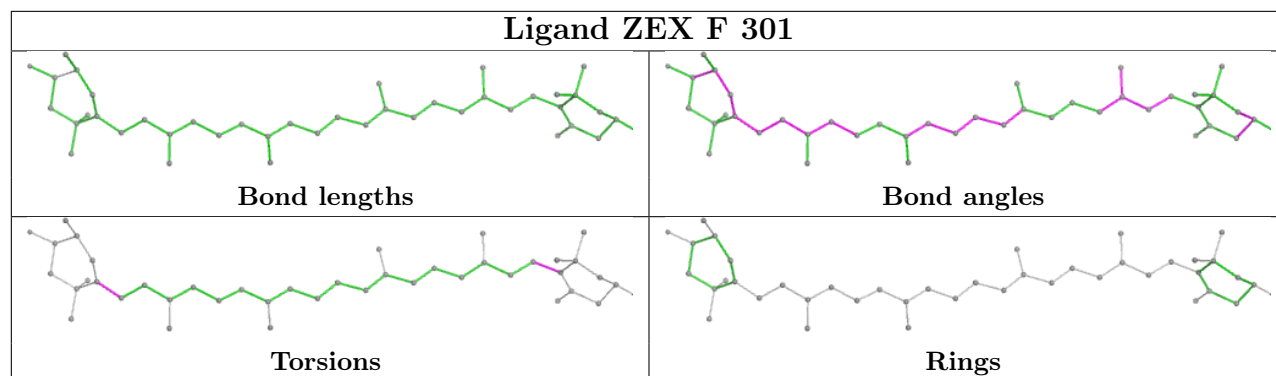
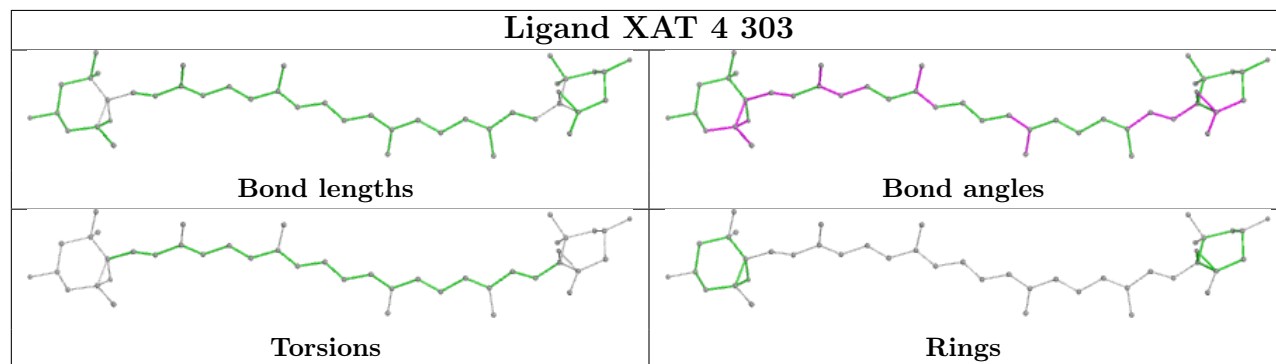


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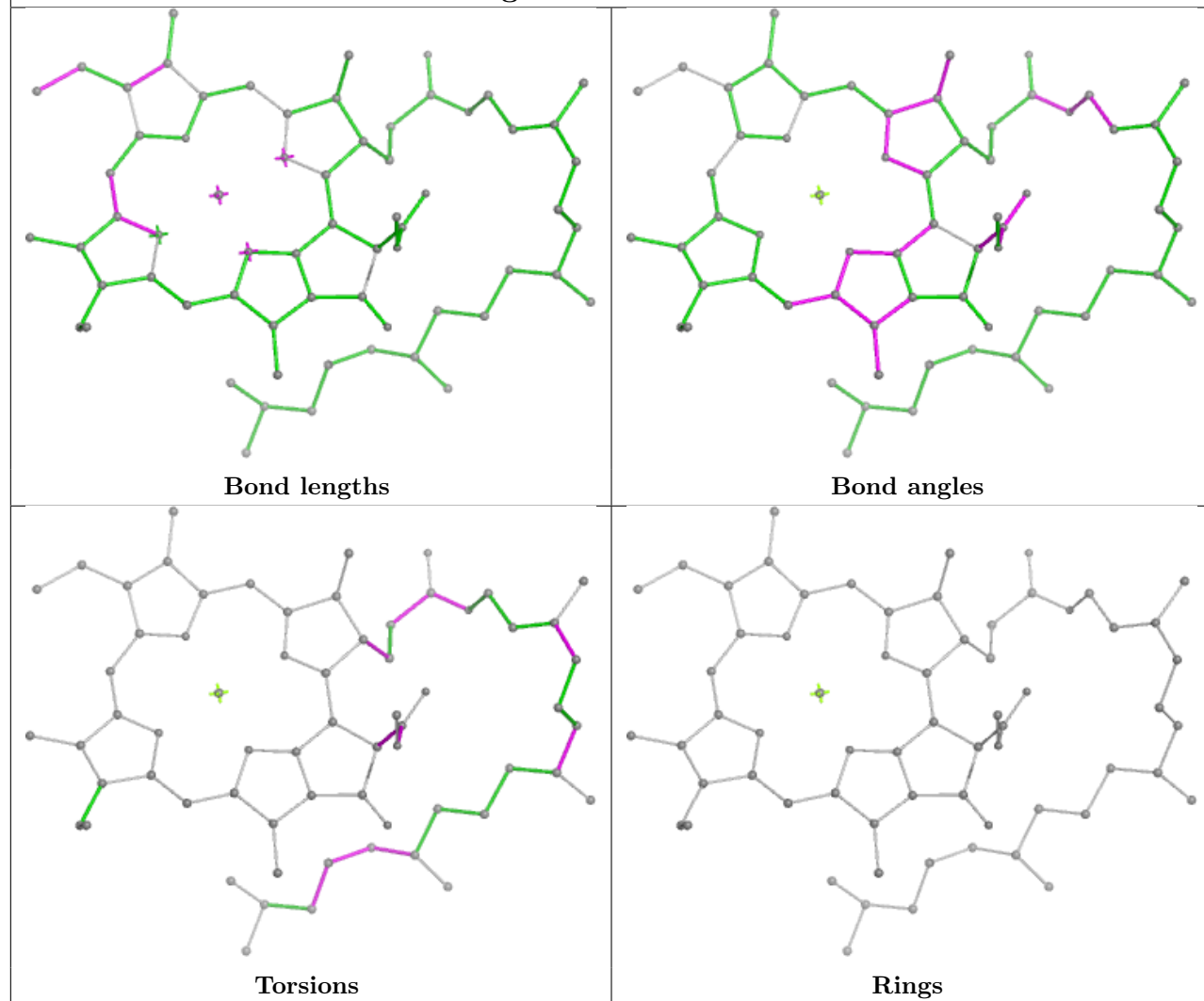




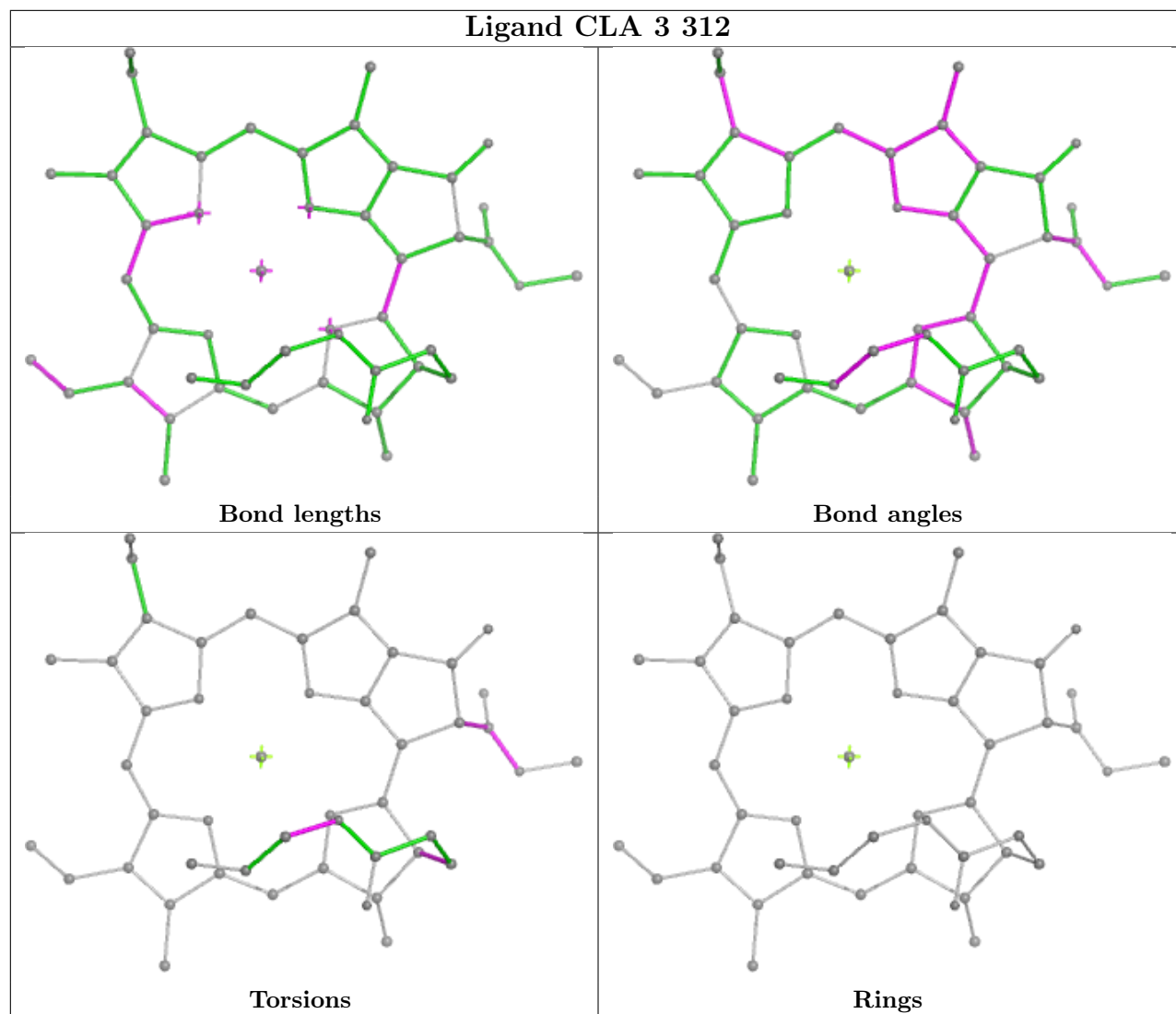


Ligand ZEX F 301**Ligand XAT 4 303**

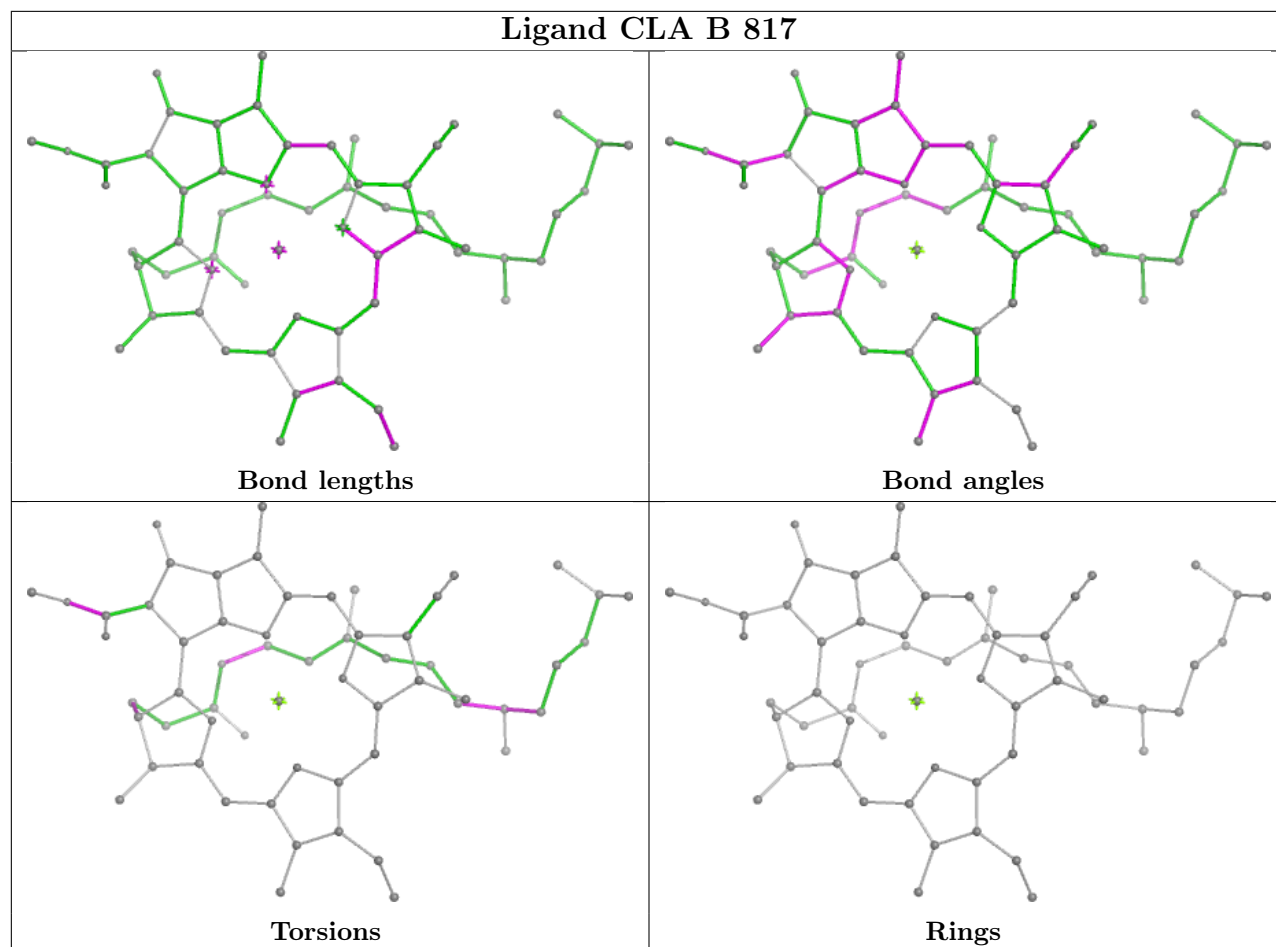
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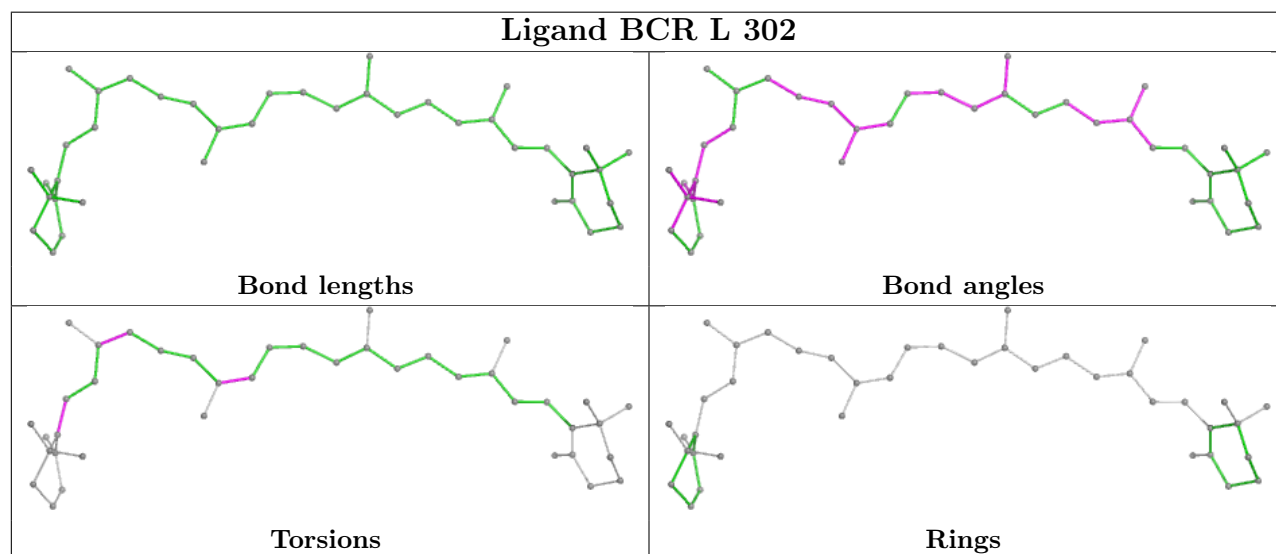
Ligand CLA 3 312



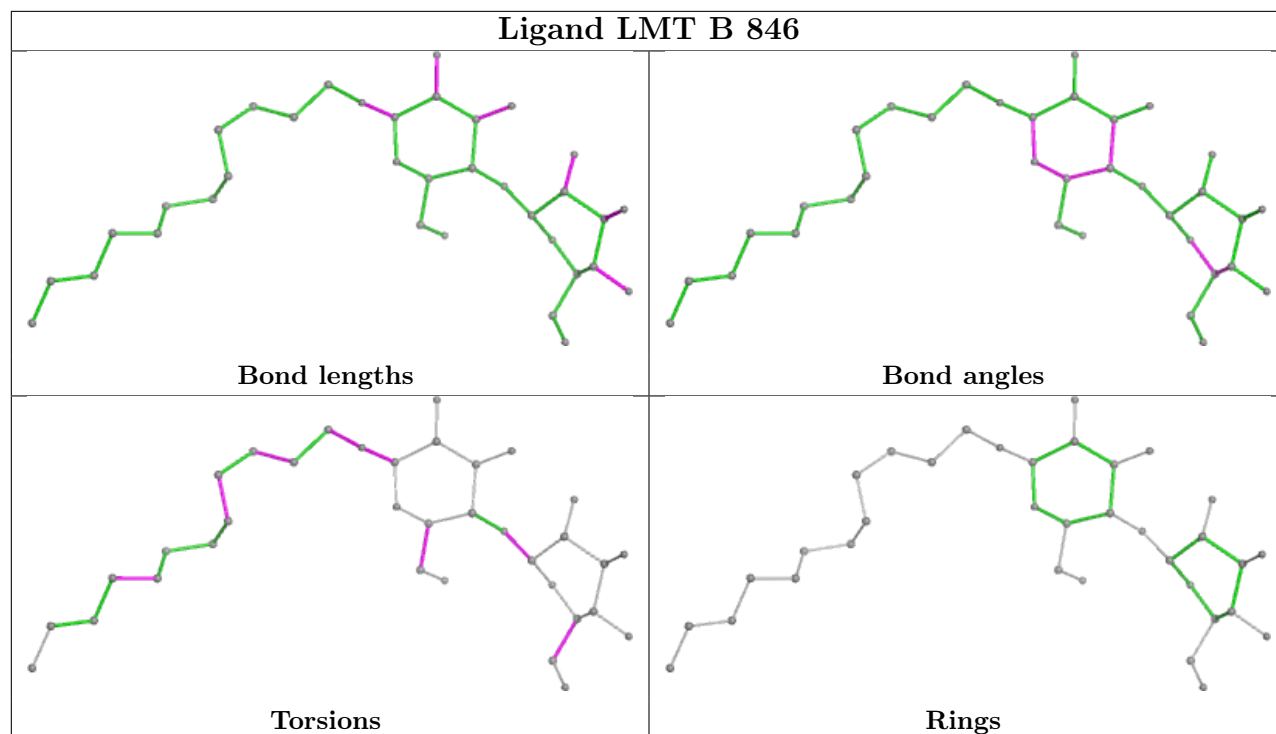
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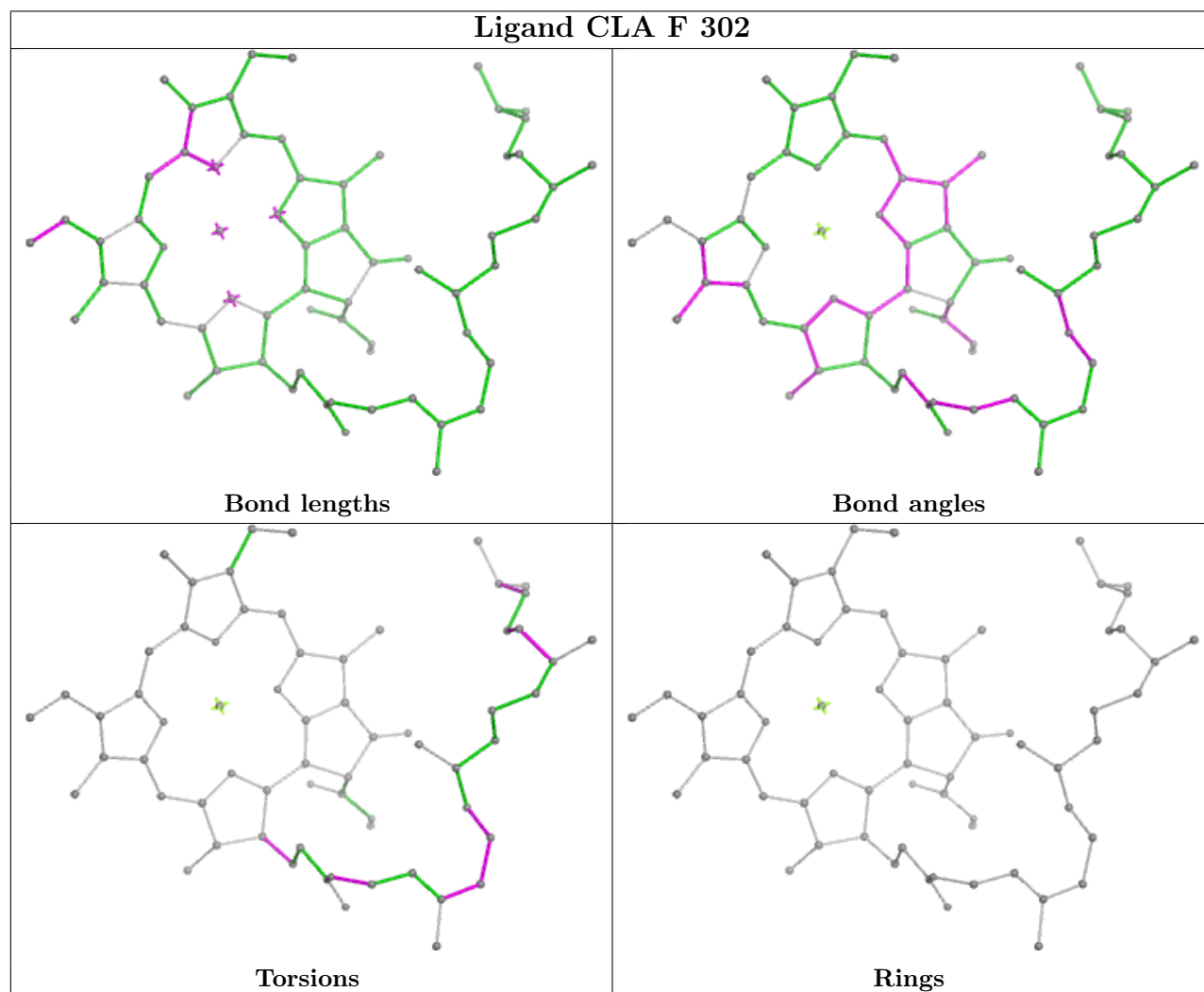
Ligand BCR L 302

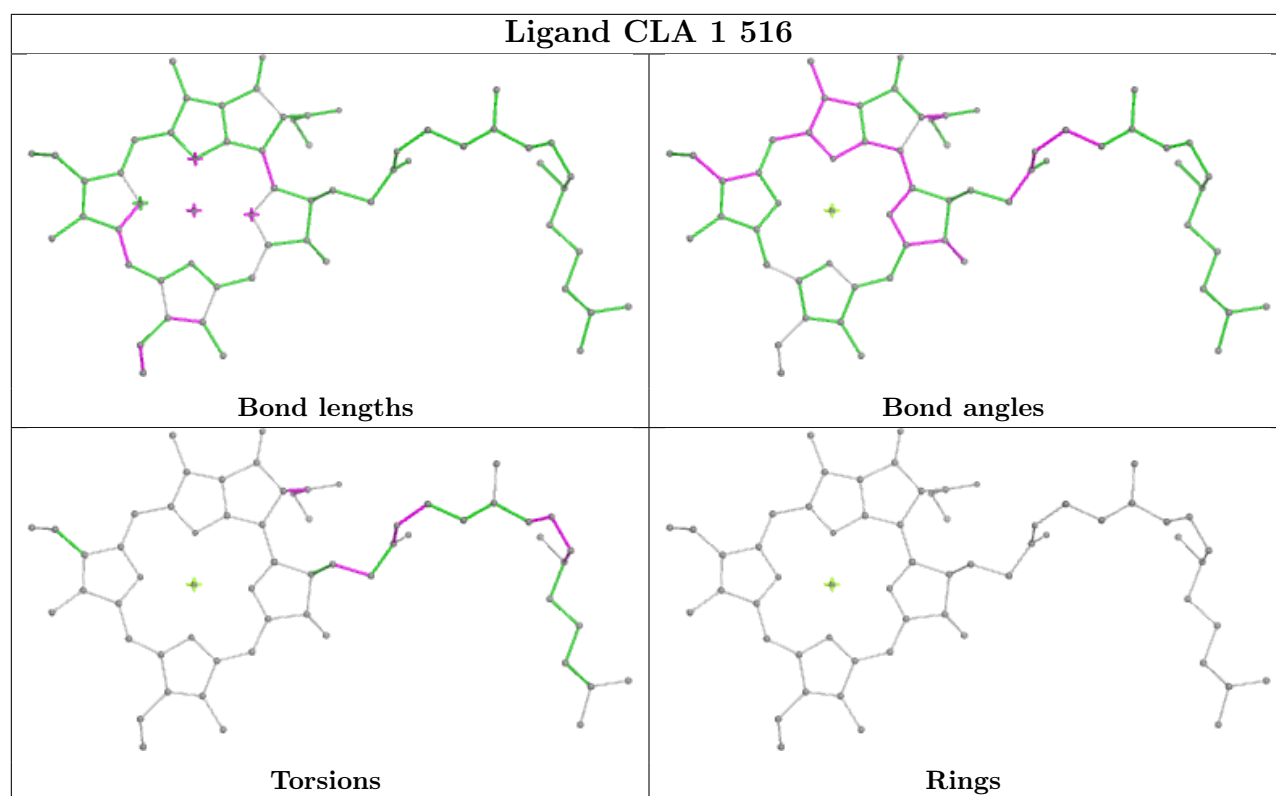


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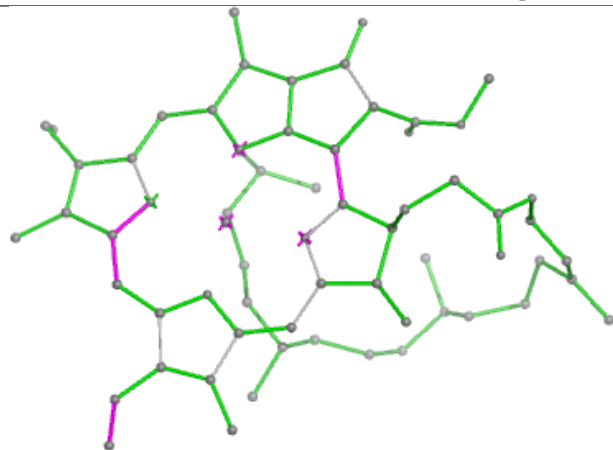


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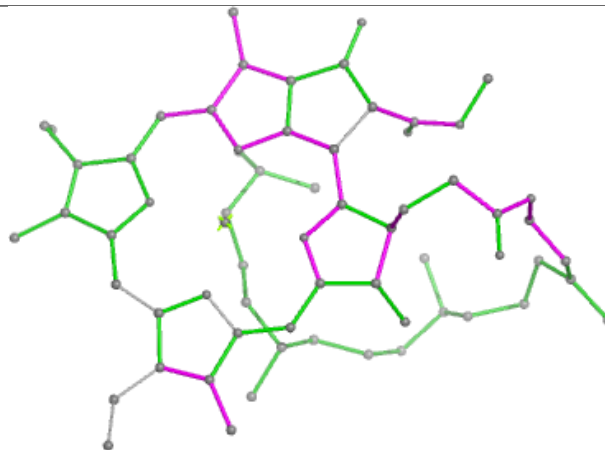




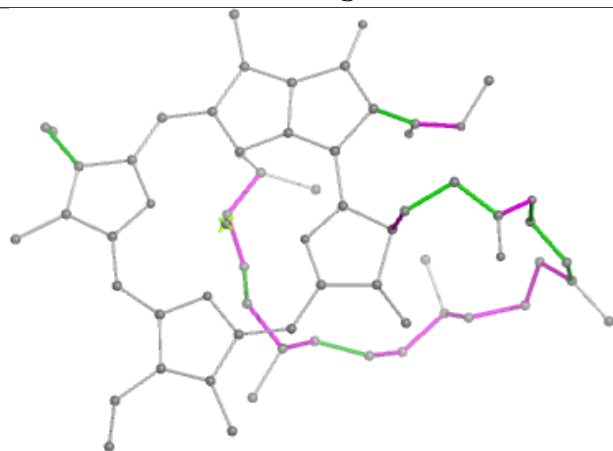
Ligand CLA A 806



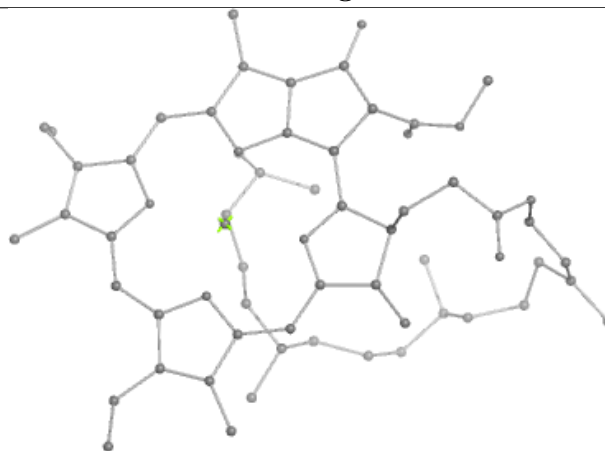
Bond lengths



Bond angles

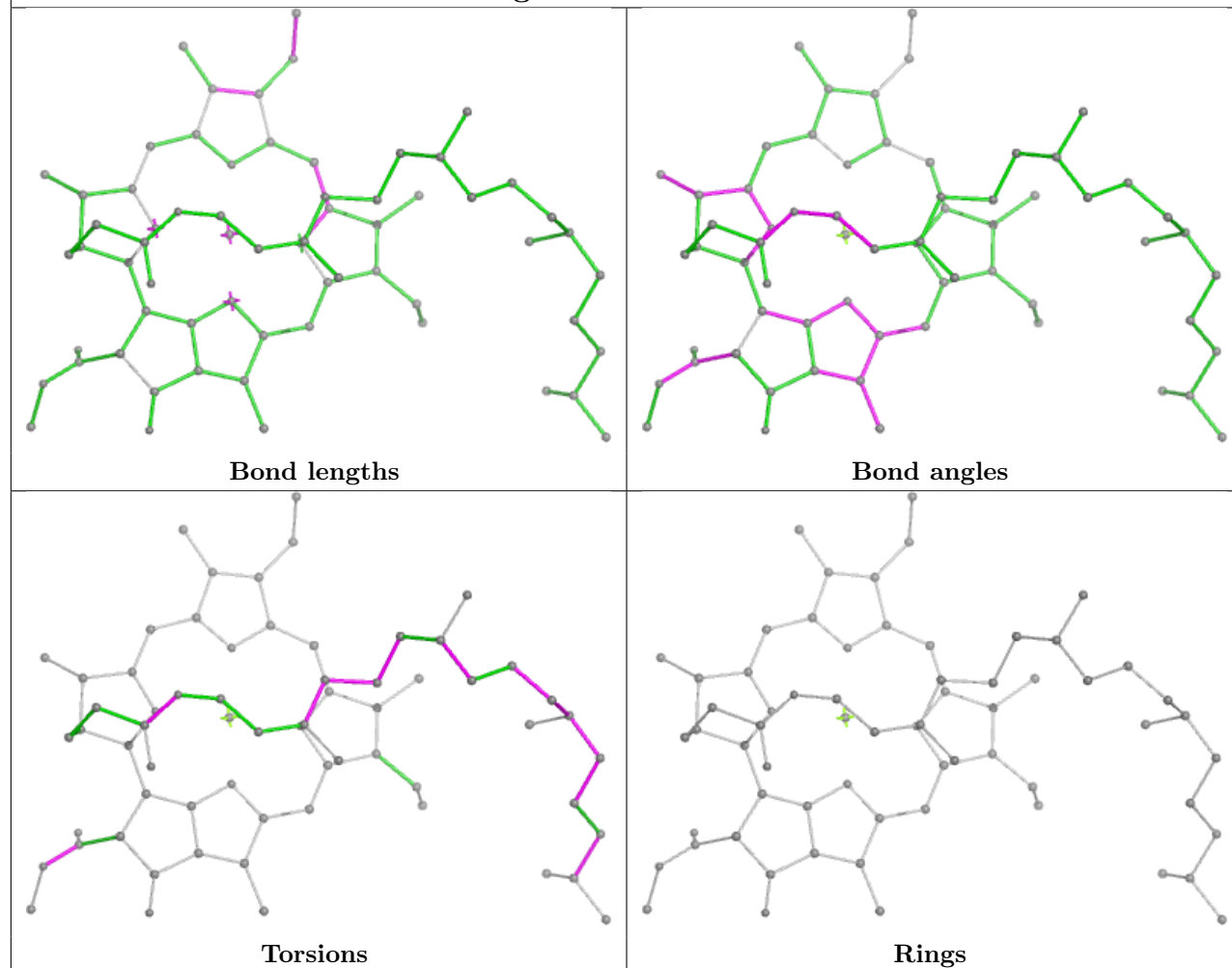


Torsions

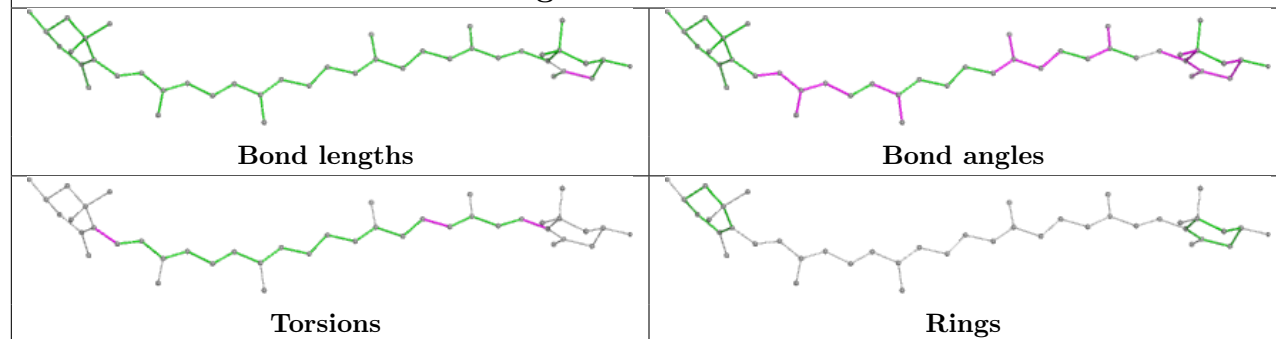


Rings

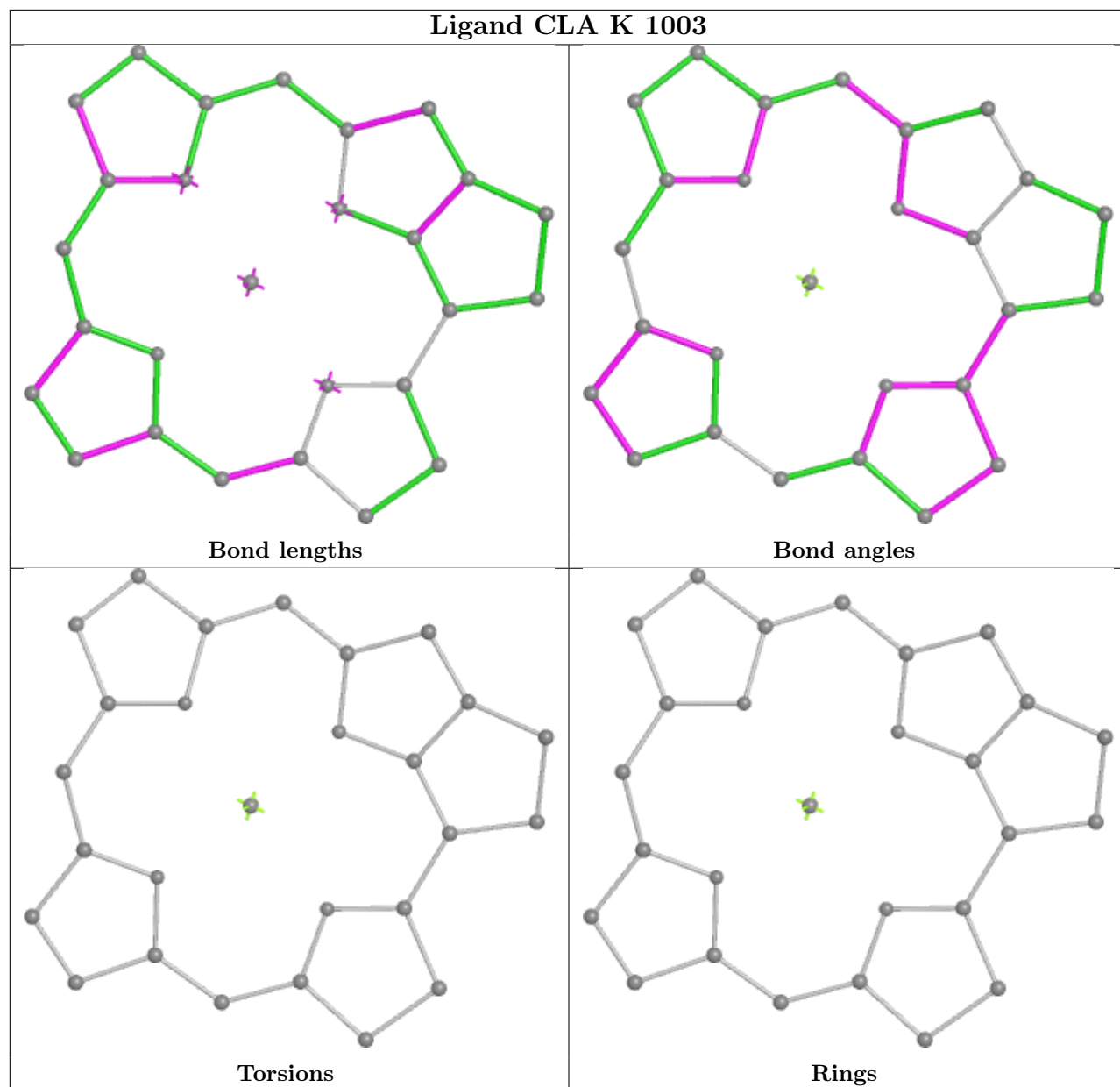
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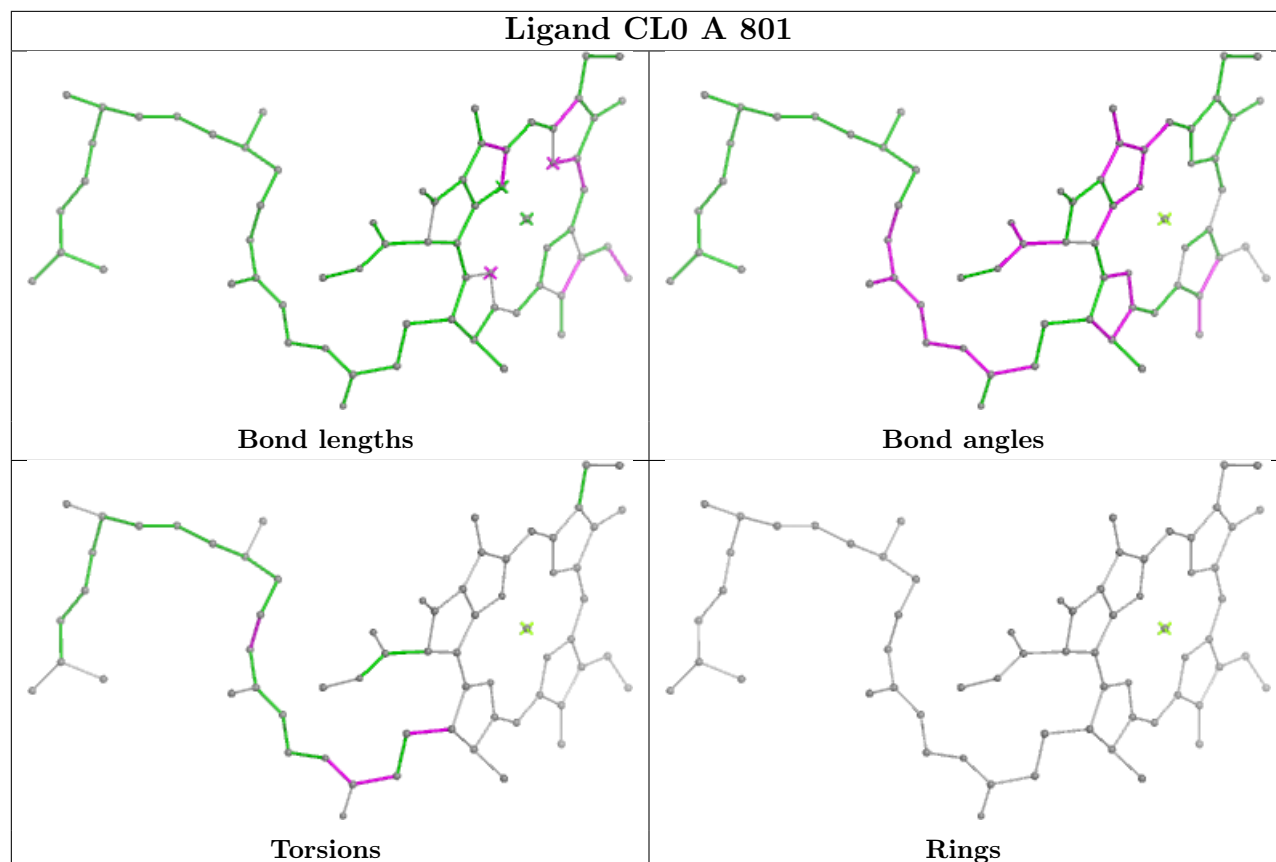
Ligand LUT 4 302



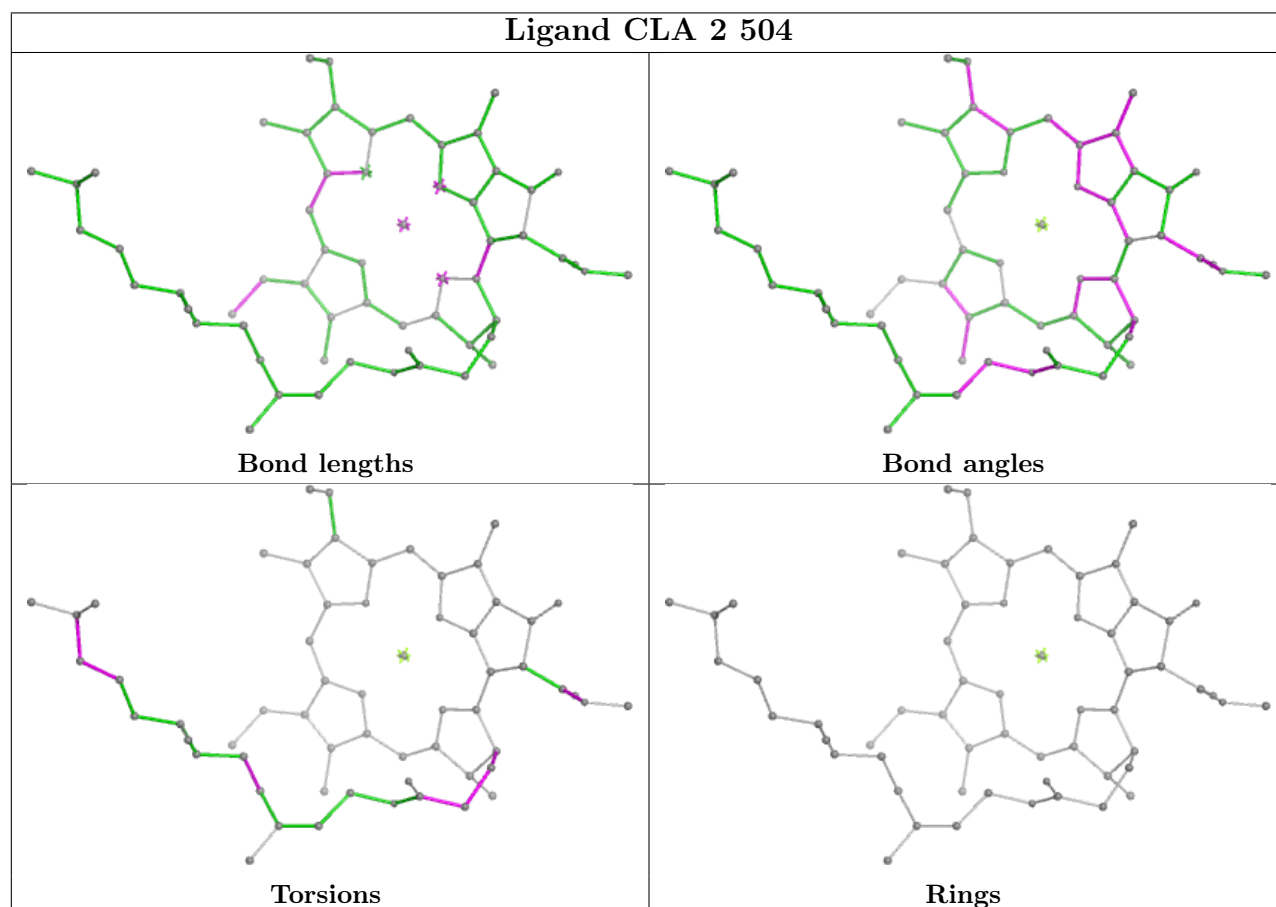
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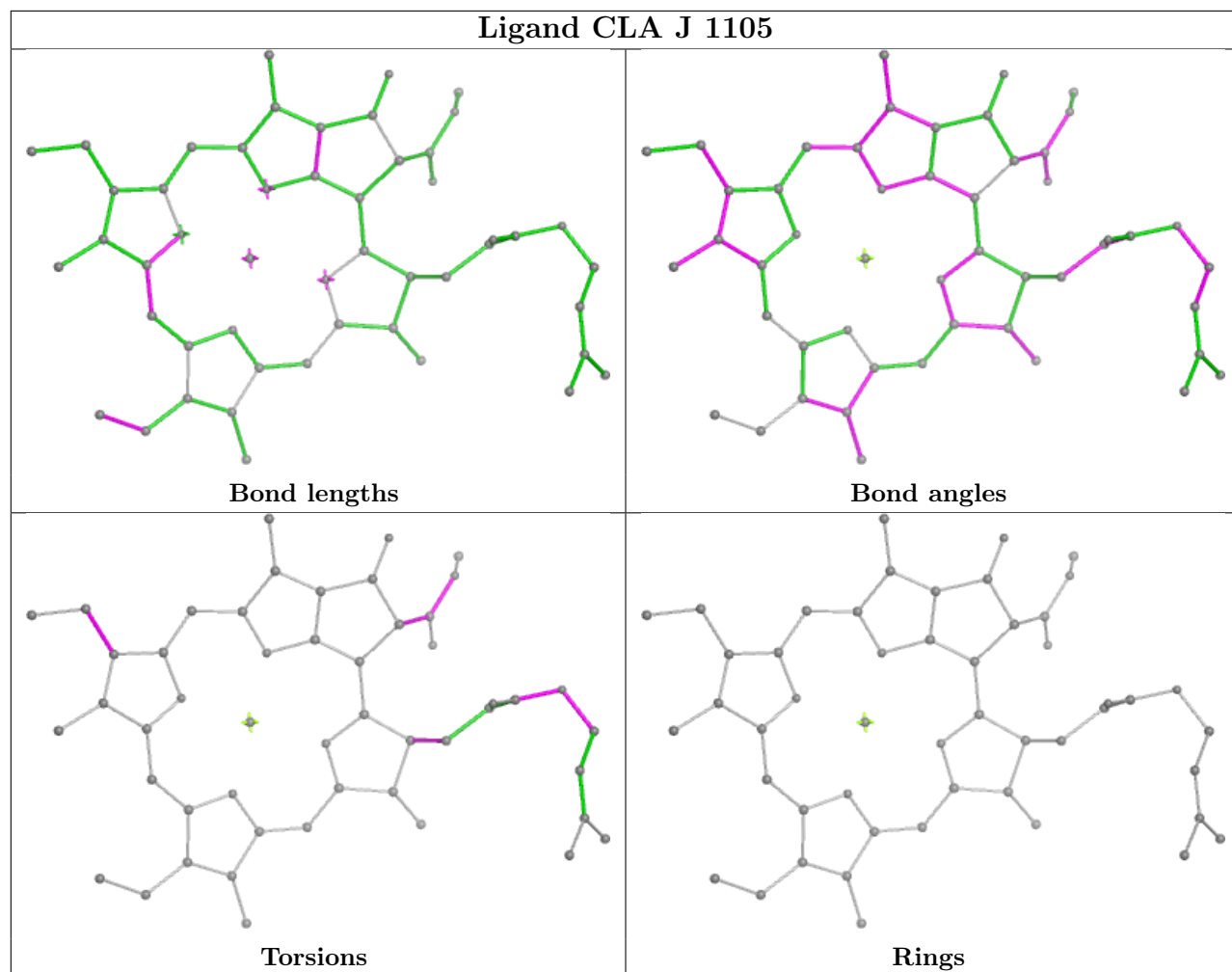


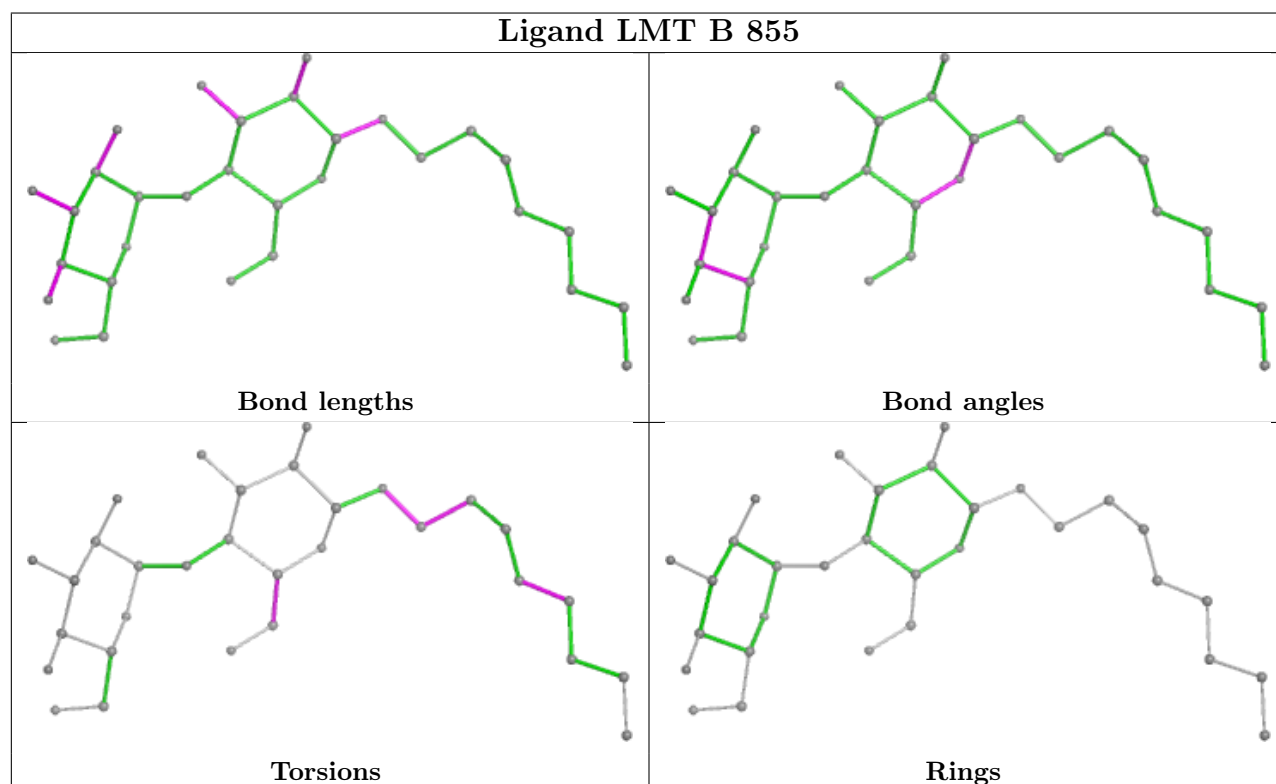
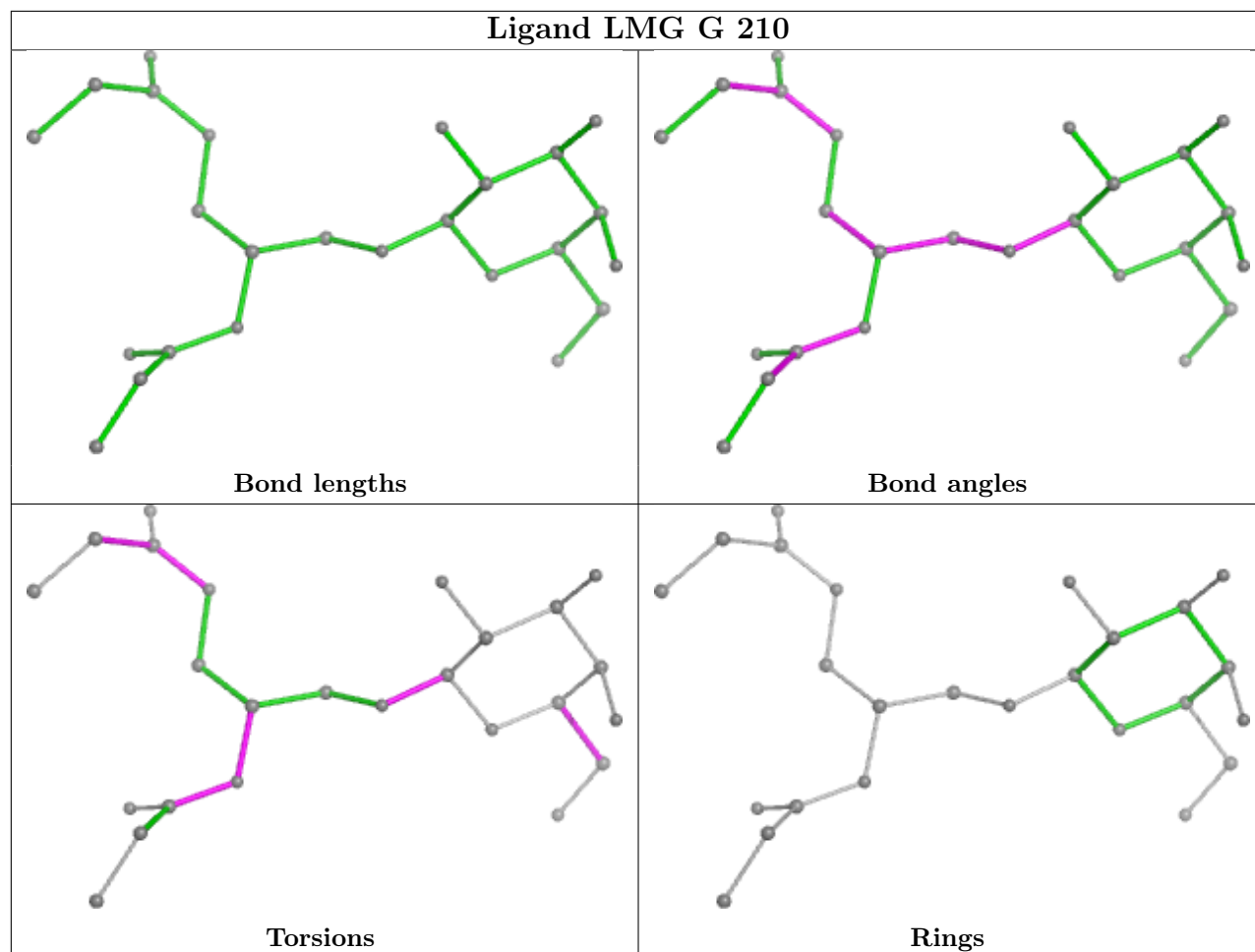
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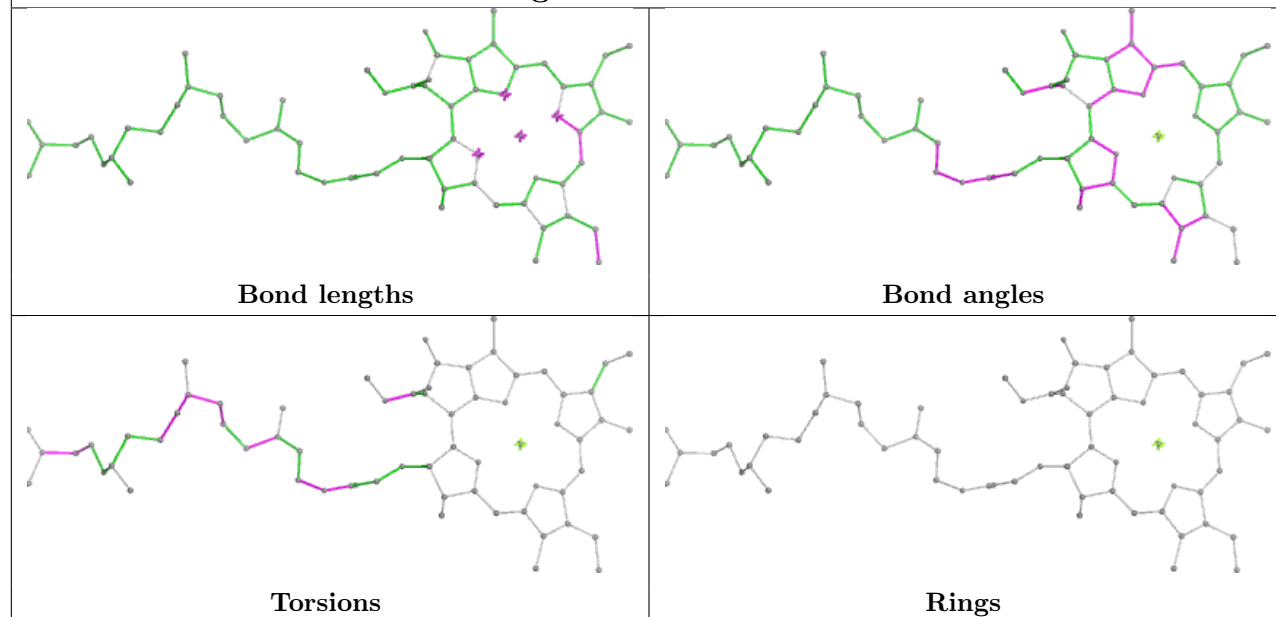
Ligand CLA 2 504



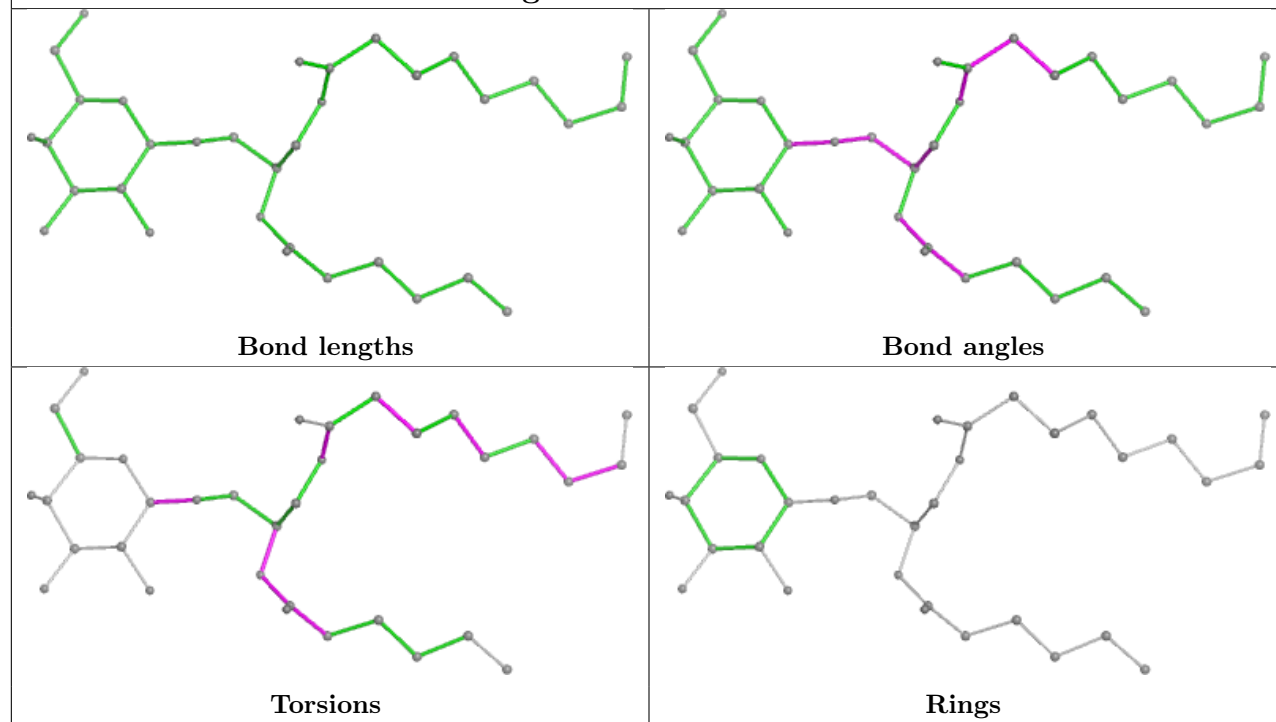




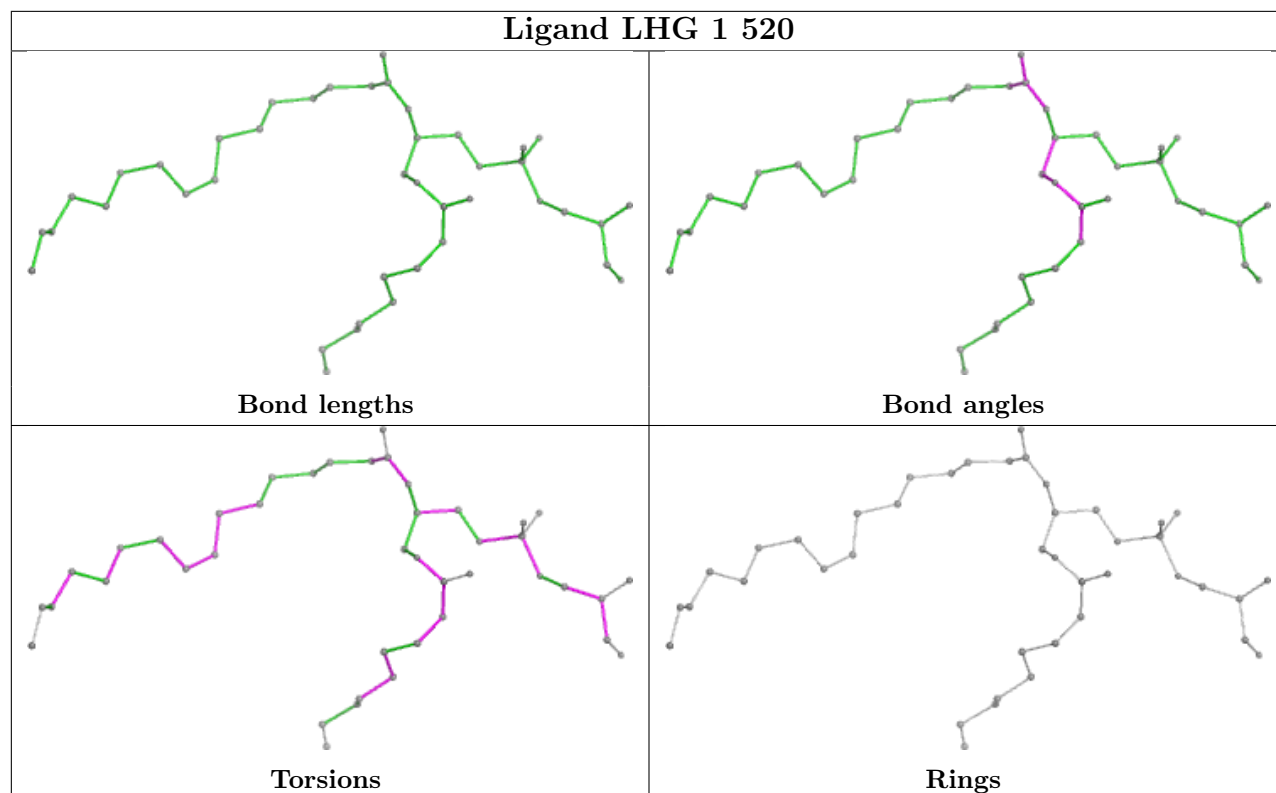
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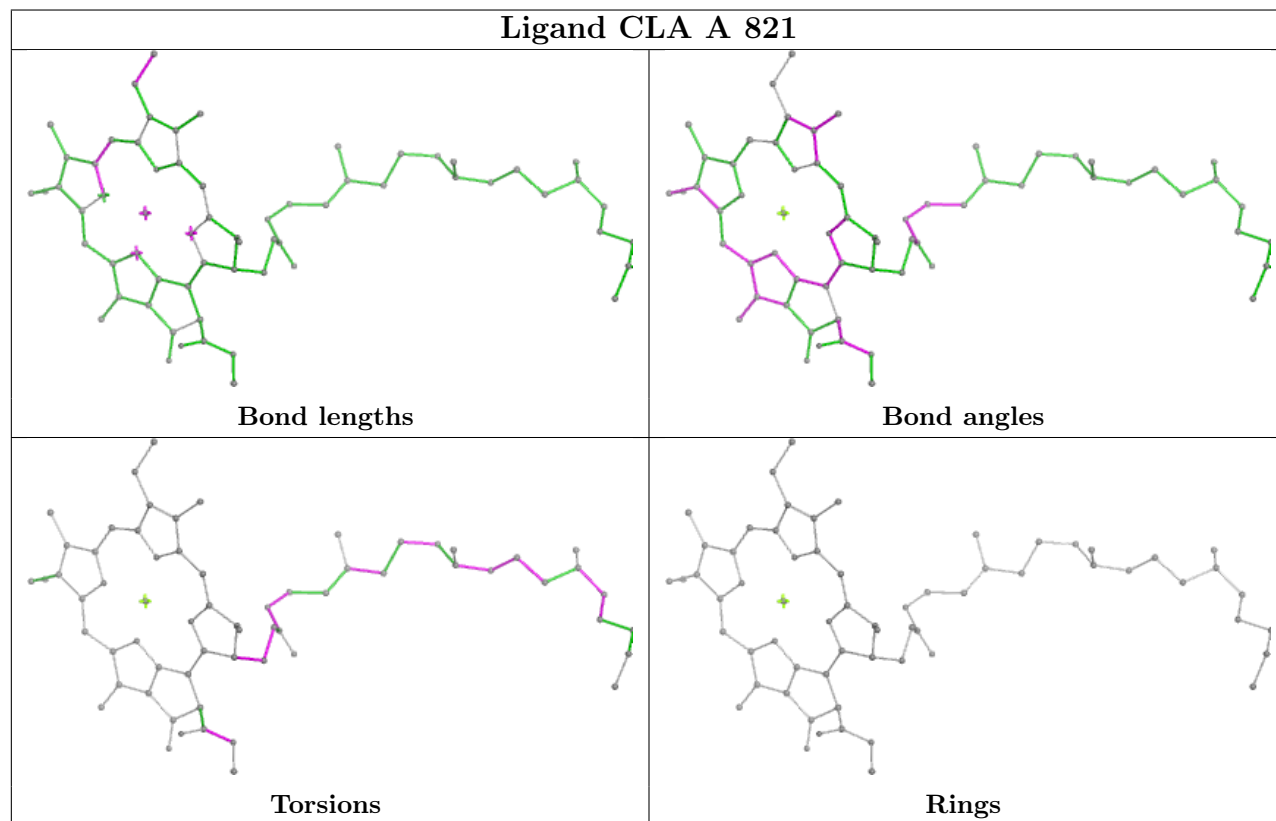
Ligand LMG J 1104



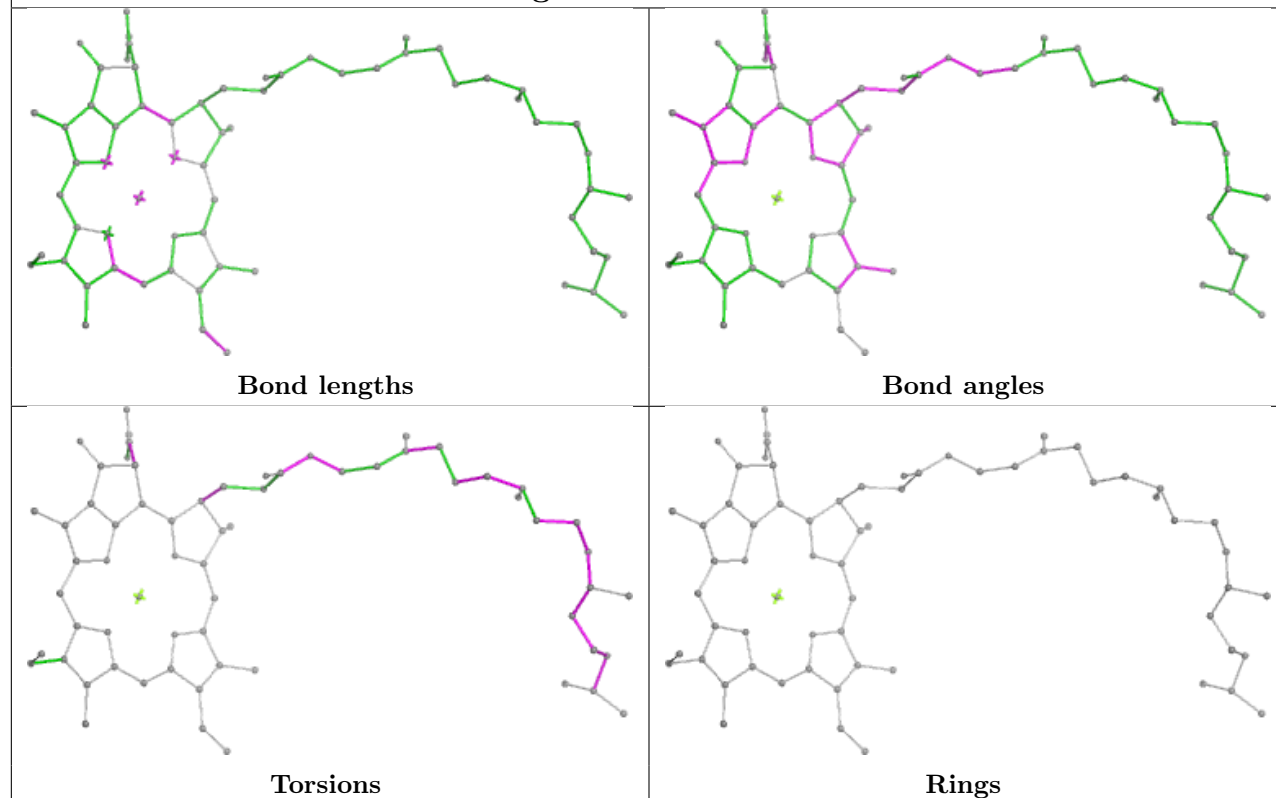
Ligand LHG 1 520



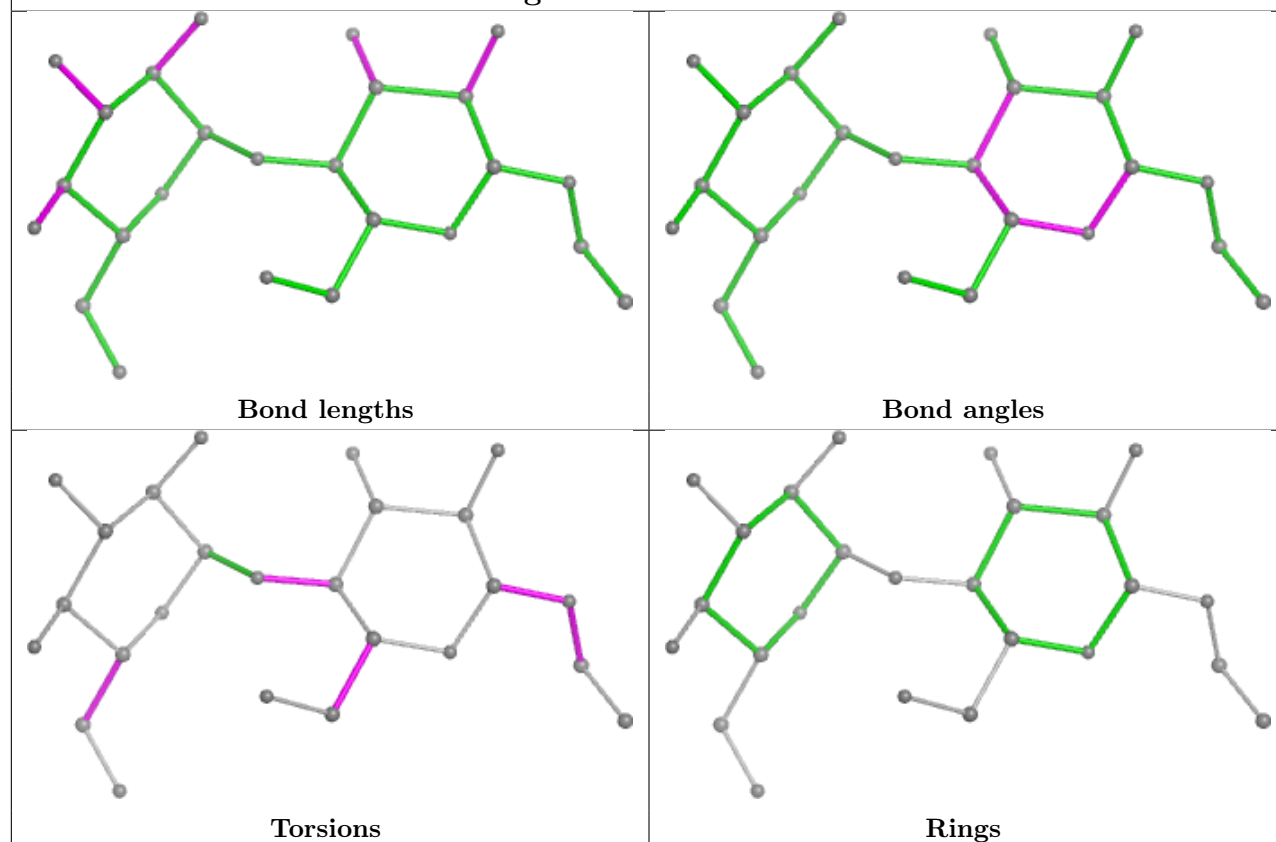
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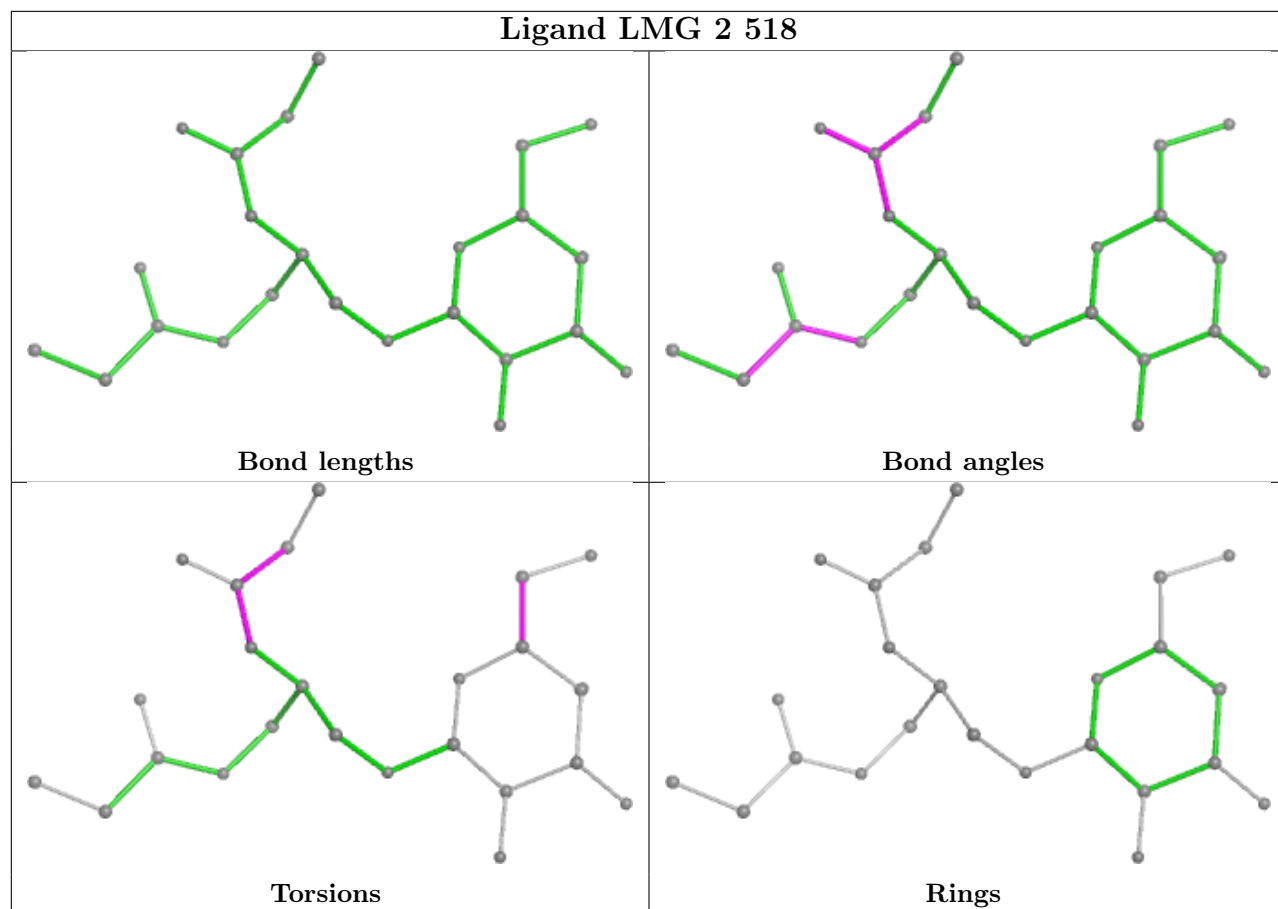


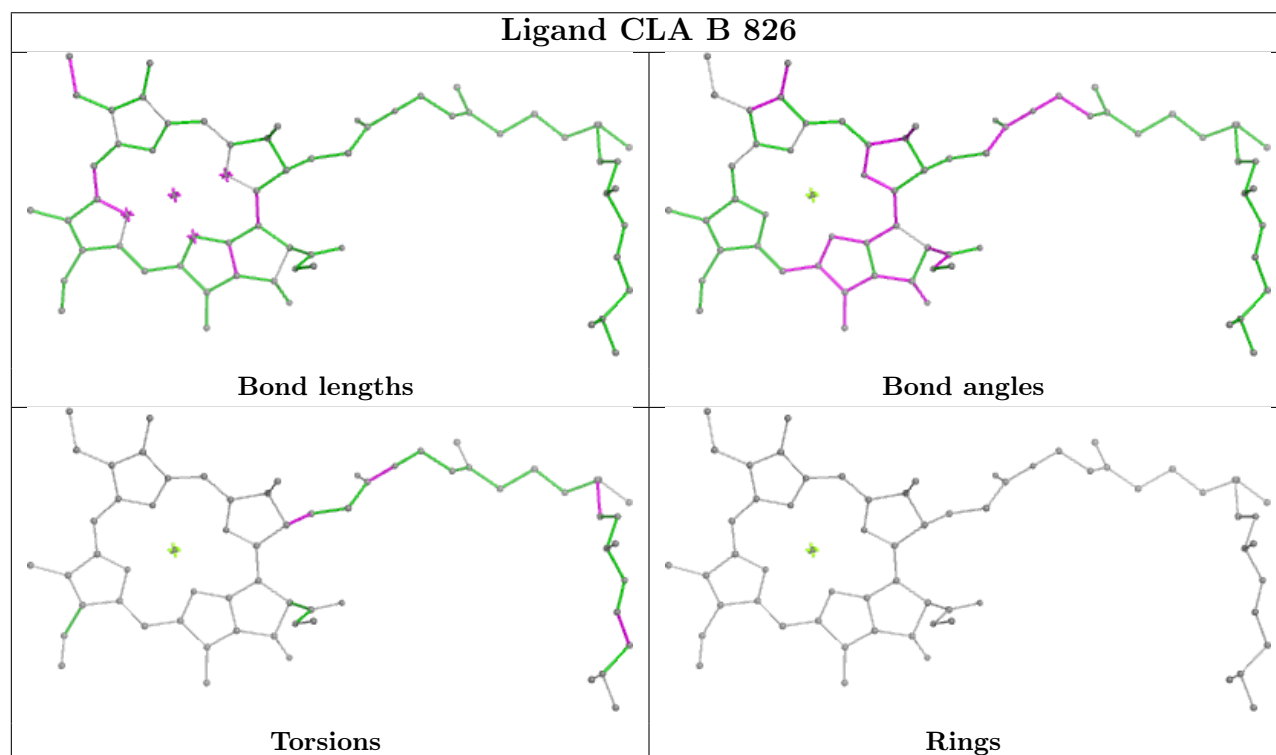
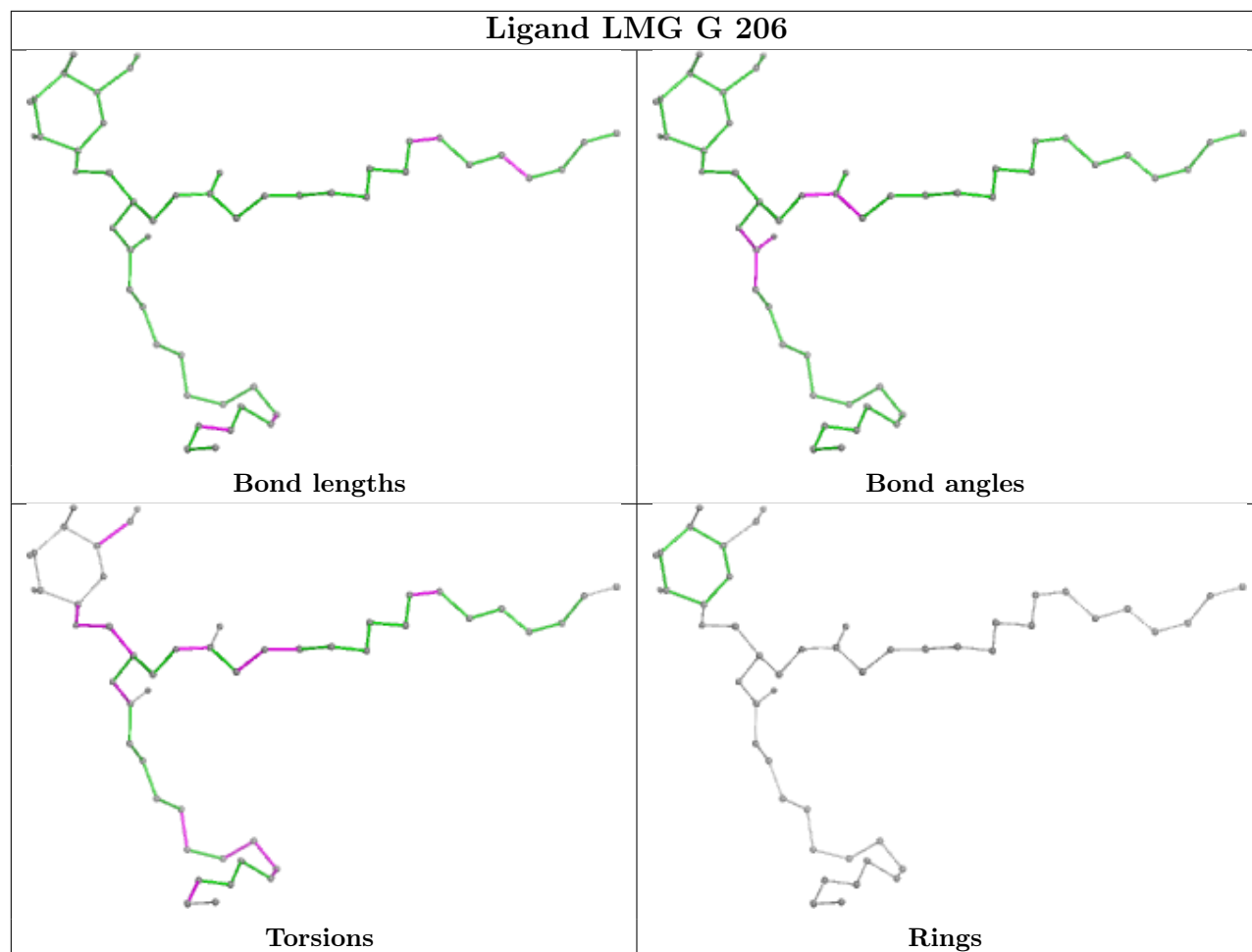
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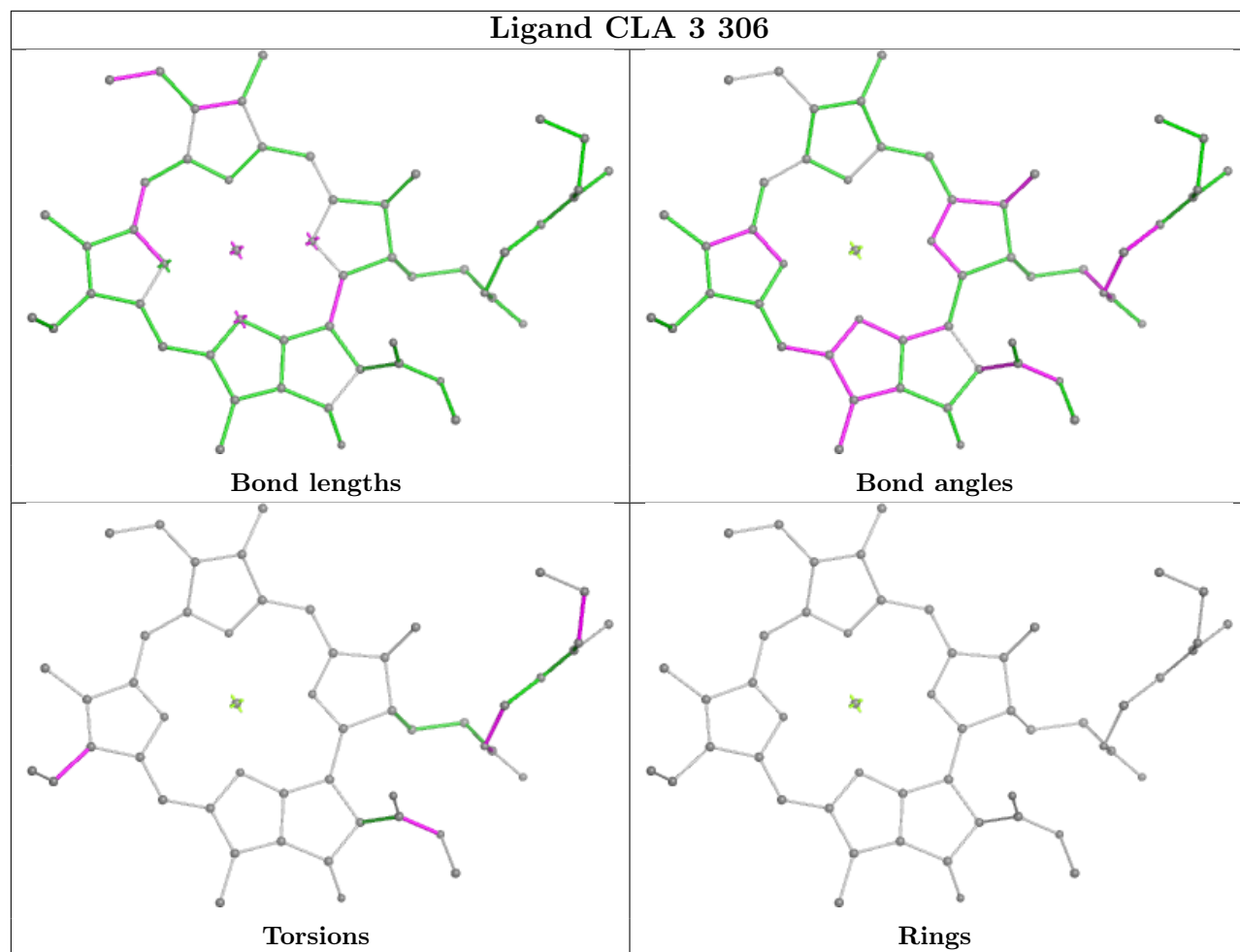
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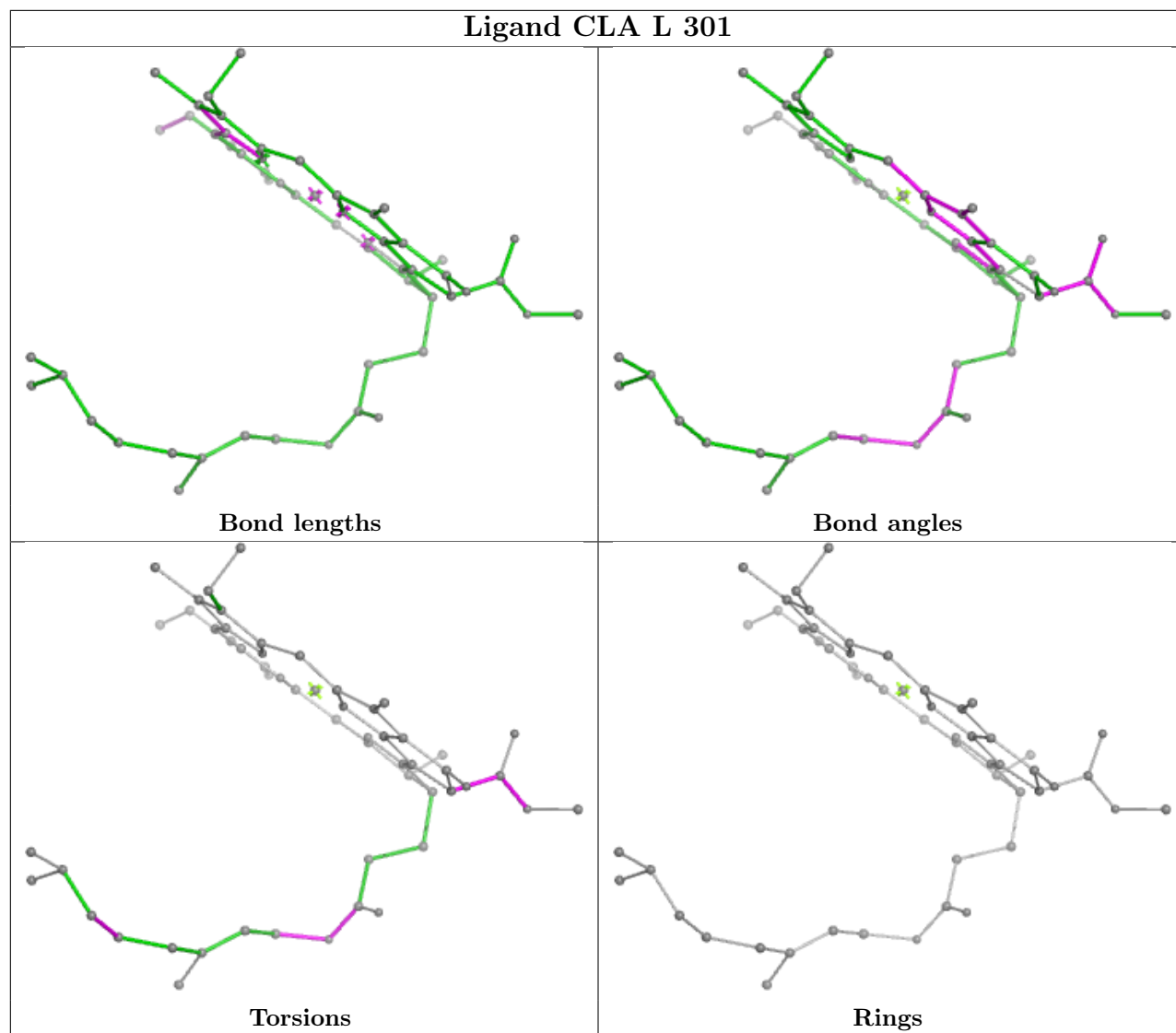




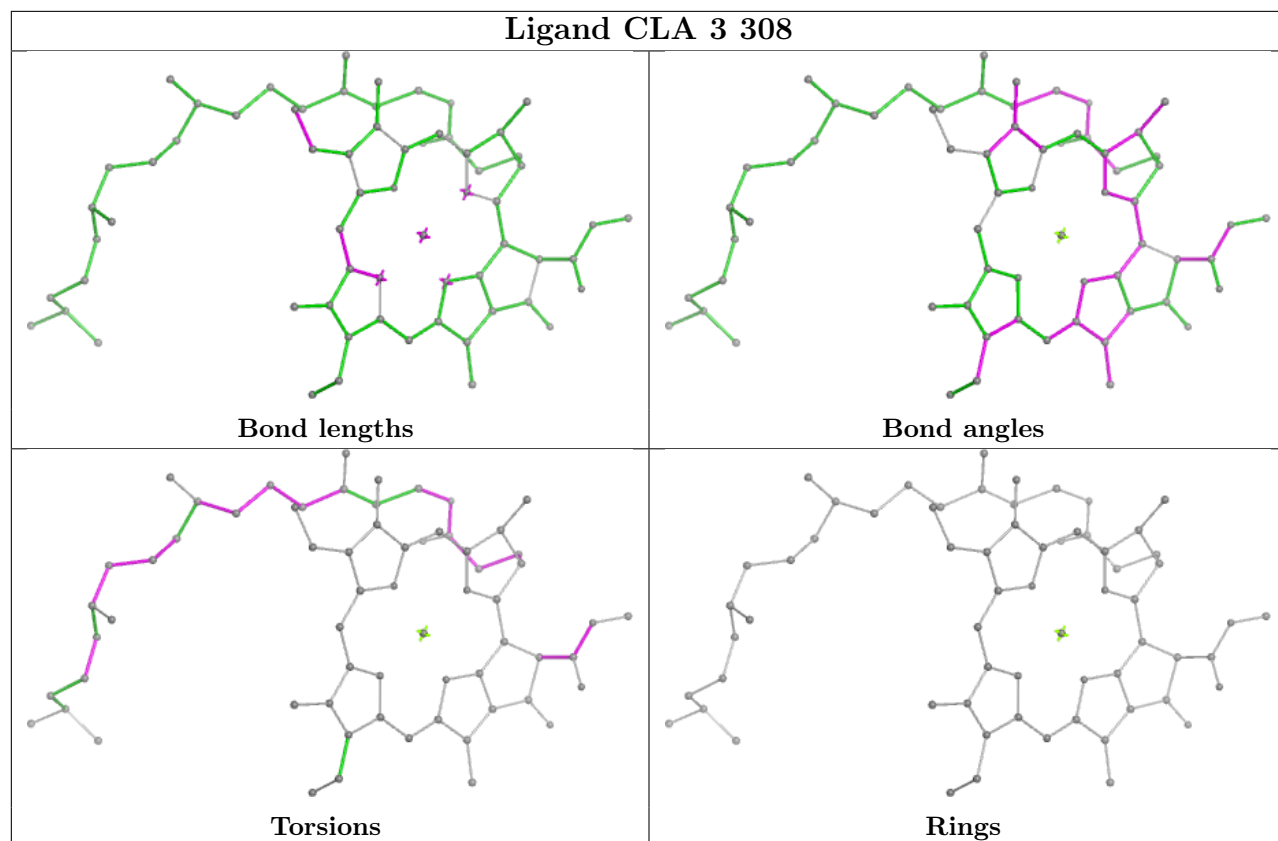
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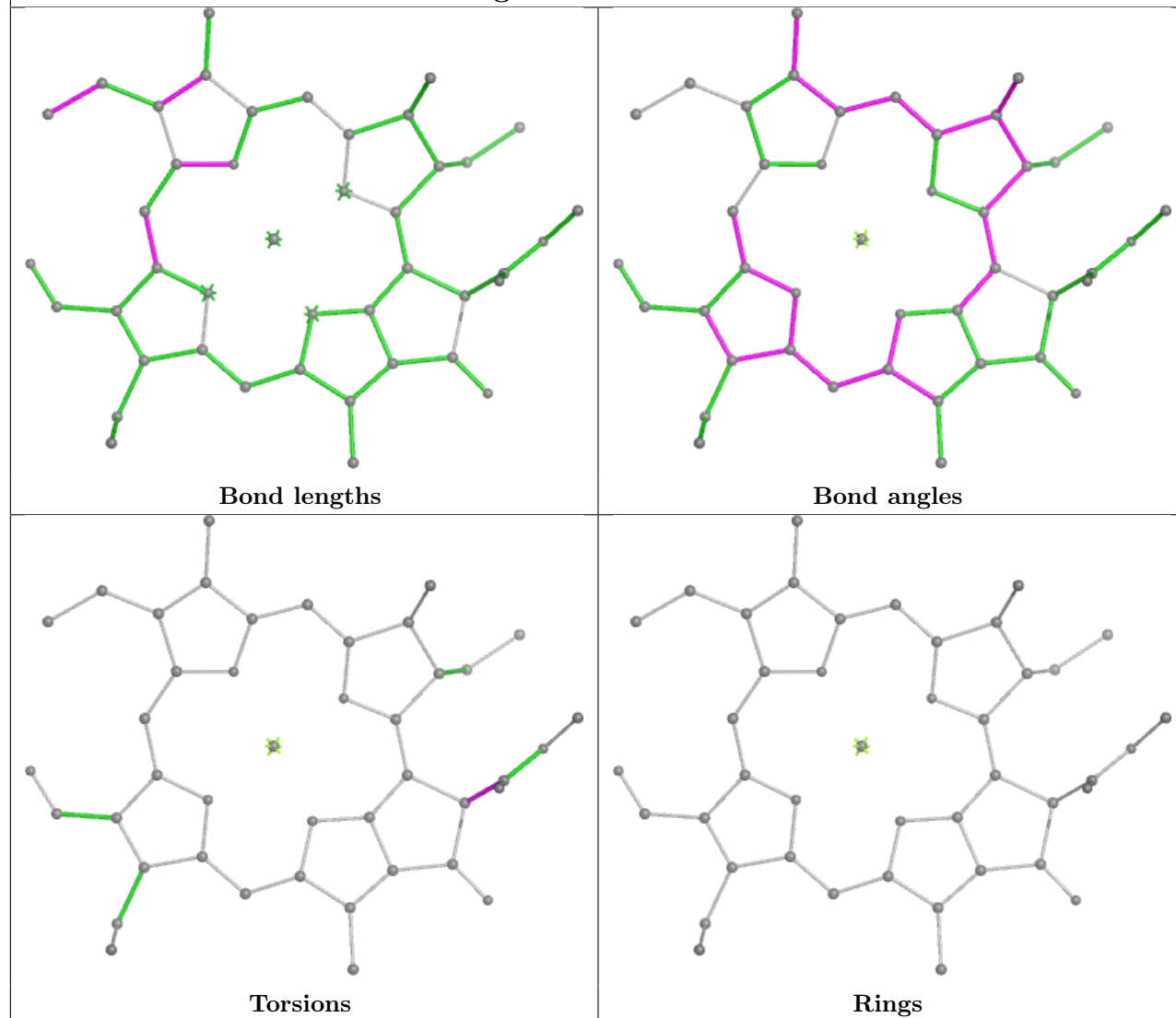
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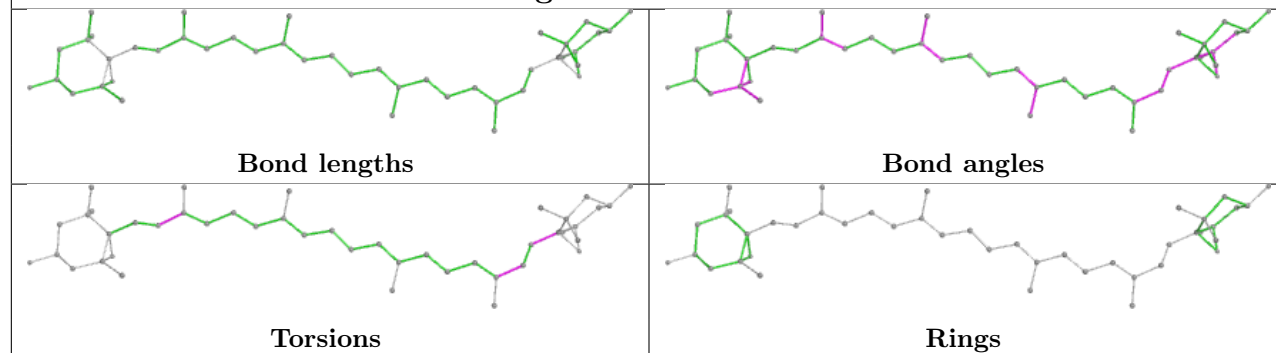
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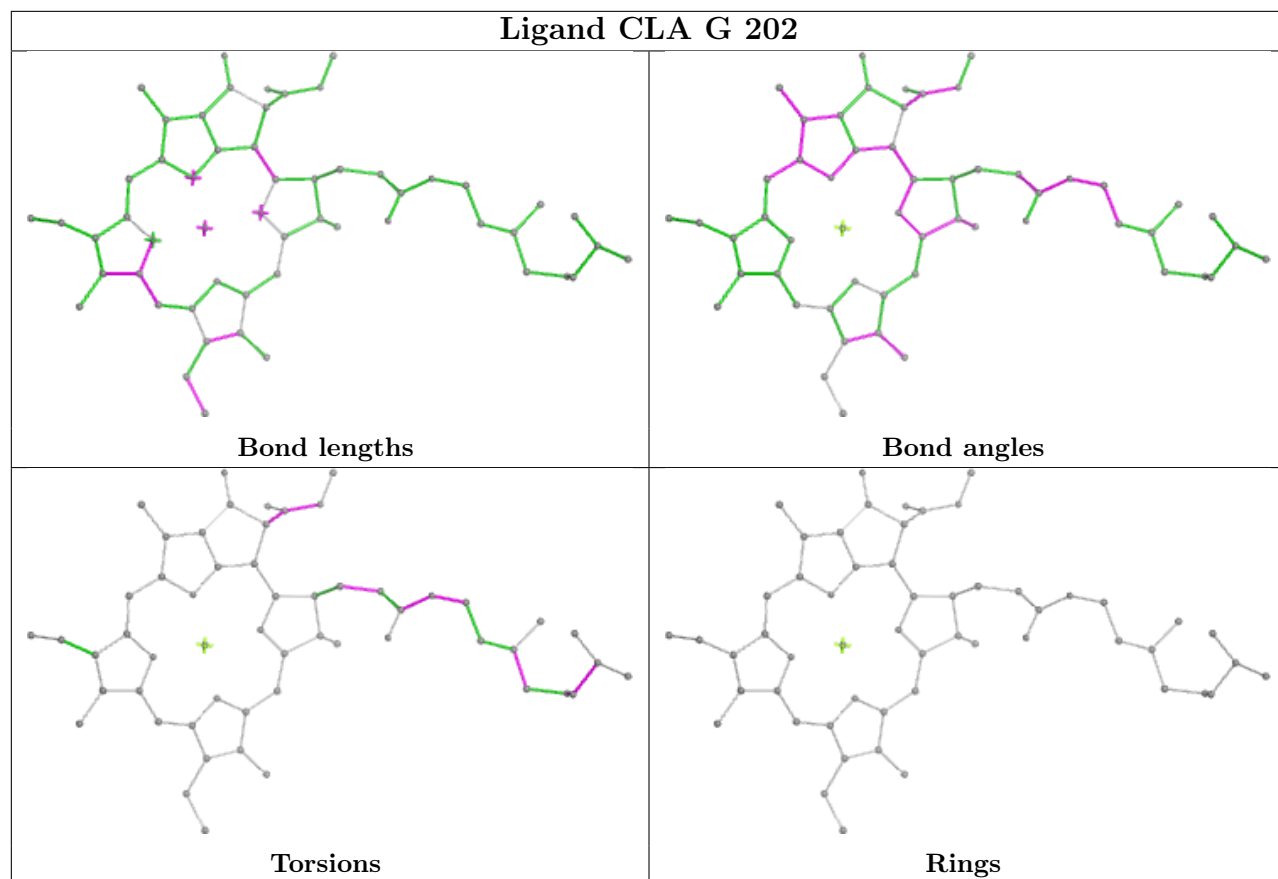


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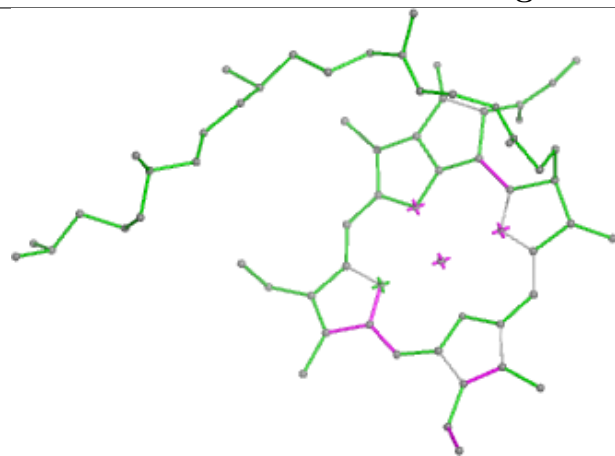


Ligand XAT 2 502

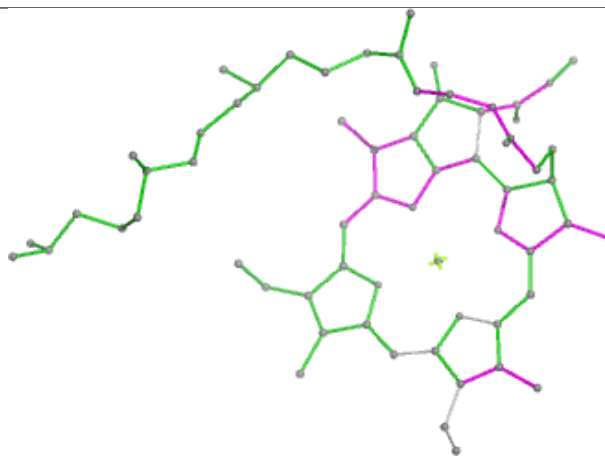




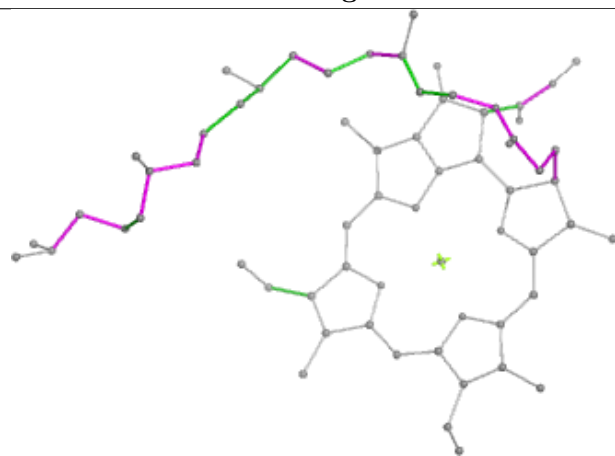
Ligand CLA A 829



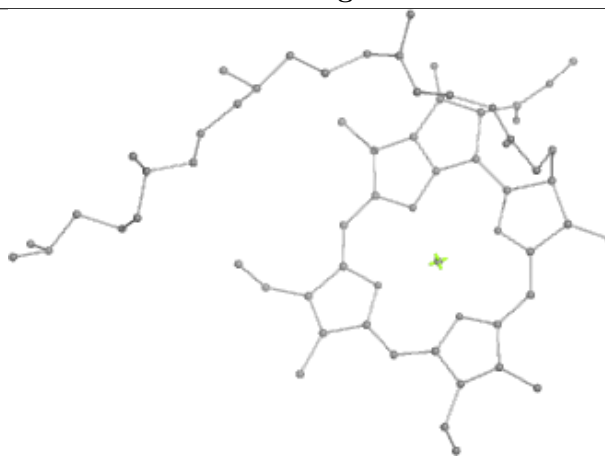
Bond lengths



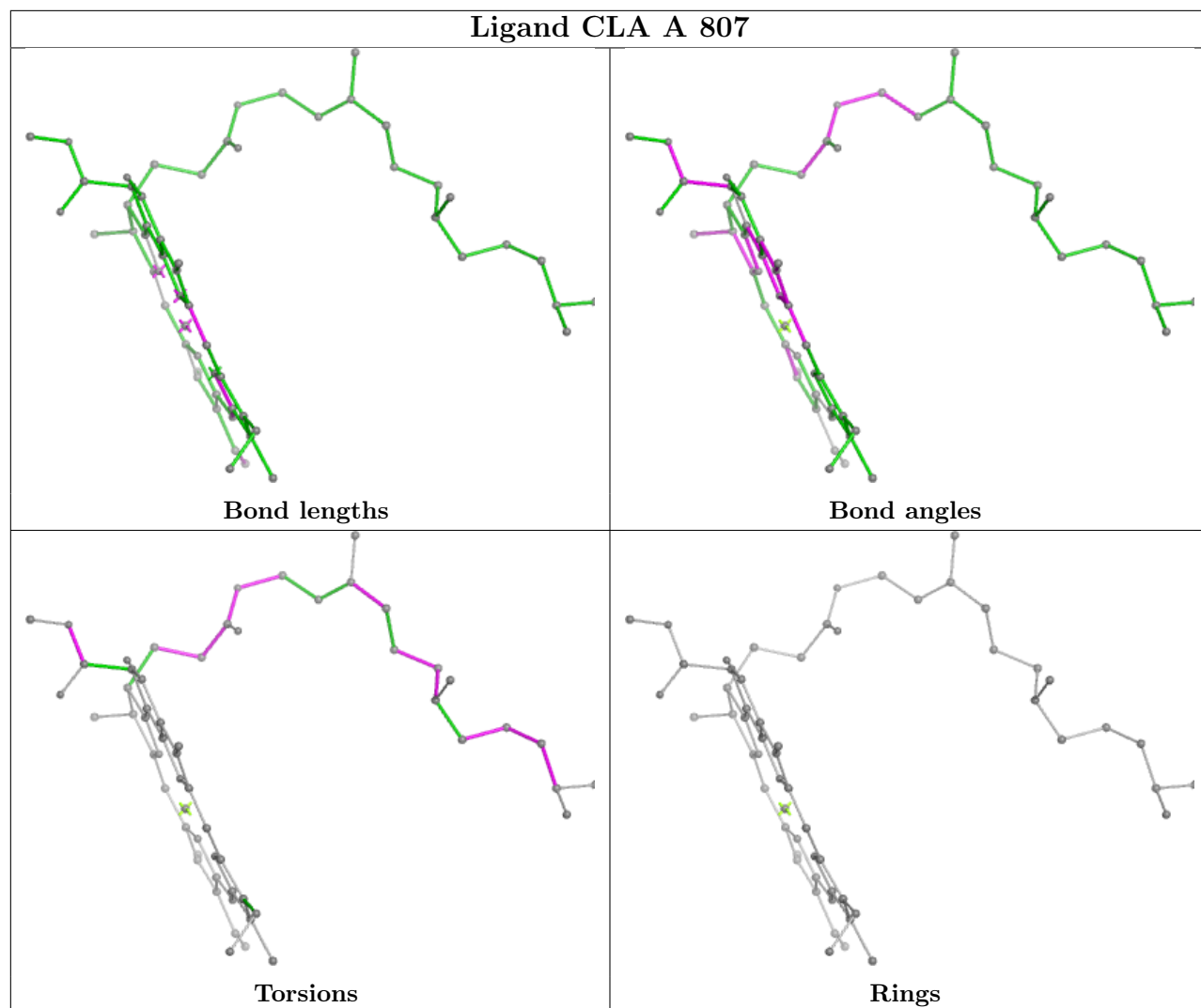
Bond angles



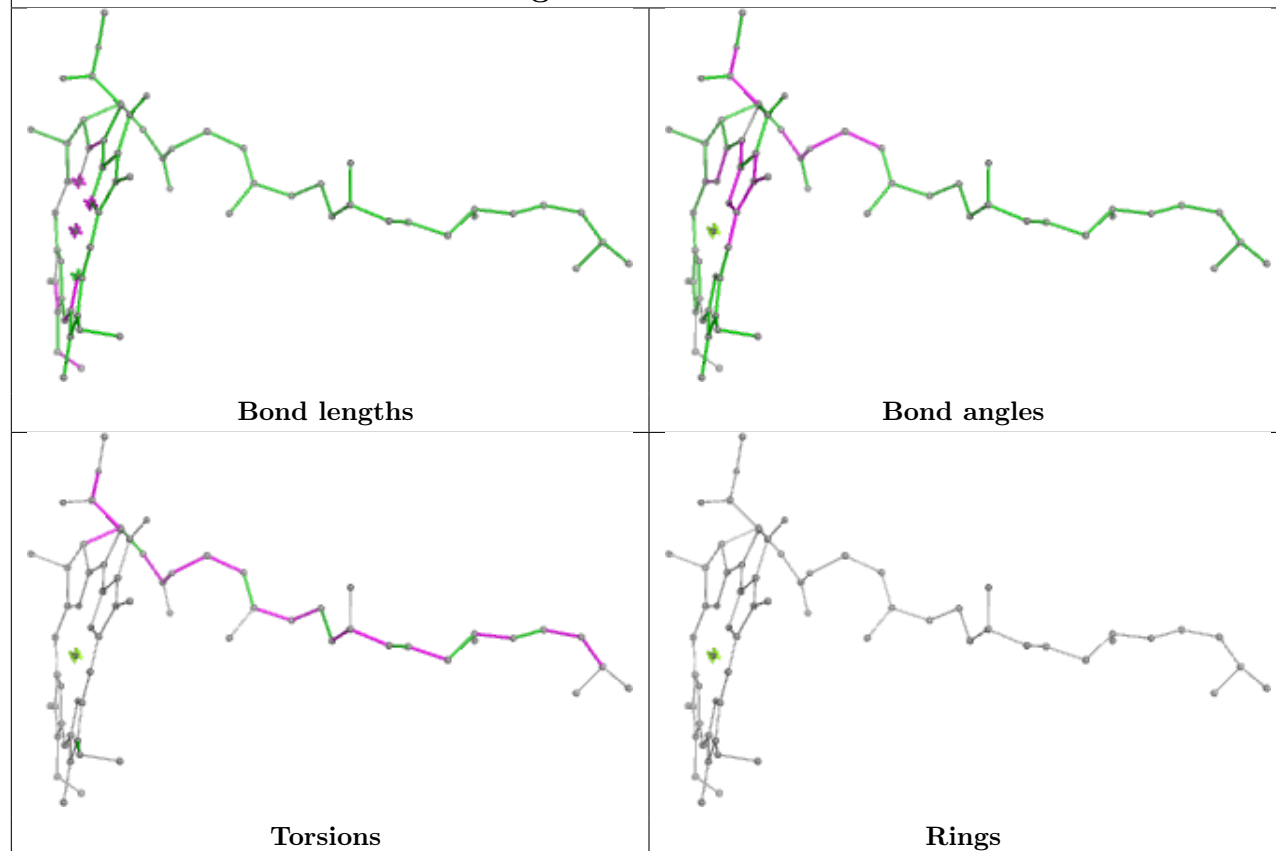
Torsions



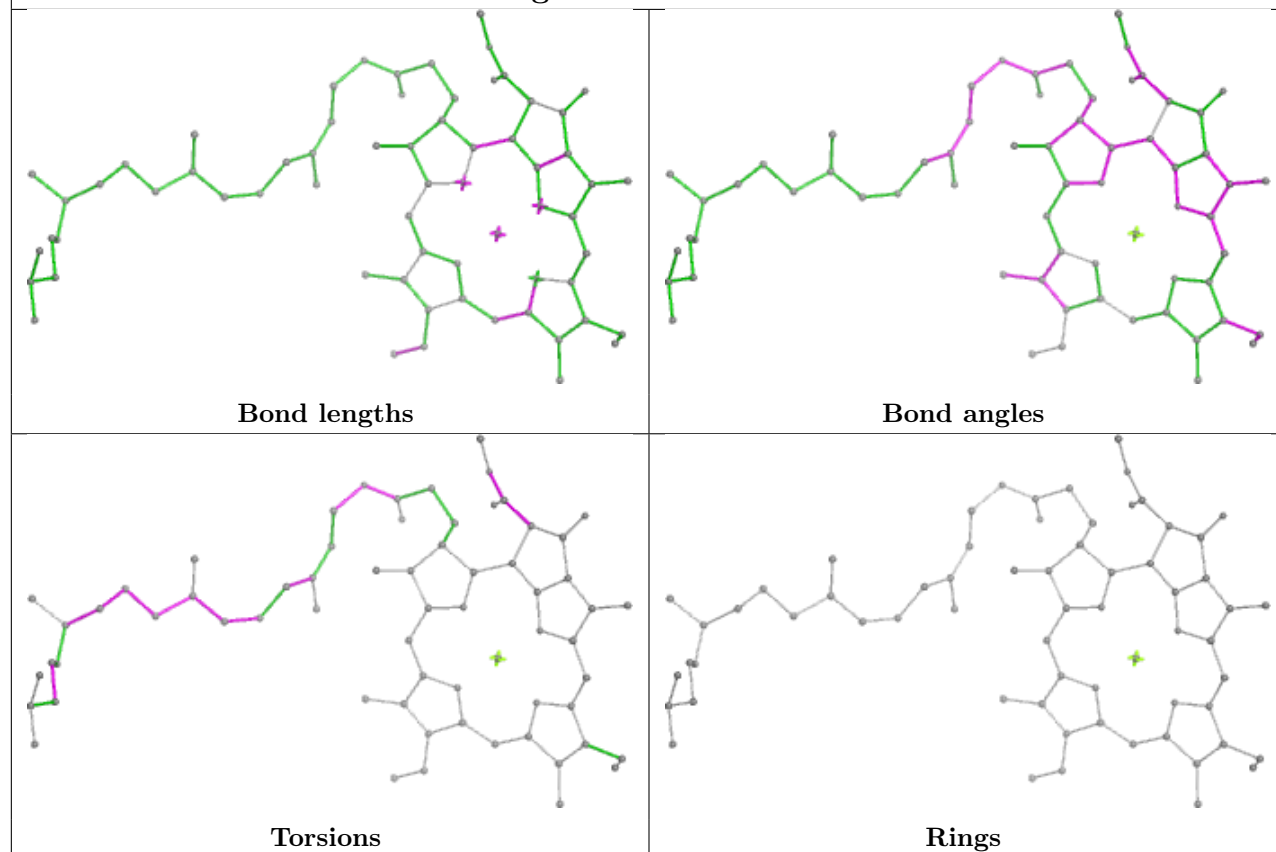
Rings



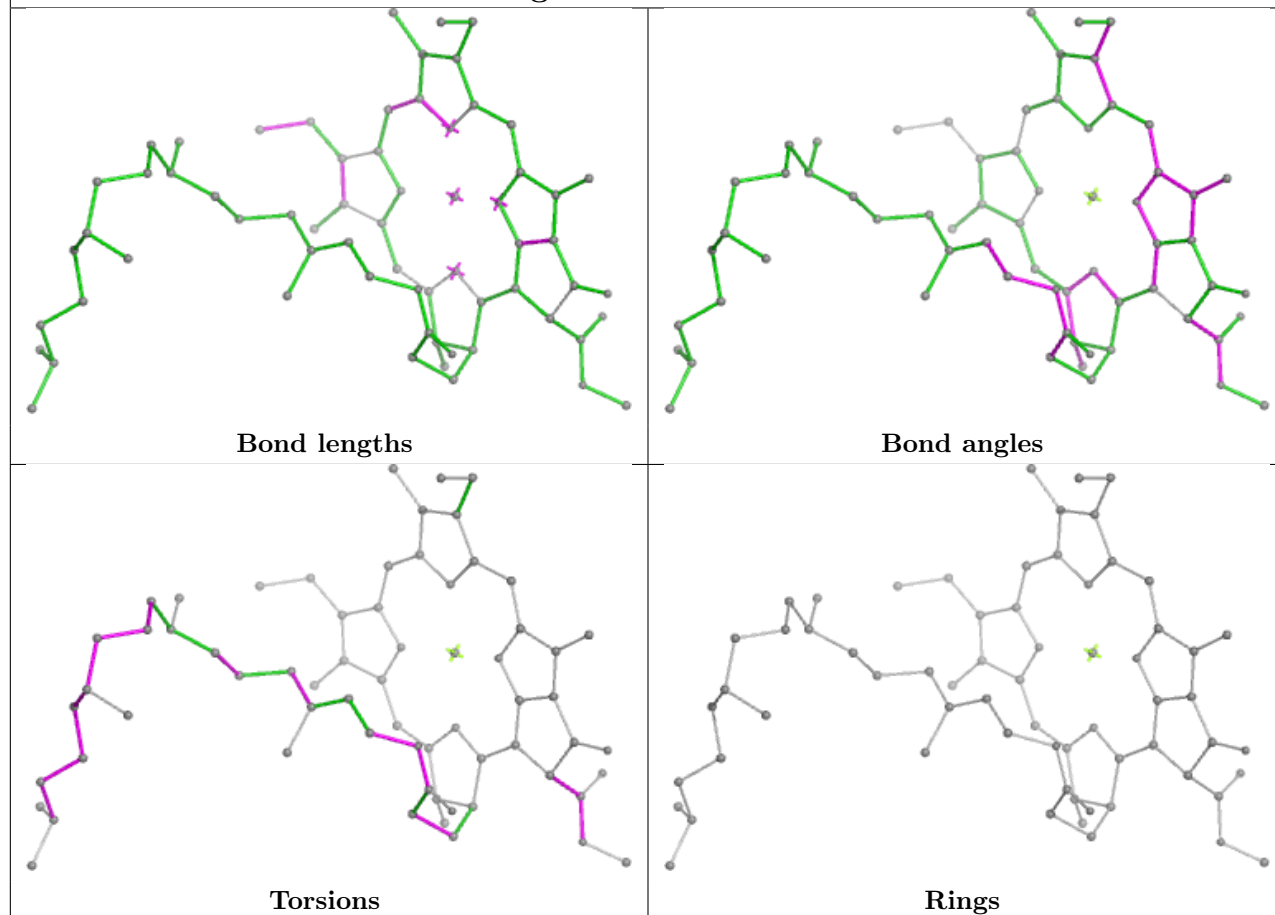
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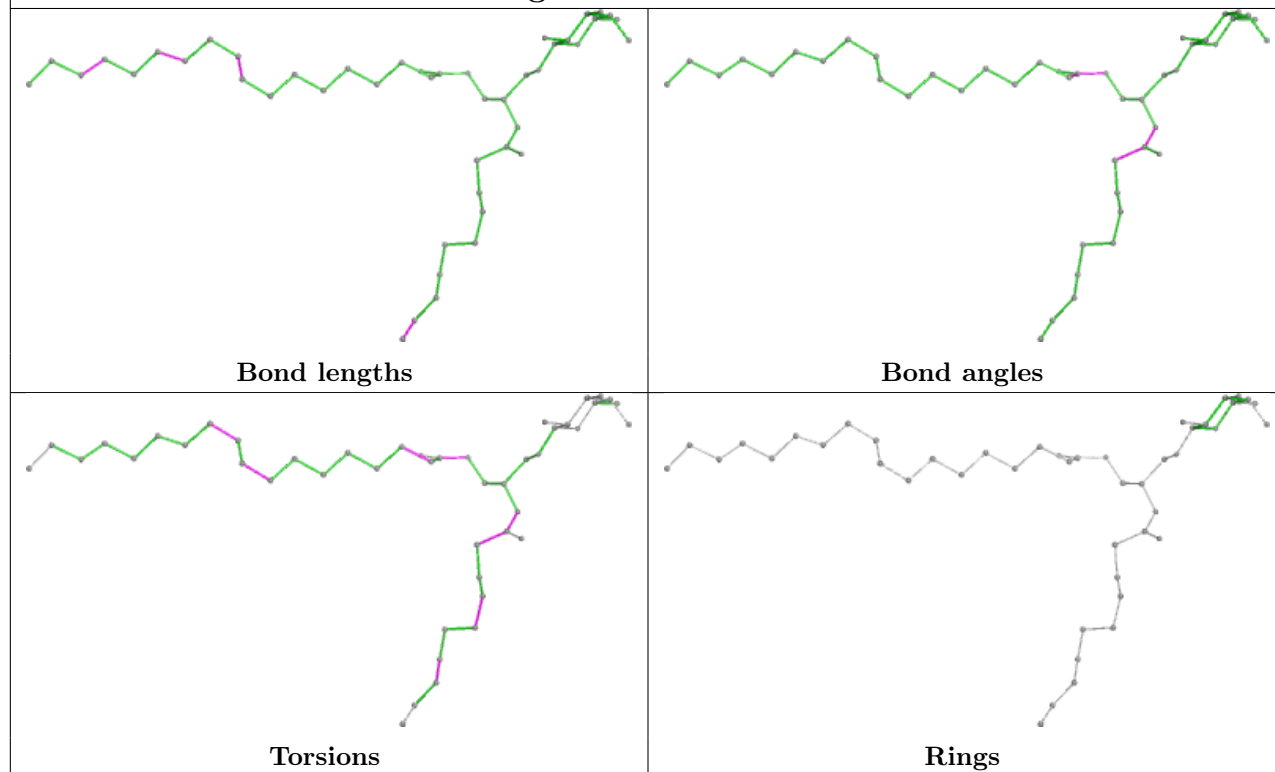
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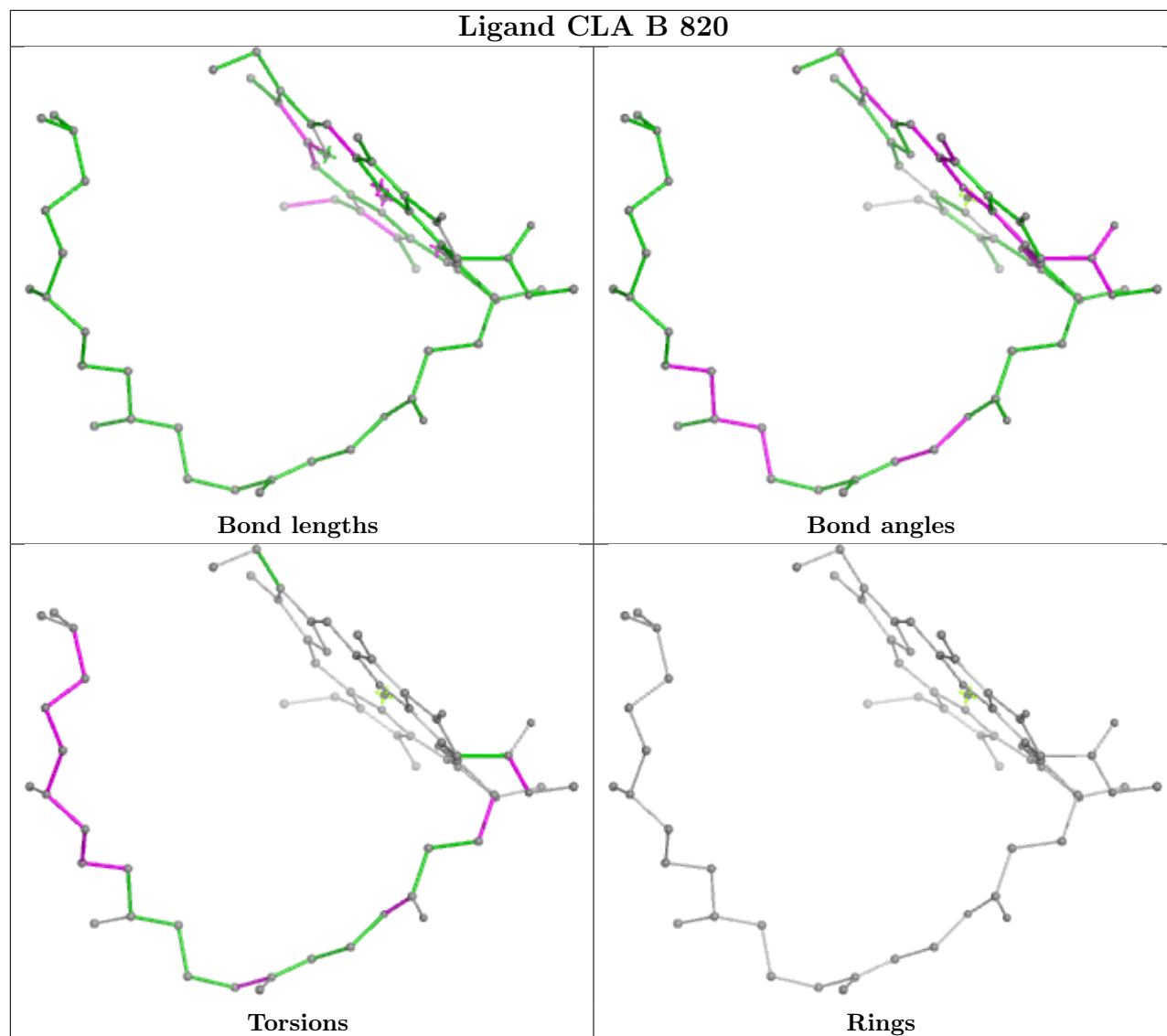


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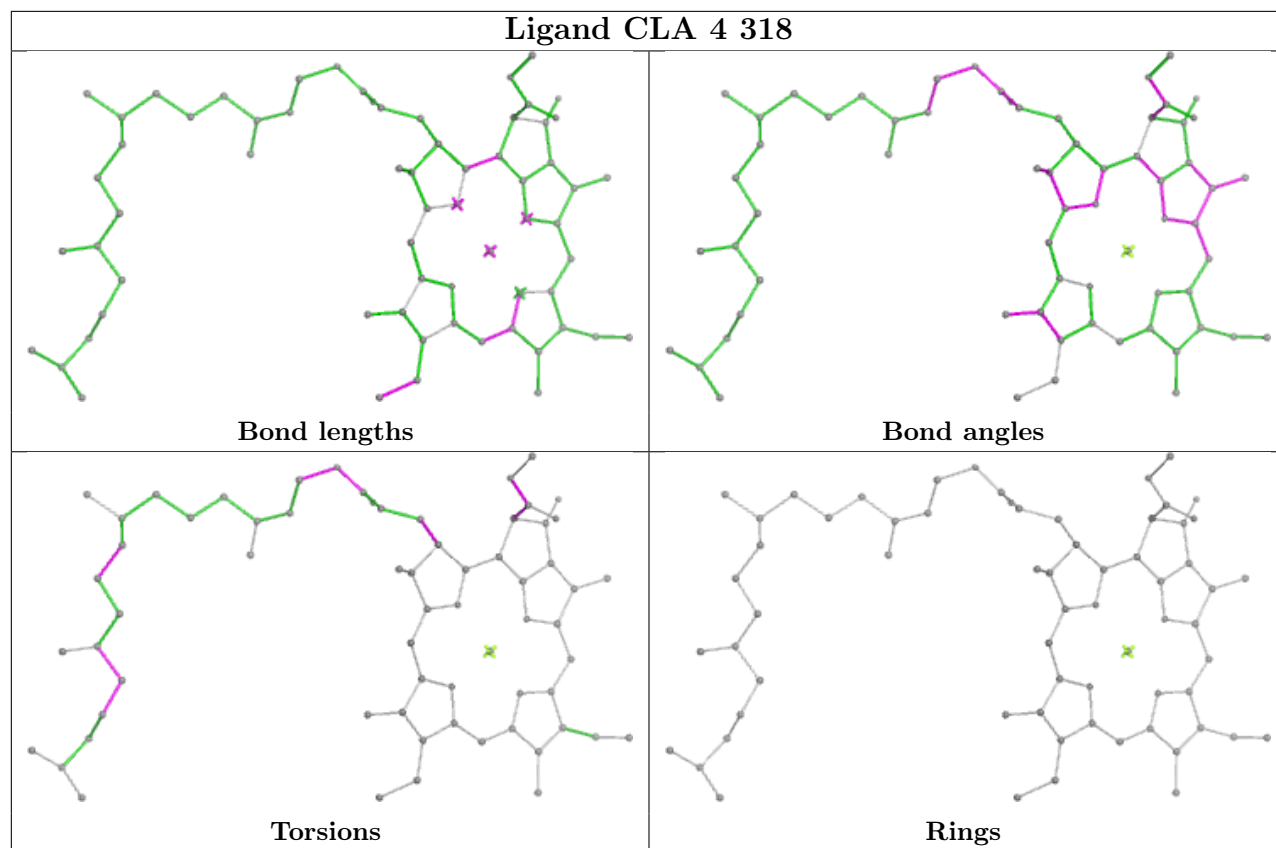


Ligand LMG F 304

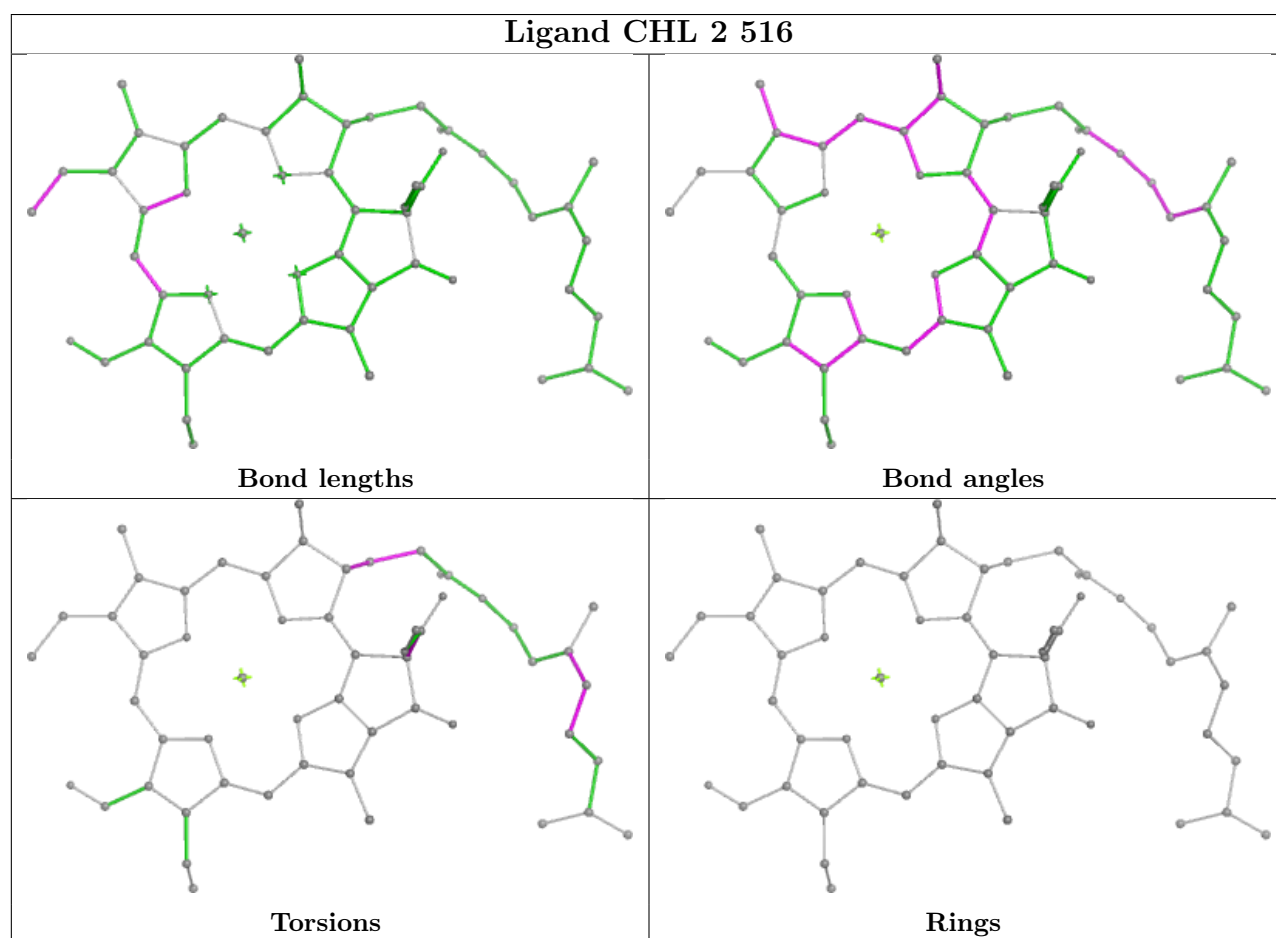




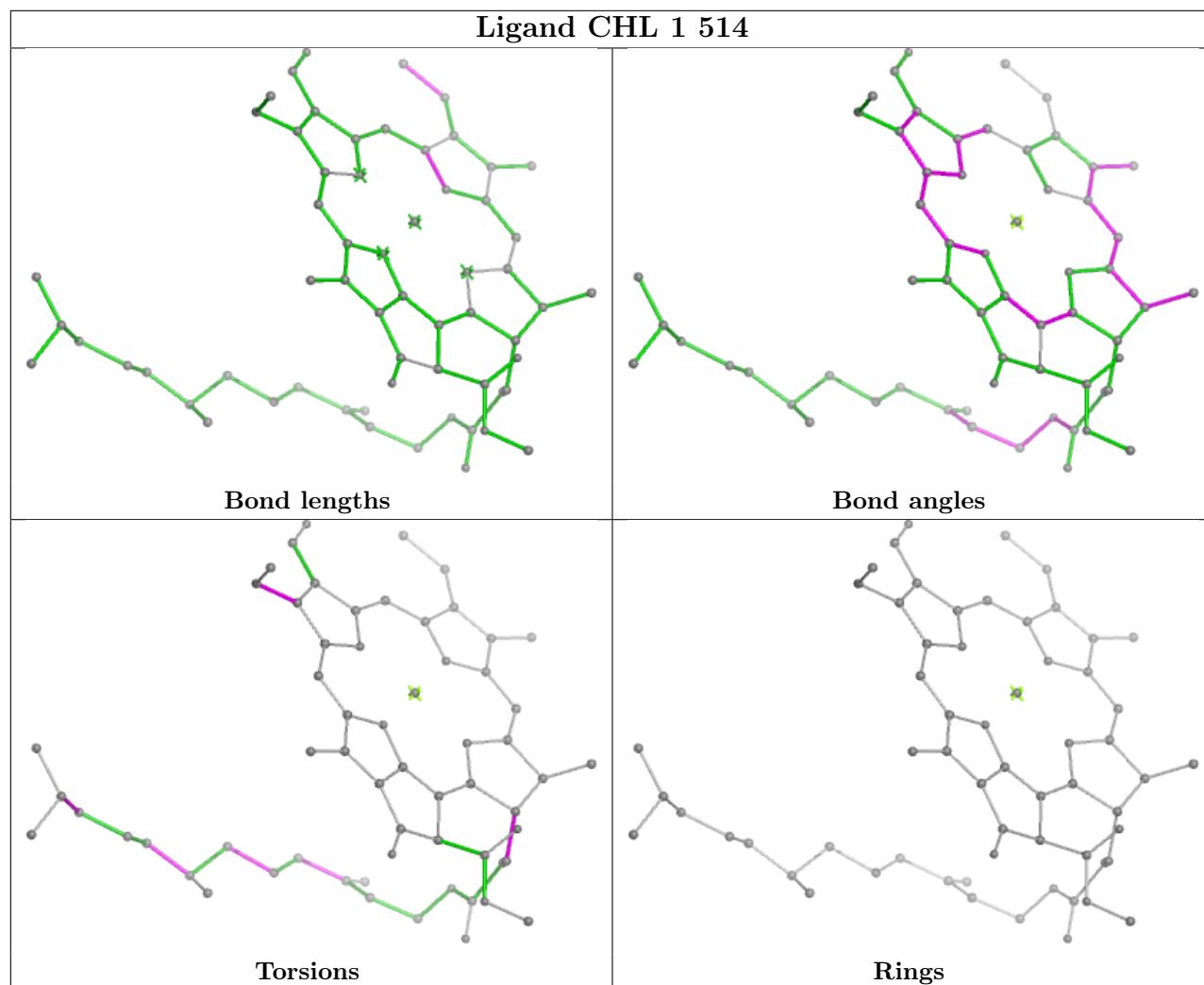
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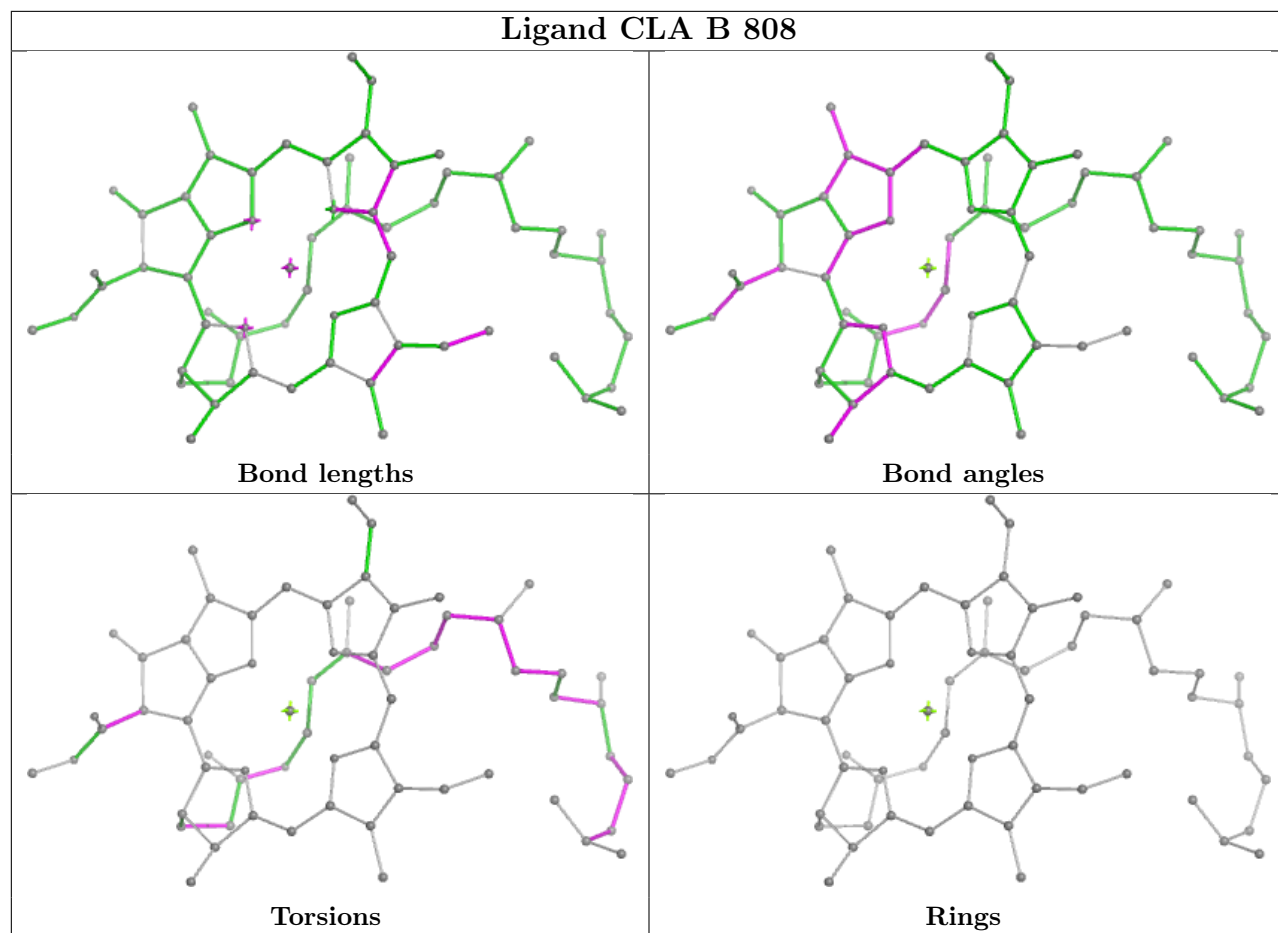
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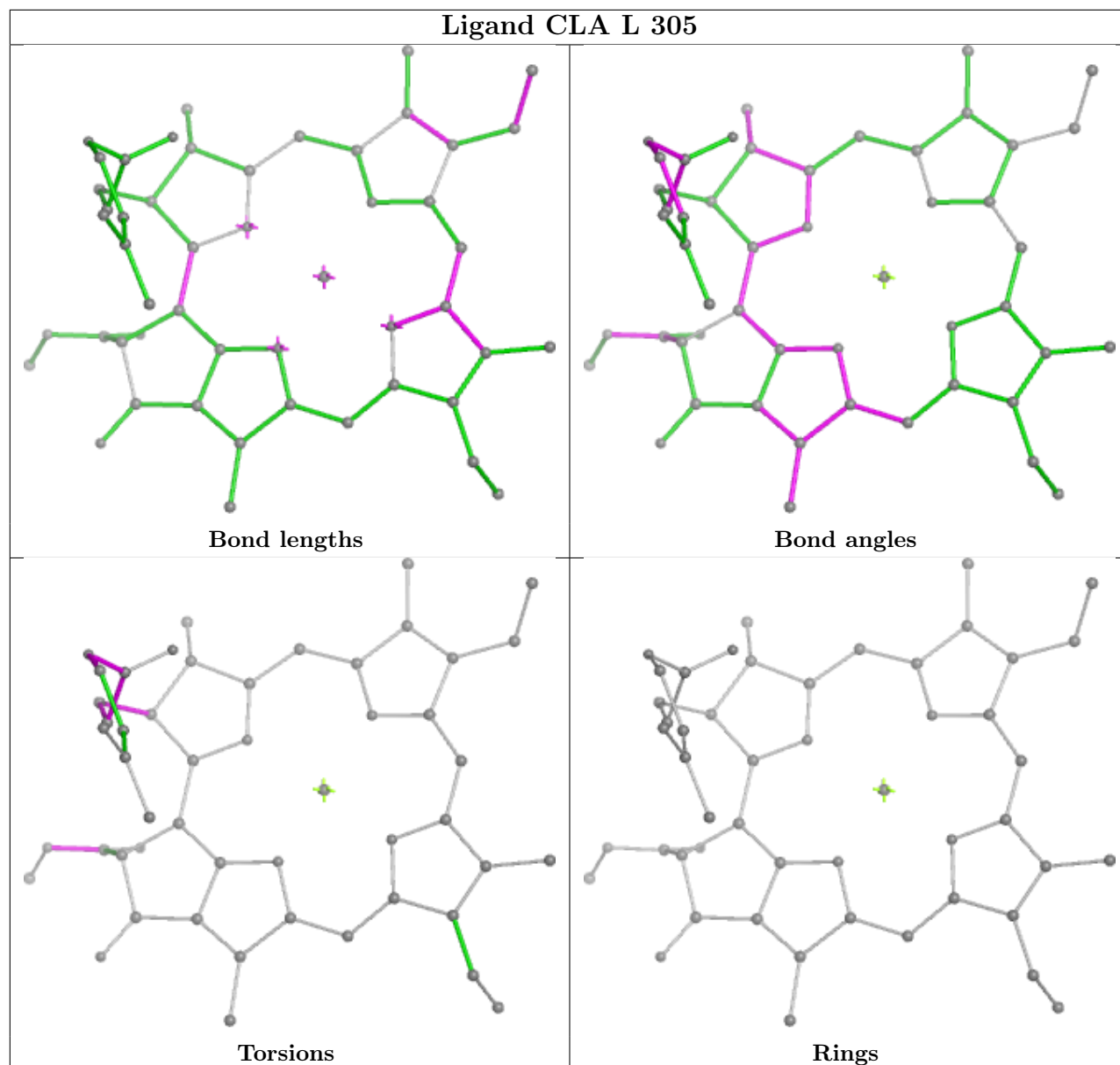
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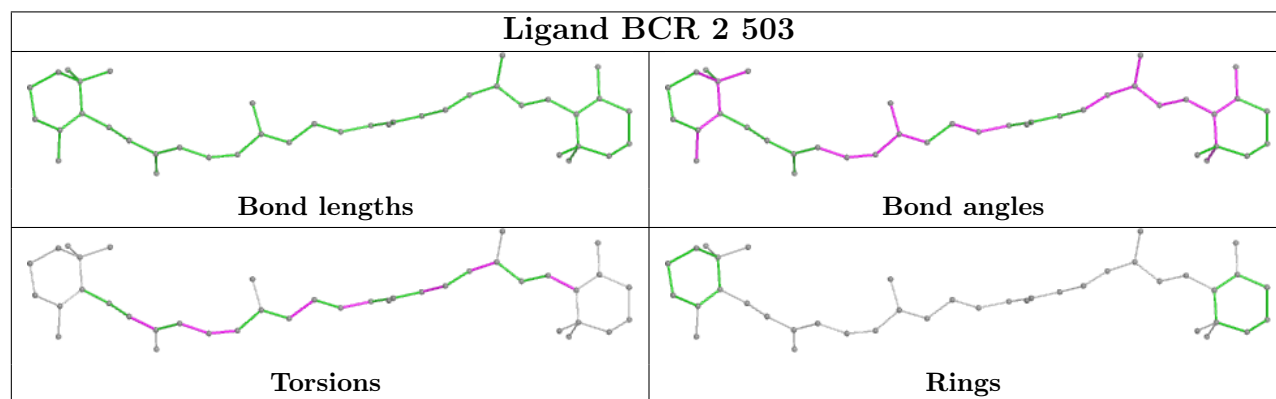
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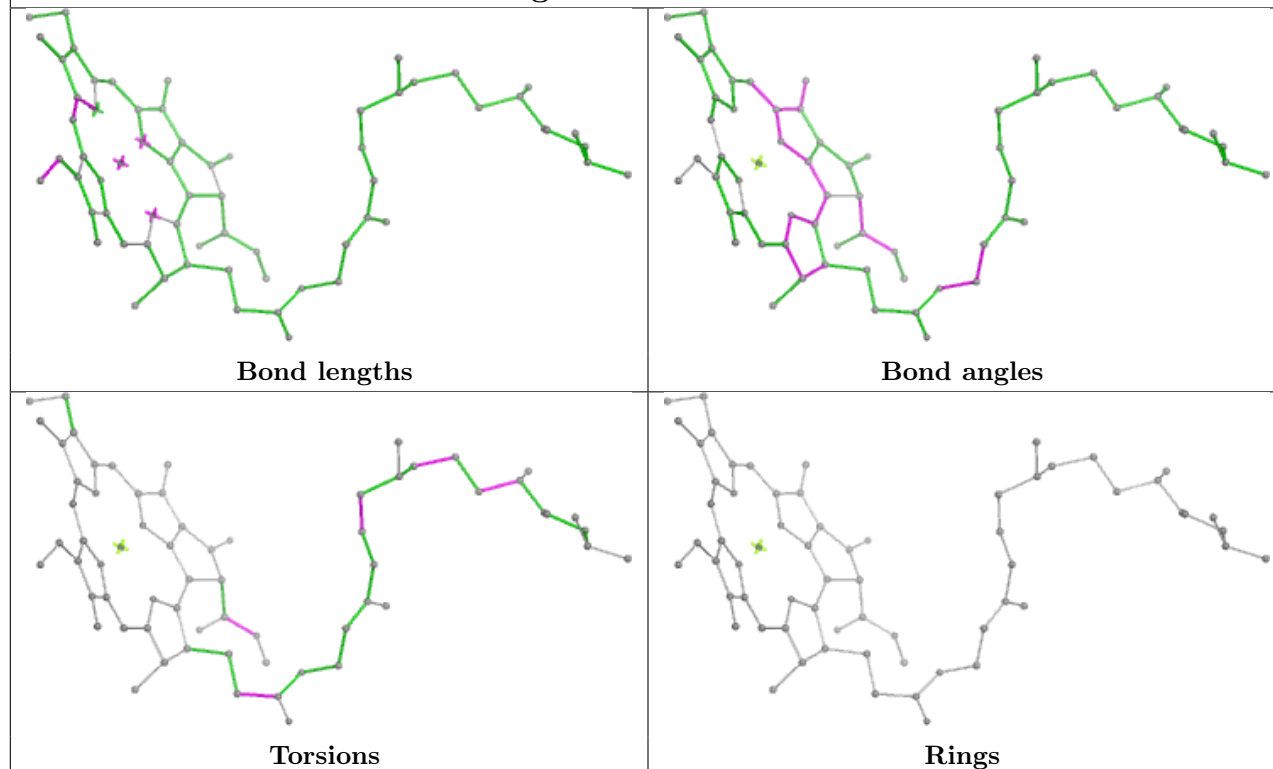
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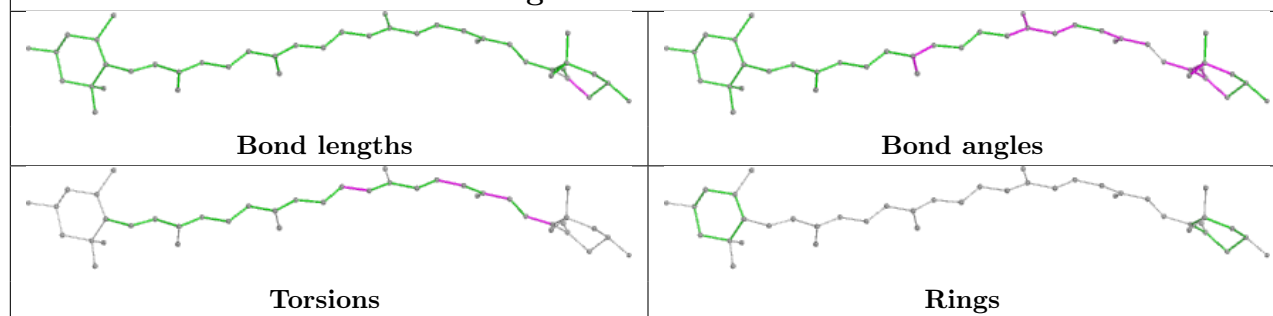
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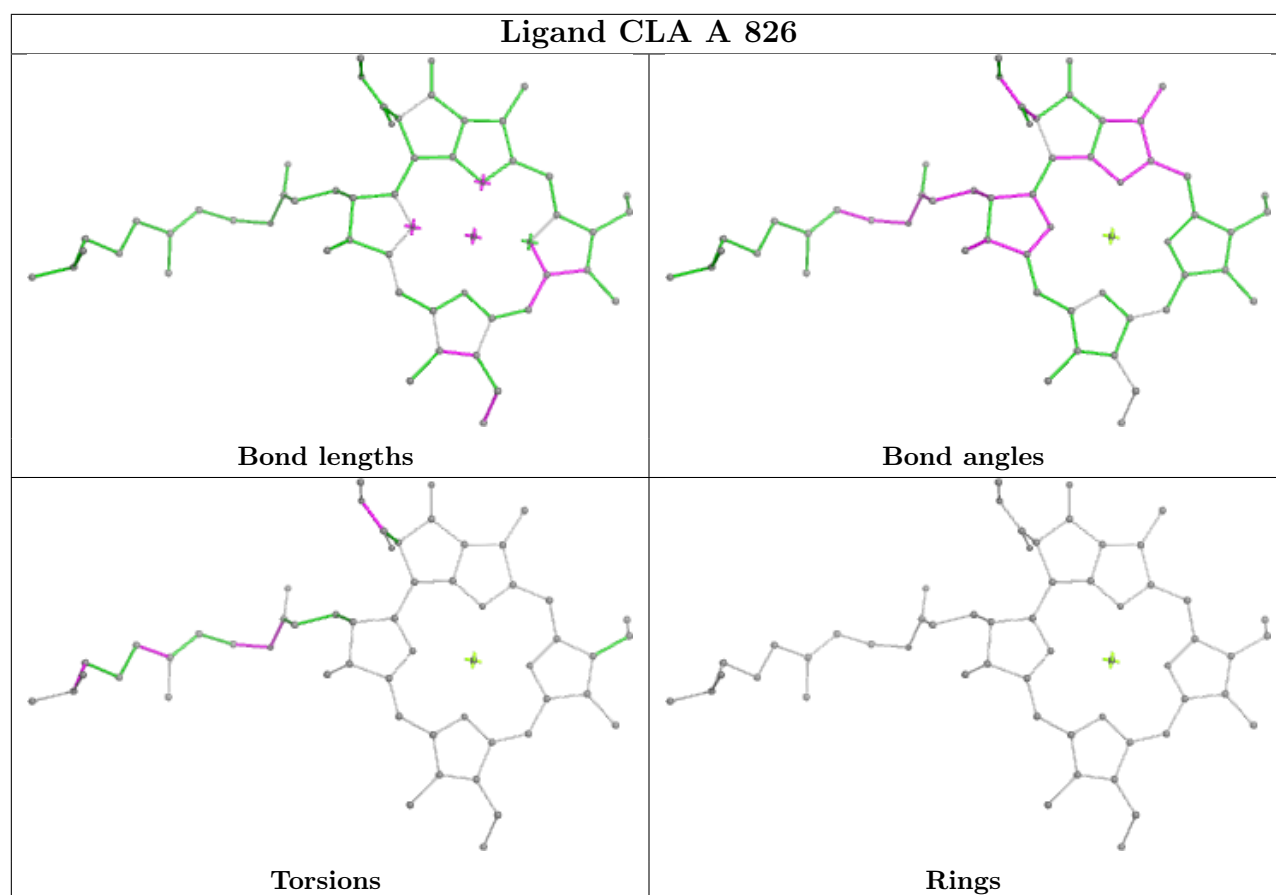


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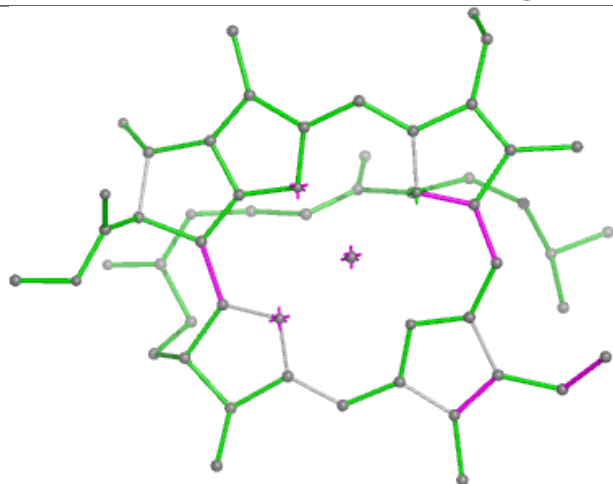


Ligand LUT J 1109

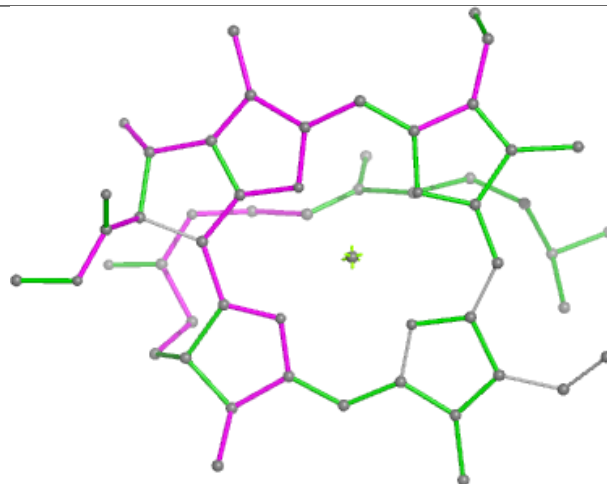




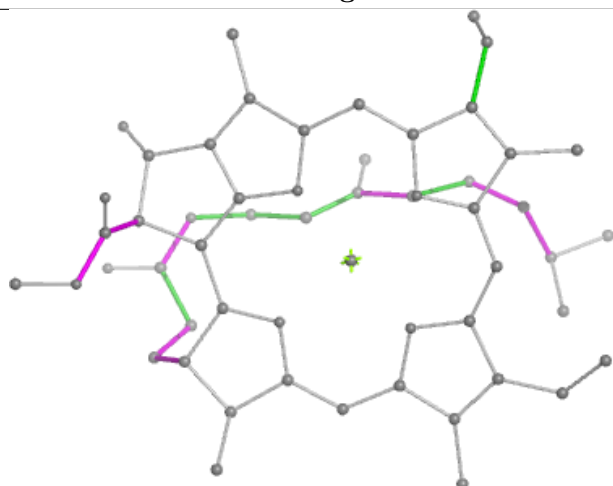
Ligand CLA 3 307



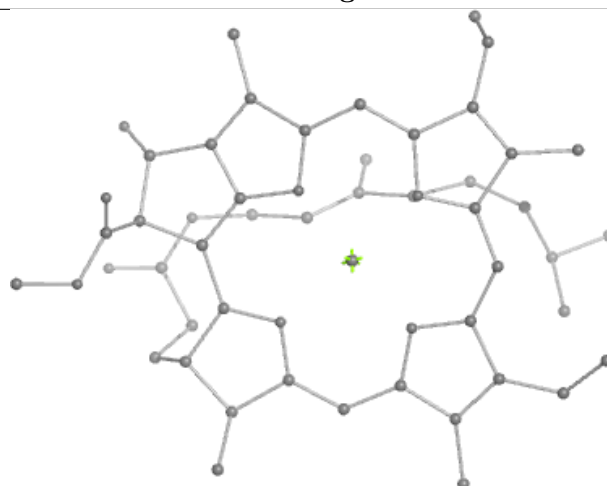
Bond lengths



Bond angles

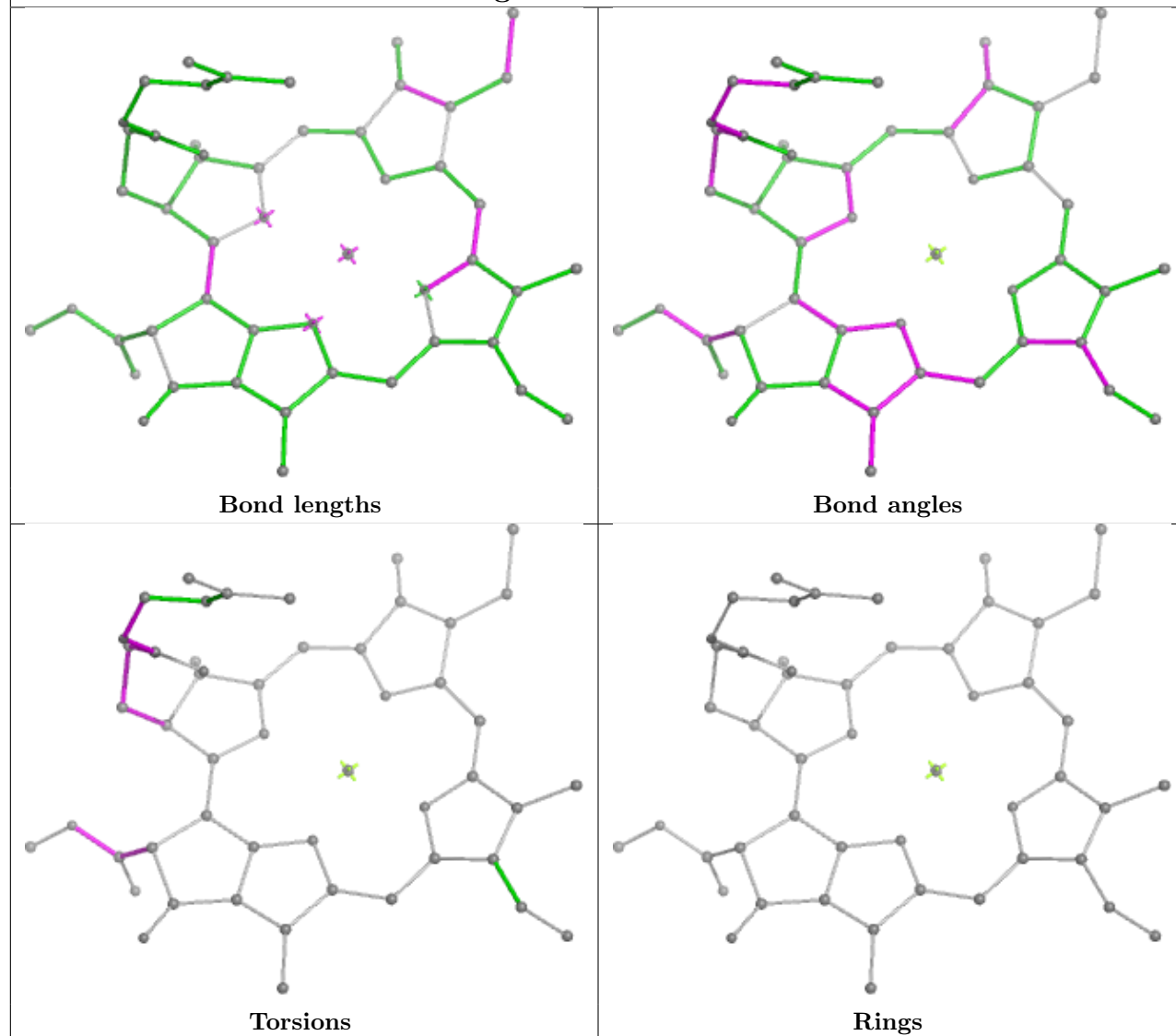


Torsions

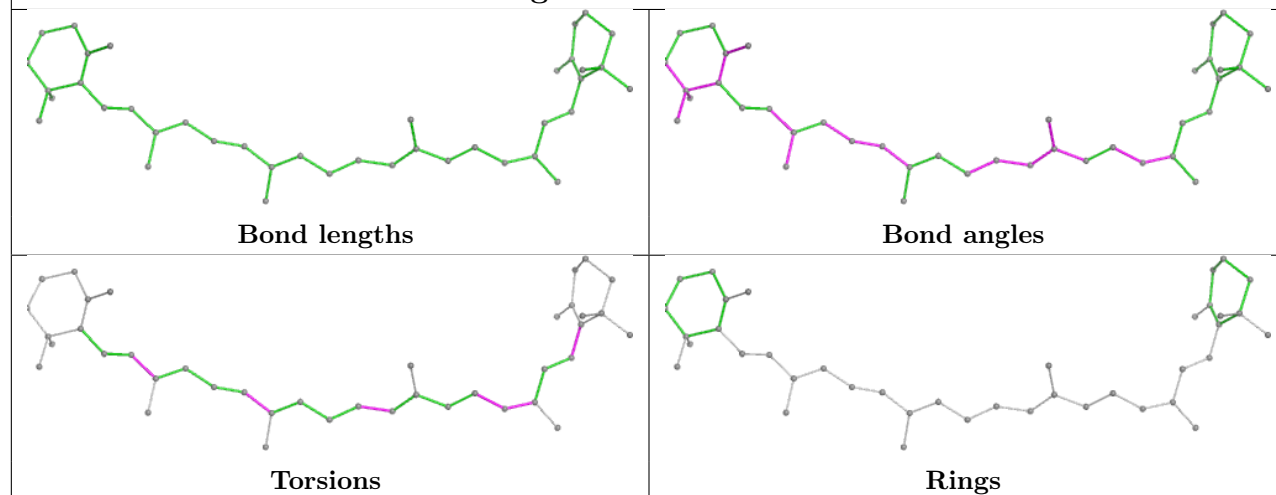


Rings

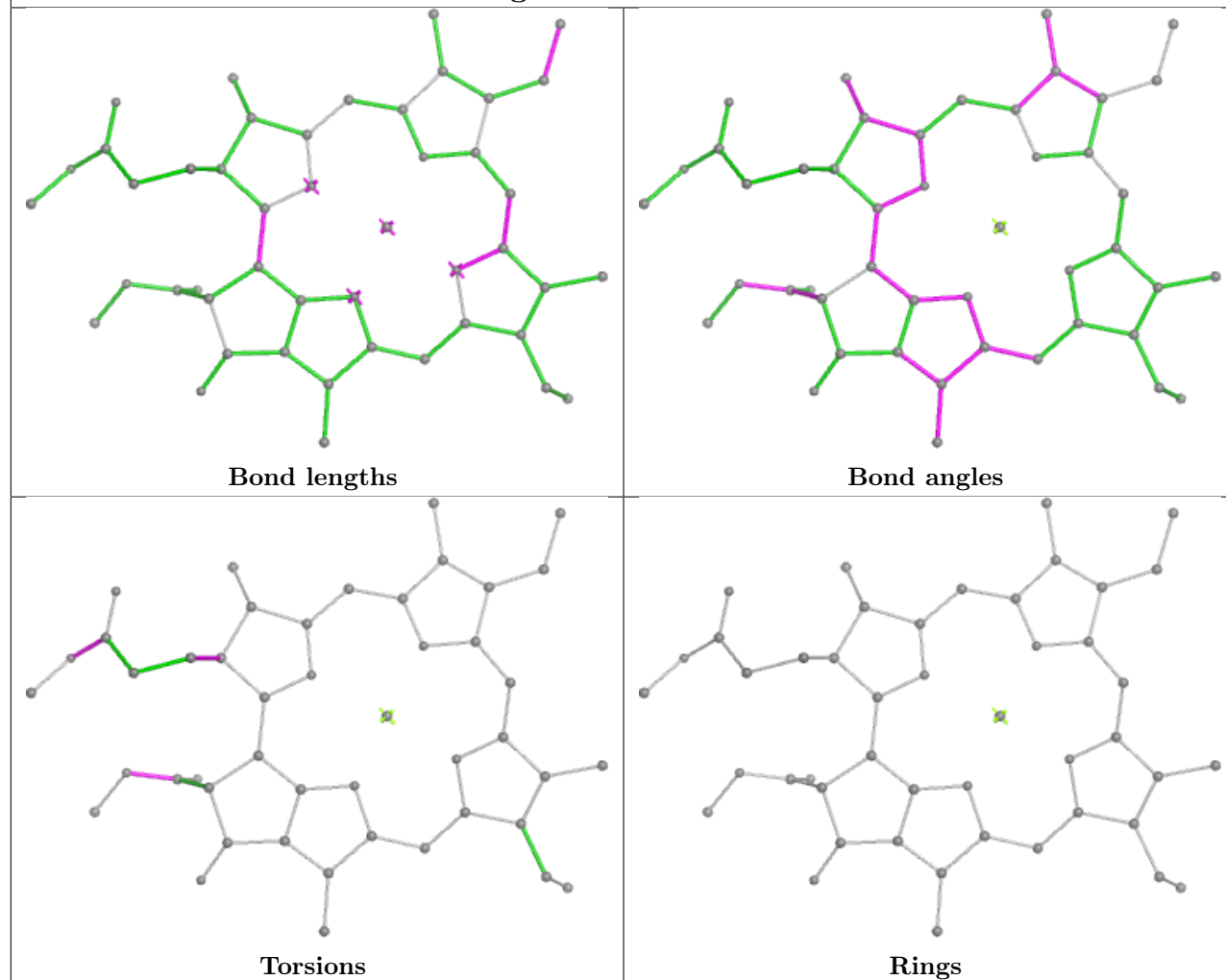
Ligand CLA 4 309



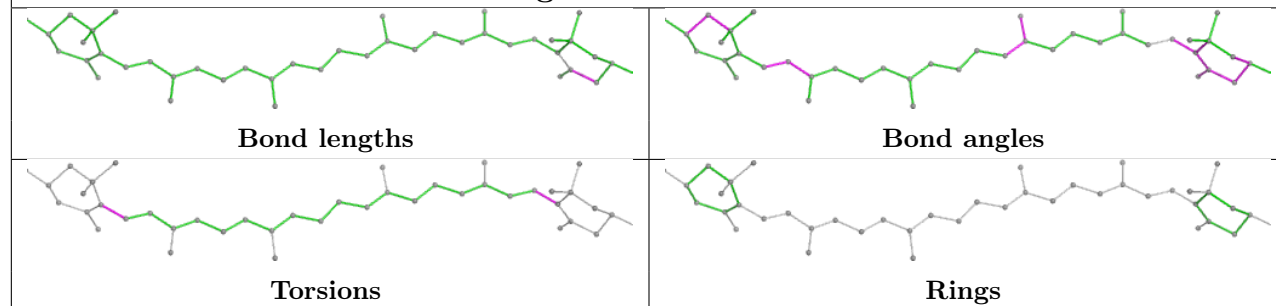
Ligand BCR B 850

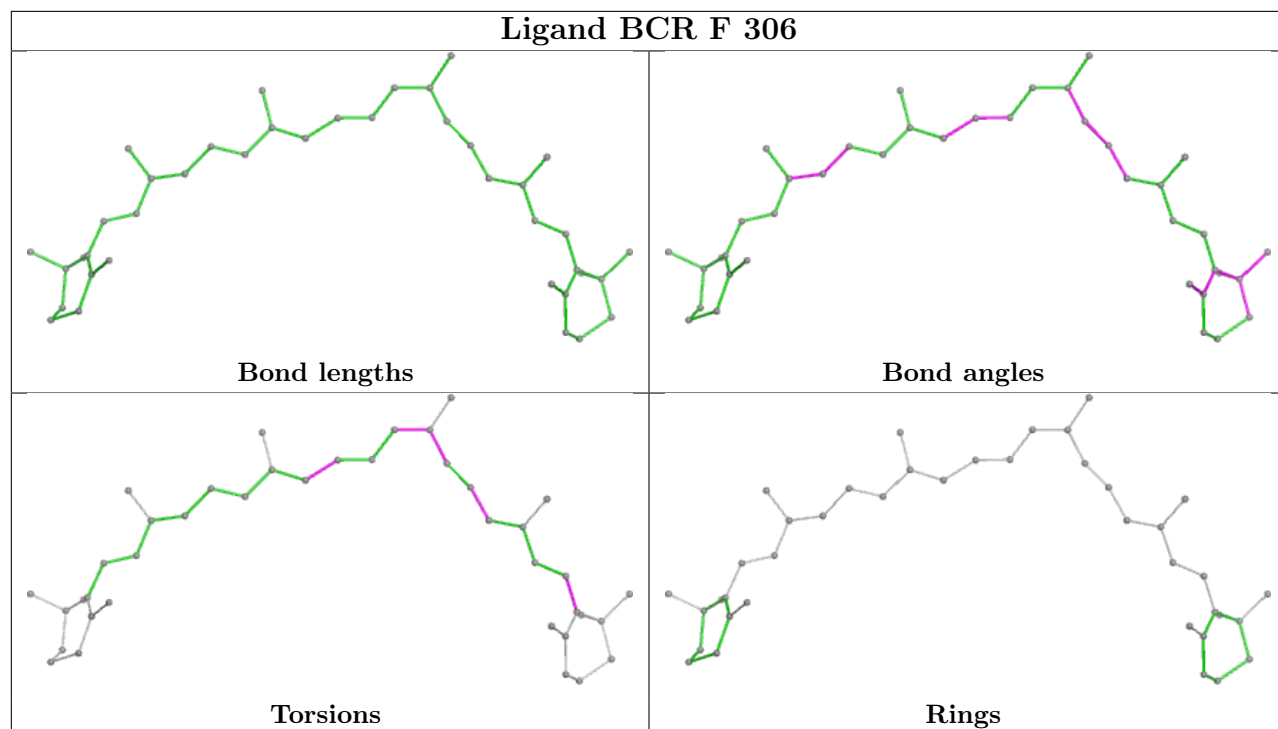


Ligand CLA G 203

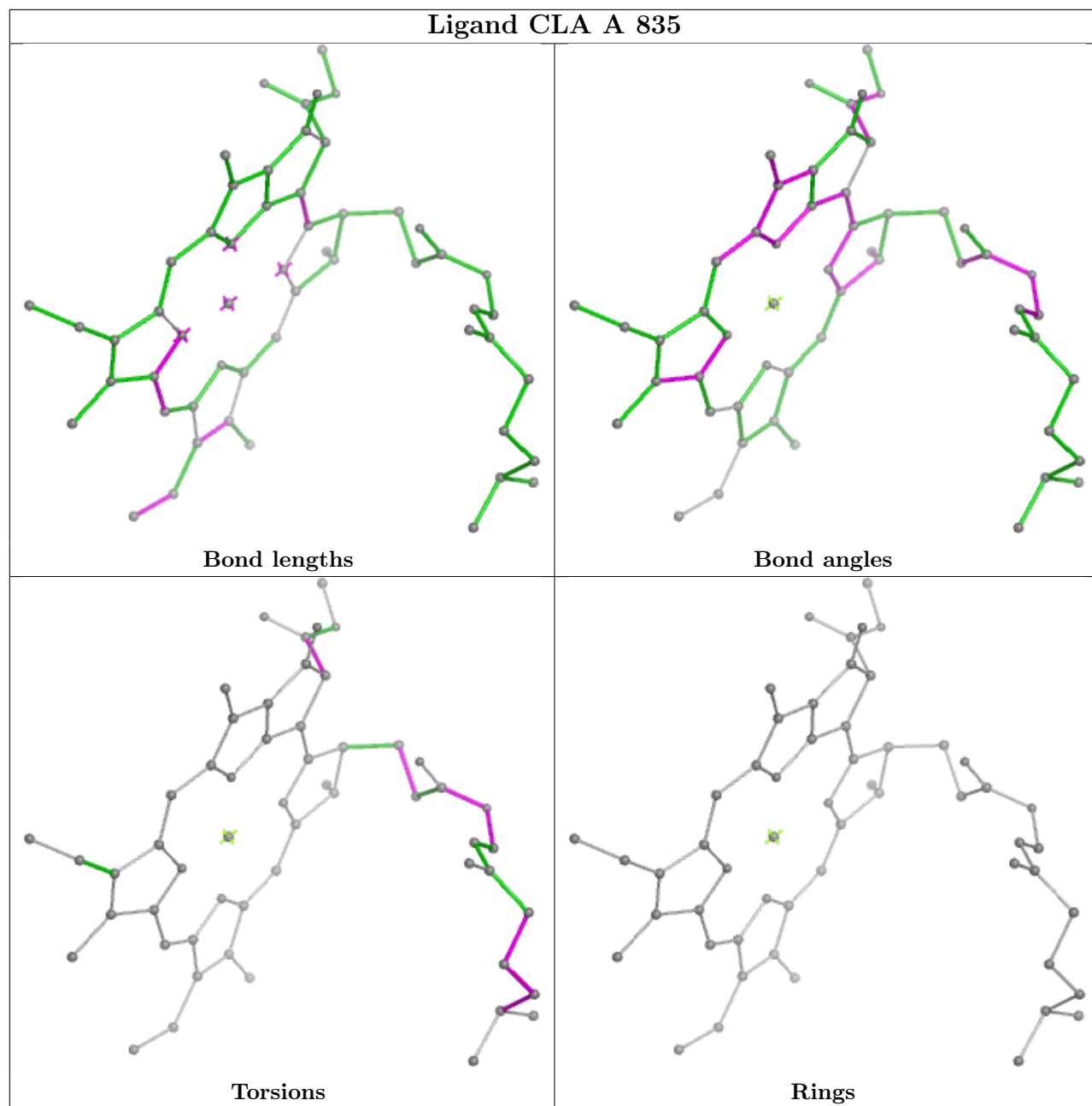


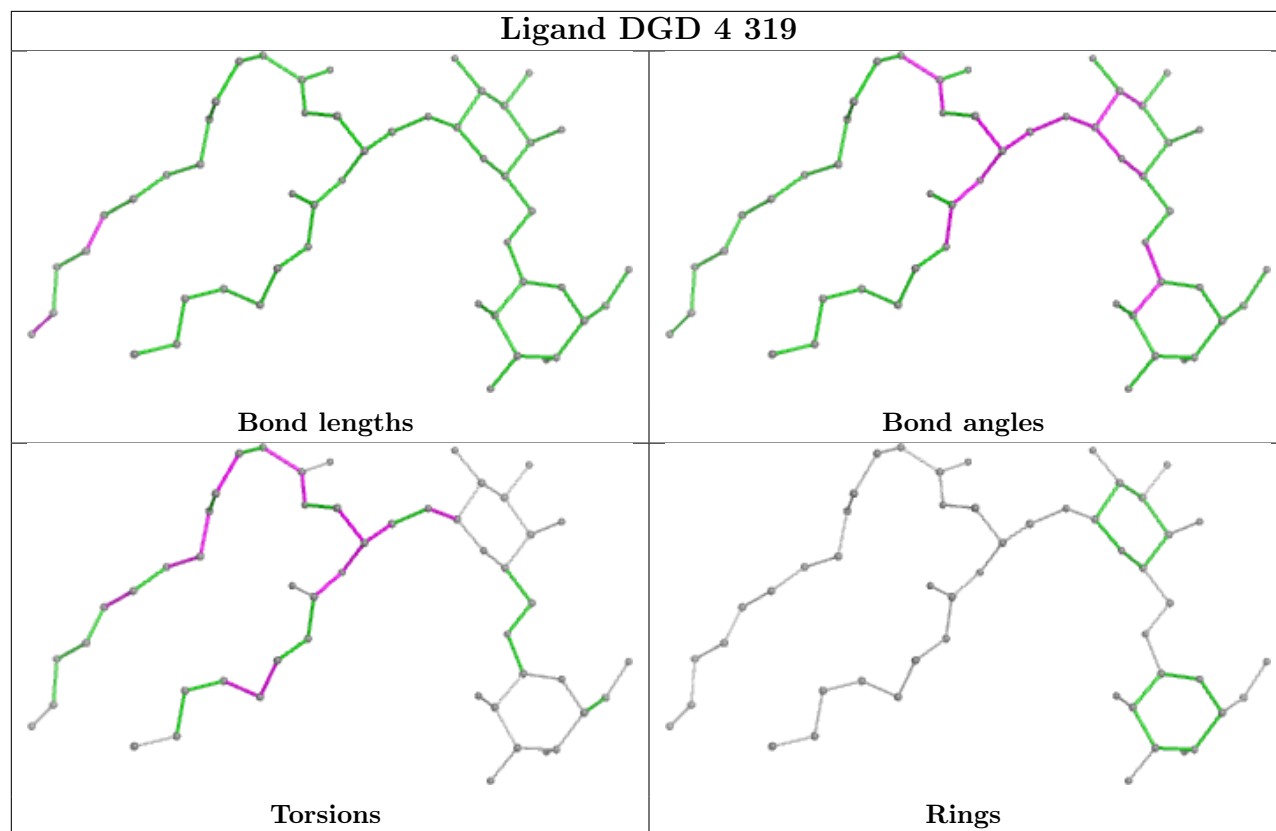
Ligand LUT 3 301



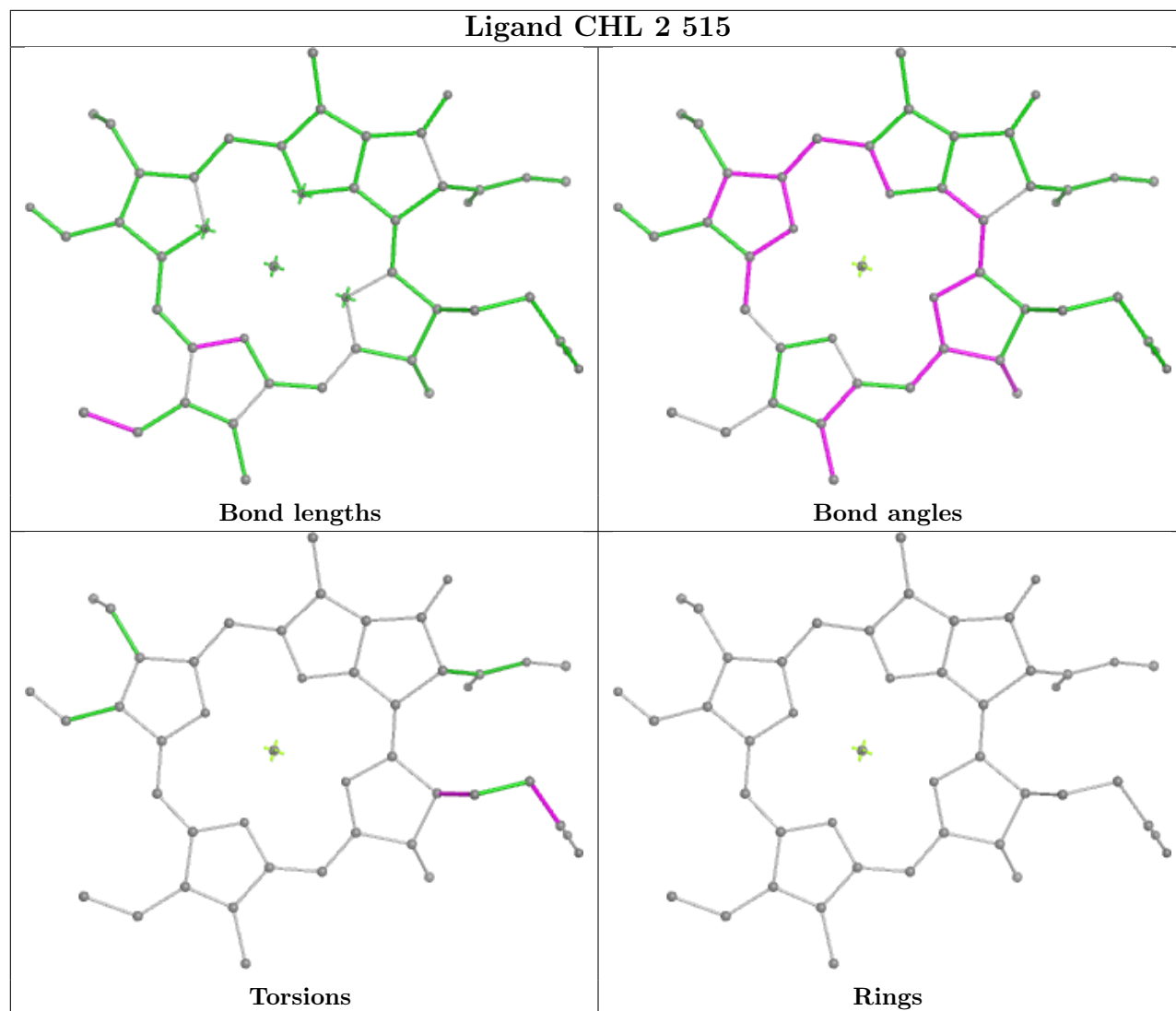


Ligand CLA A 835

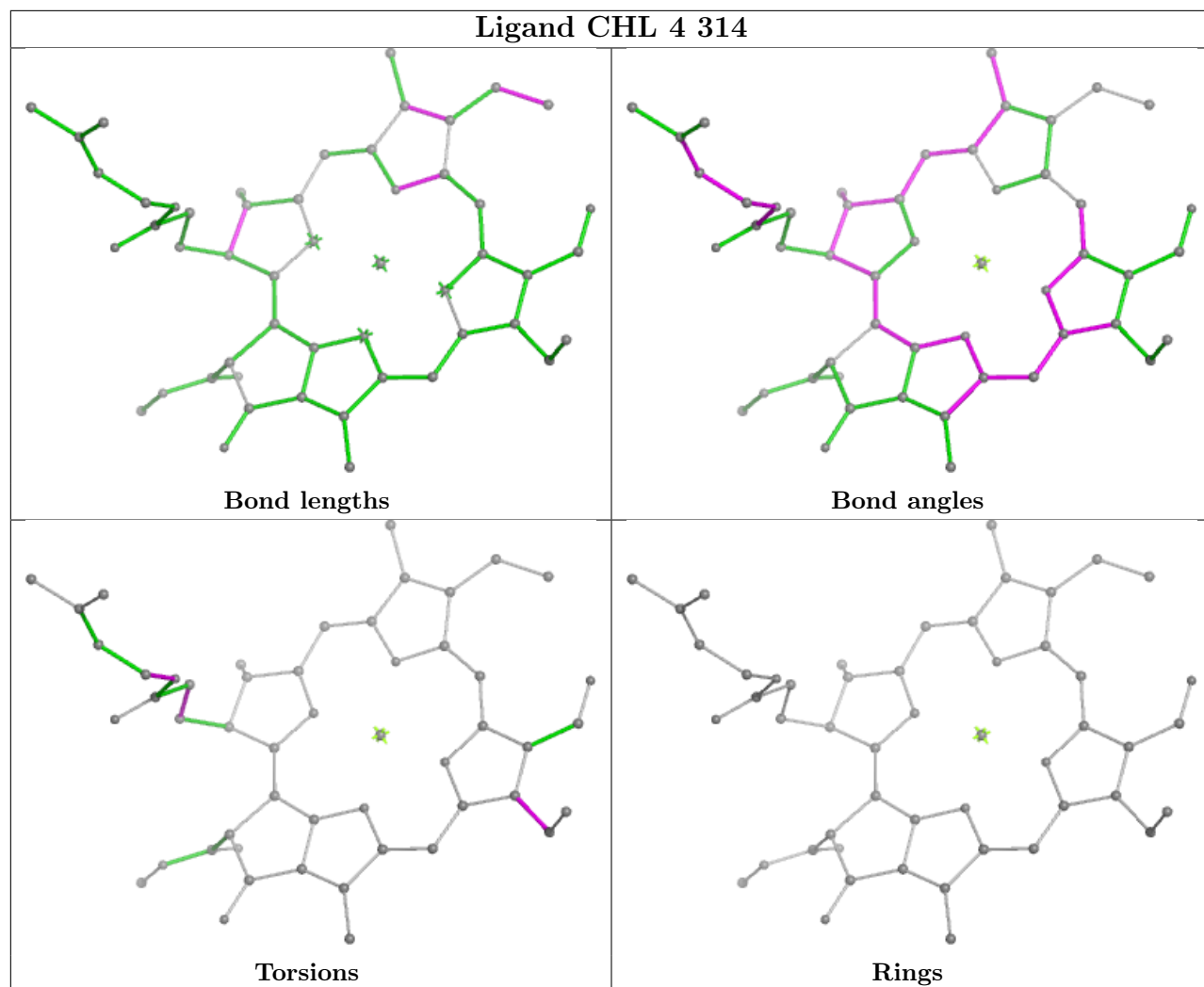




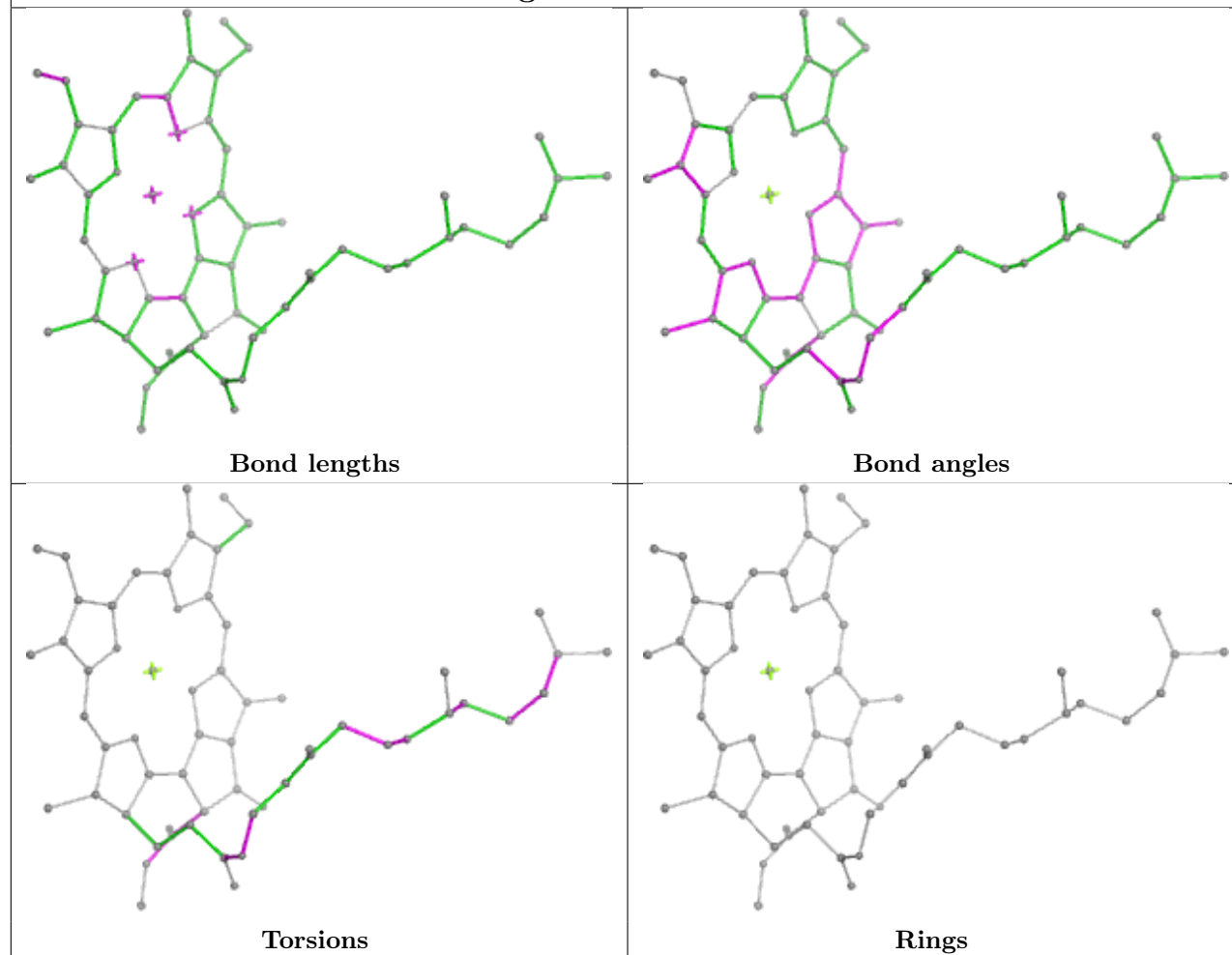
Ligand CHL 2 515



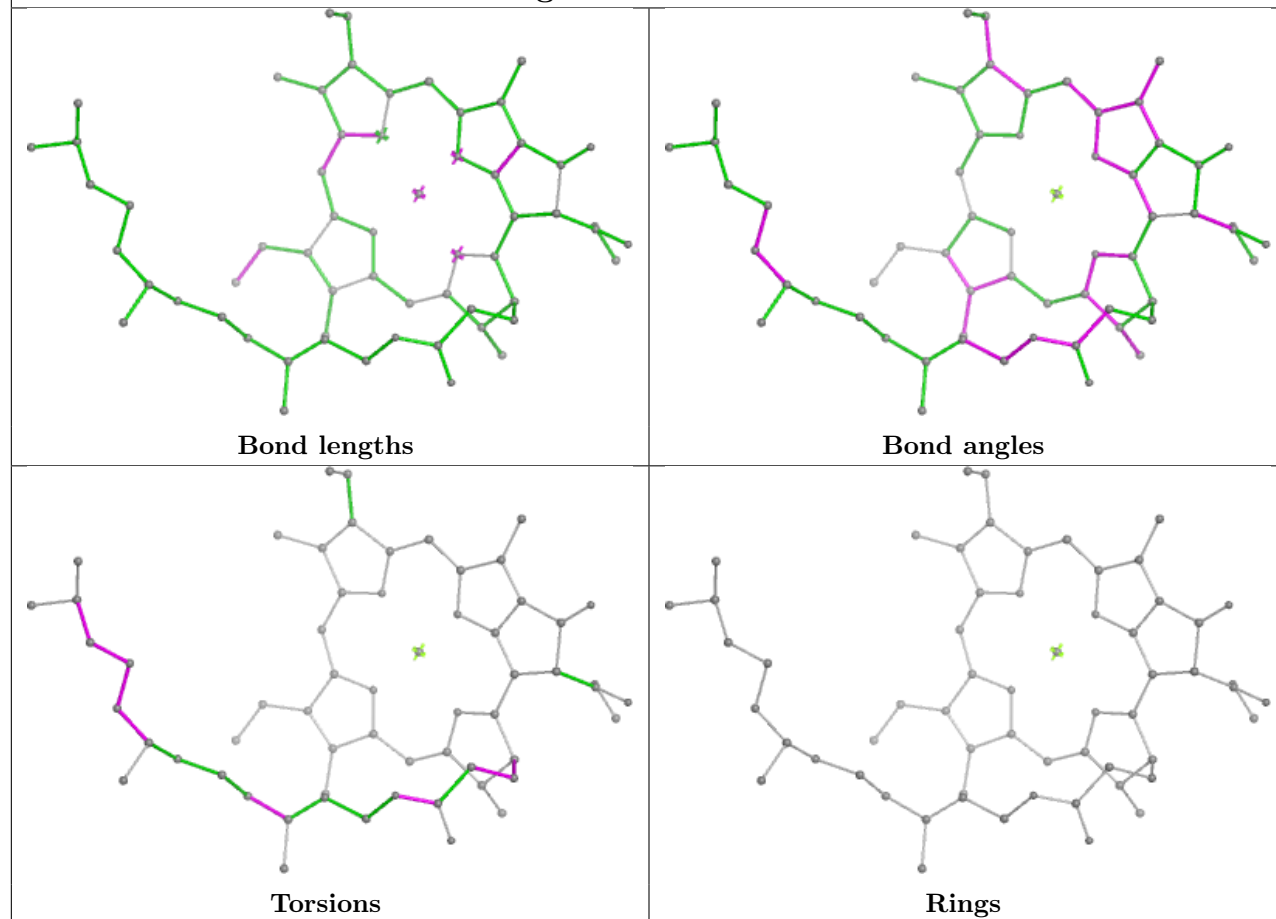
Ligand CHL 4 314



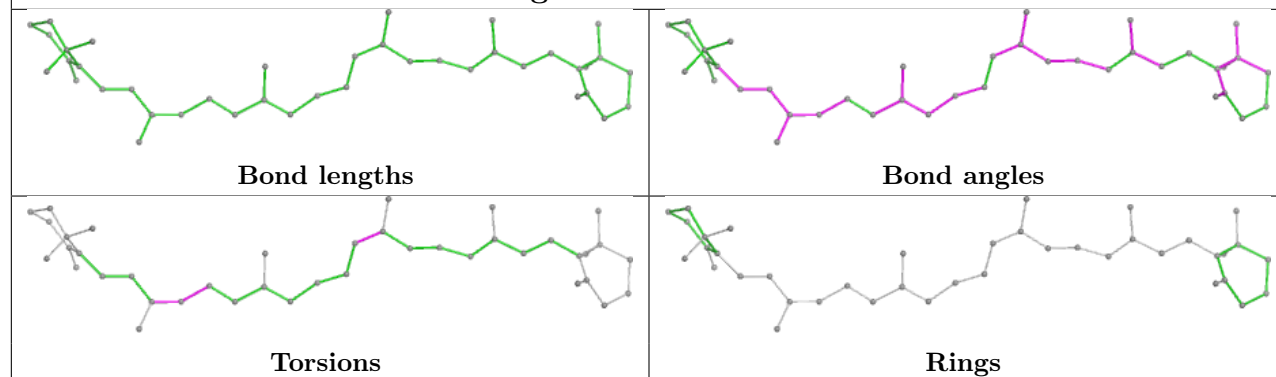
Ligand CLA 2 510



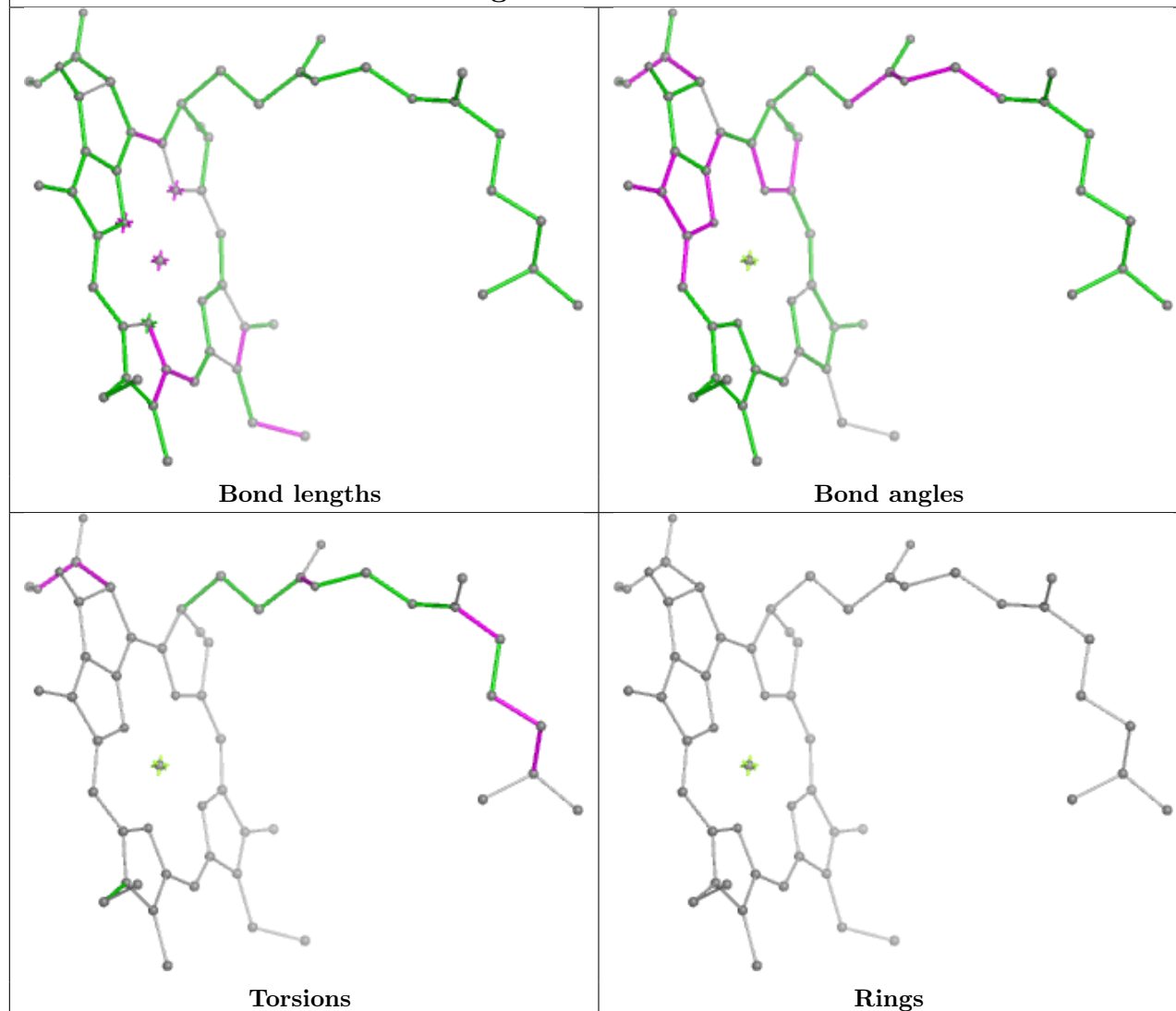
Ligand CLA 4 307



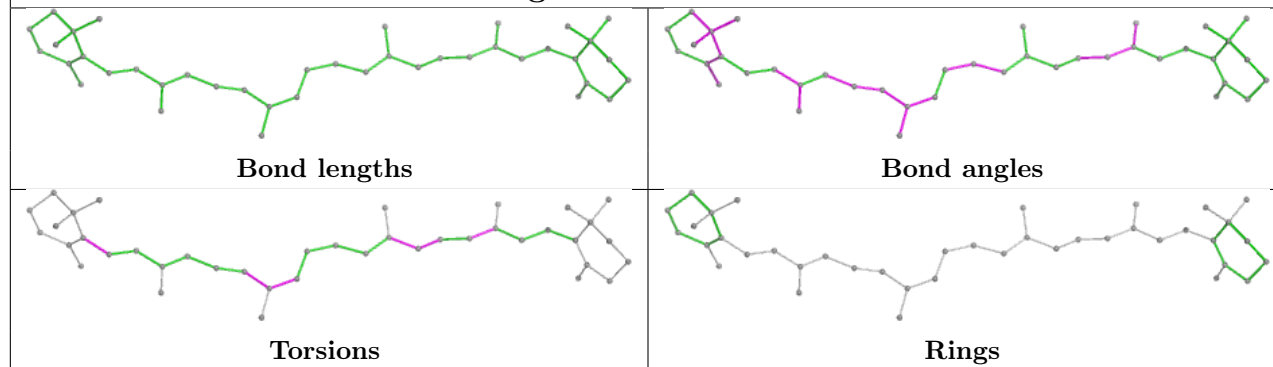
Ligand BCR B 802



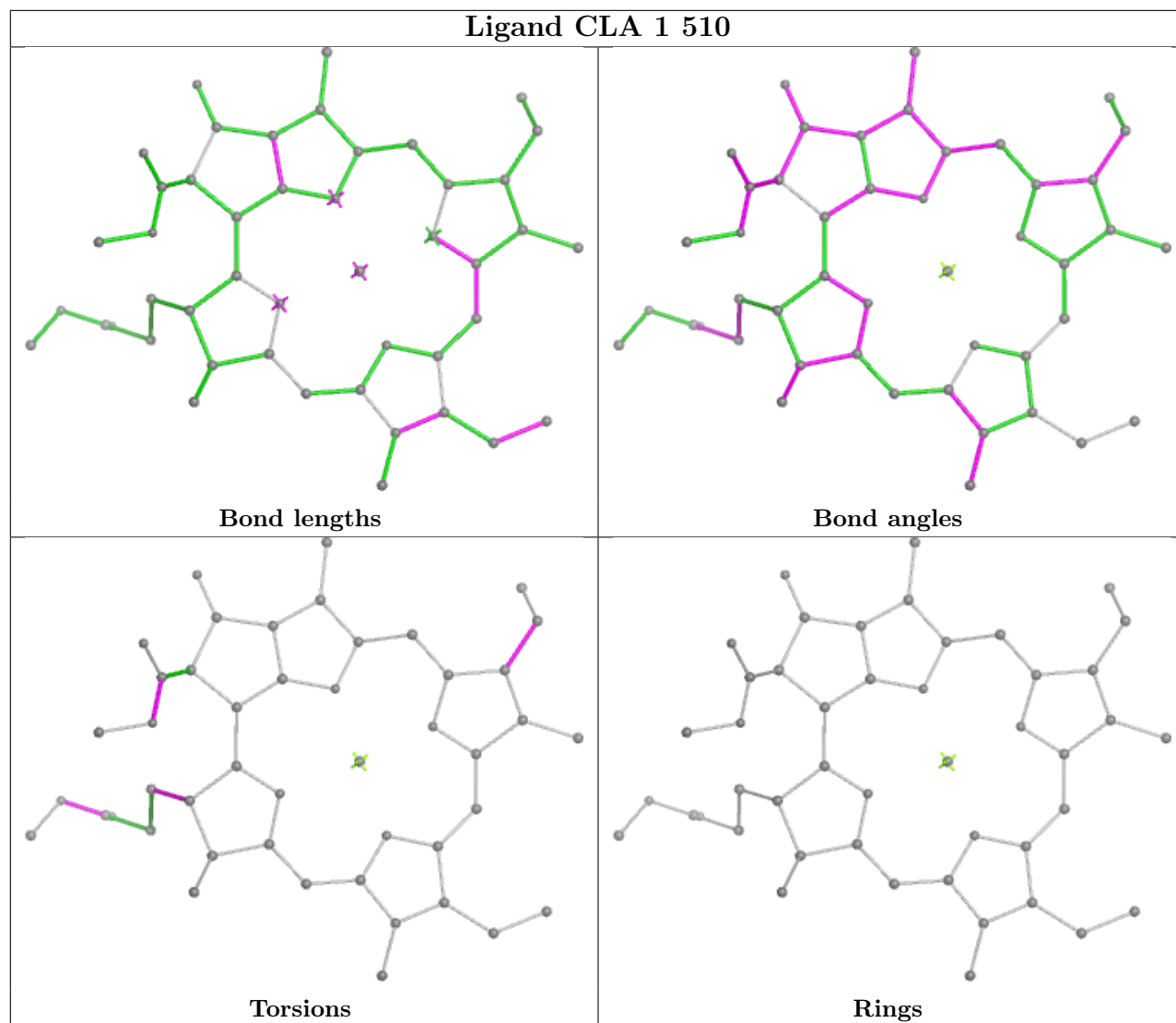
Ligand CLA B 816

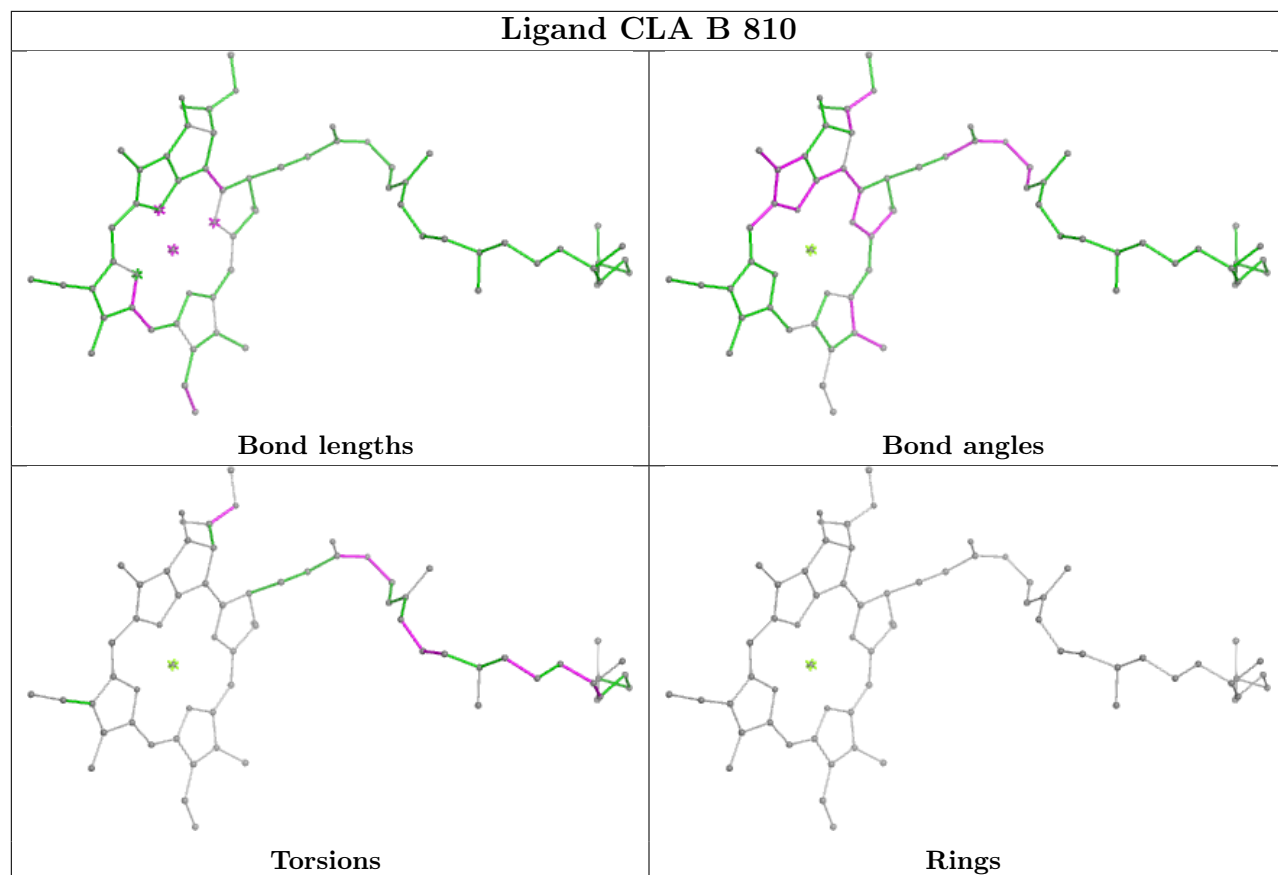


Ligand BCR G 205

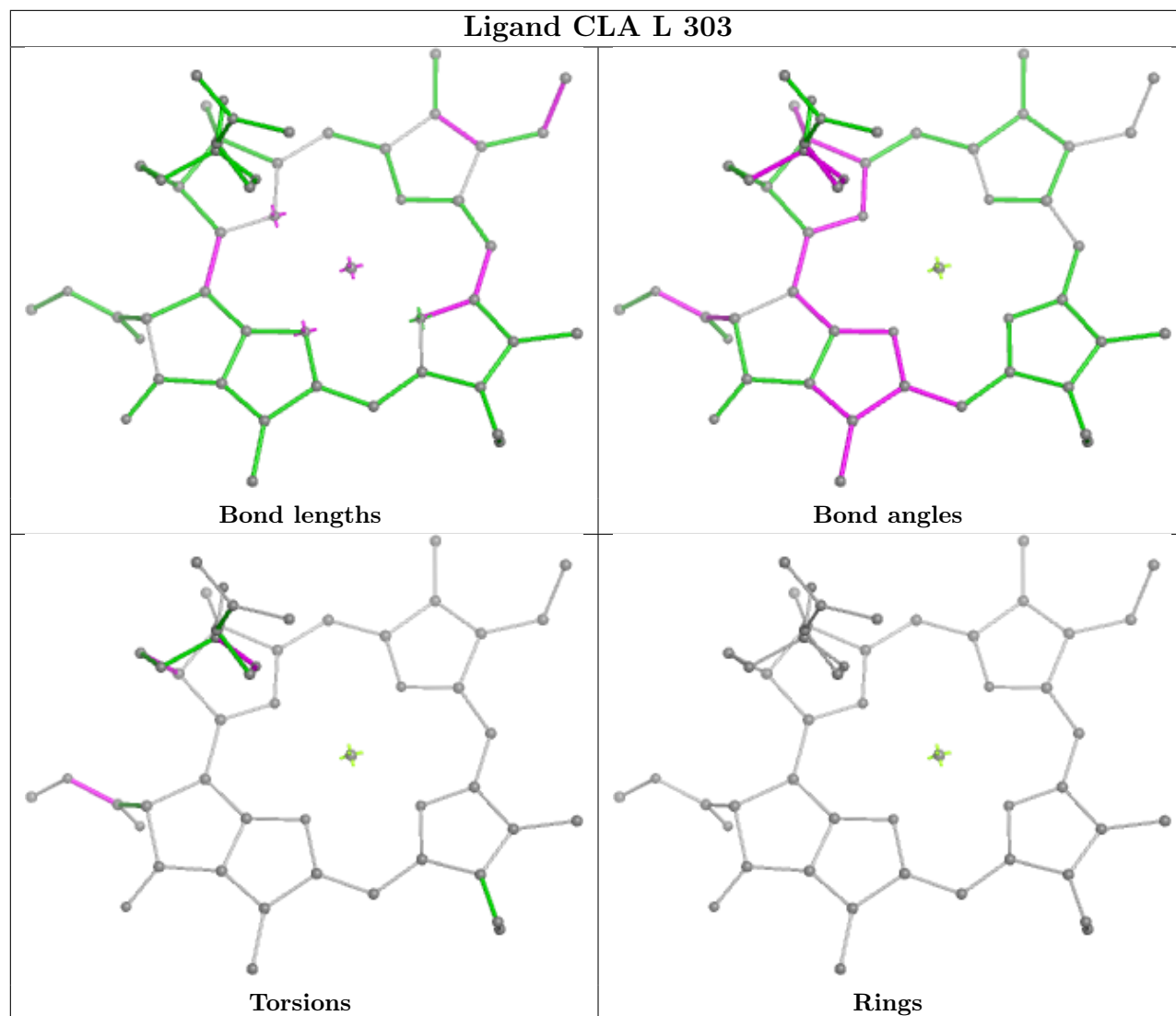


Ligand CLA 1 510

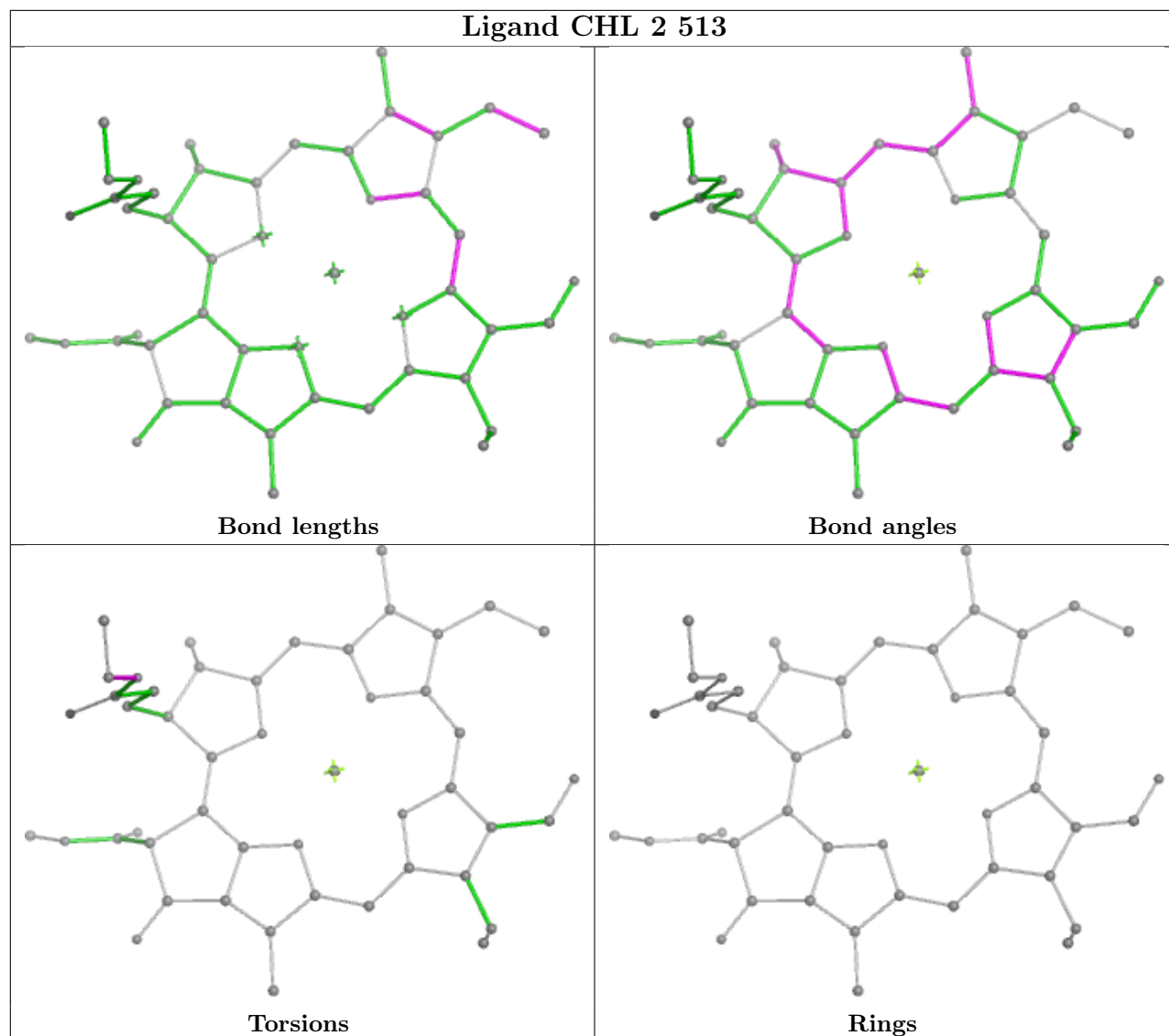




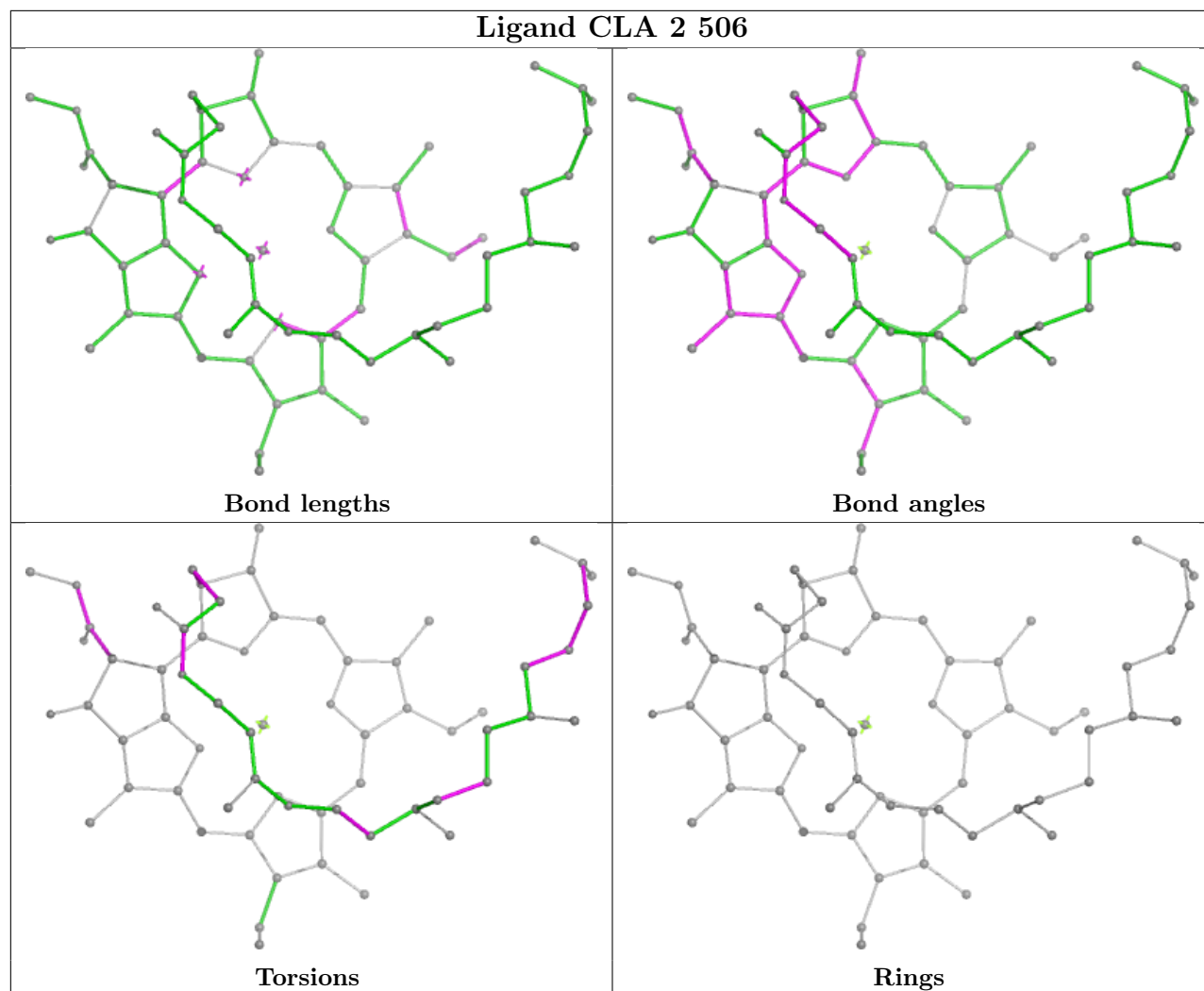
Ligand CLA L 303



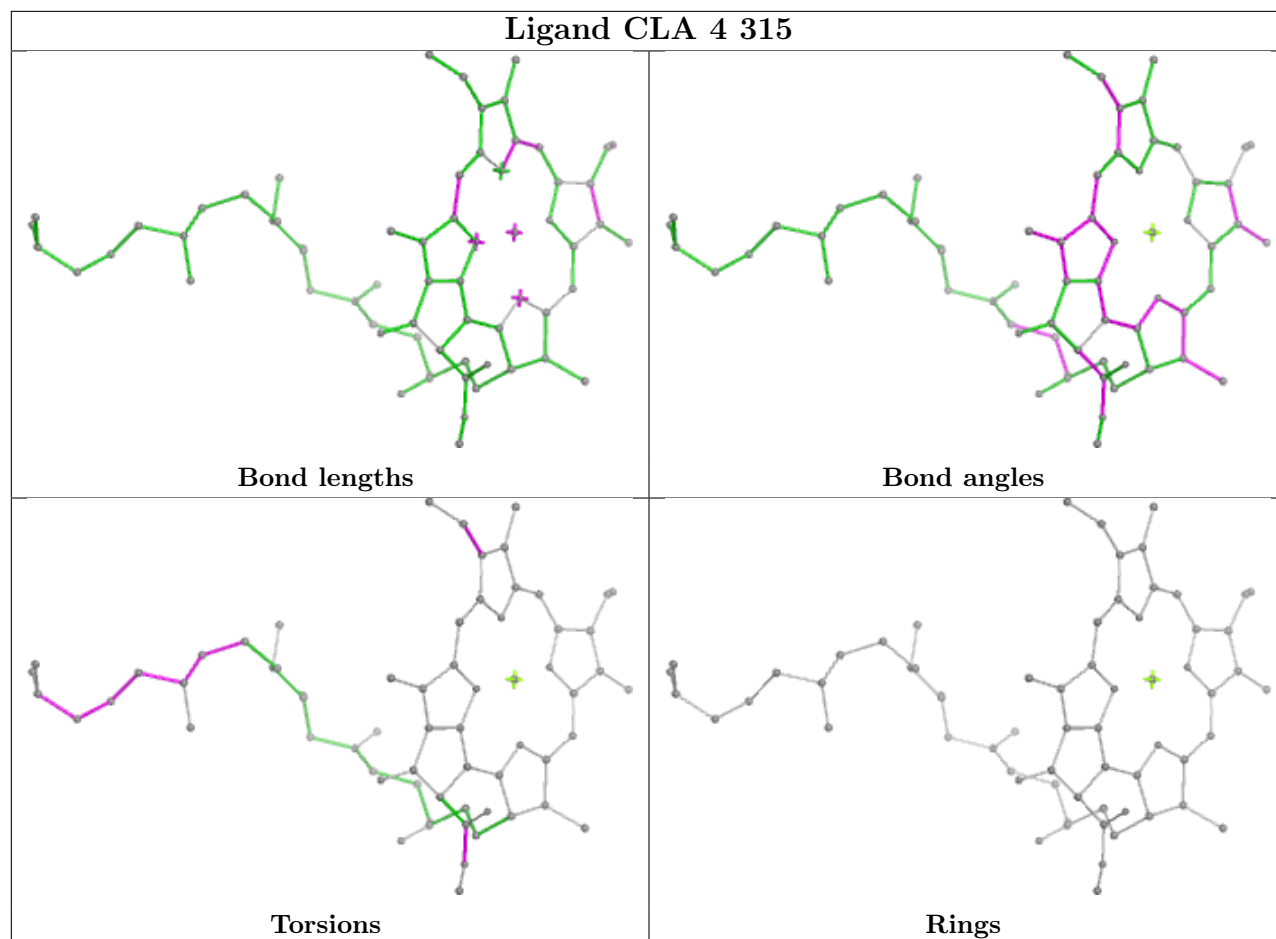
Ligand CHL 2 513



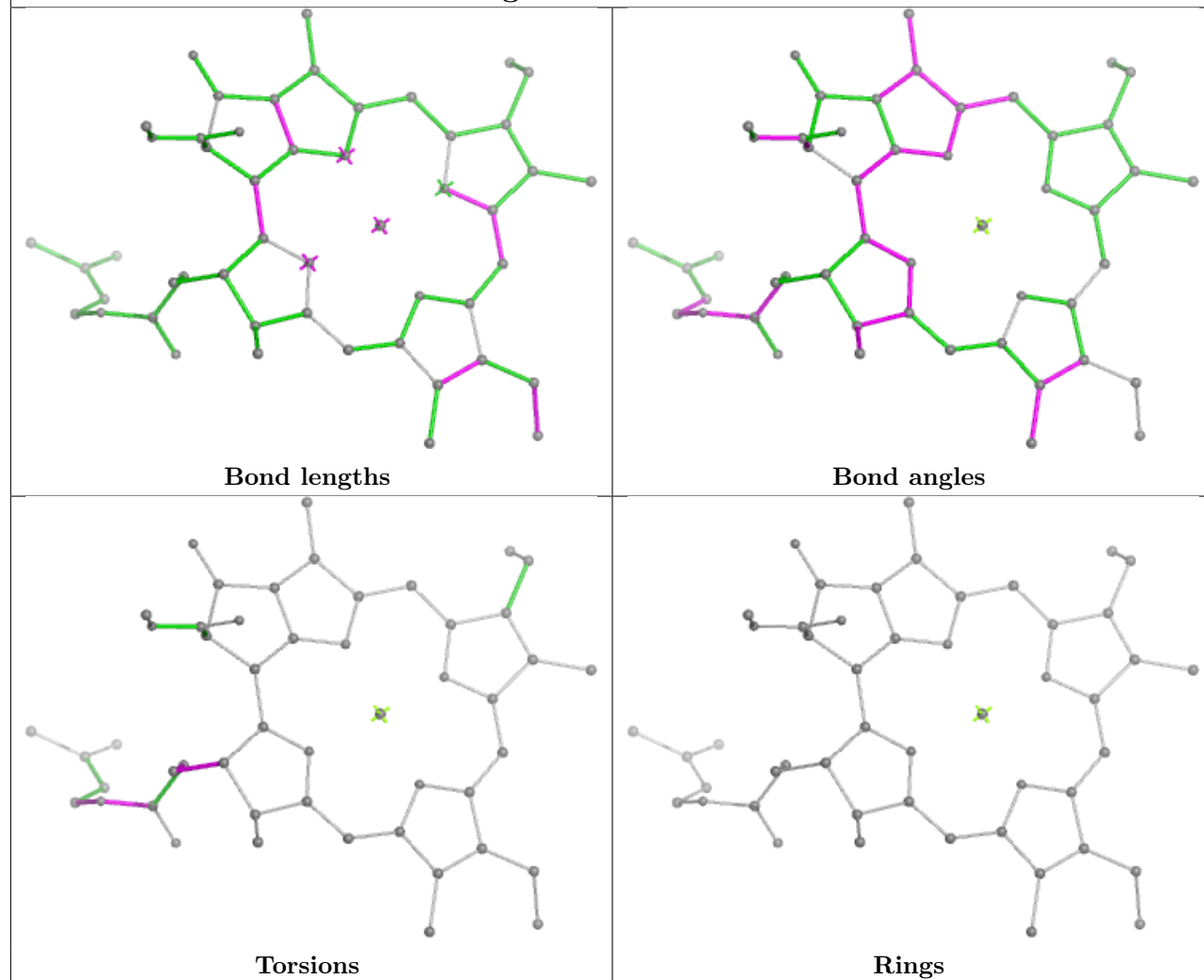
Ligand CLA 2 506



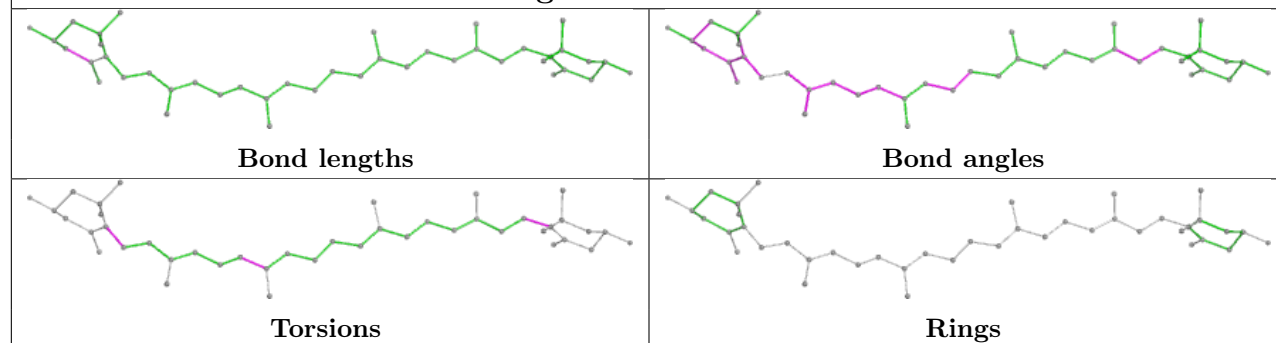
Ligand CLA 4 315

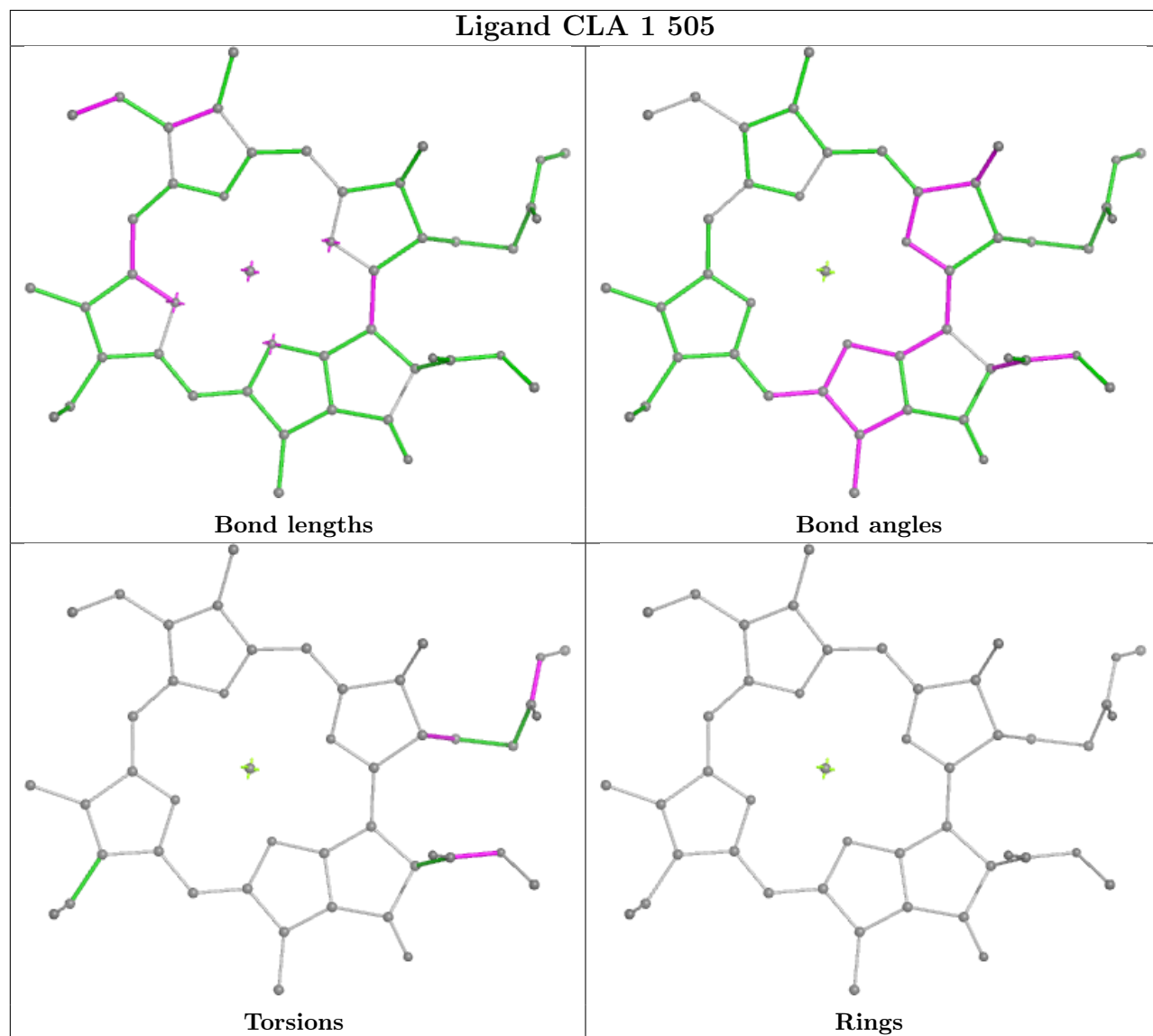
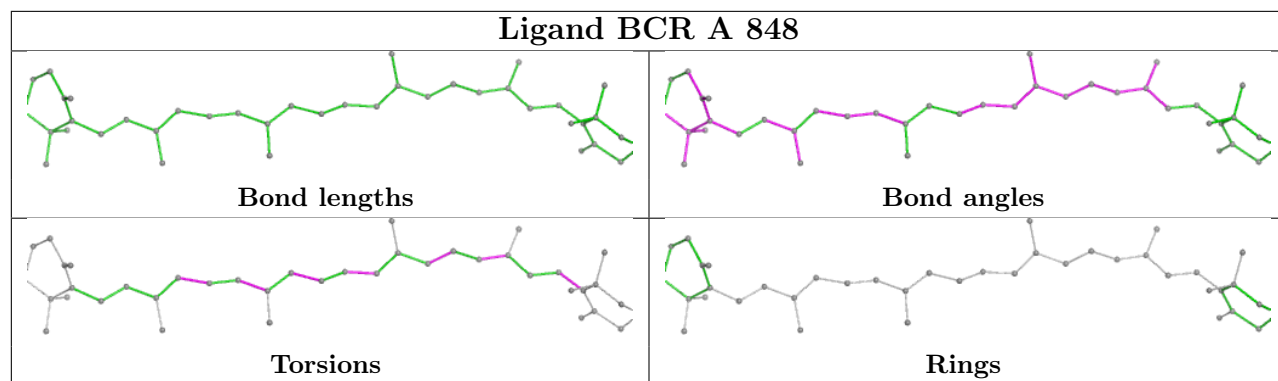


Ligand CLA B 837

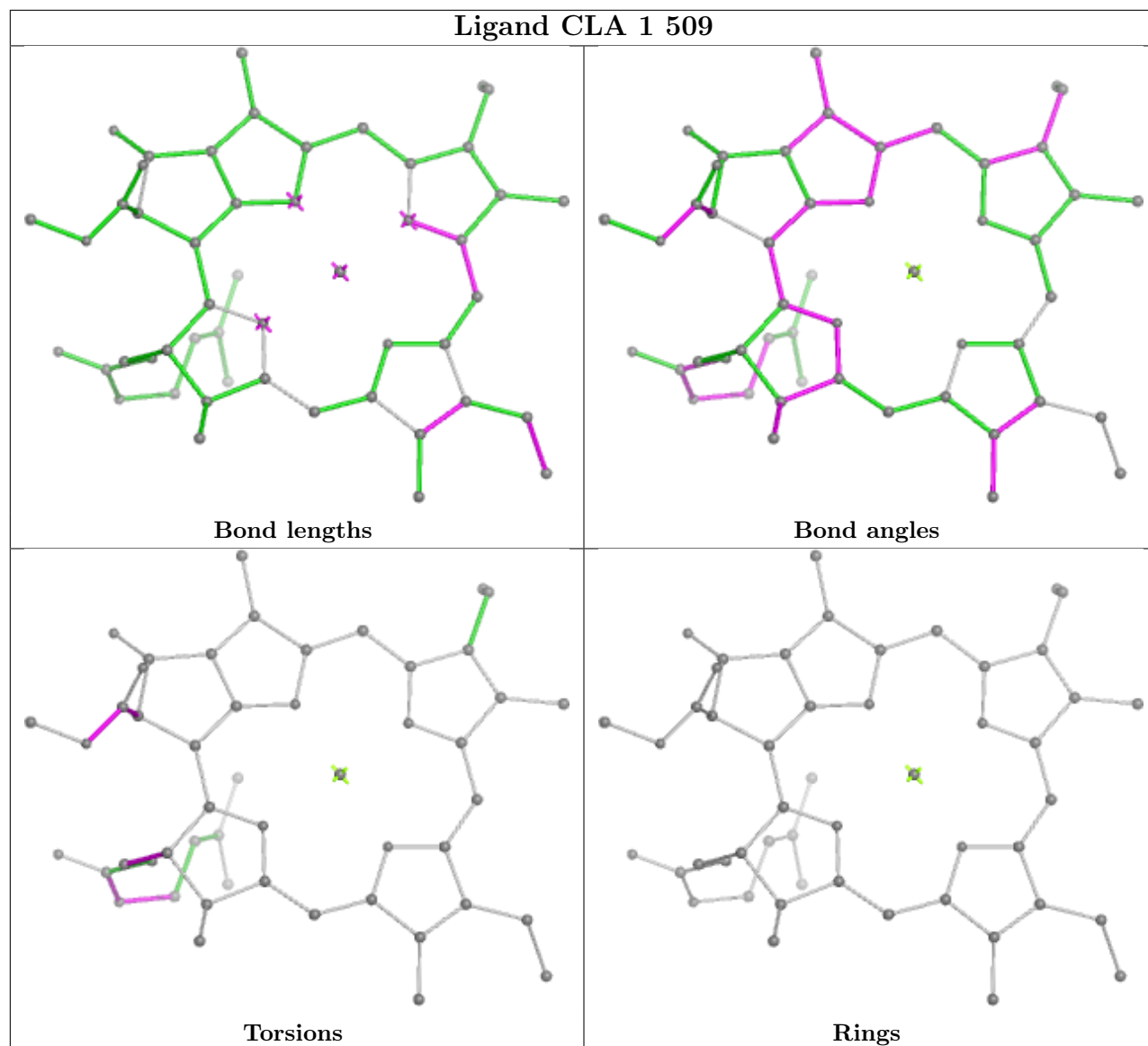


Ligand LUT 2 501

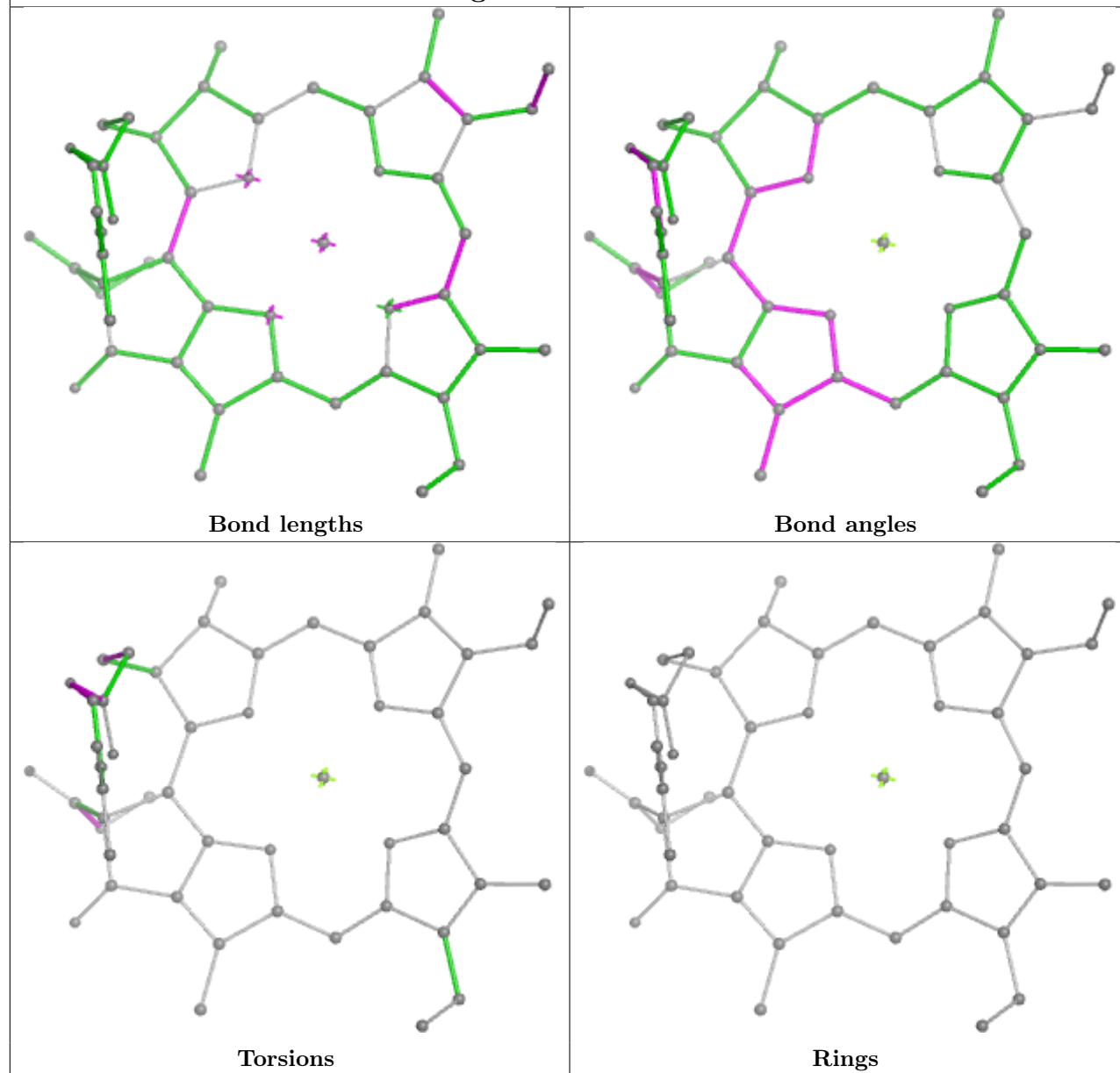




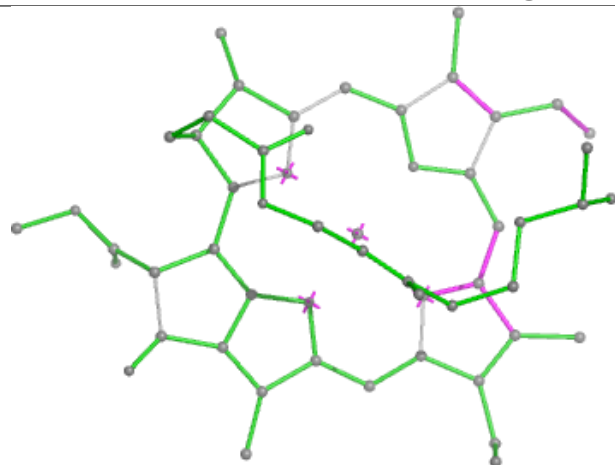
Ligand CLA 1 509



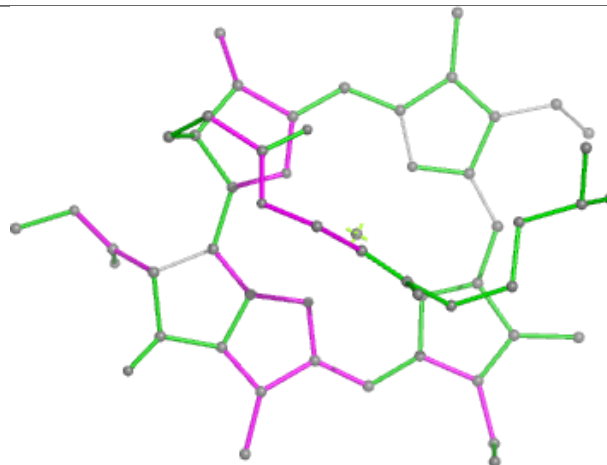
Ligand CLA 3 310



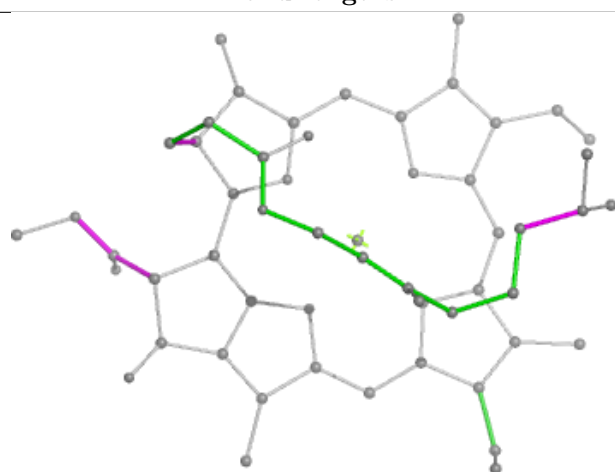
Ligand CLA 1 506



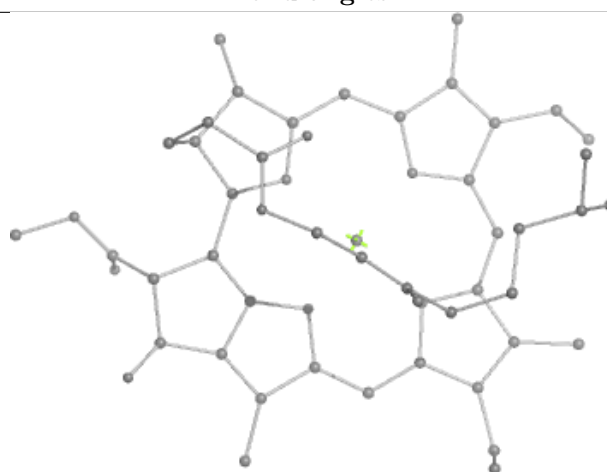
Bond lengths



Bond angles

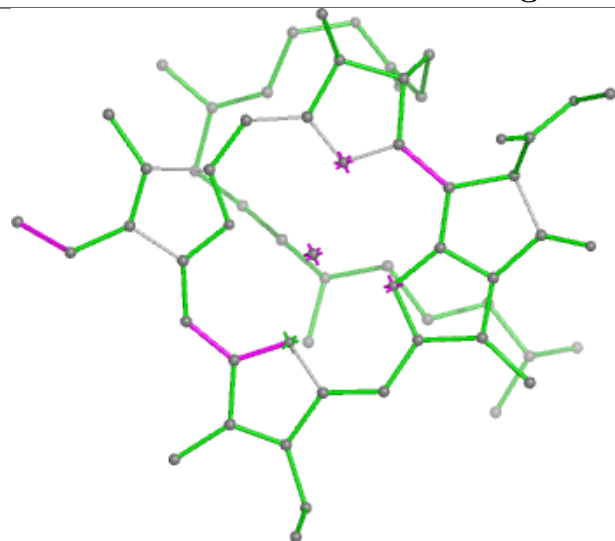


Torsions

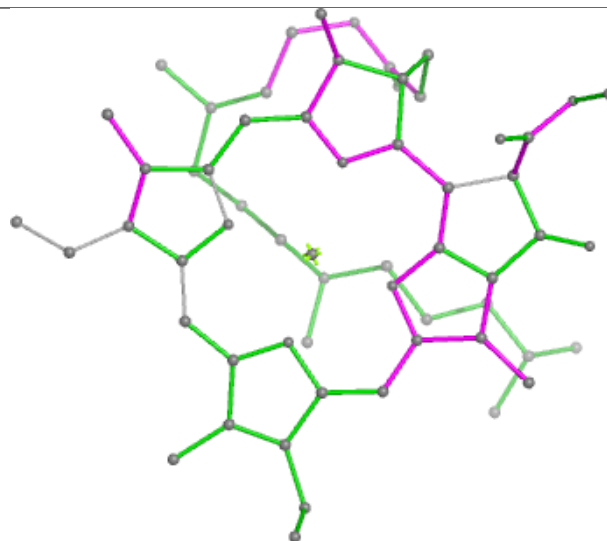


Rings

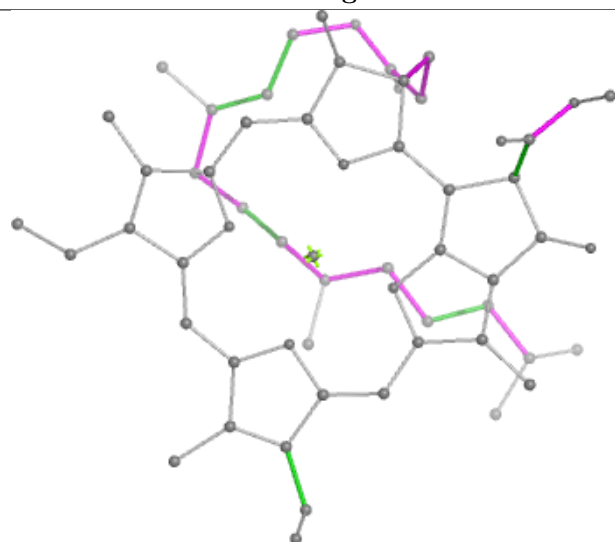
Ligand CLA 3 313



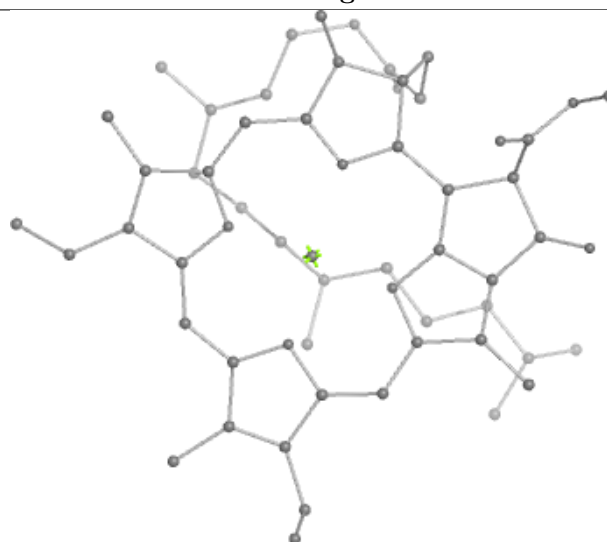
Bond lengths



Bond angles

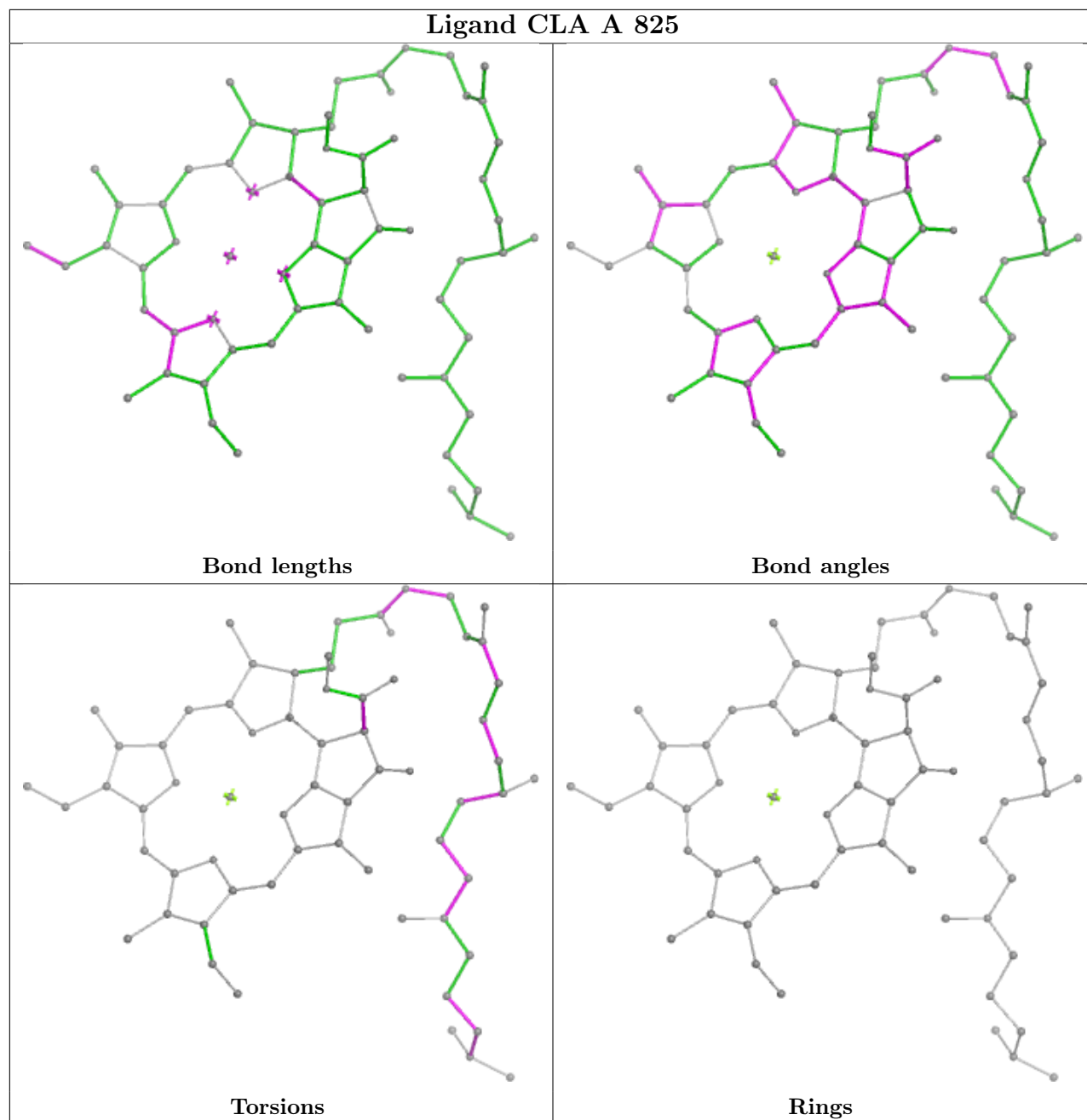


Torsions

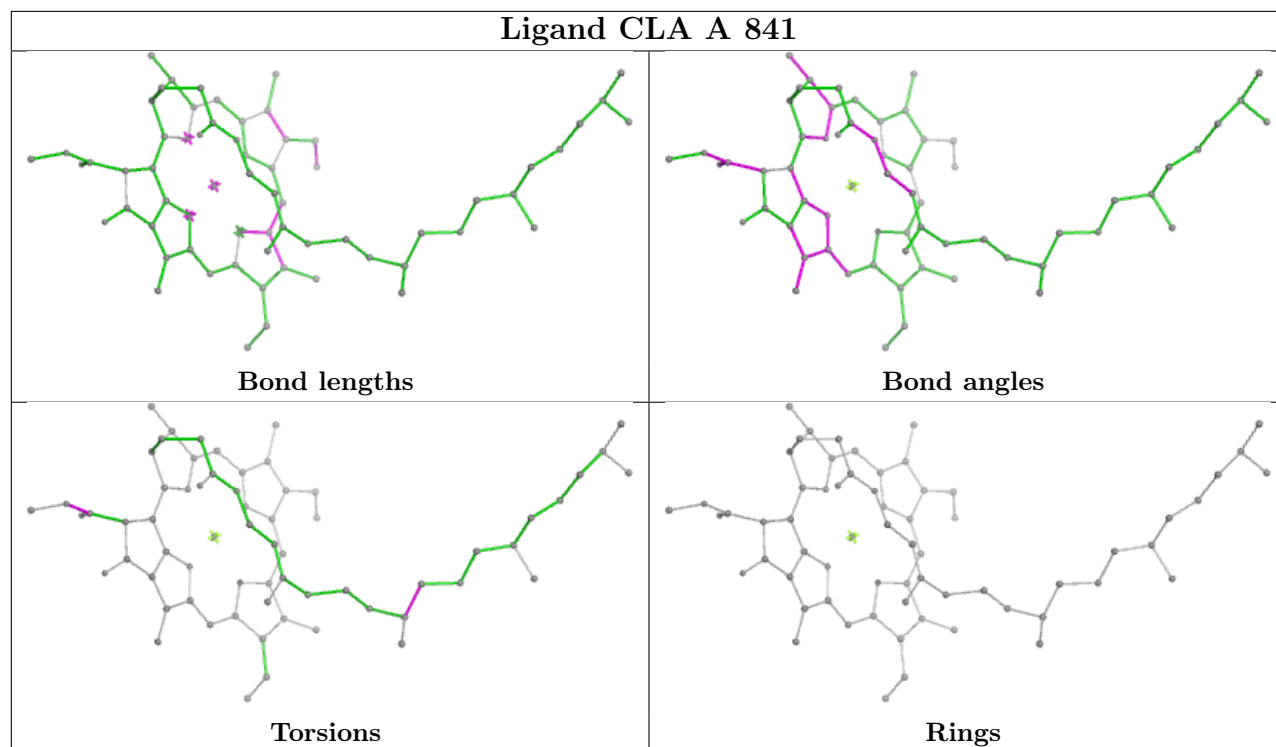


Rings

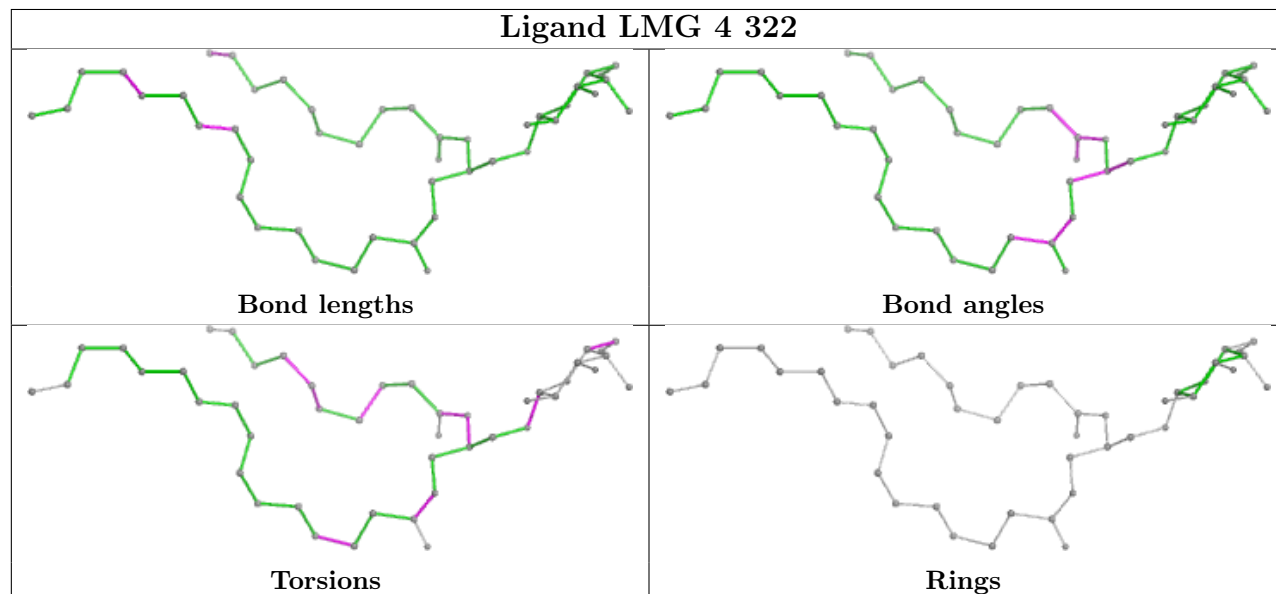
Ligand CLA A 825

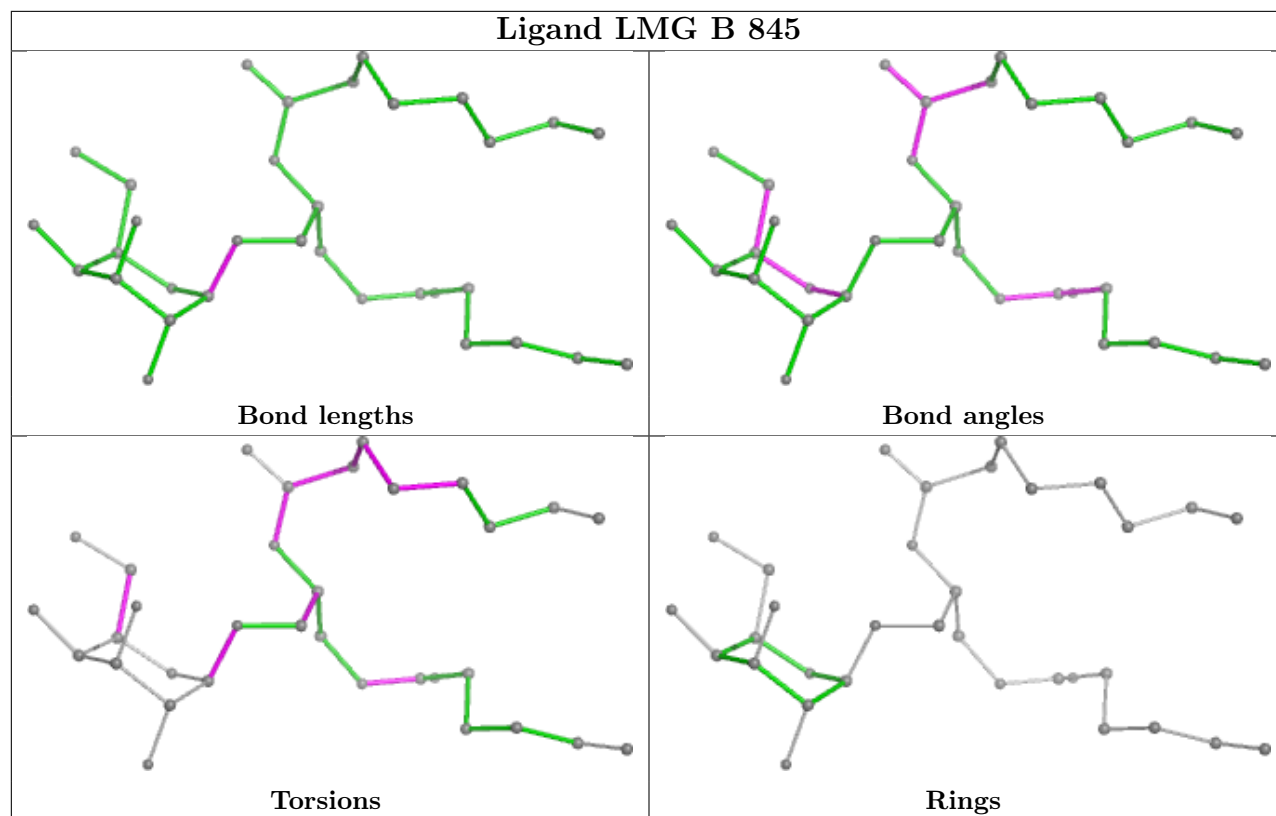


Ligand CLA A 841

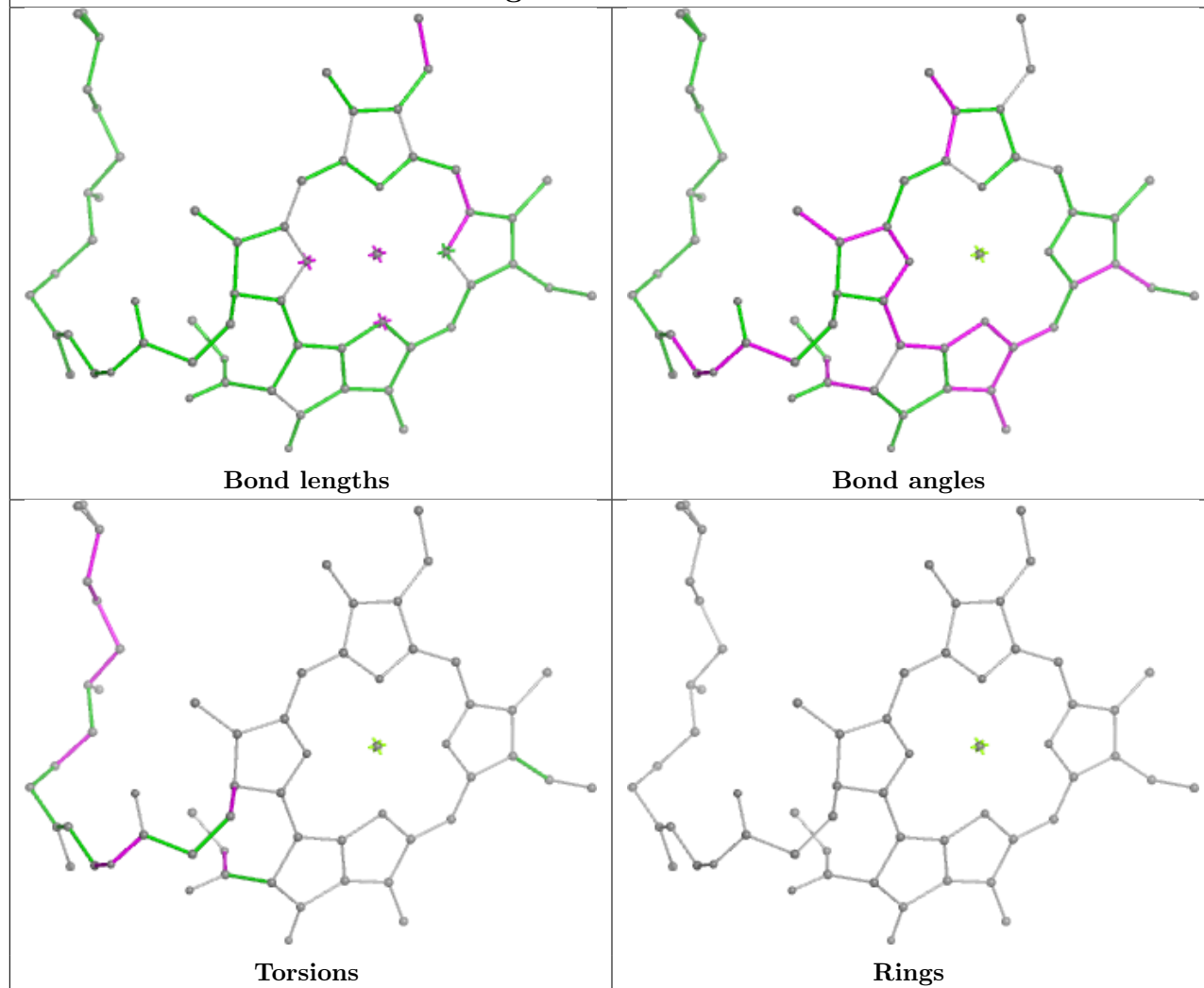


Ligand LMG 4 322

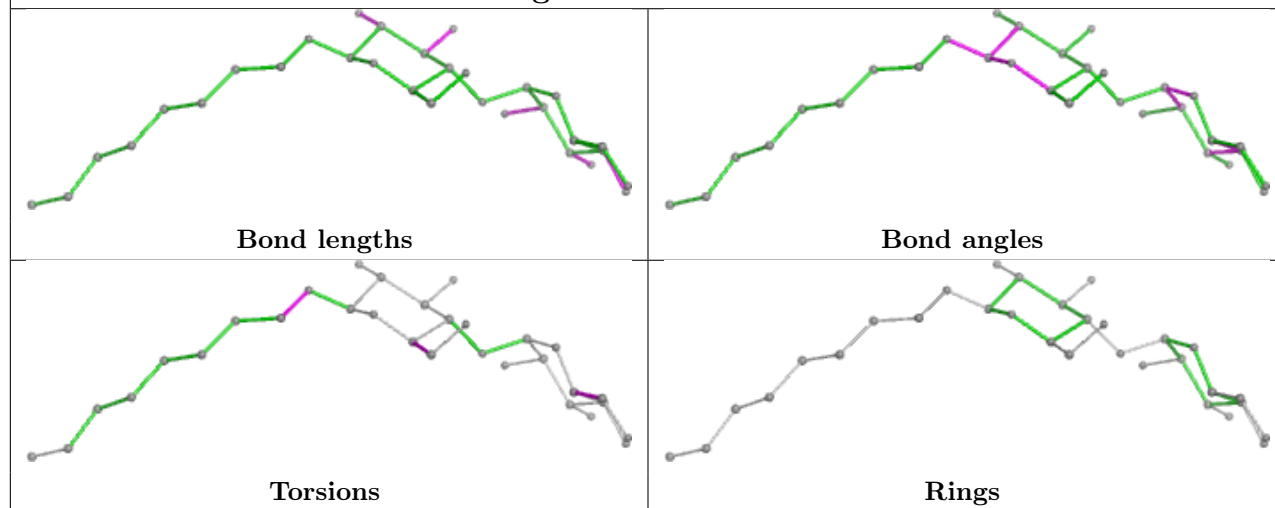




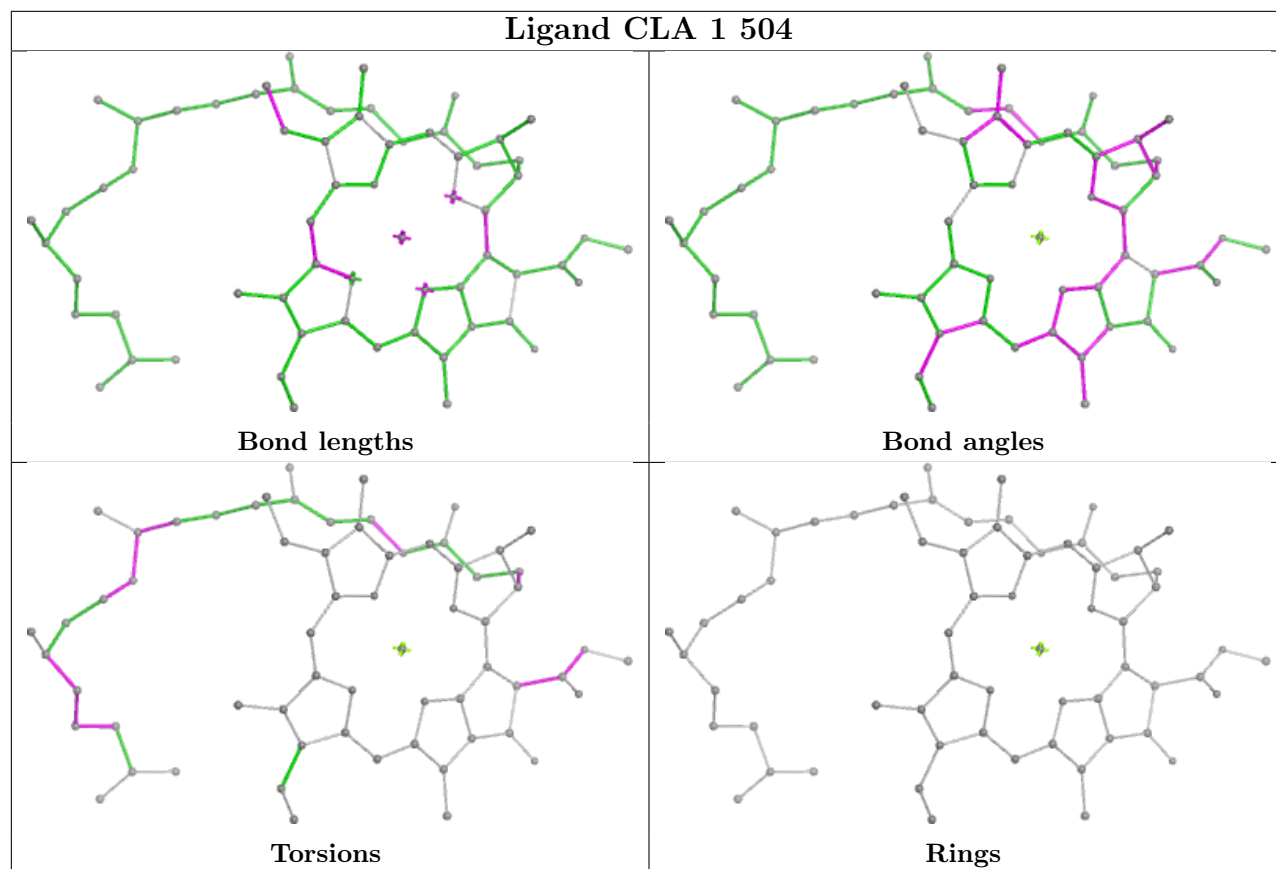
Ligand CLA 4 308



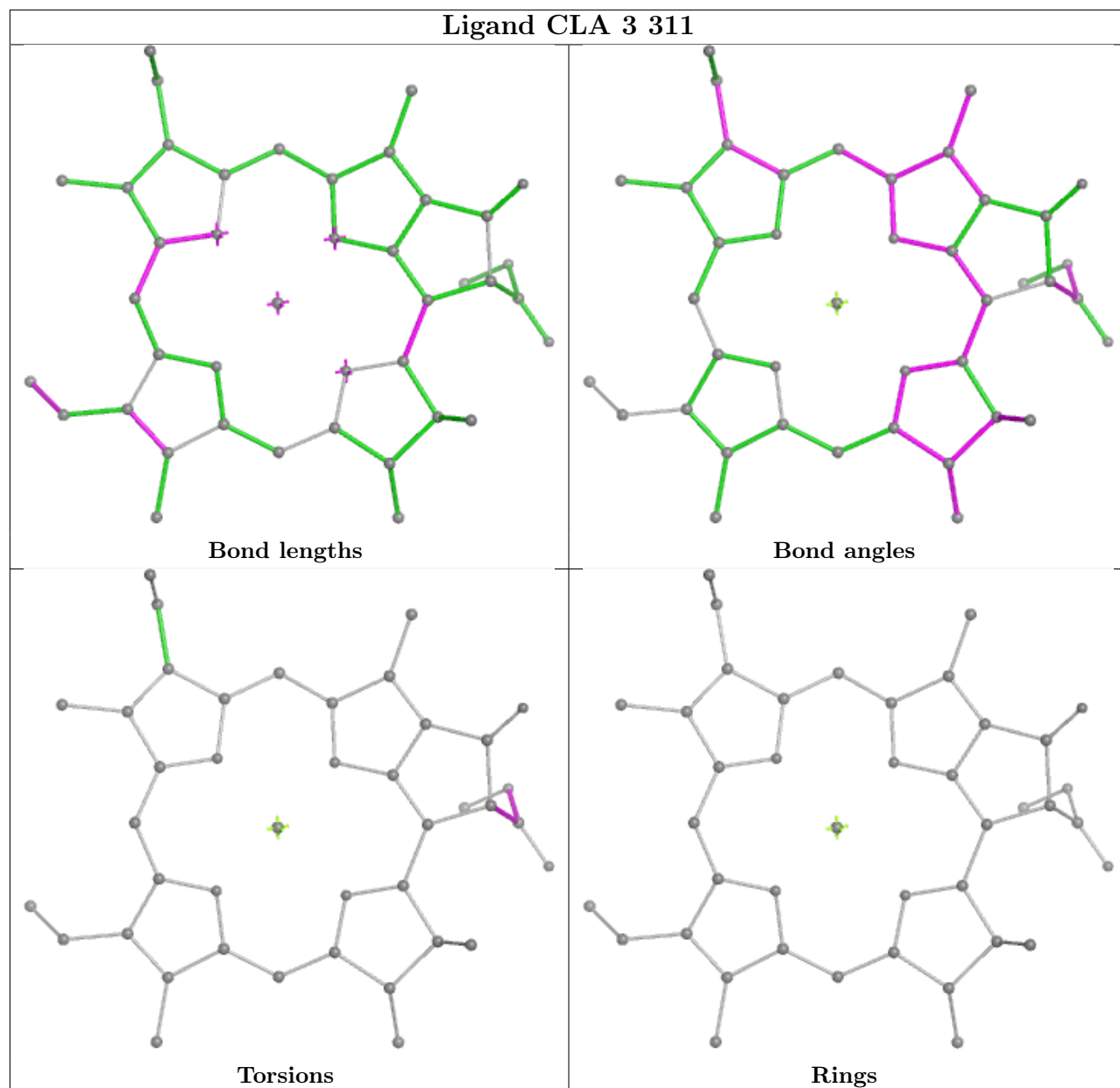
Ligand LMT 3 318

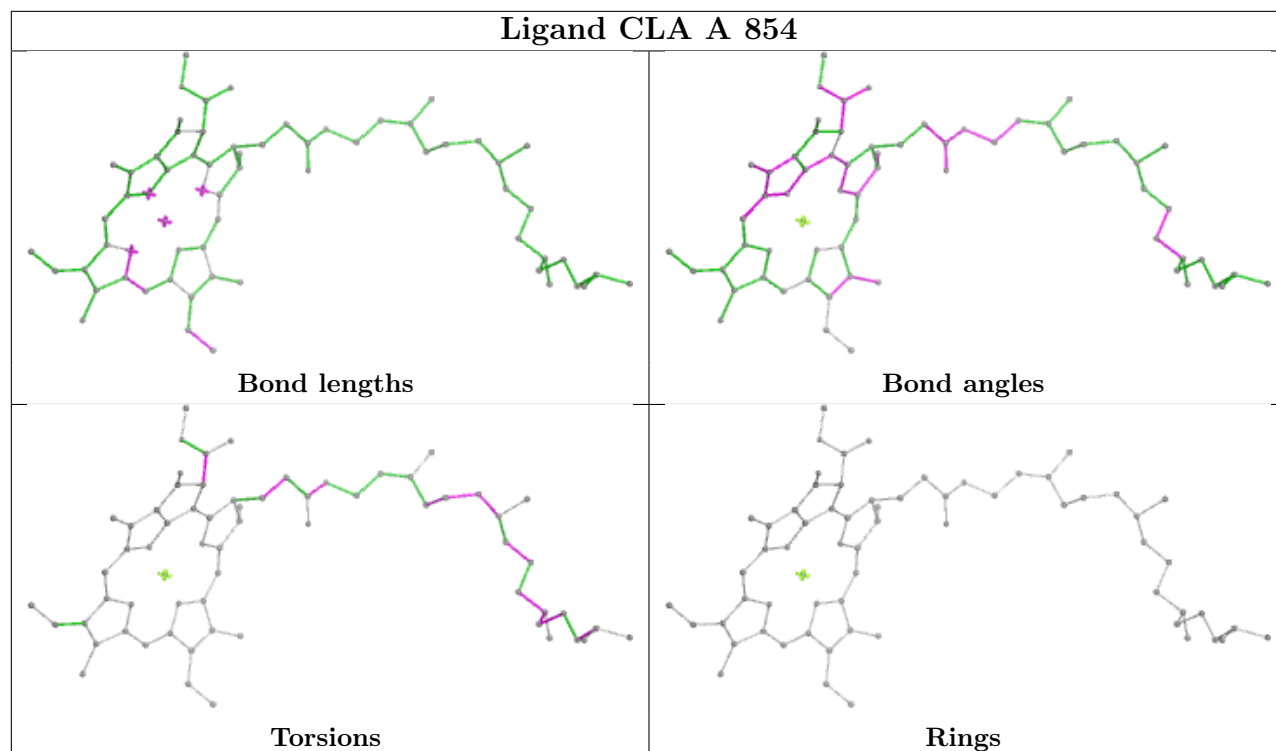
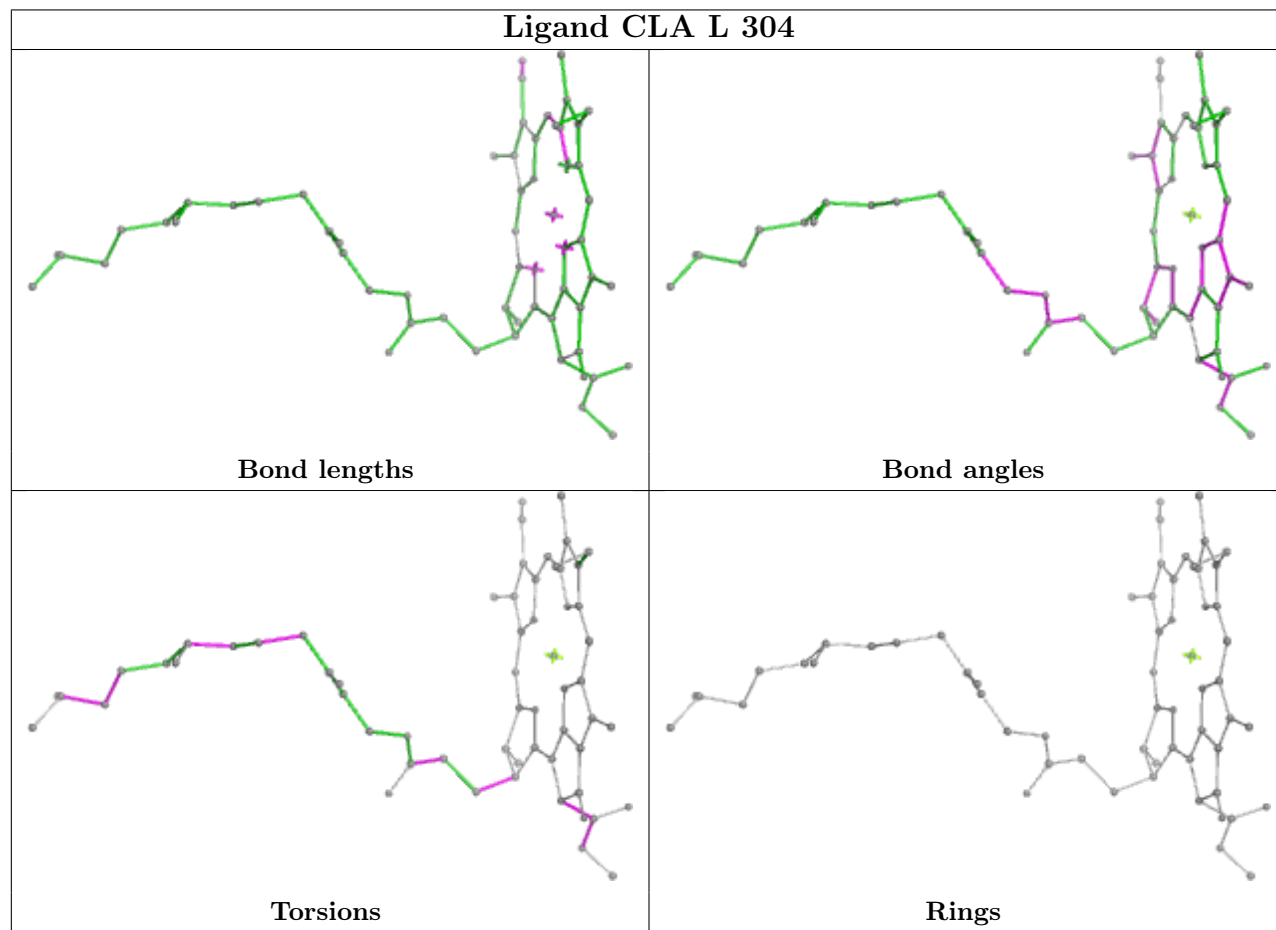


Ligand CLA 1 504

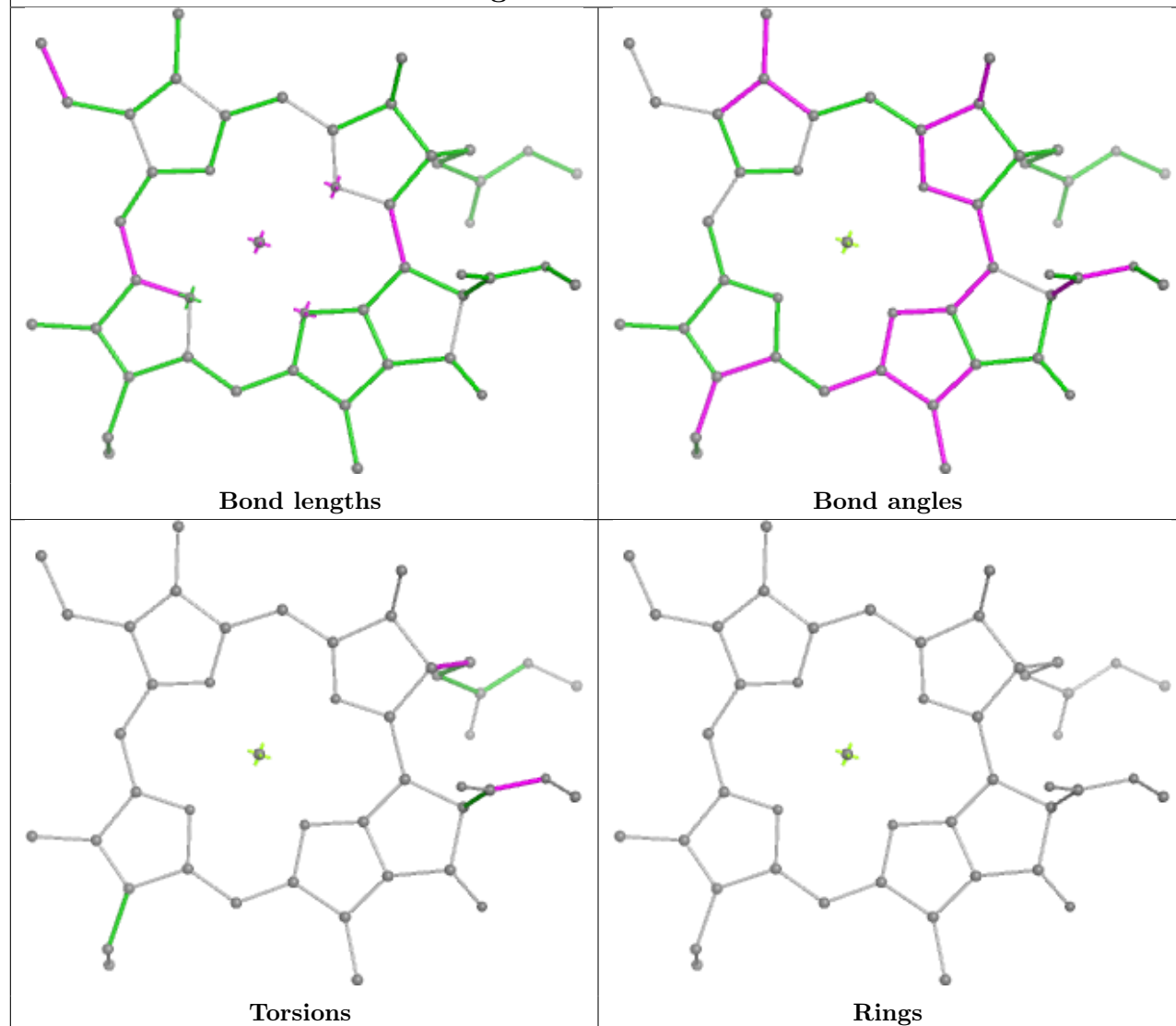


Ligand CLA 3 311

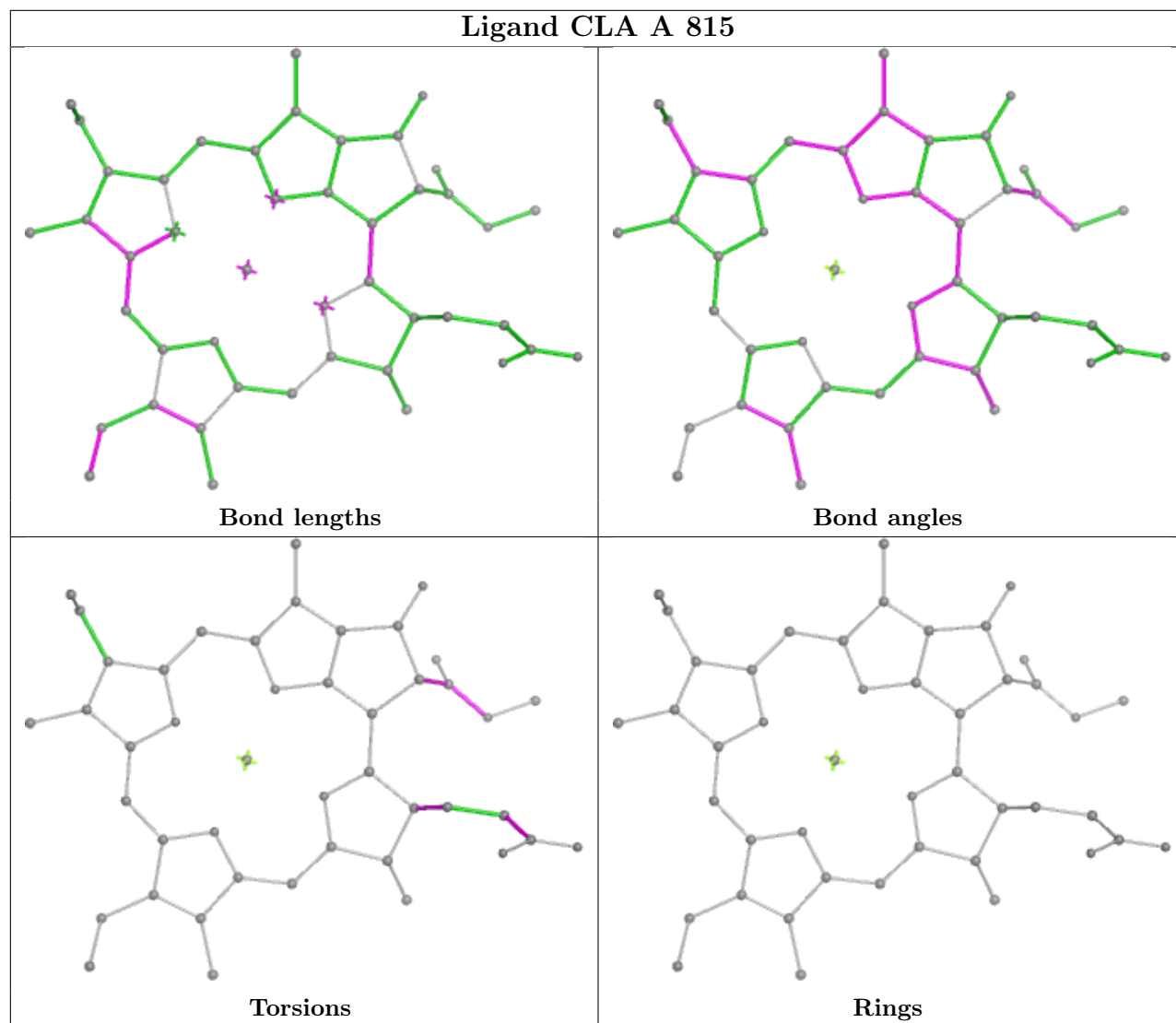


Ligand CLA A 854**Ligand CLA L 304**

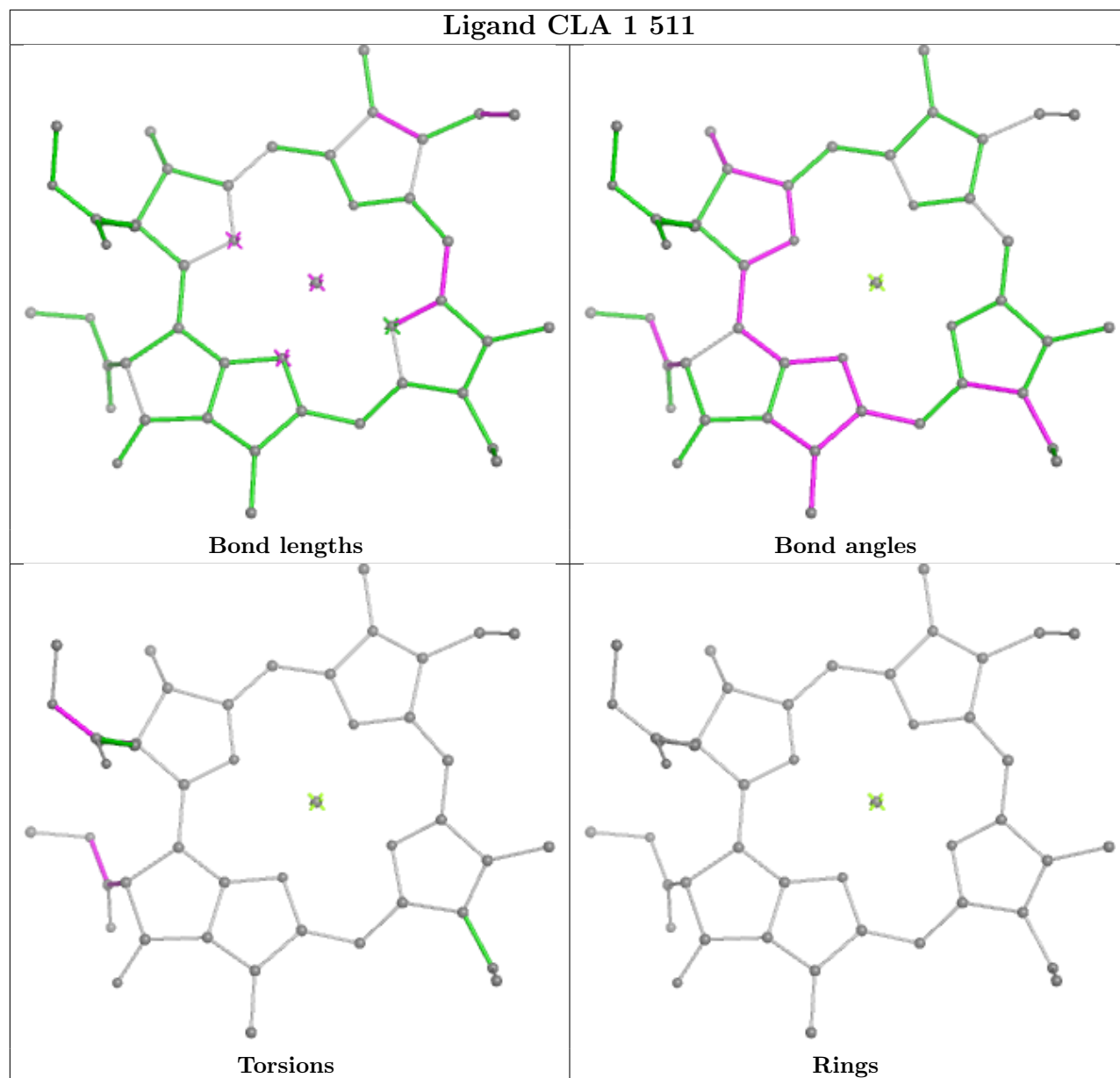
Ligand CLA B 813

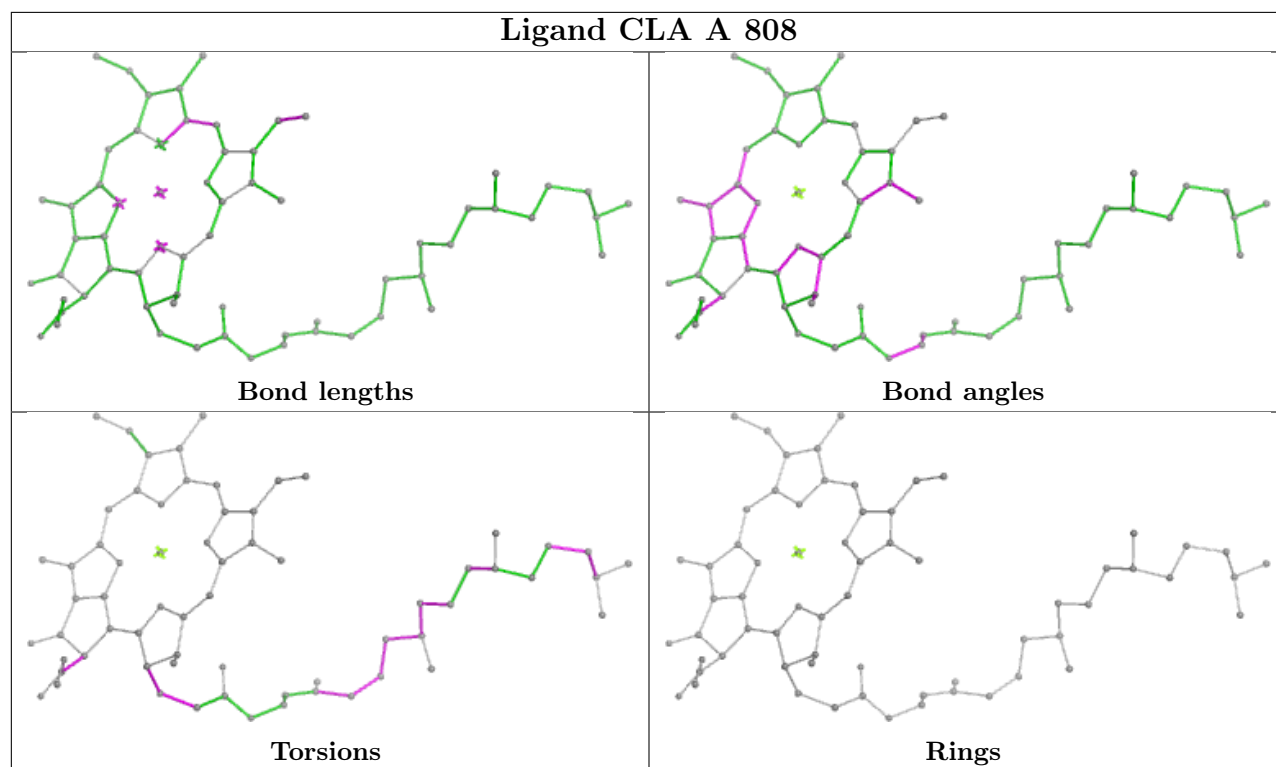
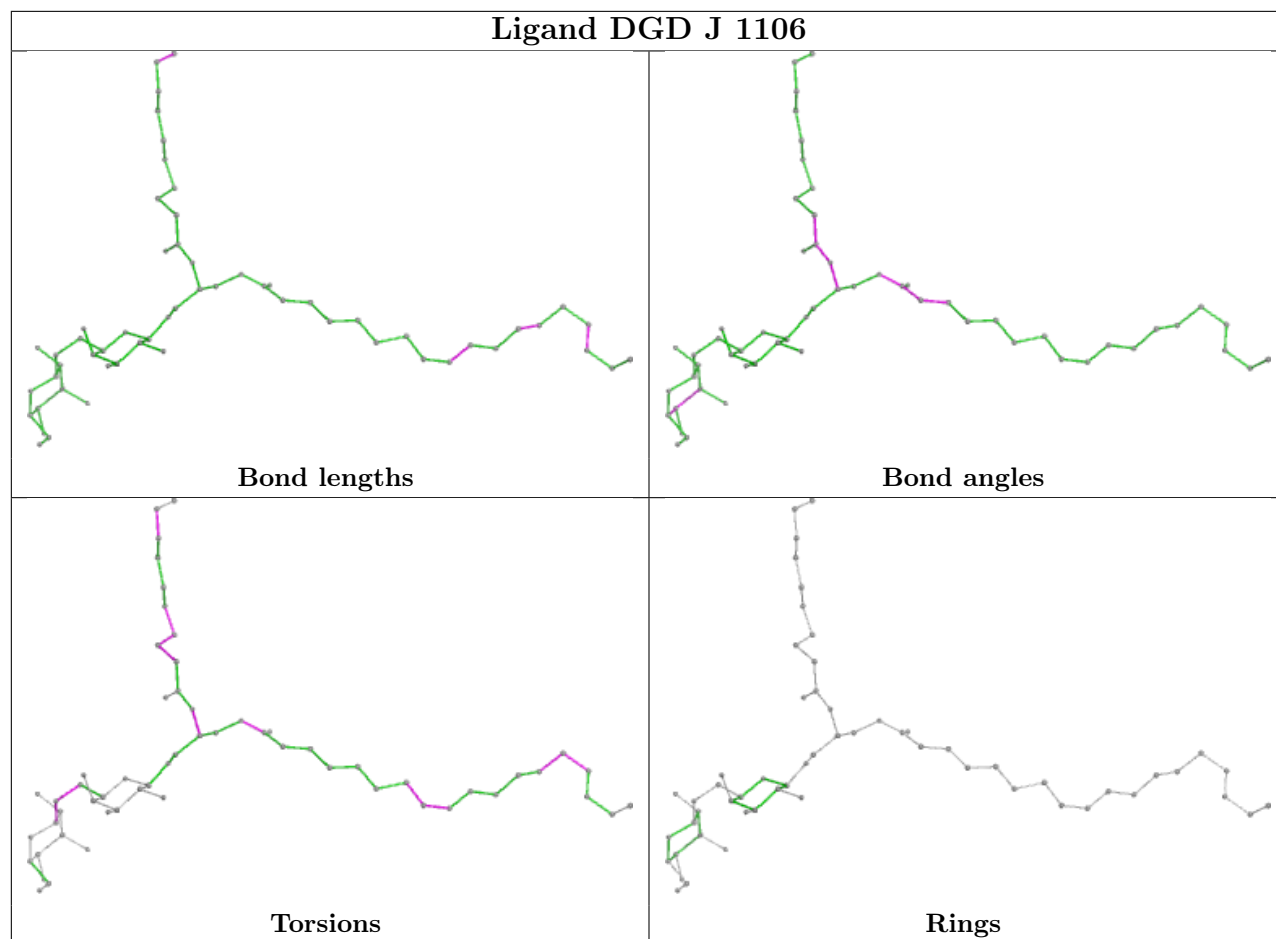


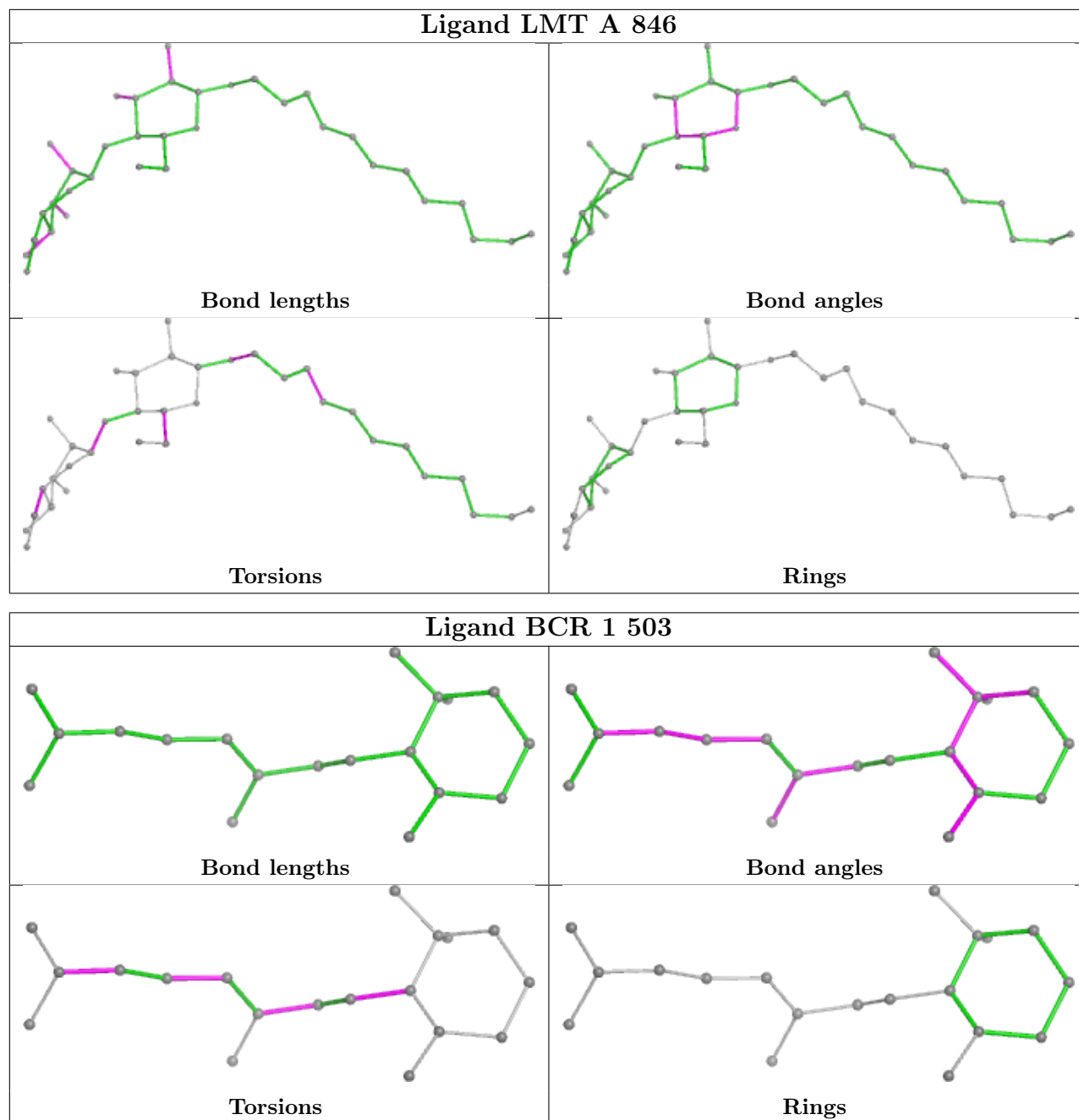
Ligand CLA A 815



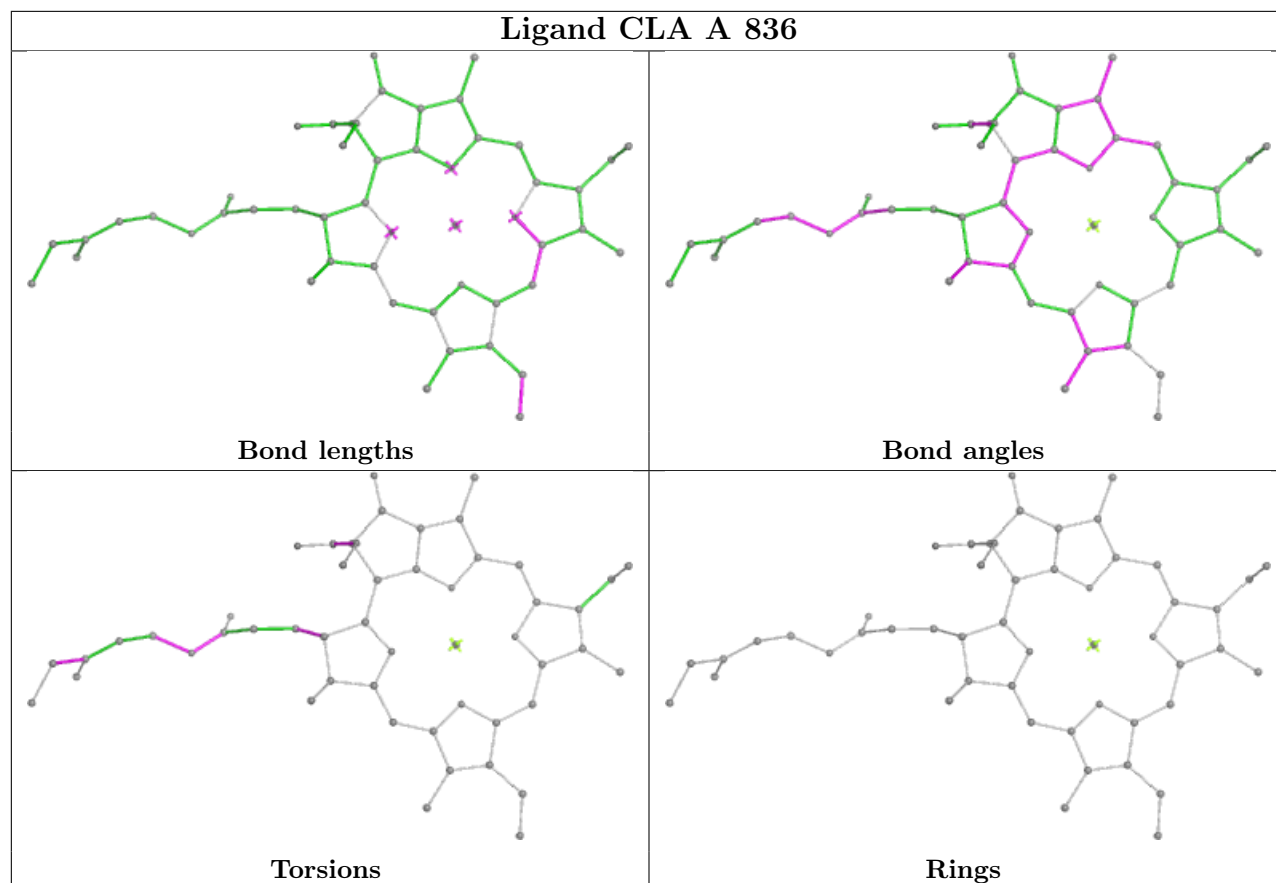
Ligand CLA 1 511



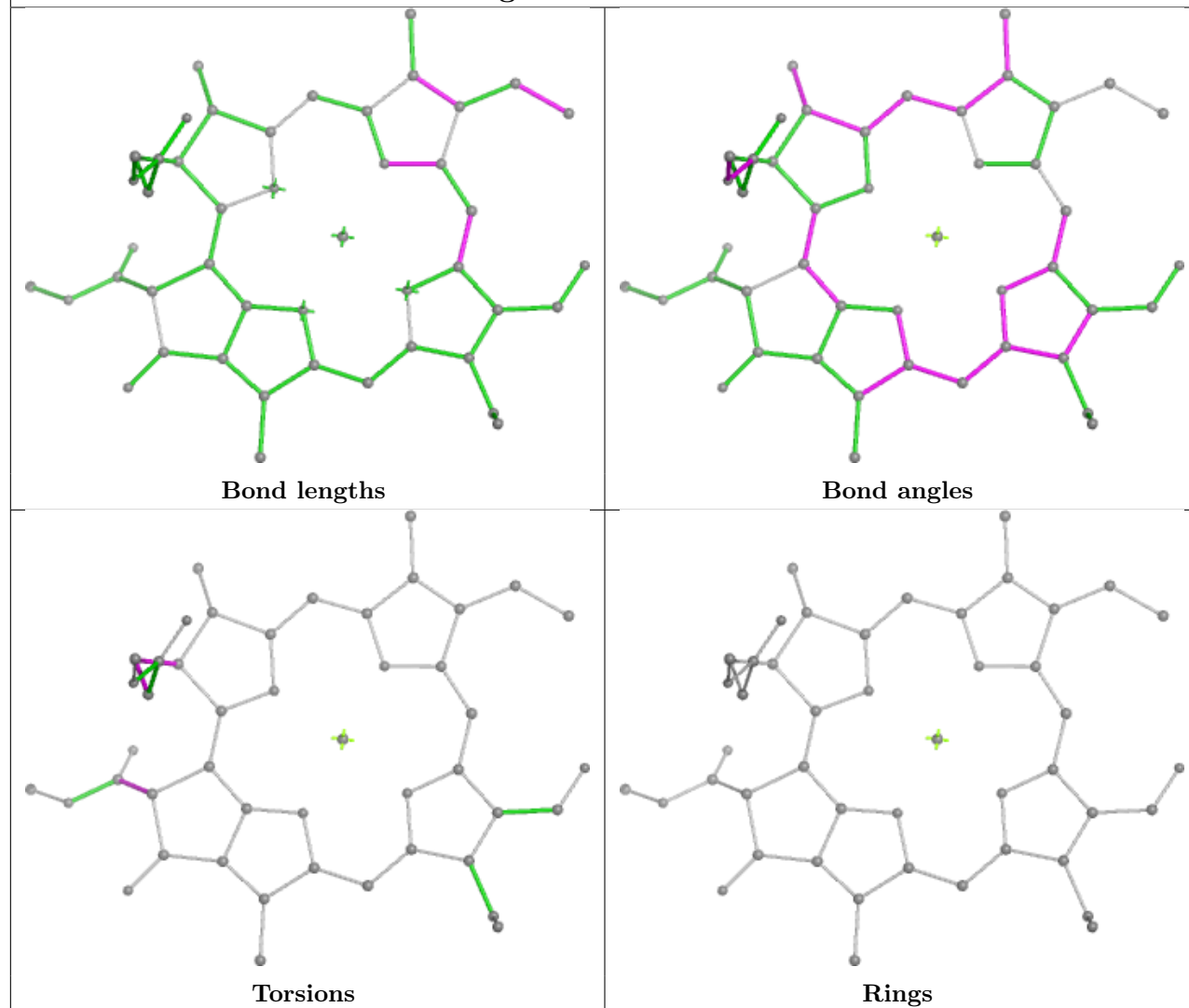




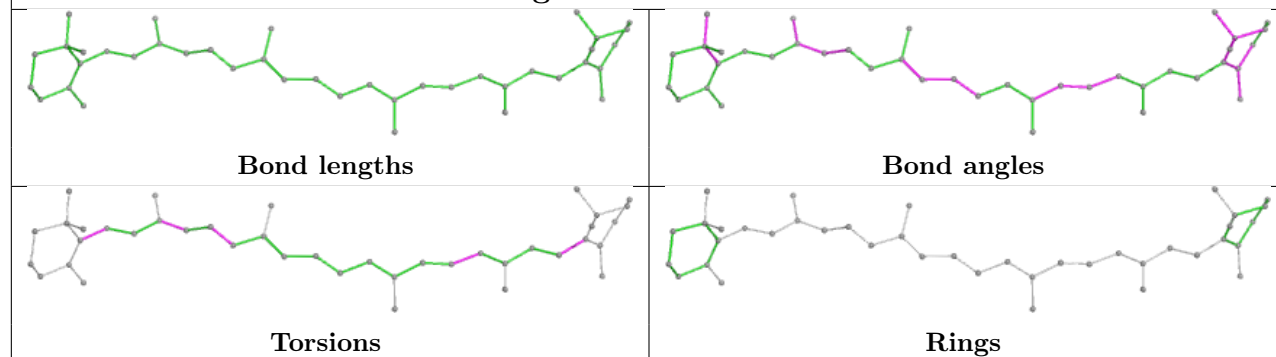
Ligand CLA A 836



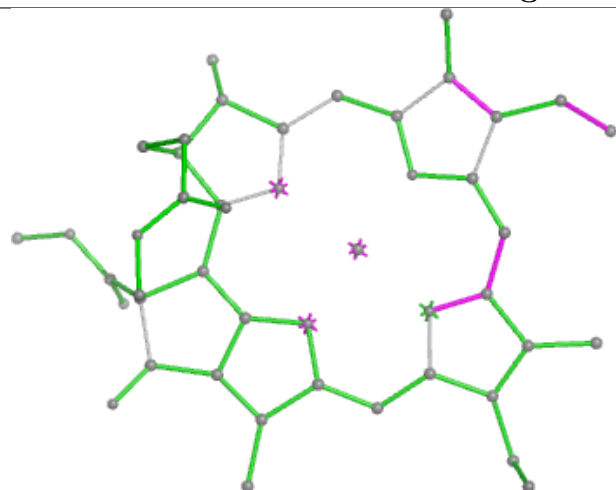
Ligand CHL 3 314



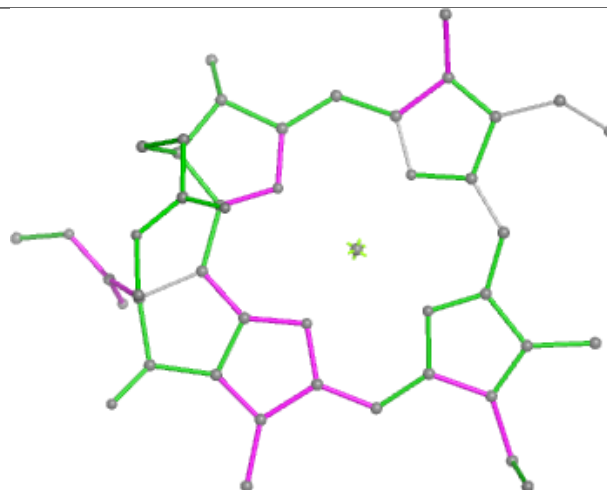
Ligand BCR L 306



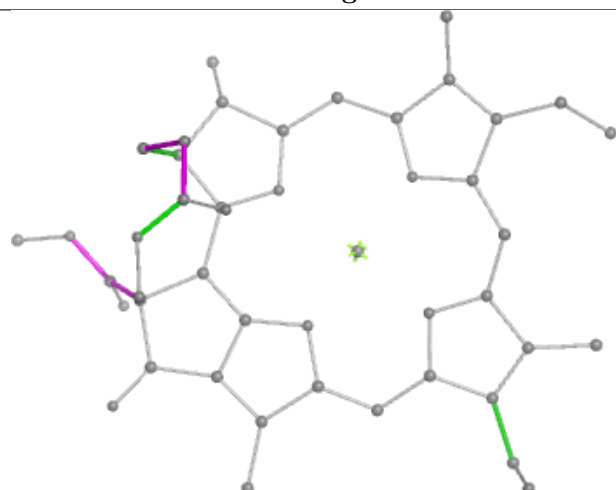
Ligand CLA 4 311



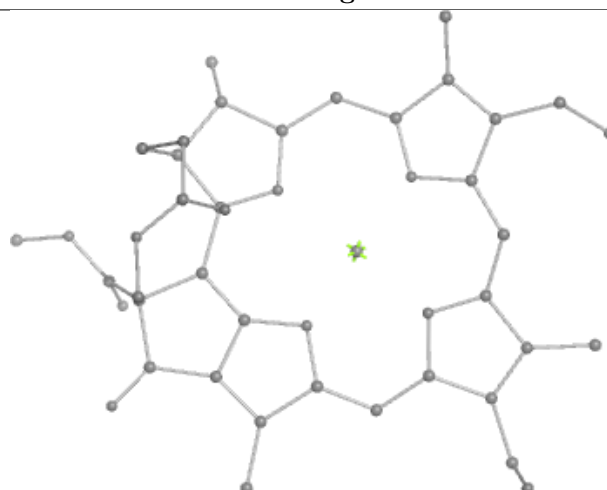
Bond lengths



Bond angles



Torsions

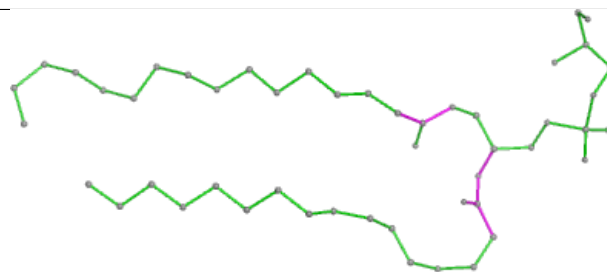


Rings

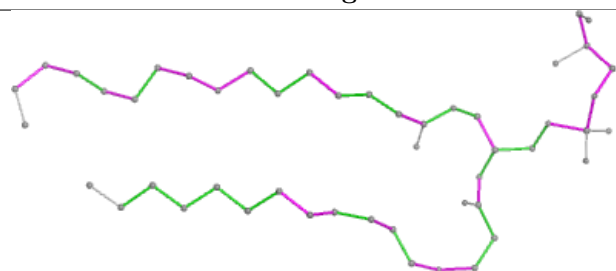
Ligand LHG 1 517



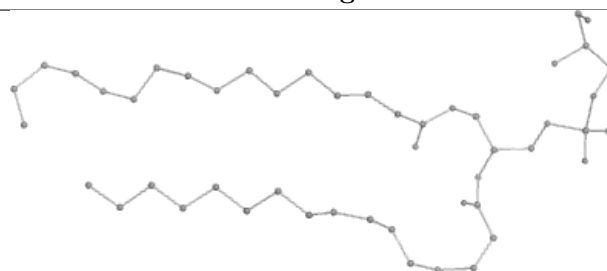
Bond lengths



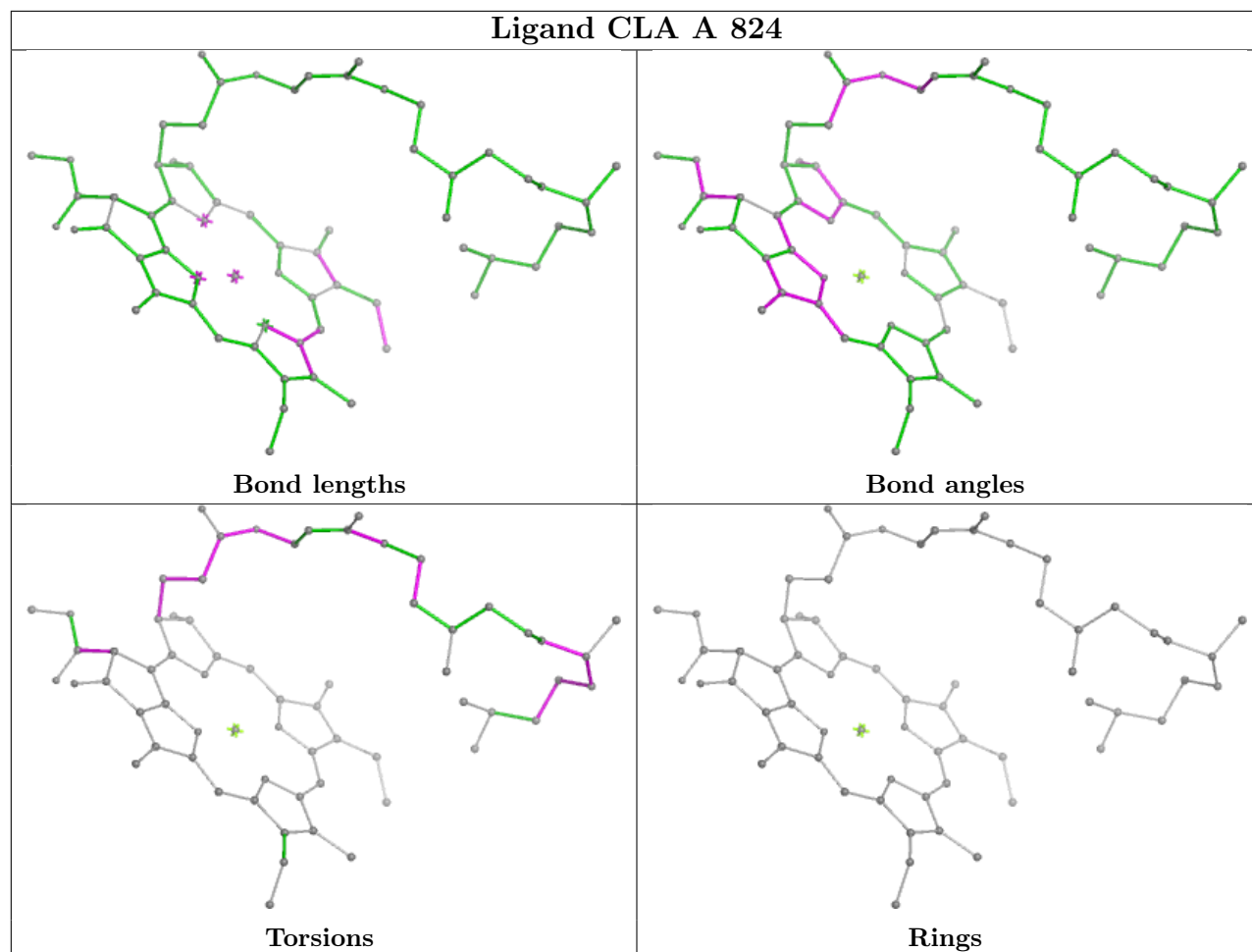
Bond angles



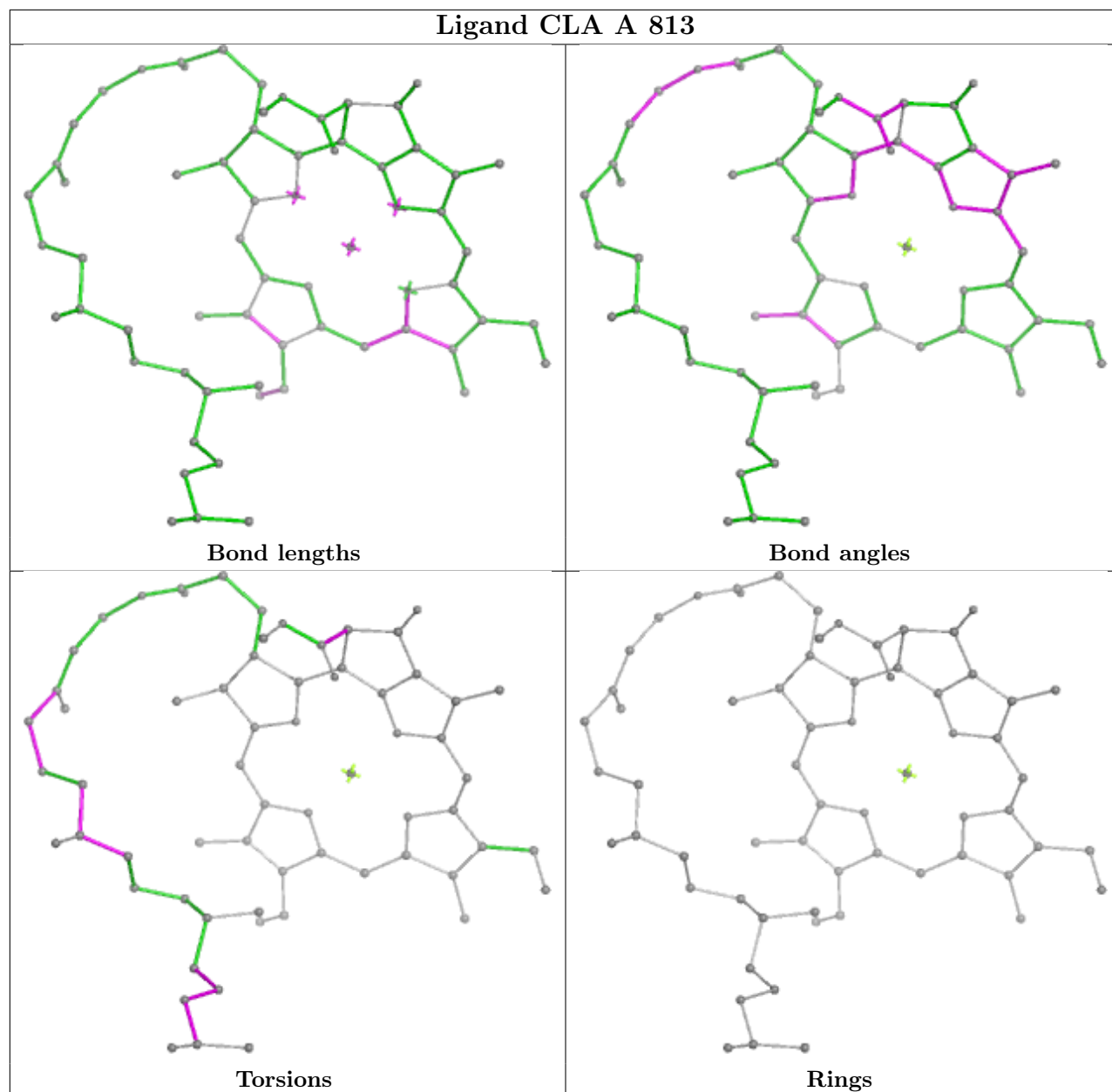
Torsions



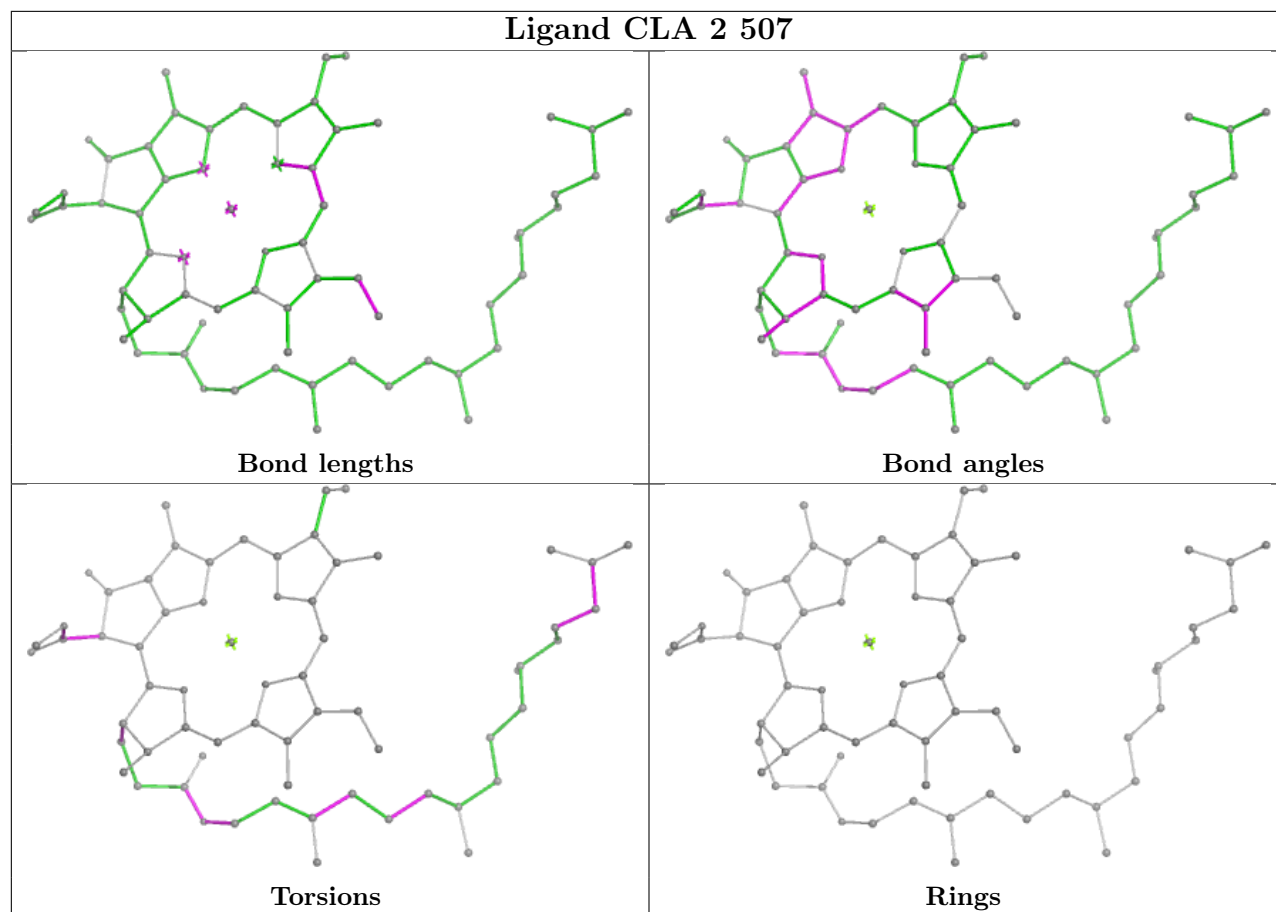
Rings



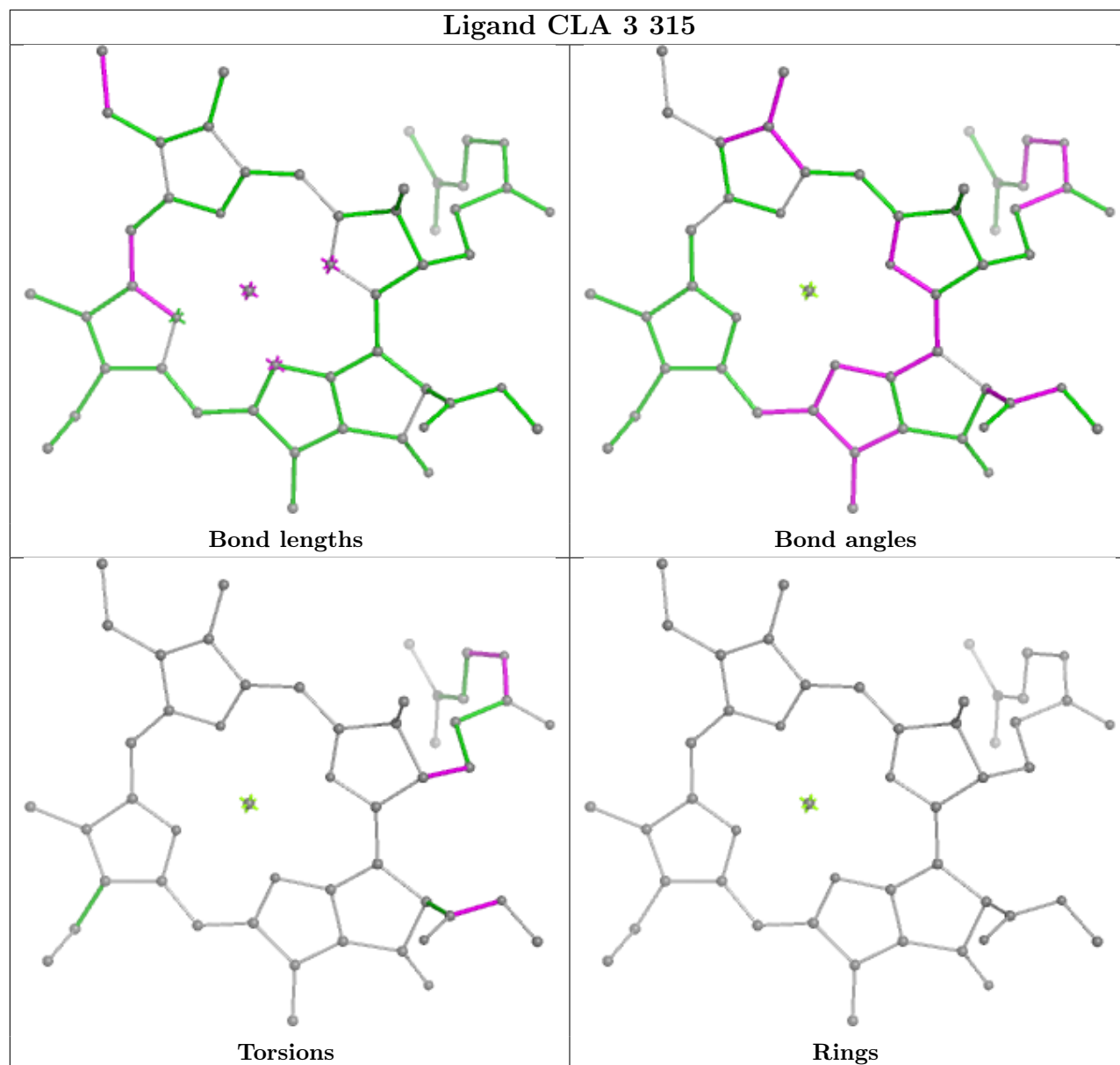
Ligand CLA A 813



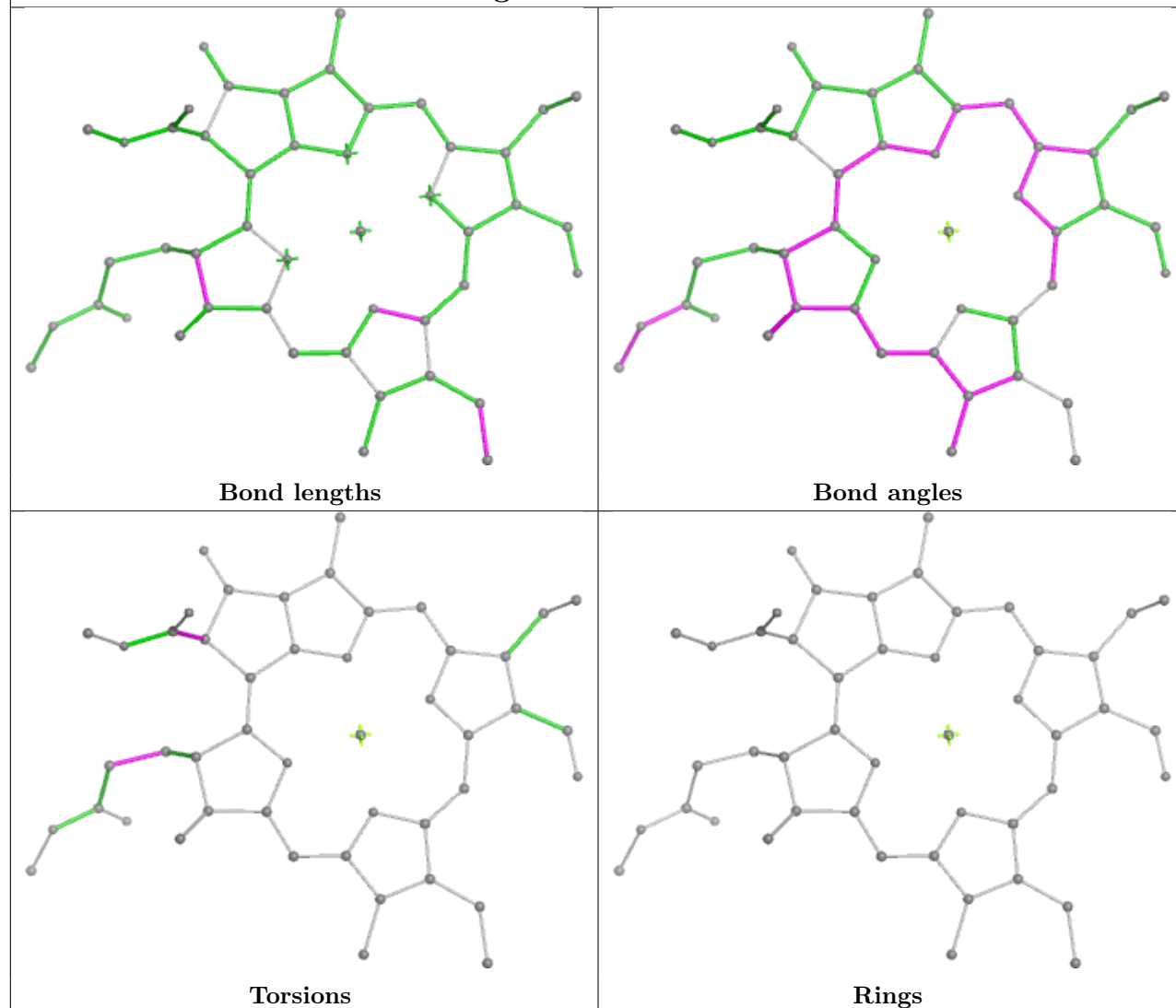
Ligand CLA 2 507



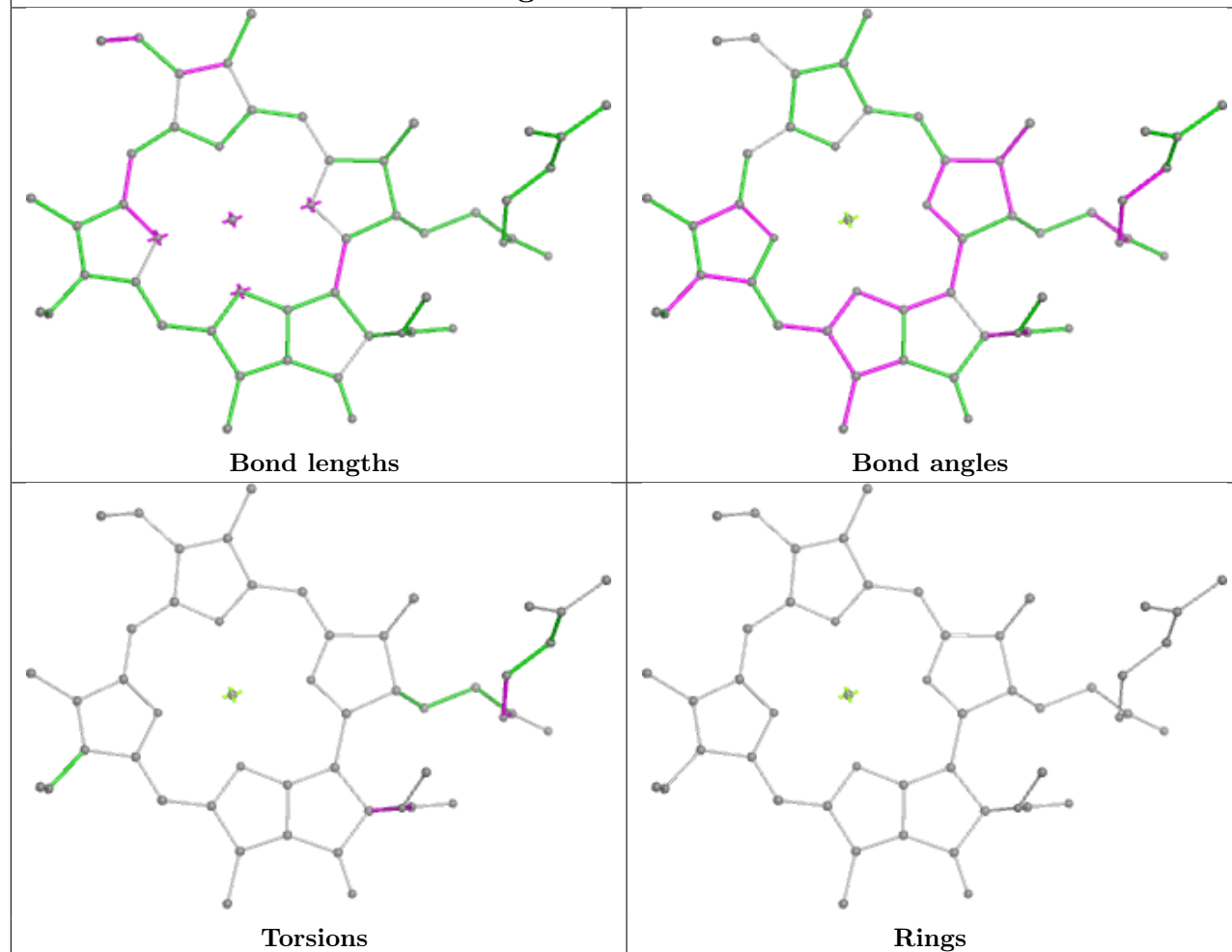
Ligand CLA 3 315



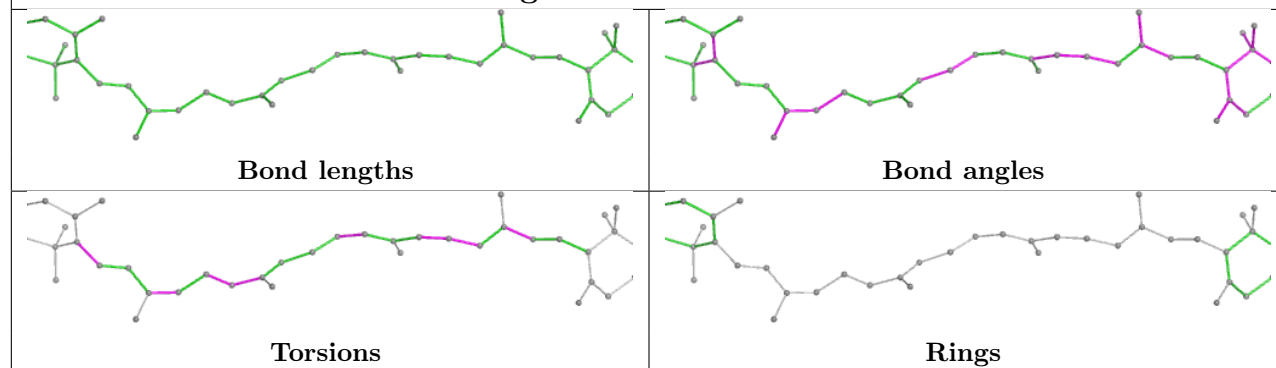
Ligand CHL 2 512



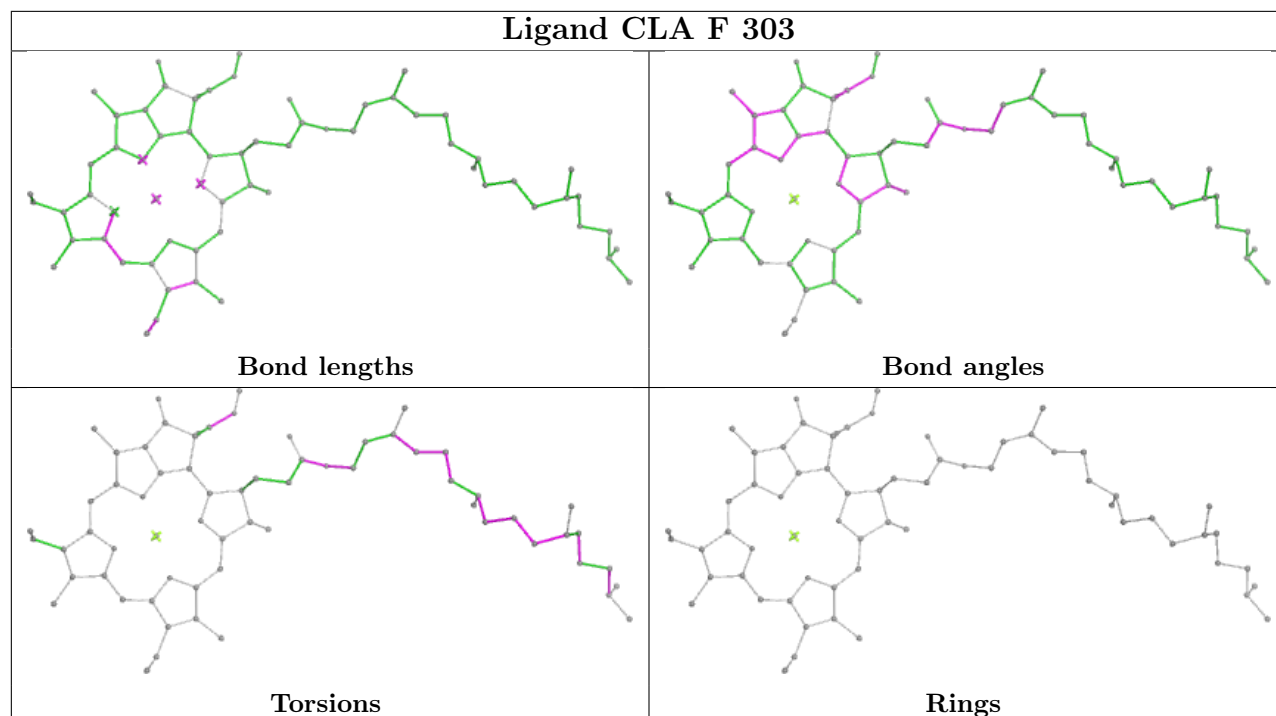
Ligand CLA 4 305



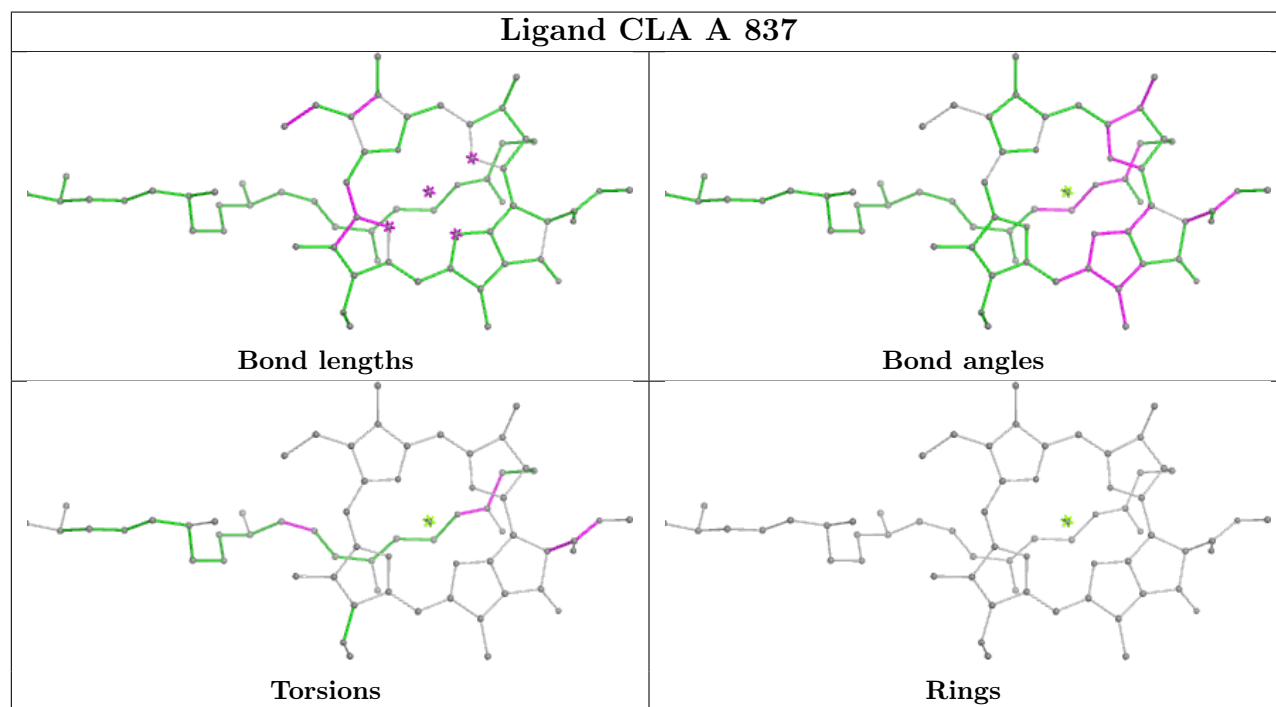
Ligand BCR K 1005

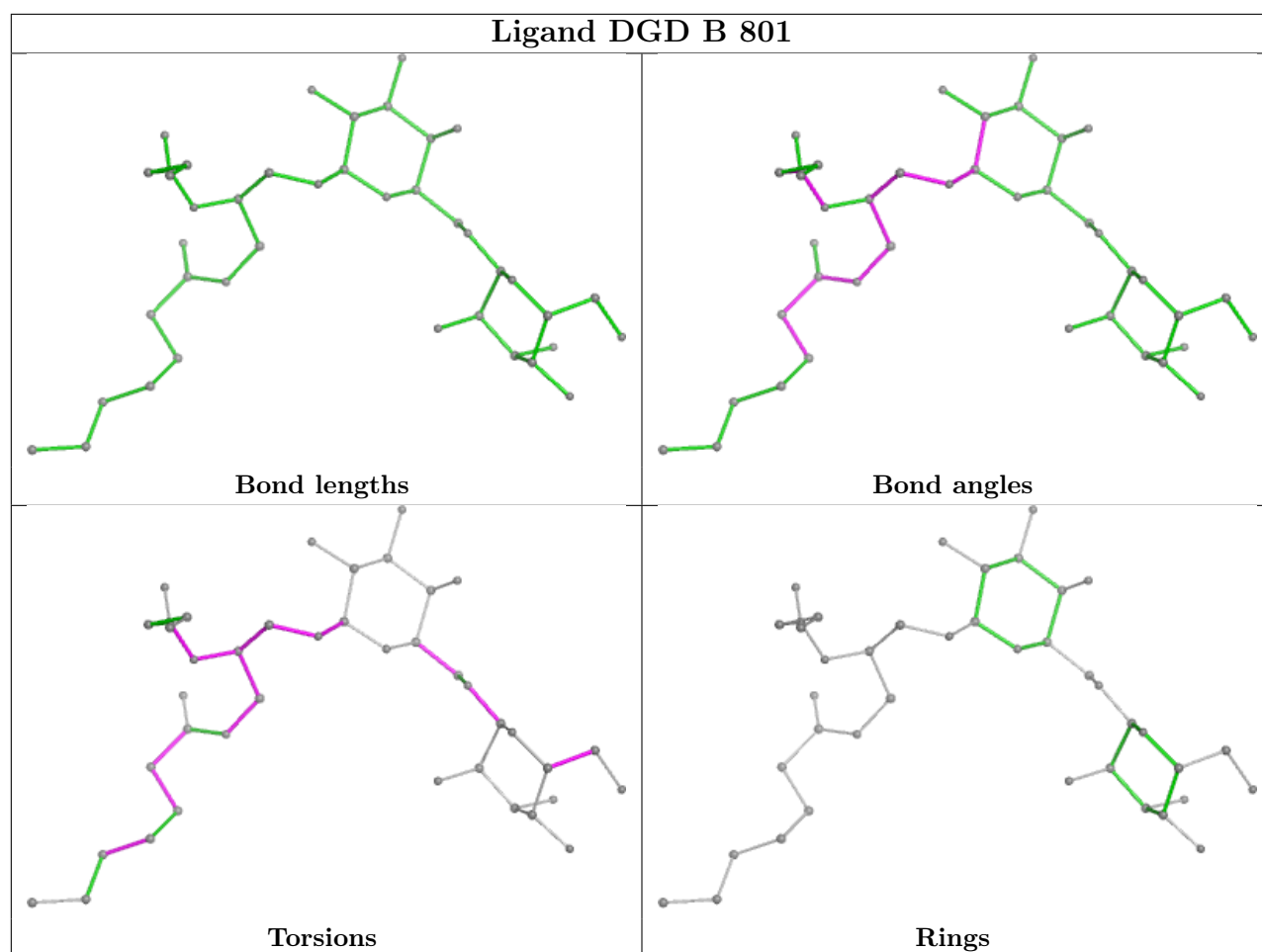


Ligand CLA F 303

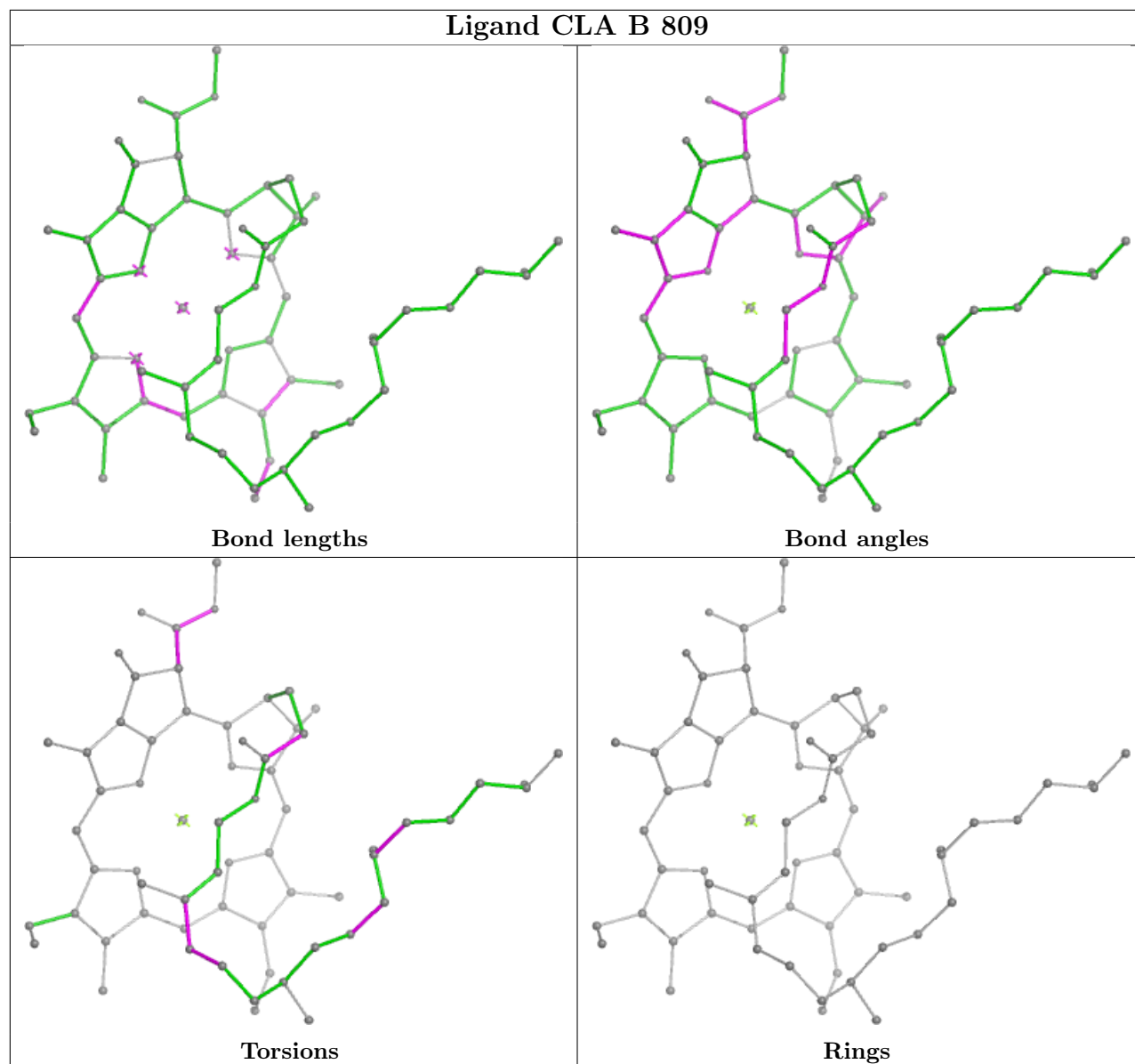


Ligand CLA A 837

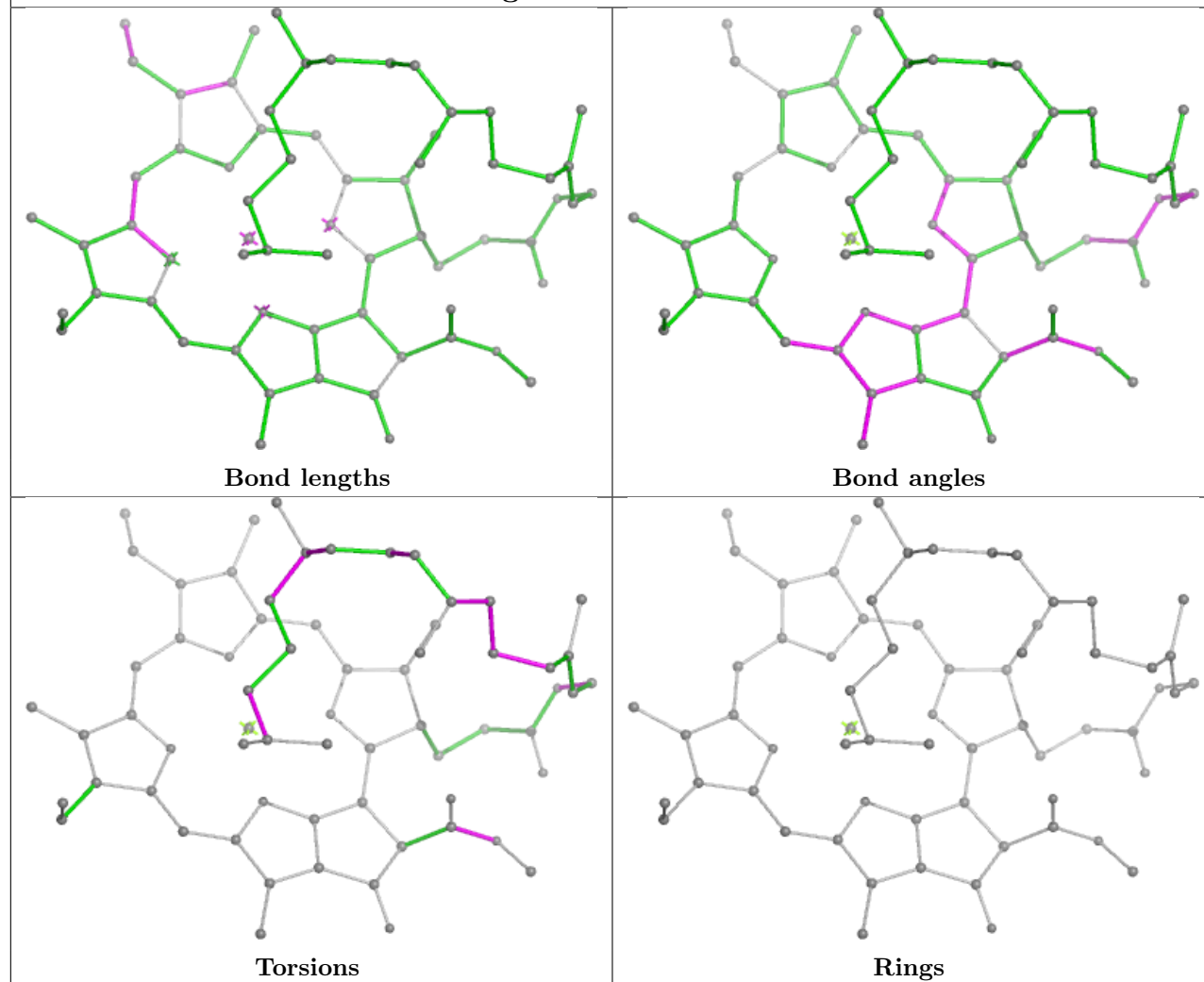




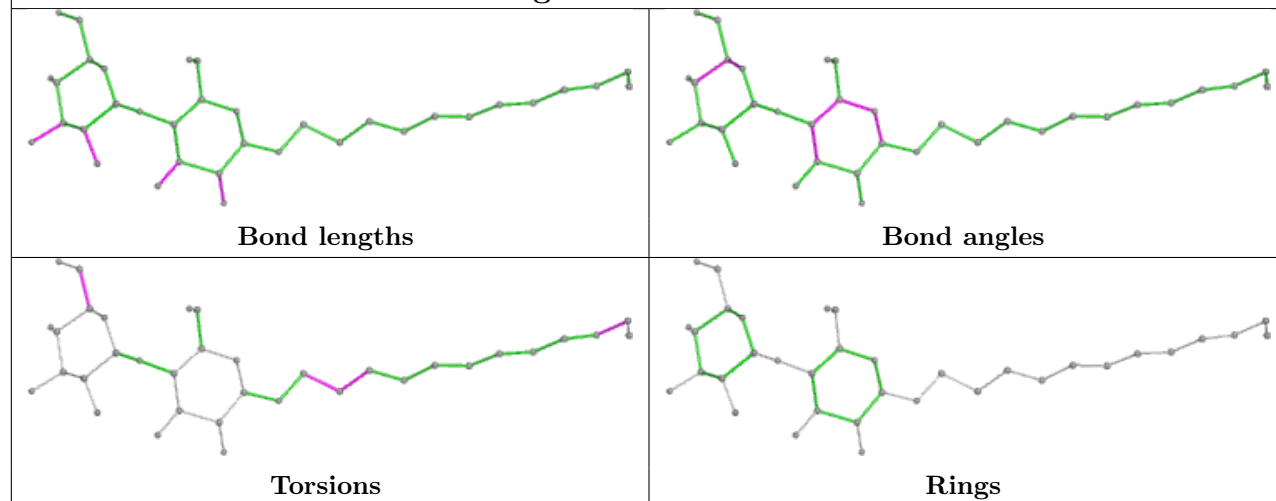
Ligand CLA B 809

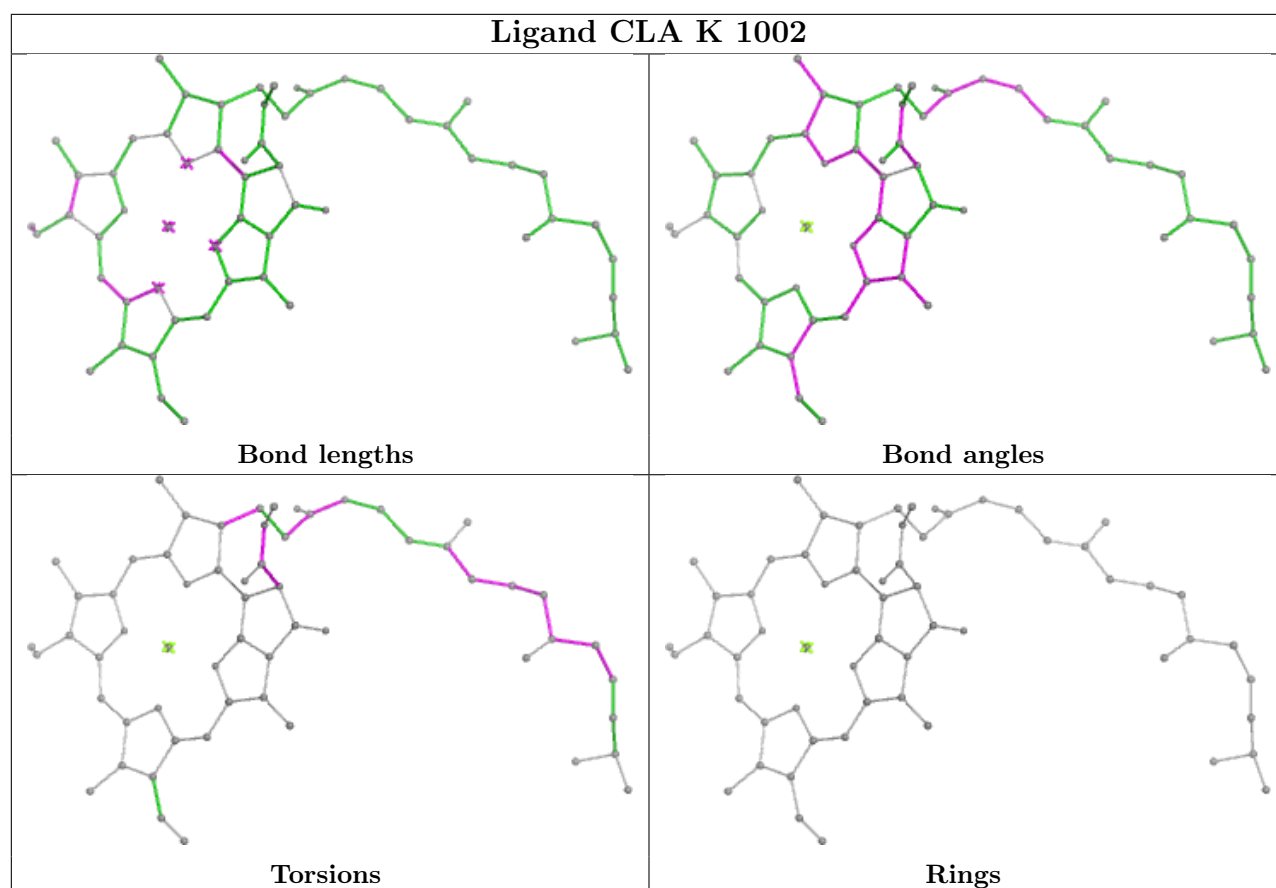


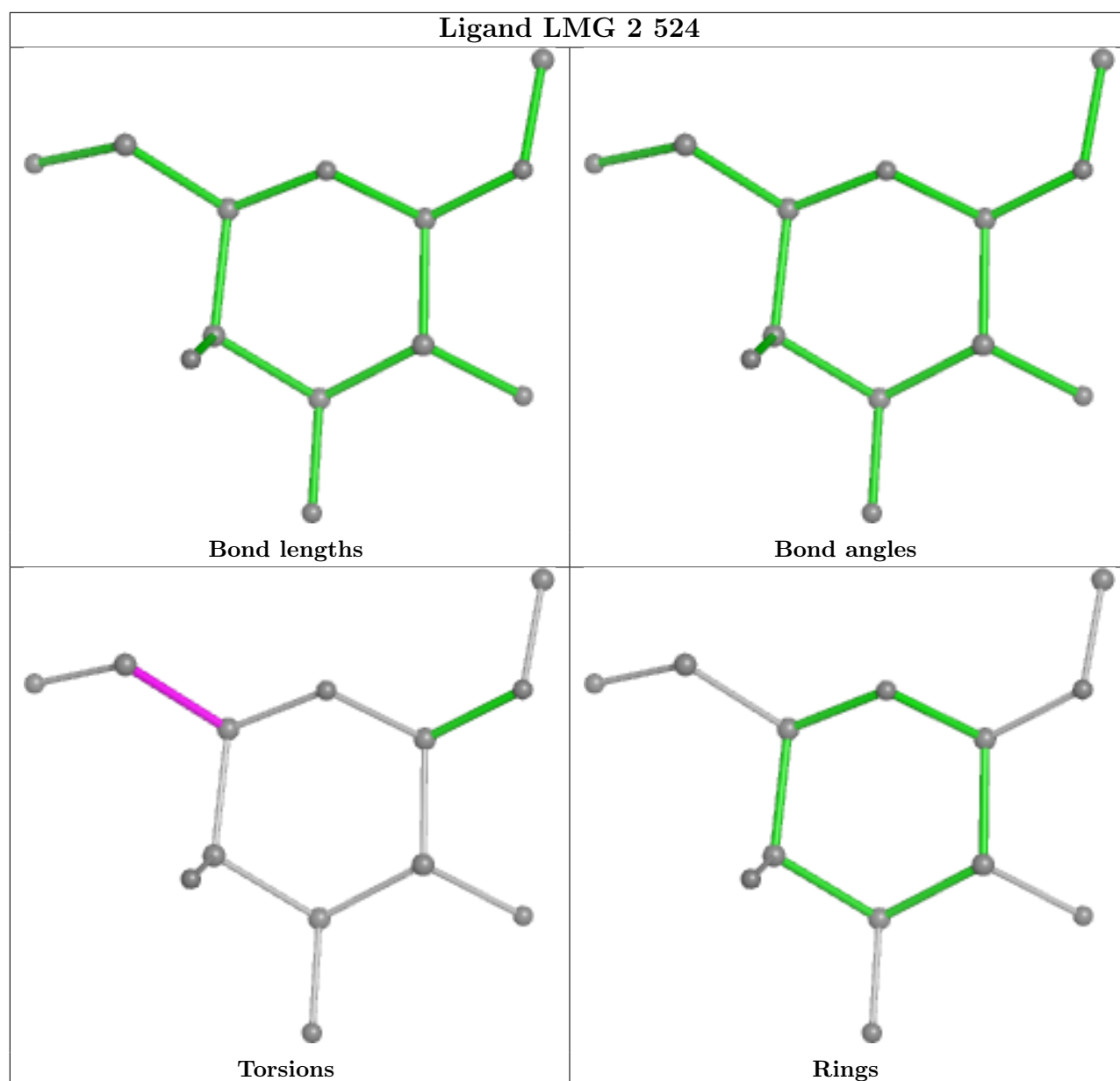
Ligand CLA B 807



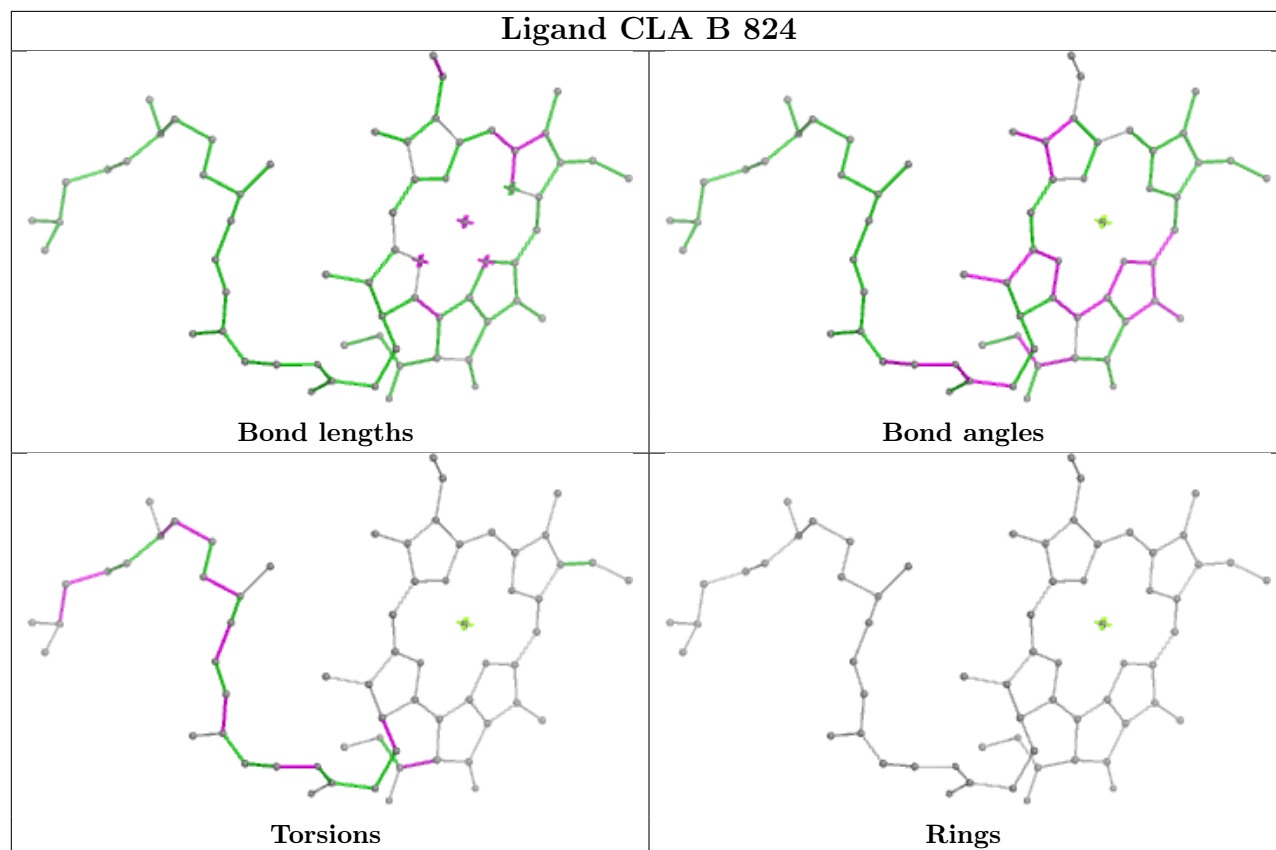
Ligand LMT 4 320



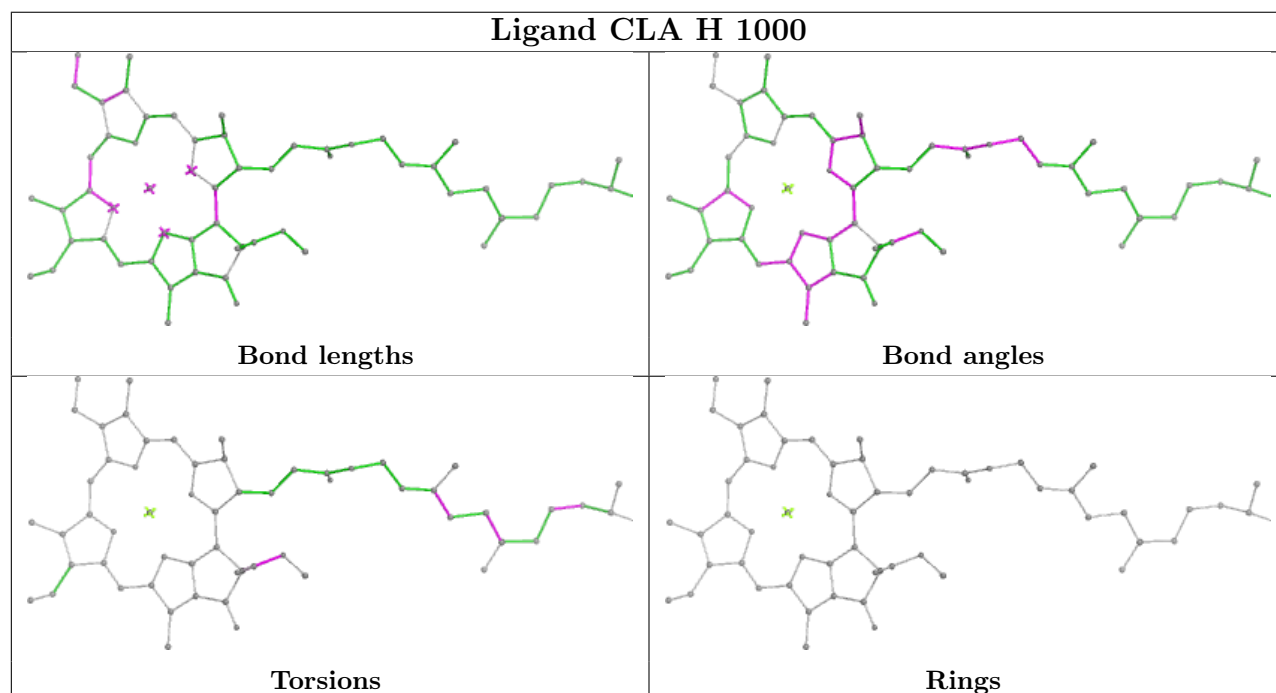


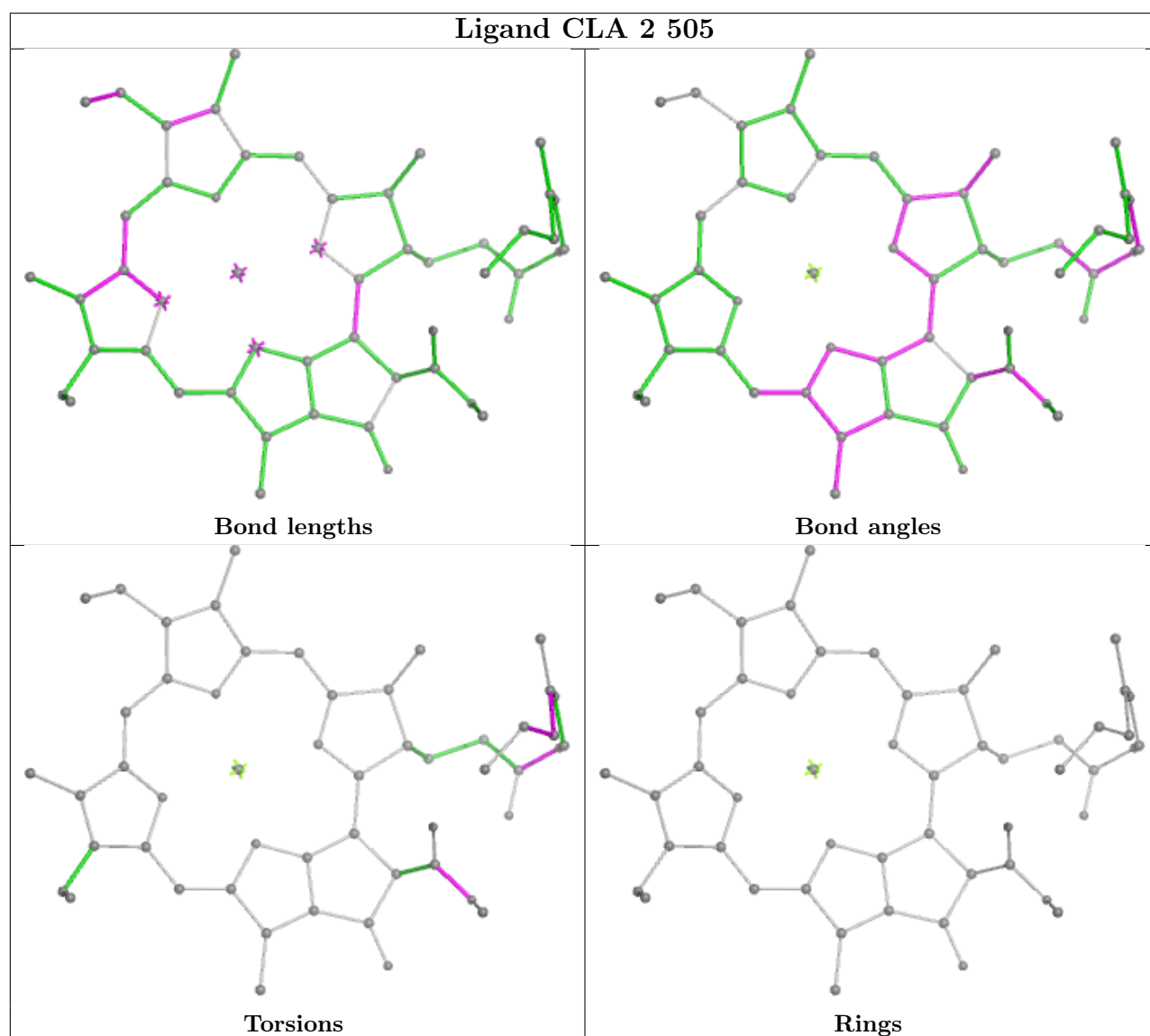
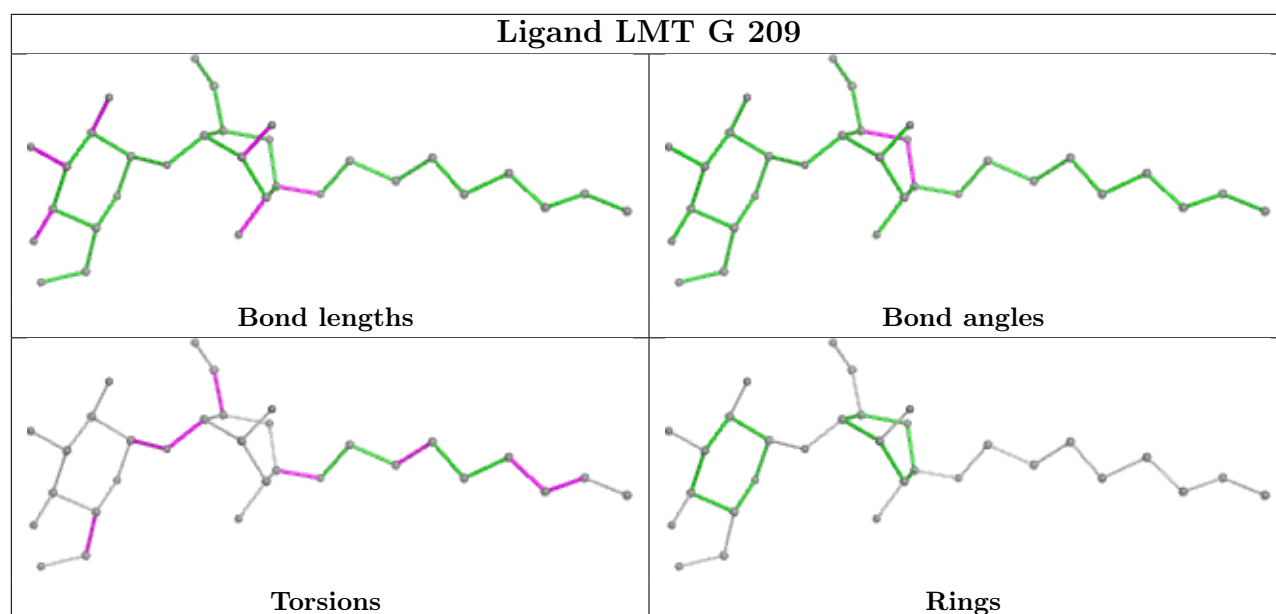


Ligand CLA B 824

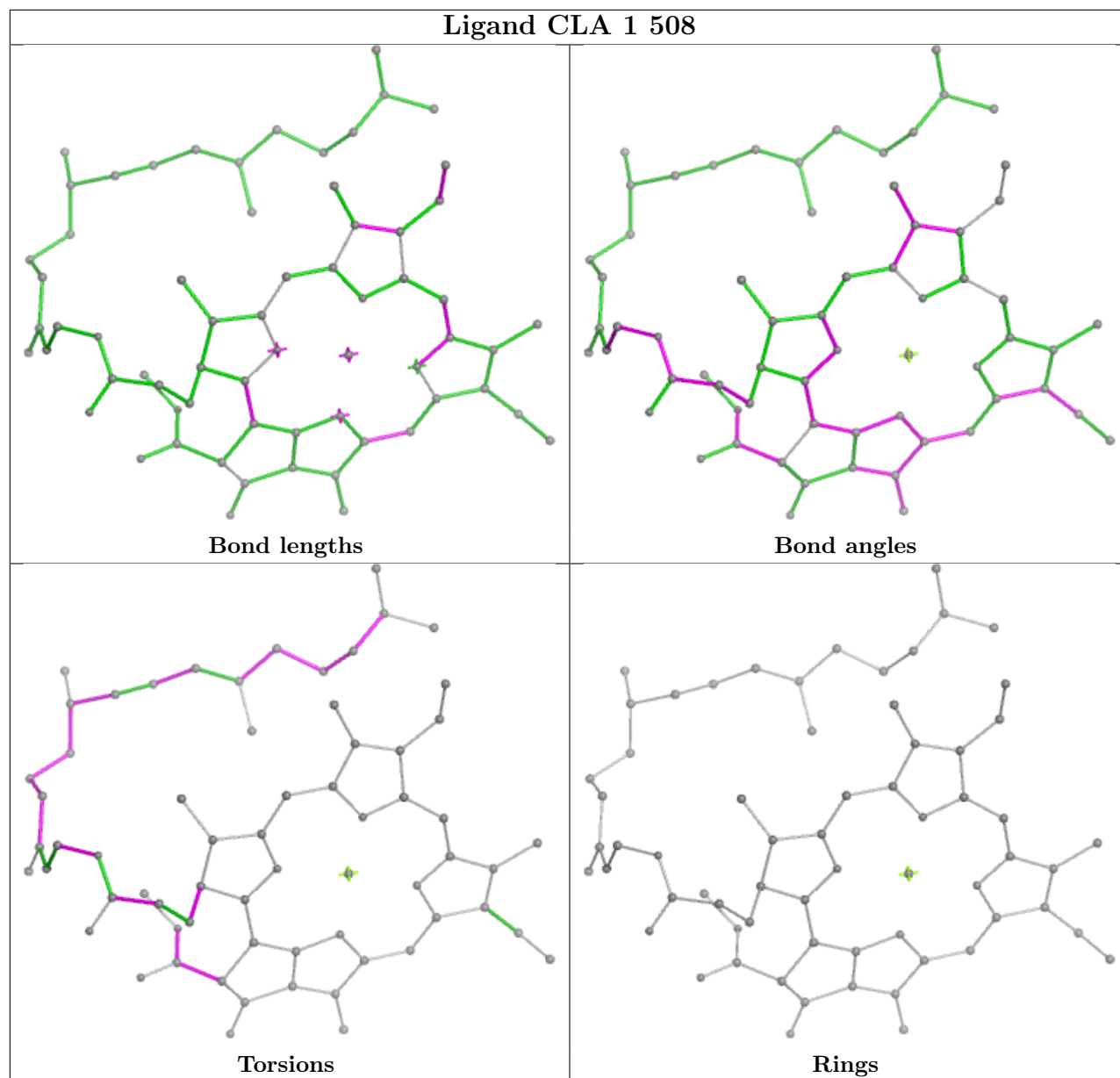


Ligand CLA H 1000

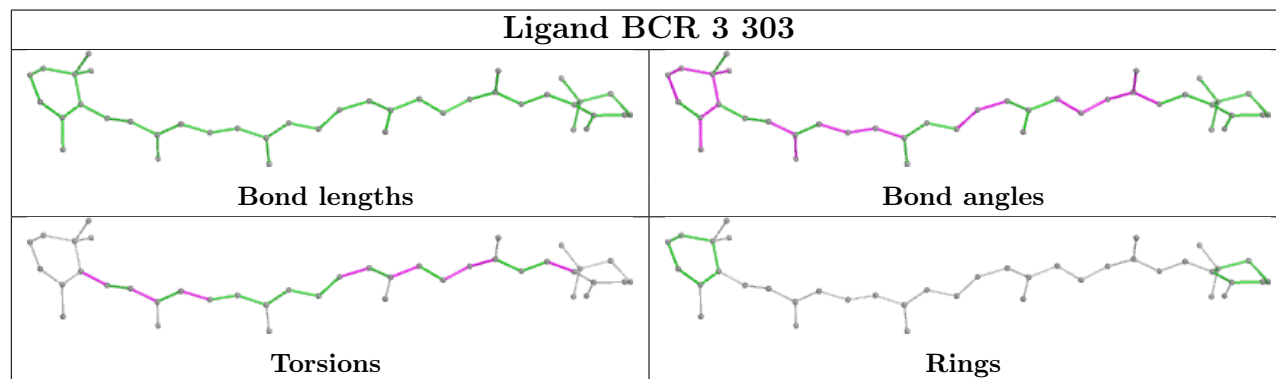




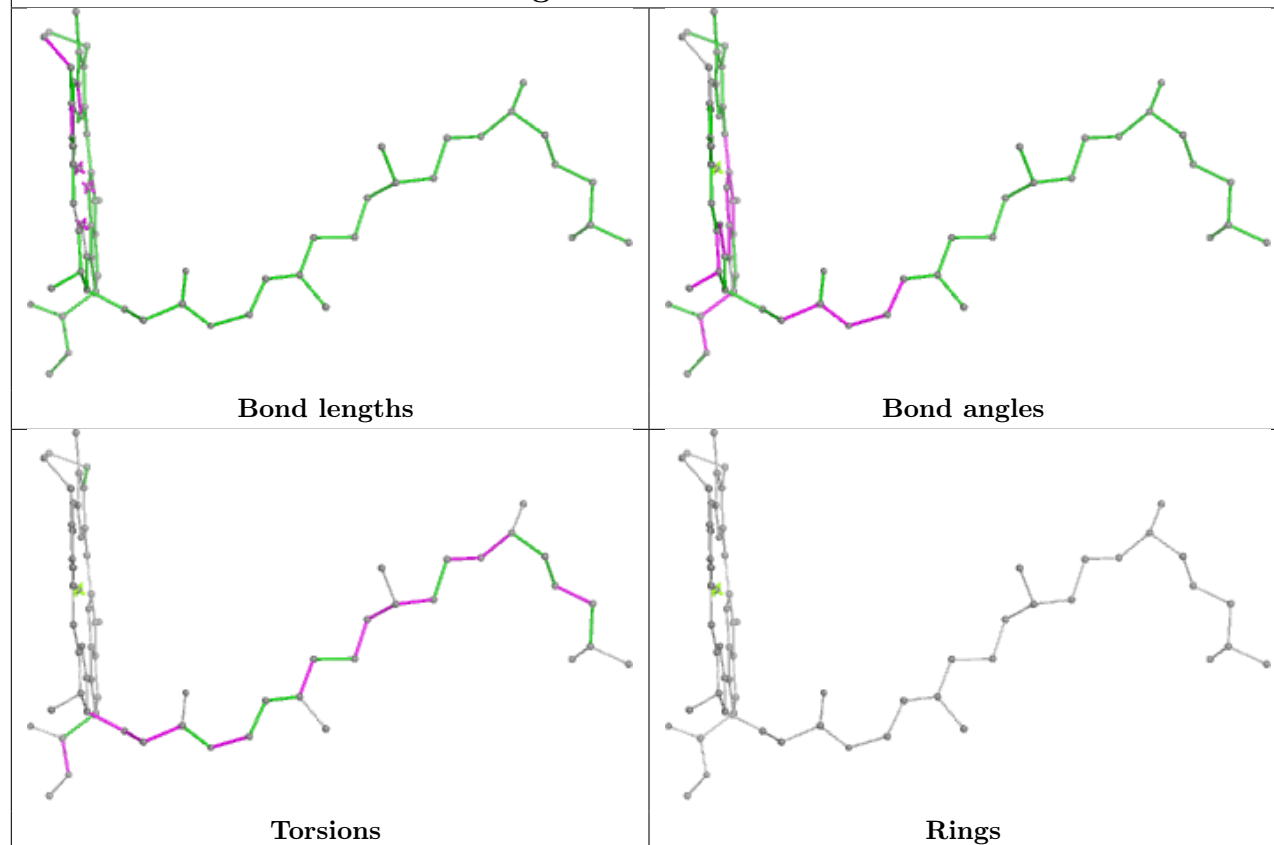
Ligand CLA 1 508



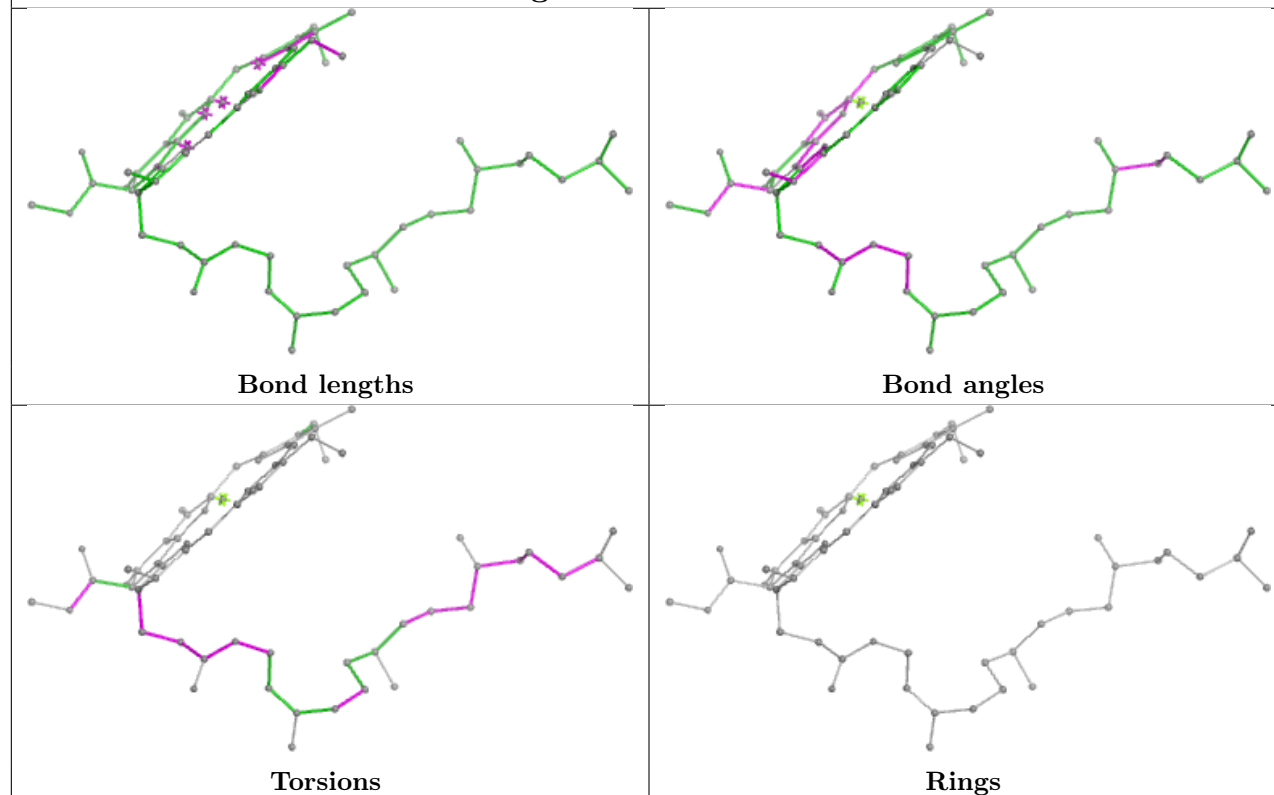
Ligand BCR 3 303



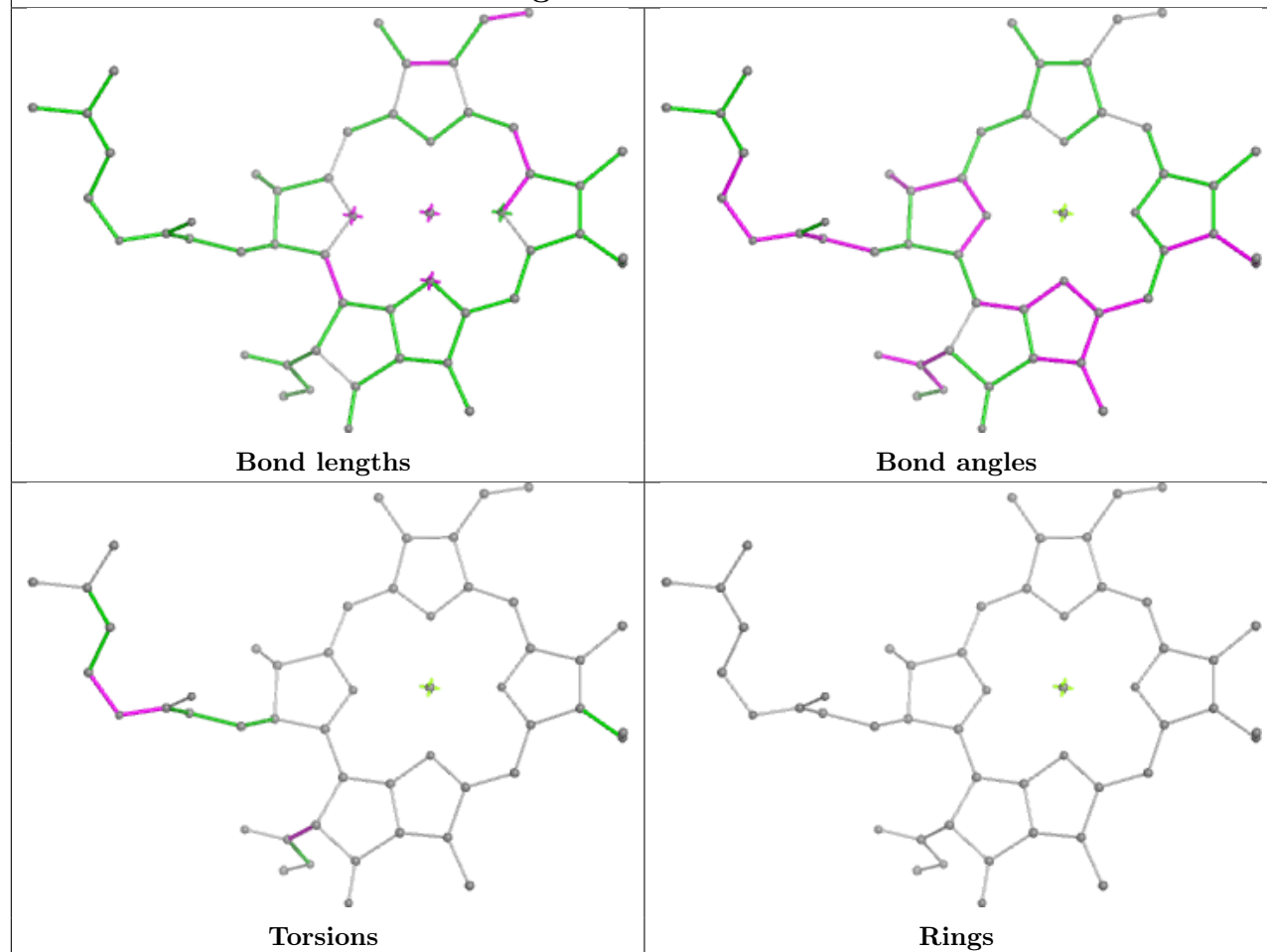
Ligand CLA B 839



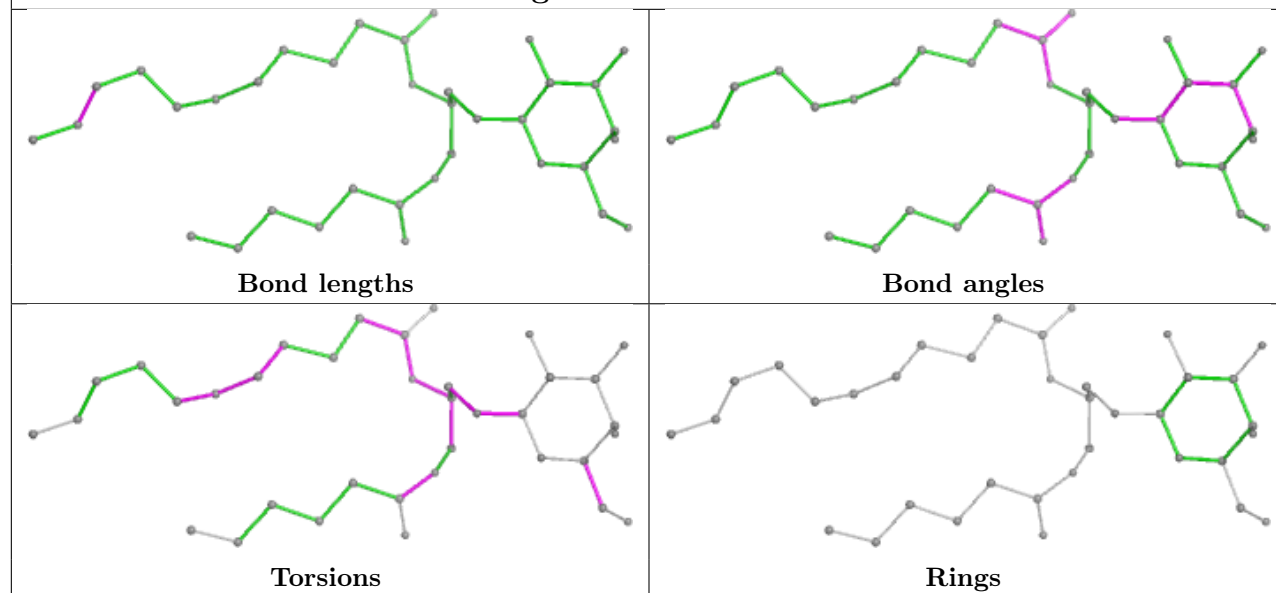
Ligand CLA G 204



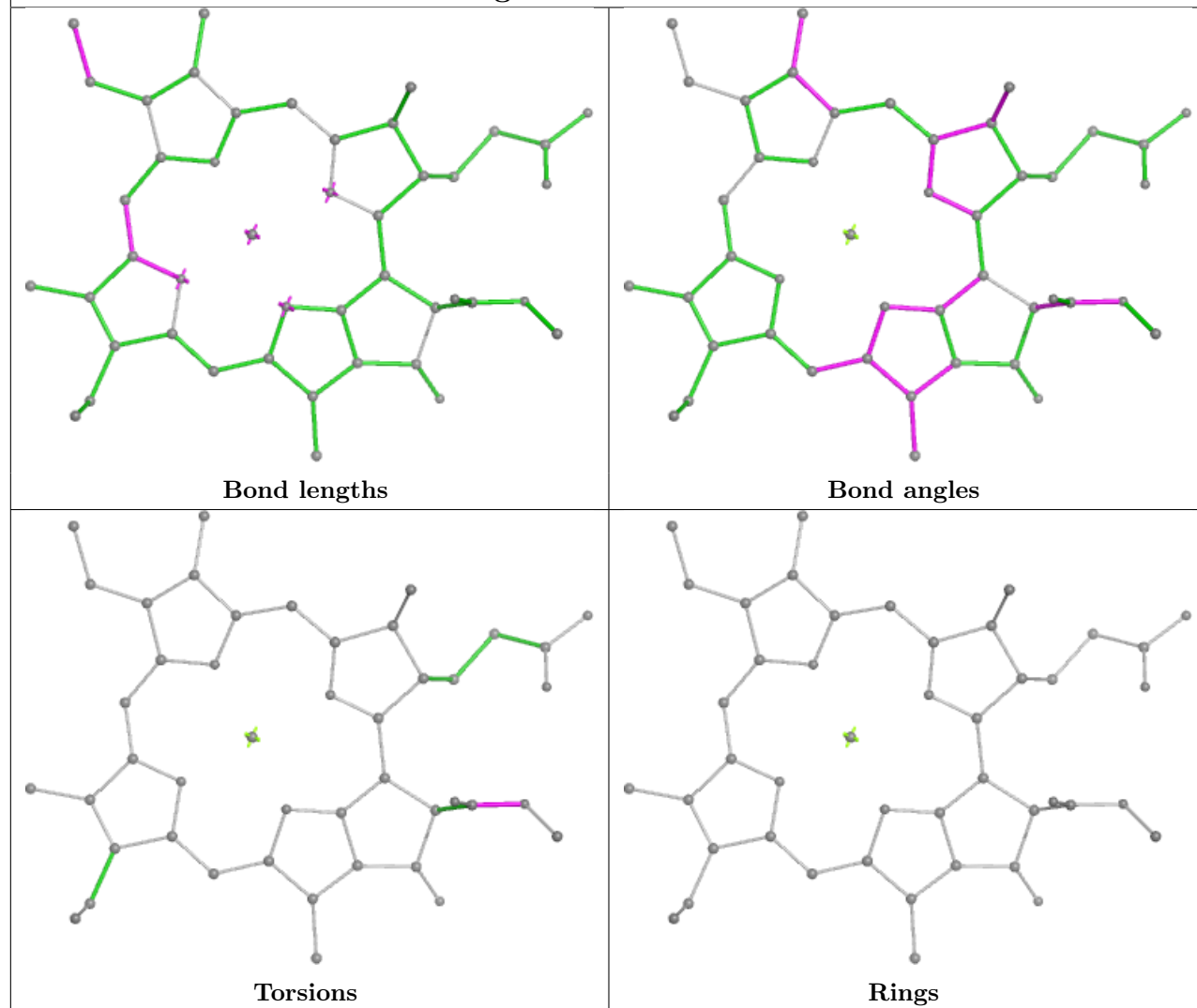
Ligand CLA 4 312

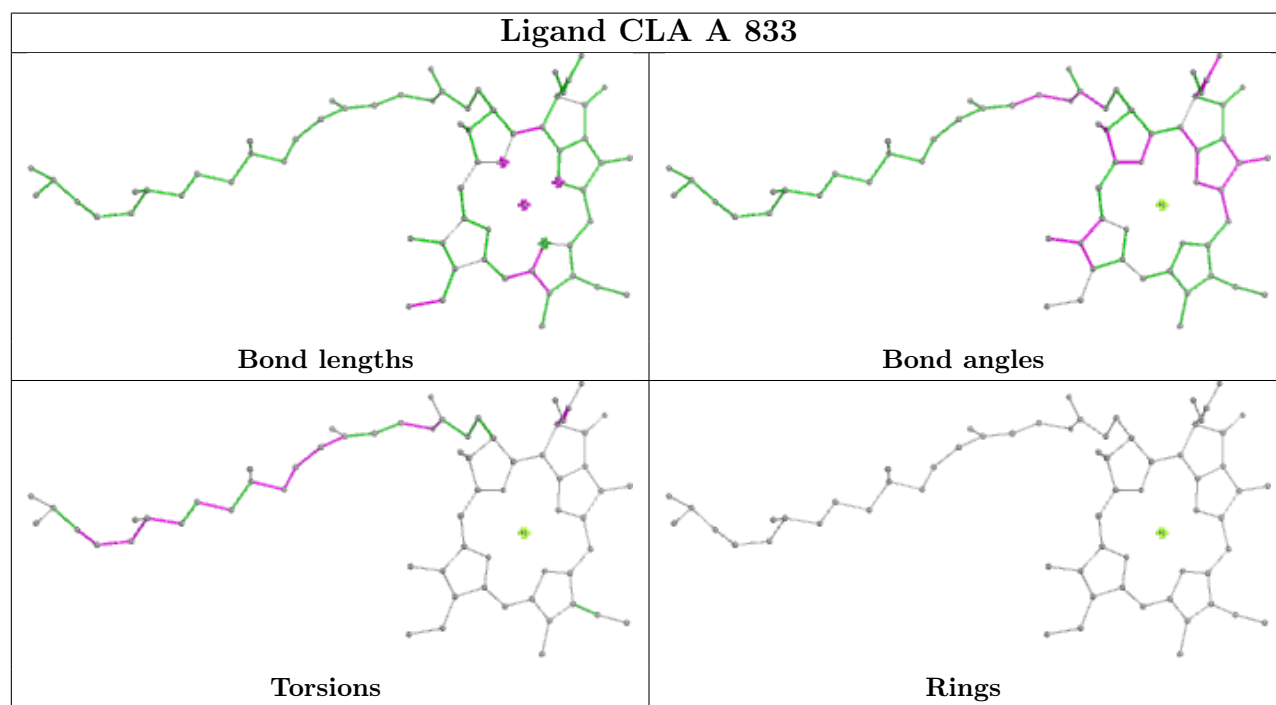
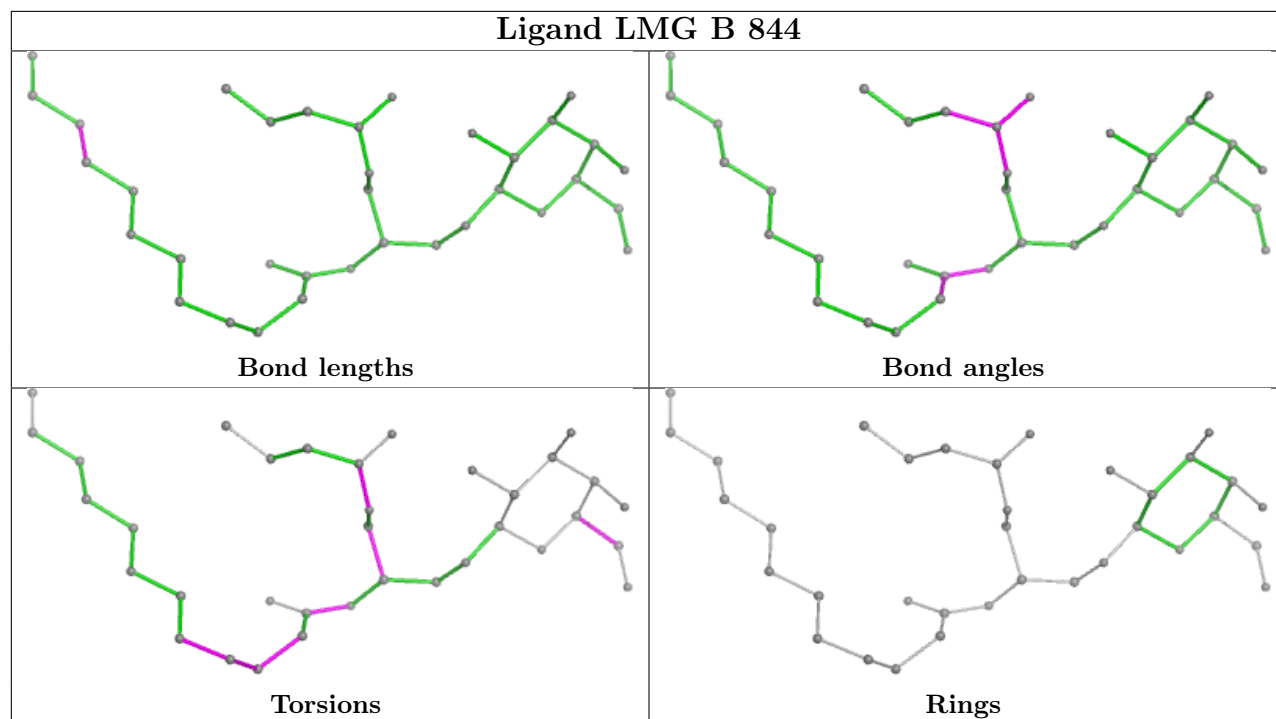


Ligand LMG 2 519

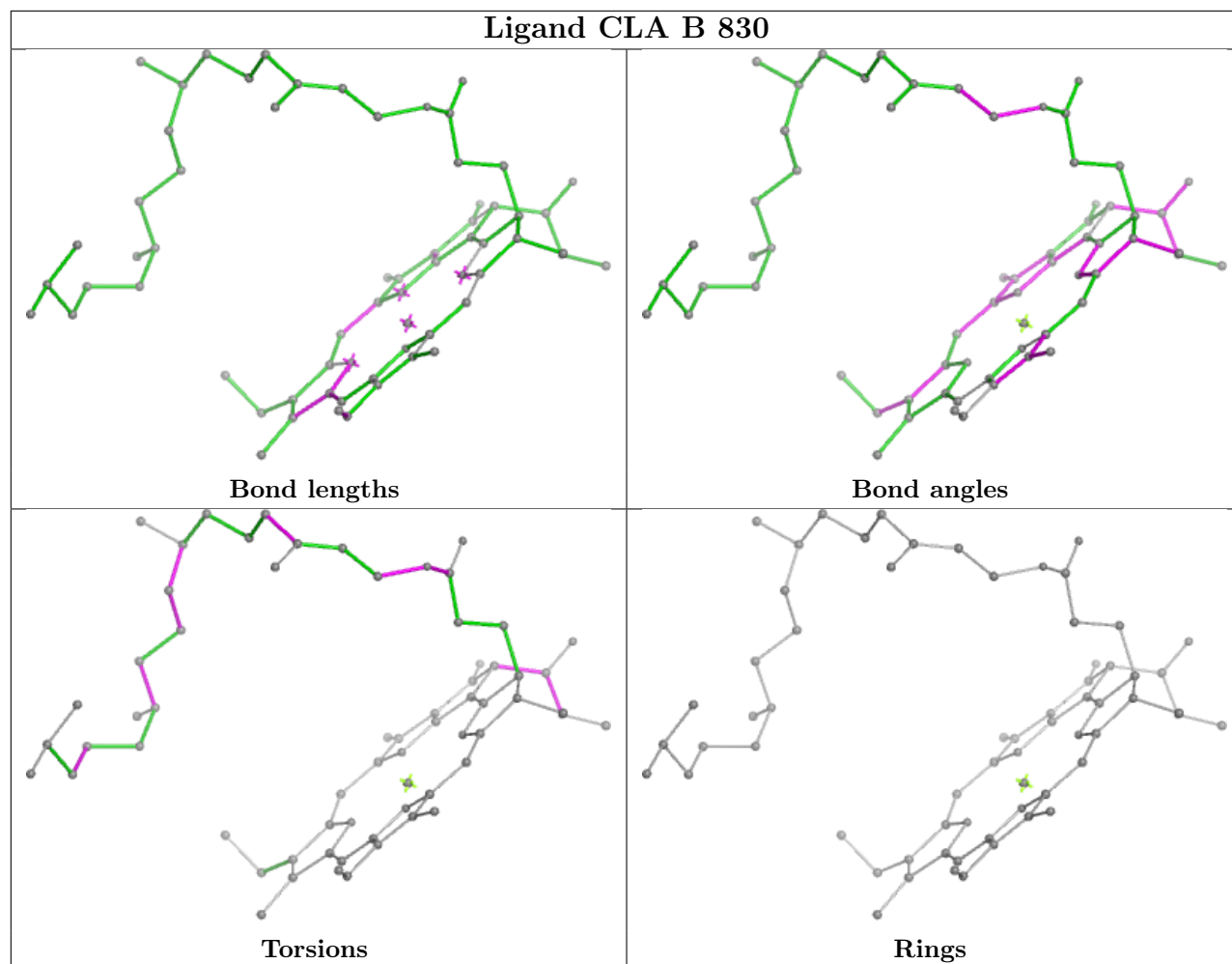


Ligand CLA J 1102

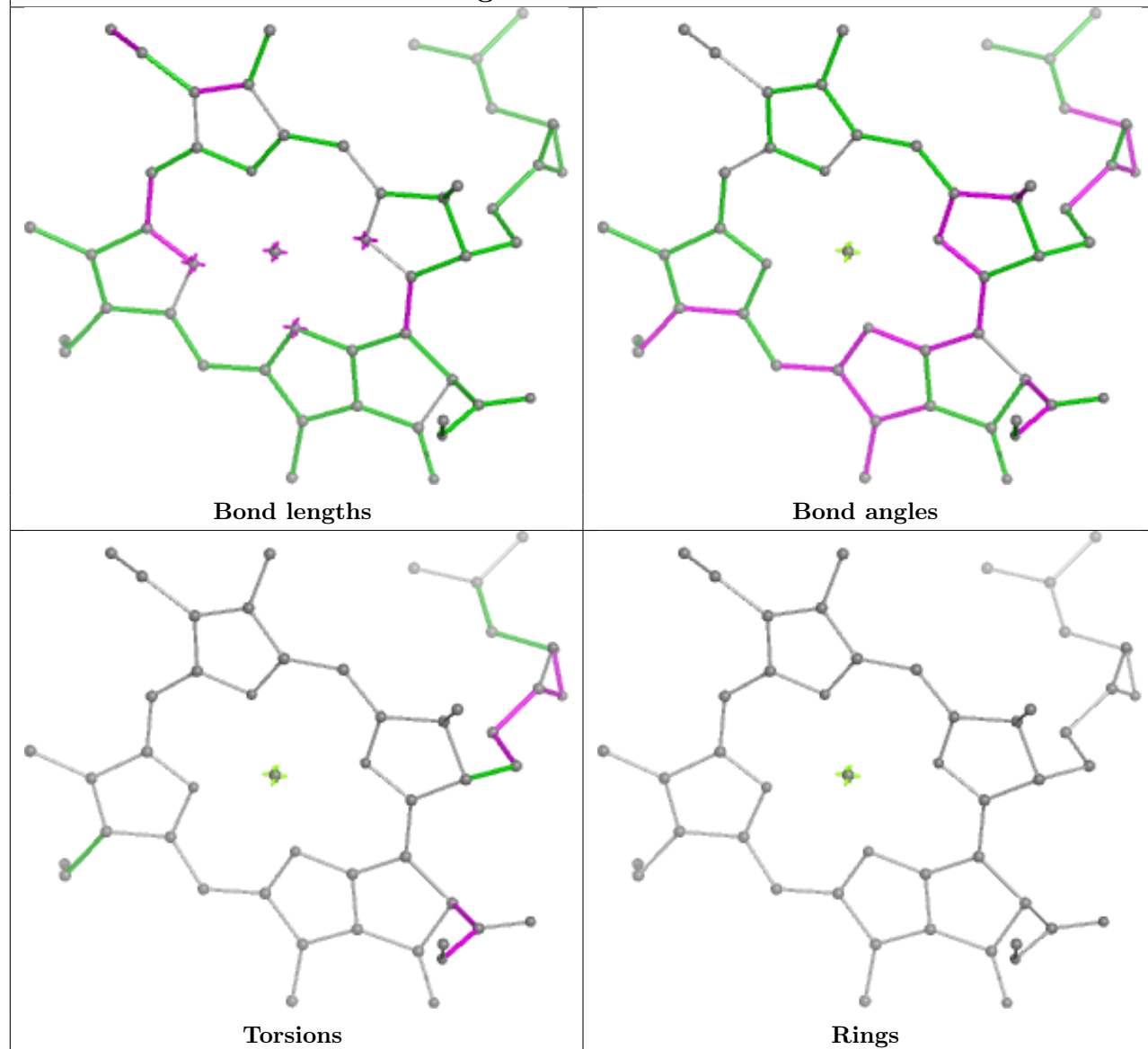


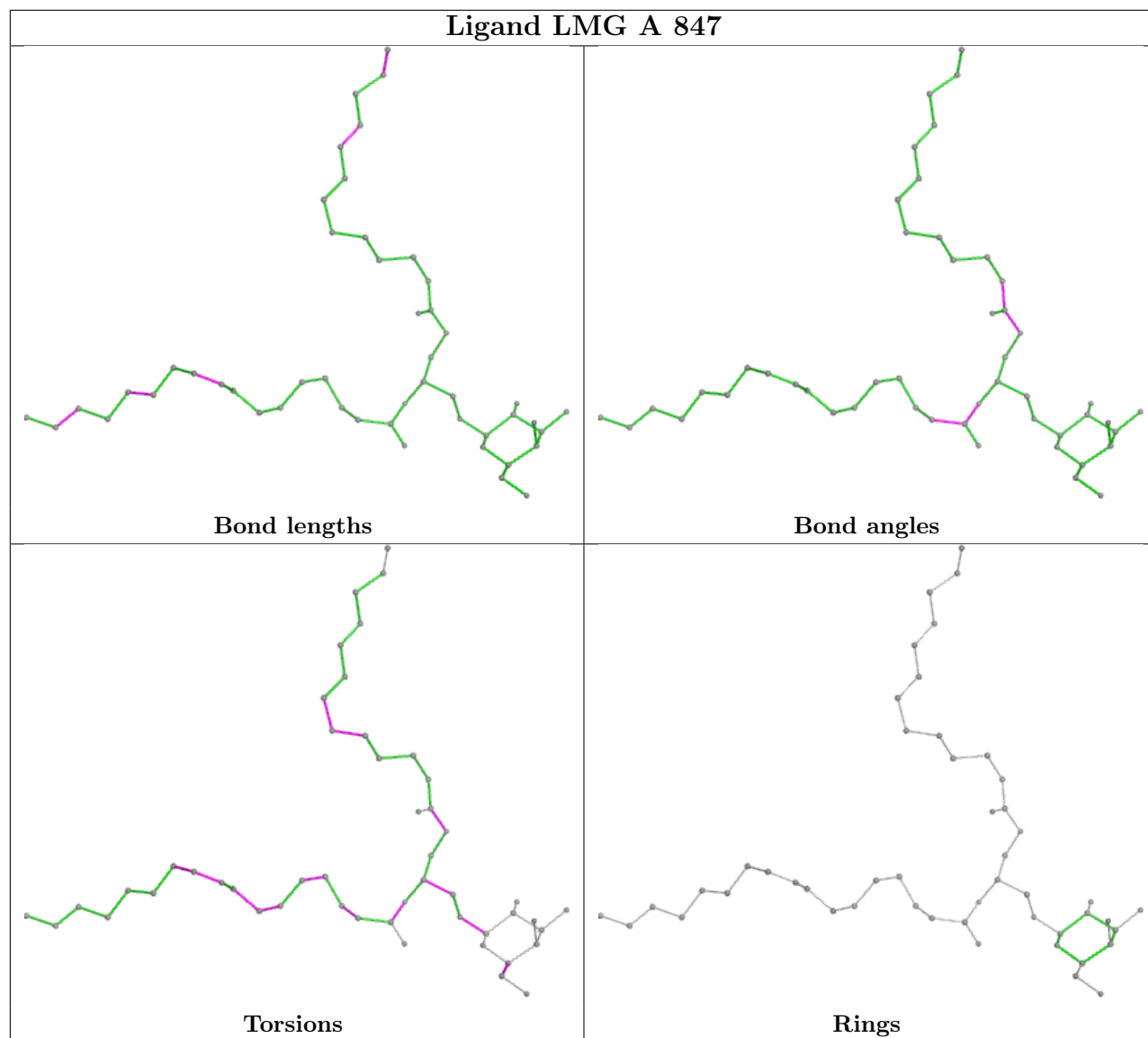


Ligand CLA B 830

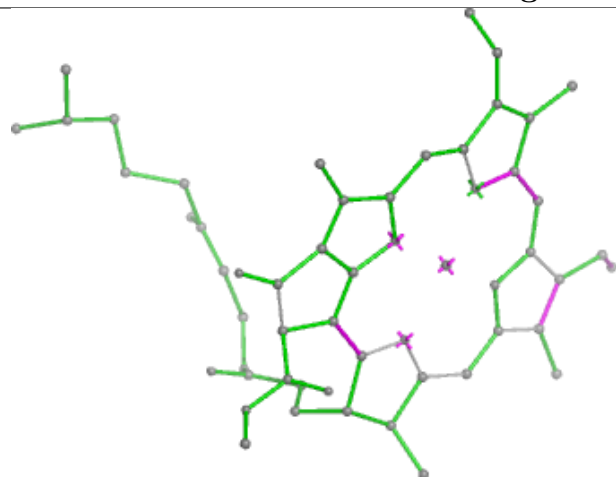


Ligand CLA A 820

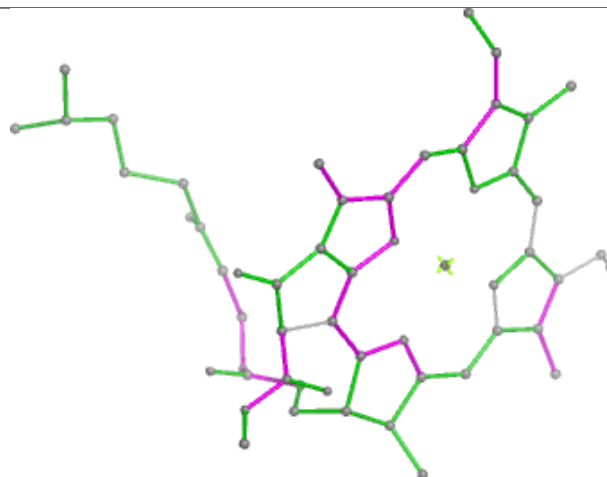




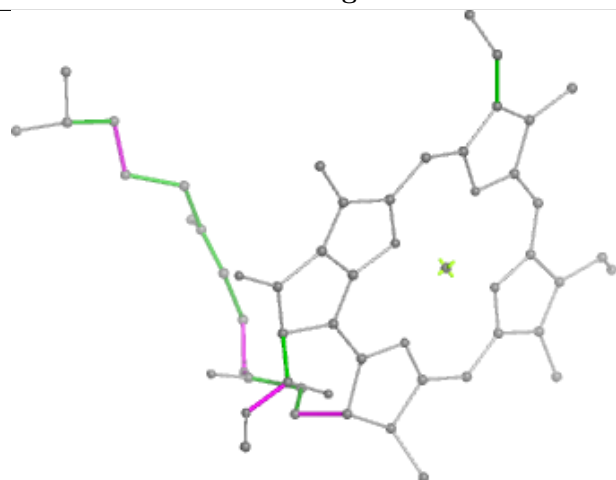
Ligand CLA 2 514



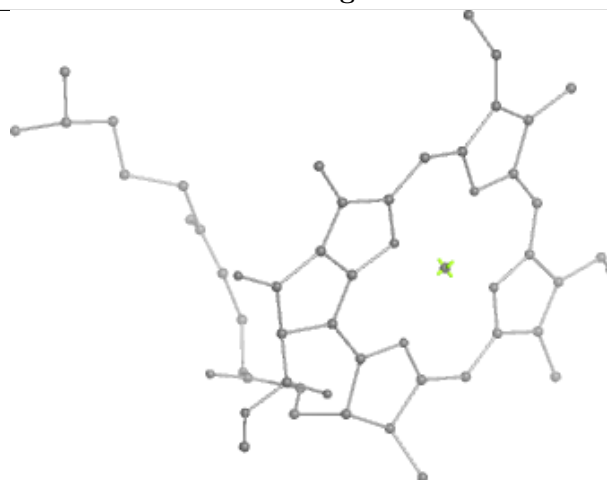
Bond lengths



Bond angles

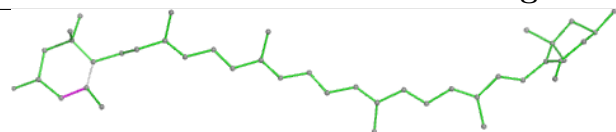


Torsions

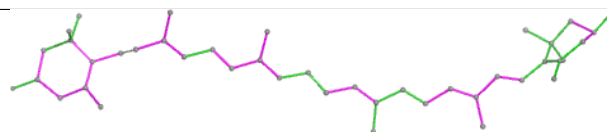


Rings

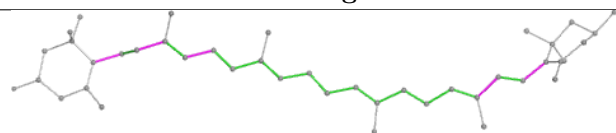
Ligand LUT 3 302



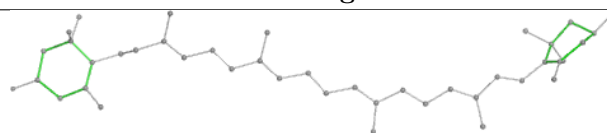
Bond lengths



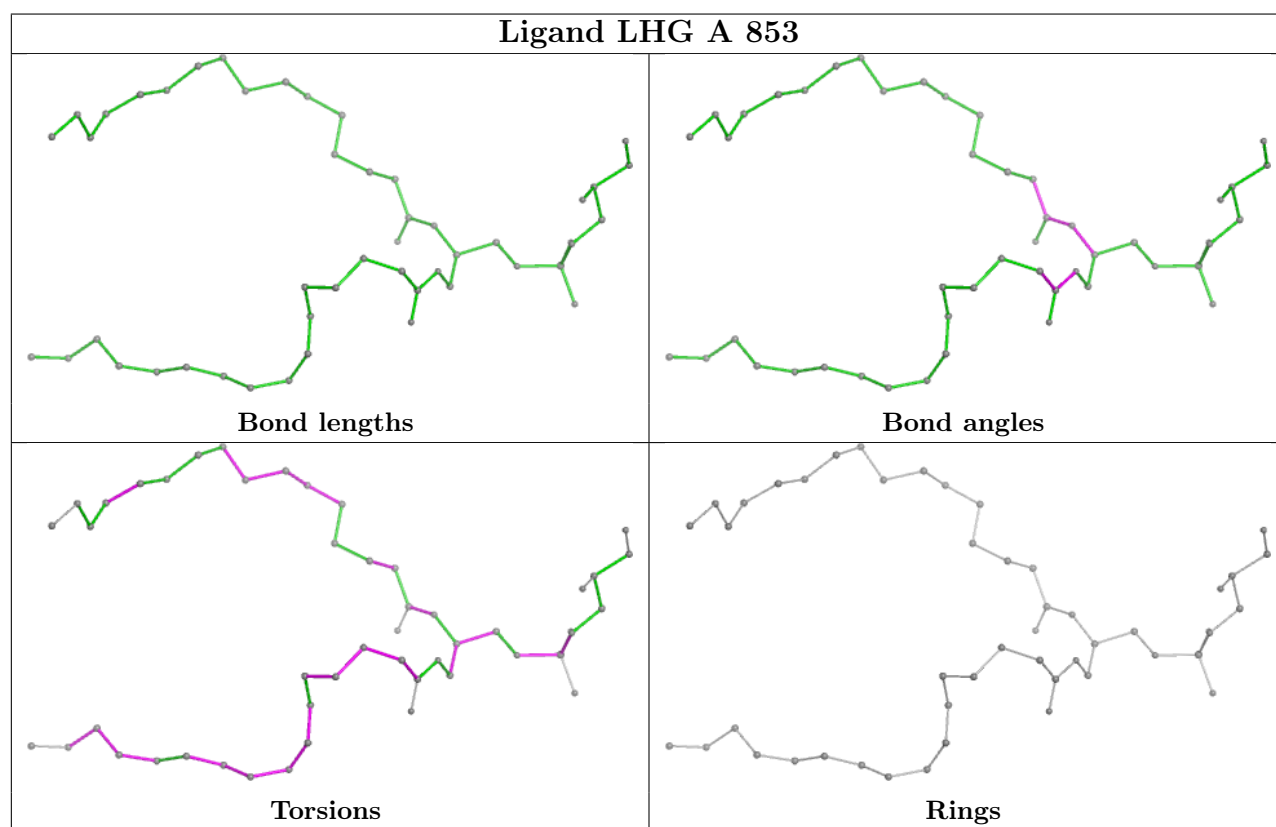
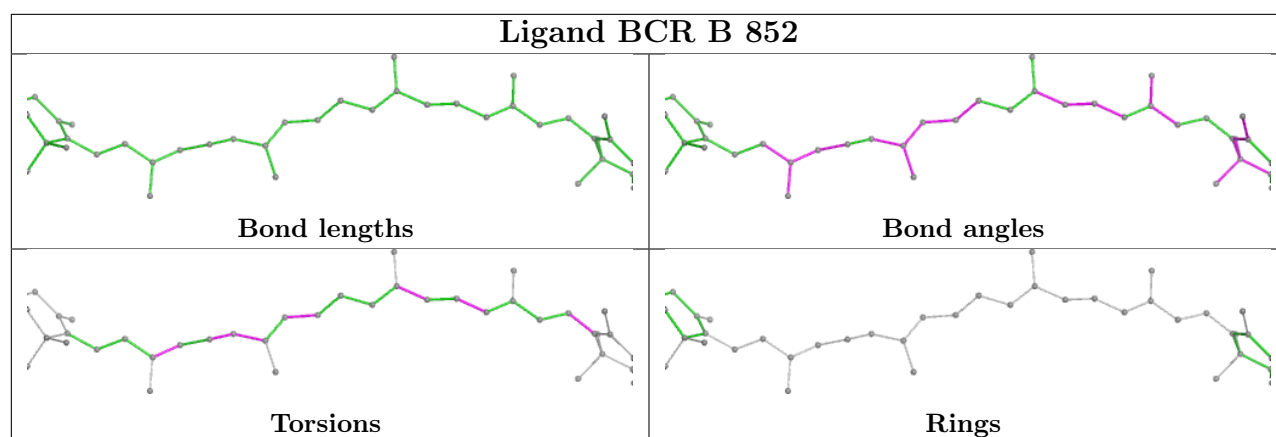
Bond angles

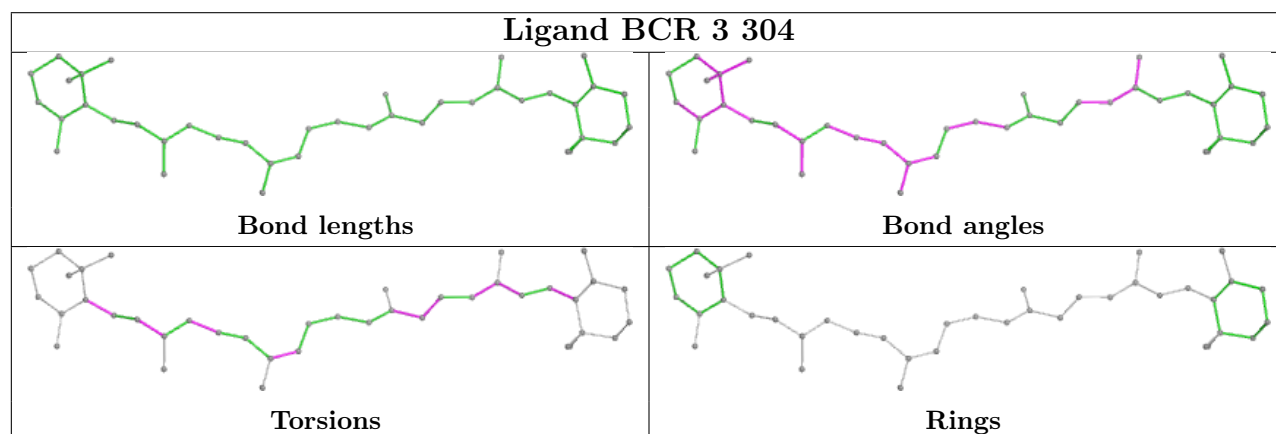
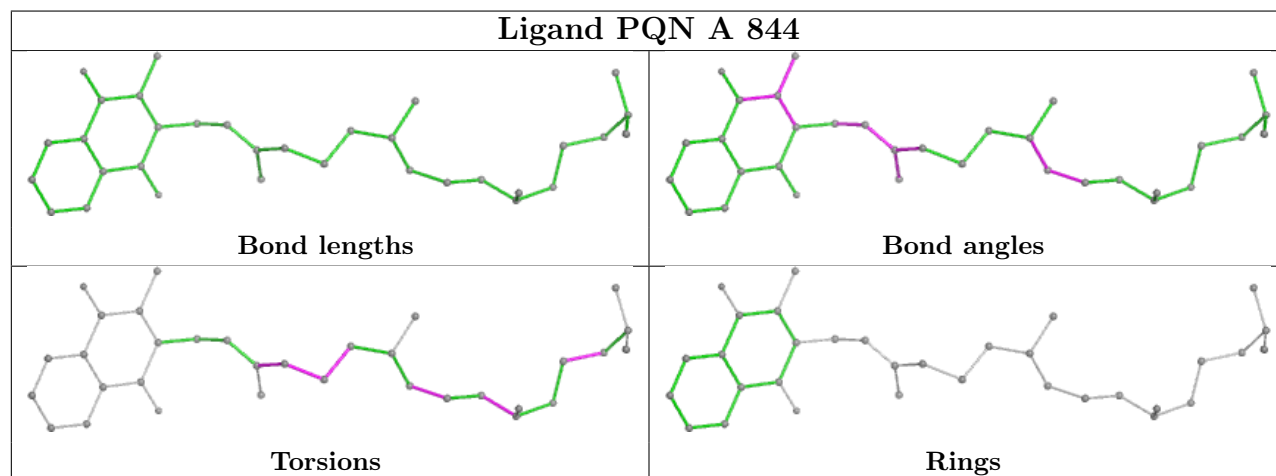
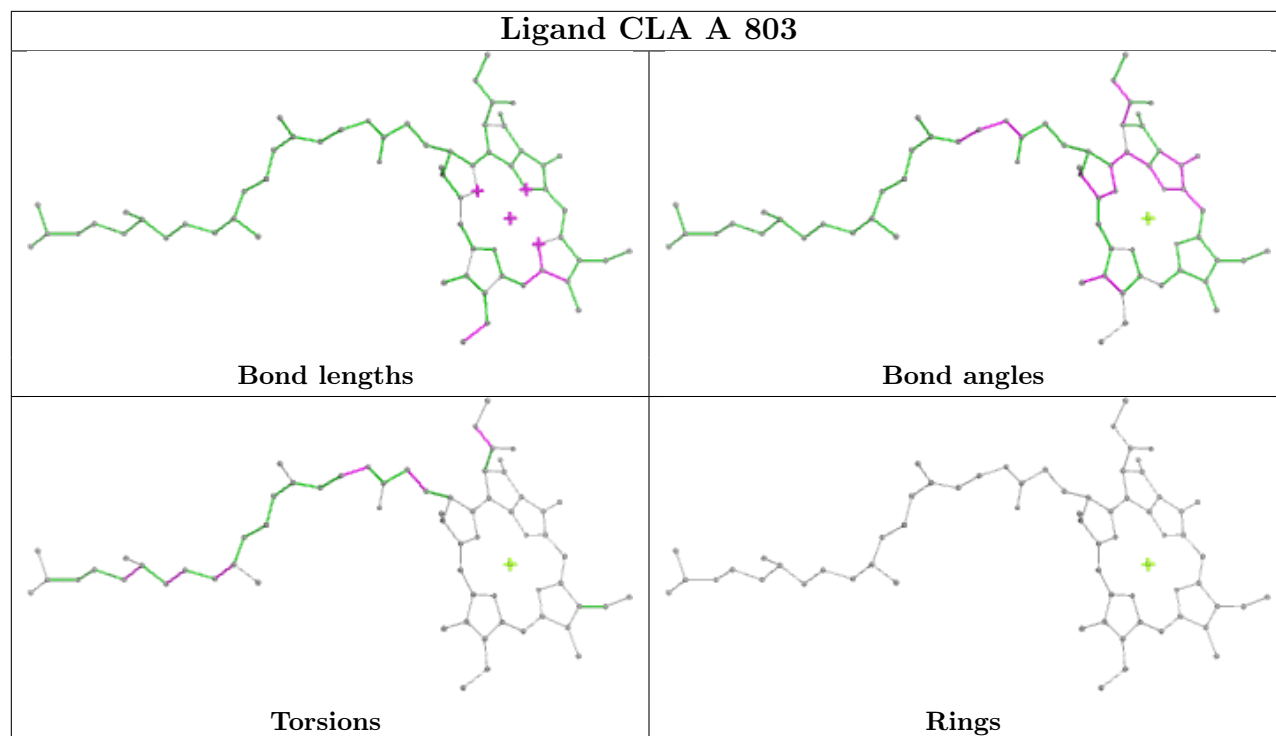


Torsions

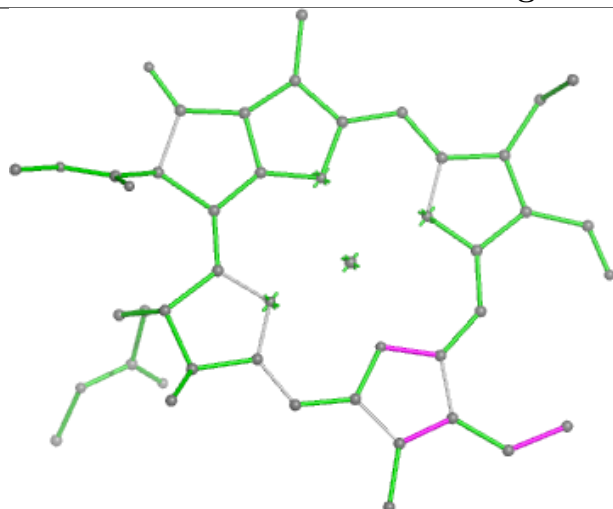


Rings

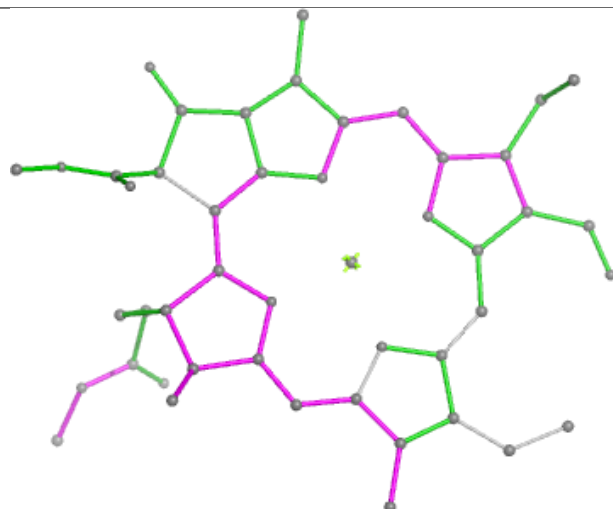




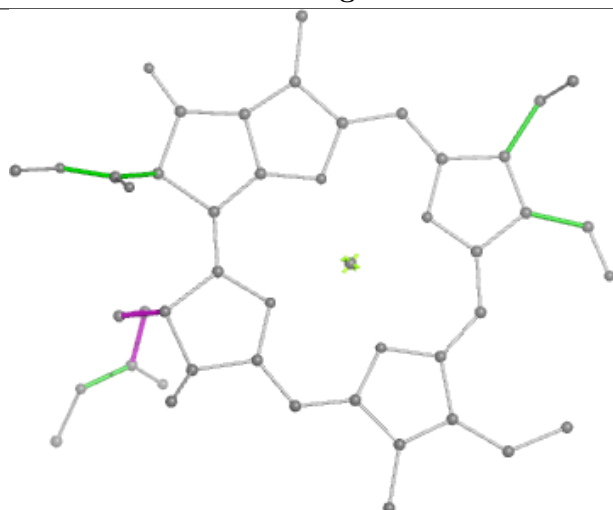
Ligand CHL 1 512



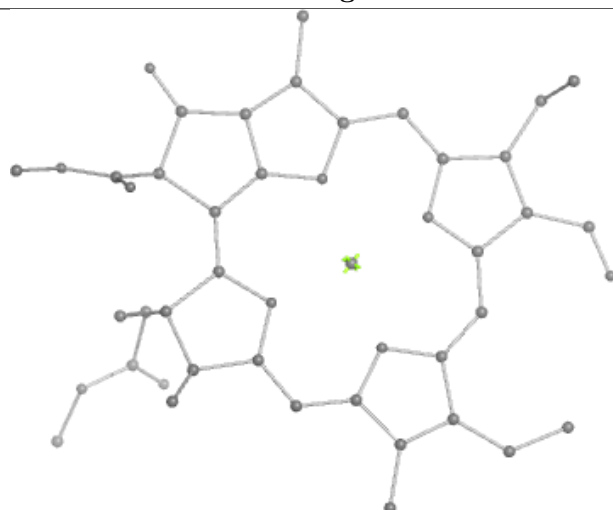
Bond lengths



Bond angles

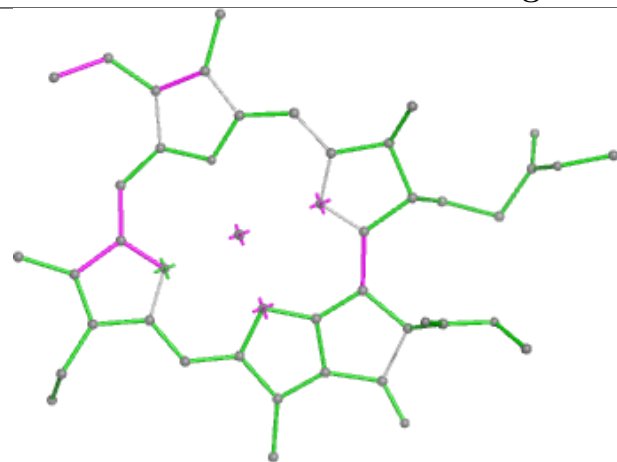


Torsions

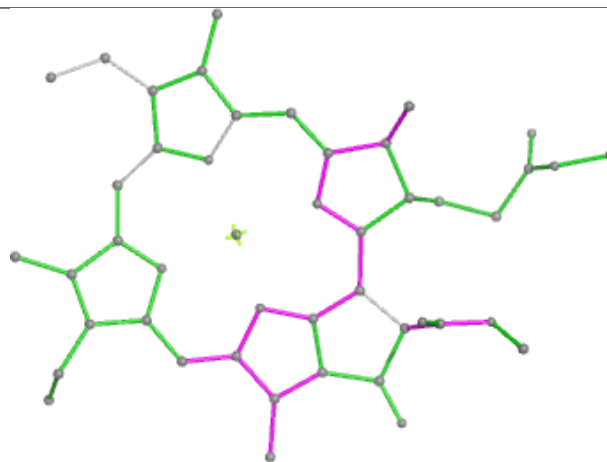


Rings

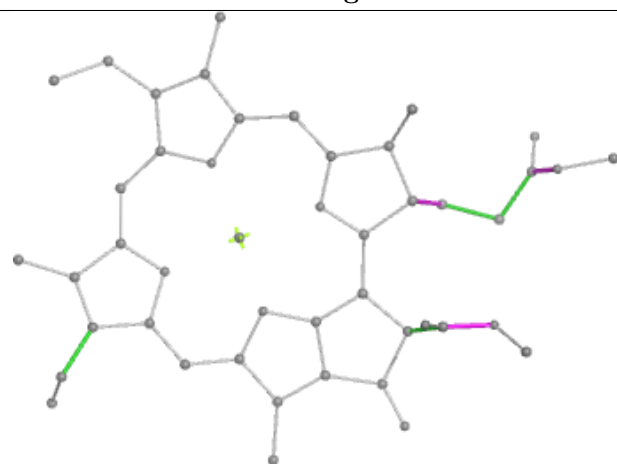
Ligand CLA 3 317



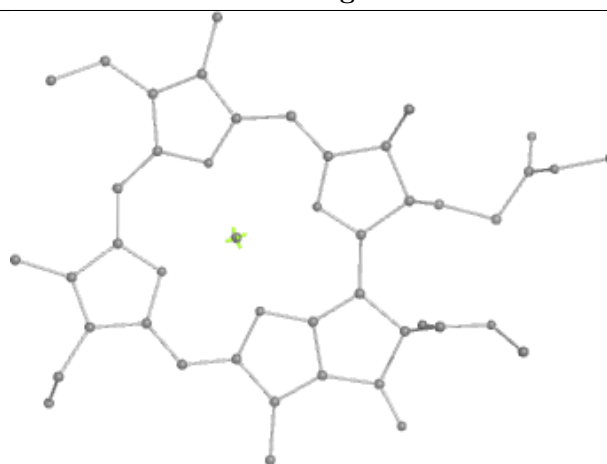
Bond lengths



Bond angles

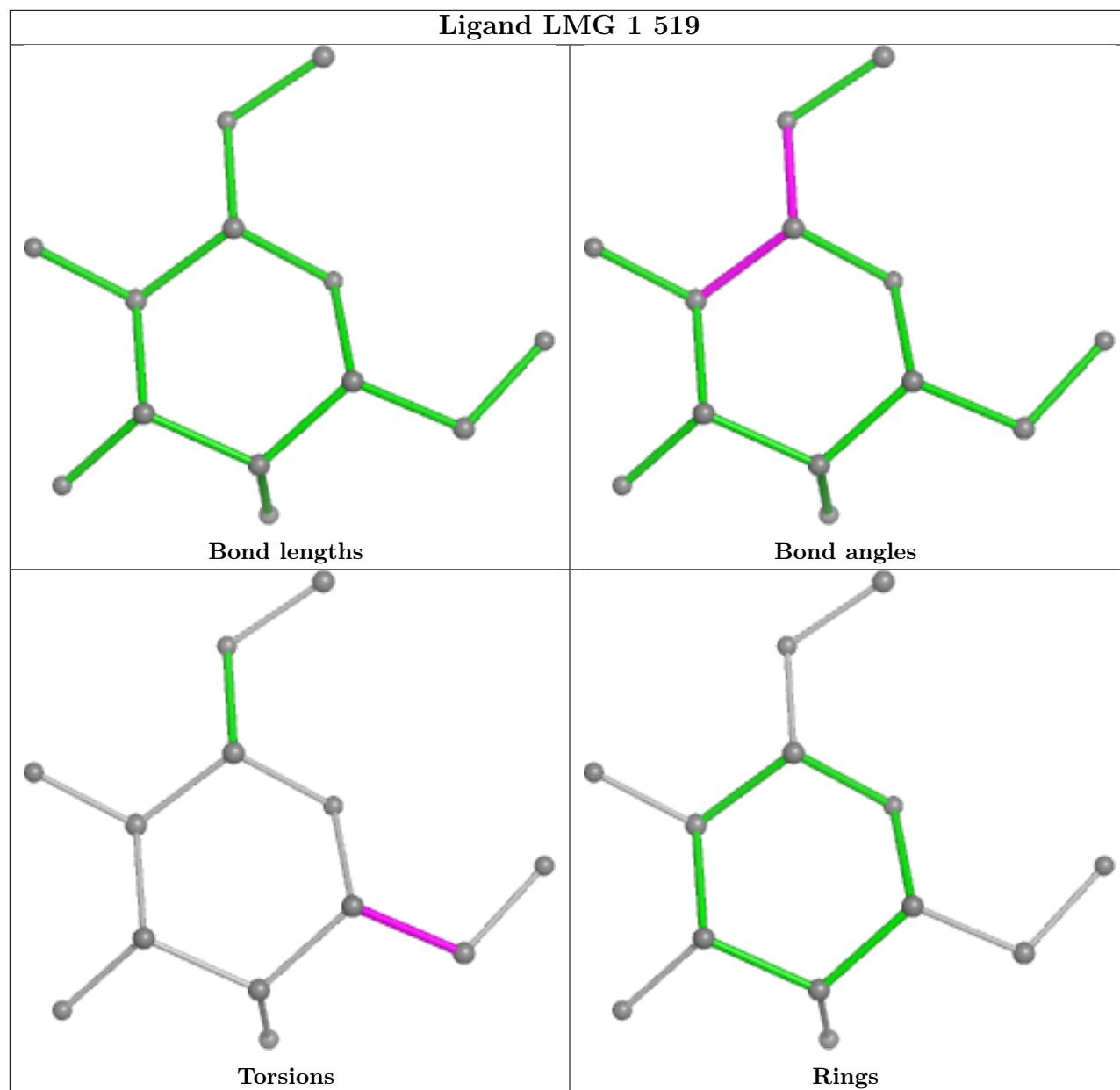


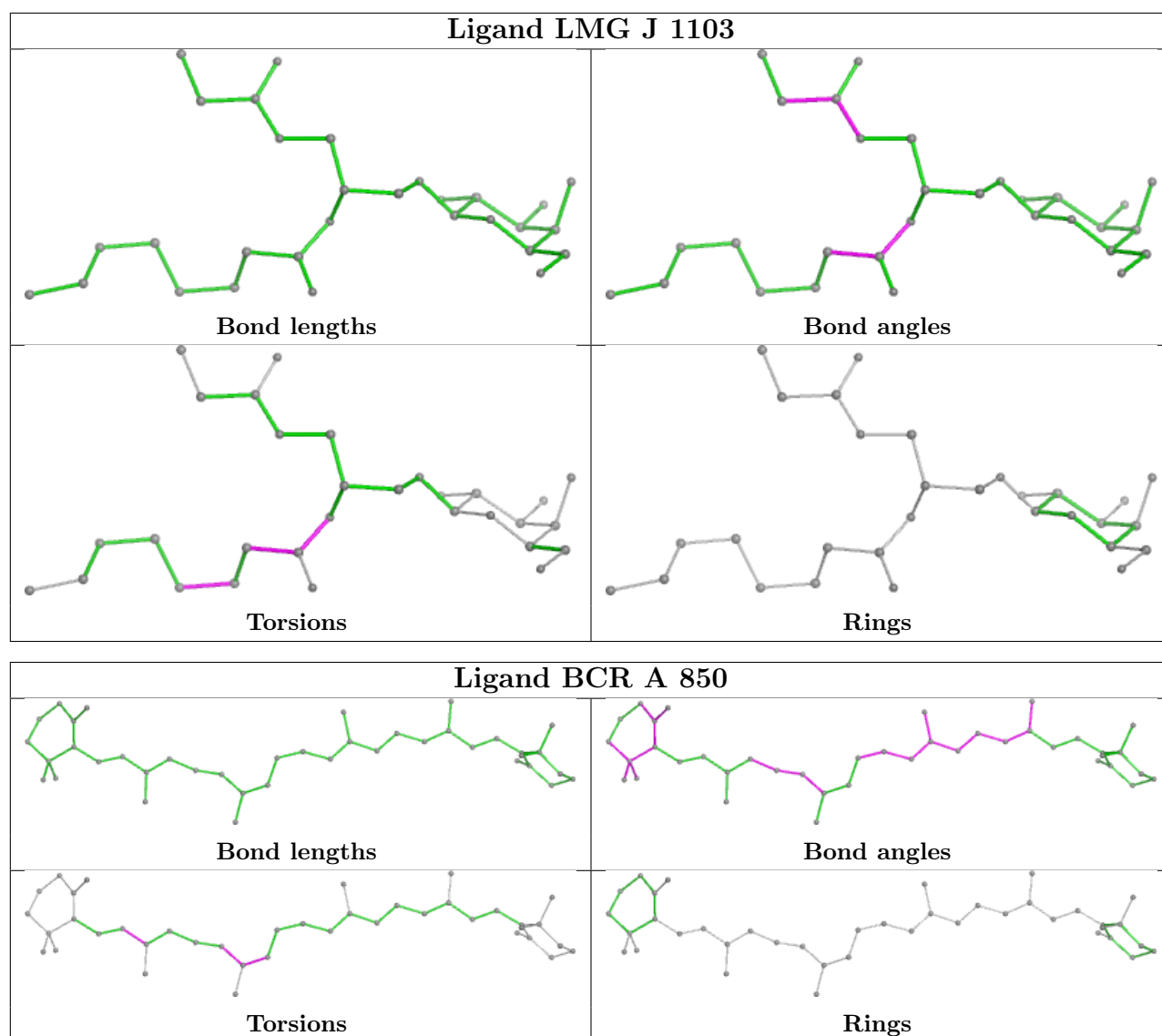
Torsions



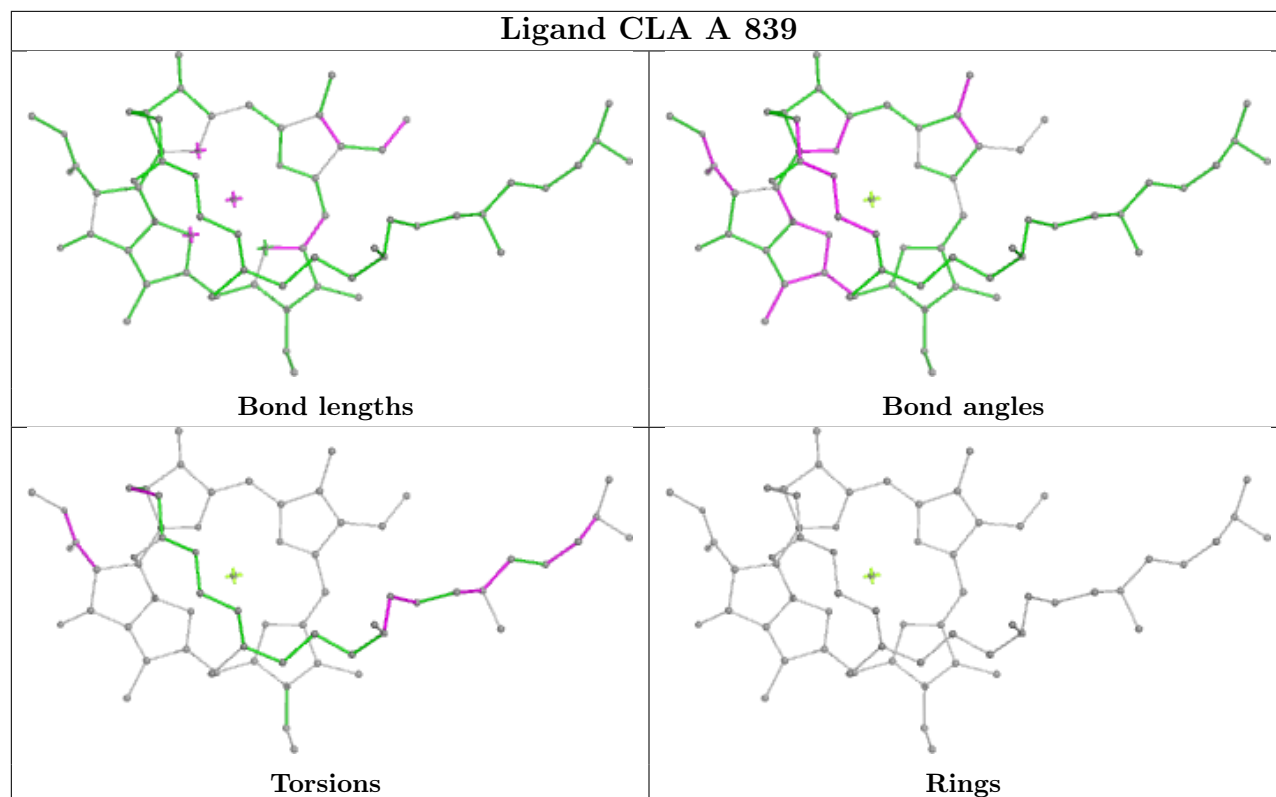
Rings

Ligand LMG 1 519

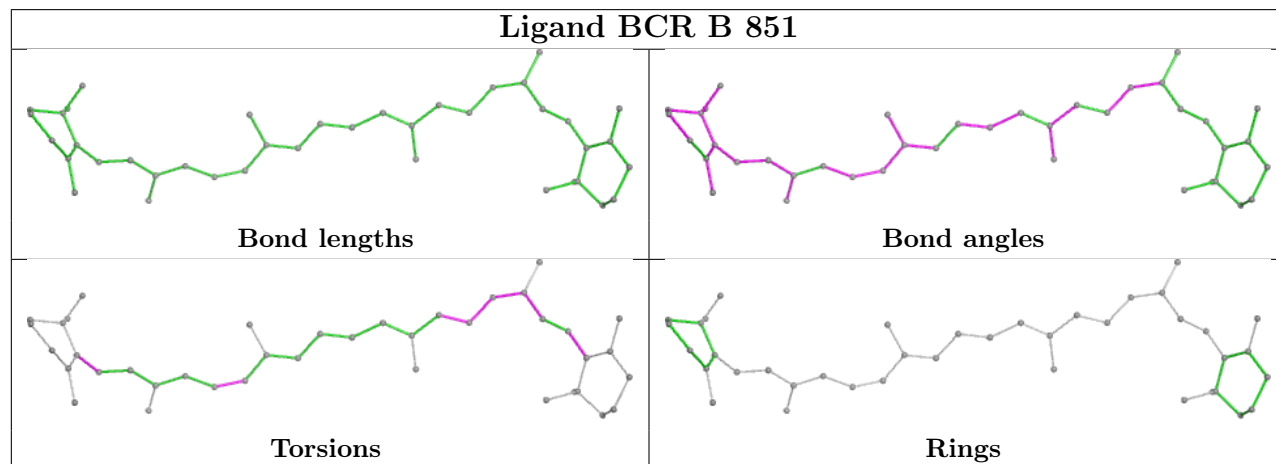




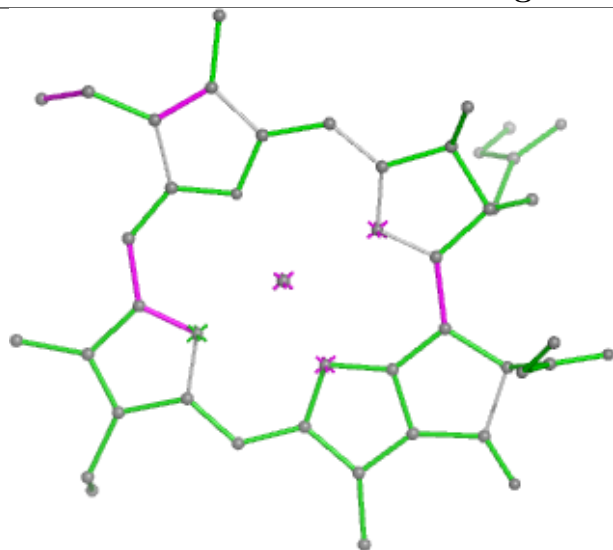
Ligand CLA A 839



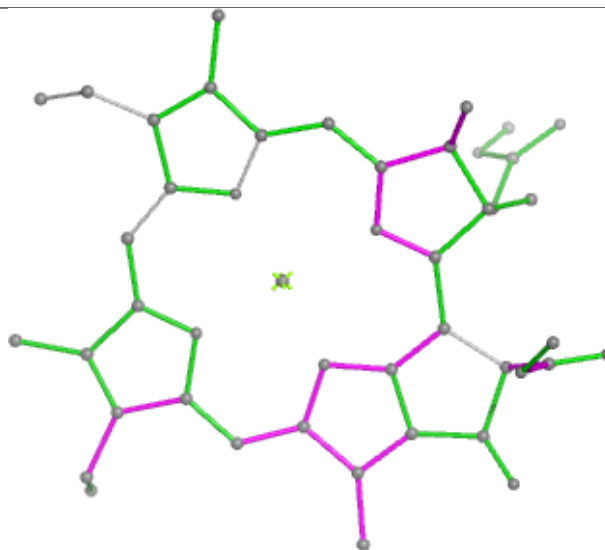
Ligand BCR B 851



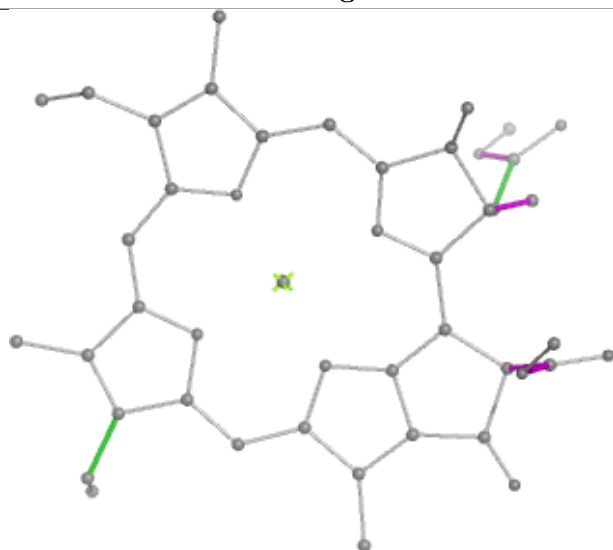
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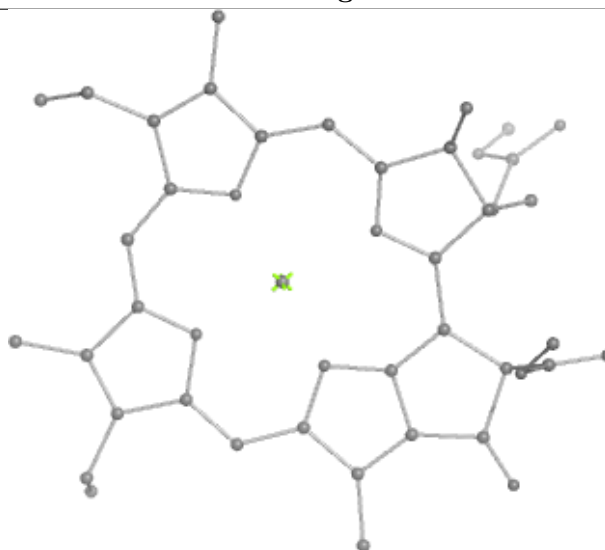
Bond lengths



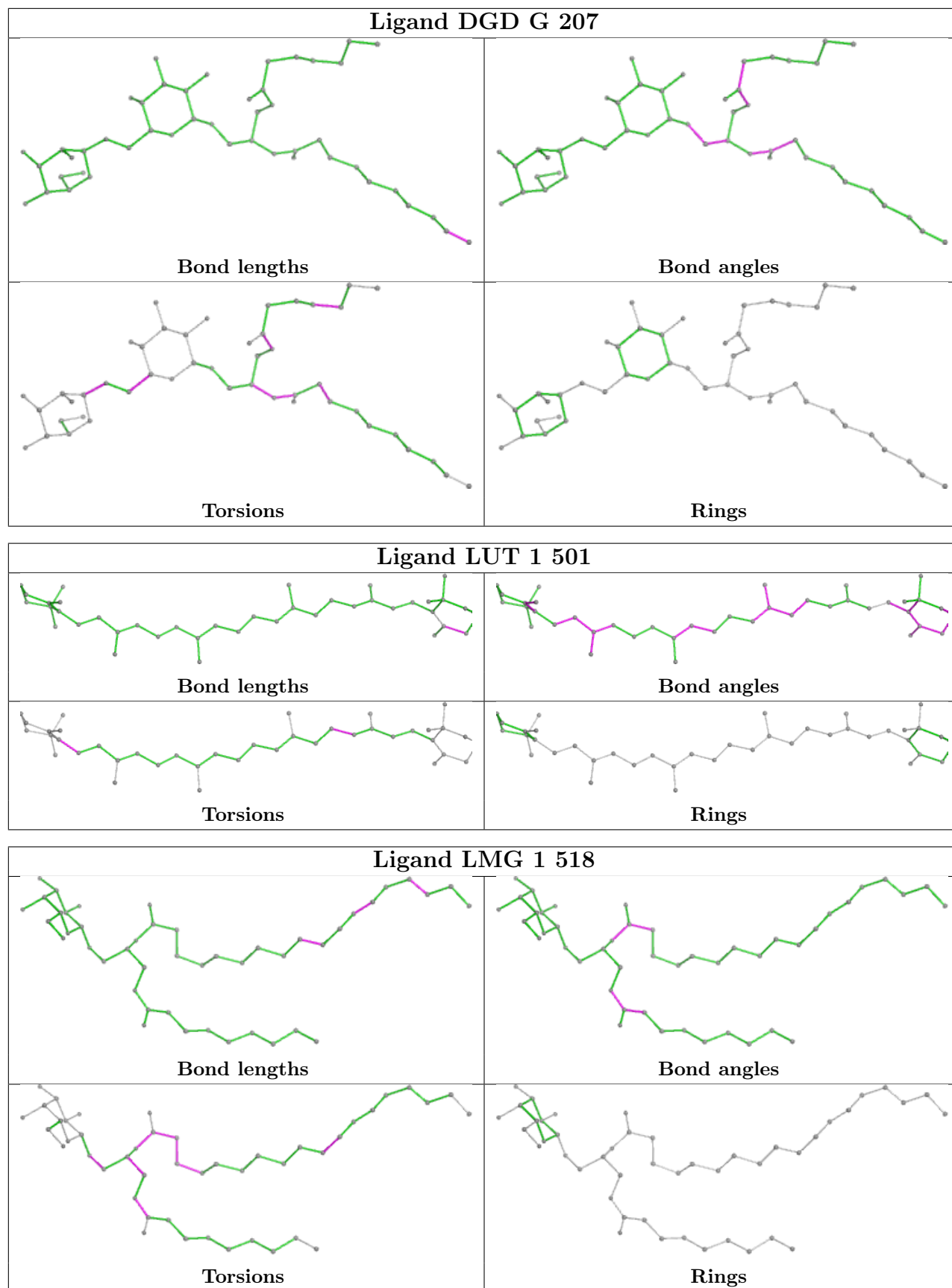
Bond angles

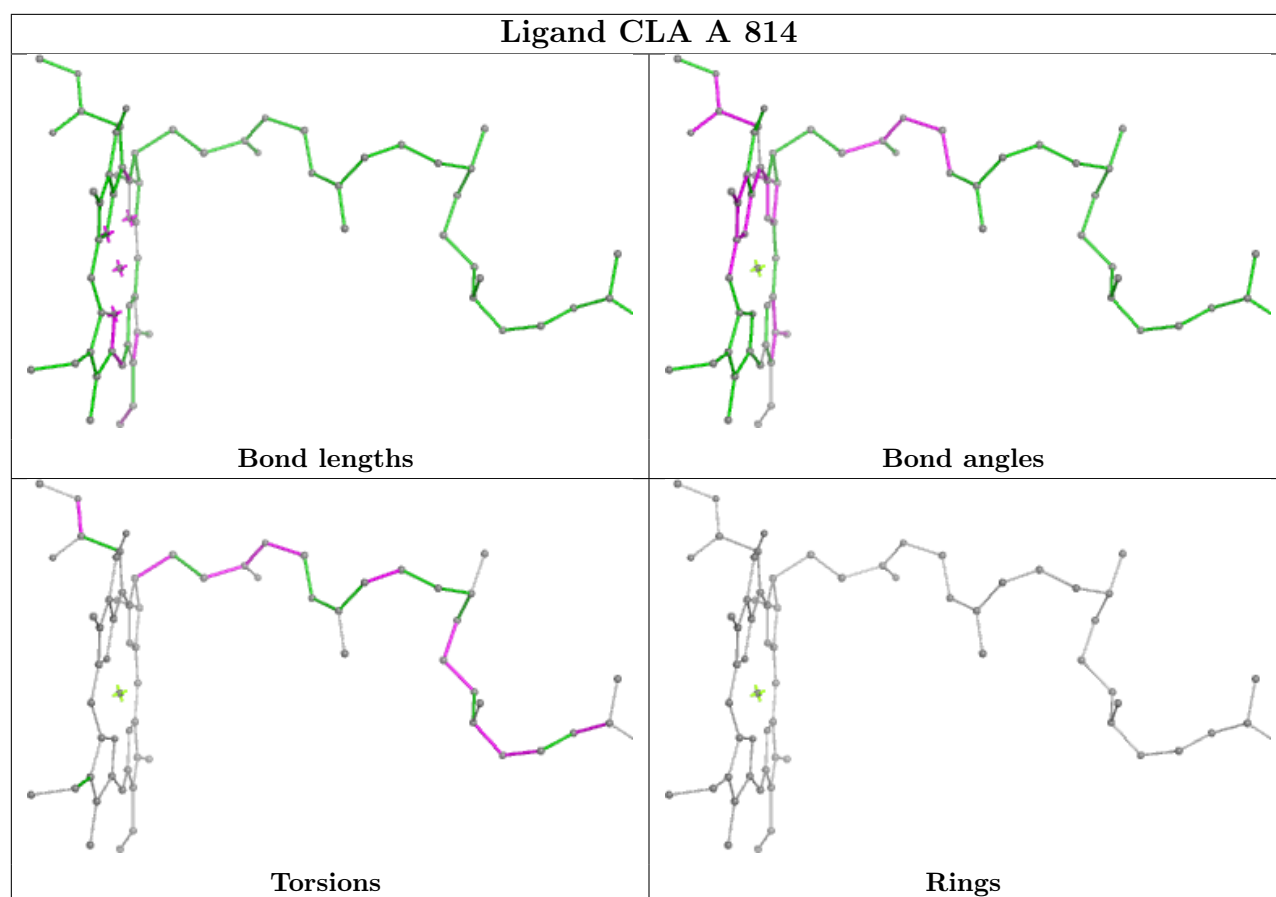


Torsions

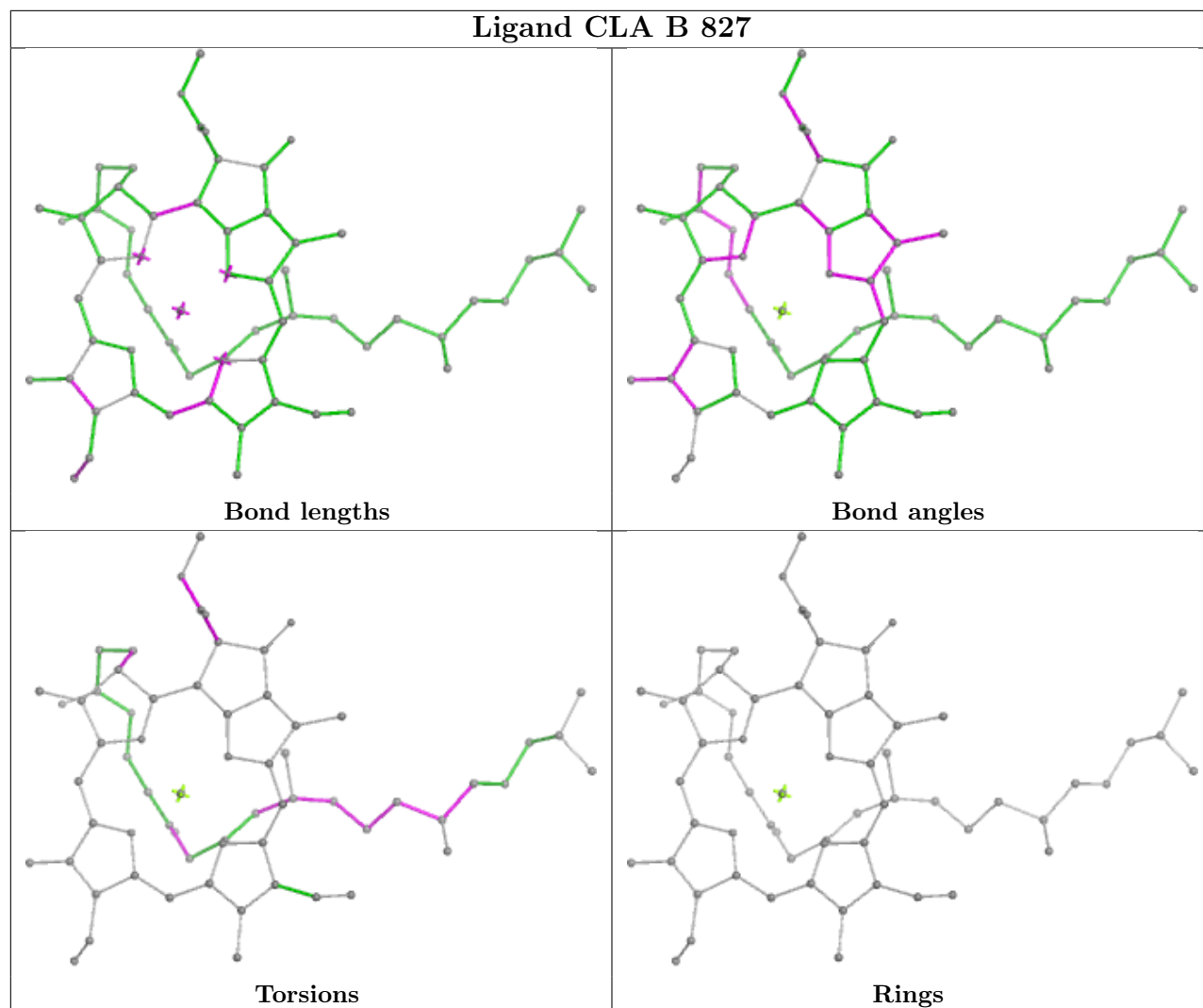


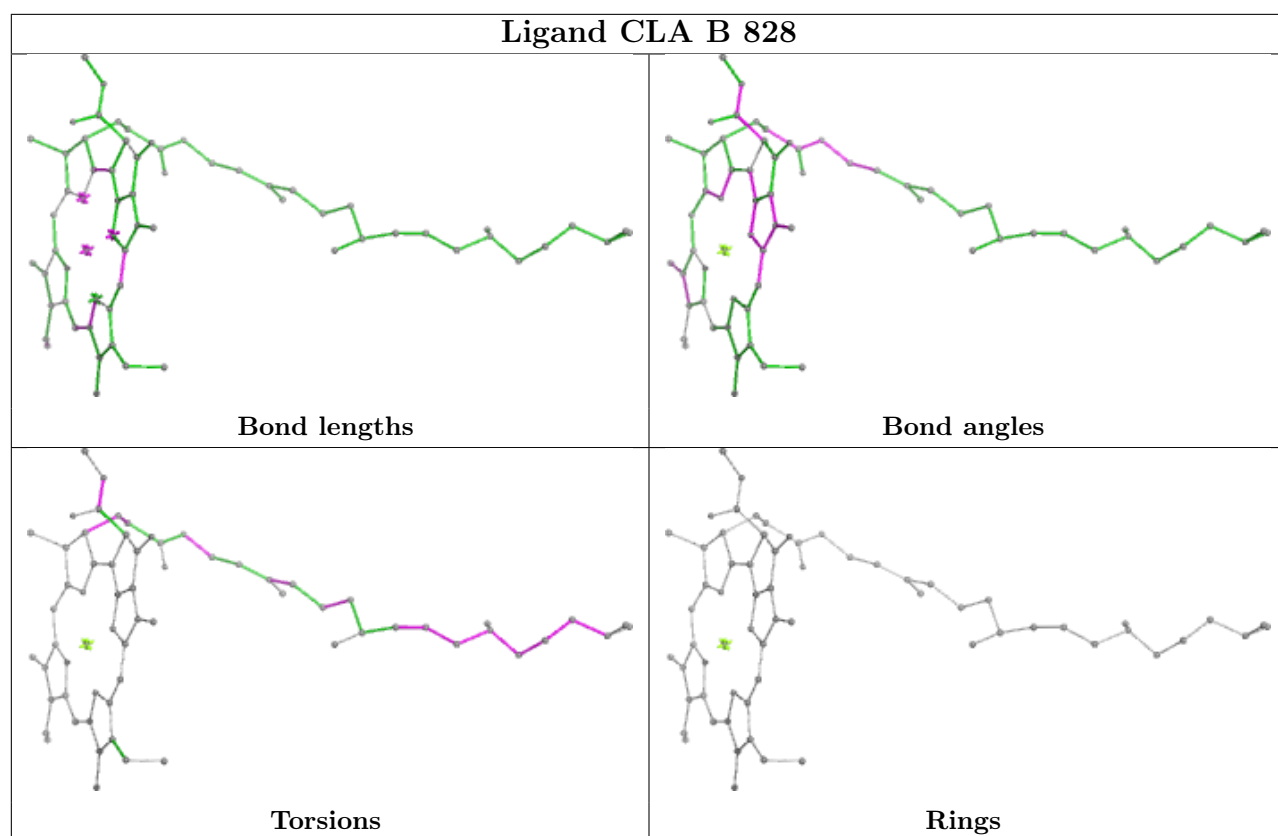
Rings



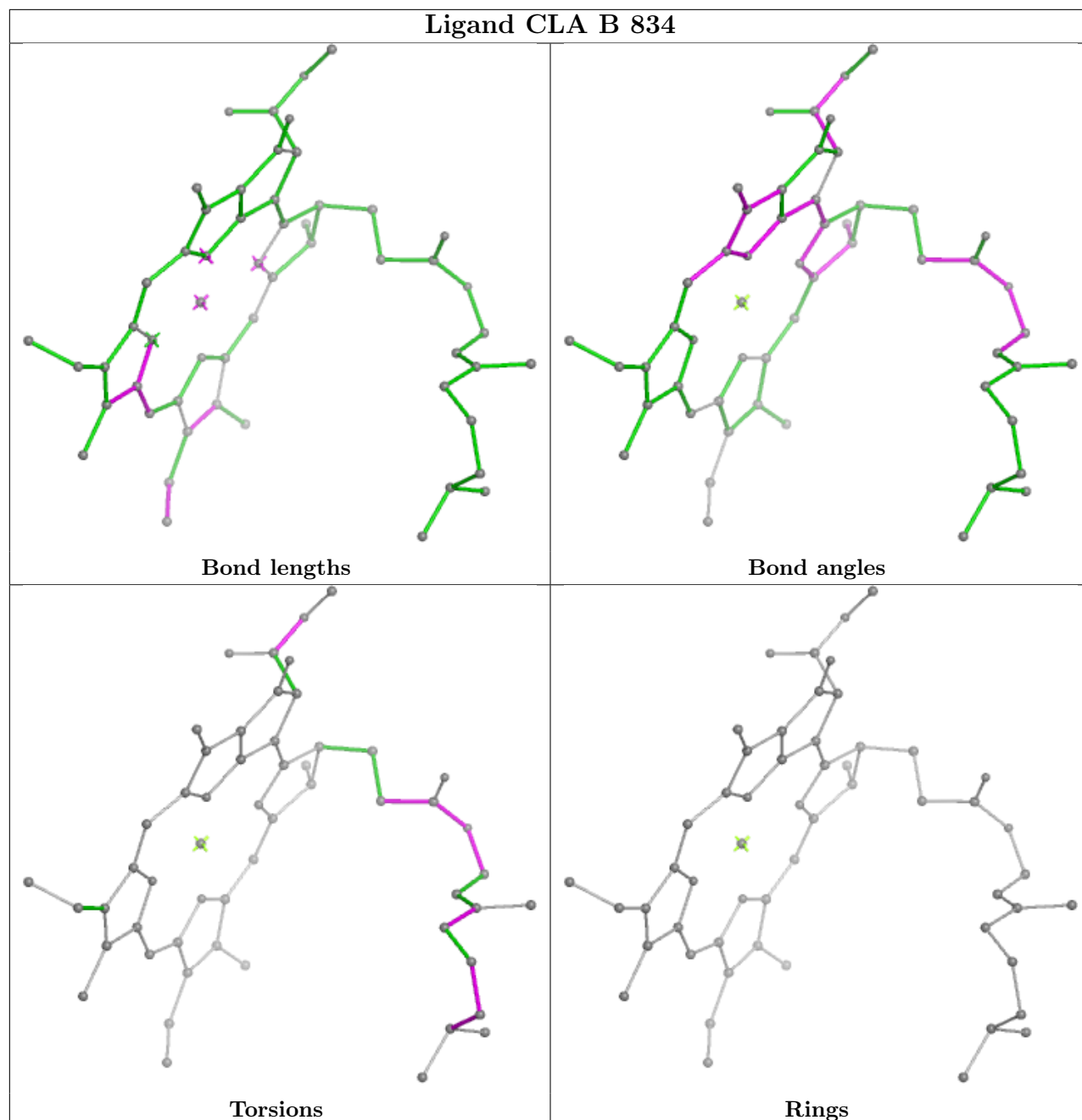


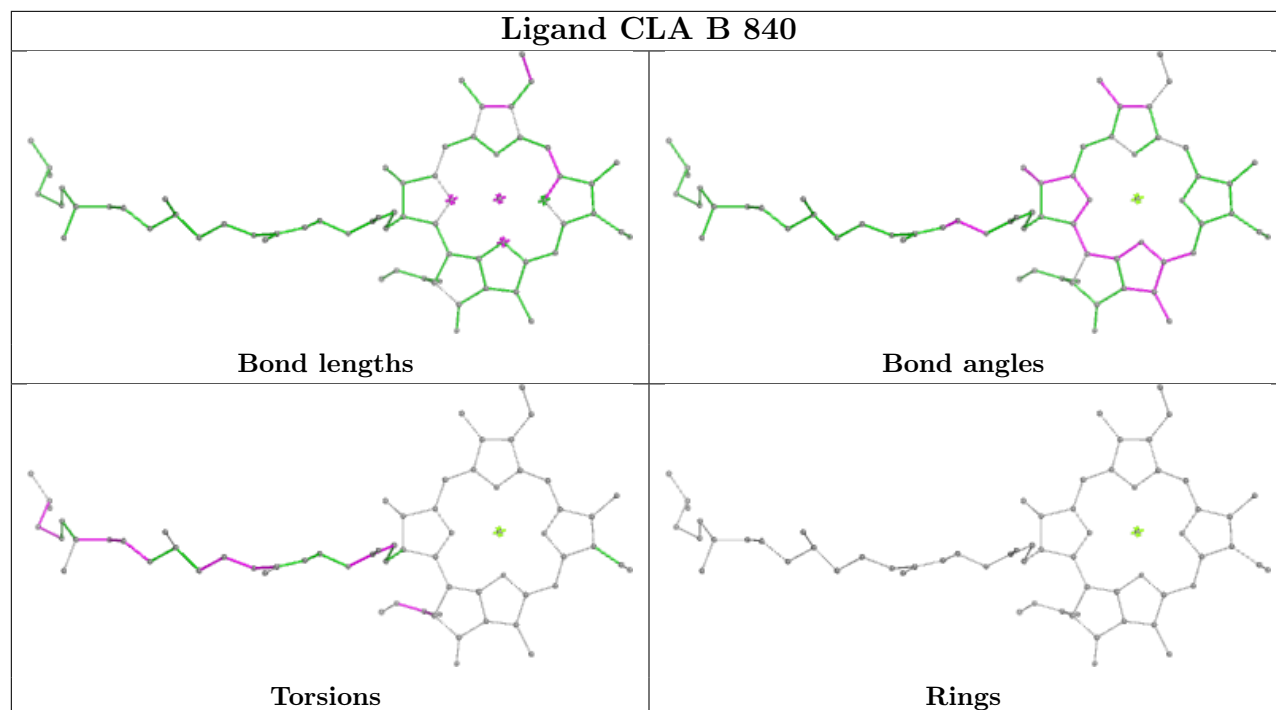
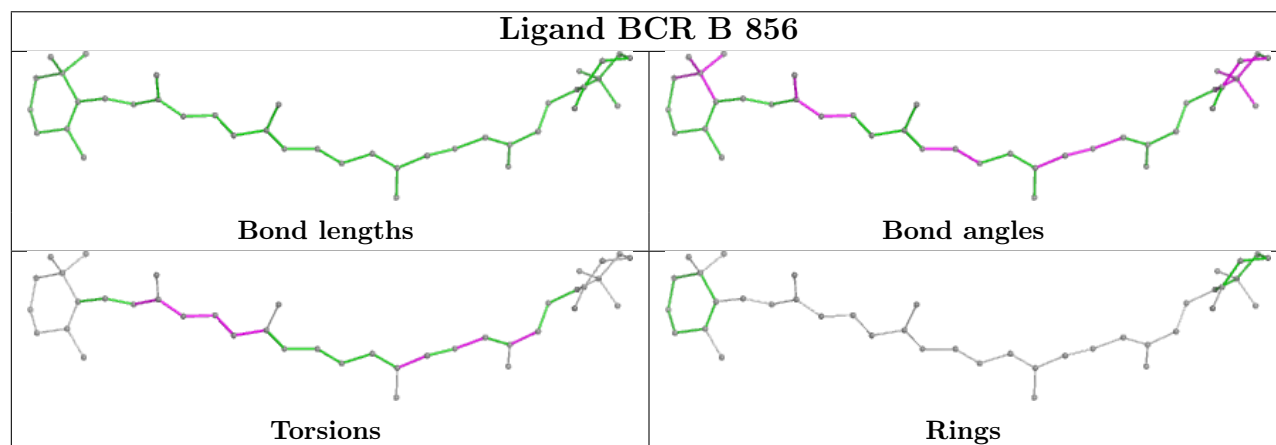
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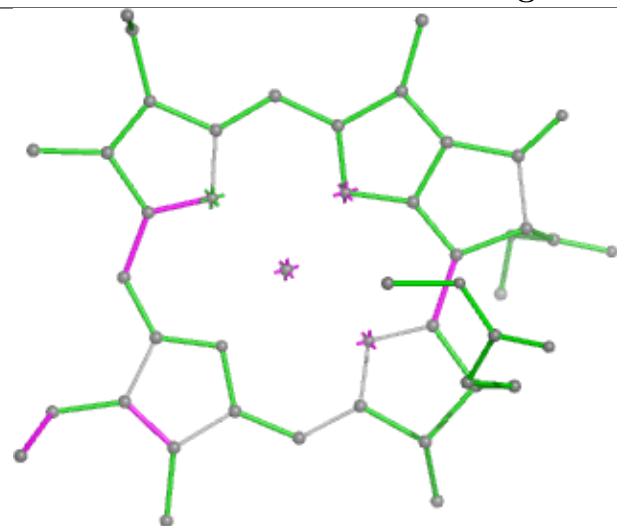


Ligand CLA B 834

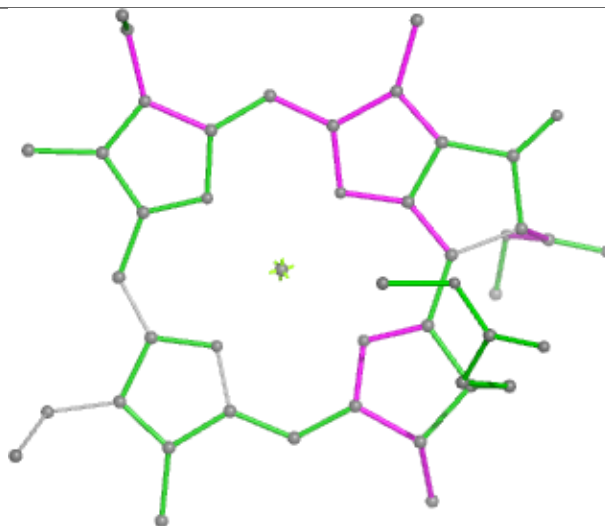


Ligand CLA B 840**Ligand BCR B 856**

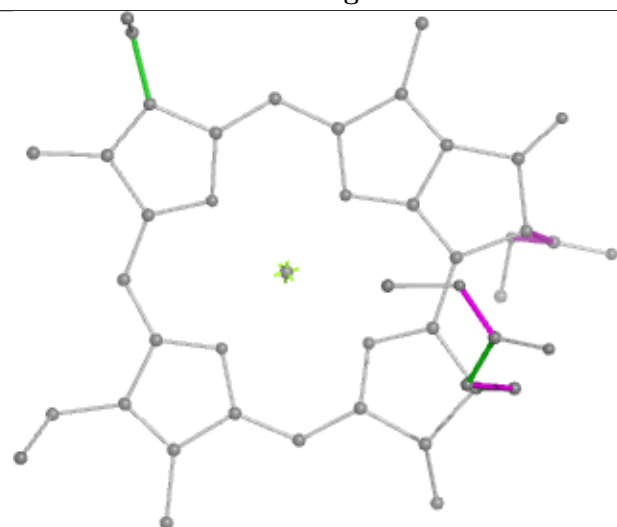
Ligand CLA A 816



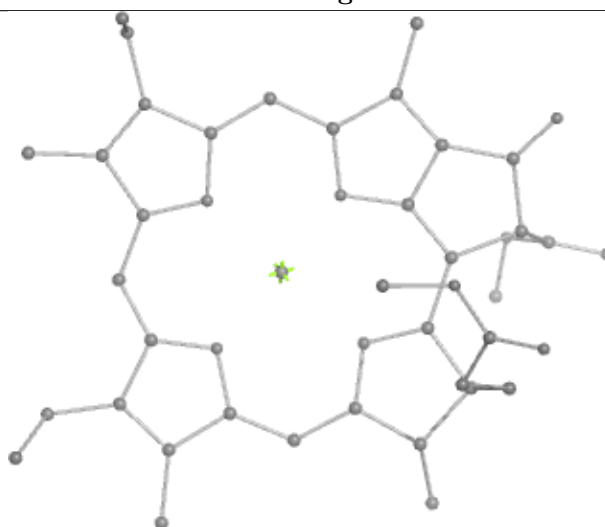
Bond lengths



Bond angles

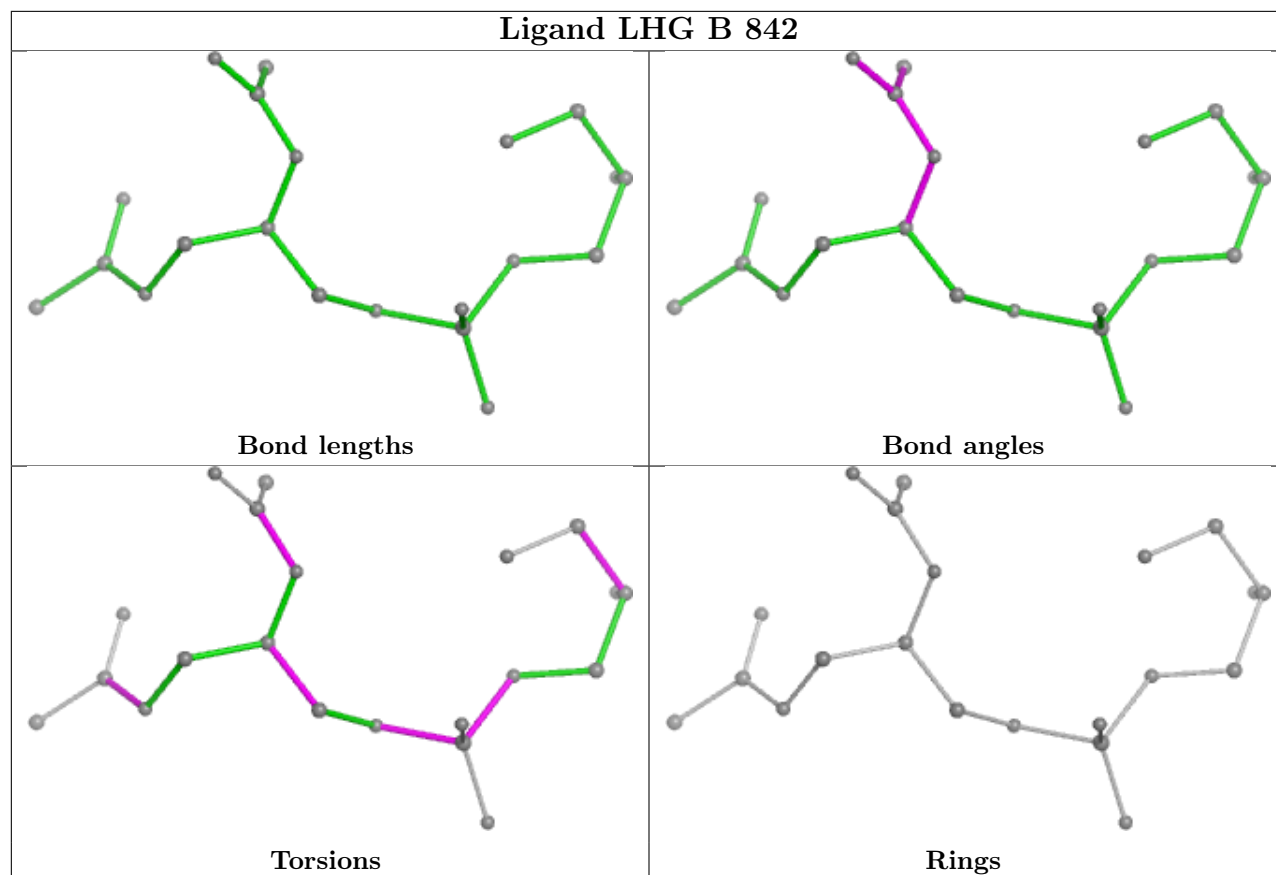


Torsions

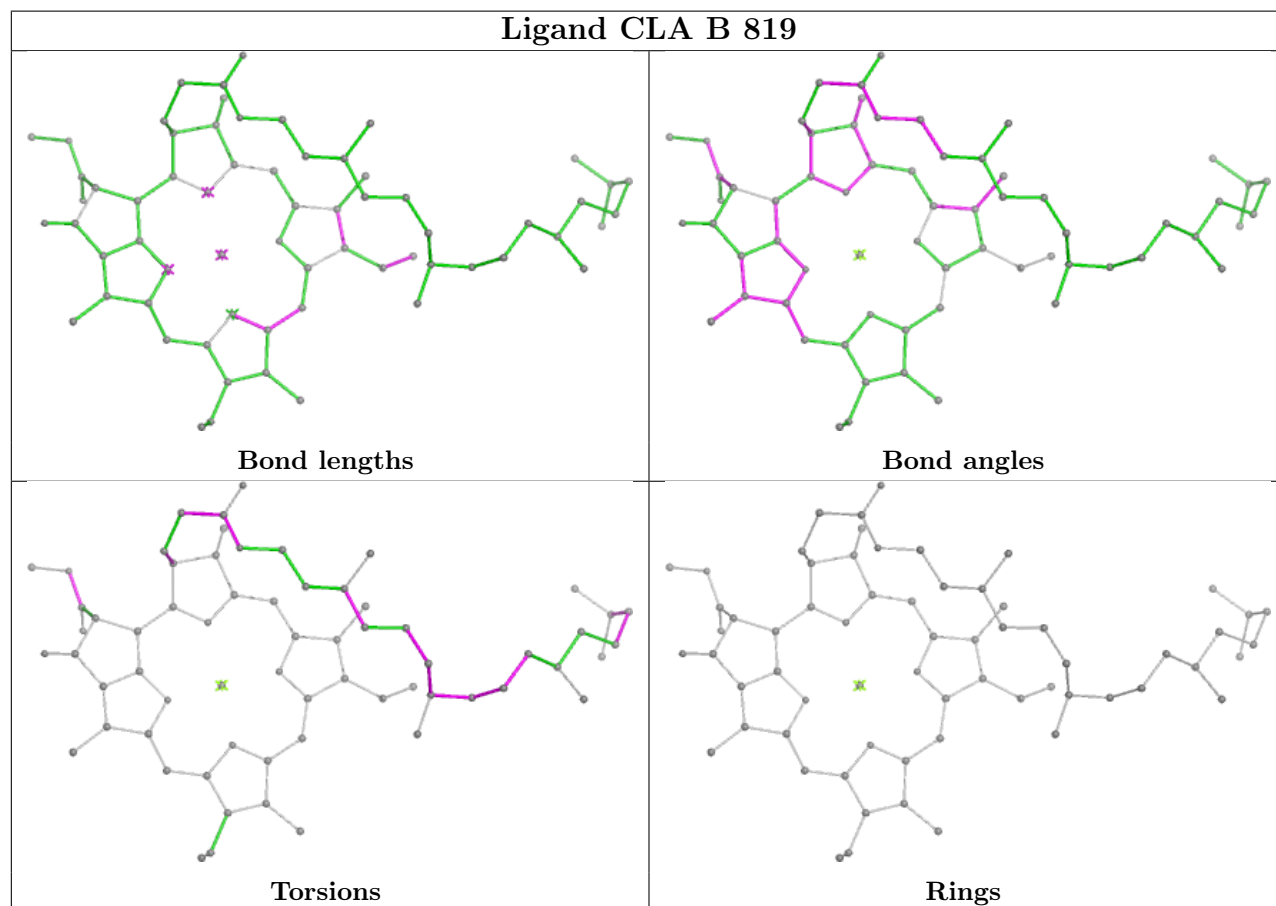


Rings

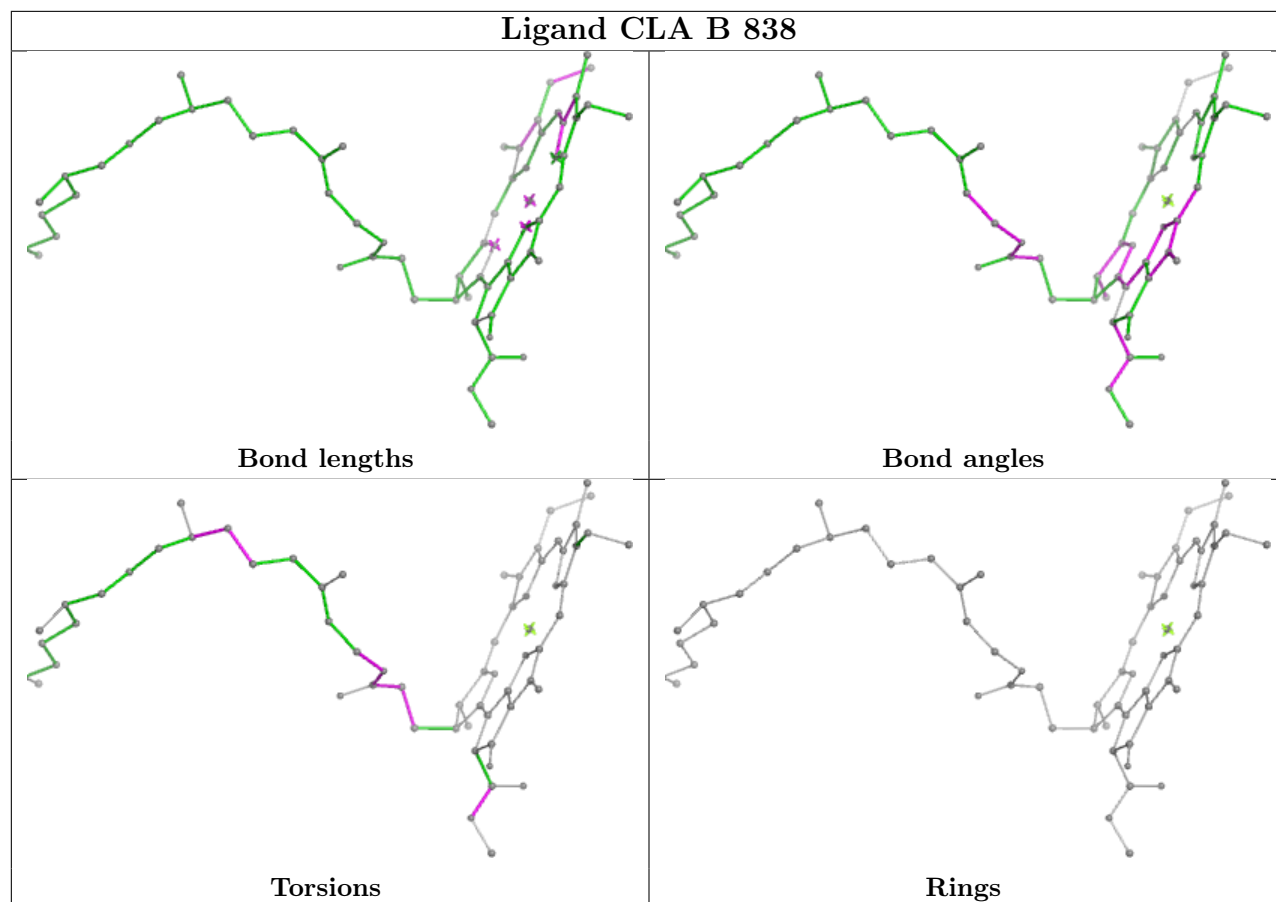
Ligand LHG B 842



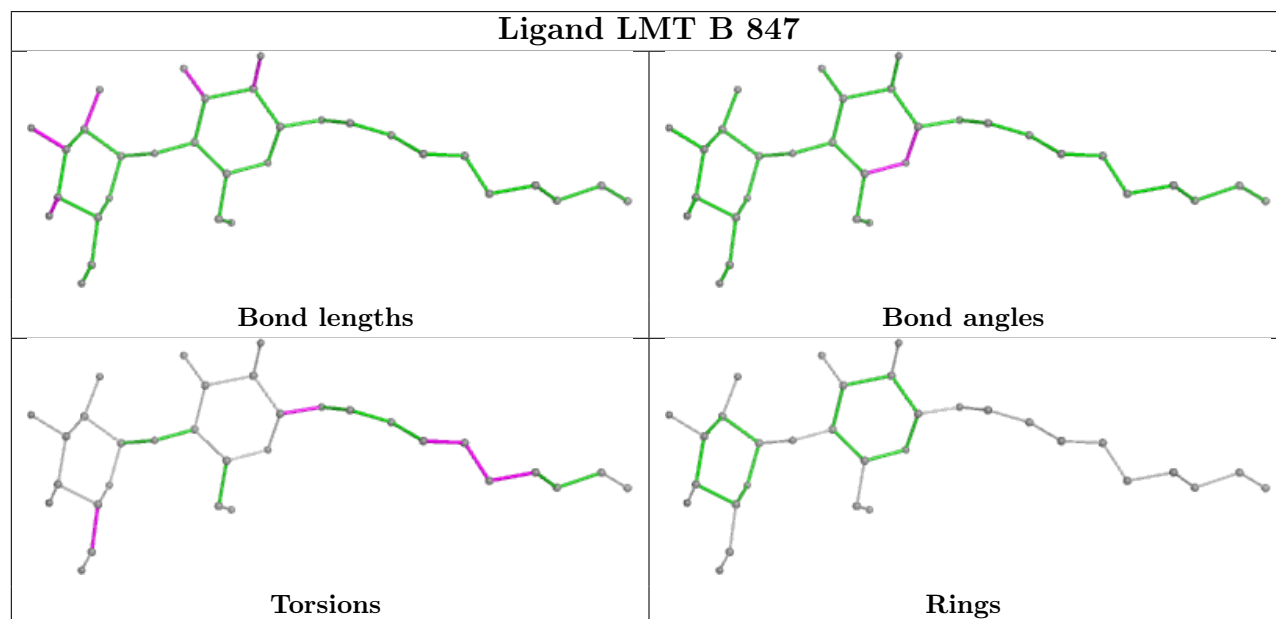
Ligand CLA B 819

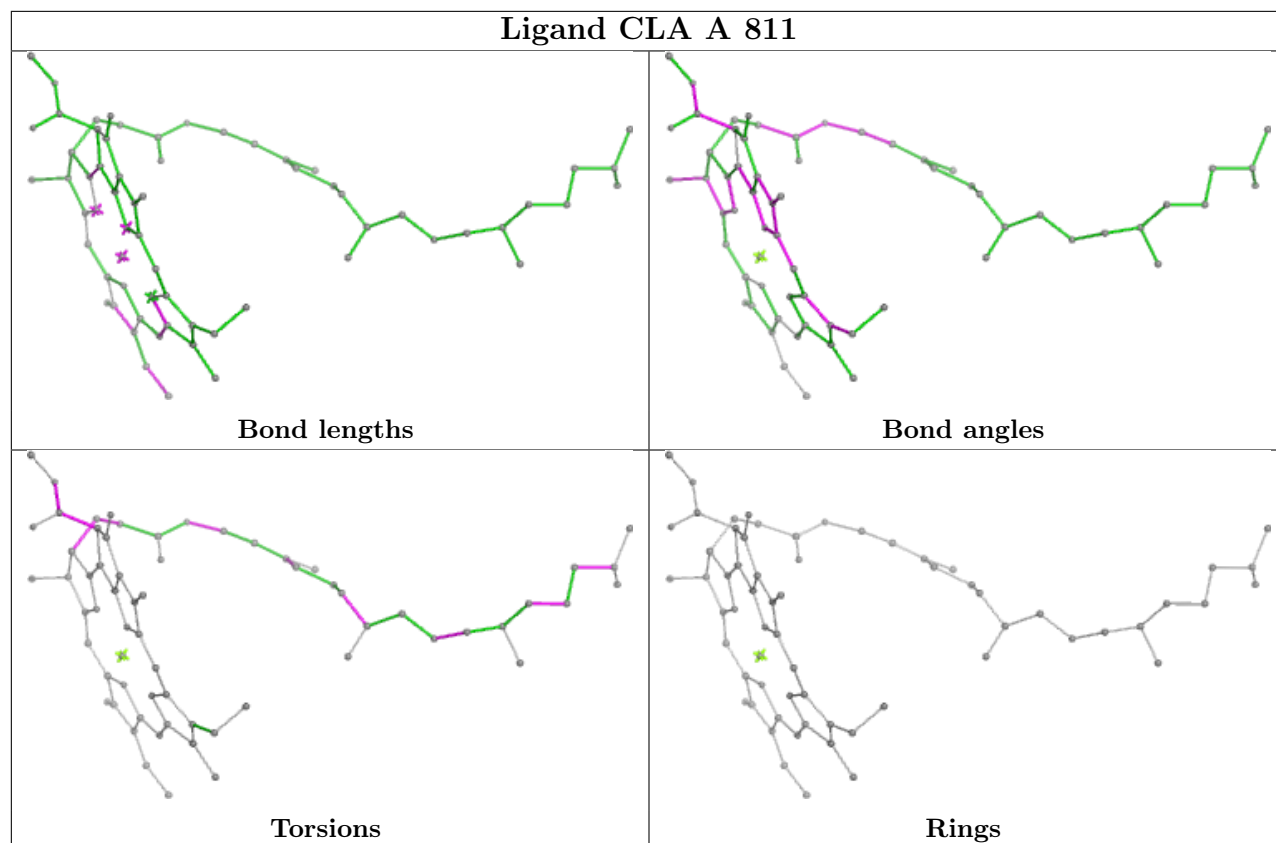


Ligand CLA B 838

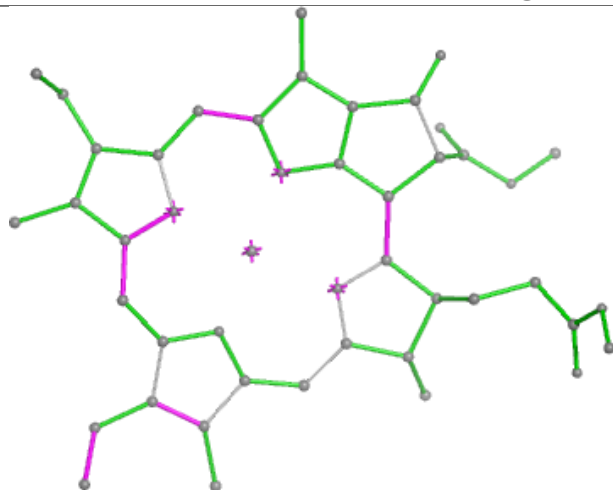


Ligand LMT B 847

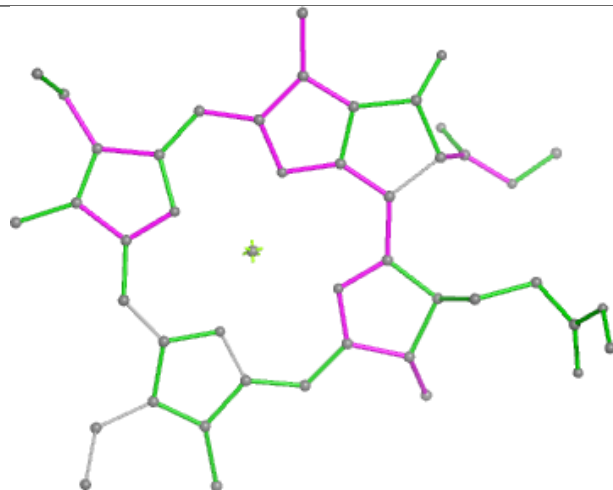




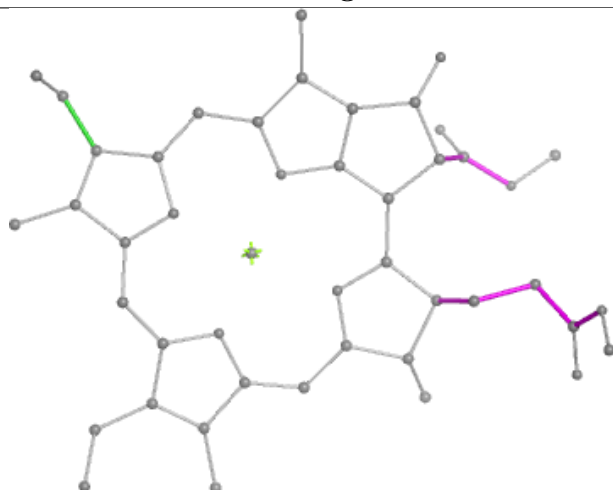
Ligand CLA 3 316



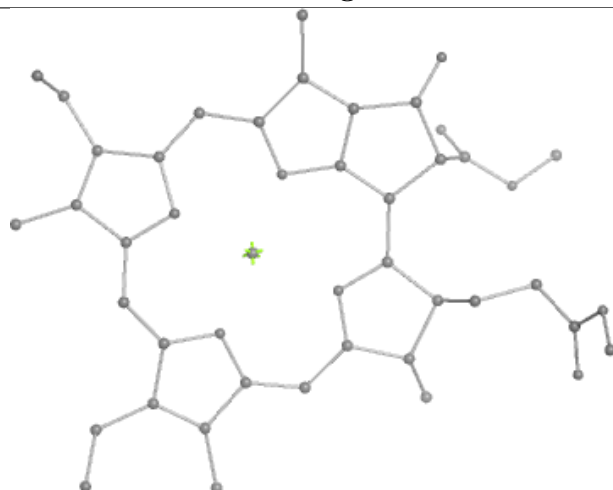
Bond lengths



Bond angles

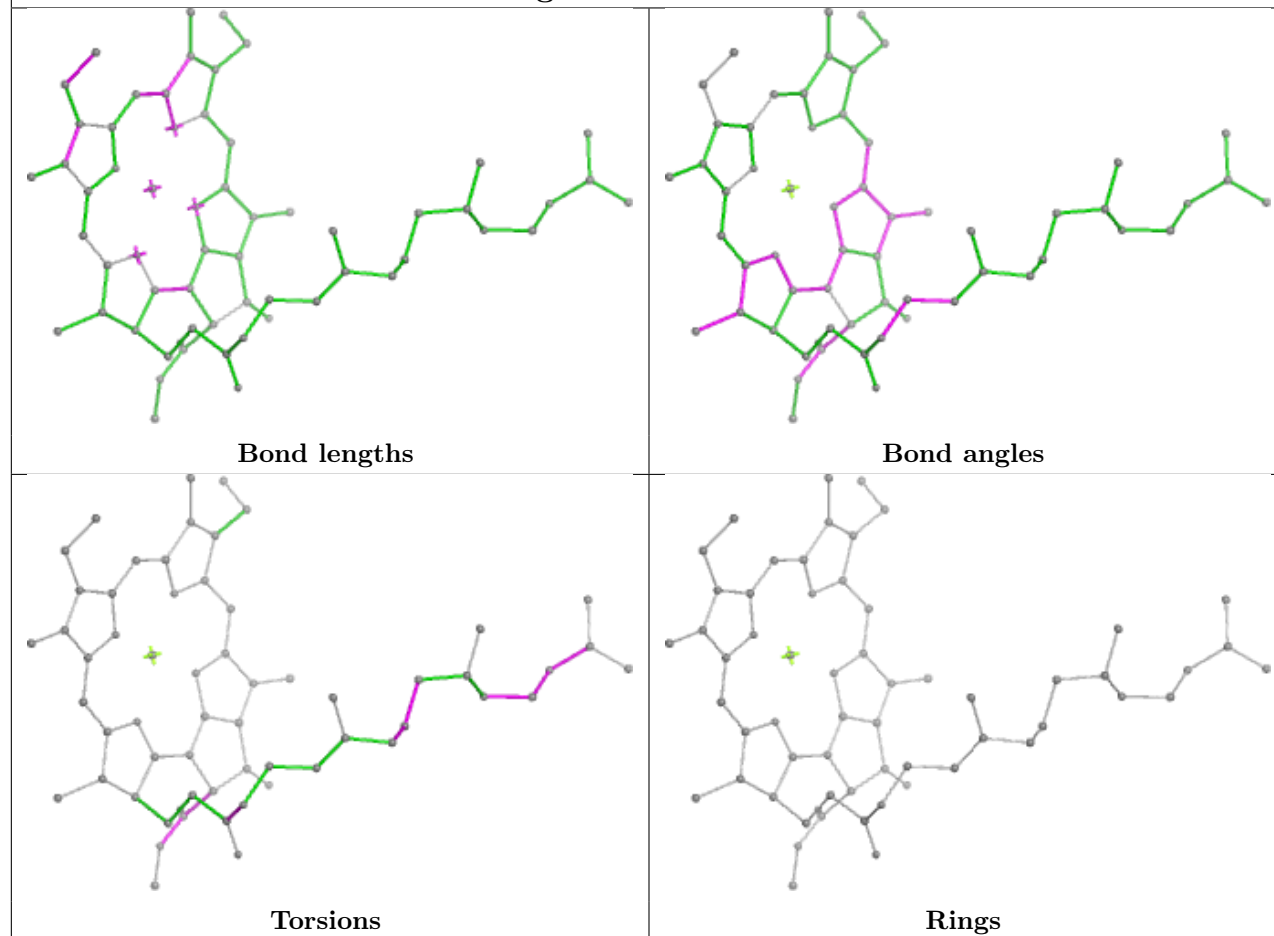


Torsions

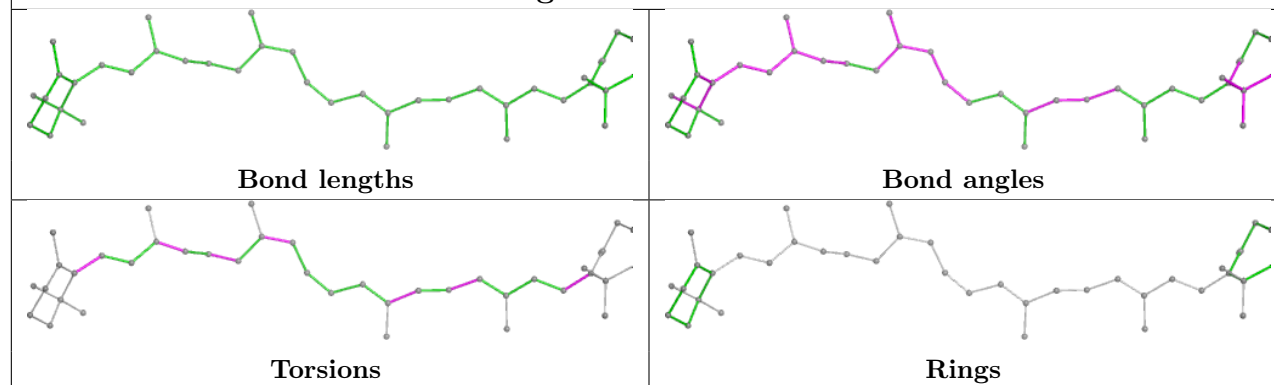


Rings

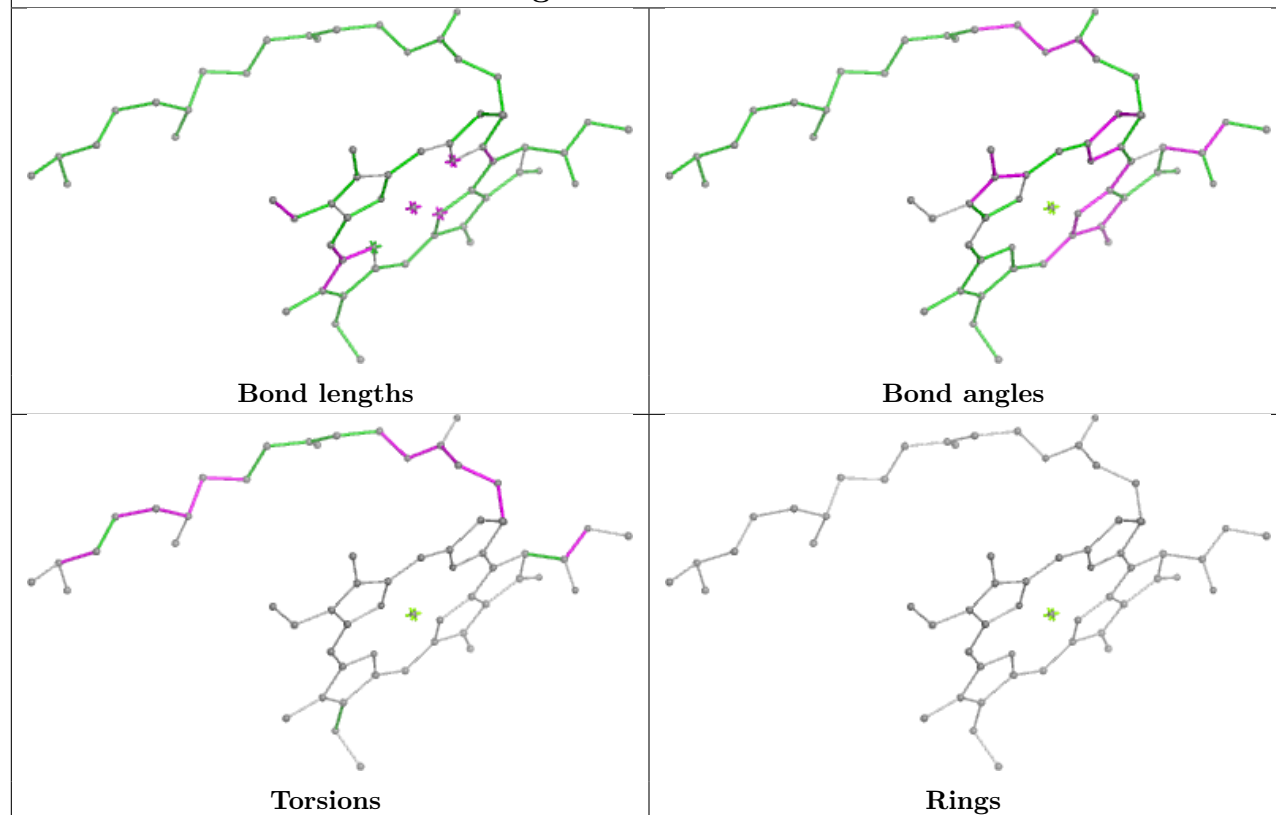
Ligand CLA 4 310



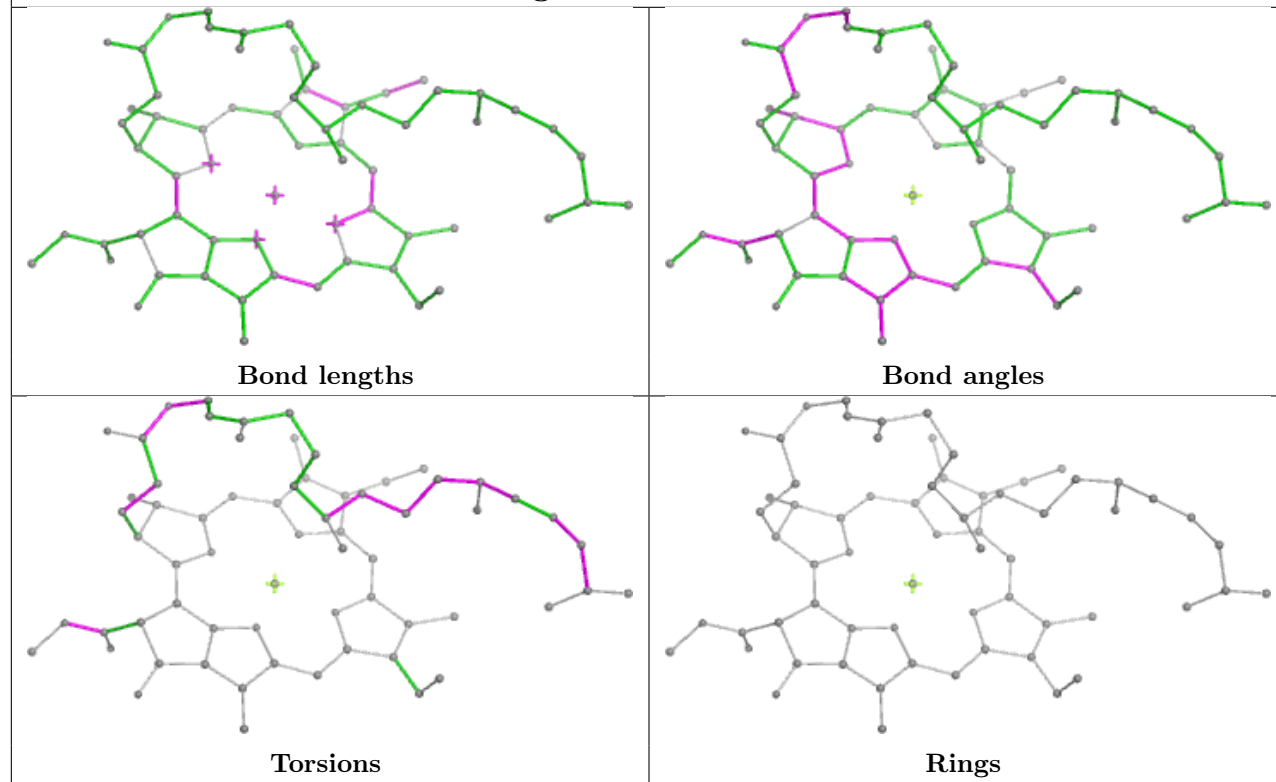
Ligand BCR I 101



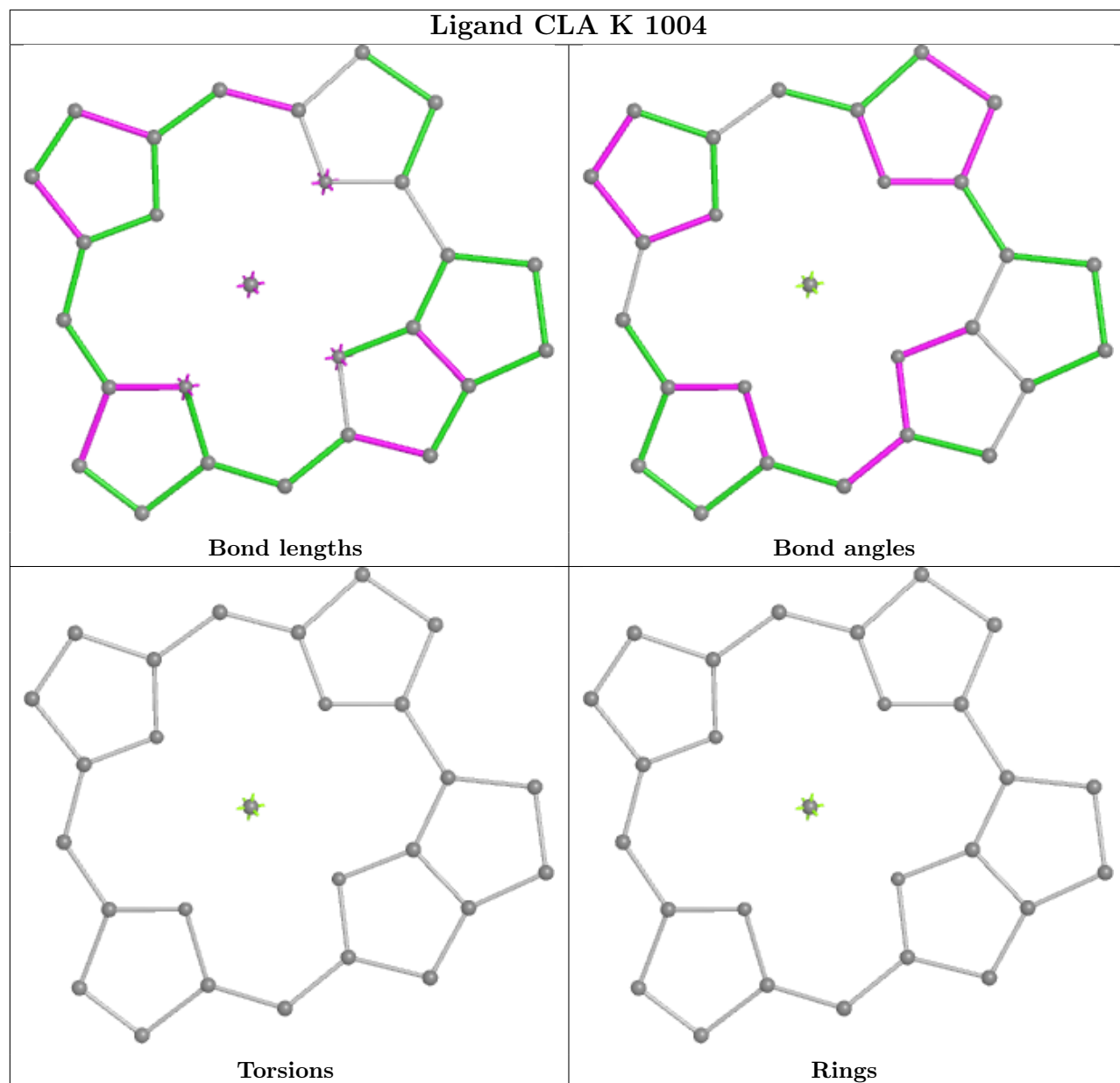
Ligand CLA B 831

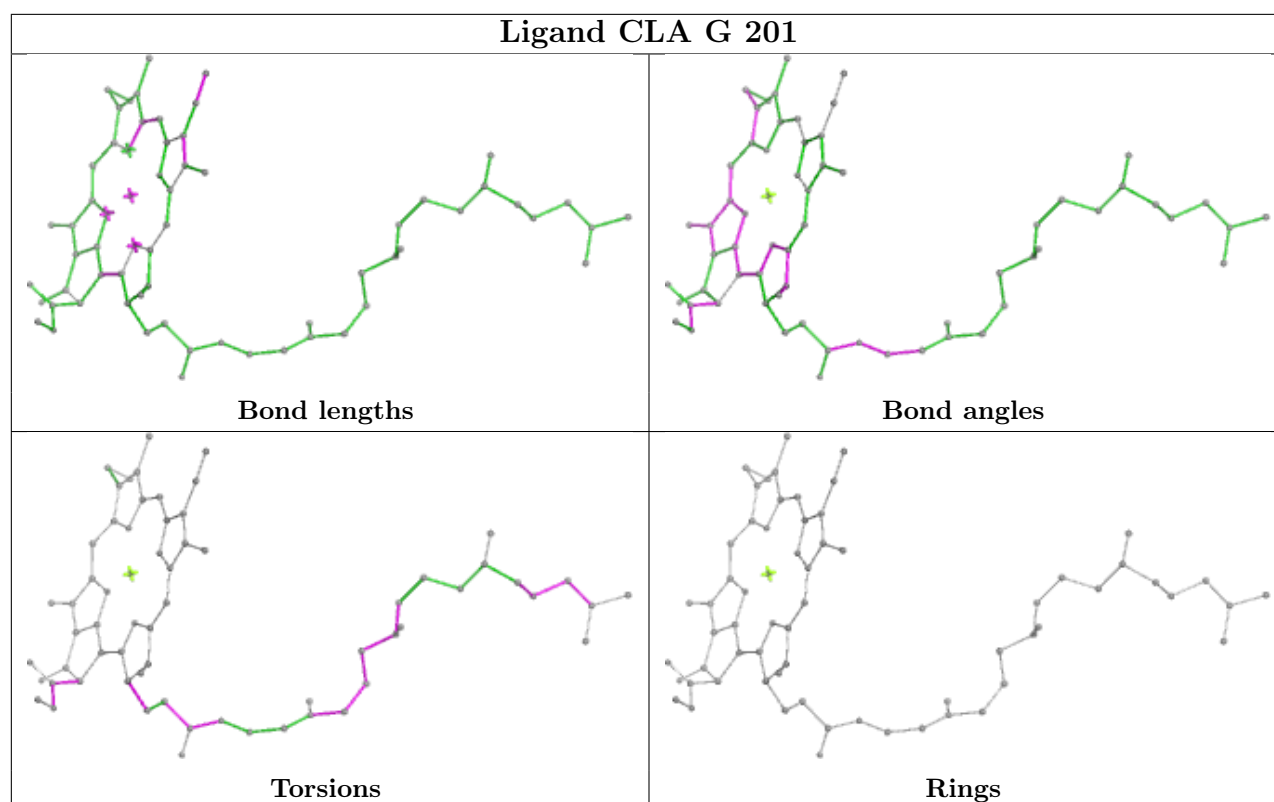


Ligand CLA B 818

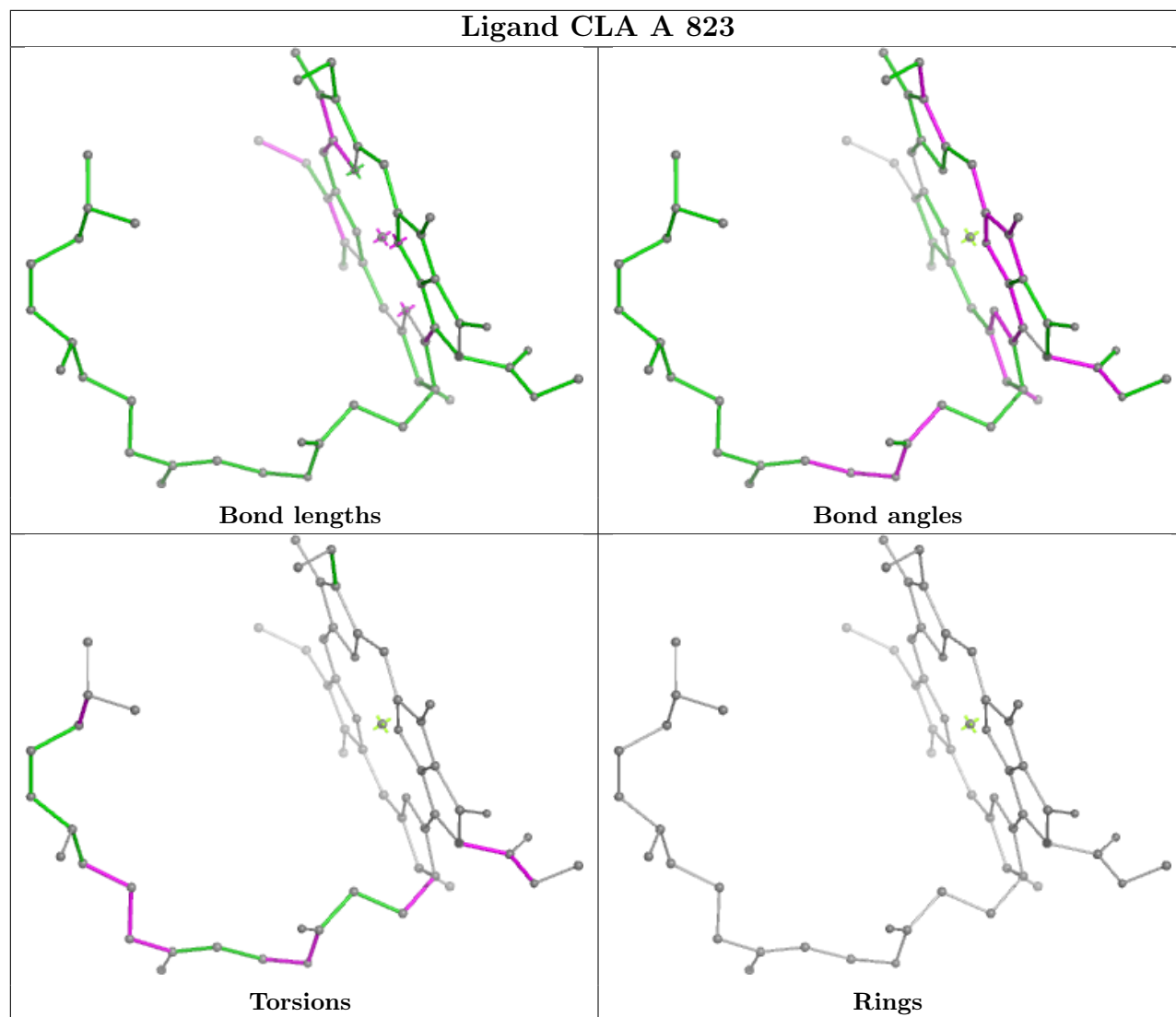


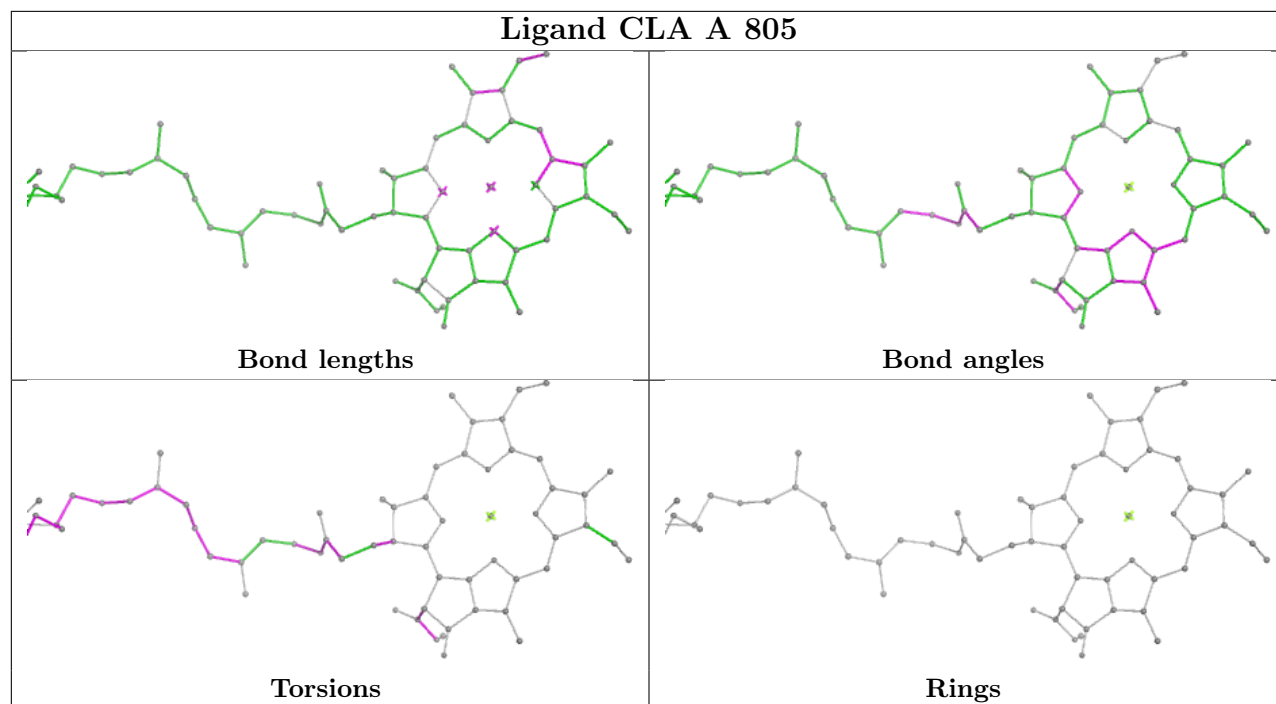
Ligand CLA K 1004



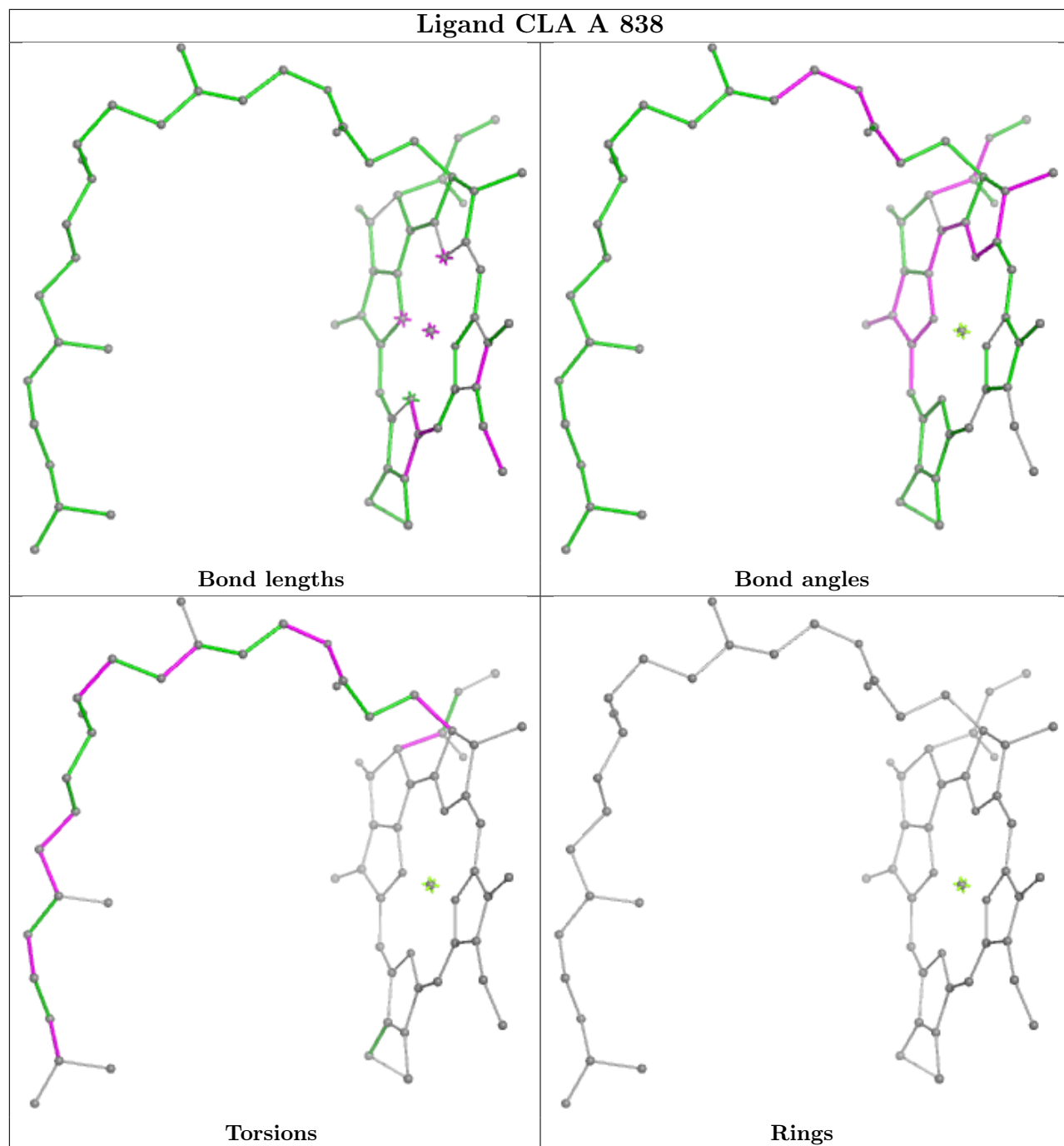


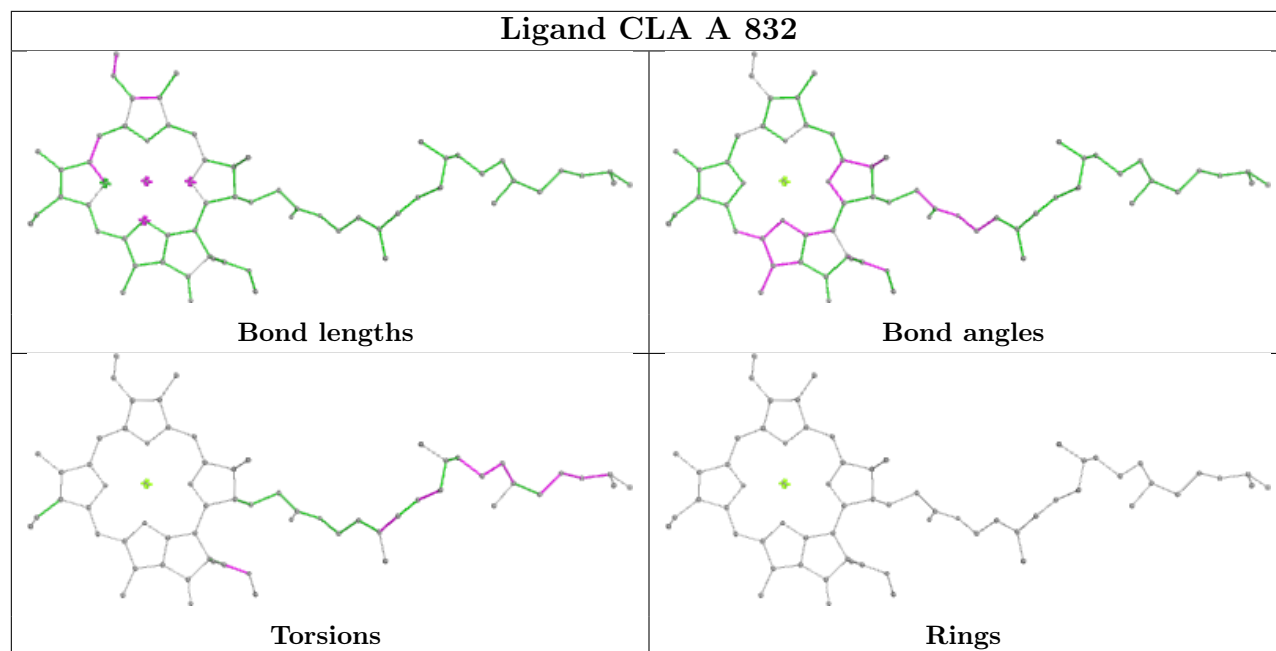
Ligand CLA A 823



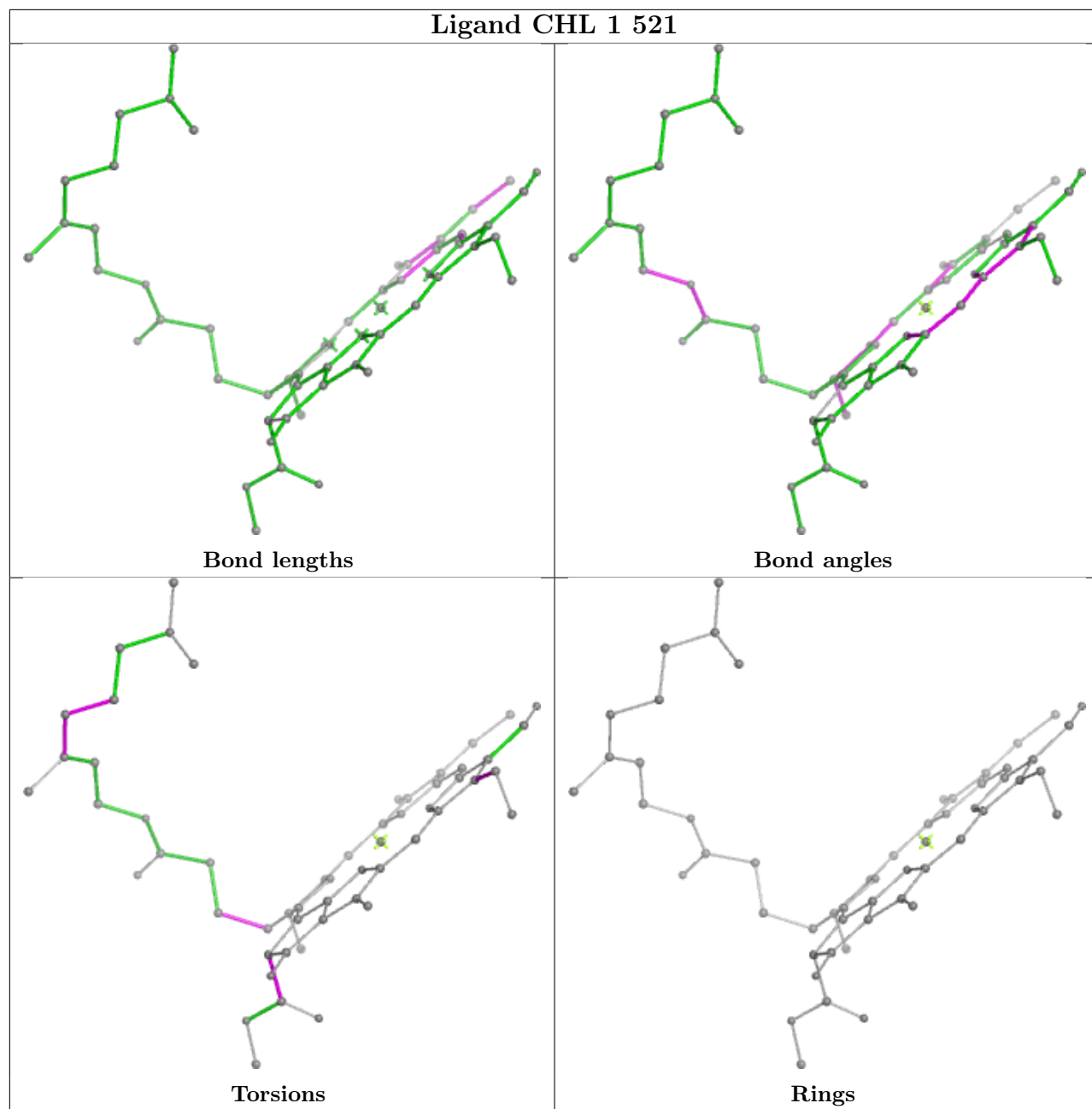


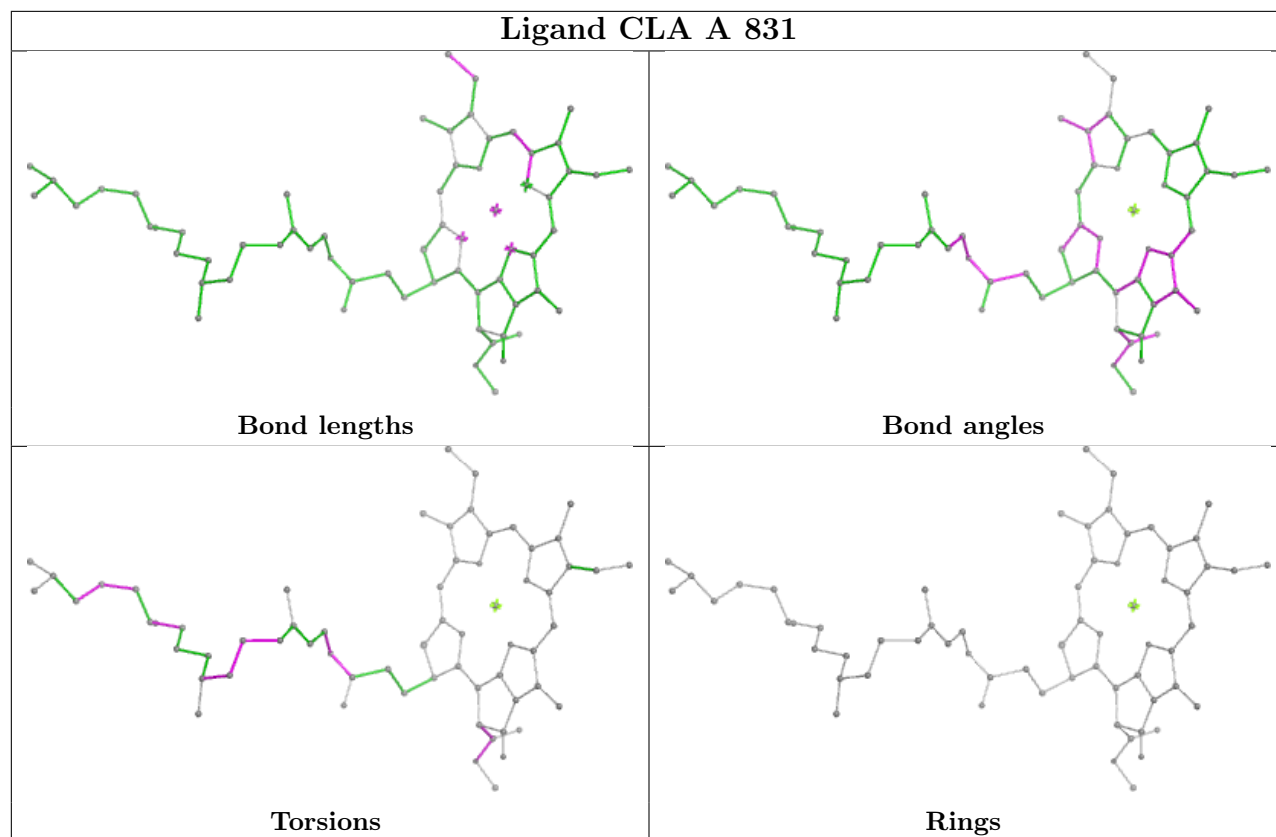
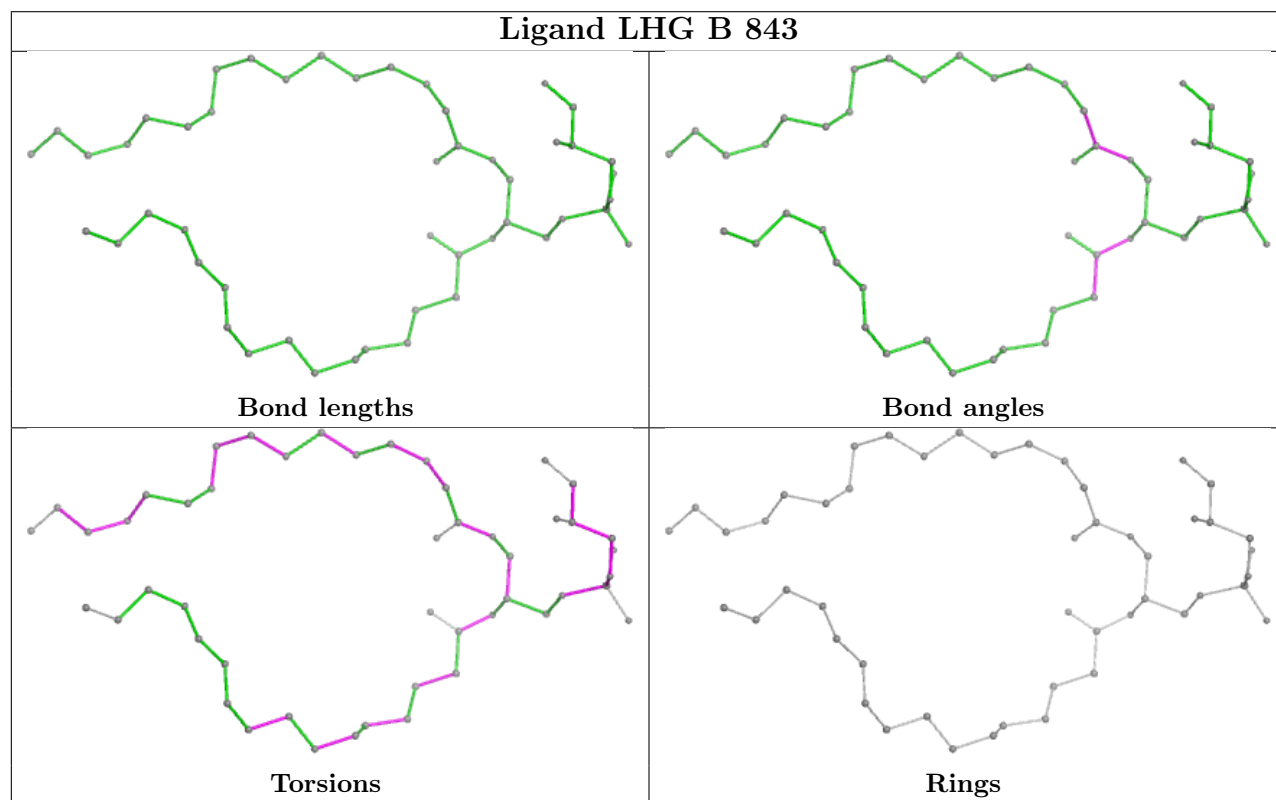
Ligand CLA A 838

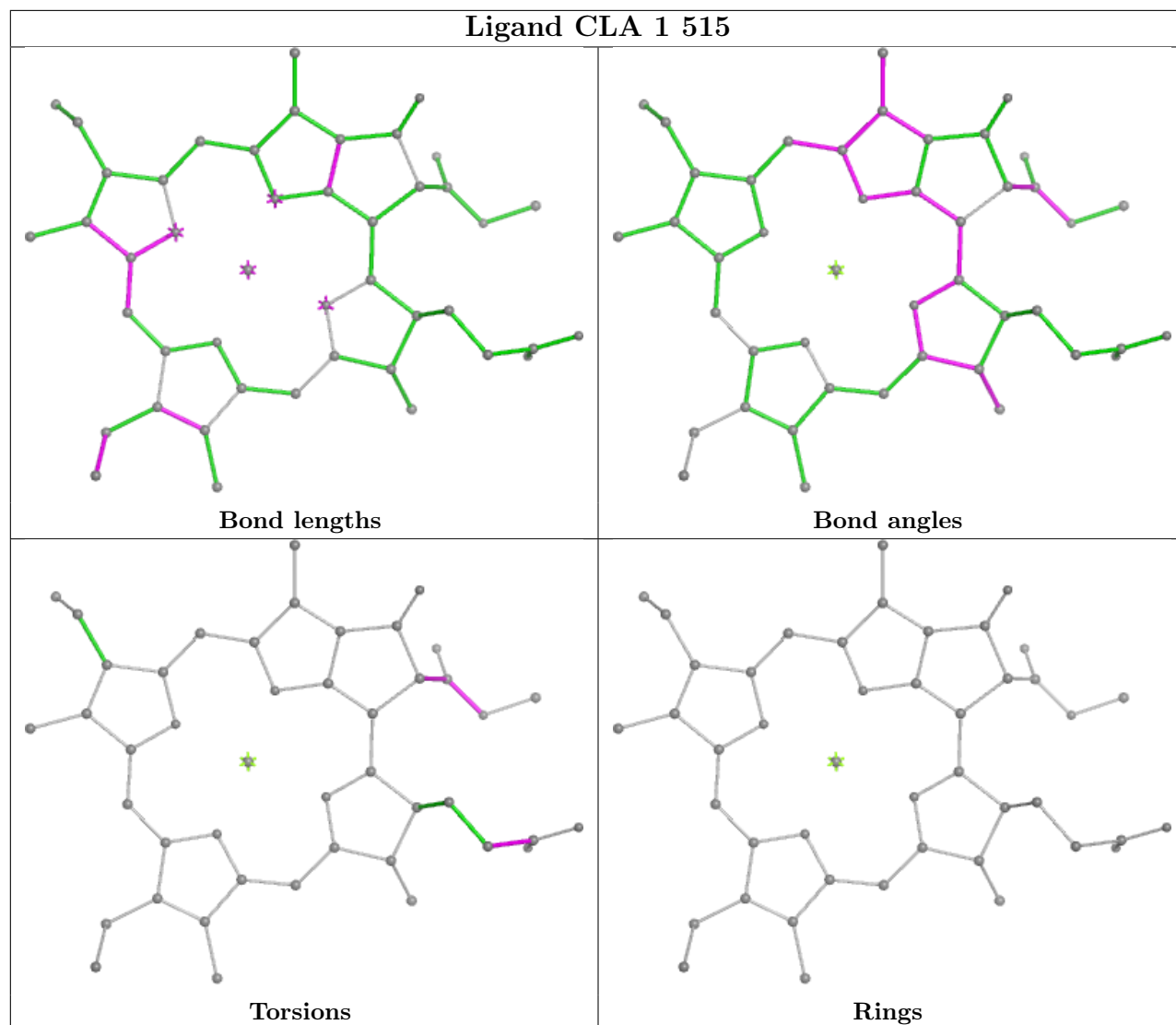
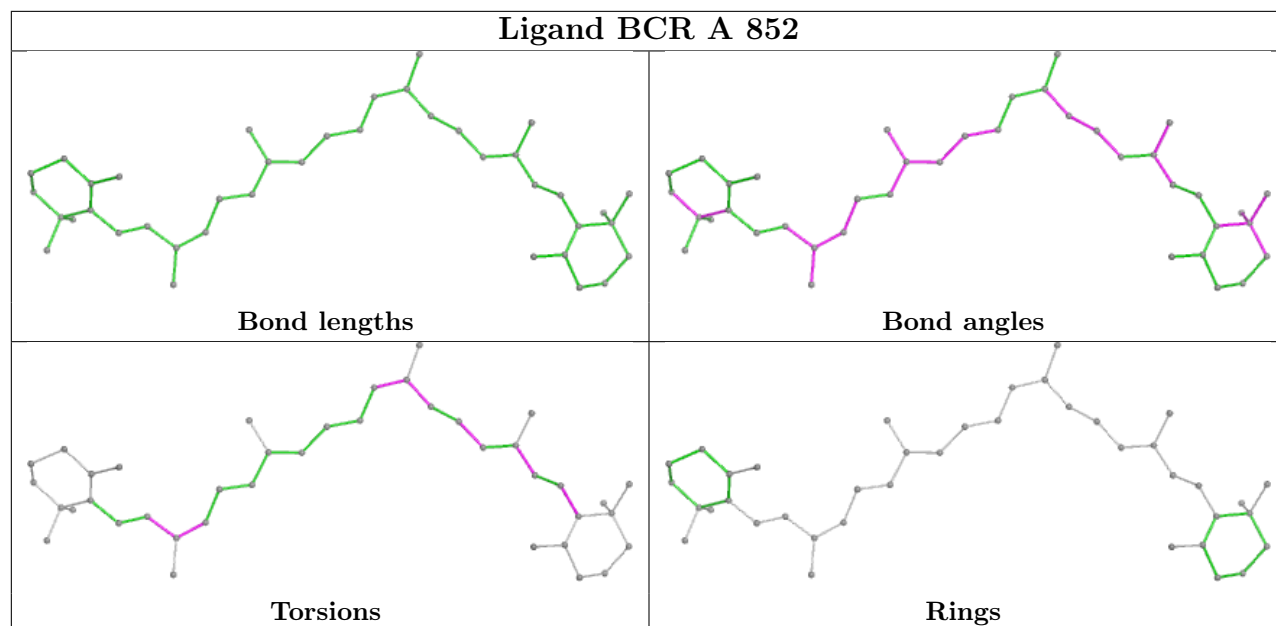


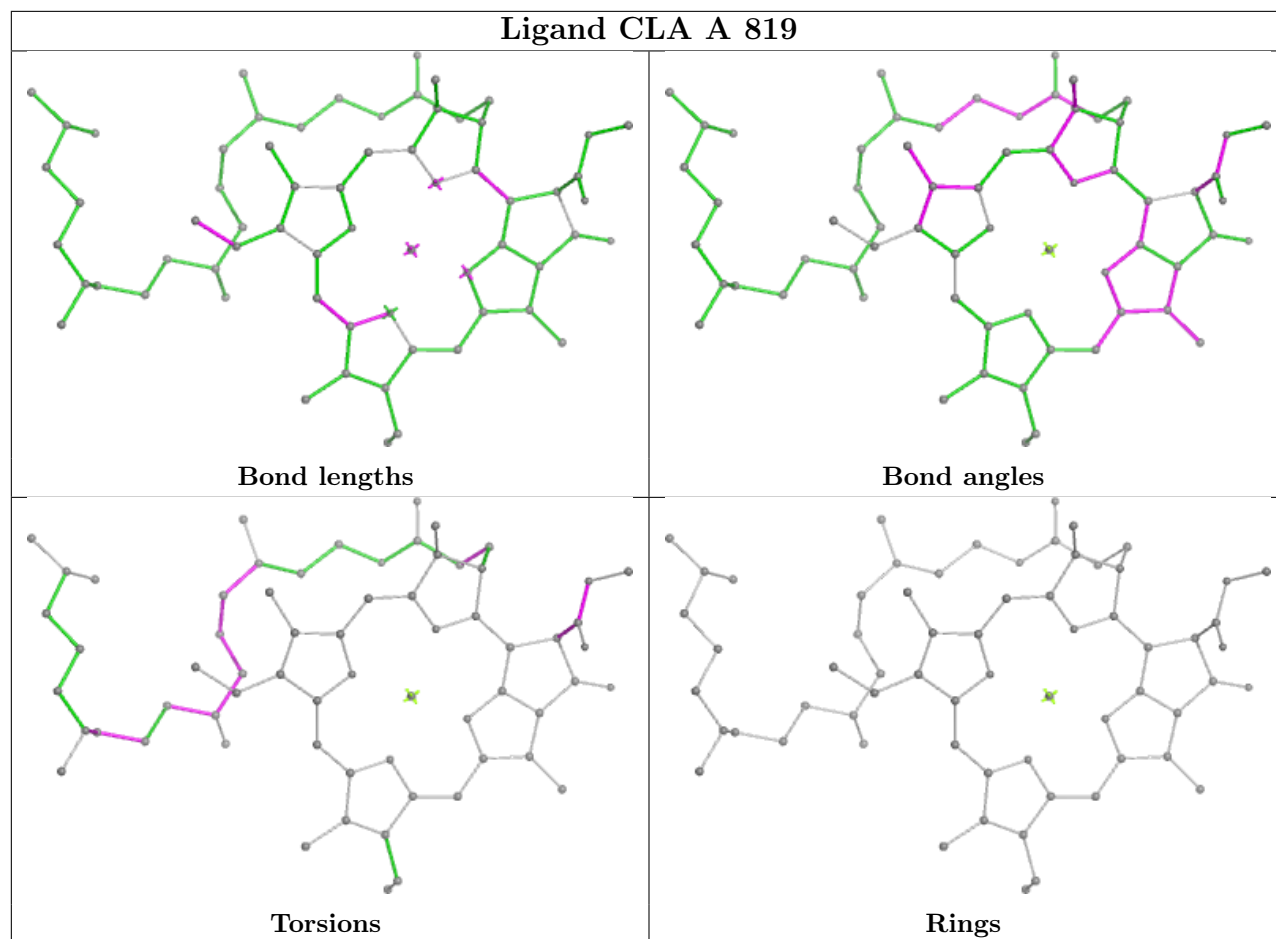


Ligand CHL 1 521

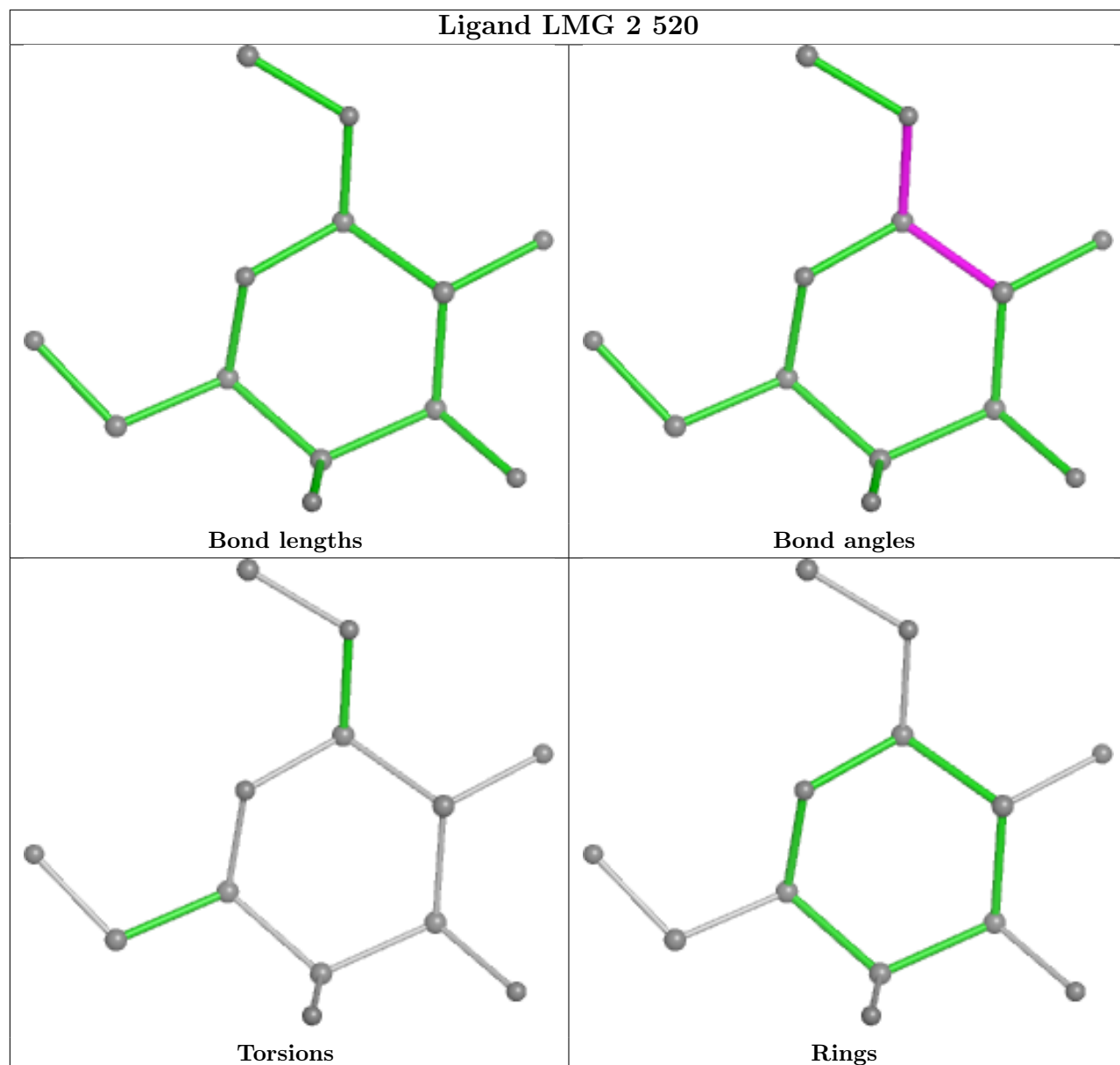


Ligand CLA A 831**Ligand LHG B 843**

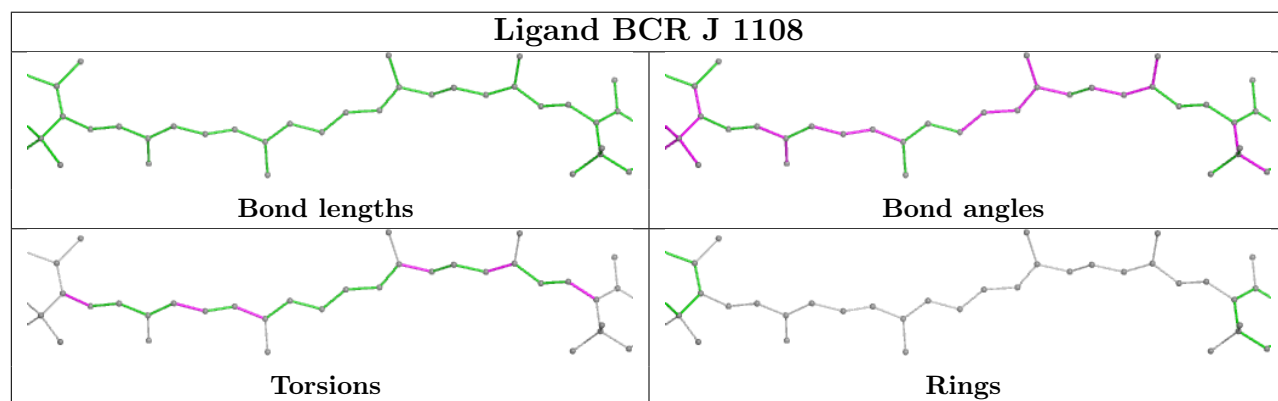


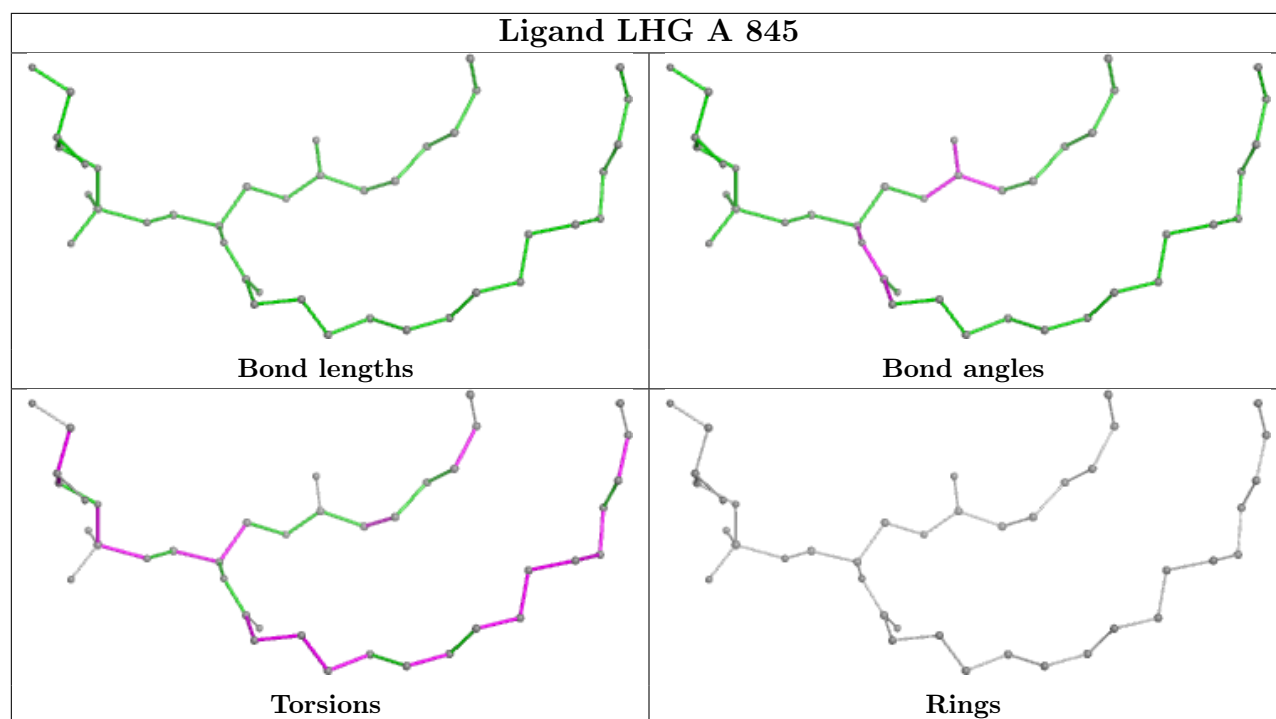
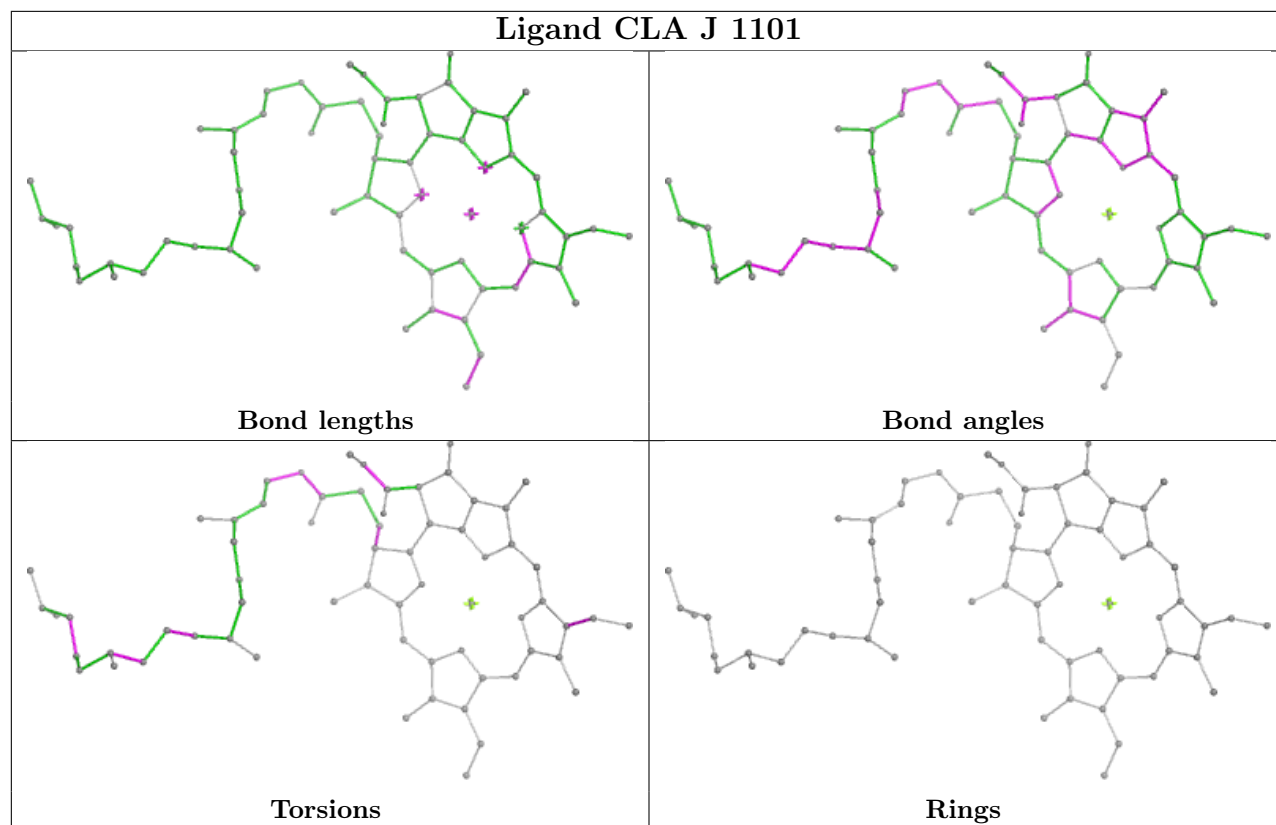


Ligand LMG 2 520

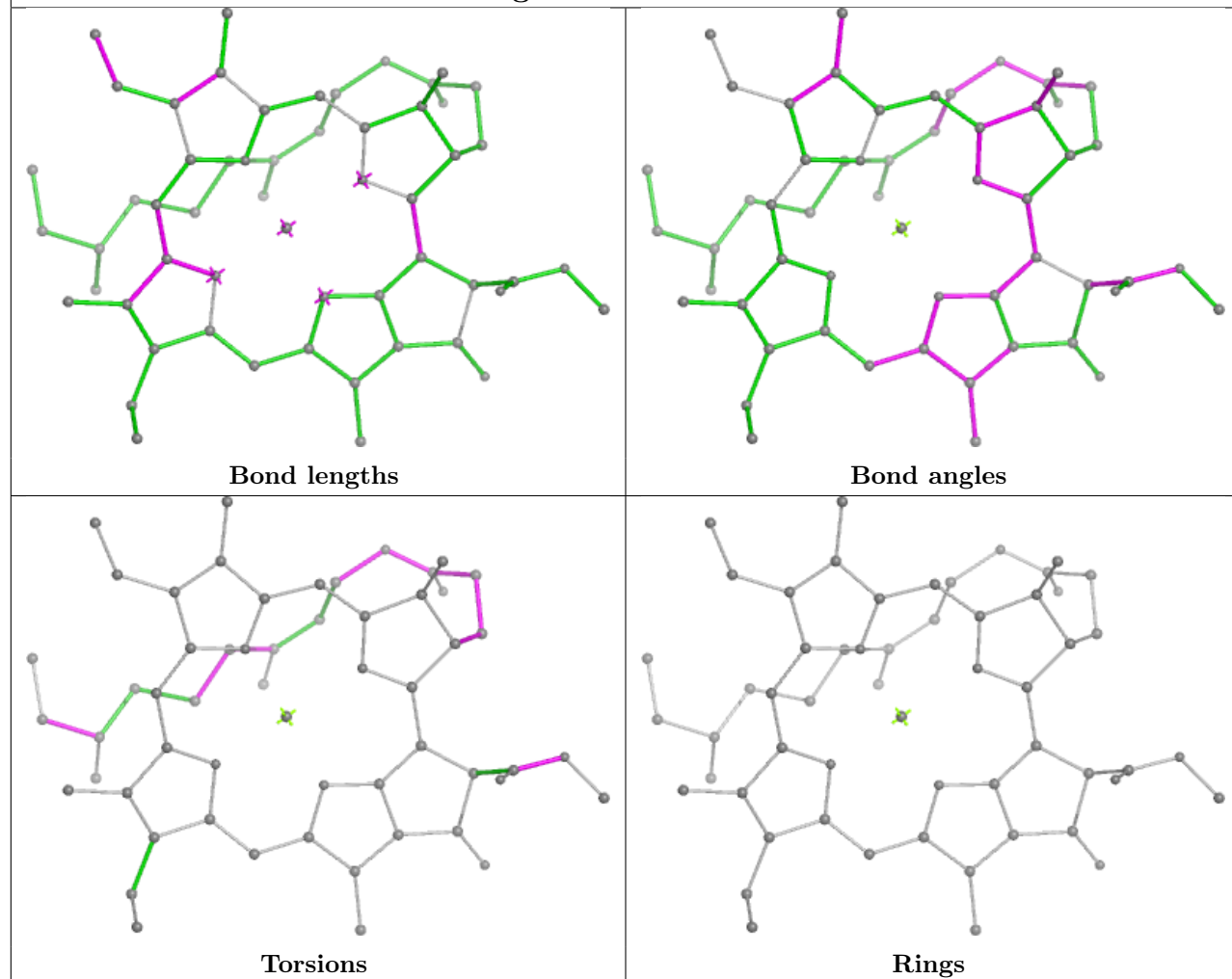


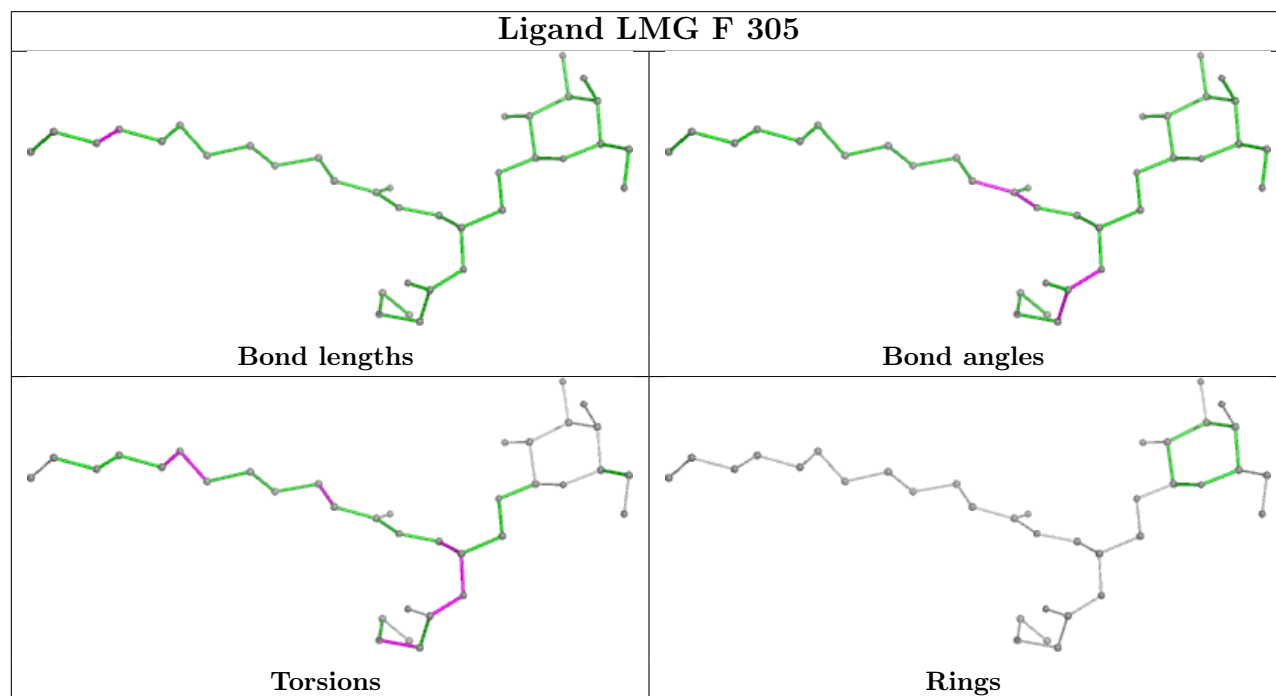
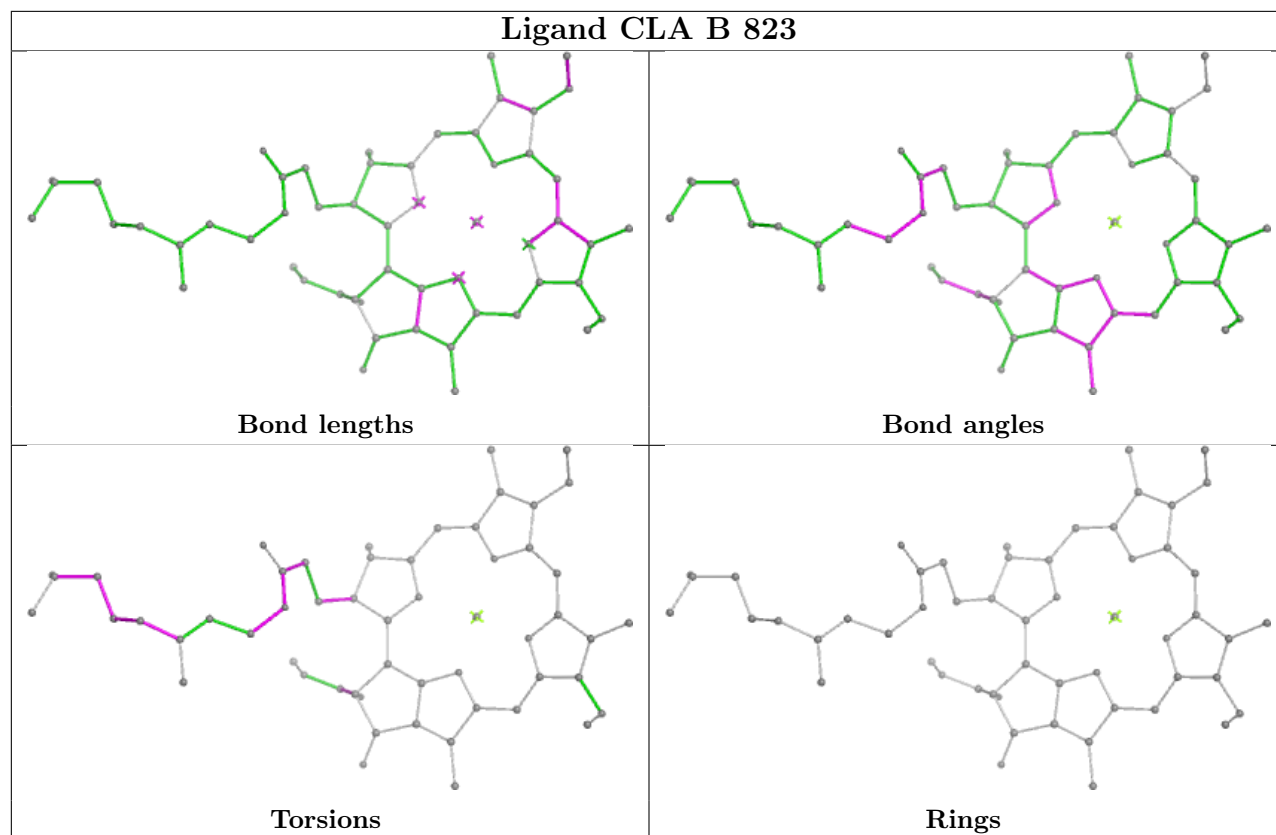
Ligand BCR J 1108

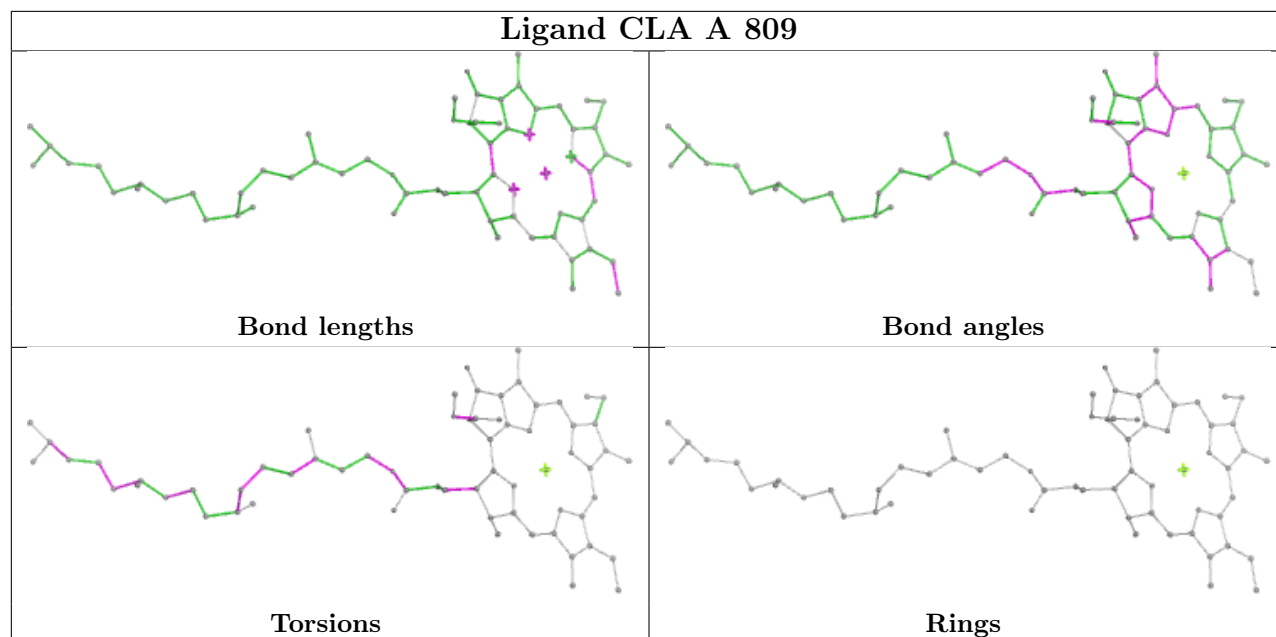
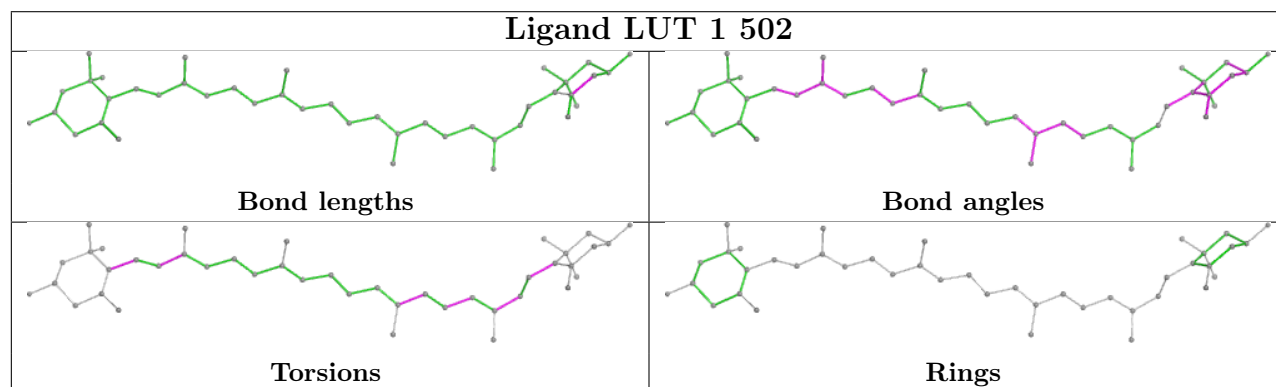




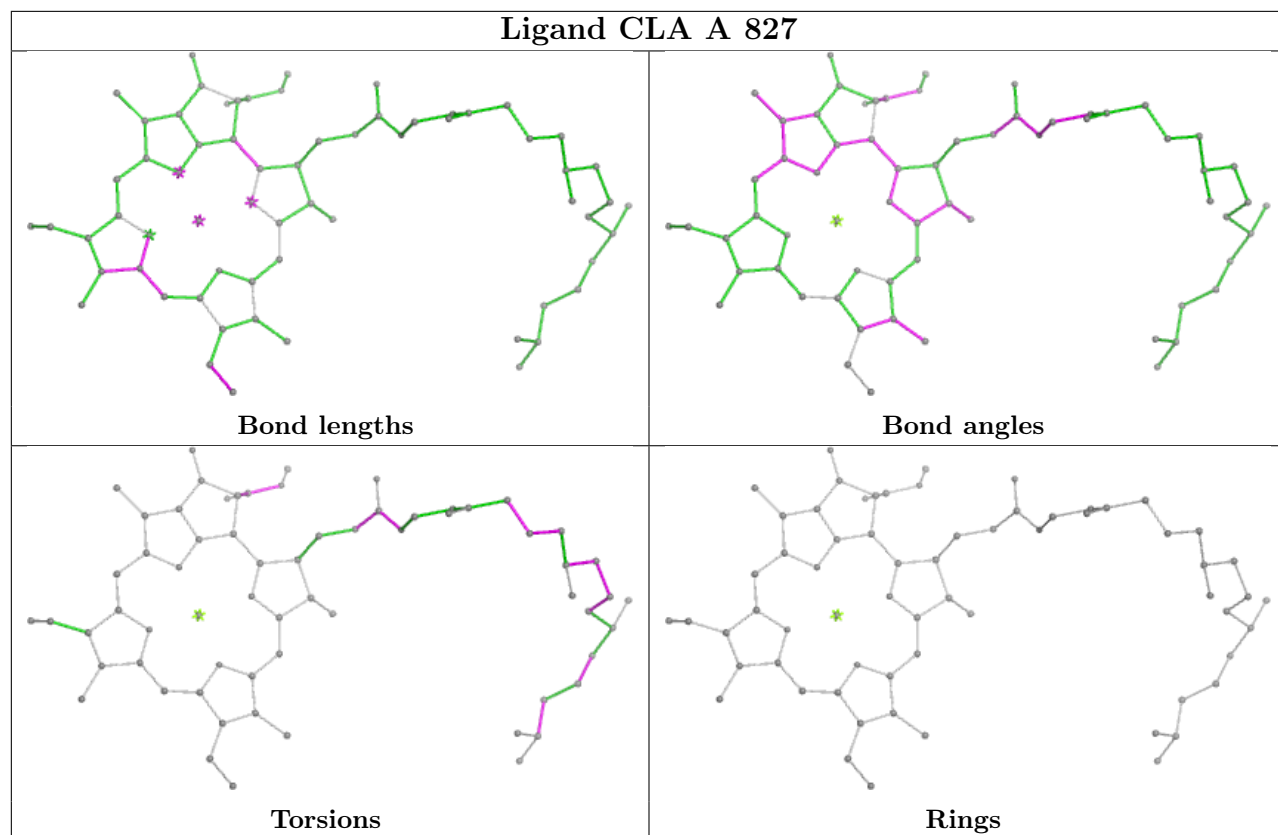
Ligand CLA A 818



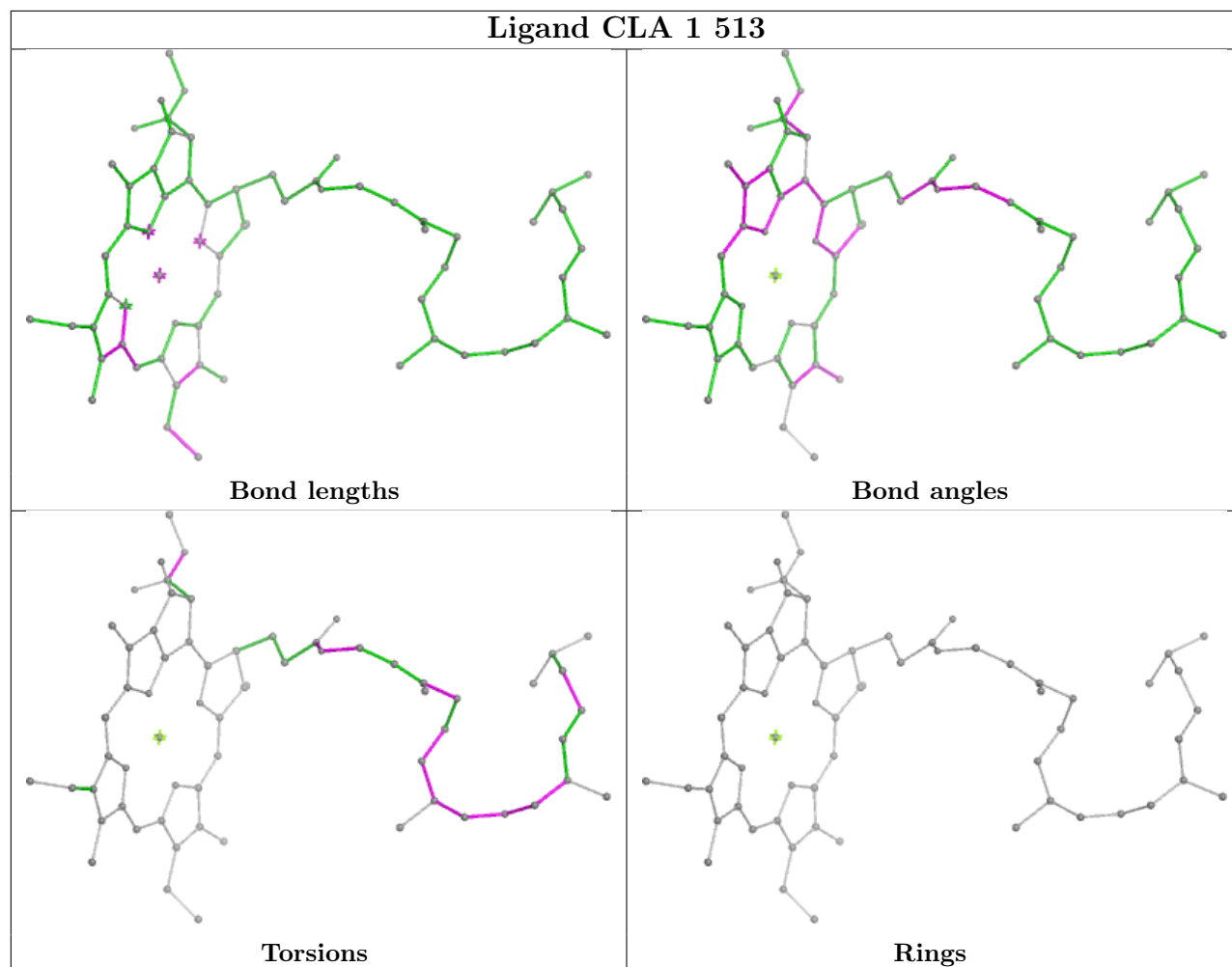


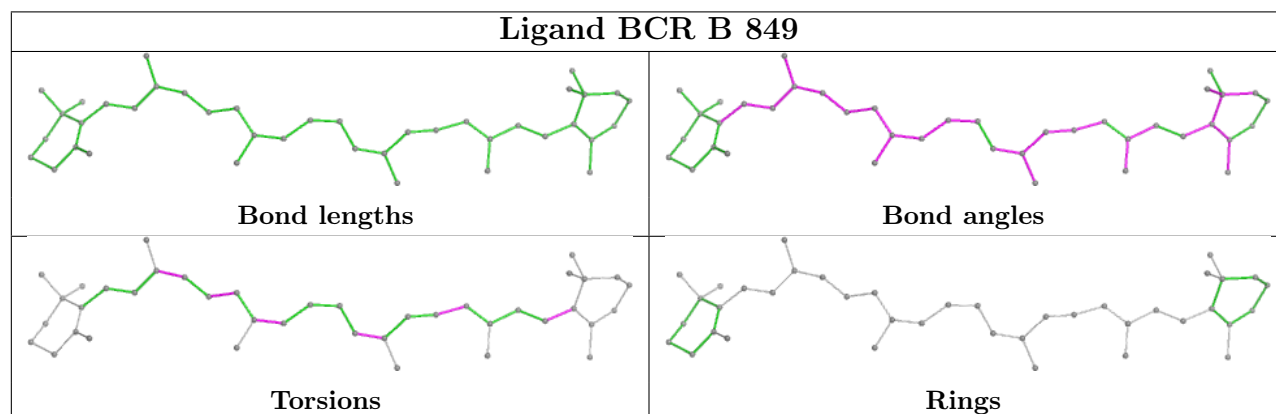
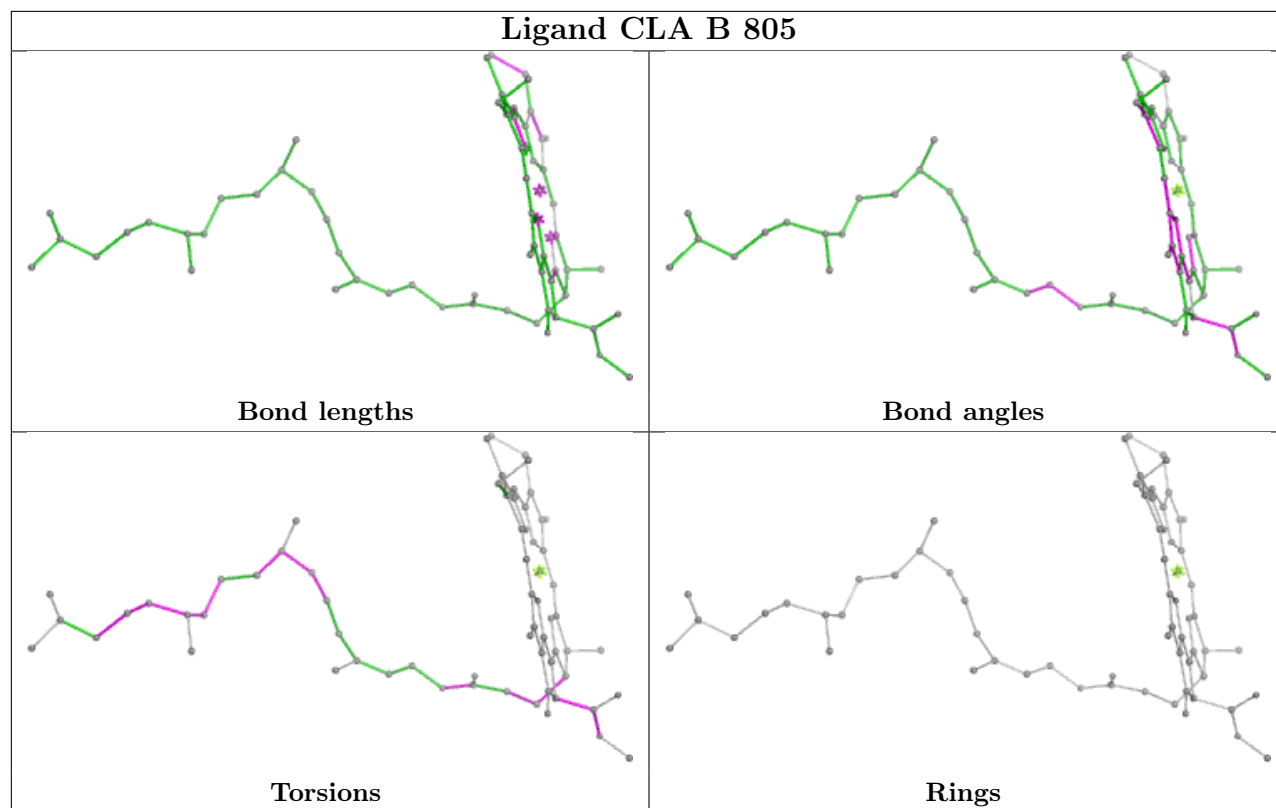
Ligand CLA A 809**Ligand LUT 1 502**

Ligand CLA A 827

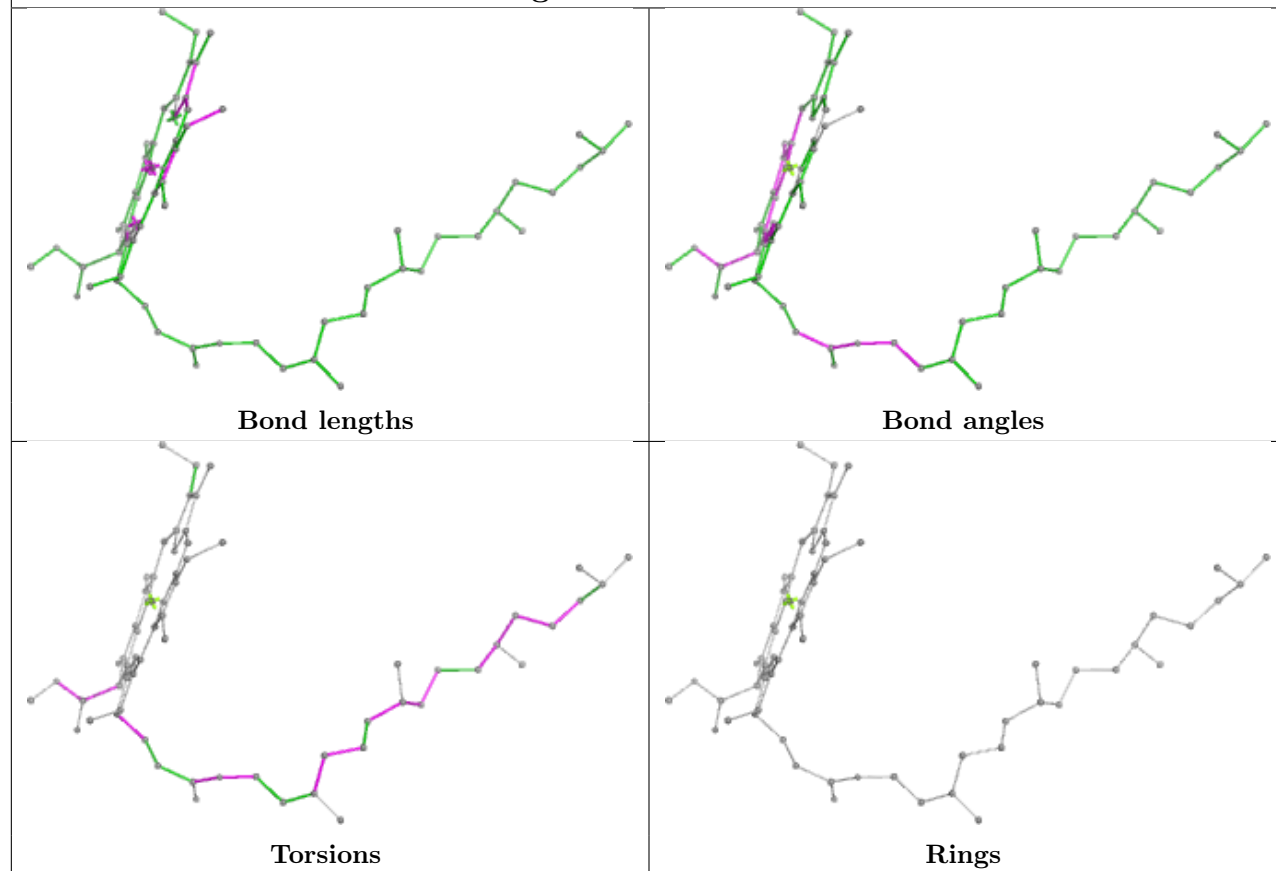


Ligand CLA 1 513

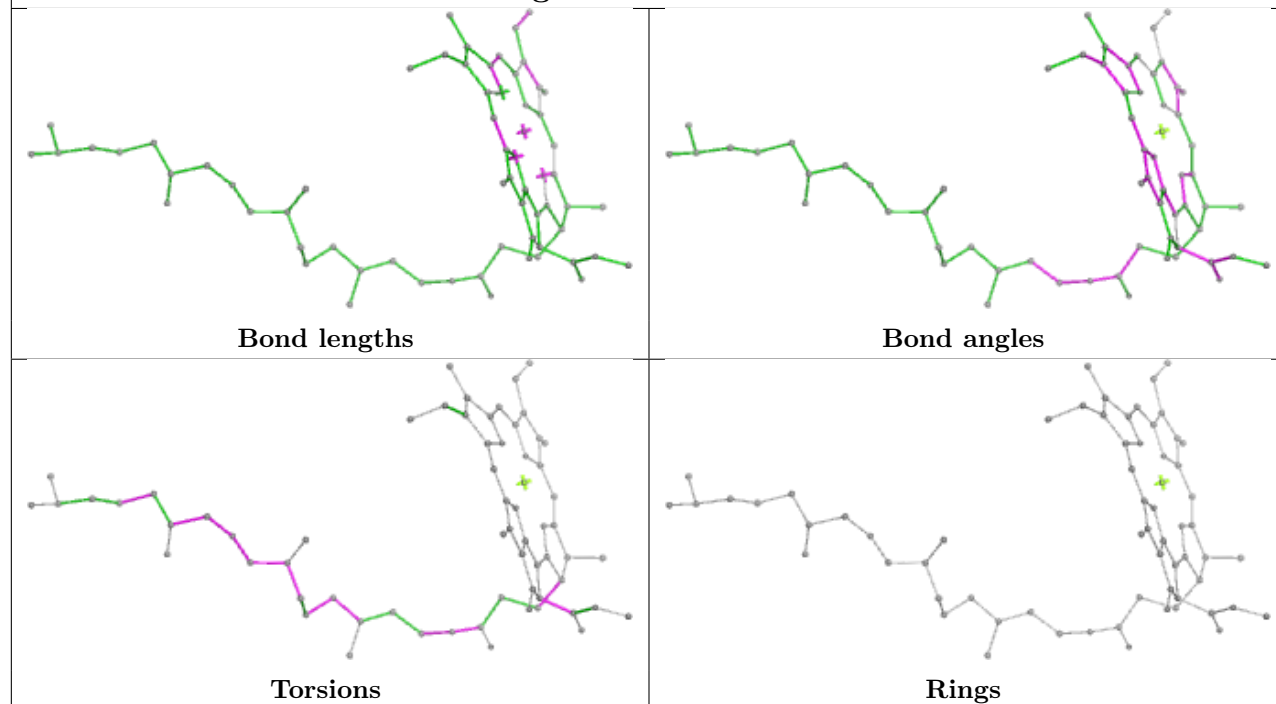




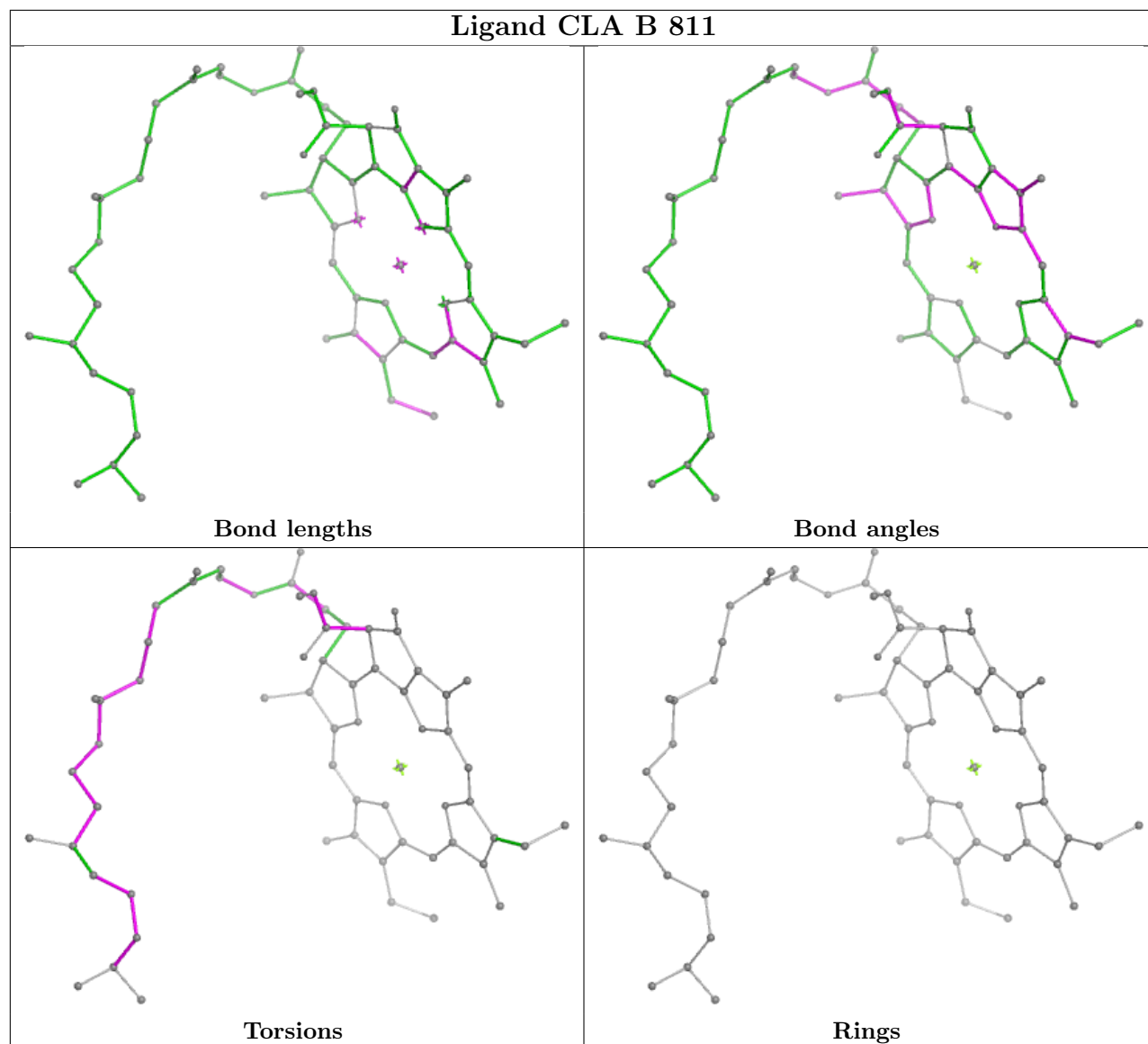
Ligand CLA A 804



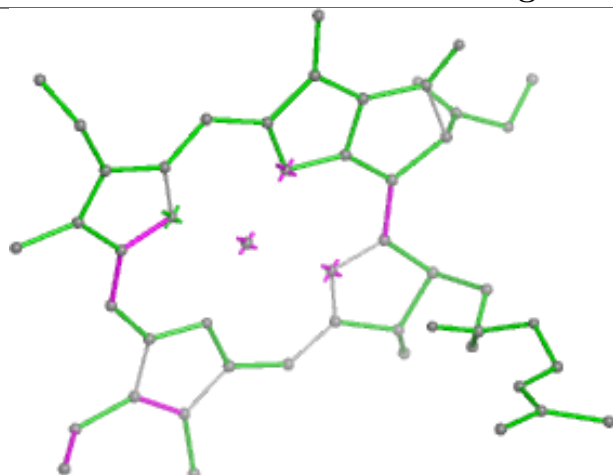
Ligand CLA B 829



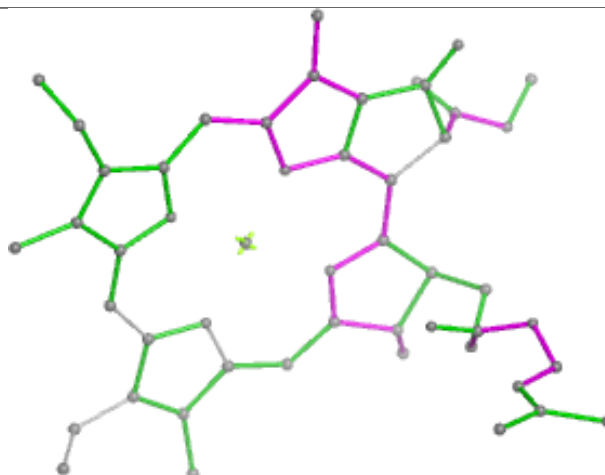
Ligand CLA B 811



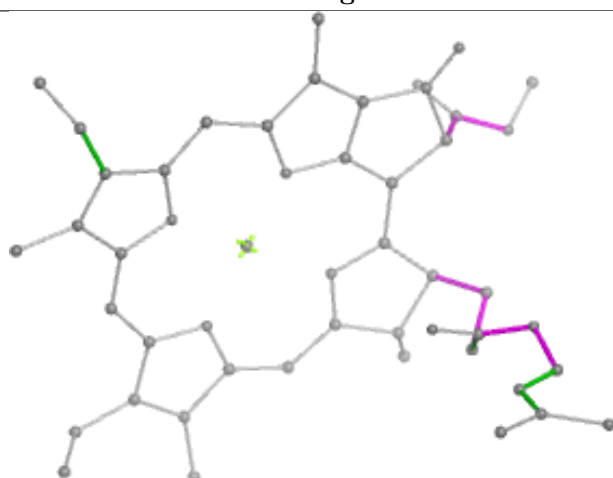
Ligand CLA 2 511



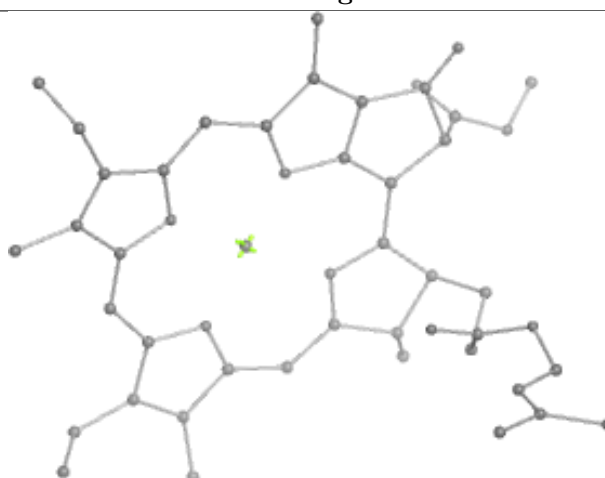
Bond lengths



Bond angles

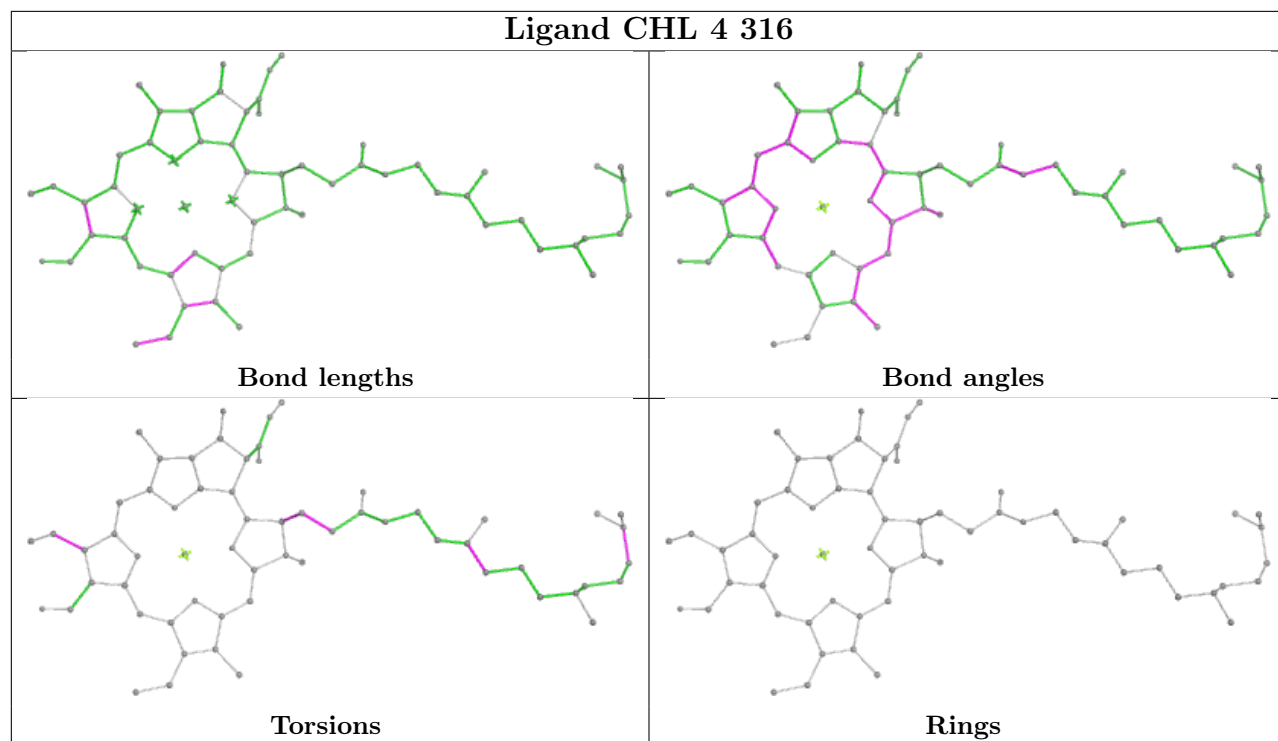


Torsions

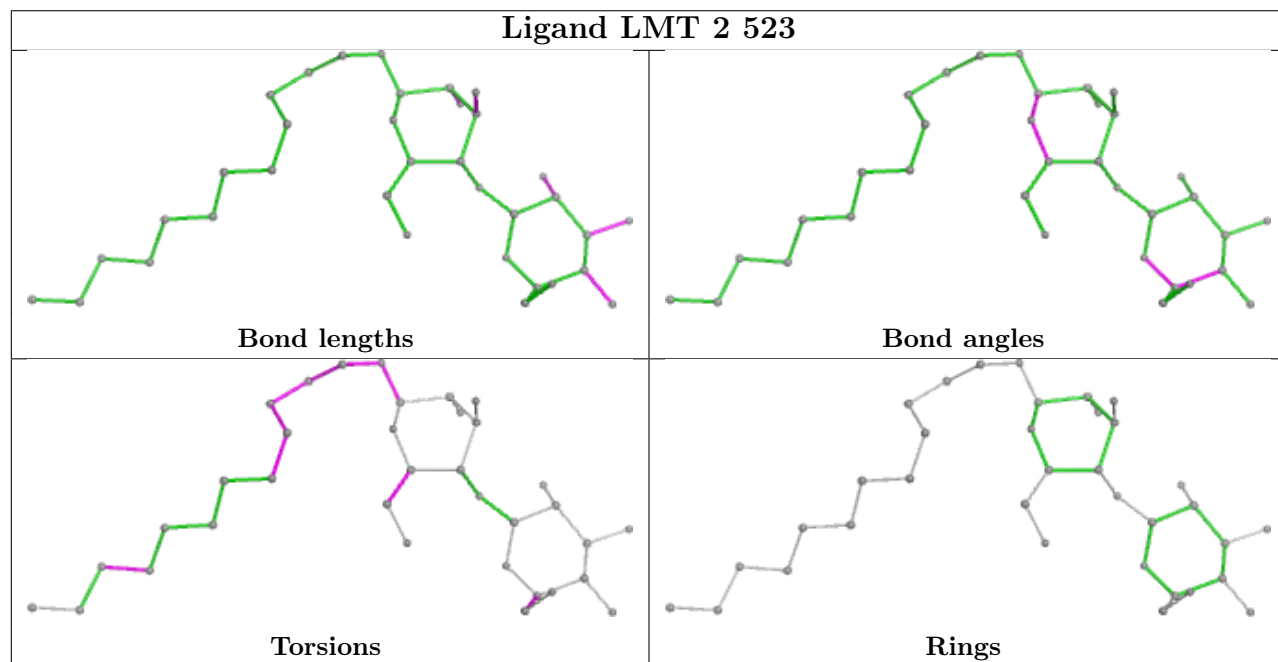


Rings

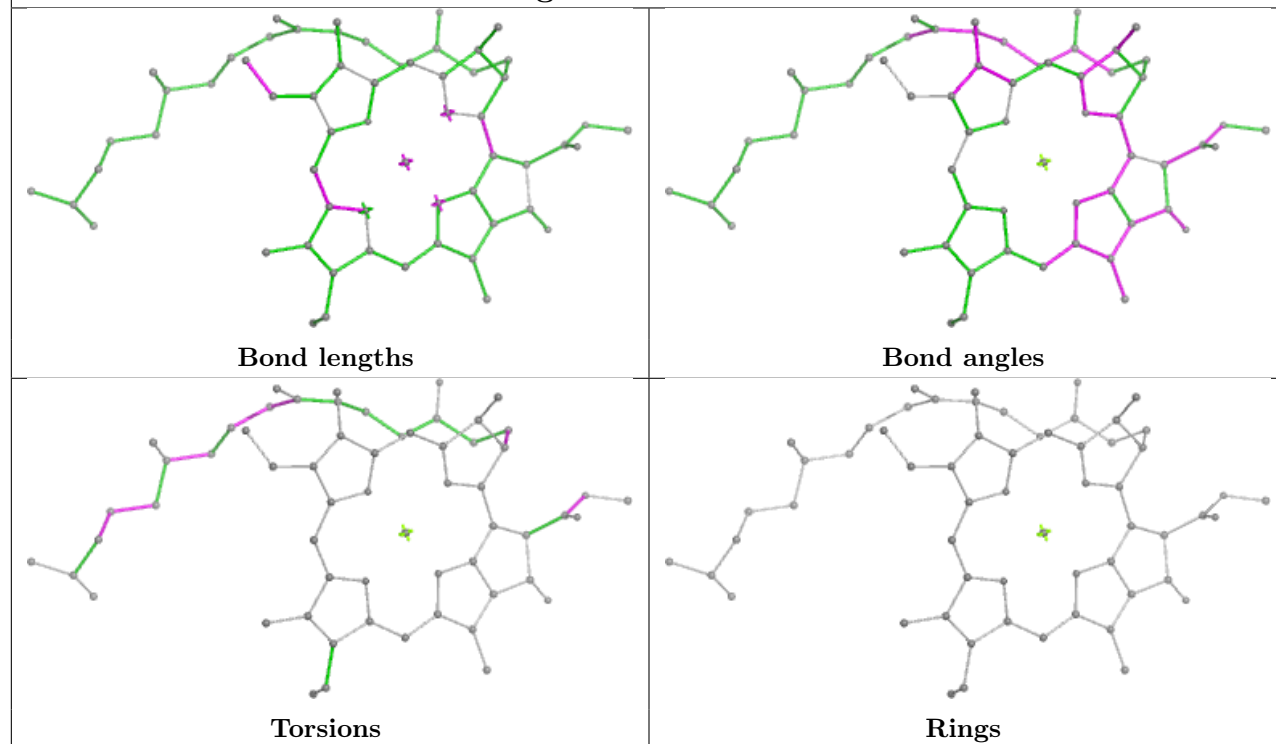
Ligand CHL 4 316



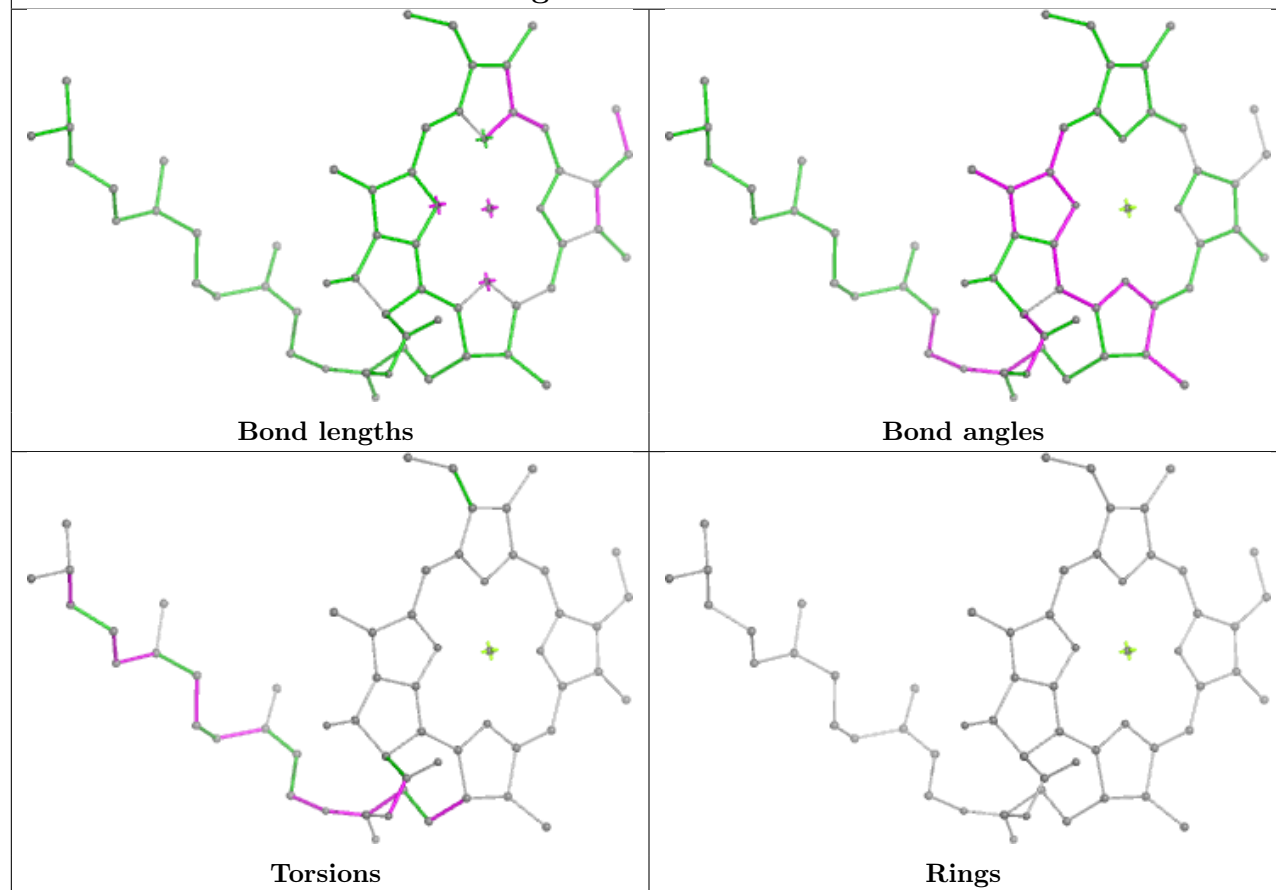
Ligand LMT 2 523



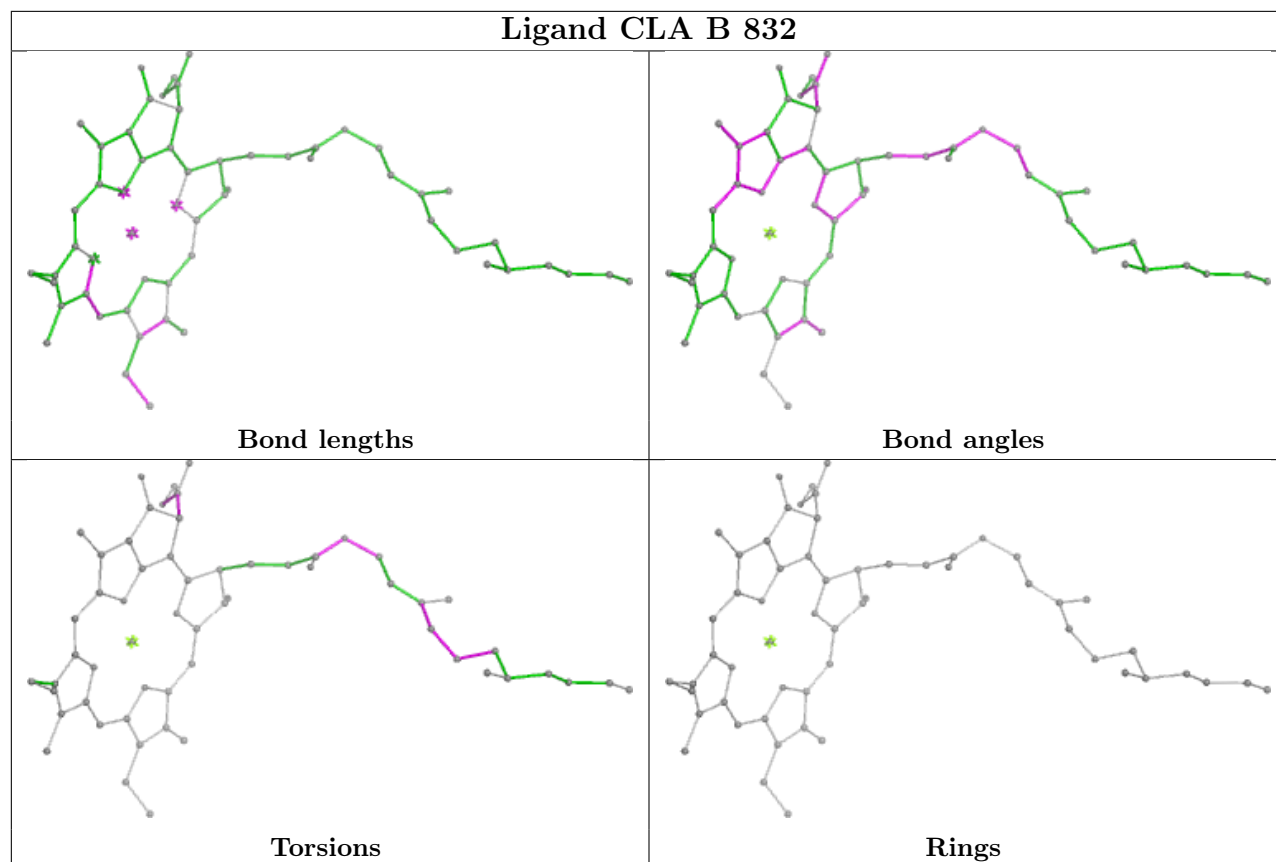
Ligand CLA 4 304



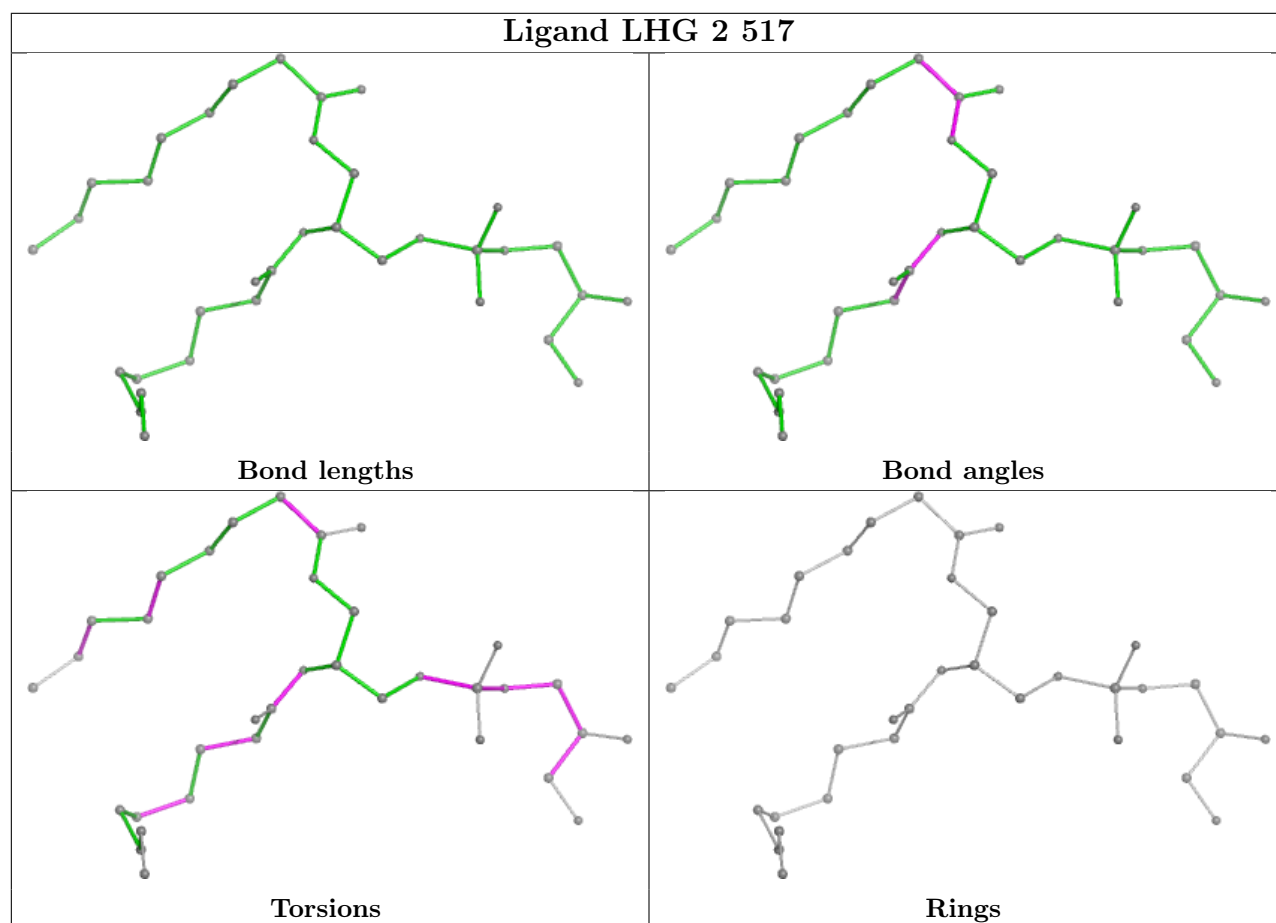
Ligand CLA A 822



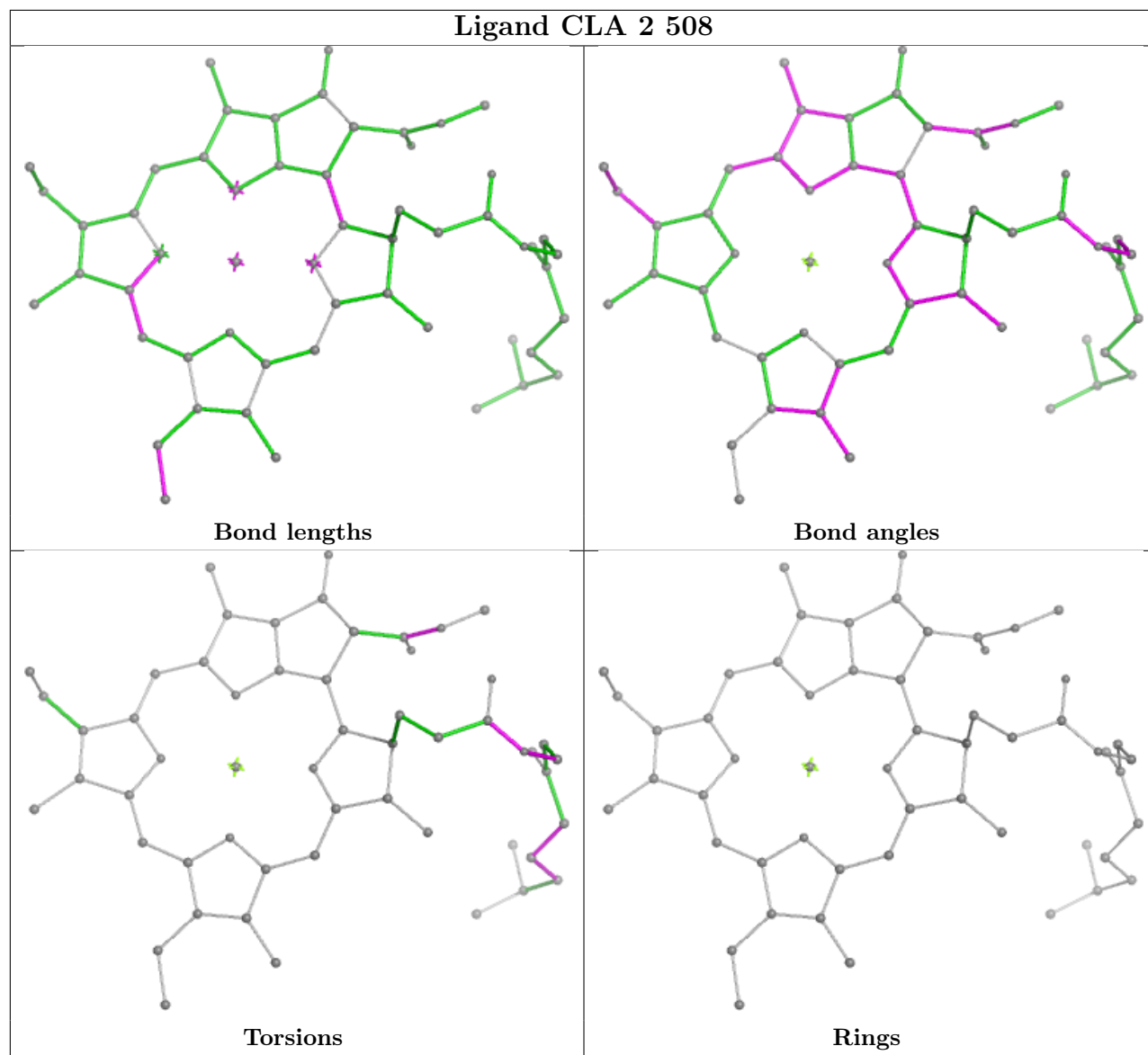
Ligand CLA B 832

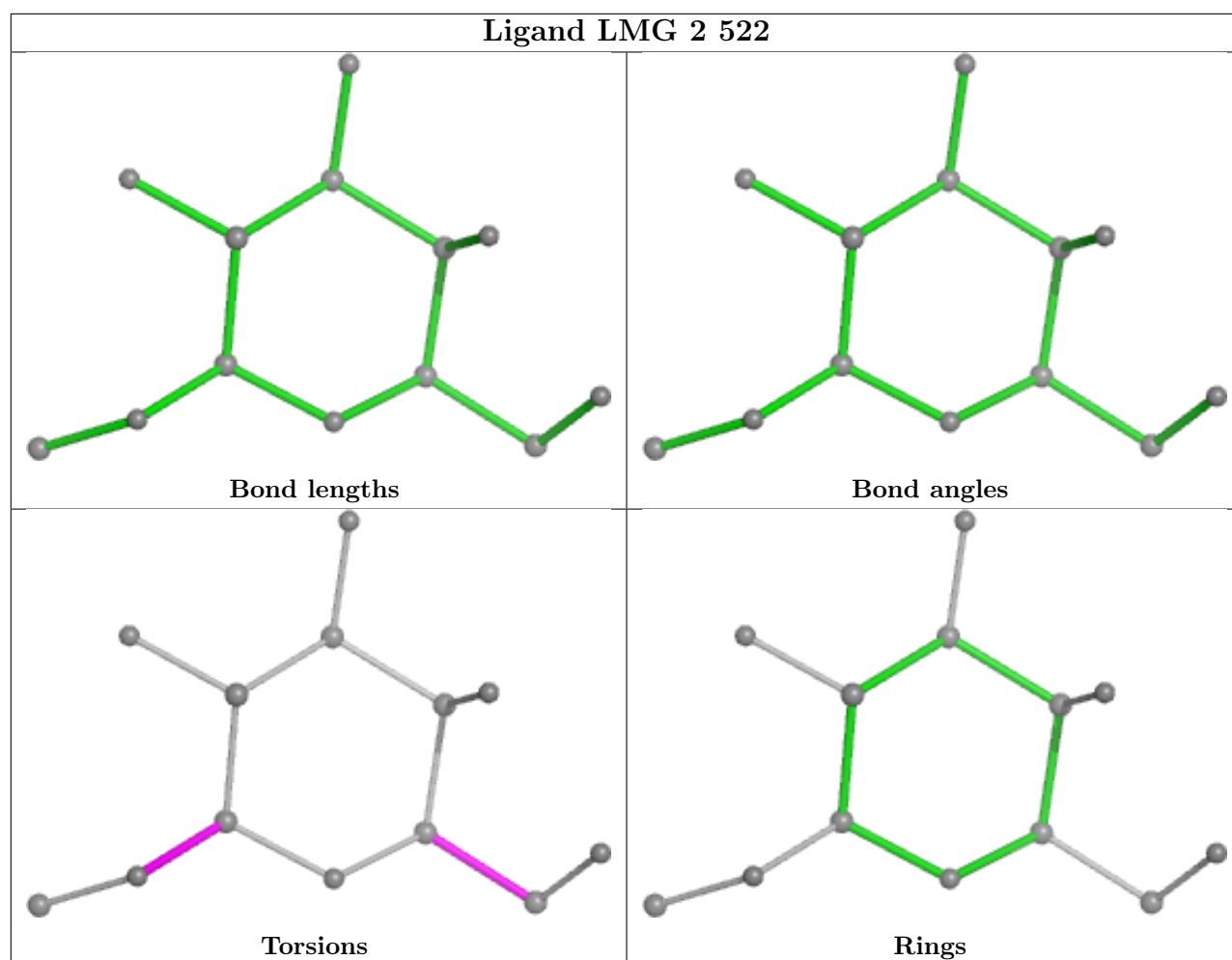


Ligand LHG 2 517

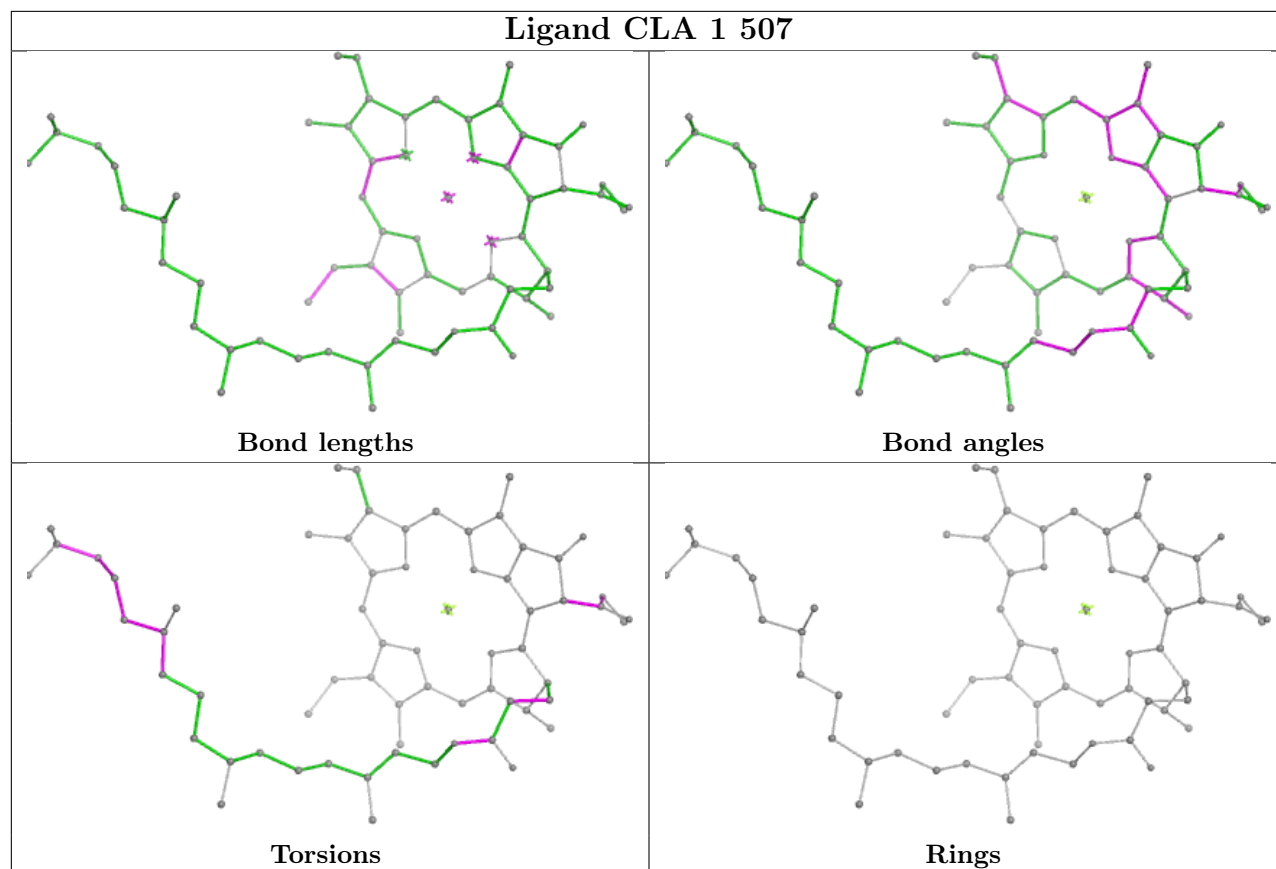


Ligand CLA 2 508

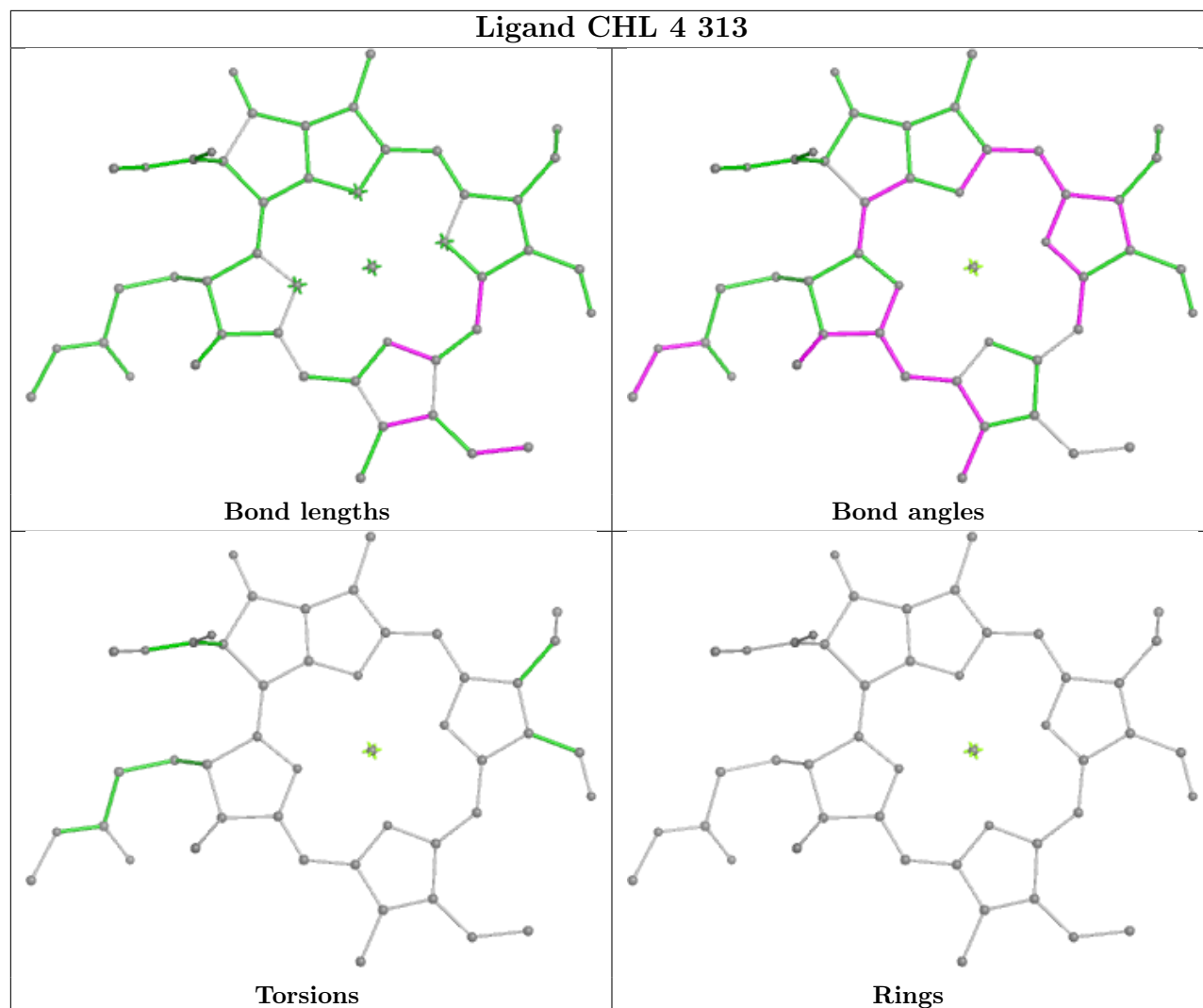


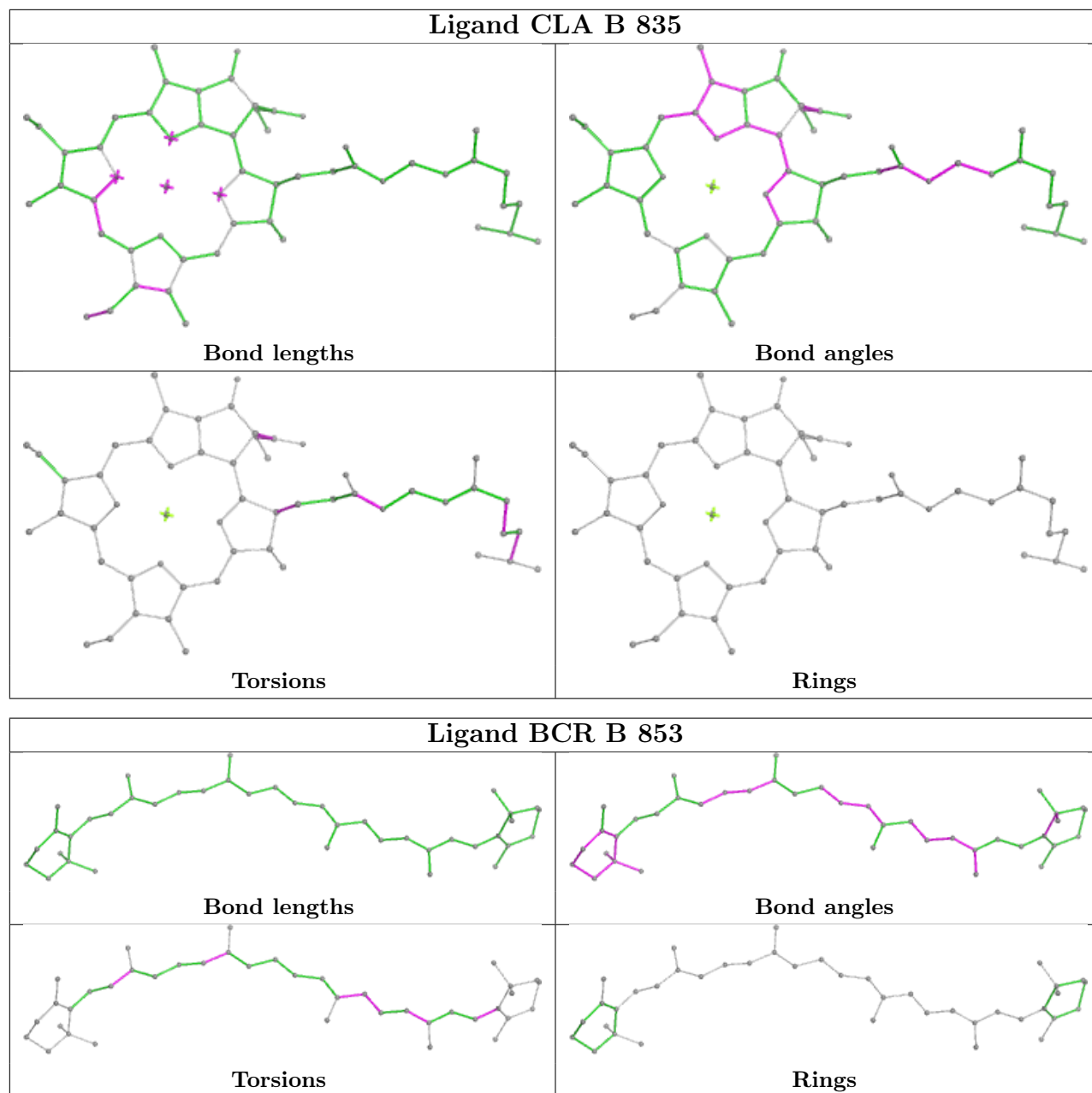


Ligand CLA 1 507

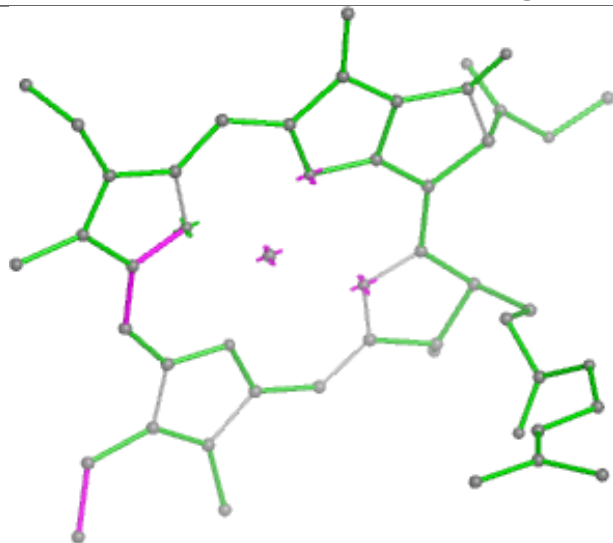


Ligand CHL 4 313

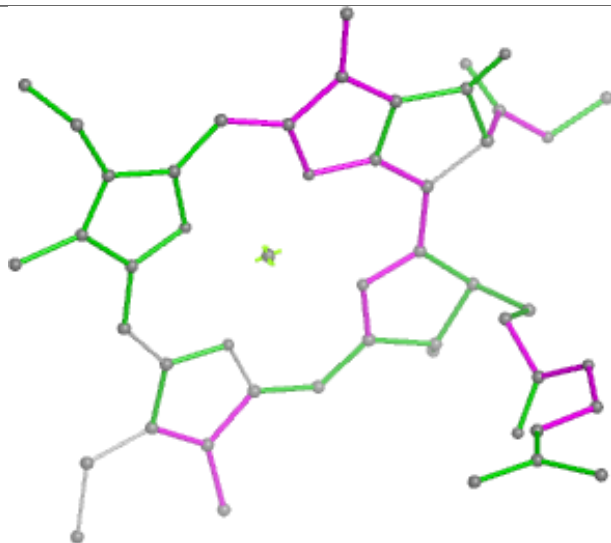




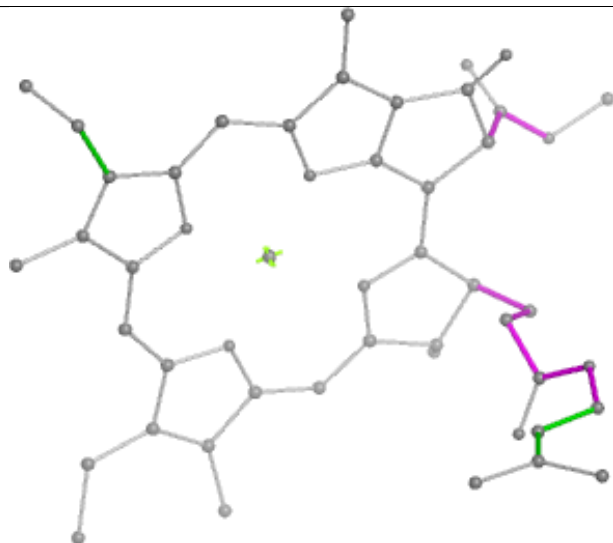
Ligand CLA 2 509



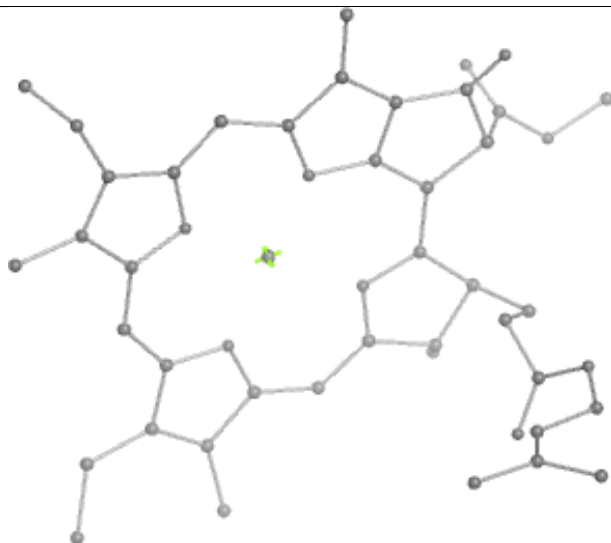
Bond lengths



Bond angles

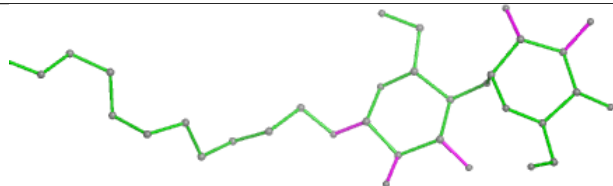


Torsions

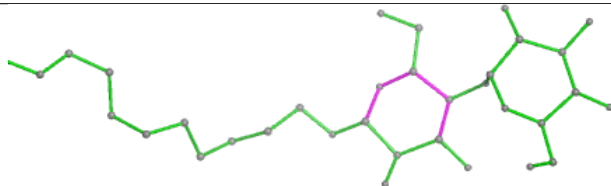


Rings

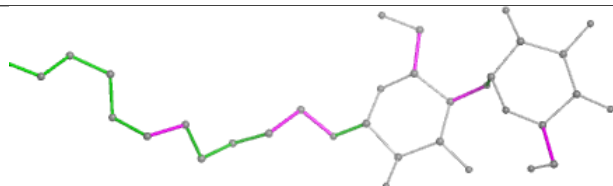
Ligand LMT G 208



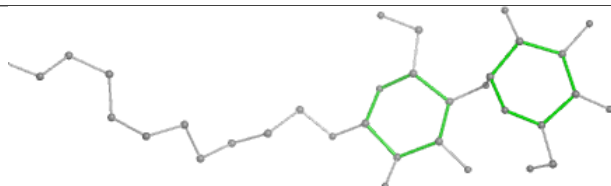
Bond lengths



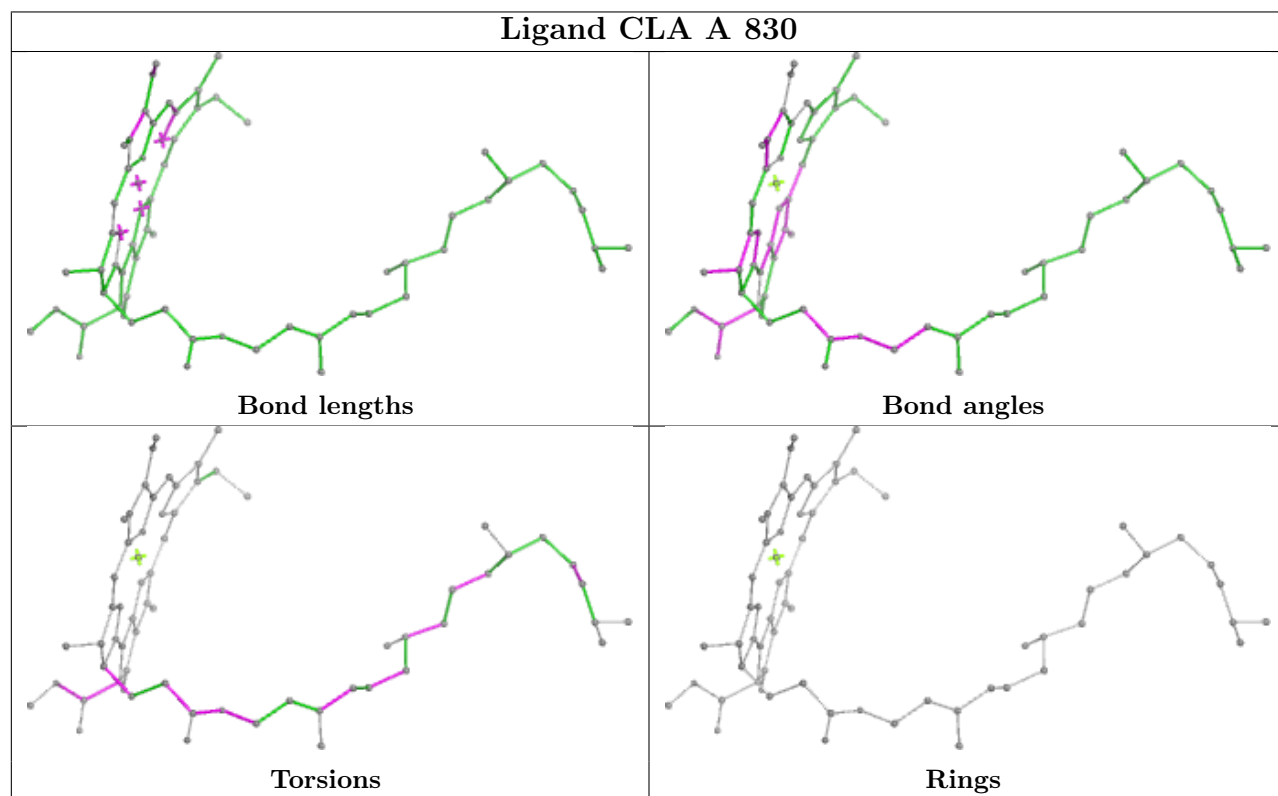
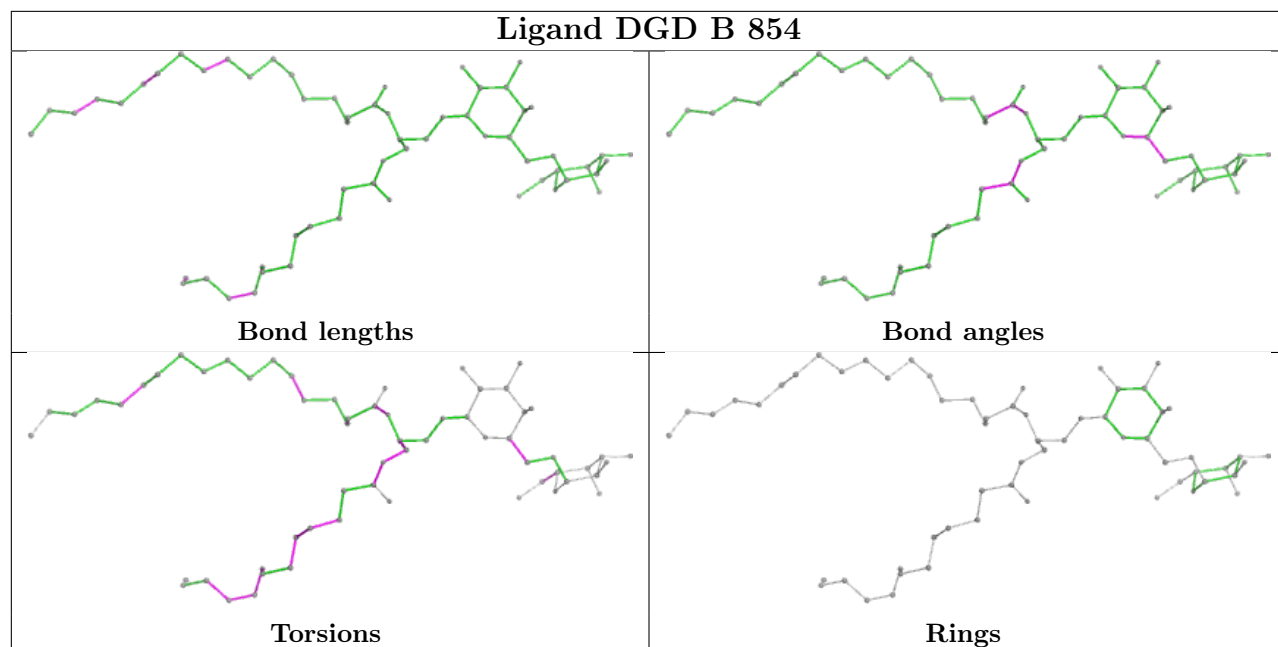
Bond angles

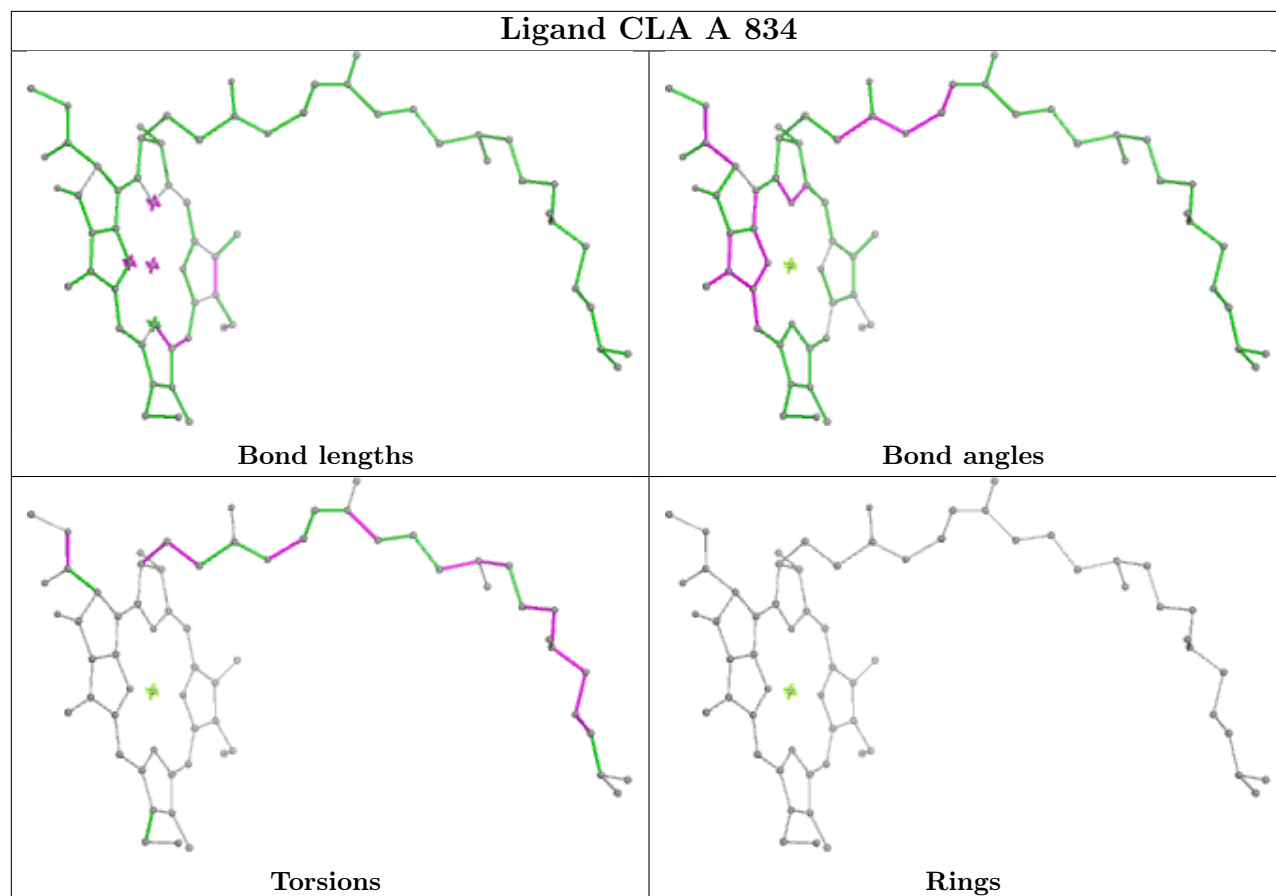


Torsions

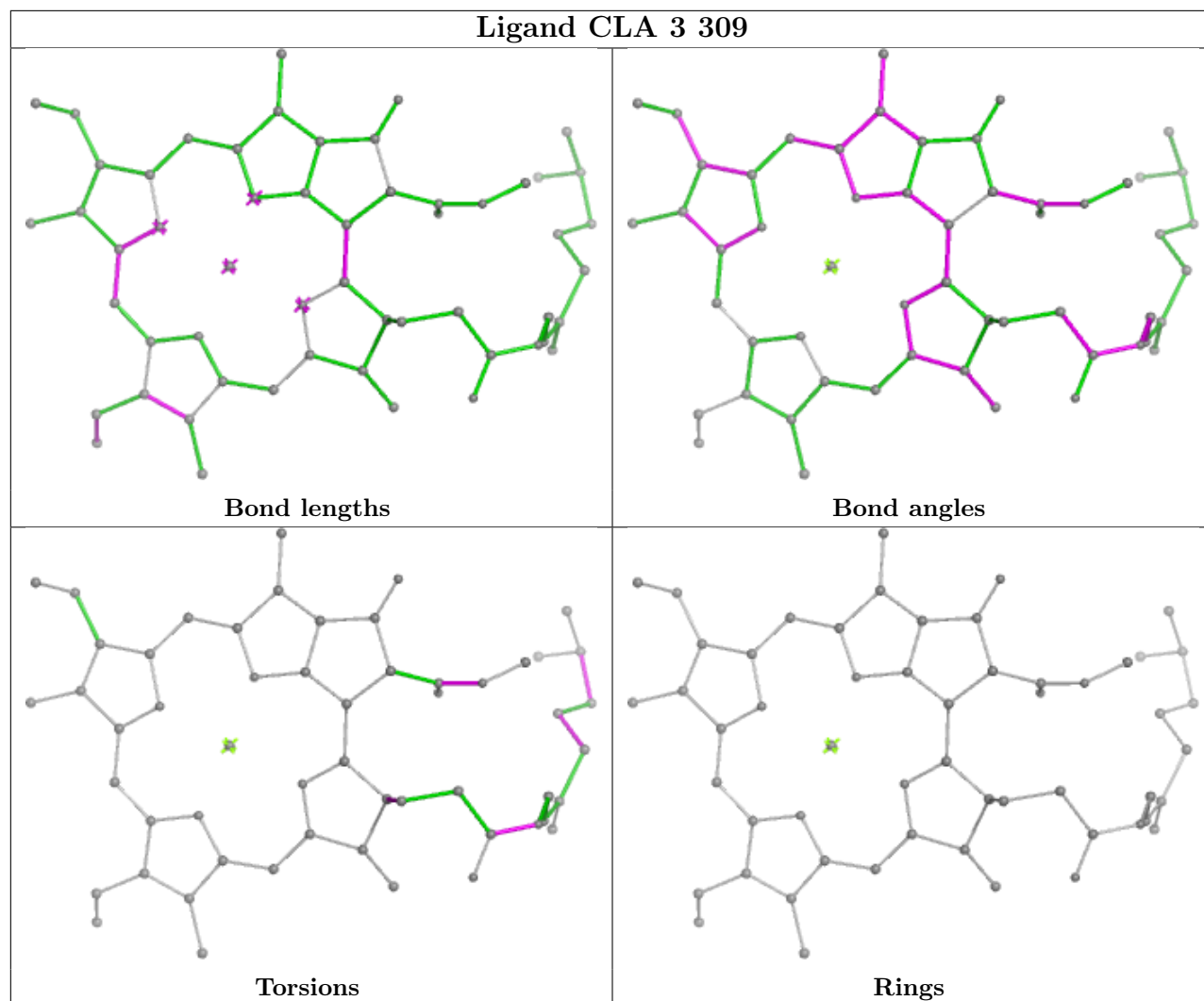


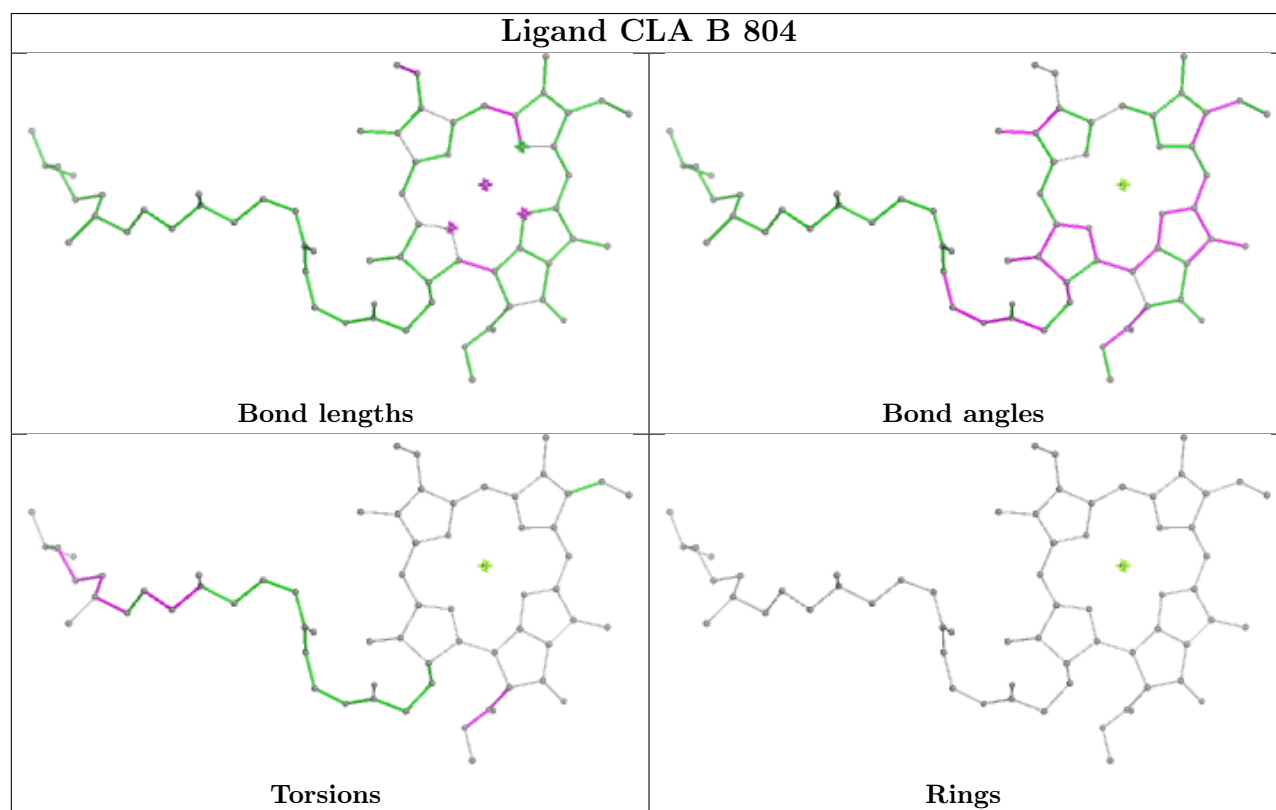
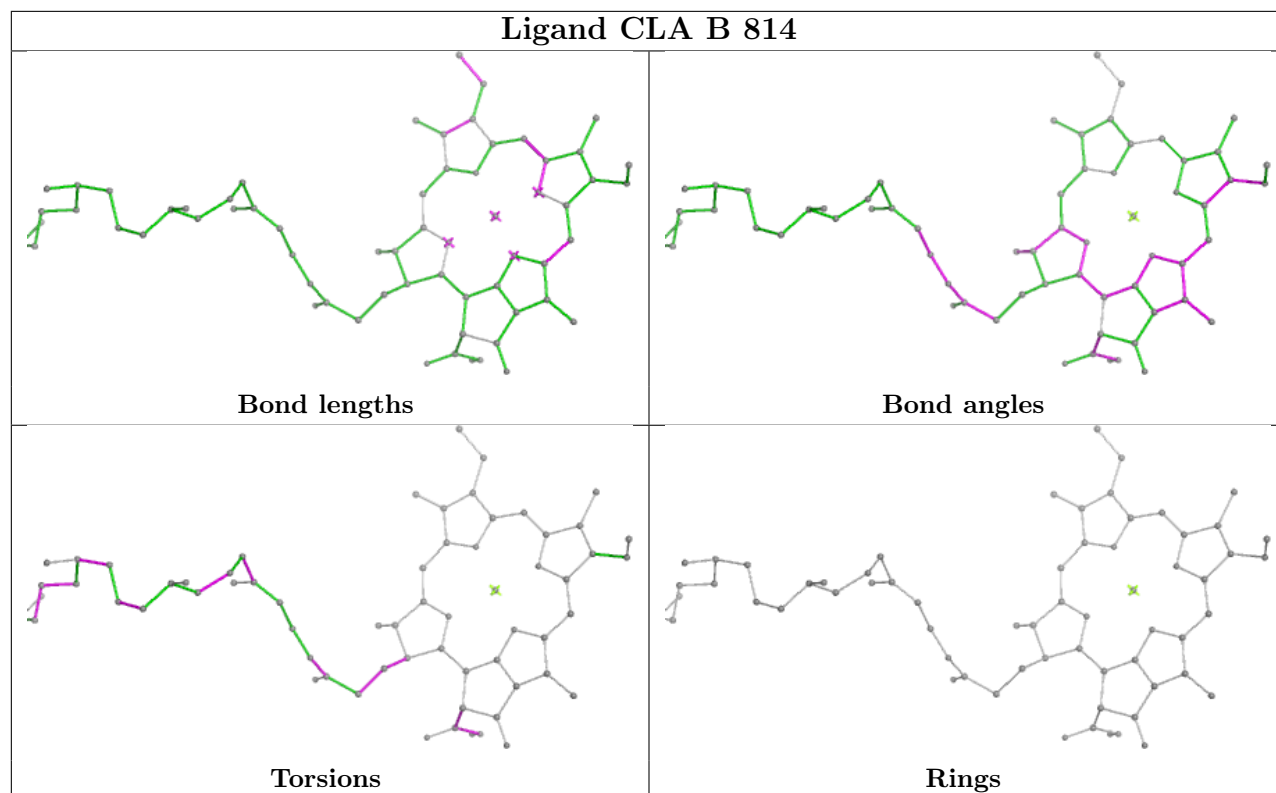
Rings



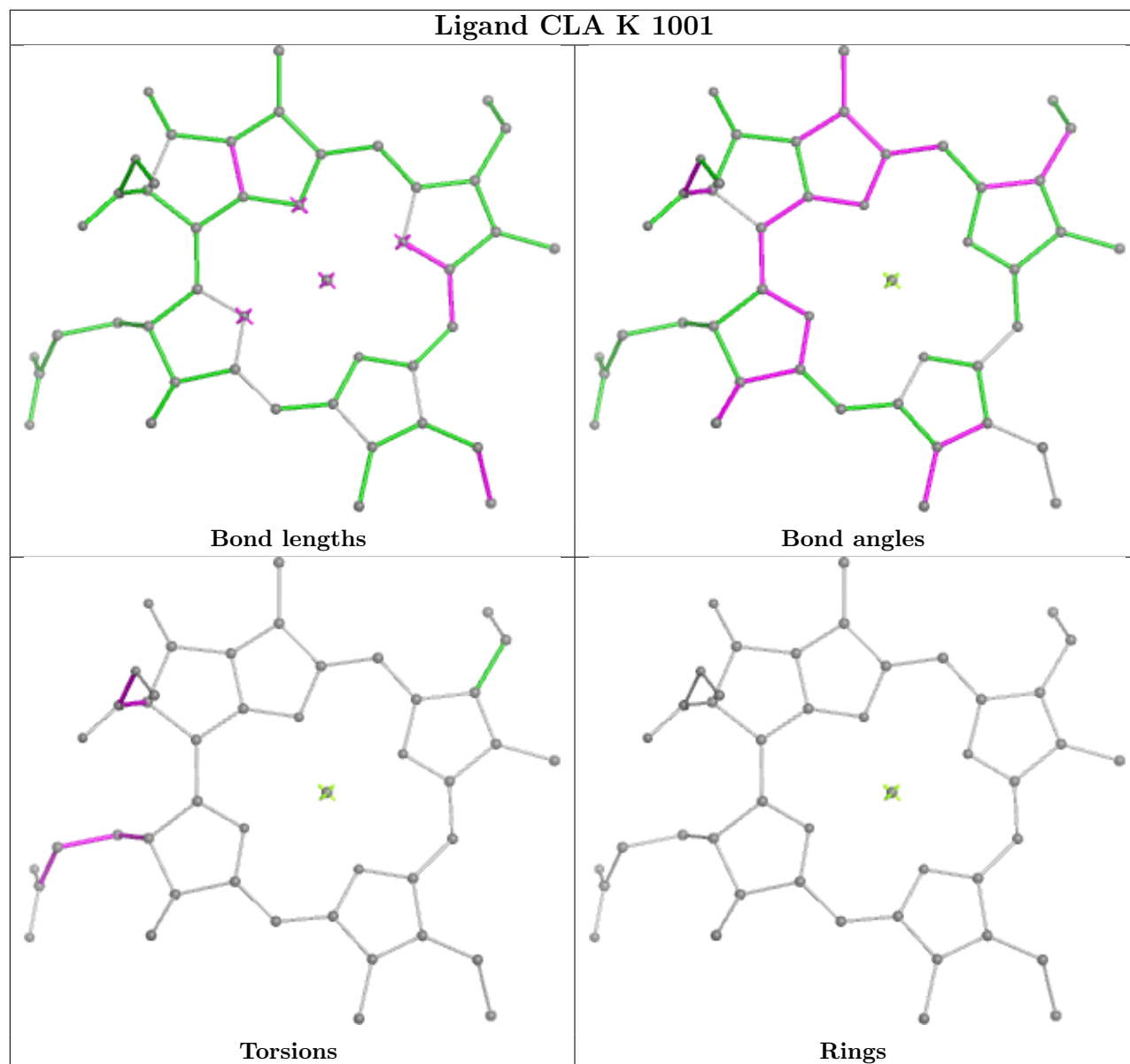


Ligand CLA 3 309

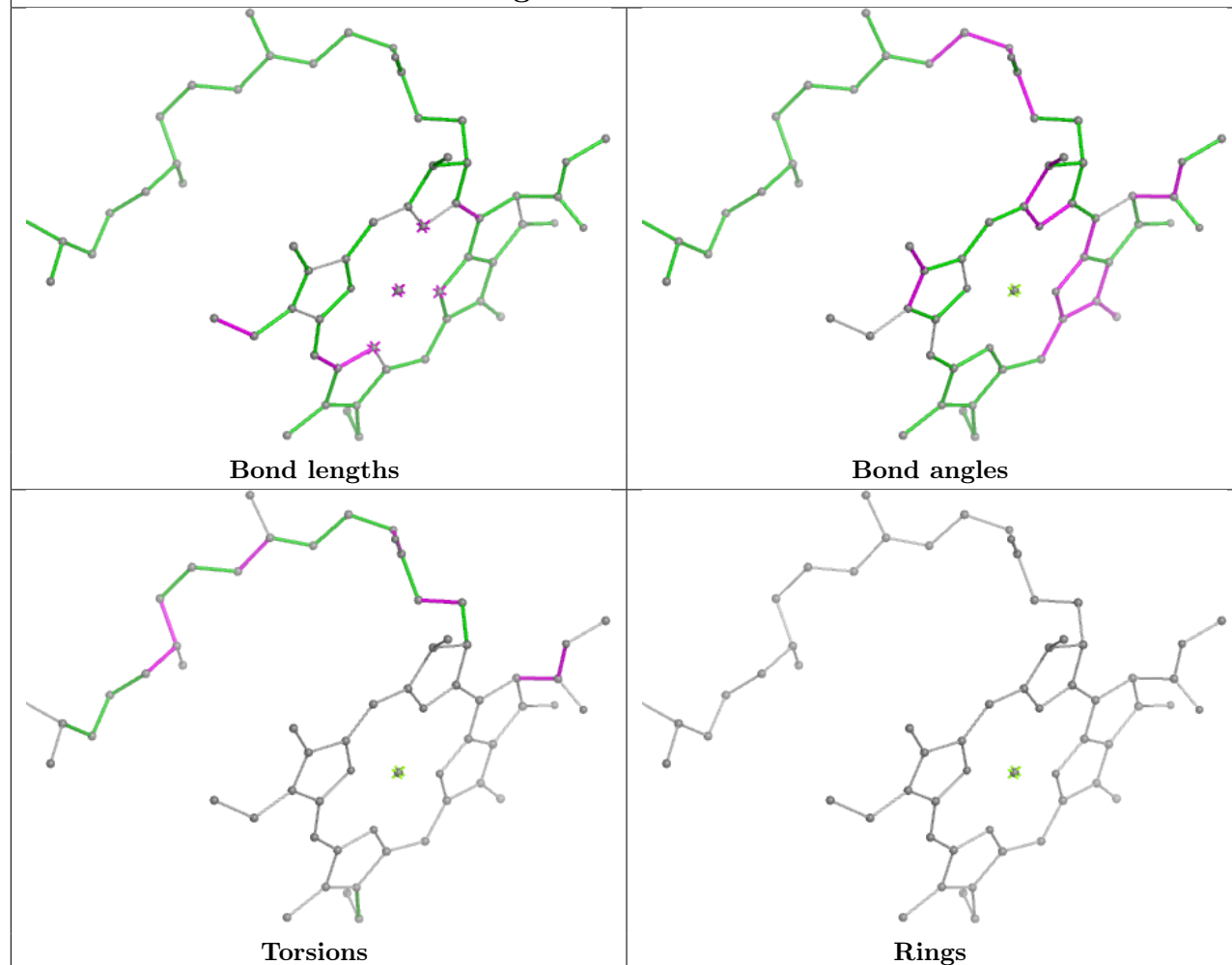




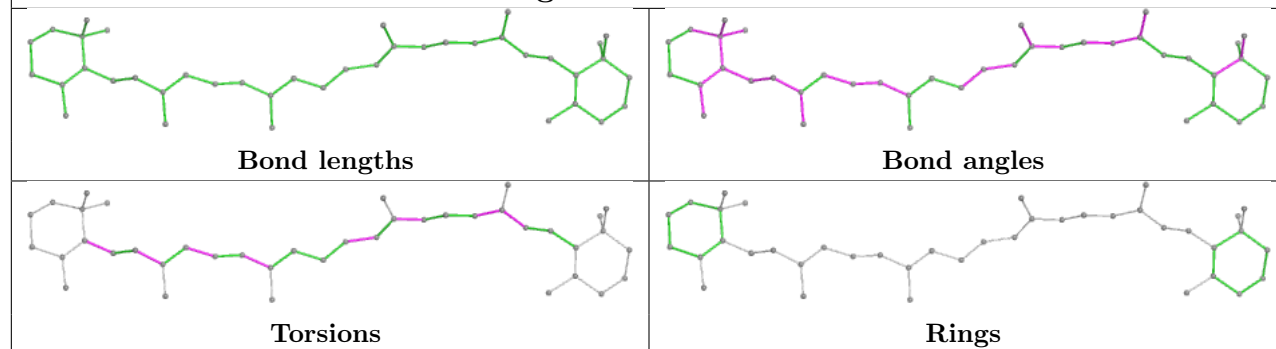
Ligand CLA K 1001



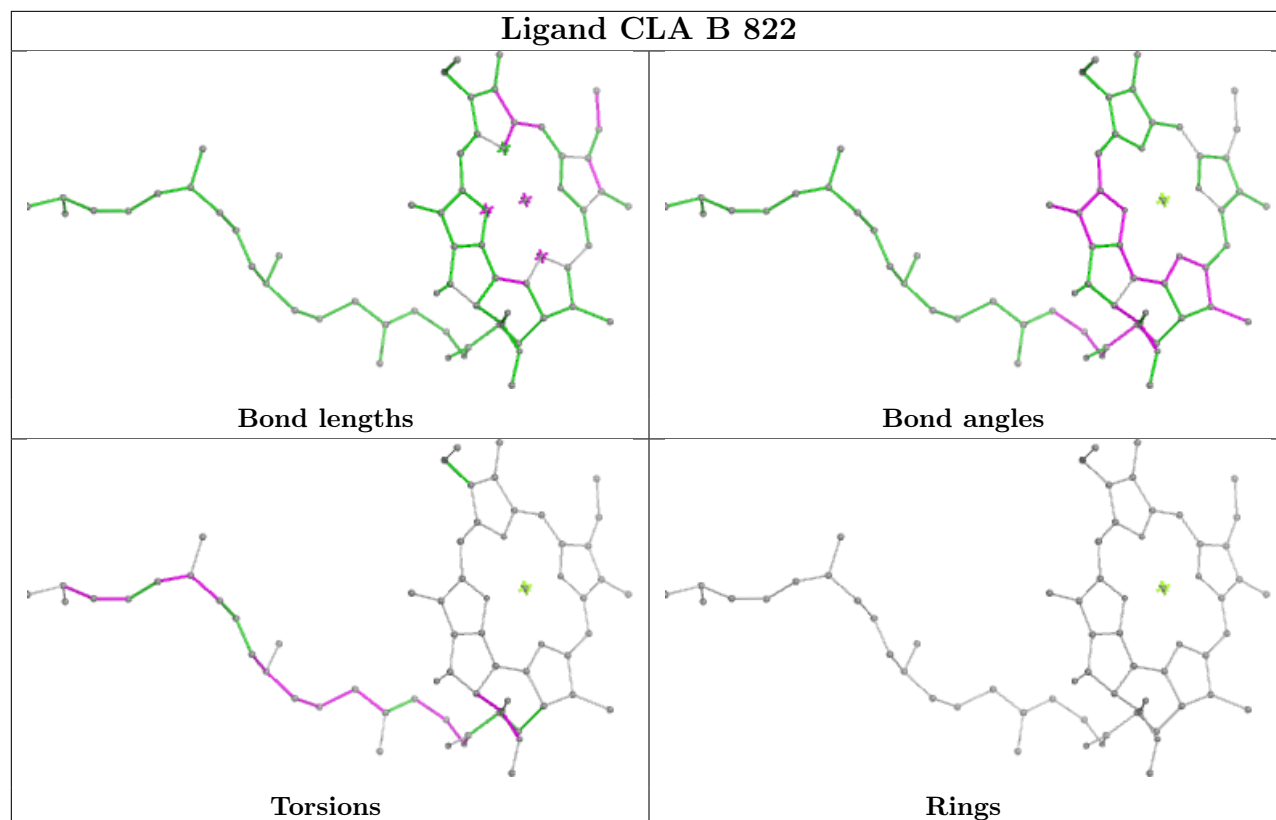
Ligand CLA A 842



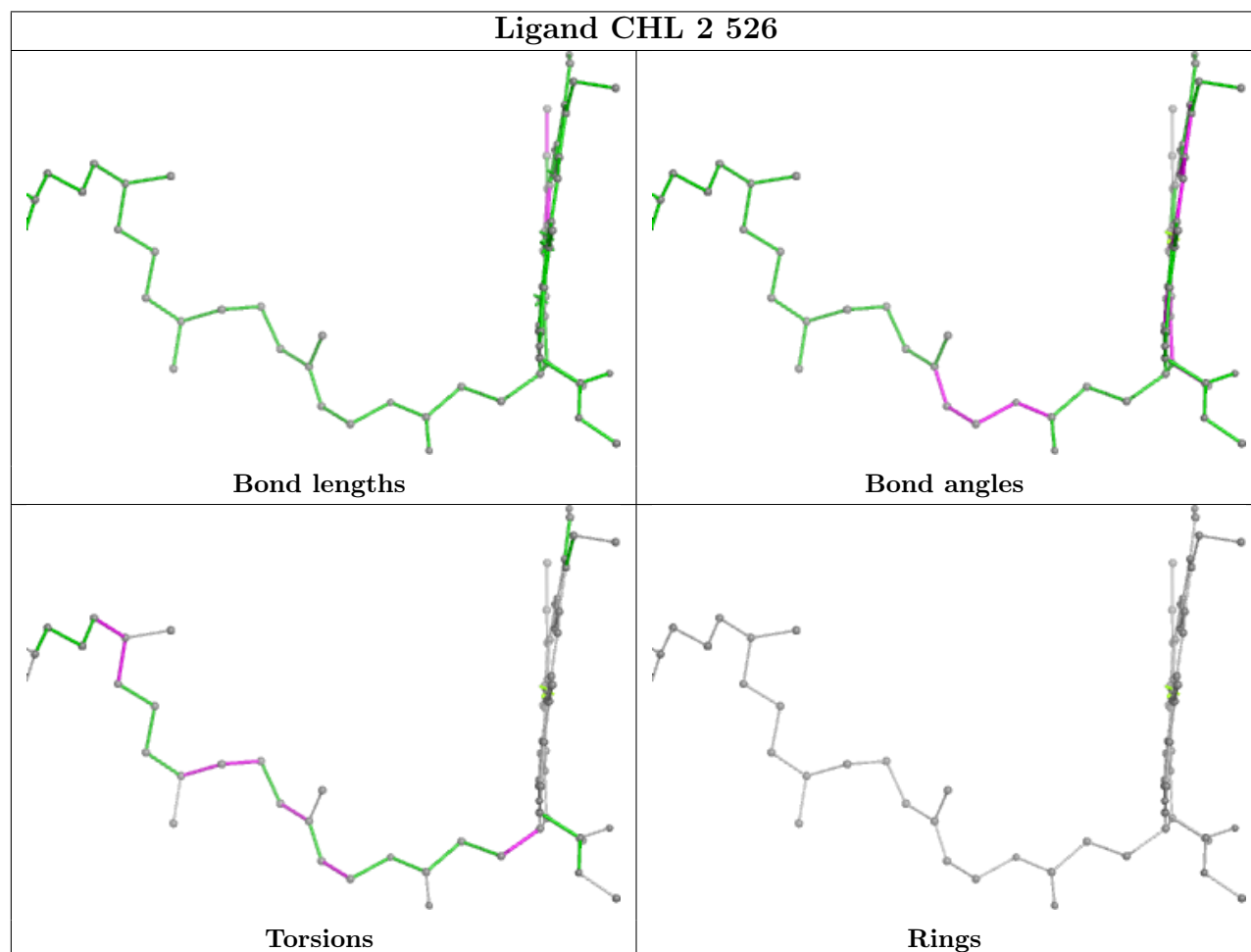
Ligand BCR I 102



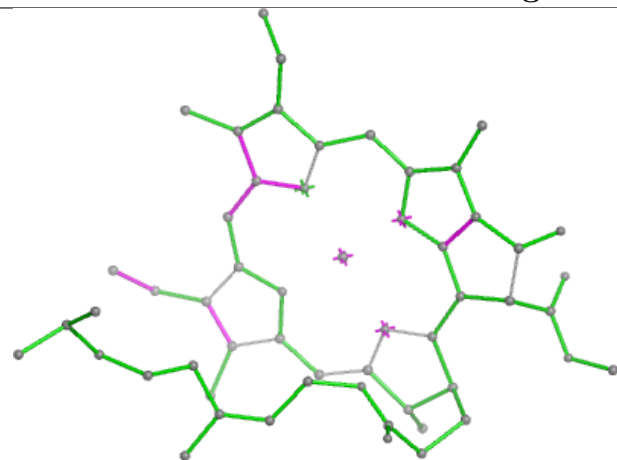
Ligand CLA B 822



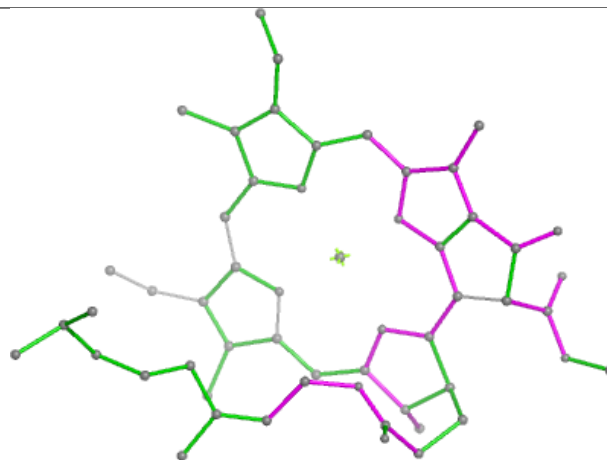
Ligand CHL 2 526



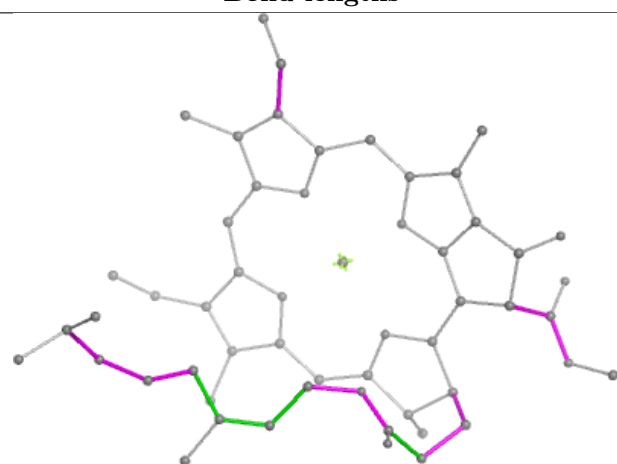
Ligand CLA 3 305



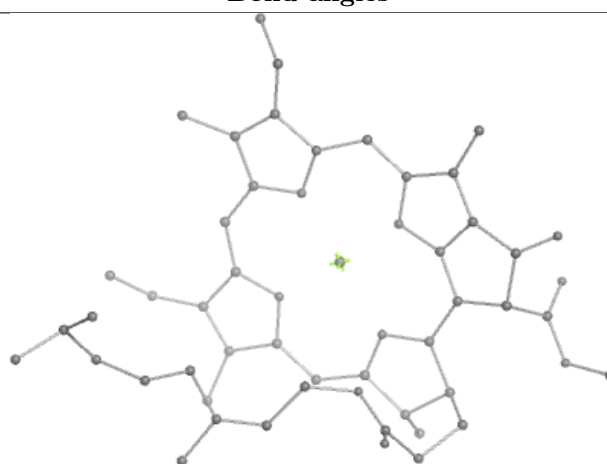
Bond lengths



Bond angles

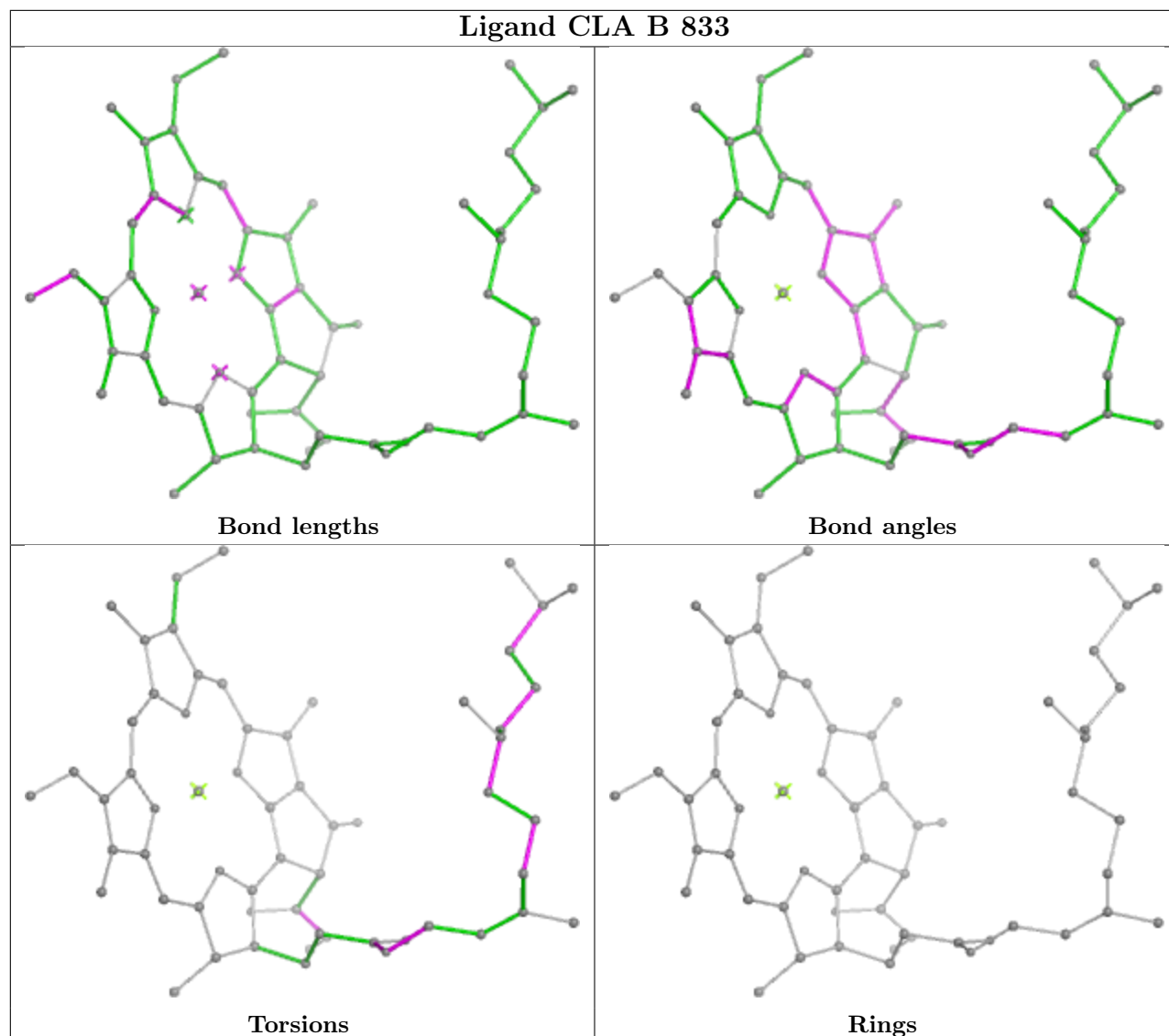


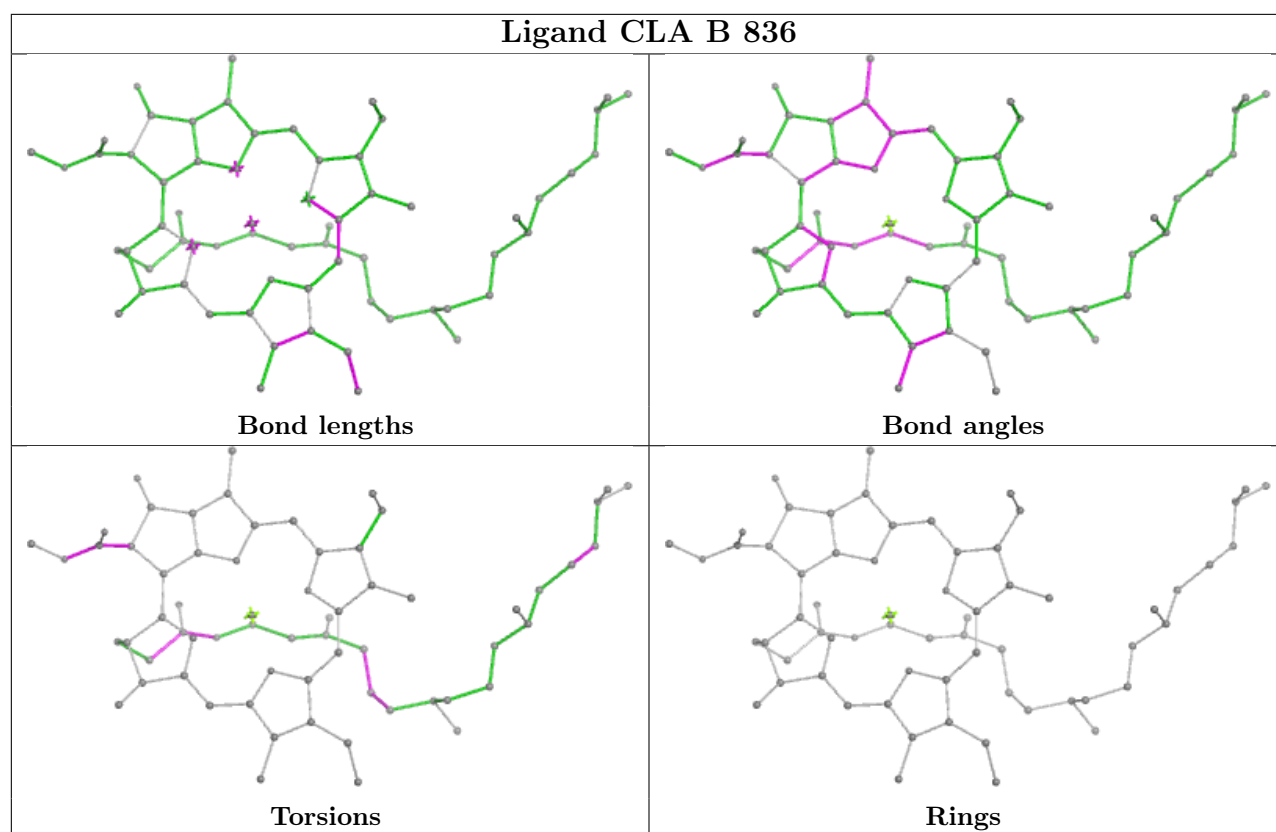
Torsions



Rings

Ligand CLA B 833





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%)	0.96	33 (17%) 5 4	86, 127, 178, 218	0
2	2	208/269 (77%)	0.22	10 (4%) 36 31	82, 113, 154, 201	0
3	3	221/275 (80%)	0.73	31 (14%) 7 6	101, 148, 202, 253	0
4	4	198/198 (100%)	0.22	12 (6%) 28 23	73, 107, 149, 196	0
5	A	743/758 (98%)	0.22	39 (5%) 34 28	47, 79, 137, 192	0
6	B	733/734 (99%)	0.16	45 (6%) 28 23	49, 76, 116, 160	0
7	C	80/81 (98%)	0.29	6 (7%) 22 17	55, 66, 89, 121	0
8	D	143/143 (100%)	0.65	18 (12%) 9 7	60, 77, 107, 153	0
9	E	66/66 (100%)	0.24	4 (6%) 28 23	51, 81, 122, 147	0
10	F	154/154 (100%)	-0.11	4 (2%) 57 51	54, 76, 116, 168	0
11	G	97/97 (100%)	0.55	10 (10%) 13 11	76, 113, 151, 161	0
12	H	88/88 (100%)	0.53	8 (9%) 16 13	80, 112, 146, 178	0
13	I	30/40 (75%)	0.20	2 (6%) 25 20	76, 99, 136, 138	0
14	J	42/42 (100%)	-0.07	2 (4%) 36 31	57, 69, 96, 145	0
15	K	77/80 (96%)	1.09	13 (16%) 5 4	131, 168, 192, 218	0
16	L	157/157 (100%)	0.65	18 (11%) 11 8	77, 105, 151, 209	0
All	All	3230/3375 (95%)	0.35	255 (7%) 20 16	47, 94, 164, 253	0

All (255) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	103	GLY	11.0
1	1	101	GLY	10.8
8	D	196	VAL	9.7
8	D	200	GLU	8.6
3	3	177	ALA	8.2

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Mol	Chain	Res	Type	RSRZ
8	D	208	PRO	8.1
11	G	153	LYS	7.8
5	A	263	ALA	7.8
12	H	53	VAL	7.5
11	G	110	GLU	7.1
8	D	206	LYS	7.0
6	B	294	ASN	7.0
1	1	102	LEU	6.8
9	E	98	ASN	6.6
6	B	70	TRP	6.4
6	B	295	PHE	6.2
8	D	197	SER	6.1
16	L	172	GLN	6.0
16	L	163	SER	5.9
1	1	161	PRO	5.7
1	1	100	LEU	5.5
2	2	58	THR	5.5
6	B	92	TRP	5.3
5	A	264	GLU	5.2
8	D	201	VAL	5.0
6	B	211	ASN	5.0
7	C	35	LYS	5.0
7	C	13	GLY	5.0
8	D	211	LEU	5.0
11	G	58	LEU	4.9
11	G	111	TYR	4.9
3	3	92	PHE	4.9
8	D	207	GLN	4.9
1	1	225	THR	4.9
3	3	173	PHE	4.9
16	L	186	THR	4.8
3	3	96	ARG	4.7
15	K	80	ALA	4.6
3	3	176	TRP	4.6
3	3	269	LEU	4.4
5	A	261	SER	4.3
14	J	42	PHE	4.3
15	K	47	ILE	4.2
6	B	136	TYR	4.2
1	1	226	ILE	4.2
6	B	566	GLY	4.1
15	K	90	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
5	A	262	PHE	4.1
15	K	50	PRO	4.1
1	1	98	GLU	4.1
12	H	78	TYR	4.0
9	E	64	PRO	3.9
2	2	168	TRP	3.9
3	3	127	LEU	3.9
6	B	165	VAL	3.9
5	A	278	ALA	3.8
3	3	125	VAL	3.8
16	L	205	TYR	3.8
2	2	206	TRP	3.8
1	1	99	ALA	3.8
10	F	231	VAL	3.8
1	1	131	LEU	3.8
6	B	505	SER	3.8
12	H	115	SER	3.7
5	A	277	TYR	3.7
10	F	227	VAL	3.7
6	B	552	ASP	3.7
5	A	519	ASP	3.6
1	1	228	ASN	3.6
1	1	219	ALA	3.6
9	E	91	VAL	3.6
16	L	115	VAL	3.6
15	K	51	THR	3.6
6	B	293	THR	3.6
1	1	96	VAL	3.6
3	3	178	LYS	3.5
16	L	171	LYS	3.5
11	G	106	THR	3.5
3	3	192	LYS	3.4
4	4	52	LYS	3.4
4	4	53	LYS	3.4
16	L	173	PRO	3.4
6	B	291	TYR	3.4
16	L	111	VAL	3.4
8	D	205	GLY	3.4
3	3	272	LEU	3.3
5	A	139	GLY	3.3
7	C	34	CYS	3.3
5	A	276	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
4	4	191	PRO	3.3
2	2	59	VAL	3.3
3	3	264	VAL	3.3
6	B	266	GLN	3.3
12	H	73	ASP	3.3
11	G	104	GLY	3.3
1	1	229	VAL	3.2
1	1	218	LEU	3.2
15	K	105	ALA	3.2
3	3	174	GLN	3.1
3	3	275	HIS	3.1
16	L	125	ILE	3.1
16	L	128	GLN	3.1
5	A	203	LEU	3.1
3	3	59	PHE	3.1
6	B	487	ASN	3.1
6	B	604	GLY	3.1
3	3	141	VAL	3.0
1	1	227	GLY	3.0
7	C	32	GLY	3.0
16	L	96	LEU	3.0
1	1	160	TYR	3.0
6	B	296	GLY	3.0
5	A	141	ARG	3.0
3	3	149	ASN	2.9
6	B	734	GLY	2.9
8	D	193	GLY	2.9
12	H	133	PRO	2.9
15	K	125	GLY	2.9
8	D	183	GLN	2.9
6	B	212	PHE	2.8
8	D	195	ASN	2.8
8	D	199	ILE	2.8
1	1	57	GLY	2.8
11	G	115	LEU	2.8
6	B	491	SER	2.7
12	H	81	LEU	2.7
16	L	184	LYS	2.7
1	1	125	PRO	2.7
13	I	6	SER	2.7
5	A	657	LEU	2.7
1	1	72	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
5	A	180	PHE	2.7
5	A	618	TRP	2.7
6	B	554	GLY	2.7
8	D	210	ASP	2.7
16	L	109	LEU	2.7
16	L	162	PRO	2.7
5	A	401	TRP	2.7
5	A	249	ILE	2.7
6	B	490	ARG	2.6
8	D	78	ASN	2.6
9	E	65	PRO	2.6
5	A	386	ALA	2.6
5	A	374	HIS	2.6
6	B	259	GLY	2.6
1	1	153	LYS	2.6
13	I	3	ASN	2.6
15	K	53	LEU	2.6
5	A	259	TYR	2.6
5	A	198	ASP	2.6
5	A	511	THR	2.5
6	B	669	GLY	2.5
16	L	116	LYS	2.5
3	3	98	LEU	2.5
15	K	103	THR	2.5
1	1	150	SER	2.5
3	3	252	PRO	2.5
1	1	201	GLN	2.5
4	4	193	ASN	2.5
8	D	133	ALA	2.5
2	2	207	GLY	2.5
5	A	179	LEU	2.4
5	A	396	PHE	2.4
4	4	67	THR	2.4
1	1	71	GLU	2.4
3	3	268	VAL	2.4
4	4	173	LYS	2.4
1	1	144	PHE	2.4
6	B	292	ARG	2.4
5	A	46	LYS	2.4
6	B	89	HIS	2.4
1	1	60	GLY	2.4
3	3	87	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
3	3	103	VAL	2.4
12	H	76	SER	2.4
6	B	87	ILE	2.4
6	B	330	ILE	2.4
10	F	228	ALA	2.4
6	B	66	PHE	2.3
15	K	102	ASP	2.3
5	A	387	THR	2.3
2	2	251	PHE	2.3
3	3	116	ALA	2.3
4	4	66	LEU	2.3
6	B	61	THR	2.3
6	B	88	ALA	2.3
6	B	300	SER	2.3
1	1	59	PHE	2.3
5	A	614	PHE	2.3
3	3	81	LEU	2.3
7	C	15	THR	2.2
1	1	40	ASP	2.2
2	2	246	PRO	2.2
5	A	493	GLN	2.2
15	K	85	ALA	2.2
5	A	453	LEU	2.2
6	B	298	GLY	2.2
2	2	208	SER	2.2
15	K	49	SER	2.2
6	B	177	HIS	2.2
1	1	162	GLY	2.2
6	B	166	SER	2.2
6	B	214	SER	2.2
5	A	494	ASN	2.2
6	B	357	ALA	2.2
16	L	209	LEU	2.2
6	B	154	TRP	2.2
3	3	86	PRO	2.2
3	3	271	SER	2.2
4	4	190	ASN	2.2
5	A	111	ASN	2.2
10	F	230	ASP	2.2
4	4	143	VAL	2.2
6	B	551	LYS	2.2
4	4	213	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	2	130	GLY	2.2
3	3	123	GLY	2.2
16	L	130	GLY	2.2
1	1	232	PRO	2.1
5	A	107	GLU	2.1
6	B	164	SER	2.1
5	A	550	HIS	2.1
1	1	58	ASP	2.1
6	B	244	PHE	2.1
6	B	361	ILE	2.1
3	3	261	ALA	2.1
5	A	546	ALA	2.1
3	3	245	GLY	2.1
6	B	401	GLU	2.1
1	1	95	LEU	2.1
6	B	2	ALA	2.1
3	3	129	PRO	2.1
5	A	260	PRO	2.1
12	H	132	PRO	2.1
3	3	121	TYR	2.1
11	G	151	ASP	2.1
5	A	373	ALA	2.1
4	4	64	GLY	2.1
6	B	558	PRO	2.1
15	K	122	LYS	2.1
5	A	407	ILE	2.1
2	2	212	GLN	2.1
7	C	36	ALA	2.1
1	1	157	LYS	2.0
11	G	109	LYS	2.0
5	A	140	PHE	2.0
4	4	192	LEU	2.0
5	A	258	LEU	2.0
14	J	7	TYR	2.0
6	B	565	GLY	2.0
8	D	194	LYS	2.0
5	A	644	GLN	2.0
11	G	112	VAL	2.0
16	L	108	PHE	2.0
8	D	209	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 monosaccharides 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(\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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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
25	CA	3	319	1/1	0.88	0.11	118,118,118,118	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
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
19	CLA	A	835	55/65	0.89	0.13	107,124,142,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	ZEX	F	301	42/42	0.89	0.17	84,105,116,122	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
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	A	823	60/65	0.90	0.12	106,123,152,160	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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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	0.10	83,83,83,83	0
19	CLA	A	802	65/65	0.97	0.09	42,50,63,75	0

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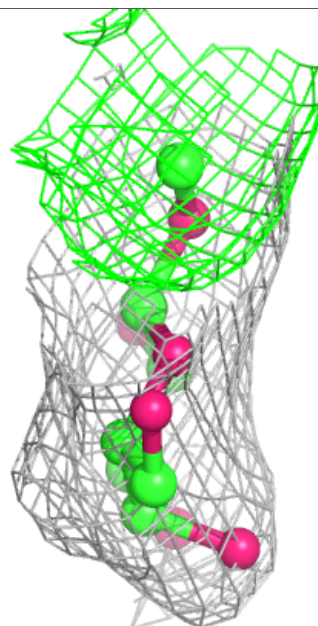
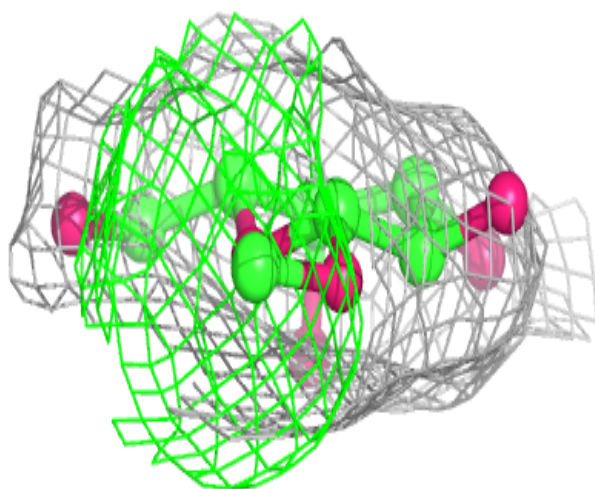
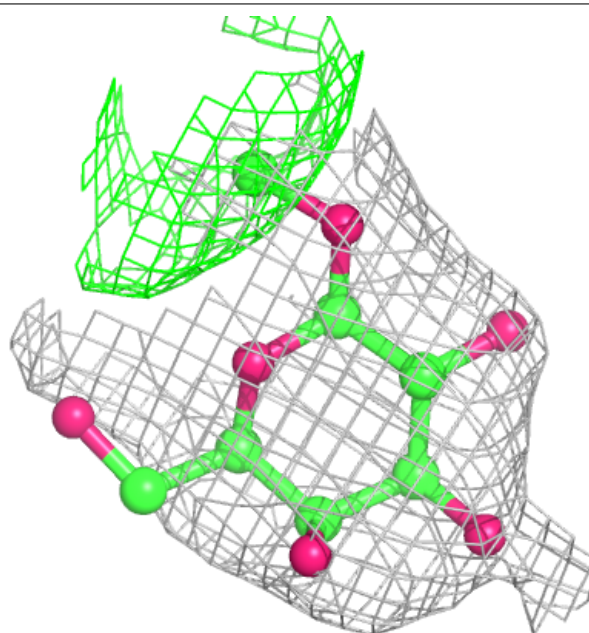
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	CLA	B	814	65/65	0.97	0.10	71,80,87,92	0
29	PQN	A	844	33/33	0.97	0.09	42,54,68,74	0
19	CLA	B	819	65/65	0.97	0.10	69,76,96,101	0
19	CLA	A	841	65/65	0.97	0.09	44,57,65,67	0
28	SF4	C	101	8/8	0.99	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.

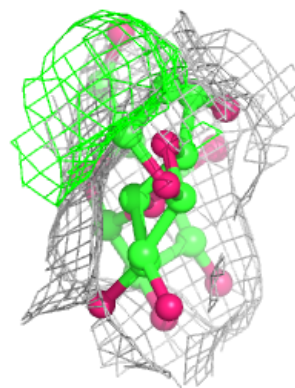
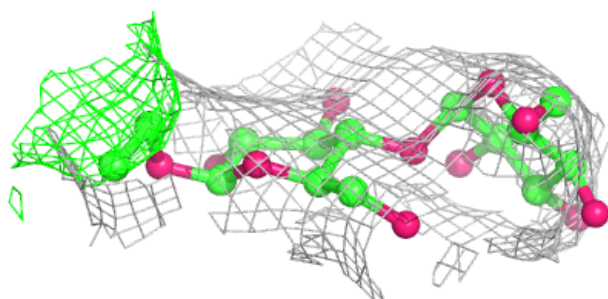
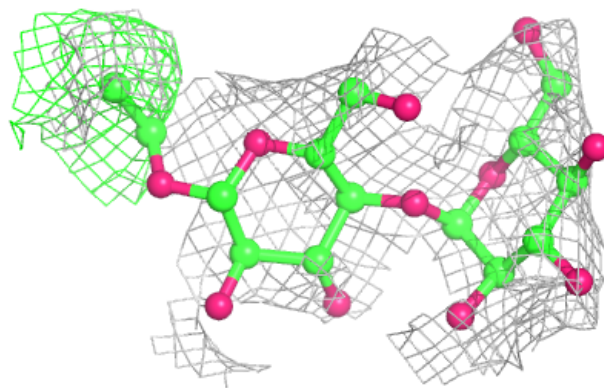
Electron density around LMG 2 520:

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

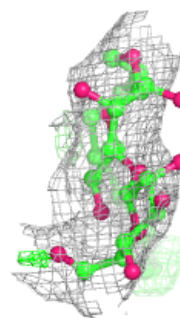
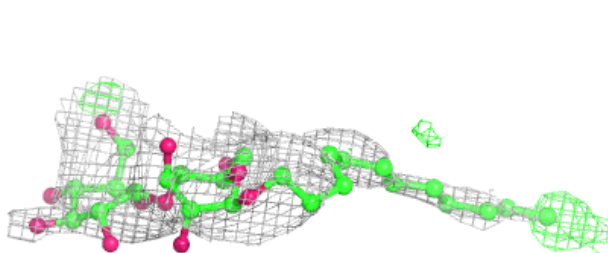
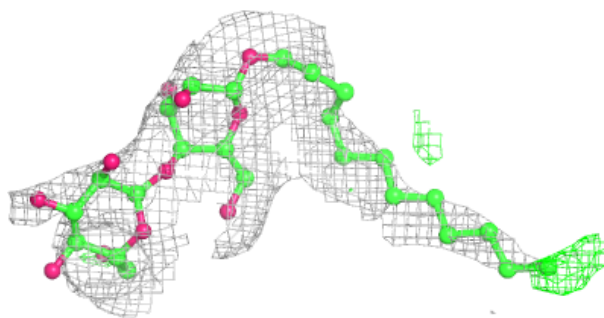


Electron density around LMT J 1107:

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

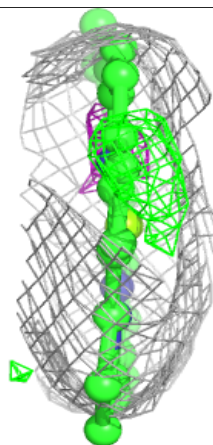
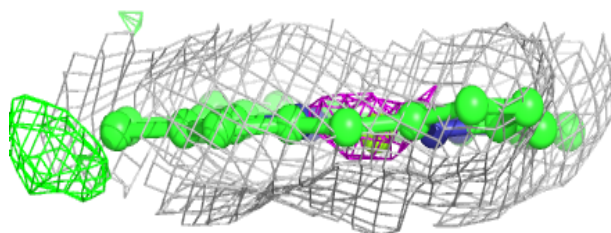
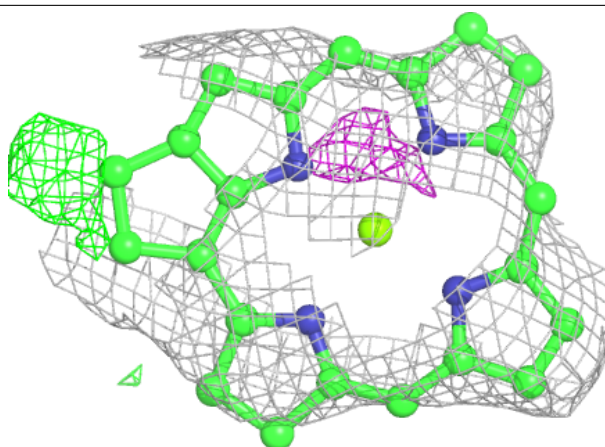
**Electron density around LMT 2 523:**

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

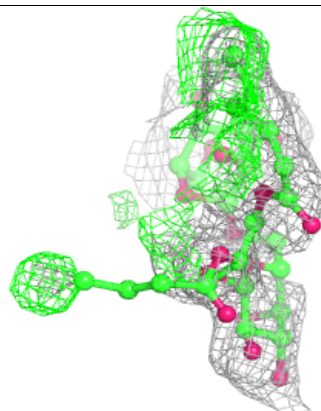
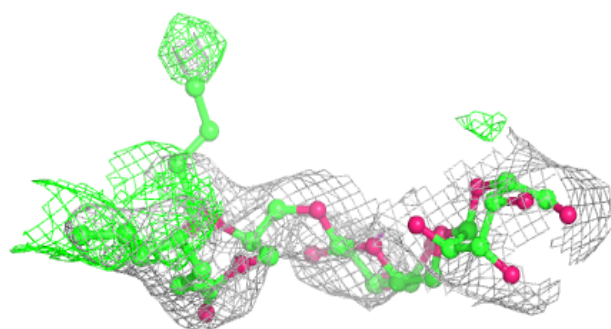
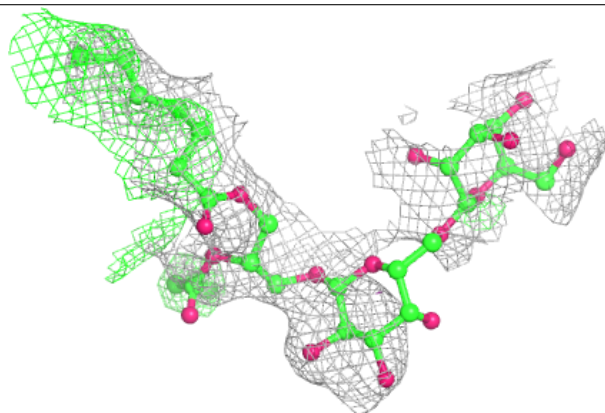


Electron density around CLA K 1004:

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

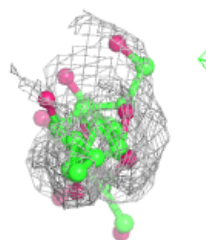
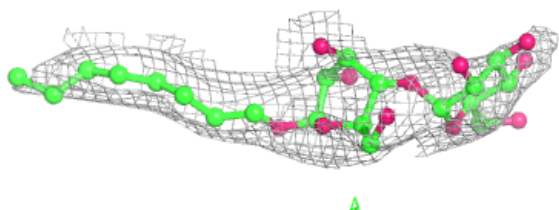
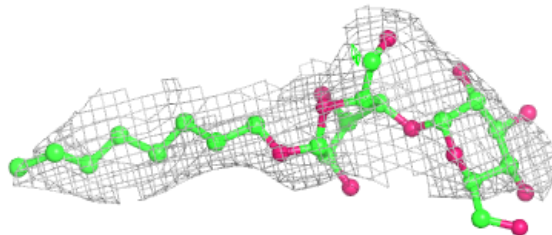
**Electron density around DGD B 801:**

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



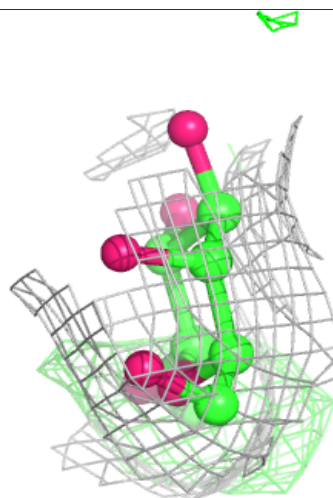
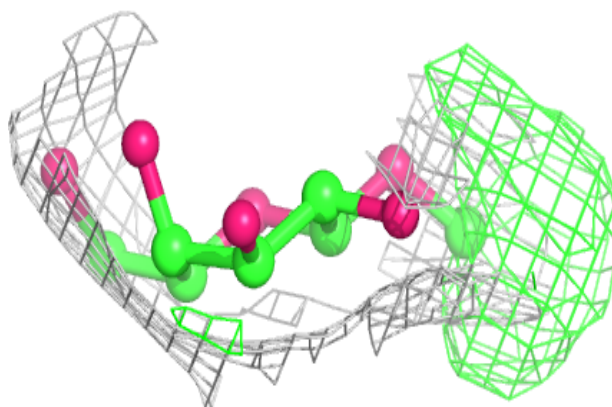
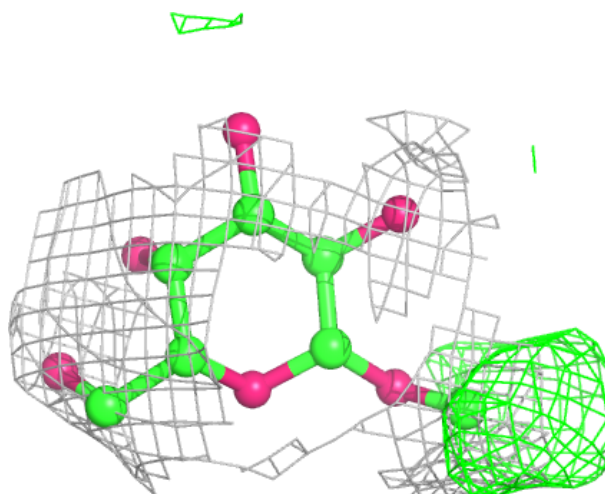
Electron density around LMT G 209:

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



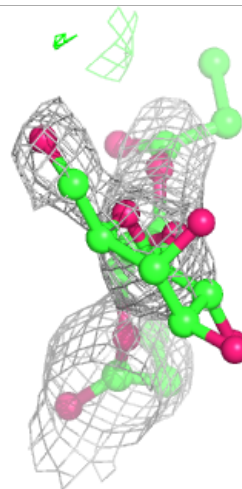
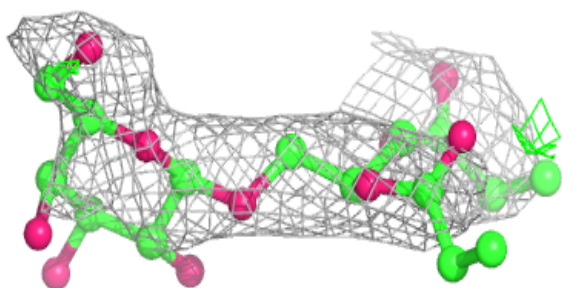
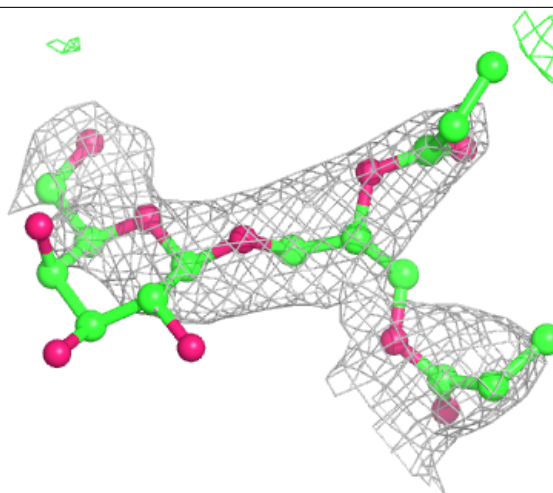
Electron density around LMG 2 522:

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



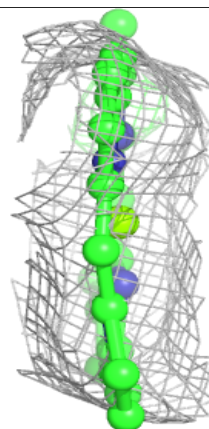
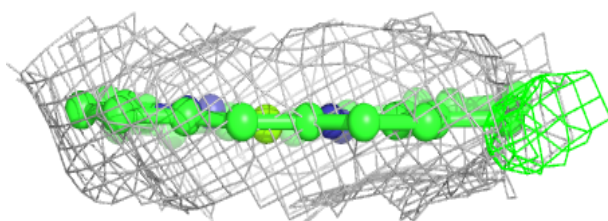
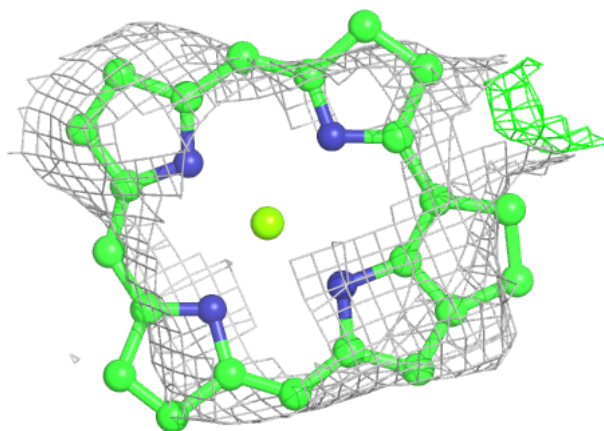
Electron density around LMG G 210:

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

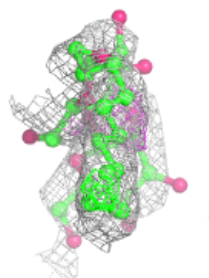
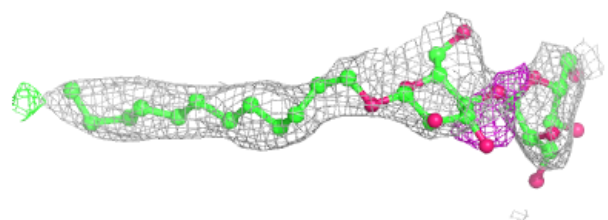
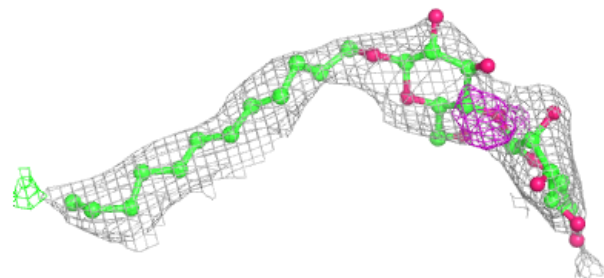


Electron density around CLA K 1003:

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

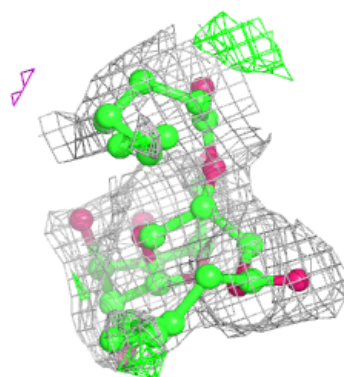
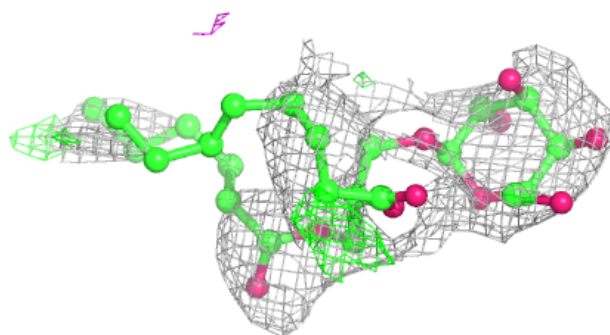
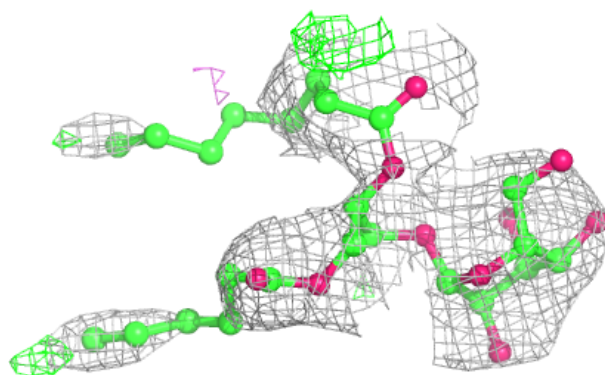
**Electron density around LMT A 846:**

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



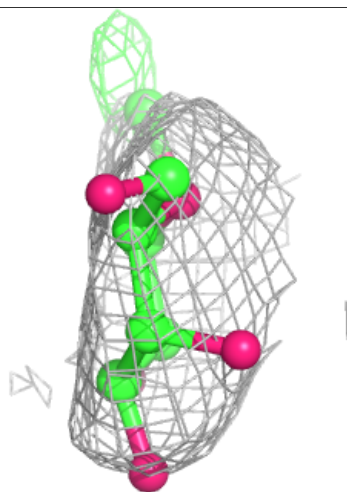
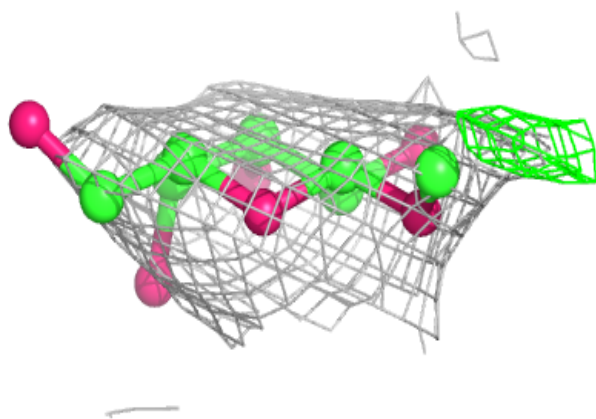
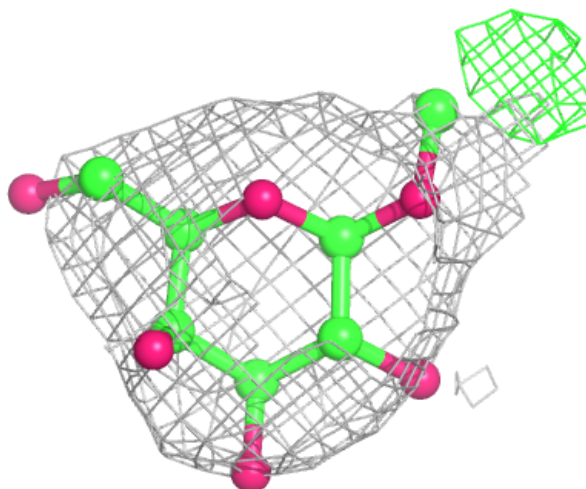
Electron density around LMG B 845:

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



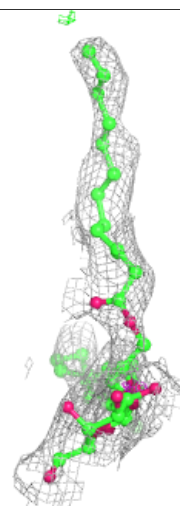
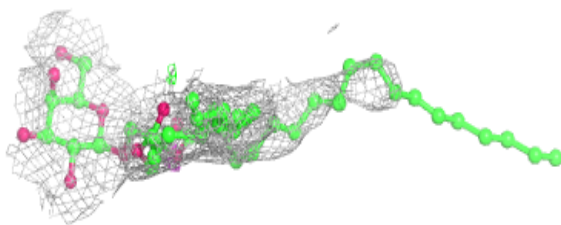
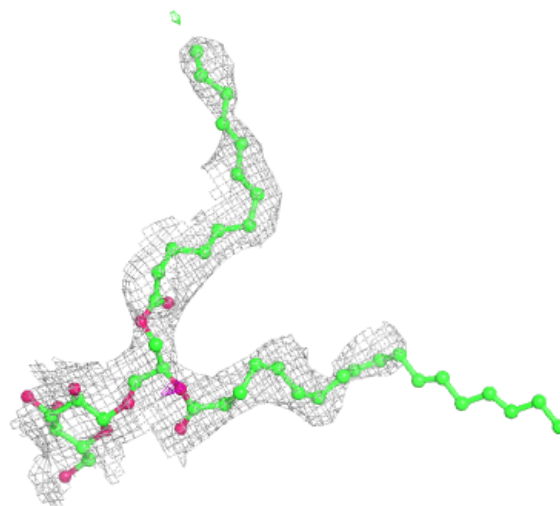
Electron density around LMG 2 524:

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



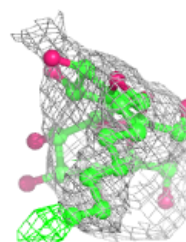
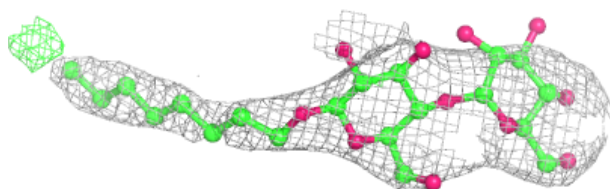
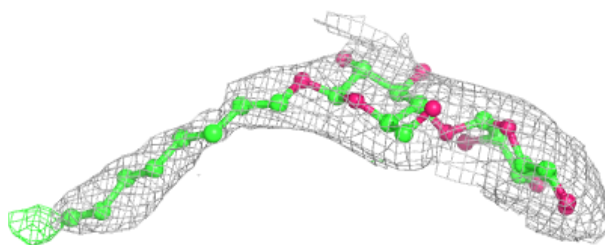
Electron density around LMG A 847:

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

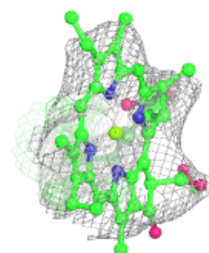
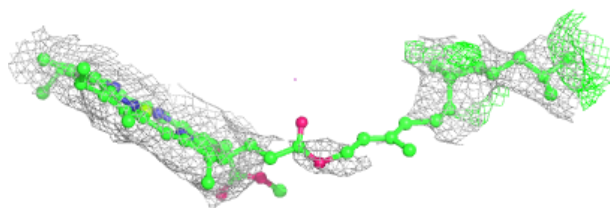
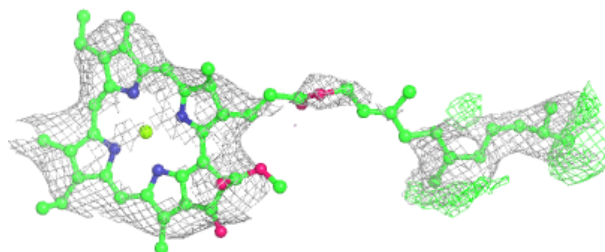


Electron density around LMT 3 318:

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

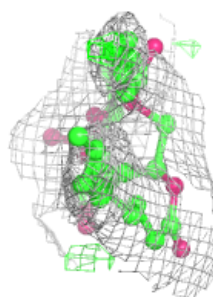
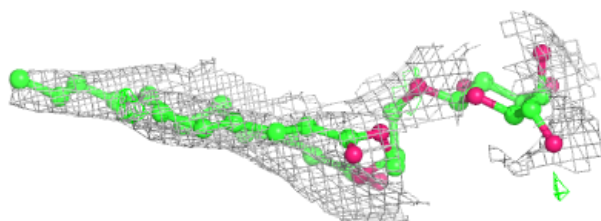
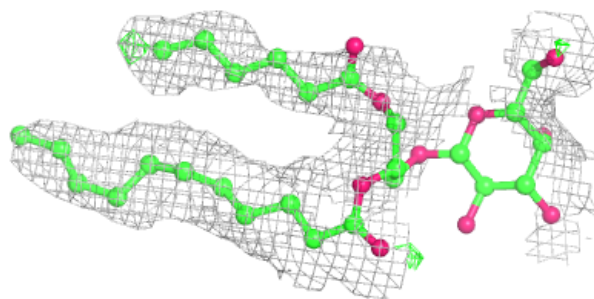
**Electron density around CLA H 1000:**

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



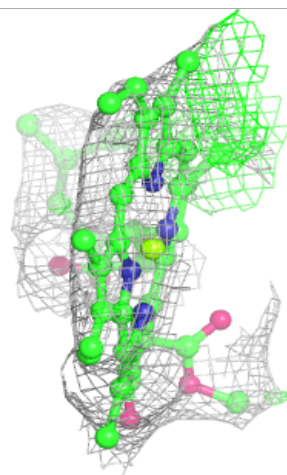
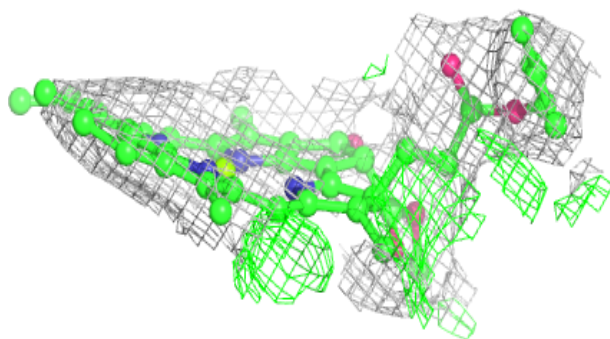
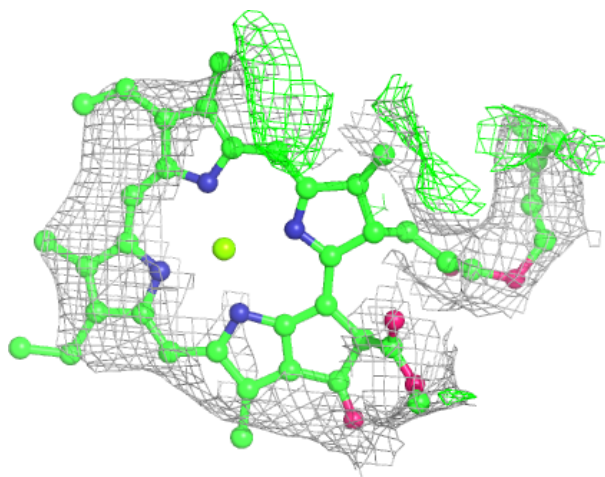
Electron density around LMG 2 519:

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



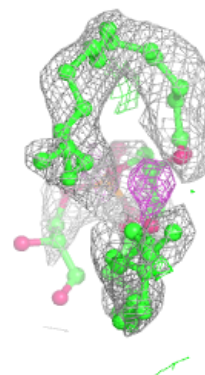
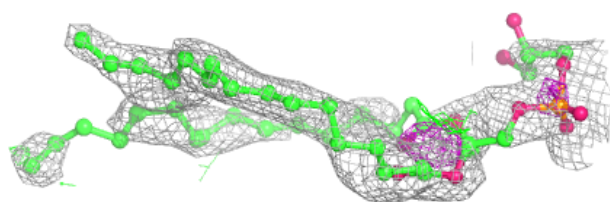
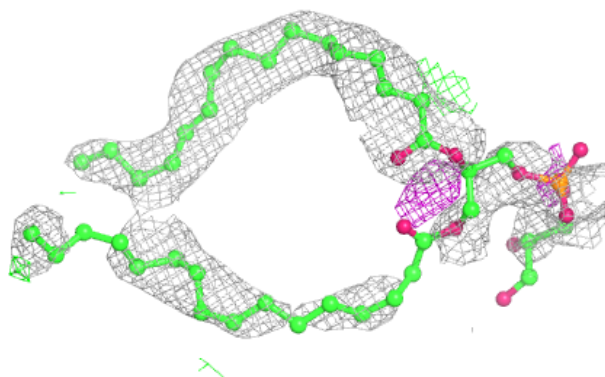
Electron density around CLA J 1105:

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



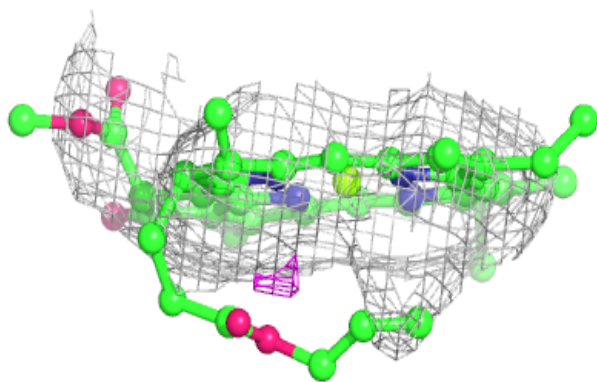
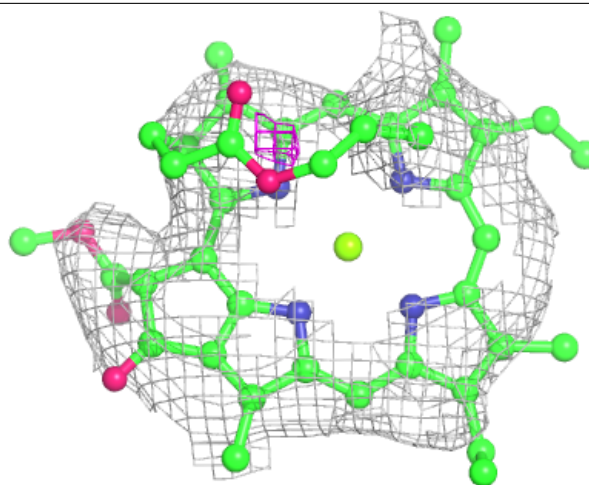
Electron density around LHG B 843:

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



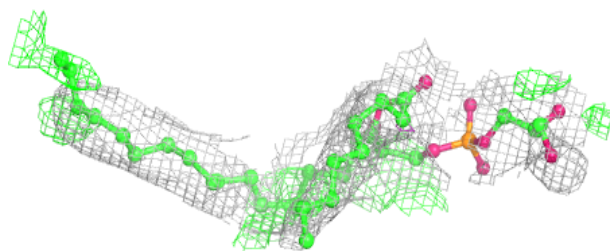
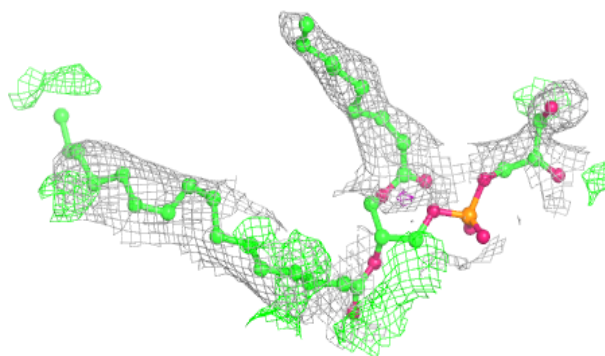
Electron density around CLA 3 312:

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

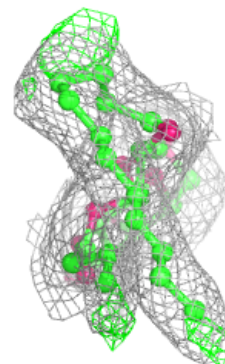
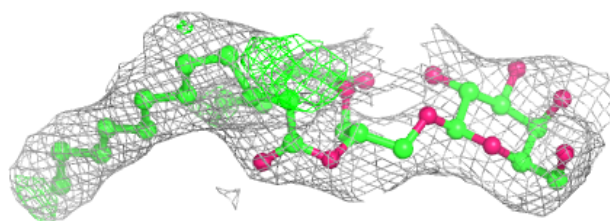
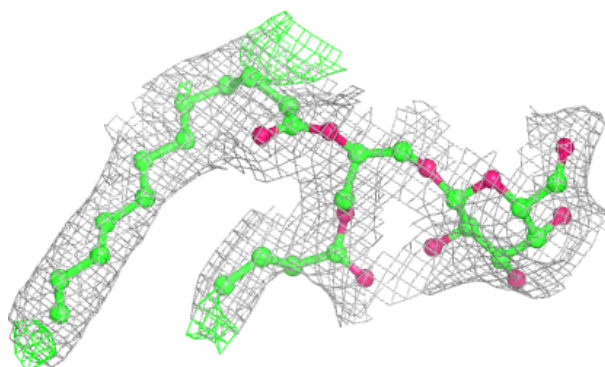


Electron density around LHG 1 520:

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

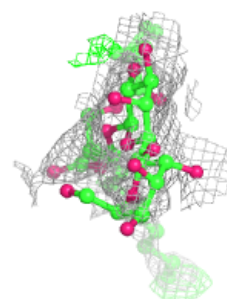
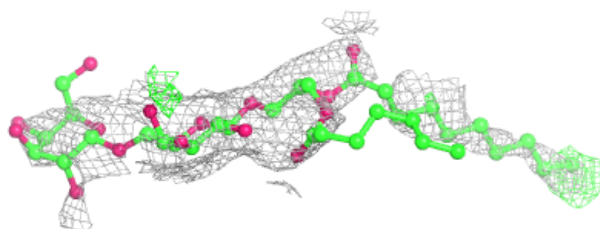
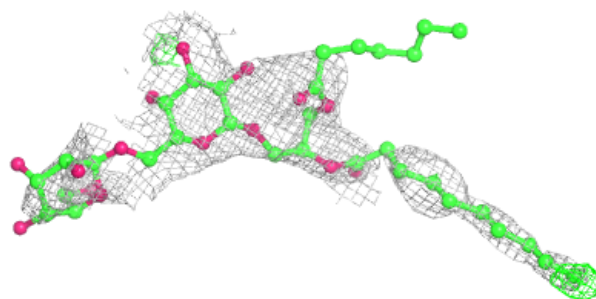
**Electron density around LMG B 844:**

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

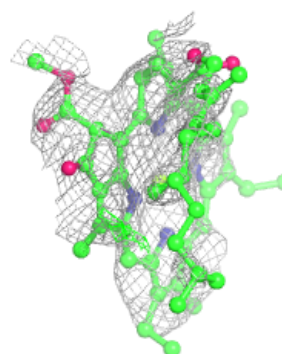
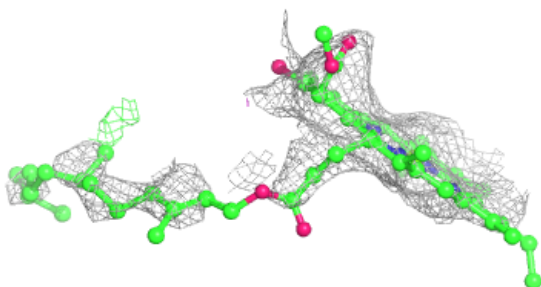
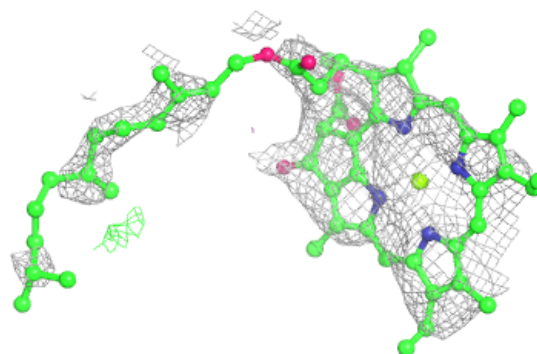


Electron density around DGD G 207:

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

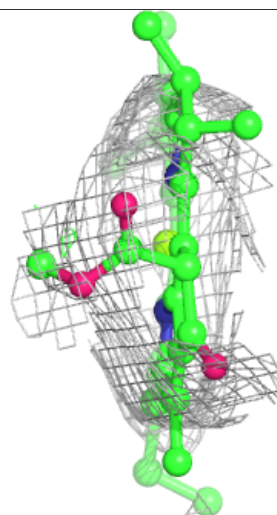
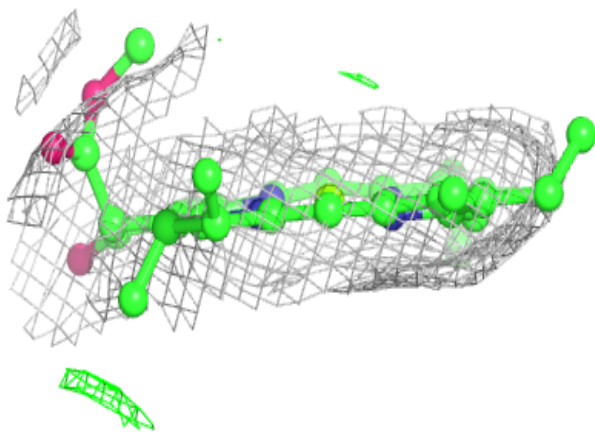
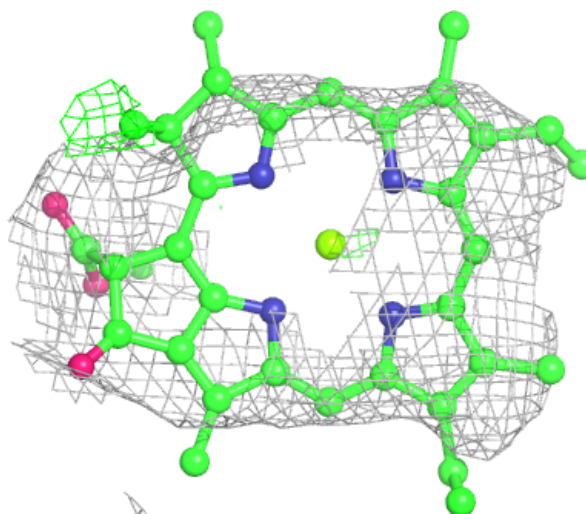
**Electron density around CLA K 1002:**

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



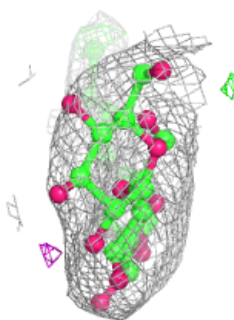
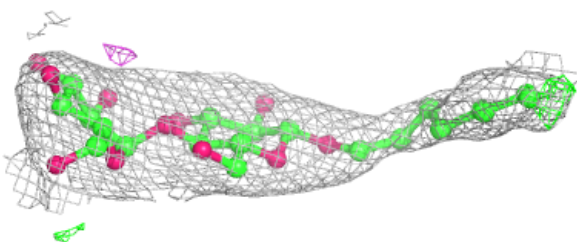
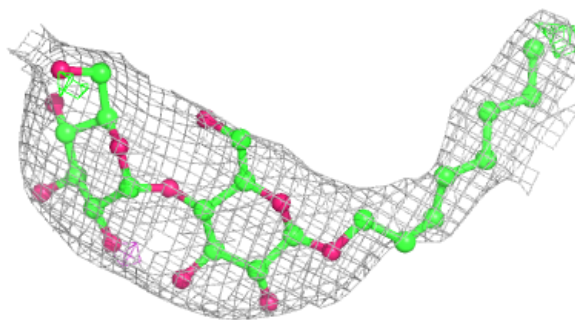
Electron density around CLA 3 311:

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

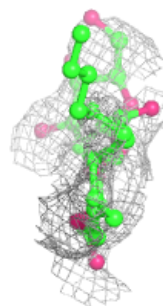
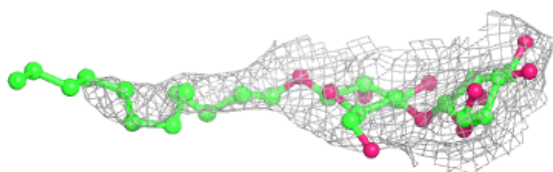
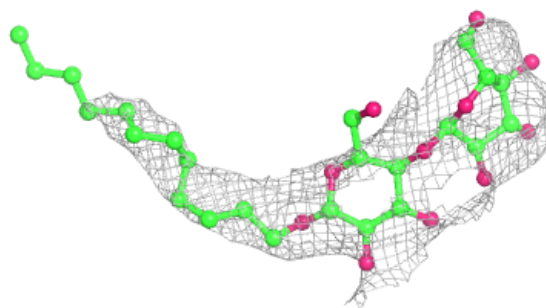


Electron density around LMT B 855:

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

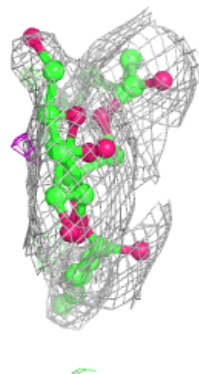
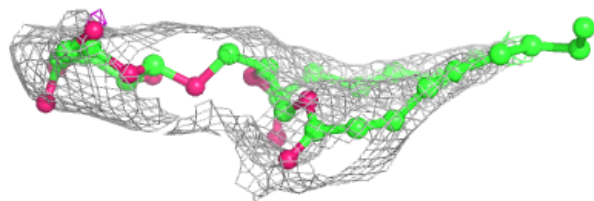
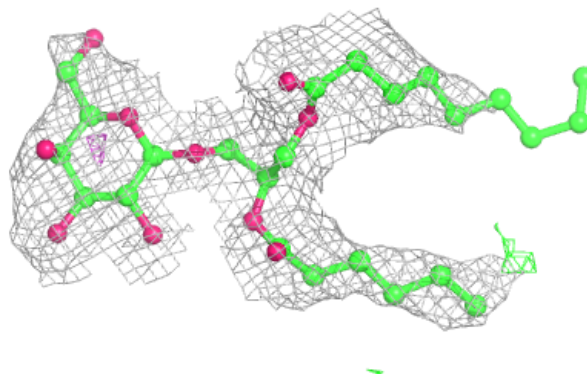
**Electron density around LMT B 846:**

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

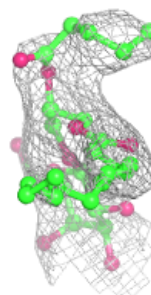
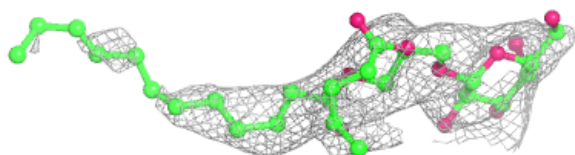
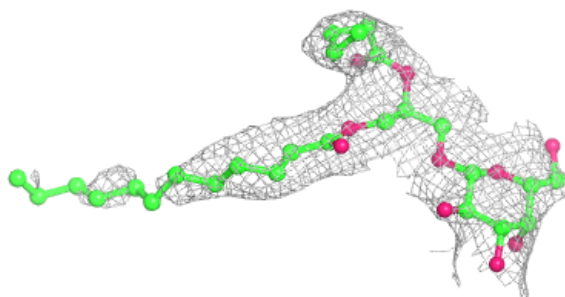


Electron density around LMG J 1104:

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

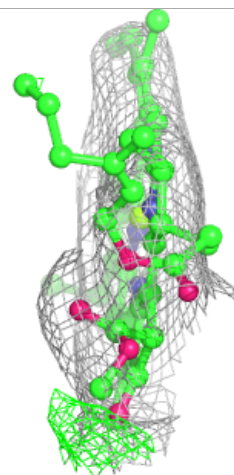
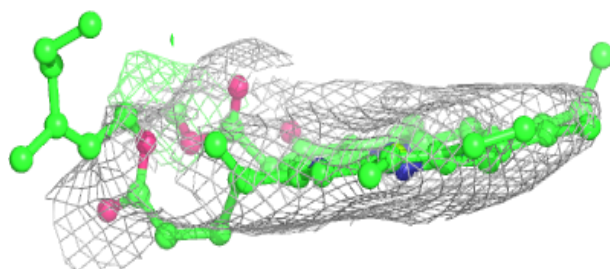
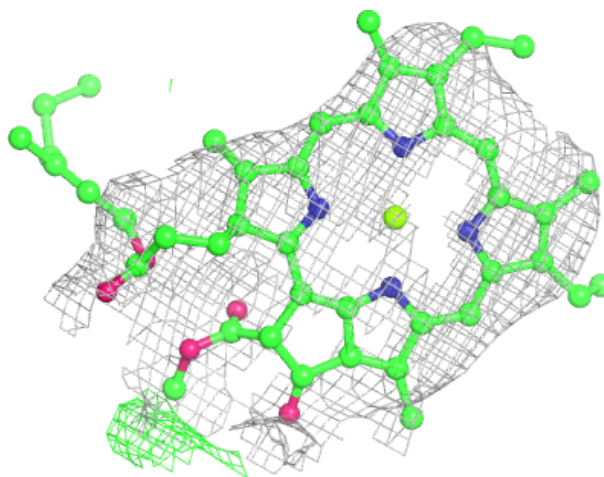
**Electron density around LMG F 305:**

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



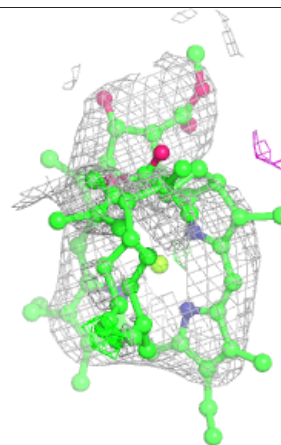
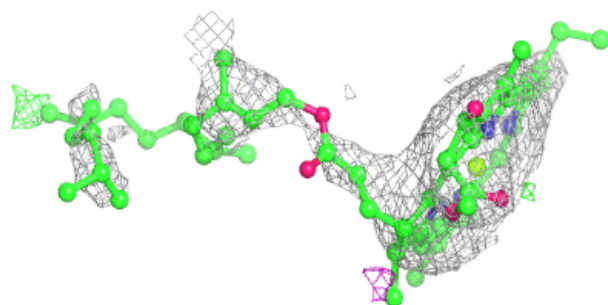
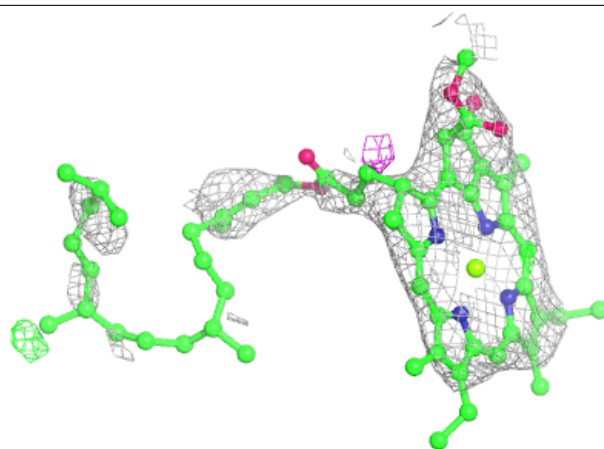
Electron density around CLA 3 306:

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



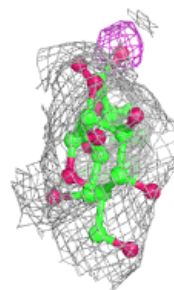
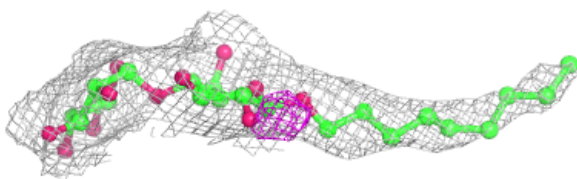
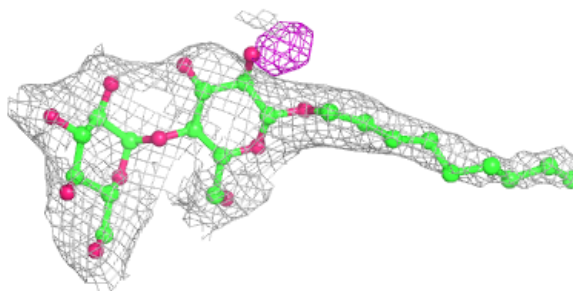
Electron density around CLA 1 513:

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



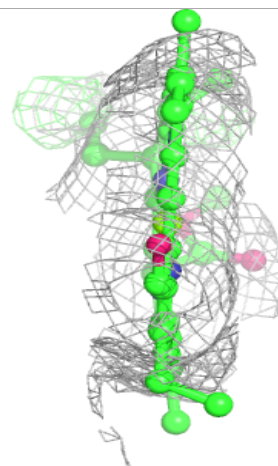
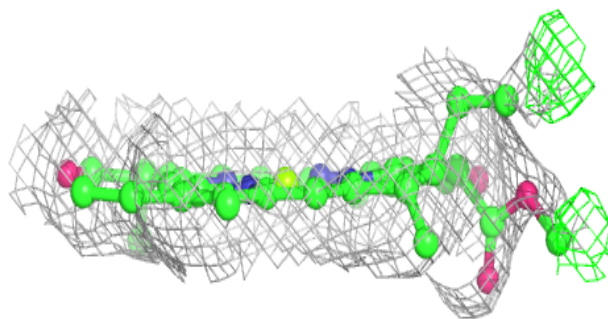
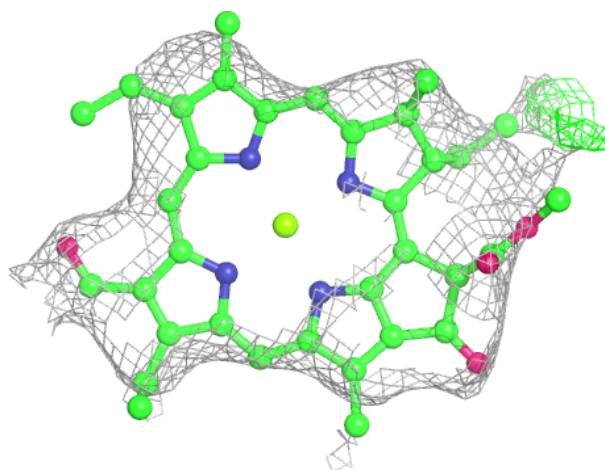
Electron density around LMT B 847:

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



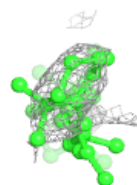
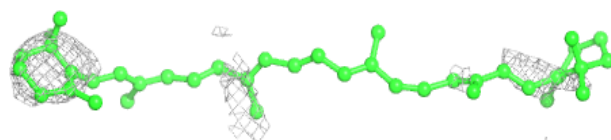
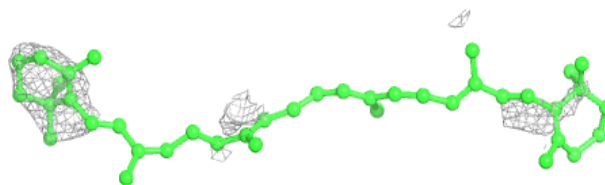
Electron density around CHL 4 317:

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



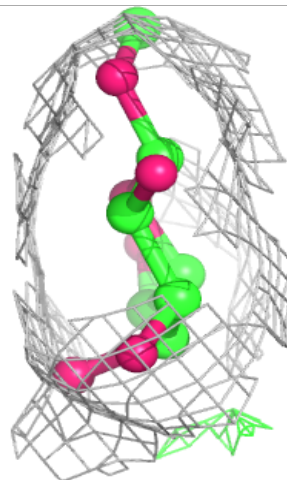
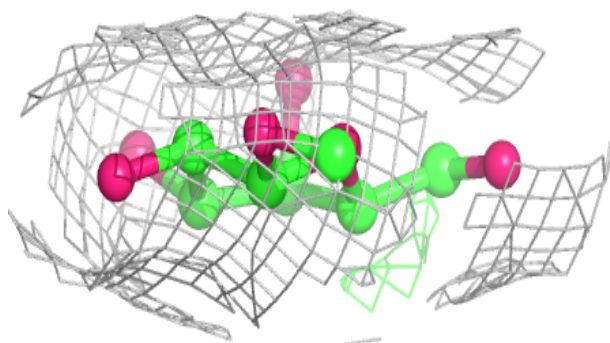
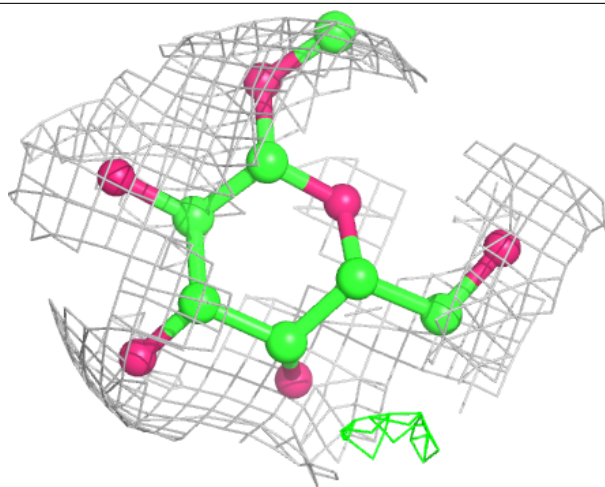
Electron density around BCR K 1005:

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



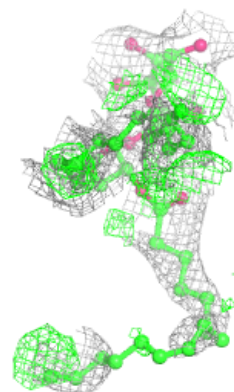
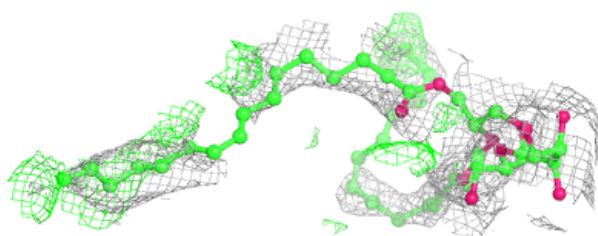
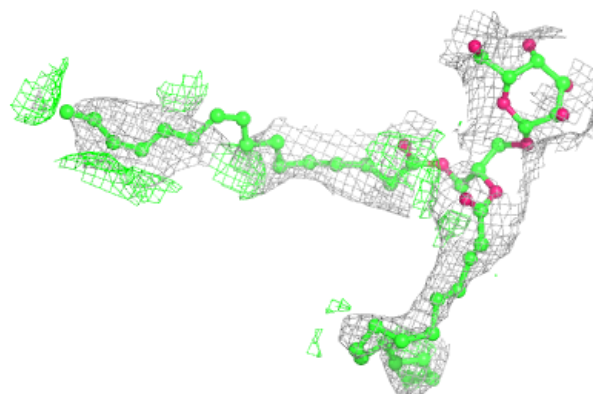
Electron density around LMG 1 519:

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

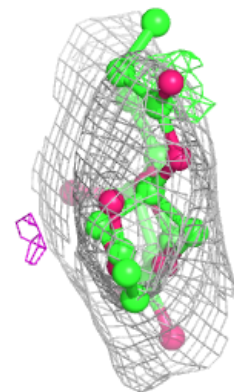
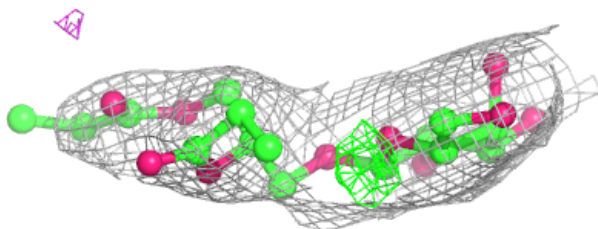
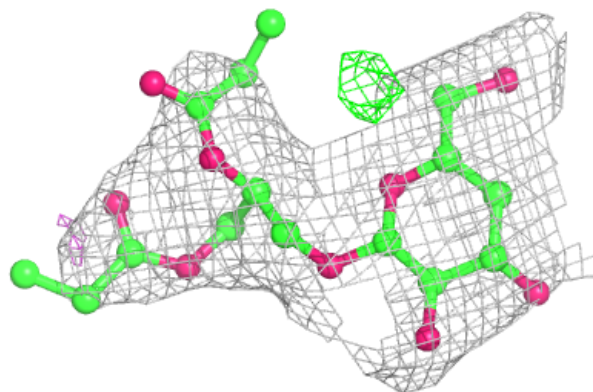


Electron density around LMG G 206:

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

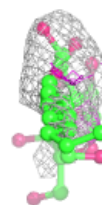
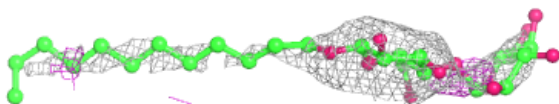
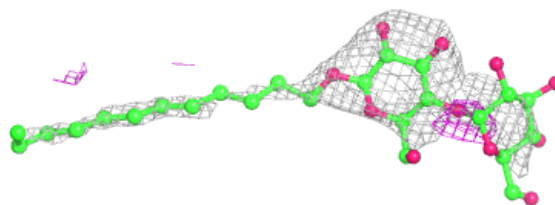
**Electron density around LMG 2 518:**

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



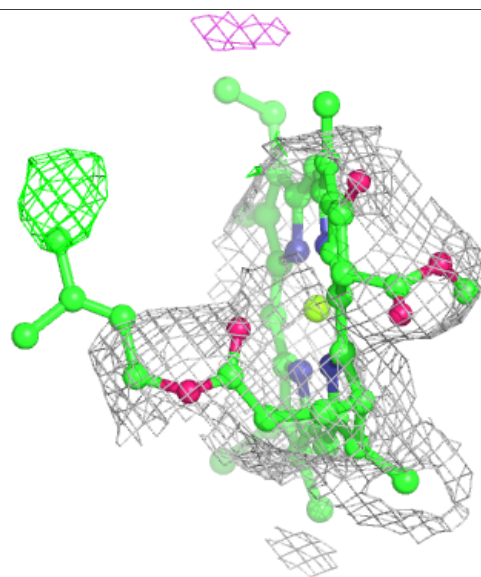
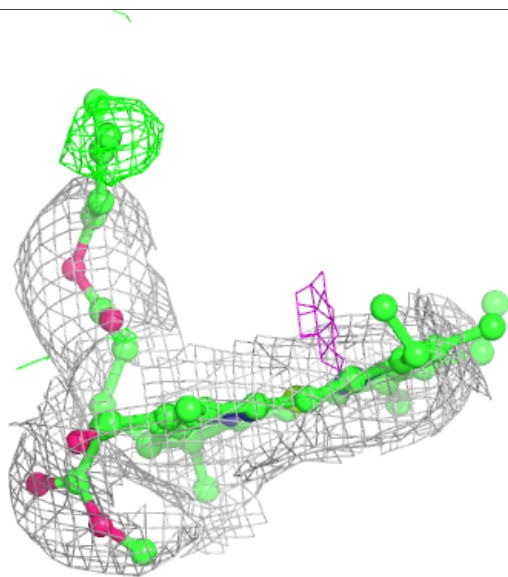
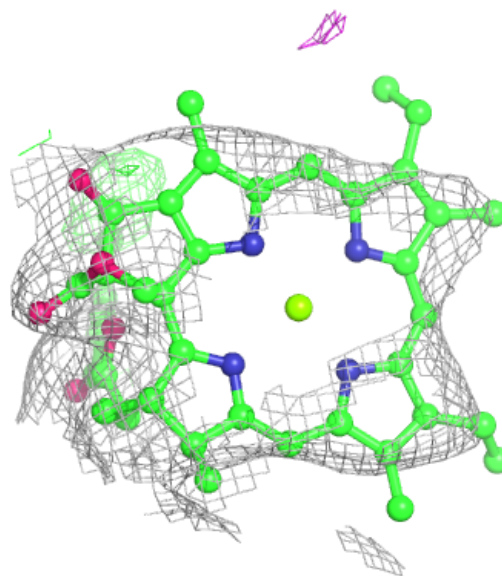
Electron density around LMT 4 320:

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



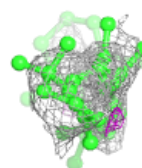
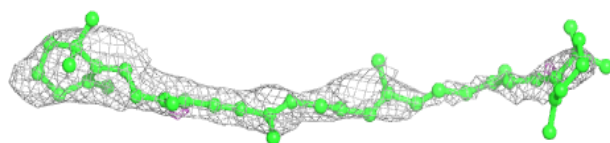
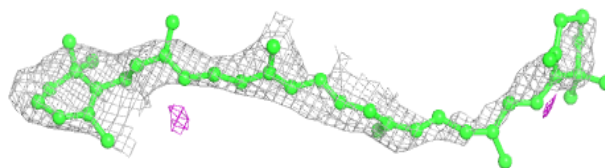
Electron density around CLA 3 310:

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



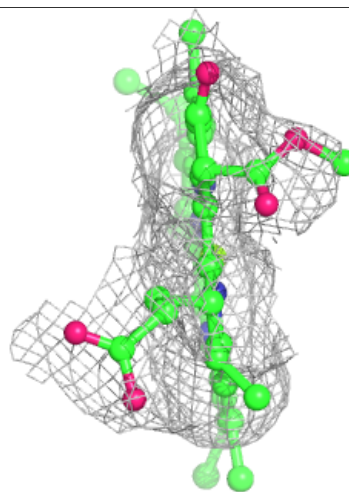
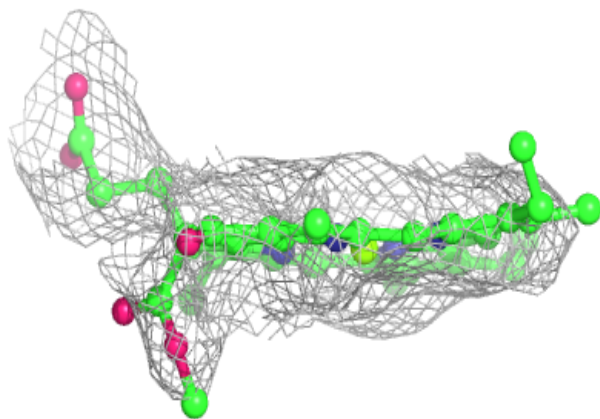
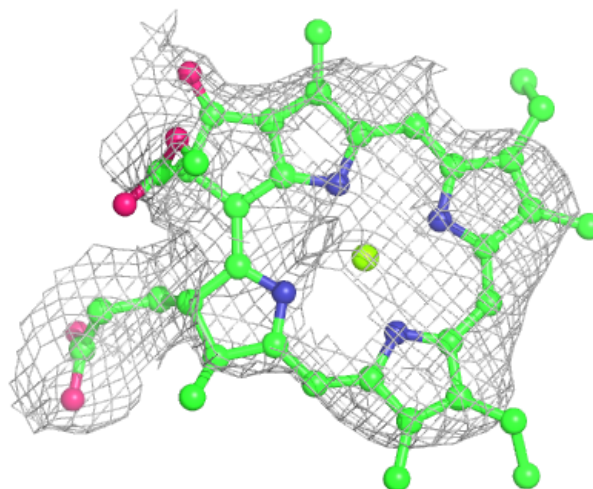
Electron density around BCR L 307:

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



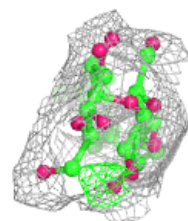
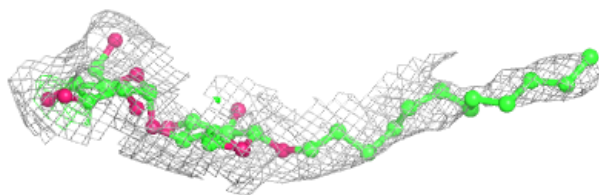
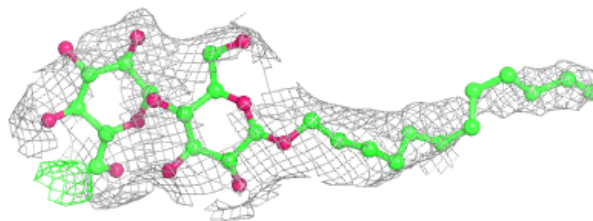
Electron density around CLA K 1001:

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

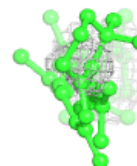
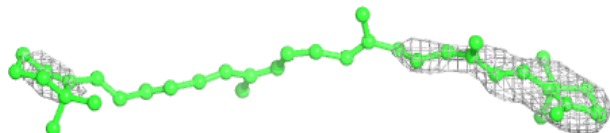
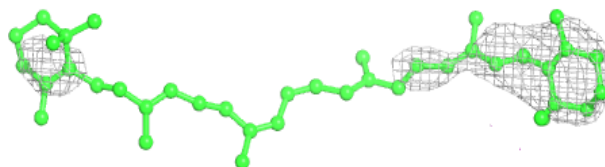


Electron density around LMT G 208:

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

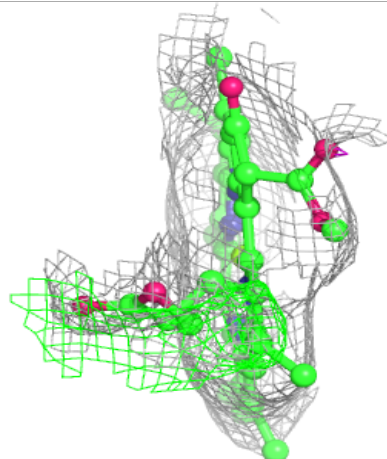
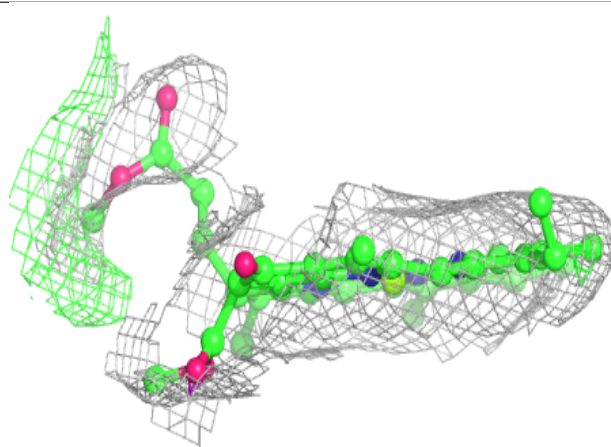
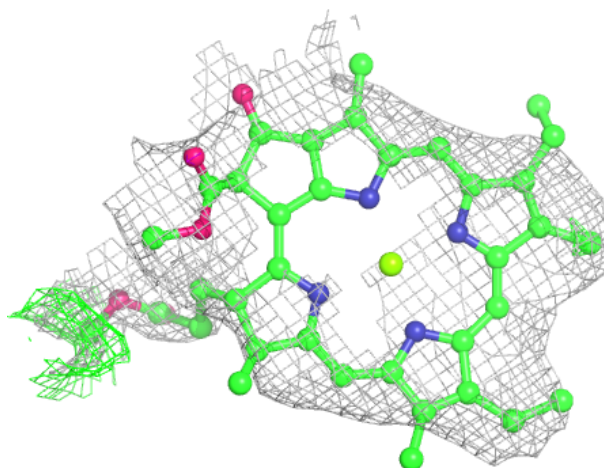
**Electron density around BCR 3 304:**

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



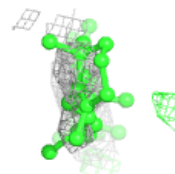
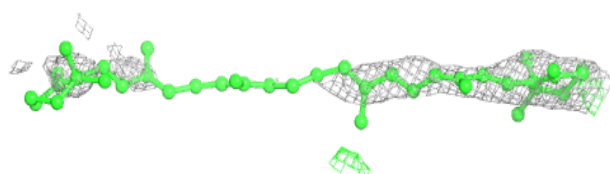
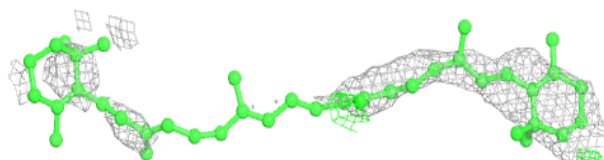
Electron density around CLA 1 510:

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

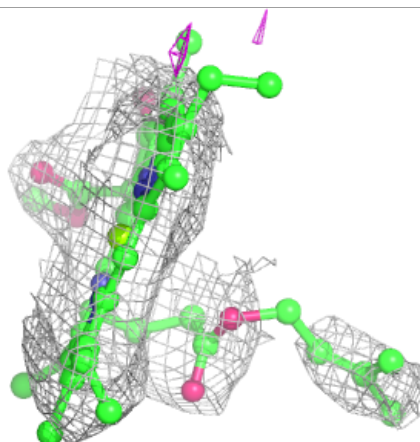
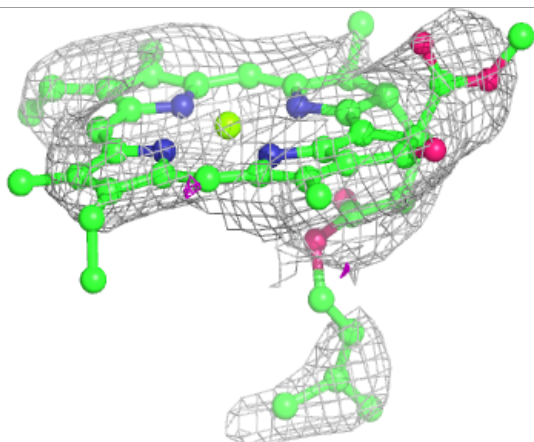
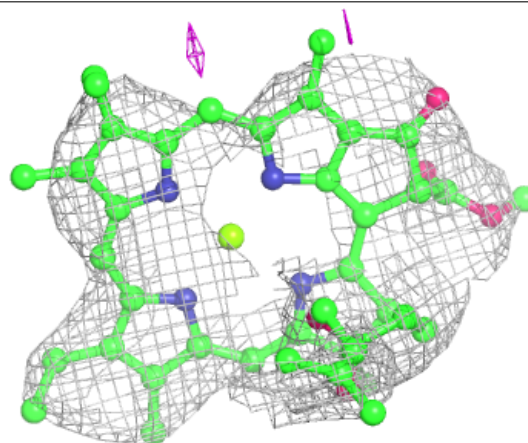


Electron density around BCR 2 503:

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

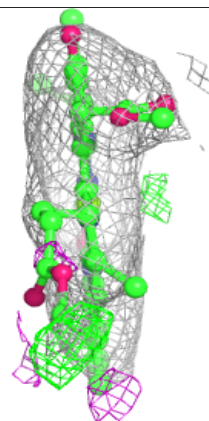
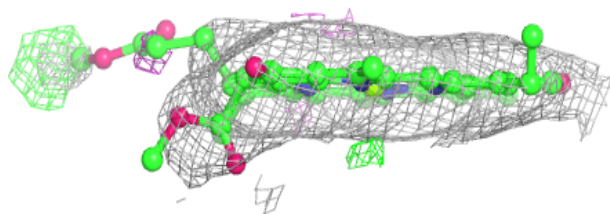
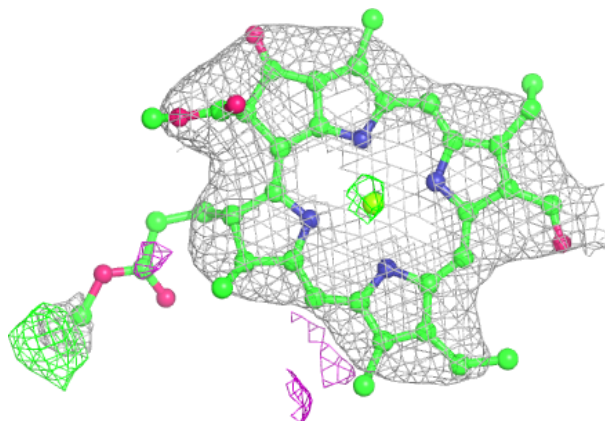
**Electron density around CLA L 303:**

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



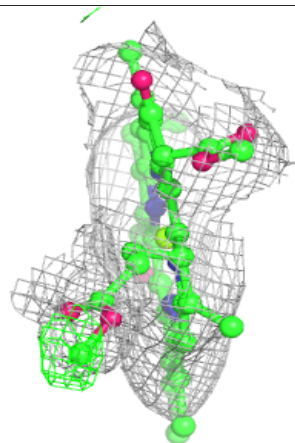
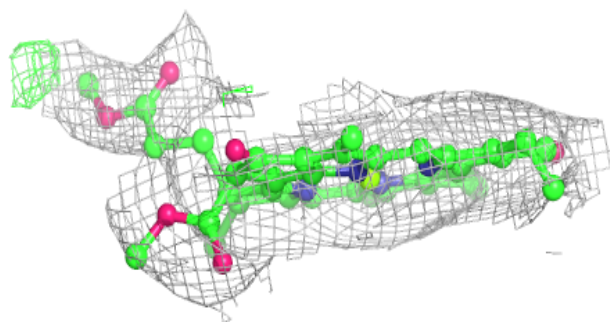
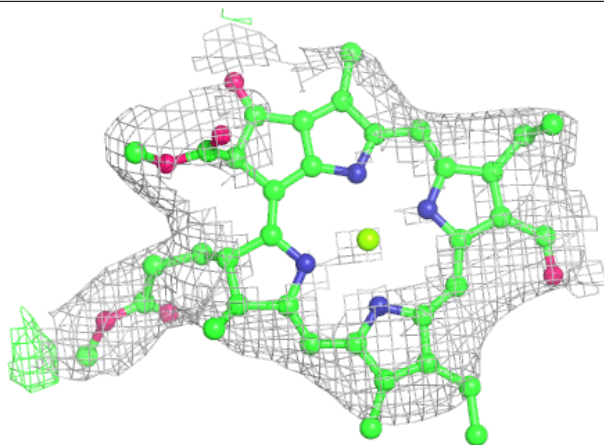
Electron density around CHL 4 313:

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

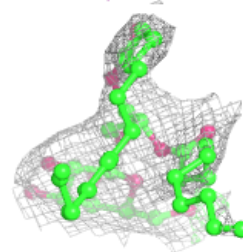
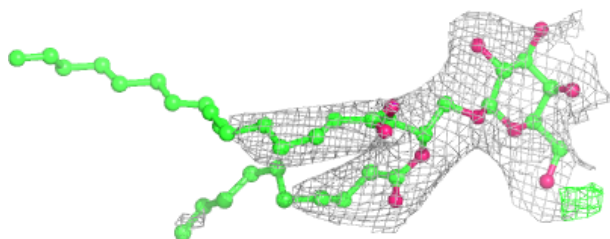
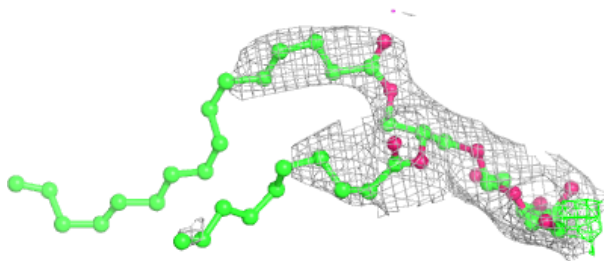


Electron density around CHL 2 512:

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

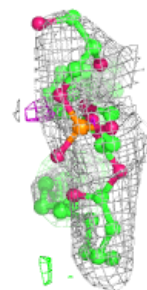
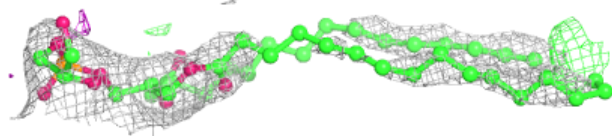
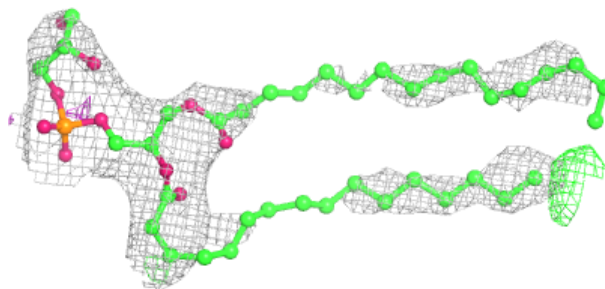
**Electron density around LMG 4 322:**

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

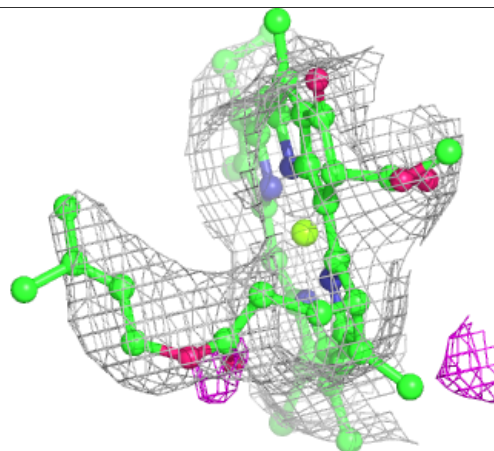
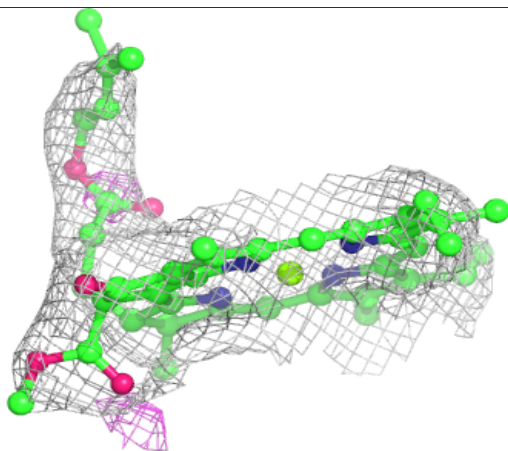
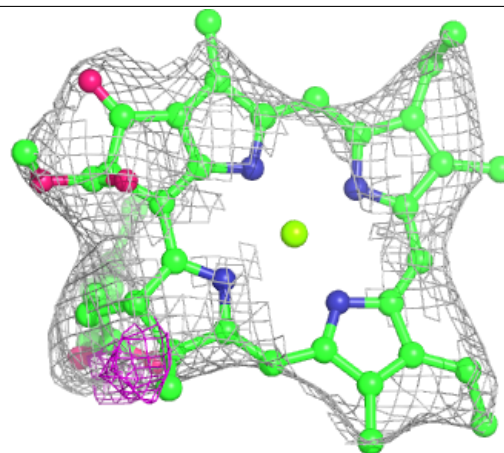


Electron density around LHG 1 517:

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

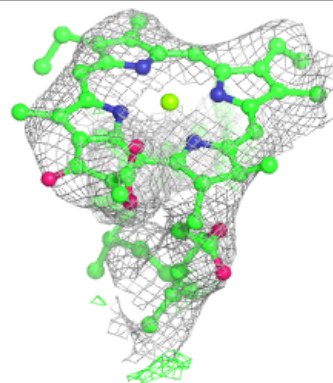
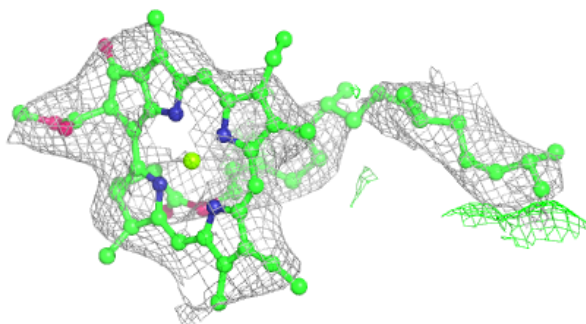
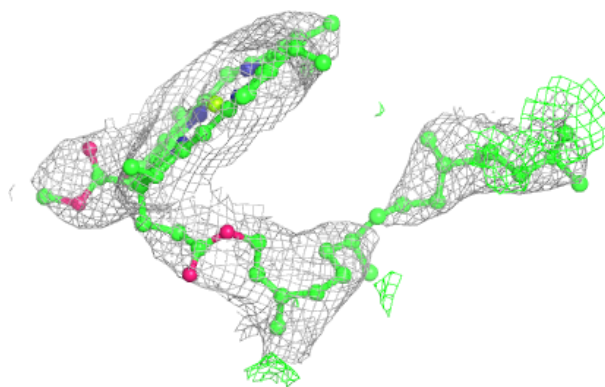
**Electron density around CLA L 305:**

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



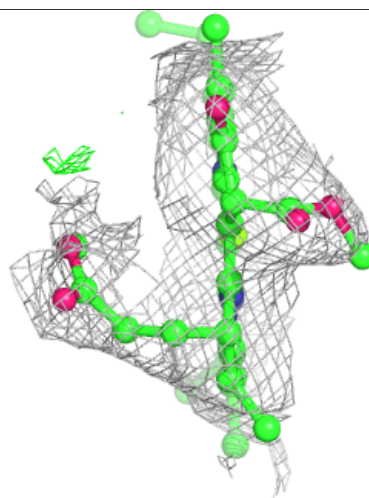
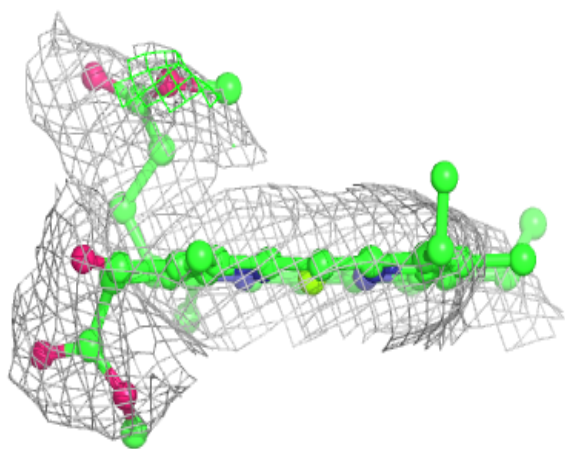
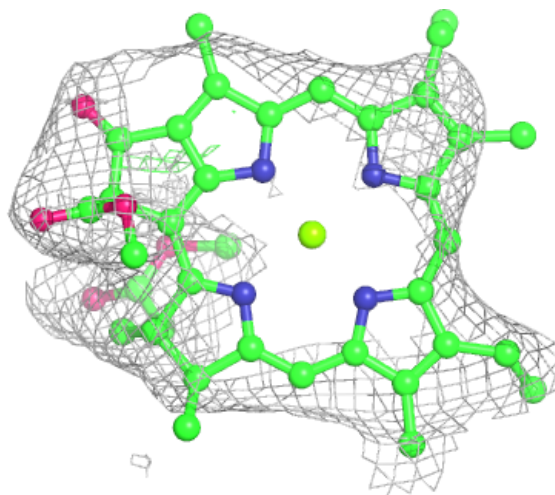
Electron density around CLA G 204:

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



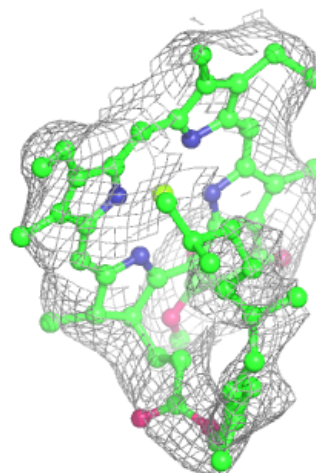
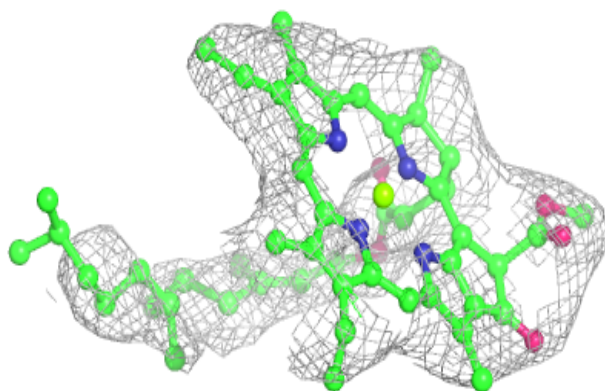
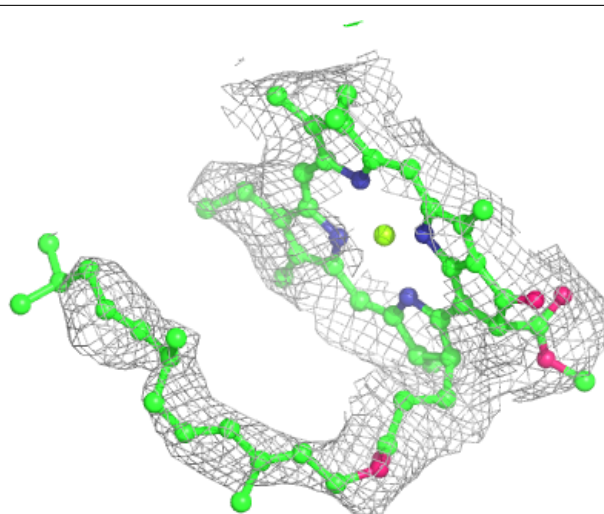
Electron density around CLA A 816:

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



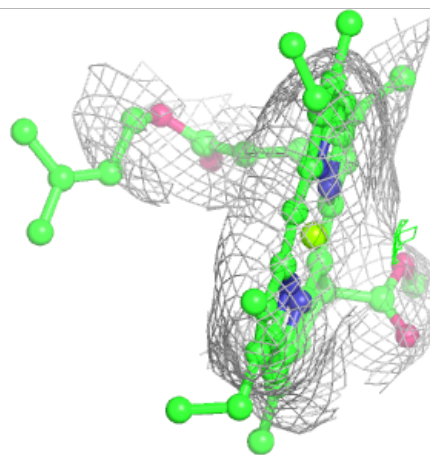
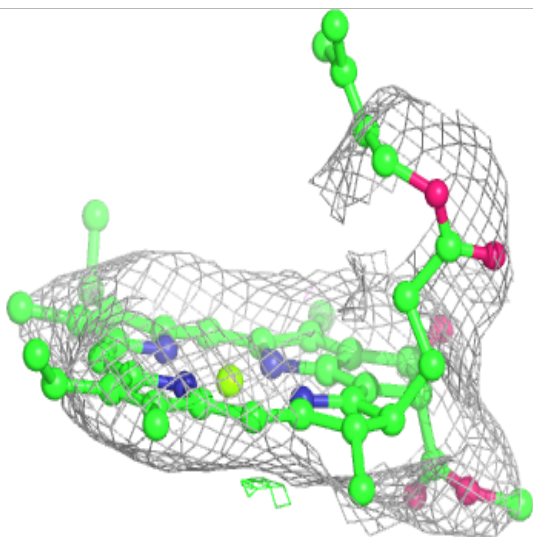
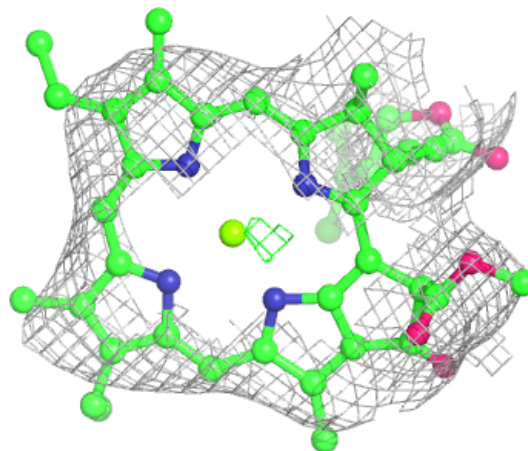
Electron density around CLA A 842:

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



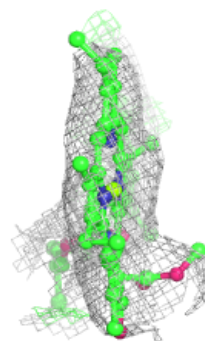
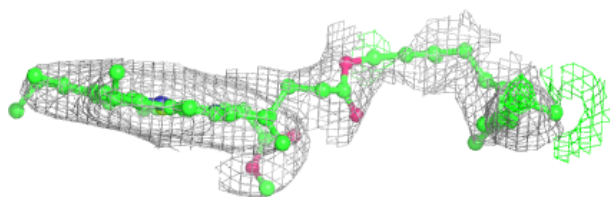
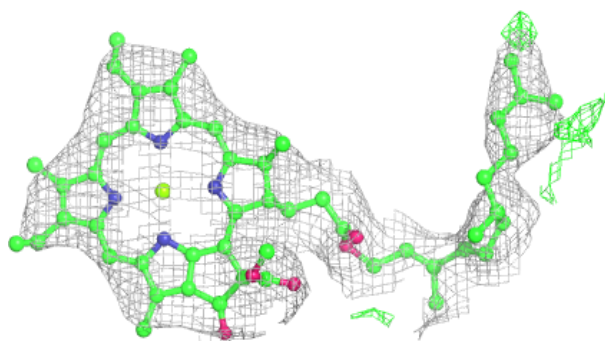
Electron density around CLA 1 509:

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

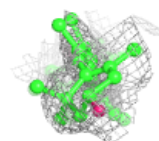
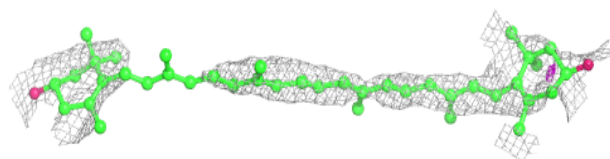
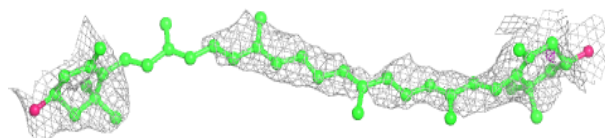


Electron density around CLA 1 516:

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

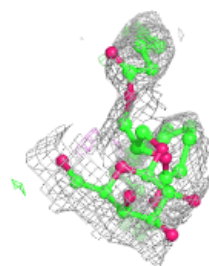
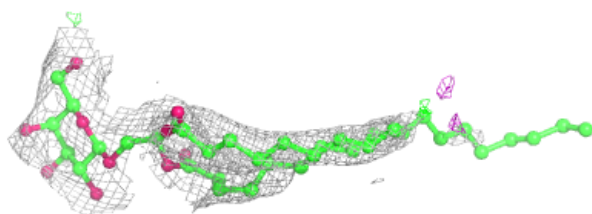
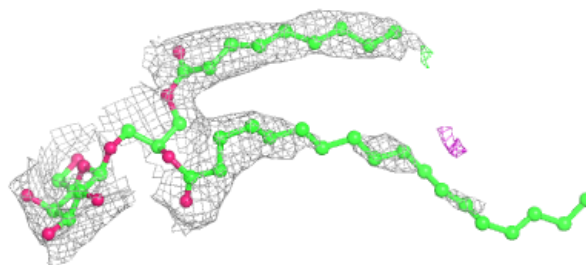
**Electron density around LUT 3 301:**

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



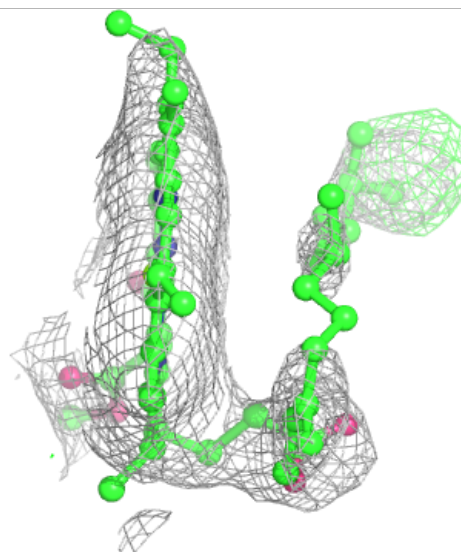
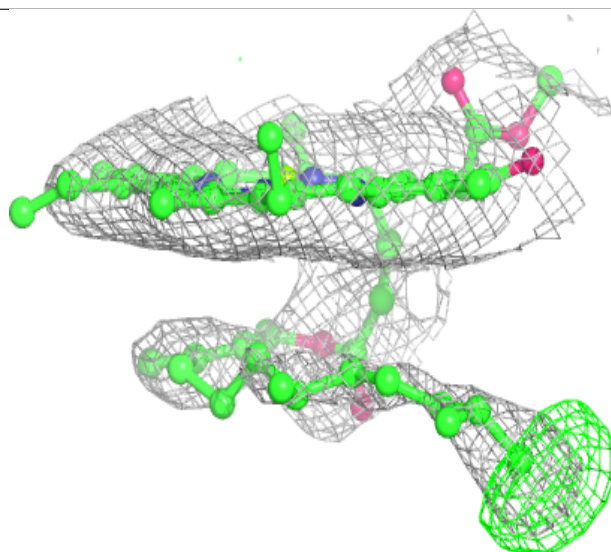
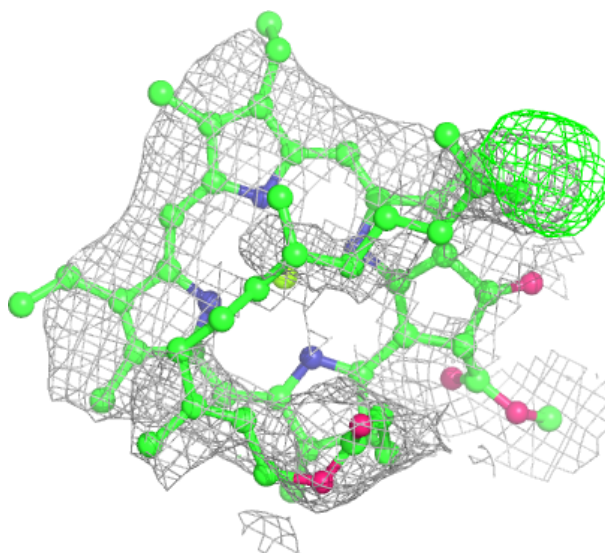
Electron density around LMG 1 518:

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



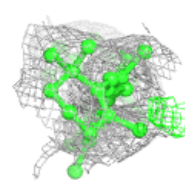
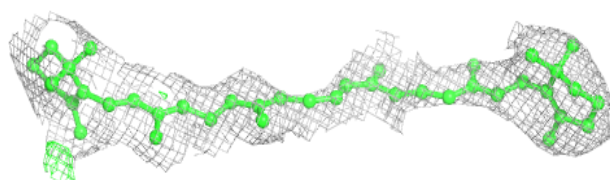
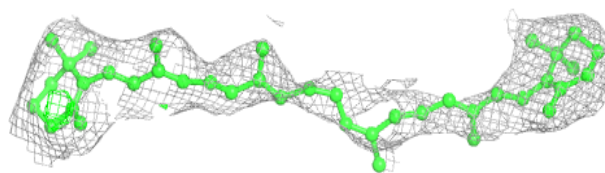
Electron density around CLA 3 313:

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

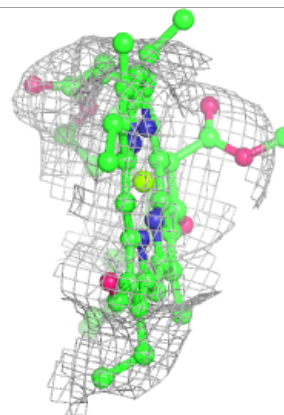
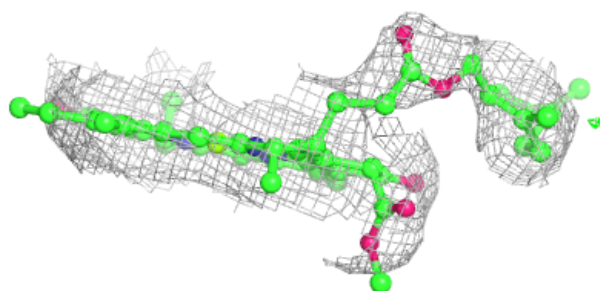
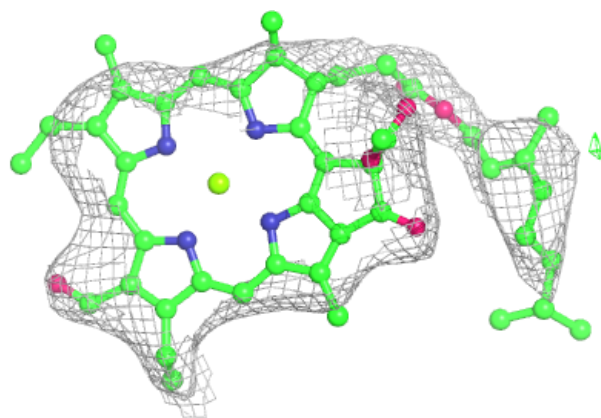


Electron density around BCR G 205:

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

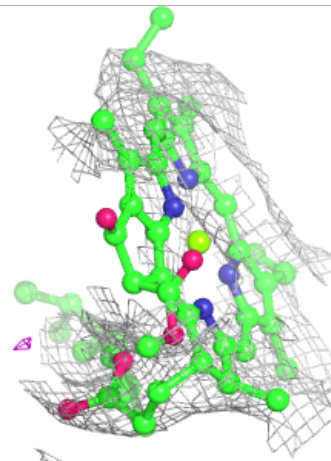
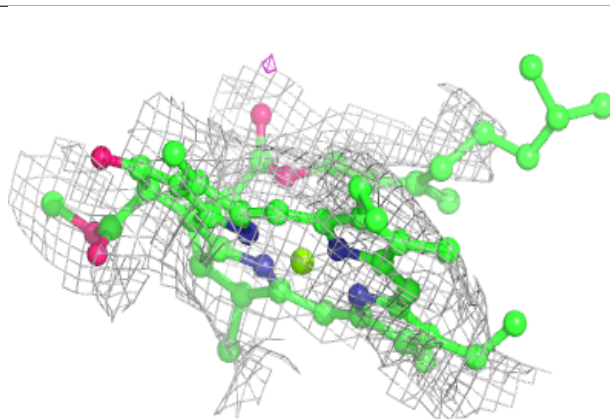
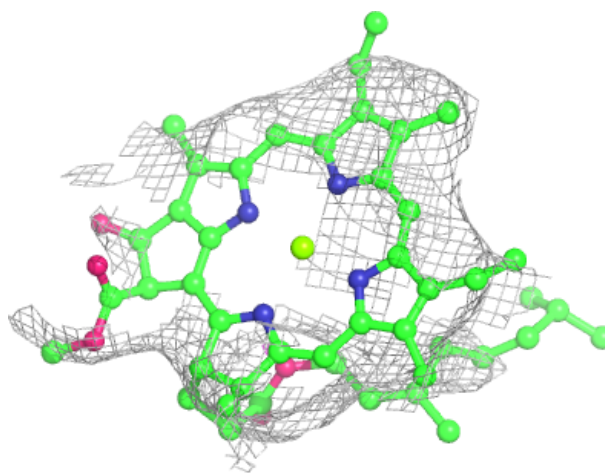
**Electron density around CHL 2 516:**

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



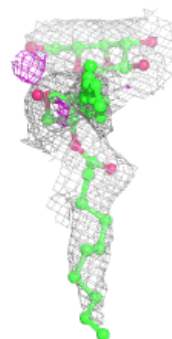
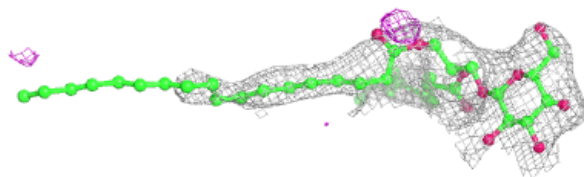
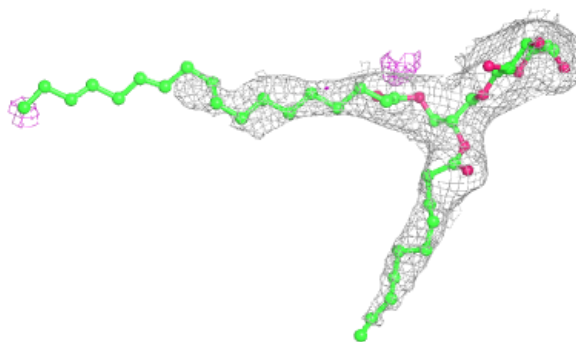
Electron density around CLA 3 305:

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

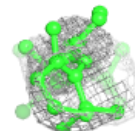
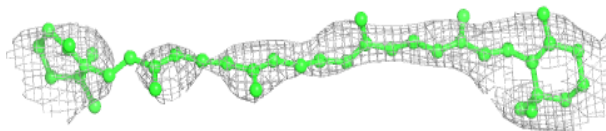
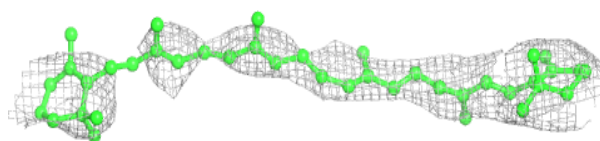


Electron density around LMG F 304:

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

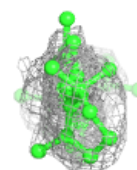
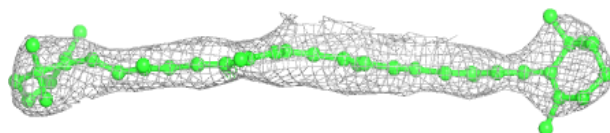
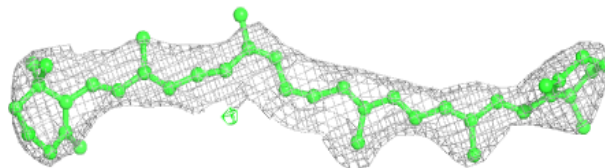
**Electron density around BCR 3 303:**

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



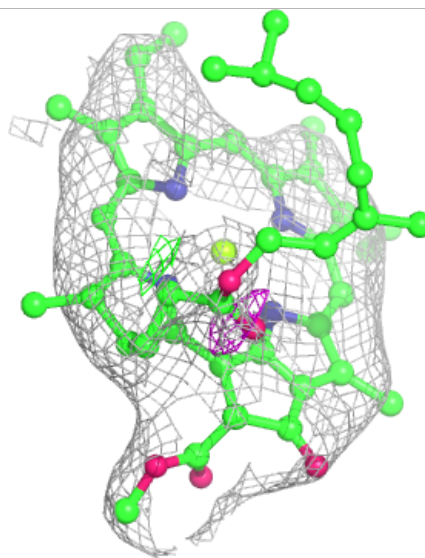
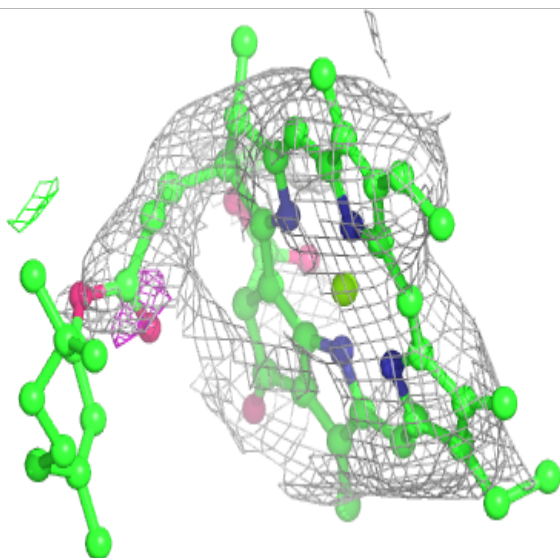
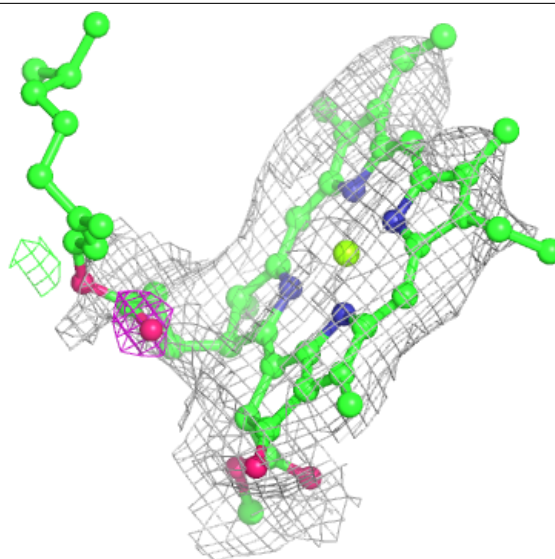
Electron density around BCR A 850:

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



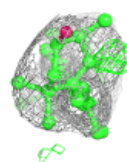
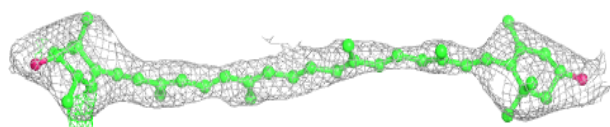
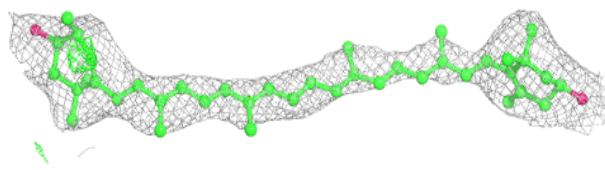
Electron density around CLA A 835:

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

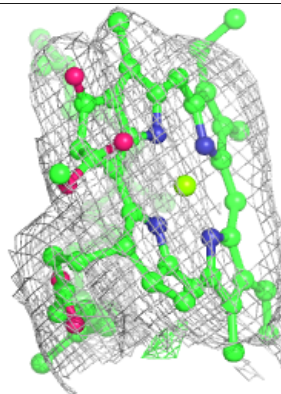
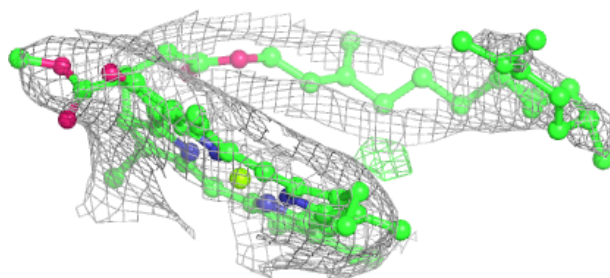
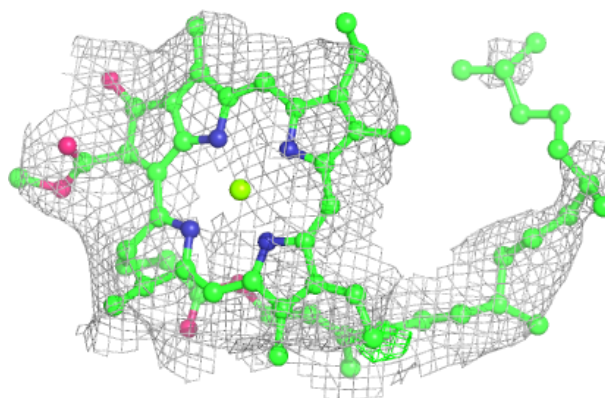


Electron density around ZEX F 301:

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

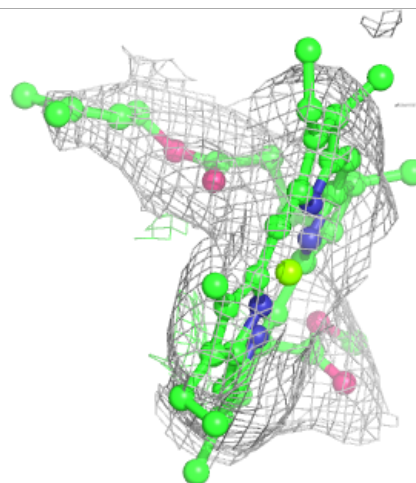
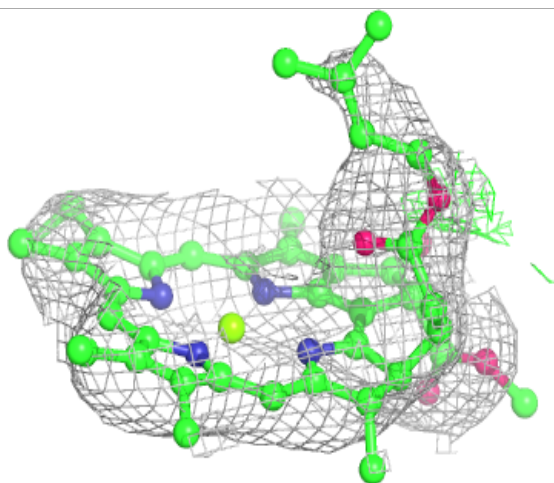
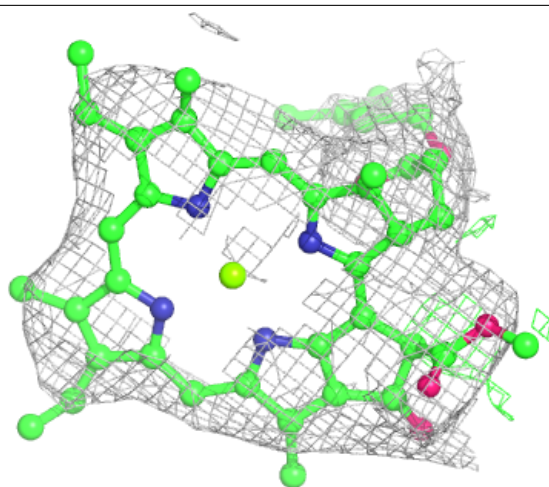
**Electron density around CLA 1 504:**

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



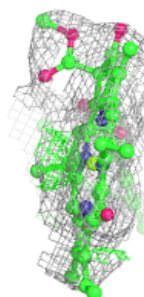
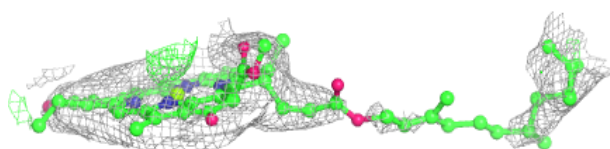
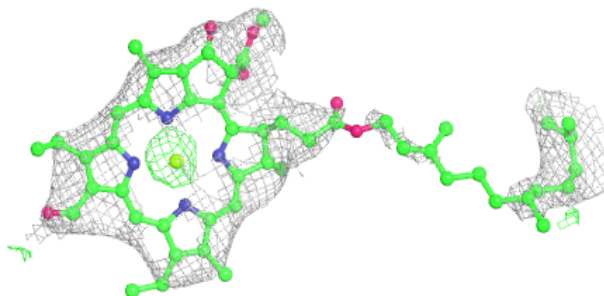
Electron density around CLA 4 309:

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

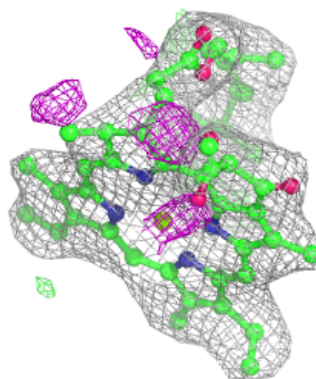
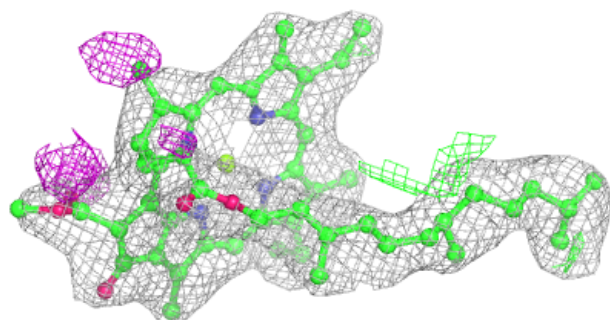
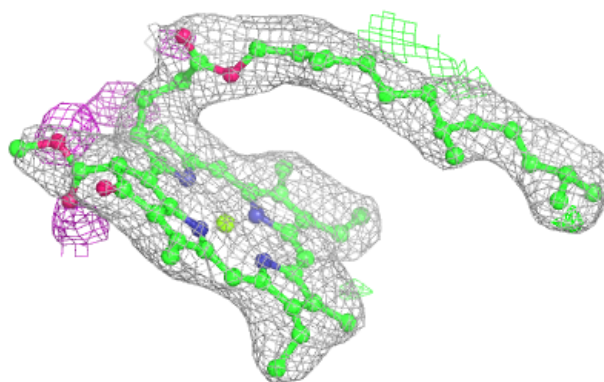


Electron density around CHL 4 316:

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

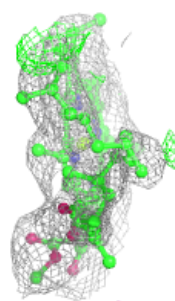
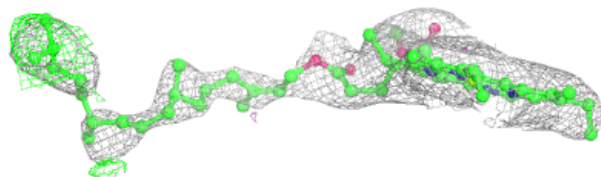
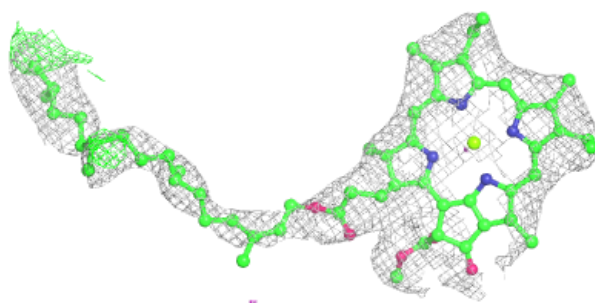
**Electron density around CLA B 831:**

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

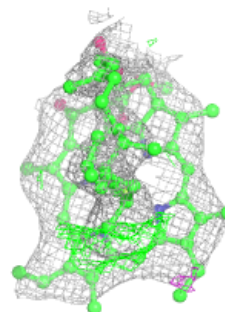
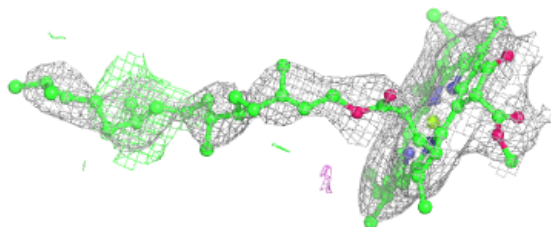
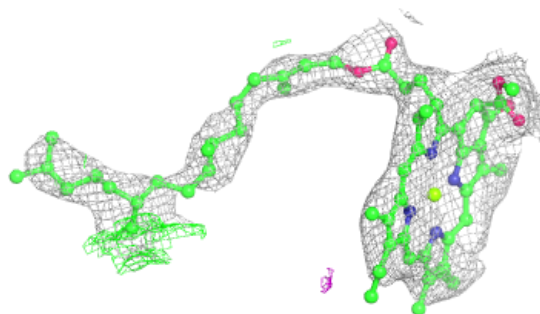


Electron density around CLA F 303:

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

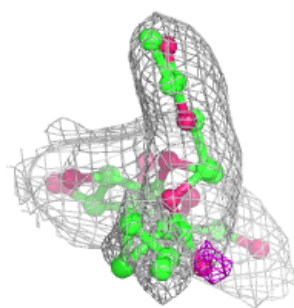
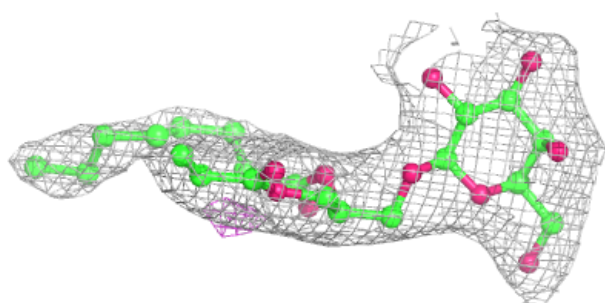
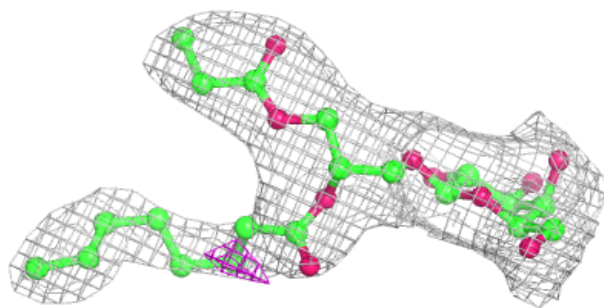
**Electron density around CLA G 201:**

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

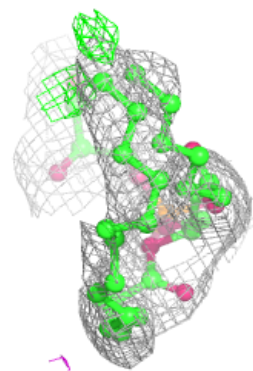
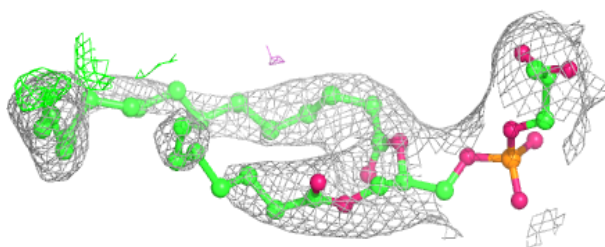
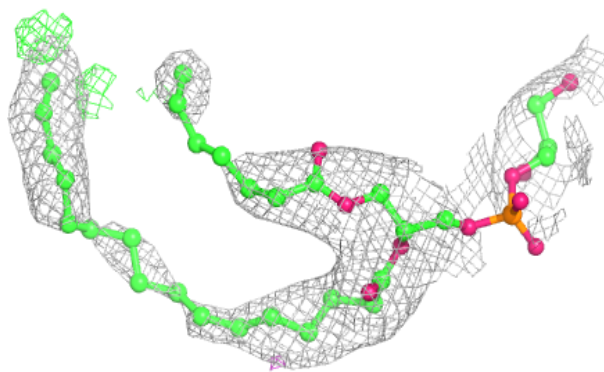


Electron density around LMG J 1103:

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

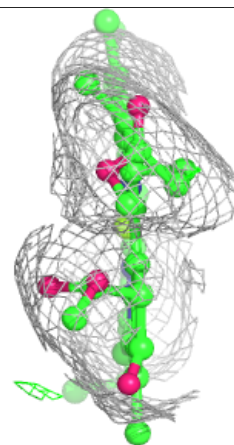
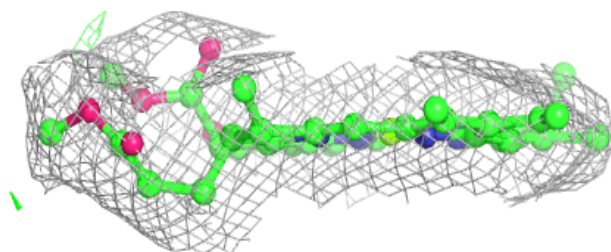
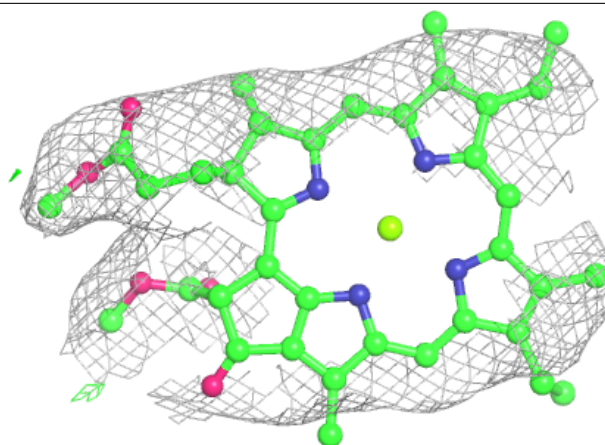
**Electron density around LHG A 845:**

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

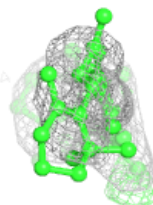
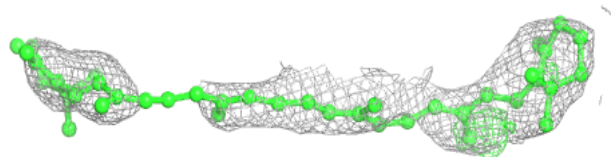
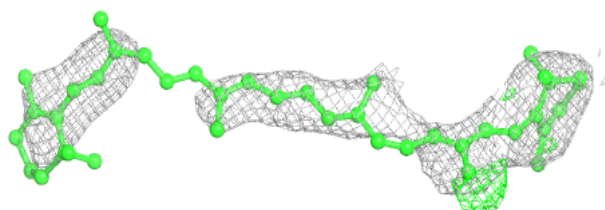


Electron density around CLA G 203:

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

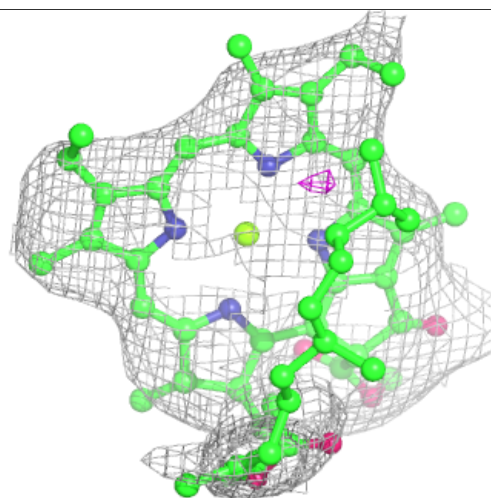
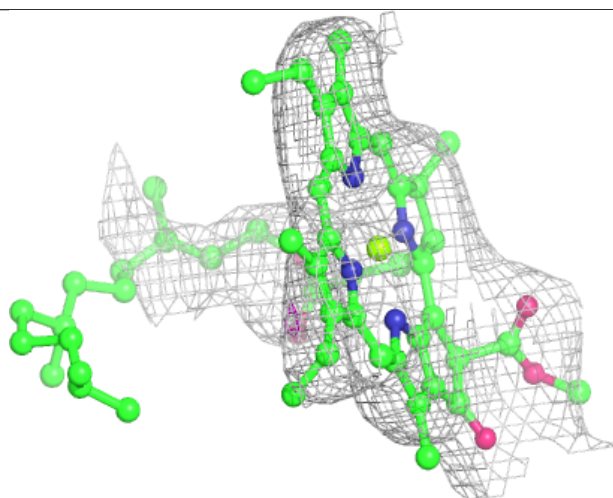
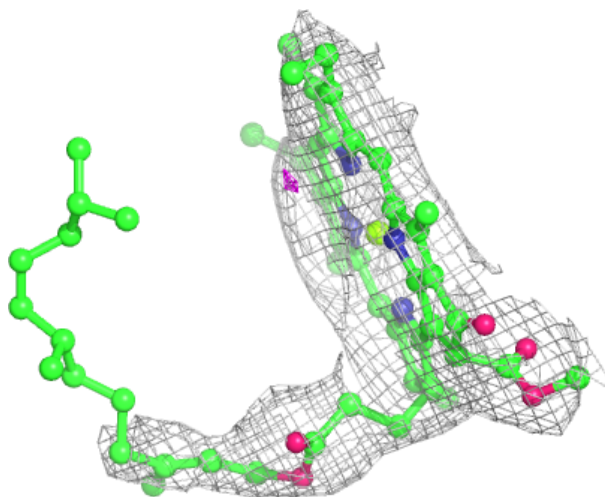
**Electron density around BCR B 851:**

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



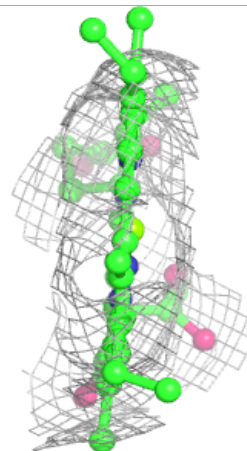
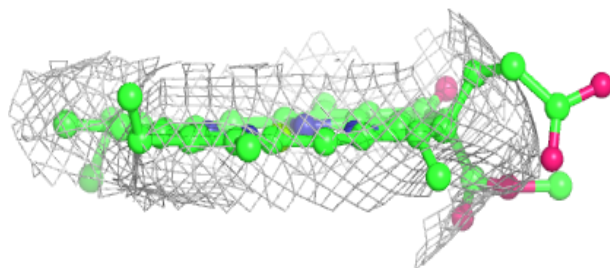
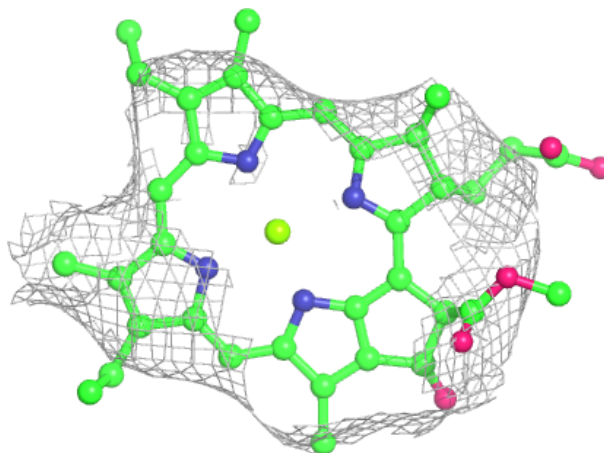
Electron density around CLA A 823:

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



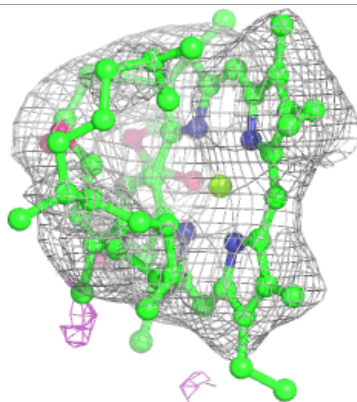
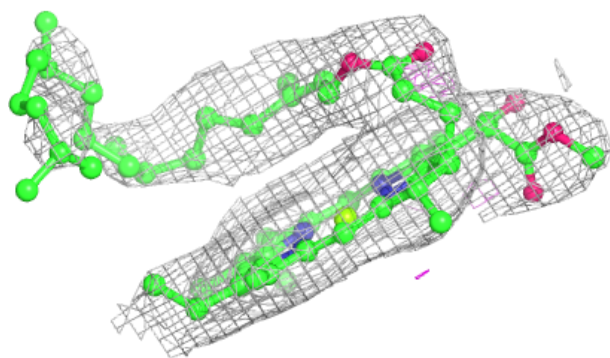
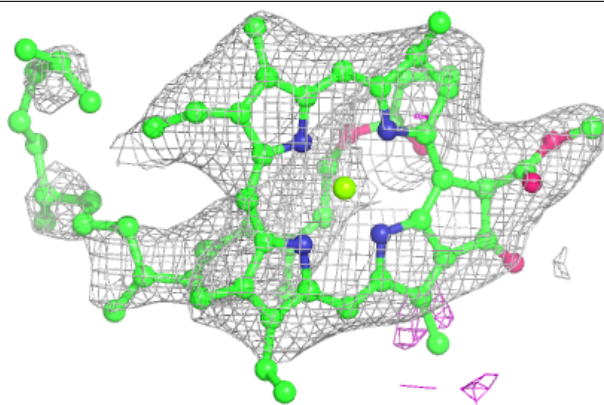
Electron density around CLA 1 515:

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

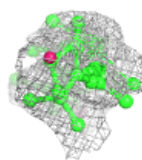
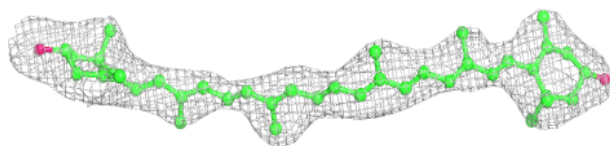
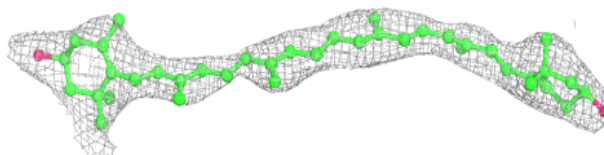


Electron density around CLA B 808:

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

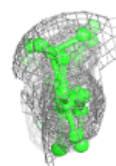
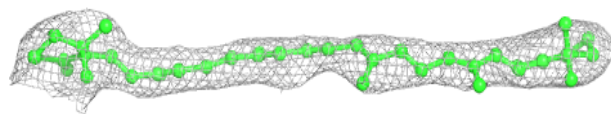
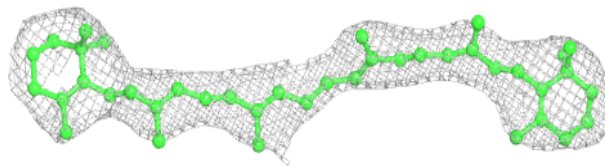
**Electron density around LUT J 1109:**

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

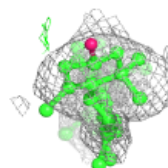
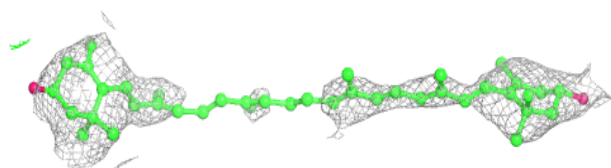
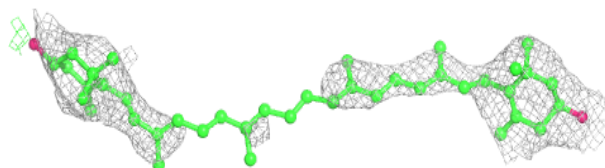


Electron density around BCR I 102:

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

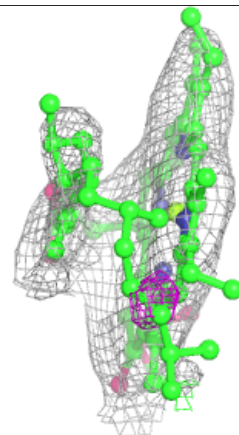
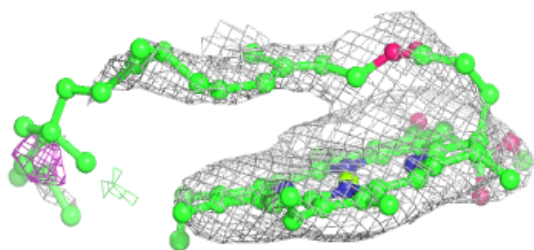
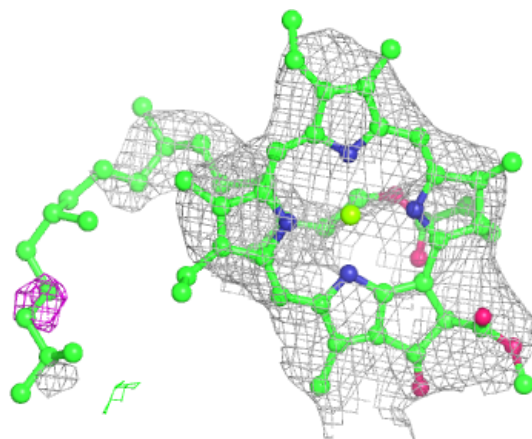
**Electron density around LUT 1 502:**

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



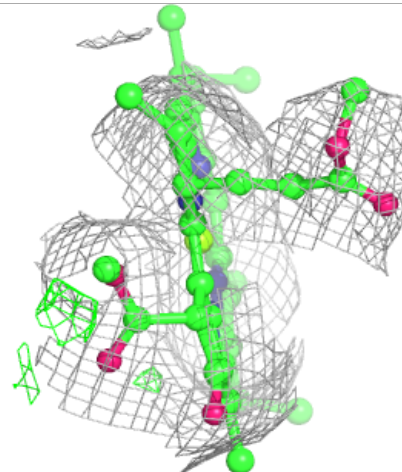
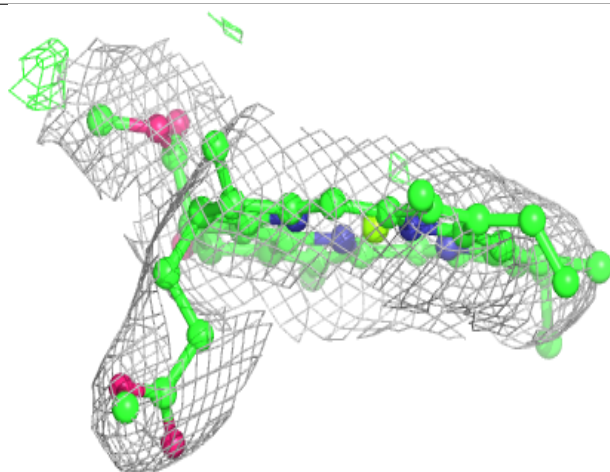
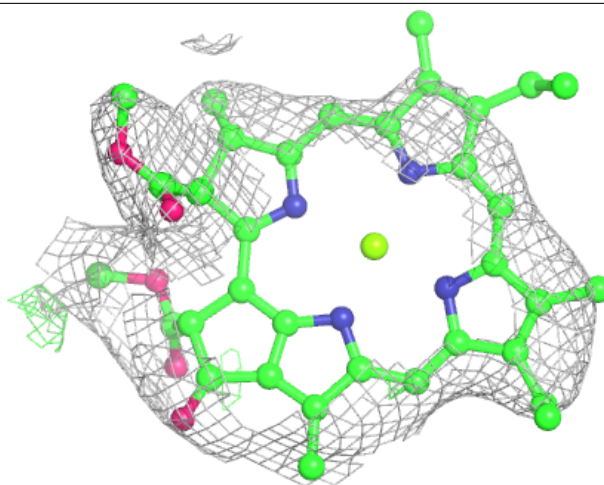
Electron density around CLA A 817:

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



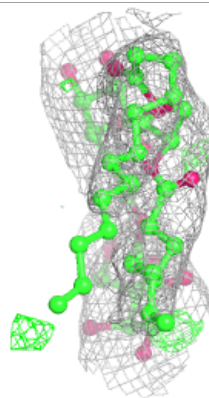
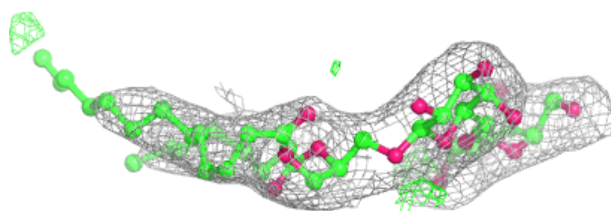
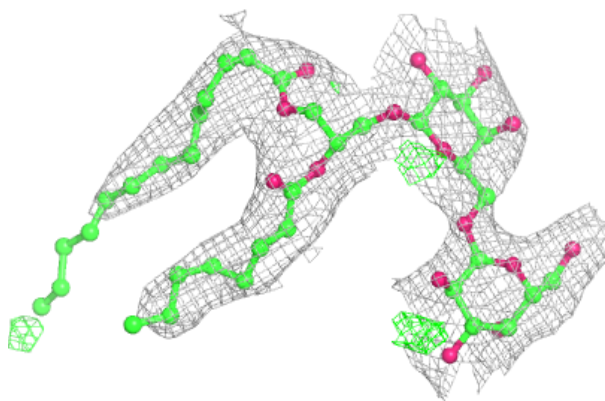
Electron density around CLA 1 511:

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

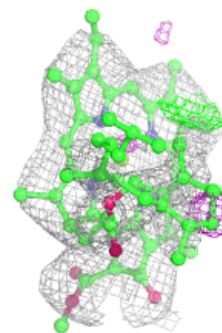
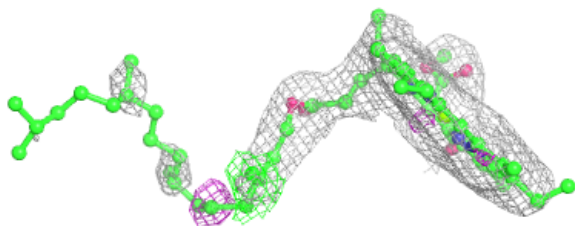
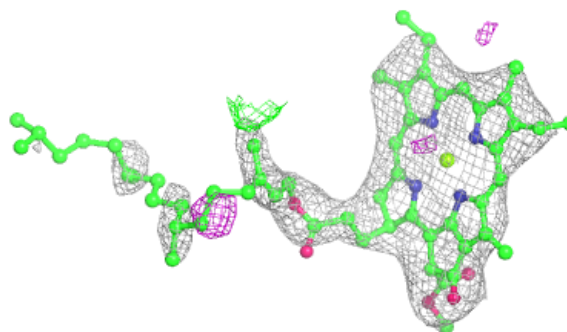


Electron density around DGD 4 319:

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

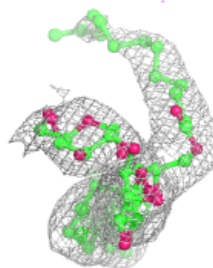
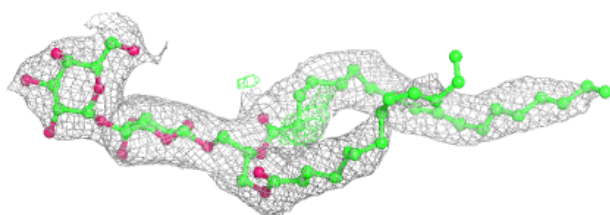
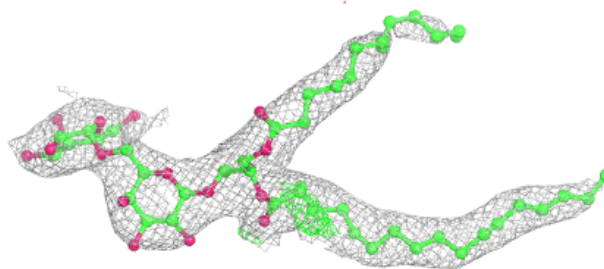
**Electron density around CLA A 831:**

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

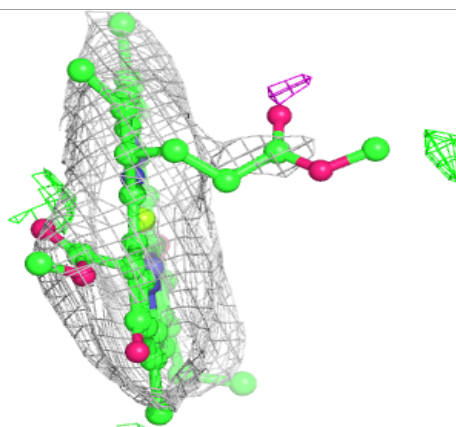
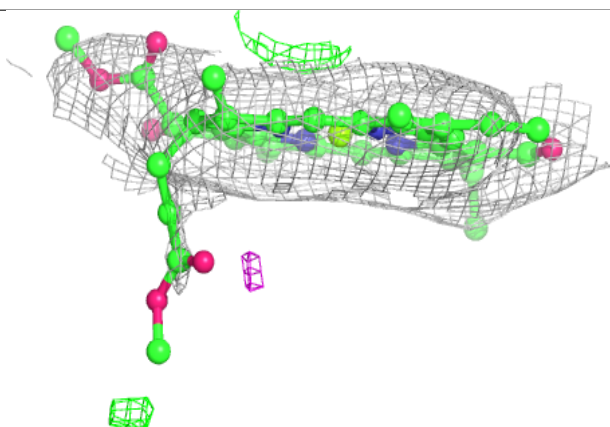
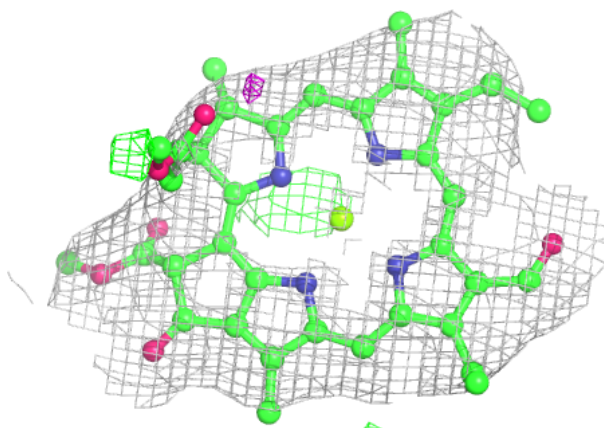


Electron density around DGD B 854:

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

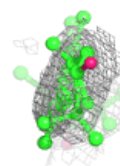
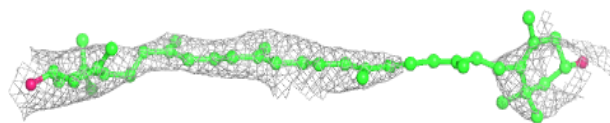
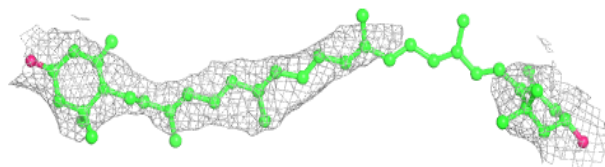
**Electron density around CHL 3 314:**

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



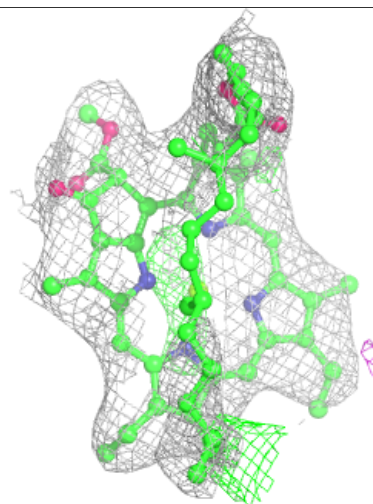
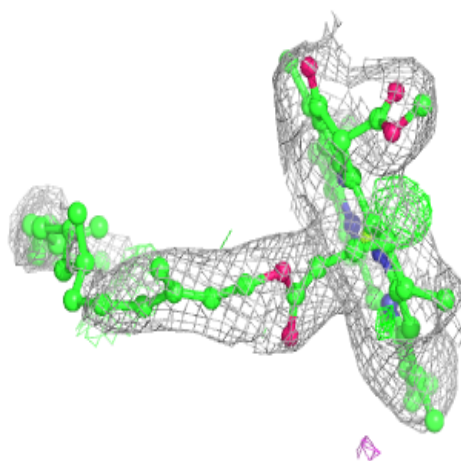
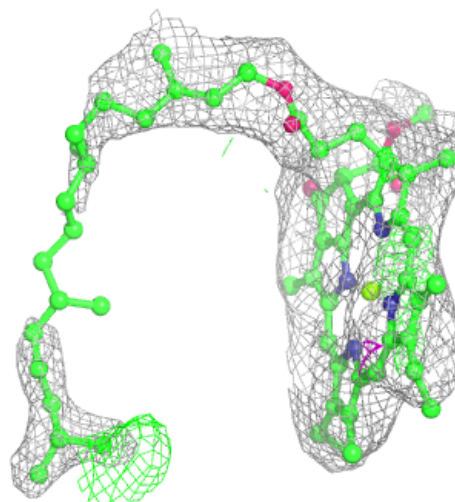
Electron density around LUT 3 302:

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



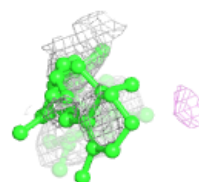
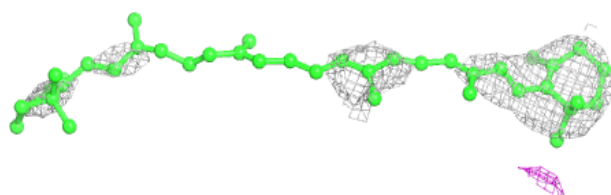
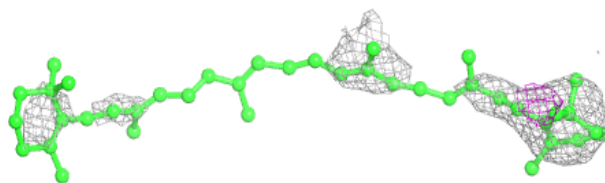
Electron density around CLA A 838:

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



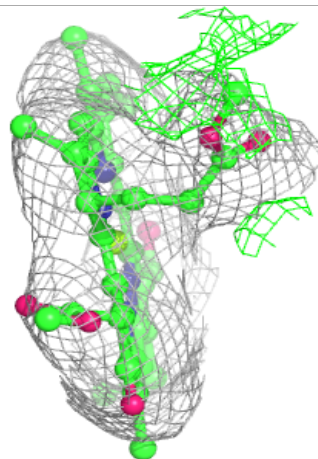
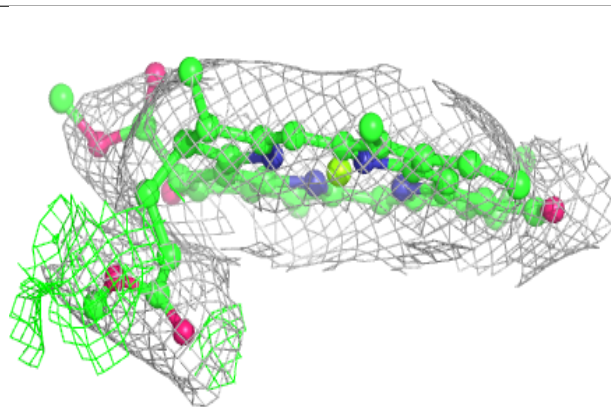
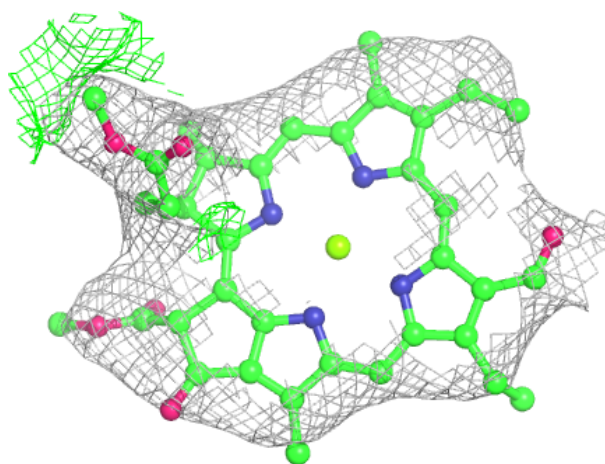
Electron density around BCR A 856:

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



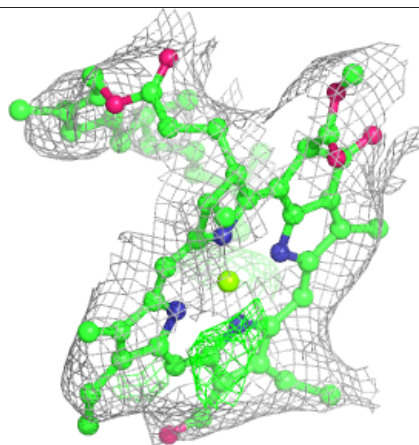
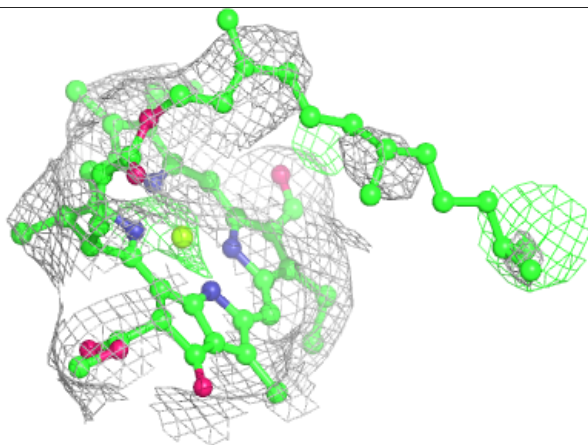
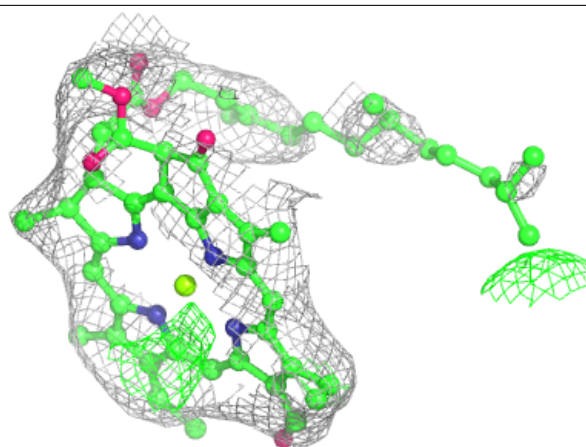
Electron density around CHL 1 512:

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



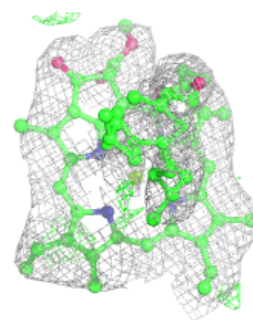
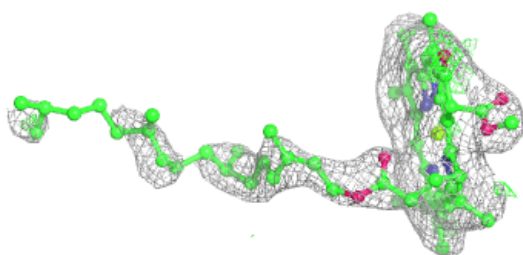
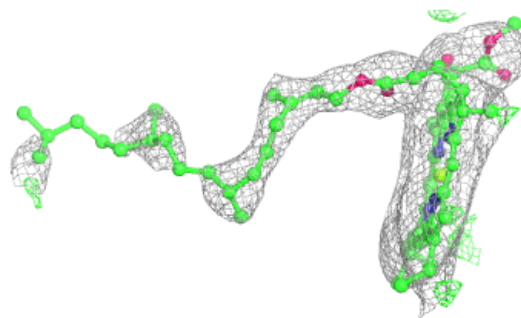
Electron density around CHL 1 514:

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



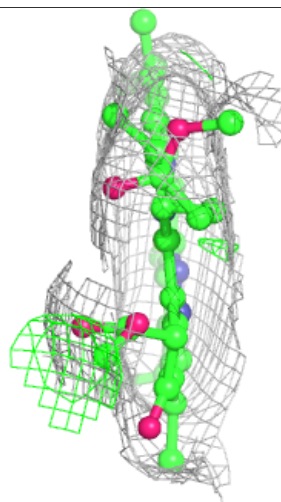
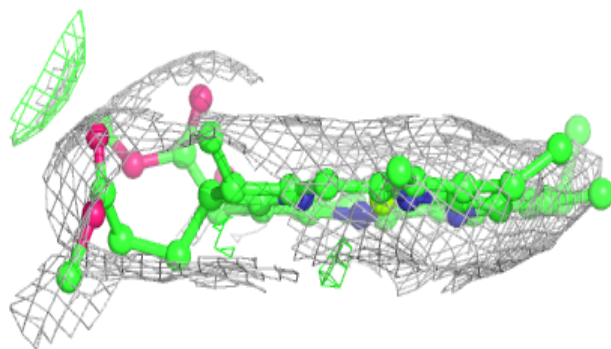
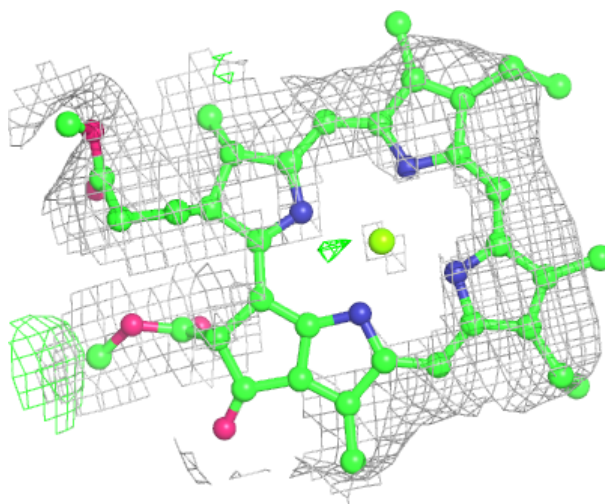
Electron density around CLA B 805:

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



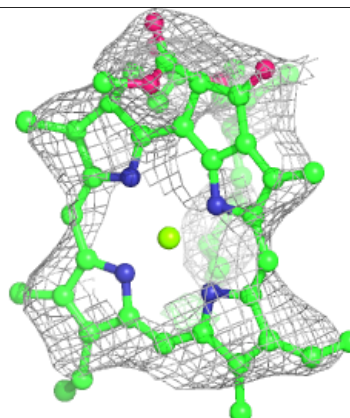
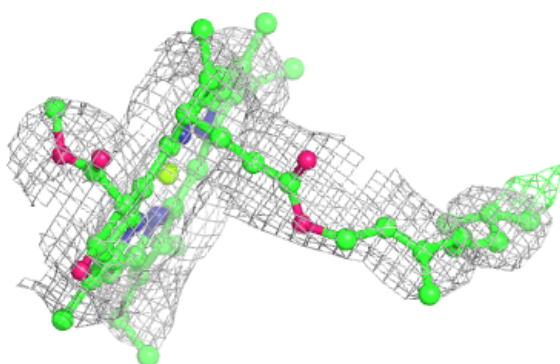
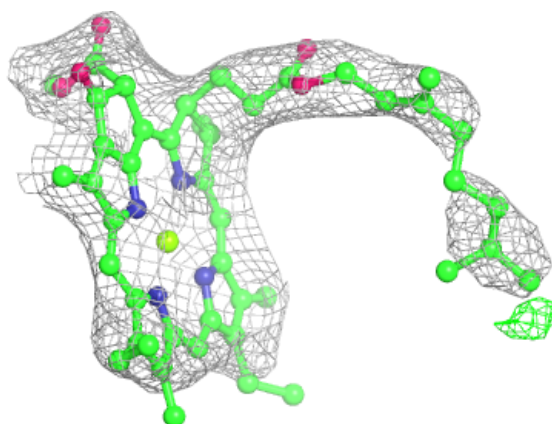
Electron density around CLA 1 505:

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

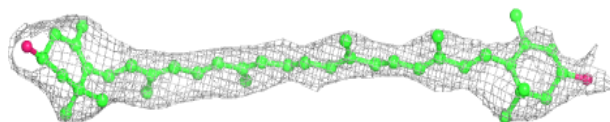
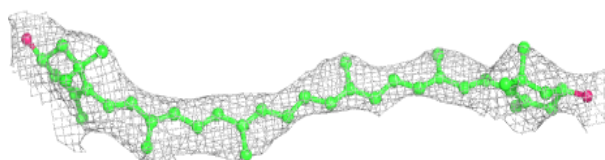


Electron density around CLA B 816:

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

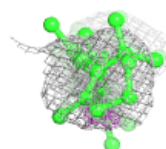
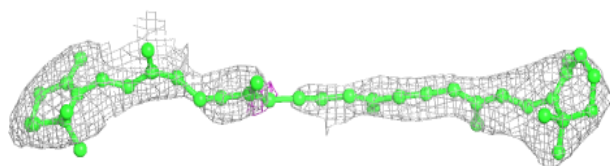
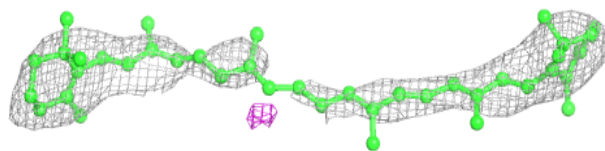
**Electron density around LUT 4 302:**

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

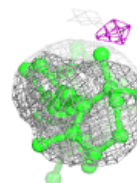
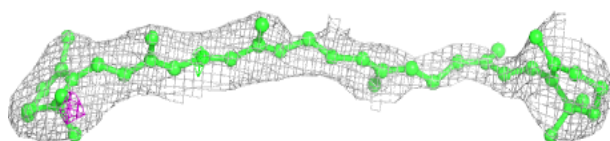
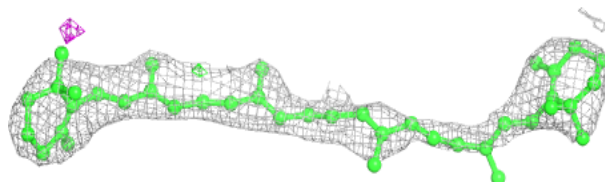


Electron density around BCR L 306:

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

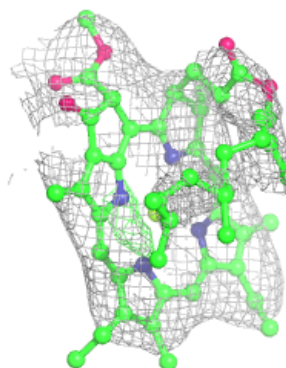
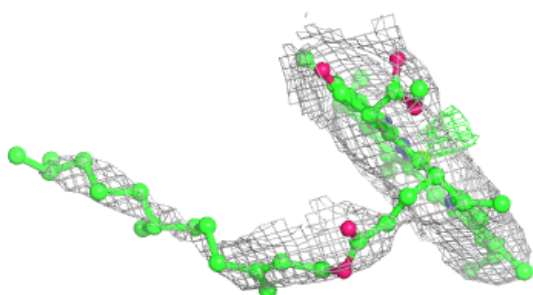
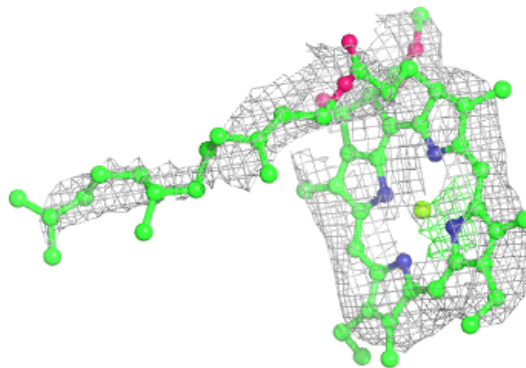
**Electron density around BCR A 851:**

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

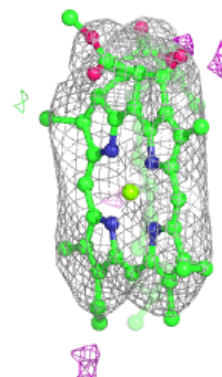
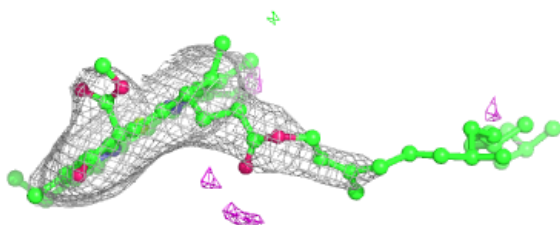
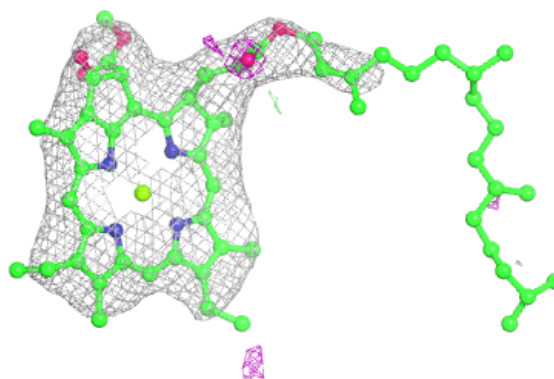


Electron density around CLA 4 310:

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

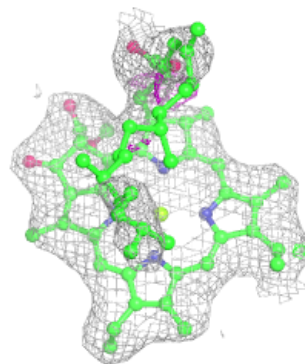
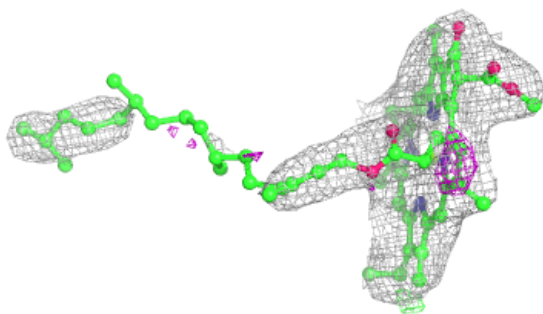
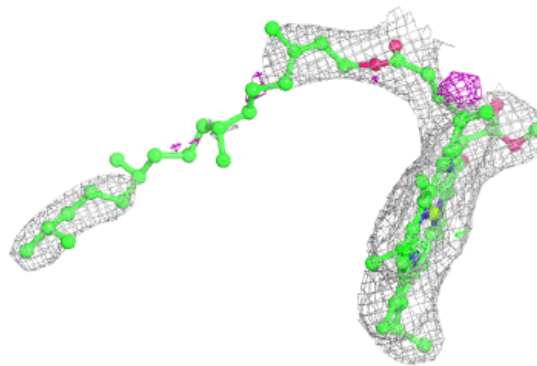
**Electron density around CLA 4 318:**

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



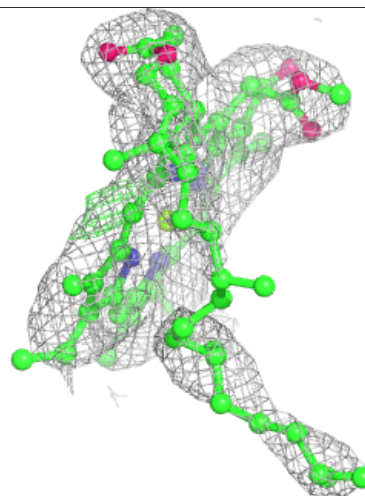
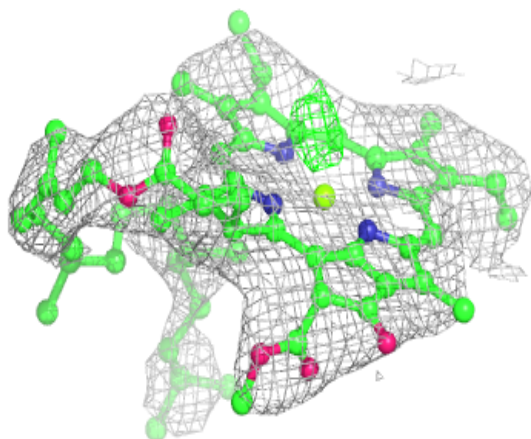
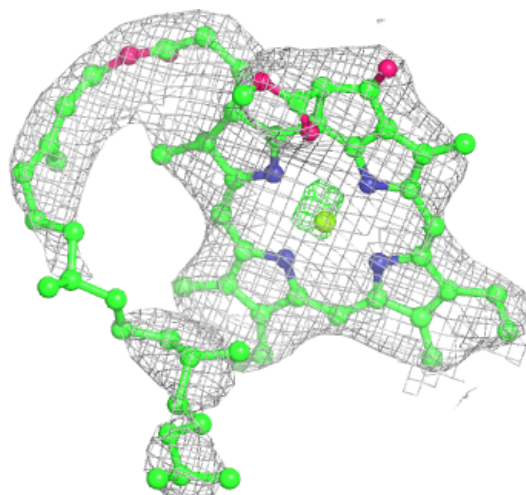
Electron density around CLA A 804:

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



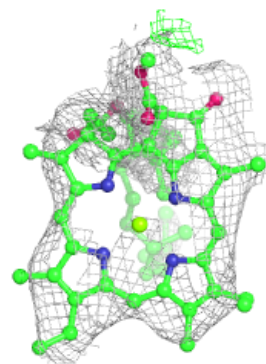
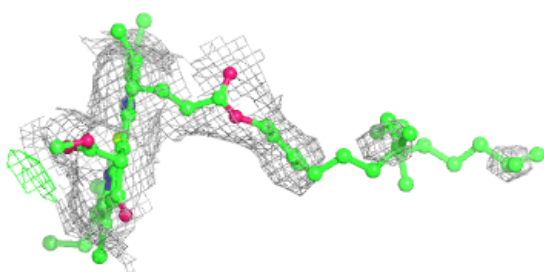
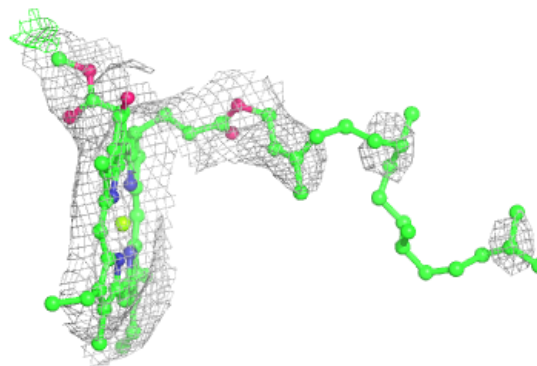
Electron density around CLA A 813:

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

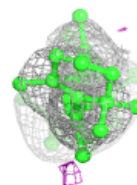
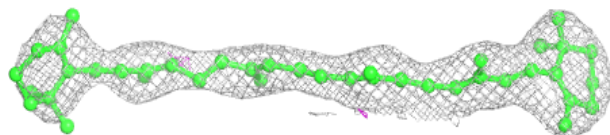
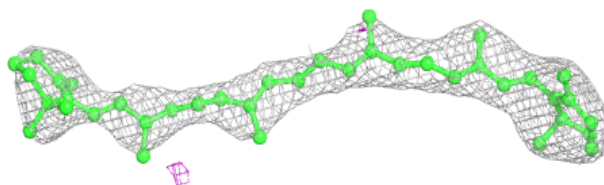


Electron density around CLA A 814:

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

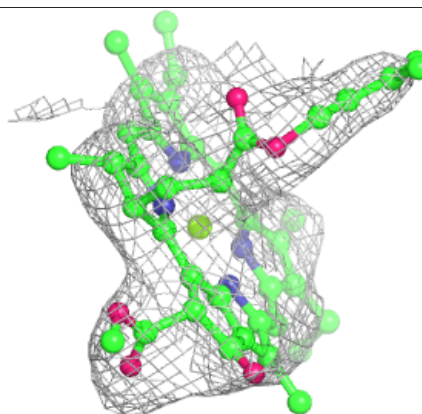
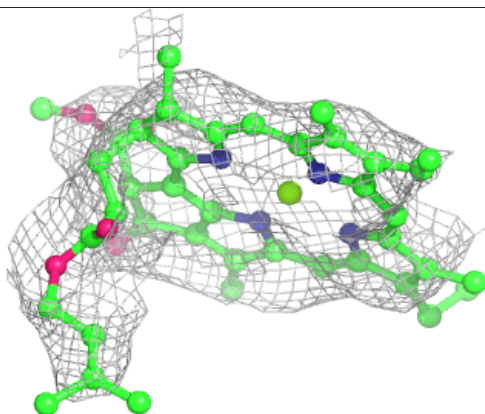
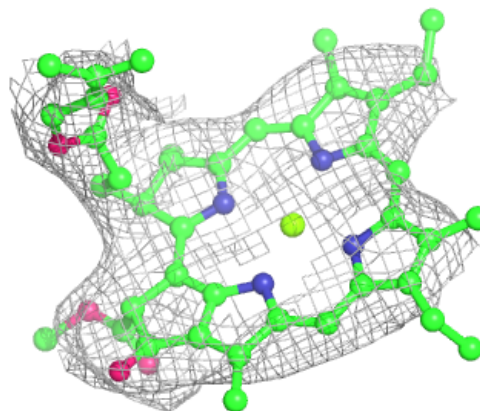
**Electron density around BCR B 852:**

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

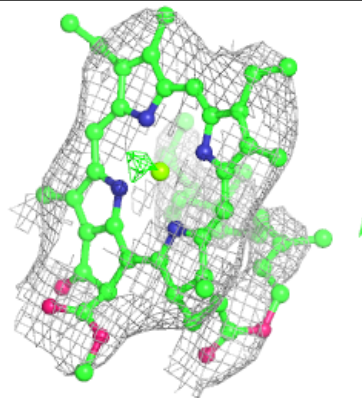
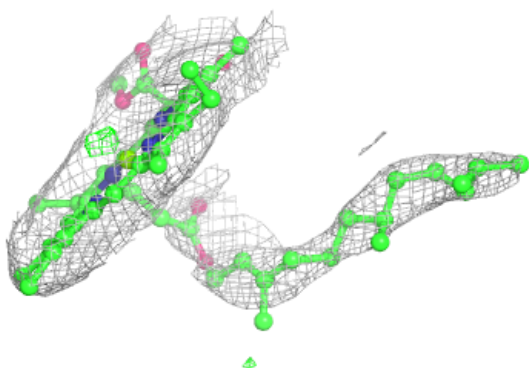
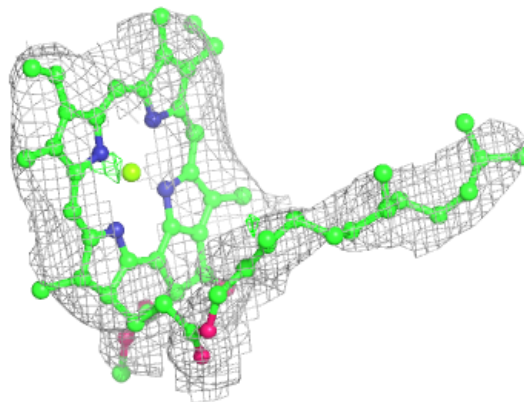


Electron density around CLA 2 509:

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

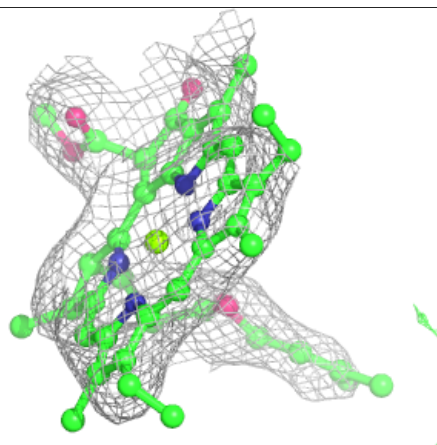
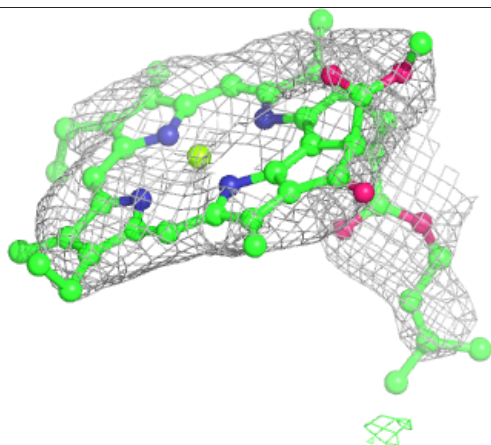
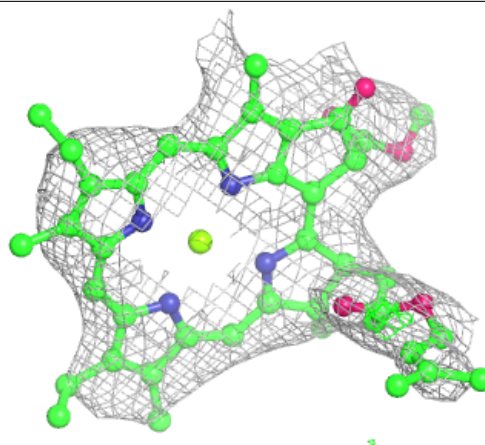
**Electron density around CLA 2 510:**

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



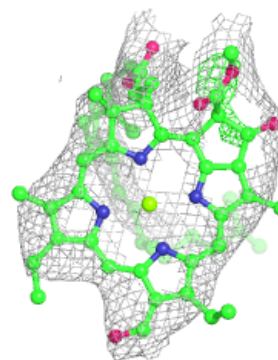
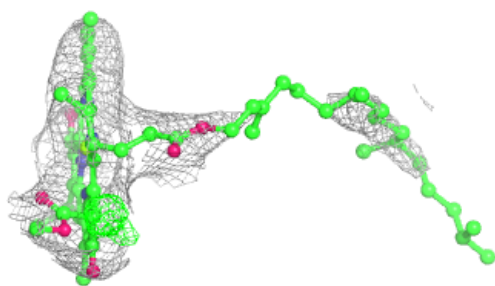
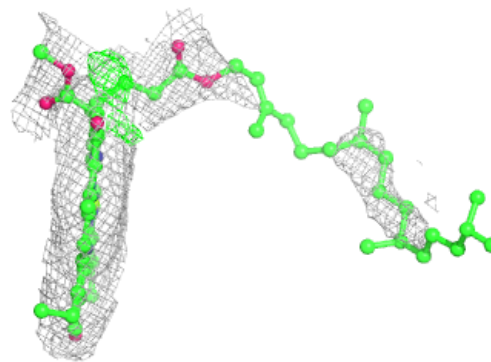
Electron density around CLA 2 511:

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



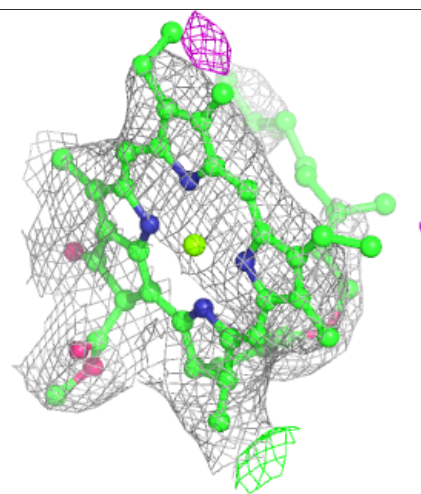
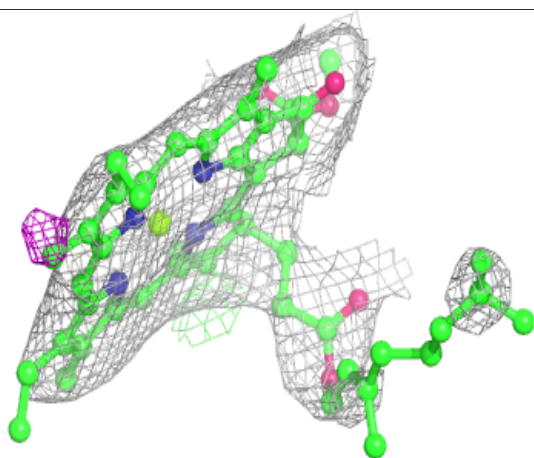
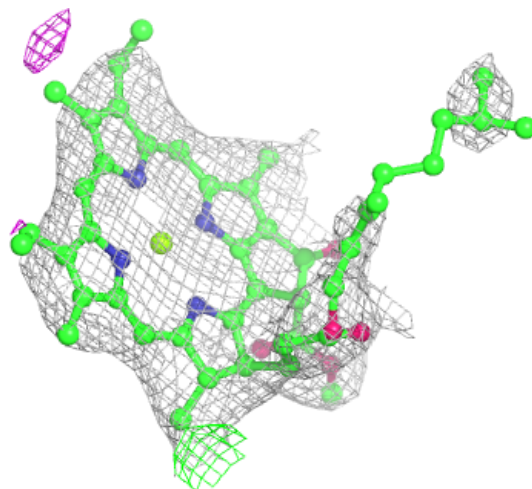
Electron density around CHL 2 526:

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



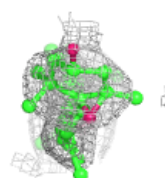
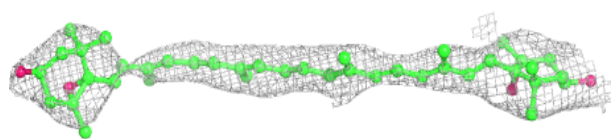
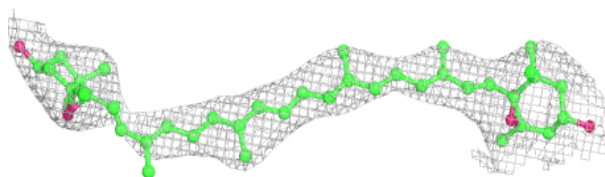
Electron density around CLA 2 514:

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

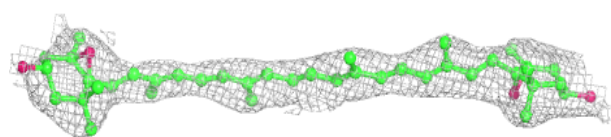
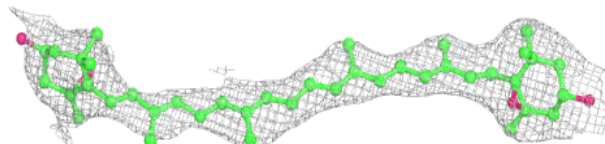


Electron density around XAT 2 502:

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

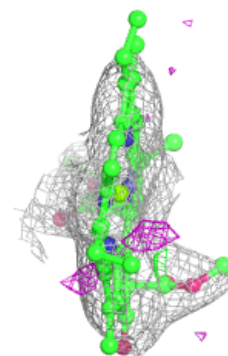
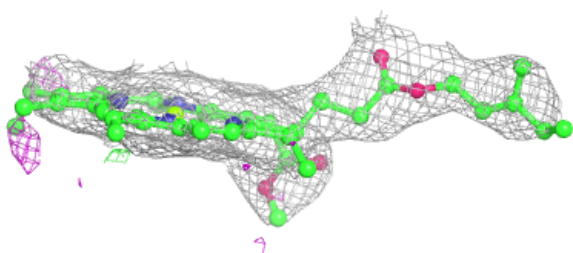
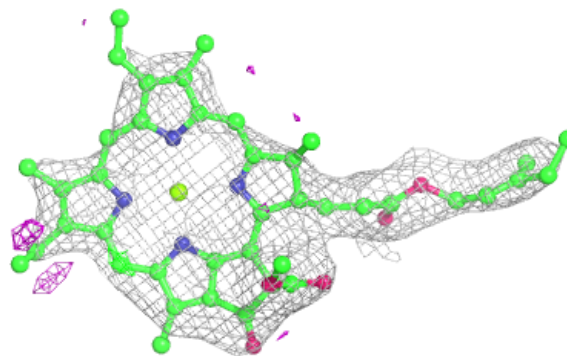
**Electron density around XAT 4 303:**

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

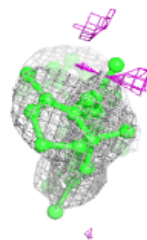
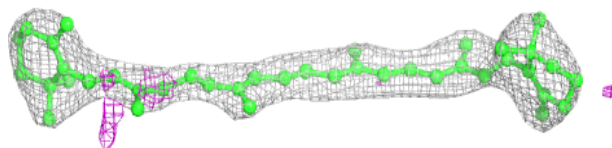
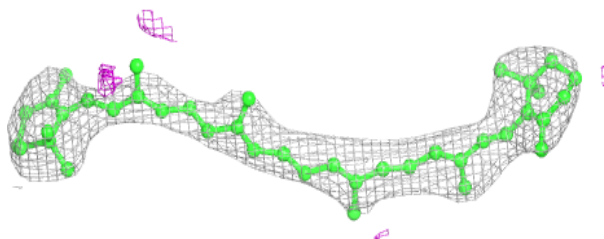


Electron density around CLA A 836:

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

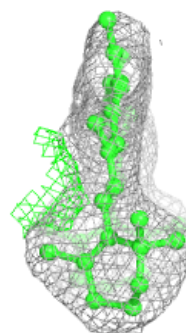
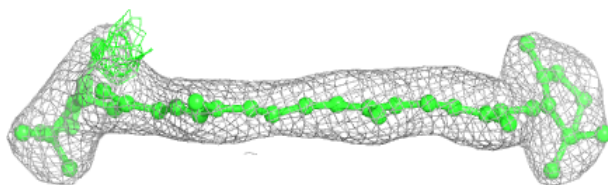
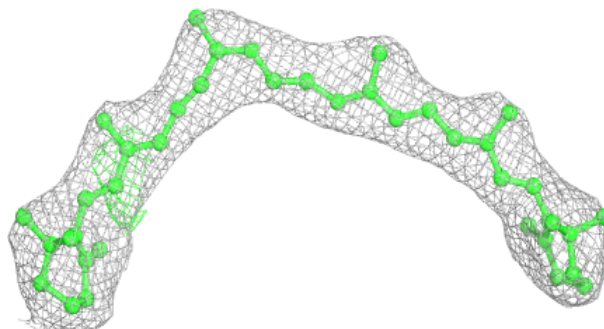
**Electron density around BCR B 853:**

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



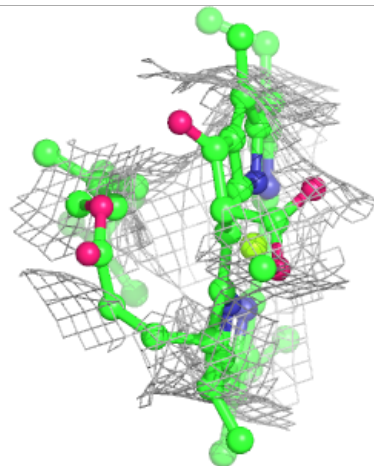
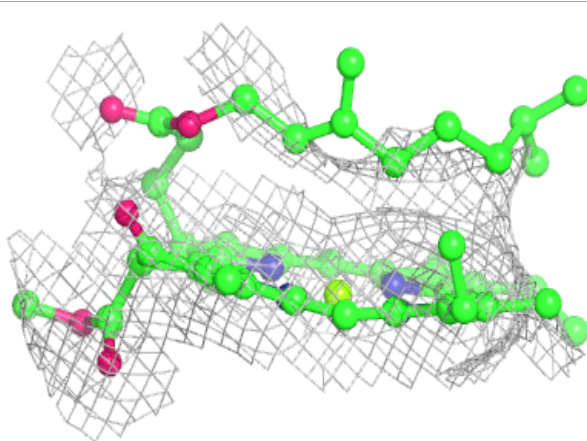
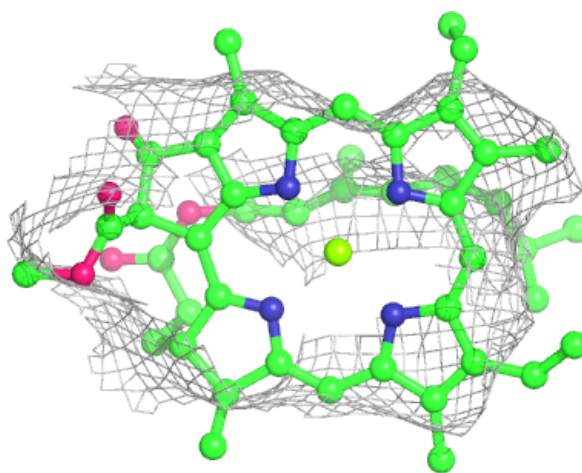
Electron density around BCR F 306:

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



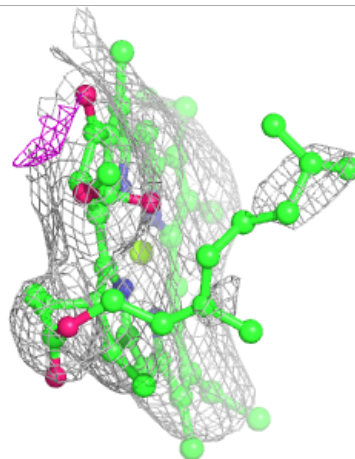
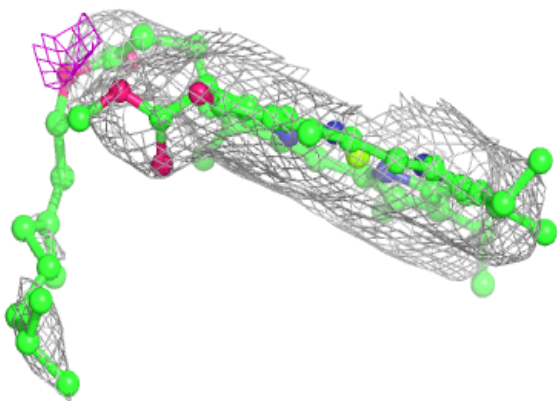
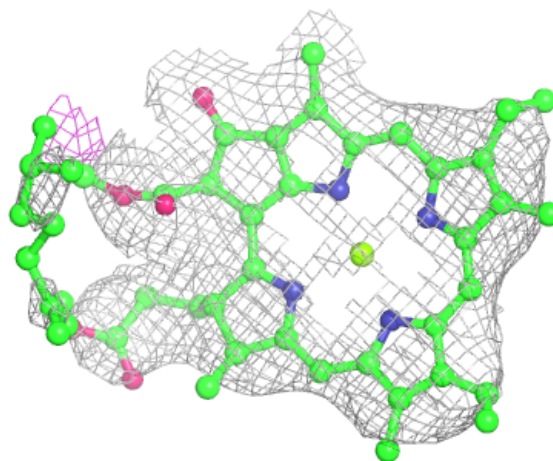
Electron density around CLA 3 307:

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



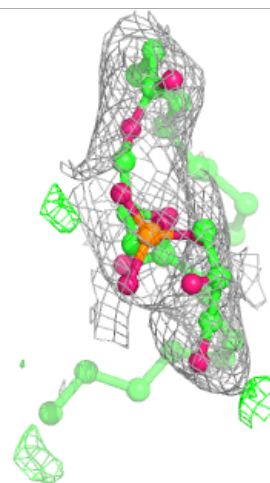
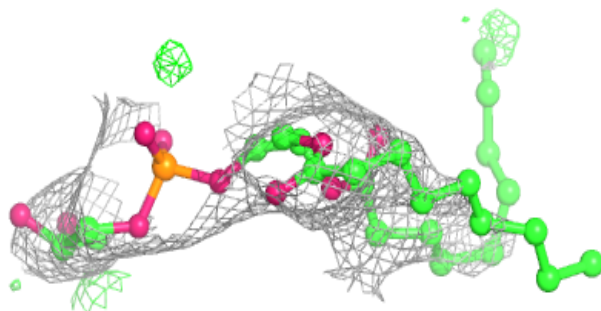
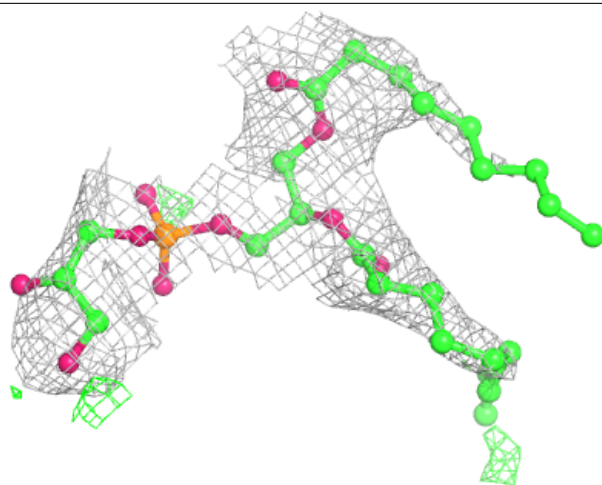
Electron density around CLA 3 309:

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



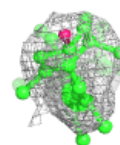
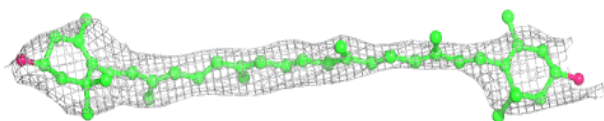
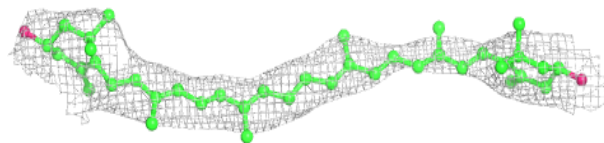
Electron density around LHG 2 517:

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

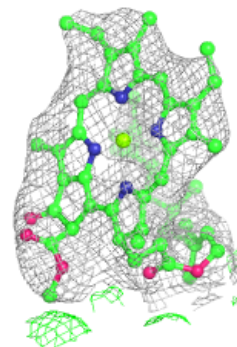
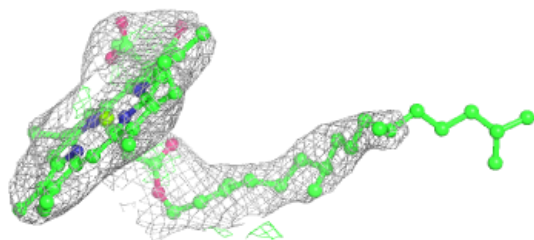
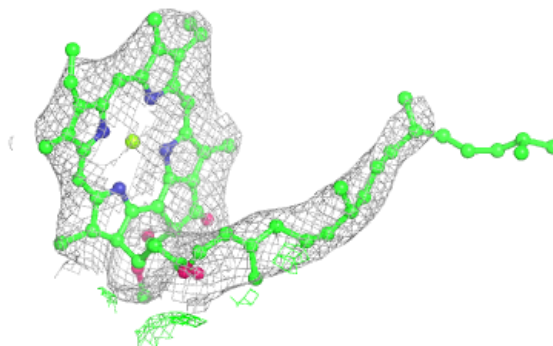


Electron density around LUT 2 501:

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

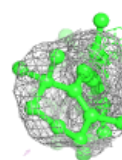
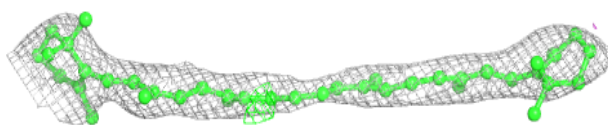
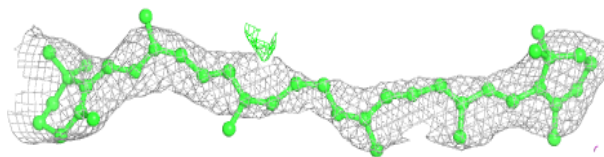
**Electron density around CLA B 822:**

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

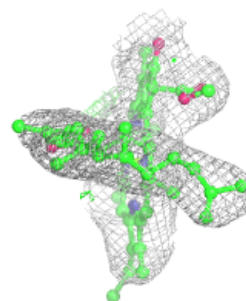
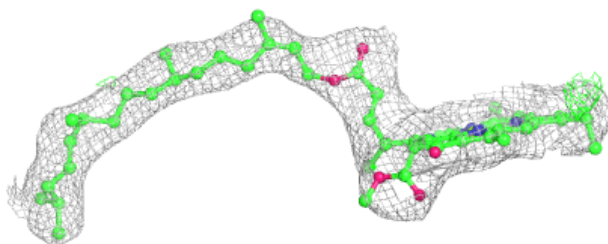
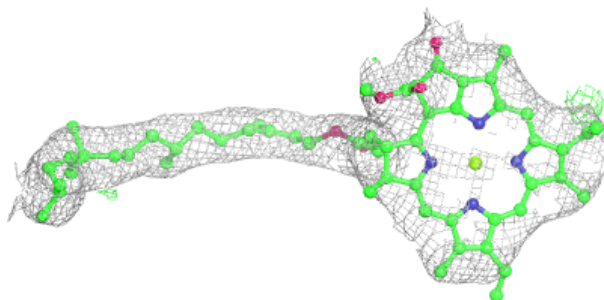


Electron density around BCR B 849:

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

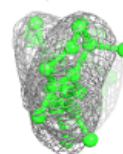
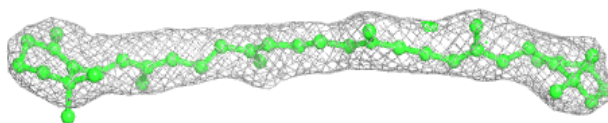
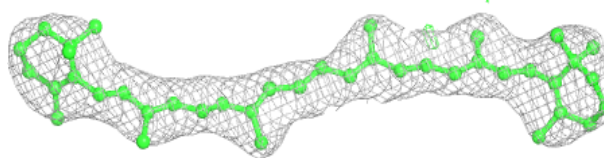
**Electron density around CLA B 840:**

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

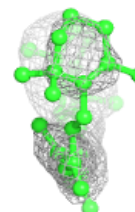
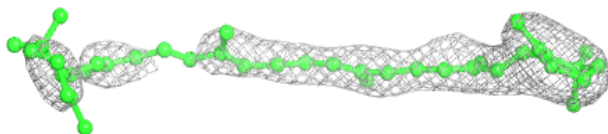
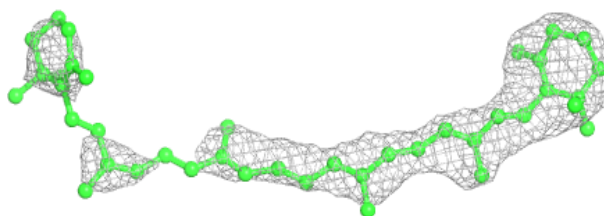


Electron density around BCR J 1108:

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

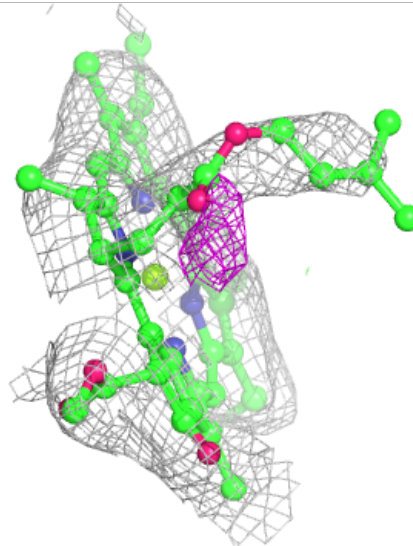
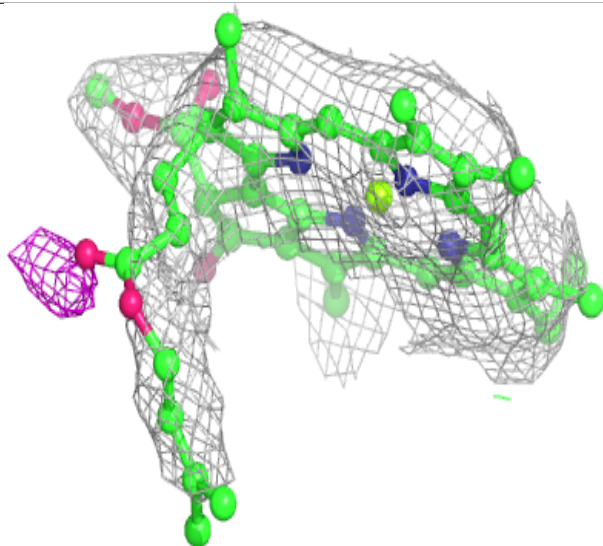
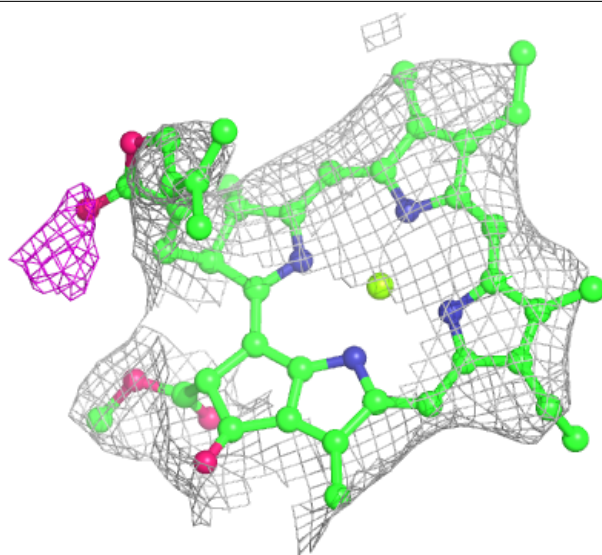
**Electron density around BCR B 850:**

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



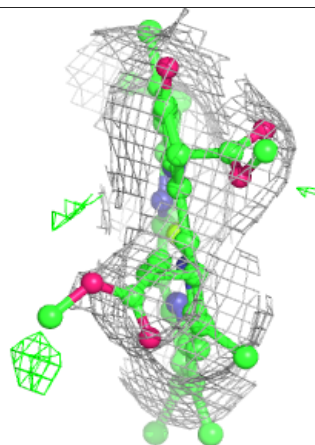
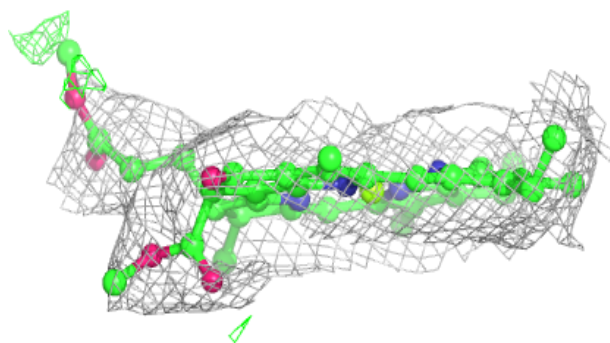
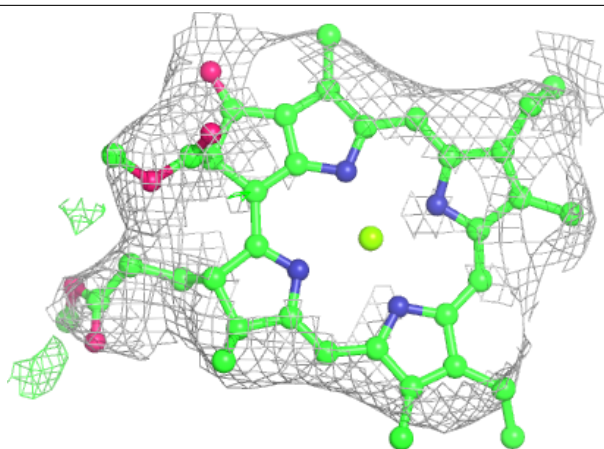
Electron density around CLA 3 315:

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



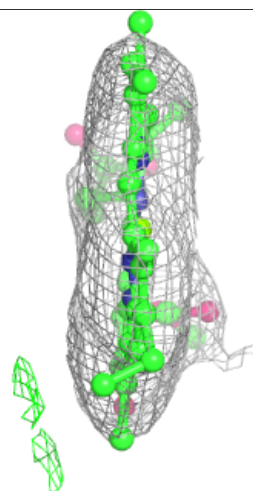
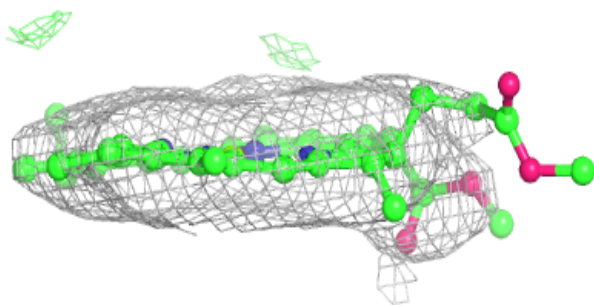
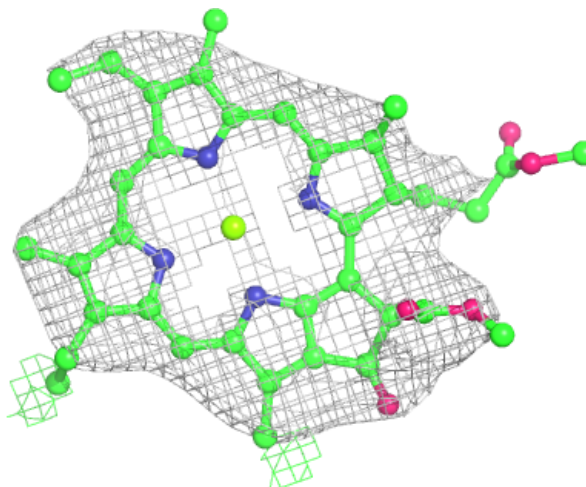
Electron density around CLA 3 316:

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



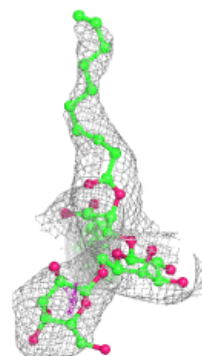
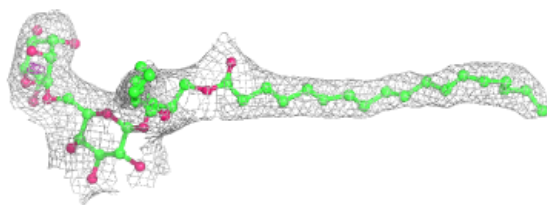
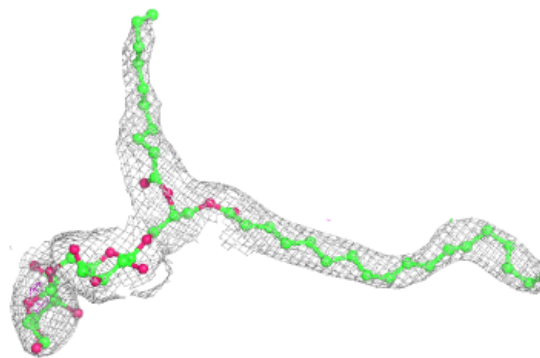
Electron density around CLA 3 317:

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



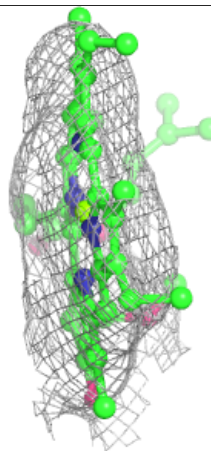
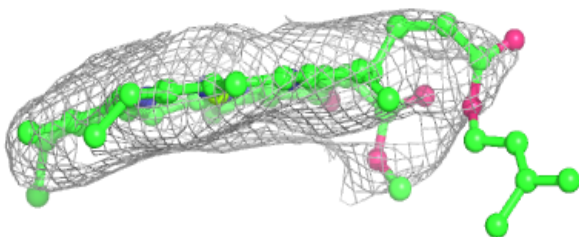
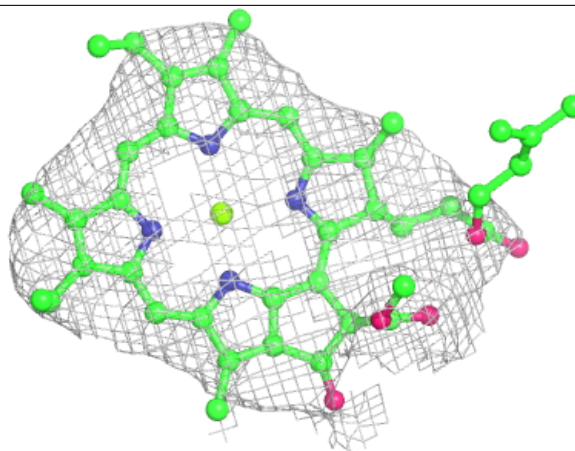
Electron density around DGD J 1106:

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

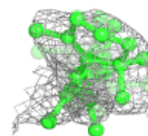
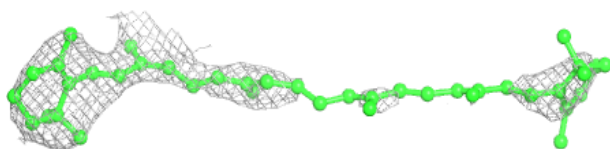
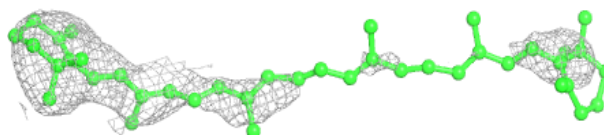


Electron density around CLA 4 305:

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

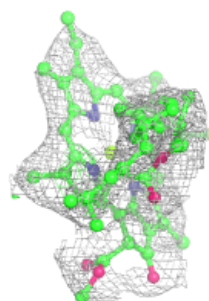
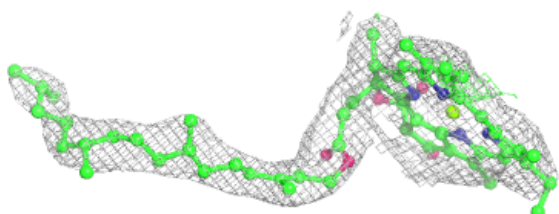
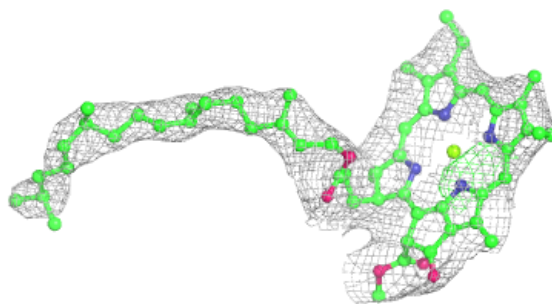
**Electron density around BCR A 848:**

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

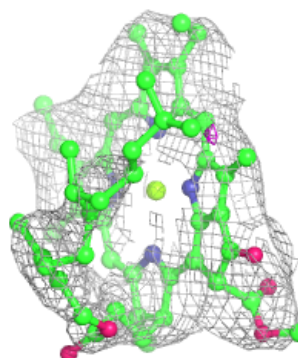
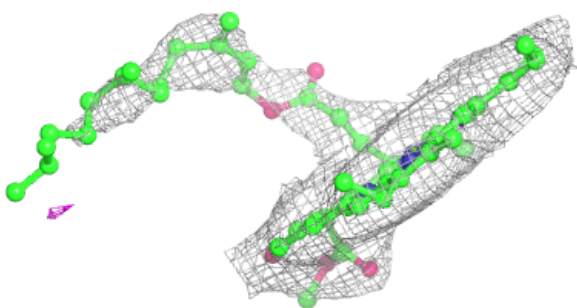
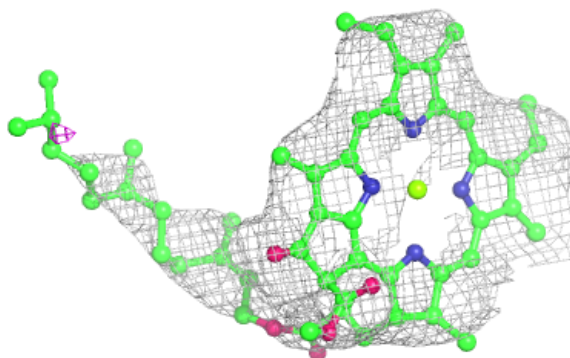


Electron density around CLA A 821:

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

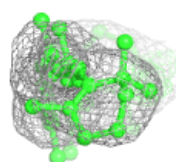
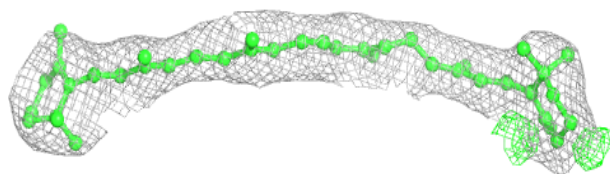
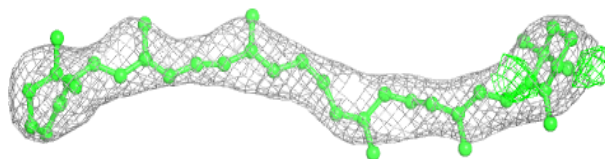
**Electron density around CLA A 822:**

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

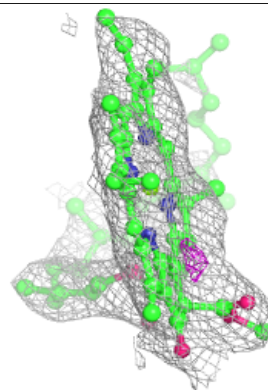
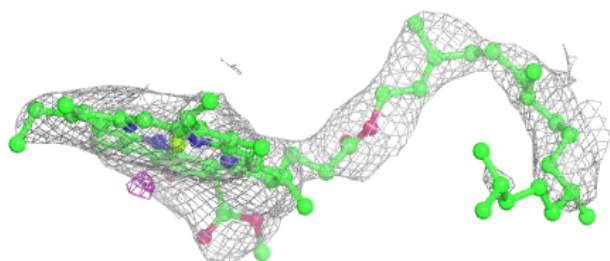
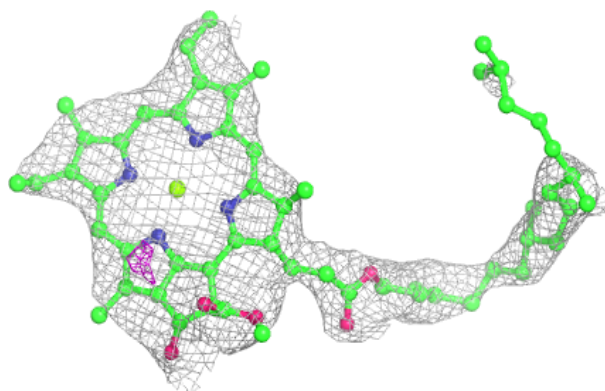


Electron density around BCR I 101:

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

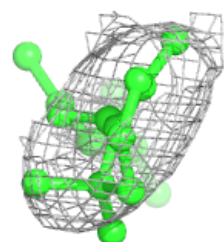
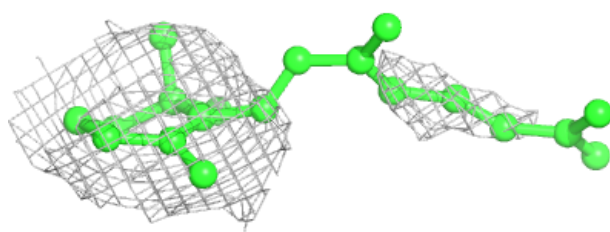
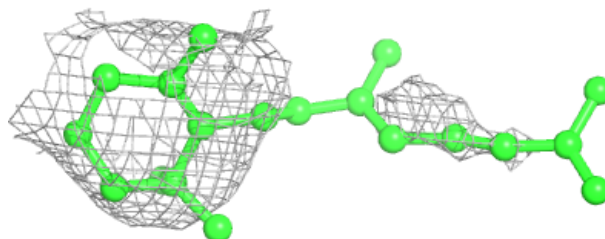
**Electron density around CLA A 827:**

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

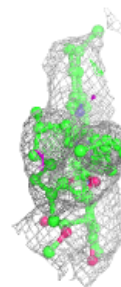
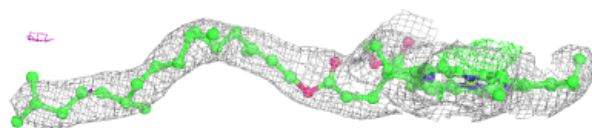
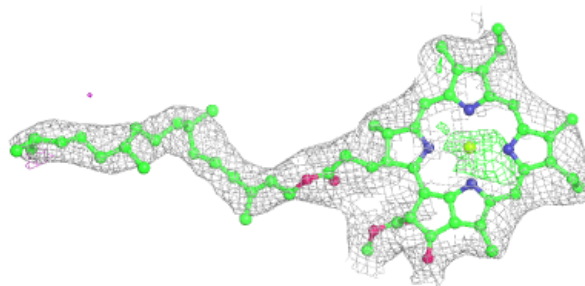


Electron density around BCR 1 503:

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

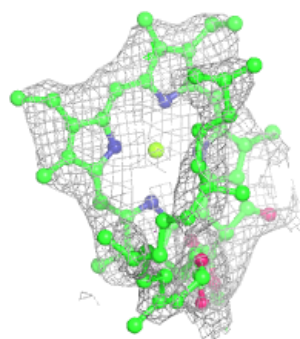
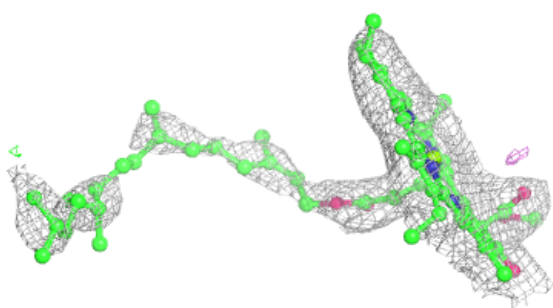
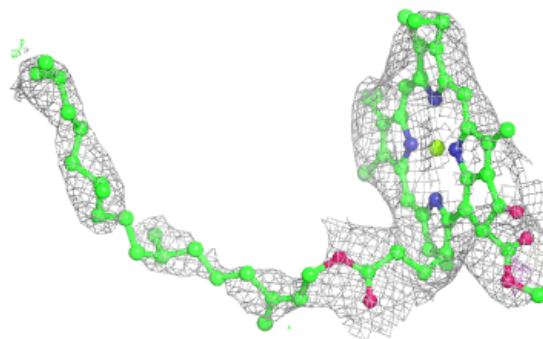
**Electron density around CLA A 832:**

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

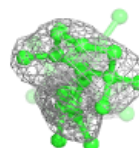
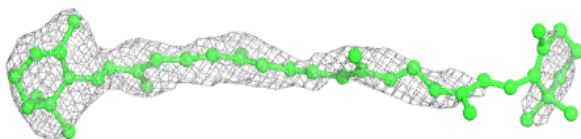
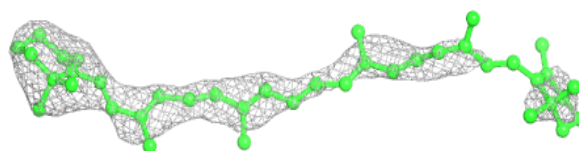


Electron density around CLA A 834:

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

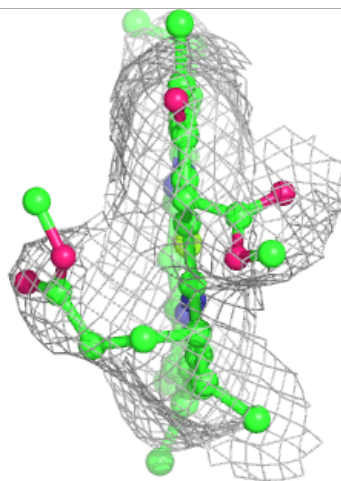
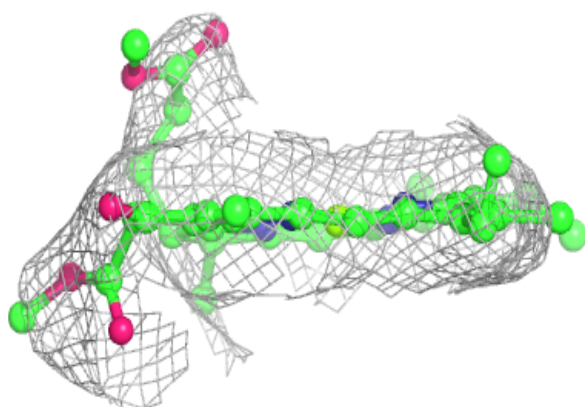
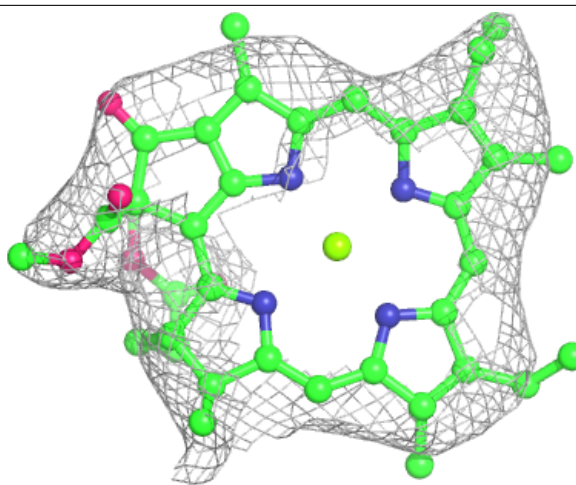
**Electron density around BCR A 849:**

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



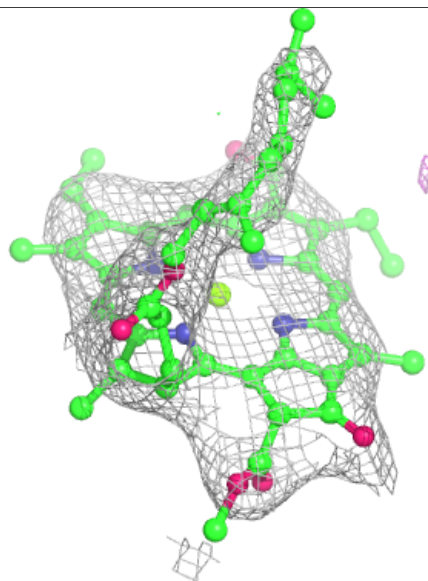
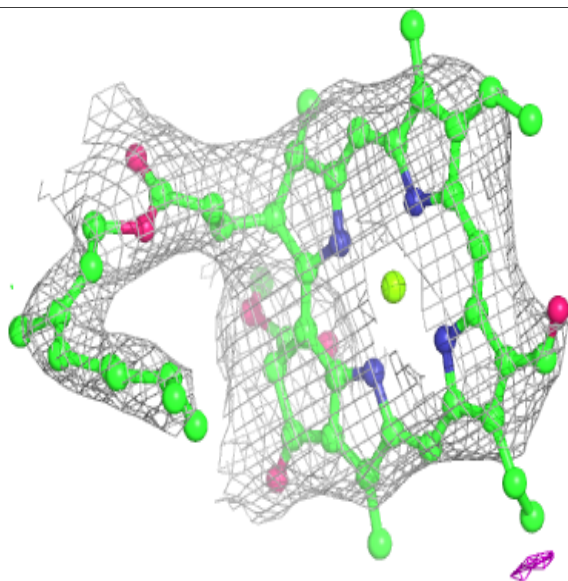
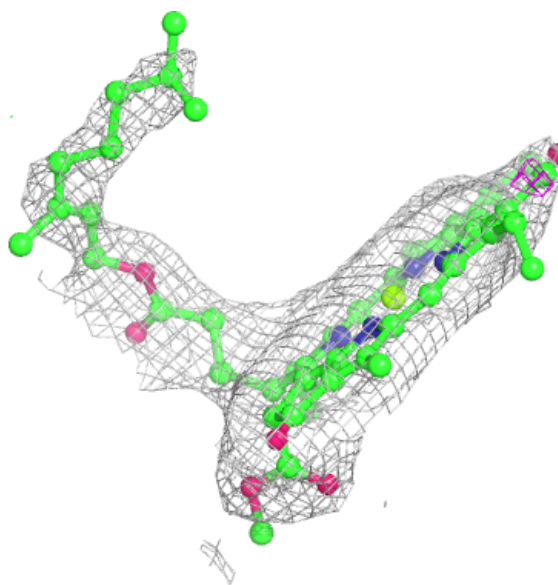
Electron density around CLA 4 311:

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



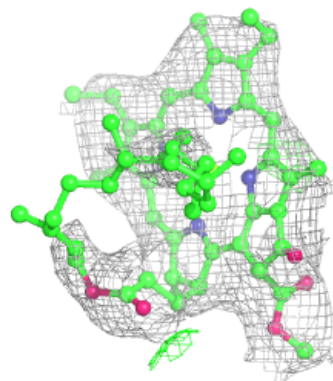
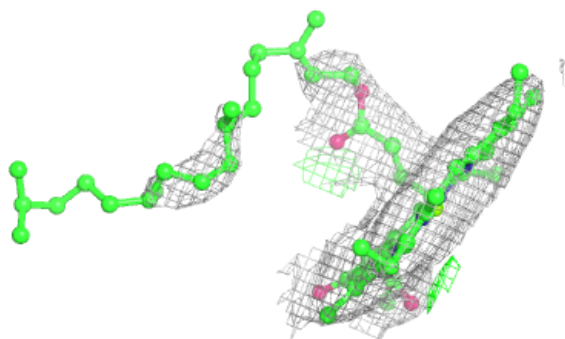
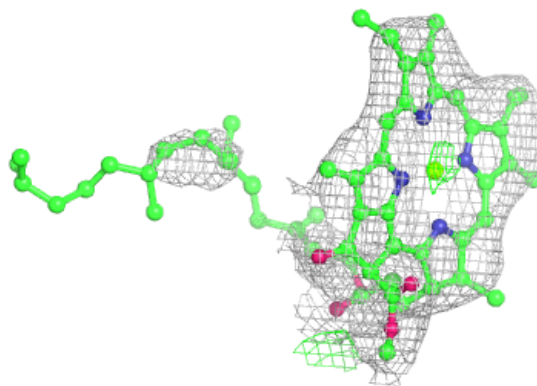
Electron density around CHL 1 521:

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

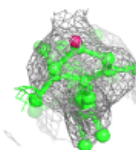
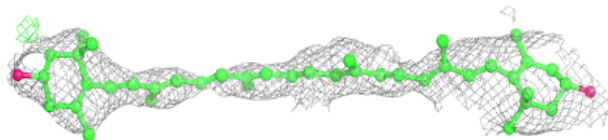
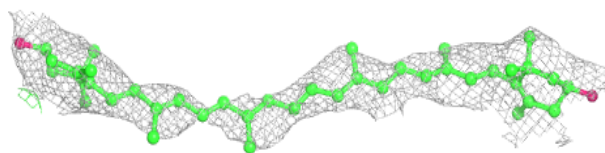


Electron density around CLA 4 315:

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

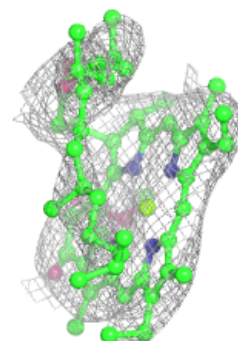
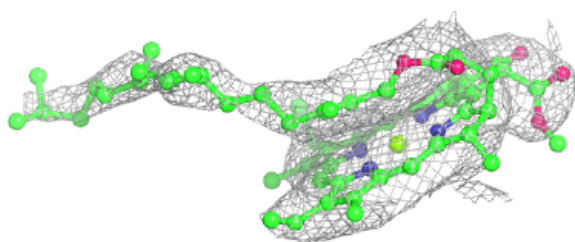
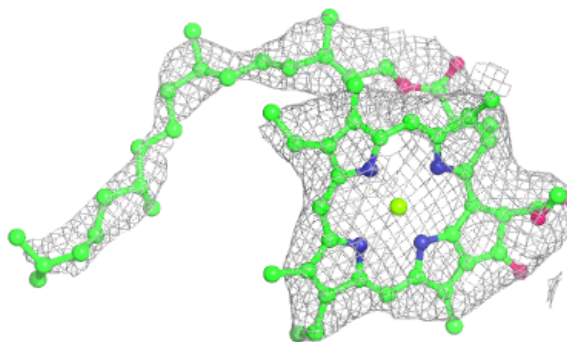
**Electron density around LUT 1 501:**

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

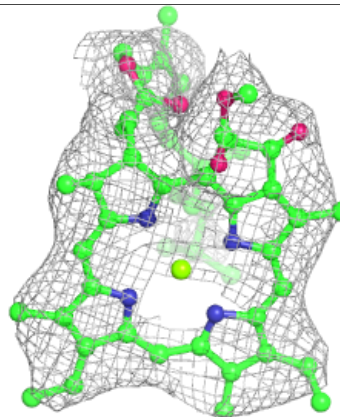
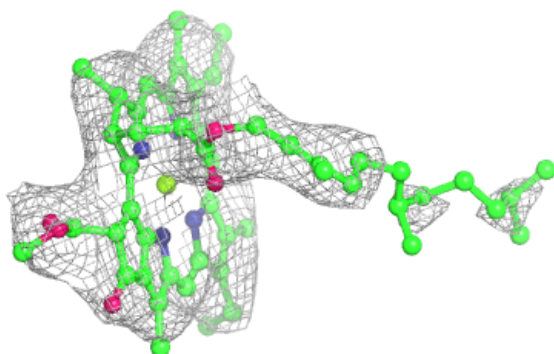
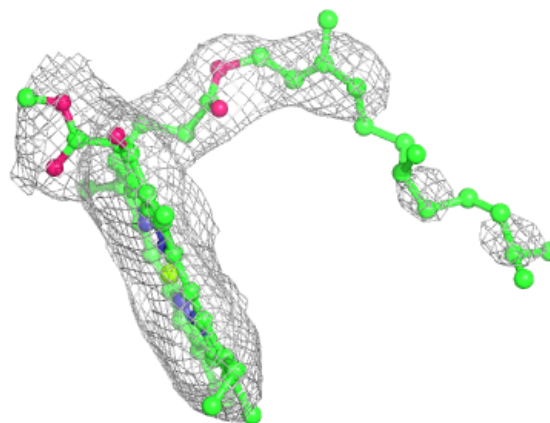


Electron density around CLA 1 507:

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

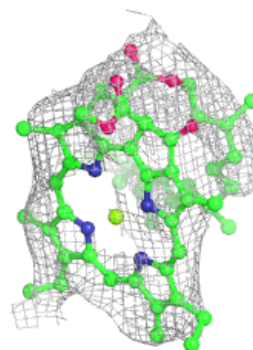
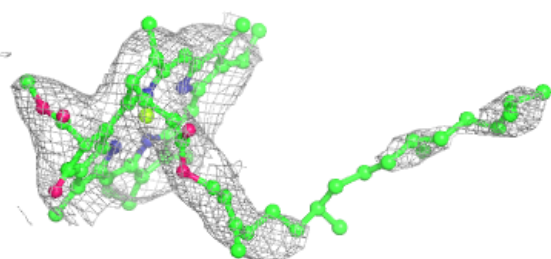
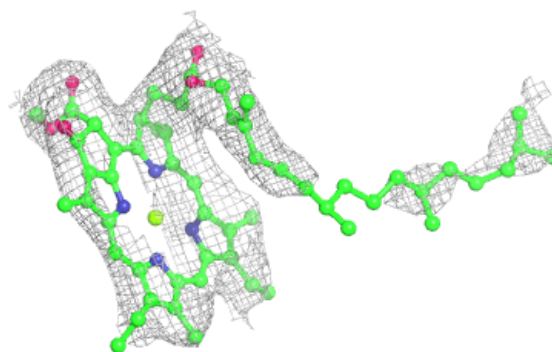
**Electron density around CLA A 807:**

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

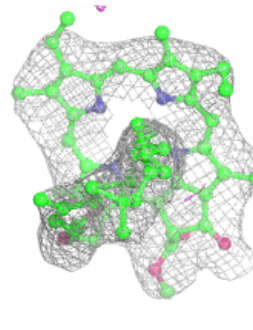
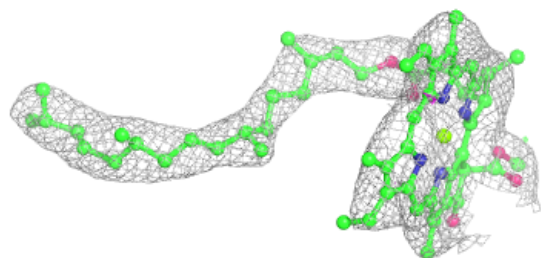
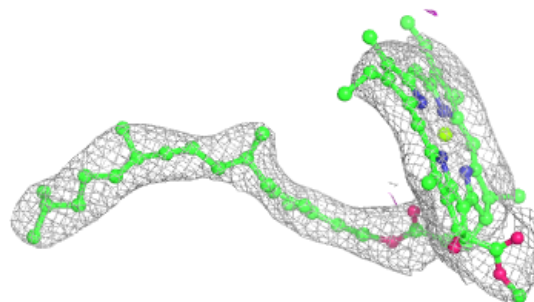


Electron density around CLA B 815:

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

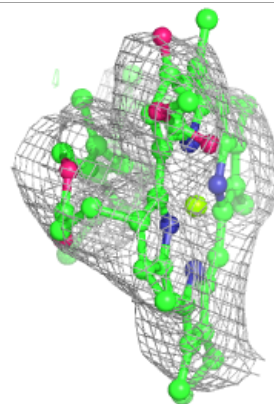
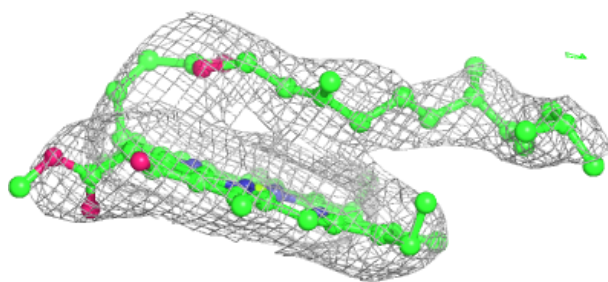
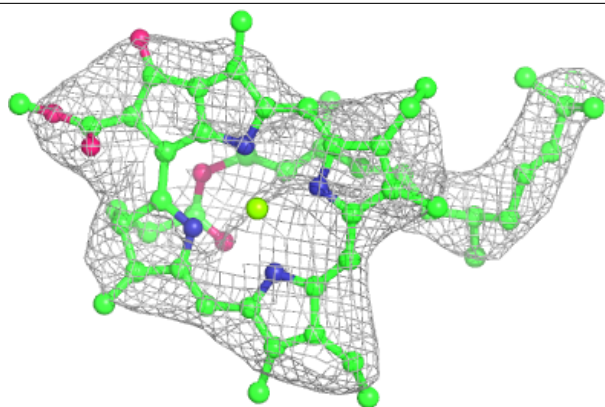
**Electron density around CLA A 811:**

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



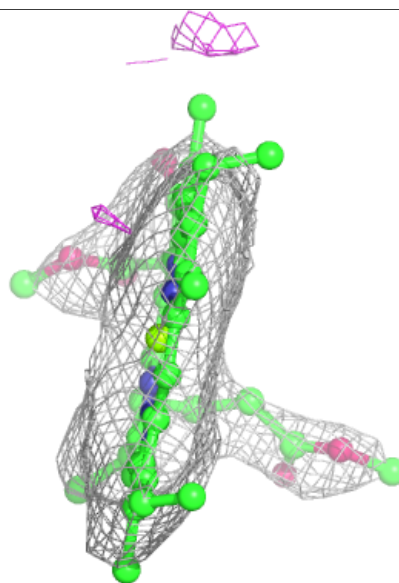
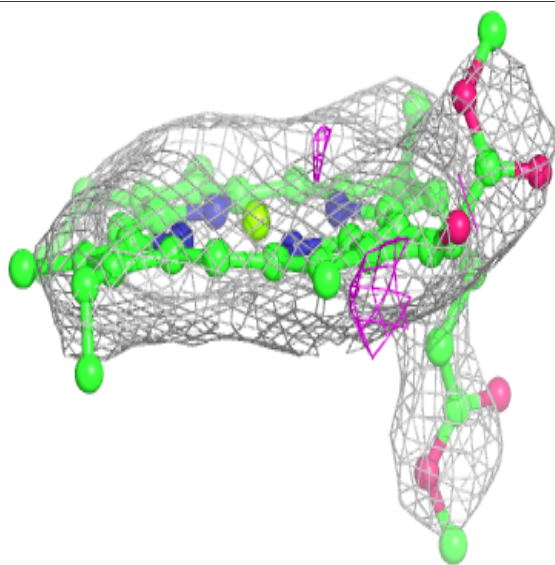
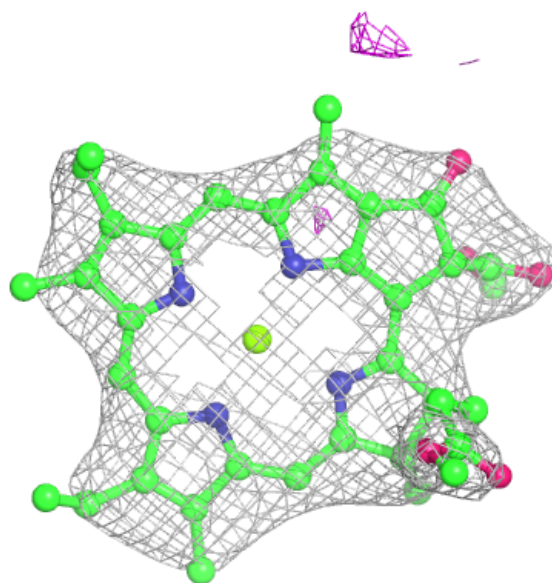
Electron density around CLA B 817:

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



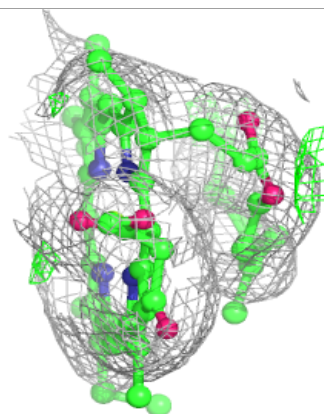
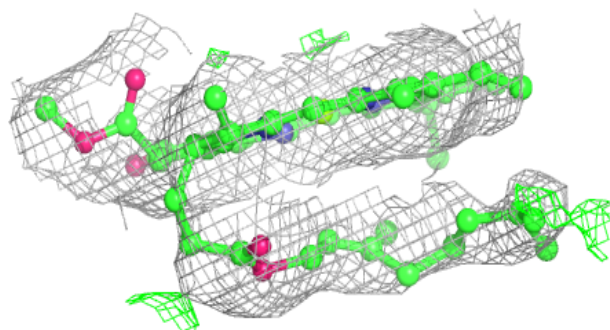
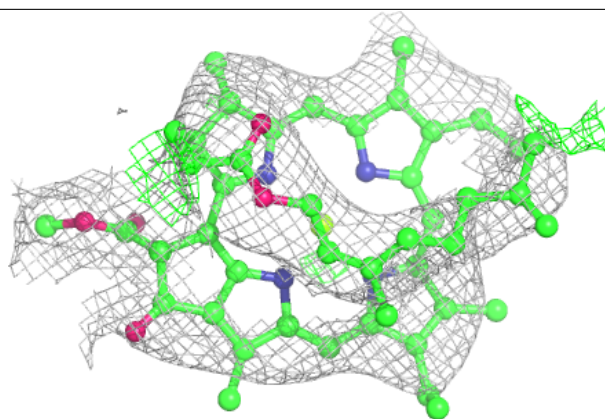
Electron density around CLA B 821:

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

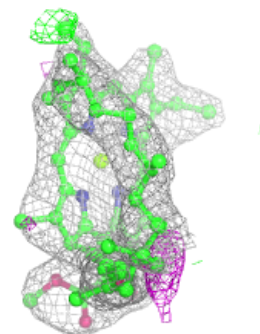
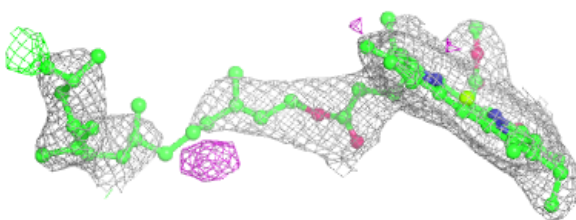
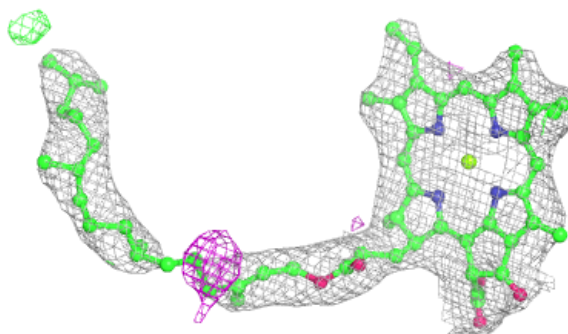


Electron density around CLA A 812:

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

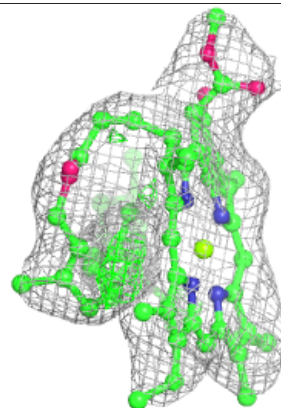
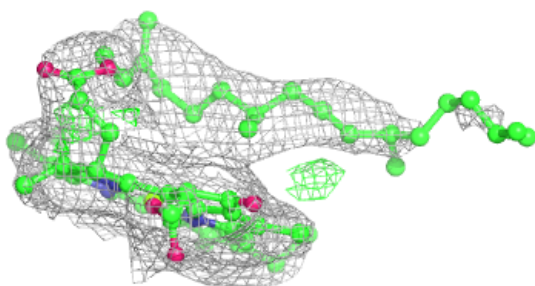
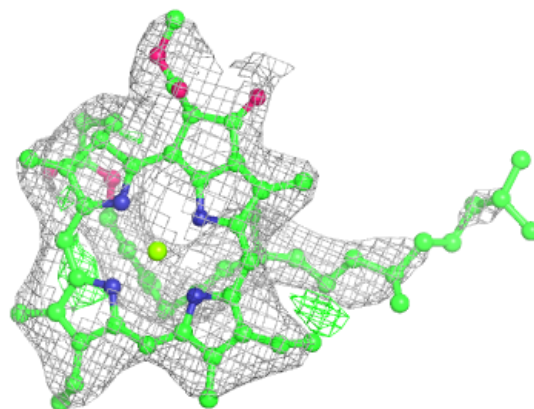
**Electron density around CLA B 825:**

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



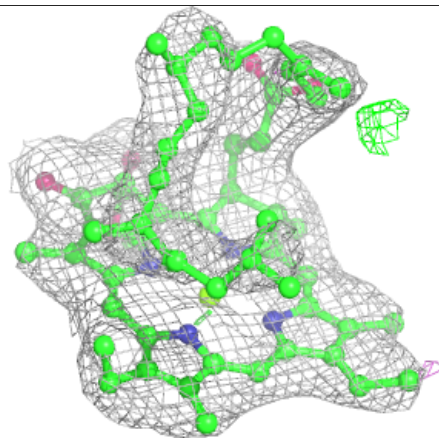
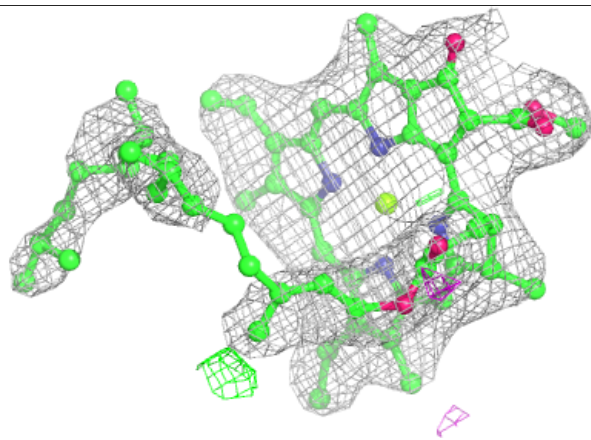
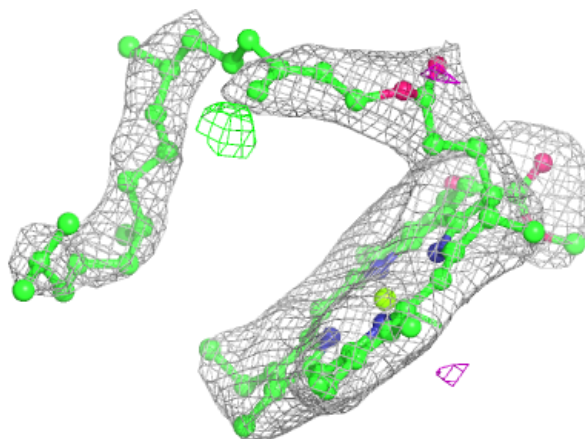
Electron density around CLA B 827:

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



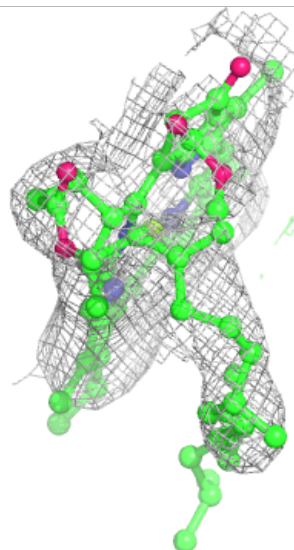
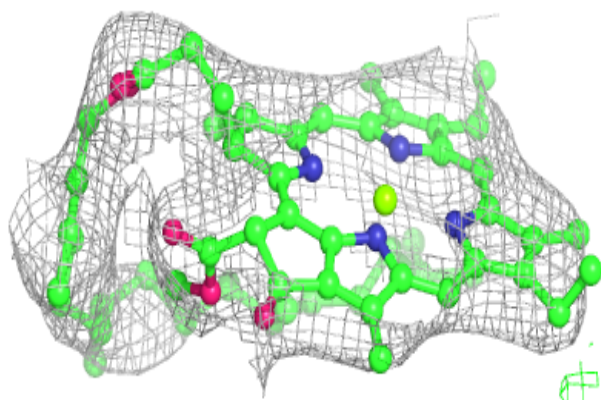
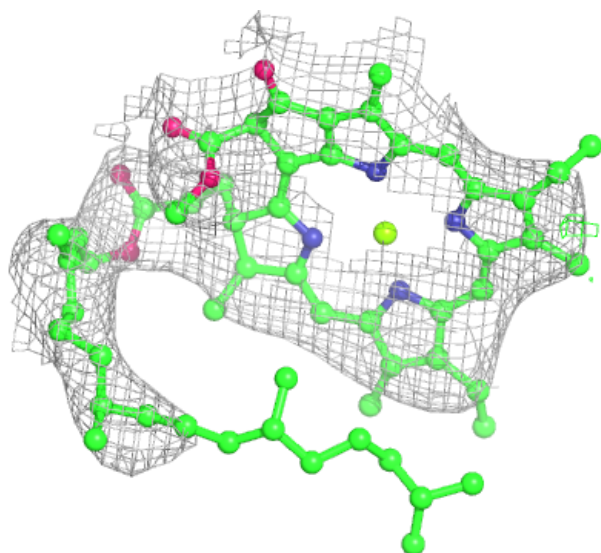
Electron density around CLA B 830:

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



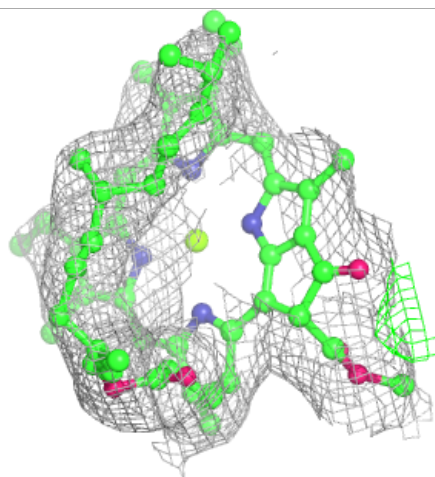
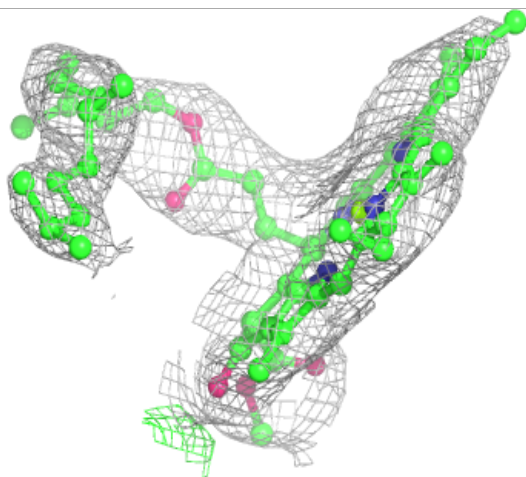
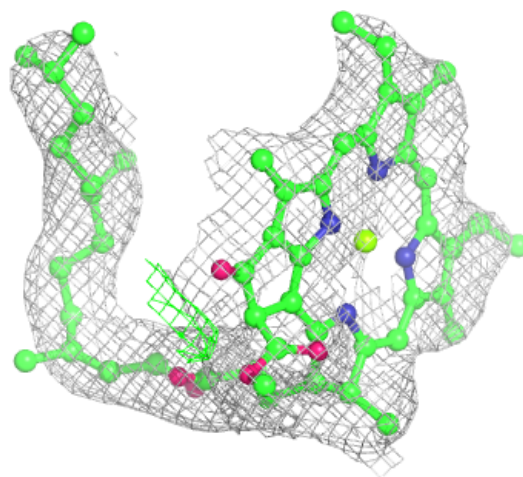
Electron density around CLA 1 508:

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



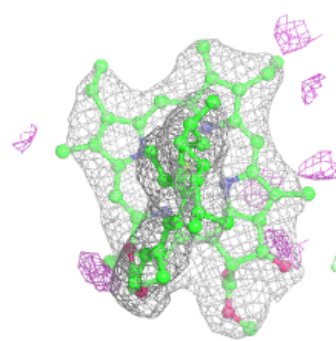
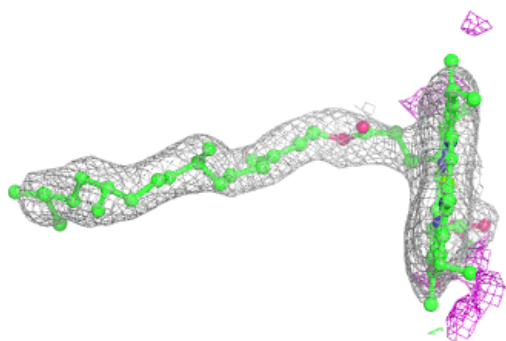
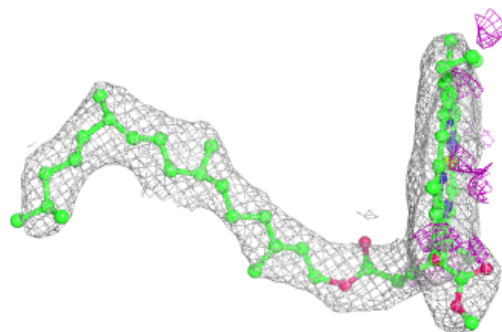
Electron density around CLA B 833:

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

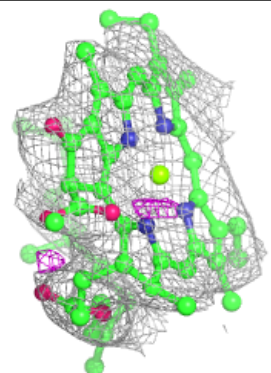
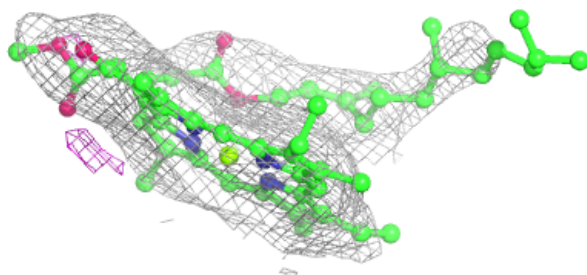
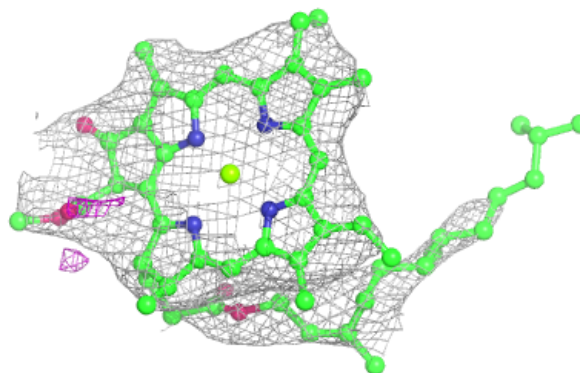


Electron density around CLA B 839:

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

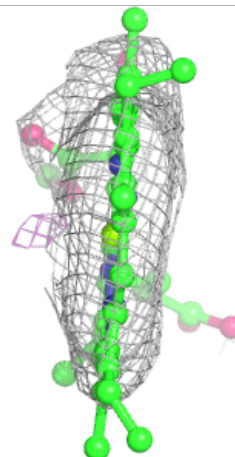
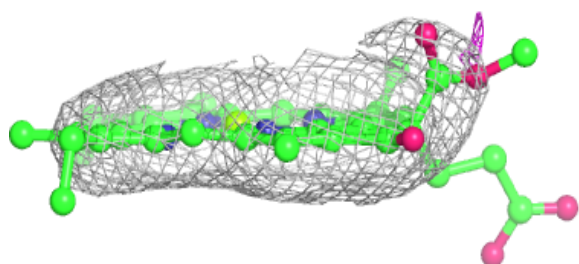
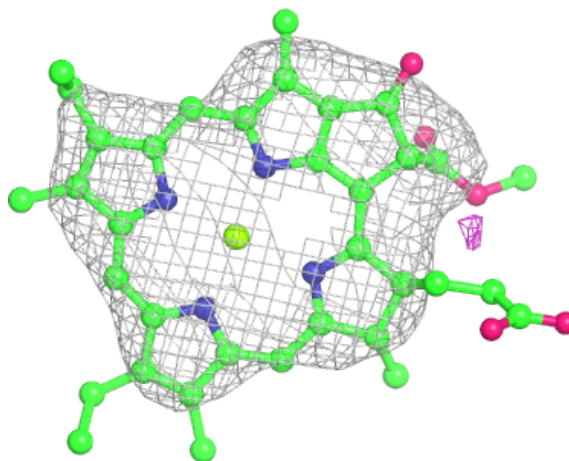
**Electron density around CLA 2 504:**

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



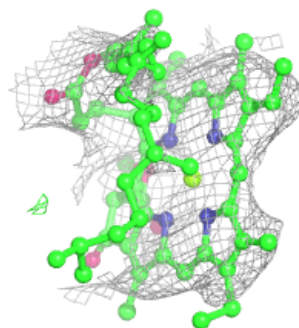
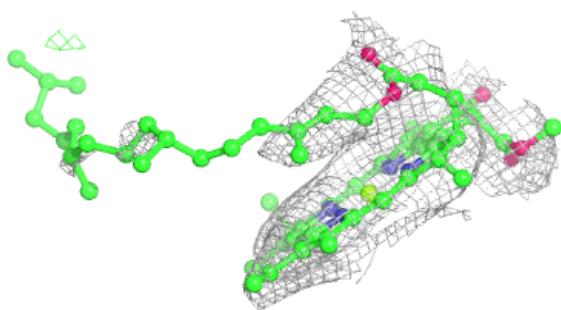
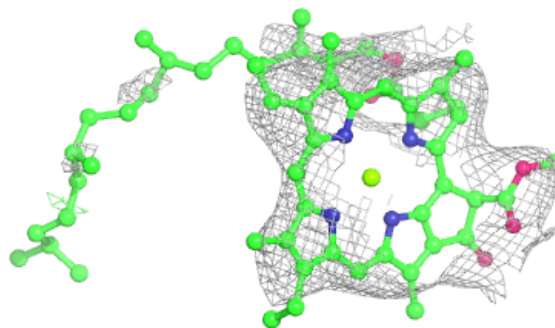
Electron density around CLA A 815:

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

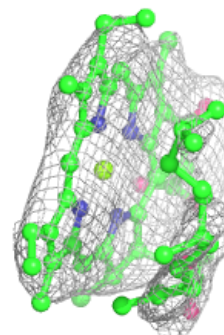
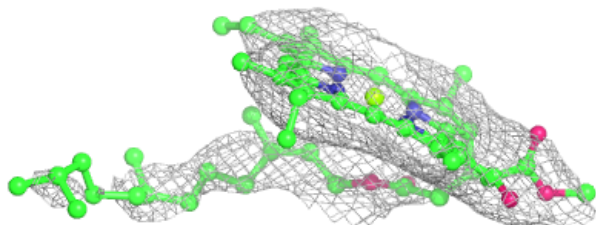
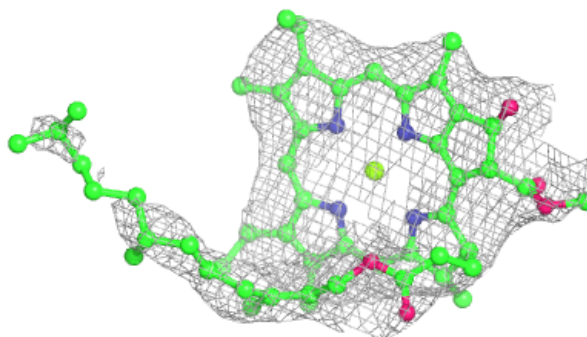


Electron density around CLA 3 308:

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

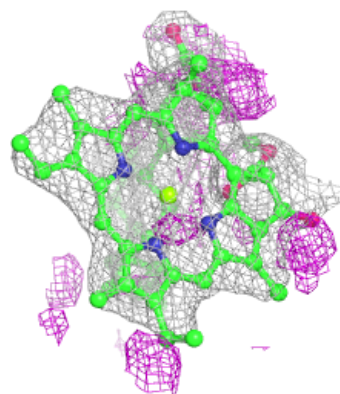
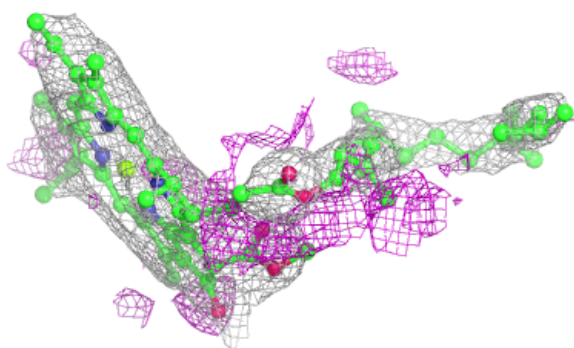
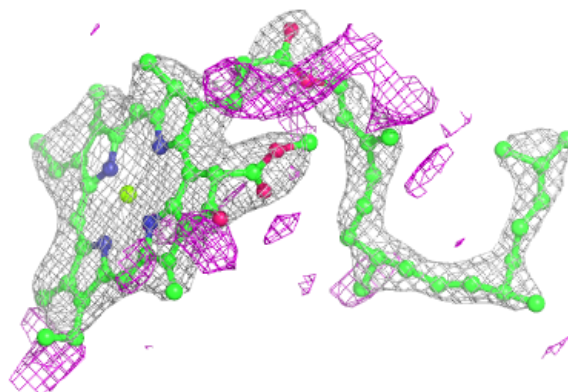
**Electron density around CLA 4 304:**

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

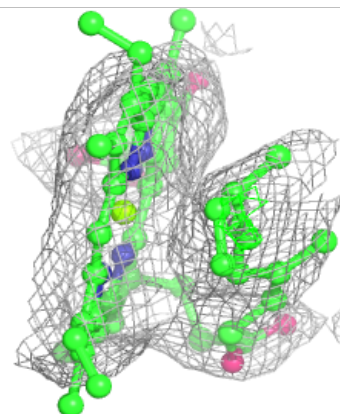
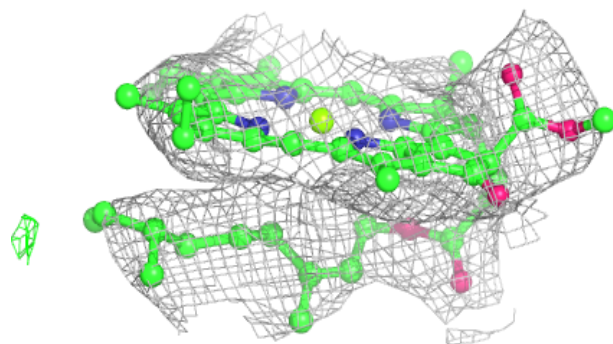
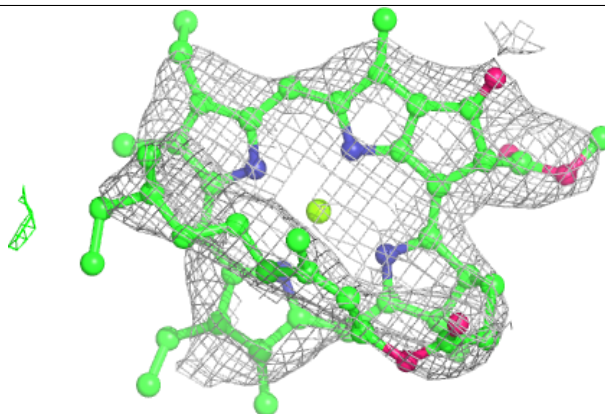


Electron density around CL0 A 801:

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

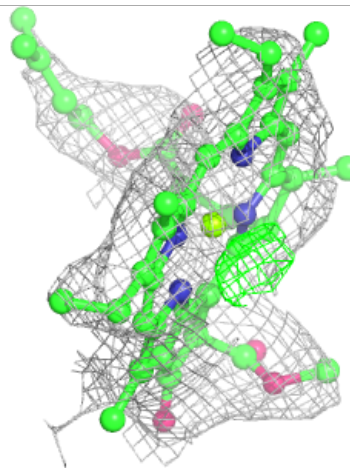
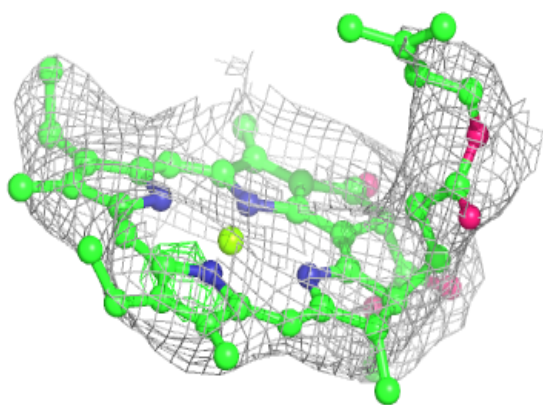
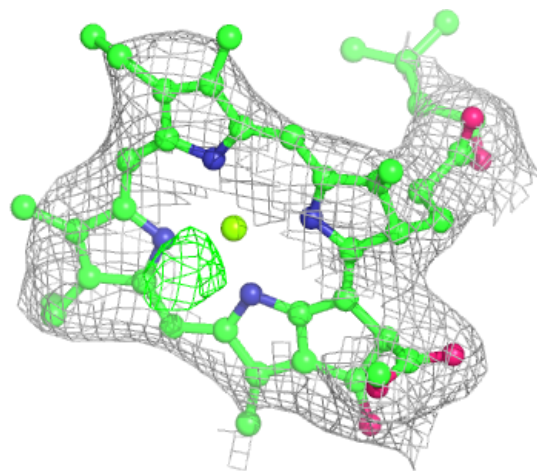
**Electron density around CLA A 818:**

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



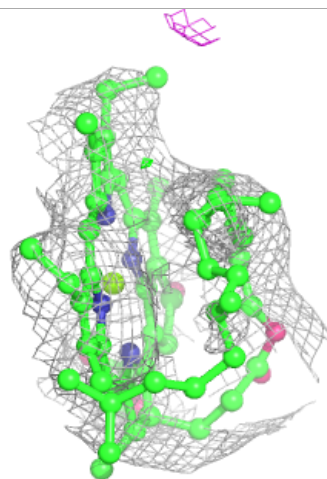
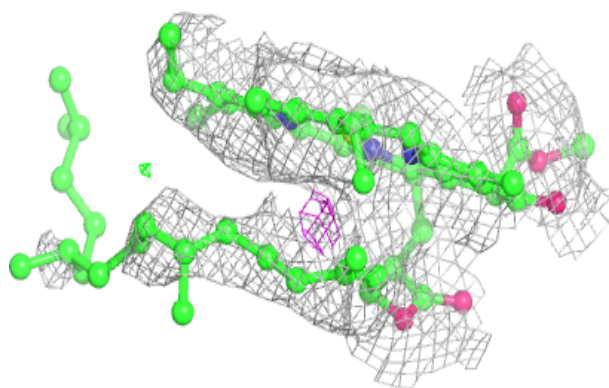
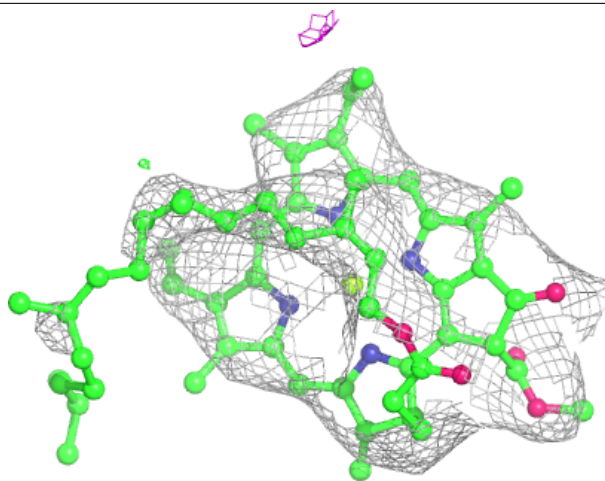
Electron density around CLA A 820:

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



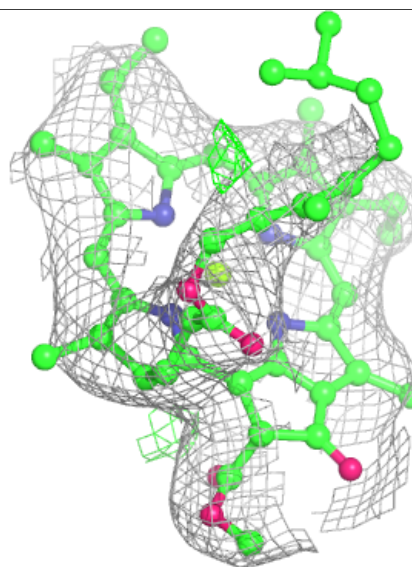
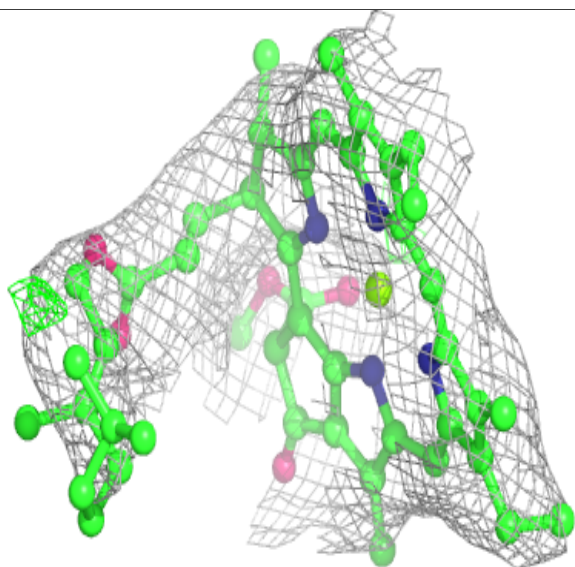
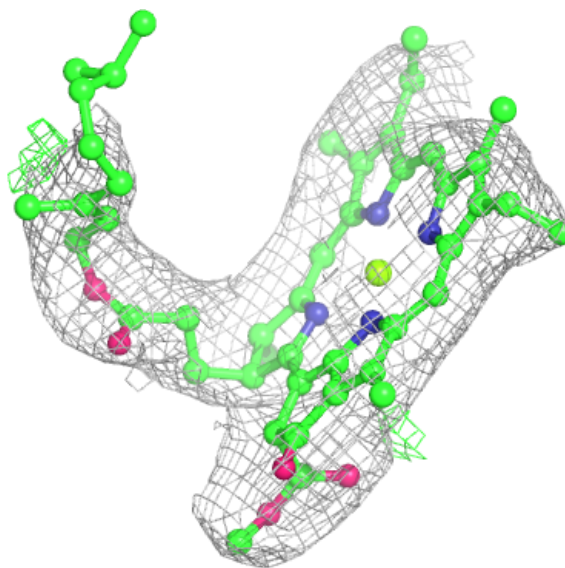
Electron density around CLA 4 306:

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



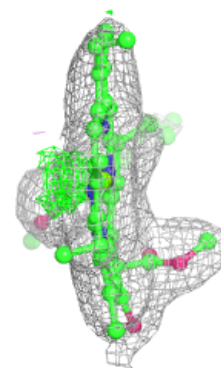
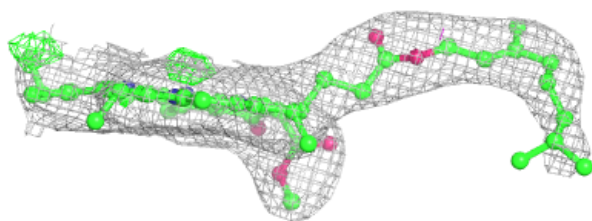
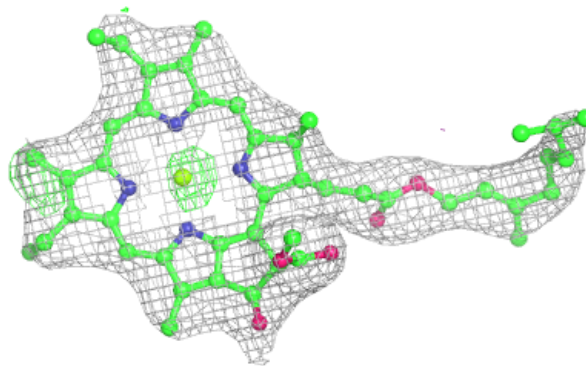
Electron density around CLA B 834:

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

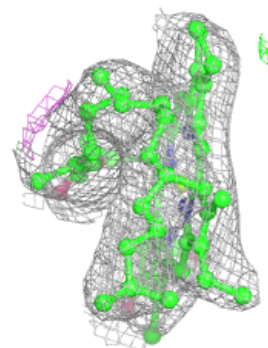
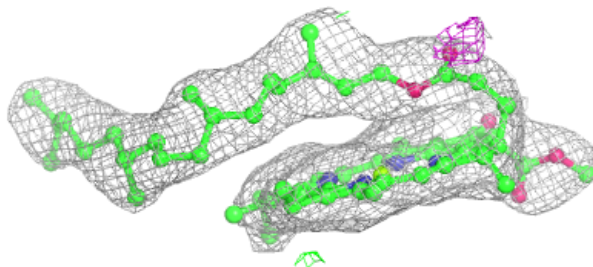
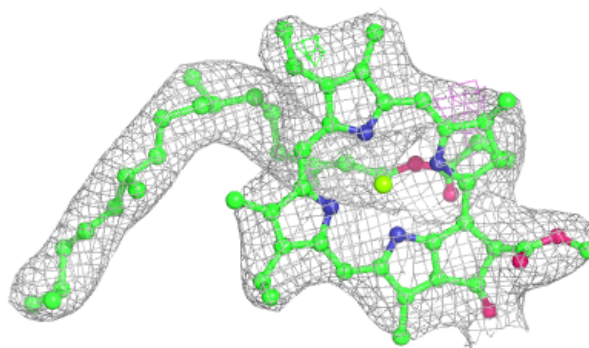


Electron density around CLA B 835:

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

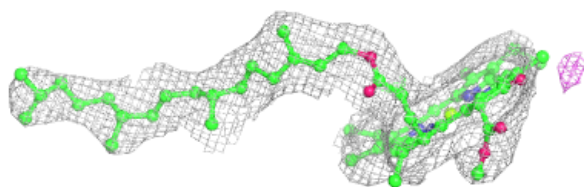
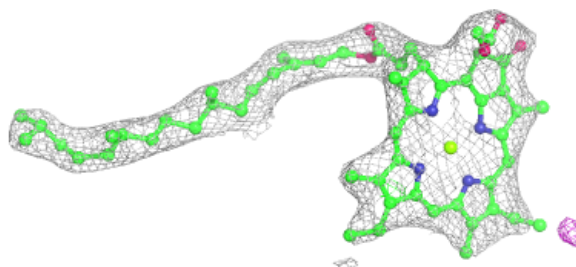
**Electron density around CLA B 836:**

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



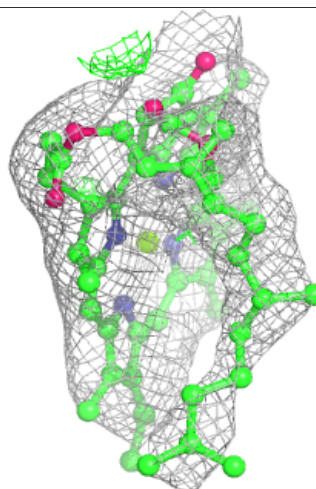
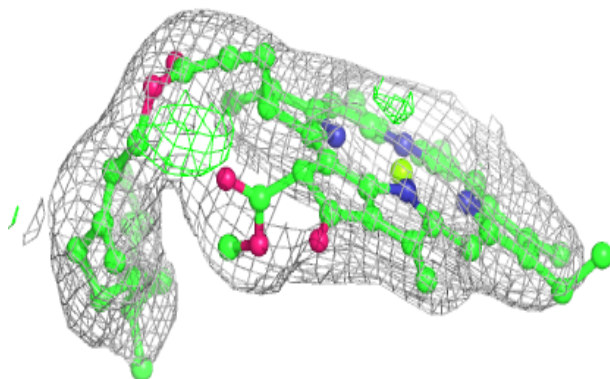
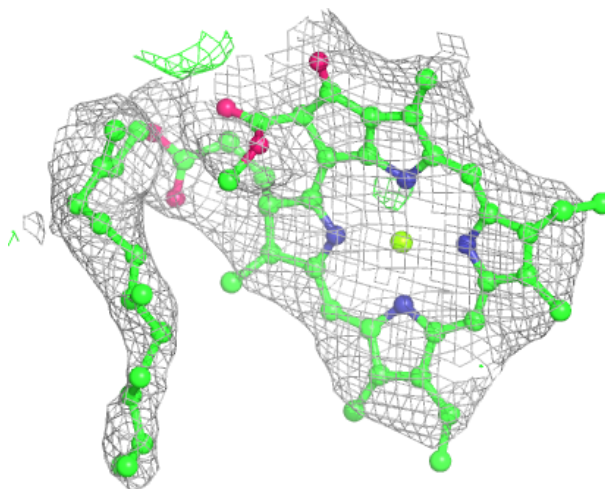
Electron density around CLA A 833:

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



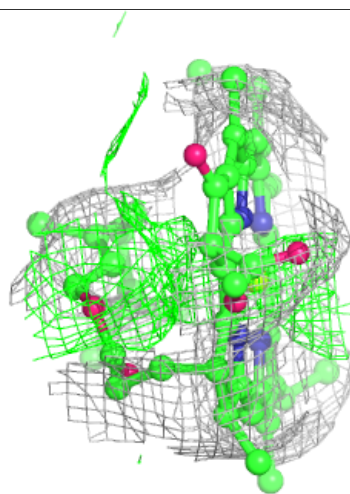
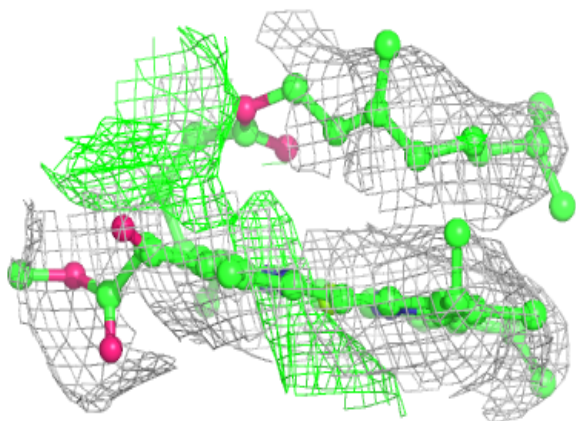
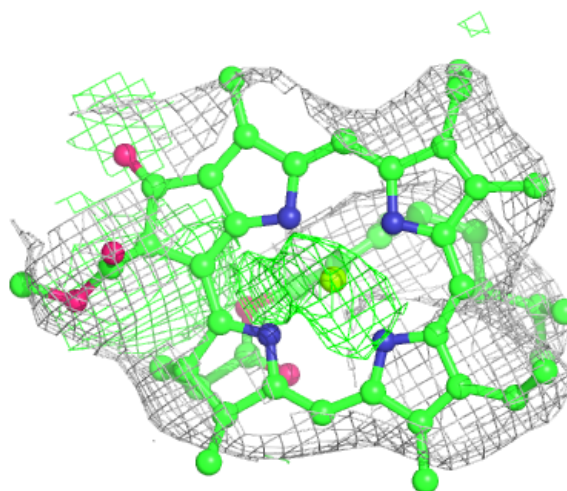
Electron density around CLA 4 308:

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



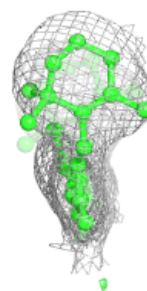
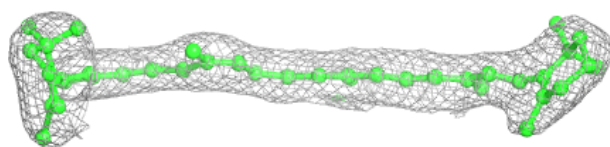
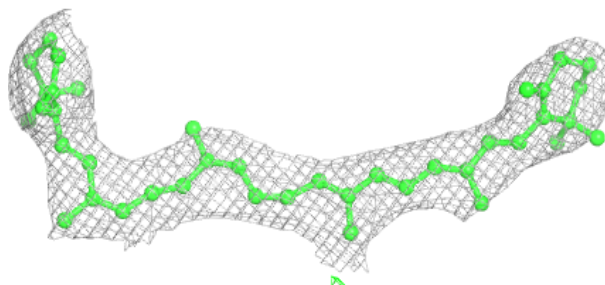
Electron density around CLA 1 506:

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

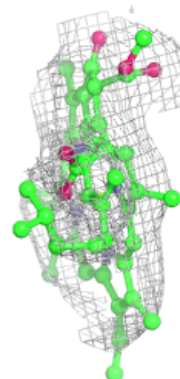
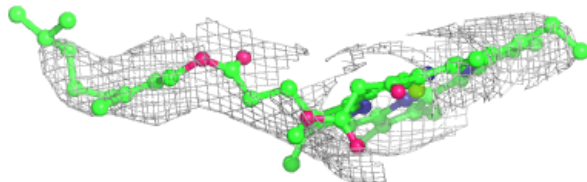
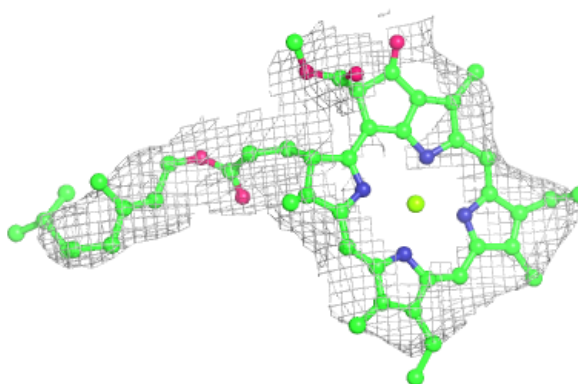


Electron density around BCR L 302:

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

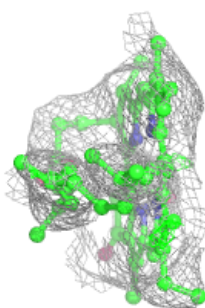
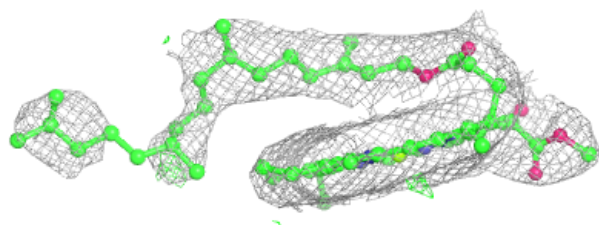
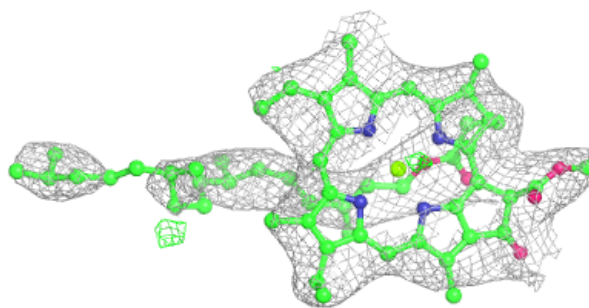
**Electron density around CLA G 202:**

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

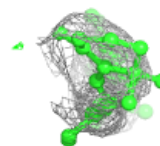
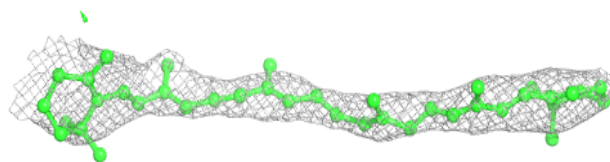
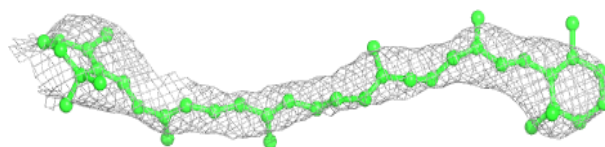


Electron density around CLA A 837:

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

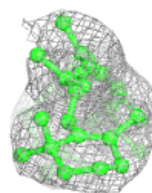
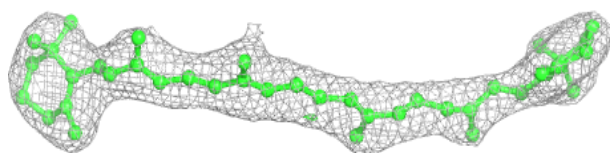
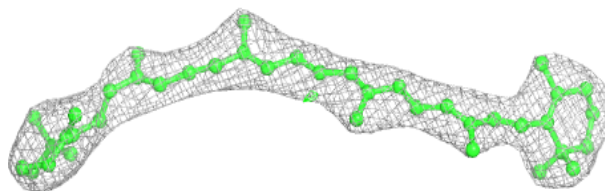
**Electron density around BCR 4 301:**

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



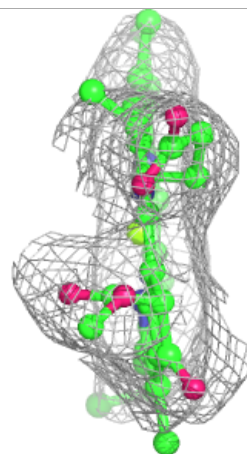
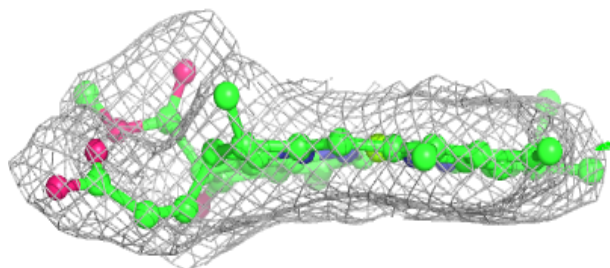
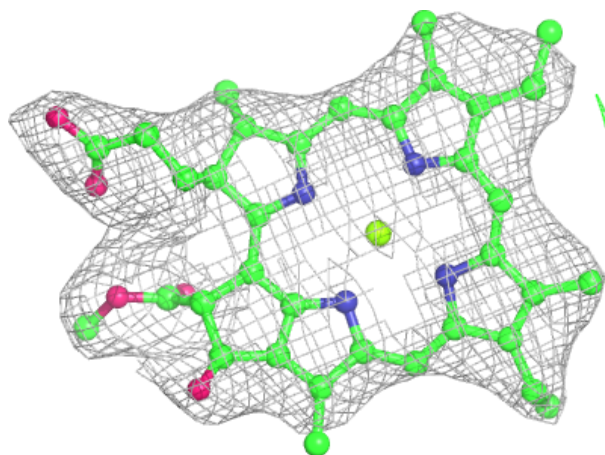
Electron density around BCR B 856:

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



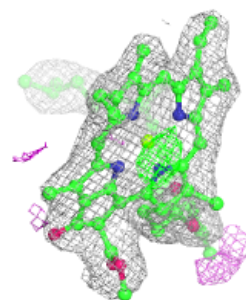
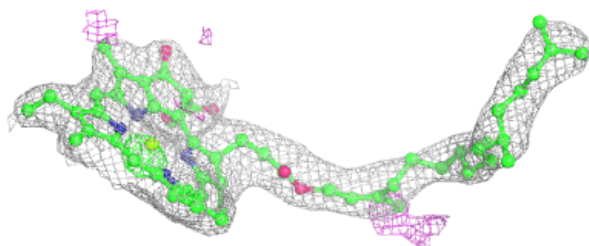
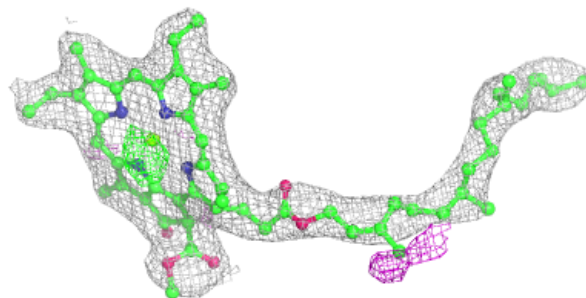
Electron density around CLA J 1102:

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



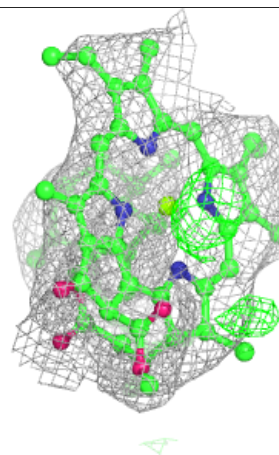
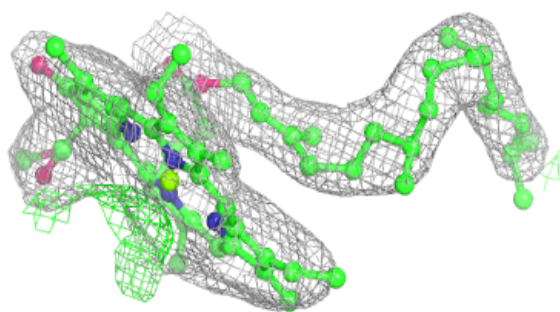
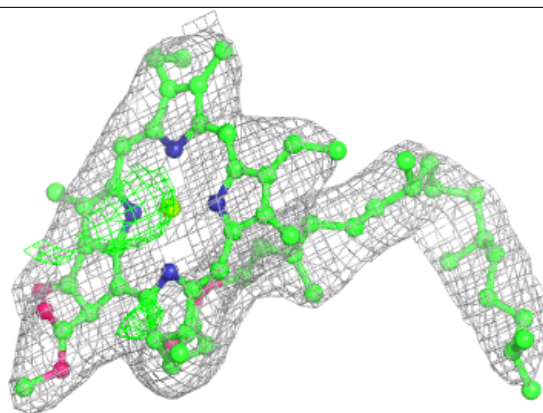
Electron density around CLA A 854:

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



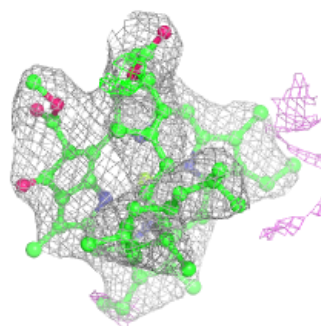
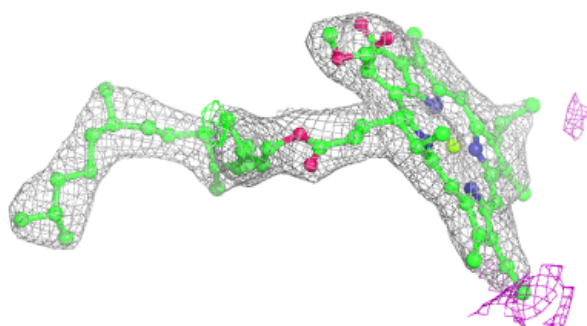
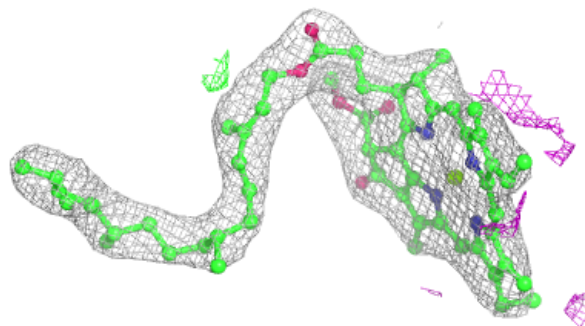
Electron density around CLA A 855:

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

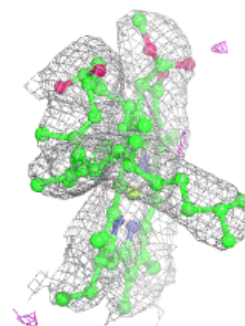
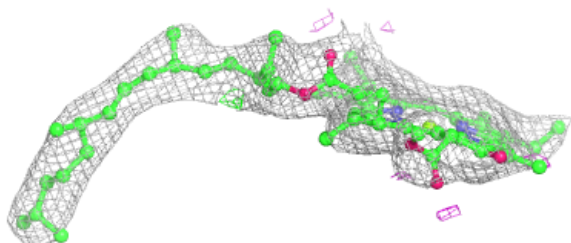
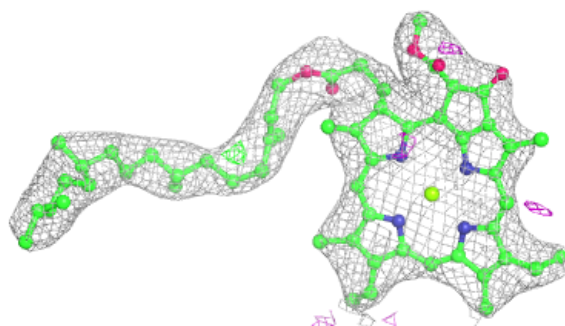


Electron density around CLA B 803:

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

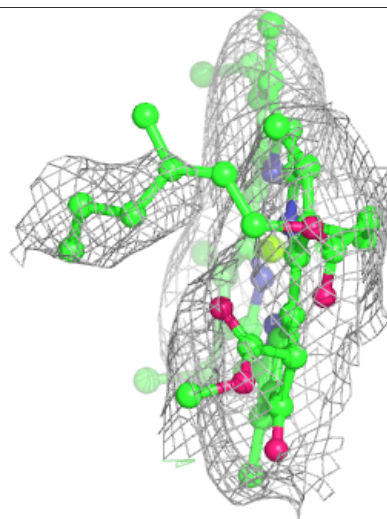
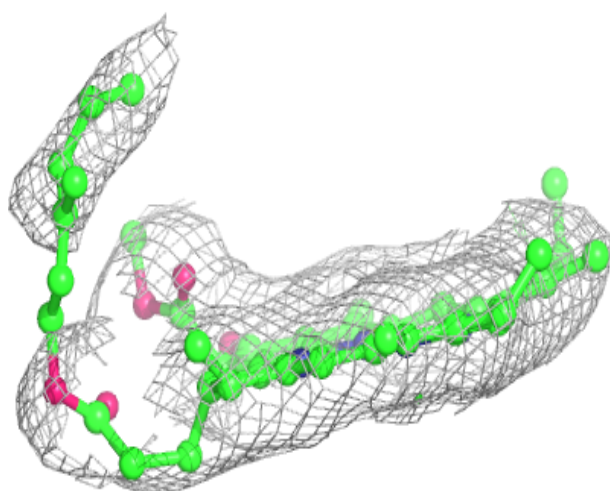
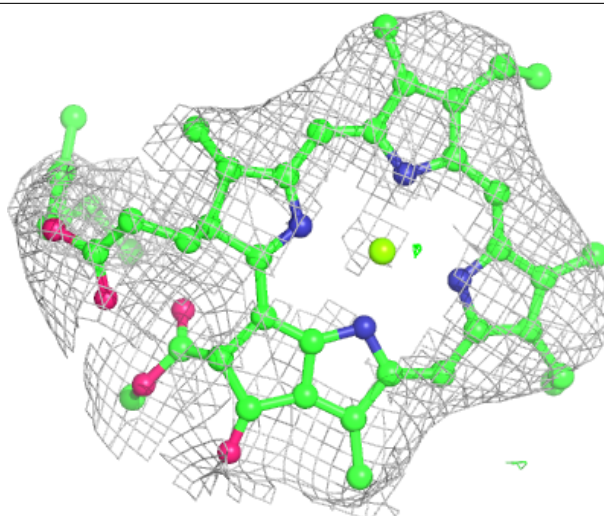
**Electron density around CLA B 804:**

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



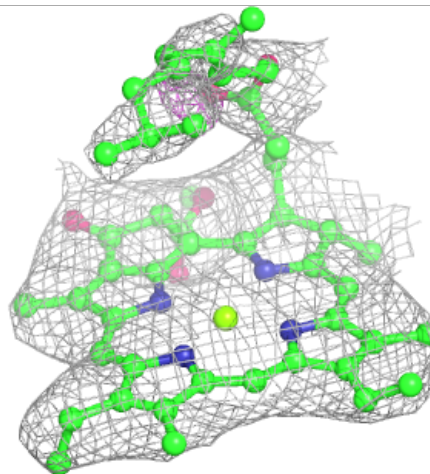
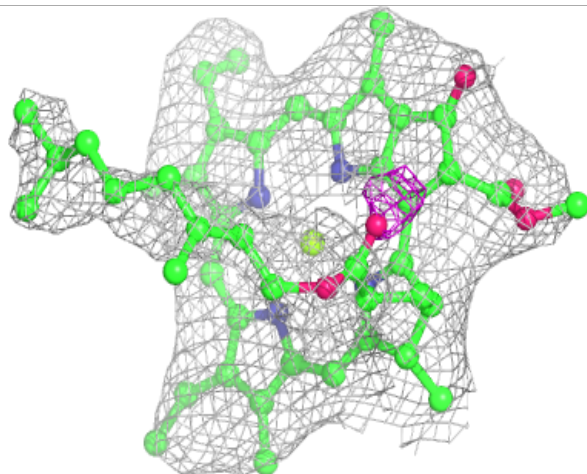
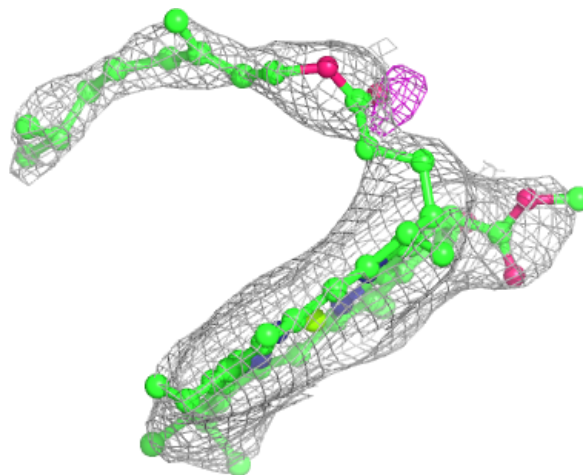
Electron density around CLA 2 505:

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



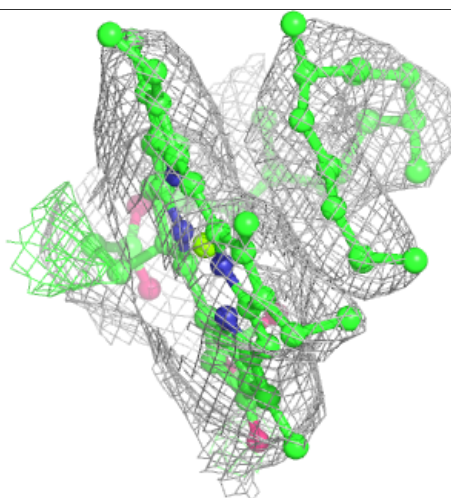
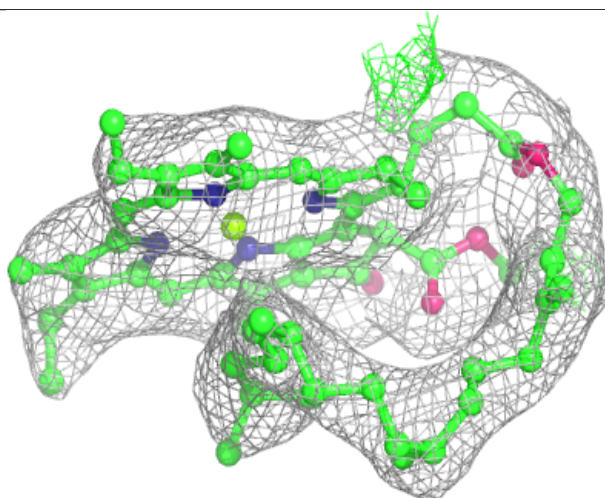
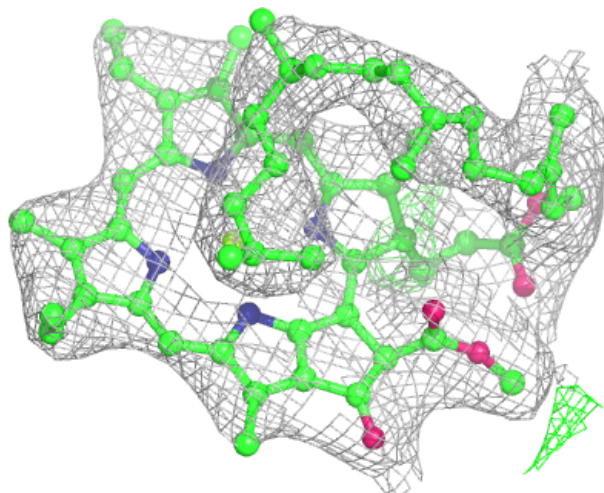
Electron density around CLA L 301:

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



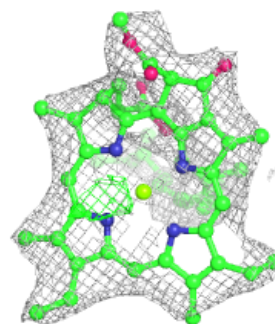
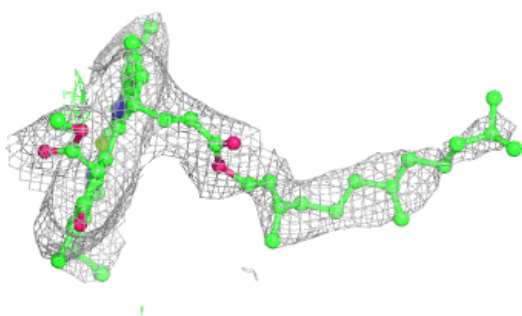
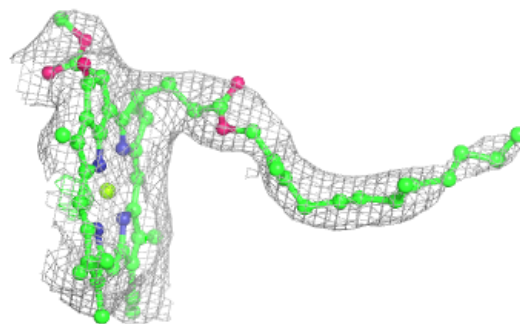
Electron density around CLA B 807:

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



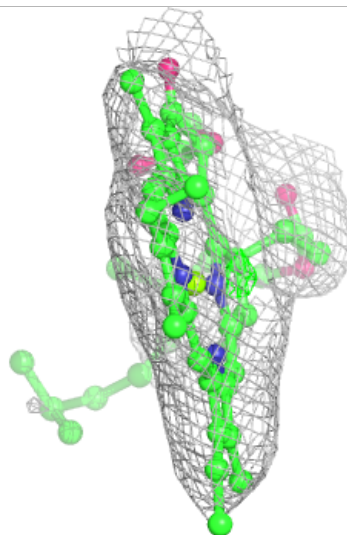
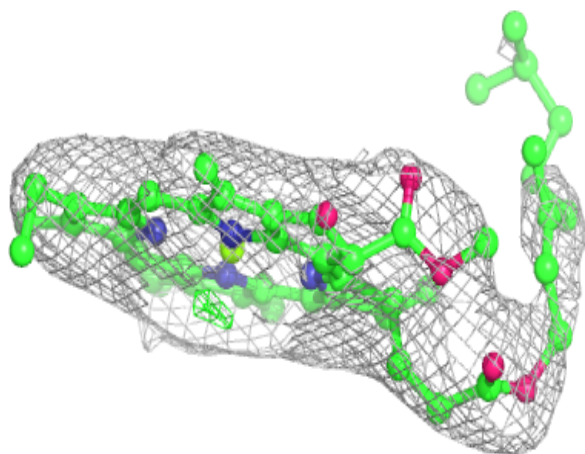
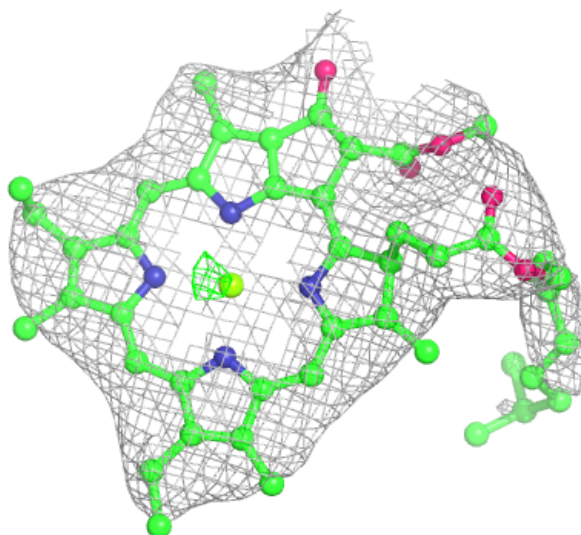
Electron density around CLA L 304:

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



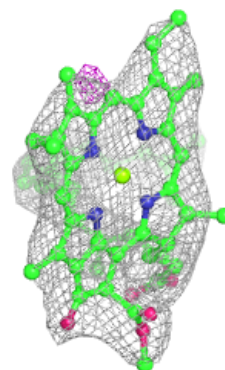
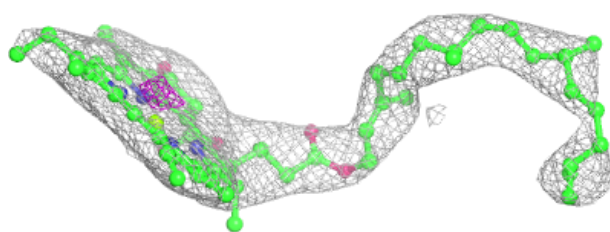
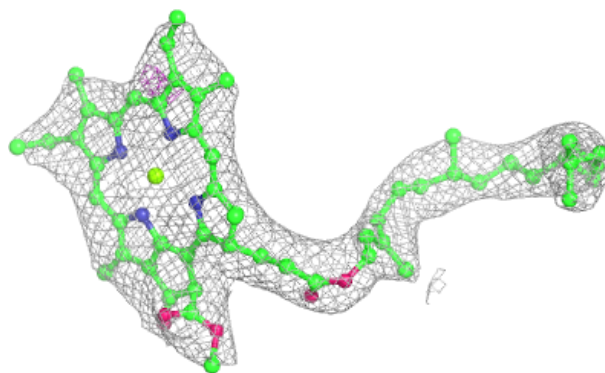
Electron density around CLA 2 508:

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



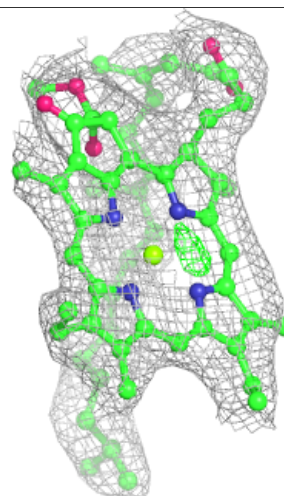
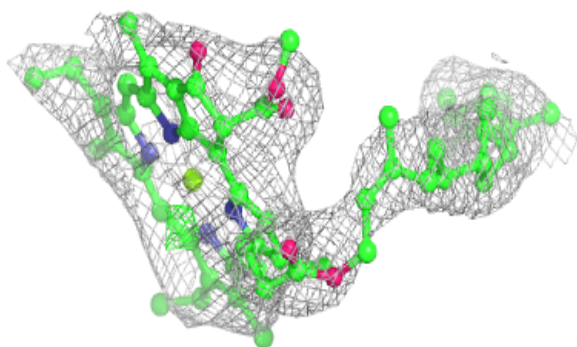
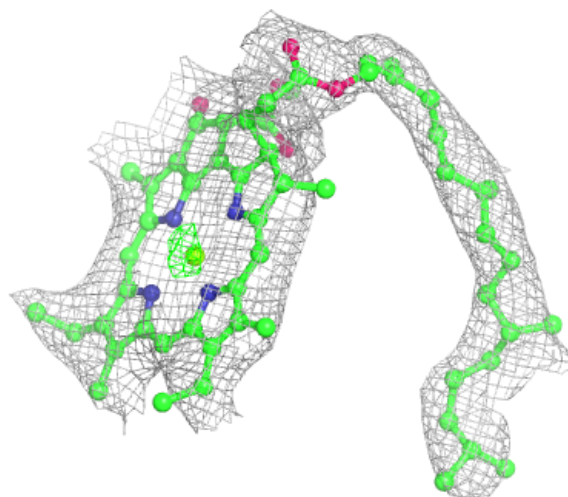
Electron density around CLA B 810:

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



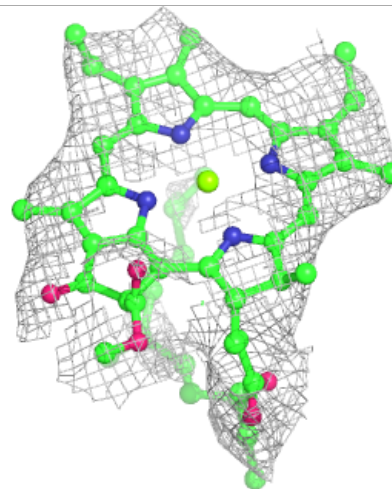
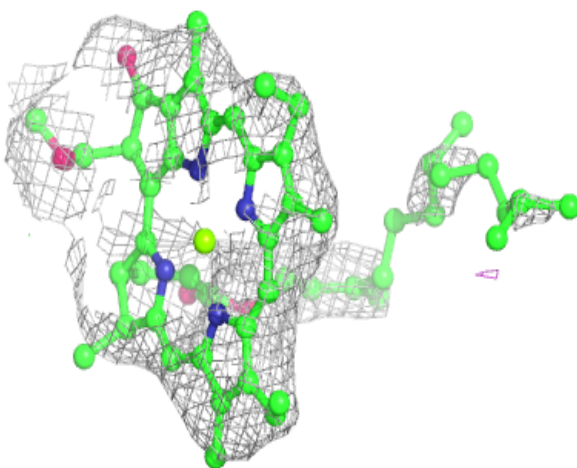
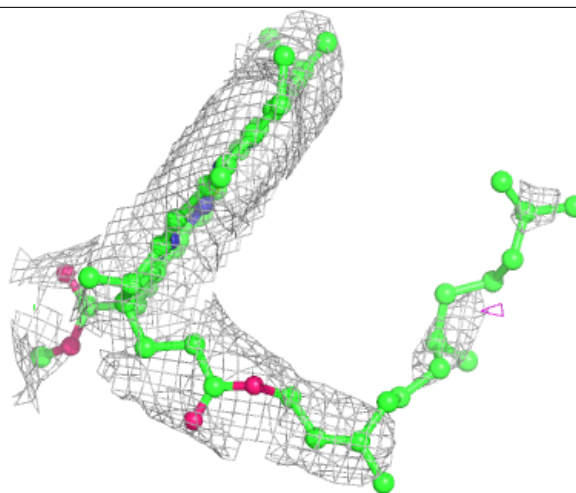
Electron density around CLA B 811:

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



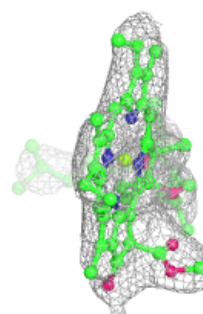
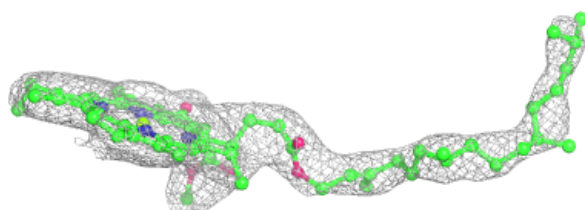
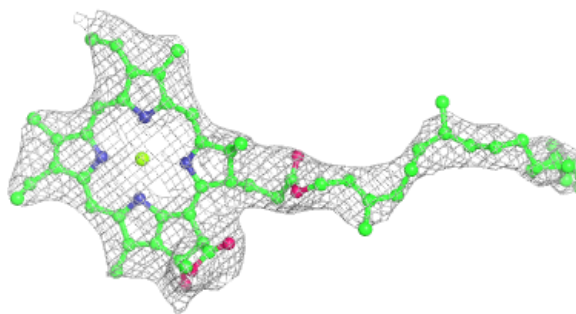
Electron density around CLA B 812:

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



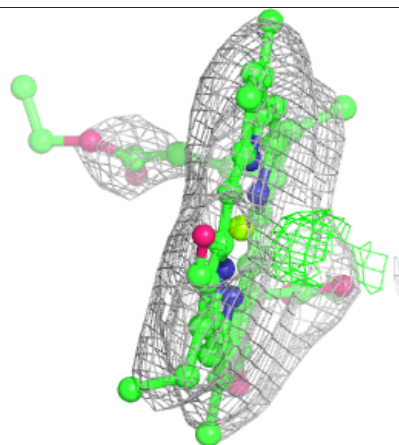
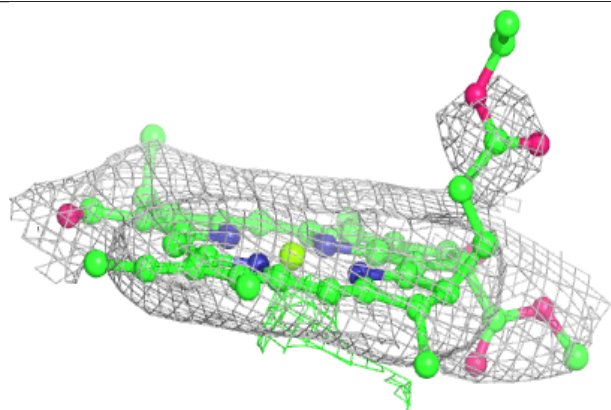
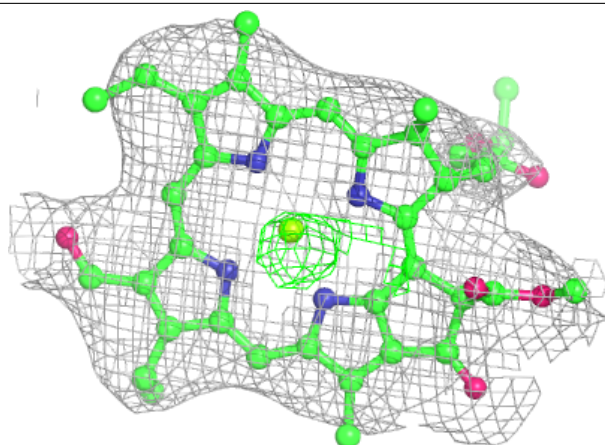
Electron density around CLA A 805:

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



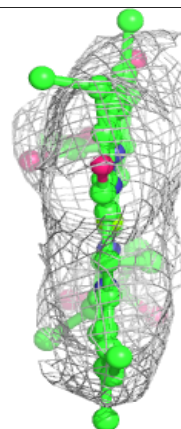
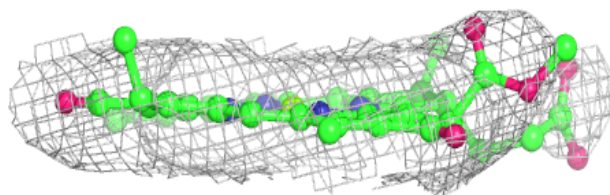
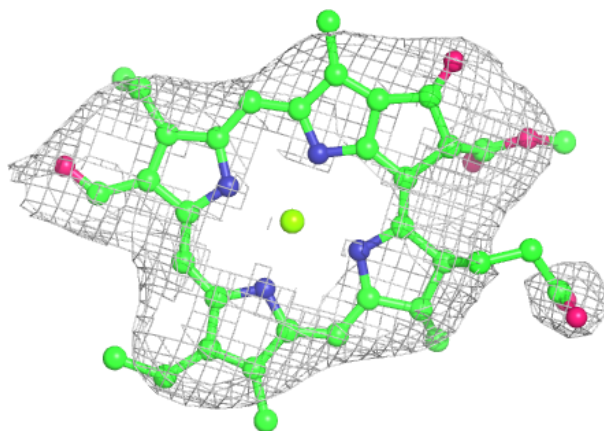
Electron density around CHL 2 513:

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

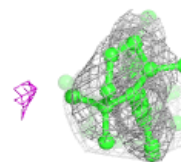
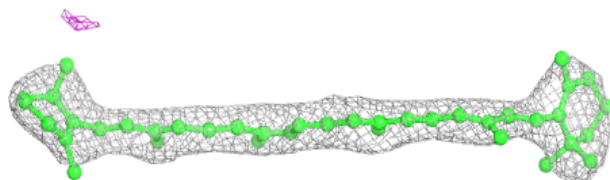
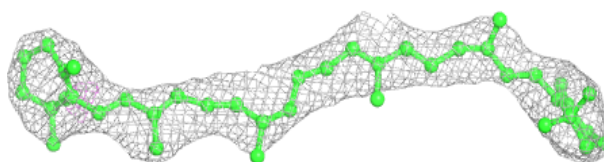


Electron density around CHL 2 515:

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

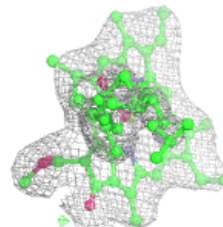
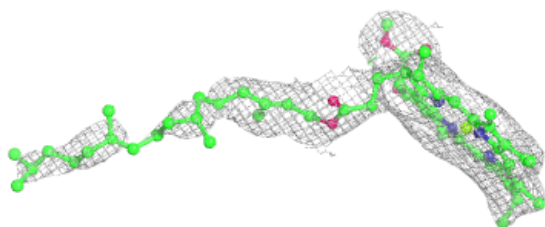
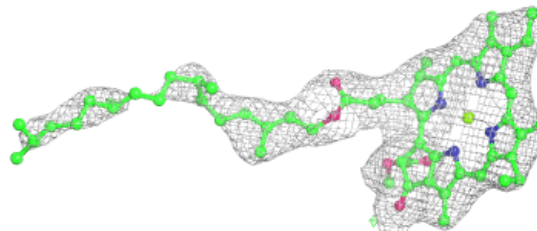
**Electron density around BCR B 802:**

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

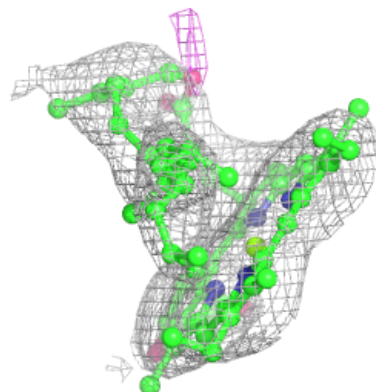
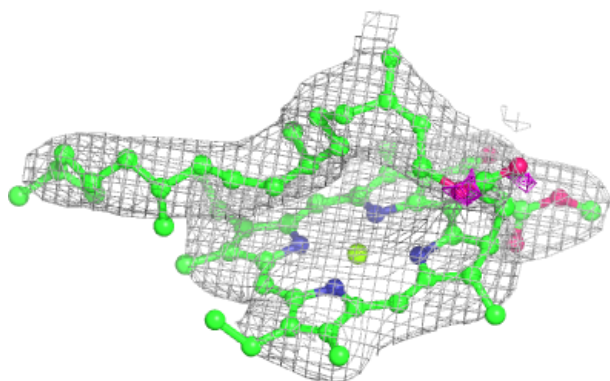
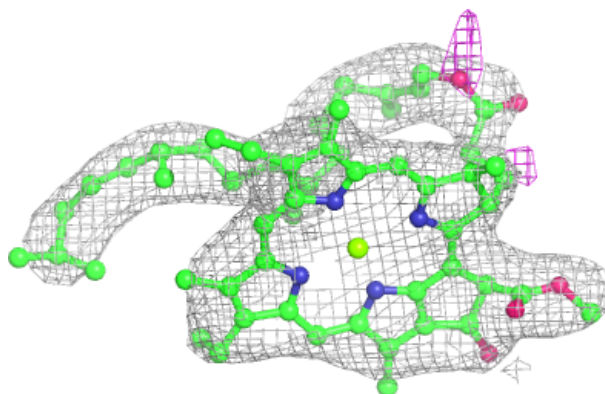


Electron density around CLA A 809:

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

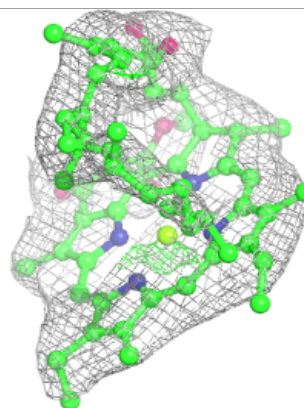
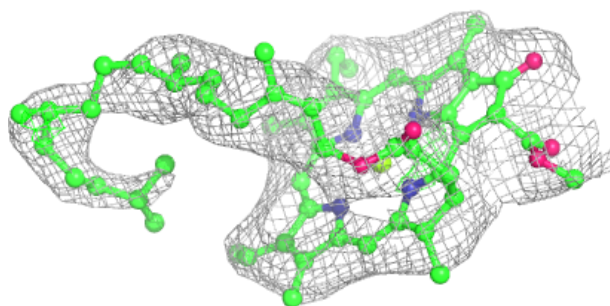
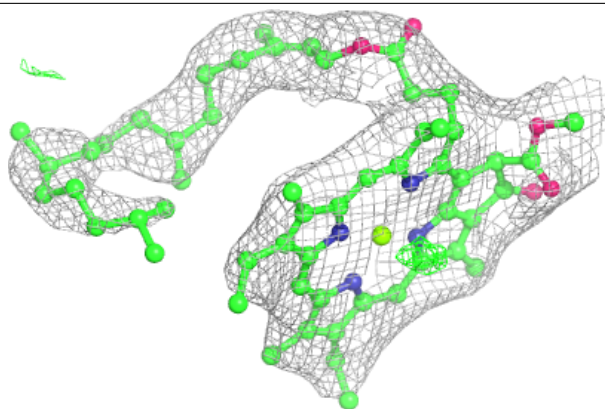
**Electron density around CLA B 818:**

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

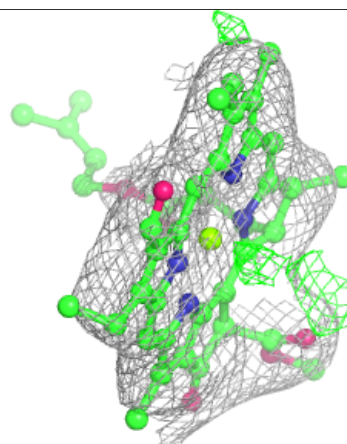
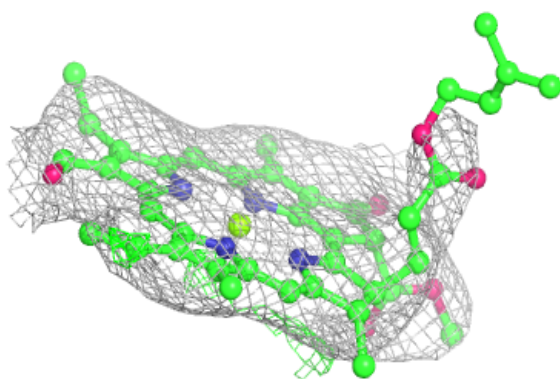
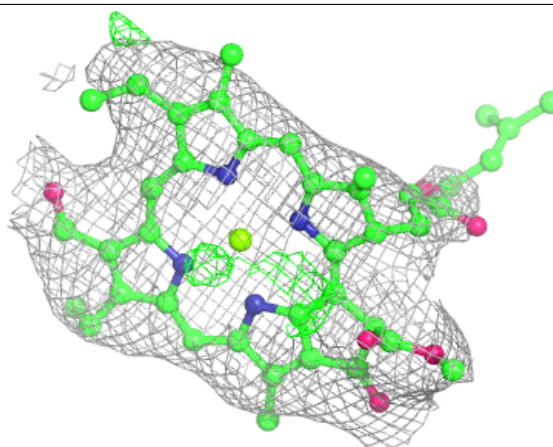


Electron density around CLA A 824:

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

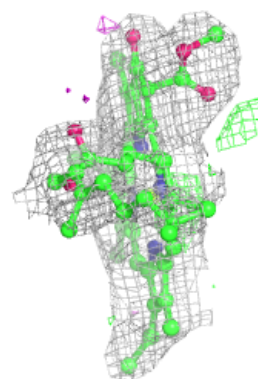
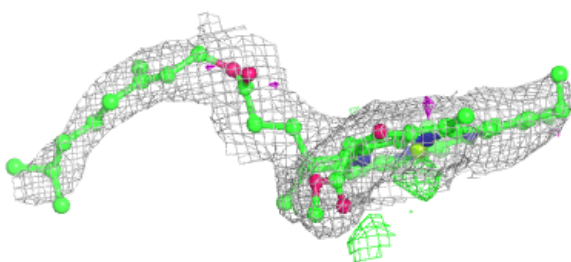
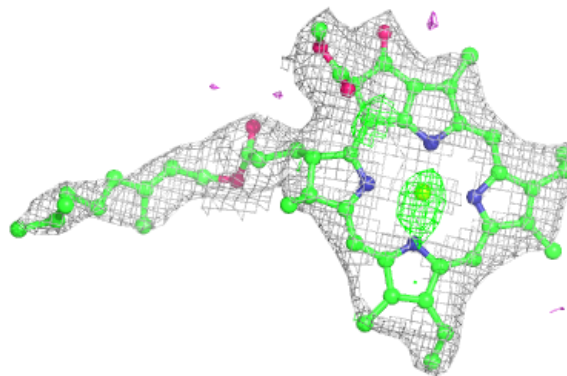
**Electron density around CHL 4 314:**

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

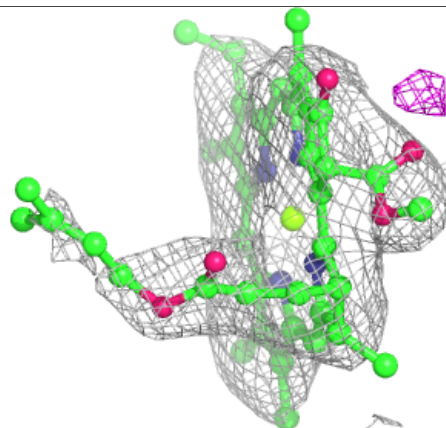
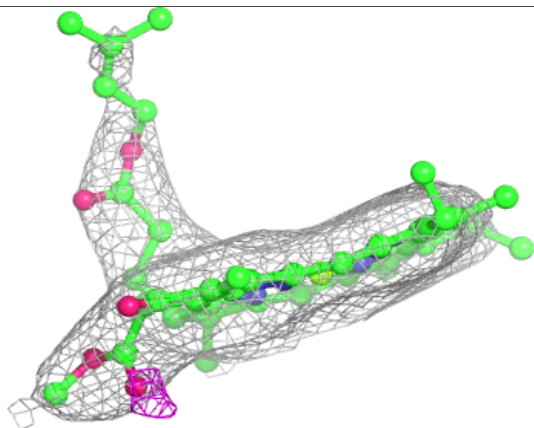
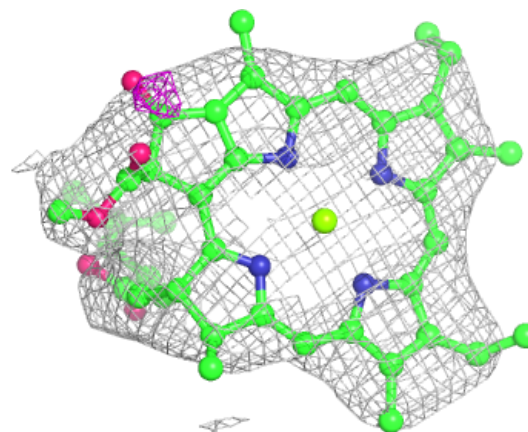


Electron density around CLA A 826:

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

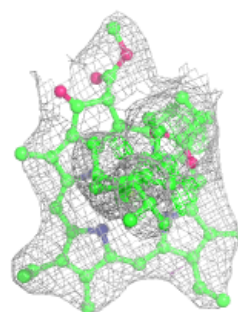
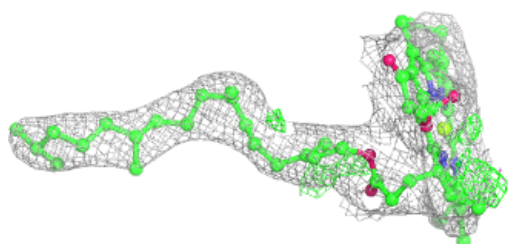
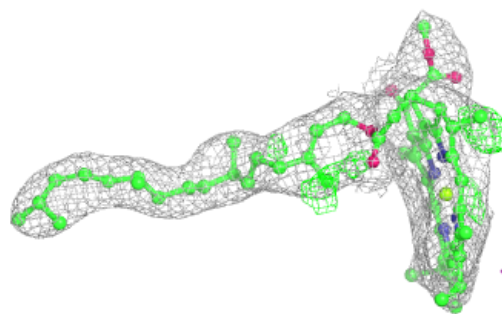
**Electron density around CLA A 810:**

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

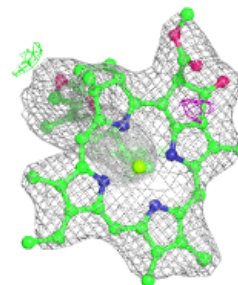
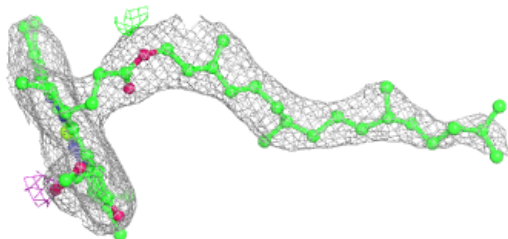
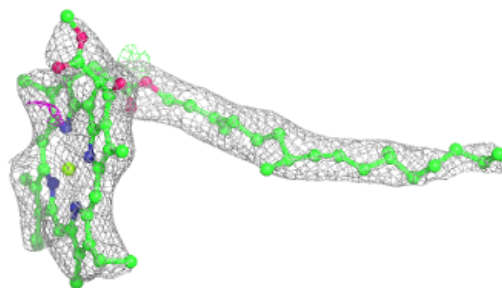


Electron density around CLA A 828:

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

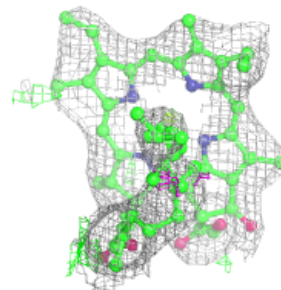
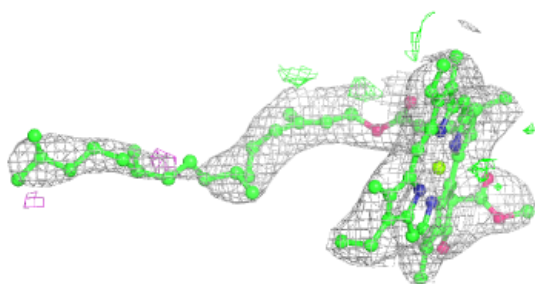
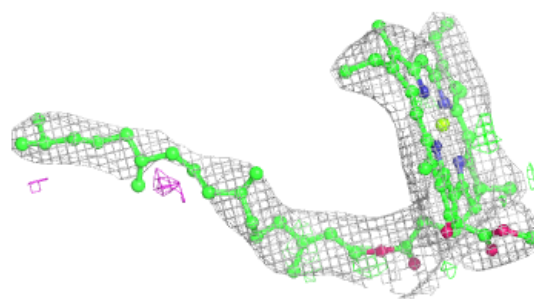
**Electron density around CLA B 828:**

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

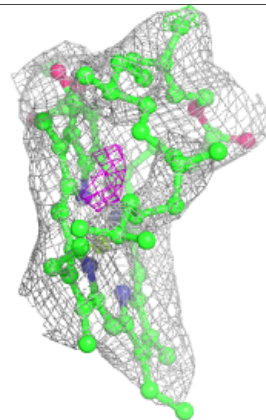
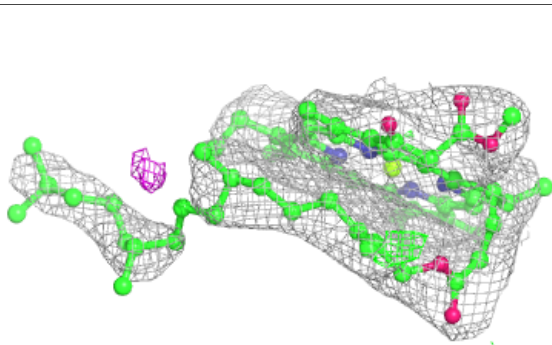
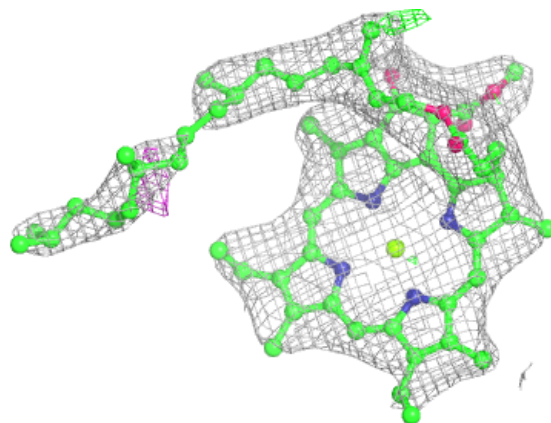


Electron density around CLA B 829:

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

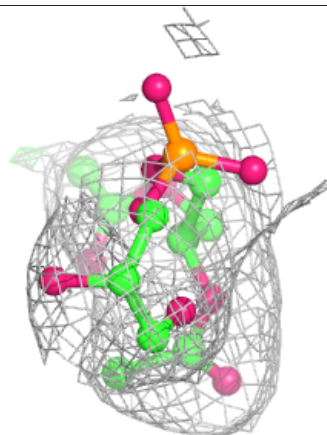
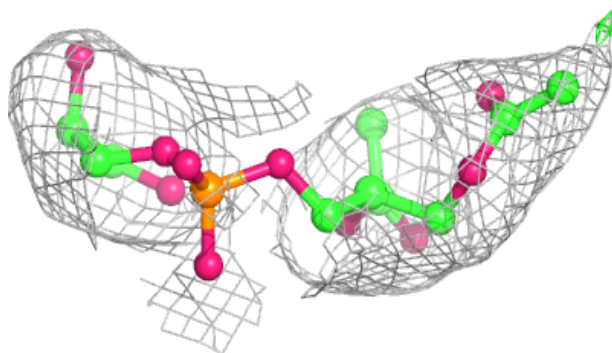
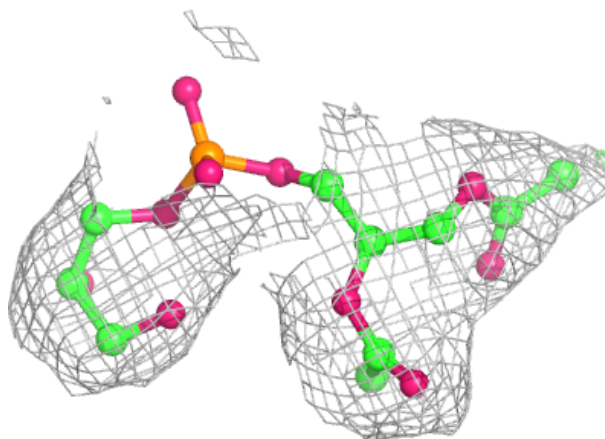
**Electron density around CLA A 829:**

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

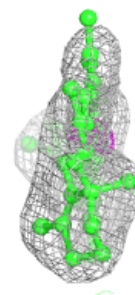
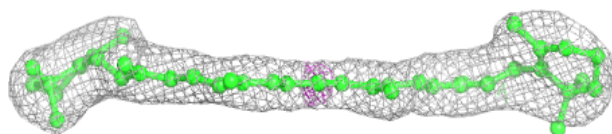
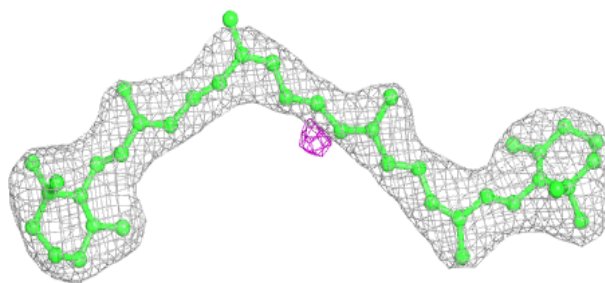


Electron density around LHG B 842:

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

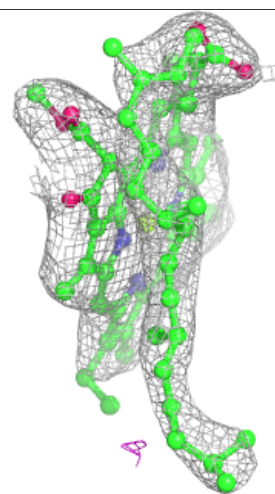
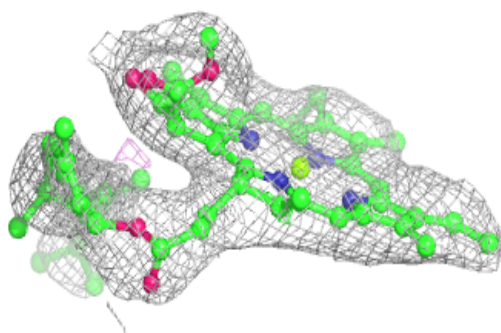
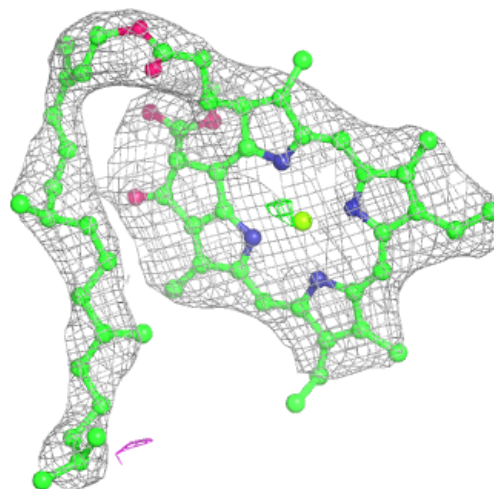
**Electron density around BCR A 852:**

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



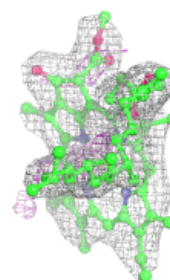
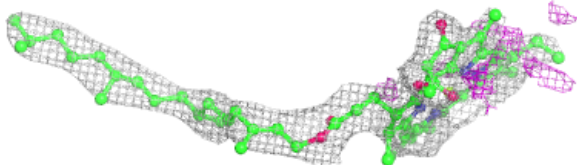
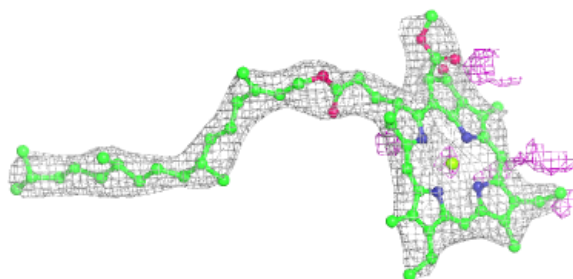
Electron density around CLA A 825:

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



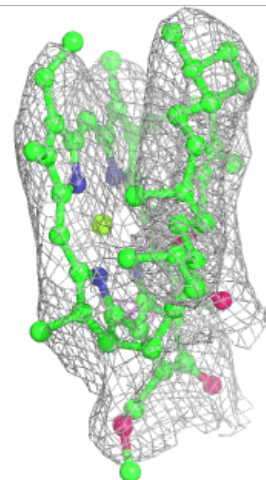
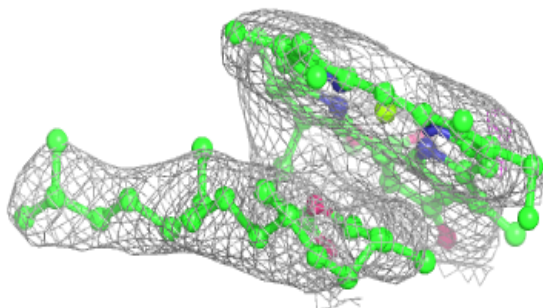
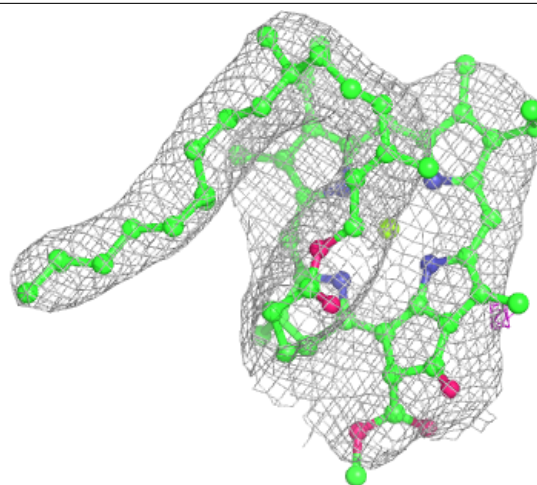
Electron density around CLA A 803:

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



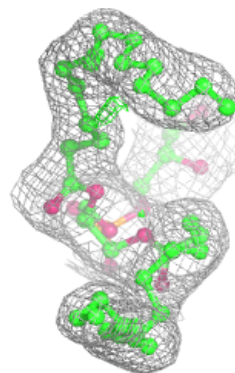
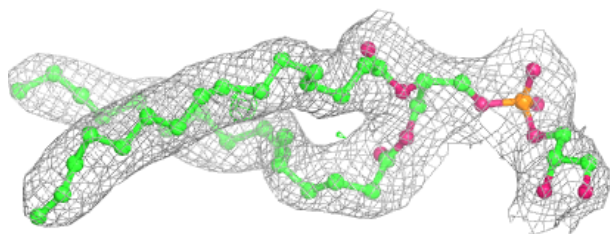
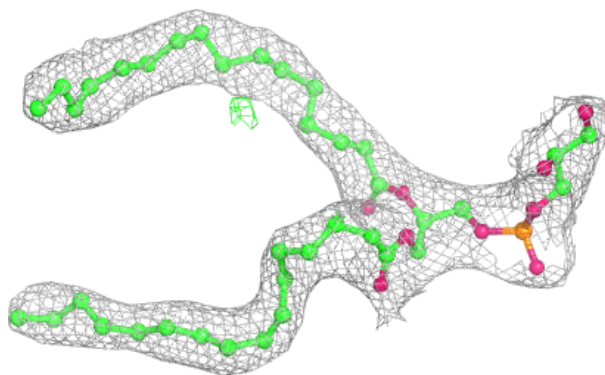
Electron density around CLA B 809:

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

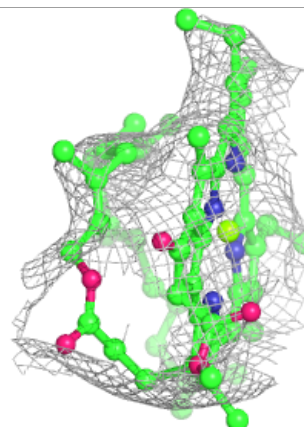
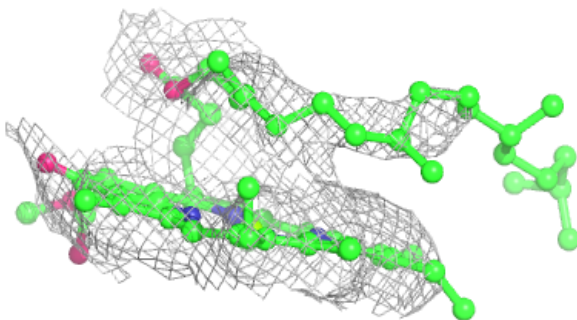
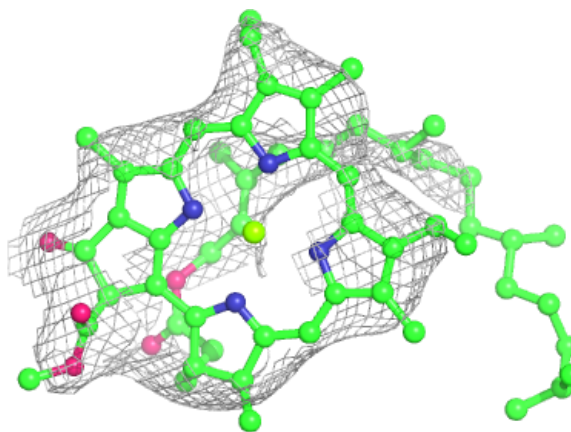


Electron density around LHG A 853:

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

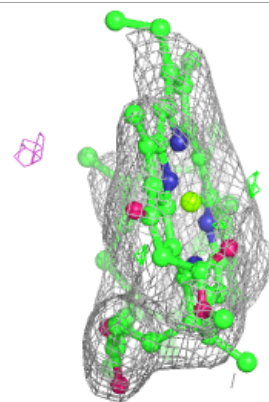
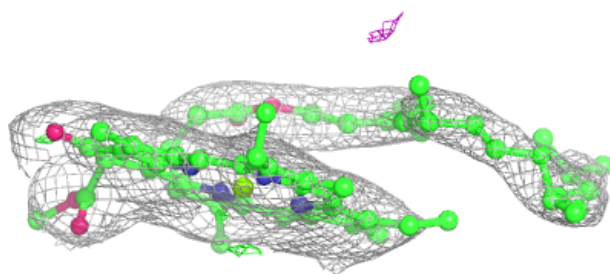
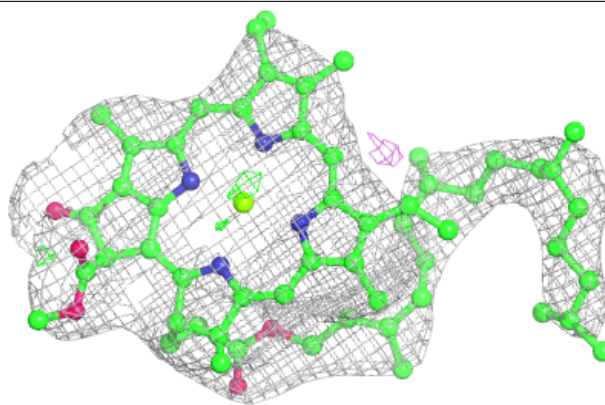
**Electron density around CLA 2 506:**

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

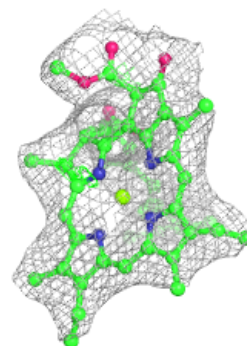
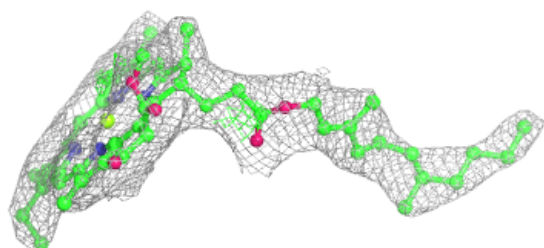
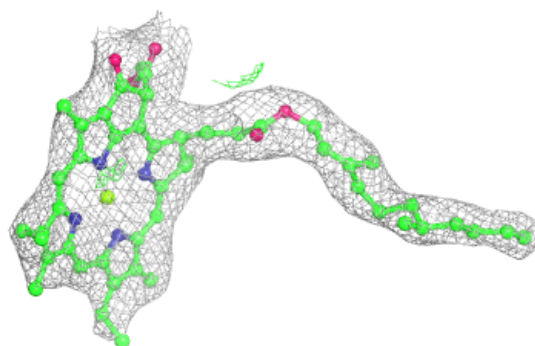


Electron density around CLA A 819:

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

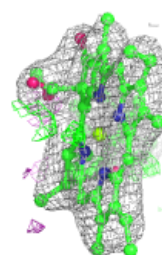
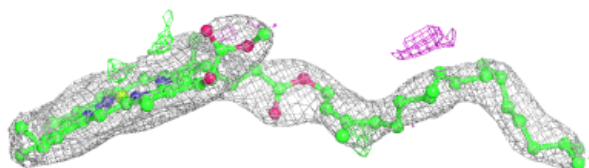
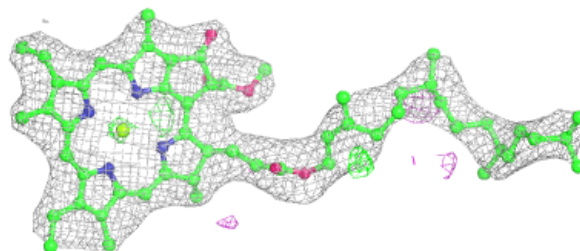
**Electron density around CLA B 832:**

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



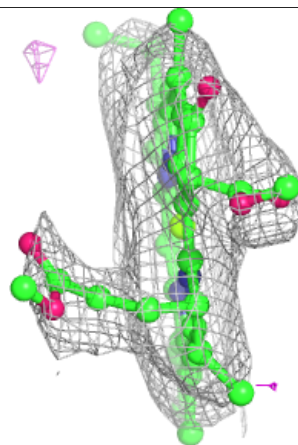
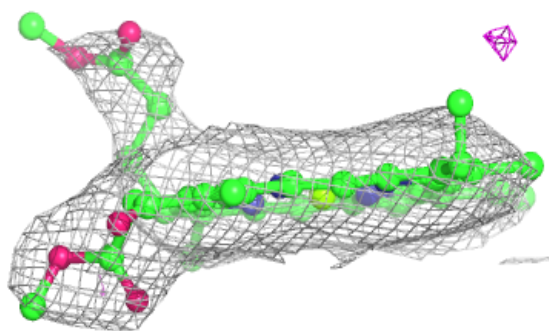
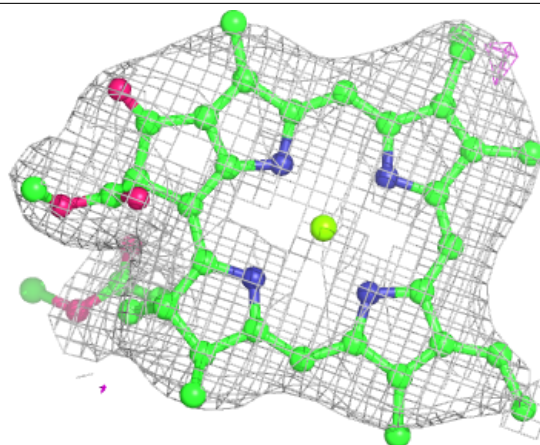
Electron density around CLA A 840:

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



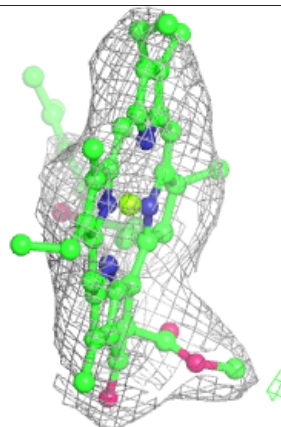
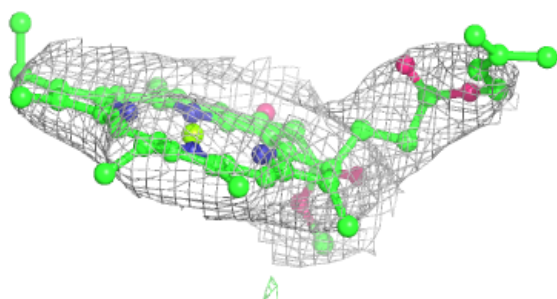
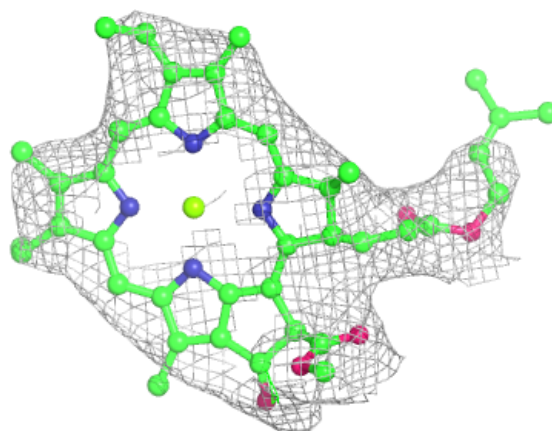
Electron density around CLA B 813:

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

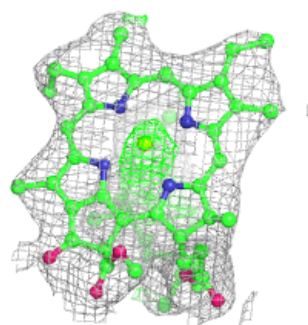
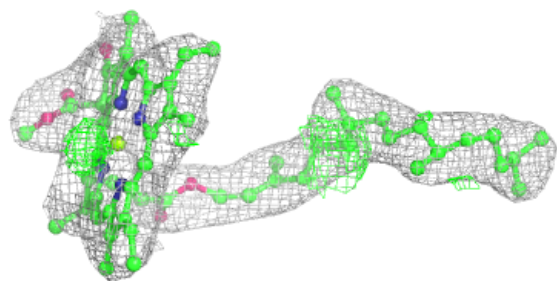
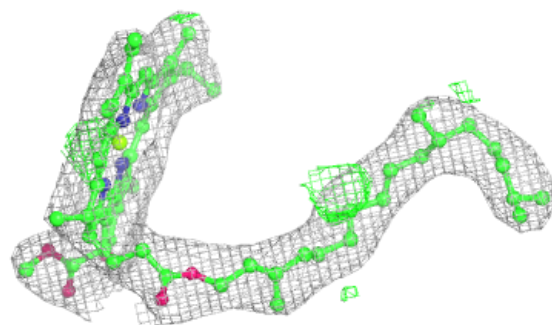


Electron density around CLA 4 312:

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

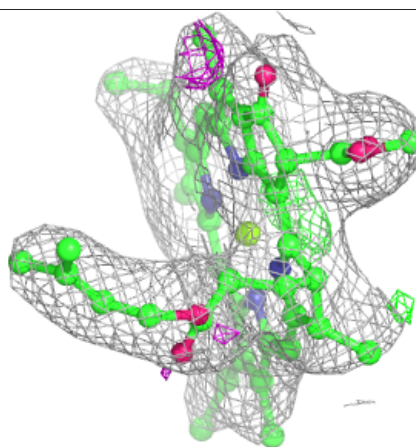
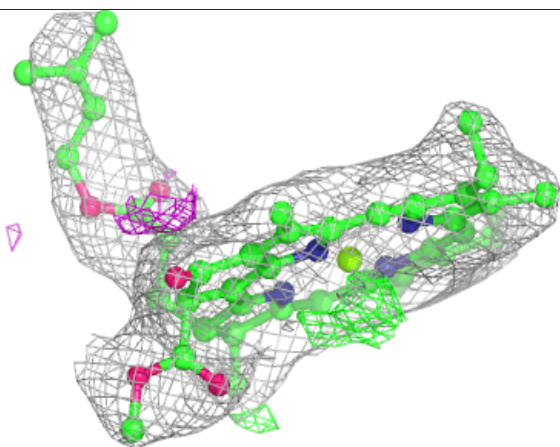
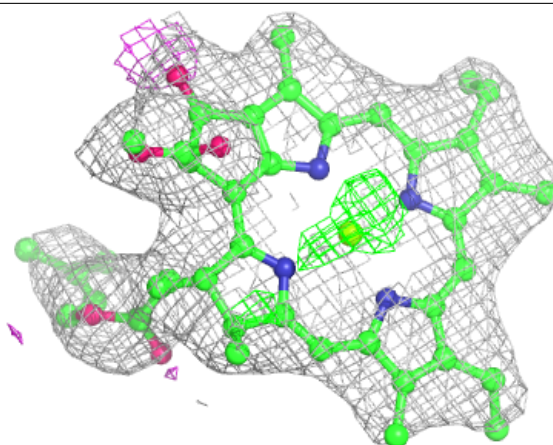
**Electron density around CLA A 830:**

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



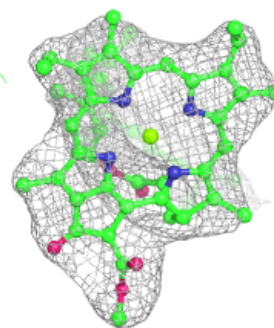
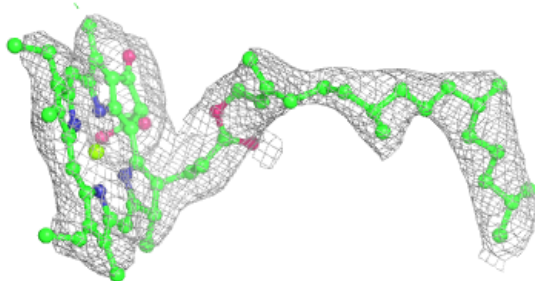
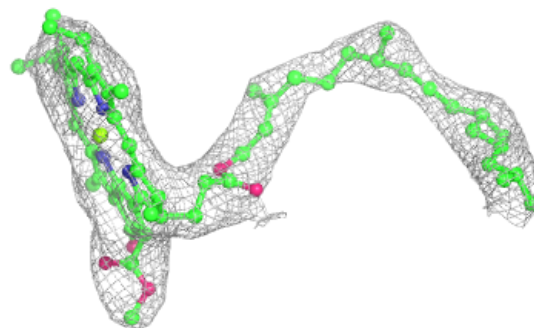
Electron density around CLA B 837:

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



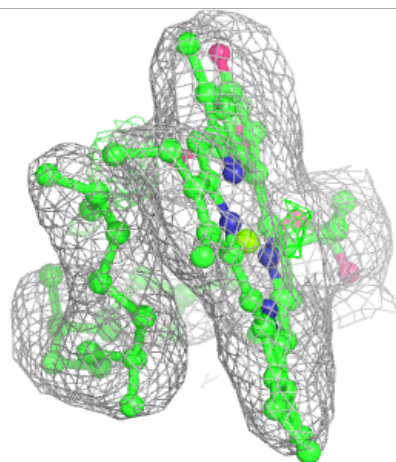
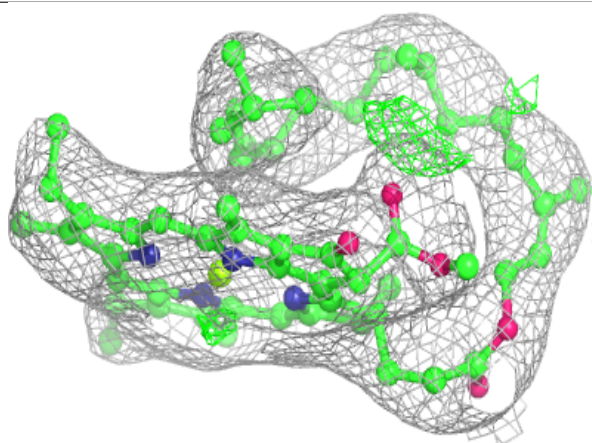
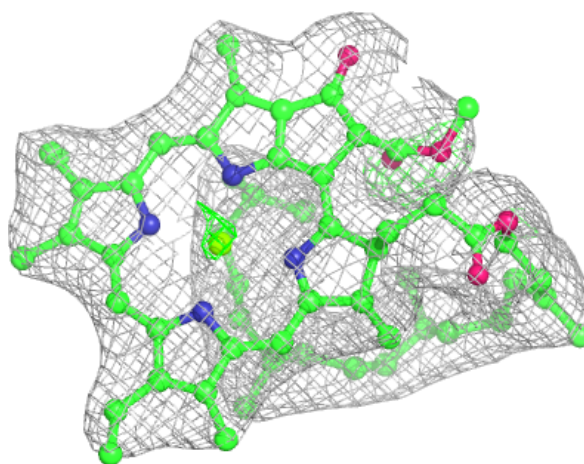
Electron density around CLA B 838:

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



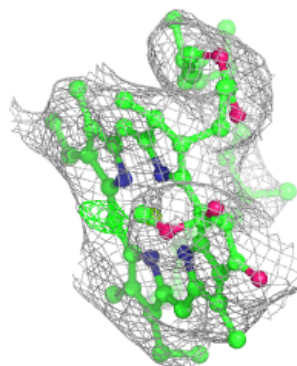
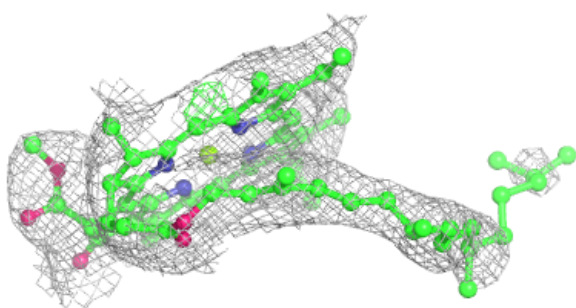
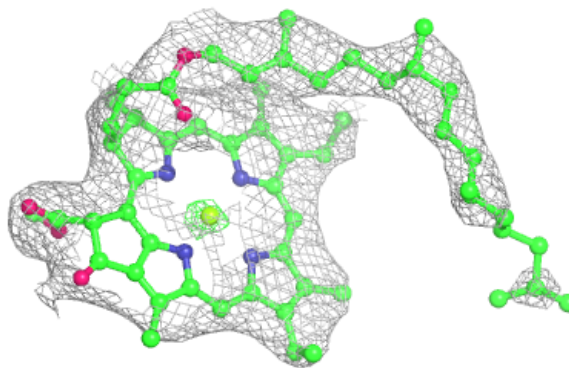
Electron density around CLA A 806:

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

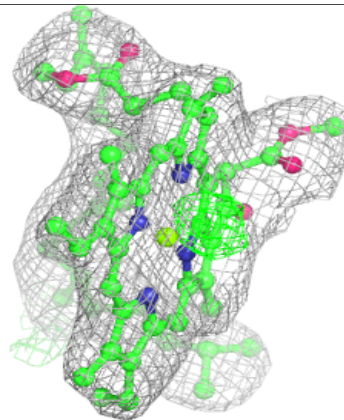
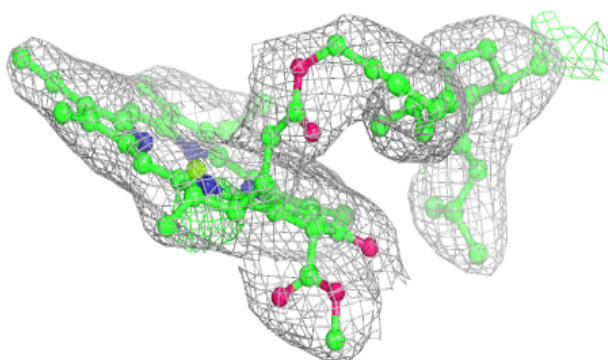
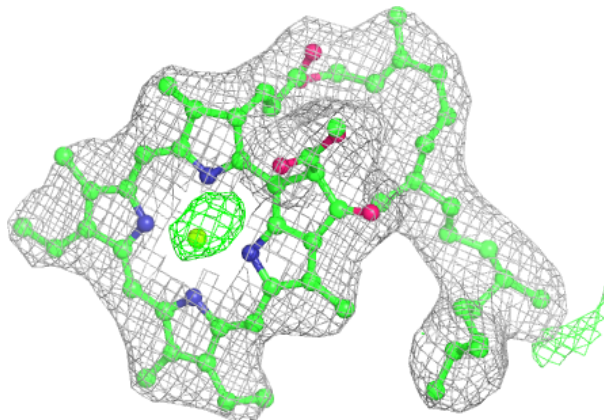


Electron density around CLA 2 507:

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

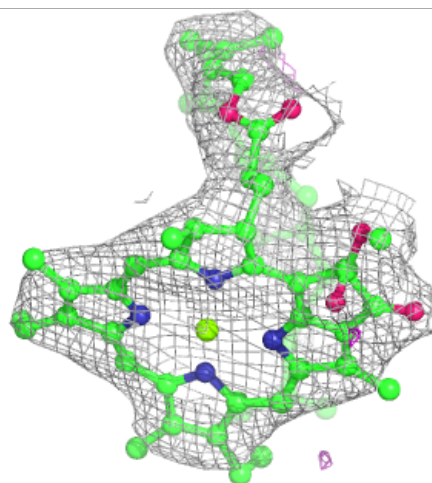
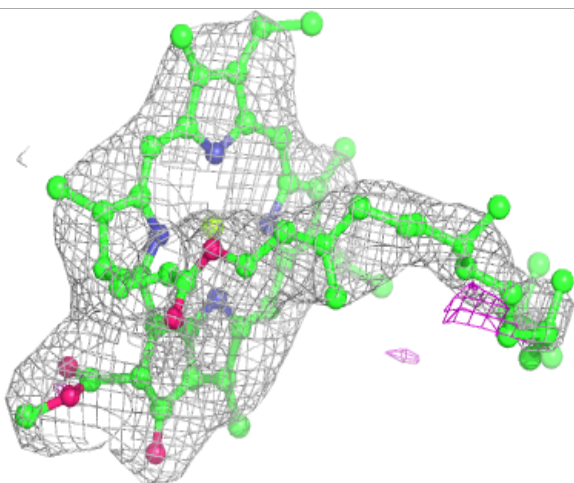
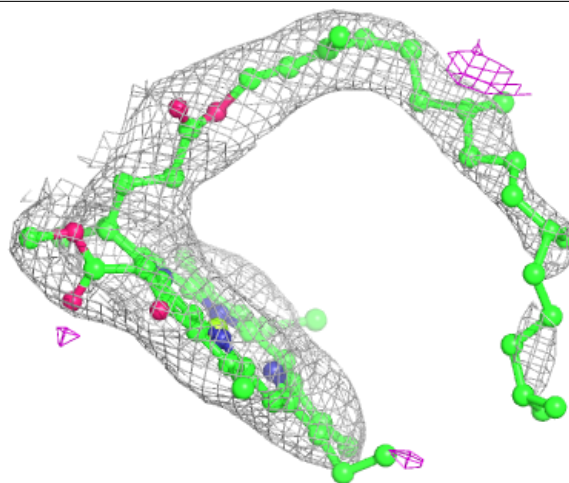
**Electron density around CLA F 302:**

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



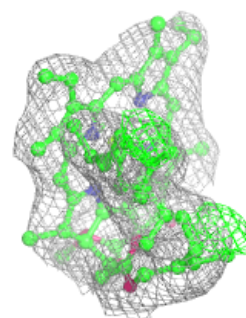
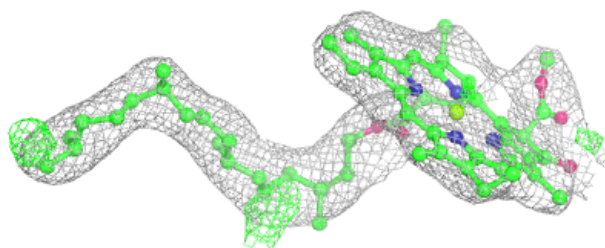
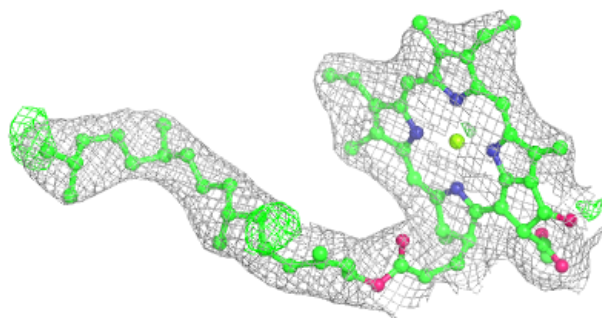
Electron density around CLA B 820:

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

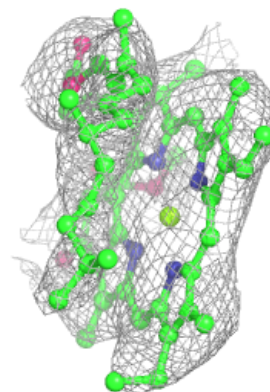
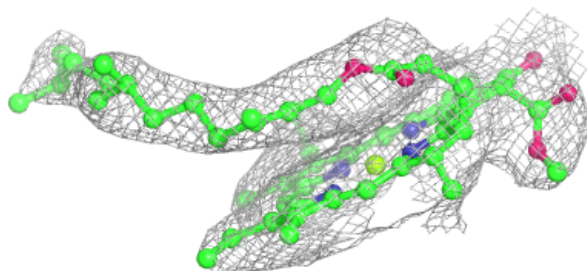
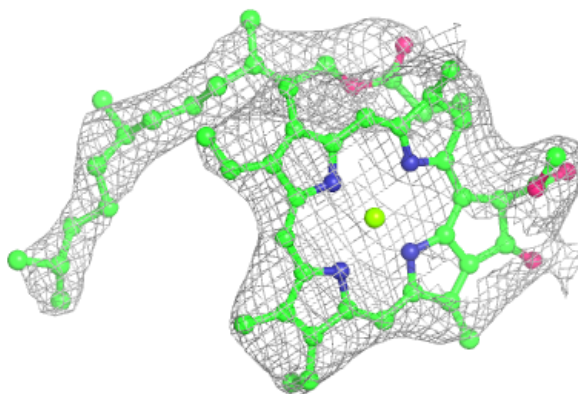


Electron density around CLA A 808:

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

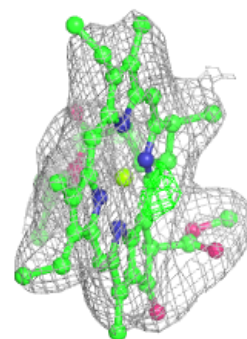
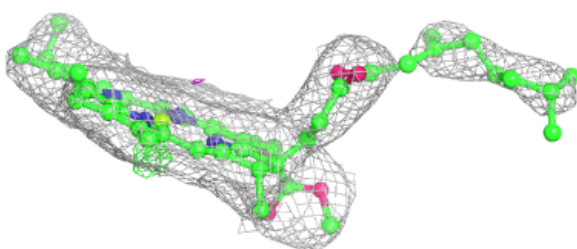
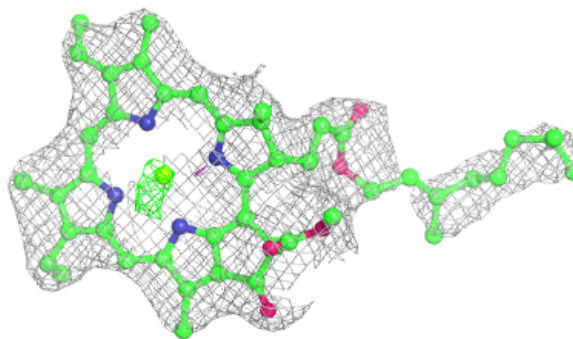
**Electron density around CLA 4 307:**

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

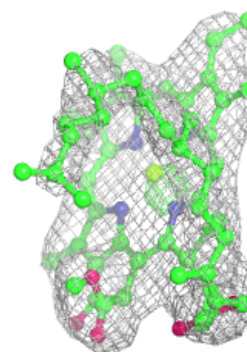
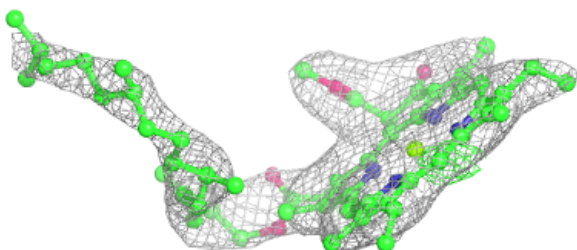
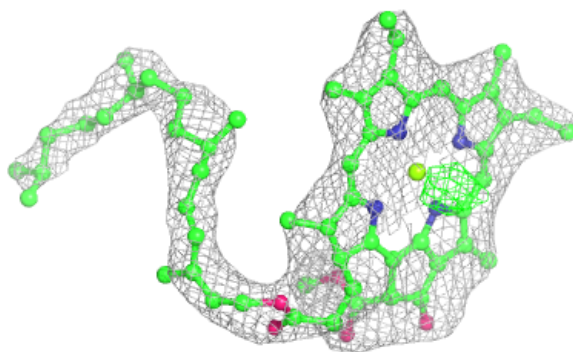


Electron density around CLA B 823:

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

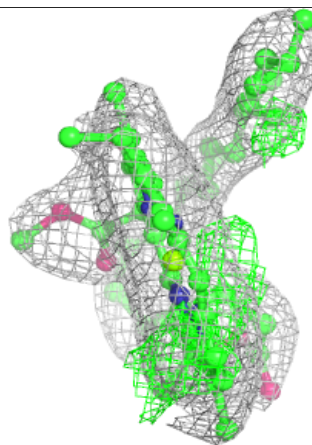
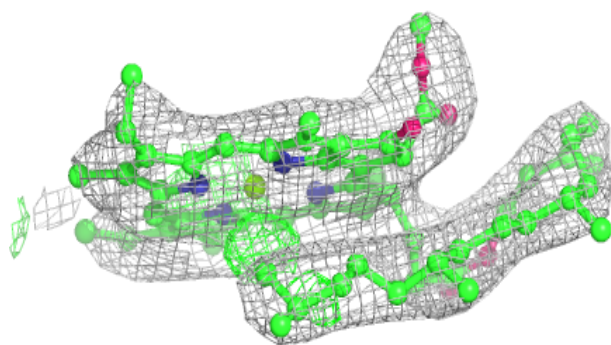
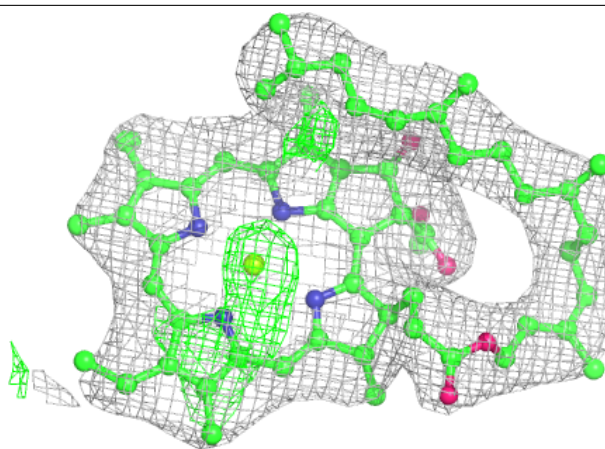
**Electron density around CLA B 824:**

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

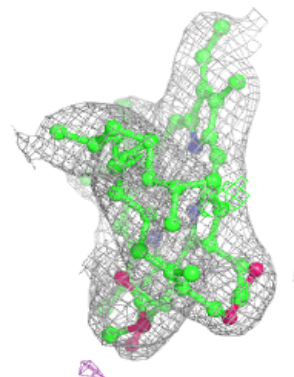
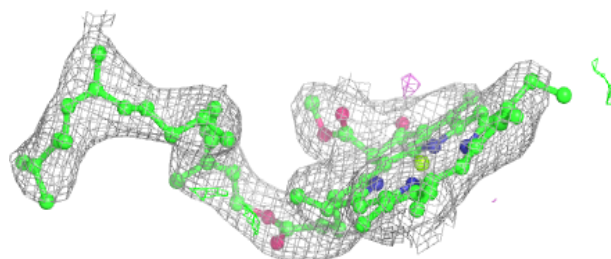
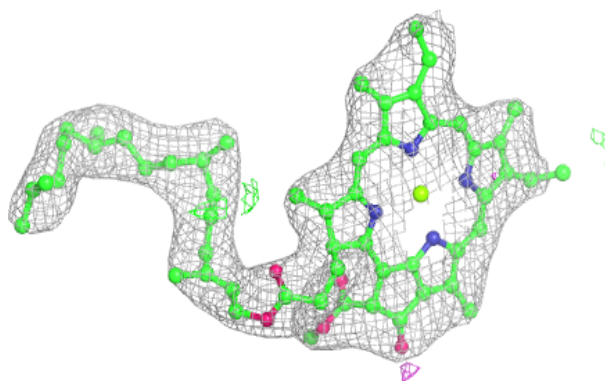


Electron density around CLA B 806:

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

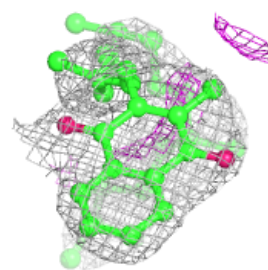
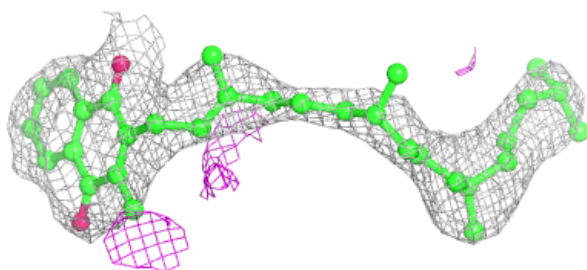
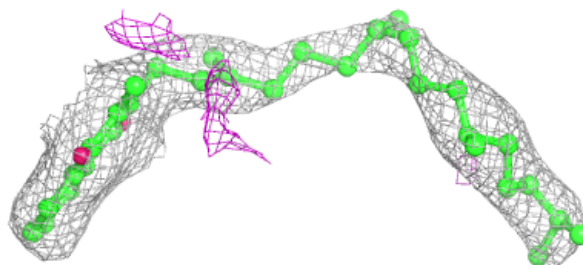
**Electron density around CLA J 1101:**

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

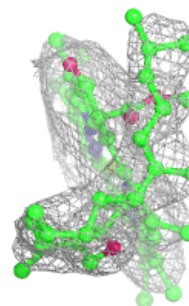
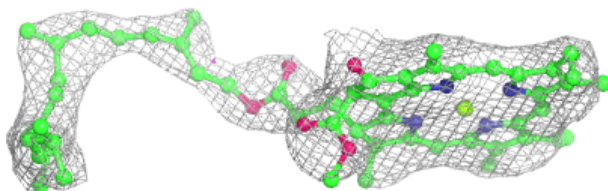
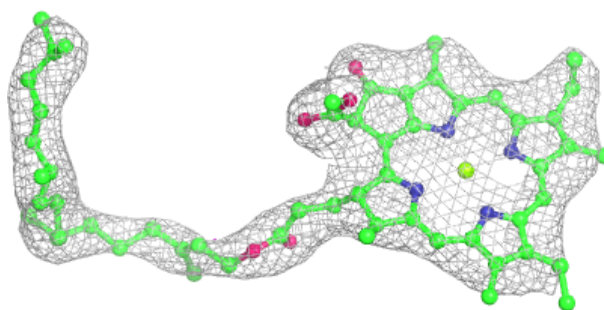


Electron density around PQN B 841:

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

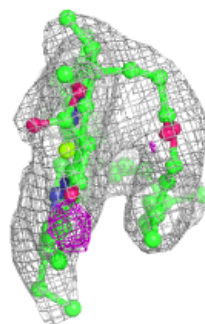
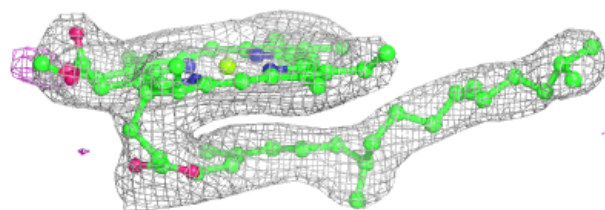
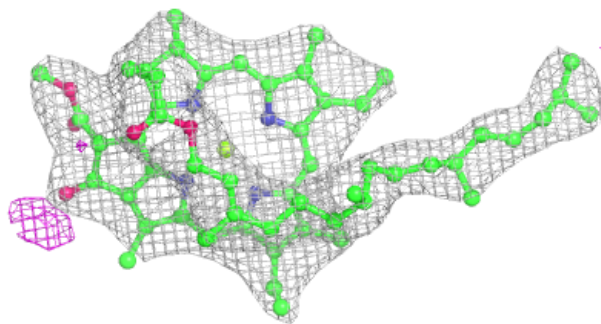
**Electron density around CLA B 826:**

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

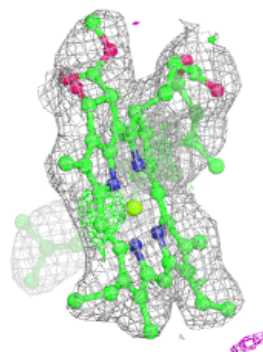
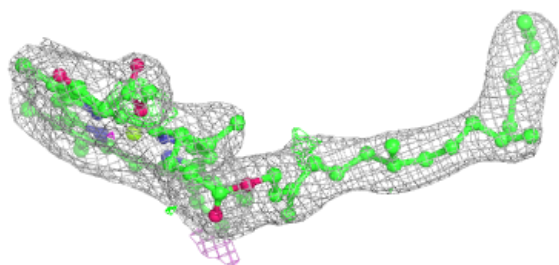
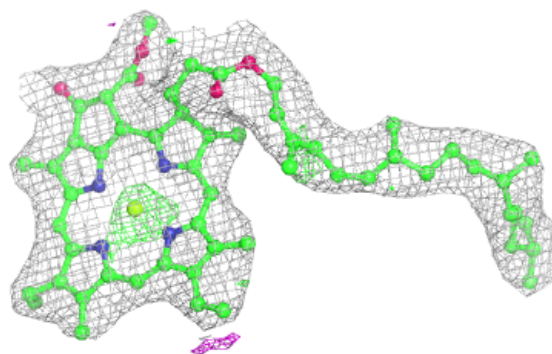


Electron density around CLA A 839:

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

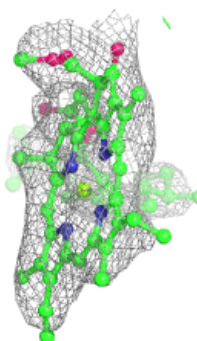
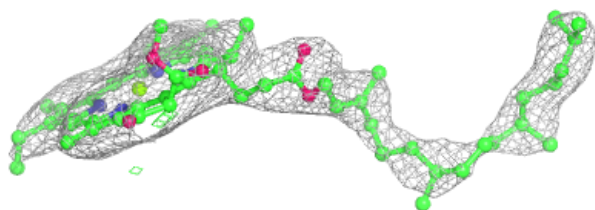
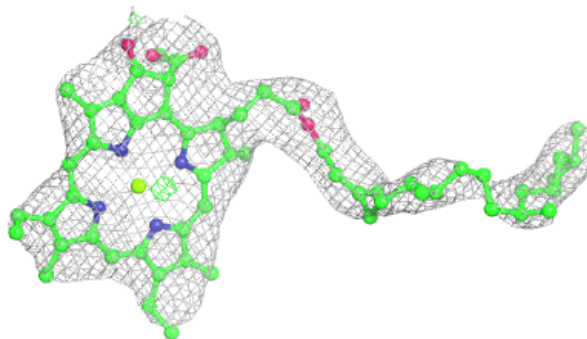
**Electron density around CLA A 802:**

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

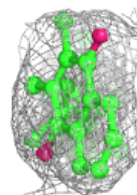
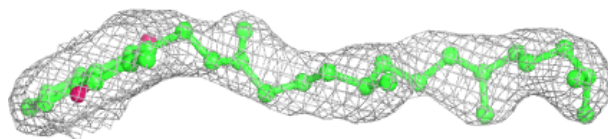
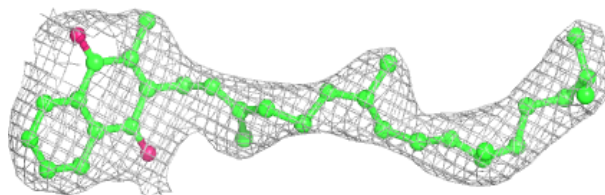


Electron density around CLA B 814:

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

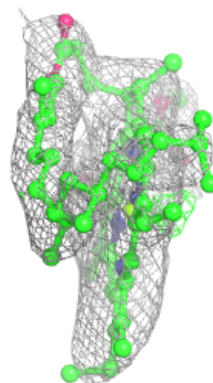
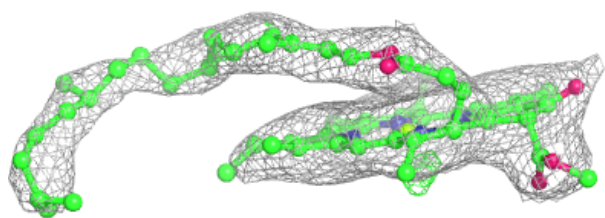
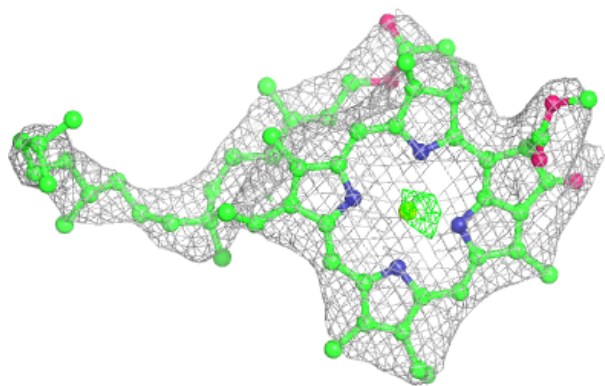
**Electron density around PQN A 844:**

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

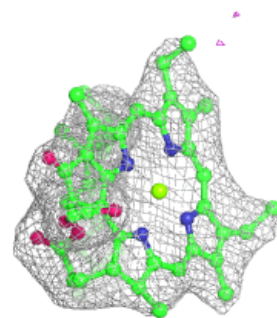
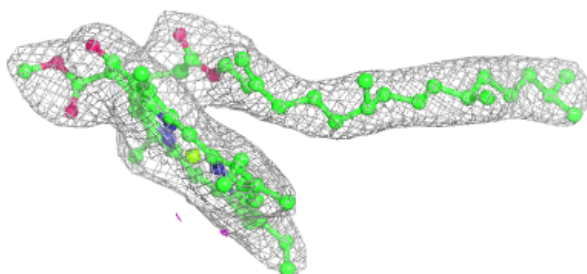
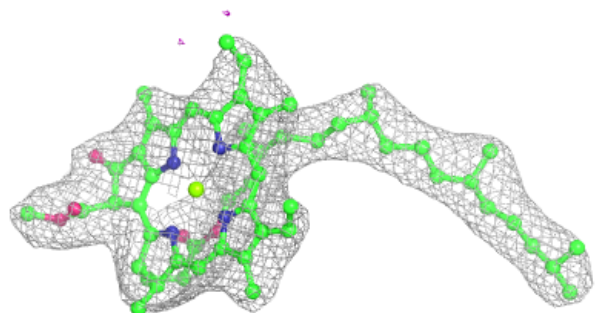


Electron density around CLA B 819:

$2mF_o-DF_c$ (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.