



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 21, 2024 – 12:47 am GMT

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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 : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

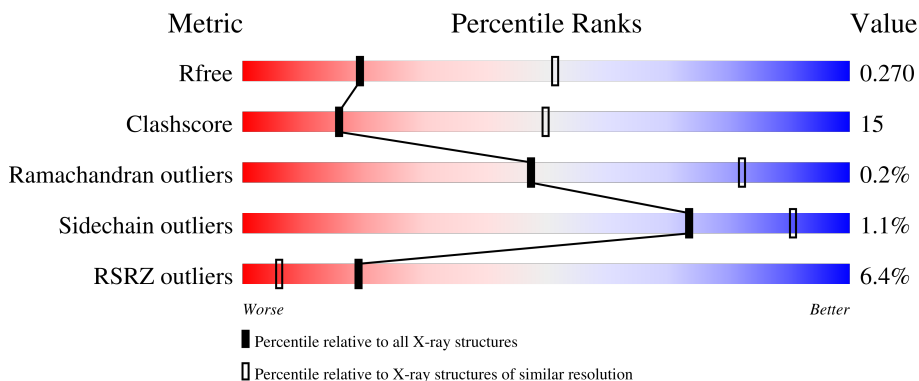
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	743	 3% 77% 23%
2	B	733	 3% 76% 24%
3	C	80	 5% 85% 15%
4	D	143	 8% 78% 22%
5	E	66	 17% 92% 8%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CL0	A	801	X	-	-	-
18	CLA	1	5006	X	-	-	-
18	CLA	1	5007	X	-	-	-
18	CLA	1	5008	X	-	-	-
18	CLA	1	5009	X	-	-	-
18	CLA	1	5010	X	-	-	-
18	CLA	1	5011	X	-	-	-
18	CLA	1	5012	X	-	-	-
18	CLA	1	5013	X	-	-	-
18	CLA	1	5015	X	-	-	-
18	CLA	1	5017	X	-	-	-
18	CLA	1	5018	X	-	-	-
18	CLA	2	306	X	-	-	-
18	CLA	2	307	X	-	-	-
18	CLA	2	308	X	-	-	-
18	CLA	2	309	X	-	-	-
18	CLA	2	310	X	-	-	-
18	CLA	2	311	X	-	-	-

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	822	X	-	-	-
18	CLA	B	823	X	-	-	-
18	CLA	B	824	X	-	-	-
18	CLA	B	825	X	-	-	-
18	CLA	B	826	X	-	-	-
18	CLA	B	827	X	-	-	-
18	CLA	B	828	X	-	-	-
18	CLA	B	829	X	-	-	-
18	CLA	B	830	X	-	-	-
18	CLA	B	831	X	-	-	-
18	CLA	B	832	X	-	-	-
18	CLA	B	833	X	-	-	-
18	CLA	B	834	X	-	-	-
18	CLA	B	835	X	-	-	-
18	CLA	B	836	X	-	-	-
18	CLA	B	837	X	-	-	-
18	CLA	B	838	X	-	-	-
18	CLA	B	839	X	-	-	-
18	CLA	B	840	X	-	-	-
18	CLA	B	841	X	-	-	-
18	CLA	F	301	X	-	-	-
18	CLA	F	302	X	-	-	-
18	CLA	F	303	X	-	-	-
18	CLA	G	1601	X	-	-	-
18	CLA	G	1602	X	-	-	-
18	CLA	G	1603	X	-	-	-
18	CLA	H	1701	X	-	-	-
18	CLA	J	1101	X	-	-	-
18	CLA	J	1103	X	-	-	-
18	CLA	K	1401	X	-	-	-
18	CLA	K	1402	X	-	-	-
18	CLA	K	1403	X	-	-	-
18	CLA	K	1404	X	-	-	X
18	CLA	L	301	X	-	-	-
18	CLA	L	304	X	-	-	-
18	CLA	L	305	X	-	-	-
18	CLA	L	306	X	-	-	-
21	BCR	1	5005	-	-	-	X
21	BCR	2	305	-	-	-	X
21	BCR	3	306	-	-	-	X
21	BCR	B	845	-	-	-	X
21	BCR	K	1405	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	BCR	L	302	-	-	-	X
22	LHG	B	849	-	-	-	X
23	LMT	A	850	-	-	-	X
23	LMT	B	852	-	-	-	X
23	LMT	G	1606	-	-	-	X
23	LMT	J	1107	-	-	-	X
24	LMG	1	5020	-	-	-	X
24	LMG	2	301	-	-	-	X
24	LMG	4	320	-	-	-	X
24	LMG	A	851	-	-	-	X
25	GOL	4	321	-	-	-	X
26	DGD	1	5002	-	-	-	X
29	LUT	1	5004	X	-	-	-
29	LUT	2	303	X	-	-	-
29	LUT	3	304	X	-	-	-
29	LUT	J	1105	X	-	-	-
30	CHL	1	5014	X	-	-	-
30	CHL	1	5016	X	-	-	-
30	CHL	2	314	X	-	-	-
30	CHL	2	315	X	-	-	-
30	CHL	2	316	X	-	-	-
30	CHL	2	318	X	-	-	-
30	CHL	2	319	X	-	-	-
30	CHL	3	310	X	-	-	-
30	CHL	3	312	X	-	-	-
30	CHL	3	313	X	-	-	-
30	CHL	3	316	X	-	-	-
30	CHL	4	302	X	-	-	-
30	CHL	4	313	X	-	-	-
30	CHL	4	314	X	-	-	-
30	CHL	4	316	X	-	-	-
30	CHL	4	317	X	-	-	-
30	CHL	4	318	X	-	-	-
31	XAT	2	304	X	-	-	-
31	XAT	4	304	X	-	-	-

## 2 Entry composition [i](#)

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

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

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

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

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

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

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

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

- Molecule 4 is a protein called PsaD.

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

- Molecule 5 is a protein called PsaE.

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

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

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



There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 7 is a protein called PsaG.

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

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

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

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	42	338	231	51	55	1	0	0	0

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 9 discrepancies between the modelled and reference sequences:

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

- Molecule 13 is a protein called Lhca1.

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

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

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

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

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

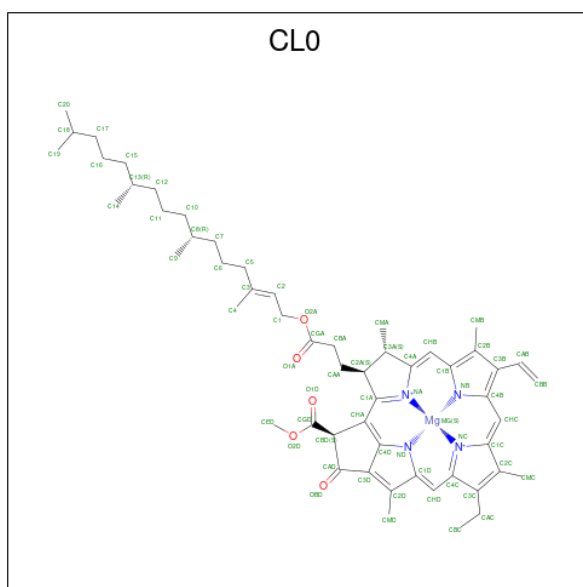
- Molecule 16 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

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

There are 3 discrepancies between the modelled and reference sequences:

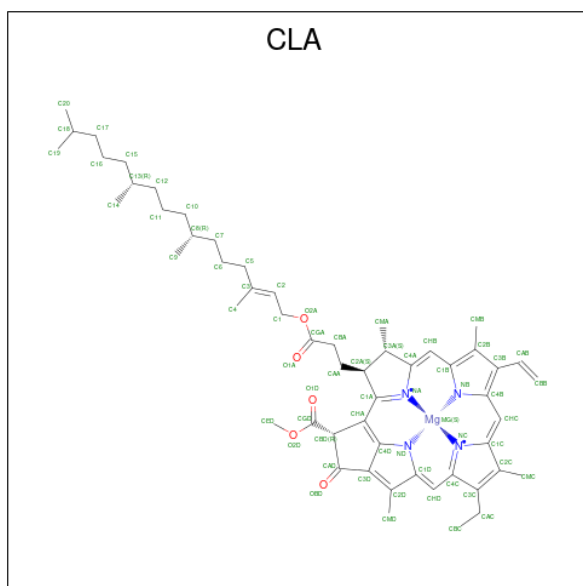
Chain	Residue	Modelled	Actual	Comment	Reference
4	89	LYS	ARG	conflict	UNP Q9SQL2
4	128	ASP	ALA	conflict	UNP Q9SQL2
4	149	PHE	SER	conflict	UNP Q9SQL2

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



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

- Molecule 18 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



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

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

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

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

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

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

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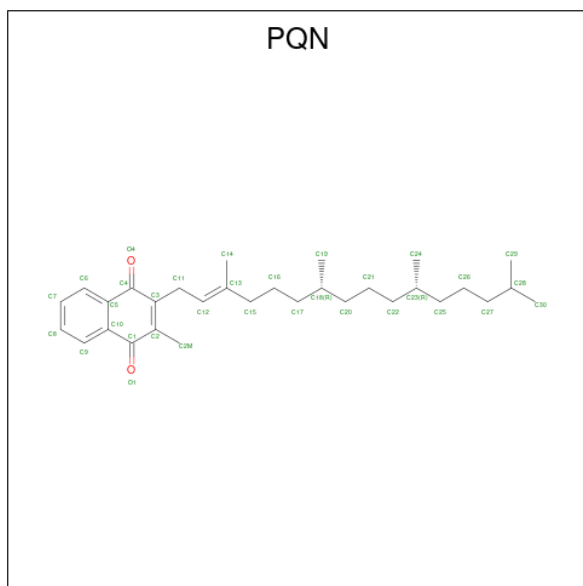
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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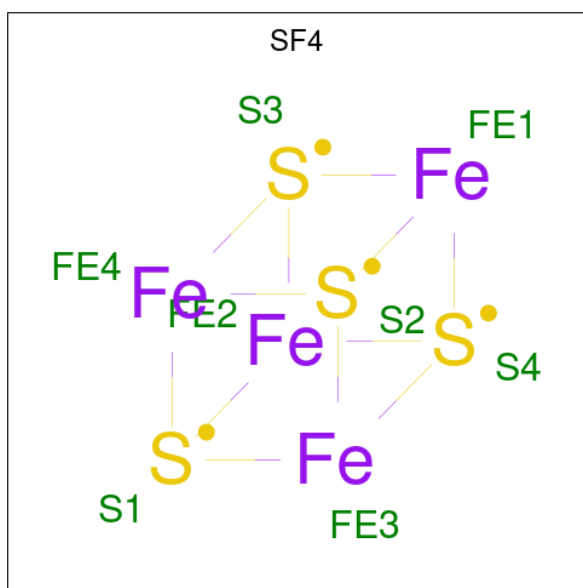
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5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

- Molecule 19 is PHYLLOQUINONE (three-letter code: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



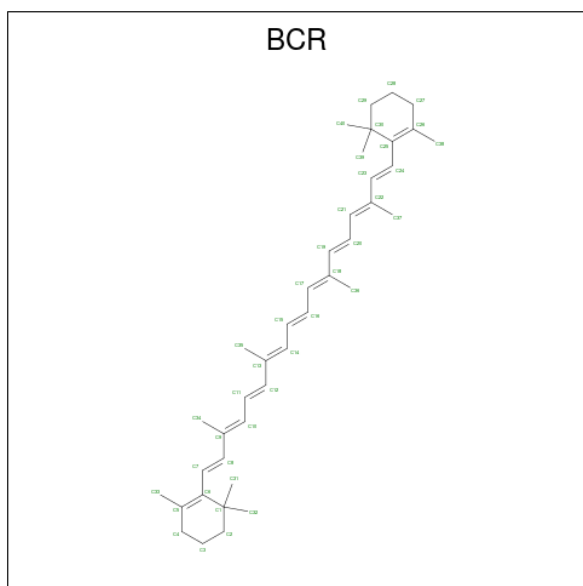
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			33	31	2		
19	B	1	Total	C	O	0	0
			33	31	2		

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



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

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



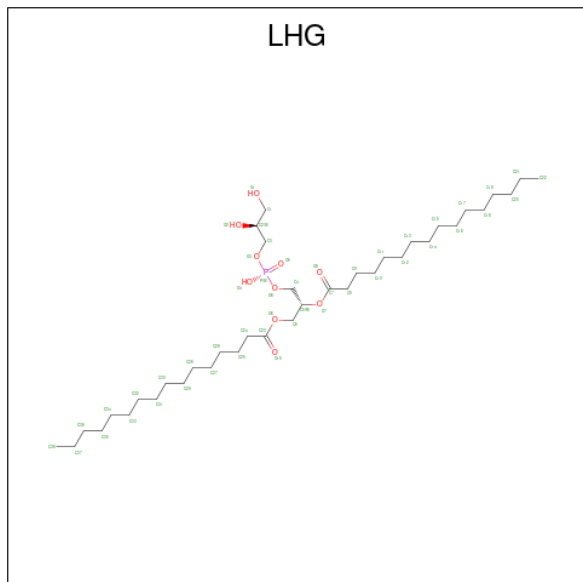
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total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

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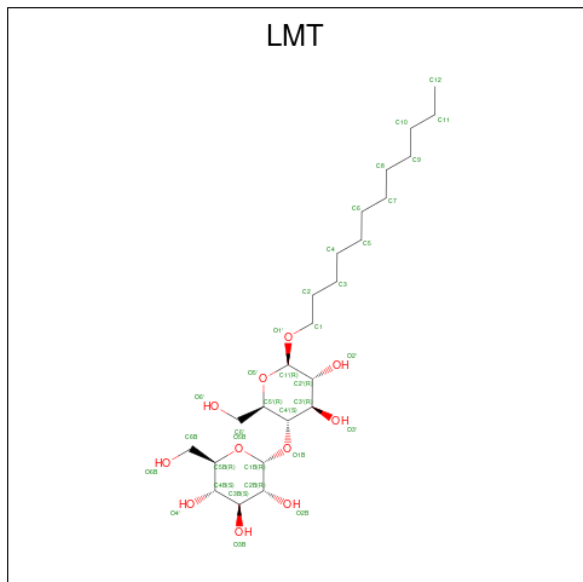
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	1	1	Total C 40 40	0	0
21	2	1	Total C 40 40	0	0
21	3	1	Total C 40 40	0	0
21	3	1	Total C 40 40	0	0
21	4	1	Total C 40 40	0	0

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



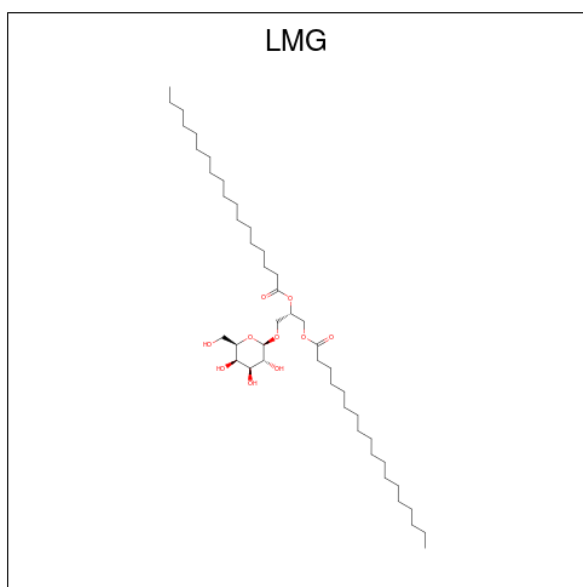
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C O P 49 38 10 1	0	0
22	A	1	Total C O P 40 29 10 1	0	0
22	B	1	Total C O P 21 10 10 1	0	0
22	B	1	Total C O P 49 38 10 1	0	0
22	1	1	Total C O P 49 38 10 1	0	0
22	2	1	Total C O P 35 24 10 1	0	0

- Molecule 23 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



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

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



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

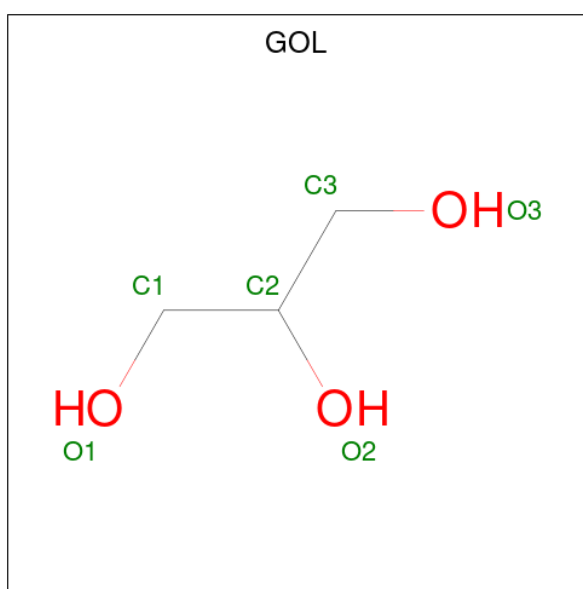
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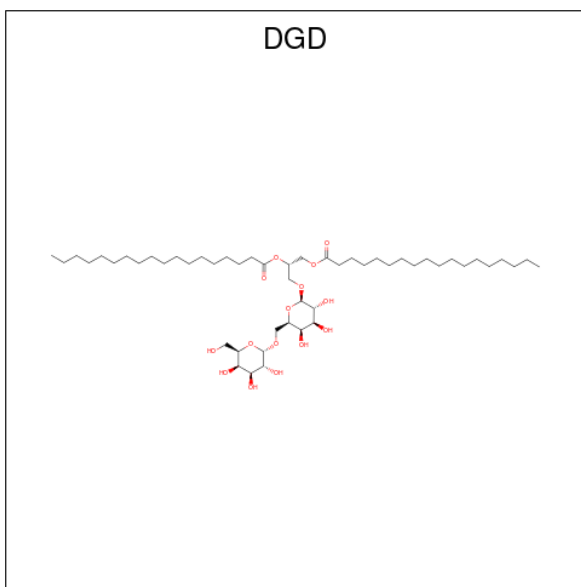
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	2	1	Total	C	O	0	0
			36	26	10		
24	2	1	Total	C	O	0	0
			13	7	6		
24	2	1	Total	C	O	0	0
			13	7	6		
24	4	1	Total	C	O	0	0
			13	7	6		

- Molecule 25 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>).

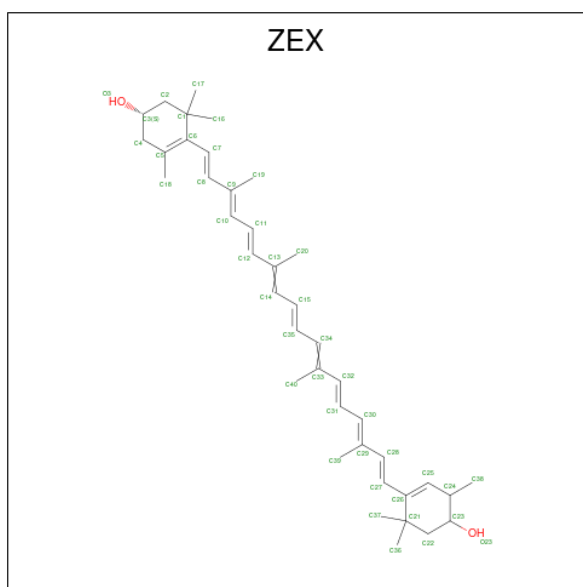


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	B	1	Total	C	O	0	0
			61	46	15		
26	F	1	Total	C	O	0	0
			57	42	15		
26	J	1	Total	C	O	0	0
			58	43	15		
26	1	1	Total	C	O	0	0
			35	26	9		
26	2	1	Total	C	O	0	0
			51	36	15		

- Molecule 27 is CALCIUM ION (three-letter code: CA) (formula: Ca).

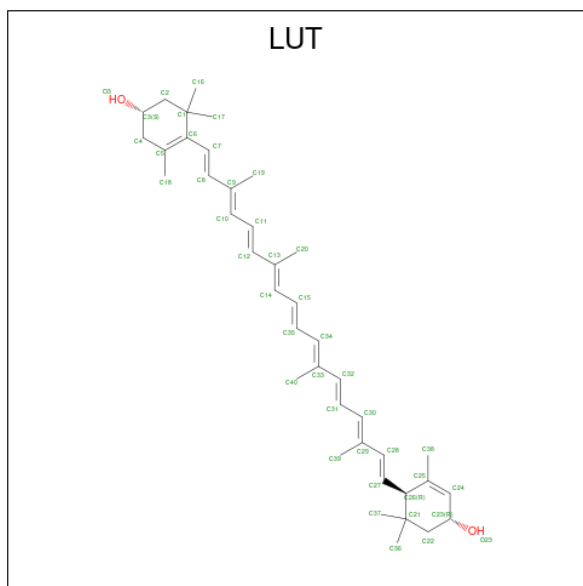
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	B	1	Total	Ca	0	0
			1	1		
27	3	1	Total	Ca	0	0
			1	1		

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



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

- Molecule 29 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula:  $C_{40}H_{56}O_2$ ).



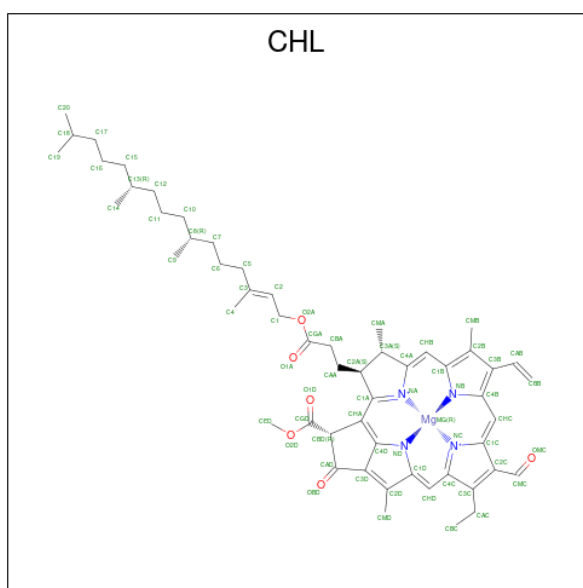
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	J	1	Total	C O	0	0
			42	40 2		
29	1	1	Total	C O	0	0
			42	40 2		

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

- Molecule 30 is CHLOROPHYLL B (three-letter code: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ).



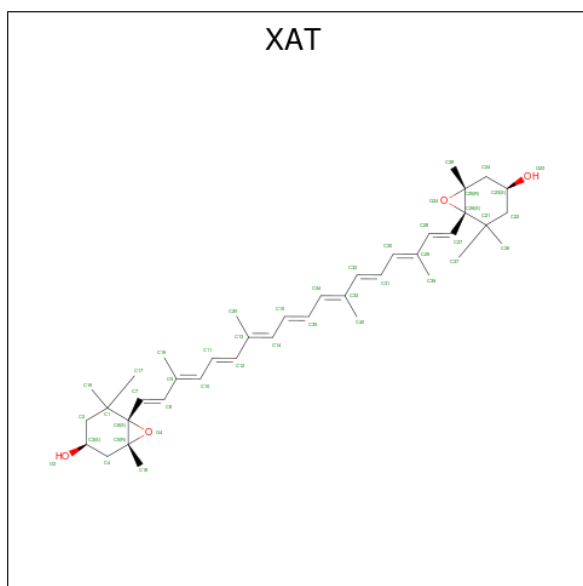
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
30	1	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
30	1	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
30	2	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
30	2	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
30	2	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
30	2	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		

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

- Molecule 31 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'-TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).

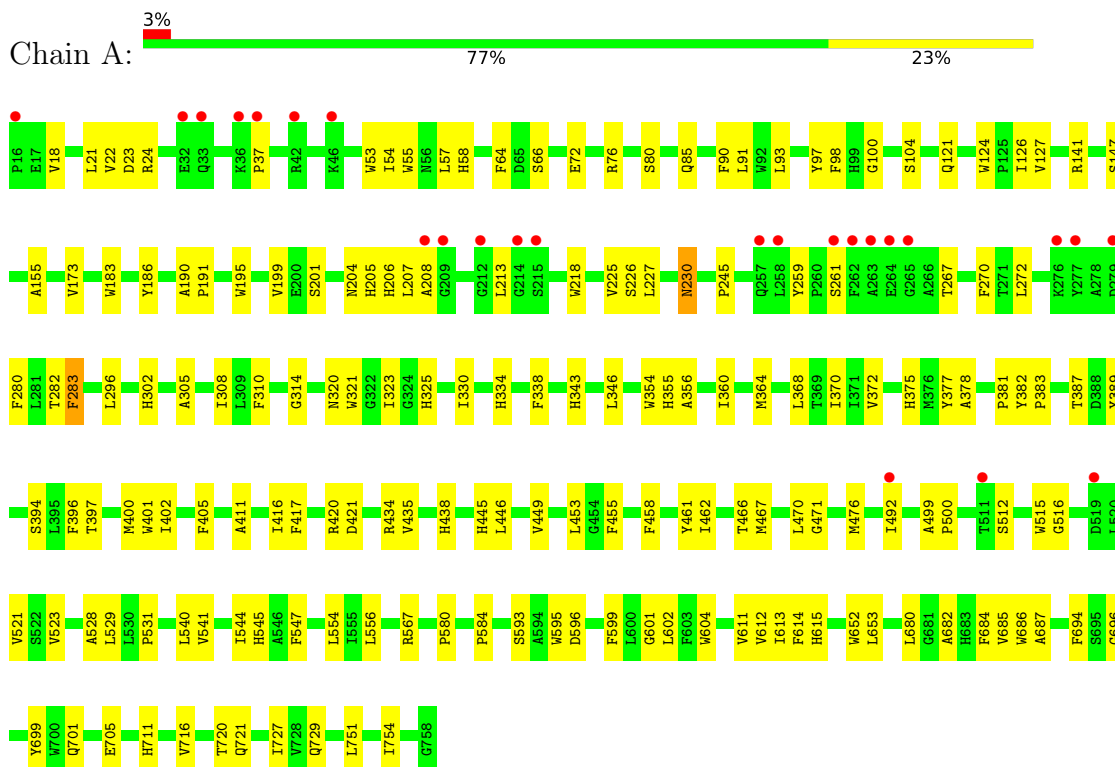


<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>			<b>ZeroOcc</b>	<b>AltConf</b>
31	2	1	Total	C	O	0	0
			44	40	4		
31	4	1	Total	C	O	0	0
			44	40	4		

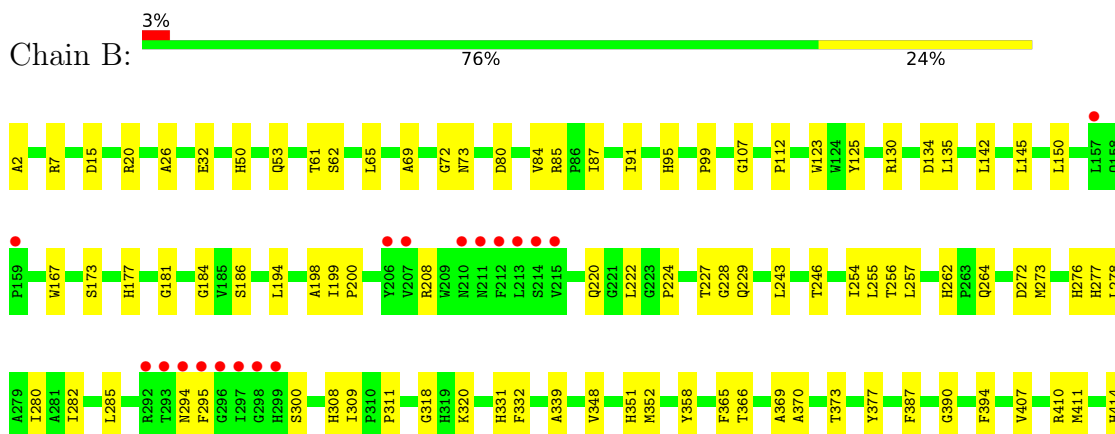
### 3 Residue-property plots [i](#)

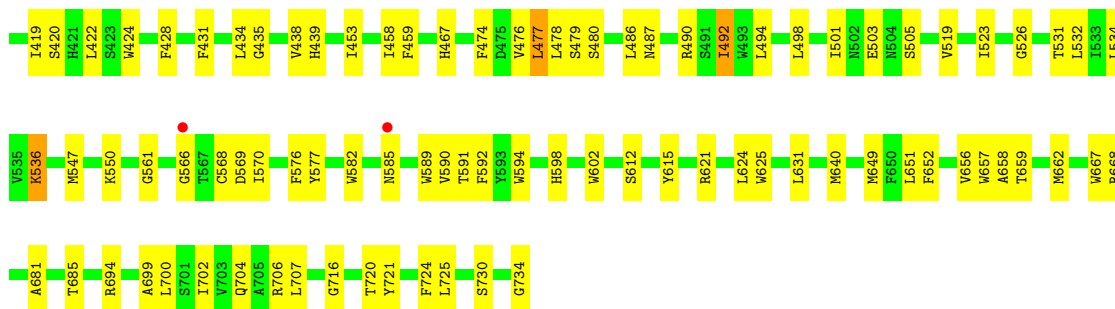
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Photosystem I P700 chlorophyll a apoprotein A1

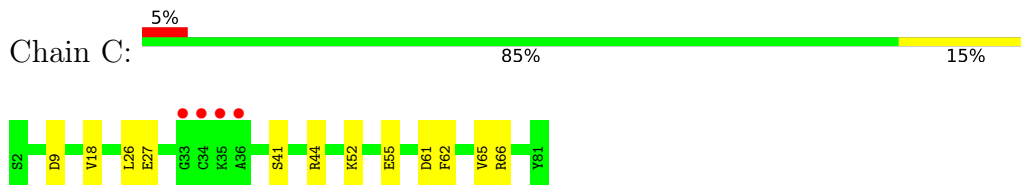


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

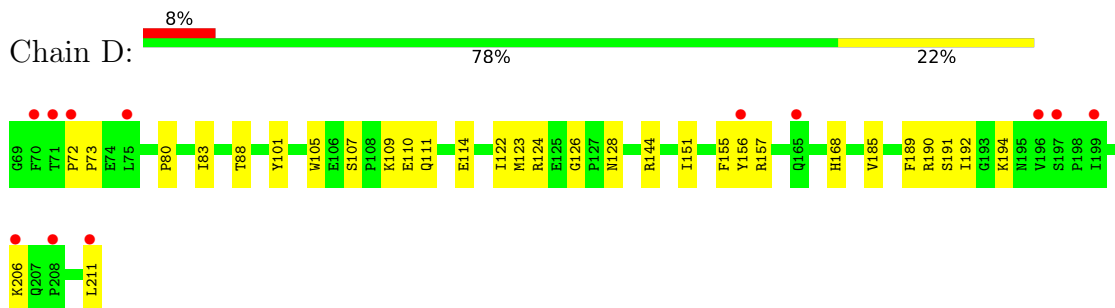




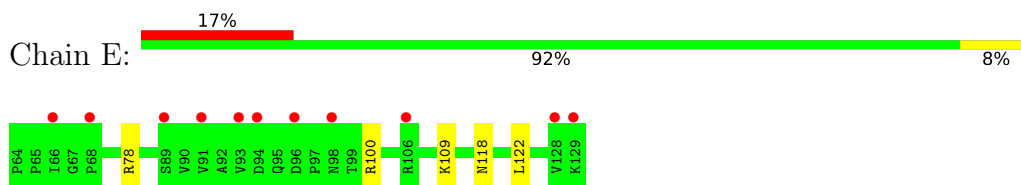
- Molecule 3: Photosystem I iron-sulfur center



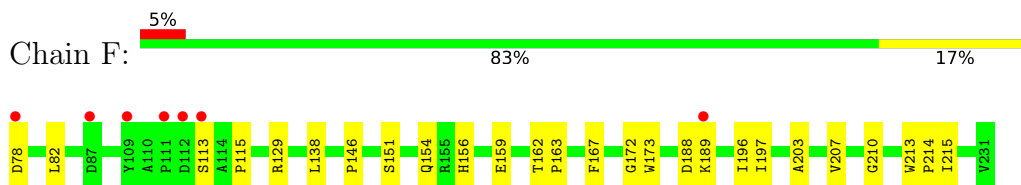
- Molecule 4: PsaD



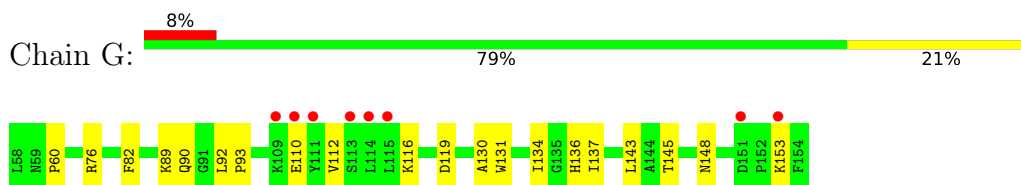
- Molecule 5: PsaE



- Molecule 6: Photosystem I reaction center subunit III

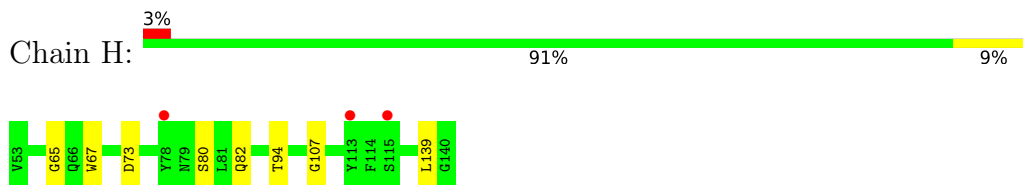


- Molecule 7: PsaG

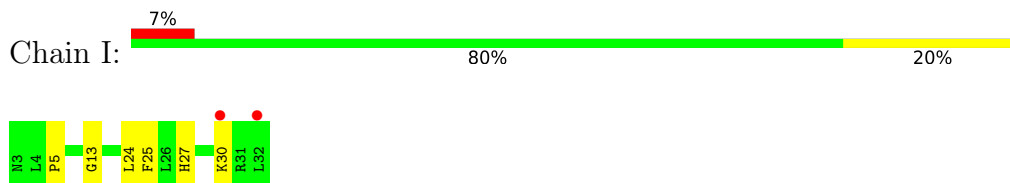




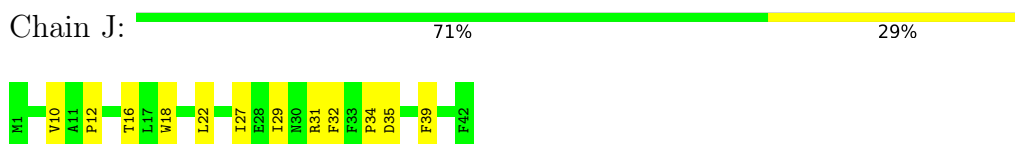
- Molecule 8: Photosystem I reaction center subunit VI



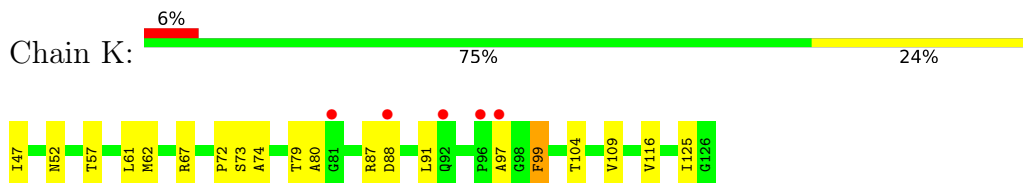
- Molecule 9: Photosystem I reaction center subunit VIII



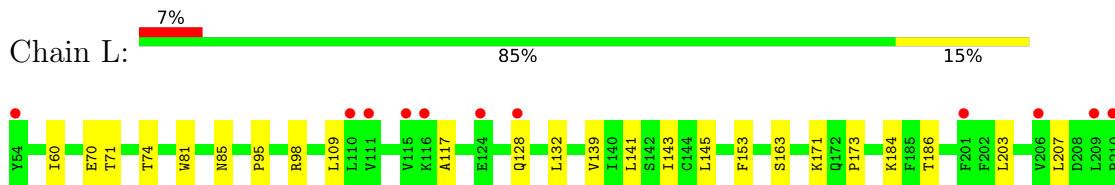
- Molecule 10: Photosystem I reaction center subunit IX



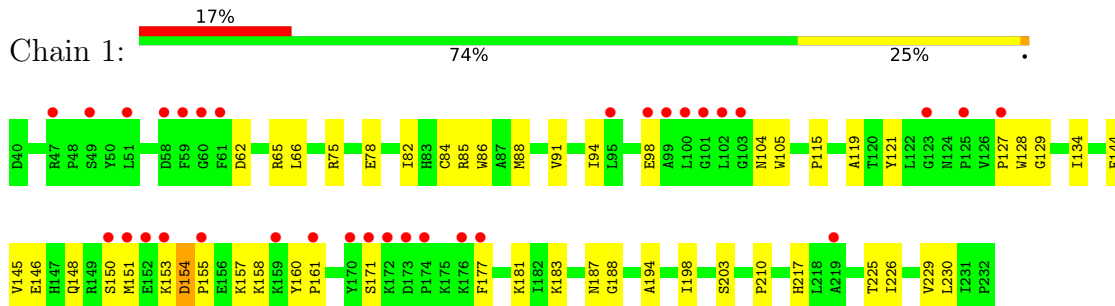
- Molecule 11: Photosystem I reaction center subunit X psaK



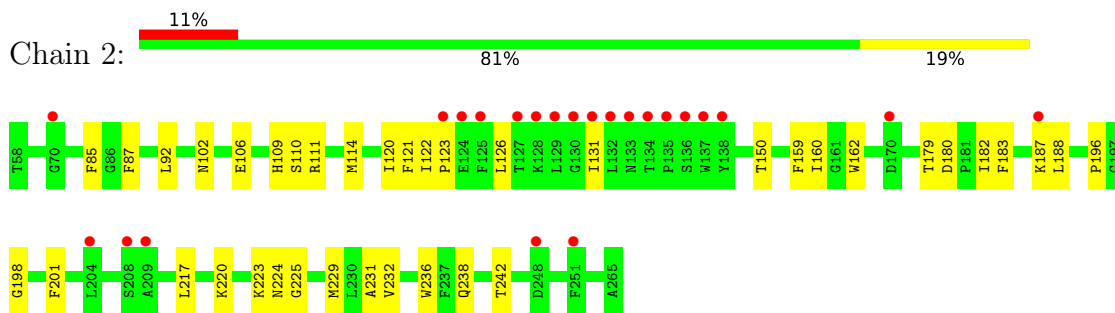
- Molecule 12: PsaL domain-containing protein



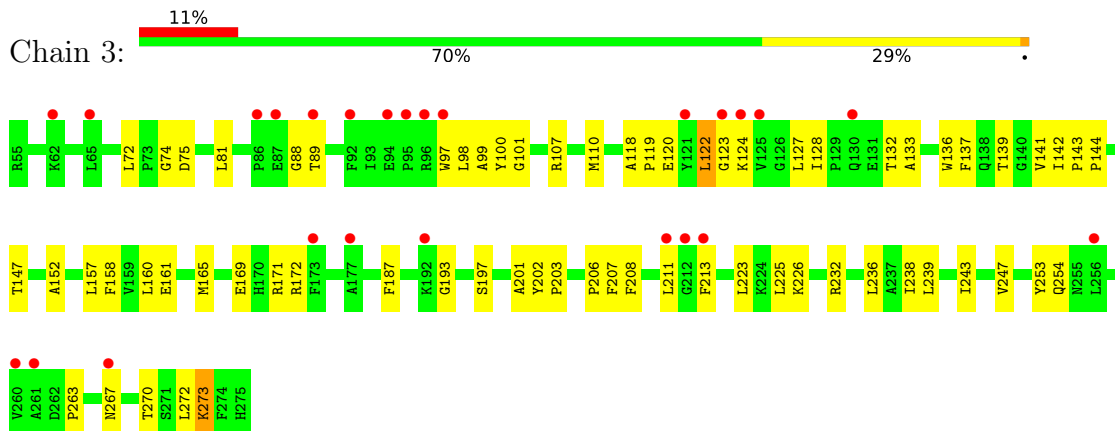
- Molecule 13: Lhca1



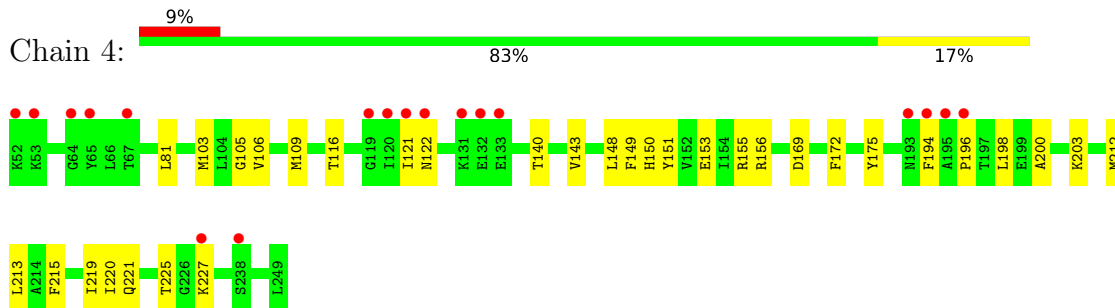
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	190.20Å 201.79Å 213.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 3.00 49.63 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.7 (49.63-3.00) 91.7 (49.63-3.00)	Depositor EDS
$R_{merge}$	0.33	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.04 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.239 , 0.270 0.239 , 0.270	Depositor DCC
$R_{free}$ test set	3139 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	96.1	Xtrriage
Anisotropy	0.450	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 58.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	37423	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	123.0	wwPDB-VP

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

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/6057	0.40	0/8264
2	B	0.24	0/6069	0.39	0/8286
3	C	0.24	0/625	0.44	0/846
4	D	0.24	0/1163	0.43	0/1572
5	E	0.24	0/540	0.40	0/734
6	F	0.24	0/1234	0.38	0/1670
7	G	0.24	0/776	0.37	0/1054
8	H	0.25	0/693	0.40	0/942
9	I	0.25	0/238	0.38	0/324
10	J	0.26	0/349	0.39	0/476
11	K	0.24	0/564	0.47	0/763
12	L	0.25	0/1207	0.41	0/1651
13	1	0.24	0/1558	0.38	0/2125
14	2	0.24	0/1679	0.39	0/2302
15	3	0.25	0/1760	0.40	0/2390
16	4	0.24	0/1608	0.37	0/2191
All	All	0.25	0/26120	0.40	0/35590

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5858	0	5717	154	0
2	B	5857	0	5653	141	0
3	C	612	0	591	11	0
4	D	1132	0	1141	16	0
5	E	528	0	528	6	0
6	F	1206	0	1231	20	0
7	G	757	0	743	16	0
8	H	673	0	667	7	0
9	I	232	0	253	5	0
10	J	338	0	345	13	0
11	K	558	0	587	17	0
12	L	1174	0	1183	18	0
13	1	1508	0	1489	45	0
14	2	1620	0	1554	35	0
15	3	1706	0	1659	59	0
16	4	1559	0	1524	28	0
17	A	65	0	72	9	0
18	1	608	0	562	43	0
18	2	572	0	538	41	0
18	3	531	0	456	33	0
18	4	516	0	488	22	0
18	A	2543	0	2661	237	0
18	B	2480	0	2602	214	0
18	F	195	0	215	16	0
18	G	166	0	152	6	0
18	H	60	0	59	8	0
18	J	115	0	110	9	0
18	K	199	0	158	15	0
18	L	215	0	183	7	0
19	A	33	0	46	4	0
19	B	33	0	46	2	0
20	A	8	0	0	0	0
20	C	16	0	0	1	0
21	1	40	0	53	3	0
21	2	40	0	53	11	0
21	3	80	0	106	6	0
21	4	40	0	52	6	0
21	A	240	0	317	38	0
21	B	240	0	317	29	0
21	F	80	0	105	11	0
21	G	40	0	53	4	0
21	I	80	0	105	4	0
21	J	40	0	53	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	K	40	0	53	2	0
21	L	120	0	159	8	0
22	1	49	0	74	3	0
22	2	35	0	40	1	0
22	A	89	0	127	16	0
22	B	70	0	86	8	0
23	2	35	0	46	1	0
23	4	35	0	46	0	0
23	A	35	0	45	0	0
23	B	98	0	118	5	0
23	G	66	0	80	3	0
23	J	25	0	22	0	0
24	1	95	0	136	10	0
24	2	113	0	106	5	0
24	4	13	0	11	0	0
24	A	50	0	73	5	0
24	B	81	0	87	2	0
24	F	117	0	147	5	0
24	G	25	0	20	1	0
24	J	30	0	30	0	0
25	4	6	0	8	0	0
25	A	6	0	8	1	0
26	1	35	0	39	0	0
26	2	51	0	60	5	0
26	B	61	0	83	8	0
26	F	57	0	75	0	0
26	J	58	0	77	4	0
27	3	1	0	0	0	0
27	B	1	0	0	0	0
28	F	42	0	56	3	0
29	1	84	0	110	15	0
29	2	42	0	55	6	0
29	3	84	0	110	12	0
29	4	42	0	55	2	0
29	J	42	0	55	9	0
30	1	108	0	87	14	0
30	2	272	0	224	18	0
30	3	215	0	172	24	0
30	4	314	0	243	19	0
31	2	44	0	56	7	0
31	4	44	0	56	6	0
All	All	37423	0	37562	1094	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 15.

All (1094) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:61:LEU:HB3	18:K:1403:CLA:HAB	1.45	0.97
31:2:304:XAT:H8	18:2:311:CLA:HBB1	1.50	0.94
1:A:401:TRP:CD1	18:A:826:CLA:HAB	2.10	0.87
18:B:807:CLA:H152	18:B:829:CLA:HBB2	1.58	0.85
21:2:305:BCR:H333	18:4:311:CLA:HMC3	1.58	0.84
24:1:5001:LMG:H122	30:1:5016:CHL:HBA1	1.61	0.83
18:A:853:CLA:H141	21:L:303:BCR:H17C	1.62	0.82
18:2:308:CLA:HMA1	18:2:313:CLA:HBC3	1.60	0.81
18:A:822:CLA:HMA1	18:A:840:CLA:HAB	1.62	0.80
18:4:310:CLA:HMA2	30:4:316:CHL:HBC3	1.62	0.79
18:A:829:CLA:HMA2	12:L:71:THR:HG21	1.64	0.79
2:B:582:TRP:CH2	18:B:801:CLA:HAB	2.17	0.79
29:3:304:LUT:H32	30:3:310:CHL:HAB	1.64	0.79
14:2:159:PHE:HB3	21:2:305:BCR:H16C	1.65	0.78
1:A:401:TRP:HD1	18:A:826:CLA:HAB	1.48	0.77
24:2:301:LMG:HC2	24:2:302:LMG:HC5	1.68	0.76
14:2:232:VAL:HG11	31:2:304:XAT:H12	1.68	0.76
12:L:145:LEU:HB3	12:L:186:THR:HG22	1.68	0.76
29:J:1105:LUT:H181	29:J:1105:LUT:H8	1.68	0.75
18:B:805:CLA:HBC1	26:B:855:DGD:HA92	1.69	0.75
4:D:83:ILE:HB	4:D:122:ILE:HB	1.68	0.75
18:B:836:CLA:HMB2	18:B:838:CLA:HED1	1.68	0.75
21:B:843:BCR:HC31	21:B:845:BCR:H333	1.68	0.74
13:1:85:ARG:HB3	18:1:5006:CLA:HBC2	1.69	0.74
2:B:311:PRO:HG2	22:B:848:LHG:HC32	1.69	0.73
18:F:303:CLA:HAB	24:F:306:LMG:H382	1.71	0.73
2:B:656:VAL:HG22	18:B:840:CLA:HMB3	1.70	0.73
1:A:310:PHE:HE1	18:A:819:CLA:HAB	1.53	0.73
18:A:804:CLA:H61	21:A:844:BCR:H24C	1.68	0.73
18:B:803:CLA:HMB1	18:B:803:CLA:HBB1	1.71	0.73
18:B:812:CLA:HHC	18:B:812:CLA:HBB1	1.72	0.72
18:B:801:CLA:HED2	18:B:803:CLA:H71	1.71	0.72
18:A:803:CLA:HBB1	18:A:810:CLA:H122	1.69	0.72
22:A:848:LHG:H161	18:J:1101:CLA:HMB2	1.70	0.72
15:3:239:LEU:HD13	18:3:311:CLA:HBB2	1.70	0.72
1:A:270:PHE:HA	18:K:1401:CLA:HAC2	1.72	0.72
3:C:18:VAL:HG22	3:C:26:LEU:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:2:303:LUT:H362	18:2:313:CLA:HBC1	1.70	0.71
2:B:477:LEU:HD13	18:B:834:CLA:HMD3	1.72	0.71
15:3:110:MET:SD	18:3:307:CLA:HAB	2.31	0.71
18:B:823:CLA:HHC	18:B:823:CLA:HBB1	1.71	0.70
18:B:815:CLA:HMB1	18:B:815:CLA:HBB1	1.72	0.70
18:B:813:CLA:HMC1	21:B:844:BCR:H10C	1.73	0.70
30:1:5014:CHL:HHC	30:1:5014:CHL:HBB1	1.73	0.70
30:2:315:CHL:HMB1	30:2:315:CHL:HBB1	1.73	0.70
18:A:814:CLA:HHC	18:A:814:CLA:HBB1	1.72	0.70
10:J:34:PRO:O	26:J:1106:DGD:O2D	2.10	0.69
9:I:25:PHE:HB2	21:I:102:BCR:H14C	1.74	0.69
18:B:830:CLA:H143	26:B:855:DGD:HAW1	1.74	0.69
18:A:802:CLA:H111	21:A:847:BCR:H23C	1.74	0.69
18:A:822:CLA:HHC	18:A:822:CLA:HBB1	1.73	0.69
18:B:830:CLA:HMB1	18:B:830:CLA:HBB1	1.75	0.69
14:2:120:ILE:HG13	31:2:304:XAT:H163	1.72	0.69
18:2:312:CLA:HMB1	18:2:312:CLA:HBB1	1.74	0.69
29:3:303:LUT:H31	21:3:306:BCR:H363	1.75	0.69
29:1:5003:LUT:H30	18:1:5006:CLA:H52	1.74	0.68
18:A:852:CLA:H122	21:B:802:BCR:H352	1.75	0.68
2:B:2:ALA:HB1	2:B:7:ARG:HE	1.57	0.68
2:B:255:LEU:HD11	18:B:816:CLA:HBC1	1.74	0.68
18:G:1601:CLA:HMB1	18:G:1601:CLA:HBB1	1.74	0.68
18:B:829:CLA:HBB1	18:B:829:CLA:HMB1	1.75	0.68
18:K:1401:CLA:HMB1	18:K:1401:CLA:HBB1	1.75	0.68
2:B:615:TYR:OH	2:B:621:ARG:NH2	2.26	0.68
18:A:834:CLA:HBB1	18:A:834:CLA:HMB1	1.75	0.68
18:2:313:CLA:HBA1	15:3:160:LEU:HD13	1.76	0.68
18:B:834:CLA:H143	18:B:835:CLA:H71	1.75	0.68
13:1:88:MET:SD	18:1:5006:CLA:HAB	2.34	0.68
2:B:373:THR:HG23	2:B:591:THR:HG21	1.75	0.68
18:2:310:CLA:HBB1	18:2:310:CLA:HMB1	1.75	0.68
18:A:805:CLA:HED1	18:A:828:CLA:H2	1.75	0.67
18:A:828:CLA:HBB1	18:A:828:CLA:HMB1	1.76	0.67
18:A:813:CLA:C2B	21:A:843:BCR:H10C	2.24	0.67
16:4:151:TYR:HB2	30:4:302:CHL:H11	1.75	0.67
18:B:834:CLA:HMB1	18:B:834:CLA:HBB1	1.77	0.67
21:A:845:BCR:H24C	24:A:851:LMG:H362	1.75	0.67
21:A:847:BCR:H16C	18:B:801:CLA:H122	1.76	0.67
6:F:196:ILE:HD12	6:F:197:ILE:HG13	1.76	0.66
15:3:139:THR:HG23	30:3:312:CHL:HED2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:805:CLA:HMB1	18:B:805:CLA:HBB1	1.76	0.66
18:G:1602:CLA:HMB1	18:G:1602:CLA:HBB1	1.77	0.66
18:A:810:CLA:H202	22:A:848:LHG:H211	1.78	0.66
18:A:820:CLA:H62	18:A:821:CLA:H12	1.76	0.66
18:B:813:CLA:HMB1	18:B:813:CLA:HBB1	1.76	0.66
21:A:847:BCR:H24C	18:B:833:CLA:HMC2	1.77	0.66
30:3:310:CHL:HBB1	30:3:310:CHL:HMB1	1.78	0.66
1:A:492:ILE:HD13	18:A:832:CLA:HBB1	1.77	0.65
21:4:301:BCR:H403	21:4:301:BCR:H23C	1.77	0.65
18:A:808:CLA:HBB1	18:A:808:CLA:HMB1	1.76	0.65
18:K:1404:CLA:HHC	18:K:1404:CLA:HBB1	1.77	0.65
14:2:110:SER:HB3	14:2:225:GLY:HA3	1.79	0.65
24:F:307:LMG:H131	24:F:307:LMG:HC91	1.78	0.65
22:1:5019:LHG:H171	30:4:318:CHL:HED1	1.78	0.65
30:3:312:CHL:HMB1	30:3:312:CHL:HBB1	1.79	0.65
15:3:160:LEU:HD21	18:3:318:CLA:HED3	1.77	0.65
7:G:131:TRP:HA	7:G:134:ILE:HD12	1.78	0.64
1:A:453:LEU:HB3	1:A:547:PHE:HB2	1.78	0.64
18:B:826:CLA:H191	18:B:841:CLA:H122	1.78	0.64
21:A:846:BCR:HC7	18:K:1402:CLA:H122	1.79	0.64
18:B:833:CLA:H91	18:F:302:CLA:HMA1	1.80	0.64
30:2:318:CHL:HHC	30:2:318:CHL:HBB1	1.80	0.64
18:A:820:CLA:H2	24:A:851:LMG:H162	1.79	0.64
18:B:826:CLA:H51	18:B:837:CLA:HBA1	1.79	0.64
18:B:841:CLA:HBA1	22:B:848:LHG:HC42	1.78	0.64
1:A:37:PRO:HA	18:J:1101:CLA:HBC1	1.80	0.64
18:A:807:CLA:HBB1	18:A:807:CLA:HMB1	1.79	0.64
18:1:5010:CLA:HBC1	30:1:5014:CHL:HBB2	1.78	0.64
18:B:811:CLA:H92	12:L:132:LEU:HB3	1.80	0.64
1:A:602:LEU:HD21	18:A:828:CLA:HBC1	1.79	0.63
1:A:462:ILE:HG22	18:A:831:CLA:HBC2	1.80	0.63
13:1:154:ASP:H	13:1:155:PRO:HA	1.64	0.63
1:A:330:ILE:O	1:A:334:HIS:ND1	2.32	0.63
21:3:306:BCR:H10C	30:3:316:CHL:O1A	1.99	0.63
15:3:247:VAL:HA	15:3:273:LYS:HG3	1.81	0.63
30:3:313:CHL:HHC	30:3:313:CHL:HBB1	1.81	0.63
18:A:806:CLA:HAB	21:J:1104:BCR:H271	1.80	0.62
18:3:307:CLA:H71	18:3:308:CLA:HMA1	1.80	0.62
1:A:183:TRP:HB2	18:A:810:CLA:HMC3	1.81	0.62
1:A:434:ARG:HH11	18:A:829:CLA:HED2	1.63	0.62
2:B:721:TYR:HB2	18:B:803:CLA:HED3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:370:ALA:HB1	18:B:828:CLA:HMA1	1.81	0.62
1:A:173:VAL:HG21	18:A:813:CLA:H91	1.80	0.62
18:B:832:CLA:H2	21:F:305:BCR:H372	1.82	0.62
1:A:76:ARG:HD2	1:A:190:ALA:HB1	1.82	0.62
18:F:301:CLA:HBB1	18:F:301:CLA:HMB1	1.81	0.62
2:B:576:PHE:HE1	18:B:830:CLA:HAC2	1.65	0.62
13:1:75:ARG:NH1	18:1:5010:CLA:O1A	2.33	0.62
15:3:165:MET:HG3	18:3:317:CLA:HMC3	1.81	0.62
1:A:126:ILE:HG13	1:A:127:VAL:HG13	1.81	0.61
14:2:114:MET:SD	18:2:306:CLA:HAB	2.40	0.61
21:4:301:BCR:H10C	30:4:317:CHL:HBB2	1.82	0.61
18:3:307:CLA:HMD2	30:3:316:CHL:HBA2	1.82	0.61
2:B:65:LEU:HD11	21:B:845:BCR:H291	1.82	0.61
18:B:806:CLA:H93	18:B:814:CLA:H2	1.83	0.61
18:B:831:CLA:HAB	18:B:838:CLA:CBB	2.29	0.61
18:1:5010:CLA:HMB1	18:1:5010:CLA:HBB1	1.81	0.61
30:1:5016:CHL:HHC	30:1:5016:CHL:HBB1	1.81	0.61
2:B:309:ILE:HG22	2:B:318:GLY:HA3	1.83	0.61
18:2:309:CLA:H71	18:2:310:CLA:HMA1	1.82	0.61
18:B:824:CLA:HMD2	18:B:825:CLA:HAB	1.83	0.61
30:2:315:CHL:HAB	30:2:318:CHL:HBB2	1.83	0.61
30:4:318:CHL:HHC	30:4:318:CHL:HBB1	1.81	0.61
1:A:687:ALA:HB3	18:A:802:CLA:HBB2	1.83	0.61
18:B:807:CLA:H43	26:B:855:DGD:HB61	1.83	0.61
14:2:121:PHE:HE2	14:2:231:ALA:HB1	1.66	0.61
26:2:327:DGD:HA31	16:4:213:LEU:HD12	1.82	0.61
15:3:202:TYR:HB3	18:3:307:CLA:HED3	1.82	0.61
15:3:236:LEU:HG	30:3:310:CHL:HMC	1.82	0.61
2:B:69:ALA:HB2	2:B:135:LEU:HB2	1.83	0.60
14:2:162:TRP:HH2	21:2:305:BCR:H321	1.65	0.60
2:B:410:ARG:HH22	24:B:850:LMG:HC61	1.66	0.60
18:1:5013:CLA:HED1	16:4:140:THR:HG23	1.82	0.60
18:2:326:CLA:HBC3	26:2:327:DGD:HG32	1.83	0.60
1:A:375:HIS:ND1	18:A:816:CLA:OBD	2.34	0.60
1:A:458:PHE:HE2	18:A:852:CLA:HMA1	1.66	0.60
1:A:226:SER:O	1:A:230:ASN:HB2	2.01	0.60
18:A:819:CLA:H111	21:A:845:BCR:H10C	1.82	0.60
18:B:818:CLA:H142	18:B:818:CLA:HBB1	1.81	0.60
30:4:302:CHL:HHC	30:4:302:CHL:HBB1	1.84	0.60
18:B:818:CLA:HBA2	18:B:827:CLA:HBB2	1.83	0.60
12:L:85:ASN:HB3	18:L:304:CLA:HAC1	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:310:CLA:H12	24:2:321:LMG:HC72	1.82	0.60
1:A:593:SER:OG	1:A:596:ASP:OD1	2.18	0.60
18:A:824:CLA:HAB	21:A:846:BCR:C23	2.32	0.60
15:3:203:PRO:HG3	30:3:316:CHL:HMD2	1.84	0.60
2:B:228:GLY:HA3	7:G:143:LEU:HB3	1.83	0.60
1:A:85:GLN:HG2	18:A:804:CLA:HMA1	1.83	0.60
1:A:321:TRP:HD1	11:K:91:LEU:HD22	1.66	0.60
18:B:812:CLA:HBD	23:G:1605:LMT:H1'	1.84	0.60
30:2:316:CHL:HHC	30:2:316:CHL:HBB1	1.82	0.60
2:B:582:TRP:HH2	18:B:801:CLA:HAB	1.67	0.60
21:B:843:BCR:H332	21:B:844:BCR:HC31	1.83	0.60
18:B:837:CLA:H52	21:F:305:BCR:H343	1.84	0.59
30:2:319:CHL:HHC	30:2:319:CHL:HBB1	1.84	0.59
18:H:1701:CLA:H121	12:L:81:TRP:HE1	1.66	0.59
18:2:326:CLA:HHC	18:2:326:CLA:HBB1	1.84	0.59
2:B:458:ILE:HG21	6:F:151:SER:HB3	1.83	0.59
18:B:820:CLA:HMB2	18:B:825:CLA:HMA3	1.83	0.59
2:B:707:LEU:HD22	26:B:855:DGD:HB21	1.85	0.59
18:B:819:CLA:H3A	18:B:819:CLA:CGA	2.32	0.59
4:D:114:GLU:O	4:D:144:ARG:NH2	2.36	0.59
16:4:203:LYS:HD2	18:4:306:CLA:HAA2	1.85	0.59
18:B:815:CLA:H2	21:B:845:BCR:H362	1.84	0.59
13:1:154:ASP:HB3	13:1:157:LYS:H	1.66	0.59
15:3:152:ALA:HB3	15:3:157:LEU:HG	1.85	0.59
18:H:1701:CLA:HMB3	21:L:302:BCR:H372	1.83	0.59
1:A:205:HIS:CG	18:A:812:CLA:HMC2	2.38	0.59
2:B:181:GLY:HA3	18:B:814:CLA:HBB1	1.85	0.59
1:A:308:ILE:HD11	21:A:855:BCR:H341	1.83	0.58
18:B:826:CLA:HED2	18:B:827:CLA:HBD	1.85	0.58
29:4:303:LUT:H373	18:4:305:CLA:H51	1.85	0.58
18:H:1701:CLA:HAB	21:L:307:BCR:H321	1.84	0.58
18:A:816:CLA:H71	18:A:833:CLA:HMA2	1.84	0.58
18:A:839:CLA:HAC1	19:A:841:PQN:H171	1.85	0.58
2:B:167:TRP:CZ2	18:B:812:CLA:HMA1	2.38	0.58
21:B:802:BCR:H362	18:B:804:CLA:H122	1.84	0.58
30:4:317:CHL:HHC	30:4:317:CHL:HBB1	1.85	0.58
1:A:394:SER:HB3	18:A:826:CLA:HMA1	1.85	0.58
18:A:828:CLA:H122	18:A:839:CLA:HMA2	1.84	0.58
1:A:360:ILE:HD11	21:A:845:BCR:HC7	1.86	0.58
18:F:303:CLA:HMB2	21:F:305:BCR:HC7	1.85	0.58
12:L:71:THR:H	12:L:74:THR:HG1	1.49	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:91:VAL:HG11	29:1:5003:LUT:H10	1.83	0.58
16:4:149:PHE:CG	18:4:315:CLA:HMC3	2.38	0.58
1:A:245:PRO:HG3	18:A:813:CLA:HED2	1.84	0.58
18:A:822:CLA:H161	22:A:849:LHG:H161	1.84	0.58
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.86	0.58
2:B:150:LEU:HD21	22:B:849:LHG:H371	1.86	0.58
18:F:303:CLA:H3A	21:F:305:BCR:H333	1.85	0.58
18:3:317:CLA:H12	18:3:319:CLA:CBB	2.33	0.58
2:B:73:ASN:ND2	2:B:107:GLY:O	2.30	0.58
18:B:810:CLA:H112	18:B:828:CLA:H192	1.85	0.58
1:A:684:PHE:CG	21:A:847:BCR:H363	2.39	0.58
4:D:80:PRO:HB3	4:D:124:ARG:HH21	1.68	0.58
1:A:716:VAL:HG21	18:A:837:CLA:HMB3	1.86	0.58
12:L:81:TRP:O	12:L:85:ASN:ND2	2.28	0.58
18:A:837:CLA:HBB1	18:A:837:CLA:HMB1	1.86	0.57
2:B:387:PHE:CZ	18:B:826:CLA:HAB	2.39	0.57
1:A:21:LEU:HA	15:3:88:GLY:HA3	1.87	0.57
11:K:125:ILE:HD11	18:K:1402:CLA:HMA1	1.86	0.57
12:L:95:PRO:HA	12:L:98:ARG:HD3	1.86	0.57
1:A:141:ARG:HE	25:A:854:GOL:H11	1.70	0.57
1:A:567:ARG:NH2	4:D:88:THR:O	2.37	0.57
2:B:32:GLU:OE2	2:B:331:HIS:NE2	2.37	0.57
2:B:438:VAL:HG22	18:B:801:CLA:H42	1.86	0.57
18:2:310:CLA:H192	30:2:315:CHL:H8	1.86	0.57
2:B:254:ILE:HG13	2:B:255:LEU:HG	1.85	0.57
2:B:668:ARG:NH1	2:B:699:ALA:O	2.38	0.57
15:3:193:GLY:HA2	15:3:206:PRO:HD2	1.86	0.57
18:A:813:CLA:C1B	21:A:843:BCR:H10C	2.35	0.57
18:B:819:CLA:H193	18:B:820:CLA:H143	1.85	0.57
14:2:126:LEU:HD23	14:2:131:ILE:HG21	1.86	0.57
1:A:372:VAL:HG22	18:A:817:CLA:H42	1.87	0.57
18:B:839:CLA:H161	21:I:101:BCR:H353	1.86	0.57
12:L:163:SER:HB3	12:L:173:PRO:HG3	1.87	0.57
13:1:128:TRP:HD1	13:1:134:ILE:HD11	1.70	0.57
1:A:604:TRP:CH2	18:A:852:CLA:HAB	2.40	0.56
18:B:823:CLA:HMA2	24:1:5001:LMG:HC61	1.87	0.56
2:B:486:LEU:HD12	2:B:494:LEU:HD13	1.86	0.56
6:F:78:ASP:N	6:F:82:LEU:O	2.38	0.56
18:A:822:CLA:HMD2	21:A:845:BCR:H343	1.87	0.56
2:B:428:PHE:CE1	18:B:837:CLA:HAB	2.40	0.56
13:1:98:GLU:HG2	13:1:104:ASN:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:315:CHL:CAB	30:2:318:CHL:HBB2	2.35	0.56
30:4:314:CHL:HHC	30:4:314:CHL:HBB1	1.87	0.56
18:A:806:CLA:HMA1	18:A:807:CLA:HMB3	1.88	0.56
18:B:826:CLA:HAA2	18:B:827:CLA:OBD	2.05	0.56
2:B:276:HIS:HB2	18:B:818:CLA:C1B	2.36	0.56
22:B:848:LHG:O3	22:B:848:LHG:O1	2.24	0.56
2:B:681:ALA:O	2:B:685:THR:OG1	2.20	0.56
30:4:316:CHL:HHC	30:4:316:CHL:HBB1	1.88	0.56
1:A:653:LEU:HD22	2:B:651:LEU:HD21	1.88	0.56
18:A:831:CLA:HMA2	12:L:117:ALA:HB1	1.88	0.56
18:B:824:CLA:CMD	18:B:825:CLA:HAB	2.35	0.56
18:A:802:CLA:H92	2:B:431:PHE:HE1	1.69	0.56
18:A:816:CLA:HAC1	18:A:832:CLA:H42	1.86	0.56
2:B:576:PHE:CE1	18:B:830:CLA:HAC2	2.41	0.56
2:B:351:HIS:HB3	18:B:818:CLA:HED2	1.87	0.55
18:B:821:CLA:HAB	21:B:843:BCR:H351	1.88	0.55
1:A:201:SER:O	1:A:205:HIS:ND1	2.21	0.55
2:B:434:LEU:O	2:B:438:VAL:HG23	2.06	0.55
18:A:838:CLA:H161	10:J:18:TRP:HE3	1.72	0.55
18:B:805:CLA:HAB	18:B:807:CLA:CAD	2.37	0.55
18:B:824:CLA:HBA2	21:B:846:BCR:H16C	1.86	0.55
1:A:80:SER:OG	1:A:186:TYR:HB2	2.07	0.55
2:B:387:PHE:HZ	18:B:826:CLA:HAB	1.71	0.55
18:A:811:CLA:H8	18:A:811:CLA:HBB1	1.88	0.55
3:C:62:PHE:HD1	4:D:192:ILE:HD13	1.71	0.55
18:A:838:CLA:HBB1	18:A:838:CLA:HMB1	1.87	0.55
18:B:841:CLA:HBB2	13:1:66:LEU:HD13	1.88	0.55
2:B:273:MET:O	2:B:277:HIS:ND1	2.31	0.55
17:A:801:CL0:H13	18:B:801:CLA:OBD	2.06	0.55
18:A:828:CLA:H91	22:A:848:LHG:H331	1.89	0.55
18:A:837:CLA:H92	21:F:304:BCR:H16C	1.88	0.55
18:A:853:CLA:H111	18:B:839:CLA:H102	1.87	0.55
30:2:314:CHL:HHC	30:2:314:CHL:HBB1	1.88	0.55
1:A:512:SER:H	1:A:515:TRP:HD1	1.53	0.55
2:B:657:TRP:CE3	18:B:803:CLA:HMA1	2.42	0.55
10:J:32:PHE:CZ	18:J:1103:CLA:HMA3	2.42	0.55
18:A:825:CLA:HBB1	18:A:825:CLA:HMB1	1.89	0.55
18:A:852:CLA:CAD	18:B:803:CLA:HMB3	2.37	0.55
18:3:319:CLA:H2A	18:3:319:CLA:HED2	1.88	0.55
18:A:837:CLA:HED3	2:B:420:SER:HB2	1.88	0.54
14:2:121:PHE:CE2	14:2:231:ALA:HB1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:804:CLA:H203	18:A:812:CLA:H62	1.89	0.54
16:4:212:MET:SD	18:4:308:CLA:HAB	2.47	0.54
1:A:72:GLU:O	1:A:76:ARG:HG3	2.08	0.54
18:A:833:CLA:H2	18:K:1402:CLA:HBA2	1.89	0.54
18:B:839:CLA:H111	18:B:840:CLA:H13	1.90	0.54
12:L:60:ILE:HA	12:L:70:GLU:HG3	1.89	0.54
24:2:322:LMG:HC71	24:2:322:LMG:H122	1.89	0.54
18:A:822:CLA:H18	21:A:845:BCR:H363	1.89	0.54
18:A:853:CLA:H71	18:B:839:CLA:H43	1.90	0.54
18:3:317:CLA:H12	18:3:319:CLA:HBB2	1.90	0.54
10:J:16:THR:HG22	18:J:1101:CLA:H8	1.90	0.54
18:A:805:CLA:HMB1	18:A:805:CLA:HBB1	1.89	0.54
18:B:809:CLA:O1A	18:B:828:CLA:HBD	2.08	0.54
11:K:79:THR:OG1	11:K:80:ALA:N	2.39	0.54
22:B:849:LHG:H201	22:B:849:LHG:H361	1.89	0.54
18:A:806:CLA:HBA1	18:A:808:CLA:H12	1.90	0.54
18:B:822:CLA:C1D	21:B:843:BCR:H402	2.38	0.54
15:3:122:LEU:HD12	15:3:128:ILE:HB	1.90	0.54
1:A:302:HIS:HB2	18:A:816:CLA:C1B	2.38	0.53
18:B:828:CLA:CGA	18:B:828:CLA:H3A	2.38	0.53
18:B:825:CLA:HMB1	18:B:825:CLA:HBB1	1.89	0.53
15:3:211:LEU:HD12	29:3:303:LUT:H222	1.91	0.53
18:B:831:CLA:H191	24:F:306:LMG:H451	1.91	0.53
14:2:182:ILE:HD11	21:2:305:BCR:H312	1.89	0.53
18:A:840:CLA:HMB1	18:A:840:CLA:HBB1	1.89	0.53
1:A:310:PHE:CE1	18:A:819:CLA:HAB	2.39	0.53
1:A:261:SER:HB2	1:A:280:PHE:HE2	1.72	0.53
18:A:823:CLA:HBA1	18:A:827:CLA:H191	1.91	0.53
18:B:816:CLA:HBB1	18:B:816:CLA:HMB1	1.90	0.53
18:B:840:CLA:HED2	26:B:855:DGD:HA52	1.90	0.53
14:2:111:ARG:NH1	30:2:316:CHL:OBD	2.40	0.53
1:A:199:VAL:HG11	18:A:823:CLA:HAC2	1.90	0.53
1:A:356:ALA:HB1	21:A:845:BCR:H312	1.91	0.53
2:B:487:ASN:O	7:G:153:LYS:NZ	2.42	0.53
18:B:829:CLA:H142	21:B:845:BCR:H372	1.91	0.53
15:3:187:PHE:HE2	30:3:316:CHL:HBB2	1.74	0.53
18:B:811:CLA:HAB	9:I:13:GLY:HA3	1.89	0.53
18:B:828:CLA:O1D	18:B:829:CLA:HMA1	2.09	0.53
18:2:312:CLA:HBB2	21:3:305:BCR:HC7	1.90	0.53
1:A:208:ALA:HB2	1:A:314:GLY:HA3	1.91	0.53
17:A:801:CL0:H13	18:B:801:CLA:CAD	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:822:CLA:H12	21:A:845:BCR:H15C	1.91	0.53
18:A:852:CLA:H172	21:B:802:BCR:H343	1.91	0.53
2:B:276:HIS:CE1	2:B:280:ILE:HD13	2.44	0.53
13:1:226:ILE:HG12	13:1:230:LEU:HG	1.91	0.53
30:4:313:CHL:HHC	30:4:313:CHL:HBB1	1.91	0.53
8:H:80:SER:O	8:H:82:GLN:N	2.41	0.52
15:3:107:ARG:HB3	18:3:307:CLA:HBC3	1.89	0.52
2:B:125:TYR:O	2:B:130:ARG:NH1	2.38	0.52
18:2:310:CLA:H111	18:2:317:CLA:H91	1.90	0.52
30:3:316:CHL:HHC	30:3:316:CHL:HBB1	1.91	0.52
16:4:155:ARG:NH1	30:4:302:CHL:OBD	2.42	0.52
18:A:852:CLA:OBD	18:B:803:CLA:HMB3	2.10	0.52
18:B:815:CLA:CHB	21:B:845:BCR:H21C	2.40	0.52
14:2:179:THR:HG22	14:2:187:LYS:HG2	1.91	0.52
1:A:124:TRP:HB3	29:J:1105:LUT:H183	1.90	0.52
1:A:195:TRP:CE2	18:A:812:CLA:HBC3	2.44	0.52
18:A:822:CLA:H8	18:A:822:CLA:H202	1.92	0.52
18:A:837:CLA:H52	21:F:304:BCR:H14C	1.92	0.52
2:B:435:GLY:HA3	18:B:833:CLA:HAB	1.92	0.52
1:A:368:LEU:HD11	18:A:817:CLA:H62	1.92	0.52
1:A:727:ILE:HD11	2:B:566:GLY:HA3	1.92	0.52
18:A:803:CLA:HAA1	18:A:810:CLA:H51	1.91	0.52
18:B:833:CLA:H122	18:F:302:CLA:H43	1.91	0.52
9:I:24:LEU:HD13	21:I:102:BCR:HC8	1.92	0.52
18:1:5009:CLA:HHD	30:4:302:CHL:HBB2	1.90	0.52
18:1:5012:CLA:HBB1	21:4:301:BCR:HC42	1.91	0.52
14:2:196:PRO:HB3	30:2:316:CHL:HBC2	1.91	0.52
18:A:811:CLA:HMC1	21:A:844:BCR:H342	1.92	0.52
13:1:153:LYS:HE3	13:1:158:LYS:HE3	1.91	0.52
30:1:5014:CHL:OMC	18:1:5017:CLA:HAB	2.10	0.52
18:2:309:CLA:HHD	30:2:314:CHL:HBB2	1.92	0.52
1:A:354:TRP:HB3	18:A:804:CLA:HAC1	1.92	0.52
1:A:435:VAL:HA	1:A:438:HIS:CE1	2.45	0.52
13:1:146:GLU:HG2	30:1:5016:CHL:NB	2.25	0.52
18:2:308:CLA:H92	18:2:308:CLA:HMC2	1.92	0.52
18:A:839:CLA:H91	19:A:841:PQN:H292	1.92	0.52
4:D:126:GLY:O	4:D:128:ASN:ND2	2.42	0.52
13:1:128:TRP:NE1	18:1:5017:CLA:OBD	2.40	0.52
15:3:141:VAL:HG21	29:3:304:LUT:H22	1.92	0.52
21:A:855:BCR:H353	21:K:1405:BCR:H323	1.91	0.51
1:A:121:GLN:NE2	18:A:808:CLA:OBD	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:853:CLA:HAA2	18:L:301:CLA:HMB1	1.91	0.51
24:1:5001:LMG:H142	30:1:5016:CHL:HMB2	1.91	0.51
2:B:272:ASP:HB3	18:B:818:CLA:HMA1	1.93	0.51
2:B:585:ASN:HB2	18:B:801:CLA:HBC2	1.93	0.51
10:J:16:THR:HG21	29:J:1105:LUT:H371	1.92	0.51
18:A:824:CLA:HMB3	21:A:846:BCR:H19C	1.92	0.51
2:B:631:LEU:HD22	2:B:724:PHE:HA	1.92	0.51
18:B:828:CLA:HBC3	26:B:855:DGD:HGB3	1.92	0.51
1:A:541:VAL:HG11	1:A:615:HIS:CG	2.45	0.51
22:1:5019:LHG:H192	24:1:5020:LMG:H251	1.92	0.51
18:A:828:CLA:H13	22:A:848:LHG:H202	1.92	0.51
13:1:183:LYS:HG2	18:1:5007:CLA:HBD	1.93	0.51
18:A:829:CLA:HBB2	18:A:836:CLA:HMC2	1.92	0.51
18:A:837:CLA:H72	21:F:304:BCR:H14C	1.93	0.51
13:1:183:LYS:O	13:1:187:ASN:ND2	2.28	0.51
1:A:90:PHE:HE2	21:A:843:BCR:HC21	1.76	0.51
18:A:830:CLA:HAB	18:A:831:CLA:HHB	1.93	0.51
16:4:225:THR:HG23	16:4:227:LYS:H	1.76	0.51
18:B:824:CLA:H71	24:1:5001:LMG:H421	1.91	0.51
18:B:835:CLA:O1A	18:G:1603:CLA:HHB	2.10	0.51
4:D:155:PHE:CZ	4:D:168:HIS:HB3	2.45	0.51
18:A:803:CLA:H201	18:A:808:CLA:H8	1.93	0.51
18:A:803:CLA:HBD	18:A:810:CLA:H12	1.93	0.50
2:B:459:PHE:HB3	18:B:836:CLA:H42	1.93	0.50
3:C:27:GLU:HG3	3:C:44:ARG:HH22	1.76	0.50
13:1:86:TRP:HD1	30:1:5016:CHL:HMD3	1.76	0.50
1:A:302:HIS:HB2	18:A:816:CLA:CHB	2.40	0.50
1:A:687:ALA:O	18:A:802:CLA:HAB	2.11	0.50
18:A:819:CLA:H193	18:A:822:CLA:HAC2	1.94	0.50
18:A:822:CLA:HBB1	18:A:829:CLA:HMD2	1.94	0.50
2:B:658:ALA:HB3	18:B:804:CLA:HBB2	1.91	0.50
1:A:580:PRO:HB3	1:A:727:ILE:HB	1.92	0.50
18:B:831:CLA:HAB	18:B:838:CLA:HBB2	1.94	0.50
1:A:57:LEU:HD21	18:J:1101:CLA:HBC2	1.93	0.50
1:A:98:PHE:CG	18:A:806:CLA:HBC3	2.47	0.50
2:B:547:MET:HE3	2:B:550:LYS:HG3	1.92	0.50
13:1:66:LEU:HD12	29:1:5004:LUT:H41	1.92	0.50
13:1:145:VAL:HG21	21:1:5005:BCR:H16C	1.92	0.50
15:3:232:ARG:NH1	30:3:310:CHL:O1D	2.45	0.50
18:3:317:CLA:HMB2	18:3:319:CLA:C4B	2.41	0.50
2:B:26:ALA:HB1	26:B:855:DGD:HB22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:422:LEU:HD13	2:B:532:LEU:HA	1.93	0.50
29:2:303:LUT:C31	18:2:307:CLA:HMC2	2.42	0.50
18:B:805:CLA:H92	18:B:808:CLA:H172	1.94	0.50
13:1:84:CYS:HB3	13:1:188:GLY:HA3	1.93	0.50
14:2:150:THR:HG23	24:2:322:LMG:HC61	1.93	0.50
15:3:267:ASN:HB3	18:3:309:CLA:OBD	2.11	0.50
1:A:100:GLY:O	1:A:104:SER:OG	2.29	0.50
18:A:819:CLA:HBC3	18:A:825:CLA:H18	1.93	0.50
18:A:826:CLA:O1D	18:A:827:CLA:HMA1	2.12	0.50
13:1:62:ASP:O	13:1:65:ARG:NH1	2.43	0.50
13:1:145:VAL:CG2	21:1:5005:BCR:H16C	2.41	0.50
14:2:85:PHE:HZ	14:2:223:LYS:HE2	1.76	0.50
1:A:195:TRP:CZ2	18:A:809:CLA:HMA1	2.47	0.49
29:J:1105:LUT:H28	29:J:1105:LUT:H361	1.93	0.49
29:1:5003:LUT:H32	18:1:5006:CLA:CAB	2.42	0.49
15:3:187:PHE:CE2	30:3:316:CHL:HBB2	2.47	0.49
21:4:301:BCR:H342	30:4:302:CHL:H51	1.94	0.49
1:A:18:VAL:N	1:A:320:ASN:OD1	2.40	0.49
1:A:24:ARG:HH21	15:3:89:THR:HB	1.76	0.49
18:B:823:CLA:HBB2	21:B:846:BCR:H343	1.93	0.49
18:B:841:CLA:HED1	21:B:846:BCR:H353	1.94	0.49
13:1:105:TRP:HE3	29:1:5004:LUT:H221	1.77	0.49
2:B:194:LEU:HA	2:B:198:ALA:HB3	1.94	0.49
2:B:474:PHE:HD1	23:B:853:LMT:H6E	1.77	0.49
1:A:397:THR:HG23	1:A:613:ILE:HG21	1.95	0.49
14:2:217:LEU:HB3	18:2:306:CLA:HMA1	1.95	0.49
15:3:124:LYS:NZ	15:3:254:GLN:OE1	2.45	0.49
2:B:65:LEU:HD21	21:B:845:BCR:H291	1.94	0.49
14:2:220:LYS:O	14:2:224:ASN:ND2	2.43	0.49
18:A:811:CLA:C4C	18:A:811:CLA:H42	2.43	0.49
2:B:222:LEU:HD12	23:B:856:LMT:H3B	1.93	0.49
15:3:74:GLY:H	15:3:225:LEU:HD12	1.78	0.49
18:A:819:CLA:H101	21:A:846:BCR:H21C	1.94	0.49
18:A:822:CLA:HMA1	18:A:840:CLA:CAB	2.37	0.49
21:A:855:BCR:H362	11:K:109:VAL:HG21	1.93	0.49
3:C:65:VAL:HG23	20:C:102:SF4:S1	2.53	0.49
18:H:1701:CLA:HMB2	18:L:304:CLA:HAA1	1.94	0.49
10:J:10:VAL:HG13	10:J:12:PRO:HD2	1.94	0.49
29:1:5003:LUT:H373	18:1:5006:CLA:H42	1.94	0.49
1:A:305:ALA:CB	18:A:816:CLA:HAB	2.43	0.49
1:A:604:TRP:HE1	18:B:804:CLA:C1D	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:526:GLY:HA2	2:B:582:TRP:CZ3	2.48	0.49
18:A:824:CLA:HBA1	18:A:825:CLA:HED2	1.94	0.48
2:B:123:TRP:CH2	21:B:845:BCR:H272	2.48	0.48
18:B:833:CLA:HMB2	18:F:301:CLA:CAB	2.43	0.48
18:B:836:CLA:H61	18:B:836:CLA:H2	1.63	0.48
14:2:122:ILE:HB	14:2:123:PRO:HD3	1.94	0.48
1:A:387:THR:HG21	1:A:523:VAL:HB	1.95	0.48
1:A:596:ASP:HA	1:A:599:PHE:HB3	1.94	0.48
2:B:243:LEU:HB2	2:B:246:THR:OG1	2.13	0.48
2:B:369:ALA:HB1	2:B:725:LEU:HD11	1.96	0.48
13:1:144:PHE:O	13:1:148:GLN:HG2	2.12	0.48
14:2:159:PHE:HB3	21:2:305:BCR:H363	1.95	0.48
15:3:98:LEU:HD22	30:3:310:CHL:H11	1.95	0.48
16:4:105:GLY:HA2	31:4:304:XAT:H181	1.94	0.48
1:A:458:PHE:CE2	18:A:852:CLA:HMA1	2.48	0.48
18:B:834:CLA:H61	18:B:835:CLA:H12	1.96	0.48
4:D:189:PHE:HB3	5:E:100:ARG:HH12	1.78	0.48
6:F:163:PRO:HG3	10:J:39:PHE:HB2	1.96	0.48
15:3:107:ARG:NH2	15:3:201:ALA:O	2.45	0.48
18:4:308:CLA:H72	18:4:309:CLA:HMA1	1.93	0.48
18:A:806:CLA:H12	18:A:808:CLA:H2	1.95	0.48
19:A:841:PQN:H241	18:J:1101:CLA:HED1	1.94	0.48
2:B:309:ILE:HD13	2:B:320:LYS:HE3	1.95	0.48
18:B:805:CLA:HMA2	22:B:849:LHG:H262	1.94	0.48
18:A:811:CLA:H52	15:3:81:LEU:HD13	1.96	0.48
18:A:819:CLA:HMA2	18:A:823:CLA:C1C	2.43	0.48
22:A:849:LHG:H202	22:A:849:LHG:H172	1.68	0.48
18:B:825:CLA:H72	18:B:827:CLA:H42	1.94	0.48
14:2:162:TRP:CH2	21:2:305:BCR:H321	2.48	0.48
18:A:821:CLA:CBB	24:A:851:LMG:H192	2.44	0.48
2:B:224:PRO:HB3	2:B:229:GLN:HG3	1.95	0.48
18:B:816:CLA:HBB1	21:B:844:BCR:HC42	1.96	0.48
4:D:109:LYS:HG3	4:D:111:GLN:HG3	1.96	0.48
11:K:57:THR:O	11:K:61:LEU:HB2	2.14	0.48
1:A:147:SER:HB2	18:A:827:CLA:HMA2	1.94	0.48
18:A:822:CLA:H43	21:A:846:BCR:H351	1.95	0.48
18:A:840:CLA:CHB	22:A:849:LHG:HC62	2.43	0.48
18:B:811:CLA:H91	18:B:811:CLA:H112	1.70	0.48
18:B:835:CLA:HAA1	18:G:1603:CLA:HMA1	1.94	0.48
14:2:201:PHE:HA	30:2:316:CHL:H11	1.96	0.48
18:A:802:CLA:H143	18:A:802:CLA:H162	1.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:810:CLA:H141	18:A:810:CLA:H161	1.73	0.48
2:B:612:SER:HA	2:B:615:TYR:HE1	1.78	0.48
18:B:830:CLA:C2D	26:B:855:DGD:HB62	2.43	0.48
18:B:808:CLA:H203	18:B:808:CLA:H161	1.70	0.48
18:B:841:CLA:C4B	18:1:5010:CLA:H52	2.44	0.48
18:1:5010:CLA:H62	18:1:5010:CLA:H41	1.43	0.48
18:1:5012:CLA:HBB1	18:1:5012:CLA:HHC	1.96	0.48
1:A:261:SER:HB2	1:A:280:PHE:CE2	2.48	0.48
2:B:167:TRP:CE2	18:B:812:CLA:HMA1	2.49	0.48
18:B:826:CLA:HBA2	18:B:838:CLA:HAA1	1.96	0.48
1:A:259:TYR:CD1	1:A:280:PHE:HB3	2.49	0.47
1:A:338:PHE:CD2	22:A:849:LHG:HC42	2.48	0.47
7:G:136:HIS:CE1	21:G:1604:BCR:H16C	2.48	0.47
24:2:321:LMG:H112	24:2:321:LMG:HC8	1.51	0.47
31:4:304:XAT:H183	18:4:310:CLA:C3B	2.44	0.47
1:A:696:GLY:HA3	2:B:568:CYS:HB2	1.95	0.47
2:B:142:LEU:HG	21:B:845:BCR:H402	1.96	0.47
7:G:92:LEU:HD12	7:G:93:PRO:HD2	1.96	0.47
11:K:61:LEU:HB3	18:K:1403:CLA:CAB	2.32	0.47
13:1:217:HIS:CG	18:1:5008:CLA:HAA2	2.49	0.47
1:A:195:TRP:CZ2	18:A:812:CLA:HBC3	2.49	0.47
1:A:381:PRO:HB3	18:A:817:CLA:HMA2	1.96	0.47
18:A:826:CLA:H8	21:A:847:BCR:H343	1.95	0.47
18:A:832:CLA:H72	21:A:846:BCR:H10C	1.95	0.47
18:B:831:CLA:H61	18:B:831:CLA:H102	1.60	0.47
21:2:305:BCR:HC41	26:2:327:DGD:HB21	1.96	0.47
18:A:829:CLA:H102	18:A:829:CLA:H61	1.49	0.47
2:B:352:MET:HG2	18:B:819:CLA:O1A	2.14	0.47
18:B:806:CLA:HED2	18:B:830:CLA:HBB2	1.96	0.47
18:H:1701:CLA:H41	18:H:1701:CLA:H61	1.55	0.47
10:J:31:ARG:HD2	29:J:1105:LUT:H41	1.96	0.47
18:1:5009:CLA:H71	18:1:5010:CLA:HMA1	1.97	0.47
1:A:614:PHE:HB3	1:A:652:TRP:HZ3	1.79	0.47
2:B:476:VAL:O	2:B:480:SER:N	2.48	0.47
18:B:813:CLA:HMC1	21:B:844:BCR:C10	2.44	0.47
16:4:106:VAL:HA	16:4:109:MET:HE3	1.97	0.47
18:A:802:CLA:HBB1	18:A:802:CLA:HMB1	1.95	0.47
18:A:824:CLA:HAA2	18:A:825:CLA:OBD	2.14	0.47
18:A:826:CLA:H71	18:A:826:CLA:H112	1.58	0.47
18:B:810:CLA:H91	18:B:810:CLA:H111	1.75	0.47
18:B:812:CLA:HBA2	23:G:1605:LMT:H11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:823:CLA:HMB3	18:B:841:CLA:C1D	2.44	0.47
16:4:150:HIS:HD2	18:4:315:CLA:HMB1	1.79	0.47
18:A:817:CLA:H203	18:A:825:CLA:H11	1.95	0.47
6:F:113:SER:OG	6:F:115:PRO:HD2	2.14	0.47
28:F:310:ZEX:O3	18:1:5018:CLA:H2	2.14	0.47
13:1:119:ALA:H	13:1:129:GLY:HA3	1.79	0.47
18:2:312:CLA:H8	18:2:312:CLA:H122	1.52	0.47
1:A:91:LEU:HD23	21:J:1104:BCR:H282	1.96	0.47
1:A:370:ILE:HG22	18:A:824:CLA:HED2	1.97	0.47
1:A:467:MET:HB2	1:A:476:MET:HG2	1.96	0.47
1:A:470:LEU:HG	18:B:810:CLA:HMC3	1.97	0.47
1:A:547:PHE:HZ	18:A:852:CLA:HBB2	1.80	0.47
18:A:809:CLA:H42	18:3:311:CLA:H2	1.97	0.47
15:3:197:SER:OG	15:3:202:TYR:O	2.33	0.47
18:A:810:CLA:H61	18:A:810:CLA:H41	1.57	0.47
18:A:853:CLA:H171	12:L:141:LEU:HD11	1.95	0.47
18:B:806:CLA:H122	18:B:806:CLA:HBD	1.96	0.47
4:D:206:LYS:HD3	4:D:211:LEU:HD21	1.96	0.47
13:1:121:TYR:CD1	18:1:5011:CLA:H2	2.50	0.47
18:1:5006:CLA:H41	18:1:5006:CLA:H61	1.48	0.47
15:3:72:LEU:HD21	15:3:99:ALA:HB2	1.97	0.47
30:4:316:CHL:HBA1	30:4:316:CHL:H3A	1.61	0.47
4:D:110:GLU:HA	4:D:123:MET:O	2.14	0.46
15:3:142:ILE:HG22	15:3:144:PRO:HG2	1.97	0.46
1:A:402:ILE:HD12	18:A:805:CLA:H143	1.96	0.46
1:A:446:LEU:HB3	1:A:554:LEU:HD13	1.97	0.46
18:A:803:CLA:H91	18:A:803:CLA:H111	1.65	0.46
18:A:808:CLA:HMA1	10:J:27:ILE:HD13	1.96	0.46
18:B:826:CLA:HBA1	18:B:826:CLA:H3A	1.51	0.46
18:A:803:CLA:H11	18:A:810:CLA:H62	1.97	0.46
2:B:50:HIS:HE1	18:B:806:CLA:H161	1.80	0.46
2:B:184:GLY:HA3	2:B:285:LEU:HD12	1.97	0.46
18:B:815:CLA:H3A	21:B:845:BCR:H392	1.96	0.46
18:F:302:CLA:H3A	18:F:302:CLA:HBA1	1.64	0.46
21:G:1604:BCR:H351	21:G:1604:BCR:H15C	1.60	0.46
15:3:98:LEU:HB3	30:3:310:CHL:H11	1.97	0.46
18:A:805:CLA:H162	18:A:805:CLA:H122	1.65	0.46
2:B:300:SER:H	7:G:90:GLN:HE21	1.62	0.46
6:F:154:GLN:NE2	24:F:306:LMG:O9	2.48	0.46
6:F:188:ASP:OD1	6:F:189:LYS:N	2.46	0.46
1:A:155:ALA:HB2	1:A:383:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:835:CLA:H13	18:A:835:CLA:H102	1.58	0.46
21:L:303:BCR:H351	21:L:303:BCR:H15C	1.76	0.46
29:1:5004:LUT:H12	18:1:5009:CLA:CBB	2.46	0.46
18:2:312:CLA:H61	18:2:312:CLA:H41	1.44	0.46
30:2:314:CHL:H62	30:2:314:CHL:H41	1.56	0.46
15:3:213:PHE:HB2	18:3:307:CLA:HBA1	1.97	0.46
18:4:315:CLA:H162	18:4:315:CLA:H203	1.69	0.46
18:A:811:CLA:H11	15:3:81:LEU:HD13	1.98	0.46
18:B:814:CLA:H151	18:B:814:CLA:H111	1.70	0.46
18:F:303:CLA:H112	18:F:303:CLA:H143	1.73	0.46
28:F:310:ZEX:H191	30:4:318:CHL:H2	1.97	0.46
18:K:1403:CLA:O1D	18:K:1403:CLA:H2	2.15	0.46
31:4:304:XAT:H31	31:4:304:XAT:H391	1.70	0.46
1:A:93:LEU:O	1:A:97:TYR:HD2	1.99	0.46
1:A:206:HIS:HB3	18:A:823:CLA:HED3	1.98	0.46
1:A:283:PHE:HZ	18:A:816:CLA:H51	1.81	0.46
1:A:321:TRP:CD1	11:K:91:LEU:HD22	2.49	0.46
1:A:389:TYR:HB3	1:A:754:ILE:HD11	1.98	0.46
1:A:686:TRP:CD2	17:A:801:CL0:H5	2.50	0.46
18:A:802:CLA:H203	18:A:839:CLA:H2	1.97	0.46
18:A:815:CLA:H101	18:K:1402:CLA:HMD3	1.97	0.46
18:A:820:CLA:H111	18:A:820:CLA:H93	1.74	0.46
18:A:822:CLA:H41	18:A:822:CLA:H61	1.56	0.46
2:B:142:LEU:HD23	2:B:145:LEU:HD12	1.97	0.46
2:B:428:PHE:CD1	18:B:837:CLA:HAB	2.51	0.46
18:1:5006:CLA:H92	18:1:5006:CLA:H62	1.67	0.46
29:2:303:LUT:H15	29:2:303:LUT:H201	1.74	0.46
6:F:167:PHE:HB2	21:F:304:BCR:H403	1.98	0.46
18:1:5006:CLA:HAC1	18:1:5015:CLA:O1A	2.15	0.46
1:A:521:VAL:HG12	1:A:528:ALA:HB3	1.98	0.46
1:A:611:VAL:HG21	17:A:801:CL0:H64	1.98	0.46
1:A:711:HIS:NE2	18:A:838:CLA:HAC1	2.31	0.46
18:A:819:CLA:H72	18:A:822:CLA:H42	1.98	0.46
18:B:820:CLA:HED2	18:B:824:CLA:HED2	1.98	0.46
18:1:5006:CLA:H192	18:1:5015:CLA:H201	1.98	0.46
16:4:203:LYS:HG3	18:4:311:CLA:HED2	1.98	0.46
1:A:218:TRP:NE1	18:A:817:CLA:O1D	2.38	0.45
18:B:806:CLA:H3A	18:B:806:CLA:HBA1	1.46	0.45
18:B:820:CLA:H203	18:B:820:CLA:H161	1.75	0.45
13:1:229:VAL:HG21	18:1:5008:CLA:HMD1	1.98	0.45
15:3:263:PRO:HG3	18:3:314:CLA:HMB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:TRP:O	1:A:323:ILE:N	2.47	0.45
18:A:822:CLA:H141	22:A:849:LHG:H202	1.99	0.45
2:B:519:VAL:O	2:B:523:ILE:HG12	2.17	0.45
2:B:594:TRP:HB2	18:B:836:CLA:HMC1	1.97	0.45
29:1:5004:LUT:H28	29:1:5004:LUT:H361	1.98	0.45
18:1:5018:CLA:H2A	18:1:5018:CLA:HED2	1.98	0.45
1:A:417:PHE:CD1	1:A:421:ASP:HB2	2.51	0.45
18:B:805:CLA:H61	22:B:849:LHG:H191	1.97	0.45
3:C:61:ASP:O	5:E:118:ASN:ND2	2.46	0.45
26:2:327:DGD:HG11	18:4:311:CLA:CHD	2.47	0.45
16:4:175:TYR:HB3	30:4:317:CHL:C3D	2.47	0.45
1:A:461:TYR:CE2	1:A:540:LEU:HB3	2.52	0.45
1:A:471:GLY:HA3	2:B:99:PRO:HG2	1.97	0.45
18:A:834:CLA:H11	18:A:835:CLA:O1A	2.16	0.45
2:B:612:SER:HA	2:B:615:TYR:CE1	2.52	0.45
21:B:802:BCR:H363	18:B:804:CLA:H72	1.97	0.45
18:B:808:CLA:HED2	9:I:5:PRO:HB3	1.99	0.45
18:H:1701:CLA:H121	12:L:81:TRP:NE1	2.32	0.45
29:3:304:LUT:H24	30:3:310:CHL:O1A	2.16	0.45
18:A:819:CLA:H2	18:A:823:CLA:HBB1	1.99	0.45
18:A:832:CLA:HBA2	18:A:833:CLA:HMB3	1.98	0.45
18:B:806:CLA:H161	18:B:806:CLA:H202	1.73	0.45
18:B:835:CLA:H62	18:B:835:CLA:H41	1.60	0.45
18:K:1402:CLA:H61	18:K:1402:CLA:H41	1.52	0.45
14:2:111:ARG:HA	14:2:114:MET:HE3	1.98	0.45
18:3:311:CLA:HED2	18:3:317:CLA:H2	1.98	0.45
1:A:321:TRP:CZ3	18:A:811:CLA:HMA1	2.52	0.45
1:A:453:LEU:HD21	18:A:835:CLA:HAB	1.98	0.45
18:A:819:CLA:HBA1	18:A:823:CLA:C3B	2.46	0.45
18:A:835:CLA:H111	18:A:835:CLA:H72	1.82	0.45
18:A:835:CLA:H161	18:A:835:CLA:H122	1.68	0.45
18:A:835:CLA:HBB2	18:A:836:CLA:HBC3	1.99	0.45
18:A:853:CLA:H102	18:B:839:CLA:H61	1.99	0.45
2:B:498:LEU:HA	2:B:501:ILE:HG22	1.98	0.45
6:F:213:TRP:CG	6:F:214:PRO:HD3	2.52	0.45
13:1:177:PHE:CE2	13:1:181:LYS:HE3	2.52	0.45
29:3:303:LUT:H401	29:3:303:LUT:H35	1.80	0.45
1:A:411:ALA:HB2	21:A:846:BCR:H402	1.99	0.45
18:A:806:CLA:CAB	21:J:1104:BCR:H271	2.44	0.45
18:A:811:CLA:H62	18:A:811:CLA:H92	1.83	0.45
16:4:215:PHE:CD2	31:4:304:XAT:H12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:813:CLA:H62	18:A:813:CLA:H102	1.64	0.45
18:A:828:CLA:H122	18:A:828:CLA:H162	1.52	0.45
2:B:173:SER:O	2:B:177:HIS:ND1	2.33	0.45
24:G:1607:LMG:HC71	24:G:1607:LMG:HC2	1.42	0.45
13:1:225:THR:HG22	13:1:226:ILE:H	1.82	0.45
29:3:304:LUT:H32	30:3:310:CHL:CAB	2.42	0.45
18:A:840:CLA:H93	18:A:840:CLA:H111	1.70	0.45
3:C:9:ASP:OD2	5:E:100:ARG:NH1	2.48	0.45
18:F:303:CLA:H3A	18:F:303:CLA:HBA1	1.76	0.45
18:G:1603:CLA:H111	18:G:1603:CLA:H142	1.69	0.45
18:J:1101:CLA:HBB1	29:J:1105:LUT:H383	1.98	0.45
1:A:55:TRP:HE3	22:A:848:LHG:H111	1.81	0.45
18:A:816:CLA:H62	18:A:816:CLA:H41	1.55	0.45
2:B:486:LEU:O	2:B:490:ARG:HG3	2.17	0.45
18:B:803:CLA:H3A	18:B:803:CLA:HBA2	1.75	0.45
23:B:856:LMT:H51	23:G:1606:LMT:H52	1.99	0.45
13:1:85:ARG:HB3	18:1:5006:CLA:CBC	2.43	0.45
17:A:801:CL0:H21	2:B:625:TRP:HD1	1.82	0.44
18:A:802:CLA:H91	18:A:802:CLA:H112	1.56	0.44
18:A:825:CLA:H91	18:A:825:CLA:H111	1.69	0.44
2:B:199:ILE:HB	2:B:200:PRO:HD3	1.99	0.44
2:B:348:VAL:O	2:B:352:MET:HG3	2.17	0.44
2:B:351:HIS:ND1	18:B:818:CLA:OBD	2.48	0.44
2:B:365:PHE:HD2	2:B:734:GLY:HA2	1.82	0.44
18:B:807:CLA:H161	18:B:807:CLA:H122	1.75	0.44
18:B:819:CLA:H41	18:B:819:CLA:H61	1.46	0.44
26:J:1106:DGD:HAS1	26:J:1106:DGD:HAH2	1.68	0.44
18:2:307:CLA:OBD	18:2:312:CLA:H2	2.17	0.44
15:3:223:LEU:HA	15:3:226:LYS:HD2	1.98	0.44
15:3:238:ILE:HG21	29:3:304:LUT:H14	1.99	0.44
18:A:815:CLA:H41	18:A:815:CLA:H62	1.47	0.44
18:A:831:CLA:H141	18:A:831:CLA:H161	1.80	0.44
2:B:662:MET:HB2	18:B:804:CLA:C1C	2.47	0.44
18:B:809:CLA:CGA	18:B:809:CLA:C1A	2.95	0.44
15:3:132:THR:O	30:3:312:CHL:HED3	2.16	0.44
29:3:304:LUT:H35	29:3:304:LUT:H401	1.72	0.44
2:B:526:GLY:HA2	2:B:582:TRP:HZ3	1.81	0.44
13:1:121:TYR:CE1	18:1:5011:CLA:H2	2.52	0.44
18:3:315:CLA:H161	18:3:315:CLA:H122	1.45	0.44
1:A:394:SER:CB	18:A:826:CLA:HMA1	2.47	0.44
18:A:804:CLA:H121	21:A:843:BCR:HC41	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:806:CLA:H151	18:B:814:CLA:CAD	2.48	0.44
18:B:816:CLA:CAB	21:B:843:BCR:H333	2.48	0.44
1:A:23:ASP:HB2	1:A:76:ARG:HH12	1.83	0.44
1:A:682:ALA:HA	1:A:685:VAL:HG22	1.99	0.44
18:A:807:CLA:HMC3	18:A:808:CLA:HMD2	1.99	0.44
21:A:847:BCR:H391	18:F:301:CLA:HMA1	1.99	0.44
2:B:80:ASP:HB2	2:B:84:VAL:HG23	2.00	0.44
2:B:366:THR:HG21	2:B:730:SER:HB3	1.98	0.44
18:B:840:CLA:H3A	18:B:840:CLA:HBA2	1.52	0.44
18:1:5009:CLA:H202	18:1:5009:CLA:H162	1.74	0.44
18:2:306:CLA:H41	18:2:307:CLA:HMA2	2.00	0.44
15:3:208:PHE:HB3	18:3:307:CLA:HMD1	1.98	0.44
18:3:314:CLA:CHA	18:3:314:CLA:HBA1	2.48	0.44
16:4:116:THR:HA	16:4:121:ILE:O	2.17	0.44
21:4:301:BCR:H271	18:4:310:CLA:NB	2.32	0.44
1:A:227:LEU:HB3	1:A:259:TYR:CE2	2.53	0.44
1:A:378:ALA:CB	18:A:825:CLA:HAC2	2.48	0.44
1:A:466:THR:HG21	18:B:810:CLA:HAB	1.99	0.44
18:A:832:CLA:HMD2	18:A:833:CLA:HAB	2.00	0.44
2:B:257:LEU:HD13	18:B:818:CLA:HMB2	2.00	0.44
2:B:365:PHE:CD2	2:B:734:GLY:HA2	2.53	0.44
18:B:809:CLA:H8	18:B:809:CLA:H51	1.58	0.44
6:F:172:GLY:HA3	6:F:213:TRP:CE2	2.53	0.44
6:F:203:ALA:O	6:F:207:VAL:HG13	2.17	0.44
8:H:65:GLY:HA2	8:H:67:TRP:CE2	2.53	0.44
21:2:305:BCR:H402	30:2:318:CHL:HAA2	1.99	0.44
18:3:311:CLA:HMD2	18:3:317:CLA:C1D	2.48	0.44
18:A:808:CLA:H62	18:A:808:CLA:H41	1.87	0.44
2:B:294:ASN:HB3	7:G:110:GLU:HA	1.99	0.44
13:1:150:SER:HB2	30:1:5016:CHL:HMA1	1.99	0.44
16:4:148:LEU:HB3	21:4:301:BCR:C16	2.47	0.44
18:B:808:CLA:H62	18:B:808:CLA:H101	1.65	0.44
18:B:841:CLA:HMB1	18:B:841:CLA:HBB1	2.00	0.44
13:1:94:ILE:HG21	13:1:198:ILE:HD13	1.99	0.44
14:2:160:ILE:HG21	18:2:317:CLA:HMC3	1.99	0.44
18:4:315:CLA:H3A	18:4:315:CLA:HBA1	1.57	0.44
1:A:751:LEU:HD23	1:A:751:LEU:HA	1.81	0.44
2:B:91:ILE:HB	2:B:112:PRO:HB2	1.99	0.44
6:F:213:TRP:CD1	6:F:214:PRO:HD3	2.53	0.44
29:1:5003:LUT:H35	29:1:5003:LUT:H401	1.75	0.44
29:1:5004:LUT:H363	18:1:5017:CLA:HMC2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:3:136:TRP:CE2	15:3:137:PHE:HD1	2.35	0.44
18:A:813:CLA:C3B	21:A:843:BCR:H10C	2.47	0.43
2:B:547:MET:HE2	2:B:570:ILE:HD13	2.00	0.43
18:B:823:CLA:H41	18:B:823:CLA:H61	1.43	0.43
3:C:66:ARG:HD3	3:C:66:ARG:HA	1.76	0.43
10:J:12:PRO:HB2	29:J:1105:LUT:H372	1.99	0.43
1:A:195:TRP:CD1	18:A:811:CLA:HED2	2.52	0.43
1:A:355:HIS:CE1	1:A:416:ILE:HG21	2.53	0.43
1:A:394:SER:HA	18:A:826:CLA:HMB3	2.00	0.43
1:A:396:PHE:O	1:A:400:MET:HG2	2.18	0.43
1:A:684:PHE:CD2	21:A:847:BCR:H363	2.53	0.43
18:A:832:CLA:C2D	18:A:833:CLA:HAB	2.48	0.43
2:B:377:TYR:CD2	18:B:828:CLA:HAB	2.53	0.43
13:1:65:ARG:HH21	24:1:5020:LMG:HC3	1.83	0.43
18:2:309:CLA:H3A	18:2:309:CLA:HBA2	1.62	0.43
18:2:317:CLA:H3A	18:2:317:CLA:HBA1	1.61	0.43
21:3:306:BCR:H392	21:3:306:BCR:H23C	2.00	0.43
1:A:66:SER:HB3	1:A:420:ARG:HH22	1.82	0.43
1:A:544:ILE:HG21	17:A:801:CL0:H60	2.01	0.43
2:B:72:GLY:HA2	2:B:87:ILE:HB	1.99	0.43
18:B:823:CLA:H203	7:G:134:ILE:HA	1.99	0.43
18:2:306:CLA:H3A	18:2:306:CLA:HBA2	1.44	0.43
16:4:215:PHE:CE2	31:4:304:XAT:H10	2.53	0.43
29:4:303:LUT:H11	29:4:303:LUT:H191	1.92	0.43
1:A:53:TRP:HE3	1:A:54:ILE:HG13	1.84	0.43
1:A:64:PHE:CD1	18:A:804:CLA:HMC2	2.53	0.43
18:A:803:CLA:H11	18:A:803:CLA:H52	1.63	0.43
18:A:813:CLA:HMB1	18:A:813:CLA:HBB1	2.01	0.43
2:B:62:SER:HA	2:B:65:LEU:HD12	2.00	0.43
21:B:843:BCR:H382	7:G:130:ALA:HB1	2.00	0.43
11:K:62:MET:SD	18:K:1403:CLA:HMC2	2.58	0.43
18:2:307:CLA:H41	18:2:307:CLA:H61	1.57	0.43
15:3:139:THR:HG21	30:3:312:CHL:HMA3	2.00	0.43
1:A:225:VAL:HG13	1:A:245:PRO:HB3	2.00	0.43
17:A:801:CL0:H58	17:A:801:CL0:H50	1.78	0.43
2:B:390:GLY:HA2	21:B:847:BCR:H393	1.99	0.43
7:G:137:ILE:HG12	21:G:1604:BCR:H392	2.00	0.43
18:K:1403:CLA:H2A	18:K:1403:CLA:HED2	2.00	0.43
13:1:127:PRO:HG2	13:1:128:TRP:CE3	2.53	0.43
1:A:604:TRP:HH2	18:A:852:CLA:HAB	1.83	0.43
18:A:840:CLA:H62	24:A:851:LMG:H332	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:811:CLA:H51	18:B:811:CLA:H11	1.79	0.43
18:B:841:CLA:H62	18:B:841:CLA:H41	1.60	0.43
18:B:841:CLA:HBC1	24:1:5001:LMG:HC62	1.99	0.43
30:2:315:CHL:HMB1	30:2:315:CHL:CBB	2.47	0.43
1:A:58:HIS:HB2	22:A:848:LHG:H112	2.01	0.43
1:A:499:ALA:N	1:A:500:PRO:HD2	2.34	0.43
1:A:680:LEU:HD13	18:B:801:CLA:H2	2.01	0.43
1:A:699:TYR:OH	18:A:802:CLA:OBD	2.27	0.43
18:A:816:CLA:HBA2	18:A:816:CLA:H3A	1.44	0.43
18:A:822:CLA:HBB	18:A:840:CLA:CAB	2.49	0.43
2:B:262:HIS:CE1	2:B:264:GLN:HB3	2.53	0.43
18:B:806:CLA:HHC	18:B:806:CLA:HBB1	2.00	0.43
4:D:191:SER:HB2	4:D:194:LYS:HG3	2.01	0.43
13:1:198:ILE:HG23	13:1:210:PRO:HG3	2.00	0.43
18:1:5009:CLA:HED2	18:1:5009:CLA:H2A	2.01	0.43
30:1:5014:CHL:C2C	18:1:5017:CLA:HMC3	2.49	0.43
15:3:75:ASP:HA	30:3:310:CHL:HED2	2.01	0.43
16:4:220:ILE:HD12	18:4:307:CLA:HAC2	2.01	0.43
18:4:307:CLA:H61	18:4:307:CLA:H41	1.83	0.43
1:A:272:LEU:HD21	11:K:116:VAL:HG22	1.99	0.43
18:A:821:CLA:HMD2	21:A:855:BCR:H23C	2.01	0.43
18:A:836:CLA:H111	18:A:836:CLA:H142	1.68	0.43
19:A:841:PQN:H161	19:A:841:PQN:H141	1.57	0.43
18:B:811:CLA:H141	8:H:107:GLY:HA2	2.01	0.43
18:B:826:CLA:HBB1	18:B:826:CLA:HMB1	1.99	0.43
4:D:72:PRO:HA	4:D:73:PRO:HD3	1.93	0.43
24:1:5001:LMG:H162	30:1:5016:CHL:C2B	2.48	0.43
15:3:158:PHE:HA	15:3:161:GLU:HG2	2.01	0.43
30:4:318:CHL:H61	30:4:318:CHL:H41	1.67	0.43
18:A:803:CLA:H3A	18:A:803:CLA:HBA2	1.40	0.43
18:A:808:CLA:CBB	21:J:1104:BCR:HC8	2.49	0.43
18:A:811:CLA:HBD	18:A:811:CLA:HBA1	1.99	0.43
2:B:467:HIS:HA	2:B:478:LEU:HD12	2.01	0.43
18:B:809:CLA:HBB1	18:B:809:CLA:H91	2.00	0.43
18:B:826:CLA:H71	18:B:837:CLA:H12	2.01	0.43
3:C:61:ASP:O	5:E:78:ARG:NH1	2.50	0.43
18:F:303:CLA:H11	18:F:303:CLA:H52	1.82	0.43
8:H:73:ASP:HB2	12:L:171:LYS:HE2	2.01	0.43
1:A:55:TRP:CE3	22:A:848:LHG:H111	2.53	0.43
18:A:805:CLA:H41	18:A:805:CLA:H61	1.40	0.43
18:A:823:CLA:H62	18:A:823:CLA:H102	1.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:839:CLA:H192	10:J:22:LEU:HD23	2.01	0.43
21:A:845:BCR:H15C	21:A:845:BCR:H351	1.69	0.43
2:B:295:PHE:HE1	18:B:813:CLA:HMA1	1.84	0.43
18:B:818:CLA:H143	18:B:818:CLA:H111	1.68	0.43
6:F:215:ILE:HG12	18:4:309:CLA:H2	2.00	0.43
11:K:67:ARG:HD2	11:K:99:PHE:HB2	2.01	0.43
13:1:171:SER:HA	13:1:177:PHE:HB2	2.00	0.43
18:2:313:CLA:CAD	30:2:314:CHL:H102	2.48	0.43
1:A:405:PHE:O	18:A:828:CLA:HMC1	2.18	0.42
18:A:833:CLA:C2	18:K:1402:CLA:H2	2.49	0.42
2:B:61:THR:HB	2:B:142:LEU:HD13	2.00	0.42
3:C:41:SER:HB2	4:D:185:VAL:H	1.84	0.42
15:3:202:TYR:HA	18:3:307:CLA:O1D	2.19	0.42
18:A:819:CLA:HMB2	18:A:823:CLA:HMA3	2.00	0.42
18:A:840:CLA:HBA1	24:A:851:LMG:H321	2.01	0.42
2:B:186:SER:O	18:B:815:CLA:HBB2	2.20	0.42
2:B:531:THR:HG21	18:B:838:CLA:HMB3	2.01	0.42
18:B:801:CLA:H161	18:B:801:CLA:H202	1.74	0.42
18:B:828:CLA:H193	18:B:828:CLA:H162	1.71	0.42
23:B:853:LMT:H52	18:F:303:CLA:HMC3	2.00	0.42
5:E:122:LEU:HD23	5:E:122:LEU:HA	1.86	0.42
23:2:325:LMT:H11	23:2:325:LMT:H41	1.87	0.42
15:3:123:GLY:HA3	15:3:133:ALA:HB1	2.01	0.42
16:4:103:MET:SD	18:4:305:CLA:HAB	2.59	0.42
2:B:53:GLN:HG2	18:B:806:CLA:HMA1	2.01	0.42
2:B:95:HIS:CE1	18:B:810:CLA:HMB3	2.54	0.42
2:B:308:HIS:HA	18:B:841:CLA:HMD1	2.01	0.42
2:B:659:THR:HA	18:B:804:CLA:HAB	2.00	0.42
2:B:667:TRP:HA	19:B:842:PQN:H8	2.01	0.42
22:B:848:LHG:HC12	13:1:66:LEU:HA	2.01	0.42
7:G:82:PHE:HB2	13:1:151:MET:SD	2.59	0.42
29:J:1105:LUT:H181	29:J:1105:LUT:C8	2.45	0.42
18:1:5010:CLA:H43	18:1:5010:CLA:HED3	2.01	0.42
21:2:305:BCR:H392	21:2:305:BCR:H282	1.33	0.42
15:3:101:GLY:HA2	18:3:317:CLA:HED2	2.01	0.42
15:3:169:GLU:OE1	15:3:172:ARG:NH2	2.41	0.42
16:4:153:GLU:OE2	16:4:156:ARG:NH2	2.49	0.42
1:A:516:GLY:O	1:A:531:PRO:HG3	2.19	0.42
2:B:339:ALA:HB2	21:B:847:BCR:H372	2.02	0.42
2:B:407:VAL:O	2:B:411:MET:HG2	2.20	0.42
2:B:410:ARG:O	2:B:414:HIS:ND1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:700:LEU:HD22	2:B:704:GLN:NE2	2.34	0.42
18:B:818:CLA:H193	18:B:818:CLA:H162	1.84	0.42
18:B:823:CLA:HBC2	18:B:824:CLA:HAA2	2.01	0.42
7:G:145:THR:HA	7:G:148:ASN:ND2	2.34	0.42
14:2:180:ASP:HB3	14:2:183:PHE:O	2.20	0.42
14:2:236:TRP:CZ3	30:2:315:CHL:HHB	2.54	0.42
15:3:193:GLY:HA3	15:3:207:PHE:CD2	2.54	0.42
18:A:812:CLA:H41	18:A:812:CLA:H61	1.70	0.42
18:A:817:CLA:H71	18:A:817:CLA:C3B	2.50	0.42
18:A:828:CLA:H61	18:A:828:CLA:H92	1.67	0.42
18:A:837:CLA:HED2	2:B:424:TRP:HB2	2.02	0.42
18:B:831:CLA:HMC3	18:B:838:CLA:HBB1	2.02	0.42
21:K:1405:BCR:H351	21:K:1405:BCR:H15C	1.81	0.42
12:L:203:LEU:HD11	21:L:302:BCR:H381	2.02	0.42
14:2:92:LEU:HD13	18:2:309:CLA:H42	2.01	0.42
18:2:310:CLA:HMD2	18:2:317:CLA:C1D	2.49	0.42
2:B:278:LEU:O	2:B:282:ILE:HG22	2.19	0.42
7:G:76:ARG:NH1	7:G:119:ASP:OD2	2.53	0.42
14:2:109:HIS:HB3	14:2:229:MET:SD	2.60	0.42
29:2:303:LUT:H11	29:2:303:LUT:H191	1.88	0.42
15:3:273:LYS:HG2	18:3:301:CLA:CGA	2.49	0.42
29:3:304:LUT:H31	29:3:304:LUT:H391	1.85	0.42
18:3:309:CLA:H12	18:3:314:CLA:CAD	2.50	0.42
18:3:319:CLA:H41	18:3:319:CLA:H61	1.45	0.42
16:4:169:ASP:HB3	16:4:172:PHE:O	2.19	0.42
1:A:321:TRP:HZ3	18:A:811:CLA:HMA1	1.84	0.42
18:A:803:CLA:HMC3	18:A:805:CLA:HED2	2.02	0.42
18:A:807:CLA:H192	18:A:807:CLA:H162	1.74	0.42
18:A:809:CLA:H11	18:A:811:CLA:H43	2.01	0.42
21:A:844:BCR:H351	21:A:844:BCR:H15C	1.92	0.42
18:A:853:CLA:HMC3	18:B:839:CLA:ND	2.34	0.42
2:B:589:TRP:CE2	18:B:803:CLA:H161	2.54	0.42
18:B:823:CLA:HED1	7:G:89:LYS:HE3	2.01	0.42
18:B:833:CLA:HBA2	18:B:833:CLA:H3A	1.77	0.42
18:B:837:CLA:H91	18:B:837:CLA:H111	1.78	0.42
18:B:841:CLA:HMC3	18:1:5010:CLA:H12	2.01	0.42
6:F:138:LEU:HD13	6:F:146:PRO:HB3	2.02	0.42
30:4:316:CHL:H62	30:4:316:CHL:H101	1.87	0.42
18:A:802:CLA:H201	18:A:807:CLA:H202	2.02	0.42
2:B:478:LEU:HA	2:B:486:LEU:HD13	2.02	0.42
18:B:822:CLA:HMB1	24:1:5001:LMG:H362	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:105:TRP:CD1	4:D:151:ILE:HG21	2.54	0.42
18:F:302:CLA:H61	18:F:302:CLA:H41	1.70	0.42
11:K:67:ARG:HH12	11:K:97:ALA:HB3	1.85	0.42
29:1:5004:LUT:H12	18:1:5009:CLA:CAB	2.49	0.42
15:3:270:THR:HG22	15:3:272:LEU:H	1.85	0.42
1:A:595:TRP:CD1	18:A:828:CLA:HMD1	2.54	0.42
18:A:811:CLA:HBB1	18:A:811:CLA:HHC	2.02	0.42
18:A:822:CLA:H151	18:A:829:CLA:HMC2	2.02	0.42
18:B:811:CLA:H3A	18:B:811:CLA:HBA1	1.67	0.42
18:B:820:CLA:HMA2	18:B:825:CLA:C1C	2.49	0.42
6:F:156:HIS:HB3	6:F:159:GLU:CD	2.40	0.42
7:G:112:VAL:O	7:G:116:LYS:HG3	2.19	0.42
18:G:1603:CLA:H92	18:G:1603:CLA:H62	1.70	0.42
29:1:5003:LUT:H11	29:1:5003:LUT:H191	1.86	0.42
18:1:5015:CLA:H203	18:1:5015:CLA:H161	1.71	0.42
14:2:106:GLU:HB2	18:2:309:CLA:CHB	2.50	0.42
15:3:107:ARG:HB3	18:3:307:CLA:CBC	2.50	0.42
18:4:305:CLA:HMD2	30:4:314:CHL:CGA	2.50	0.42
1:A:22:VAL:HA	1:A:191:PRO:HA	2.02	0.42
1:A:584:PRO:HD3	2:B:561:GLY:HA2	2.02	0.42
18:A:819:CLA:C2	18:A:823:CLA:HBB1	2.50	0.42
18:A:824:CLA:O1A	18:A:834:CLA:HMA1	2.19	0.42
18:A:838:CLA:H93	6:F:203:ALA:HB1	2.02	0.42
2:B:282:ILE:HD11	21:G:1604:BCR:H393	2.01	0.42
18:B:824:CLA:HBA1	18:B:824:CLA:H3A	1.80	0.42
11:K:87:ARG:HG2	11:K:88:ASP:N	2.35	0.42
21:L:303:BCR:C19	18:L:305:CLA:HAB	2.50	0.42
13:1:78:GLU:O	13:1:82:ILE:HG12	2.20	0.42
14:2:220:LYS:HG3	18:2:312:CLA:HED2	2.01	0.42
31:2:304:XAT:H391	31:2:304:XAT:H31	1.67	0.42
15:3:171:ARG:HD3	30:3:316:CHL:CBB	2.50	0.42
18:4:309:CLA:HMD2	18:4:315:CLA:C1D	2.50	0.42
1:A:595:TRP:NE1	18:A:828:CLA:HMD1	2.34	0.41
18:B:807:CLA:H91	18:B:828:CLA:HBC1	2.01	0.41
18:B:827:CLA:HBB1	18:B:827:CLA:HMB1	2.02	0.41
21:2:305:BCR:HC32	26:2:327:DGD:O2E	2.20	0.41
15:3:143:PRO:N	15:3:144:PRO:HD2	2.35	0.41
15:3:158:PHE:CD1	18:3:315:CLA:HBD	2.55	0.41
1:A:343:HIS:HA	1:A:346:LEU:HD12	2.01	0.41
1:A:701:GLN:O	1:A:705:GLU:HG3	2.21	0.41
18:A:811:CLA:H52	18:A:811:CLA:H11	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:822:CLA:HMD2	21:B:843:BCR:H24C	2.02	0.41
18:B:829:CLA:H62	18:B:829:CLA:H41	1.95	0.41
6:F:162:THR:HB	6:F:163:PRO:HD3	2.00	0.41
6:F:173:TRP:CD1	6:F:210:GLY:HA3	2.55	0.41
18:J:1101:CLA:H71	18:J:1101:CLA:H112	1.86	0.41
16:4:198:LEU:O	16:4:200:ALA:N	2.51	0.41
2:B:503:GLU:HG3	2:B:505:SER:H	1.85	0.41
18:B:829:CLA:H8	21:B:844:BCR:H21C	2.02	0.41
18:F:303:CLA:ND	24:F:306:LMG:H302	2.35	0.41
18:H:1701:CLA:HBB2	21:L:307:BCR:H311	2.02	0.41
18:L:306:CLA:CHA	18:L:306:CLA:HBA1	2.48	0.41
14:2:102:ASN:C	18:2:309:CLA:HMA1	2.40	0.41
14:2:188:LEU:HD23	14:2:198:GLY:HA3	2.02	0.41
18:2:326:CLA:H3A	18:2:326:CLA:HBA2	1.58	0.41
16:4:221:GLN:O	16:4:225:THR:HG22	2.20	0.41
18:A:822:CLA:H161	22:A:849:LHG:H142	2.03	0.41
18:A:840:CLA:HMC3	22:A:849:LHG:O1	2.21	0.41
2:B:590:VAL:HG22	18:B:836:CLA:HAB	2.03	0.41
18:B:801:CLA:HMA1	18:B:803:CLA:H202	2.03	0.41
18:B:812:CLA:H41	18:B:812:CLA:H62	1.78	0.41
18:B:822:CLA:H111	18:B:822:CLA:H91	1.84	0.41
18:B:833:CLA:H61	18:B:833:CLA:H41	1.75	0.41
18:B:841:CLA:H143	18:B:841:CLA:H161	1.84	0.41
8:H:94:THR:HG22	12:L:184:LYS:HA	2.02	0.41
10:J:29:ILE:HG23	26:J:1106:DGD:HB22	2.03	0.41
29:J:1105:LUT:H35	29:J:1105:LUT:H401	1.73	0.41
29:1:5004:LUT:H11	29:1:5004:LUT:H191	1.79	0.41
29:2:303:LUT:H173	18:2:306:CLA:H12	2.03	0.41
21:2:305:BCR:H322	18:2:326:CLA:HMD2	2.02	0.41
30:2:314:CHL:H71	30:2:314:CHL:H112	1.55	0.41
18:A:823:CLA:H142	18:A:823:CLA:H111	1.83	0.41
18:A:830:CLA:H143	19:B:842:PQN:H191	2.02	0.41
18:A:837:CLA:H62	18:A:837:CLA:H102	1.89	0.41
18:A:839:CLA:H18	18:J:1101:CLA:H193	2.02	0.41
21:A:855:BCR:H351	21:A:855:BCR:H15C	1.68	0.41
18:B:812:CLA:HMD2	23:B:852:LMT:H62	2.03	0.41
6:F:129:ARG:HB2	10:J:35:ASP:OD2	2.20	0.41
11:K:47:ILE:HD12	11:K:47:ILE:HA	1.92	0.41
30:1:5014:CHL:C1C	18:1:5017:CLA:HMC3	2.51	0.41
15:3:97:TRP:CZ2	18:3:317:CLA:HAA2	2.55	0.41
1:A:204:ASN:HB3	18:A:818:CLA:HMD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:807:CLA:H3A	18:A:807:CLA:HBA2	1.40	0.41
18:A:815:CLA:H3A	18:A:815:CLA:HBA2	1.87	0.41
2:B:222:LEU:HD11	18:B:816:CLA:HBA2	2.01	0.41
18:B:819:CLA:HBB2	18:B:825:CLA:H191	2.03	0.41
4:D:101:TYR:CE1	4:D:157:ARG:HD3	2.56	0.41
11:K:73:SER:OG	11:K:74:ALA:N	2.54	0.41
18:A:803:CLA:HMA2	18:A:810:CLA:HMD2	2.03	0.41
18:A:819:CLA:H41	18:A:819:CLA:H62	1.56	0.41
18:A:832:CLA:C7	21:A:846:BCR:H10C	2.51	0.41
18:A:836:CLA:HHC	18:A:836:CLA:HBB1	2.02	0.41
18:B:818:CLA:H162	18:B:818:CLA:H141	1.83	0.41
21:F:304:BCR:H351	21:F:304:BCR:H15C	1.74	0.41
13:1:194:ALA:HB1	29:1:5003:LUT:H171	2.01	0.41
29:1:5003:LUT:H15	29:1:5003:LUT:H201	1.86	0.41
14:2:110:SER:CB	14:2:225:GLY:HA3	2.49	0.41
18:2:312:CLA:HBC3	22:2:320:LHG:H252	2.02	0.41
15:3:123:GLY:HA3	15:3:133:ALA:CB	2.51	0.41
18:3:315:CLA:HMD1	18:3:318:CLA:HAB	2.01	0.41
16:4:81:LEU:HD13	18:4:308:CLA:H42	2.03	0.41
1:A:729:GLN:HB2	22:A:848:LHG:HC41	2.02	0.41
18:A:838:CLA:H62	18:A:838:CLA:H41	1.39	0.41
2:B:134:ASP:OD2	2:B:208:ARG:NH2	2.50	0.41
2:B:358:TYR:CE2	18:B:829:CLA:HED2	2.55	0.41
2:B:439:HIS:CD2	2:B:453:ILE:HG13	2.55	0.41
2:B:694:ARG:HG3	18:B:839:CLA:HED3	2.03	0.41
18:B:806:CLA:H102	18:B:806:CLA:H61	1.90	0.41
18:B:821:CLA:HAB	21:B:843:BCR:H14C	2.02	0.41
18:B:831:CLA:H122	18:B:831:CLA:H202	2.03	0.41
14:2:201:PHE:HB3	18:2:306:CLA:HMD1	2.03	0.41
16:4:121:ILE:HG22	16:4:122:ASN:H	1.86	0.41
1:A:207:LEU:O	1:A:310:PHE:HB3	2.20	0.41
1:A:213:LEU:HD22	21:A:843:BCR:H361	2.03	0.41
1:A:721:GLN:NE2	5:E:109:LYS:HB2	2.36	0.41
17:A:801:CL0:H10	17:A:801:CL0:H72	1.65	0.41
18:A:807:CLA:CAD	18:A:826:CLA:HAA2	2.50	0.41
21:A:855:BCR:H291	11:K:72:PRO:HB2	2.02	0.41
2:B:419:ILE:HG21	2:B:536:LYS:HG3	2.03	0.41
2:B:716:GLY:O	2:B:720:THR:OG1	2.29	0.41
18:B:825:CLA:H61	18:B:825:CLA:H41	1.96	0.41
3:C:52:LYS:HD3	3:C:55:GLU:OE2	2.20	0.41
3:C:61:ASP:HA	3:C:62:PHE:HA	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:F:301:CLA:H61	21:F:305:BCR:H393	2.01	0.41
28:F:310:ZEX:H27	28:F:310:ZEX:H391	1.88	0.41
8:H:65:GLY:HA2	8:H:67:TRP:CZ2	2.56	0.41
12:L:139:VAL:O	12:L:143:ILE:HG13	2.20	0.41
18:L:304:CLA:HAA2	21:L:307:BCR:H352	2.02	0.41
13:1:150:SER:HB2	30:1:5016:CHL:CMA	2.51	0.41
13:1:154:ASP:N	13:1:155:PRO:HA	2.33	0.41
13:1:203:SER:OG	18:1:5018:CLA:H71	2.21	0.41
14:2:238:GLN:HE21	18:2:308:CLA:C1A	2.34	0.41
1:A:296:LEU:HD23	1:A:296:LEU:HA	1.90	0.41
1:A:364:MET:HG3	18:A:823:CLA:HHB	2.03	0.41
18:A:853:CLA:H61	18:A:853:CLA:H41	1.49	0.41
2:B:453:ILE:HD13	26:J:1106:DGD:HA82	2.03	0.41
2:B:592:PHE:CE2	2:B:624:LEU:HD21	2.56	0.41
18:B:826:CLA:CAD	18:B:836:CLA:HBB1	2.51	0.41
14:2:87:PHE:HZ	31:2:304:XAT:H362	1.85	0.41
21:3:305:BCR:H402	30:3:312:CHL:C1B	2.51	0.41
18:4:305:CLA:H61	18:4:305:CLA:H41	1.95	0.41
1:A:325:HIS:CG	1:A:330:ILE:HD11	2.56	0.40
1:A:545:HIS:CE1	1:A:612:VAL:HA	2.56	0.40
2:B:477:LEU:C	2:B:479:SER:H	2.24	0.40
2:B:649:MET:HA	2:B:652:PHE:HB3	2.03	0.40
11:K:104:THR:CG2	18:K:1404:CLA:HAB	2.51	0.40
13:1:160:TYR:HB3	18:1:5006:CLA:HED3	2.02	0.40
31:2:304:XAT:H15	31:2:304:XAT:H201	1.72	0.40
31:2:304:XAT:H28	18:2:309:CLA:H61	2.03	0.40
15:3:118:ALA:HB3	15:3:119:PRO:HD3	2.04	0.40
29:3:304:LUT:H15	29:3:304:LUT:H201	1.97	0.40
31:4:304:XAT:H201	31:4:304:XAT:H15	1.77	0.40
1:A:85:GLN:HG2	18:A:804:CLA:CMA	2.50	0.40
1:A:205:HIS:ND1	18:A:812:CLA:HMC2	2.36	0.40
1:A:445:HIS:O	1:A:449:VAL:HG23	2.20	0.40
1:A:556:LEU:HD21	1:A:601:GLY:HA3	2.02	0.40
17:A:801:CL0:H11	17:A:801:CL0:H15	2.03	0.40
18:A:830:CLA:H143	18:A:830:CLA:H111	1.85	0.40
2:B:387:PHE:HB2	2:B:534:LEU:HD13	2.03	0.40
18:B:804:CLA:H193	18:B:811:CLA:HMC1	2.03	0.40
18:B:814:CLA:H193	18:B:814:CLA:H161	1.85	0.40
18:B:834:CLA:HMB3	18:B:836:CLA:HED3	2.04	0.40
6:F:213:TRP:CZ3	21:F:305:BCR:H381	2.56	0.40
18:H:1701:CLA:HHB	18:L:304:CLA:HBA2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:27:HIS:HA	9:I:30:LYS:HE3	2.03	0.40
21:1:5005:BCR:H351	21:1:5005:BCR:H15C	1.79	0.40
15:3:120:GLU:HG2	15:3:253:TYR:HB3	2.02	0.40
15:3:243:ILE:HG13	18:3:309:CLA:HAC2	2.04	0.40
1:A:529:LEU:HD23	1:A:529:LEU:HA	1.95	0.40
1:A:694:PHE:HB2	18:A:802:CLA:HBC2	2.03	0.40
2:B:227:THR:HG23	7:G:60:PRO:HG3	2.03	0.40
18:B:810:CLA:H193	21:I:101:BCR:H372	2.02	0.40
18:B:837:CLA:H3A	18:B:837:CLA:HBA2	1.80	0.40
12:L:128:GLN:H	12:L:128:GLN:HG2	1.63	0.40
18:1:5012:CLA:NC	22:1:5019:LHG:HC42	2.35	0.40
18:1:5013:CLA:HED3	16:4:143:VAL:HB	2.03	0.40
21:3:305:BCR:H383	30:3:312:CHL:CAB	2.50	0.40
1:A:455:PHE:HB3	18:A:831:CLA:HBB2	2.04	0.40
18:A:836:CLA:H102	22:A:849:LHG:H281	2.02	0.40
2:B:410:ARG:HH22	24:B:850:LMG:C6	2.33	0.40
2:B:569:ASP:OD1	2:B:706:ARG:NE	2.54	0.40
18:B:805:CLA:H162	18:B:805:CLA:H141	1.70	0.40
18:B:808:CLA:H112	18:B:808:CLA:H93	1.77	0.40
18:B:822:CLA:H92	24:1:5001:LMG:H161	2.03	0.40
15:3:141:VAL:HG22	18:3:318:CLA:HMC1	2.02	0.40
18:3:307:CLA:H3A	18:3:307:CLA:HBA2	1.41	0.40
16:4:215:PHE:O	16:4:219:ILE:HG12	2.21	0.40
1:A:382:TYR:CE1	18:A:827:CLA:HED2	2.57	0.40
1:A:416:ILE:HG23	1:A:420:ARG:HD3	2.03	0.40
2:B:85:ARG:HG3	8:H:139:LEU:HB2	2.03	0.40
2:B:598:HIS:HB3	2:B:602:TRP:CZ2	2.57	0.40
18:B:805:CLA:H3A	18:B:805:CLA:HBA2	1.55	0.40
30:1:5014:CHL:HHC	30:1:5014:CHL:CBB	2.48	0.40
29:2:303:LUT:H381	18:2:308:CLA:HBB1	2.04	0.40
29:3:304:LUT:H183	30:3:312:CHL:C3B	2.51	0.40
16:4:194:PHE:O	16:4:196:PRO:HD3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	741/743 (100%)	700 (94%)	40 (5%)	1 (0%)	51	85
2	B	731/733 (100%)	707 (97%)	23 (3%)	1 (0%)	51	85
3	C	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
4	D	141/143 (99%)	131 (93%)	9 (6%)	1 (1%)	22	60
5	E	64/66 (97%)	59 (92%)	5 (8%)	0	100	100
6	F	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
7	G	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
8	H	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
9	I	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
10	J	40/42 (95%)	38 (95%)	2 (5%)	0	100	100
11	K	78/80 (98%)	70 (90%)	8 (10%)	0	100	100
12	L	155/157 (99%)	147 (95%)	8 (5%)	0	100	100
13	1	191/193 (99%)	181 (95%)	7 (4%)	3 (2%)	9	40
14	2	206/208 (99%)	189 (92%)	17 (8%)	0	100	100
15	3	219/221 (99%)	201 (92%)	18 (8%)	0	100	100
16	4	196/198 (99%)	188 (96%)	8 (4%)	0	100	100
All	All	3201/3233 (99%)	3034 (95%)	161 (5%)	6 (0%)	47	82

All (6) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	604/604 (100%)	599 (99%)	5 (1%)	81	93
2	B	598/598 (100%)	588 (98%)	10 (2%)	60	85
3	C	69/69 (100%)	69 (100%)	0	100	100
4	D	122/122 (100%)	120 (98%)	2 (2%)	62	86
5	E	58/58 (100%)	58 (100%)	0	100	100
6	F	125/126 (99%)	125 (100%)	0	100	100
7	G	82/82 (100%)	82 (100%)	0	100	100
8	H	71/71 (100%)	71 (100%)	0	100	100
9	I	26/26 (100%)	26 (100%)	0	100	100
10	J	35/35 (100%)	35 (100%)	0	100	100
11	K	58/58 (100%)	56 (97%)	2 (3%)	37	72
12	L	124/124 (100%)	121 (98%)	3 (2%)	49	79
13	1	158/158 (100%)	158 (100%)	0	100	100
14	2	167/167 (100%)	166 (99%)	1 (1%)	86	95
15	3	171/172 (99%)	166 (97%)	5 (3%)	42	76
16	4	164/164 (100%)	164 (100%)	0	100	100
All	All	2632/2634 (100%)	2604 (99%)	28 (1%)	73	90

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	230	ASN
1	A	267	THR
1	A	282	THR
1	A	283	PHE
1	A	377	TYR
2	B	220	GLN
2	B	256	THR
2	B	332	PHE
2	B	394	PHE
2	B	477	LEU
2	B	492	ILE
2	B	536	LYS
2	B	577	TYR
2	B	640	MET

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Mol	Chain	Res	Type
2	B	702	ILE
4	D	156	TYR
4	D	190	ARG
11	K	52	ASN
11	K	99	PHE
12	L	109	LEU
12	L	153	PHE
12	L	207	LEU
14	2	242	THR
15	3	100	TYR
15	3	122	LEU
15	3	127	LEU
15	3	147	THR
15	3	273	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	2	306	-	60,68,73	1.40	8 (13%)	70,107,113	2.04	17 (24%)
18	CLA	A	832	-	65,73,73	1.37	8 (12%)	76,113,113	1.89	17 (22%)
18	CLA	4	308	-	60,68,73	1.40	8 (13%)	70,107,113	2.09	18 (25%)
21	BCR	B	845	-	41,41,41	1.83	4 (9%)	56,56,56	4.09	20 (35%)
18	CLA	B	825	-	65,73,73	1.35	7 (10%)	76,113,113	2.06	17 (22%)
24	LMG	F	306	-	47,47,55	0.97	3 (6%)	55,55,63	1.11	4 (7%)
18	CLA	A	839	-	65,73,73	1.37	10 (15%)	76,113,113	1.88	14 (18%)
19	PQN	B	842	-	34,34,34	0.40	0	42,45,45	1.08	3 (7%)
30	CHL	3	310	-	66,74,74	0.81	3 (4%)	73,114,114	1.39	10 (13%)
30	CHL	4	313	-	47,55,74	0.97	3 (6%)	50,91,114	1.40	11 (22%)
22	LHG	A	849	18	39,39,48	0.42	0	42,45,54	1.25	3 (7%)
26	DGD	1	5002	-	35,35,67	0.95	2 (5%)	43,43,81	1.10	3 (6%)
18	CLA	A	816	-	56,64,73	1.46	9 (16%)	65,102,113	2.09	18 (27%)
18	CLA	A	805	-	65,73,73	1.35	6 (9%)	76,113,113	1.94	19 (25%)
31	XAT	4	304	-	39,47,47	0.69	1 (2%)	54,74,74	1.92	12 (22%)
21	BCR	L	307	-	41,41,41	1.85	4 (9%)	56,56,56	4.33	15 (26%)
18	CLA	B	804	-	65,73,73	1.35	8 (12%)	76,113,113	1.92	17 (22%)
18	CLA	1	5007	13	46,54,73	1.61	8 (17%)	53,90,113	2.10	14 (26%)
18	CLA	1	5010	-	65,73,73	1.34	7 (10%)	76,113,113	2.02	19 (25%)
18	CLA	A	802	-	65,73,73	1.34	8 (12%)	76,113,113	1.86	16 (21%)
18	CLA	B	829	-	65,73,73	1.35	8 (12%)	76,113,113	1.94	17 (22%)
24	LMG	G	1607	-	25,25,55	0.68	1 (4%)	33,33,63	1.36	5 (15%)
18	CLA	3	319	-	60,68,73	1.43	9 (15%)	70,107,113	1.99	15 (21%)
21	BCR	F	304	-	41,41,41	1.84	4 (9%)	56,56,56	4.33	17 (30%)
24	LMG	2	322	-	36,36,55	0.64	1 (2%)	44,44,63	1.06	2 (4%)
30	CHL	3	312	-	51,59,74	0.89	2 (3%)	55,96,114	1.48	12 (21%)
18	CLA	A	808	1	65,73,73	1.35	7 (10%)	76,113,113	1.97	19 (25%)
18	CLA	A	813	-	65,73,73	1.34	7 (10%)	76,113,113	2.02	19 (25%)
18	CLA	A	820	-	60,68,73	1.42	9 (15%)	70,107,113	2.02	15 (21%)
18	CLA	B	801	-	65,73,73	1.38	10 (15%)	76,113,113	1.98	16 (21%)
18	CLA	B	826	-	65,73,73	1.34	7 (10%)	76,113,113	2.04	17 (22%)
18	CLA	L	305	-	60,68,73	1.42	8 (13%)	70,107,113	2.05	15 (21%)
18	CLA	A	825	-	65,73,73	1.35	7 (10%)	76,113,113	2.03	18 (23%)
18	CLA	A	804	-	65,73,73	1.34	9 (13%)	76,113,113	2.01	17 (22%)
24	LMG	1	5020	-	46,46,55	0.93	3 (6%)	54,54,63	1.07	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	A	836	-	65,73,73	1.36	9 (13%)	76,113,113	1.93	17 (22%)
18	CLA	2	312	22	60,68,73	1.41	8 (13%)	70,107,113	2.04	17 (24%)
24	LMG	F	307	-	36,36,55	0.73	1 (2%)	44,44,63	1.04	2 (4%)
18	CLA	1	5008	-	55,63,73	1.48	9 (16%)	64,101,113	2.13	15 (23%)
21	BCR	G	1604	-	41,41,41	1.85	4 (9%)	56,56,56	4.35	15 (26%)
18	CLA	B	834	-	60,68,73	1.40	8 (13%)	70,107,113	2.01	16 (22%)
30	CHL	2	314	14	66,74,74	0.83	3 (4%)	73,114,114	1.22	10 (13%)
18	CLA	F	303	6	65,73,73	1.37	9 (13%)	76,113,113	1.91	17 (22%)
18	CLA	3	301	-	45,53,73	1.62	8 (17%)	52,89,113	2.09	14 (26%)
23	LMT	G	1605	-	36,36,36	1.15	5 (13%)	47,47,47	1.00	1 (2%)
23	LMT	4	319	-	36,36,36	1.14	5 (13%)	47,47,47	0.97	2 (4%)
24	LMG	B	850	-	35,35,55	0.72	1 (2%)	43,43,63	1.14	3 (6%)
21	BCR	2	305	-	41,41,41	1.87	4 (9%)	56,56,56	4.93	27 (48%)
18	CLA	4	309	-	60,68,73	1.41	9 (15%)	70,107,113	2.04	17 (24%)
18	CLA	A	809	-	50,58,73	1.54	8 (16%)	58,95,113	2.16	15 (25%)
18	CLA	B	816	-	55,63,73	1.46	7 (12%)	64,101,113	2.21	20 (31%)
21	BCR	B	843	-	41,41,41	1.90	4 (9%)	56,56,56	4.66	21 (37%)
18	CLA	2	317	-	55,63,73	1.47	8 (14%)	64,101,113	2.08	15 (23%)
18	CLA	A	806	-	60,68,73	1.42	9 (15%)	70,107,113	2.00	15 (21%)
23	LMT	A	850	-	36,36,36	1.12	5 (13%)	47,47,47	1.15	1 (2%)
24	LMG	A	851	-	50,50,55	1.05	5 (10%)	58,58,63	1.05	3 (5%)
30	CHL	3	316	15	47,55,74	1.01	3 (6%)	50,91,114	1.48	10 (20%)
18	CLA	B	831	-	65,73,73	1.36	8 (12%)	76,113,113	1.99	16 (21%)
18	CLA	A	810	1	65,73,73	1.36	9 (13%)	76,113,113	1.93	14 (18%)
18	CLA	A	837	-	65,73,73	1.35	8 (12%)	76,113,113	1.96	16 (21%)
18	CLA	B	810	2	65,73,73	1.35	8 (12%)	76,113,113	1.91	15 (19%)
18	CLA	A	838	-	65,73,73	1.36	8 (12%)	76,113,113	1.94	17 (22%)
28	ZEX	F	310	-	42,43,43	0.80	0	55,60,60	1.90	12 (21%)
25	GOL	4	321	-	5,5,5	0.55	0	5,5,5	0.26	0
18	CLA	A	803	-	65,73,73	1.36	9 (13%)	76,113,113	1.97	18 (23%)
24	LMG	1	5001	-	49,49,55	1.02	5 (10%)	57,57,63	1.12	4 (7%)
18	CLA	A	826	-	65,73,73	1.37	8 (12%)	76,113,113	1.92	16 (21%)
21	BCR	K	1405	-	41,41,41	1.86	4 (9%)	56,56,56	4.28	18 (32%)
18	CLA	B	808	-	65,73,73	1.36	9 (13%)	76,113,113	1.92	14 (18%)
18	CLA	B	814	-	65,73,73	1.36	7 (10%)	76,113,113	2.02	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	B	820	-	65,73,73	1.36	8 (12%)	76,113,113	1.89	16 (21%)
18	CLA	4	312	-	46,54,73	1.61	9 (19%)	53,90,113	2.14	14 (26%)
26	DGD	B	855	-	62,62,67	1.11	6 (9%)	76,76,81	0.98	3 (3%)
18	CLA	3	314	-	48,56,73	1.59	10 (20%)	55,92,113	2.17	14 (25%)
24	LMG	2	324	-	13,13,55	0.57	0	18,18,63	0.67	0
18	CLA	B	828	-	65,73,73	1.36	8 (12%)	76,113,113	1.99	17 (22%)
18	CLA	B	837	-	65,73,73	1.34	9 (13%)	76,113,113	2.00	16 (21%)
18	CLA	A	818	-	50,58,73	1.55	9 (18%)	58,95,113	2.19	15 (25%)
18	CLA	4	306	16	50,58,73	1.56	10 (20%)	58,95,113	2.25	17 (29%)
21	BCR	B	844	-	41,41,41	1.85	4 (9%)	56,56,56	4.35	17 (30%)
18	CLA	A	815	-	65,73,73	1.34	9 (13%)	76,113,113	1.94	16 (21%)
18	CLA	K	1402	-	60,68,73	1.43	10 (16%)	70,107,113	2.00	16 (22%)
18	CLA	B	819	-	65,73,73	1.34	9 (13%)	76,113,113	2.04	17 (22%)
21	BCR	A	847	-	41,41,41	1.83	4 (9%)	56,56,56	4.32	20 (35%)
18	CLA	1	5018	13	60,68,73	1.42	10 (16%)	70,107,113	2.00	18 (25%)
24	LMG	2	301	-	13,13,55	0.57	0	18,18,63	0.58	0
24	LMG	2	323	-	13,13,55	0.62	0	18,18,63	0.93	1 (5%)
18	CLA	4	305	-	60,68,73	1.41	8 (13%)	70,107,113	2.02	20 (28%)
30	CHL	1	5014	-	47,55,74	0.94	2 (4%)	50,91,114	1.38	11 (22%)
18	CLA	B	841	22	65,73,73	1.35	8 (12%)	76,113,113	1.93	18 (23%)
29	LUT	2	303	-	42,43,43	2.33	1 (2%)	51,60,60	2.01	17 (33%)
18	CLA	4	310	-	50,58,73	1.54	8 (16%)	58,95,113	2.18	15 (25%)
21	BCR	A	846	-	41,41,41	1.85	4 (9%)	56,56,56	4.25	15 (26%)
18	CLA	A	823	-	65,73,73	1.35	8 (12%)	76,113,113	2.06	19 (25%)
18	CLA	3	308	-	52,60,73	1.52	9 (17%)	60,97,113	2.17	17 (28%)
25	GOL	A	854	-	5,5,5	0.55	0	5,5,5	0.27	0
20	SF4	C	102	3	0,12,12	-	-	-	-	-
18	CLA	1	5006	13	65,73,73	1.37	9 (13%)	76,113,113	1.95	18 (23%)
18	CLA	L	306	-	50,58,73	1.54	9 (18%)	58,95,113	2.19	17 (29%)
24	LMG	4	320	-	13,13,55	0.55	0	18,18,63	0.67	0
30	CHL	4	317	-	43,51,74	1.01	3 (6%)	45,86,114	1.48	9 (20%)
18	CLA	L	301	-	55,63,73	1.47	7 (12%)	64,101,113	2.09	18 (28%)
18	CLA	B	805	-	65,73,73	1.34	7 (10%)	76,113,113	1.96	18 (23%)
30	CHL	2	315	-	56,64,74	0.83	2 (3%)	61,102,114	1.33	11 (18%)
18	CLA	A	830	-	65,73,73	1.36	8 (12%)	76,113,113	1.91	15 (19%)
18	CLA	F	301	-	65,73,73	1.35	7 (10%)	76,113,113	1.95	19 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	LMG	F	308	-	34,34,55	0.50	0	42,42,63	1.09	2 (4%)
24	LMG	J	1102	-	30,30,55	0.54	0	38,38,63	1.13	3 (7%)
18	CLA	K	1401	-	45,53,73	1.61	8 (17%)	52,89,113	2.18	16 (30%)
18	CLA	J	1101	-	65,73,73	1.34	8 (12%)	76,113,113	2.03	19 (25%)
18	CLA	K	1403	-	48,56,73	1.58	8 (16%)	55,92,113	2.29	16 (29%)
18	CLA	2	308	-	65,73,73	1.36	9 (13%)	76,113,113	2.04	15 (19%)
18	CLA	1	5009	-	65,73,73	1.36	8 (12%)	76,113,113	1.99	17 (22%)
30	CHL	1	5016	-	61,69,74	0.86	2 (3%)	67,108,114	1.33	13 (19%)
18	CLA	4	311	-	60,68,73	1.42	9 (15%)	70,107,113	2.01	16 (22%)
18	CLA	2	309	14	65,73,73	1.36	9 (13%)	76,113,113	2.00	16 (21%)
18	CLA	A	834	-	51,59,73	1.52	7 (13%)	59,96,113	2.22	18 (30%)
18	CLA	B	830	-	65,73,73	1.37	9 (13%)	76,113,113	2.05	17 (22%)
21	BCR	F	305	-	41,41,41	1.84	4 (9%)	56,56,56	4.44	20 (35%)
30	CHL	2	318	-	46,54,74	0.97	3 (6%)	49,90,114	1.36	9 (18%)
18	CLA	1	5017	-	45,53,73	1.64	9 (20%)	52,89,113	2.10	12 (23%)
24	LMG	2	321	-	25,25,55	0.56	0	33,33,63	1.19	3 (9%)
21	BCR	B	802	-	41,41,41	1.88	4 (9%)	56,56,56	4.72	18 (32%)
26	DGD	F	309	-	58,58,67	1.04	4 (6%)	72,72,81	1.07	3 (4%)
24	LMG	B	854	-	13,13,55	0.55	0	18,18,63	0.73	0
18	CLA	A	812	-	65,73,73	1.33	7 (10%)	76,113,113	2.00	19 (25%)
18	CLA	B	812	-	60,68,73	1.42	8 (13%)	70,107,113	1.95	16 (22%)
18	CLA	1	5012	-	46,54,73	1.62	9 (19%)	53,90,113	2.11	13 (24%)
18	CLA	A	807	1	65,73,73	1.34	8 (12%)	76,113,113	2.01	18 (23%)
18	CLA	A	835	-	65,73,73	1.36	9 (13%)	76,113,113	1.96	15 (19%)
18	CLA	3	307	-	55,63,73	1.49	9 (16%)	64,101,113	2.08	19 (29%)
30	CHL	2	316	-	48,56,74	1.00	3 (6%)	51,92,114	1.40	11 (21%)
21	BCR	B	847	-	41,41,41	1.85	4 (9%)	56,56,56	4.37	14 (25%)
18	CLA	B	835	-	55,63,73	1.49	9 (16%)	64,101,113	2.10	18 (28%)
18	CLA	3	315	15	65,73,73	1.35	8 (12%)	76,113,113	1.91	16 (21%)
22	LHG	2	320	18	34,34,48	0.45	0	37,40,54	1.14	3 (8%)
18	CLA	1	5011	-	50,58,73	1.54	10 (20%)	58,95,113	2.20	17 (29%)
21	BCR	4	301	-	41,41,41	1.85	4 (9%)	56,56,56	4.29	17 (30%)
18	CLA	B	840	-	65,73,73	1.36	8 (12%)	76,113,113	1.97	17 (22%)
18	CLA	A	853	-	65,73,73	1.36	8 (12%)	76,113,113	2.00	15 (19%)
18	CLA	B	821	-	46,54,73	1.61	9 (19%)	53,90,113	2.14	12 (22%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	LHG	B	849	-	48,48,48	0.39	0	51,54,54	1.02	2 (3%)
21	BCR	3	306	-	41,41,41	1.89	4 (9%)	56,56,56	4.07	18 (32%)
22	LHG	1	5019	-	48,48,48	0.40	0	51,54,54	1.04	3 (5%)
18	CLA	A	821	-	60,68,73	1.41	8 (13%)	70,107,113	2.05	17 (24%)
22	LHG	B	848	18	20,20,48	0.58	0	23,26,54	1.51	2 (8%)
18	CLA	A	828	-	65,73,73	1.34	8 (12%)	76,113,113	2.04	17 (22%)
18	CLA	2	326	16,14	50,58,73	1.56	9 (18%)	58,95,113	2.16	15 (25%)
18	CLA	B	803	-	65,73,73	1.36	6 (9%)	76,113,113	1.88	16 (21%)
18	CLA	A	831	-	65,73,73	1.37	9 (13%)	76,113,113	1.95	18 (23%)
26	DGD	J	1106	-	59,59,67	1.07	5 (8%)	73,73,81	1.20	5 (6%)
18	CLA	3	309	-	55,63,73	1.49	10 (18%)	64,101,113	2.18	19 (29%)
21	BCR	A	855	-	41,41,41	1.85	4 (9%)	56,56,56	4.39	17 (30%)
18	CLA	G	1602	7	46,54,73	1.60	8 (17%)	53,90,113	2.15	14 (26%)
18	CLA	4	315	-	65,73,73	1.36	9 (13%)	76,113,113	1.98	16 (21%)
21	BCR	1	5005	-	41,41,41	1.85	4 (9%)	56,56,56	4.35	16 (28%)
21	BCR	B	846	-	41,41,41	1.85	4 (9%)	56,56,56	4.23	15 (26%)
21	BCR	L	302	-	41,41,41	1.87	4 (9%)	56,56,56	4.45	21 (37%)
23	LMT	J	1107	-	26,26,36	1.33	5 (19%)	37,37,47	1.06	2 (5%)
18	CLA	A	817	-	65,73,73	1.35	8 (12%)	76,113,113	1.93	17 (22%)
18	CLA	A	827	-	65,73,73	1.36	8 (12%)	76,113,113	1.94	14 (18%)
29	LUT	1	5004	-	42,43,43	2.38	1 (2%)	51,60,60	2.05	15 (29%)
18	CLA	B	839	-	65,73,73	1.37	9 (13%)	76,113,113	1.95	16 (21%)
18	CLA	3	311	-	55,63,73	1.48	8 (14%)	64,101,113	2.10	18 (28%)
18	CLA	B	818	-	65,73,73	1.36	9 (13%)	76,113,113	1.90	15 (19%)
23	LMT	B	852	-	36,36,36	1.14	5 (13%)	47,47,47	1.07	2 (4%)
18	CLA	4	307	-	65,73,73	1.36	9 (13%)	76,113,113	1.97	15 (19%)
18	CLA	B	815	-	65,73,73	1.34	7 (10%)	76,113,113	2.02	17 (22%)
18	CLA	A	811	-	55,63,73	1.48	9 (16%)	64,101,113	2.10	17 (26%)
18	CLA	2	310	-	65,73,73	1.32	7 (10%)	76,113,113	2.18	21 (27%)
18	CLA	A	840	22	60,68,73	1.41	7 (11%)	70,107,113	2.06	18 (25%)
18	CLA	B	813	-	46,54,73	1.59	7 (15%)	53,90,113	2.16	14 (26%)
30	CHL	4	314	16	51,59,74	0.98	3 (5%)	55,96,114	1.40	10 (18%)
21	BCR	A	844	-	41,41,41	1.82	4 (9%)	56,56,56	4.29	16 (28%)
18	CLA	L	304	12	50,58,73	1.53	8 (16%)	58,95,113	2.23	16 (27%)
20	SF4	C	101	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	XAT	2	304	-	39,47,47	0.68	1 (2%)	54,74,74	1.82	13 (24%)
18	CLA	H	1701	-	60,68,73	1.42	9 (15%)	70,107,113	2.02	15 (21%)
17	CL0	A	801	-	65,73,73	2.39	19 (29%)	76,113,113	2.52	20 (26%)
18	CLA	B	822	-	65,73,73	1.37	9 (13%)	76,113,113	1.97	16 (21%)
18	CLA	B	823	-	65,73,73	1.37	9 (13%)	76,113,113	1.93	17 (22%)
29	LUT	3	303	-	42,43,43	2.38	1 (2%)	51,60,60	1.96	16 (31%)
18	CLA	B	824	-	55,63,73	1.49	9 (16%)	64,101,113	2.02	16 (25%)
18	CLA	G	1603	-	65,73,73	1.36	10 (15%)	76,113,113	1.95	16 (21%)
18	CLA	A	814	-	46,54,73	1.62	8 (17%)	53,90,113	2.12	13 (24%)
18	CLA	B	827	-	65,73,73	1.36	8 (12%)	76,113,113	2.03	19 (25%)
18	CLA	1	5015	-	65,73,73	1.36	9 (13%)	76,113,113	1.94	15 (19%)
21	BCR	I	101	-	41,41,41	1.87	4 (9%)	56,56,56	4.29	19 (33%)
21	BCR	I	102	-	41,41,41	1.85	4 (9%)	56,56,56	4.26	15 (26%)
23	LMT	G	1606	-	32,32,36	1.22	5 (15%)	43,43,47	1.00	1 (2%)
30	CHL	3	313	-	51,59,74	0.92	2 (3%)	55,96,114	1.47	10 (18%)
18	CLA	2	311	-	50,58,73	1.53	9 (18%)	58,95,113	2.23	16 (27%)
21	BCR	A	845	-	41,41,41	1.84	4 (9%)	56,56,56	4.31	19 (33%)
18	CLA	B	836	-	55,63,73	1.48	9 (16%)	64,101,113	2.10	17 (26%)
30	CHL	4	318	-	56,64,74	0.88	2 (3%)	61,102,114	1.33	12 (19%)
18	CLA	K	1404	-	46,54,73	1.63	10 (21%)	53,90,113	2.11	12 (22%)
21	BCR	A	843	-	41,41,41	1.83	4 (9%)	56,56,56	4.31	19 (33%)
18	CLA	A	829	-	65,73,73	1.35	8 (12%)	76,113,113	2.00	18 (23%)
18	CLA	2	313	-	50,58,73	1.55	9 (18%)	58,95,113	2.25	18 (31%)
18	CLA	J	1103	-	50,58,73	1.57	10 (20%)	58,95,113	2.21	17 (29%)
26	DGD	2	327	-	52,52,67	0.92	3 (5%)	66,66,81	1.09	5 (7%)
29	LUT	J	1105	-	42,43,43	2.36	1 (2%)	51,60,60	2.17	12 (23%)
23	LMT	B	856	-	32,32,36	1.22	6 (18%)	43,43,47	1.03	3 (6%)
18	CLA	B	817	-	60,68,73	1.41	9 (15%)	70,107,113	2.02	18 (25%)
30	CHL	4	316	-	61,69,74	0.91	3 (4%)	67,108,114	1.30	12 (17%)
18	CLA	2	307	14	52,60,73	1.53	10 (19%)	60,97,113	2.17	18 (30%)
18	CLA	1	5013	-	46,54,73	1.61	9 (19%)	53,90,113	2.19	11 (20%)
29	LUT	1	5003	-	42,43,43	2.40	1 (2%)	51,60,60	1.95	14 (27%)
29	LUT	3	304	-	42,43,43	2.35	1 (2%)	51,60,60	1.99	13 (25%)
18	CLA	A	833	1	55,63,73	1.49	10 (18%)	64,101,113	2.08	16 (25%)
18	CLA	B	838	-	50,58,73	1.54	9 (18%)	58,95,113	2.21	18 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	LMT	2	325	-	36,36,36	1.16	5 (13%)	47,47,47	1.09	3 (6%)
18	CLA	B	806	-	65,73,73	1.34	9 (13%)	76,113,113	2.00	16 (21%)
24	LMG	2	302	-	13,13,55	0.57	0	18,18,63	0.61	0
30	CHL	4	302	13	56,64,74	0.89	3 (5%)	61,102,114	1.31	11 (18%)
24	LMG	B	851	-	33,33,55	0.58	0	41,41,63	1.44	8 (19%)
19	PQN	A	841	-	34,34,34	0.42	0	42,45,45	1.12	3 (7%)
20	SF4	A	842	1,2	0,12,12	-	-	-	-	-
18	CLA	A	822	-	65,73,73	1.37	9 (13%)	76,113,113	1.91	16 (21%)
18	CLA	3	317	-	50,58,73	1.53	8 (16%)	58,95,113	2.31	17 (29%)
18	CLA	B	811	-	65,73,73	1.36	8 (12%)	76,113,113	1.91	16 (21%)
18	CLA	3	318	-	46,54,73	1.60	7 (15%)	53,90,113	2.11	14 (26%)
23	LMT	B	853	-	33,33,36	1.22	6 (18%)	44,44,47	1.12	3 (6%)
18	CLA	B	809	-	65,73,73	1.37	8 (12%)	76,113,113	1.90	14 (18%)
18	CLA	B	807	2	65,73,73	1.35	9 (13%)	76,113,113	1.94	14 (18%)
18	CLA	B	832	-	60,68,73	1.41	7 (11%)	70,107,113	2.03	18 (25%)
18	CLA	F	302	-	65,73,73	1.36	9 (13%)	76,113,113	1.95	18 (23%)
21	BCR	L	303	-	41,41,41	1.86	4 (9%)	56,56,56	4.36	15 (26%)
29	LUT	4	303	-	42,43,43	2.38	1 (2%)	51,60,60	1.90	13 (25%)
18	CLA	B	833	-	58,66,73	1.43	9 (15%)	67,104,113	2.14	17 (25%)
18	CLA	A	819	-	65,73,73	1.34	7 (10%)	76,113,113	1.85	17 (22%)
18	CLA	A	852	-	65,73,73	1.38	10 (15%)	76,113,113	1.92	16 (21%)
18	CLA	G	1601	-	55,63,73	1.47	7 (12%)	64,101,113	2.12	19 (29%)
22	LHG	A	848	-	48,48,48	0.38	0	51,54,54	1.04	3 (5%)
30	CHL	2	319	-	56,64,74	0.89	2 (3%)	61,102,114	1.35	12 (19%)
21	BCR	J	1104	-	41,41,41	1.83	4 (9%)	56,56,56	4.28	15 (26%)
18	CLA	A	824	-	55,63,73	1.50	10 (18%)	64,101,113	2.03	15 (23%)
21	BCR	3	305	-	41,41,41	1.84	4 (9%)	56,56,56	4.34	15 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	2	306	-	1/1/14/20	9/31/109/115	-
18	CLA	A	832	-	1/1/15/20	18/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	4	308	-	1/1/14/20	19/31/109/115	-
21	BCR	B	845	-	-	14/29/63/63	0/2/2/2
18	CLA	B	825	-	1/1/15/20	13/37/115/115	-
24	LMG	F	306	-	-	6/42/62/70	0/1/1/1
18	CLA	A	839	-	1/1/15/20	5/37/115/115	-
30	CHL	3	310	-	4/4/20/26	10/39/137/137	-
30	CHL	4	313	-	3/3/16/26	3/17/115/137	-
19	PQN	B	842	-	-	9/23/43/43	0/2/2/2
22	LHG	A	849	18	-	23/44/44/53	-
26	DGD	1	5002	-	-	11/29/49/95	0/1/1/2
18	CLA	A	816	-	1/1/13/20	16/27/105/115	-
18	CLA	A	805	-	1/1/15/20	20/37/115/115	-
31	XAT	4	304	-	1/1/12/26	0/31/93/93	0/4/4/4
21	BCR	L	307	-	-	14/29/63/63	0/2/2/2
18	CLA	B	804	-	1/1/15/20	16/37/115/115	-
18	CLA	1	5007	13	1/1/11/20	7/15/93/115	-
18	CLA	1	5010	-	1/1/15/20	13/37/115/115	-
18	CLA	A	802	-	1/1/15/20	22/37/115/115	-
18	CLA	B	829	-	1/1/15/20	20/37/115/115	-
24	LMG	G	1607	-	-	9/20/40/70	0/1/1/1
18	CLA	3	319	-	1/1/14/20	18/31/109/115	-
21	BCR	F	304	-	-	10/29/63/63	0/2/2/2
24	LMG	2	322	-	-	17/31/51/70	0/1/1/1
30	CHL	3	312	-	3/3/17/26	2/21/119/137	-
18	CLA	A	808	1	1/1/15/20	19/37/115/115	-
18	CLA	A	813	-	1/1/15/20	15/37/115/115	-
18	CLA	A	820	-	1/1/14/20	15/31/109/115	-
18	CLA	B	801	-	1/1/15/20	17/37/115/115	-
18	CLA	B	826	-	1/1/15/20	19/37/115/115	-
18	CLA	L	305	-	1/1/14/20	18/31/109/115	-
18	CLA	A	825	-	1/1/15/20	16/37/115/115	-
18	CLA	A	804	-	1/1/15/20	27/37/115/115	-
24	LMG	1	5020	-	-	10/41/61/70	0/1/1/1
18	CLA	A	836	-	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	2	312	22	1/1/14/20	20/31/109/115	-
24	LMG	F	307	-	-	10/31/51/70	0/1/1/1
18	CLA	1	5008	-	1/1/13/20	9/25/103/115	-
30	CHL	2	314	14	4/4/20/26	10/39/137/137	-
18	CLA	B	834	-	1/1/14/20	12/31/109/115	-
21	BCR	G	1604	-	-	8/29/63/63	0/2/2/2
18	CLA	F	303	6	1/1/15/20	21/37/115/115	-
18	CLA	3	301	-	1/1/11/20	6/13/91/115	-
23	LMT	G	1605	-	-	10/21/61/61	0/2/2/2
23	LMT	4	319	-	-	4/21/61/61	0/2/2/2
24	LMG	B	850	-	-	9/30/50/70	0/1/1/1
21	BCR	2	305	-	-	10/29/63/63	0/2/2/2
18	CLA	4	309	-	1/1/14/20	12/31/109/115	-
18	CLA	A	809	-	1/1/12/20	8/19/97/115	-
18	CLA	B	816	-	1/1/13/20	6/25/103/115	-
21	BCR	B	843	-	-	10/29/63/63	0/2/2/2
18	CLA	2	317	-	1/1/13/20	10/25/103/115	-
18	CLA	A	806	-	1/1/14/20	16/31/109/115	-
23	LMT	A	850	-	-	11/21/61/61	0/2/2/2
24	LMG	A	851	-	-	19/45/65/70	0/1/1/1
30	CHL	3	316	15	3/3/16/26	5/17/115/137	-
18	CLA	B	831	-	1/1/15/20	14/37/115/115	-
18	CLA	A	810	1	1/1/15/20	19/37/115/115	-
18	CLA	A	837	-	1/1/15/20	9/37/115/115	-
18	CLA	B	810	2	1/1/15/20	14/37/115/115	-
18	CLA	A	838	-	1/1/15/20	16/37/115/115	-
28	ZEX	F	310	-	-	3/29/67/67	0/2/2/2
25	GOL	4	321	-	-	0/4/4/4	-
18	CLA	A	803	-	1/1/15/20	19/37/115/115	-
24	LMG	1	5001	-	-	15/44/64/70	0/1/1/1
18	CLA	A	826	-	1/1/15/20	22/37/115/115	-
21	BCR	K	1405	-	-	13/29/63/63	0/2/2/2
18	CLA	B	808	-	1/1/15/20	15/37/115/115	-
18	CLA	B	814	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	820	-	1/1/15/20	13/37/115/115	-
18	CLA	4	312	-	1/1/11/20	7/15/93/115	-
26	DGD	B	855	-	-	19/50/90/95	0/2/2/2
18	CLA	3	314	-	1/1/11/20	5/17/95/115	-
24	LMG	2	324	-	-	4/4/24/70	0/1/1/1
18	CLA	B	828	-	1/1/15/20	22/37/115/115	-
18	CLA	B	837	-	1/1/15/20	21/37/115/115	-
18	CLA	A	818	-	1/1/12/20	8/19/97/115	-
18	CLA	4	306	16	1/1/12/20	7/19/97/115	-
21	BCR	B	844	-	-	10/29/63/63	0/2/2/2
18	CLA	A	815	-	1/1/15/20	13/37/115/115	-
18	CLA	K	1402	-	1/1/14/20	20/31/109/115	-
18	CLA	B	819	-	1/1/15/20	18/37/115/115	-
21	BCR	A	847	-	-	14/29/63/63	0/2/2/2
18	CLA	1	5018	13	1/1/14/20	18/31/109/115	-
24	LMG	2	301	-	-	3/4/24/70	0/1/1/1
24	LMG	2	323	-	-	0/4/24/70	0/1/1/1
18	CLA	4	305	-	1/1/14/20	9/31/109/115	-
30	CHL	1	5014	-	3/3/16/26	1/17/115/137	-
18	CLA	B	841	22	1/1/15/20	17/37/115/115	-
29	LUT	2	303	-	1/1/12/27	3/29/67/67	0/2/2/2
18	CLA	4	310	-	1/1/12/20	11/19/97/115	-
21	BCR	A	846	-	-	14/29/63/63	0/2/2/2
18	CLA	A	823	-	1/1/15/20	18/37/115/115	-
18	CLA	3	308	-	1/1/12/20	8/22/100/115	-
25	GOL	A	854	-	-	2/4/4/4	-
20	SF4	C	102	3	-	-	0/6/5/5
18	CLA	1	5006	13	1/1/15/20	16/37/115/115	-
18	CLA	L	306	-	1/1/12/20	8/19/97/115	-
24	LMG	4	320	-	-	0/4/24/70	0/1/1/1
30	CHL	4	317	-	3/3/15/26	2/12/110/137	-
18	CLA	L	301	-	1/1/13/20	12/25/103/115	-
18	CLA	B	805	-	1/1/15/20	22/37/115/115	-
30	CHL	2	315	-	4/4/18/26	8/27/125/137	-
18	CLA	A	830	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	F	301	-	1/1/15/20	18/37/115/115	-
24	LMG	F	308	-	-	12/29/49/70	0/1/1/1
24	LMG	J	1102	-	-	5/25/45/70	0/1/1/1
18	CLA	K	1401	-	1/1/11/20	5/13/91/115	-
18	CLA	J	1101	-	1/1/15/20	15/37/115/115	-
18	CLA	K	1403	-	1/1/11/20	9/17/95/115	-
18	CLA	2	308	-	1/1/15/20	15/37/115/115	-
18	CLA	1	5009	-	1/1/15/20	15/37/115/115	-
30	CHL	1	5016	-	4/4/19/26	7/33/131/137	-
18	CLA	4	311	-	1/1/14/20	14/31/109/115	-
18	CLA	2	309	14	1/1/15/20	20/37/115/115	-
18	CLA	A	834	-	1/1/12/20	9/21/99/115	-
18	CLA	B	830	-	1/1/15/20	16/37/115/115	-
30	CHL	2	318	-	3/3/16/26	4/15/113/137	-
21	BCR	F	305	-	-	14/29/63/63	0/2/2/2
18	CLA	1	5017	-	1/1/11/20	7/13/91/115	-
24	LMG	2	321	-	-	5/20/40/70	0/1/1/1
21	BCR	B	802	-	-	7/29/63/63	0/2/2/2
26	DGD	F	309	-	-	18/46/86/95	0/2/2/2
24	LMG	B	854	-	-	1/4/24/70	0/1/1/1
18	CLA	A	812	-	1/1/15/20	19/37/115/115	-
18	CLA	B	812	-	1/1/14/20	10/31/109/115	-
18	CLA	1	5012	-	1/1/11/20	7/15/93/115	-
18	CLA	A	807	1	1/1/15/20	17/37/115/115	-
18	CLA	A	835	-	1/1/15/20	12/37/115/115	-
18	CLA	3	307	-	1/1/13/20	11/25/103/115	-
30	CHL	2	316	-	3/3/16/26	0/18/116/137	-
21	BCR	B	847	-	-	15/29/63/63	0/2/2/2
18	CLA	B	835	-	1/1/13/20	9/25/103/115	-
18	CLA	3	315	15	1/1/15/20	23/37/115/115	-
22	LHG	2	320	18	-	18/39/39/53	-
18	CLA	1	5011	-	1/1/12/20	7/19/97/115	-
21	BCR	4	301	-	-	13/29/63/63	0/2/2/2
18	CLA	B	840	-	1/1/15/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	853	-	1/1/15/20	17/37/115/115	-
18	CLA	B	821	-	1/1/11/20	7/15/93/115	-
22	LHG	B	849	-	-	36/53/53/53	-
21	BCR	3	306	-	-	14/29/63/63	0/2/2/2
22	LHG	1	5019	-	-	23/53/53/53	-
18	CLA	A	821	-	1/1/14/20	10/31/109/115	-
22	LHG	B	848	18	-	10/23/23/53	-
18	CLA	A	828	-	1/1/15/20	15/37/115/115	-
18	CLA	2	326	16,14	1/1/12/20	11/19/97/115	-
18	CLA	B	803	-	1/1/15/20	11/37/115/115	-
18	CLA	A	831	-	1/1/15/20	21/37/115/115	-
26	DGD	J	1106	-	-	14/47/87/95	0/2/2/2
18	CLA	3	309	-	1/1/13/20	13/25/103/115	-
21	BCR	A	855	-	-	9/29/63/63	0/2/2/2
18	CLA	G	1602	7	1/1/11/20	6/15/93/115	-
18	CLA	4	315	-	1/1/15/20	21/37/115/115	-
21	BCR	1	5005	-	-	10/29/63/63	0/2/2/2
21	BCR	B	846	-	-	8/29/63/63	0/2/2/2
21	BCR	L	302	-	-	12/29/63/63	0/2/2/2
23	LMT	J	1107	-	-	5/11/51/61	0/2/2/2
18	CLA	A	817	-	1/1/15/20	18/37/115/115	-
18	CLA	A	827	-	1/1/15/20	17/37/115/115	-
29	LUT	1	5004	-	1/1/12/27	4/29/67/67	0/2/2/2
18	CLA	B	839	-	1/1/15/20	17/37/115/115	-
18	CLA	3	311	-	1/1/13/20	7/25/103/115	-
18	CLA	B	818	-	1/1/15/20	14/37/115/115	-
23	LMT	B	852	-	-	13/21/61/61	0/2/2/2
18	CLA	4	307	-	1/1/15/20	13/37/115/115	-
18	CLA	B	815	-	1/1/15/20	16/37/115/115	-
18	CLA	A	811	-	1/1/13/20	7/25/103/115	-
18	CLA	2	310	-	1/1/15/20	15/37/115/115	-
18	CLA	A	840	22	1/1/14/20	14/31/109/115	-
18	CLA	B	813	-	1/1/11/20	3/15/93/115	-
30	CHL	4	314	16	3/3/17/26	0/21/119/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	A	844	-	-	10/29/63/63	0/2/2/2
18	CLA	L	304	12	1/1/12/20	7/19/97/115	-
20	SF4	C	101	3	-	-	0/6/5/5
31	XAT	2	304	-	1/1/12/26	4/31/93/93	0/4/4/4
18	CLA	H	1701	-	1/1/14/20	13/31/109/115	-
17	CL0	A	801	-	3/3/20/25	7/37/135/135	-
18	CLA	B	822	-	1/1/15/20	18/37/115/115	-
18	CLA	B	823	-	1/1/15/20	16/37/115/115	-
29	LUT	3	303	-	-	3/29/67/67	0/2/2/2
18	CLA	B	824	-	1/1/13/20	13/25/103/115	-
18	CLA	G	1603	-	1/1/15/20	17/37/115/115	-
18	CLA	A	814	-	1/1/11/20	9/15/93/115	-
18	CLA	B	827	-	1/1/15/20	12/37/115/115	-
18	CLA	1	5015	-	1/1/15/20	16/37/115/115	-
21	BCR	I	101	-	-	14/29/63/63	0/2/2/2
21	BCR	I	102	-	-	16/29/63/63	0/2/2/2
30	CHL	3	313	-	3/3/17/26	4/21/119/137	-
23	LMT	G	1606	-	-	13/17/57/61	0/2/2/2
18	CLA	2	311	-	1/1/12/20	9/19/97/115	-
21	BCR	A	845	-	-	12/29/63/63	0/2/2/2
18	CLA	B	836	-	1/1/13/20	9/25/103/115	-
30	CHL	4	318	-	4/4/18/26	4/27/125/137	-
18	CLA	K	1404	-	1/1/11/20	8/15/93/115	-
21	BCR	A	843	-	-	15/29/63/63	0/2/2/2
18	CLA	A	829	-	1/1/15/20	16/37/115/115	-
18	CLA	2	313	-	1/1/12/20	10/19/97/115	-
18	CLA	J	1103	-	1/1/12/20	7/19/97/115	-
26	DGD	2	327	-	-	14/40/80/95	0/2/2/2
29	LUT	J	1105	-	1/1/12/27	4/29/67/67	0/2/2/2
23	LMT	B	856	-	-	3/17/57/61	0/2/2/2
18	CLA	B	817	-	1/1/14/20	11/31/109/115	-
30	CHL	4	316	-	4/4/19/26	8/33/131/137	-
18	CLA	2	307	14	1/1/12/20	8/22/100/115	-
18	CLA	1	5013	-	1/1/11/20	6/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LUT	1	5003	-	-	6/29/67/67	0/2/2/2
29	LUT	3	304	-	1/1/12/27	9/29/67/67	0/2/2/2
18	CLA	A	833	1	1/1/13/20	9/25/103/115	-
18	CLA	B	838	-	1/1/12/20	5/19/97/115	-
23	LMT	2	325	-	-	9/21/61/61	0/2/2/2
18	CLA	B	806	-	1/1/15/20	17/37/115/115	-
30	CHL	4	302	13	4/4/18/26	8/27/125/137	-
24	LMG	2	302	-	-	0/4/24/70	0/1/1/1
24	LMG	B	851	-	-	10/28/48/70	0/1/1/1
19	PQN	A	841	-	-	6/23/43/43	0/2/2/2
20	SF4	A	842	1,2	-	-	0/6/5/5
18	CLA	A	822	-	1/1/15/20	16/37/115/115	-
18	CLA	3	317	-	1/1/12/20	10/19/97/115	-
18	CLA	B	811	-	1/1/15/20	16/37/115/115	-
18	CLA	3	318	-	1/1/11/20	8/15/93/115	-
23	LMT	B	853	-	-	9/18/58/61	0/2/2/2
18	CLA	B	809	-	1/1/15/20	9/37/115/115	-
18	CLA	B	807	2	1/1/15/20	15/37/115/115	-
18	CLA	B	832	-	1/1/14/20	21/31/109/115	-
18	CLA	F	302	-	1/1/15/20	19/37/115/115	-
21	BCR	L	303	-	-	12/29/63/63	0/2/2/2
29	LUT	4	303	-	-	4/29/67/67	0/2/2/2
18	CLA	B	833	-	1/1/13/20	14/29/107/115	-
18	CLA	A	819	-	1/1/15/20	20/37/115/115	-
18	CLA	A	852	-	1/1/15/20	13/37/115/115	-
18	CLA	G	1601	-	1/1/13/20	8/25/103/115	-
22	LHG	A	848	-	-	31/53/53/53	-
30	CHL	2	319	-	4/4/18/26	8/27/125/137	-
21	BCR	J	1104	-	-	15/29/63/63	0/2/2/2
18	CLA	A	824	-	1/1/13/20	13/25/103/115	-
21	BCR	3	305	-	-	12/29/63/63	0/2/2/2

All (1429) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	1	5003	LUT	C24-C25	14.73	1.51	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	4	303	LUT	C24-C25	14.64	1.51	1.33
29	3	303	LUT	C24-C25	14.60	1.51	1.33
29	1	5004	LUT	C24-C25	14.58	1.51	1.33
29	J	1105	LUT	C24-C25	14.44	1.51	1.33
29	3	304	LUT	C24-C25	14.43	1.51	1.33
29	2	303	LUT	C24-C25	14.33	1.51	1.33
17	A	801	CL0	MG-NA	9.11	2.27	2.06
21	B	843	BCR	C10-C9	7.79	1.46	1.35
21	B	802	BCR	C10-C9	7.71	1.46	1.35
21	L	302	BCR	C10-C9	7.66	1.45	1.35
21	3	306	BCR	C10-C9	7.63	1.45	1.35
21	I	102	BCR	C10-C9	7.37	1.45	1.35
21	L	303	BCR	C10-C9	7.35	1.45	1.35
21	1	5005	BCR	C10-C9	7.34	1.45	1.35
21	B	844	BCR	C10-C9	7.34	1.45	1.35
21	K	1405	BCR	C10-C9	7.31	1.45	1.35
21	2	305	BCR	C10-C9	7.30	1.45	1.35
21	A	846	BCR	C10-C9	7.29	1.45	1.35
21	B	847	BCR	C10-C9	7.26	1.45	1.35
21	B	846	BCR	C10-C9	7.26	1.45	1.35
21	F	304	BCR	C10-C9	7.20	1.45	1.35
21	G	1604	BCR	C10-C9	7.19	1.45	1.35
21	L	307	BCR	C10-C9	7.19	1.45	1.35
21	3	305	BCR	C10-C9	7.19	1.45	1.35
21	A	843	BCR	C10-C9	7.17	1.45	1.35
21	A	855	BCR	C10-C9	7.16	1.45	1.35
21	F	305	BCR	C10-C9	7.15	1.45	1.35
21	I	101	BCR	C10-C9	7.03	1.45	1.35
21	4	301	BCR	C10-C9	7.02	1.45	1.35
21	A	844	BCR	C10-C9	7.00	1.45	1.35
21	B	845	BCR	C10-C9	6.99	1.45	1.35
21	A	847	BCR	C10-C9	6.99	1.45	1.35
21	J	1104	BCR	C10-C9	6.95	1.45	1.35
21	A	845	BCR	C10-C9	6.63	1.44	1.35
18	K	1402	CLA	MG-NA	6.53	2.21	2.06
18	J	1103	CLA	MG-NA	6.49	2.21	2.06
18	1	5018	CLA	MG-NA	6.48	2.21	2.06
18	K	1404	CLA	MG-NA	6.47	2.21	2.06
18	B	836	CLA	MG-NA	6.47	2.21	2.06
18	K	1403	CLA	MG-NA	6.46	2.21	2.06
18	A	838	CLA	MG-NA	6.46	2.21	2.06
18	G	1603	CLA	MG-NA	6.46	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	5012	CLA	MG-NA	6.46	2.21	2.06
18	2	307	CLA	MG-NA	6.45	2.21	2.06
18	3	314	CLA	MG-NA	6.44	2.21	2.06
18	B	822	CLA	MG-NA	6.44	2.21	2.06
18	2	326	CLA	MG-NA	6.44	2.21	2.06
18	A	808	CLA	MG-NA	6.44	2.21	2.06
18	3	311	CLA	MG-NA	6.44	2.21	2.06
18	F	302	CLA	MG-NA	6.42	2.21	2.06
18	4	306	CLA	MG-NA	6.42	2.21	2.06
18	F	303	CLA	MG-NA	6.42	2.21	2.06
18	3	308	CLA	MG-NA	6.42	2.21	2.06
18	B	824	CLA	MG-NA	6.42	2.21	2.06
18	A	833	CLA	MG-NA	6.41	2.21	2.06
18	A	834	CLA	MG-NA	6.41	2.21	2.06
18	3	309	CLA	MG-NA	6.41	2.21	2.06
18	B	811	CLA	MG-NA	6.41	2.21	2.06
18	B	810	CLA	MG-NA	6.40	2.21	2.06
18	A	823	CLA	MG-NA	6.40	2.21	2.06
18	A	820	CLA	MG-NA	6.40	2.21	2.06
18	A	822	CLA	MG-NA	6.40	2.21	2.06
18	G	1601	CLA	MG-NA	6.40	2.21	2.06
18	A	814	CLA	MG-NA	6.40	2.21	2.06
18	G	1602	CLA	MG-NA	6.40	2.21	2.06
18	L	306	CLA	MG-NA	6.39	2.21	2.06
18	2	312	CLA	MG-NA	6.39	2.21	2.06
18	B	813	CLA	MG-NA	6.39	2.21	2.06
18	A	840	CLA	MG-NA	6.39	2.21	2.06
18	K	1401	CLA	MG-NA	6.39	2.21	2.06
18	3	301	CLA	MG-NA	6.38	2.21	2.06
18	1	5010	CLA	MG-NA	6.38	2.21	2.06
18	H	1701	CLA	MG-NA	6.38	2.21	2.06
18	3	315	CLA	MG-NA	6.38	2.21	2.06
18	B	827	CLA	MG-NA	6.38	2.21	2.06
18	B	823	CLA	MG-NA	6.37	2.21	2.06
18	B	801	CLA	MG-NA	6.37	2.21	2.06
18	1	5017	CLA	MG-NA	6.37	2.21	2.06
18	4	309	CLA	MG-NA	6.37	2.21	2.06
18	4	307	CLA	MG-NA	6.37	2.21	2.06
18	4	311	CLA	MG-NA	6.37	2.21	2.06
18	A	839	CLA	MG-NA	6.37	2.21	2.06
18	A	825	CLA	MG-NA	6.37	2.21	2.06
18	2	308	CLA	MG-NA	6.37	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	313	CLA	MG-NA	6.37	2.21	2.06
18	A	813	CLA	MG-NA	6.36	2.21	2.06
18	1	5007	CLA	MG-NA	6.36	2.21	2.06
18	A	816	CLA	MG-NA	6.36	2.21	2.06
18	A	852	CLA	MG-NA	6.36	2.21	2.06
18	A	836	CLA	MG-NA	6.36	2.21	2.06
18	L	301	CLA	MG-NA	6.35	2.21	2.06
18	A	806	CLA	MG-NA	6.35	2.21	2.06
18	B	841	CLA	MG-NA	6.35	2.21	2.06
18	B	821	CLA	MG-NA	6.35	2.21	2.06
18	1	5008	CLA	MG-NA	6.35	2.21	2.06
18	B	812	CLA	MG-NA	6.35	2.21	2.06
18	B	817	CLA	MG-NA	6.35	2.21	2.06
18	B	832	CLA	MG-NA	6.35	2.21	2.06
18	B	830	CLA	MG-NA	6.34	2.21	2.06
18	B	840	CLA	MG-NA	6.34	2.21	2.06
18	A	824	CLA	MG-NA	6.34	2.21	2.06
18	F	301	CLA	MG-NA	6.34	2.21	2.06
18	B	831	CLA	MG-NA	6.34	2.21	2.06
18	4	305	CLA	MG-NA	6.34	2.21	2.06
18	A	811	CLA	MG-NA	6.34	2.21	2.06
18	3	318	CLA	MG-NA	6.34	2.21	2.06
18	A	832	CLA	MG-NA	6.34	2.21	2.06
18	B	829	CLA	MG-NA	6.34	2.21	2.06
18	J	1101	CLA	MG-NA	6.34	2.21	2.06
18	1	5015	CLA	MG-NA	6.34	2.21	2.06
18	3	307	CLA	MG-NA	6.34	2.21	2.06
18	B	839	CLA	MG-NA	6.33	2.21	2.06
18	A	827	CLA	MG-NA	6.33	2.21	2.06
18	A	829	CLA	MG-NA	6.33	2.21	2.06
18	B	818	CLA	MG-NA	6.33	2.21	2.06
18	A	817	CLA	MG-NA	6.32	2.21	2.06
18	B	835	CLA	MG-NA	6.32	2.21	2.06
18	1	5009	CLA	MG-NA	6.32	2.21	2.06
18	L	304	CLA	MG-NA	6.32	2.21	2.06
18	B	828	CLA	MG-NA	6.32	2.21	2.06
18	A	818	CLA	MG-NA	6.32	2.21	2.06
18	A	803	CLA	MG-NA	6.31	2.21	2.06
18	A	821	CLA	MG-NA	6.31	2.21	2.06
18	A	810	CLA	MG-NA	6.31	2.21	2.06
18	B	833	CLA	MG-NA	6.31	2.21	2.06
18	1	5006	CLA	MG-NA	6.31	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	808	CLA	MG-NA	6.31	2.21	2.06
18	B	805	CLA	MG-NA	6.30	2.21	2.06
18	1	5011	CLA	MG-NA	6.30	2.21	2.06
18	3	319	CLA	MG-NA	6.30	2.21	2.06
18	A	837	CLA	MG-NA	6.30	2.21	2.06
18	B	816	CLA	MG-NA	6.29	2.21	2.06
18	2	309	CLA	MG-NA	6.29	2.21	2.06
18	B	814	CLA	MG-NA	6.29	2.21	2.06
18	A	815	CLA	MG-NA	6.29	2.21	2.06
18	4	308	CLA	MG-NA	6.28	2.21	2.06
18	A	805	CLA	MG-NA	6.28	2.21	2.06
18	4	312	CLA	MG-NA	6.28	2.21	2.06
18	B	825	CLA	MG-NA	6.28	2.21	2.06
18	A	830	CLA	MG-NA	6.27	2.21	2.06
18	B	834	CLA	MG-NA	6.26	2.21	2.06
18	A	804	CLA	MG-NA	6.26	2.21	2.06
18	B	838	CLA	MG-NA	6.26	2.21	2.06
18	4	315	CLA	MG-NA	6.26	2.21	2.06
18	A	802	CLA	MG-NA	6.26	2.21	2.06
18	1	5013	CLA	MG-NA	6.26	2.21	2.06
18	B	809	CLA	MG-NA	6.25	2.21	2.06
18	A	831	CLA	MG-NA	6.25	2.21	2.06
18	L	305	CLA	MG-NA	6.24	2.21	2.06
18	4	310	CLA	MG-NA	6.24	2.21	2.06
18	B	807	CLA	MG-NA	6.24	2.21	2.06
18	B	804	CLA	MG-NA	6.24	2.21	2.06
18	A	835	CLA	MG-NA	6.23	2.21	2.06
18	2	310	CLA	MG-NA	6.22	2.21	2.06
18	A	809	CLA	MG-NA	6.22	2.21	2.06
18	A	853	CLA	MG-NA	6.22	2.21	2.06
18	B	815	CLA	MG-NA	6.21	2.21	2.06
18	2	306	CLA	MG-NA	6.20	2.21	2.06
18	A	807	CLA	MG-NA	6.20	2.21	2.06
18	B	826	CLA	MG-NA	6.19	2.21	2.06
18	B	819	CLA	MG-NA	6.19	2.21	2.06
18	B	820	CLA	MG-NA	6.18	2.21	2.06
18	B	806	CLA	MG-NA	6.18	2.20	2.06
18	2	317	CLA	MG-NA	6.17	2.20	2.06
18	B	803	CLA	MG-NA	6.17	2.20	2.06
18	2	311	CLA	MG-NA	6.17	2.20	2.06
18	A	828	CLA	MG-NA	6.17	2.20	2.06
18	A	819	CLA	MG-NA	6.17	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	317	CLA	MG-NA	6.16	2.20	2.06
18	A	812	CLA	MG-NA	6.15	2.20	2.06
18	A	826	CLA	MG-NA	6.15	2.20	2.06
18	B	837	CLA	MG-NA	6.13	2.20	2.06
21	2	305	BCR	C24-C23	5.90	1.50	1.33
21	L	303	BCR	C24-C23	5.87	1.50	1.33
21	B	843	BCR	C24-C23	5.84	1.50	1.33
21	B	802	BCR	C24-C23	5.83	1.50	1.33
21	3	306	BCR	C24-C23	5.82	1.50	1.33
21	L	302	BCR	C24-C23	5.82	1.50	1.33
21	I	102	BCR	C24-C23	5.81	1.50	1.33
21	K	1405	BCR	C24-C23	5.77	1.50	1.33
21	4	301	BCR	C24-C23	5.74	1.50	1.33
21	A	845	BCR	C24-C23	5.73	1.50	1.33
21	I	101	BCR	C24-C23	5.73	1.50	1.33
21	L	307	BCR	C24-C23	5.72	1.50	1.33
21	A	855	BCR	C24-C23	5.70	1.50	1.33
21	F	304	BCR	C24-C23	5.70	1.50	1.33
21	G	1604	BCR	C24-C23	5.70	1.50	1.33
21	F	305	BCR	C24-C23	5.69	1.50	1.33
21	A	843	BCR	C24-C23	5.68	1.50	1.33
21	1	5005	BCR	C24-C23	5.66	1.50	1.33
21	A	844	BCR	C24-C23	5.64	1.50	1.33
21	A	846	BCR	C24-C23	5.63	1.50	1.33
21	B	847	BCR	C24-C23	5.63	1.50	1.33
21	J	1104	BCR	C24-C23	5.62	1.50	1.33
21	3	305	BCR	C24-C23	5.60	1.50	1.33
21	B	844	BCR	C24-C23	5.59	1.50	1.33
21	A	847	BCR	C24-C23	5.58	1.49	1.33
21	B	846	BCR	C24-C23	5.55	1.49	1.33
21	A	845	BCR	C11-C12	-5.44	1.20	1.34
21	B	845	BCR	C24-C23	5.40	1.49	1.33
21	I	101	BCR	C11-C12	-5.37	1.20	1.34
21	J	1104	BCR	C11-C12	-5.23	1.21	1.34
21	B	845	BCR	C11-C12	-5.23	1.21	1.34
21	4	301	BCR	C11-C12	-5.23	1.21	1.34
21	A	844	BCR	C11-C12	-5.19	1.21	1.34
17	A	801	CL0	O2D-CGD	5.19	1.45	1.33
21	A	847	BCR	C11-C12	-5.19	1.21	1.34
21	A	855	BCR	C11-C12	-5.18	1.21	1.34
21	F	305	BCR	C11-C12	-5.16	1.21	1.34
17	A	801	CL0	CHC-C1C	5.16	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	F	304	BCR	C11-C12	-5.15	1.21	1.34
21	3	305	BCR	C11-C12	-5.14	1.21	1.34
21	G	1604	BCR	C11-C12	-5.13	1.21	1.34
17	A	801	CL0	O2A-C1	5.13	1.60	1.46
21	L	307	BCR	C11-C12	-5.13	1.21	1.34
21	B	847	BCR	C11-C12	-5.12	1.21	1.34
21	A	846	BCR	C11-C12	-5.11	1.21	1.34
21	A	843	BCR	C11-C12	-5.11	1.21	1.34
21	B	846	BCR	C11-C12	-5.09	1.21	1.34
21	K	1405	BCR	C11-C12	-5.09	1.21	1.34
21	1	5005	BCR	C11-C12	-5.08	1.21	1.34
21	B	844	BCR	C11-C12	-5.07	1.21	1.34
21	L	303	BCR	C11-C12	-5.02	1.21	1.34
21	2	305	BCR	C11-C12	-5.01	1.21	1.34
21	I	102	BCR	C11-C12	-4.98	1.21	1.34
21	3	306	BCR	C11-C12	-4.89	1.22	1.34
21	L	302	BCR	C11-C12	-4.87	1.22	1.34
17	A	801	CL0	CHD-C1D	4.85	1.47	1.38
21	B	802	BCR	C11-C12	-4.83	1.22	1.34
21	B	843	BCR	C11-C12	-4.82	1.22	1.34
17	A	801	CL0	C3B-C2B	4.79	1.47	1.40
17	A	801	CL0	C3C-C2C	4.71	1.46	1.36
21	B	846	BCR	C16-C17	-4.44	1.29	1.43
21	4	301	BCR	C16-C17	-4.42	1.29	1.43
21	J	1104	BCR	C16-C17	-4.37	1.29	1.43
21	B	847	BCR	C16-C17	-4.36	1.29	1.43
21	B	845	BCR	C16-C17	-4.34	1.30	1.43
21	3	306	BCR	C16-C17	-4.32	1.30	1.43
26	B	855	DGD	O1G-C1A	4.32	1.46	1.33
21	F	304	BCR	C16-C17	-4.32	1.30	1.43
21	A	845	BCR	C16-C17	-4.31	1.30	1.43
21	A	847	BCR	C16-C17	-4.31	1.30	1.43
21	1	5005	BCR	C16-C17	-4.30	1.30	1.43
21	3	305	BCR	C16-C17	-4.28	1.30	1.43
26	F	309	DGD	O1G-C1A	4.28	1.45	1.33
26	1	5002	DGD	O1G-C1A	4.28	1.45	1.33
21	A	844	BCR	C16-C17	-4.27	1.30	1.43
21	A	843	BCR	C16-C17	-4.27	1.30	1.43
21	G	1604	BCR	C16-C17	-4.26	1.30	1.43
21	A	846	BCR	C16-C17	-4.26	1.30	1.43
21	A	855	BCR	C16-C17	-4.26	1.30	1.43
21	L	307	BCR	C16-C17	-4.24	1.30	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	844	BCR	C16-C17	-4.22	1.30	1.43
21	K	1405	BCR	C16-C17	-4.22	1.30	1.43
17	A	801	CL0	C3D-C4D	-4.22	1.34	1.44
26	J	1106	DGD	O1G-C1A	4.19	1.45	1.33
21	2	305	BCR	C16-C17	-4.19	1.30	1.43
21	F	305	BCR	C16-C17	-4.19	1.30	1.43
21	L	303	BCR	C16-C17	-4.17	1.30	1.43
21	I	101	BCR	C16-C17	-4.17	1.30	1.43
21	B	802	BCR	C16-C17	-4.17	1.30	1.43
17	A	801	CL0	CHD-C4C	4.16	1.48	1.39
26	2	327	DGD	O1G-C1A	4.15	1.45	1.33
21	I	102	BCR	C16-C17	-4.13	1.30	1.43
21	L	302	BCR	C16-C17	-4.09	1.30	1.43
21	B	843	BCR	C16-C17	-4.07	1.30	1.43
18	B	830	CLA	MG-ND	-4.02	1.97	2.05
18	B	803	CLA	MG-ND	-3.96	1.97	2.05
18	A	824	CLA	MG-ND	-3.92	1.98	2.05
18	B	828	CLA	MG-ND	-3.92	1.98	2.05
18	B	827	CLA	MG-ND	-3.91	1.98	2.05
18	A	828	CLA	MG-ND	-3.90	1.98	2.05
18	B	801	CLA	MG-ND	-3.89	1.98	2.05
18	A	827	CLA	MG-ND	-3.89	1.98	2.05
18	A	818	CLA	MG-ND	-3.87	1.98	2.05
18	L	301	CLA	MG-ND	-3.86	1.98	2.05
18	B	825	CLA	MG-ND	-3.85	1.98	2.05
18	B	804	CLA	MG-ND	-3.84	1.98	2.05
18	A	852	CLA	MG-ND	-3.84	1.98	2.05
18	A	802	CLA	MG-ND	-3.83	1.98	2.05
18	B	809	CLA	MG-ND	-3.83	1.98	2.05
18	3	311	CLA	MG-ND	-3.81	1.98	2.05
18	4	309	CLA	MG-ND	-3.81	1.98	2.05
18	B	838	CLA	MG-ND	-3.81	1.98	2.05
18	1	5017	CLA	MG-ND	-3.81	1.98	2.05
17	A	801	CL0	OBD-CAD	3.81	1.29	1.22
18	B	814	CLA	MG-ND	-3.80	1.98	2.05
18	B	821	CLA	MG-ND	-3.80	1.98	2.05
18	2	312	CLA	MG-ND	-3.80	1.98	2.05
18	A	826	CLA	MG-ND	-3.80	1.98	2.05
18	A	825	CLA	MG-ND	-3.80	1.98	2.05
18	B	810	CLA	MG-ND	-3.79	1.98	2.05
18	A	808	CLA	MG-ND	-3.79	1.98	2.05
18	3	318	CLA	MG-ND	-3.79	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	831	CLA	MG-ND	-3.79	1.98	2.05
18	B	835	CLA	MG-ND	-3.78	1.98	2.05
18	A	820	CLA	MG-ND	-3.78	1.98	2.05
18	A	831	CLA	MG-ND	-3.77	1.98	2.05
18	A	819	CLA	MG-ND	-3.77	1.98	2.05
18	A	840	CLA	MG-ND	-3.76	1.98	2.05
18	B	811	CLA	MG-ND	-3.76	1.98	2.05
18	L	305	CLA	MG-ND	-3.76	1.98	2.05
18	A	816	CLA	MG-ND	-3.76	1.98	2.05
18	A	823	CLA	MG-ND	-3.76	1.98	2.05
18	A	838	CLA	MG-ND	-3.76	1.98	2.05
18	A	803	CLA	MG-ND	-3.76	1.98	2.05
18	3	307	CLA	MG-ND	-3.75	1.98	2.05
18	A	830	CLA	MG-ND	-3.75	1.98	2.05
18	B	815	CLA	MG-ND	-3.75	1.98	2.05
18	K	1404	CLA	MG-ND	-3.75	1.98	2.05
18	H	1701	CLA	MG-ND	-3.74	1.98	2.05
18	3	319	CLA	MG-ND	-3.74	1.98	2.05
18	A	817	CLA	MG-ND	-3.74	1.98	2.05
18	4	315	CLA	MG-ND	-3.74	1.98	2.05
18	4	305	CLA	MG-ND	-3.74	1.98	2.05
18	3	301	CLA	MG-ND	-3.74	1.98	2.05
18	A	837	CLA	MG-ND	-3.74	1.98	2.05
18	B	826	CLA	MG-ND	-3.74	1.98	2.05
18	4	306	CLA	MG-ND	-3.74	1.98	2.05
18	B	836	CLA	MG-ND	-3.74	1.98	2.05
18	2	317	CLA	MG-ND	-3.74	1.98	2.05
18	1	5006	CLA	MG-ND	-3.74	1.98	2.05
18	1	5013	CLA	MG-ND	-3.73	1.98	2.05
18	A	806	CLA	MG-ND	-3.73	1.98	2.05
18	B	820	CLA	MG-ND	-3.73	1.98	2.05
18	B	818	CLA	MG-ND	-3.73	1.98	2.05
18	A	811	CLA	MG-ND	-3.73	1.98	2.05
18	3	309	CLA	MG-ND	-3.73	1.98	2.05
18	K	1401	CLA	MG-ND	-3.73	1.98	2.05
18	A	821	CLA	MG-ND	-3.73	1.98	2.05
18	2	307	CLA	MG-ND	-3.73	1.98	2.05
18	B	819	CLA	MG-ND	-3.73	1.98	2.05
18	A	839	CLA	MG-ND	-3.72	1.98	2.05
18	B	805	CLA	MG-ND	-3.72	1.98	2.05
18	B	822	CLA	MG-ND	-3.72	1.98	2.05
18	B	841	CLA	MG-ND	-3.72	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	836	CLA	MG-ND	-3.72	1.98	2.05
18	B	834	CLA	MG-ND	-3.72	1.98	2.05
18	4	312	CLA	MG-ND	-3.72	1.98	2.05
18	B	823	CLA	MG-ND	-3.72	1.98	2.05
18	1	5015	CLA	MG-ND	-3.72	1.98	2.05
18	B	813	CLA	MG-ND	-3.71	1.98	2.05
18	1	5010	CLA	MG-ND	-3.71	1.98	2.05
18	3	314	CLA	MG-ND	-3.71	1.98	2.05
18	G	1602	CLA	MG-ND	-3.71	1.98	2.05
18	A	814	CLA	MG-ND	-3.71	1.98	2.05
18	A	829	CLA	MG-ND	-3.71	1.98	2.05
18	1	5007	CLA	MG-ND	-3.71	1.98	2.05
18	2	326	CLA	MG-ND	-3.71	1.98	2.05
18	4	311	CLA	MG-ND	-3.71	1.98	2.05
18	B	824	CLA	MG-ND	-3.71	1.98	2.05
18	B	816	CLA	MG-ND	-3.71	1.98	2.05
18	B	832	CLA	MG-ND	-3.70	1.98	2.05
18	4	308	CLA	MG-ND	-3.70	1.98	2.05
18	A	807	CLA	MG-ND	-3.70	1.98	2.05
18	G	1603	CLA	MG-ND	-3.70	1.98	2.05
18	A	815	CLA	MG-ND	-3.70	1.98	2.05
18	A	805	CLA	MG-ND	-3.70	1.98	2.05
18	B	808	CLA	MG-ND	-3.70	1.98	2.05
18	B	839	CLA	MG-ND	-3.70	1.98	2.05
18	A	853	CLA	MG-ND	-3.70	1.98	2.05
18	B	807	CLA	MG-ND	-3.70	1.98	2.05
18	2	311	CLA	MG-ND	-3.70	1.98	2.05
18	L	304	CLA	MG-ND	-3.70	1.98	2.05
18	2	309	CLA	MG-ND	-3.70	1.98	2.05
18	A	813	CLA	MG-ND	-3.69	1.98	2.05
18	1	5008	CLA	MG-ND	-3.69	1.98	2.05
18	4	310	CLA	MG-ND	-3.69	1.98	2.05
18	2	310	CLA	MG-ND	-3.69	1.98	2.05
18	A	834	CLA	MG-ND	-3.69	1.98	2.05
18	2	308	CLA	MG-ND	-3.69	1.98	2.05
18	1	5018	CLA	MG-ND	-3.69	1.98	2.05
18	G	1601	CLA	MG-ND	-3.69	1.98	2.05
18	F	302	CLA	MG-ND	-3.69	1.98	2.05
18	3	315	CLA	MG-ND	-3.69	1.98	2.05
18	J	1103	CLA	MG-ND	-3.69	1.98	2.05
18	B	833	CLA	MG-ND	-3.69	1.98	2.05
18	K	1403	CLA	MG-ND	-3.69	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	308	CLA	MG-ND	-3.69	1.98	2.05
18	A	833	CLA	MG-ND	-3.69	1.98	2.05
18	A	812	CLA	MG-ND	-3.69	1.98	2.05
18	A	804	CLA	MG-ND	-3.68	1.98	2.05
18	2	313	CLA	MG-ND	-3.68	1.98	2.05
18	F	301	CLA	MG-ND	-3.68	1.98	2.05
18	L	306	CLA	MG-ND	-3.68	1.98	2.05
18	K	1402	CLA	MG-ND	-3.68	1.98	2.05
18	1	5011	CLA	MG-ND	-3.68	1.98	2.05
18	4	307	CLA	MG-ND	-3.67	1.98	2.05
18	B	840	CLA	MG-ND	-3.67	1.98	2.05
18	B	829	CLA	MG-ND	-3.67	1.98	2.05
18	1	5012	CLA	MG-ND	-3.67	1.98	2.05
18	B	837	CLA	MG-ND	-3.66	1.98	2.05
18	2	306	CLA	MG-ND	-3.66	1.98	2.05
18	A	809	CLA	MG-ND	-3.66	1.98	2.05
18	1	5009	CLA	MG-ND	-3.66	1.98	2.05
18	A	832	CLA	MG-ND	-3.65	1.98	2.05
18	A	835	CLA	MG-ND	-3.65	1.98	2.05
18	B	817	CLA	MG-ND	-3.65	1.98	2.05
18	3	317	CLA	MG-ND	-3.65	1.98	2.05
18	F	303	CLA	MG-ND	-3.64	1.98	2.05
18	B	812	CLA	MG-ND	-3.64	1.98	2.05
18	J	1101	CLA	MG-ND	-3.64	1.98	2.05
18	A	822	CLA	MG-ND	-3.63	1.98	2.05
18	B	806	CLA	MG-ND	-3.63	1.98	2.05
18	A	810	CLA	MG-ND	-3.61	1.98	2.05
17	A	801	CLO	MG-NC	3.50	2.14	2.06
18	A	828	CLA	C1C-NC	-3.45	1.32	1.37
18	B	814	CLA	C1C-NC	-3.40	1.32	1.37
30	3	312	CHL	CBB-CAB	3.40	1.51	1.29
30	3	310	CHL	CBB-CAB	3.39	1.51	1.29
18	B	811	CLA	CBB-CAB	3.37	1.51	1.29
18	B	826	CLA	CBB-CAB	3.37	1.51	1.29
18	J	1103	CLA	CBB-CAB	3.37	1.51	1.29
18	A	805	CLA	CBB-CAB	3.37	1.51	1.29
30	4	318	CHL	CBB-CAB	3.37	1.51	1.29
18	B	801	CLA	CBB-CAB	3.37	1.51	1.29
18	A	828	CLA	CBB-CAB	3.37	1.51	1.29
18	A	837	CLA	CBB-CAB	3.37	1.51	1.29
18	B	832	CLA	CBB-CAB	3.37	1.51	1.29
18	A	817	CLA	CBB-CAB	3.37	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	1402	CLA	CBB-CAB	3.37	1.51	1.29
18	2	306	CLA	CBB-CAB	3.37	1.51	1.29
18	K	1403	CLA	CBB-CAB	3.37	1.51	1.29
18	B	830	CLA	CBB-CAB	3.37	1.51	1.29
18	G	1602	CLA	CBB-CAB	3.37	1.51	1.29
18	4	308	CLA	CBB-CAB	3.37	1.51	1.29
18	4	310	CLA	CBB-CAB	3.37	1.51	1.29
18	K	1404	CLA	CBB-CAB	3.37	1.51	1.29
18	3	317	CLA	CBB-CAB	3.37	1.51	1.29
18	B	833	CLA	CBB-CAB	3.37	1.51	1.29
18	1	5009	CLA	CBB-CAB	3.37	1.51	1.29
18	B	838	CLA	CBB-CAB	3.37	1.51	1.29
18	F	301	CLA	CBB-CAB	3.37	1.51	1.29
18	A	819	CLA	CBB-CAB	3.37	1.51	1.29
18	A	802	CLA	CBB-CAB	3.37	1.51	1.29
18	B	816	CLA	CBB-CAB	3.37	1.51	1.29
18	B	812	CLA	CBB-CAB	3.37	1.51	1.29
18	3	315	CLA	CBB-CAB	3.37	1.51	1.29
18	A	814	CLA	CBB-CAB	3.37	1.51	1.29
30	3	313	CHL	CBB-CAB	3.37	1.51	1.29
18	A	834	CLA	CBB-CAB	3.37	1.51	1.29
18	1	5017	CLA	CBB-CAB	3.37	1.51	1.29
18	2	310	CLA	CBB-CAB	3.37	1.51	1.29
18	B	840	CLA	CBB-CAB	3.36	1.51	1.29
18	K	1401	CLA	CBB-CAB	3.36	1.51	1.29
18	A	839	CLA	CBB-CAB	3.36	1.51	1.29
18	1	5008	CLA	CBB-CAB	3.36	1.51	1.29
18	3	307	CLA	CBB-CAB	3.36	1.51	1.29
30	1	5016	CHL	CBB-CAB	3.36	1.51	1.29
18	A	807	CLA	CBB-CAB	3.36	1.51	1.29
18	B	805	CLA	CBB-CAB	3.36	1.51	1.29
18	B	807	CLA	CBB-CAB	3.36	1.51	1.29
18	B	813	CLA	CBB-CAB	3.36	1.51	1.29
18	L	304	CLA	CBB-CAB	3.36	1.51	1.29
18	1	5010	CLA	CBB-CAB	3.36	1.51	1.29
18	L	306	CLA	CBB-CAB	3.36	1.51	1.29
18	1	5018	CLA	CBB-CAB	3.36	1.51	1.29
18	A	811	CLA	CBB-CAB	3.36	1.51	1.29
18	B	819	CLA	CBB-CAB	3.36	1.51	1.29
18	L	301	CLA	CBB-CAB	3.36	1.51	1.29
18	1	5007	CLA	CBB-CAB	3.36	1.51	1.29
18	1	5011	CLA	CBB-CAB	3.36	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	1601	CLA	CBB-CAB	3.36	1.51	1.29
18	2	317	CLA	CBB-CAB	3.36	1.51	1.29
18	B	822	CLA	CBB-CAB	3.36	1.51	1.29
18	B	825	CLA	CBB-CAB	3.36	1.51	1.29
18	2	326	CLA	CBB-CAB	3.36	1.51	1.29
18	3	311	CLA	CBB-CAB	3.36	1.51	1.29
18	A	812	CLA	CBB-CAB	3.36	1.51	1.29
18	4	311	CLA	CBB-CAB	3.36	1.51	1.29
18	K	1404	CLA	C1C-NC	-3.36	1.32	1.37
18	L	305	CLA	CBB-CAB	3.36	1.51	1.29
18	3	309	CLA	CBB-CAB	3.36	1.51	1.29
18	B	827	CLA	CBB-CAB	3.36	1.51	1.29
18	B	810	CLA	CBB-CAB	3.36	1.51	1.29
18	B	821	CLA	CBB-CAB	3.36	1.51	1.29
18	2	307	CLA	CBB-CAB	3.36	1.51	1.29
18	1	5015	CLA	CBB-CAB	3.36	1.51	1.29
18	A	827	CLA	CBB-CAB	3.36	1.51	1.29
18	B	804	CLA	CBB-CAB	3.36	1.51	1.29
18	3	308	CLA	CBB-CAB	3.36	1.51	1.29
18	A	825	CLA	CBB-CAB	3.36	1.51	1.29
18	B	835	CLA	CBB-CAB	3.36	1.51	1.29
18	F	302	CLA	CBB-CAB	3.36	1.51	1.29
18	J	1101	CLA	CBB-CAB	3.36	1.51	1.29
18	3	318	CLA	CBB-CAB	3.36	1.51	1.29
18	A	831	CLA	CBB-CAB	3.36	1.51	1.29
18	B	834	CLA	CBB-CAB	3.36	1.51	1.29
18	A	816	CLA	CBB-CAB	3.36	1.51	1.29
18	A	853	CLA	CBB-CAB	3.35	1.51	1.29
18	B	837	CLA	CBB-CAB	3.35	1.51	1.29
18	G	1603	CLA	CBB-CAB	3.35	1.51	1.29
18	A	804	CLA	CBB-CAB	3.35	1.51	1.29
18	A	838	CLA	CBB-CAB	3.35	1.51	1.29
18	A	826	CLA	CBB-CAB	3.35	1.51	1.29
18	B	803	CLA	CBB-CAB	3.35	1.51	1.29
18	A	818	CLA	CBB-CAB	3.35	1.51	1.29
18	A	836	CLA	CBB-CAB	3.35	1.51	1.29
18	2	309	CLA	CBB-CAB	3.35	1.51	1.29
18	B	831	CLA	CBB-CAB	3.35	1.51	1.29
18	A	810	CLA	CBB-CAB	3.35	1.51	1.29
18	B	828	CLA	CBB-CAB	3.35	1.51	1.29
18	A	806	CLA	CBB-CAB	3.35	1.51	1.29
18	1	5006	CLA	CBB-CAB	3.35	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	307	CLA	CBB-CAB	3.35	1.51	1.29
18	A	823	CLA	CBB-CAB	3.35	1.51	1.29
30	4	313	CHL	C4B-NB	3.35	1.38	1.35
18	3	301	CLA	CBB-CAB	3.35	1.51	1.29
18	4	306	CLA	CBB-CAB	3.35	1.51	1.29
18	B	814	CLA	CBB-CAB	3.35	1.51	1.29
18	B	836	CLA	CBB-CAB	3.35	1.51	1.29
18	A	840	CLA	CBB-CAB	3.35	1.51	1.29
18	4	305	CLA	CBB-CAB	3.35	1.51	1.29
18	B	841	CLA	CBB-CAB	3.35	1.51	1.29
18	2	313	CLA	CBB-CAB	3.35	1.51	1.29
18	A	813	CLA	CBB-CAB	3.35	1.51	1.29
18	B	808	CLA	CBB-CAB	3.35	1.51	1.29
18	4	312	CLA	CBB-CAB	3.35	1.51	1.29
18	A	808	CLA	CBB-CAB	3.35	1.51	1.29
18	B	817	CLA	CBB-CAB	3.35	1.51	1.29
18	4	315	CLA	CBB-CAB	3.34	1.51	1.29
18	B	809	CLA	CBB-CAB	3.34	1.51	1.29
18	B	815	CLA	CBB-CAB	3.34	1.51	1.29
18	4	309	CLA	CBB-CAB	3.34	1.51	1.29
18	3	314	CLA	CBB-CAB	3.34	1.51	1.29
30	2	319	CHL	CBB-CAB	3.34	1.51	1.29
18	B	818	CLA	CBB-CAB	3.34	1.51	1.29
18	A	824	CLA	CBB-CAB	3.34	1.51	1.29
18	1	5013	CLA	CBB-CAB	3.34	1.51	1.29
18	A	833	CLA	CBB-CAB	3.34	1.51	1.29
18	A	852	CLA	CBB-CAB	3.34	1.51	1.29
18	A	830	CLA	CBB-CAB	3.34	1.51	1.29
18	A	835	CLA	CBB-CAB	3.34	1.51	1.29
18	F	303	CLA	CBB-CAB	3.34	1.51	1.29
18	A	809	CLA	CBB-CAB	3.34	1.51	1.29
18	B	824	CLA	CBB-CAB	3.34	1.51	1.29
18	B	839	CLA	CBB-CAB	3.34	1.51	1.29
18	B	806	CLA	CBB-CAB	3.33	1.51	1.29
18	2	312	CLA	CBB-CAB	3.33	1.51	1.29
18	B	829	CLA	CBB-CAB	3.33	1.51	1.29
18	B	823	CLA	CBB-CAB	3.33	1.51	1.29
18	A	821	CLA	CBB-CAB	3.33	1.51	1.29
18	B	820	CLA	CBB-CAB	3.33	1.51	1.29
18	A	815	CLA	CBB-CAB	3.33	1.51	1.29
18	2	308	CLA	CBB-CAB	3.33	1.51	1.29
18	1	5012	CLA	CBB-CAB	3.32	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	313	CHL	CBB-CAB	3.32	1.51	1.29
18	H	1701	CLA	CBB-CAB	3.31	1.51	1.29
18	A	829	CLA	CBB-CAB	3.31	1.51	1.29
18	A	832	CLA	CBB-CAB	3.31	1.51	1.29
18	A	811	CLA	C1C-NC	-3.31	1.32	1.37
18	4	311	CLA	C1C-NC	-3.31	1.32	1.37
18	B	827	CLA	C1C-NC	-3.31	1.32	1.37
18	A	820	CLA	CBB-CAB	3.31	1.51	1.29
30	1	5014	CHL	CBB-CAB	3.31	1.51	1.29
18	2	311	CLA	CBB-CAB	3.30	1.51	1.29
30	3	316	CHL	C4B-NB	3.30	1.38	1.35
30	4	302	CHL	CBB-CAB	3.30	1.51	1.29
18	B	812	CLA	C1C-NC	-3.30	1.32	1.37
26	J	1106	DGD	CDA-CCA	-3.30	1.33	1.51
30	2	314	CHL	CBB-CAB	3.30	1.51	1.29
30	4	317	CHL	C4B-NB	3.29	1.38	1.35
18	A	822	CLA	CBB-CAB	3.29	1.51	1.29
30	4	317	CHL	CBB-CAB	3.29	1.51	1.29
30	4	316	CHL	C4B-NB	3.29	1.38	1.35
18	B	840	CLA	C1C-NC	-3.29	1.32	1.37
30	4	314	CHL	C4B-NB	3.29	1.38	1.35
18	A	853	CLA	C1C-NC	-3.29	1.32	1.37
18	A	822	CLA	C1C-NC	-3.29	1.32	1.37
26	J	1106	DGD	CAA-C9A	-3.28	1.33	1.51
18	A	839	CLA	C1C-NC	-3.28	1.32	1.37
30	2	319	CHL	C4B-NB	3.28	1.38	1.35
18	A	803	CLA	CBB-CAB	3.28	1.51	1.29
18	A	812	CLA	C1C-NC	-3.28	1.32	1.37
30	2	318	CHL	CBB-CAB	3.27	1.51	1.29
18	A	836	CLA	C1C-NC	-3.27	1.32	1.37
17	A	801	CL0	C1D-ND	-3.27	1.33	1.37
30	4	318	CHL	C4B-NB	3.27	1.38	1.35
24	F	306	LMG	C40-C39	-3.26	1.33	1.51
18	B	823	CLA	C1C-NC	-3.26	1.32	1.37
24	F	306	LMG	C43-C42	-3.26	1.33	1.51
18	1	5006	CLA	C1C-NC	-3.26	1.32	1.37
18	3	318	CLA	C1C-NC	-3.26	1.32	1.37
18	B	830	CLA	C1C-NC	-3.26	1.32	1.37
18	A	806	CLA	C1C-NC	-3.25	1.32	1.37
18	A	824	CLA	C1C-NC	-3.25	1.32	1.37
30	4	302	CHL	C4B-NB	3.25	1.38	1.35
18	1	5007	CLA	C1C-NC	-3.25	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	855	DGD	CAB-C9B	-3.25	1.33	1.51
18	A	825	CLA	C1C-NC	-3.25	1.33	1.37
18	A	813	CLA	C1C-NC	-3.24	1.33	1.37
18	1	5008	CLA	C1C-NC	-3.24	1.33	1.37
18	4	309	CLA	C1C-NC	-3.24	1.33	1.37
18	A	814	CLA	C1C-NC	-3.24	1.33	1.37
24	1	5020	LMG	C19-C18	-3.24	1.33	1.51
18	A	807	CLA	C1C-NC	-3.24	1.33	1.37
24	F	306	LMG	C37-C36	-3.23	1.33	1.51
18	B	833	CLA	C1C-NC	-3.23	1.33	1.37
18	B	809	CLA	C1C-NC	-3.23	1.33	1.37
24	A	851	LMG	C22-C21	-3.23	1.33	1.51
26	F	309	DGD	CGA-CFA	-3.23	1.33	1.51
26	B	855	DGD	CGB-CFB	-3.23	1.33	1.51
30	3	313	CHL	C4B-NB	3.23	1.38	1.35
26	J	1106	DGD	CGA-CFA	-3.23	1.33	1.51
18	3	319	CLA	CBB-CAB	3.23	1.50	1.29
24	1	5001	LMG	C19-C18	-3.23	1.33	1.51
24	A	851	LMG	C25-C24	-3.23	1.33	1.51
30	2	314	CHL	C4B-NB	3.23	1.38	1.35
24	1	5020	LMG	C25-C24	-3.22	1.33	1.51
18	J	1103	CLA	C1C-NC	-3.22	1.33	1.37
18	B	832	CLA	C1C-NC	-3.22	1.33	1.37
18	2	311	CLA	C1C-NC	-3.22	1.33	1.37
26	2	327	DGD	CAA-C9A	-3.22	1.33	1.51
26	B	855	DGD	CDB-CCB	-3.22	1.33	1.51
18	4	315	CLA	C1C-NC	-3.22	1.33	1.37
18	B	811	CLA	C1C-NC	-3.22	1.33	1.37
18	B	806	CLA	C1C-NC	-3.22	1.33	1.37
24	A	851	LMG	C37-C36	-3.22	1.33	1.51
18	L	301	CLA	C1C-NC	-3.21	1.33	1.37
24	F	307	LMG	C37-C36	-3.21	1.33	1.51
18	3	317	CLA	C1C-NC	-3.21	1.33	1.37
24	1	5020	LMG	C22-C21	-3.21	1.33	1.51
18	B	813	CLA	C1C-NC	-3.21	1.33	1.37
18	B	803	CLA	C1C-NC	-3.21	1.33	1.37
18	B	804	CLA	C1C-NC	-3.21	1.33	1.37
26	F	309	DGD	CAA-C9A	-3.21	1.33	1.51
24	1	5001	LMG	C43-C42	-3.21	1.33	1.51
26	F	309	DGD	CDA-CCA	-3.21	1.33	1.51
24	A	851	LMG	C19-C18	-3.21	1.33	1.51
18	A	831	CLA	C1C-NC	-3.20	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	H	1701	CLA	C1C-NC	-3.20	1.33	1.37
18	4	305	CLA	C1C-NC	-3.20	1.33	1.37
18	B	815	CLA	C1C-NC	-3.20	1.33	1.37
18	B	835	CLA	C1C-NC	-3.20	1.33	1.37
18	B	819	CLA	C1C-NC	-3.20	1.33	1.37
18	L	305	CLA	C1C-NC	-3.20	1.33	1.37
18	B	826	CLA	C1C-NC	-3.20	1.33	1.37
18	B	839	CLA	C1C-NC	-3.20	1.33	1.37
18	2	306	CLA	C1C-NC	-3.20	1.33	1.37
18	2	317	CLA	C1C-NC	-3.20	1.33	1.37
24	1	5001	LMG	C37-C36	-3.20	1.33	1.51
24	B	850	LMG	C19-C18	-3.20	1.33	1.51
30	1	5016	CHL	C4B-NB	3.19	1.38	1.35
18	G	1601	CLA	C1C-NC	-3.19	1.33	1.37
18	3	309	CLA	C1C-NC	-3.19	1.33	1.37
18	B	818	CLA	C1C-NC	-3.19	1.33	1.37
18	F	301	CLA	C1C-NC	-3.19	1.33	1.37
18	B	822	CLA	C1C-NC	-3.19	1.33	1.37
24	1	5001	LMG	C40-C39	-3.19	1.33	1.51
26	B	855	DGD	CAA-C9A	-3.19	1.33	1.51
18	B	841	CLA	C1C-NC	-3.18	1.33	1.37
18	1	5009	CLA	C1C-NC	-3.18	1.33	1.37
18	3	307	CLA	C1C-NC	-3.18	1.33	1.37
18	A	835	CLA	C1C-NC	-3.18	1.33	1.37
18	A	821	CLA	C1C-NC	-3.18	1.33	1.37
18	A	827	CLA	C1C-NC	-3.18	1.33	1.37
18	K	1403	CLA	C1C-NC	-3.18	1.33	1.37
30	2	318	CHL	C4B-NB	3.18	1.38	1.35
18	B	807	CLA	C1C-NC	-3.18	1.33	1.37
18	F	303	CLA	C1C-NC	-3.17	1.33	1.37
18	A	808	CLA	C1C-NC	-3.17	1.33	1.37
18	A	826	CLA	C1C-NC	-3.17	1.33	1.37
18	L	304	CLA	C1C-NC	-3.17	1.33	1.37
18	A	810	CLA	C1C-NC	-3.17	1.33	1.37
18	A	815	CLA	C1C-NC	-3.17	1.33	1.37
18	A	820	CLA	C1C-NC	-3.17	1.33	1.37
30	3	316	CHL	CBB-CAB	3.17	1.50	1.29
30	2	315	CHL	CBB-CAB	3.17	1.50	1.29
18	A	804	CLA	C1C-NC	-3.17	1.33	1.37
18	K	1402	CLA	C1C-NC	-3.17	1.33	1.37
18	A	805	CLA	C1C-NC	-3.17	1.33	1.37
18	B	808	CLA	C1C-NC	-3.16	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	810	CLA	C1C-NC	-3.16	1.33	1.37
18	L	306	CLA	C1C-NC	-3.16	1.33	1.37
18	J	1101	CLA	C1C-NC	-3.16	1.33	1.37
18	K	1401	CLA	C1C-NC	-3.16	1.33	1.37
30	1	5014	CHL	C4B-NB	3.16	1.38	1.35
18	2	310	CLA	C1C-NC	-3.16	1.33	1.37
30	3	310	CHL	C4B-NB	3.16	1.38	1.35
18	B	816	CLA	C1C-NC	-3.16	1.33	1.37
18	1	5010	CLA	C1C-NC	-3.16	1.33	1.37
18	A	809	CLA	C1C-NC	-3.16	1.33	1.37
18	2	308	CLA	C1C-NC	-3.16	1.33	1.37
18	4	308	CLA	C1C-NC	-3.15	1.33	1.37
18	2	326	CLA	C1C-NC	-3.15	1.33	1.37
18	B	829	CLA	C1C-NC	-3.15	1.33	1.37
18	F	302	CLA	C1C-NC	-3.15	1.33	1.37
30	2	316	CHL	C3B-C2B	-3.15	1.36	1.40
18	3	301	CLA	C1C-NC	-3.15	1.33	1.37
30	2	316	CHL	CBB-CAB	3.15	1.50	1.29
30	4	316	CHL	CBB-CAB	3.15	1.50	1.29
18	3	308	CLA	C1C-NC	-3.15	1.33	1.37
18	1	5012	CLA	C1C-NC	-3.15	1.33	1.37
18	4	312	CLA	C1C-NC	-3.15	1.33	1.37
18	A	819	CLA	C1C-NC	-3.15	1.33	1.37
18	B	837	CLA	C1C-NC	-3.15	1.33	1.37
18	2	307	CLA	C1C-NC	-3.15	1.33	1.37
18	A	840	CLA	C1C-NC	-3.14	1.33	1.37
18	A	837	CLA	C1C-NC	-3.14	1.33	1.37
18	2	312	CLA	C1C-NC	-3.14	1.33	1.37
18	B	821	CLA	C1C-NC	-3.14	1.33	1.37
18	3	311	CLA	C1C-NC	-3.14	1.33	1.37
18	1	5015	CLA	C1C-NC	-3.13	1.33	1.37
18	B	824	CLA	C1C-NC	-3.13	1.33	1.37
18	4	310	CLA	C1C-NC	-3.13	1.33	1.37
18	1	5013	CLA	C1C-NC	-3.13	1.33	1.37
18	3	315	CLA	C1C-NC	-3.13	1.33	1.37
18	3	319	CLA	C1C-NC	-3.13	1.33	1.37
18	A	852	CLA	C1C-NC	-3.13	1.33	1.37
18	B	828	CLA	C1C-NC	-3.13	1.33	1.37
18	A	838	CLA	C1C-NC	-3.13	1.33	1.37
18	A	818	CLA	C1C-NC	-3.12	1.33	1.37
18	2	313	CLA	C1C-NC	-3.12	1.33	1.37
18	2	309	CLA	C1C-NC	-3.12	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	316	CHL	C3B-C2B	-3.12	1.36	1.40
18	B	831	CLA	C1C-NC	-3.12	1.33	1.37
18	A	832	CLA	C1C-NC	-3.12	1.33	1.37
18	4	306	CLA	C1C-NC	-3.12	1.33	1.37
18	B	838	CLA	C1C-NC	-3.12	1.33	1.37
18	A	816	CLA	C1C-NC	-3.11	1.33	1.37
18	B	834	CLA	C1C-NC	-3.11	1.33	1.37
18	A	829	CLA	C1C-NC	-3.11	1.33	1.37
18	B	836	CLA	C1C-NC	-3.11	1.33	1.37
18	A	830	CLA	C1C-NC	-3.11	1.33	1.37
30	4	314	CHL	CBB-CAB	3.11	1.49	1.29
18	G	1602	CLA	C1C-NC	-3.11	1.33	1.37
30	2	316	CHL	C4B-NB	3.10	1.38	1.35
18	1	5018	CLA	C1C-NC	-3.10	1.33	1.37
18	B	820	CLA	C1C-NC	-3.09	1.33	1.37
18	3	314	CLA	C1C-NC	-3.09	1.33	1.37
18	1	5011	CLA	C1C-NC	-3.09	1.33	1.37
18	B	805	CLA	C1C-NC	-3.09	1.33	1.37
18	G	1603	CLA	C1C-NC	-3.09	1.33	1.37
18	A	802	CLA	C1C-NC	-3.09	1.33	1.37
18	A	803	CLA	C1C-NC	-3.09	1.33	1.37
18	A	817	CLA	C1C-NC	-3.09	1.33	1.37
18	B	817	CLA	C1C-NC	-3.09	1.33	1.37
18	A	833	CLA	C1C-NC	-3.08	1.33	1.37
18	1	5017	CLA	C1C-NC	-3.08	1.33	1.37
18	4	307	CLA	C1C-NC	-3.08	1.33	1.37
18	A	834	CLA	C1C-NC	-3.07	1.33	1.37
17	A	801	CLO	C3D-C2D	3.05	1.47	1.39
30	2	315	CHL	C4B-NB	3.01	1.37	1.35
18	B	801	CLA	C1C-NC	-3.01	1.33	1.37
18	B	825	CLA	C1C-NC	-3.00	1.33	1.37
30	3	312	CHL	C4B-NB	2.97	1.37	1.35
18	A	823	CLA	C1C-NC	-2.94	1.33	1.37
17	A	801	CLO	C4D-CHA	2.88	1.48	1.38
30	3	316	CHL	C3B-C2B	-2.84	1.36	1.40
18	B	801	CLA	C3B-C2B	-2.84	1.36	1.40
18	3	319	CLA	C3B-C2B	-2.81	1.36	1.40
18	A	832	CLA	CHC-C1C	2.81	1.42	1.35
18	3	307	CLA	CHC-C1C	2.80	1.42	1.35
30	4	314	CHL	C3B-C2B	-2.79	1.36	1.40
18	B	826	CLA	CHC-C1C	2.79	1.42	1.35
18	F	301	CLA	CHC-C1C	2.78	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	817	CLA	CHC-C1C	2.78	1.42	1.35
18	B	841	CLA	CHC-C1C	2.78	1.42	1.35
18	A	816	CLA	CHC-C1C	2.77	1.42	1.35
18	L	305	CLA	CHC-C1C	2.77	1.42	1.35
18	B	801	CLA	CHC-C1C	2.76	1.42	1.35
18	A	805	CLA	CHC-C1C	2.76	1.42	1.35
18	A	802	CLA	CHC-C1C	2.75	1.42	1.35
18	1	5018	CLA	CHC-C1C	2.75	1.42	1.35
18	1	5009	CLA	CHC-C1C	2.75	1.42	1.35
18	1	5017	CLA	CHC-C1C	2.75	1.42	1.35
18	2	306	CLA	CHC-C1C	2.74	1.42	1.35
18	A	835	CLA	CHC-C1C	2.74	1.42	1.35
18	A	829	CLA	CHC-C1C	2.74	1.42	1.35
18	A	809	CLA	CHC-C1C	2.74	1.42	1.35
18	A	825	CLA	CHC-C1C	2.73	1.42	1.35
18	A	831	CLA	CHC-C1C	2.73	1.42	1.35
18	B	837	CLA	CHC-C1C	2.73	1.42	1.35
18	L	301	CLA	CHC-C1C	2.73	1.42	1.35
18	3	319	CLA	CHC-C1C	2.73	1.42	1.35
18	A	852	CLA	C3B-C2B	-2.73	1.36	1.40
18	A	824	CLA	CHC-C1C	2.73	1.42	1.35
18	B	820	CLA	CHC-C1C	2.73	1.42	1.35
18	B	805	CLA	CHC-C1C	2.72	1.41	1.35
18	A	837	CLA	CHC-C1C	2.72	1.41	1.35
18	A	817	CLA	CHC-C1C	2.72	1.41	1.35
18	3	315	CLA	CHC-C1C	2.72	1.41	1.35
18	B	832	CLA	CHC-C1C	2.72	1.41	1.35
18	3	317	CLA	CHC-C1C	2.71	1.41	1.35
18	B	824	CLA	CHC-C1C	2.71	1.41	1.35
18	A	822	CLA	CHC-C1C	2.71	1.41	1.35
18	B	804	CLA	CHC-C1C	2.71	1.41	1.35
18	1	5006	CLA	CHC-C1C	2.71	1.41	1.35
18	A	819	CLA	CHC-C1C	2.71	1.41	1.35
18	A	803	CLA	CHC-C1C	2.71	1.41	1.35
18	A	834	CLA	CHC-C1C	2.70	1.41	1.35
18	F	303	CLA	CHC-C1C	2.70	1.41	1.35
18	A	826	CLA	CHC-C1C	2.70	1.41	1.35
18	4	310	CLA	CHC-C1C	2.70	1.41	1.35
18	4	305	CLA	CHC-C1C	2.70	1.41	1.35
18	B	834	CLA	CHC-C1C	2.70	1.41	1.35
18	2	309	CLA	CHC-C1C	2.70	1.41	1.35
18	B	807	CLA	CHC-C1C	2.70	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	306	CLA	CHC-C1C	2.69	1.41	1.35
18	B	838	CLA	CHC-C1C	2.69	1.41	1.35
18	1	5011	CLA	CHC-C1C	2.69	1.41	1.35
18	3	311	CLA	CHC-C1C	2.69	1.41	1.35
18	B	825	CLA	CHC-C1C	2.69	1.41	1.35
18	A	836	CLA	CHC-C1C	2.68	1.41	1.35
18	A	830	CLA	CHC-C1C	2.68	1.41	1.35
18	A	814	CLA	C3B-C2B	-2.68	1.36	1.40
18	A	810	CLA	CHC-C1C	2.68	1.41	1.35
18	4	306	CLA	CHC-C1C	2.68	1.41	1.35
18	B	815	CLA	CHC-C1C	2.68	1.41	1.35
18	G	1602	CLA	CHC-C1C	2.68	1.41	1.35
18	A	812	CLA	CHC-C1C	2.68	1.41	1.35
18	B	812	CLA	CHC-C1C	2.68	1.41	1.35
18	K	1401	CLA	CHC-C1C	2.68	1.41	1.35
18	1	5015	CLA	CHC-C1C	2.67	1.41	1.35
18	4	312	CLA	CHC-C1C	2.67	1.41	1.35
18	B	811	CLA	CHC-C1C	2.67	1.41	1.35
18	B	839	CLA	CHC-C1C	2.67	1.41	1.35
18	A	833	CLA	CHC-C1C	2.67	1.41	1.35
18	4	308	CLA	CHC-C1C	2.67	1.41	1.35
18	B	835	CLA	CHC-C1C	2.67	1.41	1.35
18	1	5007	CLA	CHC-C1C	2.67	1.41	1.35
18	B	816	CLA	CHC-C1C	2.66	1.41	1.35
23	G	1605	LMT	O3'-C3'	-2.66	1.36	1.43
18	2	307	CLA	CHC-C1C	2.66	1.41	1.35
18	A	806	CLA	CHC-C1C	2.66	1.41	1.35
18	4	311	CLA	CHC-C1C	2.66	1.41	1.35
18	4	307	CLA	CHC-C1C	2.66	1.41	1.35
18	3	314	CLA	CHC-C1C	2.66	1.41	1.35
18	2	313	CLA	CHC-C1C	2.66	1.41	1.35
18	3	308	CLA	CHC-C1C	2.65	1.41	1.35
18	A	804	CLA	CHC-C1C	2.65	1.41	1.35
18	G	1603	CLA	CHC-C1C	2.65	1.41	1.35
18	3	301	CLA	CHC-C1C	2.65	1.41	1.35
18	B	831	CLA	CHC-C1C	2.65	1.41	1.35
18	F	302	CLA	CHC-C1C	2.65	1.41	1.35
18	A	807	CLA	CHC-C1C	2.65	1.41	1.35
18	3	309	CLA	CHC-C1C	2.65	1.41	1.35
18	A	852	CLA	CHC-C1C	2.65	1.41	1.35
18	B	820	CLA	C3B-C2B	-2.65	1.36	1.40
18	B	823	CLA	CHC-C1C	2.65	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	836	CLA	CHC-C1C	2.64	1.41	1.35
18	1	5012	CLA	CHC-C1C	2.64	1.41	1.35
18	2	312	CLA	CHC-C1C	2.64	1.41	1.35
18	A	803	CLA	C3B-C2B	-2.64	1.36	1.40
18	B	803	CLA	CHC-C1C	2.64	1.41	1.35
18	B	835	CLA	C3B-C2B	-2.64	1.36	1.40
18	A	821	CLA	CHC-C1C	2.64	1.41	1.35
18	K	1402	CLA	CHC-C1C	2.64	1.41	1.35
18	A	840	CLA	CHC-C1C	2.64	1.41	1.35
18	B	823	CLA	C3B-C2B	-2.64	1.36	1.40
18	B	833	CLA	CHC-C1C	2.63	1.41	1.35
18	G	1601	CLA	CHC-C1C	2.63	1.41	1.35
18	A	815	CLA	CHC-C1C	2.63	1.41	1.35
18	B	808	CLA	CHC-C1C	2.63	1.41	1.35
18	A	827	CLA	CHC-C1C	2.63	1.41	1.35
18	A	822	CLA	C3B-C2B	-2.63	1.36	1.40
18	B	827	CLA	CHC-C1C	2.63	1.41	1.35
18	B	828	CLA	CHC-C1C	2.63	1.41	1.35
18	2	310	CLA	CHC-C1C	2.63	1.41	1.35
18	B	829	CLA	CHC-C1C	2.62	1.41	1.35
23	A	850	LMT	O3'-C3'	-2.62	1.36	1.43
18	3	318	CLA	CHC-C1C	2.62	1.41	1.35
18	B	822	CLA	CHC-C1C	2.62	1.41	1.35
18	B	806	CLA	CHC-C1C	2.62	1.41	1.35
23	J	1107	LMT	O3'-C3'	-2.62	1.36	1.43
18	A	818	CLA	CHC-C1C	2.61	1.41	1.35
18	J	1103	CLA	CHC-C1C	2.61	1.41	1.35
18	A	811	CLA	CHC-C1C	2.61	1.41	1.35
18	A	838	CLA	CHC-C1C	2.61	1.41	1.35
18	2	326	CLA	CHC-C1C	2.61	1.41	1.35
18	J	1101	CLA	CHC-C1C	2.61	1.41	1.35
18	A	839	CLA	CHC-C1C	2.61	1.41	1.35
23	4	319	LMT	O3'-C3'	-2.61	1.36	1.43
23	B	856	LMT	O3'-C3'	-2.61	1.36	1.43
18	L	304	CLA	CHC-C1C	2.61	1.41	1.35
18	2	308	CLA	CHC-C1C	2.60	1.41	1.35
18	1	5013	CLA	CHC-C1C	2.60	1.41	1.35
18	B	819	CLA	CHC-C1C	2.60	1.41	1.35
18	4	309	CLA	CHC-C1C	2.60	1.41	1.35
18	A	808	CLA	CHC-C1C	2.60	1.41	1.35
18	A	853	CLA	CHC-C1C	2.60	1.41	1.35
17	A	801	CL0	C4B-CHC	2.60	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	821	CLA	CHC-C1C	2.60	1.41	1.35
18	B	840	CLA	C3B-C2B	-2.60	1.36	1.40
18	B	813	CLA	CHC-C1C	2.59	1.41	1.35
18	A	820	CLA	CHC-C1C	2.59	1.41	1.35
17	A	801	CL0	C1B-CHB	2.58	1.48	1.41
18	A	813	CLA	CHC-C1C	2.58	1.41	1.35
18	1	5010	CLA	CHC-C1C	2.58	1.41	1.35
18	1	5008	CLA	CHC-C1C	2.58	1.41	1.35
18	2	311	CLA	CHC-C1C	2.58	1.41	1.35
18	A	814	CLA	CHC-C1C	2.58	1.41	1.35
18	H	1701	CLA	CHC-C1C	2.57	1.41	1.35
18	B	806	CLA	C3B-C2B	-2.57	1.36	1.40
18	B	818	CLA	CHC-C1C	2.57	1.41	1.35
18	A	823	CLA	CHC-C1C	2.57	1.41	1.35
18	2	317	CLA	CHC-C1C	2.57	1.41	1.35
18	B	810	CLA	CHC-C1C	2.56	1.41	1.35
24	2	322	LMG	C19-C18	-2.56	1.33	1.51
18	B	814	CLA	CHC-C1C	2.56	1.41	1.35
18	4	315	CLA	CHC-C1C	2.56	1.41	1.35
18	A	826	CLA	C3B-C2B	-2.56	1.36	1.40
23	B	852	LMT	O3'-C3'	-2.56	1.37	1.43
18	A	832	CLA	C3B-C2B	-2.55	1.36	1.40
18	A	831	CLA	C3B-C2B	-2.54	1.36	1.40
23	G	1606	LMT	O3'-C3'	-2.54	1.37	1.43
18	B	809	CLA	CHC-C1C	2.53	1.41	1.35
18	1	5012	CLA	C3B-C2B	-2.53	1.36	1.40
23	B	853	LMT	O3'-C3'	-2.53	1.37	1.43
18	B	818	CLA	C3B-C2B	-2.52	1.36	1.40
18	L	305	CLA	C3B-C2B	-2.51	1.36	1.40
18	K	1404	CLA	CHC-C1C	2.51	1.41	1.35
18	B	812	CLA	C3B-C2B	-2.50	1.36	1.40
18	A	811	CLA	C3B-C2B	-2.49	1.36	1.40
18	A	836	CLA	C3B-C2B	-2.49	1.36	1.40
23	2	325	LMT	O3'-C3'	-2.49	1.37	1.43
18	1	5013	CLA	C3B-C2B	-2.49	1.36	1.40
18	2	326	CLA	C3B-C2B	-2.49	1.36	1.40
18	B	840	CLA	CHC-C1C	2.49	1.41	1.35
17	A	801	CL0	C1C-NC	-2.49	1.34	1.37
18	1	5008	CLA	C3B-C2B	-2.48	1.36	1.40
18	3	314	CLA	C3B-C2B	-2.48	1.36	1.40
18	A	830	CLA	C3B-C2B	-2.48	1.36	1.40
18	B	809	CLA	C3B-C2B	-2.48	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	833	CLA	C3B-C2B	-2.48	1.36	1.40
18	4	312	CLA	C3B-C2B	-2.47	1.36	1.40
18	A	828	CLA	CHC-C1C	2.47	1.41	1.35
18	1	5007	CLA	C3B-C2B	-2.47	1.36	1.40
18	K	1403	CLA	CHC-C1C	2.47	1.41	1.35
18	4	306	CLA	C3B-C2B	-2.46	1.37	1.40
18	A	839	CLA	C3B-C2B	-2.46	1.37	1.40
18	B	824	CLA	C3B-C2B	-2.46	1.37	1.40
18	A	835	CLA	C3B-C2B	-2.46	1.37	1.40
18	F	303	CLA	C3B-C2B	-2.45	1.37	1.40
18	A	810	CLA	C3B-C2B	-2.45	1.37	1.40
18	K	1404	CLA	C3B-C2B	-2.45	1.37	1.40
24	G	1607	LMG	O1-C1	2.44	1.44	1.40
18	3	309	CLA	C3B-C2B	-2.44	1.37	1.40
18	B	830	CLA	CHC-C1C	2.43	1.41	1.35
18	2	307	CLA	C3B-C2B	-2.43	1.37	1.40
18	4	311	CLA	C3B-C2B	-2.43	1.37	1.40
17	A	801	CL0	C1D-C2D	2.43	1.50	1.45
18	4	307	CLA	C3B-C2B	-2.41	1.37	1.40
18	H	1701	CLA	C3B-C2B	-2.41	1.37	1.40
18	B	811	CLA	C3B-C2B	-2.41	1.37	1.40
18	K	1403	CLA	C3B-C2B	-2.39	1.37	1.40
18	3	308	CLA	C3B-C2B	-2.39	1.37	1.40
18	A	824	CLA	C1C-C2C	2.38	1.49	1.44
18	B	822	CLA	C3B-C2B	-2.38	1.37	1.40
18	2	308	CLA	C3B-C2B	-2.37	1.37	1.40
18	K	1402	CLA	C3B-C2B	-2.37	1.37	1.40
18	A	824	CLA	C3B-C2B	-2.34	1.37	1.40
18	4	315	CLA	C3B-C2B	-2.34	1.37	1.40
23	B	856	LMT	O2'-C2'	-2.33	1.37	1.43
18	J	1103	CLA	C3B-C2B	-2.32	1.37	1.40
18	B	809	CLA	C1B-NB	2.32	1.37	1.35
18	A	853	CLA	C3B-C2B	-2.32	1.37	1.40
18	2	308	CLA	C1B-NB	2.32	1.37	1.35
23	B	856	LMT	O3B-C3B	-2.32	1.37	1.43
18	A	816	CLA	C1C-C2C	2.31	1.49	1.44
18	1	5017	CLA	C3B-C2B	-2.31	1.37	1.40
18	A	809	CLA	C3B-C2B	-2.31	1.37	1.40
18	B	821	CLA	C3B-C2B	-2.31	1.37	1.40
18	A	806	CLA	C1B-NB	2.31	1.37	1.35
23	B	852	LMT	O3B-C3B	-2.31	1.37	1.43
23	B	856	LMT	O2B-C2B	-2.31	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	808	CLA	C1B-NB	2.31	1.37	1.35
23	G	1605	LMT	O2B-C2B	-2.31	1.37	1.43
18	2	313	CLA	C3B-C2B	-2.31	1.37	1.40
23	4	319	LMT	O2B-C2B	-2.30	1.37	1.43
18	1	5018	CLA	C1C-C2C	2.30	1.49	1.44
18	3	307	CLA	C1C-C2C	2.30	1.49	1.44
18	4	309	CLA	C3B-C2B	-2.30	1.37	1.40
18	A	826	CLA	C1B-NB	2.30	1.37	1.35
23	J	1107	LMT	O2B-C2B	-2.30	1.37	1.43
18	F	301	CLA	C1C-C2C	2.30	1.49	1.44
23	G	1605	LMT	O3B-C3B	-2.30	1.37	1.43
23	G	1606	LMT	O3B-C3B	-2.30	1.37	1.43
23	2	325	LMT	O2B-C2B	-2.29	1.37	1.43
23	B	852	LMT	O2B-C2B	-2.29	1.37	1.43
18	2	311	CLA	C3B-C2B	-2.28	1.37	1.40
23	4	319	LMT	O3B-C3B	-2.28	1.37	1.43
18	B	801	CLA	C1C-C2C	2.28	1.49	1.44
18	B	839	CLA	C3B-C2B	-2.28	1.37	1.40
18	B	831	CLA	C3B-C2B	-2.28	1.37	1.40
23	B	853	LMT	O3B-C3B	-2.28	1.37	1.43
18	2	309	CLA	C3B-C2B	-2.28	1.37	1.40
18	L	304	CLA	C3B-C2B	-2.28	1.37	1.40
18	1	5017	CLA	C1C-C2C	2.27	1.49	1.44
18	B	817	CLA	C1C-C2C	2.27	1.49	1.44
18	4	311	CLA	C1C-C2C	2.27	1.49	1.44
18	A	833	CLA	C1B-NB	2.27	1.37	1.35
23	J	1107	LMT	O2'-C2'	-2.27	1.37	1.43
23	4	319	LMT	O2'-C2'	-2.27	1.37	1.43
18	A	830	CLA	C1B-NB	2.26	1.37	1.35
18	2	313	CLA	C1B-NB	2.26	1.37	1.35
18	A	825	CLA	C1C-C2C	2.26	1.48	1.44
18	B	839	CLA	C1B-NB	2.26	1.37	1.35
18	A	852	CLA	C1B-NB	2.26	1.37	1.35
18	4	312	CLA	C1B-NB	2.26	1.37	1.35
18	B	812	CLA	C1C-C2C	2.26	1.48	1.44
23	B	853	LMT	O2B-C2B	-2.25	1.37	1.43
23	A	850	LMT	O3B-C3B	-2.25	1.37	1.43
31	2	304	XAT	O24-C25	-2.25	1.43	1.46
18	A	836	CLA	C1C-C2C	2.25	1.48	1.44
23	G	1606	LMT	O2'-C2'	-2.25	1.37	1.43
18	A	822	CLA	C1C-C2C	2.25	1.48	1.44
18	3	319	CLA	C1B-NB	2.24	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	305	CLA	C1B-NB	2.24	1.37	1.35
18	B	828	CLA	C3B-C2B	-2.24	1.37	1.40
18	A	832	CLA	C1C-C2C	2.24	1.48	1.44
18	L	301	CLA	C1C-C2C	2.24	1.48	1.44
23	J	1107	LMT	O3B-C3B	-2.24	1.37	1.43
18	B	841	CLA	C1C-C2C	2.24	1.48	1.44
18	A	835	CLA	C1B-NB	2.23	1.37	1.35
18	A	823	CLA	MG-NC	2.23	2.11	2.06
18	A	835	CLA	C1C-C2C	2.23	1.48	1.44
18	B	805	CLA	C1C-C2C	2.23	1.48	1.44
18	A	838	CLA	C1C-C2C	2.23	1.48	1.44
23	G	1605	LMT	O2'-C2'	-2.23	1.37	1.43
23	2	325	LMT	O3B-C3B	-2.23	1.37	1.43
23	B	852	LMT	O2'-C2'	-2.23	1.37	1.43
18	A	824	CLA	C1B-NB	2.23	1.37	1.35
18	A	853	CLA	C1B-NB	2.23	1.37	1.35
18	3	314	CLA	C1B-NB	2.23	1.37	1.35
18	A	831	CLA	C1B-NB	2.22	1.37	1.35
18	A	820	CLA	C3B-C2B	-2.22	1.37	1.40
18	3	319	CLA	C1C-C2C	2.22	1.48	1.44
18	2	317	CLA	C3B-C2B	-2.22	1.37	1.40
18	F	303	CLA	C1C-C2C	2.22	1.48	1.44
18	A	810	CLA	C1B-NB	2.22	1.37	1.35
18	B	824	CLA	C1B-NB	2.22	1.37	1.35
18	B	830	CLA	CHD-C1D	2.22	1.42	1.38
18	B	819	CLA	C3B-C2B	-2.22	1.37	1.40
18	A	834	CLA	C1C-C2C	2.22	1.48	1.44
18	J	1103	CLA	C1C-C2C	2.22	1.48	1.44
18	B	835	CLA	C1C-C2C	2.21	1.48	1.44
18	A	809	CLA	C1B-NB	2.21	1.37	1.35
18	2	308	CLA	C1C-C2C	2.21	1.48	1.44
18	A	807	CLA	C1C-C2C	2.21	1.48	1.44
18	A	802	CLA	C1C-C2C	2.21	1.48	1.44
18	B	839	CLA	C1C-C2C	2.21	1.48	1.44
18	B	804	CLA	C3B-C2B	-2.21	1.37	1.40
18	3	308	CLA	C1C-C2C	2.21	1.48	1.44
18	1	5008	CLA	C1B-NB	2.21	1.37	1.35
18	A	803	CLA	C1C-C2C	2.21	1.48	1.44
18	B	823	CLA	C1C-C2C	2.21	1.48	1.44
18	B	826	CLA	C1C-C2C	2.21	1.48	1.44
18	A	837	CLA	C1C-C2C	2.21	1.48	1.44
18	A	832	CLA	C1B-NB	2.21	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	5009	CLA	C1C-C2C	2.20	1.48	1.44
18	3	309	CLA	C1C-C2C	2.20	1.48	1.44
18	1	5015	CLA	C1B-NB	2.20	1.37	1.35
18	1	5006	CLA	C1C-C2C	2.20	1.48	1.44
18	3	315	CLA	C1C-C2C	2.20	1.48	1.44
18	A	830	CLA	C1C-C2C	2.20	1.48	1.44
18	B	822	CLA	C1B-NB	2.20	1.37	1.35
18	F	303	CLA	C1B-NB	2.20	1.37	1.35
18	B	838	CLA	C1C-C2C	2.20	1.48	1.44
18	L	305	CLA	C1C-C2C	2.20	1.48	1.44
18	1	5007	CLA	C1C-C2C	2.20	1.48	1.44
18	1	5013	CLA	C1B-NB	2.20	1.37	1.35
23	2	325	LMT	O2'-C2'	-2.20	1.37	1.43
23	B	853	LMT	O2'-C2'	-2.20	1.37	1.43
18	A	806	CLA	C1C-C2C	2.20	1.48	1.44
18	2	326	CLA	C1A-CHA	2.19	1.52	1.43
18	J	1103	CLA	C1A-CHA	2.19	1.52	1.43
18	2	309	CLA	C1C-C2C	2.19	1.48	1.44
18	A	805	CLA	C1C-C2C	2.19	1.48	1.44
18	B	817	CLA	C1B-NB	2.19	1.37	1.35
18	A	829	CLA	C1C-C2C	2.19	1.48	1.44
18	K	1402	CLA	C1C-C2C	2.19	1.48	1.44
23	G	1606	LMT	O2B-C2B	-2.19	1.37	1.43
18	J	1103	CLA	C1B-NB	2.19	1.37	1.35
18	A	852	CLA	C1C-C2C	2.19	1.48	1.44
18	B	837	CLA	C1B-NB	2.18	1.37	1.35
18	A	836	CLA	C1B-NB	2.18	1.37	1.35
18	4	307	CLA	C1B-NB	2.18	1.37	1.35
18	4	305	CLA	C1C-C2C	2.18	1.48	1.44
18	2	312	CLA	C1C-C2C	2.18	1.48	1.44
18	A	817	CLA	C1C-C2C	2.18	1.48	1.44
18	1	5015	CLA	C1C-C2C	2.18	1.48	1.44
18	2	307	CLA	C1C-C2C	2.18	1.48	1.44
18	2	311	CLA	C1B-NB	2.18	1.37	1.35
18	G	1603	CLA	C1C-C2C	2.18	1.48	1.44
18	B	838	CLA	C3B-C2B	-2.18	1.37	1.40
18	1	5015	CLA	C3B-C2B	-2.18	1.37	1.40
18	3	307	CLA	C3B-C2B	-2.18	1.37	1.40
18	B	837	CLA	C3B-C2B	-2.17	1.37	1.40
18	B	810	CLA	C3B-C2B	-2.17	1.37	1.40
18	G	1602	CLA	C1C-C2C	2.17	1.48	1.44
18	A	809	CLA	C1C-C2C	2.17	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	839	CLA	C1B-NB	2.17	1.37	1.35
18	2	309	CLA	C1B-NB	2.17	1.37	1.35
18	A	833	CLA	C1C-C2C	2.17	1.48	1.44
18	B	810	CLA	C1A-CHA	2.17	1.52	1.43
18	3	314	CLA	C1C-C2C	2.17	1.48	1.44
18	B	818	CLA	C1B-NB	2.17	1.37	1.35
18	3	317	CLA	C3B-C2B	-2.17	1.37	1.40
18	H	1701	CLA	C1B-NB	2.17	1.37	1.35
18	A	810	CLA	C1C-C2C	2.17	1.48	1.44
18	4	315	CLA	C1B-NB	2.17	1.37	1.35
18	4	308	CLA	C1C-C2C	2.17	1.48	1.44
18	3	301	CLA	C1A-CHA	2.17	1.52	1.43
18	A	803	CLA	C1B-NB	2.17	1.37	1.35
18	B	837	CLA	C1C-C2C	2.17	1.48	1.44
18	2	312	CLA	C1A-CHA	2.17	1.52	1.43
18	B	816	CLA	C1C-C2C	2.16	1.48	1.44
18	A	815	CLA	C1B-NB	2.16	1.37	1.35
18	3	309	CLA	C1B-NB	2.16	1.37	1.35
18	3	318	CLA	C3B-C2B	-2.16	1.37	1.40
18	4	311	CLA	C1B-NB	2.16	1.37	1.35
18	K	1402	CLA	C1B-NB	2.16	1.37	1.35
31	4	304	XAT	O24-C25	-2.16	1.43	1.46
18	1	5012	CLA	C1C-C2C	2.16	1.48	1.44
18	A	823	CLA	C1A-CHA	2.16	1.52	1.43
18	A	806	CLA	C3B-C2B	-2.16	1.37	1.40
18	A	840	CLA	C1C-C2C	2.16	1.48	1.44
18	B	824	CLA	C1C-C2C	2.16	1.48	1.44
18	B	808	CLA	C3B-C2B	-2.16	1.37	1.40
18	2	313	CLA	C1C-C2C	2.15	1.48	1.44
18	4	307	CLA	C1C-C2C	2.15	1.48	1.44
18	K	1404	CLA	C1C-C2C	2.15	1.48	1.44
18	2	326	CLA	C1C-C2C	2.15	1.48	1.44
18	A	822	CLA	C1B-NB	2.15	1.37	1.35
18	1	5009	CLA	C1B-NB	2.15	1.37	1.35
23	A	850	LMT	O2'-C2'	-2.15	1.37	1.43
18	3	314	CLA	C1A-CHA	2.15	1.52	1.43
18	A	808	CLA	C1C-C2C	2.15	1.48	1.44
18	L	306	CLA	C1C-C2C	2.15	1.48	1.44
18	B	816	CLA	C1A-CHA	2.15	1.52	1.43
18	B	822	CLA	C1C-C2C	2.15	1.48	1.44
18	K	1403	CLA	C1B-NB	2.15	1.37	1.35
18	K	1404	CLA	C1B-NB	2.15	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	306	CLA	C1A-CHA	2.15	1.52	1.43
18	B	825	CLA	C1A-CHA	2.15	1.52	1.43
18	K	1401	CLA	C1C-C2C	2.15	1.48	1.44
18	3	309	CLA	C1A-CHA	2.15	1.52	1.43
18	1	5010	CLA	C1A-CHA	2.15	1.52	1.43
18	2	310	CLA	C1C-C2C	2.14	1.48	1.44
18	B	812	CLA	C1B-NB	2.14	1.37	1.35
18	A	819	CLA	C1C-C2C	2.14	1.48	1.44
18	B	808	CLA	C1C-C2C	2.14	1.48	1.44
18	F	302	CLA	C1C-C2C	2.14	1.48	1.44
18	B	807	CLA	C3B-C2B	-2.14	1.37	1.40
18	A	826	CLA	C1C-C2C	2.14	1.48	1.44
18	B	815	CLA	C1C-C2C	2.14	1.48	1.44
18	A	821	CLA	C1A-CHA	2.14	1.52	1.43
18	3	311	CLA	C1C-C2C	2.14	1.48	1.44
18	1	5011	CLA	C1C-C2C	2.14	1.48	1.44
18	A	818	CLA	C1C-C2C	2.14	1.48	1.44
18	B	828	CLA	C1A-CHA	2.14	1.52	1.43
18	4	305	CLA	C1A-CHA	2.14	1.52	1.43
18	A	827	CLA	C1C-C2C	2.14	1.48	1.44
18	4	306	CLA	C1C-C2C	2.14	1.48	1.44
18	A	831	CLA	C1C-C2C	2.14	1.48	1.44
18	4	312	CLA	C1C-C2C	2.14	1.48	1.44
30	4	313	CHL	C3B-C2B	-2.14	1.37	1.40
18	A	829	CLA	C3B-C2B	-2.14	1.37	1.40
18	L	306	CLA	C1A-CHA	2.14	1.52	1.43
18	A	818	CLA	C3B-C2B	-2.14	1.37	1.40
18	4	310	CLA	C1C-C2C	2.13	1.48	1.44
18	G	1603	CLA	C3B-C2B	-2.13	1.37	1.40
18	1	5008	CLA	C1C-C2C	2.13	1.48	1.44
18	B	813	CLA	C1A-CHA	2.13	1.52	1.43
18	3	308	CLA	C1A-CHA	2.13	1.52	1.43
18	B	831	CLA	C1C-C2C	2.13	1.48	1.44
18	2	306	CLA	C1C-C2C	2.13	1.48	1.44
18	B	811	CLA	C1C-C2C	2.13	1.48	1.44
18	B	820	CLA	C1C-C2C	2.13	1.48	1.44
18	3	301	CLA	C1C-C2C	2.13	1.48	1.44
18	B	804	CLA	C1A-CHA	2.13	1.51	1.43
18	A	821	CLA	C1C-C2C	2.13	1.48	1.44
18	A	804	CLA	C1B-NB	2.13	1.37	1.35
18	B	833	CLA	C1A-CHA	2.13	1.51	1.43
18	4	310	CLA	C1A-CHA	2.13	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	825	CLA	C1C-C2C	2.13	1.48	1.44
18	A	810	CLA	C1A-CHA	2.13	1.51	1.43
18	1	5017	CLA	C1A-CHA	2.12	1.51	1.43
18	1	5012	CLA	C1B-NB	2.12	1.37	1.35
18	B	814	CLA	C3B-C2B	-2.12	1.37	1.40
18	G	1601	CLA	C1A-CHA	2.12	1.51	1.43
18	2	306	CLA	C1A-CHA	2.12	1.51	1.43
18	G	1601	CLA	C1C-C2C	2.12	1.48	1.44
18	B	836	CLA	C1C-C2C	2.12	1.48	1.44
18	A	840	CLA	C1A-CHA	2.12	1.51	1.43
18	A	827	CLA	C3B-C2B	-2.12	1.37	1.40
18	A	828	CLA	C3B-C2B	-2.12	1.37	1.40
18	B	803	CLA	C1C-C2C	2.12	1.48	1.44
18	B	829	CLA	C1C-C2C	2.12	1.48	1.44
18	4	310	CLA	C3B-C2B	-2.12	1.37	1.40
18	B	822	CLA	C1A-CHA	2.12	1.51	1.43
18	B	834	CLA	C1C-C2C	2.12	1.48	1.44
18	B	821	CLA	C1A-CHA	2.11	1.51	1.43
18	1	5006	CLA	C1B-NB	2.11	1.37	1.35
18	A	838	CLA	C1A-CHA	2.11	1.51	1.43
18	2	308	CLA	C1A-CHA	2.11	1.51	1.43
18	2	311	CLA	C1A-CHA	2.11	1.51	1.43
18	3	317	CLA	C1C-C2C	2.11	1.48	1.44
18	A	803	CLA	C1A-CHA	2.11	1.51	1.43
18	K	1404	CLA	C1A-CHA	2.11	1.51	1.43
18	B	806	CLA	C1C-C2C	2.11	1.48	1.44
18	A	837	CLA	C1A-CHA	2.11	1.51	1.43
18	1	5012	CLA	C1A-CHA	2.11	1.51	1.43
18	A	816	CLA	C1B-NB	2.11	1.37	1.35
18	B	830	CLA	C3B-C2B	-2.11	1.37	1.40
23	G	1605	LMT	O4'-C4B	-2.11	1.38	1.43
18	4	311	CLA	C1A-CHA	2.11	1.51	1.43
18	G	1602	CLA	C1A-CHA	2.11	1.51	1.43
18	A	839	CLA	C1C-C2C	2.11	1.48	1.44
18	L	304	CLA	C1A-CHA	2.11	1.51	1.43
18	B	840	CLA	C1A-CHA	2.11	1.51	1.43
18	B	826	CLA	C1A-CHA	2.11	1.51	1.43
18	B	806	CLA	C1B-NB	2.10	1.37	1.35
18	G	1603	CLA	C1B-NB	2.10	1.37	1.35
18	A	823	CLA	C1C-C2C	2.10	1.48	1.44
18	K	1403	CLA	C1A-CHA	2.10	1.51	1.43
18	1	5013	CLA	C1A-CHA	2.10	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	833	CLA	C1A-CHA	2.10	1.51	1.43
18	A	814	CLA	C1C-C2C	2.10	1.48	1.44
18	A	820	CLA	C1C-C2C	2.10	1.48	1.44
18	B	835	CLA	C1A-CHA	2.10	1.51	1.43
18	A	812	CLA	C1C-C2C	2.10	1.48	1.44
18	2	317	CLA	CHD-C1D	2.10	1.42	1.38
18	B	810	CLA	C1C-C2C	2.10	1.48	1.44
18	H	1701	CLA	C1A-CHA	2.10	1.51	1.43
30	2	318	CHL	C3B-C2B	-2.10	1.37	1.40
18	A	816	CLA	C1A-CHA	2.10	1.51	1.43
18	F	302	CLA	C1A-CHA	2.10	1.51	1.43
18	A	802	CLA	C1A-CHA	2.10	1.51	1.43
18	B	807	CLA	C1C-C2C	2.10	1.48	1.44
18	B	821	CLA	C1C-C2C	2.10	1.48	1.44
18	4	306	CLA	C1B-NB	2.10	1.37	1.35
18	1	5018	CLA	C1A-CHA	2.10	1.51	1.43
18	B	832	CLA	C1A-CHA	2.10	1.51	1.43
18	B	801	CLA	C1A-CHA	2.09	1.51	1.43
18	2	307	CLA	C1A-CHA	2.09	1.51	1.43
23	B	856	LMT	O4 <sup>2</sup> -C4B	-2.09	1.38	1.43
18	A	807	CLA	C1A-CHA	2.09	1.51	1.43
18	A	820	CLA	C1B-NB	2.09	1.37	1.35
18	A	813	CLA	C1A-CHA	2.09	1.51	1.43
18	F	302	CLA	C1B-NB	2.09	1.37	1.35
18	1	5006	CLA	C3B-C2B	-2.09	1.37	1.40
18	2	306	CLA	C3B-C2B	-2.09	1.37	1.40
18	4	307	CLA	C1A-CHA	2.09	1.51	1.43
18	A	815	CLA	C1C-C2C	2.09	1.48	1.44
18	2	311	CLA	C1C-C2C	2.09	1.48	1.44
18	B	815	CLA	C1A-CHA	2.09	1.51	1.43
18	4	315	CLA	C1A-CHA	2.09	1.51	1.43
18	B	809	CLA	C1A-CHA	2.09	1.51	1.43
18	2	310	CLA	C1A-CHA	2.09	1.51	1.43
18	A	825	CLA	C1A-CHA	2.09	1.51	1.43
18	B	823	CLA	C1B-NB	2.09	1.37	1.35
18	3	315	CLA	C1A-CHA	2.09	1.51	1.43
18	1	5015	CLA	C1A-CHA	2.09	1.51	1.43
18	A	802	CLA	C3B-C2B	-2.09	1.37	1.40
18	3	308	CLA	C1B-NB	2.09	1.37	1.35
18	B	819	CLA	C1C-C2C	2.09	1.48	1.44
18	B	827	CLA	C1A-CHA	2.09	1.51	1.43
18	2	326	CLA	MG-NC	2.08	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	801	CL0	C4C-C3C	2.08	1.48	1.45
18	B	817	CLA	C3B-C2B	-2.08	1.37	1.40
18	A	804	CLA	C1C-C2C	2.08	1.48	1.44
18	A	831	CLA	C1A-CHA	2.08	1.51	1.43
23	B	853	LMT	O4'-C4B	-2.08	1.38	1.43
18	1	5008	CLA	C1A-CHA	2.08	1.51	1.43
18	B	838	CLA	C1A-CHA	2.08	1.51	1.43
18	B	833	CLA	C1B-NB	2.08	1.37	1.35
18	B	833	CLA	C3B-C2B	-2.08	1.37	1.40
18	K	1401	CLA	C1A-CHA	2.08	1.51	1.43
18	1	5007	CLA	C1A-CHA	2.08	1.51	1.43
18	1	5018	CLA	C1B-NB	2.08	1.37	1.35
18	A	828	CLA	CHD-C1D	2.07	1.42	1.38
18	2	313	CLA	C1A-CHA	2.07	1.51	1.43
18	1	5013	CLA	C1C-C2C	2.07	1.48	1.44
18	B	823	CLA	C1A-CHA	2.07	1.51	1.43
18	J	1103	CLA	MG-NC	2.07	2.11	2.06
18	B	830	CLA	C1A-CHA	2.07	1.51	1.43
18	A	820	CLA	C1A-CHA	2.07	1.51	1.43
18	A	817	CLA	C1A-CHA	2.07	1.51	1.43
18	3	307	CLA	C1A-CHA	2.07	1.51	1.43
30	3	310	CHL	CHC-C1C	2.07	1.40	1.35
18	B	832	CLA	C1C-C2C	2.07	1.48	1.44
18	1	5011	CLA	C3B-C2B	-2.07	1.37	1.40
30	2	314	CHL	C3B-C2B	-2.07	1.37	1.40
18	B	831	CLA	C1A-CHA	2.07	1.51	1.43
18	3	317	CLA	C1A-CHA	2.07	1.51	1.43
18	A	818	CLA	C1A-CHA	2.07	1.51	1.43
26	J	1106	DGD	O5D-C1E	2.07	1.43	1.40
18	2	307	CLA	C1B-NB	2.07	1.37	1.35
18	1	5010	CLA	C1C-C2C	2.07	1.48	1.44
23	B	856	LMT	O1'-C1'	-2.07	1.36	1.40
18	3	307	CLA	C1B-NB	2.06	1.37	1.35
18	B	829	CLA	C1A-CHA	2.06	1.51	1.43
18	A	811	CLA	C1A-CHA	2.06	1.51	1.43
30	4	302	CHL	C3B-C2B	-2.06	1.37	1.40
18	B	840	CLA	C1B-NB	2.06	1.37	1.35
18	A	822	CLA	C1A-CHA	2.06	1.51	1.43
18	B	805	CLA	C1A-CHA	2.06	1.51	1.43
18	B	836	CLA	MG-NC	2.06	2.11	2.06
18	A	814	CLA	C1A-CHA	2.06	1.51	1.43
18	A	839	CLA	C1A-CHA	2.06	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	838	CLA	C1B-NB	2.06	1.37	1.35
18	B	841	CLA	C1B-NB	2.06	1.37	1.35
18	A	815	CLA	C3B-C2B	-2.06	1.37	1.40
23	4	319	LMT	O4'-C4B	-2.06	1.38	1.43
18	B	827	CLA	C3D-C4D	-2.06	1.39	1.44
18	B	818	CLA	C1A-CHA	2.06	1.51	1.43
18	A	821	CLA	C1B-NB	2.06	1.37	1.35
18	B	834	CLA	CHD-C1D	2.06	1.42	1.38
23	G	1606	LMT	O4'-C4B	-2.06	1.38	1.43
18	A	838	CLA	MG-NC	2.06	2.11	2.06
18	B	828	CLA	C1C-C2C	2.05	1.48	1.44
18	F	303	CLA	C1A-CHA	2.05	1.51	1.43
18	B	806	CLA	C1A-CHA	2.05	1.51	1.43
18	1	5011	CLA	C1B-NB	2.05	1.37	1.35
18	A	808	CLA	C1A-CHA	2.05	1.51	1.43
18	B	824	CLA	C1A-CHA	2.05	1.51	1.43
18	A	824	CLA	C1A-CHA	2.05	1.51	1.43
18	B	833	CLA	C1C-C2C	2.05	1.48	1.44
23	A	850	LMT	O2B-C2B	-2.05	1.38	1.43
18	A	811	CLA	C1B-NB	2.05	1.37	1.35
23	J	1107	LMT	O4'-C4B	-2.05	1.38	1.43
18	K	1404	CLA	MG-NC	2.05	2.11	2.06
18	B	830	CLA	C3D-C4D	-2.04	1.39	1.44
18	A	816	CLA	C3B-C2B	-2.04	1.37	1.40
18	A	817	CLA	C3B-C2B	-2.04	1.37	1.40
18	A	834	CLA	C1A-CHA	2.04	1.51	1.43
18	1	5011	CLA	C1A-CHA	2.04	1.51	1.43
18	L	306	CLA	C1B-NB	2.04	1.37	1.35
18	A	818	CLA	C1B-NB	2.04	1.37	1.35
18	1	5006	CLA	C1A-CHA	2.04	1.51	1.43
18	4	312	CLA	C1A-CHA	2.04	1.51	1.43
18	K	1402	CLA	MG-NC	2.04	2.11	2.06
18	L	301	CLA	C1A-CHA	2.04	1.51	1.43
18	3	319	CLA	C1A-CHA	2.04	1.51	1.43
18	A	829	CLA	C1B-NB	2.04	1.37	1.35
18	3	318	CLA	C1A-CHA	2.04	1.51	1.43
23	2	325	LMT	O4'-C4B	-2.04	1.38	1.43
18	1	5018	CLA	C3B-C2B	-2.04	1.37	1.40
18	B	837	CLA	C1A-CHA	2.04	1.51	1.43
18	H	1701	CLA	C1C-C2C	2.04	1.48	1.44
18	4	308	CLA	C1B-NB	2.03	1.37	1.35
18	K	1402	CLA	C1A-CHA	2.03	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	309	CLA	C1A-CHA	2.03	1.51	1.43
18	L	304	CLA	C1C-C2C	2.03	1.48	1.44
18	3	315	CLA	C1B-NB	2.03	1.37	1.35
18	G	1603	CLA	C1A-CHA	2.03	1.51	1.43
18	B	819	CLA	C1A-CHA	2.03	1.51	1.43
18	4	308	CLA	C1A-CHA	2.03	1.51	1.43
18	A	833	CLA	MG-NC	2.03	2.11	2.06
18	4	305	CLA	C3B-C2B	-2.03	1.37	1.40
18	B	801	CLA	MG-NC	2.03	2.11	2.06
18	4	315	CLA	CHD-C1D	2.03	1.42	1.38
23	B	853	LMT	O5'-C5'	-2.03	1.39	1.44
23	A	850	LMT	O4'-C4B	-2.03	1.38	1.43
18	B	804	CLA	C1C-C2C	2.03	1.48	1.44
18	F	301	CLA	C1A-CHA	2.03	1.51	1.43
18	B	835	CLA	C1B-NB	2.03	1.37	1.35
18	B	820	CLA	C1A-CHA	2.03	1.51	1.43
18	3	314	CLA	MG-NC	2.02	2.11	2.06
18	A	811	CLA	C1C-C2C	2.02	1.48	1.44
18	1	5017	CLA	C1B-NB	2.02	1.37	1.35
30	4	317	CHL	C3B-C2B	-2.02	1.37	1.40
18	J	1101	CLA	C3B-C2B	-2.02	1.37	1.40
18	B	819	CLA	C1B-NB	2.02	1.37	1.35
18	J	1101	CLA	C1C-C2C	2.02	1.48	1.44
18	2	307	CLA	MG-NC	2.02	2.11	2.06
18	A	804	CLA	C1A-CHA	2.02	1.51	1.43
18	A	853	CLA	C1C-C2C	2.02	1.48	1.44
18	B	827	CLA	C1C-C2C	2.02	1.48	1.44
18	2	317	CLA	C1A-CHA	2.02	1.51	1.43
18	A	852	CLA	MG-NC	2.02	2.11	2.06
18	A	806	CLA	C1A-CHA	2.02	1.51	1.43
23	B	852	LMT	O4'-C4B	-2.02	1.38	1.43
18	1	5009	CLA	C3B-C2B	-2.02	1.37	1.40
18	B	836	CLA	C1A-CHA	2.02	1.51	1.43
18	B	841	CLA	C1A-CHA	2.02	1.51	1.43
18	A	837	CLA	C1B-NB	2.02	1.37	1.35
18	B	811	CLA	C1A-CHA	2.02	1.51	1.43
18	G	1602	CLA	MG-NC	2.02	2.11	2.06
24	1	5001	LMG	O1-C1	2.02	1.43	1.40
18	F	302	CLA	MG-NC	2.02	2.11	2.06
18	B	834	CLA	C1A-CHA	2.02	1.51	1.43
18	A	815	CLA	C1A-CHA	2.02	1.51	1.43
18	K	1401	CLA	MG-NC	2.02	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	839	CLA	CHD-C1D	2.01	1.42	1.38
18	3	311	CLA	C1A-CHA	2.01	1.51	1.43
18	A	807	CLA	C1B-NB	2.01	1.37	1.35
18	2	312	CLA	MG-NC	2.01	2.11	2.06
18	A	804	CLA	C3B-C2B	-2.01	1.37	1.40
18	A	824	CLA	MG-NC	2.01	2.11	2.06
18	1	5018	CLA	MG-NC	2.01	2.11	2.06
18	A	813	CLA	C1B-NB	2.01	1.37	1.35
18	B	836	CLA	C1B-NB	2.01	1.37	1.35
18	A	812	CLA	C1A-CHA	2.01	1.51	1.43
18	3	311	CLA	C3D-C4D	-2.01	1.39	1.44
18	B	807	CLA	C1B-NB	2.01	1.37	1.35
18	B	821	CLA	C1B-NB	2.01	1.37	1.35
18	A	835	CLA	C1A-CHA	2.01	1.51	1.43
18	G	1603	CLA	MG-NC	2.01	2.11	2.06
18	A	827	CLA	C1A-CHA	2.01	1.51	1.43
18	B	818	CLA	C1C-C2C	2.01	1.48	1.44
18	B	817	CLA	C1A-CHA	2.01	1.51	1.43
18	A	836	CLA	C1A-CHA	2.01	1.51	1.43
18	J	1101	CLA	C1A-CHA	2.01	1.51	1.43
18	B	801	CLA	C1B-NB	2.01	1.37	1.35
18	L	306	CLA	C3B-C2B	-2.01	1.37	1.40
18	4	309	CLA	C3D-C4D	-2.01	1.39	1.44
18	B	839	CLA	C1A-CHA	2.01	1.51	1.43
18	B	813	CLA	C1C-C2C	2.01	1.48	1.44
18	2	309	CLA	C3D-C4D	-2.01	1.39	1.44
18	4	306	CLA	MG-NC	2.01	2.11	2.06
26	1	5002	DGD	CAB-C9B	-2.01	1.33	1.49
18	B	814	CLA	C1A-CHA	2.00	1.51	1.43
18	A	819	CLA	C3D-C4D	-2.00	1.39	1.44
26	2	327	DGD	CDA-CCA	-2.00	1.33	1.49
24	A	851	LMG	C40-C39	-2.00	1.33	1.49
18	B	808	CLA	C1A-CHA	2.00	1.51	1.43
18	B	807	CLA	C3D-C4D	-2.00	1.39	1.44
18	4	309	CLA	C1B-NB	2.00	1.37	1.35
18	1	5011	CLA	CHD-C1D	2.00	1.42	1.38
18	A	828	CLA	C1A-CHA	2.00	1.51	1.43
18	A	852	CLA	C3D-C4D	-2.00	1.39	1.44
18	B	829	CLA	MG-NC	2.00	2.11	2.06
18	3	309	CLA	MG-NC	2.00	2.11	2.06
18	3	301	CLA	C3B-C2B	-2.00	1.37	1.40
26	B	855	DGD	CDA-CCA	-2.00	1.33	1.49

All (3182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	I	101	BCR	C10-C11-C12	18.19	180.00	123.22
21	G	1604	BCR	C10-C11-C12	17.83	178.87	123.22
21	K	1405	BCR	C10-C11-C12	17.69	178.43	123.22
21	F	304	BCR	C10-C11-C12	17.57	178.06	123.22
21	A	855	BCR	C10-C11-C12	17.55	177.97	123.22
21	A	845	BCR	C10-C11-C12	17.50	177.84	123.22
21	F	305	BCR	C10-C11-C12	17.38	177.46	123.22
21	B	845	BCR	C10-C11-C12	17.31	177.25	123.22
21	B	843	BCR	C10-C11-C12	17.26	177.09	123.22
21	A	846	BCR	C10-C11-C12	17.20	176.90	123.22
21	I	102	BCR	C10-C11-C12	17.19	176.85	123.22
21	3	305	BCR	C10-C11-C12	17.14	176.70	123.22
21	B	802	BCR	C10-C11-C12	17.13	176.68	123.22
21	B	846	BCR	C10-C11-C12	17.11	176.61	123.22
21	2	305	BCR	C10-C11-C12	17.09	176.56	123.22
21	1	5005	BCR	C10-C11-C12	17.05	176.41	123.22
21	B	847	BCR	C10-C11-C12	17.04	176.38	123.22
21	3	306	BCR	C10-C11-C12	17.02	176.32	123.22
21	B	802	BCR	C16-C15-C14	16.95	158.19	123.47
21	L	303	BCR	C10-C11-C12	16.92	176.03	123.22
21	A	843	BCR	C10-C11-C12	16.84	175.78	123.22
21	L	302	BCR	C10-C11-C12	16.82	175.71	123.22
21	L	307	BCR	C10-C11-C12	16.78	175.60	123.22
21	A	844	BCR	C10-C11-C12	16.78	175.59	123.22
21	4	301	BCR	C10-C11-C12	16.77	175.55	123.22
21	J	1104	BCR	C10-C11-C12	16.54	174.83	123.22
21	B	844	BCR	C10-C11-C12	16.38	174.32	123.22
21	A	847	BCR	C10-C11-C12	16.20	173.78	123.22
21	B	843	BCR	C11-C10-C9	15.57	149.53	127.31
21	B	844	BCR	C11-C10-C9	14.45	147.93	127.31
21	B	843	BCR	C21-C20-C19	14.39	168.12	123.22
21	F	305	BCR	C16-C15-C14	14.38	152.94	123.47
21	2	305	BCR	C29-C30-C25	-14.23	88.57	110.48
21	L	307	BCR	C11-C10-C9	14.18	147.54	127.31
21	L	302	BCR	C11-C10-C9	13.89	147.13	127.31
21	A	846	BCR	C11-C10-C9	13.87	147.11	127.31
21	1	5005	BCR	C11-C10-C9	13.82	147.03	127.31
21	L	303	BCR	C11-C10-C9	13.70	146.86	127.31
21	J	1104	BCR	C11-C10-C9	13.65	146.79	127.31
21	4	301	BCR	C11-C10-C9	13.63	146.77	127.31
21	A	855	BCR	C21-C20-C19	13.47	165.24	123.22
21	A	847	BCR	C11-C10-C9	13.38	146.41	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	G	1604	BCR	C16-C15-C14	13.38	150.87	123.47
21	A	843	BCR	C11-C10-C9	13.36	146.38	127.31
21	B	847	BCR	C16-C15-C14	13.33	150.78	123.47
21	B	847	BCR	C11-C10-C9	13.25	146.22	127.31
21	B	802	BCR	C11-C10-C9	13.19	146.13	127.31
21	I	101	BCR	C16-C15-C14	13.13	150.37	123.47
21	3	305	BCR	C16-C15-C14	13.10	150.32	123.47
21	3	305	BCR	C11-C10-C9	12.94	145.78	127.31
21	F	305	BCR	C11-C10-C9	12.92	145.74	127.31
21	F	304	BCR	C16-C15-C14	12.88	149.85	123.47
21	A	844	BCR	C21-C20-C19	12.86	163.36	123.22
21	A	844	BCR	C11-C10-C9	12.85	145.65	127.31
21	B	846	BCR	C11-C10-C9	12.68	145.41	127.31
21	1	5005	BCR	C16-C15-C14	12.67	149.44	123.47
21	3	306	BCR	C21-C20-C19	12.67	162.77	123.22
21	A	855	BCR	C16-C15-C14	12.66	149.40	123.47
21	I	102	BCR	C16-C15-C14	12.63	149.34	123.47
21	A	847	BCR	C11-C12-C13	12.61	161.84	126.42
21	L	307	BCR	C16-C15-C14	12.53	149.15	123.47
21	I	102	BCR	C11-C10-C9	12.52	145.18	127.31
21	2	305	BCR	C11-C10-C9	12.49	145.14	127.31
21	B	802	BCR	C21-C20-C19	12.49	162.20	123.22
21	A	843	BCR	C21-C20-C19	12.45	162.07	123.22
21	A	855	BCR	C11-C10-C9	12.44	145.07	127.31
21	A	845	BCR	C21-C20-C19	12.38	161.84	123.22
21	F	304	BCR	C11-C10-C9	12.26	144.81	127.31
21	A	845	BCR	C16-C15-C14	12.23	148.52	123.47
21	J	1104	BCR	C21-C20-C19	12.14	161.10	123.22
21	G	1604	BCR	C21-C20-C19	12.14	161.09	123.22
21	K	1405	BCR	C16-C15-C14	12.13	148.33	123.47
21	L	303	BCR	C16-C15-C14	12.11	148.29	123.47
21	K	1405	BCR	C11-C10-C9	12.08	144.55	127.31
21	L	302	BCR	C16-C15-C14	12.01	148.07	123.47
21	A	845	BCR	C11-C10-C9	12.00	144.43	127.31
21	L	303	BCR	C21-C20-C19	11.97	160.58	123.22
21	B	844	BCR	C11-C12-C13	11.94	159.96	126.42
21	L	302	BCR	C21-C20-C19	11.78	159.99	123.22
21	A	843	BCR	C16-C15-C14	11.77	147.59	123.47
21	A	844	BCR	C11-C12-C13	11.74	159.38	126.42
21	B	845	BCR	C11-C10-C9	11.72	144.04	127.31
21	B	844	BCR	C16-C15-C14	11.61	147.25	123.47
21	3	306	BCR	C16-C15-C14	11.61	147.25	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	L	307	BCR	C21-C20-C19	11.56	159.29	123.22
21	L	302	BCR	C11-C12-C13	11.50	158.73	126.42
21	G	1604	BCR	C11-C10-C9	11.45	143.66	127.31
21	B	846	BCR	C11-C12-C13	11.45	158.59	126.42
21	I	102	BCR	C21-C20-C19	11.42	158.87	123.22
21	B	846	BCR	C16-C15-C14	11.39	146.81	123.47
21	J	1104	BCR	C16-C15-C14	11.37	146.77	123.47
21	2	305	BCR	C11-C12-C13	11.33	158.25	126.42
21	B	847	BCR	C21-C20-C19	11.33	158.57	123.22
21	A	846	BCR	C21-C20-C19	11.31	158.52	123.22
21	K	1405	BCR	C21-C20-C19	11.26	158.36	123.22
21	A	847	BCR	C16-C15-C14	11.15	146.31	123.47
21	F	305	BCR	C21-C20-C19	11.13	157.96	123.22
21	4	301	BCR	C11-C12-C13	11.13	157.68	126.42
21	B	847	BCR	C11-C12-C13	11.12	157.66	126.42
21	4	301	BCR	C16-C15-C14	11.08	146.16	123.47
21	L	303	BCR	C11-C12-C13	11.05	157.46	126.42
21	A	846	BCR	C16-C15-C14	11.02	146.04	123.47
21	3	305	BCR	C21-C20-C19	11.00	157.56	123.22
21	1	5005	BCR	C21-C20-C19	10.98	157.48	123.22
21	3	305	BCR	C11-C12-C13	10.94	157.14	126.42
21	I	102	BCR	C11-C12-C13	10.92	157.09	126.42
21	B	845	BCR	C16-C15-C14	10.92	145.84	123.47
21	B	844	BCR	C21-C20-C19	10.91	157.27	123.22
21	1	5005	BCR	C11-C12-C13	10.91	157.06	126.42
21	K	1405	BCR	C11-C12-C13	10.89	157.02	126.42
21	I	101	BCR	C21-C20-C19	10.84	157.03	123.22
21	F	304	BCR	C21-C20-C19	10.79	156.91	123.22
21	2	305	BCR	C21-C20-C19	10.78	156.87	123.22
21	I	101	BCR	C11-C10-C9	10.78	142.70	127.31
21	J	1104	BCR	C11-C12-C13	10.73	156.57	126.42
21	B	845	BCR	C11-C12-C13	10.70	156.48	126.42
21	F	304	BCR	C11-C12-C13	10.67	156.39	126.42
21	A	843	BCR	C11-C12-C13	10.65	156.33	126.42
21	A	855	BCR	C11-C12-C13	10.62	156.25	126.42
21	L	307	BCR	C11-C12-C13	10.54	156.01	126.42
21	B	846	BCR	C21-C20-C19	10.50	155.99	123.22
21	A	845	BCR	C11-C12-C13	10.47	155.84	126.42
21	G	1604	BCR	C11-C12-C13	10.37	155.54	126.42
21	A	844	BCR	C16-C15-C14	10.36	144.70	123.47
21	2	305	BCR	C16-C15-C14	10.33	144.64	123.47
21	F	305	BCR	C11-C12-C13	10.33	155.44	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	847	BCR	C21-C20-C19	10.28	155.30	123.22
21	B	802	BCR	C11-C12-C13	10.27	155.26	126.42
21	A	846	BCR	C11-C12-C13	9.99	154.47	126.42
21	4	301	BCR	C21-C20-C19	9.68	153.43	123.22
21	4	301	BCR	C20-C19-C18	9.63	153.48	126.42
21	A	847	BCR	C20-C19-C18	9.50	153.11	126.42
21	I	101	BCR	C20-C19-C18	9.33	152.61	126.42
18	A	823	CLA	C4A-NA-C1A	9.22	110.85	106.71
21	F	305	BCR	C20-C19-C18	9.21	152.30	126.42
18	2	311	CLA	C4A-NA-C1A	9.18	110.83	106.71
18	K	1403	CLA	C4A-NA-C1A	9.18	110.83	106.71
18	B	837	CLA	C4A-NA-C1A	9.11	110.80	106.71
18	B	806	CLA	C4A-NA-C1A	9.09	110.79	106.71
18	1	5008	CLA	C4A-NA-C1A	9.09	110.79	106.71
18	3	317	CLA	C4A-NA-C1A	9.09	110.79	106.71
18	B	809	CLA	C4A-NA-C1A	9.08	110.79	106.71
18	L	304	CLA	C4A-NA-C1A	9.04	110.77	106.71
18	B	833	CLA	C4A-NA-C1A	9.03	110.77	106.71
18	J	1103	CLA	C4A-NA-C1A	9.02	110.76	106.71
18	2	308	CLA	C4A-NA-C1A	9.02	110.76	106.71
18	A	812	CLA	C4A-NA-C1A	9.00	110.75	106.71
18	L	306	CLA	C4A-NA-C1A	8.98	110.74	106.71
18	B	816	CLA	C4A-NA-C1A	8.95	110.73	106.71
18	2	310	CLA	C4A-NA-C1A	8.92	110.72	106.71
18	A	813	CLA	C4A-NA-C1A	8.92	110.72	106.71
18	A	825	CLA	C4A-NA-C1A	8.92	110.72	106.71
18	A	807	CLA	C4A-NA-C1A	8.92	110.72	106.71
18	4	315	CLA	C4A-NA-C1A	8.91	110.71	106.71
18	B	825	CLA	C4A-NA-C1A	8.90	110.71	106.71
18	1	5015	CLA	C4A-NA-C1A	8.90	110.71	106.71
18	3	308	CLA	C4A-NA-C1A	8.89	110.70	106.71
18	2	312	CLA	C4A-NA-C1A	8.88	110.70	106.71
18	3	314	CLA	C4A-NA-C1A	8.86	110.69	106.71
18	1	5013	CLA	C4A-NA-C1A	8.85	110.69	106.71
18	3	309	CLA	C4A-NA-C1A	8.85	110.69	106.71
18	B	826	CLA	C4A-NA-C1A	8.85	110.69	106.71
18	B	810	CLA	C4A-NA-C1A	8.84	110.68	106.71
18	B	813	CLA	C4A-NA-C1A	8.82	110.67	106.71
18	B	840	CLA	C4A-NA-C1A	8.81	110.67	106.71
18	4	306	CLA	C4A-NA-C1A	8.81	110.67	106.71
18	2	306	CLA	C4A-NA-C1A	8.75	110.64	106.71
18	H	1701	CLA	C4A-NA-C1A	8.75	110.64	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	853	CLA	C4A-NA-C1A	8.74	110.64	106.71
18	B	815	CLA	C4A-NA-C1A	8.74	110.64	106.71
18	A	810	CLA	C4A-NA-C1A	8.74	110.64	106.71
18	4	310	CLA	C4A-NA-C1A	8.74	110.63	106.71
18	A	815	CLA	C4A-NA-C1A	8.73	110.63	106.71
18	A	821	CLA	C4A-NA-C1A	8.73	110.63	106.71
21	F	304	BCR	C20-C19-C18	8.72	150.91	126.42
18	A	804	CLA	C4A-NA-C1A	8.72	110.62	106.71
18	A	837	CLA	C4A-NA-C1A	8.71	110.62	106.71
18	A	820	CLA	C4A-NA-C1A	8.71	110.62	106.71
18	4	311	CLA	C4A-NA-C1A	8.70	110.62	106.71
21	B	846	BCR	C20-C19-C18	8.70	150.86	126.42
18	4	307	CLA	C4A-NA-C1A	8.70	110.62	106.71
18	B	804	CLA	C4A-NA-C1A	8.69	110.61	106.71
18	K	1401	CLA	C4A-NA-C1A	8.69	110.61	106.71
18	1	5010	CLA	C4A-NA-C1A	8.69	110.61	106.71
18	B	821	CLA	C4A-NA-C1A	8.69	110.61	106.71
18	4	305	CLA	C4A-NA-C1A	8.69	110.61	106.71
18	B	819	CLA	C4A-NA-C1A	8.68	110.61	106.71
18	B	822	CLA	C4A-NA-C1A	8.68	110.61	106.71
18	2	313	CLA	C4A-NA-C1A	8.68	110.61	106.71
18	B	808	CLA	C4A-NA-C1A	8.67	110.60	106.71
18	G	1602	CLA	C4A-NA-C1A	8.66	110.60	106.71
18	2	317	CLA	C4A-NA-C1A	8.66	110.60	106.71
18	B	829	CLA	C4A-NA-C1A	8.65	110.60	106.71
18	A	808	CLA	C4A-NA-C1A	8.65	110.59	106.71
18	B	838	CLA	C4A-NA-C1A	8.65	110.59	106.71
18	A	818	CLA	C4A-NA-C1A	8.64	110.59	106.71
18	A	840	CLA	C4A-NA-C1A	8.64	110.59	106.71
18	A	811	CLA	C4A-NA-C1A	8.64	110.59	106.71
18	A	835	CLA	C4A-NA-C1A	8.64	110.59	106.71
18	A	833	CLA	C4A-NA-C1A	8.63	110.58	106.71
18	B	827	CLA	C4A-NA-C1A	8.63	110.58	106.71
21	B	844	BCR	C20-C19-C18	8.61	150.62	126.42
18	3	301	CLA	C4A-NA-C1A	8.59	110.57	106.71
18	A	828	CLA	C4A-NA-C1A	8.59	110.57	106.71
18	J	1101	CLA	C4A-NA-C1A	8.59	110.57	106.71
18	A	831	CLA	C4A-NA-C1A	8.58	110.56	106.71
18	K	1404	CLA	C4A-NA-C1A	8.58	110.56	106.71
18	A	816	CLA	C4A-NA-C1A	8.55	110.55	106.71
18	B	831	CLA	C4A-NA-C1A	8.54	110.55	106.71
21	B	843	BCR	C16-C15-C14	8.54	140.96	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	806	CLA	C4A-NA-C1A	8.53	110.54	106.71
18	B	832	CLA	C4A-NA-C1A	8.53	110.54	106.71
21	L	307	BCR	C20-C19-C18	8.53	150.38	126.42
18	1	5017	CLA	C4A-NA-C1A	8.53	110.54	106.71
18	1	5007	CLA	C4A-NA-C1A	8.53	110.54	106.71
18	B	805	CLA	C4A-NA-C1A	8.52	110.54	106.71
18	4	312	CLA	C4A-NA-C1A	8.52	110.53	106.71
21	I	101	BCR	C11-C12-C13	8.51	150.33	126.42
18	G	1603	CLA	C4A-NA-C1A	8.50	110.53	106.71
18	A	803	CLA	C4A-NA-C1A	8.49	110.53	106.71
18	F	302	CLA	C4A-NA-C1A	8.47	110.52	106.71
18	4	308	CLA	C4A-NA-C1A	8.47	110.51	106.71
18	G	1601	CLA	C4A-NA-C1A	8.47	110.51	106.71
18	B	834	CLA	C4A-NA-C1A	8.46	110.51	106.71
21	1	5005	BCR	C20-C19-C18	8.46	150.18	126.42
18	A	824	CLA	C4A-NA-C1A	8.45	110.50	106.71
18	1	5012	CLA	C4A-NA-C1A	8.45	110.50	106.71
18	A	814	CLA	C4A-NA-C1A	8.43	110.50	106.71
18	4	309	CLA	C4A-NA-C1A	8.42	110.49	106.71
18	3	318	CLA	C4A-NA-C1A	8.42	110.49	106.71
18	B	817	CLA	C4A-NA-C1A	8.41	110.49	106.71
18	1	5011	CLA	C4A-NA-C1A	8.41	110.49	106.71
18	3	315	CLA	C4A-NA-C1A	8.41	110.49	106.71
18	A	838	CLA	C4A-NA-C1A	8.41	110.48	106.71
18	2	326	CLA	C4A-NA-C1A	8.41	110.48	106.71
18	B	814	CLA	C4A-NA-C1A	8.39	110.48	106.71
18	A	834	CLA	C4A-NA-C1A	8.39	110.48	106.71
18	B	835	CLA	C4A-NA-C1A	8.38	110.47	106.71
18	B	803	CLA	C4A-NA-C1A	8.38	110.47	106.71
18	B	818	CLA	C4A-NA-C1A	8.38	110.47	106.71
18	3	319	CLA	C4A-NA-C1A	8.37	110.47	106.71
18	A	827	CLA	C4A-NA-C1A	8.37	110.47	106.71
18	2	307	CLA	C4A-NA-C1A	8.37	110.47	106.71
18	B	828	CLA	C4A-NA-C1A	8.36	110.47	106.71
18	A	839	CLA	C4A-NA-C1A	8.36	110.47	106.71
21	B	847	BCR	C20-C19-C18	8.35	149.88	126.42
18	A	826	CLA	C4A-NA-C1A	8.34	110.46	106.71
18	B	823	CLA	C4A-NA-C1A	8.31	110.44	106.71
18	1	5018	CLA	C4A-NA-C1A	8.31	110.44	106.71
18	L	305	CLA	C4A-NA-C1A	8.30	110.44	106.71
18	F	301	CLA	C4A-NA-C1A	8.30	110.44	106.71
21	3	305	BCR	C20-C19-C18	8.30	149.74	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	307	CLA	C4A-NA-C1A	8.27	110.42	106.71
18	B	839	CLA	C4A-NA-C1A	8.27	110.42	106.71
18	B	824	CLA	C4A-NA-C1A	8.26	110.42	106.71
18	2	309	CLA	C4A-NA-C1A	8.24	110.41	106.71
18	B	841	CLA	C4A-NA-C1A	8.24	110.41	106.71
18	B	836	CLA	C4A-NA-C1A	8.23	110.41	106.71
18	A	829	CLA	C4A-NA-C1A	8.23	110.41	106.71
21	I	102	BCR	C20-C19-C18	8.22	149.51	126.42
18	A	836	CLA	C4A-NA-C1A	8.22	110.40	106.71
18	A	809	CLA	C4A-NA-C1A	8.21	110.40	106.71
18	A	819	CLA	C4A-NA-C1A	8.19	110.39	106.71
18	B	801	CLA	C4A-NA-C1A	8.18	110.38	106.71
18	1	5009	CLA	C4A-NA-C1A	8.17	110.38	106.71
18	L	301	CLA	C4A-NA-C1A	8.17	110.38	106.71
18	K	1402	CLA	C4A-NA-C1A	8.16	110.38	106.71
18	F	303	CLA	C4A-NA-C1A	8.14	110.36	106.71
18	B	807	CLA	C4A-NA-C1A	8.13	110.36	106.71
18	A	817	CLA	C4A-NA-C1A	8.11	110.35	106.71
18	A	802	CLA	C4A-NA-C1A	8.11	110.35	106.71
18	A	830	CLA	C4A-NA-C1A	8.11	110.35	106.71
18	B	830	CLA	C4A-NA-C1A	8.11	110.35	106.71
21	B	843	BCR	C11-C12-C13	8.09	149.14	126.42
18	B	820	CLA	C4A-NA-C1A	8.08	110.34	106.71
18	A	852	CLA	C4A-NA-C1A	8.08	110.34	106.71
21	A	846	BCR	C20-C19-C18	8.07	149.08	126.42
18	1	5006	CLA	C4A-NA-C1A	8.06	110.33	106.71
21	3	306	BCR	C11-C10-C9	7.95	138.65	127.31
18	B	811	CLA	C4A-NA-C1A	7.89	110.25	106.71
18	A	805	CLA	C4A-NA-C1A	7.87	110.25	106.71
18	3	311	CLA	C4A-NA-C1A	7.85	110.24	106.71
21	J	1104	BCR	C20-C19-C18	7.84	148.45	126.42
18	A	832	CLA	C4A-NA-C1A	7.82	110.22	106.71
17	A	801	CL0	CMD-C2D-C1D	7.81	138.48	124.71
18	A	822	CLA	C4A-NA-C1A	7.78	110.20	106.71
21	L	302	BCR	C20-C19-C18	7.77	148.24	126.42
18	B	812	CLA	C4A-NA-C1A	7.72	110.18	106.71
21	B	843	BCR	C19-C18-C17	7.67	130.72	118.94
21	B	845	BCR	C21-C20-C19	7.63	147.03	123.22
21	A	845	BCR	C20-C19-C18	7.55	147.63	126.42
29	J	1105	LUT	C21-C26-C27	7.53	122.23	112.70
21	3	306	BCR	C20-C19-C18	7.45	147.34	126.42
21	G	1604	BCR	C20-C19-C18	7.41	147.24	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	305	BCR	C40-C30-C29	-7.40	79.32	108.91
21	K	1405	BCR	C20-C19-C18	7.40	147.19	126.42
21	L	303	BCR	C20-C19-C18	7.36	147.09	126.42
21	A	843	BCR	C20-C19-C18	7.27	146.83	126.42
21	B	802	BCR	C15-C14-C13	-6.77	117.66	127.31
17	A	801	CL0	C4A-NA-C1A	6.71	109.72	106.71
21	B	802	BCR	C20-C19-C18	6.59	144.93	126.42
21	2	305	BCR	C20-C19-C18	6.56	144.84	126.42
21	A	844	BCR	C20-C19-C18	6.54	144.78	126.42
21	3	306	BCR	C12-C13-C14	6.46	128.85	118.94
21	B	843	BCR	C12-C13-C14	6.33	128.65	118.94
21	A	855	BCR	C20-C19-C18	6.24	143.96	126.42
18	B	814	CLA	O2D-CGD-CBD	6.20	122.29	111.27
21	2	305	BCR	C40-C30-C25	6.19	120.35	110.30
18	K	1403	CLA	CMD-C2D-C1D	6.18	135.61	124.71
29	2	303	LUT	C21-C26-C25	6.15	122.44	111.42
17	A	801	CL0	C2C-C1C-NC	6.12	115.70	109.97
21	3	306	BCR	C11-C12-C13	6.12	143.60	126.42
18	B	834	CLA	CMD-C2D-C1D	6.11	135.49	124.71
18	B	833	CLA	O2D-CGD-CBD	6.04	122.00	111.27
18	B	830	CLA	CMD-C2D-C1D	6.02	135.32	124.71
18	2	310	CLA	O2A-C1-C2	6.02	124.44	108.64
18	A	820	CLA	CMD-C2D-C1D	5.99	135.26	124.71
18	A	829	CLA	CMD-C2D-C1D	5.98	135.24	124.71
29	J	1105	LUT	C31-C30-C29	-5.90	118.88	127.31
18	B	825	CLA	O2A-C1-C2	5.88	124.09	108.64
18	2	309	CLA	CMD-C2D-C1D	5.87	135.05	124.71
18	3	317	CLA	O2A-C1-C2	5.86	124.05	108.64
31	2	304	XAT	C31-C30-C29	-5.85	118.97	127.31
18	1	5009	CLA	CMD-C2D-C1D	5.83	135.00	124.71
18	A	828	CLA	O2D-CGD-CBD	5.81	121.60	111.27
18	B	828	CLA	CMD-C2D-C1D	5.81	134.95	124.71
18	A	823	CLA	O2D-CGD-CBD	5.79	121.56	111.27
18	3	307	CLA	CMD-C2D-C1D	5.76	134.87	124.71
18	1	5013	CLA	O2D-CGD-CBD	5.76	121.50	111.27
18	A	805	CLA	CMD-C2D-C1D	5.75	134.85	124.71
18	1	5006	CLA	CMD-C2D-C1D	5.74	134.83	124.71
18	4	308	CLA	O2D-CGD-CBD	5.72	121.43	111.27
17	A	801	CL0	C2D-C1D-ND	5.71	114.31	110.10
18	B	819	CLA	O2A-C1-C2	5.71	123.64	108.64
29	3	303	LUT	C21-C26-C25	5.69	121.62	111.42
18	A	807	CLA	O2D-CGD-CBD	5.69	121.38	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	835	CLA	O2A-C1-C2	5.69	123.59	108.64
18	A	822	CLA	CMD-C2D-C1D	5.69	134.74	124.71
18	J	1101	CLA	O2A-C1-C2	5.69	123.58	108.64
18	A	813	CLA	O2D-CGD-CBD	5.67	121.35	111.27
28	F	310	ZEX	C15-C14-C13	-5.67	119.22	127.31
18	4	312	CLA	CMD-C2D-C1D	5.67	134.70	124.71
18	B	826	CLA	CMD-C2D-C1D	5.66	134.69	124.71
18	J	1101	CLA	CMD-C2D-C1D	5.65	134.67	124.71
18	2	313	CLA	CMD-C2D-C1D	5.64	134.66	124.71
18	A	809	CLA	CMD-C2D-C1D	5.64	134.66	124.71
18	B	837	CLA	CMD-C2D-C1D	5.64	134.66	124.71
18	G	1601	CLA	CMD-C2D-C1D	5.64	134.65	124.71
18	B	830	CLA	O2D-CGD-CBD	5.63	121.28	111.27
18	A	825	CLA	CMD-C2D-C1D	5.62	134.62	124.71
18	B	801	CLA	O2D-CGD-CBD	5.62	121.26	111.27
18	1	5017	CLA	CMD-C2D-C1D	5.62	134.62	124.71
18	A	831	CLA	O2D-CGD-CBD	5.61	121.23	111.27
18	4	309	CLA	CMD-C2D-C1D	5.60	134.58	124.71
18	B	831	CLA	O2D-CGD-CBD	5.60	121.22	111.27
18	B	811	CLA	CMD-C2D-C1D	5.60	134.58	124.71
18	H	1701	CLA	CMD-C2D-C1D	5.60	134.58	124.71
18	1	5009	CLA	O2D-CGD-CBD	5.60	121.21	111.27
18	B	825	CLA	CMD-C2D-C1D	5.60	134.58	124.71
18	B	840	CLA	CMD-C2D-C1D	5.59	134.56	124.71
18	4	305	CLA	CMD-C2D-C1D	5.59	134.56	124.71
18	A	823	CLA	CMD-C2D-C1D	5.58	134.56	124.71
18	B	827	CLA	CMD-C2D-C1D	5.58	134.56	124.71
18	B	816	CLA	O2A-C1-C2	5.58	123.31	108.64
18	3	309	CLA	CMD-C2D-C1D	5.58	134.55	124.71
18	B	815	CLA	O2D-CGD-CBD	5.58	121.18	111.27
18	A	810	CLA	CMD-C2D-C1D	5.58	134.55	124.71
18	3	311	CLA	CMD-C2D-C1D	5.58	134.54	124.71
18	4	308	CLA	CMD-C2D-C1D	5.57	134.53	124.71
18	B	807	CLA	CMD-C2D-C1D	5.56	134.51	124.71
18	1	5015	CLA	CMD-C2D-C1D	5.56	134.51	124.71
18	4	307	CLA	CMD-C2D-C1D	5.56	134.51	124.71
18	A	829	CLA	O2D-CGD-CBD	5.55	121.14	111.27
29	1	5004	LUT	C21-C26-C27	5.55	119.72	112.70
18	3	308	CLA	CMD-C2D-C1D	5.55	134.49	124.71
18	A	834	CLA	O2A-C1-C2	5.54	123.20	108.64
18	1	5013	CLA	CMD-C2D-C1D	5.54	134.48	124.71
17	A	801	CL0	C1C-C2C-C3C	-5.54	101.14	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	308	CLA	CMD-C2D-C1D	5.54	134.47	124.71
18	B	831	CLA	CMD-C2D-C1D	5.53	134.46	124.71
18	F	302	CLA	CMD-C2D-C1D	5.53	134.46	124.71
18	A	814	CLA	CMD-C2D-C1D	5.52	134.45	124.71
18	2	310	CLA	CMD-C2D-C1D	5.52	134.44	124.71
18	K	1402	CLA	CMD-C2D-C1D	5.52	134.44	124.71
18	L	306	CLA	CMD-C2D-C1D	5.52	134.44	124.71
18	A	835	CLA	CMD-C2D-C1D	5.52	134.44	124.71
18	A	832	CLA	CMD-C2D-C1D	5.52	134.44	124.71
18	F	302	CLA	O2A-C1-C2	5.51	123.13	108.64
18	B	814	CLA	CMD-C2D-C1D	5.51	134.43	124.71
18	L	305	CLA	CMD-C2D-C1D	5.51	134.42	124.71
18	L	304	CLA	CMD-C2D-C1D	5.51	134.42	124.71
18	3	318	CLA	CMD-C2D-C1D	5.51	134.42	124.71
18	2	311	CLA	CMD-C2D-C1D	5.51	134.42	124.71
18	A	813	CLA	CMD-C2D-C1D	5.51	134.42	124.71
18	B	839	CLA	CMD-C2D-C1D	5.50	134.41	124.71
18	J	1101	CLA	O2D-CGD-CBD	5.50	121.05	111.27
18	A	834	CLA	CMD-C2D-C1D	5.50	134.41	124.71
18	B	819	CLA	CMD-C2D-C1D	5.50	134.41	124.71
18	A	812	CLA	CMD-C2D-C1D	5.50	134.40	124.71
18	B	839	CLA	O2A-C1-C2	5.50	123.08	108.64
18	A	840	CLA	CMD-C2D-C1D	5.50	134.40	124.71
18	B	817	CLA	CMD-C2D-C1D	5.50	134.40	124.71
18	G	1603	CLA	CMD-C2D-C1D	5.50	134.40	124.71
18	G	1602	CLA	CMD-C2D-C1D	5.49	134.39	124.71
18	2	326	CLA	O2D-CGD-CBD	5.49	121.02	111.27
18	K	1401	CLA	CMD-C2D-C1D	5.49	134.38	124.71
18	A	807	CLA	CMD-C2D-C1D	5.49	134.38	124.71
18	B	822	CLA	CMD-C2D-C1D	5.49	134.38	124.71
18	A	819	CLA	CMD-C2D-C1D	5.48	134.38	124.71
18	K	1404	CLA	CMD-C2D-C1D	5.48	134.37	124.71
18	2	309	CLA	O2A-C1-C2	5.48	123.04	108.64
18	A	826	CLA	CMD-C2D-C1D	5.48	134.37	124.71
18	B	823	CLA	O2A-C1-C2	5.48	123.03	108.64
18	B	805	CLA	CMD-C2D-C1D	5.48	134.37	124.71
18	A	833	CLA	CMD-C2D-C1D	5.48	134.37	124.71
18	A	812	CLA	O2D-CGD-CBD	5.48	121.00	111.27
18	B	826	CLA	O2D-CGD-CBD	5.47	121.00	111.27
18	A	806	CLA	CMD-C2D-C1D	5.47	134.35	124.71
18	F	303	CLA	CMD-C2D-C1D	5.47	134.35	124.71
18	2	307	CLA	CMD-C2D-C1D	5.47	134.35	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	319	CLA	CMD-C2D-C1D	5.47	134.35	124.71
18	1	5011	CLA	CMD-C2D-C1D	5.47	134.35	124.71
18	B	818	CLA	CMD-C2D-C1D	5.47	134.35	124.71
18	B	821	CLA	O2D-CGD-CBD	5.46	120.98	111.27
18	B	823	CLA	CMD-C2D-C1D	5.46	134.34	124.71
18	A	804	CLA	CMD-C2D-C1D	5.46	134.34	124.71
18	B	806	CLA	CMD-C2D-C1D	5.46	134.34	124.71
18	A	817	CLA	CMD-C2D-C1D	5.46	134.34	124.71
18	A	831	CLA	CMD-C2D-C1D	5.46	134.34	124.71
18	B	813	CLA	CMD-C2D-C1D	5.46	134.34	124.71
18	1	5010	CLA	CMD-C2D-C1D	5.46	134.34	124.71
18	1	5018	CLA	CMD-C2D-C1D	5.46	134.33	124.71
18	4	306	CLA	CMD-C2D-C1D	5.46	134.33	124.71
18	A	838	CLA	CMD-C2D-C1D	5.46	134.33	124.71
18	B	812	CLA	CMD-C2D-C1D	5.46	134.33	124.71
18	A	803	CLA	O2D-CGD-CBD	5.45	120.96	111.27
18	1	5012	CLA	CMD-C2D-C1D	5.45	134.32	124.71
18	3	315	CLA	CMD-C2D-C1D	5.45	134.32	124.71
18	B	833	CLA	CMD-C2D-C1D	5.45	134.32	124.71
18	3	311	CLA	O2A-C1-C2	5.44	122.94	108.64
18	B	824	CLA	CMD-C2D-C1D	5.44	134.31	124.71
18	B	808	CLA	CMD-C2D-C1D	5.44	134.30	124.71
18	1	5010	CLA	O2A-C1-C2	5.44	122.94	108.64
18	A	830	CLA	CMD-C2D-C1D	5.44	134.30	124.71
18	L	304	CLA	O2D-CGD-CBD	5.44	120.93	111.27
18	B	815	CLA	O2A-C1-C2	5.44	122.92	108.64
18	2	306	CLA	CMD-C2D-C1D	5.44	134.29	124.71
18	4	310	CLA	CMD-C2D-C1D	5.43	134.29	124.71
18	1	5017	CLA	O2D-CGD-CBD	5.43	120.92	111.27
18	A	815	CLA	CMD-C2D-C1D	5.43	134.28	124.71
18	B	827	CLA	O2D-CGD-CBD	5.42	120.91	111.27
21	B	843	BCR	C15-C14-C13	5.42	135.04	127.31
18	A	836	CLA	CMD-C2D-C1D	5.42	134.26	124.71
18	A	837	CLA	CMD-C2D-C1D	5.42	134.26	124.71
18	3	301	CLA	CMD-C2D-C1D	5.41	134.26	124.71
18	B	819	CLA	O2D-CGD-CBD	5.41	120.88	111.27
18	J	1103	CLA	CMD-C2D-C1D	5.41	134.24	124.71
18	A	853	CLA	CMD-C2D-C1D	5.40	134.24	124.71
18	B	820	CLA	CMD-C2D-C1D	5.40	134.23	124.71
18	A	816	CLA	CMD-C2D-C1D	5.39	134.21	124.71
18	A	803	CLA	CMD-C2D-C1D	5.39	134.21	124.71
18	2	313	CLA	O2D-CGD-CBD	5.39	120.84	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	832	CLA	CMD-C2D-C1D	5.38	134.19	124.71
18	2	326	CLA	CMD-C2D-C1D	5.38	134.19	124.71
18	B	815	CLA	CMD-C2D-C1D	5.38	134.19	124.71
18	A	806	CLA	O2A-C1-C2	5.38	122.76	108.64
18	A	811	CLA	CMD-C2D-C1D	5.37	134.17	124.71
18	3	314	CLA	CMD-C2D-C1D	5.37	134.17	124.71
18	A	852	CLA	CMD-C2D-C1D	5.36	134.17	124.71
18	B	817	CLA	O2A-C1-C2	5.36	122.72	108.64
18	4	306	CLA	O2D-CGD-CBD	5.36	120.79	111.27
18	B	821	CLA	CMD-C2D-C1D	5.36	134.16	124.71
18	2	313	CLA	O2A-C1-C2	5.36	122.71	108.64
18	4	312	CLA	O2D-CGD-CBD	5.35	120.78	111.27
18	B	835	CLA	CMD-C2D-C1D	5.35	134.13	124.71
18	3	317	CLA	CMD-C2D-C1D	5.34	134.13	124.71
18	B	829	CLA	CMD-C2D-C1D	5.34	134.13	124.71
18	A	821	CLA	CMD-C2D-C1D	5.34	134.12	124.71
31	4	304	XAT	C31-C30-C29	-5.33	119.70	127.31
29	3	304	LUT	C21-C26-C27	5.33	119.44	112.70
18	L	305	CLA	O2A-C1-C2	5.33	122.64	108.64
18	A	808	CLA	CMD-C2D-C1D	5.33	134.10	124.71
18	B	816	CLA	CMD-C2D-C1D	5.33	134.10	124.71
18	B	816	CLA	O2D-CGD-CBD	5.33	120.73	111.27
18	B	836	CLA	CMD-C2D-C1D	5.32	134.10	124.71
18	F	301	CLA	CMD-C2D-C1D	5.32	134.10	124.71
18	1	5008	CLA	O2A-C1-C2	5.32	122.63	108.64
18	B	841	CLA	CMD-C2D-C1D	5.32	134.09	124.71
18	G	1603	CLA	O2D-CGD-CBD	5.32	120.72	111.27
18	B	836	CLA	O2A-C1-C2	5.32	122.61	108.64
18	B	810	CLA	CMD-C2D-C1D	5.31	134.07	124.71
18	A	803	CLA	O2A-C1-C2	5.31	122.59	108.64
18	B	838	CLA	CMD-C2D-C1D	5.31	134.06	124.71
18	A	808	CLA	O2D-CGD-CBD	5.30	120.69	111.27
18	A	804	CLA	O2A-C1-C2	5.30	122.57	108.64
18	1	5008	CLA	CMD-C2D-C1D	5.30	134.06	124.71
18	B	807	CLA	O2A-C1-C2	5.30	122.56	108.64
18	A	825	CLA	O2A-C1-C2	5.30	122.56	108.64
18	4	311	CLA	CMD-C2D-C1D	5.30	134.05	124.71
18	3	318	CLA	O2D-CGD-CBD	5.30	120.68	111.27
18	A	832	CLA	O2A-C1-C2	5.29	122.55	108.64
18	B	837	CLA	O2D-CGD-CBD	5.29	120.67	111.27
18	B	828	CLA	O2D-CGD-CBD	5.29	120.67	111.27
18	B	825	CLA	O2D-CGD-CBD	5.29	120.66	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	806	CLA	O2D-CGD-CBD	5.28	120.66	111.27
18	A	816	CLA	O2A-C1-C2	5.28	122.52	108.64
18	3	309	CLA	O2A-C1-C2	5.28	122.51	108.64
18	A	853	CLA	O2A-C1-C2	5.28	122.50	108.64
18	A	830	CLA	O2D-CGD-CBD	5.28	120.64	111.27
18	A	805	CLA	O2A-C1-C2	5.27	122.50	108.64
18	2	317	CLA	CMD-C2D-C1D	5.27	134.00	124.71
18	A	818	CLA	O2D-CGD-CBD	5.27	120.63	111.27
18	1	5007	CLA	CMD-C2D-C1D	5.26	133.99	124.71
21	B	843	BCR	C36-C18-C17	-5.25	115.57	122.92
18	4	315	CLA	CMD-C2D-C1D	5.24	133.95	124.71
18	B	831	CLA	O2A-C1-C2	5.24	122.42	108.64
18	3	311	CLA	O2D-CGD-CBD	5.24	120.58	111.27
18	B	809	CLA	CMD-C2D-C1D	5.24	133.94	124.71
18	A	815	CLA	O2A-C1-C2	5.24	122.39	108.64
18	A	839	CLA	CMD-C2D-C1D	5.23	133.93	124.71
18	4	306	CLA	O2A-C1-C2	5.23	122.38	108.64
18	B	801	CLA	CMD-C2D-C1D	5.23	133.93	124.71
18	B	817	CLA	O2D-CGD-CBD	5.23	120.56	111.27
18	L	301	CLA	CMD-C2D-C1D	5.22	133.91	124.71
18	A	840	CLA	O2A-C1-C2	5.22	122.35	108.64
18	B	804	CLA	O2A-C1-C2	5.22	122.34	108.64
18	A	804	CLA	O2D-CGD-CBD	5.21	120.53	111.27
18	1	5010	CLA	O2D-CGD-CBD	5.21	120.52	111.27
18	1	5011	CLA	O2A-C1-C2	5.19	122.27	108.64
18	L	305	CLA	O2D-CGD-CBD	5.19	120.49	111.27
29	1	5003	LUT	C21-C26-C25	5.19	120.71	111.42
18	A	829	CLA	O2A-C1-C2	5.18	122.26	108.64
18	2	309	CLA	O2D-CGD-CBD	5.18	120.47	111.27
18	A	824	CLA	O2D-CGD-CBD	5.18	120.46	111.27
18	1	5006	CLA	O2A-C1-C2	5.17	122.23	108.64
18	2	312	CLA	CMD-C2D-C1D	5.17	133.82	124.71
18	3	315	CLA	O2D-CGD-CBD	5.17	120.45	111.27
18	B	804	CLA	CMD-C2D-C1D	5.17	133.82	124.71
18	2	307	CLA	O2D-CGD-CBD	5.17	120.45	111.27
18	3	319	CLA	O2A-C1-C2	5.17	122.21	108.64
18	B	811	CLA	O2D-CGD-CBD	5.16	120.44	111.27
18	B	822	CLA	O2D-CGD-CBD	5.16	120.44	111.27
18	2	312	CLA	O2D-CGD-CBD	5.16	120.44	111.27
18	B	808	CLA	O2A-C1-C2	5.16	122.19	108.64
18	2	317	CLA	O2A-C1-C2	5.15	122.18	108.64
18	B	805	CLA	O2D-CGD-CBD	5.15	120.43	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	309	CLA	O2A-C1-C2	5.15	122.16	108.64
18	A	825	CLA	O2D-CGD-CBD	5.15	120.41	111.27
18	A	827	CLA	O2A-C1-C2	5.14	122.16	108.64
21	2	305	BCR	C39-C30-C25	5.14	118.64	110.30
18	A	834	CLA	O2D-CGD-CBD	5.14	120.40	111.27
18	B	832	CLA	O2A-C1-C2	5.14	122.15	108.64
18	1	5007	CLA	O2D-CGD-CBD	5.13	120.39	111.27
18	B	824	CLA	O2A-C1-C2	5.13	122.12	108.64
18	A	835	CLA	O2D-CGD-CBD	5.13	120.38	111.27
18	A	818	CLA	CMD-C2D-C1D	5.13	133.75	124.71
17	A	801	CL0	O2A-CGA-O1A	-5.13	110.66	123.59
18	B	840	CLA	O2D-CGD-CBD	5.12	120.36	111.27
18	A	836	CLA	O2A-C1-C2	5.12	122.09	108.64
18	B	836	CLA	O2D-CGD-CBD	5.12	120.36	111.27
18	B	801	CLA	O2A-C1-C2	5.11	122.07	108.64
18	L	301	CLA	O2A-C1-C2	5.11	122.07	108.64
18	A	828	CLA	CMD-C2D-C1D	5.11	133.72	124.71
18	A	816	CLA	O2D-CGD-CBD	5.11	120.35	111.27
17	A	801	CL0	CHD-C1D-ND	-5.11	119.76	124.45
18	H	1701	CLA	O2D-CGD-CBD	5.11	120.34	111.27
18	1	5018	CLA	O2D-CGD-CBD	5.10	120.33	111.27
18	B	840	CLA	O2A-C1-C2	5.10	122.03	108.64
18	A	822	CLA	O2A-C1-C2	5.10	122.03	108.64
18	A	828	CLA	O2A-C1-C2	5.09	122.02	108.64
18	1	5018	CLA	O2A-C1-C2	5.09	122.01	108.64
18	B	818	CLA	O2D-CGD-CBD	5.08	120.30	111.27
18	A	853	CLA	O2D-CGD-CBD	5.08	120.30	111.27
18	4	308	CLA	O2A-C1-C2	5.07	121.97	108.64
18	1	5011	CLA	O2D-CGD-CBD	5.07	120.28	111.27
18	F	301	CLA	O2D-CGD-CBD	5.07	120.28	111.27
18	A	808	CLA	O2A-C1-C2	5.07	121.95	108.64
18	B	814	CLA	O2A-C1-C2	5.07	121.95	108.64
18	B	829	CLA	O2A-C1-C2	5.06	121.94	108.64
21	3	306	BCR	C35-C13-C14	-5.06	115.83	122.92
18	4	311	CLA	O2A-C1-C2	5.06	121.94	108.64
18	3	309	CLA	O2D-CGD-CBD	5.06	120.26	111.27
18	B	839	CLA	O2D-CGD-CBD	5.06	120.25	111.27
18	A	827	CLA	O2D-CGD-CBD	5.06	120.25	111.27
18	F	303	CLA	O2D-CGD-CBD	5.05	120.25	111.27
18	A	831	CLA	O2A-C1-C2	5.05	121.91	108.64
29	J	1105	LUT	C35-C34-C33	-5.05	120.10	127.31
18	4	315	CLA	O2A-C1-C2	5.05	121.91	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	811	CLA	O2A-C1-C2	5.05	121.91	108.64
18	A	839	CLA	O2D-CGD-CBD	5.05	120.24	111.27
21	B	843	BCR	C35-C13-C14	-5.05	115.85	122.92
18	A	821	CLA	O2A-C1-C2	5.05	121.90	108.64
18	1	5009	CLA	O2A-C1-C2	5.05	121.90	108.64
22	B	848	LHG	O7-C7-C8	5.05	120.37	111.09
18	2	311	CLA	O2A-C1-C2	5.05	121.89	108.64
18	A	836	CLA	O2D-CGD-CBD	5.04	120.22	111.27
18	A	833	CLA	O2D-CGD-CBD	5.04	120.22	111.27
18	A	832	CLA	O2D-CGD-CBD	5.04	120.22	111.27
18	B	811	CLA	O2A-C1-C2	5.04	121.87	108.64
18	4	305	CLA	O2A-C1-C2	5.03	121.87	108.64
18	3	314	CLA	O2D-CGD-CBD	5.03	120.21	111.27
18	1	5015	CLA	O2D-CGD-CBD	5.03	120.21	111.27
18	A	807	CLA	O2A-C1-C2	5.03	121.85	108.64
17	A	801	CL0	O2A-C1-C2	5.03	121.85	108.64
29	4	303	LUT	C21-C26-C25	5.02	120.41	111.42
18	2	308	CLA	O2D-CGD-CBD	5.02	120.18	111.27
18	B	813	CLA	O2D-CGD-CBD	5.02	120.18	111.27
18	4	310	CLA	O2A-C1-C2	5.02	121.82	108.64
29	3	304	LUT	C35-C34-C33	-5.00	120.17	127.31
18	2	306	CLA	O2D-CGD-CBD	5.00	120.15	111.27
18	B	805	CLA	O2A-C1-C2	5.00	121.78	108.64
18	B	826	CLA	O2A-C1-C2	5.00	121.77	108.64
18	4	309	CLA	O2D-CGD-CBD	4.98	120.12	111.27
18	B	812	CLA	O2A-C1-C2	4.98	121.72	108.64
18	4	307	CLA	O2A-C1-C2	4.98	121.72	108.64
18	B	838	CLA	O2D-CGD-CBD	4.97	120.11	111.27
17	A	801	CL0	O2D-CGD-CBD	4.96	120.09	111.27
18	A	824	CLA	O2A-C1-C2	4.96	121.68	108.64
18	A	809	CLA	O2D-CGD-CBD	4.96	120.08	111.27
18	A	806	CLA	O2D-CGD-CBD	4.96	120.08	111.27
18	A	837	CLA	O2D-CGD-CBD	4.96	120.08	111.27
18	A	840	CLA	O2D-CGD-CBD	4.96	120.08	111.27
18	3	307	CLA	O2D-CGD-CBD	4.96	120.08	111.27
18	H	1701	CLA	O2A-C1-C2	4.96	121.66	108.64
18	4	311	CLA	O2D-CGD-CBD	4.95	120.07	111.27
18	3	319	CLA	O2D-CGD-CBD	4.94	120.05	111.27
24	B	851	LMG	O7-C10-C11	4.94	122.14	111.50
18	G	1602	CLA	O2D-CGD-CBD	4.94	120.04	111.27
31	4	304	XAT	O4-C5-C18	-4.94	109.14	115.06
18	B	812	CLA	O2D-CGD-CBD	4.93	120.03	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	833	CLA	O2A-C1-C2	4.93	121.59	108.64
18	4	315	CLA	O2D-CGD-CBD	4.92	120.02	111.27
18	G	1601	CLA	O2A-C1-C2	4.92	121.56	108.64
18	3	307	CLA	O2A-C1-C2	4.92	121.56	108.64
18	A	852	CLA	O2A-C1-C2	4.92	121.56	108.64
18	K	1402	CLA	O2A-C1-C2	4.92	121.56	108.64
18	1	5012	CLA	O2D-CGD-CBD	4.92	120.00	111.27
31	2	304	XAT	C15-C14-C13	-4.91	120.30	127.31
18	K	1401	CLA	O2D-CGD-CBD	4.91	119.99	111.27
18	B	827	CLA	O2A-C1-C2	4.91	121.53	108.64
18	B	837	CLA	O2A-C1-C2	4.90	121.52	108.64
18	B	808	CLA	O2D-CGD-CBD	4.90	119.98	111.27
18	2	306	CLA	O2A-C1-C2	4.90	121.51	108.64
18	B	829	CLA	O2D-CGD-CBD	4.90	119.97	111.27
28	F	310	ZEX	C28-C27-C26	-4.88	118.75	127.09
18	B	841	CLA	O2A-C1-C2	4.88	121.47	108.64
18	2	317	CLA	O2D-CGD-CBD	4.88	119.94	111.27
18	2	307	CLA	O2A-C1-C2	4.88	121.45	108.64
18	A	815	CLA	O2D-CGD-CBD	4.88	119.93	111.27
18	2	310	CLA	O2D-CGD-CBD	4.87	119.93	111.27
18	B	830	CLA	O2A-C1-C2	4.87	121.44	108.64
18	1	5006	CLA	O2D-CGD-CBD	4.87	119.92	111.27
18	G	1601	CLA	O2D-CGD-CBD	4.86	119.91	111.27
18	2	311	CLA	O2D-CGD-CBD	4.86	119.90	111.27
29	3	304	LUT	C31-C30-C29	-4.85	120.39	127.31
18	A	824	CLA	CMD-C2D-C1D	4.84	133.25	124.71
18	A	820	CLA	O2D-CGD-CBD	4.84	119.87	111.27
29	1	5003	LUT	C35-C34-C33	-4.84	120.40	127.31
18	B	807	CLA	O2D-CGD-CBD	4.84	119.86	111.27
18	K	1403	CLA	O2D-CGD-CBD	4.83	119.86	111.27
18	2	310	CLA	C1-C2-C3	-4.83	117.69	126.04
18	A	830	CLA	O2A-C1-C2	4.83	121.32	108.64
18	A	817	CLA	O2D-CGD-CBD	4.83	119.84	111.27
18	A	821	CLA	O2D-CGD-CBD	4.82	119.84	111.27
18	A	827	CLA	CMD-C2D-C1D	4.82	133.21	124.71
18	2	308	CLA	O2A-C1-C2	4.82	121.30	108.64
18	4	307	CLA	O2D-CGD-CBD	4.82	119.83	111.27
21	B	843	BCR	C8-C9-C10	4.81	126.33	118.94
18	3	317	CLA	O2D-CGD-CBD	4.81	119.82	111.27
18	K	1402	CLA	O2D-CGD-CBD	4.81	119.81	111.27
18	K	1404	CLA	O2D-CGD-CBD	4.81	119.81	111.27
18	A	814	CLA	O2D-CGD-CBD	4.80	119.81	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	806	CLA	O2A-C1-C2	4.80	121.25	108.64
18	B	838	CLA	O2A-C1-C2	4.80	121.24	108.64
18	B	809	CLA	O2D-CGD-CBD	4.80	119.79	111.27
18	L	301	CLA	O2D-CGD-CBD	4.80	119.79	111.27
18	A	810	CLA	O2A-C1-C2	4.79	121.23	108.64
18	A	819	CLA	O2D-CGD-CBD	4.78	119.77	111.27
18	B	820	CLA	O2D-CGD-CBD	4.77	119.74	111.27
18	B	841	CLA	O2D-CGD-CBD	4.77	119.74	111.27
18	A	852	CLA	O2D-CGD-CBD	4.77	119.74	111.27
29	2	303	LUT	C15-C14-C13	-4.77	120.51	127.31
18	A	823	CLA	O2A-C1-C2	4.75	121.11	108.64
18	1	5008	CLA	O2D-CGD-CBD	4.74	119.69	111.27
18	A	826	CLA	O2D-CGD-CBD	4.74	119.69	111.27
21	2	305	BCR	C28-C27-C26	-4.74	105.62	114.08
31	2	304	XAT	C38-C25-C24	4.73	119.60	114.28
18	F	302	CLA	O2D-CGD-CBD	4.72	119.66	111.27
18	J	1103	CLA	O2D-CGD-CBD	4.72	119.65	111.27
18	3	308	CLA	O2A-C1-C2	4.71	121.02	108.64
21	B	845	BCR	C19-C18-C17	4.71	126.17	118.94
18	A	818	CLA	O2A-C1-C2	4.70	121.00	108.64
17	A	801	CL0	C3D-C2D-C1D	-4.70	99.41	105.83
18	B	834	CLA	O2A-C1-C2	4.70	120.98	108.64
18	4	305	CLA	O2D-CGD-CBD	4.69	119.61	111.27
18	B	823	CLA	O2D-CGD-CBD	4.68	119.59	111.27
18	L	306	CLA	O2A-C1-C2	4.68	120.94	108.64
18	A	805	CLA	O2D-CGD-CBD	4.68	119.59	111.27
18	B	804	CLA	O2D-CGD-CBD	4.67	119.58	111.27
18	L	306	CLA	O2D-CGD-CBD	4.67	119.57	111.27
18	A	811	CLA	O2D-CGD-CBD	4.66	119.56	111.27
18	A	835	CLA	O2A-C1-C2	4.66	120.89	108.64
18	4	310	CLA	O2D-CGD-CBD	4.66	119.55	111.27
18	A	820	CLA	O2A-C1-C2	4.65	120.86	108.64
18	B	820	CLA	O2A-C1-C2	4.64	120.84	108.64
18	A	802	CLA	CMD-C2D-C1D	4.64	132.89	124.71
18	B	828	CLA	O2A-C1-C2	4.64	120.82	108.64
18	A	838	CLA	O2A-C1-C2	4.63	120.80	108.64
18	2	312	CLA	O2A-C1-C2	4.63	120.79	108.64
30	3	310	CHL	CHD-C1D-ND	-4.61	120.22	124.45
18	F	303	CLA	O2A-C1-C2	4.60	120.72	108.64
18	A	813	CLA	O2A-C1-C2	4.59	120.71	108.64
18	A	812	CLA	O2A-C1-C2	4.59	120.69	108.64
18	B	832	CLA	O2D-CGD-CBD	4.58	119.41	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	845	BCR	C29-C30-C25	-4.58	103.42	110.48
18	3	308	CLA	O2D-CGD-CBD	4.58	119.41	111.27
31	4	304	XAT	C38-C25-C24	4.58	119.43	114.28
18	B	803	CLA	O2D-CGD-CBD	4.58	119.40	111.27
18	B	833	CLA	O2A-C1-C2	4.58	120.66	108.64
29	1	5004	LUT	C15-C14-C13	-4.57	120.78	127.31
29	1	5004	LUT	C21-C26-C25	4.57	119.61	111.42
18	A	837	CLA	O2A-C1-C2	4.57	120.63	108.64
29	4	303	LUT	C21-C26-C27	4.56	118.47	112.70
29	4	303	LUT	C35-C34-C33	-4.54	120.83	127.31
18	B	803	CLA	CMD-C2D-C1D	4.54	132.72	124.71
18	A	809	CLA	O2A-C1-C2	4.53	120.55	108.64
18	A	822	CLA	O2D-CGD-CBD	4.52	119.30	111.27
22	A	849	LHG	O7-C7-C8	4.52	121.23	111.50
18	A	817	CLA	O2A-C1-C2	4.51	120.49	108.64
18	B	835	CLA	O2D-CGD-CBD	4.51	119.28	111.27
18	B	803	CLA	O2A-C1-C2	4.51	120.48	108.64
18	A	802	CLA	O2D-CGD-CBD	4.50	119.27	111.27
18	B	810	CLA	O2D-CGD-CBD	4.50	119.27	111.27
18	2	326	CLA	O2A-C1-C2	4.50	120.46	108.64
18	J	1103	CLA	O2A-C1-C2	4.49	120.43	108.64
21	A	855	BCR	C33-C5-C6	-4.47	119.51	124.53
18	G	1603	CLA	O2A-C1-C2	4.47	120.37	108.64
21	2	305	BCR	C39-C30-C29	-4.46	91.08	108.91
29	3	303	LUT	C21-C26-C27	4.45	118.33	112.70
18	3	315	CLA	O2A-C1-C2	4.44	120.32	108.64
18	B	809	CLA	O2A-C1-C2	4.43	120.28	108.64
29	1	5004	LUT	C35-C34-C33	-4.42	121.00	127.31
18	A	810	CLA	O2D-CGD-CBD	4.41	119.11	111.27
29	J	1105	LUT	C21-C26-C25	4.40	119.31	111.42
18	A	838	CLA	O2D-CGD-CBD	4.40	119.09	111.27
18	3	317	CLA	C1-C2-C3	-4.39	119.65	126.75
18	B	810	CLA	O2A-C1-C2	4.39	120.17	108.64
24	1	5020	LMG	O7-C10-C11	4.38	120.93	111.50
18	B	822	CLA	O2A-C1-C2	4.38	120.13	108.64
18	B	834	CLA	O2D-CGD-CBD	4.37	119.04	111.27
18	F	301	CLA	O2A-C1-C2	4.36	120.10	108.64
29	3	304	LUT	C21-C26-C25	4.36	119.22	111.42
18	L	304	CLA	O2A-C1-C2	4.36	120.09	108.64
24	F	308	LMG	O7-C10-C11	4.34	120.86	111.50
21	4	301	BCR	C33-C5-C6	-4.34	119.66	124.53
21	B	843	BCR	C34-C9-C10	-4.29	116.91	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	838	CLA	C1-C2-C3	-4.28	119.82	126.75
18	A	826	CLA	O2A-C1-C2	4.25	119.80	108.64
18	1	5015	CLA	O2A-C1-C2	4.24	119.78	108.64
18	A	819	CLA	O2A-C1-C2	4.20	119.67	108.64
26	2	327	DGD	O2G-C1B-C2B	4.19	120.53	111.50
17	A	801	CL0	O2A-CGA-CBA	4.18	125.03	111.91
24	F	306	LMG	O7-C10-C11	4.15	120.45	111.50
31	4	304	XAT	C15-C14-C13	-4.15	121.38	127.31
29	2	303	LUT	C21-C26-C27	4.15	117.94	112.70
21	B	845	BCR	C33-C5-C6	-4.14	119.88	124.53
29	3	303	LUT	C35-C34-C33	-4.14	121.40	127.31
21	B	843	BCR	C20-C19-C18	4.14	138.05	126.42
18	A	839	CLA	O2A-C1-C2	4.14	119.52	108.64
26	1	5002	DGD	O2G-C1B-C2B	4.14	120.42	111.50
30	4	316	CHL	CHD-C1D-ND	-4.14	120.65	124.45
30	3	310	CHL	C1-C2-C3	-4.11	118.93	126.04
21	L	303	BCR	C36-C18-C17	-4.11	117.16	122.92
21	B	845	BCR	C36-C18-C17	-4.11	117.17	122.92
24	2	322	LMG	O7-C10-C11	4.10	120.34	111.50
21	B	802	BCR	C19-C18-C17	4.10	125.23	118.94
31	4	304	XAT	C18-C5-C4	4.10	118.89	114.28
21	2	305	BCR	C33-C5-C6	-4.08	119.94	124.53
18	A	802	CLA	O2A-C1-C2	4.08	119.36	108.64
30	3	316	CHL	CHD-C1D-ND	-4.07	120.71	124.45
18	B	806	CLA	C1-C2-C3	-4.07	119.01	126.04
29	3	303	LUT	C15-C14-C13	-4.07	121.51	127.31
30	2	319	CHL	CHD-C1D-ND	-4.06	120.72	124.45
18	B	826	CLA	C1-C2-C3	-4.06	119.03	126.04
22	1	5019	LHG	O7-C7-C8	4.06	120.24	111.50
30	3	313	CHL	CHD-C1D-ND	-4.05	120.73	124.45
29	1	5003	LUT	C21-C26-C27	4.03	117.79	112.70
22	B	849	LHG	O7-C7-C8	4.03	120.18	111.50
24	B	850	LMG	O7-C10-C11	4.02	120.16	111.50
18	4	306	CLA	C1-C2-C3	-4.01	120.27	126.75
30	2	314	CHL	CHD-C1D-ND	-4.00	120.78	124.45
30	4	317	CHL	CHD-C1D-ND	-4.00	120.78	124.45
24	2	321	LMG	O7-C10-C11	4.00	121.95	110.80
21	L	303	BCR	C33-C5-C6	-3.99	120.04	124.53
22	2	320	LHG	O7-C7-C8	3.99	120.10	111.50
28	F	310	ZEX	C35-C34-C33	-3.99	121.62	127.31
22	A	848	LHG	O7-C7-C8	3.99	120.09	111.50
18	A	803	CLA	C1-C2-C3	-3.98	119.16	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	305	BCR	C23-C24-C25	-3.98	116.02	127.20
18	A	853	CLA	C1-C2-C3	-3.98	119.16	126.04
24	J	1102	LMG	O7-C10-C11	3.97	120.06	111.50
18	A	828	CLA	C1-C2-C3	-3.97	119.18	126.04
18	B	824	CLA	O2D-CGD-CBD	3.94	118.28	111.27
21	2	305	BCR	C19-C18-C17	3.94	124.99	118.94
18	3	301	CLA	O2D-CGD-CBD	3.94	118.27	111.27
18	A	827	CLA	C1-C2-C3	-3.93	119.24	126.04
18	B	807	CLA	C1-C2-C3	-3.93	119.25	126.04
18	B	818	CLA	O2A-C1-C2	3.92	118.95	108.64
21	B	847	BCR	C33-C5-C6	-3.92	120.13	124.53
21	3	305	BCR	C33-C5-C6	-3.92	120.13	124.53
18	B	815	CLA	C1-C2-C3	-3.92	119.27	126.04
26	F	309	DGD	O2G-C1B-C2B	3.91	119.92	111.50
30	1	5016	CHL	CHD-C1D-ND	-3.90	120.87	124.45
18	A	826	CLA	C1-C2-C3	-3.90	119.30	126.04
30	3	312	CHL	CHD-C1D-ND	-3.90	120.87	124.45
24	1	5001	LMG	O7-C10-C11	3.88	119.87	111.50
31	2	304	XAT	C18-C5-C4	3.88	118.65	114.28
21	B	844	BCR	C33-C5-C6	-3.88	120.17	124.53
29	1	5004	LUT	C11-C10-C9	-3.87	121.78	127.31
24	F	307	LMG	O7-C10-C11	3.85	119.81	111.50
18	4	310	CLA	C1-C2-C3	-3.84	120.54	126.75
30	4	318	CHL	CHD-C1D-ND	-3.83	120.93	124.45
18	2	313	CLA	C1-C2-C3	-3.83	120.55	126.75
29	4	303	LUT	C18-C5-C6	-3.82	120.24	124.53
21	3	306	BCR	C33-C5-C6	-3.81	120.24	124.53
21	J	1104	BCR	C33-C5-C6	-3.81	120.25	124.53
18	2	311	CLA	C1-C2-C3	-3.81	120.59	126.75
21	B	845	BCR	C20-C19-C18	3.80	137.10	126.42
18	B	816	CLA	C1-C2-C3	-3.80	119.46	126.04
18	4	307	CLA	C1-C2-C3	-3.80	119.47	126.04
30	2	316	CHL	CHD-C1D-ND	-3.80	120.97	124.45
18	A	805	CLA	C1-C2-C3	-3.79	119.48	126.04
21	A	844	BCR	C33-C5-C6	-3.79	120.27	124.53
26	B	855	DGD	O2G-C1B-C2B	3.78	119.65	111.50
18	A	818	CLA	C1-C2-C3	-3.78	120.64	126.75
29	1	5003	LUT	C18-C5-C6	-3.77	120.29	124.53
24	A	851	LMG	O7-C10-C11	3.77	119.62	111.50
23	A	850	LMT	C3'-C4'-C5'	-3.77	102.29	110.93
18	B	824	CLA	C1-C2-C3	-3.75	119.55	126.04
21	A	844	BCR	C19-C18-C17	3.75	124.69	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	809	CLA	C1-C2-C3	-3.75	120.69	126.75
29	J	1105	LUT	C15-C14-C13	-3.75	121.97	127.31
21	A	847	BCR	C23-C24-C25	-3.74	116.69	127.20
29	3	304	LUT	C18-C5-C6	-3.74	120.33	124.53
18	A	826	CLA	CHD-C1D-ND	-3.74	121.02	124.45
18	J	1103	CLA	C1-C2-C3	-3.73	120.72	126.75
21	B	845	BCR	C23-C22-C21	-3.73	113.22	118.94
21	L	302	BCR	C19-C18-C17	3.72	124.65	118.94
30	1	5016	CHL	C3C-C4C-NC	-3.72	106.40	110.57
21	A	846	BCR	C23-C24-C25	-3.72	116.77	127.20
21	1	5005	BCR	C33-C5-C6	-3.71	120.36	124.53
30	2	315	CHL	CHD-C1D-ND	-3.71	121.04	124.45
18	B	803	CLA	C1-C2-C3	-3.69	119.66	126.04
18	2	308	CLA	C1-C2-C3	-3.69	119.66	126.04
18	2	308	CLA	CMA-C3A-C4A	3.68	121.67	111.77
31	4	304	XAT	C7-C8-C9	-3.67	119.84	125.53
30	4	314	CHL	CHD-C1D-ND	-3.67	121.08	124.45
21	L	303	BCR	C19-C18-C17	3.66	124.56	118.94
21	2	305	BCR	C40-C30-C39	3.66	119.76	108.53
21	A	844	BCR	C36-C18-C17	-3.65	117.81	122.92
18	1	5010	CLA	C1-C2-C3	-3.65	119.73	126.04
18	3	314	CLA	O2A-C1-C2	3.65	121.83	109.49
18	L	305	CLA	CHD-C1D-ND	-3.65	121.10	124.45
30	4	313	CHL	CHD-C1D-ND	-3.65	121.10	124.45
18	B	834	CLA	CHD-C1D-ND	-3.64	121.11	124.45
21	B	845	BCR	C39-C30-C25	3.63	116.19	110.30
18	G	1601	CLA	C1-C2-C3	-3.63	119.76	126.04
21	G	1604	BCR	C15-C14-C13	-3.63	122.13	127.31
18	A	823	CLA	C2C-C1C-NC	3.63	113.37	109.97
18	K	1403	CLA	C2C-C1C-NC	3.63	113.37	109.97
17	A	801	CL0	C1D-ND-C4D	-3.62	103.76	106.33
21	B	846	BCR	C23-C24-C25	-3.62	117.04	127.20
18	2	310	CLA	CAA-C2A-C3A	-3.62	102.87	112.78
18	K	1404	CLA	C2C-C1C-NC	3.61	113.35	109.97
30	2	318	CHL	CHD-C1D-ND	-3.60	121.14	124.45
18	1	5006	CLA	C1-C2-C3	-3.60	119.82	126.04
18	K	1403	CLA	O2A-C1-C2	3.60	121.65	109.49
18	A	809	CLA	CHD-C1D-ND	-3.59	121.15	124.45
21	B	843	BCR	C33-C5-C6	-3.59	120.50	124.53
18	A	820	CLA	CHD-C1D-ND	-3.59	121.15	124.45
26	J	1106	DGD	O5D-C1E-C2E	3.59	113.91	108.30
30	1	5016	CHL	C2C-C3C-C4C	3.59	109.05	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	L	302	BCR	C36-C18-C17	-3.58	117.91	122.92
30	3	316	CHL	C2C-C3C-C4C	3.58	109.04	106.49
21	G	1604	BCR	C33-C5-C6	-3.58	120.51	124.53
18	A	825	CLA	C1-C2-C3	-3.57	119.87	126.04
21	B	802	BCR	C33-C5-C6	-3.56	120.53	124.53
29	3	303	LUT	C22-C23-C24	-3.56	107.69	111.74
21	L	302	BCR	C33-C5-C4	3.55	120.44	113.62
18	2	326	CLA	C1-C2-C3	-3.55	121.01	126.75
18	A	829	CLA	CHD-C1D-ND	-3.55	121.20	124.45
21	B	844	BCR	C23-C24-C25	-3.54	117.25	127.20
30	4	302	CHL	CHD-C1D-ND	-3.53	121.21	124.45
29	2	303	LUT	C7-C8-C9	-3.53	120.91	126.23
18	A	832	CLA	CHD-C1D-ND	-3.53	121.21	124.45
18	1	5011	CLA	C1-C2-C3	-3.53	121.05	126.75
18	A	810	CLA	CHD-C1D-ND	-3.52	121.22	124.45
18	B	837	CLA	CHD-C1D-ND	-3.52	121.22	124.45
18	J	1103	CLA	CMA-C3A-C4A	3.52	121.24	111.77
18	A	812	CLA	CHD-C1D-ND	-3.52	121.22	124.45
21	B	802	BCR	C34-C9-C10	-3.52	118.00	122.92
21	2	305	BCR	C33-C5-C4	3.51	120.37	113.62
18	A	830	CLA	CHD-C1D-ND	-3.51	121.23	124.45
21	I	101	BCR	C12-C13-C14	3.51	124.32	118.94
18	A	829	CLA	C1-C2-C3	-3.50	119.98	126.04
18	L	306	CLA	C1-C2-C3	-3.50	121.09	126.75
30	4	316	CHL	C1-O2A-CGA	3.50	125.62	116.44
18	B	819	CLA	CHD-C1D-ND	-3.50	121.24	124.45
18	B	819	CLA	C1-C2-C3	-3.48	120.02	126.04
18	B	820	CLA	C1-C2-C3	-3.48	120.03	126.04
21	A	843	BCR	C33-C5-C6	-3.48	120.62	124.53
18	1	5006	CLA	CHD-C1D-ND	-3.48	121.26	124.45
17	A	801	CL0	C1-C2-C3	-3.48	120.03	126.04
18	B	840	CLA	C2C-C1C-NC	3.48	113.23	109.97
18	L	305	CLA	C1-C2-C3	-3.47	120.04	126.04
18	1	5009	CLA	C1-C2-C3	-3.47	120.05	126.04
21	2	305	BCR	C36-C18-C17	-3.47	118.07	122.92
18	3	317	CLA	CHD-C1D-ND	-3.46	121.27	124.45
29	1	5003	LUT	C15-C14-C13	-3.46	122.37	127.31
21	I	101	BCR	C33-C5-C6	-3.46	120.64	124.53
18	4	312	CLA	CHD-C1D-ND	-3.46	121.27	124.45
18	2	309	CLA	CHD-C1D-ND	-3.46	121.28	124.45
21	B	846	BCR	C33-C5-C6	-3.46	120.65	124.53
18	L	301	CLA	C1-C2-C3	-3.45	120.07	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	832	CLA	C1-C2-C3	-3.45	120.08	126.04
18	2	317	CLA	C2C-C1C-NC	3.45	113.20	109.97
18	A	836	CLA	C1-C2-C3	-3.45	120.08	126.04
29	3	303	LUT	C18-C5-C6	-3.44	120.66	124.53
30	1	5014	CHL	CHD-C1D-ND	-3.44	121.29	124.45
18	A	831	CLA	CHD-C1D-ND	-3.44	121.30	124.45
30	3	313	CHL	C4D-CHA-C1A	3.44	125.43	121.25
18	A	811	CLA	C1-C2-C3	-3.44	120.10	126.04
18	B	830	CLA	C2C-C1C-NC	3.43	113.19	109.97
21	I	101	BCR	C33-C5-C4	3.43	120.21	113.62
18	B	833	CLA	C1-C2-C3	-3.43	120.11	126.04
30	3	312	CHL	C1-C2-C3	-3.43	121.20	126.75
18	B	838	CLA	CHD-C1D-ND	-3.43	121.31	124.45
18	A	817	CLA	CHD-C1D-ND	-3.43	121.31	124.45
23	2	325	LMT	C1'-O5'-C5'	-3.42	106.97	113.69
18	2	313	CLA	CHD-C1D-ND	-3.42	121.31	124.45
28	F	310	ZEX	C11-C10-C9	-3.42	122.43	127.31
30	3	316	CHL	C3C-C4C-NC	-3.42	106.74	110.57
28	F	310	ZEX	C31-C30-C29	-3.42	122.43	127.31
18	1	5009	CLA	CHD-C1D-ND	-3.41	121.32	124.45
18	3	319	CLA	CHD-C1D-ND	-3.41	121.32	124.45
21	B	847	BCR	C23-C24-C25	-3.41	117.62	127.20
18	A	837	CLA	CHD-C1D-ND	-3.41	121.32	124.45
30	3	312	CHL	C3C-C4C-NC	-3.41	106.75	110.57
18	L	304	CLA	C1-C2-C3	-3.41	121.23	126.75
18	B	822	CLA	CHD-C1D-ND	-3.41	121.32	124.45
18	4	315	CLA	CHD-C1D-ND	-3.41	121.32	124.45
18	A	815	CLA	CHD-C1D-ND	-3.41	121.32	124.45
18	3	311	CLA	C1-C2-C3	-3.41	120.15	126.04
18	B	820	CLA	CHD-C1D-ND	-3.40	121.33	124.45
18	A	822	CLA	C1-C2-C3	-3.40	120.16	126.04
18	K	1401	CLA	CHD-C1D-ND	-3.40	121.33	124.45
18	B	817	CLA	CHD-C1D-ND	-3.40	121.33	124.45
18	J	1103	CLA	C2C-C1C-NC	3.40	113.16	109.97
21	3	306	BCR	C15-C14-C13	3.39	132.15	127.31
18	A	819	CLA	CHD-C1D-ND	-3.39	121.34	124.45
18	A	852	CLA	CHD-C1D-ND	-3.39	121.34	124.45
18	B	807	CLA	CHD-C1D-ND	-3.39	121.34	124.45
28	F	310	ZEX	C18-C5-C6	-3.38	120.73	124.53
24	G	1607	LMG	O1-C1-C2	3.38	113.58	108.30
21	A	846	BCR	C33-C5-C6	-3.38	120.73	124.53
18	A	813	CLA	CHD-C1D-ND	-3.38	121.35	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	310	CLA	CHD-C1D-ND	-3.38	121.35	124.45
18	K	1403	CLA	CHD-C1D-ND	-3.38	121.35	124.45
18	4	309	CLA	C1-C2-C3	-3.37	120.21	126.04
21	B	802	BCR	C36-C18-C17	-3.37	118.20	122.92
18	2	311	CLA	CHD-C1D-ND	-3.37	121.36	124.45
18	A	813	CLA	C2C-C1C-NC	3.37	113.12	109.97
18	4	315	CLA	C2C-C1C-NC	3.36	113.12	109.97
21	L	302	BCR	C33-C5-C6	-3.36	120.75	124.53
29	2	303	LUT	C18-C5-C6	-3.36	120.75	124.53
18	2	326	CLA	C2C-C1C-NC	3.36	113.12	109.97
21	L	307	BCR	C33-C5-C6	-3.36	120.75	124.53
18	B	828	CLA	CHD-C1D-ND	-3.36	121.37	124.45
18	B	808	CLA	CHD-C1D-ND	-3.36	121.37	124.45
18	B	810	CLA	C2C-C1C-NC	3.35	113.11	109.97
18	G	1603	CLA	CMA-C3A-C4A	3.35	120.79	111.77
18	A	853	CLA	CHD-C1D-ND	-3.35	121.37	124.45
18	3	307	CLA	CHD-C1D-ND	-3.35	121.37	124.45
18	B	836	CLA	C1-C2-C3	-3.35	120.25	126.04
18	A	835	CLA	CHD-C1D-ND	-3.35	121.38	124.45
18	A	822	CLA	CHD-C1D-ND	-3.35	121.38	124.45
18	2	306	CLA	CHD-C1D-ND	-3.35	121.38	124.45
18	J	1101	CLA	CHD-C1D-ND	-3.35	121.38	124.45
24	2	321	LMG	O8-C28-C29	3.35	120.15	111.38
18	3	309	CLA	C1-C2-C3	-3.34	120.26	126.04
18	A	823	CLA	C1-C2-C3	-3.34	120.26	126.04
18	A	823	CLA	CHD-C1D-ND	-3.34	121.39	124.45
18	B	809	CLA	C2C-C1C-NC	3.34	113.10	109.97
18	B	818	CLA	C2C-C1C-NC	3.34	113.10	109.97
18	4	308	CLA	CHD-C1D-ND	-3.34	121.39	124.45
18	H	1701	CLA	C2C-C1C-NC	3.34	113.10	109.97
18	B	826	CLA	CHD-C1D-ND	-3.34	121.39	124.45
18	A	828	CLA	CHD-C1D-ND	-3.33	121.39	124.45
18	A	834	CLA	C1-C2-C3	-3.33	120.29	126.04
18	2	317	CLA	CHD-C1D-ND	-3.33	121.40	124.45
18	B	812	CLA	CHD-C1D-ND	-3.32	121.40	124.45
21	A	845	BCR	C33-C5-C6	-3.32	120.80	124.53
18	A	805	CLA	CHD-C1D-ND	-3.32	121.40	124.45
24	G	1607	LMG	O7-C10-C11	3.32	120.06	110.80
18	B	801	CLA	C1-C2-C3	-3.32	120.31	126.04
18	F	301	CLA	CHD-C1D-ND	-3.31	121.41	124.45
30	3	310	CHL	CMA-C3A-C4A	3.31	120.67	111.77
18	A	814	CLA	C2C-C1C-NC	3.31	113.07	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	806	CLA	CHD-C1D-ND	-3.31	121.41	124.45
18	1	5013	CLA	CHD-C1D-ND	-3.31	121.41	124.45
18	B	818	CLA	CHD-C1D-ND	-3.30	121.42	124.45
18	B	836	CLA	C2C-C1C-NC	3.30	113.07	109.97
18	B	832	CLA	CHD-C1D-ND	-3.30	121.42	124.45
18	B	830	CLA	C1-C2-C3	-3.30	120.34	126.04
18	A	806	CLA	CHD-C1D-ND	-3.30	121.42	124.45
21	A	847	BCR	C12-C13-C14	-3.30	113.88	118.94
18	G	1603	CLA	CHD-C1D-ND	-3.29	121.43	124.45
18	B	805	CLA	CHD-C1D-ND	-3.29	121.43	124.45
18	A	836	CLA	CHD-C1D-ND	-3.29	121.43	124.45
18	A	833	CLA	CHD-C1D-ND	-3.29	121.43	124.45
18	L	304	CLA	CHD-C1D-ND	-3.29	121.44	124.45
30	4	317	CHL	C2C-C3C-C4C	3.28	108.83	106.49
18	A	834	CLA	CHD-C1D-ND	-3.28	121.44	124.45
30	3	310	CHL	C4D-CHA-C1A	3.28	125.24	121.25
29	1	5003	LUT	C22-C23-C24	-3.28	108.01	111.74
18	A	814	CLA	CHD-C1D-ND	-3.28	121.44	124.45
18	4	307	CLA	CHD-C1D-ND	-3.28	121.44	124.45
18	A	828	CLA	C2C-C1C-NC	3.28	113.04	109.97
18	G	1601	CLA	C2C-C1C-NC	3.28	113.04	109.97
18	J	1101	CLA	C2C-C1C-NC	3.28	113.04	109.97
18	1	5010	CLA	C2C-C1C-NC	3.28	113.04	109.97
18	4	305	CLA	CHD-C1D-ND	-3.28	121.44	124.45
18	B	839	CLA	CHD-C1D-ND	-3.27	121.45	124.45
18	3	315	CLA	CHD-C1D-ND	-3.27	121.45	124.45
18	B	825	CLA	C1-O2A-CGA	3.27	125.01	116.44
24	G	1607	LMG	O8-C28-C29	3.27	119.94	111.38
18	K	1402	CLA	C2C-C1C-NC	3.27	113.03	109.97
18	4	308	CLA	C1-C2-C3	-3.26	120.40	126.04
18	B	801	CLA	CHD-C1D-ND	-3.26	121.45	124.45
18	A	802	CLA	CHD-C1D-ND	-3.26	121.46	124.45
18	1	5011	CLA	CHD-C1D-ND	-3.26	121.46	124.45
21	F	305	BCR	C33-C5-C6	-3.26	120.87	124.53
30	1	5014	CHL	CMA-C3A-C4A	3.25	120.52	111.77
18	A	803	CLA	CHD-C1D-ND	-3.25	121.47	124.45
18	A	840	CLA	CHD-C1D-ND	-3.25	121.47	124.45
30	3	310	CHL	C1-O2A-CGA	3.25	124.97	116.44
18	B	830	CLA	CHD-C1D-ND	-3.25	121.47	124.45
18	1	5008	CLA	C1-C2-C3	-3.25	120.43	126.04
29	4	303	LUT	C7-C8-C9	-3.25	121.33	126.23
18	B	835	CLA	C1-C2-C3	-3.25	120.43	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	311	CLA	C1-C2-C3	-3.25	120.43	126.04
21	L	302	BCR	C3-C4-C5	-3.24	108.28	114.08
19	B	842	PQN	C11-C12-C13	-3.24	121.40	126.79
18	B	821	CLA	C2C-C1C-NC	3.24	113.01	109.97
18	A	816	CLA	C1-C2-C3	-3.24	120.44	126.04
19	A	841	PQN	C14-C13-C15	3.24	120.72	115.27
18	F	302	CLA	C2C-C1C-NC	3.24	113.00	109.97
23	B	853	LMT	C1'-O5'-C5'	-3.24	107.34	113.69
30	4	314	CHL	CMA-C3A-C4A	3.23	120.46	111.77
18	B	814	CLA	CHD-C1D-ND	-3.23	121.48	124.45
22	A	849	LHG	C5-O7-C7	-3.23	109.84	117.79
18	3	301	CLA	CHD-C1D-ND	-3.23	121.49	124.45
18	B	840	CLA	CHD-C1D-ND	-3.23	121.49	124.45
18	1	5015	CLA	CHD-C1D-ND	-3.23	121.49	124.45
18	A	838	CLA	C2C-C1C-NC	3.23	113.00	109.97
18	1	5008	CLA	C2C-C1C-NC	3.23	113.00	109.97
18	1	5012	CLA	C2C-C1C-NC	3.23	112.99	109.97
18	B	829	CLA	C2C-C1C-NC	3.22	112.99	109.97
24	J	1102	LMG	O8-C28-C29	3.22	119.83	111.38
21	F	304	BCR	C28-C27-C26	-3.22	108.32	114.08
18	H	1701	CLA	C1-C2-C3	-3.22	120.47	126.04
30	4	313	CHL	CMA-C3A-C4A	3.22	120.44	111.77
18	4	310	CLA	CHD-C1D-ND	-3.22	121.49	124.45
18	A	833	CLA	C2C-C1C-NC	3.22	112.99	109.97
18	2	310	CLA	C1C-C2C-C3C	-3.22	103.58	106.96
18	A	808	CLA	C2C-C1C-NC	3.22	112.98	109.97
18	2	312	CLA	C2C-C1C-NC	3.22	112.98	109.97
18	B	841	CLA	CHD-C1D-ND	-3.22	121.50	124.45
18	L	306	CLA	CHD-C1D-ND	-3.21	121.50	124.45
18	A	852	CLA	C2C-C1C-NC	3.21	112.98	109.97
18	B	808	CLA	C2C-C1C-NC	3.21	112.98	109.97
18	2	308	CLA	CHD-C1D-ND	-3.21	121.50	124.45
18	2	310	CLA	C2D-C1D-ND	3.21	112.47	110.10
30	4	302	CHL	CMA-C3A-C4A	3.21	120.40	111.77
18	A	807	CLA	CHD-C1D-ND	-3.21	121.51	124.45
18	1	5013	CLA	C2C-C1C-NC	3.21	112.98	109.97
18	A	820	CLA	C2C-C1C-NC	3.21	112.97	109.97
18	B	827	CLA	C1-C2-C3	-3.20	120.50	126.04
18	A	804	CLA	CHD-C1D-ND	-3.20	121.51	124.45
18	A	837	CLA	C1-C2-C3	-3.20	120.50	126.04
18	B	825	CLA	CHD-C1D-ND	-3.20	121.51	124.45
18	L	304	CLA	C2C-C1C-NC	3.20	112.97	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	317	CHL	C3C-C4C-NC	-3.20	106.98	110.57
18	A	840	CLA	C1-C2-C3	-3.20	120.51	126.04
18	F	302	CLA	CHD-C1D-ND	-3.20	121.52	124.45
18	A	818	CLA	C2C-C1C-NC	3.20	112.97	109.97
18	B	828	CLA	C1-C2-C3	-3.20	120.51	126.04
18	A	839	CLA	C2C-C1C-NC	3.20	112.97	109.97
18	G	1601	CLA	CHD-C1D-ND	-3.19	121.52	124.45
18	3	314	CLA	C2C-C1C-NC	3.19	112.96	109.97
18	K	1402	CLA	CHD-C1D-ND	-3.19	121.52	124.45
26	J	1106	DGD	O2G-C1B-C2B	3.19	118.38	111.50
18	3	309	CLA	CHD-C1D-ND	-3.19	121.52	124.45
18	B	812	CLA	C1-C2-C3	-3.19	120.53	126.04
18	B	827	CLA	C2C-C1C-NC	3.18	112.95	109.97
18	F	301	CLA	C2D-C1D-ND	3.18	112.45	110.10
18	B	828	CLA	C2C-C1C-NC	3.18	112.95	109.97
18	B	822	CLA	C2C-C1C-NC	3.18	112.95	109.97
18	A	807	CLA	C1-C2-C3	-3.18	120.54	126.04
18	A	813	CLA	C1-C2-C3	-3.18	120.54	126.04
18	A	838	CLA	CHD-C1D-ND	-3.18	121.53	124.45
18	B	823	CLA	CHD-C1D-ND	-3.18	121.53	124.45
18	G	1603	CLA	C2C-C1C-NC	3.18	112.95	109.97
21	B	845	BCR	C37-C22-C23	3.18	123.08	118.08
18	H	1701	CLA	CHD-C1D-ND	-3.18	121.53	124.45
18	3	314	CLA	CHD-C1D-ND	-3.18	121.53	124.45
18	G	1602	CLA	C2C-C1C-NC	3.18	112.95	109.97
18	2	309	CLA	C1-C2-C3	-3.18	120.55	126.04
21	F	304	BCR	C2-C1-C6	3.18	115.37	110.48
18	B	814	CLA	C2C-C1C-NC	3.17	112.94	109.97
18	B	824	CLA	CHD-C1D-ND	-3.17	121.54	124.45
18	F	303	CLA	CHD-C1D-ND	-3.17	121.54	124.45
18	3	318	CLA	CHD-C1D-ND	-3.17	121.54	124.45
18	3	308	CLA	C2C-C1C-NC	3.17	112.94	109.97
18	B	829	CLA	CHD-C1D-ND	-3.17	121.54	124.45
18	A	811	CLA	CHD-C1D-ND	-3.17	121.55	124.45
18	G	1602	CLA	CHD-C1D-ND	-3.17	121.55	124.45
18	1	5008	CLA	CHD-C1D-ND	-3.16	121.55	124.45
18	A	806	CLA	C2C-C1C-NC	3.16	112.94	109.97
18	B	813	CLA	C2C-C1C-NC	3.16	112.94	109.97
21	G	1604	BCR	C33-C5-C4	3.16	119.69	113.62
21	I	102	BCR	C33-C5-C6	-3.16	120.98	124.53
18	2	309	CLA	CMA-C3A-C4A	3.16	120.27	111.77
18	K	1401	CLA	C2C-C1C-NC	3.16	112.93	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	2	319	CHL	CMA-C3A-C4A	3.16	120.26	111.77
18	2	307	CLA	C2C-C1C-NC	3.16	112.93	109.97
18	A	816	CLA	CHD-C1D-ND	-3.16	121.55	124.45
30	2	315	CHL	C3C-C4C-NC	-3.16	107.03	110.57
30	4	314	CHL	C1-C2-C3	-3.16	121.64	126.75
18	A	830	CLA	C1-C2-C3	-3.16	120.58	126.04
18	A	839	CLA	CHD-C1D-ND	-3.15	121.56	124.45
18	4	306	CLA	C2C-C1C-NC	3.15	112.93	109.97
18	A	853	CLA	CMA-C3A-C4A	3.15	120.25	111.77
18	K	1401	CLA	C2D-C1D-ND	3.15	112.43	110.10
21	A	847	BCR	C35-C13-C12	3.15	123.04	118.08
18	L	301	CLA	CHD-C1D-ND	-3.15	121.56	124.45
18	A	827	CLA	C2C-C1C-NC	3.15	112.92	109.97
18	K	1402	CLA	CMA-C3A-C4A	3.15	120.23	111.77
18	B	831	CLA	CHD-C1D-ND	-3.15	121.56	124.45
18	A	838	CLA	CMA-C3A-C4A	3.15	120.23	111.77
18	2	313	CLA	C2C-C1C-NC	3.15	112.92	109.97
21	A	855	BCR	C36-C18-C17	-3.14	118.53	122.92
18	A	821	CLA	C2C-C1C-NC	3.14	112.91	109.97
18	1	5018	CLA	CHD-C1D-ND	-3.14	121.57	124.45
18	A	817	CLA	CMA-C3A-C4A	3.14	120.21	111.77
18	A	821	CLA	CHD-C1D-ND	-3.14	121.57	124.45
21	K	1405	BCR	C33-C5-C4	3.14	119.64	113.62
18	3	301	CLA	C2C-C1C-NC	3.14	112.91	109.97
18	A	815	CLA	C1-C2-C3	-3.14	120.62	126.04
21	I	101	BCR	C31-C1-C6	-3.13	105.22	110.30
18	B	813	CLA	CHD-C1D-ND	-3.13	121.58	124.45
21	A	855	BCR	C15-C14-C13	-3.13	122.84	127.31
30	4	317	CHL	CMA-C3A-C4A	3.13	120.18	111.77
18	2	311	CLA	C2C-C1C-NC	3.13	112.90	109.97
21	J	1104	BCR	C12-C13-C14	-3.13	114.14	118.94
18	2	308	CLA	C2C-C1C-NC	3.13	112.90	109.97
18	B	825	CLA	C2C-C1C-NC	3.12	112.90	109.97
18	1	5012	CLA	CHD-C1D-ND	-3.12	121.59	124.45
18	3	309	CLA	C2C-C1C-NC	3.12	112.89	109.97
18	A	810	CLA	CMA-C3A-C4A	3.12	120.16	111.77
18	4	308	CLA	CMA-C3A-C4A	3.12	120.15	111.77
18	3	318	CLA	C2C-C1C-NC	3.12	112.89	109.97
29	4	303	LUT	C22-C23-C24	-3.11	108.20	111.74
18	A	840	CLA	C2C-C1C-NC	3.11	112.89	109.97
21	F	305	BCR	C23-C24-C25	-3.11	118.46	127.20
18	B	815	CLA	CHD-C1D-ND	-3.11	121.59	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	825	CLA	C2D-C1D-ND	3.11	112.39	110.10
30	3	316	CHL	CMA-C3A-C4A	3.11	120.12	111.77
18	B	816	CLA	CHD-C1D-ND	-3.11	121.60	124.45
18	A	853	CLA	C2C-C1C-NC	3.10	112.88	109.97
29	2	303	LUT	C11-C10-C9	-3.10	122.89	127.31
18	A	804	CLA	C1-C2-C3	-3.10	120.69	126.04
18	B	819	CLA	C2C-C1C-NC	3.10	112.87	109.97
18	F	303	CLA	C1-C2-C3	-3.10	120.69	126.04
18	B	823	CLA	C2C-C1C-NC	3.09	112.87	109.97
18	3	308	CLA	C1-C2-C3	-3.09	120.69	126.04
18	B	835	CLA	CHD-C1D-ND	-3.09	121.61	124.45
21	1	5005	BCR	C34-C9-C10	-3.09	118.59	122.92
18	A	834	CLA	C2C-C1C-NC	3.09	112.87	109.97
30	4	314	CHL	C2C-C3C-C4C	3.09	108.69	106.49
18	4	307	CLA	C2C-C1C-NC	3.09	112.86	109.97
18	1	5013	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
18	4	309	CLA	CHD-C1D-ND	-3.09	121.62	124.45
21	F	304	BCR	C23-C24-C25	-3.09	118.53	127.20
29	4	303	LUT	C15-C14-C13	-3.09	122.91	127.31
18	B	806	CLA	C2C-C1C-NC	3.08	112.86	109.97
18	B	839	CLA	C2C-C1C-NC	3.08	112.86	109.97
29	3	304	LUT	C35-C15-C14	-3.08	117.16	123.47
18	B	830	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
30	2	319	CHL	C3C-C4C-NC	-3.08	107.11	110.57
18	B	831	CLA	C2C-C1C-NC	3.08	112.86	109.97
30	2	314	CHL	C3C-C4C-NC	-3.08	107.12	110.57
18	1	5007	CLA	C2C-C1C-NC	3.08	112.86	109.97
18	B	837	CLA	C1-C2-C3	-3.08	120.72	126.04
30	4	314	CHL	C3C-C4C-NC	-3.08	107.12	110.57
18	B	803	CLA	C2C-C1C-NC	3.08	112.85	109.97
18	K	1404	CLA	CMA-C3A-C4A	3.08	120.04	111.77
18	A	838	CLA	C1-C2-C3	-3.08	120.72	126.04
18	A	812	CLA	C1-C2-C3	-3.07	120.73	126.04
18	B	808	CLA	C1-C2-C3	-3.07	120.73	126.04
18	1	5015	CLA	C2C-C1C-NC	3.07	112.85	109.97
18	B	810	CLA	CHD-C1D-ND	-3.07	121.63	124.45
30	4	318	CHL	CMA-C3A-C4A	3.07	120.03	111.77
30	3	310	CHL	C3C-C4C-NC	-3.07	107.13	110.57
21	A	855	BCR	C19-C18-C17	3.07	123.65	118.94
18	B	814	CLA	C1-C2-C3	-3.07	120.74	126.04
21	B	802	BCR	C35-C13-C14	-3.07	118.63	122.92
18	4	311	CLA	CMA-C3A-C4A	3.06	120.00	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	311	CLA	C2D-C1D-ND	3.06	112.36	110.10
18	F	301	CLA	CMA-C3A-C4A	3.06	120.00	111.77
18	1	5008	CLA	CMA-C3A-C4A	3.06	119.99	111.77
18	B	835	CLA	C2C-C1C-NC	3.06	112.84	109.97
18	4	307	CLA	CMA-C3A-C4A	3.06	119.99	111.77
18	A	822	CLA	CMA-C3A-C4A	3.06	119.99	111.77
30	2	318	CHL	CMA-C3A-C4A	3.05	119.98	111.77
29	1	5003	LUT	C11-C10-C9	-3.05	122.95	127.31
18	B	801	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
18	B	816	CLA	C2C-C1C-NC	3.05	112.83	109.97
21	B	802	BCR	C8-C9-C10	3.05	123.62	118.94
30	3	313	CHL	C1-C2-C3	-3.05	121.82	126.75
30	4	318	CHL	C3C-C4C-NC	-3.05	107.15	110.57
21	A	847	BCR	C33-C5-C4	3.05	119.47	113.62
18	2	312	CLA	CMA-C3A-C4A	3.05	119.96	111.77
30	2	315	CHL	CMA-C3A-C4A	3.05	119.96	111.77
18	1	5011	CLA	C2C-C1C-NC	3.05	112.83	109.97
18	K	1403	CLA	CMA-C3A-C4A	3.04	119.95	111.77
21	A	845	BCR	C27-C26-C25	-3.04	118.31	122.73
18	L	306	CLA	C2C-C1C-NC	3.04	112.82	109.97
21	A	846	BCR	C36-C18-C17	-3.04	118.66	122.92
30	4	316	CHL	C4D-CHA-C1A	3.04	124.95	121.25
18	F	303	CLA	C2C-C1C-NC	3.04	112.82	109.97
18	1	5015	CLA	CMA-C3A-C4A	3.04	119.94	111.77
18	3	309	CLA	CMA-C3A-C4A	3.04	119.94	111.77
18	B	819	CLA	O2A-CGA-CBA	3.04	121.44	111.91
18	A	814	CLA	CMA-C3A-C4A	3.04	119.93	111.77
18	4	312	CLA	C2C-C1C-NC	3.03	112.81	109.97
18	4	315	CLA	C1-C2-C3	-3.03	120.80	126.04
18	B	815	CLA	C2C-C1C-NC	3.03	112.81	109.97
18	B	822	CLA	CMA-C3A-C4A	3.03	119.91	111.77
18	A	825	CLA	C2C-C1C-NC	3.03	112.81	109.97
18	2	312	CLA	CHD-C1D-ND	-3.03	121.67	124.45
30	2	316	CHL	CMA-C3A-C4A	3.03	119.91	111.77
18	B	834	CLA	C2C-C1C-NC	3.03	112.81	109.97
18	B	804	CLA	CHD-C1D-ND	-3.02	121.67	124.45
29	1	5003	LUT	C35-C15-C14	-3.02	117.28	123.47
18	B	838	CLA	C2C-C1C-NC	3.02	112.80	109.97
29	3	304	LUT	C22-C23-C24	-3.02	108.30	111.74
18	A	825	CLA	CHD-C1D-ND	-3.02	121.68	124.45
18	1	5012	CLA	CMA-C3A-C4A	3.02	119.89	111.77
18	A	811	CLA	C2C-C1C-NC	3.02	112.80	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	313	CHL	C3C-C4C-NC	-3.02	107.19	110.57
18	4	311	CLA	CHD-C1D-ND	-3.02	121.68	124.45
18	A	830	CLA	C2C-C1C-NC	3.01	112.79	109.97
21	J	1104	BCR	C35-C13-C12	3.01	122.82	118.08
18	A	804	CLA	C2C-C1C-NC	3.01	112.79	109.97
21	L	302	BCR	C2-C1-C6	3.01	115.11	110.48
18	2	310	CLA	CMA-C3A-C4A	3.00	119.85	111.77
26	J	1106	DGD	O1G-C1A-C2A	3.00	121.34	111.91
18	1	5010	CLA	CHD-C1D-ND	-3.00	121.69	124.45
18	B	833	CLA	C2C-C1C-NC	3.00	112.78	109.97
18	A	821	CLA	C1-C2-C3	-3.00	120.85	126.04
18	2	326	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
18	1	5007	CLA	C2D-C1D-ND	3.00	112.31	110.10
18	4	306	CLA	CHD-C1D-ND	-3.00	121.70	124.45
18	A	813	CLA	CMA-C3A-C4A	3.00	119.83	111.77
18	2	307	CLA	CHD-C1D-ND	-3.00	121.70	124.45
18	3	308	CLA	CHD-C1D-ND	-3.00	121.70	124.45
18	4	310	CLA	C2C-C1C-NC	3.00	112.78	109.97
18	B	819	CLA	CMA-C3A-C4A	3.00	119.83	111.77
18	2	307	CLA	C1-C2-C3	-2.99	120.86	126.04
18	3	307	CLA	C1-C2-C3	-2.99	120.86	126.04
22	A	849	LHG	O8-C23-C24	2.99	121.30	111.91
18	B	836	CLA	CHD-C1D-ND	-2.99	121.70	124.45
21	A	843	BCR	C36-C18-C17	-2.99	118.73	122.92
18	2	313	CLA	CMA-C3A-C4A	2.99	119.82	111.77
18	B	821	CLA	CHD-C1D-ND	-2.99	121.70	124.45
18	B	833	CLA	CHD-C1D-ND	-2.99	121.70	124.45
18	A	807	CLA	C2C-C1C-NC	2.99	112.78	109.97
18	A	827	CLA	CMA-C3A-C4A	2.99	119.81	111.77
18	B	830	CLA	CMB-C2B-C3B	2.99	130.27	124.68
18	L	301	CLA	CMA-C3A-C4A	2.99	119.80	111.77
29	1	5004	LUT	C7-C8-C9	-2.99	121.72	126.23
21	B	844	BCR	C34-C9-C10	-2.98	118.74	122.92
18	B	838	CLA	C2D-C1D-ND	2.98	112.30	110.10
18	A	808	CLA	CHD-C1D-ND	-2.98	121.71	124.45
18	A	820	CLA	CMA-C3A-C4A	2.98	119.79	111.77
21	L	302	BCR	C23-C24-C25	-2.98	118.83	127.20
29	1	5004	LUT	C22-C23-C24	-2.98	108.35	111.74
18	A	823	CLA	CMA-C3A-C4A	2.98	119.78	111.77
30	3	312	CHL	CHB-C4A-NA	2.98	128.63	124.51
18	3	311	CLA	CHD-C1D-ND	-2.98	121.72	124.45
30	4	302	CHL	C2C-C3C-C4C	2.98	108.61	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	5018	CLA	CMA-C3A-C4A	2.98	119.78	111.77
18	J	1103	CLA	CHD-C1D-ND	-2.98	121.72	124.45
30	3	313	CHL	CMA-C3A-C4A	2.97	119.77	111.77
18	1	5008	CLA	O2A-CGA-CBA	2.97	121.24	111.91
30	4	318	CHL	C2C-C3C-C4C	2.97	108.61	106.49
18	3	311	CLA	C2C-C1C-NC	2.97	112.76	109.97
18	B	839	CLA	CMA-C3A-C4A	2.97	119.77	111.77
18	B	809	CLA	CHD-C1D-ND	-2.97	121.72	124.45
18	B	811	CLA	C2C-C1C-NC	2.97	112.76	109.97
18	3	315	CLA	C2C-C1C-NC	2.97	112.76	109.97
18	A	802	CLA	C2D-C1D-ND	2.97	112.29	110.10
18	A	816	CLA	C2D-C1D-ND	2.97	112.29	110.10
18	B	816	CLA	CMA-C3A-C4A	2.97	119.76	111.77
30	3	310	CHL	C2C-C3C-C4C	2.97	108.61	106.49
18	A	812	CLA	C2D-C1D-ND	2.97	112.29	110.10
18	A	818	CLA	CHD-C1D-ND	-2.97	121.73	124.45
18	A	815	CLA	C2C-C1C-NC	2.97	112.75	109.97
18	2	309	CLA	C2C-C1C-NC	2.97	112.75	109.97
18	A	808	CLA	CMA-C3A-C4A	2.97	119.74	111.77
18	4	315	CLA	CMA-C3A-C4A	2.96	119.74	111.77
29	2	303	LUT	C15-C35-C34	-2.96	117.41	123.47
18	4	309	CLA	C2C-C1C-NC	2.96	112.74	109.97
18	B	826	CLA	CMA-C3A-C4A	2.96	119.72	111.77
18	A	821	CLA	CMA-C3A-C4A	2.96	119.72	111.77
18	B	812	CLA	CMA-C3A-C4A	2.96	119.72	111.77
18	A	828	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
18	B	830	CLA	CMD-C2D-C3D	-2.96	120.81	127.61
30	3	312	CHL	C2C-C3C-C4C	2.96	108.60	106.49
18	B	813	CLA	CMA-C3A-C4A	2.96	119.72	111.77
18	B	832	CLA	C2C-C1C-NC	2.95	112.74	109.97
18	A	833	CLA	CMA-C3A-C4A	2.95	119.71	111.77
18	B	830	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
18	B	817	CLA	O2A-CGA-CBA	2.95	121.17	111.91
18	B	801	CLA	C2C-C1C-NC	2.95	112.74	109.97
18	B	824	CLA	C2C-C1C-NC	2.95	112.74	109.97
23	J	1107	LMT	C1'-O5'-C5'	-2.95	107.90	113.69
21	4	301	BCR	C35-C13-C12	2.95	122.72	118.08
30	2	314	CHL	C2C-C3C-C4C	2.95	108.59	106.49
21	B	845	BCR	C23-C24-C25	-2.95	118.93	127.20
18	B	812	CLA	C2C-C1C-NC	2.95	112.73	109.97
18	4	311	CLA	C2C-C1C-NC	2.95	112.73	109.97
18	3	315	CLA	CMA-C3A-C4A	2.95	119.69	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	848	LHG	C5-O7-C7	-2.95	112.41	117.90
29	2	303	LUT	C22-C23-C24	-2.95	108.39	111.74
21	B	846	BCR	C33-C5-C4	2.94	119.27	113.62
30	3	313	CHL	C3C-C4C-NC	-2.94	107.27	110.57
18	A	835	CLA	CMA-C3A-C4A	2.94	119.68	111.77
24	B	850	LMG	O8-C28-C29	2.94	121.14	111.91
18	3	319	CLA	C2C-C1C-NC	2.94	112.73	109.97
21	4	301	BCR	C36-C18-C17	-2.94	118.81	122.92
23	B	852	LMT	C1'-O5'-C5'	-2.94	107.92	113.69
18	B	840	CLA	C1C-C2C-C3C	-2.94	103.87	106.96
18	A	825	CLA	CMA-C3A-C4A	2.94	119.67	111.77
18	1	5010	CLA	C1C-C2C-C3C	-2.94	103.87	106.96
18	B	832	CLA	CMA-C3A-C4A	2.94	119.66	111.77
21	K	1405	BCR	C34-C9-C10	-2.93	118.81	122.92
18	3	319	CLA	C1-C2-C3	-2.93	120.97	126.04
18	K	1404	CLA	CHD-C1D-ND	-2.93	121.76	124.45
18	2	306	CLA	C2D-C1D-ND	2.93	112.27	110.10
18	2	310	CLA	C2C-C1C-NC	2.93	112.72	109.97
18	B	811	CLA	CHD-C1D-ND	-2.93	121.76	124.45
18	G	1602	CLA	CMA-C3A-C4A	2.93	119.65	111.77
21	A	845	BCR	C23-C24-C25	-2.93	118.97	127.20
18	A	824	CLA	C2C-C1C-NC	2.93	112.72	109.97
18	3	314	CLA	CMA-C3A-C4A	2.93	119.64	111.77
18	4	308	CLA	C2C-C1C-NC	2.92	112.71	109.97
21	1	5005	BCR	C38-C26-C25	-2.92	121.25	124.53
18	A	822	CLA	C2C-C1C-NC	2.92	112.71	109.97
21	L	303	BCR	C37-C22-C21	-2.92	118.83	122.92
18	3	308	CLA	C6-C5-C3	-2.92	109.84	114.62
18	K	1403	CLA	C1C-C2C-C3C	-2.92	103.88	106.96
18	B	841	CLA	C2D-C1D-ND	2.92	112.26	110.10
18	1	5018	CLA	C2C-C1C-NC	2.92	112.71	109.97
21	4	301	BCR	C12-C13-C14	-2.92	114.46	118.94
18	B	806	CLA	C2D-C1D-ND	2.92	112.25	110.10
26	J	1106	DGD	O6D-C5D-C6D	2.92	112.56	106.67
30	4	302	CHL	C3C-C4C-NC	-2.92	107.30	110.57
21	A	844	BCR	C33-C5-C4	2.92	119.22	113.62
18	A	817	CLA	C2C-C1C-NC	2.92	112.70	109.97
21	4	301	BCR	C38-C26-C25	-2.92	121.25	124.53
18	L	305	CLA	CMA-C3A-C4A	2.91	119.61	111.77
29	1	5004	LUT	C18-C5-C6	-2.91	121.26	124.53
18	A	840	CLA	CMA-C3A-C4A	2.91	119.60	111.77
18	B	841	CLA	CMA-C3A-C4A	2.91	119.59	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	313	CHL	C2C-C3C-C4C	2.91	108.56	106.49
18	A	829	CLA	C2C-C1C-NC	2.90	112.69	109.97
18	B	836	CLA	CMA-C3A-C4A	2.90	119.58	111.77
30	2	314	CHL	CMA-C3A-C4A	2.90	119.58	111.77
24	1	5001	LMG	O8-C28-C29	2.90	121.02	111.91
19	B	842	PQN	C14-C13-C15	2.90	120.15	115.27
30	2	319	CHL	C1-O2A-CGA	2.90	124.06	116.44
18	A	819	CLA	C2C-C1C-NC	2.90	112.69	109.97
18	F	303	CLA	C2D-C1D-ND	2.90	112.24	110.10
18	A	810	CLA	C2C-C1C-NC	2.90	112.69	109.97
18	A	836	CLA	C2D-C1D-ND	2.90	112.24	110.10
18	4	305	CLA	C2D-C1D-ND	2.90	112.24	110.10
18	A	824	CLA	CMA-C3A-C4A	2.90	119.55	111.77
18	A	852	CLA	CMA-C3A-C4A	2.89	119.55	111.77
18	B	831	CLA	C1-C2-C3	-2.89	121.04	126.04
18	A	826	CLA	C2C-C1C-NC	2.89	112.68	109.97
18	3	309	CLA	C2D-C1D-ND	2.89	112.23	110.10
18	B	827	CLA	OBD-CAD-C3D	-2.89	121.56	128.52
18	B	829	CLA	CMA-C3A-C4A	2.89	119.53	111.77
18	1	5009	CLA	CMA-C3A-C4A	2.89	119.53	111.77
18	1	5017	CLA	CHD-C1D-ND	-2.89	121.80	124.45
18	A	827	CLA	CHD-C1D-ND	-2.88	121.80	124.45
30	2	315	CHL	C2C-C3C-C4C	2.88	108.54	106.49
21	3	305	BCR	C33-C5-C4	2.88	119.15	113.62
21	2	305	BCR	C27-C26-C25	-2.88	118.55	122.73
18	2	326	CLA	CHD-C1D-ND	-2.88	121.81	124.45
18	A	811	CLA	CMA-C3A-C4A	2.88	119.51	111.77
18	2	307	CLA	CMA-C3A-C4A	2.88	119.51	111.77
18	A	835	CLA	C2C-C1C-NC	2.88	112.67	109.97
18	A	812	CLA	C2C-C1C-NC	2.88	112.67	109.97
18	B	835	CLA	CMA-C3A-C4A	2.87	119.50	111.77
18	2	310	CLA	CBC-CAC-C3C	-2.87	104.51	112.43
21	A	844	BCR	C27-C26-C25	-2.87	118.56	122.73
18	1	5018	CLA	C2D-C1D-ND	2.87	112.22	110.10
31	4	304	XAT	C38-C25-C26	-2.87	117.44	122.26
21	A	845	BCR	C15-C14-C13	-2.87	123.21	127.31
18	3	315	CLA	C1-C2-C3	-2.87	121.08	126.04
18	A	823	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
18	3	308	CLA	CMA-C3A-C4A	2.87	119.49	111.77
21	4	301	BCR	C33-C5-C4	2.87	119.13	113.62
18	3	317	CLA	O2A-CGA-CBA	2.87	120.91	111.91
18	3	308	CLA	C2D-C1D-ND	2.87	112.22	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	307	CLA	C2D-C1D-ND	2.86	112.22	110.10
18	A	803	CLA	C2C-C1C-NC	2.86	112.66	109.97
18	1	5017	CLA	C2C-C1C-NC	2.86	112.66	109.97
18	B	833	CLA	CAA-CBA-CGA	-2.86	104.89	113.25
18	A	824	CLA	C2D-C1D-ND	2.86	112.21	110.10
18	K	1401	CLA	CMA-C3A-C4A	2.86	119.46	111.77
18	A	839	CLA	CMA-C3A-C4A	2.86	119.46	111.77
30	3	313	CHL	C2C-C3C-C4C	2.86	108.53	106.49
18	A	809	CLA	CMA-C3A-C4A	2.86	119.45	111.77
18	A	837	CLA	C2C-C1C-NC	2.86	112.65	109.97
21	A	844	BCR	C35-C13-C12	2.86	122.58	118.08
18	B	805	CLA	C2C-C1C-NC	2.86	112.65	109.97
18	B	839	CLA	C1-C2-C3	-2.86	121.11	126.04
18	L	306	CLA	C2D-C1D-ND	2.86	112.21	110.10
18	B	830	CLA	C1C-C2C-C3C	-2.85	103.95	106.96
18	4	305	CLA	C2C-C1C-NC	2.85	112.65	109.97
18	A	803	CLA	C2D-C1D-ND	2.85	112.21	110.10
18	2	308	CLA	O2A-CGA-CBA	2.85	120.86	111.91
18	1	5008	CLA	C2D-C1D-ND	2.85	112.21	110.10
18	B	807	CLA	C2C-C1C-NC	2.85	112.64	109.97
18	B	837	CLA	C2C-C1C-NC	2.85	112.64	109.97
30	1	5014	CHL	C3C-C4C-NC	-2.85	107.38	110.57
18	A	805	CLA	C2C-C1C-NC	2.85	112.64	109.97
21	A	847	BCR	C4-C5-C6	-2.85	118.60	122.73
18	A	806	CLA	CMA-C3A-C4A	2.85	119.42	111.77
18	A	836	CLA	C2C-C1C-NC	2.84	112.64	109.97
29	J	1105	LUT	C22-C23-C24	-2.84	108.50	111.74
18	A	833	CLA	C1-C2-C3	-2.84	121.13	126.04
21	3	306	BCR	C34-C9-C10	-2.84	118.95	122.92
18	1	5007	CLA	CHD-C1D-ND	-2.84	121.84	124.45
18	2	306	CLA	C1-C2-C3	-2.84	121.14	126.04
18	L	305	CLA	C2D-C1D-ND	2.84	112.19	110.10
26	2	327	DGD	C2G-O2G-C1B	-2.83	110.81	117.79
30	2	316	CHL	C4D-CHA-C1A	2.83	124.70	121.25
18	B	820	CLA	C2C-C1C-NC	2.83	112.63	109.97
18	G	1603	CLA	C1-C2-C3	-2.83	121.14	126.04
18	B	805	CLA	C1-C2-C3	-2.83	121.15	126.04
18	A	835	CLA	C2D-C1D-ND	2.83	112.19	110.10
18	B	834	CLA	C1-C2-C3	-2.83	121.15	126.04
18	A	809	CLA	C2D-C1D-ND	2.83	112.19	110.10
18	1	5006	CLA	C2C-C1C-NC	2.83	112.62	109.97
29	4	303	LUT	C31-C30-C29	-2.83	123.28	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	G	1604	BCR	C36-C18-C17	-2.83	118.96	122.92
18	L	304	CLA	CMA-C3A-C4A	2.83	119.37	111.77
21	G	1604	BCR	C23-C24-C25	-2.83	119.26	127.20
18	A	807	CLA	C2D-C1D-ND	2.83	112.19	110.10
18	B	810	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
21	B	844	BCR	C27-C26-C25	-2.82	118.64	122.73
18	2	311	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
18	B	831	CLA	CMA-C3A-C4A	2.82	119.35	111.77
18	B	801	CLA	OBD-CAD-C3D	-2.82	121.73	128.52
18	A	828	CLA	CMB-C2B-C3B	2.82	129.95	124.68
23	G	1606	LMT	C1'-O5'-C5'	-2.82	108.15	113.69
18	J	1101	CLA	C1C-C2C-C3C	-2.82	104.00	106.96
21	A	845	BCR	C38-C26-C27	2.81	119.02	113.62
18	B	809	CLA	O2D-CGD-O1D	-2.81	118.33	123.84
18	3	317	CLA	C2D-C1D-ND	2.81	112.18	110.10
21	3	306	BCR	C33-C5-C4	2.81	119.02	113.62
18	2	308	CLA	C2D-C1D-ND	2.81	112.18	110.10
17	A	801	CL0	CMC-C2C-C1C	2.81	129.32	125.04
18	3	307	CLA	CMA-C3A-C4A	2.81	119.33	111.77
18	A	838	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
18	2	312	CLA	CMB-C2B-C3B	2.81	129.94	124.68
18	A	831	CLA	C1-C2-C3	-2.81	121.18	126.04
18	1	5007	CLA	CMA-C3A-C4A	2.81	119.33	111.77
18	B	819	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
18	A	815	CLA	C2D-C1D-ND	2.81	112.17	110.10
31	4	304	XAT	O24-C25-C24	2.81	115.49	113.38
28	F	310	ZEX	C27-C28-C29	-2.81	121.99	126.23
18	F	301	CLA	C2C-C1C-NC	2.81	112.60	109.97
18	A	831	CLA	C2D-C1D-ND	2.81	112.17	110.10
18	4	309	CLA	C2D-C1D-ND	2.81	112.17	110.10
21	A	855	BCR	C27-C26-C25	-2.81	118.66	122.73
18	A	831	CLA	CMA-C3A-C4A	2.81	119.31	111.77
21	A	847	BCR	C3-C4-C5	-2.80	109.07	114.08
18	B	827	CLA	CMA-C3A-C4A	2.80	119.31	111.77
18	L	306	CLA	CMA-C3A-C4A	2.80	119.31	111.77
23	G	1605	LMT	C3'-C4'-C5'	-2.80	104.50	110.93
18	A	837	CLA	CMB-C2B-C3B	2.80	129.92	124.68
18	A	832	CLA	C2D-C1D-ND	2.80	112.17	110.10
18	A	806	CLA	C1-C2-C3	-2.80	121.20	126.04
18	B	834	CLA	CMD-C2D-C3D	-2.80	121.17	127.61
21	I	102	BCR	C36-C18-C17	-2.80	119.00	122.92
18	A	817	CLA	C1-C2-C3	-2.80	121.20	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	G	1601	CLA	C1C-C2C-C3C	-2.80	104.02	106.96
21	A	843	BCR	C23-C24-C25	-2.80	119.35	127.20
24	F	306	LMG	O8-C28-C29	2.80	120.68	111.91
18	A	804	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
18	B	814	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
18	A	852	CLA	OBD-CAD-C3D	-2.79	121.80	128.52
21	A	843	BCR	C35-C13-C12	2.79	122.48	118.08
21	F	305	BCR	C15-C14-C13	-2.79	123.33	127.31
18	B	818	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
30	4	316	CHL	CMA-C3A-C4A	2.79	119.27	111.77
18	A	802	CLA	C2C-C1C-NC	2.79	112.59	109.97
18	1	5009	CLA	C2C-C1C-NC	2.79	112.59	109.97
21	4	301	BCR	C24-C25-C26	-2.79	114.70	121.46
30	4	302	CHL	C1-O2A-CGA	2.79	123.76	116.44
18	B	837	CLA	C2D-C1D-ND	2.79	112.16	110.10
18	K	1404	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
18	4	305	CLA	C1-C2-C3	-2.79	121.22	126.04
18	B	834	CLA	CMB-C2B-C3B	2.79	129.89	124.68
18	A	809	CLA	C2C-C1C-NC	2.79	112.58	109.97
18	3	317	CLA	C2C-C1C-NC	2.79	112.58	109.97
18	B	822	CLA	C1-C2-C3	-2.79	121.22	126.04
18	J	1101	CLA	C1-C2-C3	-2.79	121.22	126.04
18	A	837	CLA	CMA-C3A-C4A	2.78	119.26	111.77
21	B	843	BCR	C36-C18-C19	-2.78	113.69	118.08
18	A	804	CLA	CMA-C3A-C4A	2.78	119.25	111.77
18	K	1403	CLA	CMD-C2D-C3D	-2.78	121.21	127.61
29	3	304	LUT	C10-C11-C12	-2.78	114.53	123.22
21	I	101	BCR	C1-C6-C5	-2.78	118.69	122.61
18	B	841	CLA	C1-C2-C3	-2.78	121.23	126.04
18	4	315	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
18	B	833	CLA	C2D-C1D-ND	2.78	112.15	110.10
18	B	801	CLA	C2D-C1D-ND	2.78	112.15	110.10
18	B	801	CLA	C2D-C1D-ND	2.78	112.15	110.10
18	3	314	CLA	C2D-C1D-ND	2.78	112.15	110.10
18	B	805	CLA	CMB-C2B-C3B	2.78	129.87	124.68
18	B	815	CLA	CMB-C2B-C3B	2.78	129.87	124.68
18	3	319	CLA	CMA-C3A-C4A	2.78	119.23	111.77
18	G	1603	CLA	C2D-C1D-ND	2.77	112.15	110.10
30	1	5014	CHL	C2C-C3C-C4C	2.77	108.47	106.49
18	2	311	CLA	C2D-C1D-ND	2.77	112.15	110.10
18	3	307	CLA	C2C-C1C-NC	2.77	112.57	109.97
18	B	819	CLA	C2D-C1D-ND	2.77	112.15	110.10
26	B	855	DGD	O1G-C1A-C2A	2.77	120.61	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	816	CLA	C2D-C1D-ND	2.77	112.14	110.10
18	2	307	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
18	A	835	CLA	C1-C2-C3	-2.77	121.26	126.04
18	B	826	CLA	C2D-C1D-ND	2.77	112.14	110.10
18	3	301	CLA	CMA-C3A-C4A	2.77	119.21	111.77
21	K	1405	BCR	C33-C5-C6	-2.77	121.42	124.53
18	A	814	CLA	C2D-C1D-ND	2.76	112.14	110.10
18	B	817	CLA	C2D-C1D-ND	2.76	112.14	110.10
21	A	844	BCR	C28-C27-C26	-2.76	109.14	114.08
24	A	851	LMG	O8-C28-C29	2.76	120.58	111.91
18	2	313	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
18	3	301	CLA	C2D-C1D-ND	2.76	112.14	110.10
18	2	317	CLA	C1C-C2C-C3C	-2.76	104.06	106.96
30	2	319	CHL	C2C-C3C-C4C	2.76	108.45	106.49
18	L	304	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
18	A	823	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
18	B	840	CLA	CMA-C3A-C4A	2.75	119.17	111.77
21	A	844	BCR	C12-C13-C14	-2.75	114.72	118.94
18	B	804	CLA	C2D-C1D-ND	2.75	112.13	110.10
18	B	810	CLA	C2D-C1D-ND	2.75	112.13	110.10
18	A	802	CLA	CMB-C2B-C3B	2.75	129.82	124.68
24	F	307	LMG	O8-C28-C29	2.75	120.54	111.91
18	L	301	CLA	C2C-C1C-NC	2.75	112.55	109.97
18	B	822	CLA	C2D-C1D-ND	2.75	112.13	110.10
18	1	5012	CLA	C2D-C1D-ND	2.75	112.13	110.10
18	B	829	CLA	CMB-C2B-C3B	2.74	129.81	124.68
30	4	318	CHL	C4D-CHA-C1A	2.74	124.59	121.25
18	4	307	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
21	1	5005	BCR	C33-C5-C4	2.74	118.88	113.62
18	B	821	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
18	A	813	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
18	L	304	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
18	B	840	CLA	C2D-C1D-ND	2.74	112.12	110.10
18	B	835	CLA	C2D-C1D-ND	2.74	112.12	110.10
18	B	827	CLA	CHD-C1D-ND	-2.74	121.94	124.45
18	2	308	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
30	2	316	CHL	C3C-C4C-NC	-2.73	107.51	110.57
24	B	851	LMG	C1-C2-C3	2.73	115.69	110.00
21	B	802	BCR	C23-C24-C25	-2.73	119.53	127.20
18	J	1103	CLA	C2D-C1D-ND	2.73	112.12	110.10
21	A	845	BCR	C36-C18-C17	-2.73	119.10	122.92
21	B	845	BCR	C35-C13-C12	2.73	122.38	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	5002	DGD	O1G-C1A-C2A	2.73	120.48	111.91
18	4	306	CLA	C2D-C1D-ND	2.73	112.12	110.10
18	B	823	CLA	C1-C2-C3	-2.73	121.32	126.04
18	B	812	CLA	C2D-C1D-ND	2.73	112.11	110.10
18	F	301	CLA	CMB-C2B-C3B	2.73	129.78	124.68
18	A	829	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
18	B	823	CLA	CMA-C3A-C4A	2.73	119.10	111.77
18	B	818	CLA	CMA-C3A-C4A	2.72	119.10	111.77
18	B	808	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
18	B	836	CLA	C2D-C1D-ND	2.72	112.11	110.10
29	1	5003	LUT	C8-C7-C6	-2.72	119.56	127.20
18	J	1103	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
18	4	307	CLA	C2D-C1D-ND	2.72	112.11	110.10
18	A	823	CLA	C2D-C1D-ND	2.72	112.11	110.10
18	L	301	CLA	C2D-C1D-ND	2.72	112.11	110.10
21	B	846	BCR	C38-C26-C25	-2.72	121.48	124.53
18	A	816	CLA	CMA-C3A-C4A	2.72	119.07	111.77
18	B	836	CLA	O2A-CGA-CBA	2.72	120.43	111.91
18	F	301	CLA	O2A-CGA-CBA	2.72	120.43	111.91
18	A	818	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
21	F	304	BCR	C4-C5-C6	-2.71	118.79	122.73
18	B	811	CLA	C1-C2-C3	-2.71	121.35	126.04
18	A	834	CLA	C2D-C1D-ND	2.71	112.10	110.10
18	A	814	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
18	A	834	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
18	B	813	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
18	B	824	CLA	CMA-C3A-C4A	2.71	119.06	111.77
18	B	827	CLA	C2D-C1D-ND	2.71	112.10	110.10
18	G	1601	CLA	C2D-C1D-ND	2.71	112.10	110.10
18	1	5008	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
18	A	807	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
21	K	1405	BCR	C36-C18-C17	-2.71	119.13	122.92
18	L	301	CLA	CMB-C2B-C3B	2.71	129.75	124.68
18	A	826	CLA	CMA-C3A-C4A	2.71	119.05	111.77
18	4	305	CLA	CMA-C3A-C4A	2.71	119.05	111.77
18	4	308	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
18	A	815	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
18	A	821	CLA	C2D-C1D-ND	2.70	112.10	110.10
18	L	305	CLA	C2C-C1C-NC	2.70	112.50	109.97
18	B	830	CLA	CMA-C3A-C4A	2.70	119.03	111.77
18	3	319	CLA	C2D-C1D-ND	2.70	112.09	110.10
21	B	845	BCR	C33-C5-C4	2.70	118.80	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	L	302	BCR	C4-C5-C6	-2.70	118.81	122.73
30	3	316	CHL	C4D-CHA-C1A	2.70	124.53	121.25
18	A	818	CLA	CMA-C3A-C4A	2.70	119.02	111.77
18	B	807	CLA	C2D-C1D-ND	2.70	112.09	110.10
23	4	319	LMT	C1'-O5'-C5'	-2.69	108.40	113.69
18	4	308	CLA	O2A-CGA-CBA	2.69	120.36	111.91
18	2	307	CLA	C6-C5-C3	-2.69	110.22	114.62
21	B	846	BCR	C35-C13-C12	2.69	122.32	118.08
18	B	809	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
18	A	812	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
18	B	822	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
18	A	835	CLA	O2A-CGA-CBA	2.69	120.35	111.91
18	1	5015	CLA	C2D-C1D-ND	2.69	112.08	110.10
18	2	313	CLA	C2D-C1D-ND	2.69	112.08	110.10
18	J	1101	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
18	1	5017	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
18	A	815	CLA	CMA-C3A-C4A	2.68	118.99	111.77
18	A	822	CLA	C2D-C1D-ND	2.68	112.08	110.10
18	F	302	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
30	1	5016	CHL	C1B-CHB-C4A	-2.68	124.81	130.12
18	A	813	CLA	C2D-C1D-ND	2.68	112.08	110.10
18	B	834	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
18	B	809	CLA	CMA-C3A-C4A	2.68	118.97	111.77
21	2	305	BCR	C38-C26-C27	2.68	118.76	113.62
18	J	1101	CLA	C2D-C1D-ND	2.68	112.08	110.10
18	3	308	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
30	2	315	CHL	C1-O2A-CGA	2.68	123.47	116.44
18	B	823	CLA	C2D-C1D-ND	2.68	112.08	110.10
18	2	317	CLA	C1-C2-C3	-2.68	121.42	126.04
18	4	308	CLA	C1C-C2C-C3C	-2.67	104.14	106.96
18	A	804	CLA	C2D-C1D-ND	2.67	112.08	110.10
18	B	825	CLA	C1C-C2C-C3C	-2.67	104.14	106.96
18	B	837	CLA	O2A-CGA-CBA	2.67	120.30	111.91
18	B	803	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
18	A	806	CLA	C2D-C1D-ND	2.67	112.07	110.10
18	1	5015	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
21	B	802	BCR	C33-C5-C4	2.67	118.75	113.62
24	B	850	LMG	C8-O7-C10	-2.67	111.22	117.79
18	4	308	CLA	C2D-C1D-ND	2.67	112.07	110.10
18	4	309	CLA	CMA-C3A-C4A	2.67	118.94	111.77
29	3	303	LUT	C31-C30-C29	-2.67	123.50	127.31
18	G	1603	CLA	C1C-C2C-C3C	-2.67	104.15	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	5013	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
21	L	303	BCR	C33-C5-C4	2.67	118.74	113.62
21	I	101	BCR	C35-C13-C14	-2.67	119.19	122.92
18	B	839	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
21	A	845	BCR	C33-C5-C4	2.67	118.74	113.62
18	B	803	CLA	CHD-C1D-ND	-2.67	122.00	124.45
18	A	852	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
18	B	825	CLA	CMB-C2B-C3B	2.67	129.66	124.68
18	B	835	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
22	1	5019	LHG	C5-O7-C7	-2.66	111.23	117.79
18	A	836	CLA	CMA-C3A-C4A	2.66	118.93	111.77
21	J	1104	BCR	C33-C5-C4	2.66	118.73	113.62
18	B	828	CLA	O2A-CGA-CBA	2.66	120.26	111.91
21	A	855	BCR	C37-C22-C21	-2.66	119.19	122.92
18	1	5012	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
18	2	310	CLA	CMB-C2B-C3B	2.66	129.66	124.68
19	A	841	PQN	C11-C12-C13	-2.66	122.36	126.79
18	1	5010	CLA	CMA-C3A-C4A	2.66	118.92	111.77
18	B	838	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
28	F	310	ZEX	C15-C35-C34	-2.66	118.03	123.47
18	A	831	CLA	C2C-C1C-NC	2.66	112.46	109.97
18	A	833	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
18	B	831	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
29	1	5003	LUT	C31-C30-C29	-2.66	123.52	127.31
18	A	810	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
18	2	312	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
18	G	1602	CLA	CMB-C2B-C3B	2.66	129.65	124.68
18	A	810	CLA	C2D-C1D-ND	2.66	112.06	110.10
18	A	829	CLA	CMD-C2D-C3D	-2.66	121.51	127.61
18	4	310	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
18	B	829	CLA	C2D-C1D-ND	2.65	112.06	110.10
18	G	1602	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
18	A	832	CLA	C2C-C1C-NC	2.65	112.46	109.97
18	A	808	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
18	4	312	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
18	1	5013	CLA	CMA-C3A-C4A	2.65	118.89	111.77
18	A	830	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
18	K	1402	CLA	O2A-CGA-CBA	2.65	120.22	111.91
21	G	1604	BCR	C28-C27-C26	-2.65	109.35	114.08
18	B	841	CLA	C2C-C1C-NC	2.65	112.45	109.97
18	A	817	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
18	1	5011	CLA	C1C-C2C-C3C	-2.65	104.17	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	821	CLA	CMA-C3A-C4A	2.65	118.89	111.77
18	F	302	CLA	C2D-C1D-ND	2.65	112.05	110.10
18	4	312	CLA	CMA-C3A-C4A	2.65	118.88	111.77
18	B	830	CLA	CHA-C4D-ND	2.64	138.03	132.50
18	K	1402	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
18	B	806	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
18	A	819	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
18	B	814	CLA	O2A-CGA-CBA	2.64	120.20	111.91
23	B	856	LMT	C1'-O5'-C5'	-2.64	108.50	113.69
18	3	314	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
18	A	840	CLA	C2D-C1D-ND	2.64	112.05	110.10
18	3	315	CLA	C2D-C1D-ND	2.64	112.05	110.10
18	2	306	CLA	CMA-C3A-C4A	2.64	118.87	111.77
22	B	849	LHG	O8-C23-C24	2.64	120.19	111.91
18	2	326	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
21	F	305	BCR	C38-C26-C27	2.64	118.69	113.62
18	A	840	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
30	4	316	CHL	C3C-C4C-NC	-2.64	107.61	110.57
18	B	808	CLA	C2D-C1D-ND	2.64	112.05	110.10
18	A	802	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
18	A	827	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
18	2	310	CLA	C1-O2A-CGA	2.64	123.36	116.44
18	A	828	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
18	2	309	CLA	C1C-C2C-C3C	-2.64	104.19	106.96
24	1	5020	LMG	O8-C28-C29	2.63	120.17	111.91
18	3	315	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
18	B	815	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
18	2	312	CLA	C2D-C1D-ND	2.63	112.04	110.10
18	3	317	CLA	CMA-C3A-C4A	2.63	118.85	111.77
30	1	5016	CHL	CMA-C3A-C4A	2.63	118.85	111.77
18	B	823	CLA	C1-O2A-CGA	2.63	123.35	116.44
18	1	5007	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
18	B	833	CLA	CMA-C3A-C4A	2.63	118.84	111.77
21	L	302	BCR	C32-C1-C6	-2.63	106.03	110.30
18	A	803	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
18	1	5017	CLA	CHA-C4D-ND	2.63	138.00	132.50
18	A	811	CLA	C2D-C1D-ND	2.63	112.04	110.10
18	A	840	CLA	O2A-CGA-CBA	2.63	120.15	111.91
18	H	1701	CLA	C1C-C2C-C3C	-2.63	104.20	106.96
18	1	5006	CLA	CMA-C3A-C4A	2.62	118.83	111.77
18	B	827	CLA	CHA-C4D-ND	2.62	137.99	132.50
29	1	5004	LUT	C31-C30-C29	-2.62	123.57	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	J	1105	LUT	C1-C6-C5	-2.62	118.92	122.61
18	B	806	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
21	L	302	BCR	C34-C9-C10	-2.62	119.25	122.92
21	I	101	BCR	C23-C24-C25	-2.62	119.84	127.20
30	2	316	CHL	C1B-CHB-C4A	-2.62	124.93	130.12
18	K	1401	CLA	CMB-C2B-C3B	2.62	129.58	124.68
17	A	801	CL0	C4-C3-C5	2.62	119.68	115.27
18	B	816	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
18	3	301	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
21	F	304	BCR	C34-C9-C10	-2.62	119.26	122.92
18	A	839	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
18	A	832	CLA	C1-O2A-CGA	2.62	123.31	116.44
21	2	305	BCR	C34-C9-C10	-2.62	119.26	122.92
18	B	829	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
24	2	322	LMG	O8-C28-C29	2.62	120.12	111.91
21	K	1405	BCR	C4-C5-C6	-2.62	118.93	122.73
18	B	833	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
18	A	821	CLA	C1C-C2C-C3C	-2.62	104.21	106.96
18	B	830	CLA	O2A-CGA-CBA	2.61	120.11	111.91
18	A	834	CLA	CMB-C2B-C3B	2.61	129.57	124.68
18	A	833	CLA	C2D-C1D-ND	2.61	112.03	110.10
18	A	832	CLA	C1-C2-C3	-2.61	121.52	126.04
18	F	303	CLA	CMA-C3A-C4A	2.61	118.79	111.77
18	A	805	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
18	A	828	CLA	CMA-C3A-C4A	2.61	118.79	111.77
18	2	306	CLA	C2C-C1C-NC	2.61	112.42	109.97
26	2	327	DGD	O1G-C1A-C2A	2.61	120.10	111.91
18	B	832	CLA	C2D-C1D-ND	2.61	112.03	110.10
18	B	827	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
18	A	853	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
18	B	828	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
18	A	816	CLA	C2C-C1C-NC	2.61	112.42	109.97
18	G	1601	CLA	CMA-C3A-C4A	2.61	118.78	111.77
18	4	306	CLA	CMA-C3A-C4A	2.61	118.78	111.77
18	3	319	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
18	B	837	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
18	B	826	CLA	C2C-C1C-NC	2.60	112.41	109.97
18	B	825	CLA	CHA-C4D-ND	2.60	137.95	132.50
21	A	855	BCR	C33-C5-C4	2.60	118.62	113.62
18	A	820	CLA	CMD-C2D-C3D	-2.60	121.63	127.61
18	B	812	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
18	G	1603	CLA	O2D-CGD-O1D	-2.60	118.75	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	817	CLA	CMA-C3A-C4A	2.60	118.76	111.77
30	2	319	CHL	C4D-CHA-C1A	2.60	124.41	121.25
18	3	311	CLA	CMA-C3A-C4A	2.60	118.76	111.77
18	B	821	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
21	3	306	BCR	C8-C9-C10	2.60	122.93	118.94
18	B	819	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
18	B	836	CLA	C1C-C2C-C3C	-2.60	104.23	106.96
18	1	5010	CLA	C2D-C1D-ND	2.60	112.02	110.10
18	B	813	CLA	C1C-C2C-C3C	-2.60	104.23	106.96
18	A	820	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
18	1	5018	CLA	C1-C2-C3	-2.59	121.56	126.04
29	J	1105	LUT	C11-C10-C9	-2.59	123.61	127.31
18	K	1404	CLA	C2D-C1D-ND	2.59	112.01	110.10
18	B	804	CLA	C2C-C1C-NC	2.59	112.40	109.97
18	A	806	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
18	A	835	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
18	A	805	CLA	CMB-C2B-C3B	2.59	129.53	124.68
18	3	315	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
30	1	5016	CHL	C1-O2A-CGA	2.59	123.24	116.44
21	A	847	BCR	C34-C9-C10	-2.59	119.30	122.92
18	3	309	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
18	B	815	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
18	B	840	CLA	C1-C2-C3	-2.59	121.57	126.04
18	1	5009	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
18	B	820	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
18	K	1402	CLA	C2D-C1D-ND	2.59	112.01	110.10
18	H	1701	CLA	C2D-C1D-ND	2.58	112.01	110.10
18	A	824	CLA	CHD-C1D-ND	-2.58	122.08	124.45
18	B	807	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
24	A	851	LMG	C8-O7-C10	-2.58	111.43	117.79
18	B	805	CLA	C2D-C1D-ND	2.58	112.01	110.10
21	K	1405	BCR	C27-C26-C25	-2.58	118.98	122.73
18	B	805	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
18	1	5009	CLA	O2A-CGA-CBA	2.58	120.01	111.91
30	4	316	CHL	C1B-CHB-C4A	-2.58	125.01	130.12
18	2	309	CLA	CMD-C2D-C3D	-2.58	121.68	127.61
21	L	303	BCR	C23-C22-C21	2.58	122.90	118.94
30	3	313	CHL	C1B-CHB-C4A	-2.58	125.01	130.12
18	B	826	CLA	CMB-C2B-C3B	2.58	129.50	124.68
22	2	320	LHG	O8-C23-C24	2.58	120.00	111.91
18	B	813	CLA	CMB-C2B-C3B	2.58	129.50	124.68
18	A	817	CLA	C2D-C1D-ND	2.58	112.00	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	5018	CLA	O2A-CGA-CBA	2.58	120.00	111.91
18	B	831	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
18	3	311	CLA	CHA-C4D-ND	2.58	137.89	132.50
18	A	829	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
18	A	820	CLA	C2D-C1D-ND	2.58	112.00	110.10
18	1	5013	CLA	C2D-C1D-ND	2.58	112.00	110.10
18	B	837	CLA	O2D-CGD-O1D	-2.57	118.80	123.84
18	B	812	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
29	4	303	LUT	C35-C15-C14	-2.57	118.20	123.47
18	A	853	CLA	O2A-CGA-CBA	2.57	119.98	111.91
30	2	315	CHL	C1B-CHB-C4A	-2.57	125.02	130.12
18	B	816	CLA	CMB-C2B-C3B	2.57	129.49	124.68
18	B	823	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
18	B	825	CLA	C2D-C1D-ND	2.57	112.00	110.10
18	A	825	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
18	A	828	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
21	L	303	BCR	C38-C26-C25	-2.57	121.64	124.53
18	A	807	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
18	A	806	CLA	O2A-CGA-CBA	2.57	119.97	111.91
21	B	843	BCR	C33-C5-C4	2.57	118.55	113.62
18	A	804	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
18	F	302	CLA	O2A-CGA-CBA	2.57	119.96	111.91
18	F	303	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
18	A	809	CLA	C1D-ND-C4D	-2.57	104.51	106.33
18	A	803	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
21	F	304	BCR	C33-C5-C4	2.56	118.54	113.62
18	B	841	CLA	CMB-C2B-C3B	2.56	129.47	124.68
18	A	826	CLA	C2D-C1D-ND	2.56	111.99	110.10
21	4	301	BCR	C28-C27-C26	-2.56	109.50	114.08
18	B	828	CLA	CMA-C3A-C4A	2.56	118.66	111.77
18	A	837	CLA	C2D-C1D-ND	2.56	111.99	110.10
18	A	853	CLA	C2D-C1D-ND	2.56	111.99	110.10
18	2	326	CLA	C2D-C1D-ND	2.56	111.99	110.10
18	2	312	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
18	B	840	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
30	3	310	CHL	C1B-CHB-C4A	-2.56	125.05	130.12
18	3	309	CLA	OBD-CAD-C3D	-2.56	122.36	128.52
30	1	5016	CHL	CHD-C4C-C3C	2.56	128.60	124.84
18	A	839	CLA	C1-C2-C3	-2.56	121.62	126.04
18	B	839	CLA	C2D-C1D-ND	2.56	111.99	110.10
18	4	306	CLA	O2A-CGA-CBA	2.56	119.93	111.91
30	2	314	CHL	C1-O2A-CGA	2.56	123.15	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	I	102	BCR	C34-C9-C10	-2.56	119.34	122.92
18	B	811	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
30	3	312	CHL	C1B-CHB-C4A	-2.56	125.06	130.12
18	4	306	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
18	B	803	CLA	O2A-CGA-CBA	2.56	119.93	111.91
18	1	5009	CLA	CMD-C2D-C3D	-2.55	121.74	127.61
21	B	847	BCR	C37-C22-C23	2.55	122.10	118.08
18	2	312	CLA	C1-C2-C3	-2.55	121.62	126.04
18	A	831	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
18	B	810	CLA	O2A-CGA-CBA	2.55	119.92	111.91
18	A	852	CLA	C1-C2-C3	-2.55	121.63	126.04
18	G	1602	CLA	C2D-C1D-ND	2.55	111.99	110.10
18	4	312	CLA	C2D-C1D-ND	2.55	111.99	110.10
18	2	310	CLA	C1D-ND-C4D	-2.55	104.52	106.33
18	A	822	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
18	3	311	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
18	A	805	CLA	C2D-C1D-ND	2.55	111.98	110.10
18	L	304	CLA	C2D-C1D-ND	2.55	111.98	110.10
21	3	305	BCR	C36-C18-C17	-2.55	119.35	122.92
21	F	304	BCR	C3-C4-C5	-2.55	109.52	114.08
18	B	801	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
18	B	824	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
18	2	309	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
26	2	327	DGD	C3G-O3G-C1D	-2.55	108.76	113.74
18	B	827	CLA	O2A-CGA-CBA	2.55	119.91	111.91
18	B	835	CLA	O2A-CGA-CBA	2.55	119.91	111.91
21	2	305	BCR	C32-C1-C6	-2.55	106.16	110.30
18	B	813	CLA	C2D-C1D-ND	2.55	111.98	110.10
18	2	307	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
18	G	1601	CLA	CMB-C2B-C3B	2.55	129.44	124.68
18	B	826	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
18	B	817	CLA	C2C-C1C-NC	2.55	112.36	109.97
18	A	808	CLA	CMB-C2B-C3B	2.55	129.44	124.68
18	B	814	CLA	C2D-C1D-ND	2.55	111.98	110.10
21	A	846	BCR	C38-C26-C27	2.55	118.51	113.62
18	A	802	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
18	1	5009	CLA	C2D-C1D-ND	2.54	111.98	110.10
22	1	5019	LHG	O8-C23-C24	2.54	119.89	111.91
18	A	839	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
18	B	833	CLA	O1D-CGD-CBD	-2.54	119.28	124.48
18	1	5018	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
18	A	819	CLA	CMB-C2B-C3B	2.54	129.43	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	834	CLA	CHA-C4D-ND	2.54	137.81	132.50
18	4	310	CLA	C2D-C1D-ND	2.54	111.98	110.10
18	A	816	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
18	B	828	CLA	O1D-CGD-CBD	-2.54	119.29	124.48
18	3	307	CLA	CMD-C2D-C3D	-2.54	121.77	127.61
18	B	804	CLA	C1-C2-C3	-2.54	121.65	126.04
18	A	813	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
18	A	818	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
21	K	1405	BCR	C23-C24-C25	-2.54	120.08	127.20
18	B	831	CLA	C2D-C1D-ND	2.54	111.97	110.10
18	A	808	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
18	A	812	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
18	B	828	CLA	CMD-C2D-C3D	-2.53	121.78	127.61
18	1	5011	CLA	O2A-CGA-CBA	2.53	119.86	111.91
18	A	825	CLA	CHA-C4D-ND	2.53	137.80	132.50
18	L	305	CLA	C1C-C2C-C3C	-2.53	104.29	106.96
18	A	830	CLA	C2D-C1D-ND	2.53	111.97	110.10
18	A	811	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
18	B	809	CLA	O2A-CGA-CBA	2.53	119.85	111.91
29	2	303	LUT	C30-C31-C32	-2.53	115.32	123.22
21	A	846	BCR	C19-C18-C17	2.53	122.82	118.94
18	4	309	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
21	G	1604	BCR	C19-C18-C17	2.53	122.82	118.94
18	B	836	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
30	3	312	CHL	C4D-CHA-C1A	2.53	124.33	121.25
18	A	827	CLA	C2D-C1D-ND	2.53	111.97	110.10
18	K	1403	CLA	CHA-C4D-ND	2.53	137.78	132.50
18	B	804	CLA	O2A-CGA-CBA	2.53	119.83	111.91
21	3	306	BCR	C37-C22-C21	-2.53	119.39	122.92
18	A	832	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
18	A	852	CLA	C2D-C1D-ND	2.53	111.97	110.10
21	F	304	BCR	C31-C1-C6	-2.53	106.20	110.30
18	K	1401	CLA	C1C-C2C-C3C	-2.52	104.30	106.96
18	3	309	CLA	O2A-CGA-CBA	2.52	119.83	111.91
30	2	319	CHL	C1B-CHB-C4A	-2.52	125.12	130.12
18	2	326	CLA	CHA-C4D-ND	2.52	137.78	132.50
18	A	830	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
18	A	808	CLA	C2D-C1D-ND	2.52	111.96	110.10
18	B	814	CLA	O1D-CGD-CBD	-2.52	119.33	124.48
18	K	1403	CLA	C2D-C1D-ND	2.52	111.96	110.10
18	1	5006	CLA	CAA-C2A-C3A	-2.52	105.89	112.78
18	A	835	CLA	O2D-CGD-O1D	-2.52	118.92	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	309	CLA	CHA-C4D-ND	2.52	137.76	132.50
18	A	808	CLA	C1-C2-C3	-2.52	121.69	126.04
18	4	311	CLA	C1C-C2C-C3C	-2.51	104.31	106.96
22	A	848	LHG	O8-C23-C24	2.51	119.79	111.91
18	4	306	CLA	CHA-C4D-ND	2.51	137.75	132.50
31	2	304	XAT	C38-C25-C26	-2.51	118.05	122.26
24	B	851	LMG	O8-C28-C29	2.51	119.79	111.91
18	B	808	CLA	CMA-C3A-C4A	2.51	118.52	111.77
18	A	829	CLA	CHA-C4D-ND	2.51	137.75	132.50
21	J	1104	BCR	C27-C26-C25	-2.51	119.09	122.73
18	B	828	CLA	CHA-C4D-ND	2.51	137.75	132.50
18	L	306	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
18	A	838	CLA	CMB-C2B-C3B	2.51	129.37	124.68
18	2	310	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
18	B	824	CLA	C2D-C1D-ND	2.51	111.95	110.10
18	3	309	CLA	CHA-C4D-ND	2.51	137.74	132.50
18	B	829	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
18	A	821	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
18	B	838	CLA	CMA-C3A-C4A	2.50	118.50	111.77
18	A	826	CLA	C1C-C2C-C3C	-2.50	104.32	106.96
18	1	5015	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
18	3	301	CLA	CMB-C2B-C3B	2.50	129.36	124.68
18	A	819	CLA	C2D-C1D-ND	2.50	111.95	110.10
18	A	835	CLA	C1D-ND-C4D	-2.50	104.56	106.33
21	A	843	BCR	C12-C13-C14	-2.50	115.10	118.94
18	B	811	CLA	CHA-C4D-ND	2.50	137.73	132.50
18	2	307	CLA	CHA-C4D-ND	2.50	137.73	132.50
18	A	809	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
18	1	5010	CLA	CMB-C2B-C3B	2.50	129.35	124.68
21	L	307	BCR	C33-C5-C4	2.50	118.42	113.62
18	B	811	CLA	CMA-C3A-C4A	2.50	118.49	111.77
18	A	837	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
18	A	824	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
30	2	314	CHL	CHB-C4A-NA	2.50	127.97	124.51
21	J	1104	BCR	C23-C24-C25	-2.50	120.19	127.20
18	B	837	CLA	CMA-C3A-C4A	2.50	118.49	111.77
30	2	315	CHL	C4D-CHA-C1A	2.50	124.29	121.25
18	B	818	CLA	C2D-C1D-ND	2.50	111.94	110.10
18	2	313	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
18	A	820	CLA	CHA-C4D-ND	2.49	137.72	132.50
18	4	305	CLA	C1C-C2C-C3C	-2.49	104.33	106.96
18	B	822	CLA	O2D-CGD-O1D	-2.49	118.97	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	821	CLA	CHA-C4D-ND	2.49	137.71	132.50
18	1	5006	CLA	C2D-C1D-ND	2.49	111.94	110.10
29	2	303	LUT	C35-C34-C33	-2.49	123.75	127.31
18	A	805	CLA	CMD-C2D-C3D	-2.49	121.88	127.61
18	3	311	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
18	L	305	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
18	B	803	CLA	CHA-C4D-ND	2.49	137.71	132.50
21	2	305	BCR	C35-C13-C12	2.49	122.00	118.08
18	A	834	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
18	F	301	CLA	C1D-ND-C4D	-2.49	104.57	106.33
21	I	101	BCR	C4-C5-C6	-2.49	119.12	122.73
18	A	834	CLA	O2A-CGA-CBA	2.48	119.71	111.91
18	B	820	CLA	C2D-C1D-ND	2.48	111.94	110.10
24	F	306	LMG	C8-O7-C10	-2.48	111.67	117.79
18	A	823	CLA	CHA-C4D-ND	2.48	137.69	132.50
18	A	817	CLA	CMB-C2B-C3B	2.48	129.32	124.68
18	B	805	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
18	A	810	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
18	A	836	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
21	A	846	BCR	C27-C26-C25	-2.48	119.13	122.73
18	A	817	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
18	B	811	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
19	A	841	PQN	C2M-C2-C3	-2.48	120.35	124.40
18	F	303	CLA	C1D-ND-C4D	-2.48	104.57	106.33
18	B	816	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
18	3	307	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
18	B	839	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
18	B	821	CLA	C2D-C1D-ND	2.48	111.93	110.10
18	A	853	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
18	B	801	CLA	CHA-C4D-ND	2.48	137.69	132.50
18	F	302	CLA	CMA-C3A-C4A	2.48	118.44	111.77
18	A	818	CLA	C2D-C1D-ND	2.48	111.93	110.10
18	B	831	CLA	CHA-C4D-ND	2.48	137.68	132.50
18	1	5011	CLA	C2D-C1D-ND	2.48	111.93	110.10
18	A	834	CLA	CMA-C3A-C4A	2.48	118.43	111.77
18	3	318	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
30	3	313	CHL	C1-O2A-CGA	2.47	122.94	116.44
18	A	812	CLA	C1D-ND-C4D	-2.47	104.58	106.33
18	B	809	CLA	C1-C2-C3	-2.47	121.76	126.04
18	A	825	CLA	CMB-C2B-C3B	2.47	129.31	124.68
18	2	317	CLA	O2A-CGA-CBA	2.47	119.67	111.91
18	A	829	CLA	C2D-C1D-ND	2.47	111.93	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	819	CLA	CHA-C4D-ND	2.47	137.67	132.50
21	A	843	BCR	C33-C5-C4	2.47	118.37	113.62
18	A	852	CLA	CHA-C4D-ND	2.47	137.67	132.50
30	2	318	CHL	C4D-CHA-C1A	2.47	124.26	121.25
18	3	308	CLA	CHA-C4D-ND	2.47	137.67	132.50
18	1	5011	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
18	B	826	CLA	CHA-C4D-ND	2.47	137.67	132.50
30	4	318	CHL	C1B-CHB-C4A	-2.47	125.22	130.12
31	4	304	XAT	C40-C33-C34	-2.47	119.46	122.92
18	2	309	CLA	C2D-C1D-ND	2.47	111.92	110.10
18	B	811	CLA	CMD-C2D-C3D	-2.47	121.93	127.61
23	2	325	LMT	C2'-C3'-C4'	2.47	115.32	109.68
21	L	307	BCR	C8-C7-C6	-2.47	120.27	127.20
18	1	5017	CLA	CMD-C2D-C3D	-2.47	121.94	127.61
18	A	807	CLA	CMA-C3A-C4A	2.47	118.40	111.77
21	4	301	BCR	C37-C22-C23	2.47	121.96	118.08
18	B	803	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
18	G	1602	CLA	CHA-C4D-ND	2.46	137.66	132.50
21	3	306	BCR	C30-C25-C24	2.46	122.75	115.78
18	3	307	CLA	C2D-C1D-ND	2.46	111.92	110.10
18	3	311	CLA	C2D-C1D-ND	2.46	111.92	110.10
30	1	5016	CHL	C1-C2-C3	-2.46	121.78	126.04
30	2	318	CHL	C3C-C4C-NC	-2.46	107.81	110.57
18	1	5011	CLA	CHA-C4D-ND	2.46	137.65	132.50
17	A	801	CL0	O2D-CGD-O1D	-2.46	119.02	123.84
18	1	5006	CLA	CMD-C2D-C3D	-2.46	121.95	127.61
18	1	5009	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
18	J	1103	CLA	CHA-C4D-ND	2.46	137.65	132.50
18	A	807	CLA	CMB-C2B-C3B	2.46	129.28	124.68
18	A	824	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
18	2	309	CLA	CHA-C4D-ND	2.46	137.65	132.50
18	3	311	CLA	CMB-C2B-C3B	2.46	129.28	124.68
18	1	5012	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
21	K	1405	BCR	C38-C26-C27	2.46	118.34	113.62
21	L	307	BCR	C36-C18-C17	-2.46	119.48	122.92
18	3	317	CLA	C1-O2A-CGA	2.46	122.89	116.44
18	A	837	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
18	B	815	CLA	CHA-C4D-ND	2.46	137.64	132.50
18	1	5009	CLA	CHA-C4D-ND	2.46	137.64	132.50
18	1	5012	CLA	CHA-C4D-ND	2.46	137.64	132.50
18	4	306	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
18	A	834	CLA	CHA-C4D-ND	2.46	137.64	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	801	CLA	O2A-CGA-CBA	2.46	119.61	111.91
21	A	843	BCR	C38-C26-C27	2.46	118.33	113.62
21	A	843	BCR	C19-C18-C17	2.45	122.71	118.94
29	3	303	LUT	C7-C8-C9	-2.45	122.53	126.23
18	A	831	CLA	O2A-CGA-CBA	2.45	119.61	111.91
17	A	801	CL0	CMB-C2B-C3B	2.45	129.27	124.68
18	L	301	CLA	CMB-C2B-C1B	-2.45	124.69	128.46
18	B	807	CLA	CHA-C4D-ND	2.45	137.63	132.50
18	A	825	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
18	2	306	CLA	C1D-ND-C4D	-2.45	104.59	106.33
21	1	5005	BCR	C8-C9-C10	2.45	122.70	118.94
18	B	817	CLA	C1D-ND-C4D	-2.45	104.59	106.33
18	1	5017	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
18	B	820	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
18	A	818	CLA	CHA-C4D-ND	2.45	137.62	132.50
18	B	836	CLA	CHA-C4D-ND	2.45	137.62	132.50
18	A	827	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
18	3	307	CLA	CHA-C4D-ND	2.45	137.62	132.50
30	4	313	CHL	C4D-CHA-C1A	2.45	124.23	121.25
18	3	317	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
18	1	5013	CLA	CHA-C4D-ND	2.45	137.62	132.50
18	2	312	CLA	CHA-C4D-ND	2.45	137.62	132.50
18	3	318	CLA	CHA-C4D-ND	2.45	137.62	132.50
18	1	5010	CLA	CHA-C4D-ND	2.45	137.62	132.50
18	A	840	CLA	CMB-C2B-C3B	2.45	129.26	124.68
18	B	801	CLA	CMA-C3A-C4A	2.45	118.35	111.77
18	H	1701	CLA	CHA-C4D-ND	2.45	137.62	132.50
18	B	804	CLA	CHA-C4D-ND	2.45	137.62	132.50
29	1	5004	LUT	C31-C32-C33	-2.45	119.55	126.42
18	B	832	CLA	CMB-C2B-C3B	2.45	129.25	124.68
21	A	846	BCR	C34-C9-C10	-2.45	119.50	122.92
18	B	828	CLA	CMB-C2B-C3B	2.44	129.25	124.68
21	B	844	BCR	C38-C26-C27	2.44	118.31	113.62
18	A	838	CLA	C2D-C1D-ND	2.44	111.91	110.10
21	A	847	BCR	C8-C7-C6	-2.44	120.34	127.20
18	A	805	CLA	CHA-C4D-ND	2.44	137.61	132.50
18	L	301	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
18	1	5018	CLA	CHA-C4D-ND	2.44	137.60	132.50
30	1	5014	CHL	C4D-CHA-C1A	2.44	124.22	121.25
21	J	1104	BCR	C36-C18-C17	-2.44	119.51	122.92
18	1	5007	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
18	2	307	CLA	O2A-CGA-CBA	2.44	119.56	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	310	CLA	CHA-C4D-ND	2.44	137.60	132.50
18	4	309	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
18	B	809	CLA	CHA-C4D-ND	2.44	137.59	132.50
18	4	307	CLA	CHA-C4D-ND	2.44	137.59	132.50
18	B	835	CLA	CAA-C2A-C3A	-2.44	106.11	112.78
18	B	804	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
18	G	1601	CLA	CHA-C4D-ND	2.43	137.59	132.50
18	1	5007	CLA	CHA-C4D-ND	2.43	137.59	132.50
28	F	310	ZEX	C27-C26-C25	-2.43	118.91	122.84
18	B	833	CLA	CHA-C4D-ND	2.43	137.59	132.50
18	3	314	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
18	A	840	CLA	CHA-C4D-ND	2.43	137.59	132.50
18	B	826	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
18	2	317	CLA	CHA-C4D-ND	2.43	137.58	132.50
18	A	839	CLA	C2D-C1D-ND	2.43	111.89	110.10
21	B	847	BCR	C35-C13-C12	2.43	121.91	118.08
21	3	305	BCR	C35-C13-C12	2.43	121.91	118.08
18	K	1404	CLA	CHA-C4D-ND	2.43	137.58	132.50
18	1	5006	CLA	CHA-C4D-ND	2.43	137.58	132.50
18	2	308	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
18	B	841	CLA	C1D-ND-C4D	-2.43	104.61	106.33
18	B	813	CLA	CHA-C4D-ND	2.43	137.57	132.50
18	A	833	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
18	B	833	CLA	C1C-C2C-C3C	-2.43	104.41	106.96
30	3	312	CHL	C1-O2A-CGA	2.42	122.81	116.44
18	A	802	CLA	CAA-C2A-C3A	-2.42	106.14	112.78
18	B	817	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
18	A	806	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
18	A	837	CLA	CHA-C4D-ND	2.42	137.57	132.50
18	J	1101	CLA	O2A-CGA-CBA	2.42	119.51	111.91
18	3	319	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
18	F	302	CLA	CHA-C4D-ND	2.42	137.57	132.50
18	4	305	CLA	CHA-C4D-ND	2.42	137.57	132.50
18	A	805	CLA	CAA-C2A-C3A	-2.42	106.14	112.78
18	B	810	CLA	CHA-C4D-ND	2.42	137.56	132.50
18	J	1101	CLA	CHA-C4D-ND	2.42	137.56	132.50
18	A	822	CLA	CMD-C2D-C3D	-2.42	122.05	127.61
18	A	822	CLA	CHA-C4D-ND	2.42	137.56	132.50
18	H	1701	CLA	CMA-C3A-C4A	2.42	118.28	111.77
23	B	852	LMT	O5B-C5B-C4B	2.42	114.09	109.69
31	2	304	XAT	C18-C5-C6	-2.42	118.21	122.26
30	2	318	CHL	CHB-C4A-NA	2.42	127.86	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	318	CLA	C2D-C1D-ND	2.42	111.89	110.10
21	B	847	BCR	C23-C22-C21	-2.42	115.23	118.94
18	A	808	CLA	CHA-C4D-ND	2.42	137.55	132.50
17	A	801	CL0	C3D-C4D-ND	2.42	114.14	110.24
18	A	803	CLA	CHA-C4D-ND	2.42	137.55	132.50
18	4	308	CLA	CHA-C4D-ND	2.41	137.55	132.50
18	B	837	CLA	C1D-ND-C4D	-2.41	104.62	106.33
18	B	824	CLA	CHA-C4D-ND	2.41	137.55	132.50
18	4	312	CLA	CMD-C2D-C3D	-2.41	122.06	127.61
18	B	823	CLA	CHA-C4D-ND	2.41	137.54	132.50
18	F	301	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
18	A	804	CLA	C6-C5-C3	-2.41	107.13	113.45
18	A	816	CLA	CHA-C4D-ND	2.41	137.54	132.50
18	B	822	CLA	CHA-C4D-ND	2.41	137.54	132.50
18	K	1402	CLA	CHA-C4D-ND	2.41	137.54	132.50
31	2	304	XAT	O24-C25-C24	2.41	115.19	113.38
30	2	316	CHL	CHC-C1C-NC	2.41	127.86	124.20
18	B	820	CLA	CHA-C4D-ND	2.41	137.54	132.50
18	B	811	CLA	C2D-C1D-ND	2.41	111.88	110.10
18	B	814	CLA	C1C-C2C-C3C	-2.41	104.42	106.96
18	A	814	CLA	CHA-C4D-ND	2.41	137.54	132.50
21	B	802	BCR	C27-C26-C25	-2.41	119.23	122.73
18	A	833	CLA	CHA-C4D-ND	2.41	137.53	132.50
29	4	303	LUT	C11-C10-C9	-2.41	123.88	127.31
30	4	317	CHL	C4D-CHA-C1A	2.41	124.18	121.25
18	B	804	CLA	CMA-C3A-C4A	2.41	118.24	111.77
18	A	820	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
18	B	810	CLA	C1-C2-C3	-2.40	121.88	126.04
24	1	5001	LMG	C8-O7-C10	-2.40	111.87	117.79
29	3	303	LUT	C35-C15-C14	-2.40	118.55	123.47
18	1	5010	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
18	1	5015	CLA	CHA-C4D-ND	2.40	137.53	132.50
18	B	803	CLA	CMB-C2B-C3B	2.40	129.17	124.68
18	J	1103	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
18	4	312	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
18	B	839	CLA	CHA-C4D-ND	2.40	137.52	132.50
18	A	807	CLA	CHA-C4D-ND	2.40	137.52	132.50
18	B	808	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
18	A	804	CLA	CHA-C4D-ND	2.40	137.52	132.50
18	B	805	CLA	CHA-C4D-ND	2.40	137.52	132.50
18	B	818	CLA	CHA-C4D-ND	2.40	137.52	132.50
18	A	802	CLA	CMB-C2B-C1B	-2.40	124.78	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	821	CLA	CHA-C4D-ND	2.40	137.52	132.50
18	G	1602	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
18	G	1603	CLA	CHA-C4D-ND	2.40	137.52	132.50
18	K	1401	CLA	CHA-C4D-ND	2.40	137.51	132.50
18	K	1401	CLA	C1D-ND-C4D	-2.40	104.63	106.33
18	A	838	CLA	CHA-C4D-ND	2.40	137.51	132.50
18	A	830	CLA	O2A-CGA-CBA	2.40	119.42	111.91
18	A	840	CLA	O2D-CGD-O1D	-2.40	119.16	123.84
18	B	814	CLA	CHA-C4D-ND	2.39	137.51	132.50
18	B	815	CLA	O2A-CGA-CBA	2.39	119.42	111.91
18	3	317	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
18	2	310	CLA	CHA-C4D-ND	2.39	137.50	132.50
17	A	801	CL0	CMD-C2D-C3D	-2.39	122.11	127.61
18	B	825	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
28	F	310	ZEX	C8-C7-C6	-2.39	120.48	127.20
21	K	1405	BCR	C19-C18-C17	2.39	122.61	118.94
18	B	832	CLA	C1C-C2C-C3C	-2.39	104.44	106.96
18	2	306	CLA	C1C-C2C-C3C	-2.39	104.44	106.96
18	B	806	CLA	CMA-C3A-C4A	2.39	118.20	111.77
18	B	812	CLA	C1D-ND-C4D	-2.39	104.64	106.33
18	3	314	CLA	CHA-C4D-ND	2.39	137.50	132.50
18	A	824	CLA	C1-C2-C3	-2.39	121.91	126.04
18	A	831	CLA	CHA-C4D-ND	2.39	137.49	132.50
18	4	312	CLA	CHA-C4D-ND	2.39	137.49	132.50
18	K	1402	CLA	C1-C2-C3	-2.39	121.91	126.04
18	A	828	CLA	CHA-C4D-ND	2.39	137.49	132.50
30	2	318	CHL	C4A-NA-C1A	2.39	107.78	106.71
18	3	319	CLA	CHA-C4D-ND	2.39	137.49	132.50
26	F	309	DGD	O5D-C6D-C5D	2.38	113.46	109.05
23	4	319	LMT	C3'-C4'-C5'	-2.38	105.46	110.93
18	A	852	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
18	1	5007	CLA	C1D-ND-C4D	-2.38	104.64	106.33
18	2	311	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
18	L	305	CLA	O2A-CGA-CBA	2.38	119.39	111.91
18	A	839	CLA	CHA-C4D-ND	2.38	137.48	132.50
18	2	313	CLA	CHA-C4D-ND	2.38	137.48	132.50
18	B	829	CLA	CHA-C4D-ND	2.38	137.48	132.50
18	2	326	CLA	CMA-C3A-C4A	2.38	118.17	111.77
18	L	305	CLA	C1D-ND-C4D	-2.38	104.64	106.33
26	F	309	DGD	O1G-C1A-C2A	2.38	119.38	111.91
18	H	1701	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
18	A	829	CLA	CMA-C3A-C4A	2.38	118.17	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	1401	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
30	4	314	CHL	C4D-CHA-C1A	2.38	124.15	121.25
18	B	835	CLA	CHA-C4D-ND	2.38	137.47	132.50
21	A	845	BCR	C31-C1-C6	-2.38	106.44	110.30
18	1	5018	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
18	2	317	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
18	B	817	CLA	C1C-C2C-C3C	-2.38	104.46	106.96
18	F	303	CLA	CHA-C4D-ND	2.38	137.47	132.50
30	3	312	CHL	CHD-C4C-C3C	2.38	128.34	124.84
21	A	845	BCR	C3-C4-C5	-2.38	109.83	114.08
18	3	301	CLA	CHA-C4D-ND	2.38	137.47	132.50
21	1	5005	BCR	C37-C22-C23	2.38	121.82	118.08
18	4	311	CLA	C1D-ND-C4D	-2.38	104.65	106.33
18	A	832	CLA	CHA-C4D-ND	2.38	137.47	132.50
18	B	840	CLA	CHA-C4D-ND	2.37	137.47	132.50
18	L	301	CLA	CHA-C4D-ND	2.37	137.47	132.50
30	4	302	CHL	C4D-CHA-C1A	2.37	124.14	121.25
18	L	304	CLA	CHA-C4D-ND	2.37	137.46	132.50
29	3	303	LUT	C11-C10-C9	-2.37	123.92	127.31
30	1	5014	CHL	C1B-CHB-C4A	-2.37	125.42	130.12
29	1	5004	LUT	C3-C4-C5	-2.37	107.13	111.85
30	2	314	CHL	C1-C2-C3	-2.37	121.94	126.04
18	G	1601	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
18	A	811	CLA	CHA-C4D-ND	2.37	137.46	132.50
18	J	1101	CLA	CMD-C2D-C3D	-2.37	122.16	127.61
18	A	813	CLA	O2A-CGA-CBA	2.37	119.35	111.91
18	B	829	CLA	CMB-C2B-C1B	-2.37	124.82	128.46
18	K	1403	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
18	A	806	CLA	CHA-C4D-ND	2.37	137.46	132.50
21	B	802	BCR	C38-C26-C27	2.37	118.17	113.62
18	A	832	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
18	B	827	CLA	CMB-C2B-C3B	2.37	129.11	124.68
18	B	808	CLA	CHA-C4D-ND	2.37	137.46	132.50
18	B	806	CLA	C1D-ND-C4D	-2.37	104.65	106.33
18	B	819	CLA	CHA-C4D-ND	2.37	137.45	132.50
18	B	807	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
18	3	307	CLA	C1-O2A-CGA	2.37	122.66	116.44
28	F	310	ZEX	C7-C8-C9	-2.37	122.66	126.23
18	2	311	CLA	C1D-ND-C4D	-2.37	104.65	106.33
18	F	301	CLA	C1C-C2C-C3C	-2.37	104.47	106.96
18	A	817	CLA	CHA-C4D-ND	2.37	137.45	132.50
18	A	824	CLA	CHA-C4D-ND	2.37	137.45	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	837	CLA	CHA-C4D-ND	2.37	137.45	132.50
18	B	826	CLA	CMD-C2D-C3D	-2.37	122.17	127.61
29	2	303	LUT	C39-C29-C28	2.37	121.81	118.08
18	1	5006	CLA	C1C-C2C-C3C	-2.37	104.47	106.96
18	B	805	CLA	CMA-C3A-C4A	2.37	118.13	111.77
18	1	5017	CLA	C2D-C1D-ND	2.37	111.85	110.10
18	A	813	CLA	CHA-C4D-ND	2.36	137.45	132.50
18	B	827	CLA	C1C-C2C-C3C	-2.36	104.47	106.96
18	4	315	CLA	CHA-C4D-ND	2.36	137.44	132.50
18	B	837	CLA	CMD-C2D-C3D	-2.36	122.18	127.61
18	3	311	CLA	CMD-C2D-C3D	-2.36	122.18	127.61
18	2	313	CLA	O2A-CGA-CBA	2.36	119.33	111.91
18	A	803	CLA	CMA-C3A-C4A	2.36	118.12	111.77
18	4	311	CLA	CHA-C4D-ND	2.36	137.44	132.50
18	A	828	CLA	O2A-CGA-CBA	2.36	119.32	111.91
18	4	310	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
18	2	306	CLA	C1-O2A-CGA	2.36	122.64	116.44
18	K	1402	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
18	4	307	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
29	3	303	LUT	C10-C11-C12	-2.36	115.85	123.22
18	B	841	CLA	C1C-C2C-C3C	-2.36	104.48	106.96
18	A	815	CLA	CHA-C4D-ND	2.36	137.43	132.50
18	B	806	CLA	CHA-C4D-ND	2.36	137.43	132.50
18	B	816	CLA	CHA-C4D-ND	2.36	137.43	132.50
18	A	820	CLA	O2A-CGA-CBA	2.36	119.30	111.91
18	A	836	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
30	1	5014	CHL	CHB-C4A-NA	2.36	127.77	124.51
18	B	832	CLA	CHA-C4D-ND	2.36	137.43	132.50
21	B	845	BCR	C8-C7-C6	-2.36	120.59	127.20
18	2	311	CLA	CHA-C4D-ND	2.36	137.43	132.50
18	1	5008	CLA	C1D-ND-C4D	-2.36	104.66	106.33
18	A	835	CLA	CHA-C4D-ND	2.35	137.42	132.50
31	2	304	XAT	C6-C7-C8	-2.35	121.02	125.99
18	A	836	CLA	C1D-ND-C4D	-2.35	104.66	106.33
18	L	301	CLA	O2A-CGA-CBA	2.35	119.29	111.91
18	2	308	CLA	CHA-C4D-ND	2.35	137.42	132.50
18	A	816	CLA	O2A-CGA-CBA	2.35	119.29	111.91
29	J	1105	LUT	C39-C29-C30	-2.35	119.63	122.92
21	4	301	BCR	C8-C7-C6	-2.35	120.59	127.20
31	4	304	XAT	C6-C7-C8	-2.35	121.02	125.99
21	F	305	BCR	C27-C26-C25	-2.35	119.32	122.73
30	4	314	CHL	C1-O2A-CGA	2.35	122.61	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	810	CLA	CMD-C2D-C3D	-2.35	122.21	127.61
18	B	815	CLA	C2D-C1D-ND	2.35	111.84	110.10
18	A	827	CLA	CHA-C4D-ND	2.35	137.41	132.50
18	B	833	CLA	O2A-CGA-CBA	2.35	119.28	111.91
18	A	836	CLA	CHA-C4D-ND	2.35	137.41	132.50
26	B	855	DGD	C2G-O2G-C1B	-2.35	112.01	117.79
18	A	830	CLA	CHA-C4D-ND	2.35	137.41	132.50
18	L	306	CLA	CHA-C4D-ND	2.35	137.41	132.50
18	4	315	CLA	C2D-C1D-ND	2.35	111.83	110.10
18	A	809	CLA	CMD-C2D-C3D	-2.35	122.22	127.61
18	A	819	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
18	A	837	CLA	CMB-C2B-C1B	-2.34	124.86	128.46
18	A	822	CLA	C1D-ND-C4D	-2.34	104.67	106.33
18	B	818	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
21	I	101	BCR	C34-C9-C10	-2.34	119.64	122.92
30	3	316	CHL	C1B-CHB-C4A	-2.34	125.48	130.12
18	B	828	CLA	C2D-C1D-ND	2.34	111.83	110.10
18	B	824	CLA	CMD-C2D-C3D	-2.34	122.23	127.61
18	B	838	CLA	CHA-C4D-ND	2.34	137.39	132.50
18	F	302	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
31	4	304	XAT	C26-C27-C28	-2.34	121.05	125.99
18	3	315	CLA	CMB-C2B-C3B	2.34	129.05	124.68
18	A	810	CLA	CHA-C4D-ND	2.34	137.39	132.50
23	2	325	LMT	O5B-C5B-C4B	2.34	113.94	109.69
18	A	827	CLA	O2A-CGA-CBA	2.34	119.24	111.91
21	B	845	BCR	C29-C28-C27	2.34	116.60	111.38
18	3	315	CLA	CHA-C4D-ND	2.34	137.39	132.50
29	3	304	LUT	C2-C3-C4	-2.34	107.11	110.30
18	3	308	CLA	O2A-CGA-CBA	2.34	119.24	111.91
21	J	1104	BCR	C38-C26-C27	2.33	118.10	113.62
18	B	812	CLA	CHA-C4D-ND	2.33	137.38	132.50
18	3	317	CLA	CHA-C4D-ND	2.33	137.38	132.50
18	A	814	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
18	4	311	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
18	A	809	CLA	CHA-C4D-ND	2.33	137.38	132.50
22	2	320	LHG	C5-O7-C7	-2.33	112.05	117.79
21	F	305	BCR	C33-C5-C4	2.33	118.09	113.62
18	B	818	CLA	O2A-CGA-CBA	2.33	119.22	111.91
18	A	828	CLA	O1D-CGD-CBD	-2.33	119.72	124.48
18	1	5015	CLA	C1-C2-C3	-2.33	122.01	126.04
18	A	812	CLA	CHA-C4D-ND	2.33	137.37	132.50
21	B	844	BCR	C33-C5-C4	2.33	118.09	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	1404	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
18	B	817	CLA	CHA-C4D-ND	2.33	137.37	132.50
29	3	304	LUT	C20-C13-C12	2.33	121.75	118.08
18	L	304	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
18	2	313	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
18	G	1601	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
18	B	831	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
18	L	306	CLA	O2D-CGD-O1D	-2.32	119.29	123.84
18	L	306	CLA	C1D-ND-C4D	-2.32	104.68	106.33
18	B	832	CLA	O2A-CGA-CBA	2.32	119.20	111.91
18	B	829	CLA	C1-C2-C3	-2.32	122.03	126.04
18	1	5009	CLA	C1D-ND-C4D	-2.32	104.69	106.33
21	L	302	BCR	C35-C13-C12	2.32	121.74	118.08
31	2	304	XAT	C19-C9-C10	-2.32	119.67	122.92
18	2	312	CLA	CMB-C2B-C1B	-2.32	124.89	128.46
21	A	844	BCR	C38-C26-C27	2.32	118.08	113.62
18	2	306	CLA	CHA-C4D-ND	2.32	137.35	132.50
18	1	5008	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
18	B	805	CLA	CMB-C2B-C1B	-2.32	124.90	128.46
18	H	1701	CLA	CMD-C2D-C3D	-2.32	122.28	127.61
18	1	5011	CLA	CMD-C2D-C3D	-2.32	122.28	127.61
18	J	1101	CLA	CMA-C3A-C4A	2.32	118.01	111.77
30	2	315	CHL	CHD-C4C-C3C	2.32	128.25	124.84
30	4	318	CHL	C1-C2-C3	-2.32	122.04	126.04
18	B	825	CLA	CMD-C2D-C3D	-2.32	122.29	127.61
18	A	832	CLA	C1D-ND-C4D	-2.32	104.69	106.33
21	2	305	BCR	C1-C6-C5	-2.32	119.35	122.61
18	B	838	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
18	B	815	CLA	CMD-C2D-C3D	-2.31	122.29	127.61
18	A	821	CLA	CAA-C2A-C3A	-2.31	106.44	112.78
21	B	843	BCR	C30-C25-C26	-2.31	119.36	122.61
21	A	847	BCR	C33-C5-C6	-2.31	121.93	124.53
18	B	839	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
18	B	832	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
18	1	5008	CLA	CHA-C4D-ND	2.31	137.33	132.50
18	B	840	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
23	B	856	LMT	O1'-C1'-C2'	2.31	111.91	108.30
21	A	855	BCR	C38-C26-C27	2.31	118.05	113.62
18	F	301	CLA	CHA-C4D-ND	2.31	137.32	132.50
18	A	812	CLA	CMB-C2B-C3B	2.31	128.99	124.68
21	B	843	BCR	C37-C22-C21	-2.31	119.69	122.92
18	4	308	CLA	CMD-C2D-C3D	-2.31	122.31	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	808	CLA	C1D-ND-C4D	-2.31	104.70	106.33
23	B	853	LMT	C2'-C3'-C4'	2.31	114.95	109.68
24	B	851	LMG	O6-C5-C6	2.31	112.17	106.44
21	B	846	BCR	C36-C18-C17	-2.31	119.69	122.92
18	2	308	CLA	C1D-ND-C4D	-2.30	104.70	106.33
18	A	824	CLA	O2A-CGA-CBA	2.30	119.14	111.91
18	A	812	CLA	CMA-C3A-C4A	2.30	117.96	111.77
18	4	315	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
21	F	305	BCR	C36-C18-C19	2.30	121.70	118.08
18	A	853	CLA	CHA-C4D-ND	2.30	137.31	132.50
18	B	834	CLA	O2A-CGA-CBA	2.30	119.13	111.91
21	B	844	BCR	C35-C13-C12	2.30	121.70	118.08
18	A	813	CLA	CMB-C2B-C3B	2.30	128.98	124.68
21	F	304	BCR	C36-C18-C17	-2.30	119.70	122.92
31	2	304	XAT	C40-C33-C34	-2.30	119.70	122.92
18	A	805	CLA	C1D-ND-C4D	-2.30	104.70	106.33
18	B	807	CLA	C1D-ND-C4D	-2.30	104.70	106.33
18	B	819	CLA	C1D-ND-C4D	-2.30	104.70	106.33
18	B	841	CLA	CHA-C4D-ND	2.30	137.31	132.50
18	A	853	CLA	C1D-ND-C4D	-2.30	104.70	106.33
18	A	815	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
18	B	818	CLA	C1-C2-C3	-2.30	122.07	126.04
18	1	5015	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
21	3	305	BCR	C37-C22-C23	2.30	121.70	118.08
18	2	310	CLA	CAA-C2A-C1A	-2.30	104.45	111.97
18	B	825	CLA	CHA-C1A-NA	-2.30	121.14	126.40
18	F	301	CLA	CMB-C2B-C1B	-2.30	124.94	128.46
18	B	819	CLA	CAA-C2A-C1A	-2.30	104.45	111.97
18	B	823	CLA	O2A-CGA-CBA	2.30	119.11	111.91
18	3	318	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
18	4	315	CLA	CAA-C2A-C3A	-2.30	106.49	112.78
18	J	1101	CLA	C1D-ND-C4D	-2.29	104.70	106.33
18	2	312	CLA	O2A-CGA-CBA	2.29	119.10	111.91
18	A	814	CLA	C1D-ND-C4D	-2.29	104.71	106.33
21	A	843	BCR	C27-C26-C25	-2.29	119.41	122.73
31	4	304	XAT	C39-C29-C30	-2.29	119.72	122.92
18	B	807	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
21	3	305	BCR	C38-C26-C27	2.29	118.01	113.62
18	A	823	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
18	B	834	CLA	CMB-C2B-C1B	-2.29	124.95	128.46
18	B	817	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
18	A	807	CLA	O1D-CGD-CBD	-2.29	119.80	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	819	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
21	2	305	BCR	C1-C6-C7	2.29	122.25	115.78
18	4	307	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
21	3	306	BCR	C38-C26-C27	2.29	118.01	113.62
17	A	801	CL0	C4D-C3D-CAD	2.29	110.79	108.10
18	K	1402	CLA	CMD-C2D-C3D	-2.29	122.36	127.61
18	B	838	CLA	C1D-ND-C4D	-2.28	104.71	106.33
21	4	301	BCR	C30-C25-C24	2.28	122.24	115.78
30	2	315	CHL	CHB-C4A-NA	2.28	127.67	124.51
18	A	802	CLA	CHA-C4D-ND	2.28	137.27	132.50
18	F	302	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
18	B	823	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
31	2	304	XAT	C39-C29-C30	-2.28	119.73	122.92
30	4	314	CHL	C1B-CHB-C4A	-2.28	125.60	130.12
30	4	313	CHL	C4A-NA-C1A	2.28	107.73	106.71
18	L	301	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
18	1	5013	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
18	A	838	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
18	3	317	CLA	C1D-ND-C4D	-2.28	104.72	106.33
21	3	306	BCR	C30-C25-C26	-2.28	119.40	122.61
18	A	825	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
18	A	835	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
18	3	308	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
18	A	802	CLA	CHA-C1A-NA	-2.28	121.18	126.40
18	4	309	CLA	CHA-C1A-NA	-2.28	121.18	126.40
26	J	1106	DGD	C3E-C4E-C5E	2.28	114.30	110.24
18	2	306	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
18	2	311	CLA	CMD-C2D-C3D	-2.28	122.38	127.61
18	B	829	CLA	O2A-CGA-CBA	2.28	119.05	111.91
18	1	5010	CLA	CMD-C2D-C3D	-2.27	122.38	127.61
21	B	844	BCR	C36-C18-C17	-2.27	119.74	122.92
18	G	1602	CLA	CMD-C2D-C3D	-2.27	122.38	127.61
18	A	826	CLA	CHA-C4D-ND	2.27	137.25	132.50
18	2	310	CLA	CMB-C2B-C1B	-2.27	124.97	128.46
18	B	801	CLA	CHA-C1A-NA	-2.27	121.20	126.40
30	2	314	CHL	C4D-CHA-C1A	2.27	124.01	121.25
21	I	101	BCR	C3-C4-C5	-2.27	110.02	114.08
18	B	812	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
18	A	817	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
18	K	1403	CLA	C1D-ND-C4D	-2.27	104.72	106.33
18	A	826	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
29	3	304	LUT	C7-C8-C9	-2.27	122.81	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	802	CLA	O2A-CGA-CBA	2.27	119.03	111.91
18	3	318	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
30	4	317	CHL	C4A-NA-C1A	2.27	107.72	106.71
24	F	308	LMG	O8-C28-C29	2.27	119.02	111.91
18	B	814	CLA	CHA-C1A-NA	-2.27	121.21	126.40
18	B	813	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
18	A	815	CLA	C1-O2A-CGA	2.27	122.39	116.44
18	A	853	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
18	B	804	CLA	CAC-C3C-C4C	2.27	127.75	124.81
21	B	847	BCR	C8-C7-C6	-2.26	120.84	127.20
18	B	808	CLA	CMD-C2D-C3D	-2.26	122.40	127.61
18	3	308	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
30	3	312	CHL	CHC-C1C-NC	2.26	127.64	124.20
18	4	310	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
18	A	825	CLA	C1D-ND-C4D	-2.26	104.73	106.33
18	B	822	CLA	O2A-CGA-CBA	2.26	119.01	111.91
21	B	847	BCR	C33-C5-C4	2.26	117.96	113.62
18	G	1602	CLA	CMB-C2B-C1B	-2.26	124.99	128.46
18	A	811	CLA	C1D-ND-C4D	-2.26	104.73	106.33
29	3	303	LUT	C38-C25-C24	-2.26	118.72	123.56
18	B	805	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
30	3	316	CHL	CHB-C4A-NA	2.26	127.64	124.51
18	L	305	CLA	CHA-C4D-ND	2.26	137.23	132.50
21	F	305	BCR	C38-C26-C25	-2.26	121.99	124.53
30	1	5016	CHL	C4D-CHA-C1A	2.26	124.00	121.25
18	2	306	CLA	CMB-C2B-C3B	2.26	128.90	124.68
18	A	830	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
18	2	308	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
18	A	833	CLA	O2A-CGA-CBA	2.26	118.99	111.91
18	K	1402	CLA	CHA-C1A-NA	-2.26	121.23	126.40
21	B	846	BCR	C37-C22-C23	2.26	121.63	118.08
29	2	303	LUT	C18-C5-C4	2.26	118.53	114.36
18	B	814	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
18	A	831	CLA	C1C-C2C-C3C	-2.26	104.58	106.96
21	K	1405	BCR	C1-C6-C5	-2.25	119.44	122.61
18	K	1404	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
18	3	315	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
18	B	809	CLA	C2D-C1D-ND	2.25	111.77	110.10
18	A	804	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
18	A	814	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
21	3	306	BCR	C38-C26-C25	-2.25	122.00	124.53
21	J	1104	BCR	C37-C22-C21	-2.25	119.77	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	840	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
18	B	819	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
18	A	810	CLA	O2A-CGA-CBA	2.25	118.97	111.91
18	B	812	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
21	F	304	BCR	C37-C22-C23	2.25	121.62	118.08
18	3	318	CLA	CMA-C3A-C4A	2.25	117.82	111.77
18	G	1603	CLA	C1D-ND-C4D	-2.25	104.74	106.33
18	3	308	CLA	C1D-ND-C4D	-2.25	104.74	106.33
30	4	302	CHL	C1-C2-C3	-2.25	122.16	126.04
30	4	317	CHL	CHB-C4A-NA	2.25	127.62	124.51
18	A	809	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
18	A	806	CLA	CMD-C2D-C3D	-2.24	122.45	127.61
18	A	837	CLA	O2A-CGA-CBA	2.24	118.95	111.91
18	4	305	CLA	CAA-C2A-C3A	-2.24	106.63	112.78
18	2	309	CLA	C1D-ND-C4D	-2.24	104.74	106.33
24	J	1102	LMG	C8-O7-C10	-2.24	112.27	117.79
18	B	835	CLA	C1-O2A-CGA	2.24	122.33	116.44
18	A	811	CLA	CMD-C2D-C3D	-2.24	122.45	127.61
30	4	302	CHL	CHB-C4A-NA	2.24	127.61	124.51
21	B	845	BCR	C12-C13-C14	-2.24	115.50	118.94
18	L	306	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
18	B	810	CLA	CMA-C3A-C4A	2.24	117.80	111.77
18	B	823	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
18	B	804	CLA	CMB-C2B-C3B	2.24	128.87	124.68
18	1	5018	CLA	C1D-ND-C4D	-2.24	104.74	106.33
21	I	101	BCR	C38-C26-C27	2.24	117.92	113.62
18	A	834	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
18	B	820	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
18	B	809	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
18	L	305	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
18	A	829	CLA	O2A-CGA-CBA	2.24	118.93	111.91
30	4	314	CHL	CHB-C4A-NA	2.24	127.61	124.51
18	A	833	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
18	B	825	CLA	O2A-CGA-CBA	2.24	118.93	111.91
18	A	821	CLA	CMB-C2B-C3B	2.24	128.86	124.68
21	B	802	BCR	C30-C25-C26	-2.24	119.46	122.61
21	L	307	BCR	C38-C26-C27	2.24	117.91	113.62
18	A	829	CLA	CMB-C2B-C3B	2.24	128.86	124.68
18	3	309	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
21	B	847	BCR	C28-C27-C26	-2.23	110.09	114.08
18	B	806	CLA	O2A-CGA-CBA	2.23	118.92	111.91
18	A	832	CLA	CMD-C2D-C3D	-2.23	122.48	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	848	LHG	C5-O7-C7	-2.23	112.30	117.79
18	3	318	CLA	CMB-C2B-C3B	2.23	128.85	124.68
21	A	843	BCR	C31-C1-C6	-2.23	106.68	110.30
18	3	318	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
24	G	1607	LMG	C1-O6-C5	2.23	118.07	113.69
18	B	821	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
21	L	302	BCR	C30-C25-C26	-2.23	119.47	122.61
30	3	312	CHL	C4A-NA-C1A	2.23	107.71	106.71
18	G	1603	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
18	4	310	CLA	O2A-CGA-CBA	2.23	118.91	111.91
19	B	842	PQN	C2M-C2-C3	-2.23	120.76	124.40
30	2	316	CHL	CHB-C4A-NA	2.23	127.60	124.51
18	F	303	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
18	4	305	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
18	A	816	CLA	C1C-C2C-C3C	-2.23	104.61	106.96
21	A	847	BCR	C32-C1-C6	-2.23	106.68	110.30
24	2	321	LMG	O7-C10-O9	-2.23	118.32	123.70
30	3	310	CHL	CMB-C2B-C1B	-2.23	125.04	128.46
18	4	308	CLA	CMB-C2B-C3B	2.23	128.85	124.68
18	A	831	CLA	O1D-CGD-CBD	-2.23	119.93	124.48
21	K	1405	BCR	C30-C25-C26	-2.23	119.48	122.61
30	4	318	CHL	CHB-C4A-NA	2.23	127.59	124.51
30	2	318	CHL	C1B-CHB-C4A	-2.23	125.71	130.12
18	A	834	CLA	CMB-C2B-C1B	-2.23	125.04	128.46
30	3	312	CHL	CMB-C2B-C1B	-2.23	125.04	128.46
18	A	813	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
18	3	319	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
18	B	816	CLA	CAA-C2A-C3A	-2.23	106.68	112.78
29	1	5004	LUT	C39-C29-C28	2.22	121.58	118.08
18	3	309	CLA	C1D-ND-C4D	-2.22	104.75	106.33
21	I	102	BCR	C19-C18-C17	2.22	122.35	118.94
29	3	304	LUT	C19-C9-C8	2.22	121.58	118.08
21	2	305	BCR	C12-C13-C14	-2.22	115.53	118.94
18	B	818	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
18	3	311	CLA	CHA-C1A-NA	-2.22	121.31	126.40
18	B	827	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
18	B	820	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
18	A	829	CLA	C1D-ND-C4D	-2.22	104.76	106.33
18	3	307	CLA	C1D-ND-C4D	-2.22	104.76	106.33
18	A	815	CLA	C1D-ND-C4D	-2.22	104.76	106.33
18	B	840	CLA	C1D-ND-C4D	-2.22	104.76	106.33
18	B	822	CLA	CMD-C2D-C3D	-2.22	122.52	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	814	CLA	CMA-C3A-C4A	2.22	117.73	111.77
31	2	304	XAT	C20-C13-C14	-2.22	119.82	122.92
18	A	804	CLA	C1D-ND-C4D	-2.22	104.76	106.33
18	A	824	CLA	C1D-ND-C4D	-2.21	104.76	106.33
18	K	1401	CLA	CMB-C2B-C1B	-2.21	125.06	128.46
18	A	836	CLA	O2A-CGA-CBA	2.21	118.85	111.91
18	4	309	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
30	2	315	CHL	CMB-C2B-C1B	-2.21	125.06	128.46
29	1	5003	LUT	C18-C5-C4	2.21	118.45	114.36
18	3	301	CLA	CHA-C1A-NA	-2.21	121.33	126.40
18	B	834	CLA	C2D-C1D-ND	2.21	111.73	110.10
18	A	808	CLA	O2A-CGA-CBA	2.21	118.84	111.91
18	A	816	CLA	CMB-C2B-C3B	2.21	128.81	124.68
18	B	824	CLA	C1D-ND-C4D	-2.21	104.77	106.33
18	L	306	CLA	CHA-C1A-NA	-2.21	121.34	126.40
18	2	326	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
18	A	834	CLA	CHA-C1A-NA	-2.21	121.34	126.40
18	B	811	CLA	C1D-ND-C4D	-2.21	104.77	106.33
18	B	826	CLA	C1D-ND-C4D	-2.21	104.77	106.33
30	4	313	CHL	C1B-CHB-C4A	-2.21	125.75	130.12
18	A	823	CLA	O1D-CGD-CBD	-2.21	119.97	124.48
18	B	833	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
30	1	5016	CHL	C4A-NA-C1A	2.21	107.70	106.71
30	4	313	CHL	CHB-C4A-NA	2.21	127.56	124.51
18	A	837	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
29	1	5004	LUT	C18-C5-C4	2.20	118.44	114.36
18	A	809	CLA	CAA-C2A-C3A	-2.20	106.74	112.78
18	2	317	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
18	4	306	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
18	B	839	CLA	O2A-CGA-CBA	2.20	118.83	111.91
18	A	838	CLA	O2A-CGA-CBA	2.20	118.82	111.91
18	A	805	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
21	1	5005	BCR	C36-C18-C17	-2.20	119.84	122.92
18	B	840	CLA	O2A-CGA-CBA	2.20	118.82	111.91
21	L	307	BCR	C23-C24-C25	-2.20	121.02	127.20
18	1	5012	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
18	B	838	CLA	O2A-CGA-CBA	2.20	118.82	111.91
21	B	844	BCR	C8-C9-C10	2.20	122.32	118.94
18	B	832	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
30	1	5016	CHL	CHB-C4A-NA	2.20	127.56	124.51
18	F	302	CLA	C1-C2-C3	-2.20	122.24	126.04
18	B	839	CLA	C1D-ND-C4D	-2.20	104.77	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	851	LMG	O7-C10-O9	-2.20	118.39	123.70
30	2	316	CHL	C4A-NA-C1A	2.20	107.69	106.71
24	2	323	LMG	C1-O6-C5	2.20	118.00	113.69
18	1	5015	CLA	O2A-CGA-CBA	2.20	118.81	111.91
18	A	811	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
18	4	305	CLA	C1D-ND-C4D	-2.20	104.77	106.33
18	B	831	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
18	B	810	CLA	CHA-C1A-NA	-2.20	121.36	126.40
29	4	303	LUT	C10-C11-C12	-2.20	116.36	123.22
18	A	808	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
18	B	829	CLA	C1D-ND-C4D	-2.20	104.78	106.33
18	2	311	CLA	O2A-CGA-CBA	2.20	118.80	111.91
21	G	1604	BCR	C34-C9-C10	-2.19	119.85	122.92
18	2	317	CLA	C2D-C1D-ND	2.19	111.72	110.10
18	B	836	CLA	CHA-C1A-NA	-2.19	121.38	126.40
18	3	309	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
18	4	305	CLA	CMB-C2B-C3B	2.19	128.78	124.68
18	3	307	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
18	2	306	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
30	3	313	CHL	CHC-C1C-NC	2.19	127.53	124.20
21	A	847	BCR	C2-C1-C6	2.19	113.85	110.48
18	B	810	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
18	1	5009	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
18	B	841	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
30	4	318	CHL	C4A-NA-C1A	2.19	107.69	106.71
18	L	306	CLA	O2A-CGA-CBA	2.19	118.78	111.91
18	4	305	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
18	3	314	CLA	CHA-C1A-NA	-2.19	121.39	126.40
18	1	5006	CLA	CMB-C2B-C3B	2.19	128.77	124.68
18	4	307	CLA	C1D-ND-C4D	-2.19	104.78	106.33
18	A	823	CLA	CMB-C2B-C3B	2.19	128.77	124.68
18	F	303	CLA	O2A-CGA-CBA	2.19	118.77	111.91
18	A	813	CLA	CHA-C1A-NA	-2.19	121.39	126.40
18	B	804	CLA	CHA-C1A-NA	-2.19	121.39	126.40
18	A	803	CLA	C1-O2A-CGA	2.19	122.18	116.44
18	A	821	CLA	O2A-CGA-CBA	2.19	118.77	111.91
18	B	806	CLA	CMD-C2D-C3D	-2.19	122.59	127.61
18	A	810	CLA	C1D-ND-C4D	-2.18	104.78	106.33
18	2	307	CLA	C1D-ND-C4D	-2.18	104.78	106.33
18	2	309	CLA	O2A-CGA-CBA	2.18	118.76	111.91
18	4	310	CLA	CMB-C2B-C3B	2.18	128.76	124.68
18	1	5010	CLA	C1-O2A-CGA	2.18	122.17	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	304	CLA	C1D-ND-C4D	-2.18	104.78	106.33
18	3	318	CLA	CHA-C1A-NA	-2.18	121.40	126.40
18	2	309	CLA	C1-O2A-CGA	2.18	122.17	116.44
18	B	803	CLA	CHA-C1A-NA	-2.18	121.40	126.40
18	A	812	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
30	2	316	CHL	CHD-C4C-C3C	2.18	128.05	124.84
18	A	831	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
21	I	102	BCR	C38-C26-C25	-2.18	122.08	124.53
18	B	815	CLA	CMB-C2B-C1B	-2.18	125.11	128.46
18	A	818	CLA	O2A-CGA-CBA	2.18	118.75	111.91
18	4	308	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
24	B	851	LMG	O1-C1-C2	2.18	111.71	108.30
18	2	307	CLA	CHA-C1A-NA	-2.18	121.41	126.40
18	4	308	CLA	C1D-ND-C4D	-2.18	104.79	106.33
30	4	317	CHL	C1B-CHB-C4A	-2.18	125.80	130.12
18	3	311	CLA	O2A-CGA-CBA	2.18	118.75	111.91
18	A	804	CLA	C1-O2A-CGA	2.18	122.16	116.44
18	A	826	CLA	O2A-CGA-CBA	2.18	118.74	111.91
21	A	855	BCR	C23-C24-C25	-2.18	121.09	127.20
18	A	822	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
18	A	852	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
18	1	5018	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
21	L	303	BCR	C38-C26-C27	2.18	117.80	113.62
18	A	807	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
18	B	829	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
18	K	1403	CLA	CHA-C1A-NA	-2.17	121.42	126.40
18	3	315	CLA	C1D-ND-C4D	-2.17	104.79	106.33
18	2	307	CLA	CMD-C2D-C3D	-2.17	122.61	127.61
21	I	102	BCR	C28-C27-C26	-2.17	110.19	114.08
18	B	815	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
21	L	307	BCR	C35-C13-C12	2.17	121.50	118.08
18	L	301	CLA	C1D-ND-C4D	-2.17	104.79	106.33
18	4	308	CLA	CAA-C2A-C3A	-2.17	106.83	112.78
18	1	5006	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
24	B	851	LMG	C1-O6-C5	2.17	117.95	113.69
18	A	826	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
18	F	303	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
18	B	816	CLA	C1D-ND-C4D	-2.17	104.79	106.33
18	B	823	CLA	C1D-ND-C4D	-2.17	104.79	106.33
18	1	5015	CLA	C1D-ND-C4D	-2.17	104.79	106.33
18	G	1601	CLA	O2A-CGA-CBA	2.17	118.72	111.91
18	3	319	CLA	C1D-ND-C4D	-2.17	104.79	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	825	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
18	B	827	CLA	CHA-C1A-NA	-2.17	121.43	126.40
18	A	806	CLA	C1D-ND-C4D	-2.17	104.80	106.33
18	J	1101	CLA	C1-O2A-CGA	2.17	122.13	116.44
18	B	803	CLA	C2D-C1D-ND	2.17	111.70	110.10
18	2	326	CLA	O2A-CGA-CBA	2.17	118.71	111.91
18	A	816	CLA	C1D-ND-C4D	-2.16	104.80	106.33
18	A	817	CLA	O2A-CGA-CBA	2.16	118.70	111.91
18	A	815	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
30	4	318	CHL	C1-O2A-CGA	2.16	122.12	116.44
18	B	813	CLA	CMB-C2B-C1B	-2.16	125.14	128.46
30	2	316	CHL	C1-O2A-CGA	2.16	123.01	116.73
30	4	302	CHL	C4A-NA-C1A	2.16	107.68	106.71
21	A	844	BCR	C34-C9-C10	-2.16	119.89	122.92
18	1	5017	CLA	CMA-C3A-C4A	2.16	117.58	111.77
29	1	5003	LUT	C38-C25-C24	-2.16	118.94	123.56
30	4	316	CHL	CHB-C4A-NA	2.16	127.50	124.51
18	B	827	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
18	2	310	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
21	A	847	BCR	C38-C26-C27	2.16	117.77	113.62
18	A	832	CLA	CMA-C3A-C4A	2.16	117.58	111.77
18	A	819	CLA	C1-C2-C3	-2.16	122.31	126.04
18	4	309	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
30	1	5016	CHL	CHC-C1C-NC	2.16	127.48	124.20
18	K	1402	CLA	C1D-ND-C4D	-2.16	104.80	106.33
18	L	304	CLA	O2A-CGA-CBA	2.16	118.68	111.91
21	A	846	BCR	C37-C22-C23	2.16	121.48	118.08
29	2	303	LUT	C38-C25-C24	-2.16	118.94	123.56
18	A	825	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
18	B	834	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
18	A	817	CLA	CMB-C2B-C1B	-2.16	125.15	128.46
31	2	304	XAT	O4-C5-C18	-2.16	112.47	115.06
18	A	838	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
18	B	833	CLA	C1D-ND-C4D	-2.16	104.80	106.33
18	4	312	CLA	C1D-ND-C4D	-2.16	104.80	106.33
24	1	5001	LMG	O8-C28-O10	-2.15	118.15	123.59
18	B	816	CLA	CMB-C2B-C1B	-2.15	125.15	128.46
18	B	828	CLA	CHA-C1A-NA	-2.15	121.47	126.40
18	F	302	CLA	CHA-C1A-NA	-2.15	121.47	126.40
18	F	301	CLA	C1-C2-C3	-2.15	122.32	126.04
18	A	805	CLA	CMB-C2B-C1B	-2.15	125.16	128.46
18	4	312	CLA	O1D-CGD-CBD	-2.15	120.08	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	820	CLA	O2A-CGA-CBA	2.15	118.66	111.91
18	4	305	CLA	CHA-C1A-NA	-2.15	121.47	126.40
18	3	301	CLA	CMD-C2D-C3D	-2.15	122.66	127.61
18	J	1103	CLA	CHA-C1A-NA	-2.15	121.47	126.40
18	3	317	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
18	K	1401	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
18	A	811	CLA	O2A-CGA-CBA	2.15	118.65	111.91
18	A	813	CLA	C1D-ND-C4D	-2.15	104.81	106.33
29	1	5003	LUT	C7-C8-C9	-2.15	122.99	126.23
30	4	302	CHL	C1B-CHB-C4A	-2.15	125.86	130.12
30	2	319	CHL	CHD-C4C-C3C	2.15	128.00	124.84
18	A	812	CLA	O2A-CGA-CBA	2.15	118.65	111.91
18	B	841	CLA	CHA-C1A-NA	-2.15	121.48	126.40
21	L	302	BCR	C38-C26-C27	2.15	117.74	113.62
18	1	5012	CLA	C1D-ND-C4D	-2.15	104.81	106.33
18	A	811	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
18	2	310	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
18	J	1103	CLA	CMD-C2D-C3D	-2.15	122.68	127.61
18	K	1403	CLA	O2A-CGA-CBA	2.15	118.64	111.91
18	A	834	CLA	C1D-ND-C4D	-2.15	104.81	106.33
30	4	316	CHL	CHC-C1C-NC	2.14	127.46	124.20
21	A	843	BCR	C3-C4-C5	-2.14	110.25	114.08
18	4	306	CLA	CHA-C1A-NA	-2.14	121.49	126.40
18	1	5010	CLA	C1D-ND-C4D	-2.14	104.81	106.33
30	2	315	CHL	C1-C2-C3	-2.14	122.34	126.04
18	A	839	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
18	A	819	CLA	CMB-C2B-C1B	-2.14	125.18	128.46
18	A	821	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
18	G	1601	CLA	C1D-ND-C4D	-2.14	104.82	106.33
23	J	1107	LMT	C3'-C4'-C5'	-2.14	106.03	110.93
18	A	836	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
18	1	5006	CLA	C1D-ND-C4D	-2.14	104.82	106.33
18	1	5018	CLA	CHA-C1A-NA	-2.14	121.50	126.40
18	A	822	CLA	O2A-CGA-CBA	2.14	118.61	111.91
18	A	812	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
18	A	838	CLA	CHA-C1A-NA	-2.14	121.51	126.40
18	B	816	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
18	4	315	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
18	B	822	CLA	C1D-ND-C4D	-2.13	104.82	106.33
18	4	309	CLA	C1D-ND-C4D	-2.13	104.82	106.33
21	L	307	BCR	C38-C26-C25	-2.13	122.13	124.53
30	4	313	CHL	C1-O2A-CGA	2.13	123.14	116.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	846	BCR	C33-C5-C4	2.13	117.71	113.62
18	A	828	CLA	C2D-C1D-ND	2.13	111.68	110.10
21	3	305	BCR	C34-C9-C10	-2.13	119.94	122.92
30	3	316	CHL	CHC-C1C-NC	2.13	127.44	124.20
18	3	314	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
18	A	839	CLA	O2A-CGA-CBA	2.13	118.60	111.91
18	B	835	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
18	A	827	CLA	CMB-C2B-C3B	2.13	128.67	124.68
18	F	302	CLA	CMB-C2B-C3B	2.13	128.67	124.68
18	A	803	CLA	CHA-C1A-NA	-2.13	121.52	126.40
18	A	819	CLA	C1D-ND-C4D	-2.13	104.82	106.33
24	G	1607	LMG	O6-C5-C6	2.13	111.73	106.44
18	2	313	CLA	C1D-ND-C4D	-2.13	104.82	106.33
18	B	835	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
18	1	5006	CLA	O2A-CGA-CBA	2.13	118.59	111.91
18	B	805	CLA	O2A-CGA-CBA	2.13	118.59	111.91
18	B	822	CLA	CHA-C1A-NA	-2.13	121.52	126.40
21	B	843	BCR	C30-C25-C24	2.13	121.80	115.78
18	H	1701	CLA	CHA-C1A-NA	-2.13	121.53	126.40
18	K	1401	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
29	4	303	LUT	C38-C25-C24	-2.13	119.01	123.56
21	1	5005	BCR	C15-C14-C13	-2.13	124.28	127.31
18	A	819	CLA	O2A-CGA-CBA	2.13	118.58	111.91
18	A	803	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
29	4	303	LUT	C31-C32-C33	-2.12	120.45	126.42
18	3	314	CLA	C1D-ND-C4D	-2.12	104.83	106.33
30	4	316	CHL	C2C-C3C-C4C	2.12	108.00	106.49
30	2	319	CHL	CHC-C1C-NC	2.12	127.42	124.20
18	K	1403	CLA	CBC-CAC-C3C	-2.12	106.58	112.43
30	2	314	CHL	C1B-CHB-C4A	-2.12	125.91	130.12
18	1	5008	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
18	B	826	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
30	4	313	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
30	4	317	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
18	3	311	CLA	CMB-C2B-C1B	-2.12	125.21	128.46
30	2	319	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
18	A	808	CLA	CHA-C1A-NA	-2.12	121.54	126.40
18	A	802	CLA	C1D-ND-C4D	-2.12	104.83	106.33
18	G	1603	CLA	CHA-C1A-NA	-2.12	121.55	126.40
30	2	314	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
18	A	823	CLA	O2A-CGA-CBA	2.12	118.55	111.91
21	F	305	BCR	C37-C22-C23	2.12	121.41	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	3	313	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
30	4	318	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
18	F	303	CLA	O1D-CGD-CBD	-2.12	120.16	124.48
18	1	5012	CLA	CHA-C1A-NA	-2.12	121.55	126.40
18	A	813	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
18	4	310	CLA	CHA-C1A-NA	-2.11	121.56	126.40
18	A	831	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
18	A	807	CLA	C1D-ND-C4D	-2.11	104.83	106.33
18	2	311	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
21	K	1405	BCR	C35-C13-C12	2.11	121.41	118.08
18	3	307	CLA	CMB-C2B-C3B	2.11	128.63	124.68
18	L	304	CLA	CHA-C1A-NA	-2.11	121.56	126.40
30	1	5014	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
30	3	316	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
18	B	830	CLA	CAC-C3C-C4C	2.11	127.55	124.81
21	3	305	BCR	C27-C26-C25	-2.11	119.67	122.73
21	A	843	BCR	C34-C9-C10	-2.11	119.97	122.92
18	G	1603	CLA	O2A-CGA-CBA	2.11	118.53	111.91
18	A	817	CLA	C1D-ND-C4D	-2.11	104.83	106.33
21	A	845	BCR	C37-C22-C21	-2.11	119.97	122.92
18	B	825	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
18	2	317	CLA	CHA-C1A-NA	-2.11	121.56	126.40
21	B	844	BCR	C12-C13-C14	-2.11	115.70	118.94
18	A	826	CLA	C1D-ND-C4D	-2.11	104.84	106.33
18	1	5011	CLA	C1D-ND-C4D	-2.11	104.84	106.33
18	4	306	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
21	A	845	BCR	C30-C25-C26	-2.11	119.64	122.61
21	F	305	BCR	C35-C13-C12	2.11	121.40	118.08
30	1	5014	CHL	C4A-NA-C1A	2.11	107.65	106.71
18	F	301	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
18	A	836	CLA	CHA-C1A-NA	-2.11	121.57	126.40
21	B	845	BCR	C34-C9-C10	-2.11	119.97	122.92
18	B	807	CLA	O2A-CGA-CBA	2.11	118.52	111.91
30	2	318	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
18	B	816	CLA	C1-O2A-CGA	2.11	121.97	116.44
18	A	824	CLA	C1-O2A-CGA	2.11	121.97	116.44
18	4	305	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
18	A	832	CLA	CHA-C1A-NA	-2.11	121.58	126.40
18	A	818	CLA	CMD-C2D-C3D	-2.11	122.77	127.61
30	4	302	CHL	CMB-C2B-C1B	-2.11	125.23	128.46
18	A	852	CLA	CHA-C1A-NA	-2.11	121.58	126.40
18	B	836	CLA	C1D-ND-C4D	-2.10	104.84	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	1	5016	CHL	CMB-C2B-C1B	-2.10	125.23	128.46
18	B	840	CLA	C1-O2A-CGA	2.10	121.96	116.44
29	2	303	LUT	C40-C33-C32	2.10	121.39	118.08
18	G	1601	CLA	CHA-C1A-NA	-2.10	121.58	126.40
29	2	303	LUT	C3-C4-C5	-2.10	107.67	111.85
18	B	823	CLA	CHA-C1A-NA	-2.10	121.58	126.40
18	B	810	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
18	B	836	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
18	2	312	CLA	CHA-C1A-NA	-2.10	121.59	126.40
21	F	305	BCR	C34-C9-C10	-2.10	119.98	122.92
18	1	5010	CLA	CMB-C2B-C1B	-2.10	125.23	128.46
18	B	818	CLA	CHA-C1A-NA	-2.10	121.59	126.40
18	3	309	CLA	CHA-C1A-NA	-2.10	121.59	126.40
18	A	808	CLA	CMB-C2B-C1B	-2.10	125.24	128.46
30	4	314	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
18	3	309	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
18	A	816	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
18	B	824	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
18	A	852	CLA	O2A-CGA-CBA	2.10	118.49	111.91
21	2	305	BCR	C4-C5-C6	-2.10	119.69	122.73
18	F	302	CLA	C1D-ND-C4D	-2.10	104.84	106.33
18	L	301	CLA	CMD-C2D-C3D	-2.10	122.79	127.61
24	1	5020	LMG	C8-O7-C10	-2.10	112.63	117.79
30	4	316	CHL	CHD-C4C-C3C	2.10	127.92	124.84
18	2	313	CLA	O1D-CGD-CBD	-2.10	120.20	124.48
18	J	1103	CLA	CMA-C3A-C2A	2.09	122.28	113.83
18	2	326	CLA	CHA-C1A-NA	-2.09	121.60	126.40
24	B	851	LMG	C7-O1-C1	-2.09	109.65	113.74
29	J	1105	LUT	C31-C32-C33	-2.09	120.53	126.42
29	J	1105	LUT	C40-C33-C34	-2.09	119.99	122.92
18	A	825	CLA	CHA-C1A-NA	-2.09	121.60	126.40
21	B	846	BCR	C34-C9-C10	-2.09	119.99	122.92
30	2	318	CHL	C2C-C3C-C4C	2.09	107.98	106.49
18	1	5009	CLA	CMB-C2B-C3B	2.09	128.59	124.68
18	J	1103	CLA	O2A-CGA-CBA	2.09	118.47	111.91
18	4	311	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
21	B	846	BCR	C12-C13-C14	-2.09	115.73	118.94
18	3	309	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
18	A	830	CLA	CMA-C3A-C4A	2.09	117.39	111.77
21	F	305	BCR	C30-C25-C24	2.09	121.69	115.78
18	G	1601	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
18	A	831	CLA	C1D-ND-C4D	-2.09	104.85	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	841	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
21	B	843	BCR	C38-C26-C27	2.09	117.62	113.62
18	A	807	CLA	O2A-CGA-CBA	2.09	118.45	111.91
18	A	803	CLA	C1D-ND-C4D	-2.09	104.85	106.33
18	A	828	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
18	B	817	CLA	CMB-C2B-C3B	2.09	128.58	124.68
18	4	305	CLA	C1-O2A-CGA	2.09	121.92	116.44
18	B	832	CLA	C1D-ND-C4D	-2.08	104.85	106.33
18	B	834	CLA	CHA-C1A-NA	-2.08	121.62	126.40
18	A	816	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
30	2	316	CHL	CMB-C2B-C1B	-2.08	125.26	128.46
18	A	803	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
21	1	5005	BCR	C35-C13-C12	2.08	121.36	118.08
18	A	805	CLA	CHA-C1A-NA	-2.08	121.63	126.40
21	A	855	BCR	C29-C28-C27	2.08	116.03	111.38
18	A	821	CLA	C1D-ND-C4D	-2.08	104.86	106.33
18	J	1101	CLA	CHA-C1A-NA	-2.08	121.63	126.40
29	3	303	LUT	C2-C3-C4	-2.08	107.46	110.30
29	1	5003	LUT	C31-C32-C33	-2.08	120.57	126.42
18	K	1404	CLA	CHA-C1A-NA	-2.08	121.63	126.40
29	2	303	LUT	C10-C11-C12	-2.08	116.73	123.22
18	A	825	CLA	O2A-CGA-CBA	2.08	118.43	111.91
18	4	315	CLA	CHA-C1A-NA	-2.08	121.64	126.40
18	A	826	CLA	C6-C5-C3	-2.08	108.01	113.45
18	A	812	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
18	B	805	CLA	C1D-ND-C4D	-2.07	104.86	106.33
18	L	306	CLA	CMB-C2B-C3B	2.07	128.56	124.68
18	A	833	CLA	C1D-ND-C4D	-2.07	104.86	106.33
18	B	841	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
18	A	838	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
18	4	309	CLA	CAC-C3C-C4C	2.07	127.50	124.81
18	A	814	CLA	CHA-C1A-NA	-2.07	121.66	126.40
18	B	817	CLA	CMC-C2C-C1C	2.07	128.19	125.04
18	A	833	CLA	CHA-C1A-NA	-2.07	121.66	126.40
18	A	816	CLA	CHA-C1A-NA	-2.07	121.66	126.40
21	A	847	BCR	C37-C22-C23	2.07	121.34	118.08
18	B	824	CLA	CHA-C1A-NA	-2.07	121.66	126.40
18	A	807	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
18	B	838	CLA	CHA-C1A-NA	-2.07	121.67	126.40
18	B	839	CLA	C1-O2A-CGA	2.07	121.87	116.44
18	B	821	CLA	O1D-CGD-CBD	-2.07	120.26	124.48
21	F	305	BCR	C31-C1-C6	-2.07	106.95	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	820	CLA	CHA-C1A-NA	-2.06	121.67	126.40
30	3	316	CHL	CHD-C4C-C3C	2.06	127.87	124.84
18	A	830	CLA	C1D-ND-C4D	-2.06	104.87	106.33
18	A	829	CLA	CHA-C1A-NA	-2.06	121.67	126.40
18	B	828	CLA	CMB-C2B-C1B	-2.06	125.29	128.46
18	B	831	CLA	CHA-C1A-NA	-2.06	121.67	126.40
30	4	316	CHL	C4A-NA-C1A	2.06	107.63	106.71
18	B	830	CLA	CHA-C1A-NA	-2.06	121.68	126.40
23	B	856	LMT	C3B-C4B-C5B	-2.06	106.56	110.24
28	F	310	ZEX	C20-C13-C14	-2.06	120.04	122.92
18	K	1401	CLA	CHA-C1A-NA	-2.06	121.68	126.40
18	B	812	CLA	C1-O2A-CGA	2.06	121.85	116.44
18	A	822	CLA	CHA-C1A-NA	-2.06	121.68	126.40
18	A	840	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
18	B	811	CLA	O2A-CGA-CBA	2.06	118.37	111.91
18	4	315	CLA	O2A-CGA-CBA	2.06	118.37	111.91
18	3	311	CLA	C1D-ND-C4D	-2.06	104.87	106.33
18	A	811	CLA	CHA-C1A-NA	-2.06	121.69	126.40
18	A	840	CLA	CHA-C1A-NA	-2.06	121.69	126.40
18	B	811	CLA	CHA-C1A-NA	-2.06	121.69	126.40
18	A	805	CLA	O2A-CGA-CBA	2.06	118.36	111.91
18	B	832	CLA	CHA-C1A-NA	-2.05	121.69	126.40
18	B	816	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
18	B	838	CLA	CMD-C2D-C3D	-2.05	122.89	127.61
18	1	5011	CLA	C1-O2A-CGA	2.05	121.83	116.44
30	4	313	CHL	CHC-C1C-NC	2.05	127.32	124.20
18	F	303	CLA	CHA-C1A-NA	-2.05	121.70	126.40
18	G	1602	CLA	CHA-C1A-NA	-2.05	121.70	126.40
18	B	820	CLA	C1D-ND-C4D	-2.05	104.88	106.33
18	A	820	CLA	C1D-ND-C4D	-2.05	104.88	106.33
18	A	823	CLA	C1D-ND-C4D	-2.05	104.88	106.33
18	1	5017	CLA	CHA-C1A-NA	-2.05	121.70	126.40
18	2	306	CLA	CAA-C2A-C1A	-2.05	105.26	111.97
18	2	307	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
18	1	5010	CLA	CHA-C1A-NA	-2.05	121.71	126.40
18	2	317	CLA	CMB-C2B-C3B	2.05	128.51	124.68
21	I	101	BCR	C27-C26-C25	-2.05	119.76	122.73
18	B	813	CLA	CHA-C1A-NA	-2.05	121.71	126.40
29	3	303	LUT	C19-C9-C8	2.05	121.30	118.08
18	A	836	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
18	F	302	CLA	C1-O2A-CGA	2.04	121.81	116.44
29	J	1105	LUT	C3-C4-C5	-2.04	107.78	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	814	CLA	C1D-ND-C4D	-2.04	104.88	106.33
18	A	818	CLA	CHA-C1A-NA	-2.04	121.72	126.40
18	B	835	CLA	C1D-ND-C4D	-2.04	104.88	106.33
18	1	5011	CLA	CMB-C2B-C3B	2.04	128.50	124.68
18	3	317	CLA	CMB-C2B-C3B	2.04	128.50	124.68
18	B	838	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
18	1	5018	CLA	CMB-C2B-C3B	2.04	128.50	124.68
18	1	5007	CLA	CHA-C1A-NA	-2.04	121.72	126.40
29	3	304	LUT	C39-C29-C30	-2.04	120.06	122.92
18	A	808	CLA	C1D-ND-C4D	-2.04	104.89	106.33
18	1	5007	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
18	A	823	CLA	CHA-C1A-NA	-2.04	121.73	126.40
21	A	855	BCR	C35-C13-C12	2.04	121.29	118.08
18	3	307	CLA	CHA-C1A-NA	-2.04	121.73	126.40
18	J	1101	CLA	CMB-C2B-C3B	2.04	128.49	124.68
18	B	831	CLA	O2A-CGA-CBA	2.04	118.30	111.91
18	B	835	CLA	CHA-C1A-NA	-2.04	121.73	126.40
18	A	812	CLA	CHA-C1A-NA	-2.04	121.73	126.40
18	B	832	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
30	2	319	CHL	C1-C2-C3	-2.04	122.52	126.04
18	B	804	CLA	C1C-C2C-C3C	-2.04	104.82	106.96
18	1	5006	CLA	CHA-C1A-NA	-2.04	121.74	126.40
18	4	306	CLA	C1D-ND-C4D	-2.04	104.89	106.33
18	A	808	CLA	C1-O2A-CGA	2.03	121.78	116.44
18	L	301	CLA	CHA-C1A-NA	-2.03	121.74	126.40
30	4	316	CHL	CMB-C2B-C1B	-2.03	125.34	128.46
21	I	102	BCR	C35-C13-C12	2.03	121.28	118.08
18	B	820	CLA	CHA-C1A-NA	-2.03	121.74	126.40
18	B	817	CLA	C1-C2-C3	-2.03	122.53	126.04
18	1	5018	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
18	4	311	CLA	CHA-C1A-NA	-2.03	121.75	126.40
21	1	5005	BCR	C38-C26-C27	2.03	117.52	113.62
30	1	5014	CHL	C1-O2A-CGA	2.03	122.80	116.11
24	F	306	LMG	O7-C10-O9	-2.03	118.80	123.70
21	I	101	BCR	C8-C7-C6	-2.03	121.50	127.20
18	2	311	CLA	CMA-C3A-C4A	2.03	117.23	111.77
18	H	1701	CLA	C1D-ND-C4D	-2.03	104.89	106.33
21	A	845	BCR	C8-C7-C6	-2.03	121.51	127.20
18	F	301	CLA	CMD-C2D-C3D	-2.03	122.95	127.61
30	1	5014	CHL	CHD-C4C-C3C	2.03	127.82	124.84
18	3	308	CLA	CHA-C1A-NA	-2.03	121.75	126.40
21	L	302	BCR	C30-C25-C24	2.03	121.51	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	803	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
18	A	831	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
21	F	304	BCR	C15-C14-C13	-2.03	124.42	127.31
18	1	5010	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
18	B	804	CLA	CMD-C2D-C3D	-2.03	122.95	127.61
26	2	327	DGD	O2G-C1B-O1B	-2.03	118.81	123.70
18	F	301	CLA	CHA-C1A-NA	-2.03	121.76	126.40
18	B	817	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
18	4	312	CLA	CHA-C1A-NA	-2.02	121.76	126.40
18	B	838	CLA	CMB-C2B-C3B	2.02	128.47	124.68
21	G	1604	BCR	C4-C5-C6	-2.02	119.79	122.73
18	A	805	CLA	CMA-C3A-C4A	2.02	117.21	111.77
21	I	102	BCR	C32-C1-C6	-2.02	107.02	110.30
21	A	843	BCR	C38-C26-C25	-2.02	122.26	124.53
18	B	801	CLA	CMD-C2D-C3D	-2.02	122.96	127.61
21	L	302	BCR	C27-C26-C25	-2.02	119.80	122.73
21	L	303	BCR	C31-C1-C6	-2.02	107.02	110.30
18	B	806	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
18	4	305	CLA	O2A-CGA-CBA	2.02	118.25	111.91
18	1	5011	CLA	CHA-C1A-NA	-2.02	121.77	126.40
30	2	319	CHL	C4A-NA-C1A	2.02	107.61	106.71
21	A	845	BCR	C35-C13-C12	2.02	121.26	118.08
18	B	824	CLA	O2A-CGA-CBA	2.02	118.24	111.91
26	1	5002	DGD	C2G-O2G-C1B	-2.02	112.82	117.79
18	B	803	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
21	L	307	BCR	C37-C22-C21	-2.02	120.10	122.92
18	A	829	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
18	B	805	CLA	CHA-C1A-NA	-2.02	121.78	126.40
23	B	853	LMT	C1'-C2'-C3'	2.02	114.20	110.00
18	B	819	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
18	A	819	CLA	CHA-C1A-NA	-2.02	121.78	126.40
18	B	827	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
18	3	307	CLA	O2A-CGA-CBA	2.02	118.24	111.91
18	4	311	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
18	3	315	CLA	CHA-C1A-NA	-2.02	121.78	126.40
18	A	815	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
18	J	1103	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
18	3	301	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
18	A	840	CLA	C1D-ND-C4D	-2.02	104.90	106.33
18	B	826	CLA	CMB-C2B-C1B	-2.02	125.37	128.46
18	2	313	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
18	B	836	CLA	CMB-C2B-C3B	2.01	128.45	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	815	CLA	CHA-C1A-NA	-2.01	121.78	126.40
21	A	847	BCR	C27-C26-C25	-2.01	119.81	122.73
18	B	837	CLA	CMB-C2B-C3B	2.01	128.45	124.68
18	B	840	CLA	CHA-C1A-NA	-2.01	121.79	126.40
18	A	804	CLA	CMB-C2B-C3B	2.01	128.44	124.68
18	2	312	CLA	CMD-C2D-C3D	-2.01	122.98	127.61
18	J	1101	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
18	A	813	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
18	A	832	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
18	3	301	CLA	C1D-ND-C4D	-2.01	104.91	106.33
18	3	319	CLA	O2A-CGA-CBA	2.01	118.21	111.91
18	G	1601	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
18	2	313	CLA	CHA-C1A-NA	-2.01	121.80	126.40
29	3	303	LUT	C20-C13-C12	2.01	121.24	118.08
18	1	5007	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
18	3	307	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
30	4	318	CHL	CHD-C4C-C3C	2.01	127.79	124.84
18	B	841	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
21	F	305	BCR	C30-C25-C26	-2.01	119.79	122.61
30	3	310	CHL	CHC-C1C-NC	2.01	127.25	124.20
21	I	102	BCR	C38-C26-C27	2.01	117.47	113.62
18	A	823	CLA	C3D-C2D-C1D	-2.00	103.09	105.83
18	4	307	CLA	C1-O2A-CGA	2.00	121.70	116.44
21	B	843	BCR	C38-C26-C25	-2.00	122.28	124.53
29	1	5004	LUT	C20-C13-C14	-2.00	120.12	122.92
29	3	303	LUT	C8-C7-C6	-2.00	121.58	127.20
21	B	844	BCR	C30-C25-C26	-2.00	119.79	122.61
18	B	803	CLA	C6-C5-C3	-2.00	108.20	113.45
21	2	305	BCR	C23-C24-C25	-2.00	121.58	127.20
29	1	5004	LUT	C38-C25-C24	-2.00	119.28	123.56
29	2	303	LUT	C28-C29-C30	-2.00	115.87	118.94
18	B	816	CLA	CHA-C1A-NA	-2.00	121.82	126.40

All (206) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	A	801	CL0	NA
17	A	801	CL0	ND
17	A	801	CL0	NC
18	A	802	CLA	ND
18	A	803	CLA	ND
18	A	804	CLA	ND

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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
18	B	806	CLA	ND
18	B	807	CLA	ND
18	B	808	CLA	ND
18	B	809	CLA	ND
18	B	810	CLA	ND
18	B	811	CLA	ND
18	B	812	CLA	ND
18	B	813	CLA	ND
18	B	814	CLA	ND
18	B	815	CLA	ND
18	B	816	CLA	ND
18	B	817	CLA	ND
18	B	818	CLA	ND
18	B	819	CLA	ND
18	B	820	CLA	ND
18	B	821	CLA	ND
18	B	822	CLA	ND
18	B	823	CLA	ND
18	B	824	CLA	ND
18	B	825	CLA	ND
18	B	826	CLA	ND
18	B	827	CLA	ND
18	B	828	CLA	ND
18	B	829	CLA	ND
18	B	830	CLA	ND
18	B	831	CLA	ND
18	B	832	CLA	ND
18	B	833	CLA	ND
18	B	834	CLA	ND
18	B	835	CLA	ND
18	B	836	CLA	ND
18	B	837	CLA	ND
18	B	838	CLA	ND
18	B	839	CLA	ND
18	B	840	CLA	ND
18	B	841	CLA	ND
18	F	301	CLA	ND
18	F	302	CLA	ND
18	F	303	CLA	ND
18	G	1601	CLA	ND
18	G	1602	CLA	ND
18	G	1603	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
18	H	1701	CLA	ND
18	J	1101	CLA	ND
18	J	1103	CLA	ND
18	K	1401	CLA	ND
18	K	1402	CLA	ND
18	K	1403	CLA	ND
18	K	1404	CLA	ND
18	L	301	CLA	ND
18	L	304	CLA	ND
18	L	305	CLA	ND
18	L	306	CLA	ND
18	1	5006	CLA	ND
18	1	5007	CLA	ND
18	1	5008	CLA	ND
18	1	5009	CLA	ND
18	1	5010	CLA	ND
18	1	5011	CLA	ND
18	1	5012	CLA	ND
18	1	5013	CLA	ND
18	1	5015	CLA	ND
18	1	5017	CLA	ND
18	1	5018	CLA	ND
18	2	306	CLA	ND
18	2	307	CLA	ND
18	2	308	CLA	ND
18	2	309	CLA	ND
18	2	310	CLA	ND
18	2	311	CLA	ND
18	2	312	CLA	ND
18	2	313	CLA	ND
18	2	317	CLA	ND
18	2	326	CLA	ND
18	3	301	CLA	ND
18	3	307	CLA	ND
18	3	308	CLA	ND
18	3	309	CLA	ND
18	3	311	CLA	ND
18	3	314	CLA	ND
18	3	315	CLA	ND
18	3	317	CLA	ND
18	3	318	CLA	ND
18	3	319	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
18	4	305	CLA	ND
18	4	306	CLA	ND
18	4	307	CLA	ND
18	4	308	CLA	ND
18	4	309	CLA	ND
18	4	310	CLA	ND
18	4	311	CLA	ND
18	4	312	CLA	ND
18	4	315	CLA	ND
29	J	1105	LUT	C26
29	1	5004	LUT	C26
29	2	303	LUT	C26
29	3	304	LUT	C26
30	1	5014	CHL	NA
30	1	5014	CHL	ND
30	1	5014	CHL	NC
30	1	5016	CHL	NA
30	1	5016	CHL	ND
30	1	5016	CHL	C8
30	1	5016	CHL	NC
30	2	314	CHL	NA
30	2	314	CHL	ND
30	2	314	CHL	C8
30	2	314	CHL	NC
30	2	315	CHL	NA
30	2	315	CHL	ND
30	2	315	CHL	C8
30	2	315	CHL	NC
30	2	316	CHL	NA
30	2	316	CHL	ND
30	2	316	CHL	NC
30	2	318	CHL	NA
30	2	318	CHL	ND
30	2	318	CHL	NC
30	2	319	CHL	NA
30	2	319	CHL	ND
30	2	319	CHL	C8
30	2	319	CHL	NC
30	3	310	CHL	NA
30	3	310	CHL	ND
30	3	310	CHL	C8
30	3	310	CHL	NC

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Mol	Chain	Res	Type	Atom
30	3	312	CHL	NA
30	3	312	CHL	ND
30	3	312	CHL	NC
30	3	313	CHL	NA
30	3	313	CHL	ND
30	3	313	CHL	NC
30	3	316	CHL	NA
30	3	316	CHL	ND
30	3	316	CHL	NC
30	4	302	CHL	NA
30	4	302	CHL	ND
30	4	302	CHL	C8
30	4	302	CHL	NC
30	4	313	CHL	NA
30	4	313	CHL	ND
30	4	313	CHL	NC
30	4	314	CHL	NA
30	4	314	CHL	ND
30	4	314	CHL	NC
30	4	316	CHL	NA
30	4	316	CHL	ND
30	4	316	CHL	C8
30	4	316	CHL	NC
30	4	317	CHL	NA
30	4	317	CHL	ND
30	4	317	CHL	NC
30	4	318	CHL	NA
30	4	318	CHL	ND
30	4	318	CHL	C8
30	4	318	CHL	NC
31	2	304	XAT	C6
31	4	304	XAT	C6

All (2777) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	802	CLA	C2-C1-O2A-CGA
18	A	802	CLA	CHA-CBD-CGD-O1D
18	A	802	CLA	CHA-CBD-CGD-O2D
18	A	802	CLA	C2-C3-C5-C6
18	A	802	CLA	C4-C3-C5-C6
18	A	803	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	A	803	CLA	C3A-C2A-CAA-CBA
18	A	804	CLA	C1A-C2A-CAA-CBA
18	A	804	CLA	C3A-C2A-CAA-CBA
18	A	804	CLA	C2-C1-O2A-CGA
18	A	804	CLA	CHA-CBD-CGD-O1D
18	A	804	CLA	CHA-CBD-CGD-O2D
18	A	804	CLA	CAD-CBD-CGD-O1D
18	A	805	CLA	C3A-C2A-CAA-CBA
18	A	805	CLA	CBD-CGD-O2D-CED
18	A	805	CLA	C2-C3-C5-C6
18	A	805	CLA	C4-C3-C5-C6
18	A	806	CLA	C2-C1-O2A-CGA
18	A	806	CLA	CBD-CGD-O2D-CED
18	A	807	CLA	C3A-C2A-CAA-CBA
18	A	807	CLA	CHA-CBD-CGD-O1D
18	A	807	CLA	CHA-CBD-CGD-O2D
18	A	808	CLA	CBD-CGD-O2D-CED
18	A	808	CLA	C2-C3-C5-C6
18	A	808	CLA	C4-C3-C5-C6
18	A	809	CLA	CBD-CGD-O2D-CED
18	A	810	CLA	C1A-C2A-CAA-CBA
18	A	810	CLA	C3A-C2A-CAA-CBA
18	A	810	CLA	C4-C3-C5-C6
18	A	811	CLA	C1A-C2A-CAA-CBA
18	A	811	CLA	C3A-C2A-CAA-CBA
18	A	812	CLA	CHA-CBD-CGD-O1D
18	A	812	CLA	CHA-CBD-CGD-O2D
18	A	813	CLA	C14-C13-C15-C16
18	A	814	CLA	CBD-CGD-O2D-CED
18	A	815	CLA	C4-C3-C5-C6
18	A	816	CLA	C3A-C2A-CAA-CBA
18	A	816	CLA	CBD-CGD-O2D-CED
18	A	816	CLA	C2-C3-C5-C6
18	A	816	CLA	C4-C3-C5-C6
18	A	817	CLA	CHA-CBD-CGD-O1D
18	A	817	CLA	CHA-CBD-CGD-O2D
18	A	818	CLA	C2-C1-O2A-CGA
18	A	818	CLA	CBD-CGD-O2D-CED
18	A	819	CLA	C2-C1-O2A-CGA
18	A	819	CLA	C2-C3-C5-C6
18	A	819	CLA	C4-C3-C5-C6
18	A	821	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	A	822	CLA	CHA-CBD-CGD-O1D
18	A	822	CLA	CHA-CBD-CGD-O2D
18	A	823	CLA	C2-C1-O2A-CGA
18	A	824	CLA	C1A-C2A-CAA-CBA
18	A	824	CLA	C3A-C2A-CAA-CBA
18	A	825	CLA	C1A-C2A-CAA-CBA
18	A	825	CLA	C3A-C2A-CAA-CBA
18	A	826	CLA	C1A-C2A-CAA-CBA
18	A	826	CLA	C2-C1-O2A-CGA
18	A	829	CLA	C2A-CAA-CBA-CGA
18	A	831	CLA	CHA-CBD-CGD-O1D
18	A	831	CLA	CHA-CBD-CGD-O2D
18	A	831	CLA	C2-C3-C5-C6
18	A	831	CLA	C4-C3-C5-C6
18	A	831	CLA	C14-C13-C15-C16
18	A	832	CLA	C11-C10-C8-C9
18	A	833	CLA	CHA-CBD-CGD-O1D
18	A	833	CLA	CHA-CBD-CGD-O2D
18	A	834	CLA	C1A-C2A-CAA-CBA
18	A	834	CLA	C3A-C2A-CAA-CBA
18	A	834	CLA	CBD-CGD-O2D-CED
18	A	836	CLA	CHA-CBD-CGD-O1D
18	A	836	CLA	CHA-CBD-CGD-O2D
18	A	837	CLA	CBD-CGD-O2D-CED
18	A	838	CLA	C4-C3-C5-C6
18	A	839	CLA	CBD-CGD-O2D-CED
18	A	840	CLA	C2A-CAA-CBA-CGA
18	A	840	CLA	CHA-CBD-CGD-O1D
18	A	840	CLA	CHA-CBD-CGD-O2D
18	A	853	CLA	CBD-CGD-O2D-CED
18	A	853	CLA	C2-C3-C5-C6
18	A	853	CLA	C4-C3-C5-C6
18	A	853	CLA	C11-C12-C13-C14
18	B	801	CLA	CHA-CBD-CGD-O1D
18	B	801	CLA	CAD-CBD-CGD-O1D
18	B	801	CLA	CAD-CBD-CGD-O2D
18	B	803	CLA	CHA-CBD-CGD-O1D
18	B	803	CLA	CHA-CBD-CGD-O2D
18	B	803	CLA	CBD-CGD-O2D-CED
18	B	804	CLA	CHA-CBD-CGD-O1D
18	B	804	CLA	CHA-CBD-CGD-O2D
18	B	804	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	B	805	CLA	C1A-C2A-CAA-CBA
18	B	805	CLA	C3A-C2A-CAA-CBA
18	B	805	CLA	CBD-CGD-O2D-CED
18	B	806	CLA	C3A-C2A-CAA-CBA
18	B	807	CLA	C6-C7-C8-C9
18	B	808	CLA	CHA-CBD-CGD-O1D
18	B	808	CLA	CHA-CBD-CGD-O2D
18	B	809	CLA	CHA-CBD-CGD-O1D
18	B	809	CLA	CHA-CBD-CGD-O2D
18	B	809	CLA	CBD-CGD-O2D-CED
18	B	810	CLA	C2-C1-O2A-CGA
18	B	810	CLA	CBD-CGD-O2D-CED
18	B	811	CLA	C2-C1-O2A-CGA
18	B	811	CLA	CBD-CGD-O2D-CED
18	B	811	CLA	C6-C7-C8-C9
18	B	813	CLA	CBD-CGD-O2D-CED
18	B	816	CLA	CBD-CGD-O2D-CED
18	B	818	CLA	C2-C1-O2A-CGA
18	B	818	CLA	CBD-CGD-O2D-CED
18	B	818	CLA	C11-C10-C8-C9
18	B	819	CLA	C2-C3-C5-C6
18	B	819	CLA	C4-C3-C5-C6
18	B	820	CLA	CHA-CBD-CGD-O1D
18	B	820	CLA	CHA-CBD-CGD-O2D
18	B	821	CLA	CBA-CGA-O2A-C1
18	B	821	CLA	O1A-CGA-O2A-C1
18	B	822	CLA	C4-C3-C5-C6
18	B	823	CLA	CHA-CBD-CGD-O1D
18	B	823	CLA	CHA-CBD-CGD-O2D
18	B	823	CLA	C2-C3-C5-C6
18	B	823	CLA	C4-C3-C5-C6
18	B	825	CLA	C2-C1-O2A-CGA
18	B	826	CLA	C3A-C2A-CAA-CBA
18	B	826	CLA	CHA-CBD-CGD-O1D
18	B	826	CLA	CHA-CBD-CGD-O2D
18	B	828	CLA	C1A-C2A-CAA-CBA
18	B	828	CLA	CHA-CBD-CGD-O1D
18	B	829	CLA	C1A-C2A-CAA-CBA
18	B	829	CLA	C3A-C2A-CAA-CBA
18	B	829	CLA	CHA-CBD-CGD-O1D
18	B	829	CLA	CHA-CBD-CGD-O2D
18	B	829	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
18	B	829	CLA	C4-C3-C5-C6
18	B	830	CLA	CHA-CBD-CGD-O1D
18	B	830	CLA	CHA-CBD-CGD-O2D
18	B	830	CLA	CAD-CBD-CGD-O1D
18	B	832	CLA	C1A-C2A-CAA-CBA
18	B	832	CLA	C3A-C2A-CAA-CBA
18	B	832	CLA	C11-C10-C8-C9
18	B	833	CLA	C1A-C2A-CAA-CBA
18	B	833	CLA	C3A-C2A-CAA-CBA
18	B	833	CLA	CHA-CBD-CGD-O1D
18	B	833	CLA	CHA-CBD-CGD-O2D
18	B	833	CLA	C2-C3-C5-C6
18	B	833	CLA	C4-C3-C5-C6
18	B	835	CLA	C2-C1-O2A-CGA
18	B	835	CLA	CBD-CGD-O2D-CED
18	B	836	CLA	C1A-C2A-CAA-CBA
18	B	836	CLA	CBD-CGD-O2D-CED
18	B	839	CLA	C2-C1-O2A-CGA
18	B	840	CLA	C1A-C2A-CAA-CBA
18	B	840	CLA	C3A-C2A-CAA-CBA
18	B	840	CLA	CBD-CGD-O2D-CED
18	B	841	CLA	CHA-CBD-CGD-O1D
18	B	841	CLA	CHA-CBD-CGD-O2D
18	F	301	CLA	C2-C1-O2A-CGA
18	F	301	CLA	CBD-CGD-O2D-CED
18	F	302	CLA	C1A-C2A-CAA-CBA
18	F	302	CLA	C3A-C2A-CAA-CBA
18	F	302	CLA	C2-C1-O2A-CGA
18	F	303	CLA	CHA-CBD-CGD-O1D
18	F	303	CLA	CHA-CBD-CGD-O2D
18	G	1601	CLA	CBD-CGD-O2D-CED
18	G	1602	CLA	CBA-CGA-O2A-C1
18	H	1701	CLA	CHA-CBD-CGD-O1D
18	H	1701	CLA	CHA-CBD-CGD-O2D
18	H	1701	CLA	CBD-CGD-O2D-CED
18	H	1701	CLA	C4-C3-C5-C6
18	K	1402	CLA	C1A-C2A-CAA-CBA
18	K	1402	CLA	CHA-CBD-CGD-O1D
18	K	1402	CLA	CHA-CBD-CGD-O2D
18	K	1402	CLA	C2-C3-C5-C6
18	K	1402	CLA	C4-C3-C5-C6
18	K	1403	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	L	301	CLA	CBD-CGD-O2D-CED
18	L	304	CLA	C1A-C2A-CAA-CBA
18	L	304	CLA	C2-C1-O2A-CGA
18	L	305	CLA	CHA-CBD-CGD-O1D
18	L	305	CLA	CHA-CBD-CGD-O2D
18	L	306	CLA	C1A-C2A-CAA-CBA
18	1	5006	CLA	C2-C3-C5-C6
18	1	5006	CLA	C4-C3-C5-C6
18	1	5007	CLA	CBA-CGA-O2A-C1
18	1	5007	CLA	CBD-CGD-O2D-CED
18	1	5008	CLA	C1A-C2A-CAA-CBA
18	1	5008	CLA	CBD-CGD-O2D-CED
18	1	5010	CLA	CBD-CGD-O2D-CED
18	1	5010	CLA	C2-C3-C5-C6
18	1	5010	CLA	C4-C3-C5-C6
18	1	5011	CLA	CHA-CBD-CGD-O1D
18	1	5011	CLA	CHA-CBD-CGD-O2D
18	1	5011	CLA	CBD-CGD-O2D-CED
18	1	5012	CLA	CHA-CBD-CGD-O1D
18	1	5012	CLA	CHA-CBD-CGD-O2D
18	1	5013	CLA	CBD-CGD-O2D-CED
18	1	5015	CLA	C2-C1-O2A-CGA
18	2	306	CLA	C3A-C2A-CAA-CBA
18	2	309	CLA	C3A-C2A-CAA-CBA
18	2	310	CLA	CHA-CBD-CGD-O1D
18	2	310	CLA	CHA-CBD-CGD-O2D
18	2	311	CLA	C1A-C2A-CAA-CBA
18	2	311	CLA	CHA-CBD-CGD-O1D
18	2	311	CLA	CHA-CBD-CGD-O2D
18	2	312	CLA	CBD-CGD-O2D-CED
18	2	312	CLA	C4-C3-C5-C6
18	2	313	CLA	C1A-C2A-CAA-CBA
18	2	313	CLA	C2A-CAA-CBA-CGA
18	2	326	CLA	CHA-CBD-CGD-O1D
18	2	326	CLA	CHA-CBD-CGD-O2D
18	2	326	CLA	CAD-CBD-CGD-O1D
18	2	326	CLA	CAD-CBD-CGD-O2D
18	3	301	CLA	C3A-C2A-CAA-CBA
18	3	301	CLA	CHA-CBD-CGD-O1D
18	3	301	CLA	CHA-CBD-CGD-O2D
18	3	307	CLA	C1A-C2A-CAA-CBA
18	3	307	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	3	308	CLA	C3-C5-C6-C7
18	3	309	CLA	C2-C3-C5-C6
18	3	309	CLA	C4-C3-C5-C6
18	3	314	CLA	C1A-C2A-CAA-CBA
18	3	315	CLA	C3A-C2A-CAA-CBA
18	3	317	CLA	C1A-C2A-CAA-CBA
18	3	317	CLA	C3A-C2A-CAA-CBA
18	3	317	CLA	C2-C1-O2A-CGA
18	3	317	CLA	CBD-CGD-O2D-CED
18	3	318	CLA	C1A-C2A-CAA-CBA
18	3	318	CLA	C3A-C2A-CAA-CBA
18	3	318	CLA	CBD-CGD-O2D-CED
18	3	319	CLA	C2-C1-O2A-CGA
18	3	319	CLA	CBD-CGD-O2D-CED
18	3	319	CLA	C2-C3-C5-C6
18	3	319	CLA	C4-C3-C5-C6
18	4	307	CLA	C2-C3-C5-C6
18	4	307	CLA	C4-C3-C5-C6
18	4	308	CLA	CHA-CBD-CGD-O1D
18	4	308	CLA	CHA-CBD-CGD-O2D
18	4	309	CLA	C1A-C2A-CAA-CBA
18	4	311	CLA	C1A-C2A-CAA-CBA
18	4	311	CLA	C3A-C2A-CAA-CBA
18	4	311	CLA	CHA-CBD-CGD-O1D
18	4	312	CLA	CHA-CBD-CGD-O1D
18	4	312	CLA	CHA-CBD-CGD-O2D
18	4	315	CLA	O1A-CGA-O2A-C1
18	4	315	CLA	CBD-CGD-O2D-CED
19	A	841	PQN	C12-C13-C15-C16
19	A	841	PQN	C14-C13-C15-C16
21	A	843	BCR	C1-C6-C7-C8
21	A	843	BCR	C11-C10-C9-C8
21	A	843	BCR	C11-C10-C9-C34
21	A	843	BCR	C10-C11-C12-C13
21	A	843	BCR	C11-C12-C13-C14
21	A	843	BCR	C11-C12-C13-C35
21	A	844	BCR	C11-C10-C9-C8
21	A	844	BCR	C11-C10-C9-C34
21	A	844	BCR	C36-C18-C19-C20
21	A	844	BCR	C23-C24-C25-C30
21	A	845	BCR	C11-C10-C9-C8
21	A	845	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
21	A	845	BCR	C17-C18-C19-C20
21	A	845	BCR	C36-C18-C19-C20
21	A	845	BCR	C21-C22-C23-C24
21	A	845	BCR	C37-C22-C23-C24
21	A	846	BCR	C11-C10-C9-C8
21	A	846	BCR	C11-C10-C9-C34
21	A	846	BCR	C10-C11-C12-C13
21	A	847	BCR	C7-C8-C9-C34
21	A	847	BCR	C11-C10-C9-C8
21	A	847	BCR	C11-C10-C9-C34
21	A	847	BCR	C17-C18-C19-C20
21	A	847	BCR	C36-C18-C19-C20
21	A	847	BCR	C21-C22-C23-C24
21	A	847	BCR	C37-C22-C23-C24
21	A	855	BCR	C5-C6-C7-C8
21	A	855	BCR	C7-C8-C9-C10
21	A	855	BCR	C7-C8-C9-C34
21	A	855	BCR	C11-C10-C9-C8
21	A	855	BCR	C11-C10-C9-C34
21	B	802	BCR	C11-C10-C9-C8
21	B	802	BCR	C11-C10-C9-C34
21	B	843	BCR	C11-C10-C9-C8
21	B	843	BCR	C11-C10-C9-C34
21	B	843	BCR	C23-C24-C25-C26
21	B	843	BCR	C23-C24-C25-C30
21	B	844	BCR	C11-C10-C9-C8
21	B	844	BCR	C11-C10-C9-C34
21	B	844	BCR	C17-C18-C19-C20
21	B	844	BCR	C36-C18-C19-C20
21	B	844	BCR	C21-C22-C23-C24
21	B	844	BCR	C37-C22-C23-C24
21	B	845	BCR	C11-C12-C13-C14
21	B	845	BCR	C11-C12-C13-C35
21	B	845	BCR	C23-C24-C25-C30
21	B	846	BCR	C11-C10-C9-C8
21	B	846	BCR	C11-C10-C9-C34
21	B	847	BCR	C7-C8-C9-C34
21	B	847	BCR	C11-C10-C9-C8
21	B	847	BCR	C11-C10-C9-C34
21	B	847	BCR	C10-C11-C12-C13
21	B	847	BCR	C17-C18-C19-C20
21	B	847	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
21	F	304	BCR	C7-C8-C9-C34
21	F	304	BCR	C11-C10-C9-C8
21	F	304	BCR	C11-C10-C9-C34
21	F	304	BCR	C17-C18-C19-C20
21	F	304	BCR	C36-C18-C19-C20
21	F	305	BCR	C7-C8-C9-C10
21	F	305	BCR	C7-C8-C9-C34
21	F	305	BCR	C11-C10-C9-C8
21	F	305	BCR	C11-C10-C9-C34
21	F	305	BCR	C10-C11-C12-C13
21	F	305	BCR	C23-C24-C25-C30
21	G	1604	BCR	C17-C18-C19-C20
21	G	1604	BCR	C36-C18-C19-C20
21	I	101	BCR	C1-C6-C7-C8
21	I	101	BCR	C7-C8-C9-C10
21	I	101	BCR	C7-C8-C9-C34
21	I	101	BCR	C10-C11-C12-C13
21	I	101	BCR	C17-C18-C19-C20
21	I	101	BCR	C36-C18-C19-C20
21	I	102	BCR	C7-C8-C9-C10
21	I	102	BCR	C7-C8-C9-C34
21	I	102	BCR	C11-C10-C9-C8
21	I	102	BCR	C11-C10-C9-C34
21	I	102	BCR	C10-C11-C12-C13
21	I	102	BCR	C23-C24-C25-C26
21	I	102	BCR	C23-C24-C25-C30
21	J	1104	BCR	C7-C8-C9-C10
21	J	1104	BCR	C7-C8-C9-C34
21	J	1104	BCR	C11-C10-C9-C8
21	J	1104	BCR	C11-C10-C9-C34
21	J	1104	BCR	C10-C11-C12-C13
21	J	1104	BCR	C21-C22-C23-C24
21	J	1104	BCR	C37-C22-C23-C24
21	K	1405	BCR	C11-C10-C9-C8
21	K	1405	BCR	C11-C10-C9-C34
21	K	1405	BCR	C21-C22-C23-C24
21	K	1405	BCR	C37-C22-C23-C24
21	L	302	BCR	C7-C8-C9-C10
21	L	302	BCR	C7-C8-C9-C34
21	L	302	BCR	C11-C10-C9-C8
21	L	302	BCR	C11-C10-C9-C34
21	L	302	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
21	L	303	BCR	C7-C8-C9-C10
21	L	303	BCR	C7-C8-C9-C34
21	L	307	BCR	C7-C8-C9-C10
21	L	307	BCR	C7-C8-C9-C34
21	L	307	BCR	C11-C10-C9-C8
21	L	307	BCR	C11-C10-C9-C34
21	L	307	BCR	C10-C11-C12-C13
21	L	307	BCR	C11-C12-C13-C14
21	L	307	BCR	C11-C12-C13-C35
21	1	5005	BCR	C36-C18-C19-C20
21	2	305	BCR	C11-C10-C9-C8
21	2	305	BCR	C11-C10-C9-C34
21	2	305	BCR	C11-C12-C13-C14
21	2	305	BCR	C11-C12-C13-C35
21	3	305	BCR	C5-C6-C7-C8
21	3	305	BCR	C7-C8-C9-C10
21	3	305	BCR	C7-C8-C9-C34
21	3	305	BCR	C11-C10-C9-C8
21	3	305	BCR	C11-C10-C9-C34
21	3	305	BCR	C10-C11-C12-C13
21	3	305	BCR	C23-C24-C25-C30
21	3	306	BCR	C5-C6-C7-C8
21	3	306	BCR	C11-C10-C9-C8
21	3	306	BCR	C11-C10-C9-C34
21	4	301	BCR	C5-C6-C7-C8
21	4	301	BCR	C17-C18-C19-C20
21	4	301	BCR	C36-C18-C19-C20
21	4	301	BCR	C21-C22-C23-C24
21	4	301	BCR	C37-C22-C23-C24
22	A	848	LHG	C3-O3-P-O5
22	A	848	LHG	C3-O3-P-O6
22	A	848	LHG	C4-O6-P-O4
22	A	848	LHG	C4-O6-P-O5
22	A	848	LHG	O7-C5-C6-O8
22	A	849	LHG	C3-O3-P-O5
22	A	849	LHG	C3-O3-P-O6
22	A	849	LHG	C4-O6-P-O4
22	B	848	LHG	O1-C1-C2-O2
22	B	848	LHG	O1-C1-C2-C3
22	B	848	LHG	C3-O3-P-O5
22	B	848	LHG	O9-C7-O7-C5
22	B	848	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
22	B	849	LHG	C1-C2-C3-O3
22	B	849	LHG	C3-O3-P-O4
22	B	849	LHG	C3-O3-P-O5
22	B	849	LHG	C3-O3-P-O6
22	B	849	LHG	C4-O6-P-O5
22	B	849	LHG	C8-C7-O7-C5
22	1	5019	LHG	C3-O3-P-O4
22	1	5019	LHG	C3-O3-P-O5
22	1	5019	LHG	C3-O3-P-O6
22	2	320	LHG	O1-C1-C2-C3
23	B	853	LMT	C2'-C1'-O1'-C1
23	B	853	LMT	O5'-C1'-O1'-C1
23	B	853	LMT	C2-C1-O1'-C1'
23	G	1605	LMT	C2-C1-O1'-C1'
23	2	325	LMT	O5'-C1'-O1'-C1
23	2	325	LMT	C2-C1-O1'-C1'
24	A	851	LMG	O6-C1-O1-C7
24	A	851	LMG	O9-C10-O7-C8
24	B	850	LMG	O9-C10-O7-C8
24	B	850	LMG	C11-C10-O7-C8
24	B	851	LMG	O9-C10-O7-C8
24	B	851	LMG	C11-C10-O7-C8
24	F	306	LMG	C11-C10-O7-C8
24	F	308	LMG	C2-C1-O1-C7
24	F	308	LMG	O6-C1-O1-C7
24	F	308	LMG	O9-C10-O7-C8
24	F	308	LMG	C11-C10-O7-C8
24	G	1607	LMG	C2-C1-O1-C7
24	G	1607	LMG	O6-C1-O1-C7
24	G	1607	LMG	C11-C10-O7-C8
24	J	1102	LMG	C11-C10-O7-C8
24	1	5001	LMG	O9-C10-O7-C8
24	2	321	LMG	O9-C10-O7-C8
24	2	321	LMG	C11-C10-O7-C8
26	B	855	DGD	O1B-C1B-O2G-C2G
26	F	309	DGD	C2D-C1D-O3G-C3G
26	F	309	DGD	O6D-C1D-O3G-C3G
26	F	309	DGD	C4D-C5D-C6D-O5D
26	2	327	DGD	O1G-C1G-C2G-O2G
28	F	310	ZEX	C1-C6-C7-C8
28	F	310	ZEX	C25-C26-C27-C28
29	J	1105	LUT	C21-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
29	J	1105	LUT	C27-C28-C29-C30
29	J	1105	LUT	C27-C28-C29-C39
29	J	1105	LUT	C29-C30-C31-C32
29	1	5004	LUT	C21-C26-C27-C28
29	1	5004	LUT	C27-C28-C29-C30
29	1	5004	LUT	C27-C28-C29-C39
29	2	303	LUT	C21-C26-C27-C28
29	3	303	LUT	C1-C6-C7-C8
29	3	304	LUT	C21-C26-C27-C28
29	4	303	LUT	C25-C26-C27-C28
30	2	319	CHL	CHA-CBD-CGD-O1D
30	3	310	CHL	C3A-C2A-CAA-CBA
30	4	302	CHL	C1A-C2A-CAA-CBA
30	4	302	CHL	CHA-CBD-CGD-O1D
30	4	302	CHL	CHA-CBD-CGD-O2D
30	4	316	CHL	C1A-C2A-CAA-CBA
30	4	316	CHL	C3A-C2A-CAA-CBA
30	4	317	CHL	CHA-CBD-CGD-O1D
30	4	317	CHL	CHA-CBD-CGD-O2D
30	4	318	CHL	C2-C3-C5-C6
30	4	318	CHL	C4-C3-C5-C6
31	2	304	XAT	C1-C6-C7-C8
31	2	304	XAT	O4-C6-C7-C8
31	2	304	XAT	C7-C8-C9-C10
31	2	304	XAT	C7-C8-C9-C19
18	A	805	CLA	O1D-CGD-O2D-CED
18	A	826	CLA	O1D-CGD-O2D-CED
18	A	838	CLA	O1D-CGD-O2D-CED
18	B	807	CLA	O1D-CGD-O2D-CED
18	B	810	CLA	O1D-CGD-O2D-CED
18	B	823	CLA	O1D-CGD-O2D-CED
18	B	835	CLA	O1D-CGD-O2D-CED
18	2	310	CLA	O1D-CGD-O2D-CED
18	A	810	CLA	O1D-CGD-O2D-CED
18	A	840	CLA	O1D-CGD-O2D-CED
18	B	803	CLA	O1D-CGD-O2D-CED
18	B	804	CLA	O1D-CGD-O2D-CED
18	F	303	CLA	O1D-CGD-O2D-CED
18	G	1602	CLA	O1D-CGD-O2D-CED
18	L	306	CLA	O1D-CGD-O2D-CED
18	3	308	CLA	O1D-CGD-O2D-CED
18	3	309	CLA	O1D-CGD-O2D-CED

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
18	4	310	CLA	O1D-CGD-O2D-CED
18	A	802	CLA	CBD-CGD-O2D-CED
18	A	803	CLA	CBD-CGD-O2D-CED
18	A	804	CLA	CBD-CGD-O2D-CED
18	A	810	CLA	CBD-CGD-O2D-CED
18	A	811	CLA	CBD-CGD-O2D-CED
18	A	813	CLA	CBD-CGD-O2D-CED
18	A	815	CLA	CBD-CGD-O2D-CED
18	A	819	CLA	CBD-CGD-O2D-CED
18	A	820	CLA	CBD-CGD-O2D-CED
18	A	824	CLA	CBD-CGD-O2D-CED
18	A	826	CLA	CBD-CGD-O2D-CED
18	A	830	CLA	CBD-CGD-O2D-CED
18	A	831	CLA	CBD-CGD-O2D-CED
18	A	838	CLA	CBD-CGD-O2D-CED
18	A	840	CLA	CBD-CGD-O2D-CED
18	A	852	CLA	CBD-CGD-O2D-CED
18	B	806	CLA	CBD-CGD-O2D-CED
18	B	807	CLA	CBD-CGD-O2D-CED
18	B	812	CLA	CBD-CGD-O2D-CED
18	B	815	CLA	CBD-CGD-O2D-CED
18	B	819	CLA	CBD-CGD-O2D-CED
18	B	820	CLA	CBD-CGD-O2D-CED
18	B	821	CLA	CBD-CGD-O2D-CED
18	B	823	CLA	CBD-CGD-O2D-CED
18	B	828	CLA	CBD-CGD-O2D-CED
18	B	829	CLA	CBD-CGD-O2D-CED
18	B	831	CLA	CBD-CGD-O2D-CED
18	B	832	CLA	CBD-CGD-O2D-CED
18	B	833	CLA	CBD-CGD-O2D-CED
18	B	834	CLA	CBD-CGD-O2D-CED
18	F	302	CLA	CBD-CGD-O2D-CED
18	F	303	CLA	CBD-CGD-O2D-CED
18	G	1602	CLA	CBD-CGD-O2D-CED
18	G	1603	CLA	CBD-CGD-O2D-CED
18	J	1101	CLA	CBD-CGD-O2D-CED
18	J	1103	CLA	CBD-CGD-O2D-CED
18	K	1401	CLA	CBD-CGD-O2D-CED
18	K	1404	CLA	CBD-CGD-O2D-CED
18	L	304	CLA	CBD-CGD-O2D-CED
18	L	306	CLA	CBD-CGD-O2D-CED
18	1	5006	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	1	5015	CLA	CBD-CGD-O2D-CED
18	1	5017	CLA	CBD-CGD-O2D-CED
18	1	5018	CLA	CBD-CGD-O2D-CED
18	2	308	CLA	CBD-CGD-O2D-CED
18	2	309	CLA	CBD-CGD-O2D-CED
18	2	310	CLA	CBD-CGD-O2D-CED
18	2	311	CLA	CBD-CGD-O2D-CED
18	2	313	CLA	CBD-CGD-O2D-CED
18	2	317	CLA	CBD-CGD-O2D-CED
18	3	308	CLA	CBD-CGD-O2D-CED
18	3	309	CLA	CBD-CGD-O2D-CED
18	3	311	CLA	CBD-CGD-O2D-CED
18	3	314	CLA	CBD-CGD-O2D-CED
18	3	315	CLA	CBD-CGD-O2D-CED
18	4	305	CLA	CBD-CGD-O2D-CED
18	4	307	CLA	CBD-CGD-O2D-CED
18	4	309	CLA	CBD-CGD-O2D-CED
18	4	310	CLA	CBD-CGD-O2D-CED
18	4	311	CLA	CBD-CGD-O2D-CED
18	4	312	CLA	CBD-CGD-O2D-CED
18	B	835	CLA	O1A-CGA-O2A-C1
18	G	1603	CLA	O1A-CGA-O2A-C1
18	L	301	CLA	O1A-CGA-O2A-C1
18	3	308	CLA	O1A-CGA-O2A-C1
18	3	309	CLA	O1A-CGA-O2A-C1
24	1	5001	LMG	O10-C28-O8-C9
24	2	322	LMG	O10-C28-O8-C9
18	A	814	CLA	O1A-CGA-O2A-C1
18	G	1602	CLA	O1A-CGA-O2A-C1
18	1	5007	CLA	O1A-CGA-O2A-C1
18	A	815	CLA	O1D-CGD-O2D-CED
18	A	820	CLA	O1D-CGD-O2D-CED
18	A	834	CLA	O1D-CGD-O2D-CED
18	F	302	CLA	O1D-CGD-O2D-CED
18	J	1103	CLA	O1D-CGD-O2D-CED
18	K	1404	CLA	O1D-CGD-O2D-CED
18	1	5010	CLA	O1D-CGD-O2D-CED
18	1	5015	CLA	O1D-CGD-O2D-CED
18	1	5017	CLA	O1D-CGD-O2D-CED
18	2	311	CLA	O1D-CGD-O2D-CED
18	4	305	CLA	O1D-CGD-O2D-CED
18	A	814	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	1	5013	CLA	CBA-CGA-O2A-C1
18	A	809	CLA	O1D-CGD-O2D-CED
18	A	814	CLA	O1D-CGD-O2D-CED
18	A	818	CLA	O1D-CGD-O2D-CED
18	A	837	CLA	O1D-CGD-O2D-CED
18	B	809	CLA	O1D-CGD-O2D-CED
18	B	811	CLA	O1D-CGD-O2D-CED
18	B	818	CLA	O1D-CGD-O2D-CED
18	B	828	CLA	O1D-CGD-O2D-CED
18	B	836	CLA	O1D-CGD-O2D-CED
18	B	840	CLA	O1D-CGD-O2D-CED
18	G	1601	CLA	O1D-CGD-O2D-CED
18	K	1401	CLA	O1D-CGD-O2D-CED
18	1	5007	CLA	O1D-CGD-O2D-CED
18	1	5011	CLA	O1D-CGD-O2D-CED
18	1	5013	CLA	O1D-CGD-O2D-CED
18	3	314	CLA	O1D-CGD-O2D-CED
18	3	318	CLA	O1D-CGD-O2D-CED
18	3	319	CLA	O1D-CGD-O2D-CED
18	4	307	CLA	O1D-CGD-O2D-CED
18	4	315	CLA	O1D-CGD-O2D-CED
18	A	829	CLA	CBA-CGA-O2A-C1
18	3	309	CLA	CBA-CGA-O2A-C1
18	3	311	CLA	CBA-CGA-O2A-C1
18	4	315	CLA	CBA-CGA-O2A-C1
24	2	322	LMG	C29-C28-O8-C9
18	A	807	CLA	CBD-CGD-O2D-CED
18	A	825	CLA	CBD-CGD-O2D-CED
18	A	827	CLA	CBD-CGD-O2D-CED
18	A	828	CLA	CBD-CGD-O2D-CED
18	A	829	CLA	CBD-CGD-O2D-CED
18	A	832	CLA	CBD-CGD-O2D-CED
18	A	835	CLA	CBD-CGD-O2D-CED
18	B	827	CLA	CBD-CGD-O2D-CED
18	B	839	CLA	CBD-CGD-O2D-CED
18	1	5009	CLA	CBD-CGD-O2D-CED
18	2	306	CLA	CBD-CGD-O2D-CED
18	2	307	CLA	CBD-CGD-O2D-CED
18	4	308	CLA	CBD-CGD-O2D-CED
18	A	822	CLA	O1A-CGA-O2A-C1
18	A	829	CLA	O1A-CGA-O2A-C1
18	A	853	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	B	818	CLA	O1A-CGA-O2A-C1
18	B	831	CLA	O1A-CGA-O2A-C1
18	G	1601	CLA	O1A-CGA-O2A-C1
18	J	1103	CLA	O1A-CGA-O2A-C1
18	1	5011	CLA	O1A-CGA-O2A-C1
18	2	308	CLA	O1A-CGA-O2A-C1
18	2	312	CLA	O1A-CGA-O2A-C1
18	2	317	CLA	O1A-CGA-O2A-C1
18	2	326	CLA	O1A-CGA-O2A-C1
18	3	311	CLA	O1A-CGA-O2A-C1
18	3	317	CLA	O1A-CGA-O2A-C1
18	4	306	CLA	O1A-CGA-O2A-C1
18	4	307	CLA	O1A-CGA-O2A-C1
24	A	851	LMG	O10-C28-O8-C9
18	1	5013	CLA	O1A-CGA-O2A-C1
18	A	816	CLA	O1D-CGD-O2D-CED
18	A	821	CLA	O1D-CGD-O2D-CED
18	B	816	CLA	O1D-CGD-O2D-CED
18	F	301	CLA	O1D-CGD-O2D-CED
18	H	1701	CLA	O1D-CGD-O2D-CED
18	K	1403	CLA	O1D-CGD-O2D-CED
18	1	5008	CLA	O1D-CGD-O2D-CED
18	A	806	CLA	O1D-CGD-O2D-CED
18	A	808	CLA	O1D-CGD-O2D-CED
18	A	839	CLA	O1D-CGD-O2D-CED
18	A	853	CLA	O1D-CGD-O2D-CED
18	B	805	CLA	O1D-CGD-O2D-CED
18	L	301	CLA	O1D-CGD-O2D-CED
18	2	312	CLA	O1D-CGD-O2D-CED
18	3	317	CLA	O1D-CGD-O2D-CED
18	A	836	CLA	CBD-CGD-O2D-CED
18	B	808	CLA	CBD-CGD-O2D-CED
18	B	826	CLA	CBD-CGD-O2D-CED
18	3	307	CLA	CBD-CGD-O2D-CED
18	B	813	CLA	O1D-CGD-O2D-CED
18	1	5006	CLA	O1D-CGD-O2D-CED
18	2	308	CLA	O1D-CGD-O2D-CED
18	2	309	CLA	O1D-CGD-O2D-CED
18	4	312	CLA	O1D-CGD-O2D-CED
22	B	849	LHG	O9-C7-O7-C5
24	F	306	LMG	O9-C10-O7-C8
24	J	1102	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
18	B	826	CLA	O1A-CGA-O2A-C1
18	3	315	CLA	O1A-CGA-O2A-C1
18	1	5012	CLA	O1A-CGA-O2A-C1
18	1	5018	CLA	O1D-CGD-O2D-CED
18	2	313	CLA	O1D-CGD-O2D-CED
18	A	803	CLA	C3-C5-C6-C7
18	A	807	CLA	C3-C5-C6-C7
18	A	816	CLA	C3-C5-C6-C7
18	A	821	CLA	C3-C5-C6-C7
18	A	825	CLA	C3-C5-C6-C7
18	A	829	CLA	C3-C5-C6-C7
18	A	830	CLA	C3-C5-C6-C7
18	A	852	CLA	C3-C5-C6-C7
18	B	807	CLA	C3-C5-C6-C7
18	B	808	CLA	C3-C5-C6-C7
18	B	810	CLA	C3-C5-C6-C7
18	B	815	CLA	C3-C5-C6-C7
18	B	824	CLA	C3-C5-C6-C7
18	B	832	CLA	C3-C5-C6-C7
18	B	836	CLA	C3-C5-C6-C7
18	F	302	CLA	C3-C5-C6-C7
18	K	1402	CLA	C3-C5-C6-C7
18	1	5018	CLA	C3-C5-C6-C7
18	2	306	CLA	C3-C5-C6-C7
18	2	308	CLA	C3-C5-C6-C7
18	2	309	CLA	C3-C5-C6-C7
18	3	311	CLA	C3-C5-C6-C7
18	3	319	CLA	C3-C5-C6-C7
18	4	308	CLA	C3-C5-C6-C7
30	3	310	CHL	C3-C5-C6-C7
18	A	809	CLA	CBA-CGA-O2A-C1
18	A	822	CLA	CBA-CGA-O2A-C1
18	A	826	CLA	CBA-CGA-O2A-C1
18	A	853	CLA	CBA-CGA-O2A-C1
18	B	818	CLA	CBA-CGA-O2A-C1
18	B	831	CLA	CBA-CGA-O2A-C1
18	B	835	CLA	CBA-CGA-O2A-C1
18	G	1601	CLA	CBA-CGA-O2A-C1
18	G	1603	CLA	CBA-CGA-O2A-C1
18	J	1103	CLA	CBA-CGA-O2A-C1
18	L	301	CLA	CBA-CGA-O2A-C1
18	1	5011	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	2	307	CLA	CBA-CGA-O2A-C1
18	2	308	CLA	CBA-CGA-O2A-C1
18	2	312	CLA	CBA-CGA-O2A-C1
18	2	317	CLA	CBA-CGA-O2A-C1
18	3	308	CLA	CBA-CGA-O2A-C1
18	3	317	CLA	CBA-CGA-O2A-C1
18	3	319	CLA	CBA-CGA-O2A-C1
18	4	307	CLA	CBA-CGA-O2A-C1
18	4	310	CLA	CBA-CGA-O2A-C1
18	4	311	CLA	CBA-CGA-O2A-C1
24	B	850	LMG	C29-C28-O8-C9
24	1	5001	LMG	C29-C28-O8-C9
24	1	5020	LMG	C29-C28-O8-C9
18	B	809	CLA	C5-C6-C7-C8
24	A	851	LMG	C11-C10-O7-C8
24	1	5001	LMG	C11-C10-O7-C8
26	B	855	DGD	C2B-C1B-O2G-C2G
18	A	804	CLA	O1D-CGD-O2D-CED
18	A	830	CLA	O1D-CGD-O2D-CED
18	2	317	CLA	O1D-CGD-O2D-CED
26	F	309	DGD	O6D-C5D-C6D-O5D
18	1	5012	CLA	CBA-CGA-O2A-C1
24	2	324	LMG	O6-C1-O1-C7
24	1	5020	LMG	O6-C5-C6-O5
18	A	822	CLA	C4-C3-C5-C6
18	B	840	CLA	C4-C3-C5-C6
18	2	307	CLA	C4-C3-C5-C6
18	A	810	CLA	C2-C3-C5-C6
18	A	815	CLA	C2-C3-C5-C6
18	A	822	CLA	C2-C3-C5-C6
18	B	822	CLA	C2-C3-C5-C6
18	2	312	CLA	C2-C3-C5-C6
18	A	817	CLA	CBD-CGD-O2D-CED
18	B	817	CLA	CBD-CGD-O2D-CED
18	B	822	CLA	CBD-CGD-O2D-CED
18	A	819	CLA	C2A-CAA-CBA-CGA
18	A	833	CLA	C2A-CAA-CBA-CGA
18	B	805	CLA	C2A-CAA-CBA-CGA
18	B	840	CLA	C2A-CAA-CBA-CGA
18	F	302	CLA	C2A-CAA-CBA-CGA
18	1	5018	CLA	C2A-CAA-CBA-CGA
18	2	308	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
18	2	311	CLA	C2A-CAA-CBA-CGA
18	3	309	CLA	C2A-CAA-CBA-CGA
18	4	310	CLA	C2A-CAA-CBA-CGA
18	4	312	CLA	C2A-CAA-CBA-CGA
30	1	5014	CHL	C2A-CAA-CBA-CGA
18	F	303	CLA	O1A-CGA-O2A-C1
18	A	824	CLA	O1D-CGD-O2D-CED
18	A	852	CLA	O1D-CGD-O2D-CED
18	B	819	CLA	O1D-CGD-O2D-CED
24	A	851	LMG	C17-C18-C19-C20
24	1	5001	LMG	C35-C36-C37-C38
24	1	5001	LMG	C38-C39-C40-C41
26	B	855	DGD	C8A-C9A-CAA-CBA
18	A	804	CLA	C3-C5-C6-C7
18	B	823	CLA	C3-C5-C6-C7
18	B	830	CLA	C3-C5-C6-C7
18	G	1603	CLA	C3-C5-C6-C7
18	L	301	CLA	C3-C5-C6-C7
18	2	312	CLA	C3-C5-C6-C7
18	3	315	CLA	C3-C5-C6-C7
18	A	802	CLA	CBA-CGA-O2A-C1
18	B	812	CLA	CBA-CGA-O2A-C1
18	B	822	CLA	CBA-CGA-O2A-C1
18	K	1403	CLA	CBA-CGA-O2A-C1
18	L	306	CLA	CBA-CGA-O2A-C1
18	2	326	CLA	CBA-CGA-O2A-C1
18	3	315	CLA	CBA-CGA-O2A-C1
18	4	306	CLA	CBA-CGA-O2A-C1
18	4	309	CLA	CBA-CGA-O2A-C1
24	A	851	LMG	C29-C28-O8-C9
23	B	852	LMT	O5'-C5'-C6'-O6'
23	B	853	LMT	O5B-C5B-C6B-O6B
18	B	832	CLA	O1D-CGD-O2D-CED
18	A	811	CLA	O1D-CGD-O2D-CED
18	A	819	CLA	O1D-CGD-O2D-CED
18	B	806	CLA	O1D-CGD-O2D-CED
18	B	812	CLA	O1D-CGD-O2D-CED
18	B	834	CLA	O1D-CGD-O2D-CED
18	L	304	CLA	O1D-CGD-O2D-CED
18	3	311	CLA	O1D-CGD-O2D-CED
18	4	309	CLA	O1D-CGD-O2D-CED
24	G	1607	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
23	A	850	LMT	C4B-C5B-C6B-O6B
23	G	1606	LMT	C4B-C5B-C6B-O6B
18	A	809	CLA	O1A-CGA-O2A-C1
18	A	826	CLA	O1A-CGA-O2A-C1
18	B	810	CLA	O1A-CGA-O2A-C1
18	B	812	CLA	O1A-CGA-O2A-C1
18	L	304	CLA	O1A-CGA-O2A-C1
18	L	306	CLA	O1A-CGA-O2A-C1
18	2	307	CLA	O1A-CGA-O2A-C1
18	3	319	CLA	O1A-CGA-O2A-C1
18	4	309	CLA	O1A-CGA-O2A-C1
18	4	311	CLA	O1A-CGA-O2A-C1
24	B	850	LMG	O10-C28-O8-C9
24	F	306	LMG	O10-C28-O8-C9
26	1	5002	DGD	O1A-C1A-O1G-C1G
24	2	324	LMG	C2-C1-O1-C7
21	F	305	BCR	C13-C14-C15-C16
21	K	1405	BCR	C15-C16-C17-C18
21	3	306	BCR	C19-C20-C21-C22
23	B	853	LMT	O5'-C5'-C6'-O6'
17	A	801	CL0	CBD-CGD-O2D-CED
18	B	837	CLA	CBD-CGD-O2D-CED
18	K	1402	CLA	CBD-CGD-O2D-CED
18	2	326	CLA	CBD-CGD-O2D-CED
18	B	820	CLA	O1D-CGD-O2D-CED
18	B	821	CLA	O1D-CGD-O2D-CED
18	B	831	CLA	O1D-CGD-O2D-CED
18	G	1603	CLA	O1D-CGD-O2D-CED
18	3	315	CLA	O1D-CGD-O2D-CED
18	A	813	CLA	C3-C5-C6-C7
18	A	836	CLA	C3-C5-C6-C7
18	B	811	CLA	C3-C5-C6-C7
18	F	303	CLA	C3-C5-C6-C7
18	1	5006	CLA	C3-C5-C6-C7
18	A	805	CLA	CBA-CGA-O2A-C1
18	A	816	CLA	CBA-CGA-O2A-C1
18	A	820	CLA	CBA-CGA-O2A-C1
18	A	821	CLA	CBA-CGA-O2A-C1
18	B	826	CLA	CBA-CGA-O2A-C1
18	B	833	CLA	CBA-CGA-O2A-C1
18	F	303	CLA	CBA-CGA-O2A-C1
18	L	304	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	2	309	CLA	CBA-CGA-O2A-C1
18	2	313	CLA	CBA-CGA-O2A-C1
26	1	5002	DGD	C2A-C1A-O1G-C1G
18	A	802	CLA	O1A-CGA-O2A-C1
18	A	805	CLA	O1A-CGA-O2A-C1
18	B	822	CLA	O1A-CGA-O2A-C1
18	K	1403	CLA	O1A-CGA-O2A-C1
18	4	310	CLA	O1A-CGA-O2A-C1
24	1	5020	LMG	O10-C28-O8-C9
18	A	802	CLA	O1D-CGD-O2D-CED
18	A	813	CLA	O1D-CGD-O2D-CED
18	B	815	CLA	O1D-CGD-O2D-CED
18	4	311	CLA	O1D-CGD-O2D-CED
18	3	318	CLA	CBA-CGA-O2A-C1
18	A	822	CLA	CBD-CGD-O2D-CED
18	1	5012	CLA	CBD-CGD-O2D-CED
23	2	325	LMT	O5'-C5'-C6'-O6'
23	2	325	LMT	C4'-C5'-C6'-O6'
23	G	1605	LMT	C3'-C4'-O1B-C1B
26	J	1106	DGD	O6D-C5D-C6D-O5D
23	A	850	LMT	O5B-C5B-C6B-O6B
26	F	309	DGD	O6E-C5E-C6E-O5E
26	J	1106	DGD	C4D-C5D-C6D-O5D
18	B	833	CLA	O1D-CGD-O2D-CED
18	J	1101	CLA	O1D-CGD-O2D-CED
18	A	805	CLA	C3-C5-C6-C7
18	B	833	CLA	C3-C5-C6-C7
18	B	810	CLA	CBA-CGA-O2A-C1
24	F	306	LMG	C29-C28-O8-C9
18	A	803	CLA	O1D-CGD-O2D-CED
23	G	1606	LMT	O5B-C5B-C6B-O6B
23	J	1107	LMT	O5B-C5B-C6B-O6B
23	J	1107	LMT	O5'-C5'-C6'-O6'
23	2	325	LMT	O5B-C5B-C6B-O6B
18	A	816	CLA	O1A-CGA-O2A-C1
18	A	821	CLA	O1A-CGA-O2A-C1
18	B	833	CLA	O1A-CGA-O2A-C1
23	4	319	LMT	O5B-C5B-C6B-O6B
18	A	832	CLA	C4-C3-C5-C6
30	2	314	CHL	C4-C3-C5-C6
23	B	852	LMT	C4'-C5'-C6'-O6'
23	B	853	LMT	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
24	1	5020	LMG	C4-C5-C6-O5
24	2	324	LMG	C4-C5-C6-O5
18	A	832	CLA	C2-C3-C5-C6
18	A	838	CLA	C2-C3-C5-C6
18	H	1701	CLA	C2-C3-C5-C6
30	2	314	CHL	C2-C3-C5-C6
18	B	829	CLA	O1D-CGD-O2D-CED
18	A	820	CLA	O1A-CGA-O2A-C1
18	2	313	CLA	O1A-CGA-O2A-C1
24	2	322	LMG	O6-C1-O1-C7
18	J	1101	CLA	C3-C5-C6-C7
18	A	833	CLA	CBA-CGA-O2A-C1
18	B	815	CLA	CBA-CGA-O2A-C1
18	B	830	CLA	CBA-CGA-O2A-C1
18	A	831	CLA	O1D-CGD-O2D-CED
18	K	1404	CLA	CBA-CGA-O2A-C1
18	A	807	CLA	O1D-CGD-O2D-CED
18	B	827	CLA	O1D-CGD-O2D-CED
18	B	839	CLA	O1D-CGD-O2D-CED
18	2	309	CLA	O1A-CGA-O2A-C1
18	A	829	CLA	O1D-CGD-O2D-CED
18	A	832	CLA	O1D-CGD-O2D-CED
18	2	307	CLA	O1D-CGD-O2D-CED
18	4	308	CLA	O1D-CGD-O2D-CED
18	L	305	CLA	CBD-CGD-O2D-CED
22	2	320	LHG	C1-C2-C3-O3
23	J	1107	LMT	C4'-C5'-C6'-O6'
23	2	325	LMT	C4B-C5B-C6B-O6B
18	A	833	CLA	O1A-CGA-O2A-C1
18	B	830	CLA	O1A-CGA-O2A-C1
18	1	5010	CLA	C3-C5-C6-C7
18	4	311	CLA	C3-C5-C6-C7
18	A	806	CLA	CBA-CGA-O2A-C1
18	A	808	CLA	CBA-CGA-O2A-C1
18	A	813	CLA	CBA-CGA-O2A-C1
18	A	819	CLA	CBA-CGA-O2A-C1
18	A	824	CLA	CBA-CGA-O2A-C1
18	A	827	CLA	CBA-CGA-O2A-C1
18	B	806	CLA	CBA-CGA-O2A-C1
18	B	823	CLA	CBA-CGA-O2A-C1
18	B	824	CLA	CBA-CGA-O2A-C1
18	B	834	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	B	836	CLA	CBA-CGA-O2A-C1
18	B	841	CLA	CBA-CGA-O2A-C1
18	F	301	CLA	CBA-CGA-O2A-C1
18	J	1101	CLA	CBA-CGA-O2A-C1
18	K	1402	CLA	CBA-CGA-O2A-C1
18	1	5009	CLA	CBA-CGA-O2A-C1
26	J	1106	DGD	C2A-C1A-O1G-C1G
23	B	853	LMT	C4'-C5'-C6'-O6'
26	J	1106	DGD	CDA-CEA-CFA-CGA
18	3	318	CLA	O1A-CGA-O2A-C1
18	1	5009	CLA	O1D-CGD-O2D-CED
21	I	101	BCR	C9-C10-C11-C12
21	L	302	BCR	C13-C14-C15-C16
18	B	807	CLA	C8-C10-C11-C12
18	B	823	CLA	C5-C6-C7-C8
18	3	315	CLA	C10-C11-C12-C13
23	J	1107	LMT	C4B-C5B-C6B-O6B
18	A	827	CLA	O1D-CGD-O2D-CED
18	A	807	CLA	C5-C6-C7-C8
18	A	810	CLA	C13-C15-C16-C17
18	A	831	CLA	C8-C10-C11-C12
18	A	853	CLA	C10-C11-C12-C13
18	B	801	CLA	C8-C10-C11-C12
18	B	809	CLA	C10-C11-C12-C13
18	B	830	CLA	C8-C10-C11-C12
18	F	303	CLA	C10-C11-C12-C13
18	G	1603	CLA	C10-C11-C12-C13
18	3	309	CLA	C5-C6-C7-C8
22	B	849	LHG	O2-C2-C3-O3
22	2	320	LHG	O2-C2-C3-O3
23	G	1606	LMT	C2'-C1'-O1'-C1
24	1	5001	LMG	C2-C1-O1-C7
18	B	806	CLA	O1A-CGA-O2A-C1
18	1	5009	CLA	O1A-CGA-O2A-C1
18	B	840	CLA	C2-C3-C5-C6
18	2	307	CLA	C2-C3-C5-C6
18	A	802	CLA	C14-C13-C15-C16
18	A	803	CLA	C11-C10-C8-C9
18	A	808	CLA	C6-C7-C8-C9
18	A	808	CLA	C11-C10-C8-C9
18	A	826	CLA	C6-C7-C8-C9
18	A	836	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
18	B	804	CLA	C14-C13-C15-C16
18	B	815	CLA	C14-C13-C15-C16
18	B	818	CLA	C11-C12-C13-C14
18	B	820	CLA	C14-C13-C15-C16
18	B	826	CLA	C6-C7-C8-C9
18	B	840	CLA	C11-C10-C8-C9
18	G	1603	CLA	C6-C7-C8-C9
18	L	305	CLA	C6-C7-C8-C9
18	1	5006	CLA	C6-C7-C8-C9
18	1	5010	CLA	C14-C13-C15-C16
18	1	5018	CLA	C6-C7-C8-C9
18	2	310	CLA	C6-C7-C8-C9
18	2	312	CLA	C6-C7-C8-C9
18	4	305	CLA	C6-C7-C8-C9
18	4	315	CLA	C14-C13-C15-C16
30	1	5016	CHL	C11-C10-C8-C9
18	A	828	CLA	O1D-CGD-O2D-CED
18	A	835	CLA	O1D-CGD-O2D-CED
18	A	805	CLA	C8-C10-C11-C12
18	A	820	CLA	C8-C10-C11-C12
18	A	826	CLA	C15-C16-C17-C18
18	A	832	CLA	C13-C15-C16-C17
18	B	803	CLA	C13-C15-C16-C17
18	A	814	CLA	C2A-CAA-CBA-CGA
21	A	844	BCR	C7-C8-C9-C34
21	A	846	BCR	C7-C8-C9-C34
21	A	846	BCR	C11-C12-C13-C35
21	B	844	BCR	C11-C12-C13-C35
21	B	846	BCR	C7-C8-C9-C34
21	F	305	BCR	C36-C18-C19-C20
21	I	102	BCR	C37-C22-C23-C24
21	J	1104	BCR	C11-C12-C13-C35
21	K	1405	BCR	C11-C12-C13-C35
21	L	302	BCR	C37-C22-C23-C24
21	1	5005	BCR	C37-C22-C23-C24
21	2	305	BCR	C37-C22-C23-C24
21	3	306	BCR	C37-C22-C23-C24
21	4	301	BCR	C7-C8-C9-C34
21	4	301	BCR	C11-C12-C13-C35
21	A	846	BCR	C7-C8-C9-C10
21	F	304	BCR	C7-C8-C9-C10
21	F	305	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
21	I	102	BCR	C21-C22-C23-C24
21	J	1104	BCR	C11-C12-C13-C14
21	L	302	BCR	C21-C22-C23-C24
21	1	5005	BCR	C21-C22-C23-C24
21	2	305	BCR	C21-C22-C23-C24
21	3	306	BCR	C21-C22-C23-C24
21	4	301	BCR	C7-C8-C9-C10
21	4	301	BCR	C11-C12-C13-C14
24	2	322	LMG	C10-C11-C12-C13
18	A	806	CLA	O1A-CGA-O2A-C1
18	A	824	CLA	O1A-CGA-O2A-C1
18	A	827	CLA	O1A-CGA-O2A-C1
18	B	824	CLA	O1A-CGA-O2A-C1
18	F	301	CLA	O1A-CGA-O2A-C1
18	J	1101	CLA	O1A-CGA-O2A-C1
26	J	1106	DGD	O1A-C1A-O1G-C1G
18	A	806	CLA	C8-C10-C11-C12
18	A	831	CLA	C15-C16-C17-C18
18	B	807	CLA	C5-C6-C7-C8
18	B	811	CLA	C5-C6-C7-C8
18	B	819	CLA	C8-C10-C11-C12
18	B	822	CLA	C15-C16-C17-C18
18	B	824	CLA	C5-C6-C7-C8
18	G	1603	CLA	C13-C15-C16-C17
23	4	319	LMT	C4B-C5B-C6B-O6B
18	B	808	CLA	CBA-CGA-O2A-C1
18	A	806	CLA	C5-C6-C7-C8
18	A	812	CLA	C15-C16-C17-C18
18	A	817	CLA	C13-C15-C16-C17
18	A	822	CLA	C13-C15-C16-C17
18	A	827	CLA	C15-C16-C17-C18
18	B	805	CLA	C13-C15-C16-C17
18	B	819	CLA	C15-C16-C17-C18
18	B	829	CLA	C15-C16-C17-C18
18	B	831	CLA	C15-C16-C17-C18
18	B	833	CLA	C5-C6-C7-C8
18	H	1701	CLA	C8-C10-C11-C12
18	K	1402	CLA	C8-C10-C11-C12
18	1	5015	CLA	C15-C16-C17-C18
18	1	5018	CLA	C5-C6-C7-C8
18	4	305	CLA	C8-C10-C11-C12
22	1	5019	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
18	A	819	CLA	O1A-CGA-O2A-C1
18	B	823	CLA	O1A-CGA-O2A-C1
23	G	1606	LMT	C5'-C4'-O1B-C1B
18	A	803	CLA	C8-C10-C11-C12
18	A	803	CLA	C15-C16-C17-C18
18	A	807	CLA	C15-C16-C17-C18
18	A	825	CLA	C5-C6-C7-C8
18	A	828	CLA	C5-C6-C7-C8
18	A	830	CLA	C15-C16-C17-C18
18	A	835	CLA	C5-C6-C7-C8
18	A	838	CLA	C8-C10-C11-C12
18	A	838	CLA	C13-C15-C16-C17
18	A	838	CLA	C15-C16-C17-C18
18	B	804	CLA	C13-C15-C16-C17
18	B	808	CLA	C8-C10-C11-C12
18	B	818	CLA	C10-C11-C12-C13
18	B	820	CLA	C15-C16-C17-C18
18	B	825	CLA	C10-C11-C12-C13
18	B	828	CLA	C10-C11-C12-C13
18	B	830	CLA	C10-C11-C12-C13
18	B	840	CLA	C10-C11-C12-C13
18	H	1701	CLA	C5-C6-C7-C8
18	1	5006	CLA	C5-C6-C7-C8
18	2	308	CLA	C13-C15-C16-C17
18	2	312	CLA	C8-C10-C11-C12
18	2	317	CLA	C5-C6-C7-C8
18	4	305	CLA	C10-C11-C12-C13
18	4	307	CLA	C8-C10-C11-C12
18	4	308	CLA	C10-C11-C12-C13
18	4	311	CLA	C8-C10-C11-C12
18	4	315	CLA	C13-C15-C16-C17
30	3	310	CHL	C8-C10-C11-C12
22	A	849	LHG	O1-C1-C2-O2
22	1	5019	LHG	O1-C1-C2-O2
22	A	848	LHG	C7-C8-C9-C10
22	B	849	LHG	C7-C8-C9-C10
24	A	851	LMG	C10-C11-C12-C13
24	F	307	LMG	C28-C29-C30-C31
24	1	5001	LMG	C28-C29-C30-C31
18	A	805	CLA	C5-C6-C7-C8
18	A	819	CLA	C8-C10-C11-C12
18	B	806	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
18	B	829	CLA	C10-C11-C12-C13
18	F	303	CLA	C5-C6-C7-C8
18	1	5006	CLA	C15-C16-C17-C18
23	B	852	LMT	C2B-C1B-O1B-C4'
18	A	818	CLA	CBA-CGA-O2A-C1
18	A	825	CLA	O1D-CGD-O2D-CED
18	A	808	CLA	C2-C1-O2A-CGA
18	A	813	CLA	C2-C1-O2A-CGA
18	A	821	CLA	C2-C1-O2A-CGA
18	A	824	CLA	C2-C1-O2A-CGA
18	A	838	CLA	C2-C1-O2A-CGA
18	A	852	CLA	C2-C1-O2A-CGA
18	B	807	CLA	C2-C1-O2A-CGA
18	B	823	CLA	C2-C1-O2A-CGA
18	B	833	CLA	C2-C1-O2A-CGA
18	B	838	CLA	C2-C1-O2A-CGA
18	F	303	CLA	C2-C1-O2A-CGA
18	G	1603	CLA	C2-C1-O2A-CGA
18	J	1101	CLA	C2-C1-O2A-CGA
18	K	1403	CLA	C2-C1-O2A-CGA
18	L	306	CLA	C2-C1-O2A-CGA
18	1	5010	CLA	C2-C1-O2A-CGA
18	1	5011	CLA	C2-C1-O2A-CGA
18	2	310	CLA	C2-C1-O2A-CGA
18	2	312	CLA	C2-C1-O2A-CGA
18	2	313	CLA	C2-C1-O2A-CGA
18	2	317	CLA	C2-C1-O2A-CGA
18	2	326	CLA	C2-C1-O2A-CGA
18	3	308	CLA	C2-C1-O2A-CGA
18	4	306	CLA	C2-C1-O2A-CGA
18	4	310	CLA	C2-C1-O2A-CGA
18	A	836	CLA	C10-C11-C12-C13
18	B	822	CLA	C13-C15-C16-C17
18	1	5006	CLA	C8-C10-C11-C12
18	3	319	CLA	C10-C11-C12-C13
18	4	307	CLA	C10-C11-C12-C13
18	4	309	CLA	C8-C10-C11-C12
18	2	306	CLA	O1D-CGD-O2D-CED
22	A	849	LHG	C23-C24-C25-C26
22	B	849	LHG	C23-C24-C25-C26
24	1	5020	LMG	C11-C10-O7-C8
26	F	309	DGD	C2B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
18	2	307	CLA	C3-C5-C6-C7
23	B	852	LMT	O5B-C1B-O1B-C4'
18	A	817	CLA	C10-C11-C12-C13
18	A	833	CLA	C5-C6-C7-C8
18	B	814	CLA	C15-C16-C17-C18
18	A	802	CLA	C12-C13-C15-C16
18	A	822	CLA	C6-C7-C8-C10
18	B	820	CLA	C12-C13-C15-C16
18	B	830	CLA	C6-C7-C8-C10
18	3	315	CLA	C12-C13-C15-C16
19	B	842	PQN	C21-C22-C23-C25
18	A	817	CLA	C3-C5-C6-C7
18	A	824	CLA	C3-C5-C6-C7
18	A	813	CLA	O1A-CGA-O2A-C1
18	B	808	CLA	O1A-CGA-O2A-C1
18	K	1402	CLA	O1A-CGA-O2A-C1
21	A	843	BCR	C9-C10-C11-C12
21	A	846	BCR	C9-C10-C11-C12
21	A	846	BCR	C13-C14-C15-C16
21	B	846	BCR	C19-C20-C21-C22
18	A	807	CLA	C2A-CAA-CBA-CGA
18	B	818	CLA	C2A-CAA-CBA-CGA
18	G	1603	CLA	C2A-CAA-CBA-CGA
18	A	836	CLA	O1D-CGD-O2D-CED
18	B	808	CLA	O1D-CGD-O2D-CED
18	3	307	CLA	O1D-CGD-O2D-CED
18	B	826	CLA	C5-C6-C7-C8
18	B	830	CLA	C15-C16-C17-C18
18	B	840	CLA	C15-C16-C17-C18
18	F	302	CLA	C10-C11-C12-C13
18	G	1603	CLA	C5-C6-C7-C8
18	L	301	CLA	C5-C6-C7-C8
18	A	808	CLA	O1A-CGA-O2A-C1
18	B	834	CLA	O1A-CGA-O2A-C1
18	B	836	CLA	O1A-CGA-O2A-C1
23	B	852	LMT	O5'-C1'-O1'-C1
18	A	805	CLA	C15-C16-C17-C18
18	A	852	CLA	C10-C11-C12-C13
18	B	814	CLA	C10-C11-C12-C13
19	A	841	PQN	C25-C26-C27-C28
18	B	826	CLA	O1D-CGD-O2D-CED
24	B	850	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	A	845	BCR	C10-C11-C12-C13
21	B	802	BCR	C10-C11-C12-C13
21	B	843	BCR	C10-C11-C12-C13
21	B	845	BCR	C10-C11-C12-C13
21	K	1405	BCR	C10-C11-C12-C13
21	L	303	BCR	C10-C11-C12-C13
18	F	301	CLA	C3-C5-C6-C7
18	A	823	CLA	C15-C16-C17-C18
18	A	836	CLA	C5-C6-C7-C8
18	B	834	CLA	C8-C10-C11-C12
18	1	5006	CLA	C13-C15-C16-C17
18	B	817	CLA	O1D-CGD-O2D-CED
18	B	815	CLA	O1A-CGA-O2A-C1
18	B	841	CLA	O1A-CGA-O2A-C1
24	2	324	LMG	O6-C5-C6-O5
24	B	851	LMG	C10-C11-C12-C13
18	A	802	CLA	C10-C11-C12-C13
18	A	827	CLA	C5-C6-C7-C8
18	B	812	CLA	C5-C6-C7-C8
18	B	812	CLA	C10-C11-C12-C13
18	B	822	CLA	C5-C6-C7-C8
18	B	832	CLA	C8-C10-C11-C12
18	F	301	CLA	C13-C15-C16-C17
18	2	310	CLA	C10-C11-C12-C13
18	2	310	CLA	C15-C16-C17-C18
18	2	312	CLA	C5-C6-C7-C8
18	4	308	CLA	C8-C10-C11-C12
18	4	315	CLA	C10-C11-C12-C13
18	4	315	CLA	C15-C16-C17-C18
19	A	841	PQN	C18-C20-C21-C22
26	2	327	DGD	C2B-C1B-O2G-C2G
18	A	802	CLA	C13-C15-C16-C17
18	A	807	CLA	C13-C15-C16-C17
18	A	836	CLA	C13-C15-C16-C17
18	B	806	CLA	C13-C15-C16-C17
18	B	820	CLA	C13-C15-C16-C17
18	B	837	CLA	C15-C16-C17-C18
18	B	839	CLA	C5-C6-C7-C8
18	1	5006	CLA	C10-C11-C12-C13
18	2	309	CLA	C15-C16-C17-C18
22	A	848	LHG	C4-O6-P-O3
22	A	849	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
22	B	848	LHG	C4-O6-P-O3
22	2	320	LHG	C4-O6-P-O3
18	A	834	CLA	CBA-CGA-O2A-C1
18	B	832	CLA	CBA-CGA-O2A-C1
18	1	5018	CLA	CBA-CGA-O2A-C1
18	B	837	CLA	C10-C11-C12-C13
23	G	1606	LMT	C3'-C4'-O1B-C1B
18	A	817	CLA	O1D-CGD-O2D-CED
24	1	5020	LMG	O9-C10-O7-C8
26	F	309	DGD	O1B-C1B-O2G-C2G
26	2	327	DGD	O1B-C1B-O2G-C2G
18	B	815	CLA	C4-C3-C5-C6
18	B	841	CLA	C4-C3-C5-C6
18	L	301	CLA	C4-C3-C5-C6
18	4	305	CLA	C4-C3-C5-C6
18	A	837	CLA	C8-C10-C11-C12
18	B	812	CLA	C8-C10-C11-C12
18	1	5010	CLA	C5-C6-C7-C8
18	3	315	CLA	C8-C10-C11-C12
18	A	816	CLA	C2A-CAA-CBA-CGA
18	B	829	CLA	C2A-CAA-CBA-CGA
18	4	307	CLA	C2A-CAA-CBA-CGA
30	4	316	CHL	C2A-CAA-CBA-CGA
18	B	841	CLA	C16-C17-C18-C19
23	G	1606	LMT	C4'-C5'-C6'-O6'
18	A	823	CLA	CBA-CGA-O2A-C1
18	F	302	CLA	CBA-CGA-O2A-C1
26	B	855	DGD	C2A-C1A-O1G-C1G
18	B	840	CLA	C5-C6-C7-C8
23	A	850	LMT	C2B-C1B-O1B-C4'
18	A	802	CLA	C8-C10-C11-C12
18	B	808	CLA	C15-C16-C17-C18
18	F	302	CLA	C8-C10-C11-C12
18	1	5009	CLA	C8-C10-C11-C12
29	1	5004	LUT	C29-C30-C31-C32
22	A	848	LHG	C27-C28-C29-C30
22	1	5019	LHG	C28-C29-C30-C31
22	2	320	LHG	C8-C7-O7-C5
24	2	322	LMG	C11-C10-O7-C8
18	A	819	CLA	C10-C11-C12-C13
21	G	1604	BCR	C11-C10-C9-C34
21	L	303	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
21	1	5005	BCR	C11-C10-C9-C34
18	A	812	CLA	C3-C5-C6-C7
18	A	838	CLA	C3-C5-C6-C7
22	A	848	LHG	C13-C14-C15-C16
22	B	849	LHG	C34-C35-C36-C37
18	B	822	CLA	O1D-CGD-O2D-CED
17	A	801	CL0	C16-C17-C18-C19
18	A	819	CLA	C16-C17-C18-C20
18	A	820	CLA	C11-C12-C13-C14
18	A	823	CLA	C16-C17-C18-C20
18	A	837	CLA	C16-C17-C18-C19
18	B	839	CLA	C16-C17-C18-C20
18	G	1601	CLA	C6-C7-C8-C10
18	3	315	CLA	C16-C17-C18-C19
18	4	308	CLA	C11-C12-C13-C14
18	4	311	CLA	C11-C12-C13-C14
30	1	5016	CHL	C11-C12-C13-C15
23	B	852	LMT	C7-C8-C9-C10
22	2	320	LHG	O9-C7-O7-C5
24	2	322	LMG	O9-C10-O7-C8
26	J	1106	DGD	C1B-C2B-C3B-C4B
24	F	308	LMG	C30-C31-C32-C33
23	G	1606	LMT	C2B-C1B-O1B-C4'
22	A	849	LHG	C13-C14-C15-C16
21	G	1604	BCR	C11-C10-C9-C8
21	L	303	BCR	C11-C10-C9-C8
21	1	5005	BCR	C11-C10-C9-C8
23	B	852	LMT	C2'-C1'-O1'-C1
23	J	1107	LMT	C2'-C1'-O1'-C1
24	B	851	LMG	C2-C1-O1-C7
24	2	322	LMG	C14-C15-C16-C17
18	K	1404	CLA	O1A-CGA-O2A-C1
18	A	808	CLA	C5-C6-C7-C8
18	A	805	CLA	C16-C17-C18-C20
18	A	808	CLA	C16-C17-C18-C19
18	A	810	CLA	C16-C17-C18-C20
18	A	831	CLA	C16-C17-C18-C19
18	A	833	CLA	C6-C7-C8-C10
18	A	838	CLA	C16-C17-C18-C20
18	B	826	CLA	C16-C17-C18-C19
18	B	837	CLA	C16-C17-C18-C20
18	1	5010	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
18	3	309	CLA	C6-C7-C8-C10
17	A	801	CL0	O1D-CGD-O2D-CED
18	B	837	CLA	O1D-CGD-O2D-CED
18	K	1402	CLA	O1D-CGD-O2D-CED
23	G	1606	LMT	O5'-C5'-C6'-O6'
22	1	5019	LHG	C25-C26-C27-C28
23	G	1606	LMT	C4-C5-C6-C7
24	2	322	LMG	C13-C14-C15-C16
18	B	815	CLA	C2-C3-C5-C6
18	A	815	CLA	C11-C10-C8-C9
18	A	831	CLA	C11-C12-C13-C14
18	B	805	CLA	C11-C12-C13-C14
18	B	809	CLA	C14-C13-C15-C16
18	B	828	CLA	C11-C10-C8-C9
18	F	301	CLA	C6-C7-C8-C9
18	1	5018	CLA	C11-C10-C8-C9
18	3	315	CLA	C11-C10-C8-C9
18	4	308	CLA	C6-C7-C8-C9
18	B	814	CLA	C5-C6-C7-C8
18	B	823	CLA	C8-C10-C11-C12
18	F	301	CLA	C5-C6-C7-C8
18	F	303	CLA	C13-C15-C16-C17
18	4	312	CLA	CBA-CGA-O2A-C1
18	A	802	CLA	C2A-CAA-CBA-CGA
30	3	316	CHL	C2A-CAA-CBA-CGA
18	A	818	CLA	O1A-CGA-O2A-C1
18	A	834	CLA	O1A-CGA-O2A-C1
18	F	302	CLA	O1A-CGA-O2A-C1
21	A	855	BCR	C37-C22-C23-C24
29	3	304	LUT	C27-C28-C29-C39
22	A	849	LHG	O1-C1-C2-C3
22	B	849	LHG	O1-C1-C2-C3
22	1	5019	LHG	O1-C1-C2-C3
21	A	846	BCR	C11-C12-C13-C14
21	A	855	BCR	C21-C22-C23-C24
21	1	5005	BCR	C17-C18-C19-C20
29	3	304	LUT	C27-C28-C29-C30
24	F	307	LMG	O9-C10-O7-C8
18	2	308	CLA	C15-C16-C17-C18
24	F	307	LMG	C11-C10-O7-C8
24	1	5001	LMG	C37-C38-C39-C40
24	B	851	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
18	2	326	CLA	O1D-CGD-O2D-CED
22	A	848	LHG	C12-C13-C14-C15
18	A	813	CLA	C16-C17-C18-C20
18	A	817	CLA	C16-C17-C18-C20
18	A	827	CLA	C16-C17-C18-C19
18	A	827	CLA	C16-C17-C18-C20
18	A	852	CLA	C16-C17-C18-C20
18	B	810	CLA	C16-C17-C18-C20
18	B	825	CLA	C16-C17-C18-C20
18	B	841	CLA	C16-C17-C18-C20
18	F	301	CLA	C16-C17-C18-C19
18	L	305	CLA	C11-C12-C13-C15
18	2	312	CLA	C11-C12-C13-C14
18	3	315	CLA	C16-C17-C18-C20
18	3	319	CLA	C11-C12-C13-C14
18	A	831	CLA	C13-C15-C16-C17
18	B	801	CLA	C15-C16-C17-C18
22	1	5019	LHG	C11-C10-C9-C8
24	2	301	LMG	C2-C1-O1-C7
18	B	841	CLA	C15-C16-C17-C18
18	A	823	CLA	O1A-CGA-O2A-C1
18	1	5018	CLA	O1A-CGA-O2A-C1
26	B	855	DGD	O1A-C1A-O1G-C1G
24	A	851	LMG	C11-C12-C13-C14
18	A	815	CLA	CBA-CGA-O2A-C1
18	B	837	CLA	CBA-CGA-O2A-C1
18	1	5015	CLA	CBA-CGA-O2A-C1
18	2	311	CLA	CBA-CGA-O2A-C1
18	A	826	CLA	C3A-C2A-CAA-CBA
18	B	814	CLA	C3A-C2A-CAA-CBA
18	B	825	CLA	C3A-C2A-CAA-CBA
18	B	827	CLA	C3A-C2A-CAA-CBA
18	B	836	CLA	C3A-C2A-CAA-CBA
18	G	1602	CLA	C3A-C2A-CAA-CBA
18	J	1101	CLA	C3A-C2A-CAA-CBA
18	J	1103	CLA	C3A-C2A-CAA-CBA
18	K	1403	CLA	C3A-C2A-CAA-CBA
18	K	1404	CLA	C3A-C2A-CAA-CBA
18	L	304	CLA	C3A-C2A-CAA-CBA
18	L	306	CLA	C3A-C2A-CAA-CBA
18	1	5007	CLA	C3A-C2A-CAA-CBA
18	2	310	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	2	313	CLA	C3A-C2A-CAA-CBA
18	3	311	CLA	C3A-C2A-CAA-CBA
18	3	314	CLA	C3A-C2A-CAA-CBA
18	3	319	CLA	C3A-C2A-CAA-CBA
18	4	309	CLA	C3A-C2A-CAA-CBA
30	2	318	CHL	C3A-C2A-CAA-CBA
30	2	319	CHL	C3A-C2A-CAA-CBA
18	A	820	CLA	C5-C6-C7-C8
18	A	825	CLA	C8-C10-C11-C12
18	B	805	CLA	C8-C10-C11-C12
18	B	805	CLA	C15-C16-C17-C18
18	B	837	CLA	C13-C15-C16-C17
18	1	5015	CLA	C8-C10-C11-C12
21	3	305	BCR	C13-C14-C15-C16
23	A	850	LMT	C2-C1-O1'-C1'
18	B	832	CLA	O1A-CGA-O2A-C1
18	A	807	CLA	C16-C17-C18-C20
18	A	813	CLA	C16-C17-C18-C19
18	A	819	CLA	C16-C17-C18-C19
18	A	823	CLA	C16-C17-C18-C19
18	A	829	CLA	C16-C17-C18-C19
18	A	829	CLA	C16-C17-C18-C20
18	B	825	CLA	C16-C17-C18-C19
18	B	839	CLA	C16-C17-C18-C19
18	3	309	CLA	C6-C7-C8-C9
23	B	852	LMT	C4-C5-C6-C7
18	B	841	CLA	CBD-CGD-O2D-CED
18	B	835	CLA	C4-C3-C5-C6
18	B	838	CLA	CBA-CGA-O2A-C1
22	B	849	LHG	O1-C1-C2-O2
22	A	849	LHG	C11-C10-C9-C8
22	B	849	LHG	C11-C12-C13-C14
18	B	826	CLA	C16-C17-C18-C20
18	G	1601	CLA	C6-C7-C8-C9
18	4	311	CLA	C11-C12-C13-C15
18	A	817	CLA	C5-C6-C7-C8
18	J	1101	CLA	C15-C16-C17-C18
18	B	822	CLA	C3-C5-C6-C7
19	A	841	PQN	C13-C15-C16-C17
24	A	851	LMG	C28-C29-C30-C31
23	B	852	LMT	C1-C2-C3-C4
18	A	816	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
18	A	820	CLA	C2-C1-O2A-CGA
18	A	829	CLA	C2-C1-O2A-CGA
18	A	836	CLA	C2-C1-O2A-CGA
18	B	817	CLA	C2-C1-O2A-CGA
18	B	824	CLA	C2-C1-O2A-CGA
18	B	829	CLA	C2-C1-O2A-CGA
18	B	834	CLA	C2-C1-O2A-CGA
18	B	840	CLA	C2-C1-O2A-CGA
18	J	1103	CLA	C2-C1-O2A-CGA
18	L	301	CLA	C2-C1-O2A-CGA
18	2	309	CLA	C2-C1-O2A-CGA
18	3	314	CLA	C2-C1-O2A-CGA
18	3	315	CLA	C2-C1-O2A-CGA
22	A	848	LHG	C28-C29-C30-C31
26	B	855	DGD	C2A-C3A-C4A-C5A
18	A	840	CLA	C5-C6-C7-C8
18	J	1101	CLA	C8-C10-C11-C12
18	2	312	CLA	C10-C11-C12-C13
18	4	311	CLA	C5-C6-C7-C8
18	B	837	CLA	O1A-CGA-O2A-C1
22	1	5019	LHG	C13-C14-C15-C16
21	A	843	BCR	C5-C6-C7-C8
21	A	844	BCR	C23-C24-C25-C26
21	A	855	BCR	C1-C6-C7-C8
21	B	844	BCR	C1-C6-C7-C8
21	B	844	BCR	C5-C6-C7-C8
21	B	845	BCR	C1-C6-C7-C8
21	B	845	BCR	C5-C6-C7-C8
21	B	845	BCR	C23-C24-C25-C26
21	B	847	BCR	C1-C6-C7-C8
21	B	847	BCR	C5-C6-C7-C8
21	F	305	BCR	C23-C24-C25-C26
21	I	101	BCR	C5-C6-C7-C8
21	J	1104	BCR	C1-C6-C7-C8
21	J	1104	BCR	C5-C6-C7-C8
21	K	1405	BCR	C1-C6-C7-C8
21	K	1405	BCR	C5-C6-C7-C8
21	L	303	BCR	C23-C24-C25-C26
21	L	303	BCR	C23-C24-C25-C30
21	L	307	BCR	C1-C6-C7-C8
21	L	307	BCR	C5-C6-C7-C8
21	L	307	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
21	L	307	BCR	C23-C24-C25-C30
21	1	5005	BCR	C23-C24-C25-C26
21	1	5005	BCR	C23-C24-C25-C30
21	2	305	BCR	C1-C6-C7-C8
21	2	305	BCR	C5-C6-C7-C8
21	3	305	BCR	C1-C6-C7-C8
21	3	305	BCR	C23-C24-C25-C26
21	3	306	BCR	C1-C6-C7-C8
21	3	306	BCR	C23-C24-C25-C26
21	3	306	BCR	C23-C24-C25-C30
21	4	301	BCR	C1-C6-C7-C8
21	4	301	BCR	C23-C24-C25-C26
21	4	301	BCR	C23-C24-C25-C30
28	F	310	ZEX	C5-C6-C7-C8
29	1	5003	LUT	C1-C6-C7-C8
29	1	5003	LUT	C5-C6-C7-C8
29	3	303	LUT	C5-C6-C7-C8
29	3	304	LUT	C1-C6-C7-C8
23	A	850	LMT	O5'-C5'-C6'-O6'
23	G	1605	LMT	C5'-C4'-O1B-C1B
18	1	5012	CLA	O1D-CGD-O2D-CED
18	A	803	CLA	C10-C11-C12-C13
18	A	804	CLA	C5-C6-C7-C8
18	A	807	CLA	C8-C10-C11-C12
18	A	825	CLA	C15-C16-C17-C18
18	A	826	CLA	C10-C11-C12-C13
26	1	5002	DGD	C2B-C1B-O2G-C2G
22	A	849	LHG	C15-C16-C17-C18
24	2	301	LMG	O6-C1-O1-C7
26	B	855	DGD	C2B-C3B-C4B-C5B
18	A	803	CLA	C5-C6-C7-C8
18	A	810	CLA	C10-C11-C12-C13
18	A	812	CLA	C8-C10-C11-C12
18	A	840	CLA	C8-C10-C11-C12
18	G	1603	CLA	C8-C10-C11-C12
22	A	848	LHG	C33-C34-C35-C36
18	A	806	CLA	C4-C3-C5-C6
18	3	315	CLA	C4-C3-C5-C6
30	4	302	CHL	C4-C3-C5-C6
18	A	806	CLA	C2-C3-C5-C6
18	A	813	CLA	C12-C13-C15-C16
18	A	823	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
18	A	830	CLA	C12-C13-C15-C16
18	A	831	CLA	C11-C12-C13-C15
18	A	837	CLA	C11-C10-C8-C7
18	B	804	CLA	C11-C12-C13-C15
18	B	805	CLA	C11-C12-C13-C15
18	B	818	CLA	C11-C12-C13-C15
18	B	826	CLA	C6-C7-C8-C10
18	B	828	CLA	C11-C10-C8-C7
18	B	832	CLA	C6-C7-C8-C10
18	B	834	CLA	C6-C7-C8-C10
18	F	301	CLA	C6-C7-C8-C10
18	H	1701	CLA	C6-C7-C8-C10
18	L	305	CLA	C6-C7-C8-C10
18	1	5010	CLA	C12-C13-C15-C16
18	1	5018	CLA	C11-C10-C8-C7
18	2	308	CLA	C6-C7-C8-C10
18	2	309	CLA	C12-C13-C15-C16
18	3	315	CLA	C2-C3-C5-C6
18	4	308	CLA	C6-C7-C8-C10
18	4	315	CLA	C12-C13-C15-C16
30	1	5016	CHL	C11-C10-C8-C7
30	4	302	CHL	C2-C3-C5-C6
18	B	837	CLA	C3-C5-C6-C7
18	A	815	CLA	O1A-CGA-O2A-C1
18	B	838	CLA	O1A-CGA-O2A-C1
18	1	5015	CLA	O1A-CGA-O2A-C1
18	2	311	CLA	O1A-CGA-O2A-C1
23	G	1605	LMT	C5-C6-C7-C8
18	B	818	CLA	C8-C10-C11-C12
21	4	301	BCR	C19-C20-C21-C22
17	A	801	CL0	C16-C17-C18-C20
18	A	808	CLA	C16-C17-C18-C20
18	A	810	CLA	C16-C17-C18-C19
18	A	822	CLA	C16-C17-C18-C19
30	1	5016	CHL	C11-C12-C13-C14
18	A	822	CLA	O1D-CGD-O2D-CED
18	L	305	CLA	O1D-CGD-O2D-CED
22	1	5019	LHG	O9-C7-O7-C5
26	J	1106	DGD	O1B-C1B-O2G-C2G
18	A	811	CLA	CBA-CGA-O2A-C1
18	A	835	CLA	CBA-CGA-O2A-C1
18	A	840	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	B	803	CLA	CBA-CGA-O2A-C1
18	B	805	CLA	CBA-CGA-O2A-C1
18	B	828	CLA	CBA-CGA-O2A-C1
18	4	308	CLA	CBA-CGA-O2A-C1
22	A	849	LHG	C9-C10-C11-C12
22	B	848	LHG	C24-C23-O8-C6
18	A	810	CLA	C2A-CAA-CBA-CGA
18	A	853	CLA	C2A-CAA-CBA-CGA
18	L	306	CLA	C2A-CAA-CBA-CGA
18	1	5009	CLA	C2A-CAA-CBA-CGA
18	3	315	CLA	C2A-CAA-CBA-CGA
18	J	1101	CLA	C5-C6-C7-C8
23	B	852	LMT	C6-C7-C8-C9
26	F	309	DGD	C5A-C6A-C7A-C8A
23	G	1605	LMT	C1-C2-C3-C4
18	B	823	CLA	C15-C16-C17-C18
18	4	311	CLA	C10-C11-C12-C13
22	1	5019	LHG	C33-C34-C35-C36
23	A	850	LMT	C2-C3-C4-C5
24	B	850	LMG	C11-C12-C13-C14
24	1	5020	LMG	C11-C12-C13-C14
26	B	855	DGD	C2G-C1G-O1G-C1A
18	B	804	CLA	C16-C17-C18-C19
18	1	5008	CLA	C6-C7-C8-C10
23	A	850	LMT	O5'-C1'-O1'-C1
26	1	5002	DGD	O6D-C1D-O3G-C3G
18	A	812	CLA	C10-C11-C12-C13
18	A	822	CLA	C10-C11-C12-C13
18	B	826	CLA	C8-C10-C11-C12
18	B	841	CLA	C8-C10-C11-C12
22	A	848	LHG	C11-C12-C13-C14
22	1	5019	LHG	C29-C30-C31-C32
22	A	848	LHG	C8-C7-O7-C5
22	1	5019	LHG	C8-C7-O7-C5
26	J	1106	DGD	C2B-C1B-O2G-C2G
24	A	851	LMG	C15-C16-C17-C18
24	F	306	LMG	C34-C35-C36-C37
26	2	327	DGD	C2B-C3B-C4B-C5B
26	1	5002	DGD	O1B-C1B-O2G-C2G
18	A	827	CLA	C3-C5-C6-C7
23	2	325	LMT	C11-C10-C9-C8
23	A	850	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
26	J	1106	DGD	C2E-C1E-O5D-C6D
26	1	5002	DGD	C2D-C1D-O3G-C3G
18	A	831	CLA	C16-C17-C18-C20
18	A	838	CLA	C16-C17-C18-C19
18	B	805	CLA	C16-C17-C18-C20
18	1	5010	CLA	C16-C17-C18-C20
18	A	822	CLA	C15-C16-C17-C18
18	A	823	CLA	C8-C10-C11-C12
18	A	852	CLA	C15-C16-C17-C18
18	B	835	CLA	C2-C3-C5-C6
18	B	841	CLA	C2-C3-C5-C6
18	L	301	CLA	C2-C3-C5-C6
18	4	305	CLA	C2-C3-C5-C6
18	A	802	CLA	C11-C10-C8-C9
18	A	803	CLA	C11-C12-C13-C14
18	A	804	CLA	C6-C7-C8-C9
18	A	830	CLA	C14-C13-C15-C16
18	A	837	CLA	C11-C10-C8-C9
18	B	804	CLA	C11-C12-C13-C14
18	B	823	CLA	C14-C13-C15-C16
18	B	829	CLA	C6-C7-C8-C9
18	B	829	CLA	C14-C13-C15-C16
18	B	830	CLA	C6-C7-C8-C9
18	B	832	CLA	C6-C7-C8-C9
18	B	834	CLA	C6-C7-C8-C9
18	B	839	CLA	C6-C7-C8-C9
18	H	1701	CLA	C6-C7-C8-C9
18	2	309	CLA	C14-C13-C15-C16
18	2	310	CLA	C14-C13-C15-C16
18	2	312	CLA	C11-C10-C8-C9
19	B	842	PQN	C21-C22-C23-C24
18	B	801	CLA	C3-C5-C6-C7
30	2	315	CHL	C3-C5-C6-C7
23	G	1606	LMT	O5B-C1B-O1B-C4'
18	B	821	CLA	C2A-CAA-CBA-CGA
18	B	828	CLA	C2A-CAA-CBA-CGA
26	2	327	DGD	C4A-C5A-C6A-C7A
18	B	841	CLA	C10-C11-C12-C13
22	B	849	LHG	C26-C27-C28-C29
26	B	855	DGD	C7A-C8A-C9A-CAA
21	A	844	BCR	C17-C18-C19-C20
21	A	847	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
21	B	847	BCR	C7-C8-C9-C10
21	L	302	BCR	C17-C18-C19-C20
18	A	811	CLA	O1A-CGA-O2A-C1
18	B	803	CLA	O1A-CGA-O2A-C1
18	A	805	CLA	C1A-C2A-CAA-CBA
18	A	807	CLA	C1A-C2A-CAA-CBA
18	A	808	CLA	C1A-C2A-CAA-CBA
18	A	809	CLA	C1A-C2A-CAA-CBA
18	A	813	CLA	C1A-C2A-CAA-CBA
18	A	816	CLA	C1A-C2A-CAA-CBA
18	A	820	CLA	C1A-C2A-CAA-CBA
18	A	832	CLA	C1A-C2A-CAA-CBA
18	A	836	CLA	C1A-C2A-CAA-CBA
18	B	806	CLA	C1A-C2A-CAA-CBA
18	B	812	CLA	C1A-C2A-CAA-CBA
18	B	813	CLA	C1A-C2A-CAA-CBA
18	B	814	CLA	C1A-C2A-CAA-CBA
18	B	823	CLA	C1A-C2A-CAA-CBA
18	B	825	CLA	C1A-C2A-CAA-CBA
18	B	826	CLA	C1A-C2A-CAA-CBA
18	B	838	CLA	C1A-C2A-CAA-CBA
18	F	301	CLA	C1A-C2A-CAA-CBA
18	G	1602	CLA	C1A-C2A-CAA-CBA
18	G	1603	CLA	C1A-C2A-CAA-CBA
18	J	1101	CLA	C1A-C2A-CAA-CBA
18	J	1103	CLA	C1A-C2A-CAA-CBA
18	K	1403	CLA	C1A-C2A-CAA-CBA
18	K	1404	CLA	C1A-C2A-CAA-CBA
18	1	5006	CLA	C1A-C2A-CAA-CBA
18	1	5007	CLA	C1A-C2A-CAA-CBA
18	1	5013	CLA	C1A-C2A-CAA-CBA
18	2	306	CLA	C1A-C2A-CAA-CBA
18	2	308	CLA	C1A-C2A-CAA-CBA
18	2	309	CLA	C1A-C2A-CAA-CBA
18	2	310	CLA	C1A-C2A-CAA-CBA
18	3	301	CLA	C1A-C2A-CAA-CBA
18	3	309	CLA	C1A-C2A-CAA-CBA
18	3	311	CLA	C1A-C2A-CAA-CBA
18	3	315	CLA	C1A-C2A-CAA-CBA
18	3	319	CLA	C1A-C2A-CAA-CBA
18	4	305	CLA	C1A-C2A-CAA-CBA
30	2	318	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	2	319	CHL	C1A-C2A-CAA-CBA
30	3	310	CHL	C1A-C2A-CAA-CBA
30	3	316	CHL	C1A-C2A-CAA-CBA
18	A	817	CLA	C16-C17-C18-C19
18	A	833	CLA	C6-C7-C8-C9
18	B	804	CLA	C16-C17-C18-C20
18	B	810	CLA	C16-C17-C18-C19
18	F	301	CLA	C16-C17-C18-C20
18	L	305	CLA	C11-C12-C13-C14
18	1	5008	CLA	C6-C7-C8-C9
18	2	312	CLA	C11-C12-C13-C15
21	B	845	BCR	C13-C14-C15-C16
21	F	305	BCR	C9-C10-C11-C12
18	A	803	CLA	C13-C15-C16-C17
18	A	832	CLA	C10-C11-C12-C13
18	B	815	CLA	C15-C16-C17-C18
18	B	828	CLA	C15-C16-C17-C18
18	2	306	CLA	C10-C11-C12-C13
24	B	851	LMG	C12-C13-C14-C15
18	3	307	CLA	C3-C5-C6-C7
18	A	813	CLA	C13-C15-C16-C17
18	A	815	CLA	C5-C6-C7-C8
18	A	827	CLA	C10-C11-C12-C13
18	B	807	CLA	C13-C15-C16-C17
22	1	5019	LHG	C9-C10-C11-C12
23	A	850	LMT	O1'-C1-C2-C3
18	A	820	CLA	C11-C12-C13-C15
18	4	308	CLA	C11-C12-C13-C15
22	A	848	LHG	C24-C25-C26-C27
22	A	848	LHG	C34-C35-C36-C37
23	A	850	LMT	O5B-C1B-O1B-C4'
22	A	849	LHG	C16-C17-C18-C19
18	B	835	CLA	C3-C5-C6-C7
23	G	1605	LMT	O5'-C5'-C6'-O6'
22	B	849	LHG	C24-C25-C26-C27
18	A	835	CLA	O1A-CGA-O2A-C1
18	A	840	CLA	O1A-CGA-O2A-C1
18	B	805	CLA	O1A-CGA-O2A-C1
18	A	837	CLA	C16-C17-C18-C20
18	A	853	CLA	C16-C17-C18-C19
22	A	848	LHG	C4-C5-C6-O8
24	F	308	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
24	G	1607	LMG	O1-C7-C8-C9
24	2	322	LMG	O1-C7-C8-C9
26	J	1106	DGD	O1G-C1G-C2G-C3G
26	2	327	DGD	O1G-C1G-C2G-C3G
24	1	5001	LMG	O6-C5-C6-O5
18	4	308	CLA	O1A-CGA-O2A-C1
24	1	5020	LMG	C8-C7-O1-C1
18	1	5009	CLA	C10-C11-C12-C13
26	B	855	DGD	C6A-C7A-C8A-C9A
24	F	308	LMG	C10-C11-C12-C13
24	1	5001	LMG	C10-C11-C12-C13
26	F	309	DGD	C1A-C2A-C3A-C4A
18	B	828	CLA	O1A-CGA-O2A-C1
23	G	1605	LMT	C9-C10-C11-C12
18	L	305	CLA	C3-C5-C6-C7
22	B	849	LHG	C24-C23-O8-C6
24	2	321	LMG	O6-C5-C6-O5
22	2	320	LHG	O1-C1-C2-O2
26	1	5002	DGD	C4A-C5A-C6A-C7A
18	A	829	CLA	C8-C10-C11-C12
18	F	302	CLA	C13-C15-C16-C17
18	B	835	CLA	C5-C6-C7-C8
21	B	845	BCR	C11-C10-C9-C34
23	B	852	LMT	O5B-C5B-C6B-O6B
24	B	851	LMG	O6-C5-C6-O5
24	2	322	LMG	O6-C5-C6-O5
18	B	831	CLA	C4-C3-C5-C6
18	F	301	CLA	C4-C3-C5-C6
30	1	5016	CHL	C4-C3-C5-C6
24	B	850	LMG	C12-C13-C14-C15
18	A	825	CLA	C16-C17-C18-C20
23	B	856	LMT	O5'-C5'-C6'-O6'
18	A	823	CLA	C10-C11-C12-C13
18	4	307	CLA	C13-C15-C16-C17
18	A	832	CLA	C2-C1-O2A-CGA
18	A	833	CLA	C2-C1-O2A-CGA
18	2	311	CLA	C2-C1-O2A-CGA
18	4	307	CLA	C2-C1-O2A-CGA
22	A	849	LHG	C26-C27-C28-C29
24	A	851	LMG	O6-C5-C6-O5
24	2	301	LMG	O6-C5-C6-O5
17	A	801	CL0	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	A	812	CLA	CBA-CGA-O2A-C1
18	A	831	CLA	CBA-CGA-O2A-C1
18	B	819	CLA	CBA-CGA-O2A-C1
18	3	307	CLA	C6-C7-C8-C10
24	F	307	LMG	C10-C11-C12-C13
18	A	808	CLA	C10-C11-C12-C13
18	B	808	CLA	C5-C6-C7-C8
18	B	829	CLA	C13-C15-C16-C17
23	B	852	LMT	C5-C6-C7-C8
18	A	804	CLA	C8-C10-C11-C12
18	A	824	CLA	C5-C6-C7-C8
18	A	828	CLA	C8-C10-C11-C12
18	A	853	CLA	C15-C16-C17-C18
18	B	805	CLA	C5-C6-C7-C8
18	F	301	CLA	C15-C16-C17-C18
23	2	325	LMT	C2'-C1'-O1'-C1
22	2	320	LHG	C28-C29-C30-C31
18	A	826	CLA	C5-C6-C7-C8
18	A	829	CLA	C5-C6-C7-C8
18	B	831	CLA	C5-C6-C7-C8
18	A	822	CLA	C16-C17-C18-C20
18	B	837	CLA	C16-C17-C18-C19
18	A	821	CLA	C4-C3-C5-C6
18	A	802	CLA	C6-C7-C8-C10
18	A	803	CLA	C11-C12-C13-C15
18	A	804	CLA	C6-C7-C8-C10
18	A	804	CLA	C11-C12-C13-C15
18	A	805	CLA	C12-C13-C15-C16
18	A	806	CLA	C6-C7-C8-C10
18	A	826	CLA	C6-C7-C8-C10
18	A	827	CLA	C11-C12-C13-C15
18	A	831	CLA	C6-C7-C8-C10
18	A	832	CLA	C6-C7-C8-C10
18	A	852	CLA	C11-C10-C8-C7
18	A	853	CLA	C11-C12-C13-C15
18	B	804	CLA	C11-C10-C8-C7
18	B	807	CLA	C11-C12-C13-C15
18	B	814	CLA	C11-C12-C13-C15
18	B	819	CLA	C6-C7-C8-C10
18	B	820	CLA	C6-C7-C8-C10
18	B	823	CLA	C12-C13-C15-C16
18	B	825	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
18	B	829	CLA	C6-C7-C8-C10
18	B	829	CLA	C12-C13-C15-C16
18	B	831	CLA	C2-C3-C5-C6
18	B	839	CLA	C6-C7-C8-C10
18	B	840	CLA	C11-C10-C8-C7
18	F	301	CLA	C2-C3-C5-C6
18	F	303	CLA	C11-C10-C8-C7
18	J	1101	CLA	C11-C12-C13-C15
18	K	1402	CLA	C6-C7-C8-C10
18	1	5015	CLA	C6-C7-C8-C10
18	1	5018	CLA	C6-C7-C8-C10
18	2	309	CLA	C6-C7-C8-C10
18	2	310	CLA	C6-C7-C8-C10
18	2	310	CLA	C11-C12-C13-C15
18	2	312	CLA	C6-C7-C8-C10
18	2	312	CLA	C11-C10-C8-C7
18	3	315	CLA	C6-C7-C8-C10
18	3	315	CLA	C11-C12-C13-C15
18	4	315	CLA	C11-C10-C8-C7
19	B	842	PQN	C17-C18-C20-C21
30	2	314	CHL	C11-C10-C8-C7
18	A	802	CLA	C11-C12-C13-C14
18	A	804	CLA	C11-C12-C13-C14
18	A	804	CLA	C14-C13-C15-C16
18	A	805	CLA	C11-C12-C13-C14
18	A	816	CLA	C6-C7-C8-C9
18	A	820	CLA	C11-C10-C8-C9
18	A	822	CLA	C6-C7-C8-C9
18	A	823	CLA	C11-C10-C8-C9
18	A	827	CLA	C11-C12-C13-C14
18	A	829	CLA	C14-C13-C15-C16
18	A	832	CLA	C6-C7-C8-C9
18	A	838	CLA	C6-C7-C8-C9
18	A	840	CLA	C6-C7-C8-C9
18	A	852	CLA	C6-C7-C8-C9
18	B	801	CLA	C6-C7-C8-C9
18	B	804	CLA	C11-C10-C8-C9
18	B	808	CLA	C11-C12-C13-C14
18	B	810	CLA	C6-C7-C8-C9
18	B	815	CLA	C11-C10-C8-C9
18	B	819	CLA	C6-C7-C8-C9
18	B	820	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
18	B	825	CLA	C11-C12-C13-C14
18	B	825	CLA	C14-C13-C15-C16
18	B	830	CLA	C14-C13-C15-C16
18	B	837	CLA	C14-C13-C15-C16
18	B	840	CLA	C6-C7-C8-C9
18	F	302	CLA	C6-C7-C8-C9
18	F	303	CLA	C11-C10-C8-C9
18	K	1402	CLA	C6-C7-C8-C9
18	1	5009	CLA	C11-C12-C13-C14
18	1	5015	CLA	C6-C7-C8-C9
18	2	308	CLA	C6-C7-C8-C9
18	2	310	CLA	C11-C12-C13-C14
18	3	315	CLA	C6-C7-C8-C9
18	4	307	CLA	C14-C13-C15-C16
18	4	315	CLA	C6-C7-C8-C9
22	A	848	LHG	C23-C24-C25-C26
18	A	825	CLA	CBA-CGA-O2A-C1
18	A	832	CLA	C2A-CAA-CBA-CGA
22	B	849	LHG	C35-C36-C37-C38
17	A	801	CL0	O1A-CGA-O2A-C1
21	A	843	BCR	C37-C22-C23-C24
21	A	844	BCR	C37-C22-C23-C24
18	B	805	CLA	C16-C17-C18-C19
21	A	844	BCR	C7-C8-C9-C10
21	A	844	BCR	C21-C22-C23-C24
18	A	802	CLA	C5-C6-C7-C8
18	A	808	CLA	C13-C15-C16-C17
19	A	841	PQN	C15-C16-C17-C18
22	A	848	LHG	C35-C36-C37-C38
18	A	812	CLA	O1A-CGA-O2A-C1
18	B	827	CLA	CBA-CGA-O2A-C1
22	B	849	LHG	C33-C34-C35-C36
18	A	840	CLA	C10-C11-C12-C13
18	B	801	CLA	C13-C15-C16-C17
18	4	312	CLA	O1A-CGA-O2A-C1
22	B	849	LHG	C9-C10-C11-C12
18	B	803	CLA	C16-C17-C18-C19
18	B	814	CLA	CBA-CGA-O2A-C1
18	A	830	CLA	C13-C15-C16-C17
18	A	804	CLA	C4-C3-C5-C6
18	A	824	CLA	C4-C3-C5-C6
18	B	837	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
18	F	302	CLA	C4-C3-C5-C6
18	A	804	CLA	C2-C3-C5-C6
18	A	821	CLA	C2-C3-C5-C6
30	1	5016	CHL	C2-C3-C5-C6
22	2	320	LHG	C7-C8-C9-C10
24	F	306	LMG	C28-C29-C30-C31
22	A	848	LHG	O9-C7-O7-C5
18	A	816	CLA	C11-C10-C8-C9
22	B	849	LHG	C13-C14-C15-C16
18	A	824	CLA	C6-C7-C8-C9
18	B	831	CLA	C8-C10-C11-C12
18	B	817	CLA	C3A-C2A-CAA-CBA
18	B	828	CLA	C3A-C2A-CAA-CBA
18	L	305	CLA	C3A-C2A-CAA-CBA
18	1	5008	CLA	C3A-C2A-CAA-CBA
18	2	317	CLA	C3A-C2A-CAA-CBA
18	2	326	CLA	C3A-C2A-CAA-CBA
18	4	310	CLA	C3A-C2A-CAA-CBA
18	4	315	CLA	C3A-C2A-CAA-CBA
30	4	302	CHL	C3A-C2A-CAA-CBA
21	J	1104	BCR	C9-C10-C11-C12
23	B	852	LMT	C2-C1-O1'-C1'
23	B	853	LMT	C6-C7-C8-C9
18	B	826	CLA	C13-C15-C16-C17
23	G	1605	LMT	O1'-C1-C2-C3
18	A	805	CLA	C16-C17-C18-C19
18	B	807	CLA	CBA-CGA-O2A-C1
18	B	839	CLA	CBA-CGA-O2A-C1
26	F	309	DGD	C6A-C7A-C8A-C9A
22	A	849	LHG	C4-C5-C6-O8
24	B	851	LMG	O1-C7-C8-C9
24	F	307	LMG	C7-C8-C9-O8
26	B	855	DGD	O1G-C1G-C2G-C3G
23	B	856	LMT	C1-C2-C3-C4
22	B	849	LHG	C28-C29-C30-C31
18	B	819	CLA	C3-C5-C6-C7
18	A	826	CLA	C16-C17-C18-C20
22	A	849	LHG	C11-C12-C13-C14
26	F	309	DGD	C1B-C2B-C3B-C4B
18	A	831	CLA	O1A-CGA-O2A-C1
22	B	849	LHG	O10-C23-O8-C6
22	A	848	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
18	A	853	CLA	C16-C17-C18-C20
18	1	5018	CLA	C10-C11-C12-C13
26	F	309	DGD	C4E-C5E-C6E-O5E
24	B	851	LMG	O1-C7-C8-O7
24	F	307	LMG	O7-C8-C9-O8
24	F	308	LMG	O7-C8-C9-O8
24	2	322	LMG	O7-C8-C9-O8
18	A	826	CLA	C16-C17-C18-C19
18	3	307	CLA	C6-C7-C8-C9
23	G	1606	LMT	O5'-C1'-O1'-C1
18	A	831	CLA	C5-C6-C7-C8
18	A	810	CLA	C2-C1-O2A-CGA
18	A	811	CLA	C2-C1-O2A-CGA
18	1	5009	CLA	C2-C1-O2A-CGA
18	4	308	CLA	C2-C1-O2A-CGA
18	B	837	CLA	C2-C3-C5-C6
22	A	848	LHG	C19-C20-C21-C22
18	3	319	CLA	C5-C6-C7-C8
18	A	807	CLA	C11-C12-C13-C14
18	A	810	CLA	C11-C12-C13-C14
18	A	823	CLA	C11-C12-C13-C14
18	A	831	CLA	C6-C7-C8-C9
18	B	801	CLA	C11-C12-C13-C14
18	B	805	CLA	C14-C13-C15-C16
18	F	301	CLA	C14-C13-C15-C16
18	F	302	CLA	C11-C12-C13-C14
18	J	1101	CLA	C6-C7-C8-C9
18	J	1101	CLA	C11-C12-C13-C14
18	3	315	CLA	C11-C12-C13-C14
22	A	848	LHG	C11-C10-C9-C8
22	A	849	LHG	C14-C15-C16-C17
18	A	806	CLA	C10-C11-C12-C13
18	A	827	CLA	C8-C10-C11-C12
18	A	834	CLA	C4-C3-C5-C6
26	B	855	DGD	C4A-C5A-C6A-C7A
18	A	825	CLA	C16-C17-C18-C19
18	A	852	CLA	C16-C17-C18-C19
18	4	306	CLA	CBD-CGD-O2D-CED
18	A	826	CLA	C3-C5-C6-C7
21	A	846	BCR	C1-C6-C7-C8
21	A	846	BCR	C5-C6-C7-C8
21	A	846	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
21	A	846	BCR	C23-C24-C25-C30
21	A	847	BCR	C1-C6-C7-C8
21	A	847	BCR	C5-C6-C7-C8
21	B	846	BCR	C23-C24-C25-C26
21	B	846	BCR	C23-C24-C25-C30
21	G	1604	BCR	C23-C24-C25-C26
21	G	1604	BCR	C23-C24-C25-C30
21	I	101	BCR	C23-C24-C25-C26
21	I	102	BCR	C5-C6-C7-C8
21	L	302	BCR	C1-C6-C7-C8
21	L	302	BCR	C5-C6-C7-C8
29	2	303	LUT	C1-C6-C7-C8
29	2	303	LUT	C5-C6-C7-C8
29	3	304	LUT	C5-C6-C7-C8
29	4	303	LUT	C1-C6-C7-C8
29	4	303	LUT	C5-C6-C7-C8
22	A	848	LHG	C29-C30-C31-C32
21	A	843	BCR	C36-C18-C19-C20
22	A	849	LHG	C19-C20-C21-C22
21	B	844	BCR	C11-C12-C13-C14
21	B	846	BCR	C7-C8-C9-C10
21	K	1405	BCR	C11-C12-C13-C14
18	K	1402	CLA	C10-C11-C12-C13
22	1	5019	LHG	C35-C36-C37-C38
18	A	807	CLA	C16-C17-C18-C19
30	2	315	CHL	C6-C7-C8-C10
18	A	853	CLA	C8-C10-C11-C12
18	B	819	CLA	O1A-CGA-O2A-C1
18	B	827	CLA	O1A-CGA-O2A-C1
18	1	5009	CLA	C15-C16-C17-C18
18	1	5010	CLA	C13-C15-C16-C17
22	A	848	LHG	O6-C4-C5-C6
22	2	320	LHG	O6-C4-C5-C6
18	K	1401	CLA	C2C-C3C-CAC-CBC
18	A	802	CLA	C11-C12-C13-C15
18	A	805	CLA	C11-C12-C13-C15
18	A	808	CLA	C6-C7-C8-C10
18	A	810	CLA	C11-C10-C8-C7
18	A	810	CLA	C11-C12-C13-C15
18	A	812	CLA	C6-C7-C8-C10
18	A	815	CLA	C11-C10-C8-C7
18	A	817	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
18	A	819	CLA	C11-C12-C13-C15
18	A	823	CLA	C11-C10-C8-C7
18	A	829	CLA	C12-C13-C15-C16
18	A	831	CLA	C12-C13-C15-C16
18	A	832	CLA	C11-C10-C8-C7
18	A	838	CLA	C6-C7-C8-C10
18	A	852	CLA	C6-C7-C8-C10
18	B	801	CLA	C6-C7-C8-C10
18	B	801	CLA	C11-C12-C13-C15
18	B	805	CLA	C11-C10-C8-C7
18	B	807	CLA	C6-C7-C8-C10
18	B	808	CLA	C11-C12-C13-C15
18	B	810	CLA	C6-C7-C8-C10
18	B	811	CLA	C6-C7-C8-C10
18	B	815	CLA	C11-C10-C8-C7
18	B	818	CLA	C11-C10-C8-C7
18	B	822	CLA	C6-C7-C8-C10
18	B	826	CLA	C11-C10-C8-C7
18	B	830	CLA	C12-C13-C15-C16
18	B	831	CLA	C11-C12-C13-C15
18	B	837	CLA	C12-C13-C15-C16
18	B	840	CLA	C6-C7-C8-C10
18	F	301	CLA	C12-C13-C15-C16
18	1	5009	CLA	C11-C12-C13-C15
18	4	305	CLA	C6-C7-C8-C10
18	4	307	CLA	C12-C13-C15-C16
18	4	308	CLA	C11-C10-C8-C7
18	4	309	CLA	C11-C10-C8-C7
19	B	842	PQN	C16-C17-C18-C20
30	3	310	CHL	C6-C7-C8-C10
18	B	833	CLA	C8-C10-C11-C12
21	F	304	BCR	C19-C20-C21-C22
21	I	101	BCR	C19-C20-C21-C22
21	I	102	BCR	C9-C10-C11-C12
21	J	1104	BCR	C19-C20-C21-C22
21	1	5005	BCR	C19-C20-C21-C22
29	1	5003	LUT	C29-C30-C31-C32
18	3	319	CLA	C11-C12-C13-C15
18	B	804	CLA	C15-C16-C17-C18
24	F	308	LMG	O8-C28-C29-C30
18	B	832	CLA	C2A-CAA-CBA-CGA
18	F	303	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	I	101	BCR	C11-C10-C9-C34
22	2	320	LHG	C23-C24-C25-C26
18	A	824	CLA	C6-C7-C8-C10
18	A	828	CLA	CBA-CGA-O2A-C1
18	A	816	CLA	C11-C10-C8-C7
18	B	814	CLA	O1A-CGA-O2A-C1
18	A	804	CLA	CAD-CBD-CGD-O2D
18	A	821	CLA	CAD-CBD-CGD-O2D
18	B	825	CLA	CAD-CBD-CGD-O2D
18	B	830	CLA	CAD-CBD-CGD-O2D
30	3	312	CHL	CAD-CBD-CGD-O2D
30	3	313	CHL	CAD-CBD-CGD-O2D
22	B	849	LHG	C29-C30-C31-C32
23	G	1605	LMT	C11-C10-C9-C8
18	B	824	CLA	C4-C3-C5-C6
18	B	824	CLA	C2-C3-C5-C6
22	A	848	LHG	C25-C26-C27-C28
24	B	850	LMG	C7-C8-C9-O8
24	G	1607	LMG	C7-C8-C9-O8
18	A	825	CLA	O1A-CGA-O2A-C1
18	B	839	CLA	O1A-CGA-O2A-C1
26	B	855	DGD	C6B-C7B-C8B-C9B
22	A	848	LHG	O6-C4-C5-O7
18	B	811	CLA	C10-C11-C12-C13
18	B	841	CLA	CAA-CBA-CGA-O2A
26	2	327	DGD	O1G-C1A-C2A-C3A
26	J	1106	DGD	C3A-C4A-C5A-C6A
22	B	848	LHG	O10-C23-O8-C6
18	B	803	CLA	C16-C17-C18-C20
18	B	806	CLA	C16-C17-C18-C20
18	B	834	CLA	C11-C12-C13-C14
30	2	315	CHL	C6-C7-C8-C9
18	A	803	CLA	CHA-CBD-CGD-O1D
18	A	803	CLA	CHA-CBD-CGD-O2D
18	A	818	CLA	CHA-CBD-CGD-O1D
18	A	818	CLA	CHA-CBD-CGD-O2D
18	A	837	CLA	CHA-CBD-CGD-O1D
18	A	837	CLA	CHA-CBD-CGD-O2D
18	B	801	CLA	CHA-CBD-CGD-O2D
18	B	806	CLA	CHA-CBD-CGD-O1D
18	B	806	CLA	CHA-CBD-CGD-O2D
18	B	822	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
18	B	822	CLA	CHA-CBD-CGD-O2D
18	B	831	CLA	CHA-CBD-CGD-O1D
18	1	5017	CLA	CHA-CBD-CGD-O1D
18	2	312	CLA	CHA-CBD-CGD-O1D
18	2	312	CLA	CHA-CBD-CGD-O2D
18	3	309	CLA	CHA-CBD-CGD-O1D
18	3	309	CLA	CHA-CBD-CGD-O2D
18	4	311	CLA	CHA-CBD-CGD-O2D
21	B	847	BCR	C19-C20-C21-C22
30	2	319	CHL	CHA-CBD-CGD-O2D
18	A	813	CLA	C10-C11-C12-C13
26	2	327	DGD	C2A-C3A-C4A-C5A
18	A	806	CLA	C3-C5-C6-C7
18	B	807	CLA	O1A-CGA-O2A-C1
21	B	845	BCR	C11-C10-C9-C8
18	B	810	CLA	C8-C10-C11-C12
24	B	850	LMG	O7-C8-C9-O8
24	2	322	LMG	O1-C7-C8-O7
18	F	303	CLA	C15-C16-C17-C18
18	4	309	CLA	C10-C11-C12-C13
18	A	828	CLA	O1A-CGA-O2A-C1
25	A	854	GOL	O2-C2-C3-O3
18	4	306	CLA	O1D-CGD-O2D-CED
18	A	836	CLA	C15-C16-C17-C18
18	A	817	CLA	C11-C10-C8-C9
18	A	817	CLA	C11-C12-C13-C14
18	A	825	CLA	C11-C12-C13-C14
18	A	832	CLA	C11-C12-C13-C14
18	B	827	CLA	C11-C12-C13-C14
18	H	1701	CLA	C11-C10-C8-C9
18	1	5015	CLA	C14-C13-C15-C16
18	4	308	CLA	C11-C10-C8-C9
24	2	322	LMG	C15-C16-C17-C18
18	B	841	CLA	O1D-CGD-O2D-CED
18	A	828	CLA	C13-C15-C16-C17
18	3	315	CLA	C13-C15-C16-C17
30	2	315	CHL	C2A-CAA-CBA-CGA
22	A	848	LHG	C30-C31-C32-C33
21	I	102	BCR	C36-C18-C19-C20
23	4	319	LMT	C4'-C5'-C6'-O6'
18	A	817	CLA	C1A-C2A-CAA-CBA
18	A	831	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	B	820	CLA	C1A-C2A-CAA-CBA
18	B	827	CLA	C1A-C2A-CAA-CBA
18	B	830	CLA	C1A-C2A-CAA-CBA
18	2	326	CLA	C1A-C2A-CAA-CBA
18	B	818	CLA	C16-C17-C18-C19
18	B	824	CLA	C6-C7-C8-C9
18	B	827	CLA	C8-C10-C11-C12
19	B	842	PQN	C25-C26-C27-C28
18	A	809	CLA	C2-C1-O2A-CGA
21	A	847	BCR	C19-C20-C21-C22
21	B	847	BCR	C9-C10-C11-C12
21	I	102	BCR	C13-C14-C15-C16
22	B	848	LHG	C3-O3-P-O6
22	B	849	LHG	C4-O6-P-O3
22	2	320	LHG	C3-O3-P-O6
22	B	849	LHG	C2-C3-O3-P
23	B	853	LMT	C3-C4-C5-C6
22	B	848	LHG	C4-O6-P-O5
22	2	320	LHG	C4-O6-P-O5
18	B	815	CLA	C16-C17-C18-C19
18	F	303	CLA	C16-C17-C18-C19
18	A	812	CLA	C13-C15-C16-C17
18	B	820	CLA	CBA-CGA-O2A-C1
22	B	849	LHG	O6-C4-C5-C6
23	4	319	LMT	O1'-C1-C2-C3
18	A	818	CLA	CAD-CBD-CGD-O1D
18	A	834	CLA	C2-C3-C5-C6
18	B	806	CLA	CAD-CBD-CGD-O1D
18	B	831	CLA	CAD-CBD-CGD-O1D
18	B	836	CLA	CAD-CBD-CGD-O1D
30	2	319	CHL	CAD-CBD-CGD-O1D
18	B	832	CLA	C5-C6-C7-C8
18	2	309	CLA	C13-C15-C16-C17
18	B	834	CLA	C3-C5-C6-C7
24	A	851	LMG	C18-C19-C20-C21
18	1	5009	CLA	C16-C17-C18-C20
30	2	319	CHL	C4-C3-C5-C6
18	A	808	CLA	C11-C12-C13-C15
18	A	810	CLA	C6-C7-C8-C10
18	A	817	CLA	C11-C12-C13-C15
18	A	825	CLA	C11-C12-C13-C15
18	A	826	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
18	A	828	CLA	C11-C12-C13-C15
18	A	832	CLA	C11-C12-C13-C15
18	A	832	CLA	C12-C13-C15-C16
18	A	836	CLA	C12-C13-C15-C16
18	B	815	CLA	C12-C13-C15-C16
18	B	817	CLA	C6-C7-C8-C10
18	B	828	CLA	C6-C7-C8-C10
18	B	832	CLA	C11-C10-C8-C7
18	B	837	CLA	C6-C7-C8-C10
18	B	841	CLA	C11-C12-C13-C15
18	F	302	CLA	C11-C12-C13-C15
18	G	1603	CLA	C6-C7-C8-C10
18	1	5015	CLA	C12-C13-C15-C16
18	4	315	CLA	C11-C12-C13-C15
22	B	849	LHG	O6-C4-C5-O7
22	2	320	LHG	O6-C4-C5-O7
29	1	5003	LUT	C25-C26-C27-C28
29	3	304	LUT	C25-C26-C27-C28
30	2	314	CHL	C6-C7-C8-C10
18	A	853	CLA	C3-C5-C6-C7
21	A	843	BCR	C19-C20-C21-C22
21	K	1405	BCR	C19-C20-C21-C22
18	1	5012	CLA	CAA-CBA-CGA-O2A
22	1	5019	LHG	C4-C5-C6-O8
24	2	322	LMG	C7-C8-C9-O8
22	1	5019	LHG	O7-C5-C6-O8
24	G	1607	LMG	O1-C7-C8-O7
18	A	836	CLA	C8-C10-C11-C12
18	B	818	CLA	C15-C16-C17-C18
18	B	828	CLA	C8-C10-C11-C12
24	G	1607	LMG	C8-C7-O1-C1
24	2	322	LMG	C8-C7-O1-C1
18	2	309	CLA	C16-C17-C18-C20
18	K	1402	CLA	C5-C6-C7-C8
22	B	849	LHG	C12-C13-C14-C15
18	A	825	CLA	C13-C15-C16-C17
18	A	830	CLA	C4-C3-C5-C6
18	B	806	CLA	C4-C3-C5-C6
18	B	811	CLA	CBA-CGA-O2A-C1
18	G	1603	CLA	C15-C16-C17-C18
18	A	802	CLA	C6-C7-C8-C9
18	A	810	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
18	A	819	CLA	C11-C12-C13-C14
18	A	827	CLA	C14-C13-C15-C16
18	A	828	CLA	C6-C7-C8-C9
18	A	840	CLA	C11-C10-C8-C9
18	B	805	CLA	C11-C10-C8-C9
18	B	822	CLA	C6-C7-C8-C9
18	3	315	CLA	C14-C13-C15-C16
18	4	309	CLA	C11-C10-C8-C9
19	B	842	PQN	C16-C17-C18-C19
30	2	314	CHL	C6-C7-C8-C9
30	3	310	CHL	C6-C7-C8-C9
30	2	314	CHL	C3-C5-C6-C7
21	B	845	BCR	C18-C19-C20-C21
21	K	1405	BCR	C18-C19-C20-C21
21	2	305	BCR	C18-C19-C20-C21
18	B	819	CLA	CAA-CBA-CGA-O2A
23	G	1606	LMT	O1'-C1-C2-C3
18	B	811	CLA	O1A-CGA-O2A-C1
18	A	827	CLA	C13-C15-C16-C17
18	B	837	CLA	C8-C10-C11-C12
18	2	308	CLA	C16-C17-C18-C19
23	A	850	LMT	C1-C2-C3-C4
18	A	822	CLA	C8-C10-C11-C12
24	F	307	LMG	C9-C8-O7-C10
26	J	1106	DGD	C1G-C2G-O2G-C1B
18	4	308	CLA	C2A-CAA-CBA-CGA
18	A	812	CLA	C2-C1-O2A-CGA
18	A	828	CLA	C2-C1-O2A-CGA
18	A	830	CLA	C2-C1-O2A-CGA
18	A	834	CLA	C2-C1-O2A-CGA
18	B	814	CLA	C2-C1-O2A-CGA
18	B	828	CLA	C2-C1-O2A-CGA
22	1	5019	LHG	C34-C35-C36-C37
30	3	310	CHL	CBA-CGA-O2A-C1
21	B	802	BCR	C9-C10-C11-C12
29	4	303	LUT	C29-C30-C31-C32
18	B	832	CLA	C11-C12-C13-C14
21	B	847	BCR	C23-C24-C25-C26
21	B	847	BCR	C23-C24-C25-C30
21	F	304	BCR	C23-C24-C25-C26
21	I	101	BCR	C23-C24-C25-C30
21	I	102	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
18	A	828	CLA	C10-C11-C12-C13
22	1	5019	LHG	C11-C12-C13-C14
24	B	851	LMG	O6-C1-O1-C7
26	2	327	DGD	O6D-C1D-O3G-C3G
18	G	1601	CLA	C2A-CAA-CBA-CGA
26	2	327	DGD	C2D-C1D-O3G-C3G
23	G	1605	LMT	C7-C8-C9-C10
22	1	5019	LHG	C4-O6-P-O3
18	F	302	CLA	C15-C16-C17-C18
18	B	805	CLA	C10-C11-C12-C13
24	J	1102	LMG	C11-C12-C13-C14
18	2	308	CLA	C4-C3-C5-C6
18	A	827	CLA	C12-C13-C15-C16
18	A	840	CLA	C6-C7-C8-C10
18	B	809	CLA	C12-C13-C15-C16
18	H	1701	CLA	C11-C10-C8-C7
18	J	1101	CLA	C6-C7-C8-C10
18	2	310	CLA	C12-C13-C15-C16
18	4	315	CLA	C6-C7-C8-C10
18	A	806	CLA	C6-C7-C8-C9
18	A	808	CLA	C11-C12-C13-C14
18	A	852	CLA	C11-C10-C8-C9
18	B	807	CLA	C11-C12-C13-C14
18	B	817	CLA	C6-C7-C8-C9
18	B	826	CLA	C11-C10-C8-C9
18	B	828	CLA	C6-C7-C8-C9
18	2	309	CLA	C6-C7-C8-C9
18	4	315	CLA	C11-C10-C8-C9
18	4	315	CLA	C11-C12-C13-C14
21	A	855	BCR	C19-C20-C21-C22
18	F	303	CLA	C16-C17-C18-C20
18	1	5015	CLA	C16-C17-C18-C20
18	B	828	CLA	CAA-CBA-CGA-O2A
18	K	1404	CLA	C2A-CAA-CBA-CGA
18	A	835	CLA	C10-C11-C12-C13
22	A	848	LHG	C17-C18-C19-C20
22	1	5019	LHG	C31-C32-C33-C34
24	A	851	LMG	C12-C13-C14-C15
18	B	820	CLA	O1A-CGA-O2A-C1
18	B	824	CLA	C6-C7-C8-C10
30	4	316	CHL	C11-C12-C13-C15
22	2	320	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
22	1	5019	LHG	C30-C31-C32-C33
18	F	302	CLA	CAA-CBA-CGA-O2A
18	B	817	CLA	C5-C6-C7-C8
21	A	843	BCR	C17-C18-C19-C20
21	A	843	BCR	C21-C22-C23-C24
18	A	824	CLA	C2-C3-C5-C6
18	F	302	CLA	C2-C3-C5-C6
18	L	305	CLA	CBA-CGA-O2A-C1
18	B	834	CLA	C10-C11-C12-C13
22	A	849	LHG	C7-C8-C9-C10
18	B	804	CLA	C2A-CAA-CBA-CGA
21	B	843	BCR	C19-C20-C21-C22
21	B	845	BCR	C19-C20-C21-C22
21	F	305	BCR	C19-C20-C21-C22
21	L	307	BCR	C19-C20-C21-C22
21	2	305	BCR	C19-C20-C21-C22
21	3	305	BCR	C9-C10-C11-C12
29	3	304	LUT	C29-C30-C31-C32
18	L	305	CLA	O1A-CGA-O2A-C1
22	A	849	LHG	O6-C4-C5-O7
21	F	304	BCR	C10-C11-C12-C13
21	L	302	BCR	C10-C11-C12-C13
22	B	849	LHG	C30-C31-C32-C33
18	B	825	CLA	O1D-CGD-O2D-CED
18	B	825	CLA	C4-C3-C5-C6
22	A	849	LHG	C17-C18-C19-C20
18	A	823	CLA	C2-C3-C5-C6
18	A	838	CLA	O1A-CGA-O2A-C1
18	B	822	CLA	C2-C1-O2A-CGA
18	2	308	CLA	C16-C17-C18-C20
18	B	819	CLA	C2A-CAA-CBA-CGA
18	2	306	CLA	C2A-CAA-CBA-CGA
24	A	851	LMG	O7-C8-C9-O8
30	3	313	CHL	C2A-CAA-CBA-CGA
18	A	819	CLA	C3A-C2A-CAA-CBA
18	1	5018	CLA	C3A-C2A-CAA-CBA
22	A	848	LHG	C26-C27-C28-C29
21	L	307	BCR	C9-C10-C11-C12
21	3	305	BCR	C19-C20-C21-C22
21	3	306	BCR	C15-C16-C17-C18
18	A	823	CLA	C4-C3-C5-C6
18	A	815	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
18	A	826	CLA	C14-C13-C15-C16
18	G	1603	CLA	C11-C12-C13-C14
18	1	5006	CLA	C11-C12-C13-C14
18	B	815	CLA	C16-C17-C18-C20
18	4	315	CLA	C16-C17-C18-C20
18	B	825	CLA	C15-C16-C17-C18
26	2	327	DGD	C6A-C7A-C8A-C9A
18	B	811	CLA	C8-C10-C11-C12
21	A	845	BCR	C16-C17-C18-C36
21	A	847	BCR	C16-C17-C18-C36
21	B	802	BCR	C16-C17-C18-C36
21	B	843	BCR	C35-C13-C14-C15
21	B	843	BCR	C16-C17-C18-C36
21	F	305	BCR	C16-C17-C18-C36
21	G	1604	BCR	C16-C17-C18-C36
21	I	101	BCR	C35-C13-C14-C15
21	L	303	BCR	C16-C17-C18-C36
21	L	303	BCR	C20-C21-C22-C37
21	3	306	BCR	C35-C13-C14-C15
21	3	306	BCR	C16-C17-C18-C36
18	3	301	CLA	CAA-CBA-CGA-O2A
18	B	838	CLA	C2A-CAA-CBA-CGA
18	L	305	CLA	C2A-CAA-CBA-CGA
18	A	804	CLA	O1A-CGA-O2A-C1
18	B	832	CLA	C11-C12-C13-C15
18	2	309	CLA	C16-C17-C18-C19
19	B	842	PQN	C26-C27-C28-C29
30	2	314	CHL	O2A-C1-C2-C3
29	1	5003	LUT	C7-C8-C9-C19
22	B	849	LHG	C31-C32-C33-C34
24	2	322	LMG	C7-C8-O7-C10
24	2	322	LMG	C9-C8-O7-C10
18	B	828	CLA	C4-C3-C5-C6
18	A	821	CLA	C1A-C2A-CAA-CBA
18	B	801	CLA	C1A-C2A-CAA-CBA
18	B	811	CLA	C1A-C2A-CAA-CBA
18	B	817	CLA	C1A-C2A-CAA-CBA
18	B	819	CLA	C1A-C2A-CAA-CBA
18	B	821	CLA	C1A-C2A-CAA-CBA
18	L	305	CLA	C1A-C2A-CAA-CBA
18	1	5018	CLA	C1A-C2A-CAA-CBA
18	2	317	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	4	310	CLA	C1A-C2A-CAA-CBA
18	A	804	CLA	C12-C13-C15-C16
18	A	807	CLA	C11-C12-C13-C15
18	A	807	CLA	C12-C13-C15-C16
18	A	812	CLA	C11-C10-C8-C7
18	A	836	CLA	C11-C12-C13-C15
18	B	804	CLA	C12-C13-C15-C16
18	B	805	CLA	C6-C7-C8-C10
18	B	819	CLA	C11-C10-C8-C7
18	B	827	CLA	C11-C12-C13-C15
18	B	839	CLA	C11-C10-C8-C7
18	A	823	CLA	C3-C5-C6-C7
18	3	301	CLA	CAA-CBA-CGA-O1A
24	2	321	LMG	O7-C10-C11-C12
21	A	843	BCR	C15-C16-C17-C18
21	B	846	BCR	C13-C14-C15-C16
18	B	819	CLA	C10-C11-C12-C13
18	A	815	CLA	C16-C17-C18-C20
26	B	855	DGD	C3A-C4A-C5A-C6A
18	A	812	CLA	C2A-CAA-CBA-CGA
18	B	806	CLA	C2A-CAA-CBA-CGA
18	B	827	CLA	C2A-CAA-CBA-CGA
23	2	325	LMT	C1-C2-C3-C4
18	B	840	CLA	C13-C15-C16-C17
18	1	5009	CLA	C13-C15-C16-C17
30	3	310	CHL	C5-C6-C7-C8
26	F	309	DGD	C2A-C3A-C4A-C5A
24	1	5020	LMG	O7-C10-C11-C12
18	A	819	CLA	C5-C6-C7-C8
18	B	808	CLA	C13-C15-C16-C17
18	A	838	CLA	CBA-CGA-O2A-C1
18	B	816	CLA	CBA-CGA-O2A-C1
18	A	812	CLA	C4-C3-C5-C6
18	A	817	CLA	C4-C3-C5-C6
18	1	5015	CLA	C4-C3-C5-C6
18	A	825	CLA	C10-C11-C12-C13
26	J	1106	DGD	C6B-C7B-C8B-C9B
21	A	845	BCR	C16-C17-C18-C19
21	A	847	BCR	C16-C17-C18-C19
21	B	802	BCR	C16-C17-C18-C19
21	B	843	BCR	C12-C13-C14-C15
21	B	843	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
21	F	305	BCR	C16-C17-C18-C19
21	G	1604	BCR	C16-C17-C18-C19
21	I	101	BCR	C12-C13-C14-C15
21	L	303	BCR	C16-C17-C18-C19
21	L	303	BCR	C20-C21-C22-C23
21	3	306	BCR	C12-C13-C14-C15
21	3	306	BCR	C16-C17-C18-C19
18	1	5017	CLA	CAA-CBA-CGA-O1A
22	2	320	LHG	O7-C5-C6-O8
24	A	851	LMG	O1-C7-C8-O7
24	G	1607	LMG	O7-C8-C9-O8
18	B	819	CLA	C5-C6-C7-C8
18	1	5007	CLA	C2A-CAA-CBA-CGA
30	2	319	CHL	C2A-CAA-CBA-CGA
21	A	846	BCR	C19-C20-C21-C22
21	B	845	BCR	C9-C10-C11-C12
21	I	102	BCR	C19-C20-C21-C22
21	L	303	BCR	C19-C20-C21-C22
29	3	303	LUT	C29-C30-C31-C32
18	K	1401	CLA	CAA-CBA-CGA-O1A
18	1	5017	CLA	CAA-CBA-CGA-O2A
18	1	5006	CLA	C2-C1-O2A-CGA
18	B	806	CLA	C2-C3-C5-C6
30	2	319	CHL	C2-C3-C5-C6
18	B	801	CLA	C14-C13-C15-C16
18	B	817	CLA	C11-C10-C8-C9
18	B	840	CLA	C11-C12-C13-C14
18	B	841	CLA	C11-C12-C13-C14
18	2	309	CLA	C11-C10-C8-C9
26	F	309	DGD	CCA-CDA-CEA-CFA
18	A	806	CLA	C2A-CAA-CBA-CGA
18	A	852	CLA	C2A-CAA-CBA-CGA
21	A	845	BCR	C1-C6-C7-C8
21	A	847	BCR	C23-C24-C25-C30
21	F	304	BCR	C23-C24-C25-C30
18	K	1404	CLA	CAA-CBA-CGA-O2A
24	A	851	LMG	C7-C8-C9-O8
18	K	1401	CLA	CAA-CBA-CGA-O2A
22	A	848	LHG	O1-C1-C2-C3
25	A	854	GOL	C1-C2-C3-O3
18	B	816	CLA	O1A-CGA-O2A-C1
21	L	307	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
18	A	820	CLA	C4-C3-C5-C6
18	B	814	CLA	C4-C3-C5-C6
18	B	839	CLA	C4-C3-C5-C6
18	4	308	CLA	C4-C3-C5-C6
18	B	828	CLA	C16-C17-C18-C19
18	1	5015	CLA	C16-C17-C18-C19
18	B	829	CLA	C8-C10-C11-C12
18	A	830	CLA	C2-C3-C5-C6
18	2	308	CLA	C2-C3-C5-C6
18	G	1601	CLA	C3-C5-C6-C7
18	A	804	CLA	C10-C11-C12-C13
18	B	803	CLA	C10-C11-C12-C13
22	2	320	LHG	O8-C23-C24-C25
30	2	315	CHL	CAA-CBA-CGA-O2A
18	L	301	CLA	C6-C7-C8-C10
17	A	801	CL0	C5-C6-C7-C8
18	A	827	CLA	CAA-CBA-CGA-O2A
22	A	849	LHG	O6-C4-C5-C6
18	A	826	CLA	CAA-CBA-CGA-O2A
18	B	801	CLA	C4-C3-C5-C6
18	A	820	CLA	C11-C10-C8-C7
18	A	829	CLA	C6-C7-C8-C10
18	B	806	CLA	C12-C13-C15-C16
18	B	828	CLA	C2-C3-C5-C6
18	L	305	CLA	C11-C10-C8-C7
18	1	5006	CLA	C6-C7-C8-C10
30	2	314	CHL	C12-C13-C15-C16
18	1	5015	CLA	C5-C6-C7-C8
21	K	1405	BCR	C9-C10-C11-C12
18	K	1402	CLA	CAA-CBA-CGA-O2A
26	B	855	DGD	O1G-C1G-C2G-O2G
18	A	804	CLA	CBA-CGA-O2A-C1
26	B	855	DGD	CAB-CBB-CCB-CDB
18	A	806	CLA	CAA-CBA-CGA-O2A
18	B	824	CLA	CAA-CBA-CGA-O2A
18	1	5018	CLA	CAA-CBA-CGA-O2A
18	B	830	CLA	C4-C3-C5-C6
26	1	5002	DGD	C2A-C3A-C4A-C5A
18	A	817	CLA	C2-C3-C5-C6
18	B	814	CLA	C2-C3-C5-C6
18	A	810	CLA	C6-C7-C8-C9
18	A	812	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
18	A	812	CLA	C11-C10-C8-C9
18	A	819	CLA	C6-C7-C8-C9
18	A	828	CLA	C11-C12-C13-C14
18	A	832	CLA	C14-C13-C15-C16
18	A	836	CLA	C14-C13-C15-C16
18	B	831	CLA	C11-C12-C13-C14
18	B	837	CLA	C6-C7-C8-C9
30	2	314	CHL	C14-C13-C15-C16
22	B	849	LHG	C27-C28-C29-C30
18	B	801	CLA	C3A-C2A-CAA-CBA
18	B	811	CLA	C3A-C2A-CAA-CBA
18	B	819	CLA	C3A-C2A-CAA-CBA
18	3	308	CLA	CAA-CBA-CGA-O2A
24	1	5001	LMG	O7-C10-C11-C12
18	B	821	CLA	CAD-CBD-CGD-O2D
18	B	827	CLA	CAD-CBD-CGD-O2D
18	1	5017	CLA	CAD-CBD-CGD-O2D
18	2	307	CLA	CAD-CBD-CGD-O2D
18	2	309	CLA	CAD-CBD-CGD-O2D
18	2	312	CLA	CAD-CBD-CGD-O2D
26	1	5002	DGD	C1G-C2G-O2G-C1B
26	1	5002	DGD	C3G-C2G-O2G-C1B
30	3	316	CHL	CAD-CBD-CGD-O2D
30	4	316	CHL	CAD-CBD-CGD-O2D
18	4	315	CLA	C16-C17-C18-C19
30	3	312	CHL	C2A-CAA-CBA-CGA
18	B	814	CLA	CAA-CBA-CGA-O2A
26	J	1106	DGD	CCA-CDA-CEA-CFA
18	A	826	CLA	C4-C3-C5-C6
18	B	816	CLA	C4-C3-C5-C6
18	B	839	CLA	C2-C3-C5-C6
18	1	5015	CLA	C2-C3-C5-C6
18	A	816	CLA	CAA-CBA-CGA-O2A
18	3	307	CLA	CAA-CBA-CGA-O2A
18	3	319	CLA	CAA-CBA-CGA-O2A
26	2	327	DGD	O2G-C1B-C2B-C3B
21	B	847	BCR	C21-C22-C23-C24
21	I	102	BCR	C17-C18-C19-C20
21	J	1104	BCR	C17-C18-C19-C20
22	B	849	LHG	C4-C5-C6-O8
30	2	318	CHL	CAA-CBA-CGA-O1A
26	B	855	DGD	O6D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
18	2	313	CLA	CAA-CBA-CGA-O2A
24	1	5001	LMG	O8-C28-C29-C30
30	3	313	CHL	CAA-CBA-CGA-O2A
30	3	316	CHL	CAA-CBA-CGA-O2A
30	2	318	CHL	CAA-CBA-CGA-O2A
18	A	803	CLA	C2A-CAA-CBA-CGA
18	A	803	CLA	CAA-CBA-CGA-O2A
18	B	839	CLA	CAA-CBA-CGA-O2A
18	B	840	CLA	CAA-CBA-CGA-O2A
18	L	305	CLA	CAA-CBA-CGA-O2A
18	A	819	CLA	C3-C5-C6-C7
18	A	802	CLA	C16-C17-C18-C19
19	B	842	PQN	C26-C27-C28-C30
30	4	316	CHL	C11-C12-C13-C14
18	A	805	CLA	CHA-CBD-CGD-O1D
18	A	805	CLA	CHA-CBD-CGD-O2D
18	A	809	CLA	CHA-CBD-CGD-O1D
18	A	809	CLA	CHA-CBD-CGD-O2D
18	A	810	CLA	CHA-CBD-CGD-O2D
18	A	814	CLA	CHA-CBD-CGD-O1D
18	A	814	CLA	CHA-CBD-CGD-O2D
18	A	819	CLA	CHA-CBD-CGD-O1D
18	A	819	CLA	CHA-CBD-CGD-O2D
18	A	823	CLA	CHA-CBD-CGD-O1D
18	A	823	CLA	CHA-CBD-CGD-O2D
18	A	826	CLA	CHA-CBD-CGD-O1D
18	A	826	CLA	CHA-CBD-CGD-O2D
18	A	828	CLA	CHA-CBD-CGD-O2D
18	A	835	CLA	CHA-CBD-CGD-O1D
18	A	835	CLA	CHA-CBD-CGD-O2D
18	A	853	CLA	CHA-CBD-CGD-O1D
18	A	853	CLA	CHA-CBD-CGD-O2D
18	B	805	CLA	CHA-CBD-CGD-O1D
18	B	805	CLA	CHA-CBD-CGD-O2D
18	B	807	CLA	CHA-CBD-CGD-O1D
18	B	807	CLA	CHA-CBD-CGD-O2D
18	B	814	CLA	CHA-CBD-CGD-O1D
18	B	814	CLA	CHA-CBD-CGD-O2D
18	B	824	CLA	CHA-CBD-CGD-O1D
18	B	824	CLA	CHA-CBD-CGD-O2D
18	B	828	CLA	CHA-CBD-CGD-O2D
18	B	831	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	B	832	CLA	CHA-CBD-CGD-O1D
18	B	832	CLA	CHA-CBD-CGD-O2D
18	B	836	CLA	CHA-CBD-CGD-O1D
18	B	837	CLA	CHA-CBD-CGD-O1D
18	B	837	CLA	CHA-CBD-CGD-O2D
18	K	1403	CLA	CHA-CBD-CGD-O1D
18	K	1403	CLA	CHA-CBD-CGD-O2D
18	L	301	CLA	CHA-CBD-CGD-O2D
18	1	5008	CLA	CHA-CBD-CGD-O1D
18	1	5008	CLA	CHA-CBD-CGD-O2D
18	1	5009	CLA	CHA-CBD-CGD-O1D
18	1	5009	CLA	CHA-CBD-CGD-O2D
18	1	5010	CLA	CHA-CBD-CGD-O2D
18	1	5017	CLA	CHA-CBD-CGD-O2D
18	1	5018	CLA	CHA-CBD-CGD-O1D
18	1	5018	CLA	CHA-CBD-CGD-O2D
18	2	317	CLA	CHA-CBD-CGD-O2D
18	3	307	CLA	CHA-CBD-CGD-O1D
18	3	307	CLA	CHA-CBD-CGD-O2D
18	3	317	CLA	CHA-CBD-CGD-O1D
18	3	317	CLA	CHA-CBD-CGD-O2D
18	3	318	CLA	CHA-CBD-CGD-O1D
18	3	318	CLA	CHA-CBD-CGD-O2D
18	3	319	CLA	CHA-CBD-CGD-O1D
18	3	319	CLA	CHA-CBD-CGD-O2D
18	4	306	CLA	CHA-CBD-CGD-O1D
18	4	306	CLA	CHA-CBD-CGD-O2D
18	4	309	CLA	CHA-CBD-CGD-O1D
18	4	309	CLA	CHA-CBD-CGD-O2D
18	4	310	CLA	CHA-CBD-CGD-O1D
18	4	310	CLA	CHA-CBD-CGD-O2D
18	4	315	CLA	CHA-CBD-CGD-O1D
18	4	315	CLA	CHA-CBD-CGD-O2D
21	B	845	BCR	C15-C16-C17-C18
30	2	315	CHL	CHA-CBD-CGD-O1D
30	2	315	CHL	CHA-CBD-CGD-O2D
30	4	313	CHL	CHA-CBD-CGD-O1D
30	4	313	CHL	CHA-CBD-CGD-O2D
18	A	835	CLA	CAA-CBA-CGA-O2A
18	B	832	CLA	CAA-CBA-CGA-O2A
18	B	837	CLA	CAA-CBA-CGA-O2A
18	2	306	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	J	1102	LMG	O7-C10-C11-C12
22	B	849	LHG	C25-C26-C27-C28
24	1	5020	LMG	C18-C19-C20-C21
22	B	849	LHG	O7-C5-C6-O8
24	B	854	LMG	O6-C5-C6-O5
18	H	1701	CLA	C10-C11-C12-C13
18	A	813	CLA	CAA-CBA-CGA-O2A
18	A	839	CLA	CAA-CBA-CGA-O2A
18	B	811	CLA	CAA-CBA-CGA-O2A
18	2	309	CLA	C2A-CAA-CBA-CGA
18	A	803	CLA	C11-C10-C8-C7
18	A	808	CLA	C11-C10-C8-C7
18	B	801	CLA	C12-C13-C15-C16
18	B	812	CLA	C6-C7-C8-C10
18	B	817	CLA	C11-C10-C8-C7
18	B	840	CLA	C11-C12-C13-C15
18	K	1402	CLA	C11-C10-C8-C7
18	2	309	CLA	C11-C10-C8-C7
18	A	804	CLA	C16-C17-C18-C19
18	A	804	CLA	CAA-CBA-CGA-O2A
18	1	5013	CLA	CAA-CBA-CGA-O2A
18	A	823	CLA	C6-C7-C8-C9
18	B	806	CLA	C14-C13-C15-C16
18	B	810	CLA	C11-C12-C13-C14
18	B	839	CLA	C11-C10-C8-C9
18	F	303	CLA	C14-C13-C15-C16
18	K	1402	CLA	C11-C10-C8-C9
21	A	845	BCR	C19-C20-C21-C22
26	F	309	DGD	O1G-C1A-C2A-C3A
18	B	839	CLA	C2A-CAA-CBA-CGA
18	1	5018	CLA	CAA-CBA-CGA-O1A
18	B	803	CLA	C8-C10-C11-C12
21	B	847	BCR	C37-C22-C23-C24
21	J	1104	BCR	C36-C18-C19-C20
18	A	806	CLA	CAA-CBA-CGA-O1A
18	B	814	CLA	CAA-CBA-CGA-O1A
18	K	1402	CLA	CAA-CBA-CGA-O1A
18	3	319	CLA	CAA-CBA-CGA-O1A
24	1	5001	LMG	O9-C10-C11-C12
18	A	832	CLA	C15-C16-C17-C18
30	4	318	CHL	C2C-C3C-CAC-CBC
18	B	815	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
18	A	804	CLA	C13-C15-C16-C17
24	F	307	LMG	C32-C33-C34-C35
18	B	824	CLA	CAA-CBA-CGA-O1A
18	F	303	CLA	C1A-C2A-CAA-CBA
18	4	315	CLA	C1A-C2A-CAA-CBA
30	1	5016	CHL	C1A-C2A-CAA-CBA
22	2	320	LHG	C12-C13-C14-C15
18	A	816	CLA	CAA-CBA-CGA-O1A
30	4	316	CHL	C2C-C3C-CAC-CBC
18	A	803	CLA	CAA-CBA-CGA-O1A
18	B	839	CLA	CAA-CBA-CGA-O1A
18	B	840	CLA	CAA-CBA-CGA-O1A
18	2	313	CLA	CAA-CBA-CGA-O1A
30	3	313	CHL	CAA-CBA-CGA-O1A
30	3	316	CHL	CAA-CBA-CGA-O1A
24	A	851	LMG	O1-C7-C8-C9
18	A	817	CLA	C2A-CAA-CBA-CGA
18	B	808	CLA	C2A-CAA-CBA-CGA
18	A	835	CLA	C16-C17-C18-C20
18	B	808	CLA	C16-C17-C18-C20
18	A	813	CLA	CAA-CBA-CGA-O1A
18	A	812	CLA	C2C-C3C-CAC-CBC
24	A	851	LMG	O7-C10-C11-C12
18	B	829	CLA	C5-C6-C7-C8
18	3	307	CLA	CAA-CBA-CGA-O1A
18	3	308	CLA	CAA-CBA-CGA-O1A
18	B	811	CLA	C16-C17-C18-C20
18	B	834	CLA	C11-C12-C13-C15
18	L	305	CLA	CAA-CBA-CGA-O1A
30	3	310	CHL	O1A-CGA-O2A-C1
21	A	843	BCR	C23-C24-C25-C30
18	A	812	CLA	C4C-C3C-CAC-CBC
26	1	5002	DGD	C1A-C2A-C3A-C4A
18	A	835	CLA	CAA-CBA-CGA-O1A
18	B	832	CLA	CAA-CBA-CGA-O1A
18	2	306	CLA	CAA-CBA-CGA-O1A
24	J	1102	LMG	O9-C10-C11-C12
18	A	815	CLA	C16-C17-C18-C19
26	B	855	DGD	C5A-C6A-C7A-C8A
26	2	327	DGD	O1B-C1B-C2B-C3B
26	F	309	DGD	CFA-CGA-CHA-CIA
24	1	5001	LMG	O10-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
18	4	308	CLA	C2-C3-C5-C6
18	B	816	CLA	CAD-CBD-CGD-O1D
18	B	832	CLA	CAD-CBD-CGD-O1D
18	L	301	CLA	CAD-CBD-CGD-O1D
18	2	317	CLA	CAD-CBD-CGD-O1D
18	3	317	CLA	CAD-CBD-CGD-O1D
24	F	307	LMG	C7-C8-O7-C10
24	F	308	LMG	C7-C8-O7-C10
24	F	308	LMG	C9-C8-O7-C10
18	B	841	CLA	CAA-CBA-CGA-O1A
26	2	327	DGD	C4B-C5B-C6B-C7B
18	1	5008	CLA	CAA-CBA-CGA-O2A
18	4	310	CLA	CAA-CBA-CGA-O2A
30	4	302	CHL	CAA-CBA-CGA-O2A
18	B	804	CLA	C8-C10-C11-C12
18	B	828	CLA	C13-C15-C16-C17
30	4	318	CHL	C5-C6-C7-C8
18	A	805	CLA	C14-C13-C15-C16
18	A	826	CLA	C11-C10-C8-C9
18	A	829	CLA	C11-C12-C13-C14
18	A	830	CLA	C11-C12-C13-C14
18	A	838	CLA	C11-C10-C8-C9
18	B	812	CLA	C6-C7-C8-C9
18	F	303	CLA	C11-C12-C13-C14
18	G	1603	CLA	C14-C13-C15-C16
18	L	305	CLA	C11-C10-C8-C9
18	1	5006	CLA	C14-C13-C15-C16
19	B	842	PQN	C19-C18-C20-C21
24	F	308	LMG	O10-C28-C29-C30
18	A	814	CLA	CAA-CBA-CGA-O2A
26	B	855	DGD	C1B-C2B-C3B-C4B
18	A	839	CLA	CAA-CBA-CGA-O1A
18	B	822	CLA	C8-C10-C11-C12
18	B	826	CLA	C10-C11-C12-C13
24	2	321	LMG	O9-C10-C11-C12
30	4	313	CHL	C2A-CAA-CBA-CGA
18	A	836	CLA	CAA-CBA-CGA-O2A
18	B	826	CLA	CAA-CBA-CGA-O2A
30	2	314	CHL	C5-C6-C7-C8
18	B	811	CLA	CAA-CBA-CGA-O1A
18	B	837	CLA	CAA-CBA-CGA-O1A
18	B	827	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
18	A	812	CLA	C2-C3-C5-C6
18	A	828	CLA	C12-C13-C15-C16
18	A	829	CLA	C11-C12-C13-C15
18	A	835	CLA	C11-C12-C13-C15
18	A	839	CLA	C12-C13-C15-C16
18	A	840	CLA	C11-C10-C8-C7
18	B	809	CLA	C6-C7-C8-C10
18	B	810	CLA	C11-C12-C13-C15
18	B	829	CLA	C11-C10-C8-C7
18	F	303	CLA	C12-C13-C15-C16
18	K	1402	CLA	C3A-C2A-CAA-CBA
30	3	310	CHL	C12-C13-C15-C16
18	A	804	CLA	CAA-CBA-CGA-O1A
18	B	815	CLA	CAA-CBA-CGA-O1A
18	A	820	CLA	CAA-CBA-CGA-O2A
18	B	822	CLA	CAA-CBA-CGA-O2A
22	A	849	LHG	O7-C7-C8-C9
23	G	1606	LMT	C3-C4-C5-C6
21	1	5005	BCR	C11-C12-C13-C14
29	1	5003	LUT	C7-C8-C9-C10
29	3	304	LUT	C7-C8-C9-C10
29	3	304	LUT	C31-C32-C33-C34
18	B	822	CLA	CAA-CBA-CGA-O1A
22	A	849	LHG	O9-C7-C8-C9
24	A	851	LMG	O9-C10-C11-C12
21	A	845	BCR	C15-C16-C17-C18
21	B	802	BCR	C19-C20-C21-C22
24	F	307	LMG	O7-C10-C11-C12
18	B	810	CLA	C15-C16-C17-C18
26	F	309	DGD	O1A-C1A-C2A-C3A
30	4	302	CHL	CAA-CBA-CGA-O1A
18	B	817	CLA	C8-C10-C11-C12
30	2	315	CHL	C5-C6-C7-C8
23	B	856	LMT	O5B-C5B-C6B-O6B
18	A	828	CLA	CAA-CBA-CGA-O2A
22	B	849	LHG	O8-C23-C24-C25
30	4	316	CHL	C10-C11-C12-C13
26	F	309	DGD	C7A-C8A-C9A-CAA
18	A	815	CLA	C3-C5-C6-C7
18	A	814	CLA	CAA-CBA-CGA-O1A
18	A	820	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

221 monomers are involved in 828 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	2	306	CLA	6	0
18	A	832	CLA	7	0
18	4	308	CLA	3	0
21	B	845	BCR	9	0
18	B	825	CLA	8	0
24	F	306	LMG	4	0
18	A	839	CLA	6	0
19	B	842	PQN	2	0
30	3	310	CHL	9	0
30	4	313	CHL	1	0
22	A	849	LHG	8	0
18	A	816	CLA	9	0
18	A	805	CLA	6	0
31	4	304	XAT	6	0
21	L	307	BCR	3	0
18	B	804	CLA	7	0
18	1	5007	CLA	1	0
18	1	5010	CLA	8	0
18	A	802	CLA	11	0
18	B	829	CLA	7	0
24	G	1607	LMG	1	0
18	3	319	CLA	5	0
21	F	304	BCR	5	0
24	2	322	LMG	2	0
30	3	312	CHL	7	0
18	A	808	CLA	9	0
18	A	813	CLA	7	0
18	A	820	CLA	3	0
18	B	801	CLA	11	0
18	B	826	CLA	11	0
18	L	305	CLA	1	0
18	A	825	CLA	7	0
18	A	804	CLA	7	0
24	1	5020	LMG	2	0
18	A	836	CLA	5	0
18	2	312	CLA	7	0
24	F	307	LMG	1	0
18	1	5008	CLA	2	0
21	G	1604	BCR	4	0
18	B	834	CLA	5	0
30	2	314	CHL	5	0
18	F	303	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	3	301	CLA	1	0
23	G	1605	LMT	2	0
24	B	850	LMG	2	0
21	2	305	BCR	11	0
18	4	309	CLA	3	0
18	A	809	CLA	3	0
18	B	816	CLA	5	0
21	B	843	BCR	8	0
18	2	317	CLA	4	0
18	A	806	CLA	6	0
24	A	851	LMG	5	0
30	3	316	CHL	7	0
18	B	831	CLA	6	0
18	A	810	CLA	9	0
18	A	837	CLA	8	0
18	B	810	CLA	6	0
18	A	838	CLA	5	0
28	F	310	ZEX	3	0
18	A	803	CLA	10	0
24	1	5001	LMG	8	0
18	A	826	CLA	9	0
21	K	1405	BCR	2	0
18	B	808	CLA	5	0
18	B	814	CLA	5	0
18	B	820	CLA	5	0
26	B	855	DGD	8	0
18	3	314	CLA	3	0
18	B	828	CLA	9	0
18	B	837	CLA	7	0
18	A	818	CLA	1	0
18	4	306	CLA	1	0
21	B	844	BCR	5	0
18	A	815	CLA	3	0
18	K	1402	CLA	6	0
18	B	819	CLA	5	0
21	A	847	BCR	7	0
18	1	5018	CLA	3	0
24	2	301	LMG	1	0
18	4	305	CLA	4	0
30	1	5014	CHL	6	0
18	B	841	CLA	12	0
29	2	303	LUT	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	4	310	CLA	3	0
21	A	846	BCR	8	0
18	A	823	CLA	11	0
18	3	308	CLA	1	0
25	A	854	GOL	1	0
20	C	102	SF4	1	0
18	1	5006	CLA	11	0
18	L	306	CLA	1	0
30	4	317	CHL	3	0
18	L	301	CLA	1	0
18	B	805	CLA	8	0
30	2	315	CHL	6	0
18	A	830	CLA	3	0
18	F	301	CLA	4	0
18	K	1401	CLA	2	0
18	J	1101	CLA	8	0
18	K	1403	CLA	5	0
18	2	308	CLA	4	0
18	1	5009	CLA	6	0
30	1	5016	CHL	8	0
18	4	311	CLA	3	0
18	2	309	CLA	7	0
18	A	834	CLA	3	0
18	B	830	CLA	6	0
21	F	305	BCR	6	0
30	2	318	CHL	4	0
18	1	5017	CLA	5	0
24	2	321	LMG	2	0
21	B	802	BCR	4	0
18	A	812	CLA	6	0
18	B	812	CLA	7	0
18	1	5012	CLA	3	0
18	A	807	CLA	7	0
18	A	835	CLA	6	0
18	3	307	CLA	10	0
30	2	316	CHL	4	0
21	B	847	BCR	2	0
18	B	835	CLA	5	0
18	3	315	CLA	3	0
22	2	320	LHG	1	0
18	1	5011	CLA	2	0
21	4	301	BCR	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	840	CLA	4	0
18	A	853	CLA	8	0
18	B	821	CLA	2	0
22	B	849	LHG	4	0
21	3	306	BCR	3	0
22	1	5019	LHG	3	0
18	A	821	CLA	3	0
22	B	848	LHG	4	0
18	A	828	CLA	11	0
18	2	326	CLA	4	0
18	B	803	CLA	9	0
18	A	831	CLA	5	0
26	J	1106	DGD	4	0
18	3	309	CLA	3	0
21	A	855	BCR	6	0
18	G	1602	CLA	1	0
18	4	315	CLA	5	0
21	1	5005	BCR	3	0
21	B	846	BCR	3	0
21	L	302	BCR	2	0
18	A	817	CLA	6	0
18	A	827	CLA	4	0
29	1	5004	LUT	7	0
18	B	839	CLA	7	0
18	3	311	CLA	4	0
18	B	818	CLA	10	0
23	B	852	LMT	1	0
18	4	307	CLA	2	0
18	B	815	CLA	5	0
18	A	811	CLA	13	0
18	2	310	CLA	6	0
18	A	840	CLA	9	0
18	B	813	CLA	4	0
30	4	314	CHL	2	0
21	A	844	BCR	3	0
18	L	304	CLA	4	0
31	2	304	XAT	7	0
18	H	1701	CLA	8	0
17	A	801	CL0	9	0
18	B	822	CLA	5	0
18	B	823	CLA	8	0
29	3	303	LUT	3	0

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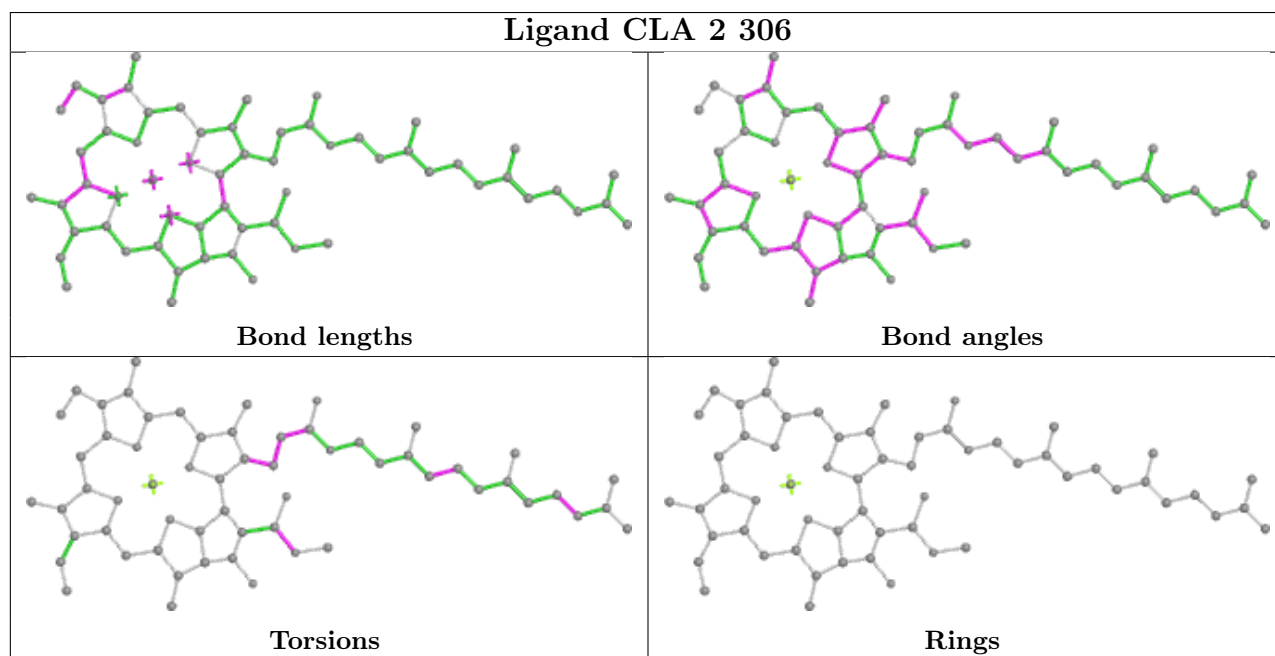
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18	1	5015	CLA	3	0
21	I	101	BCR	2	0
21	I	102	BCR	2	0
23	G	1606	LMT	1	0
30	3	313	CHL	1	0
18	2	311	CLA	1	0
21	A	845	BCR	8	0
18	B	836	CLA	7	0
30	4	318	CHL	4	0
18	K	1404	CLA	2	0
21	A	843	BCR	6	0
18	A	829	CLA	6	0
18	2	313	CLA	4	0
18	J	1103	CLA	1	0
26	2	327	DGD	5	0
29	J	1105	LUT	9	0
23	B	856	LMT	2	0
30	4	316	CHL	4	0
18	2	307	CLA	4	0
18	1	5013	CLA	2	0
29	1	5003	LUT	8	0
29	3	304	LUT	9	0
18	A	833	CLA	6	0
18	B	838	CLA	6	0
23	2	325	LMT	1	0
18	B	806	CLA	10	0
24	2	302	LMG	1	0
30	4	302	CHL	5	0
19	A	841	PQN	4	0
18	A	822	CLA	17	0
18	3	317	CLA	8	0
18	B	811	CLA	7	0
18	3	318	CLA	3	0
23	B	853	LMT	2	0
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18	B	832	CLA	1	0
18	F	302	CLA	4	0

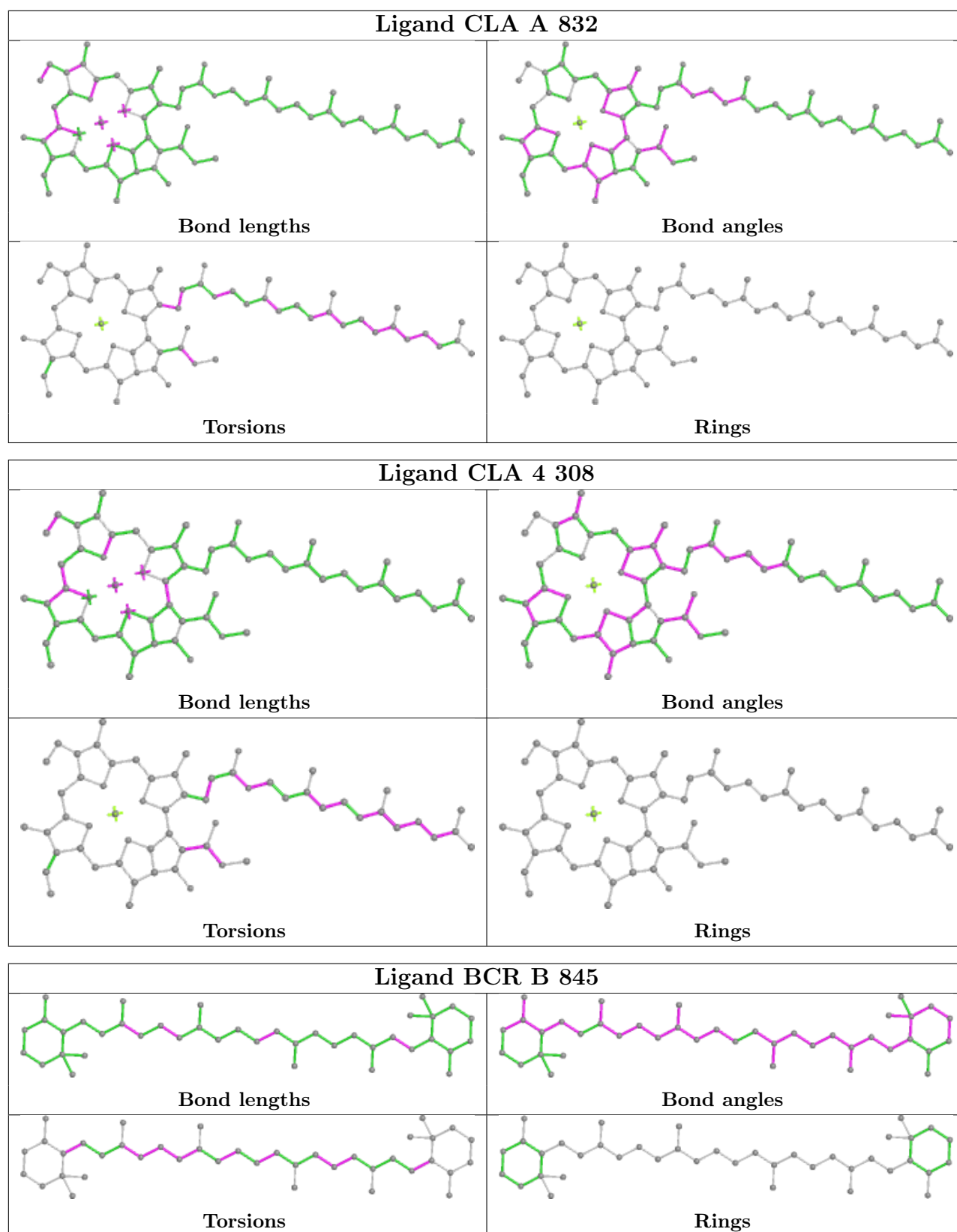
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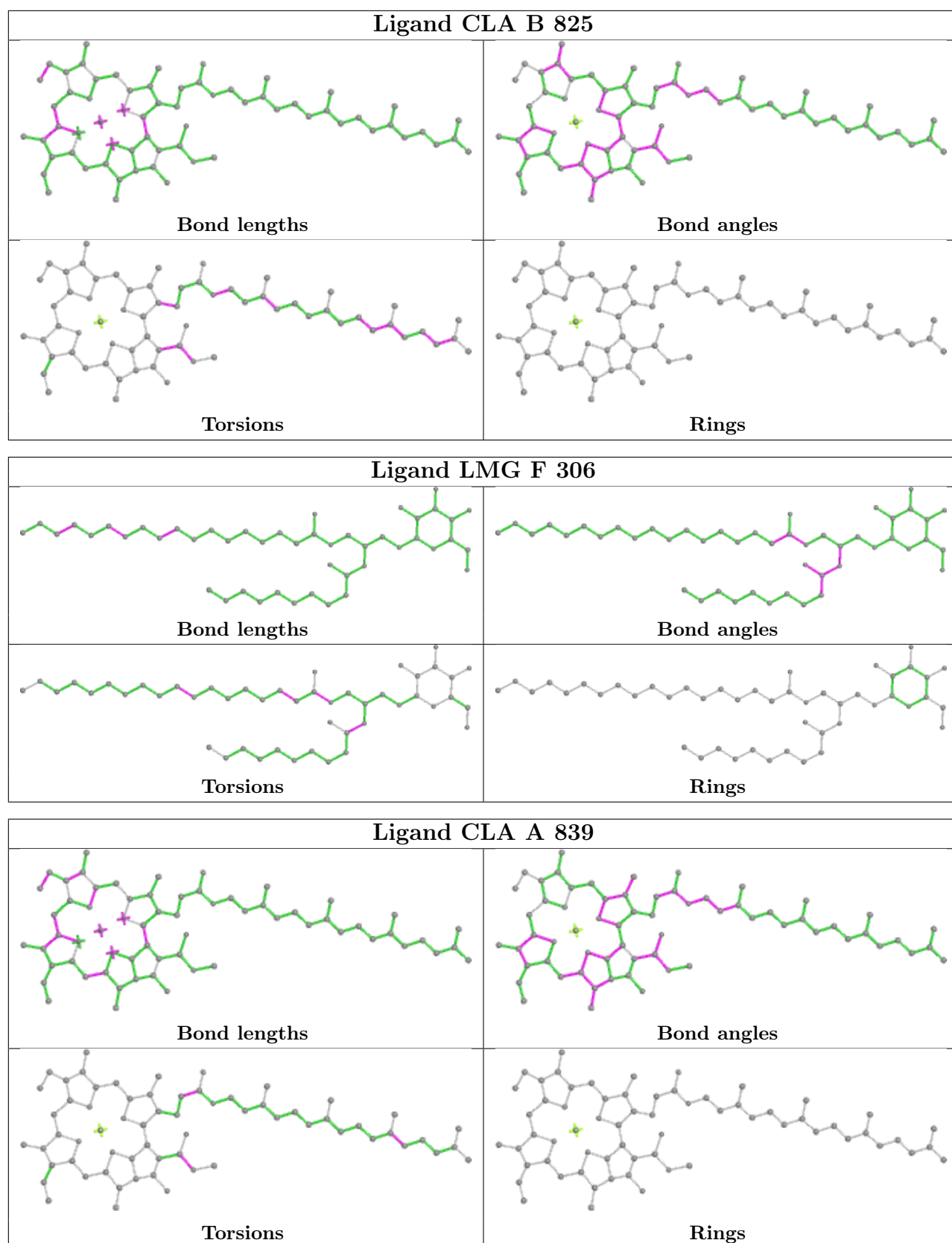
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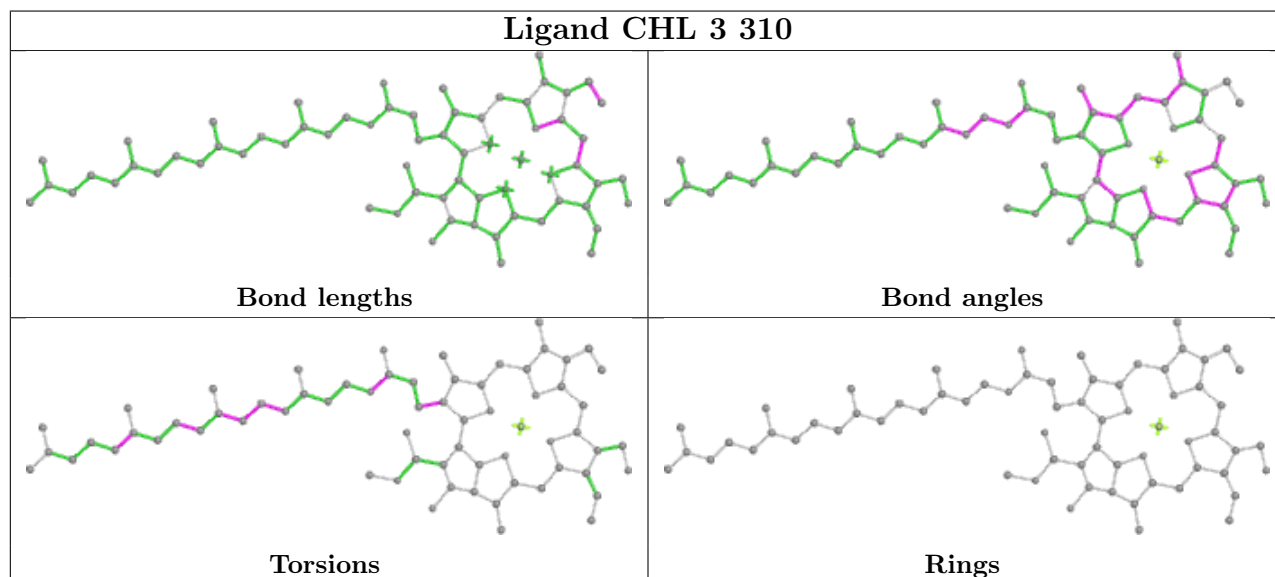
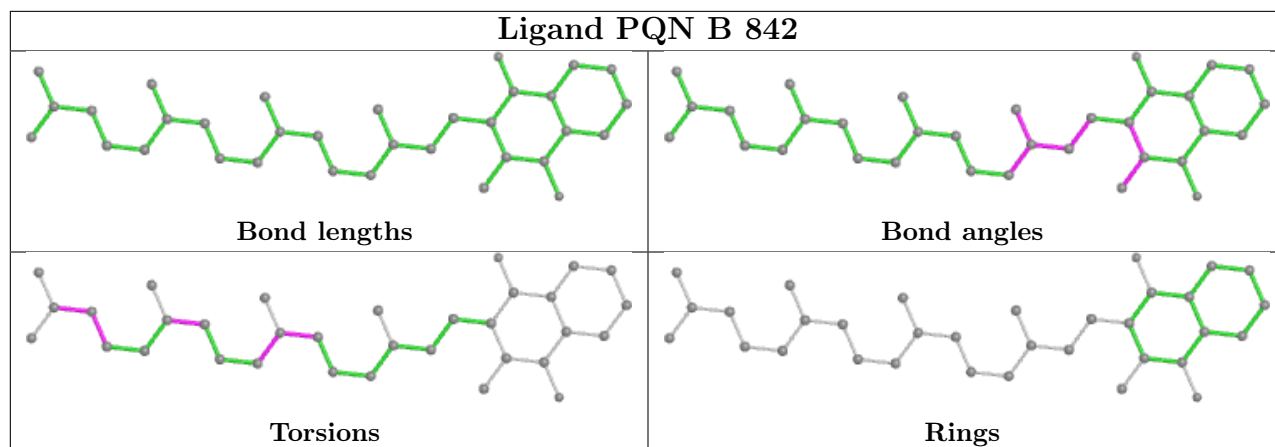
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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29	4	303	LUT	2	0
18	B	833	CLA	7	0
18	A	819	CLA	13	0
18	A	852	CLA	9	0
18	G	1601	CLA	1	0
22	A	848	LHG	8	0
30	2	319	CHL	1	0
21	J	1104	BCR	4	0
18	A	824	CLA	6	0
21	3	305	BCR	3	0

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

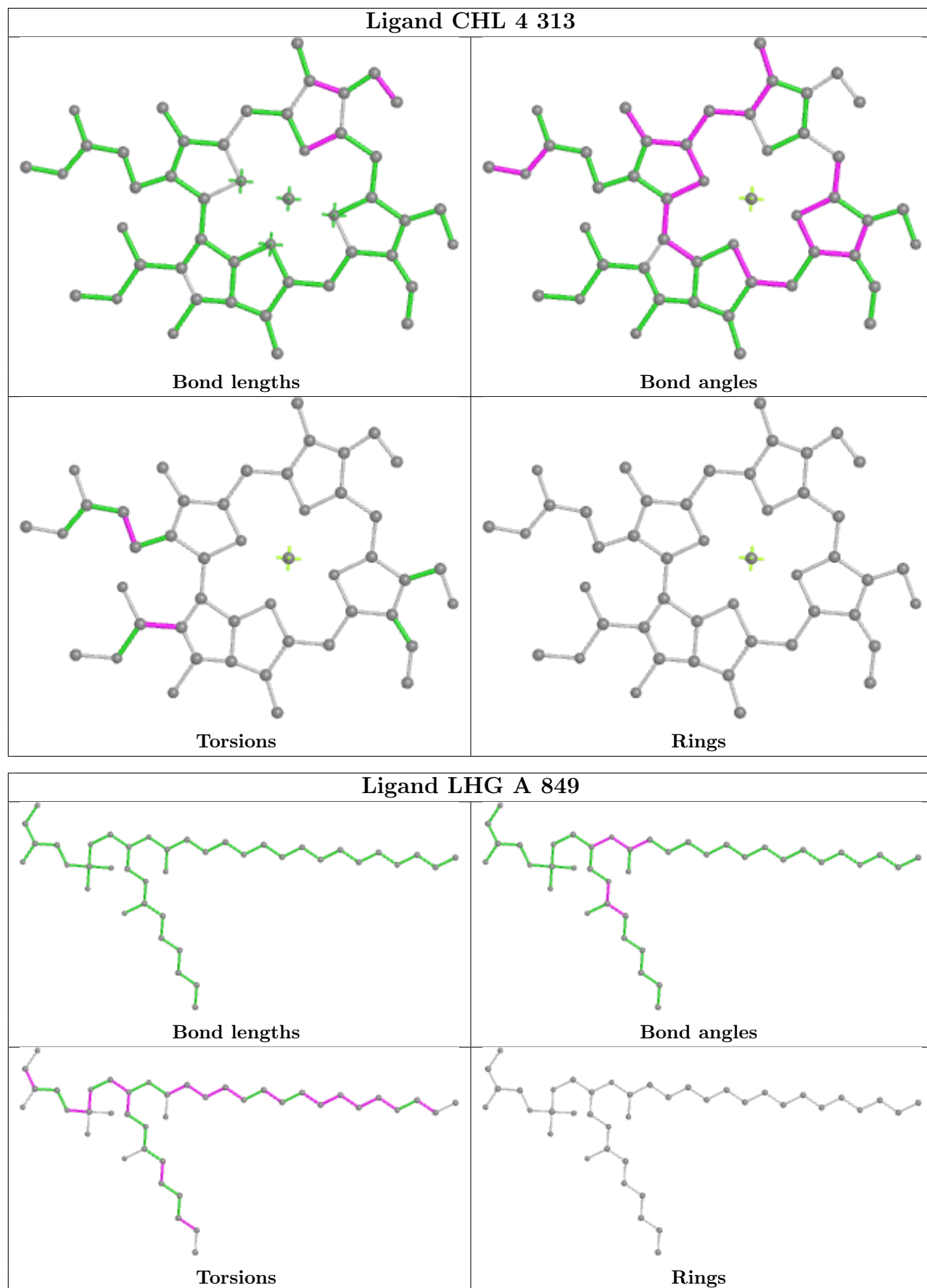


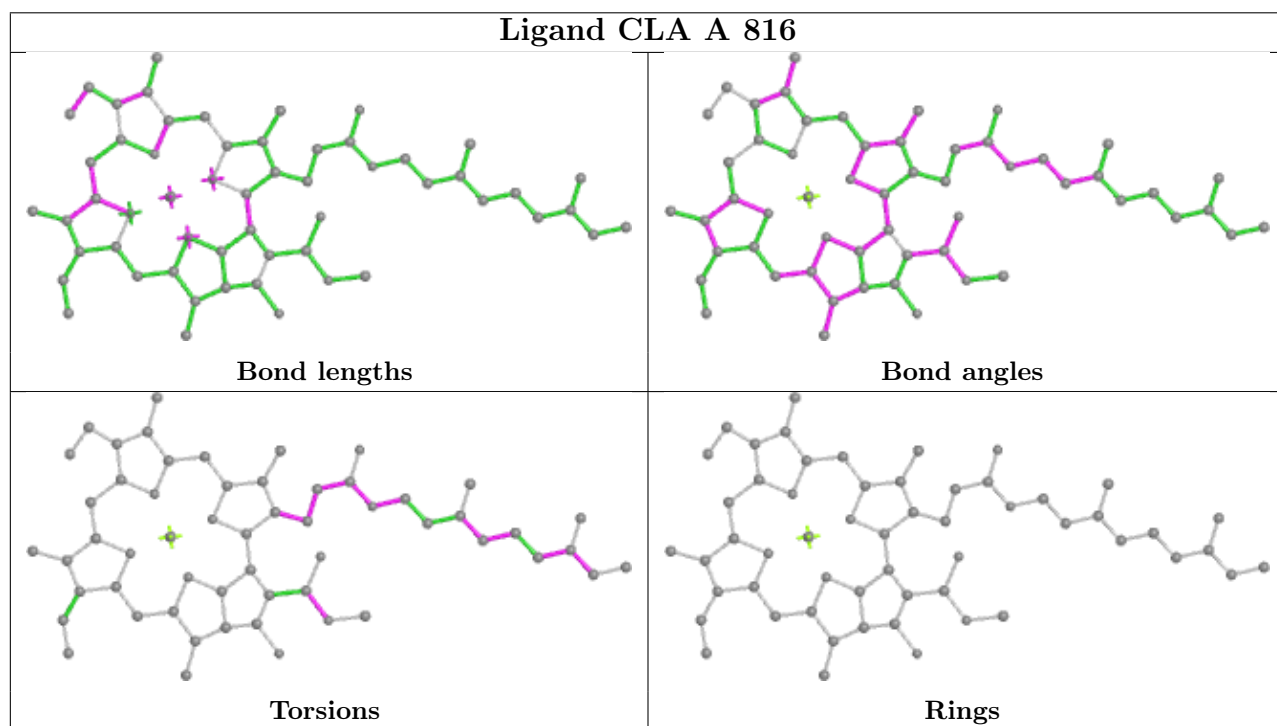
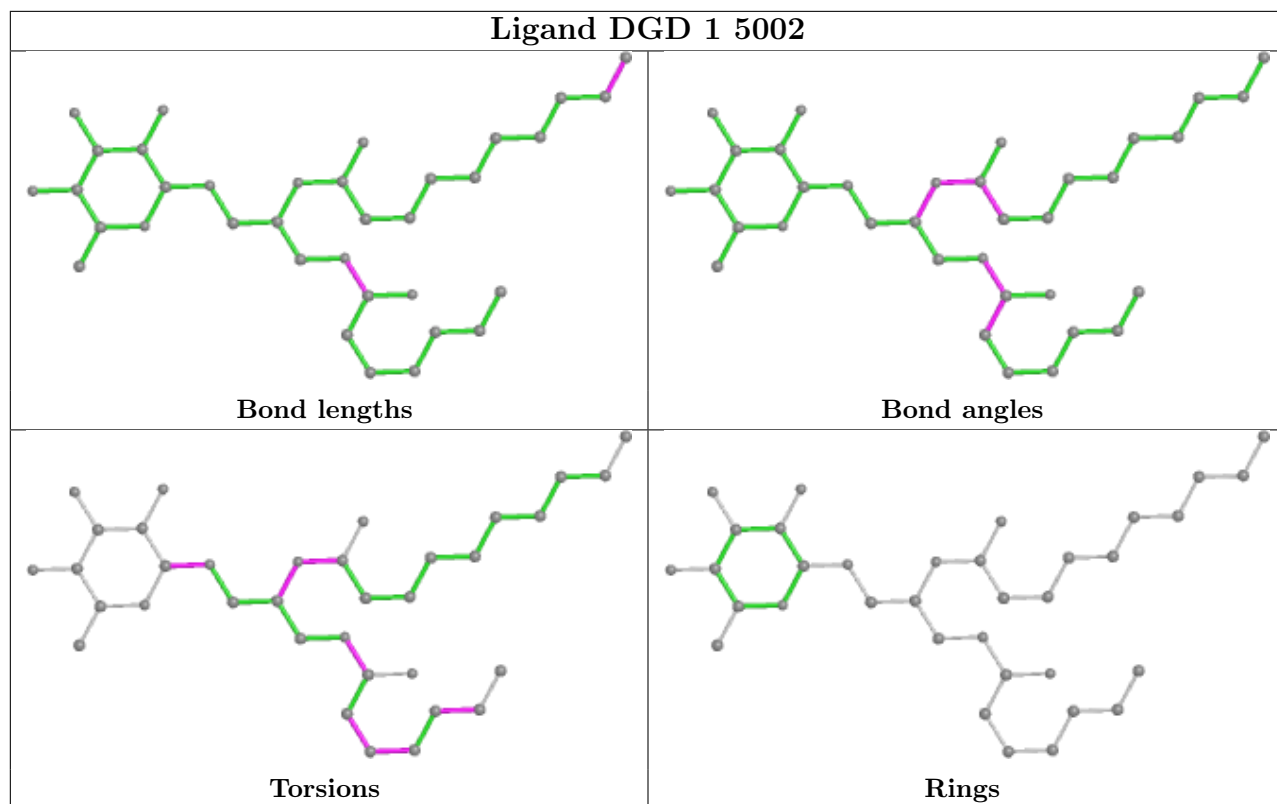


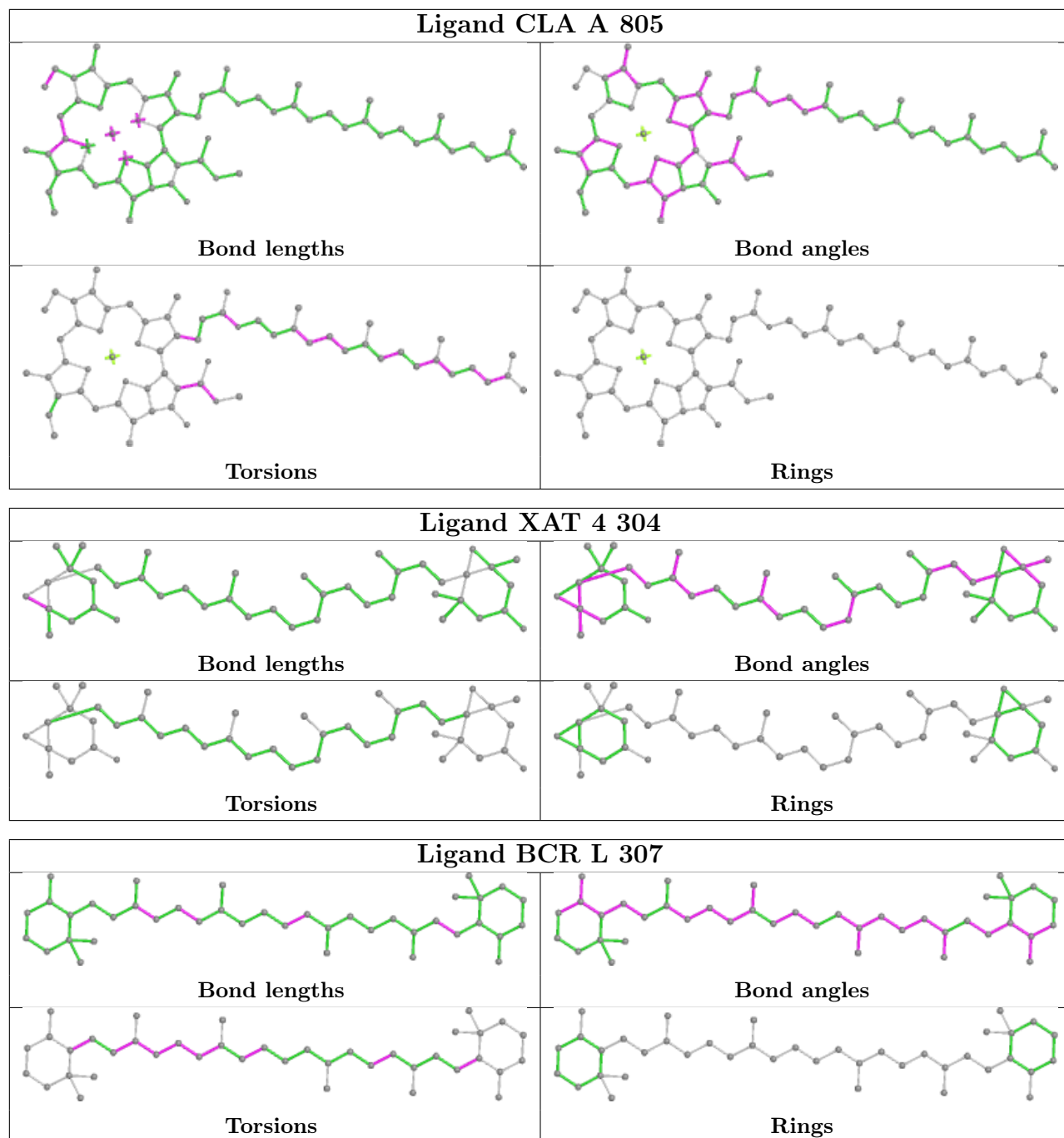


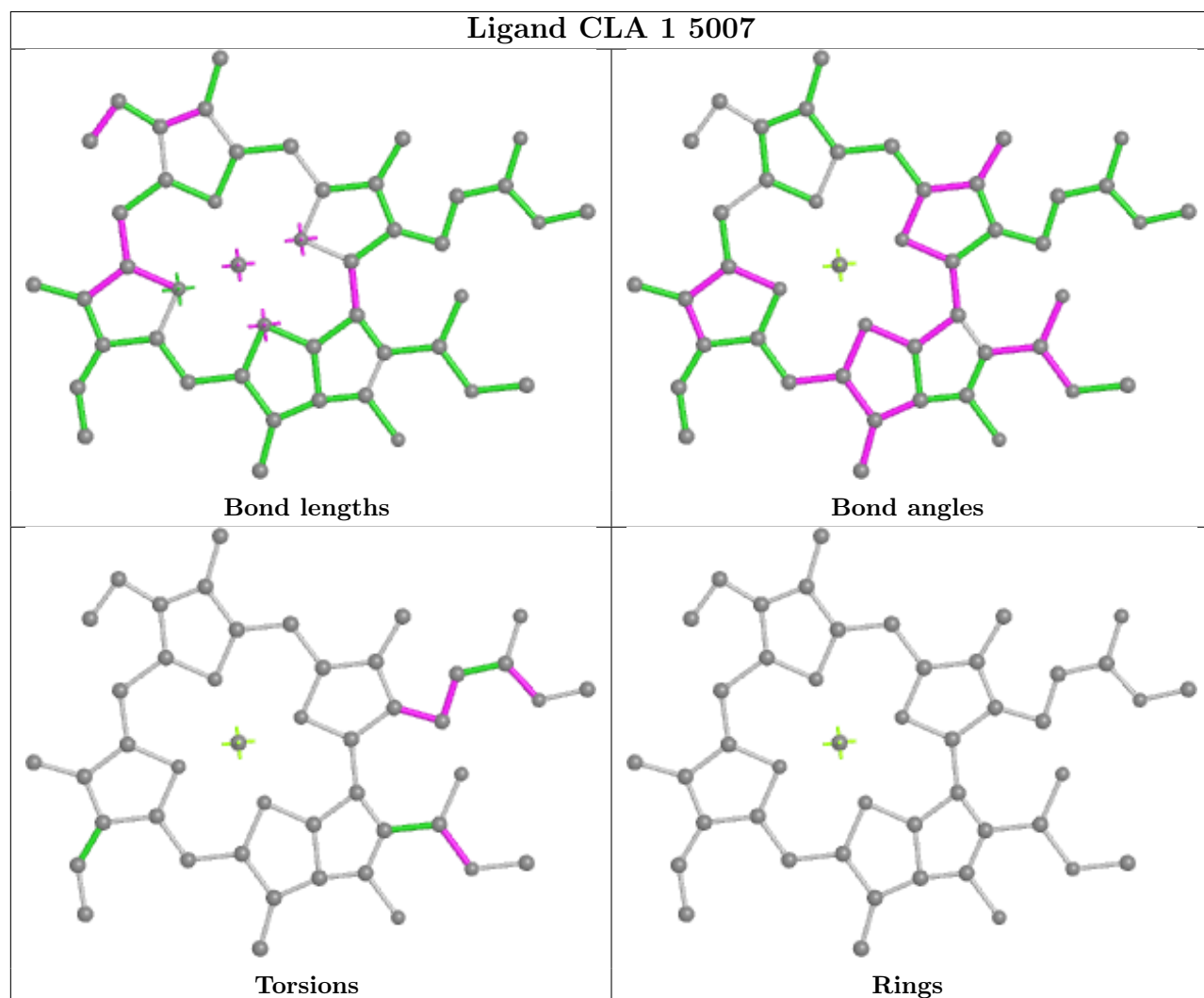
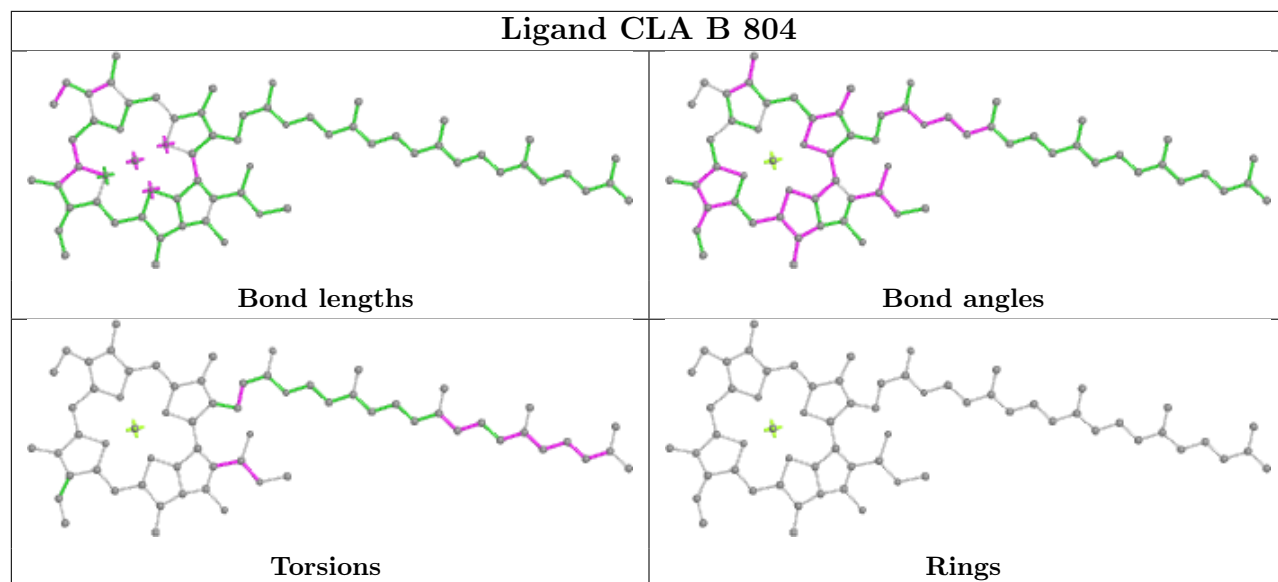


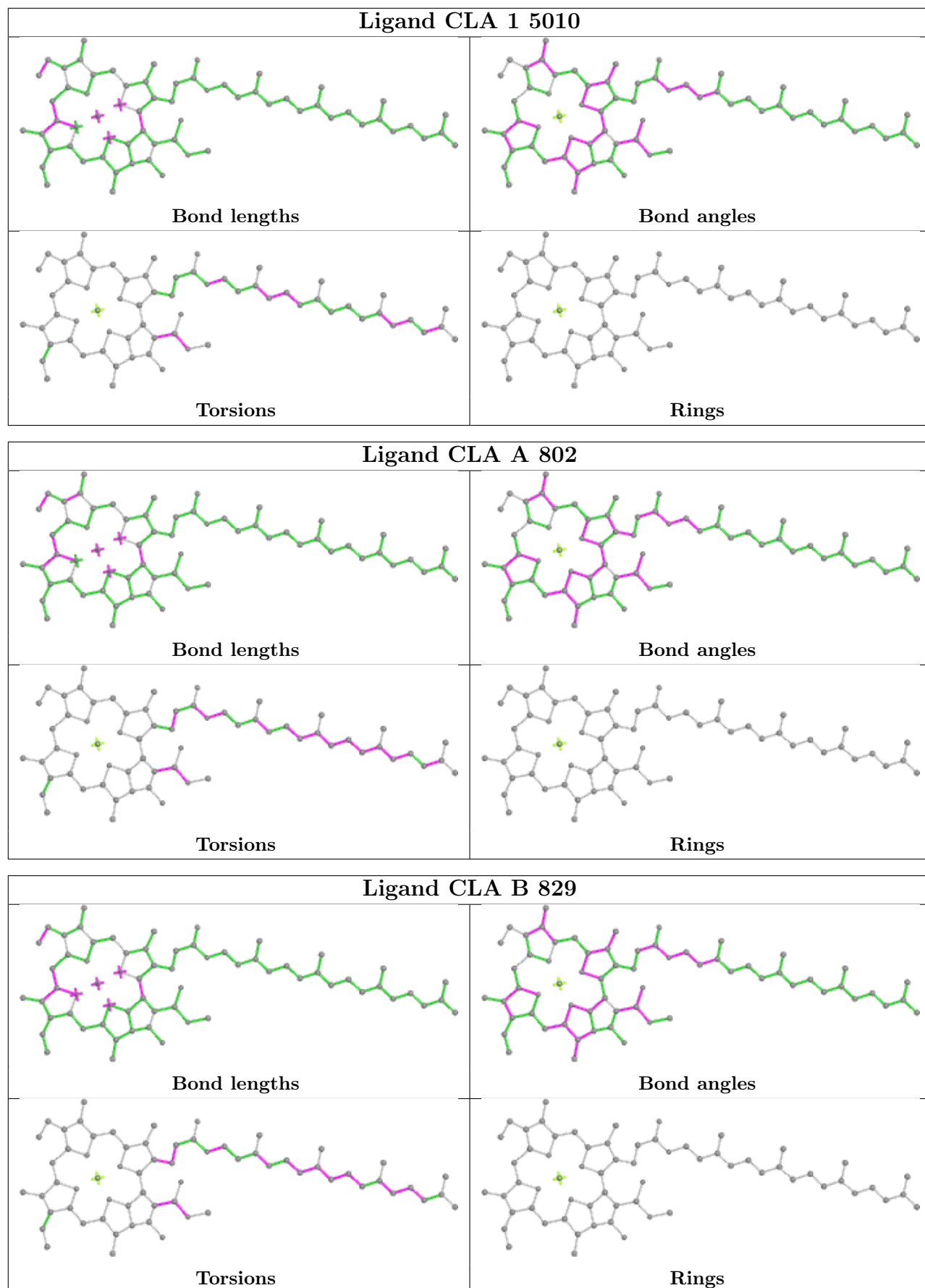


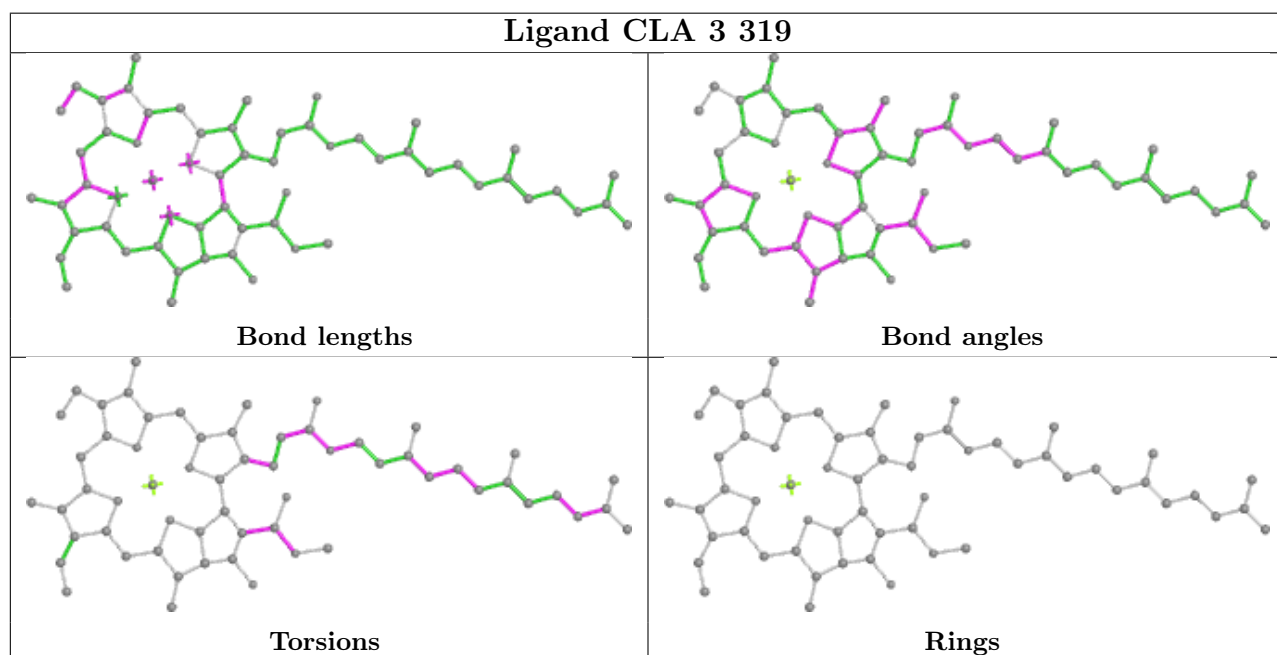
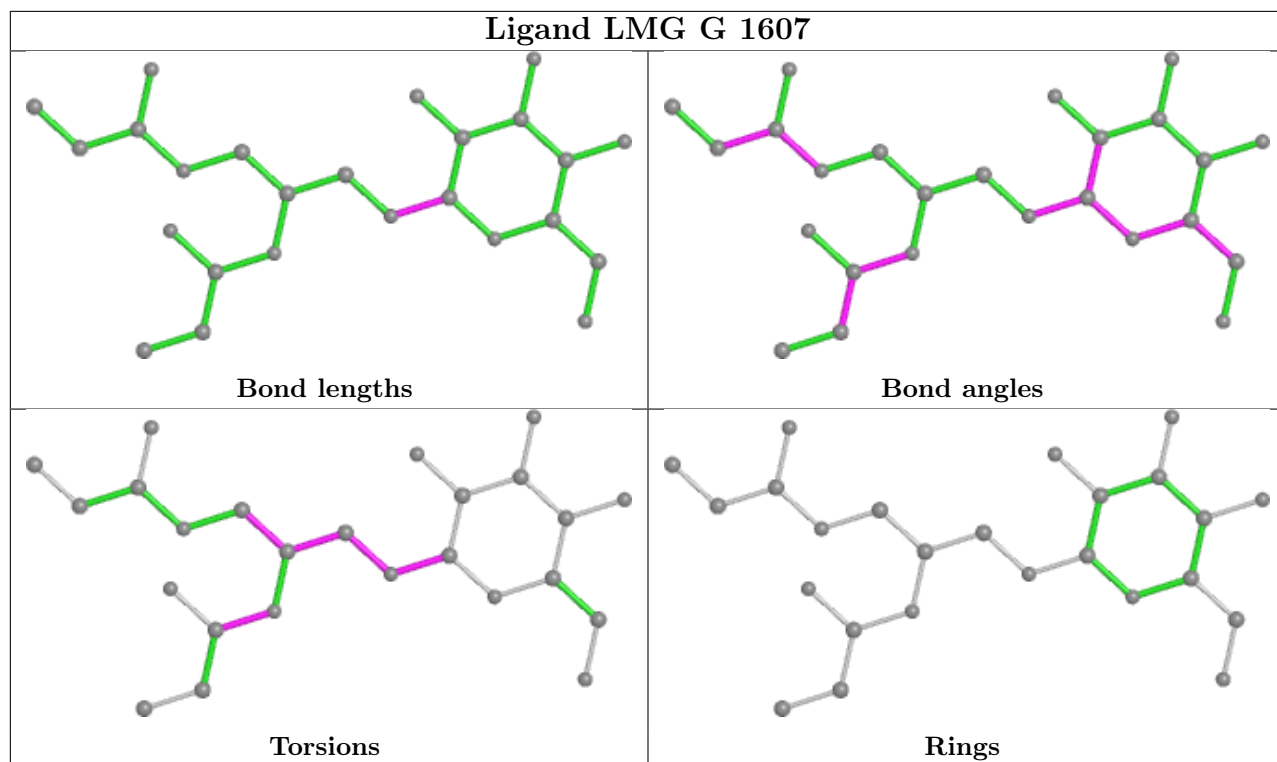


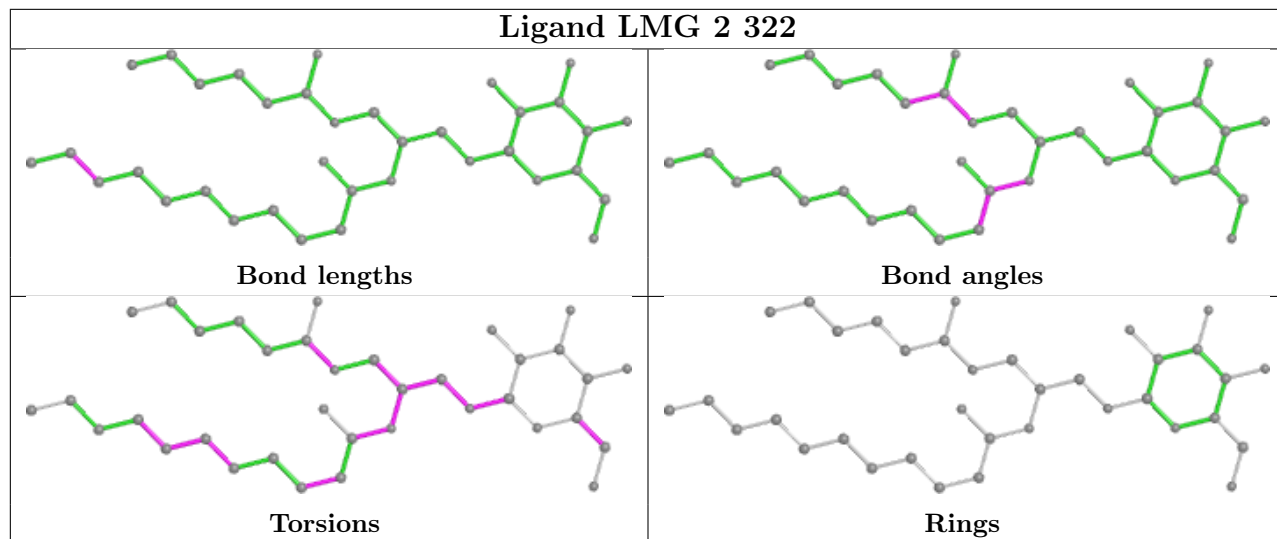
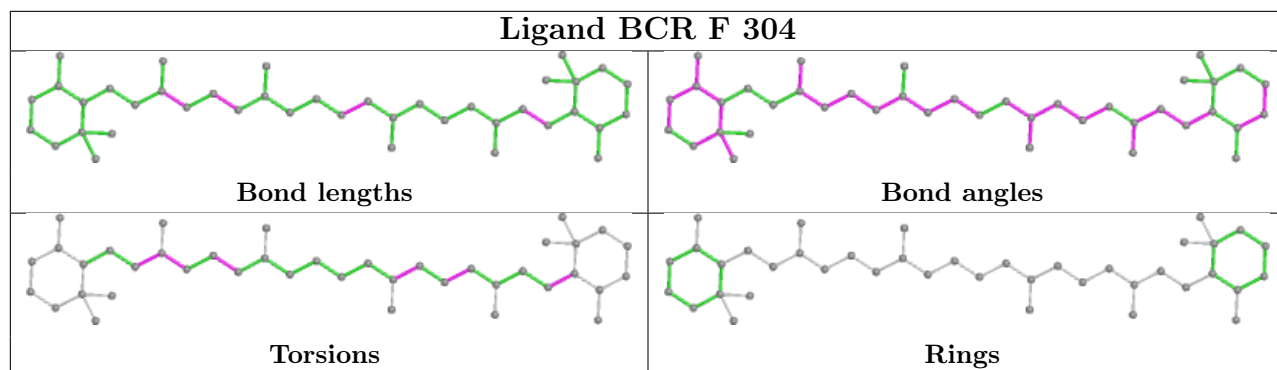


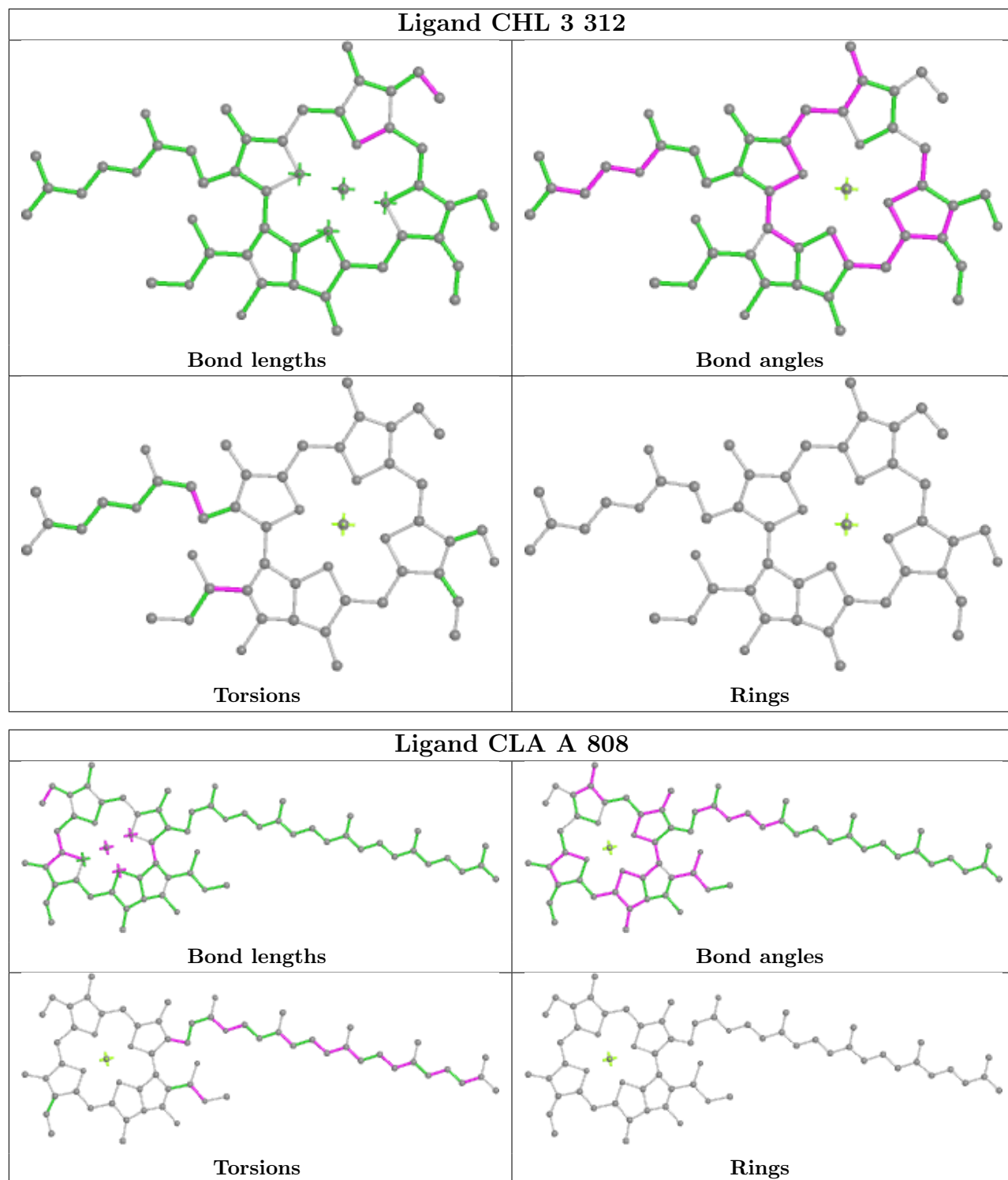




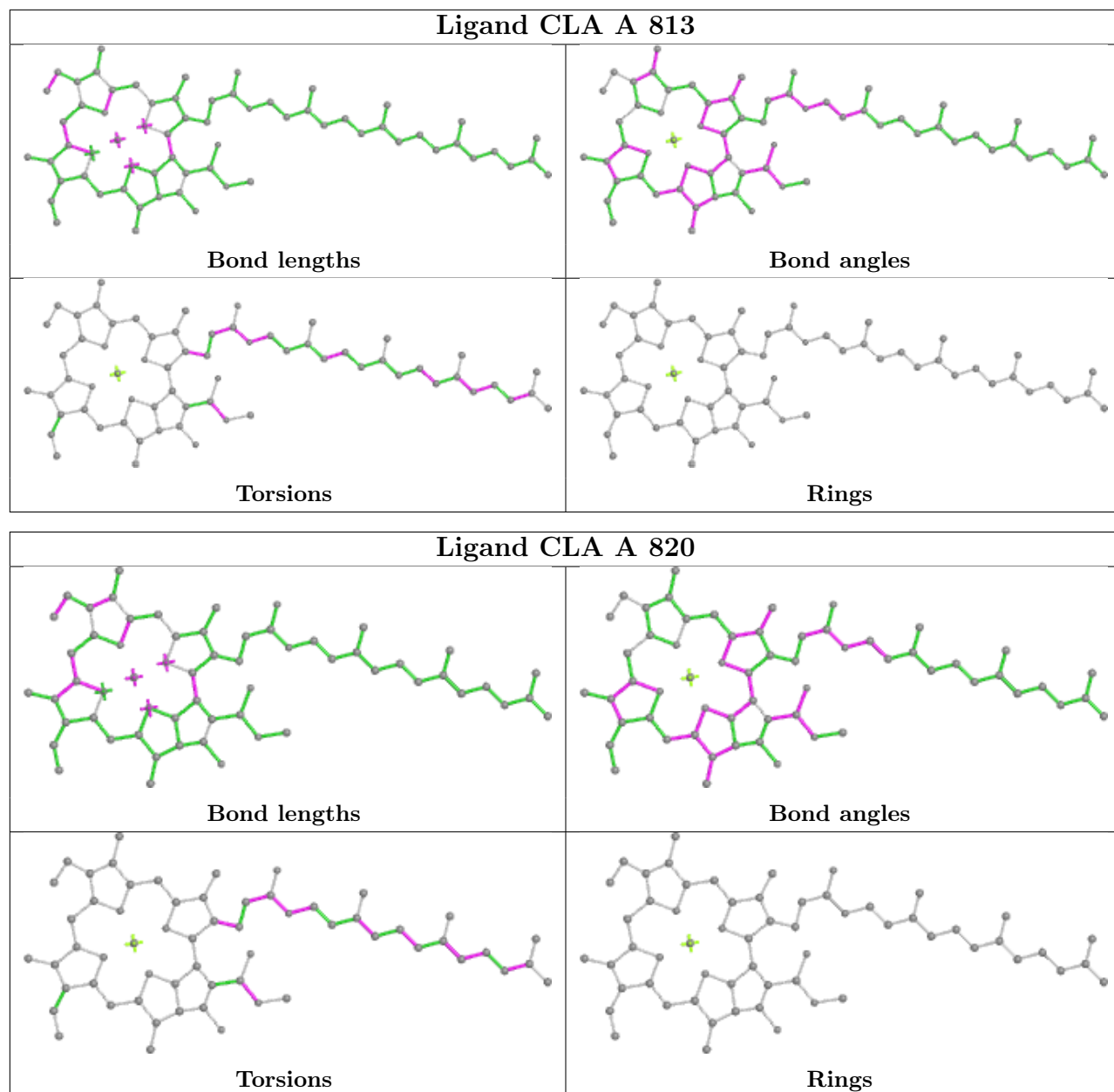


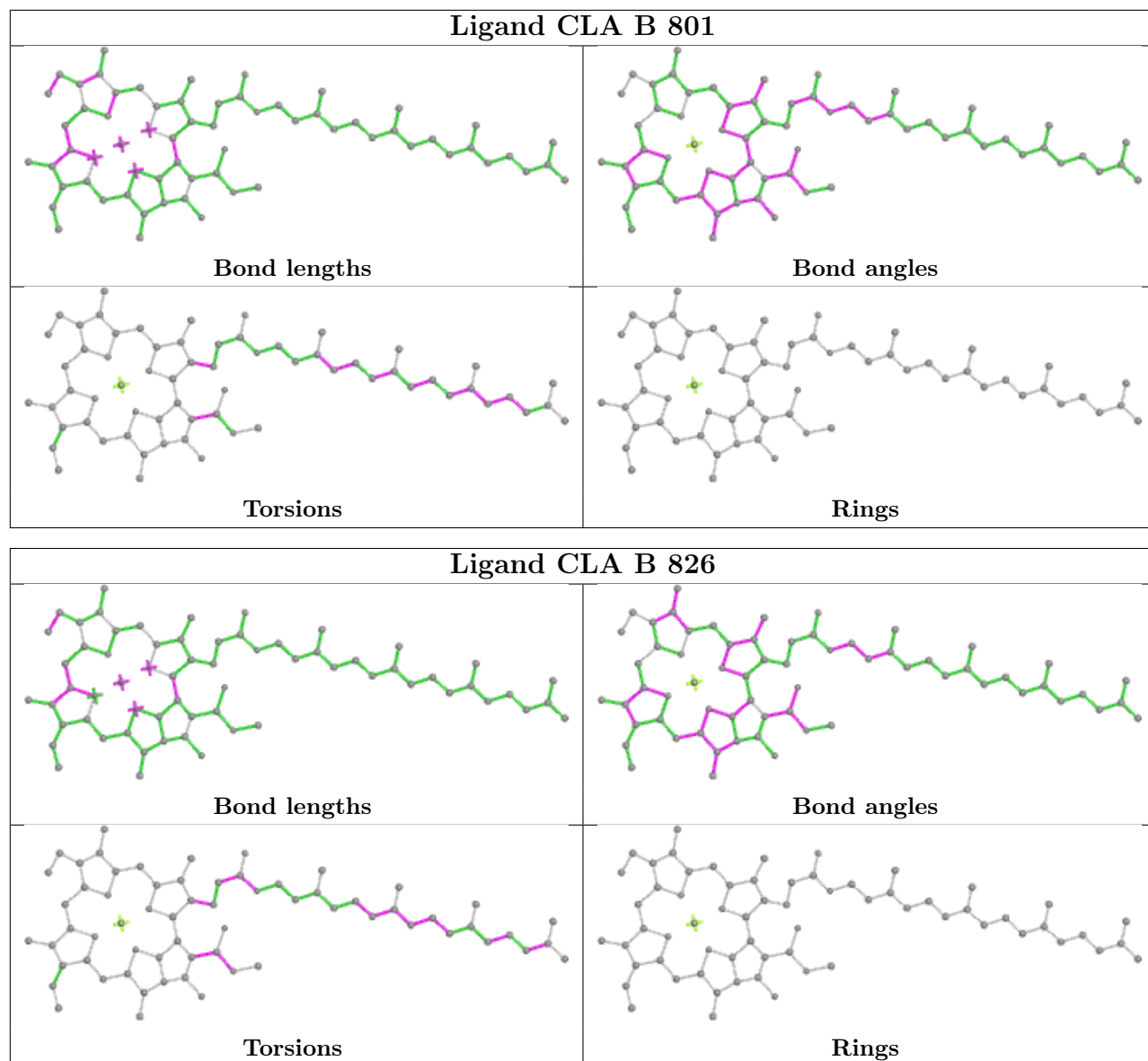


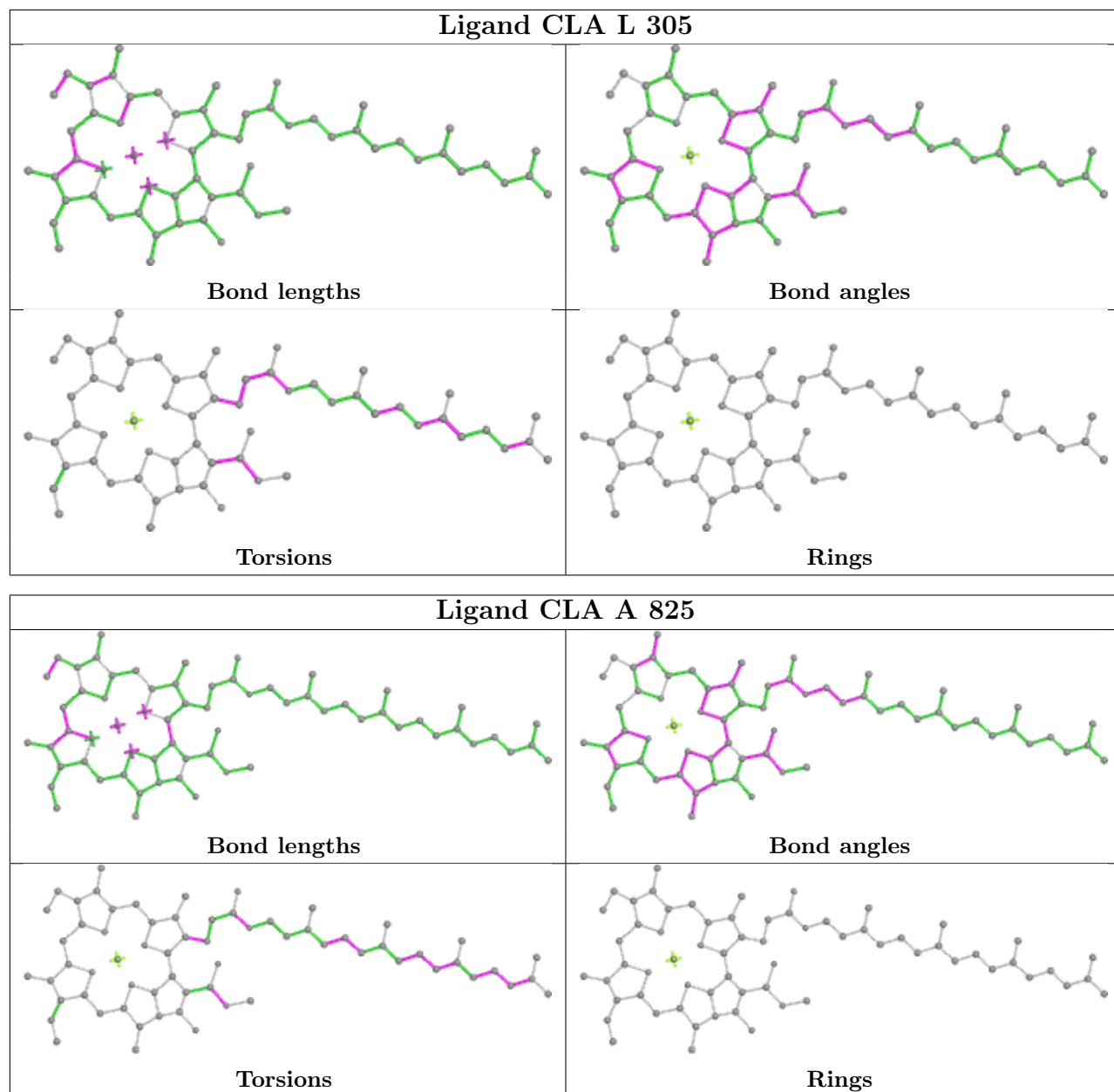


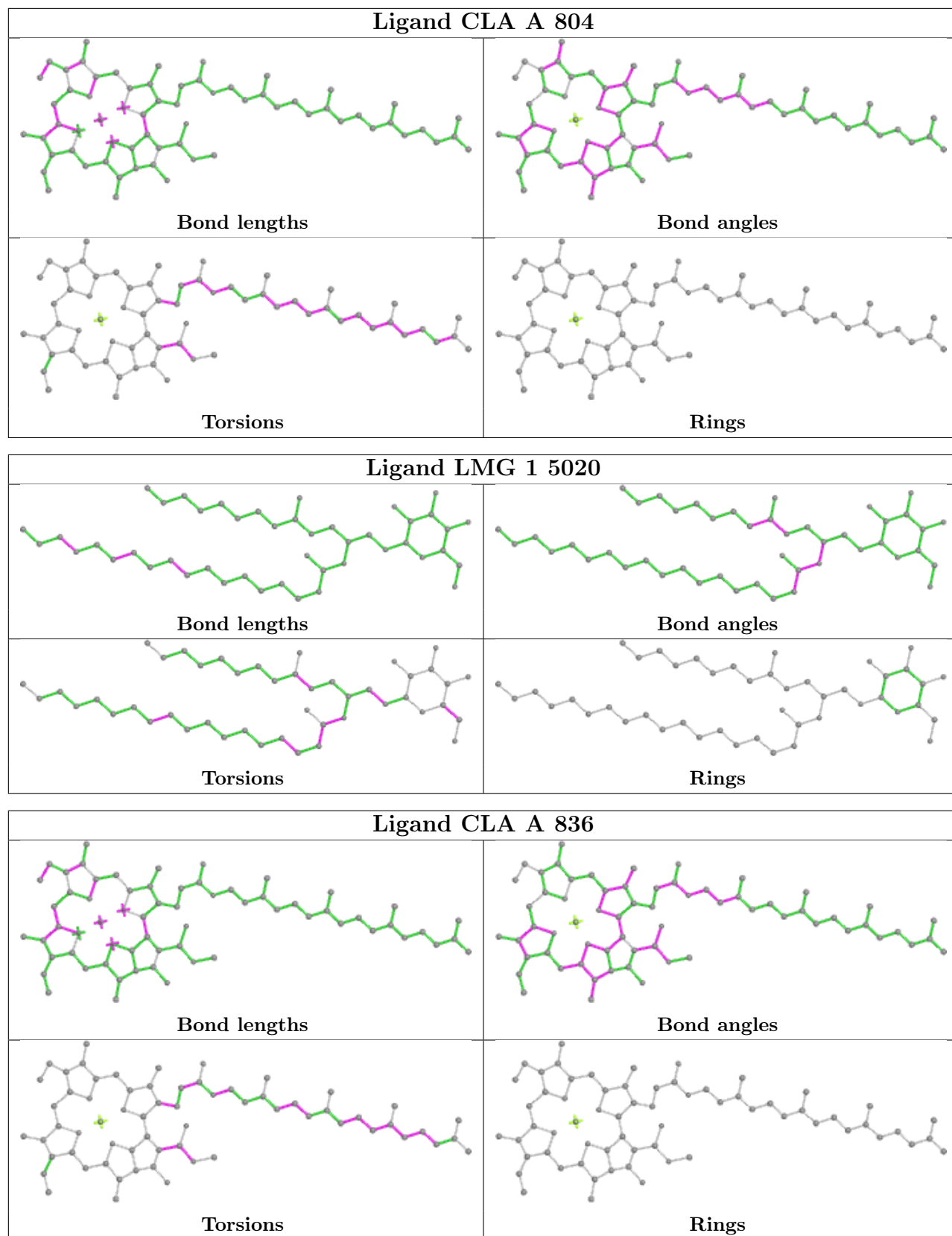


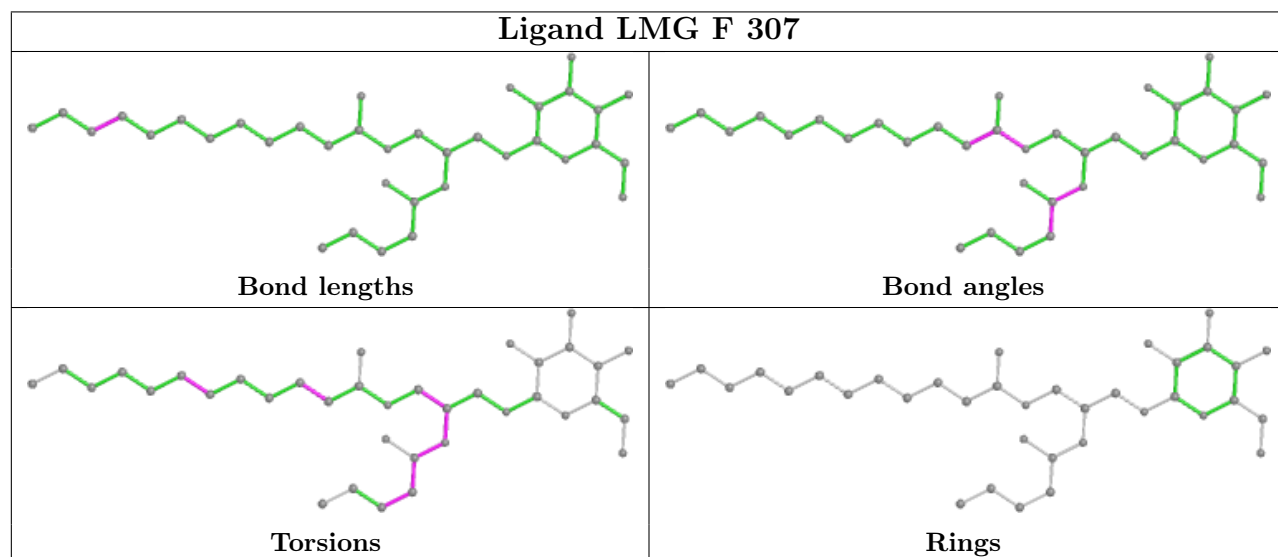
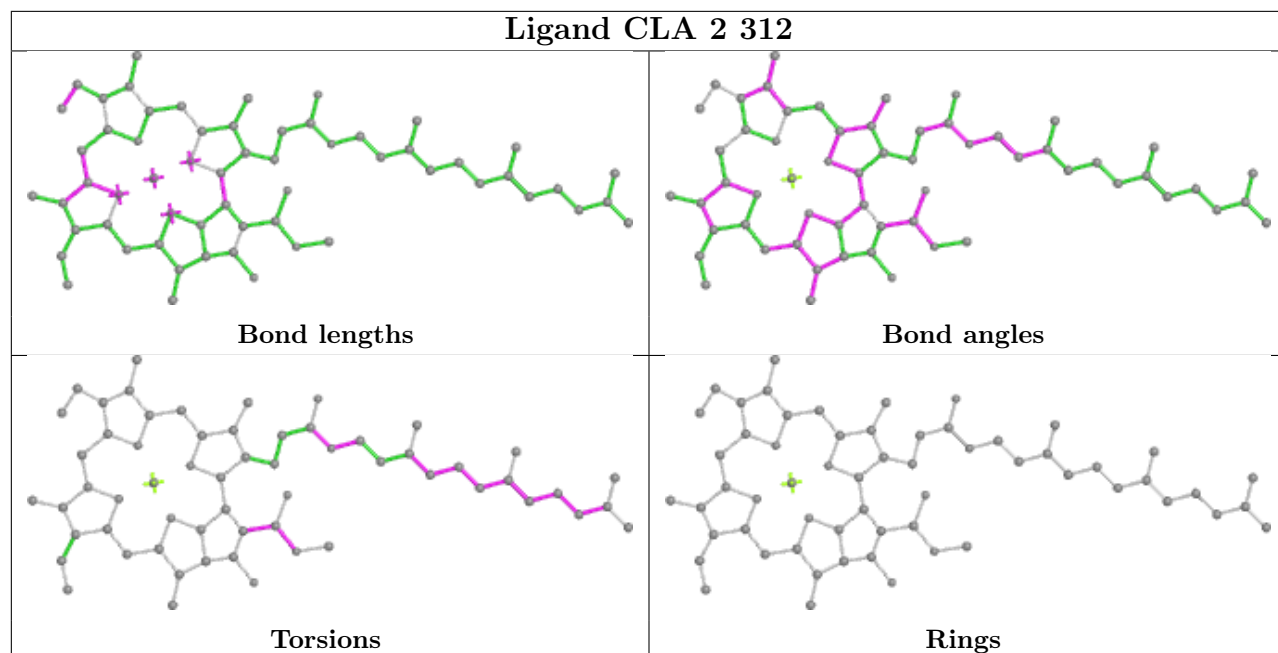


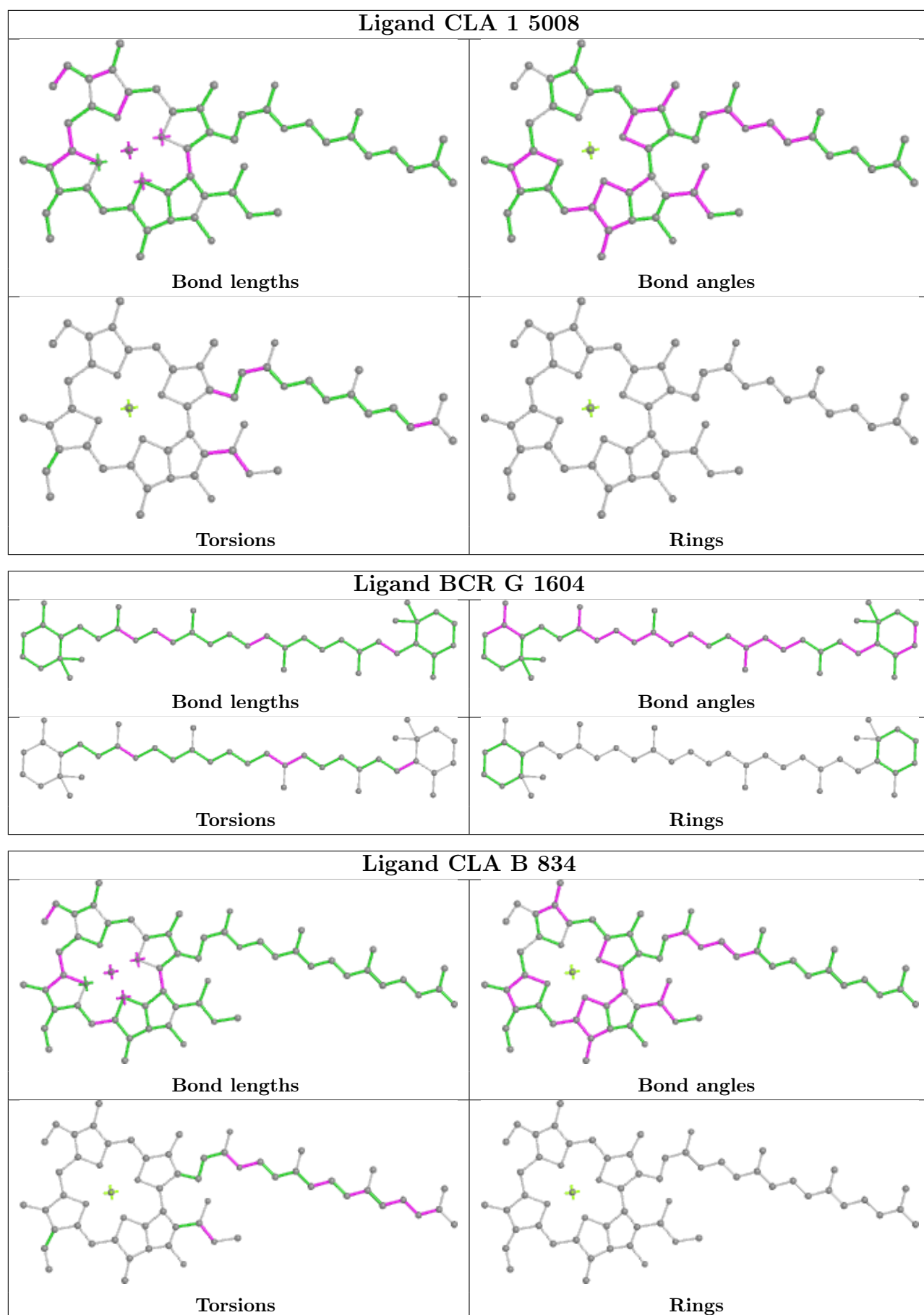


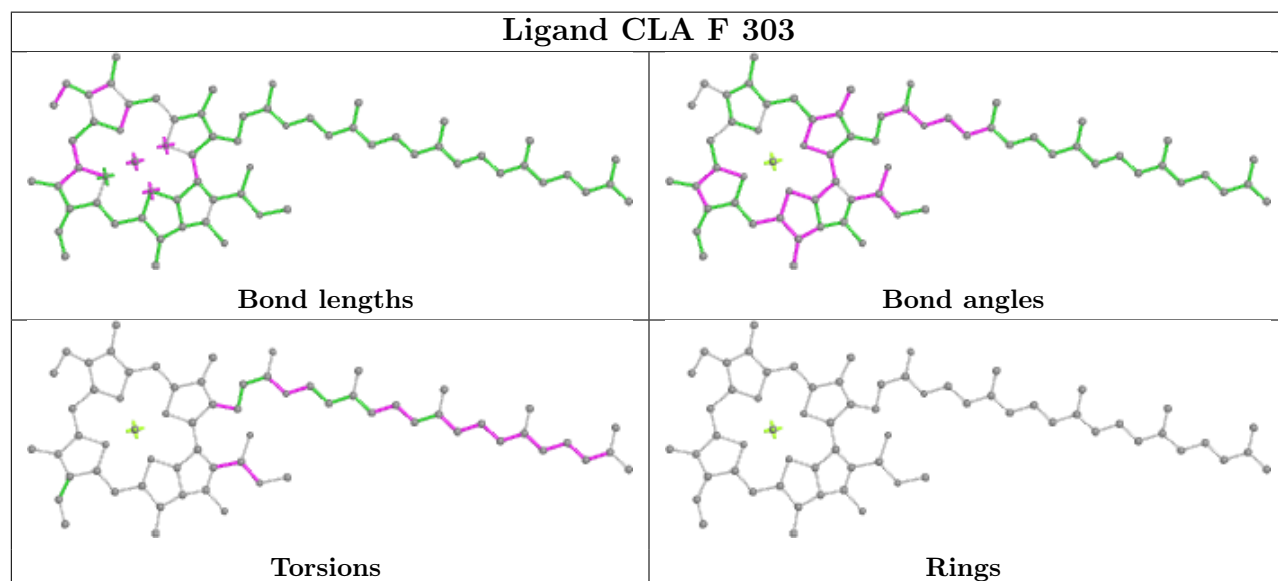
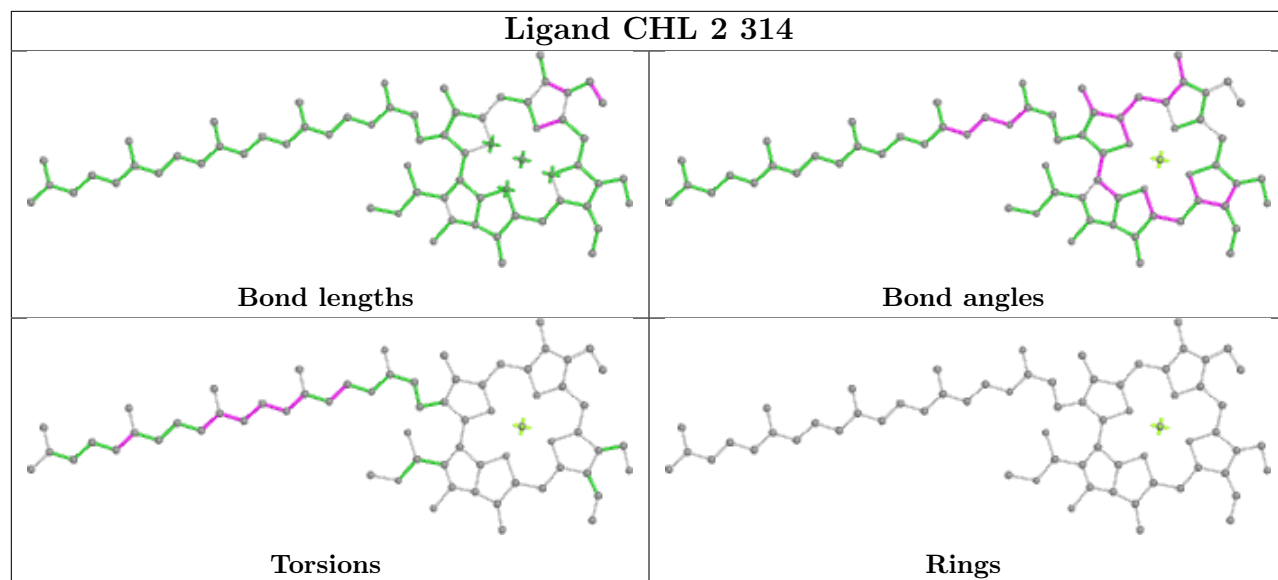


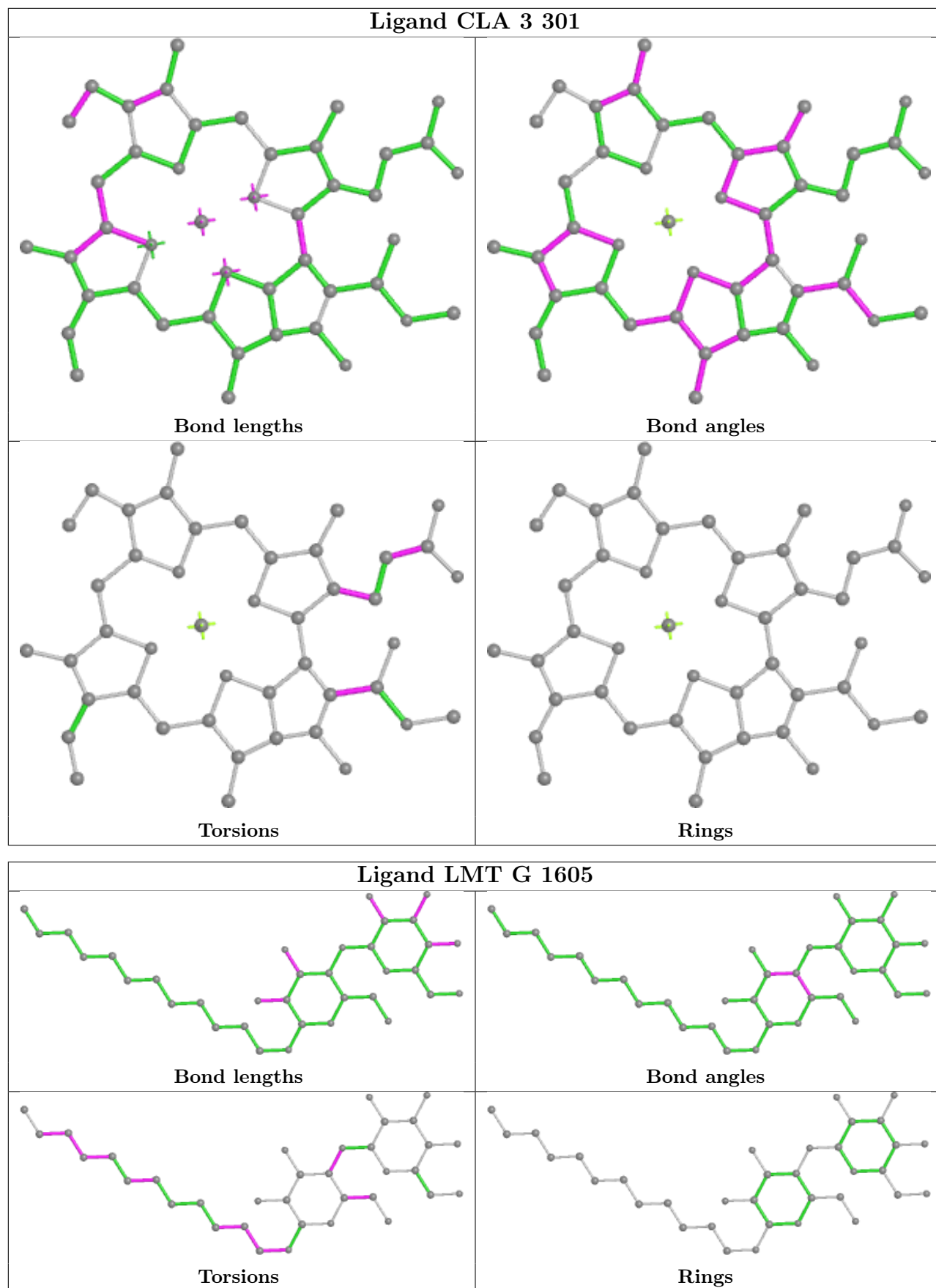




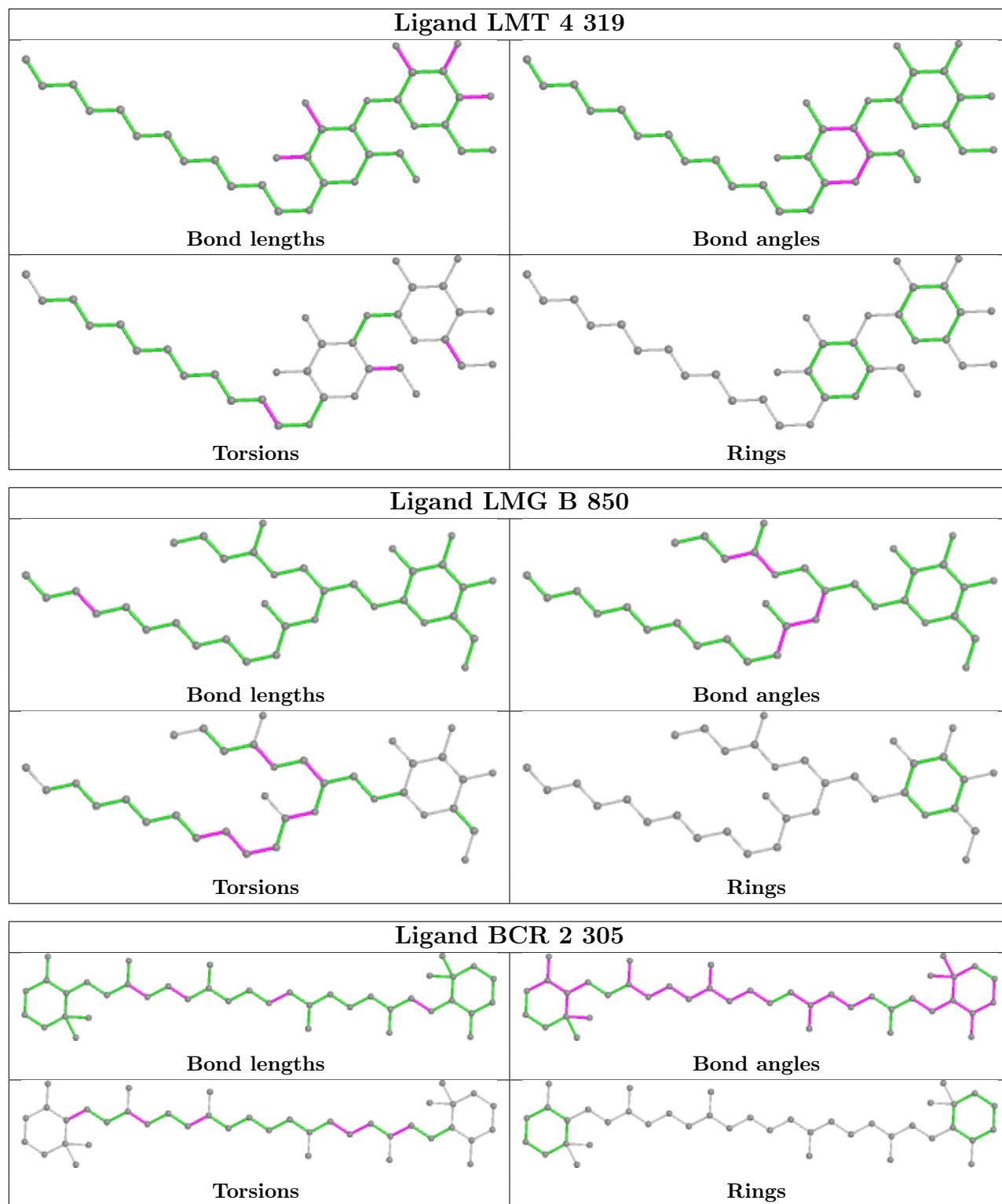


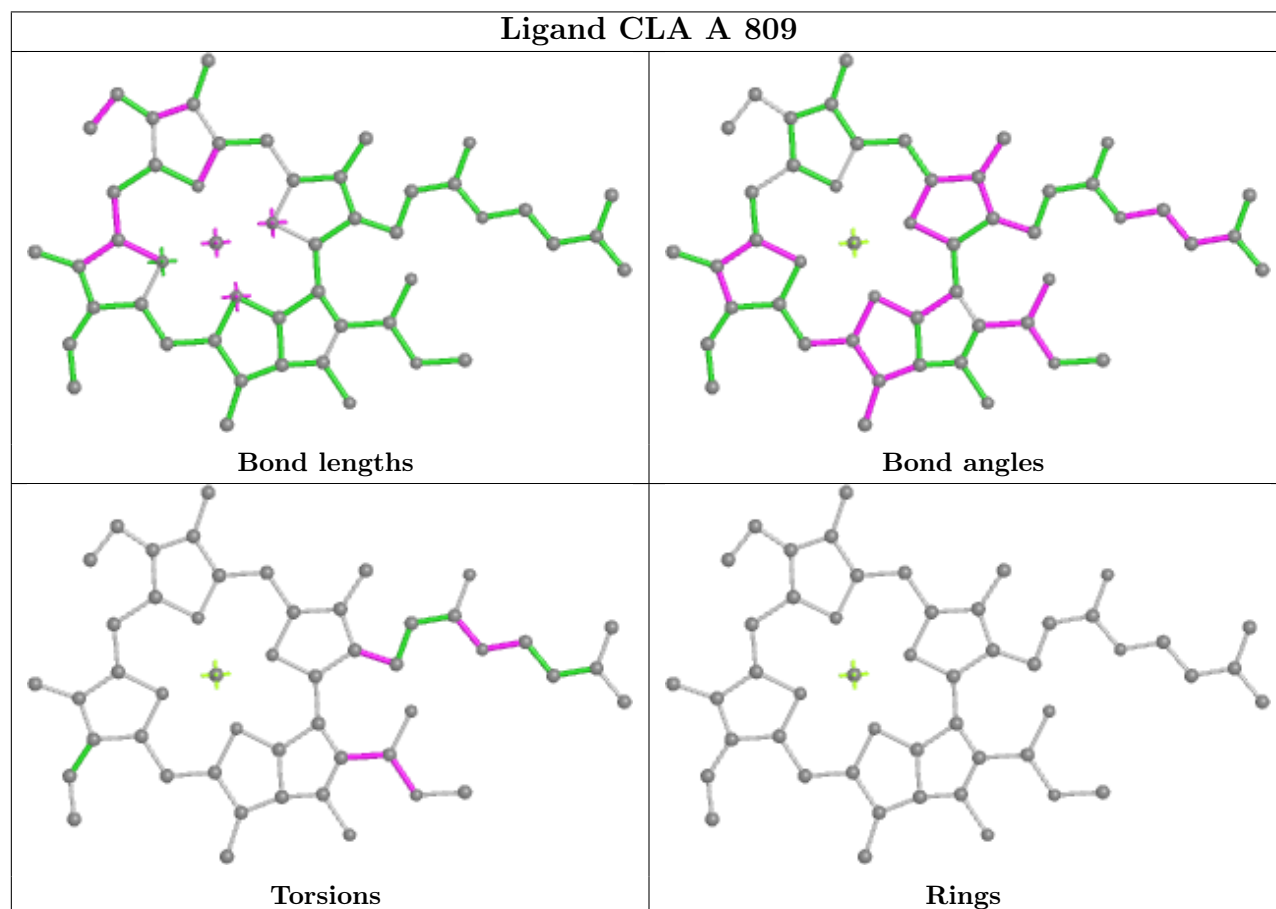
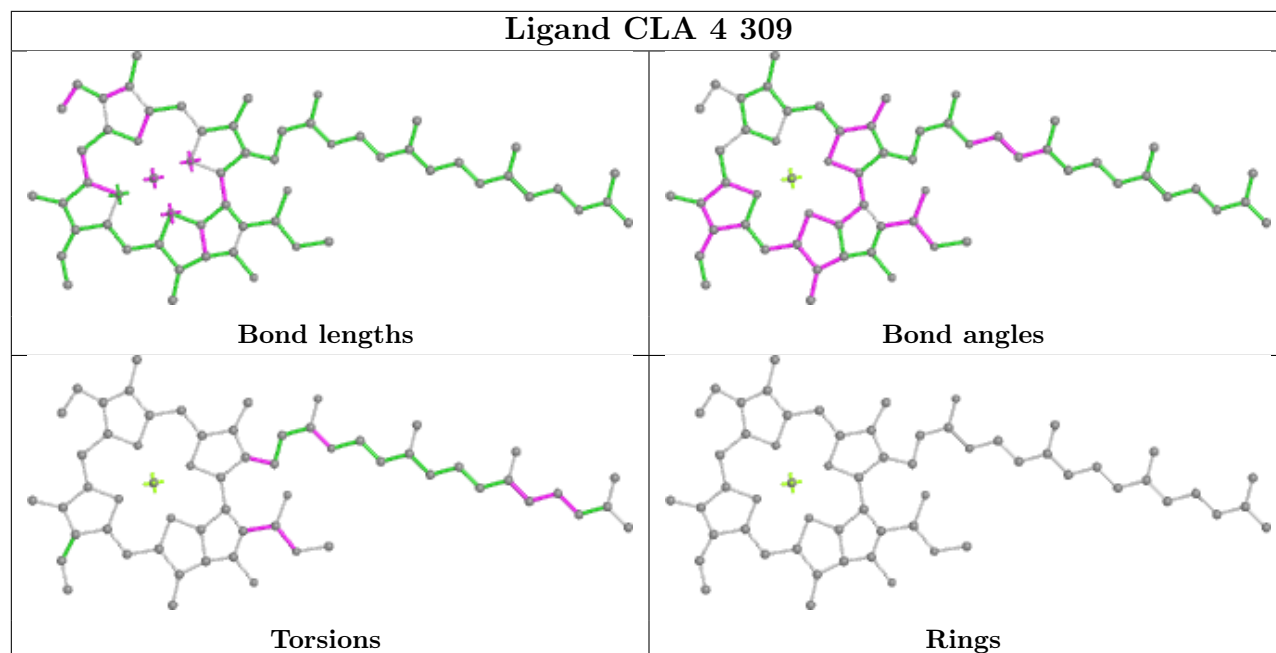


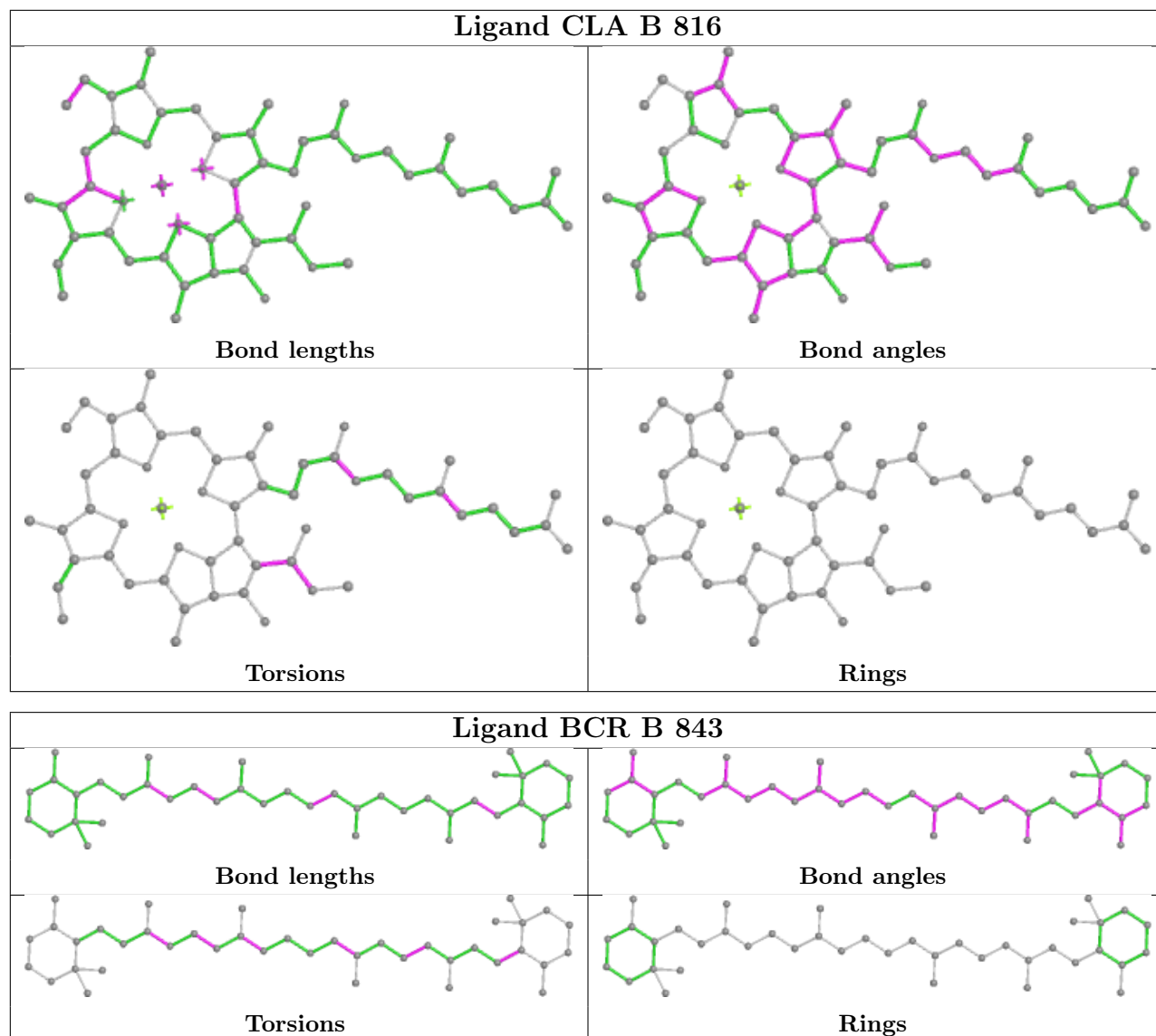




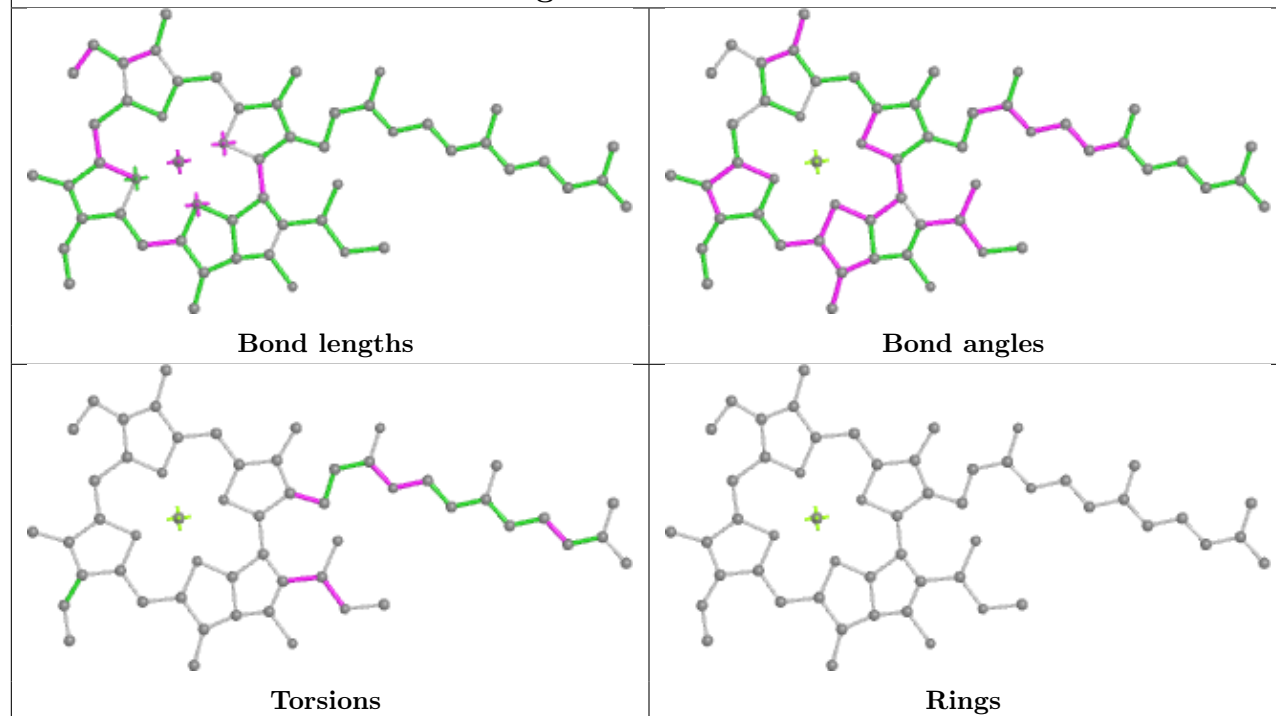




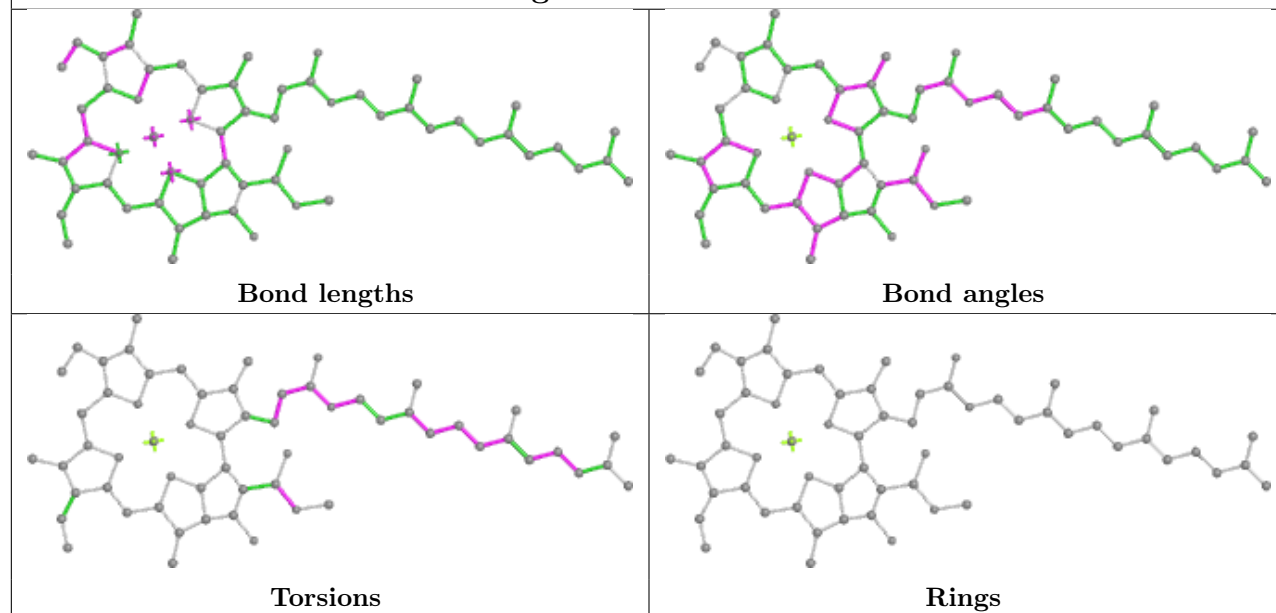


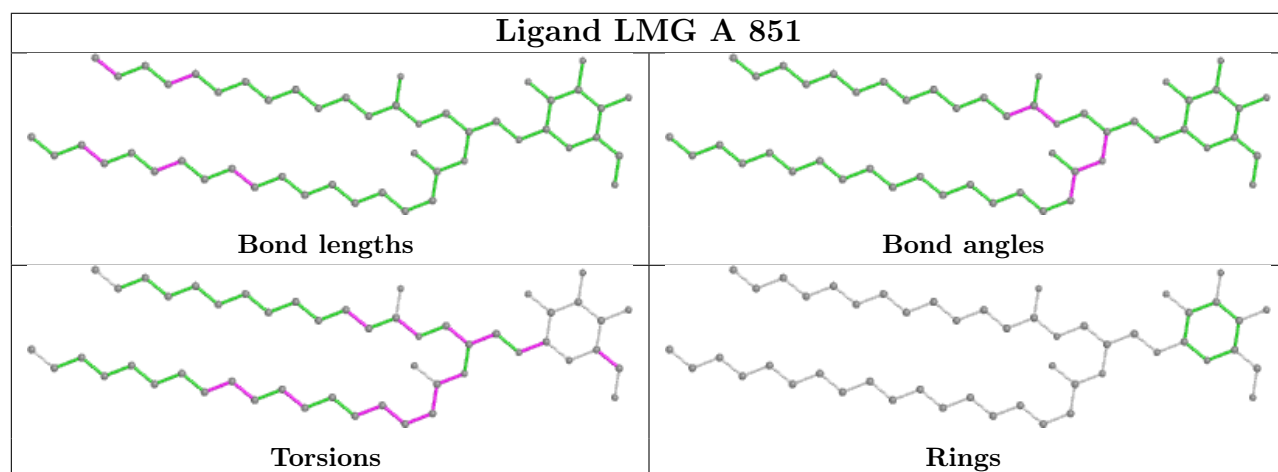
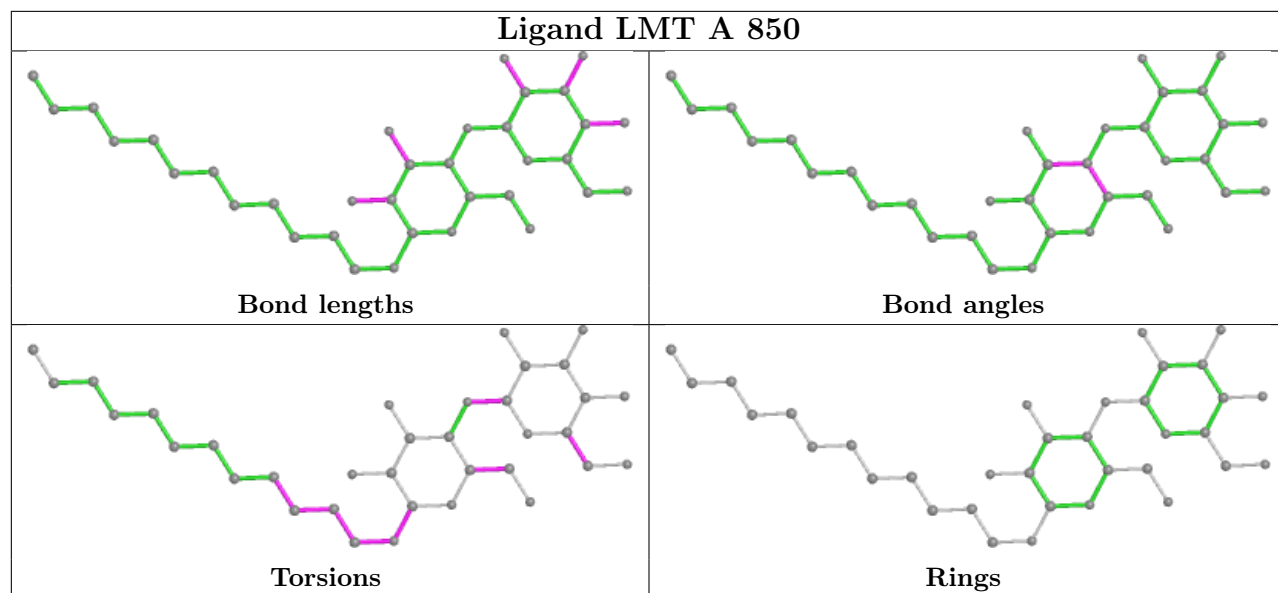


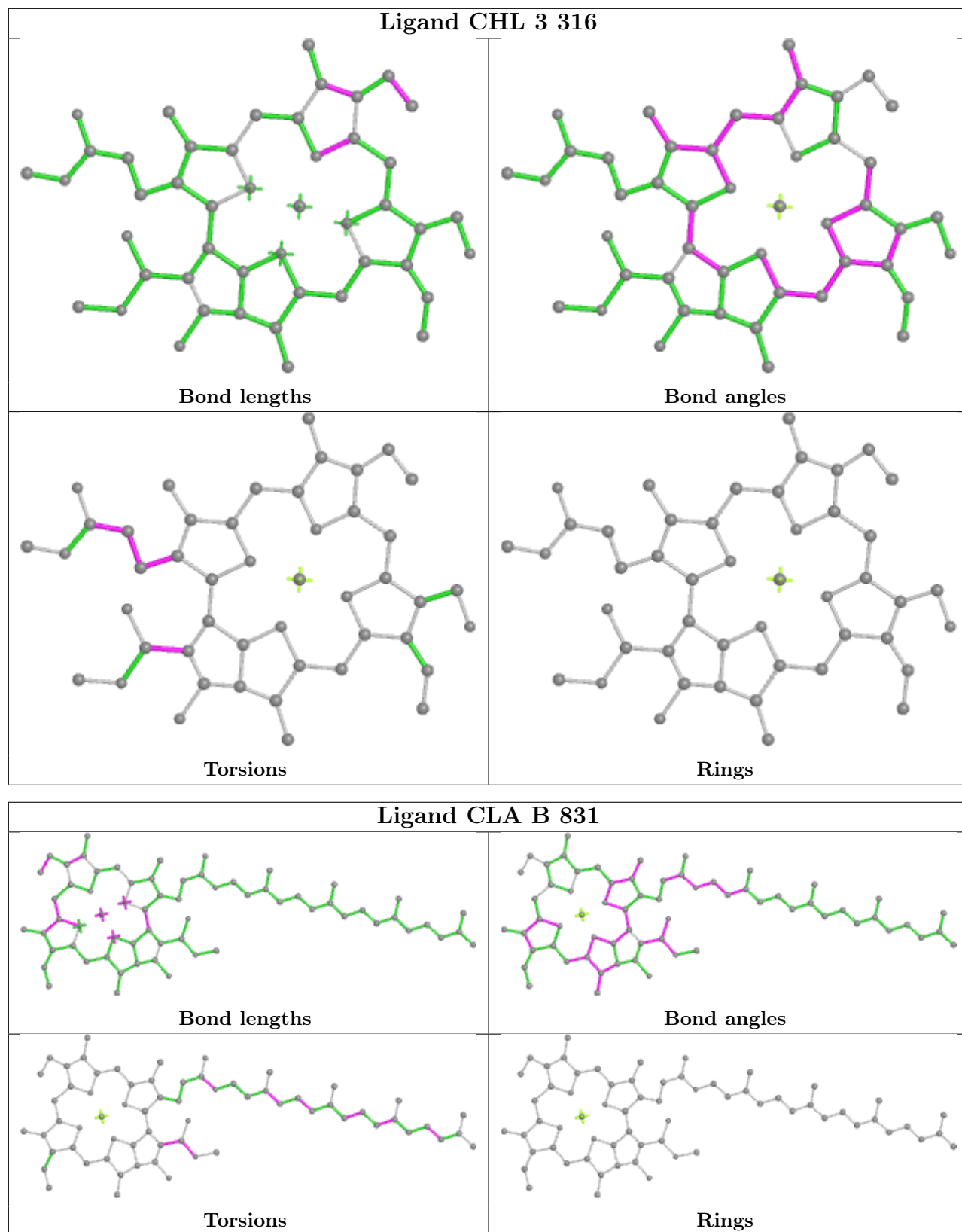
## Ligand CLA 2 317

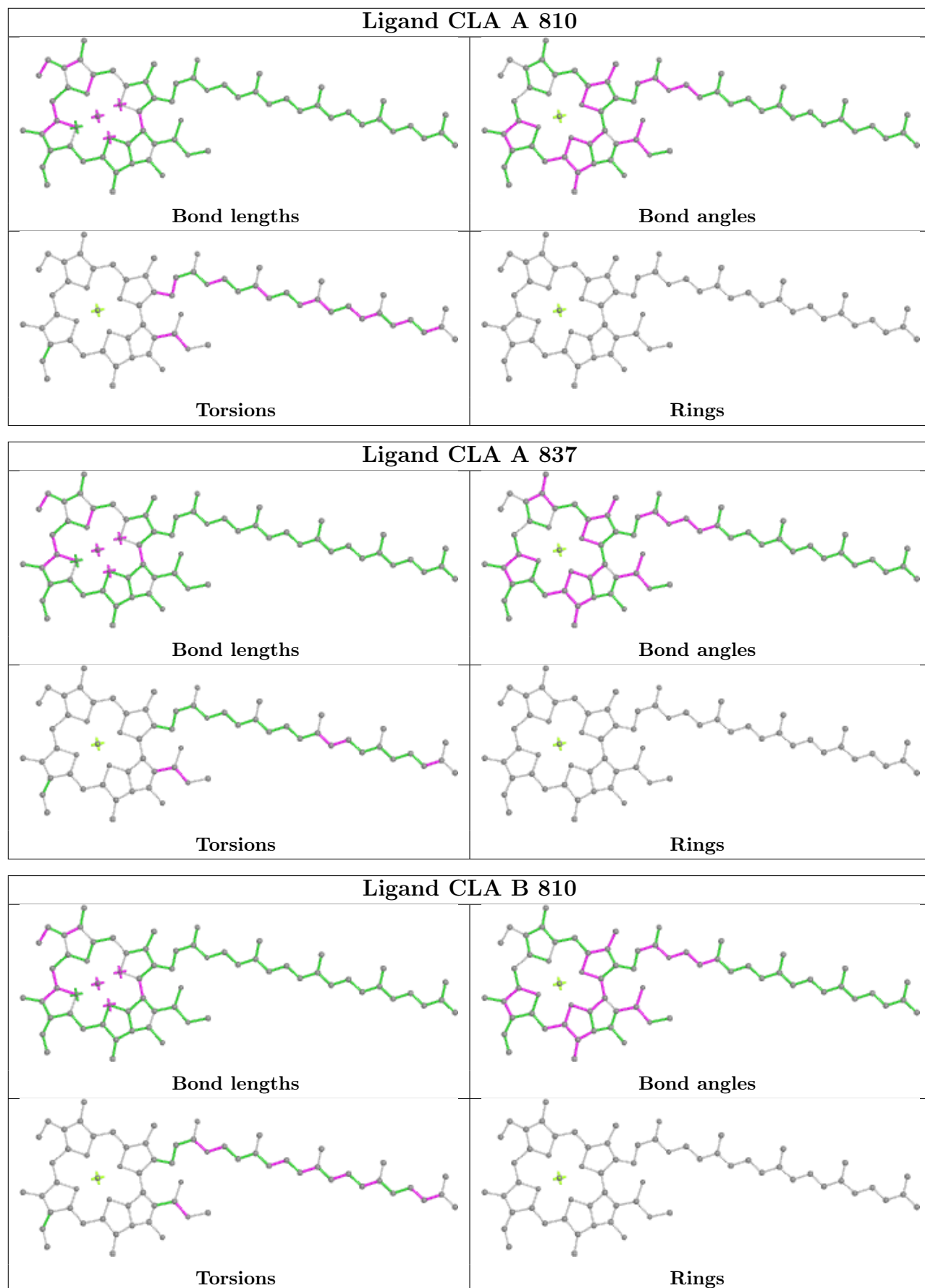


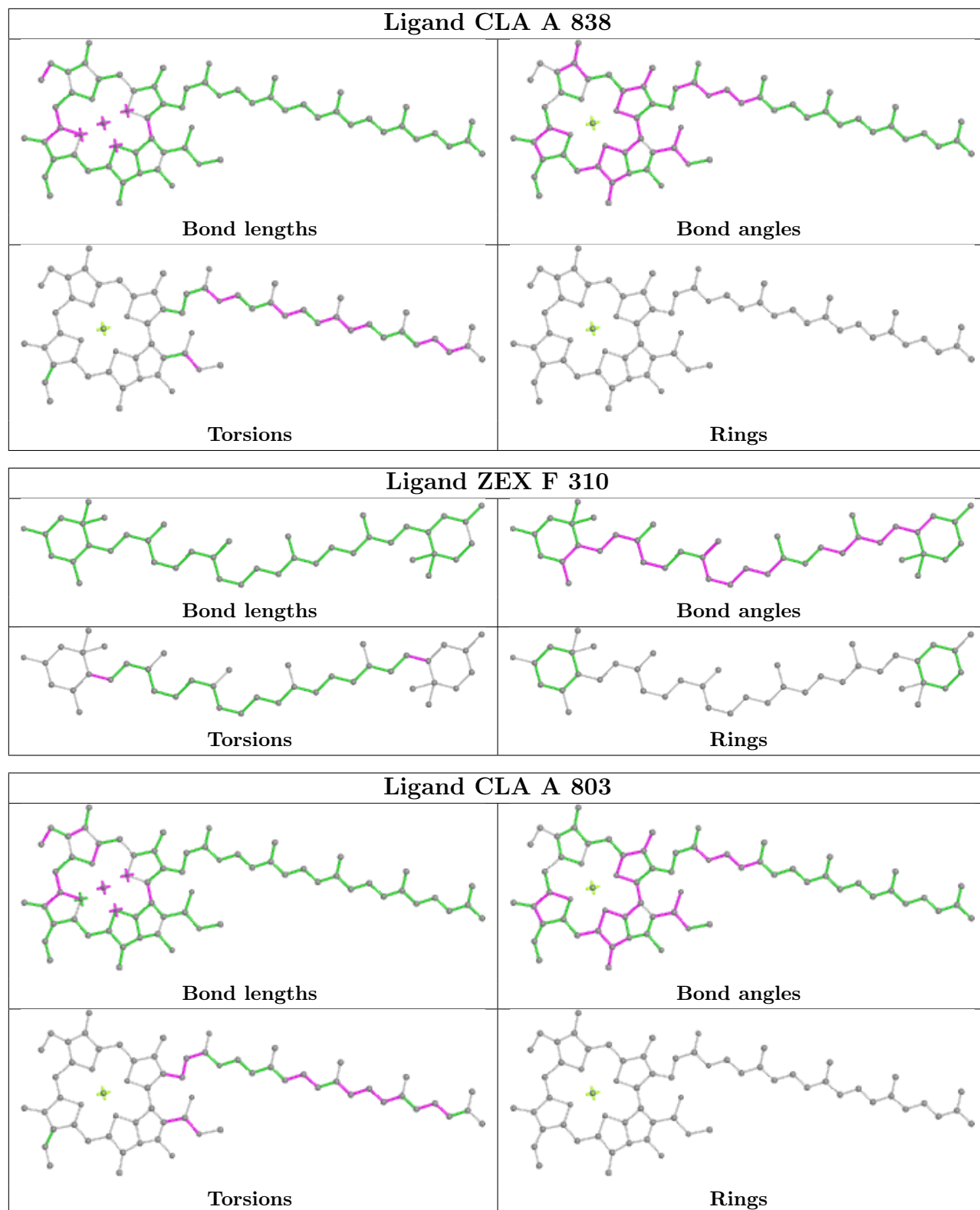
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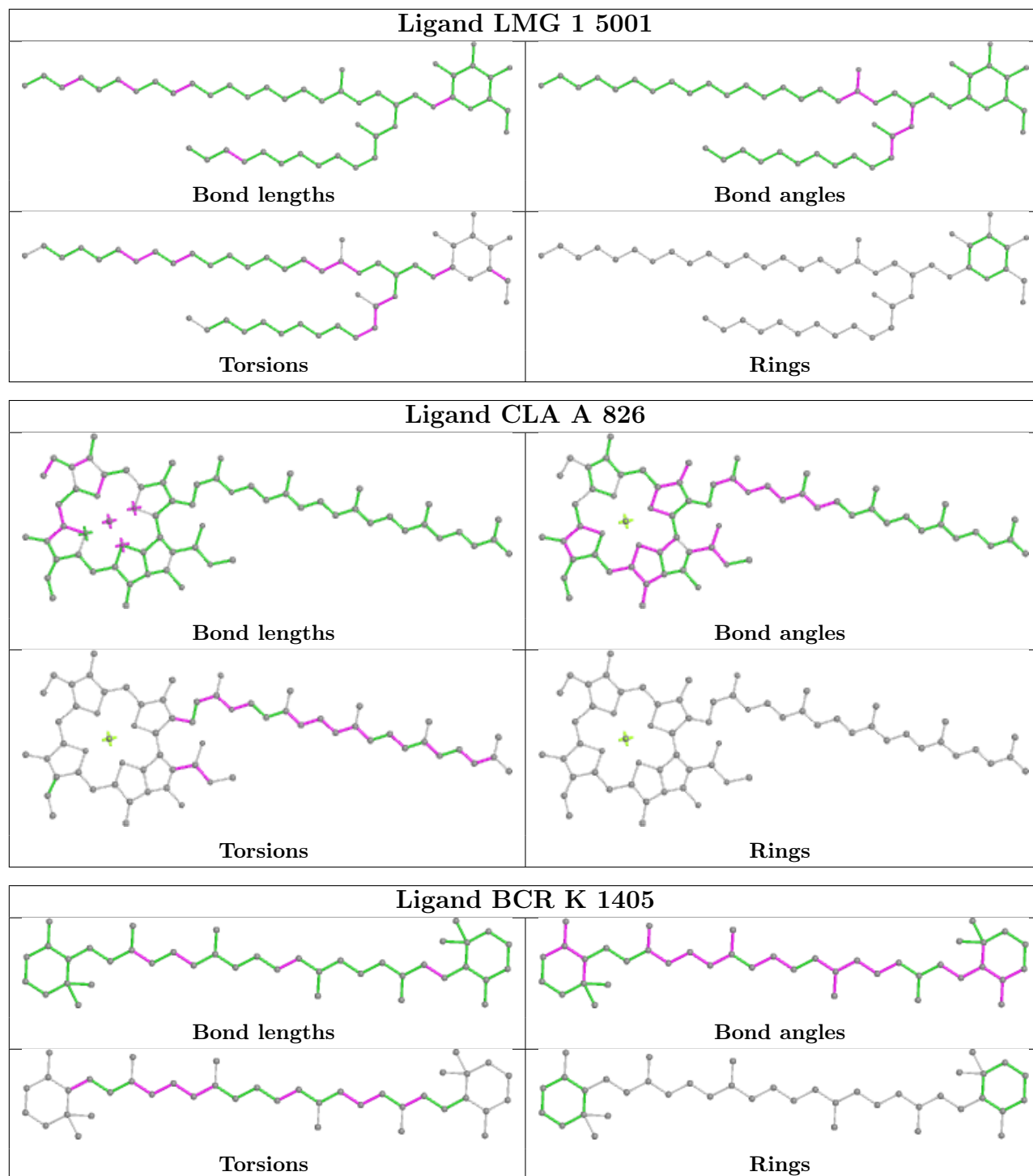


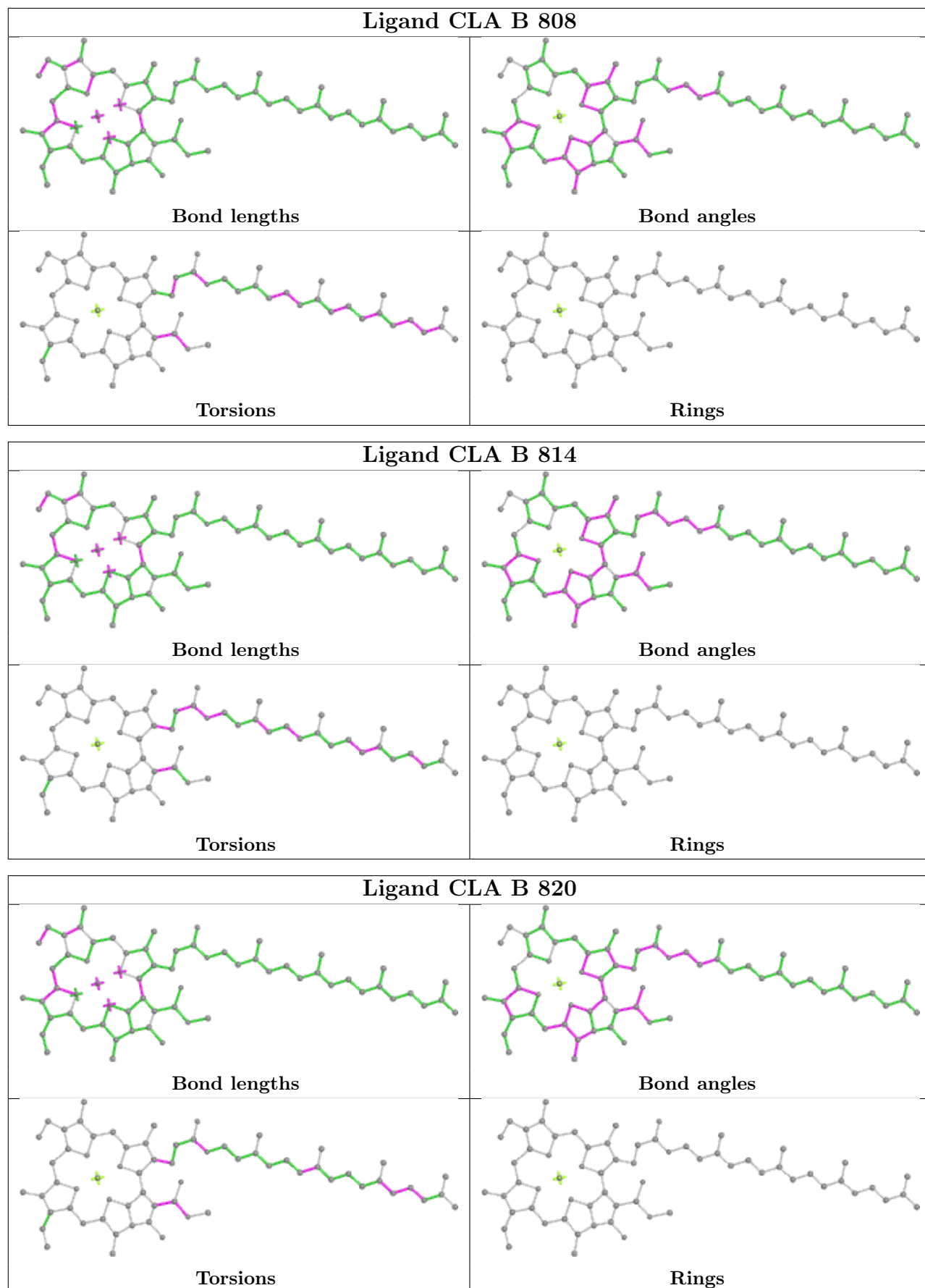


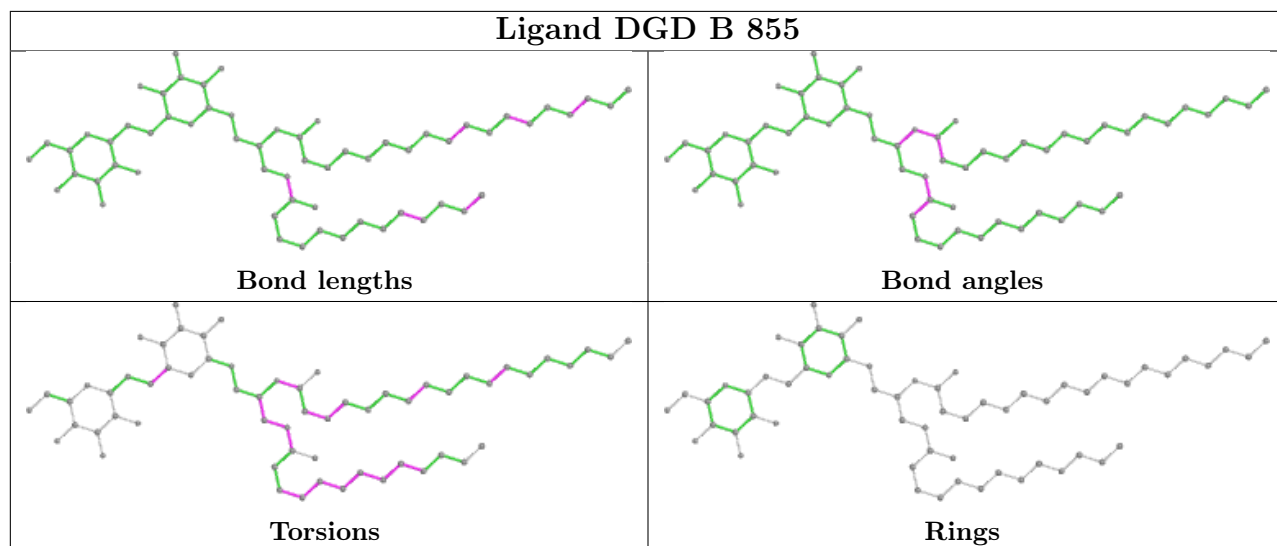
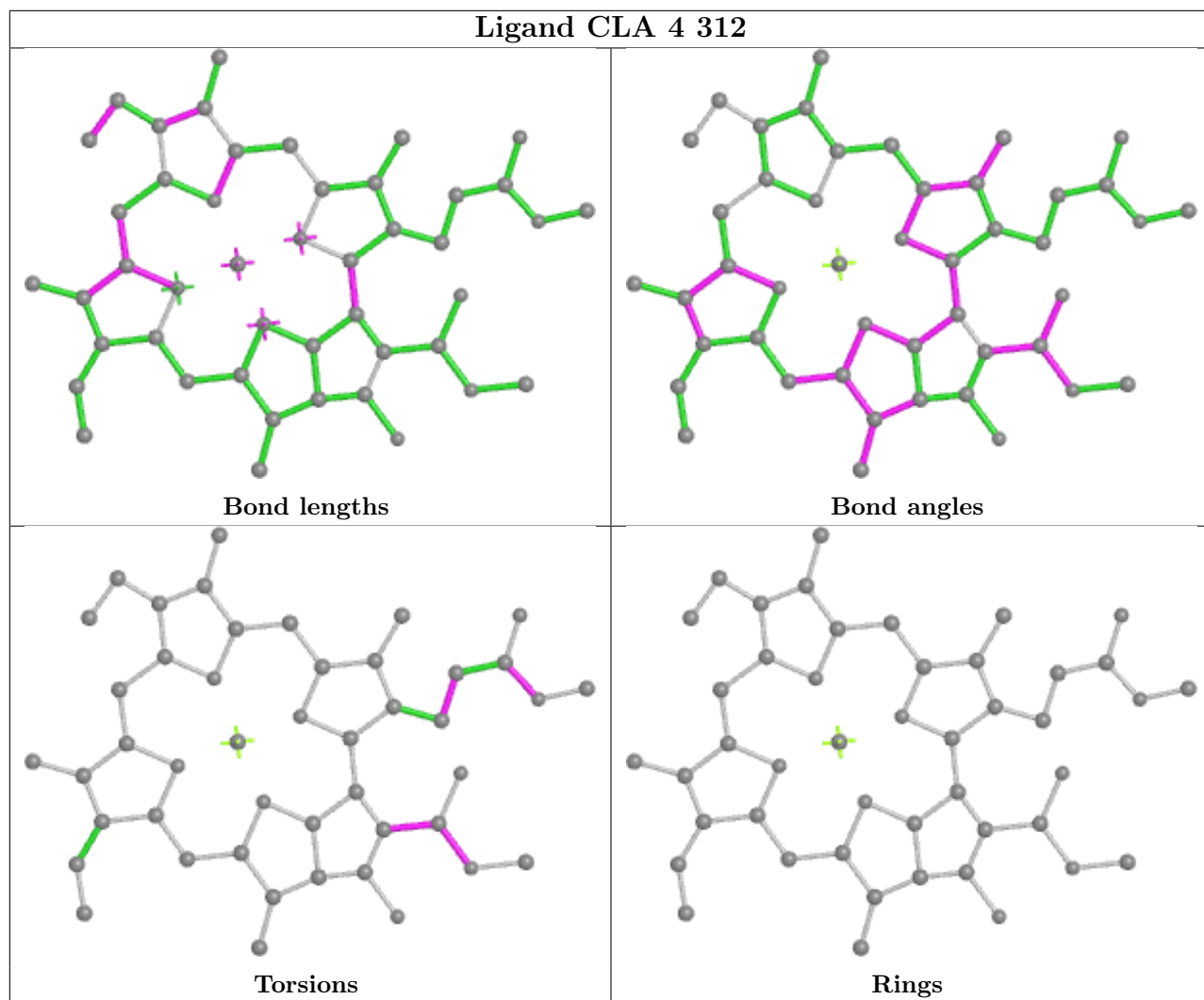


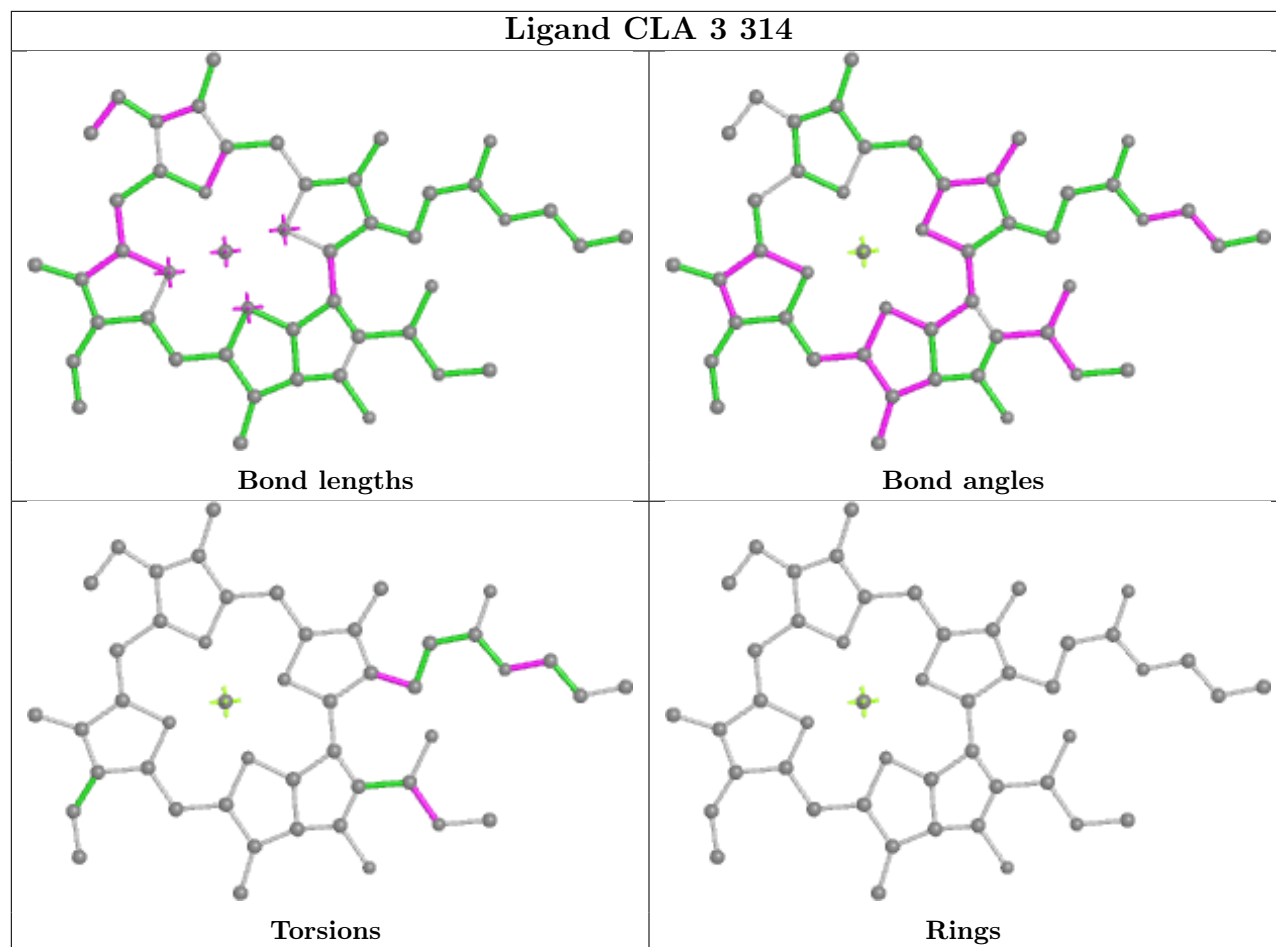


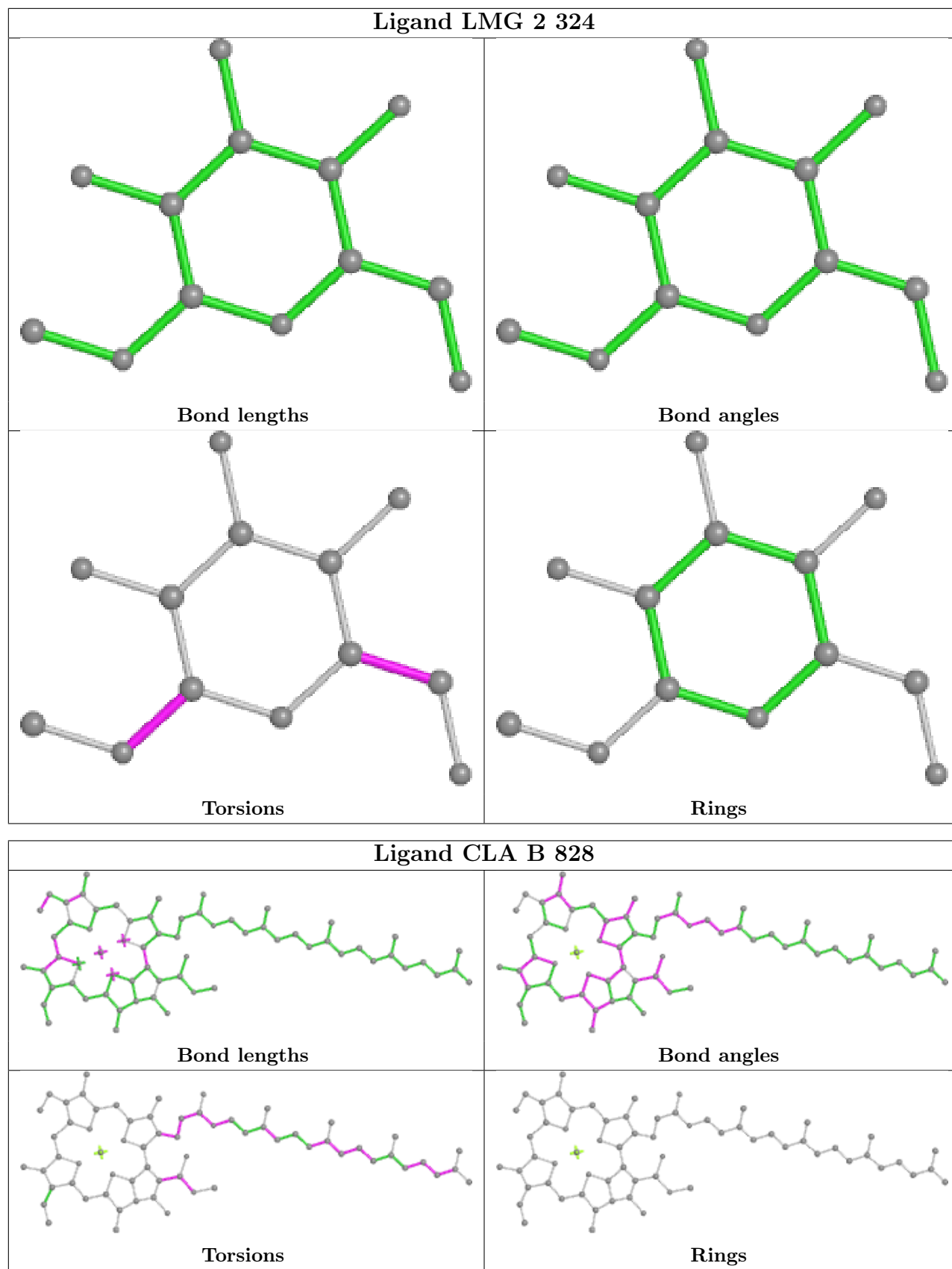


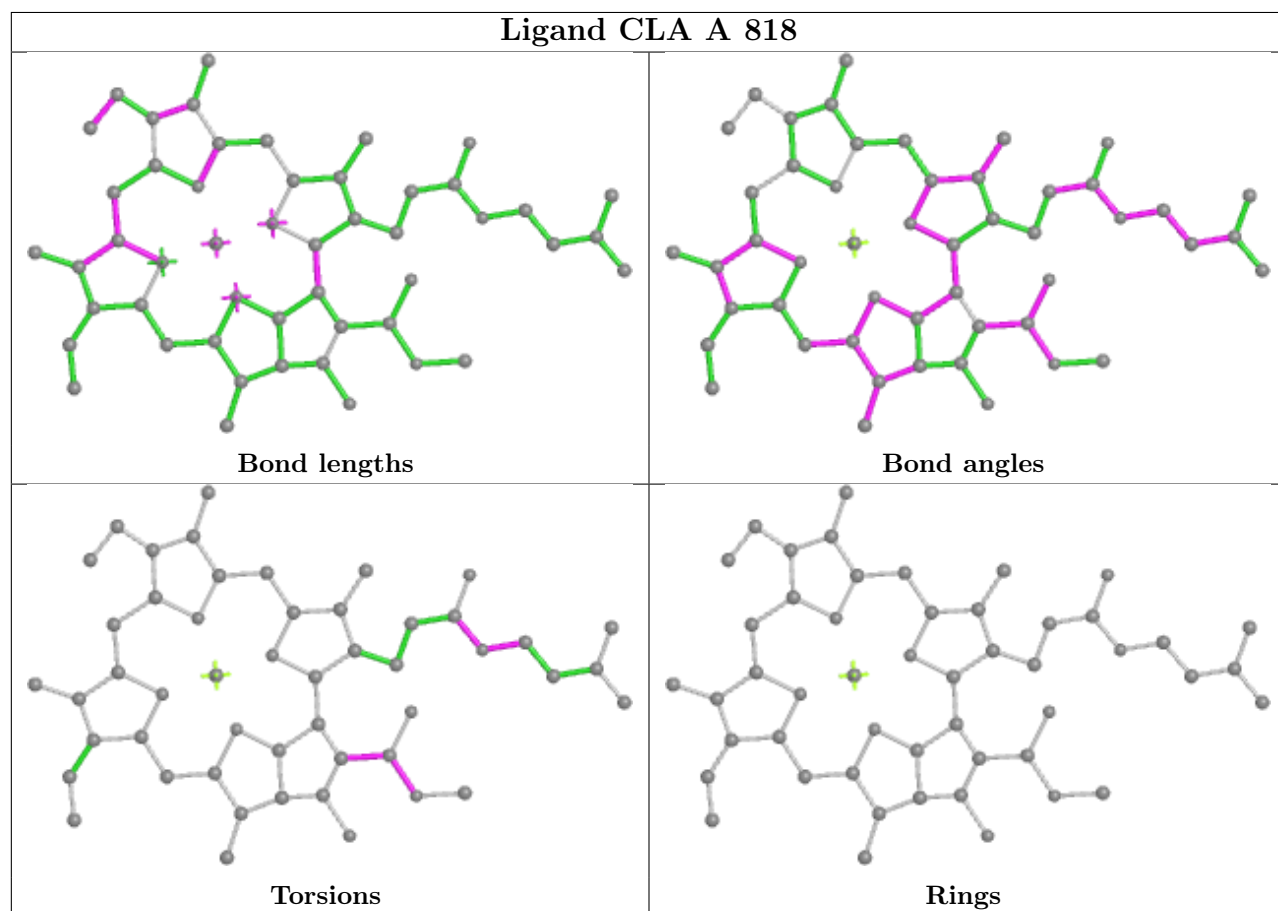
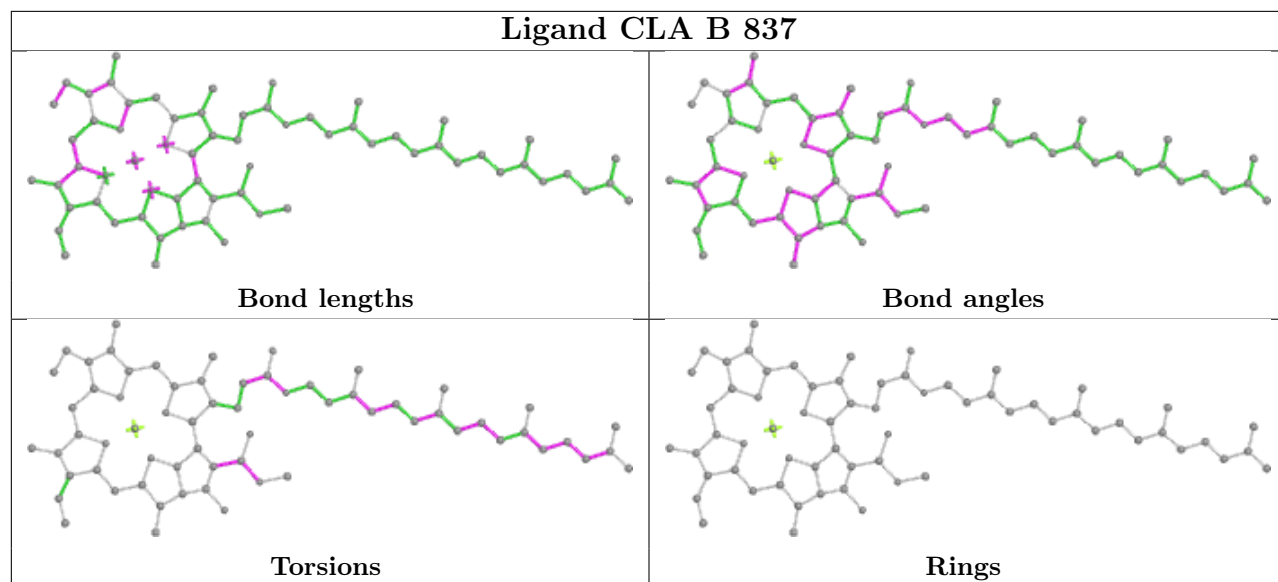


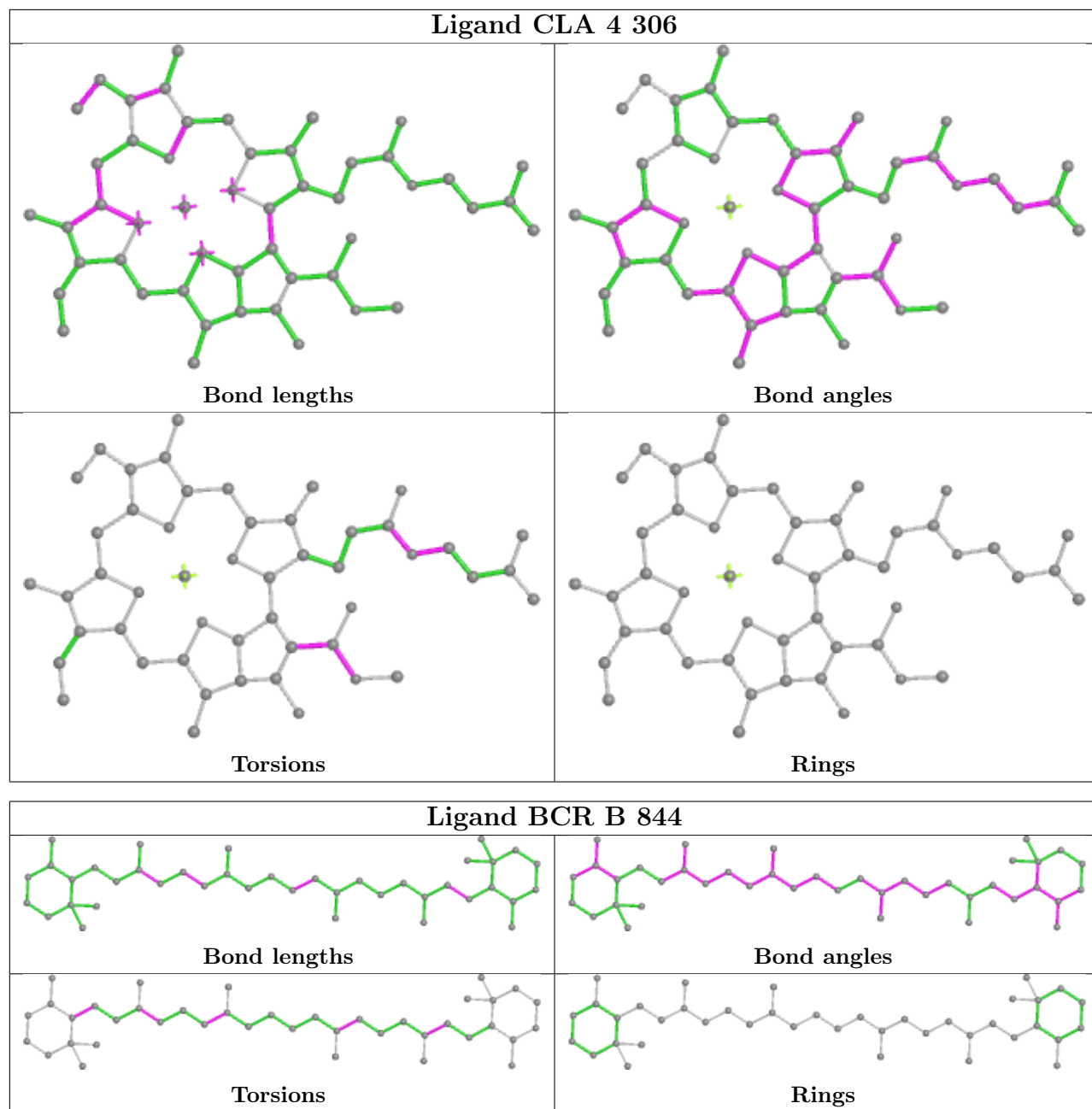


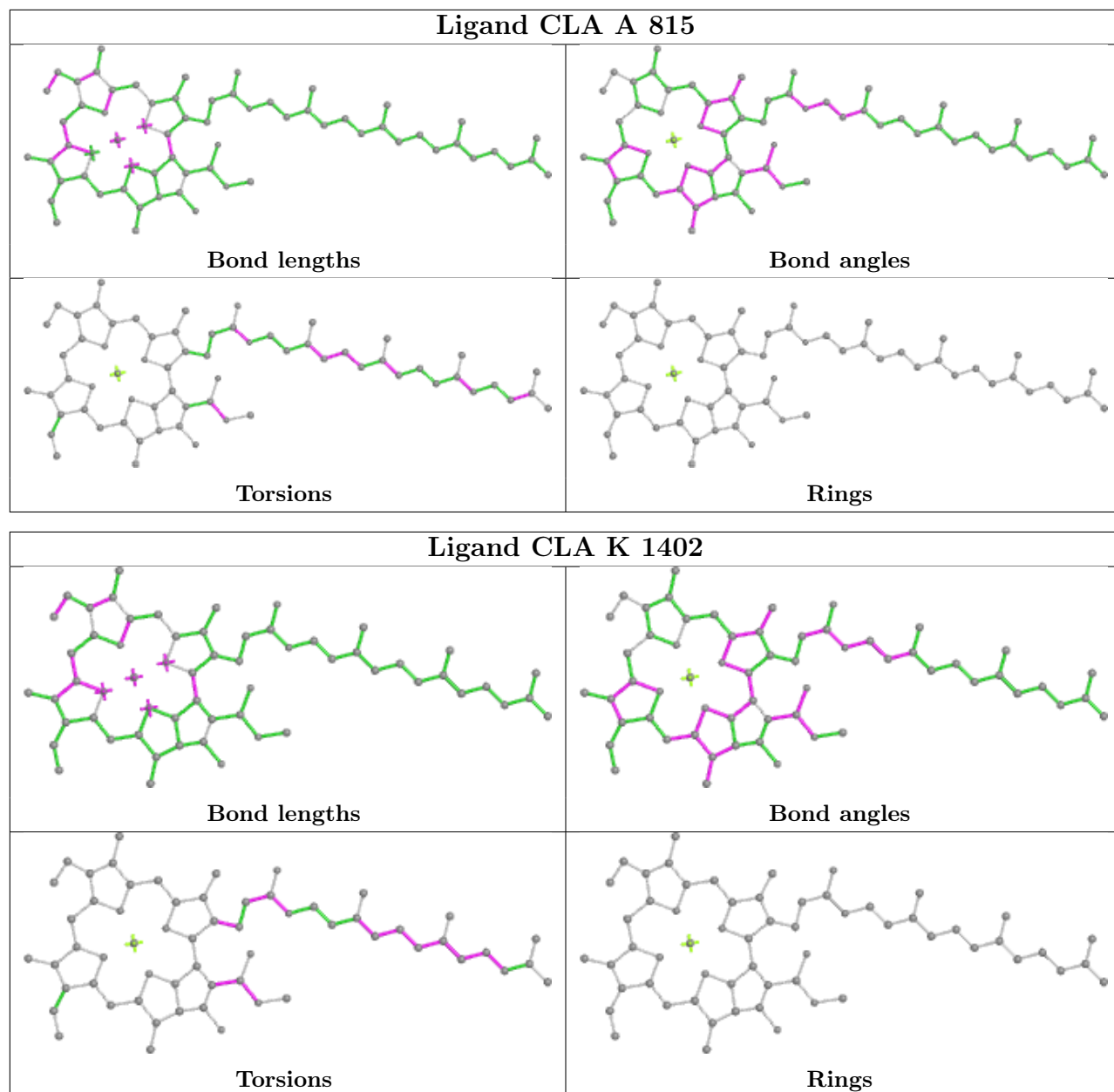




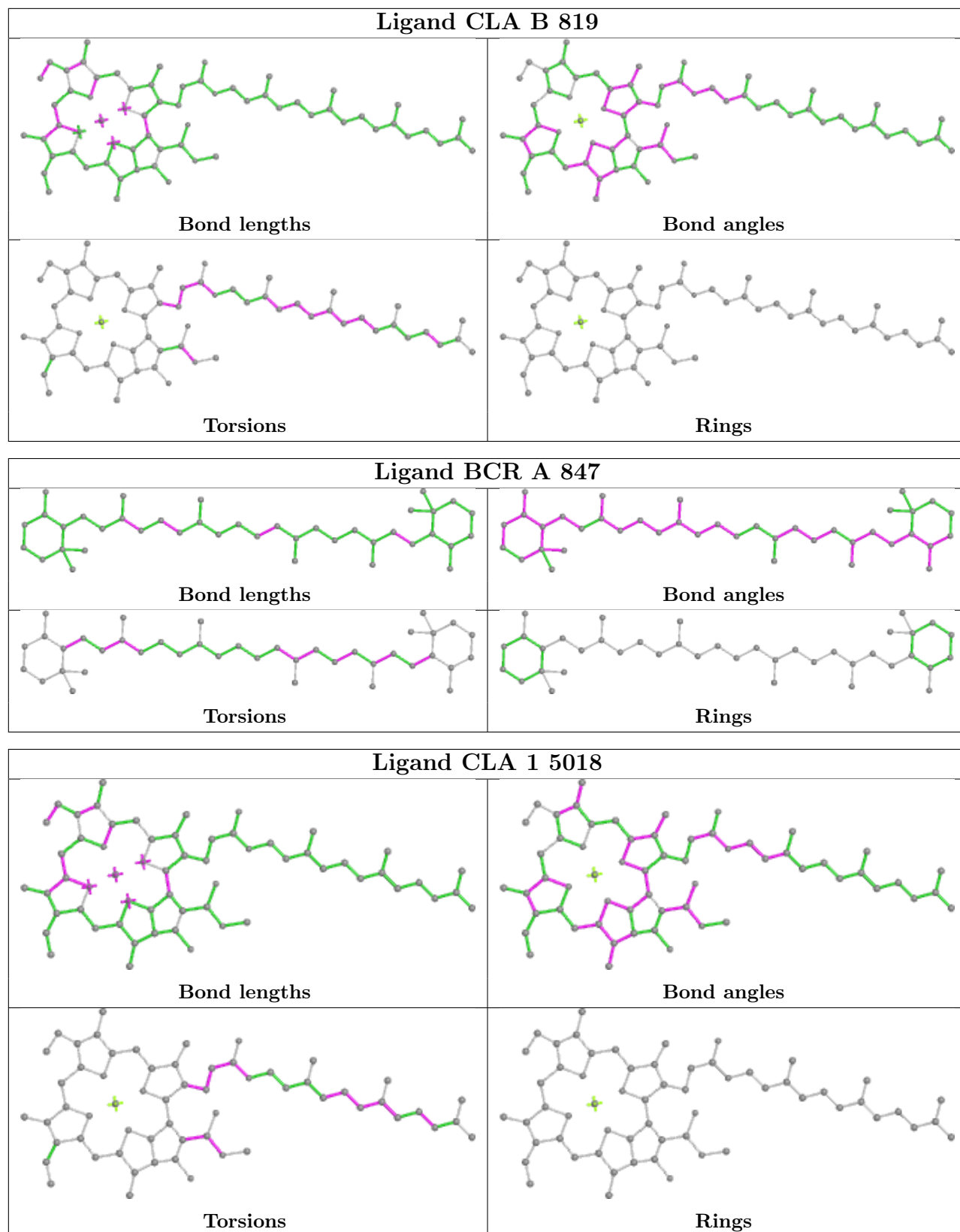


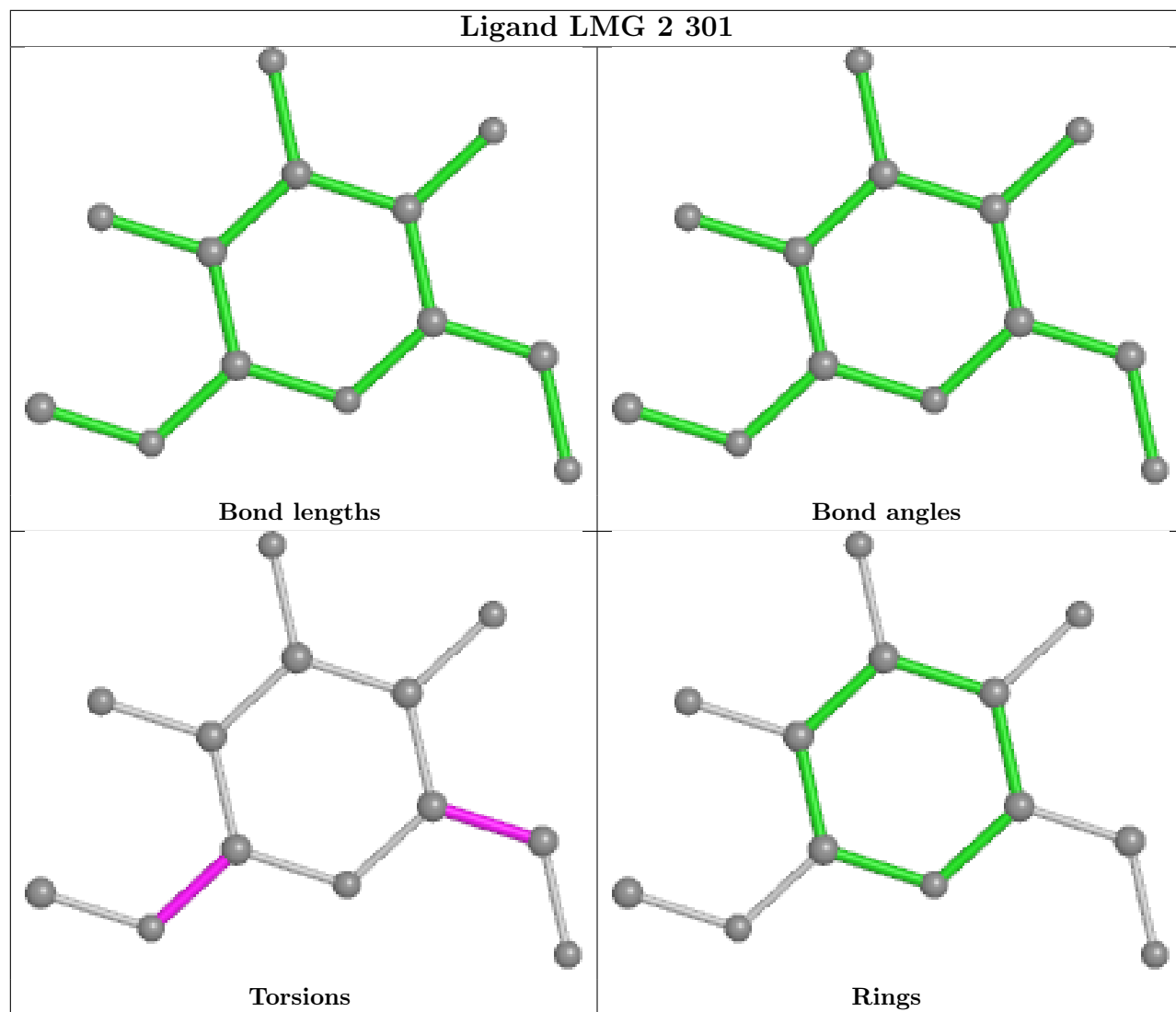


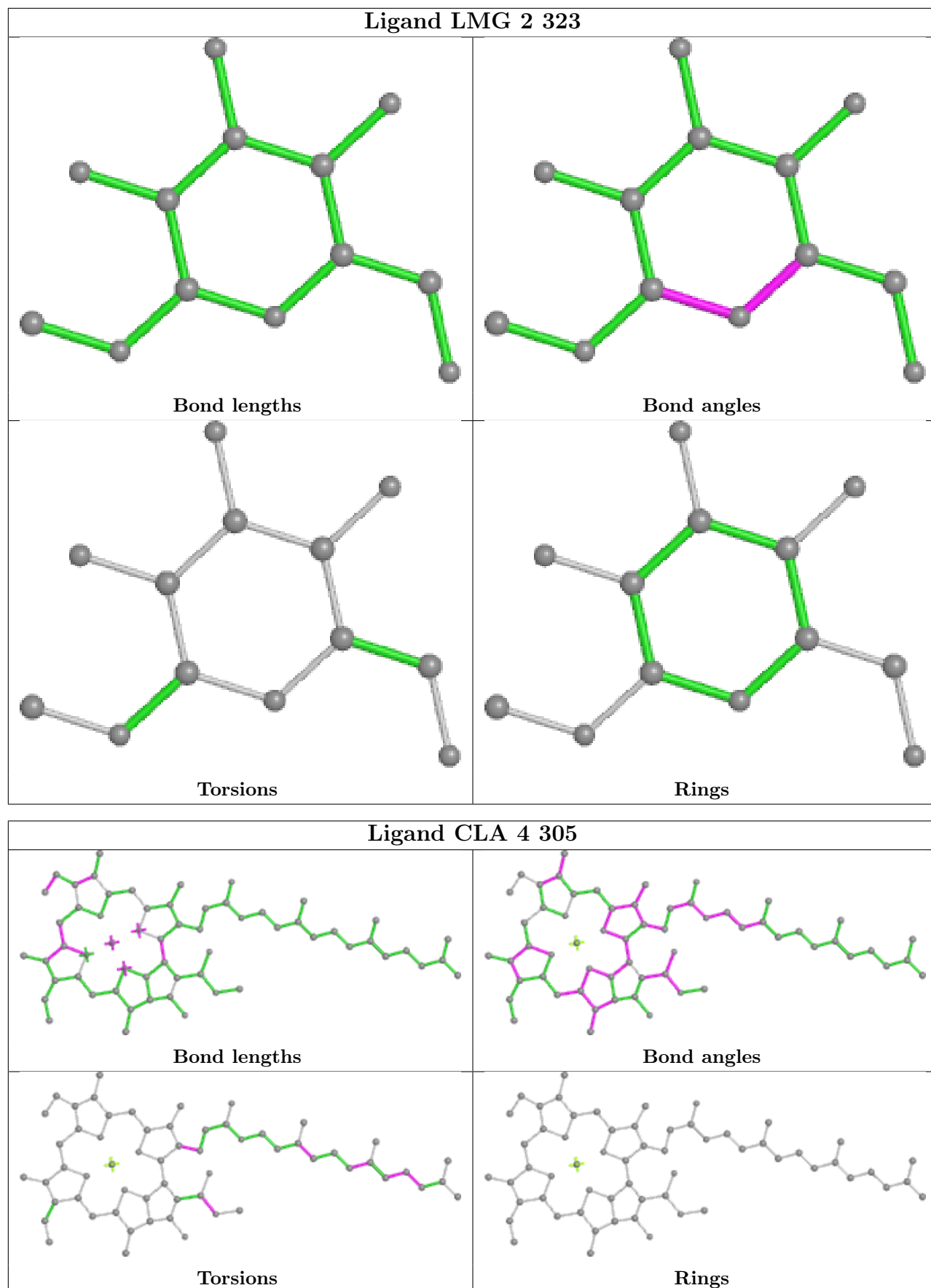


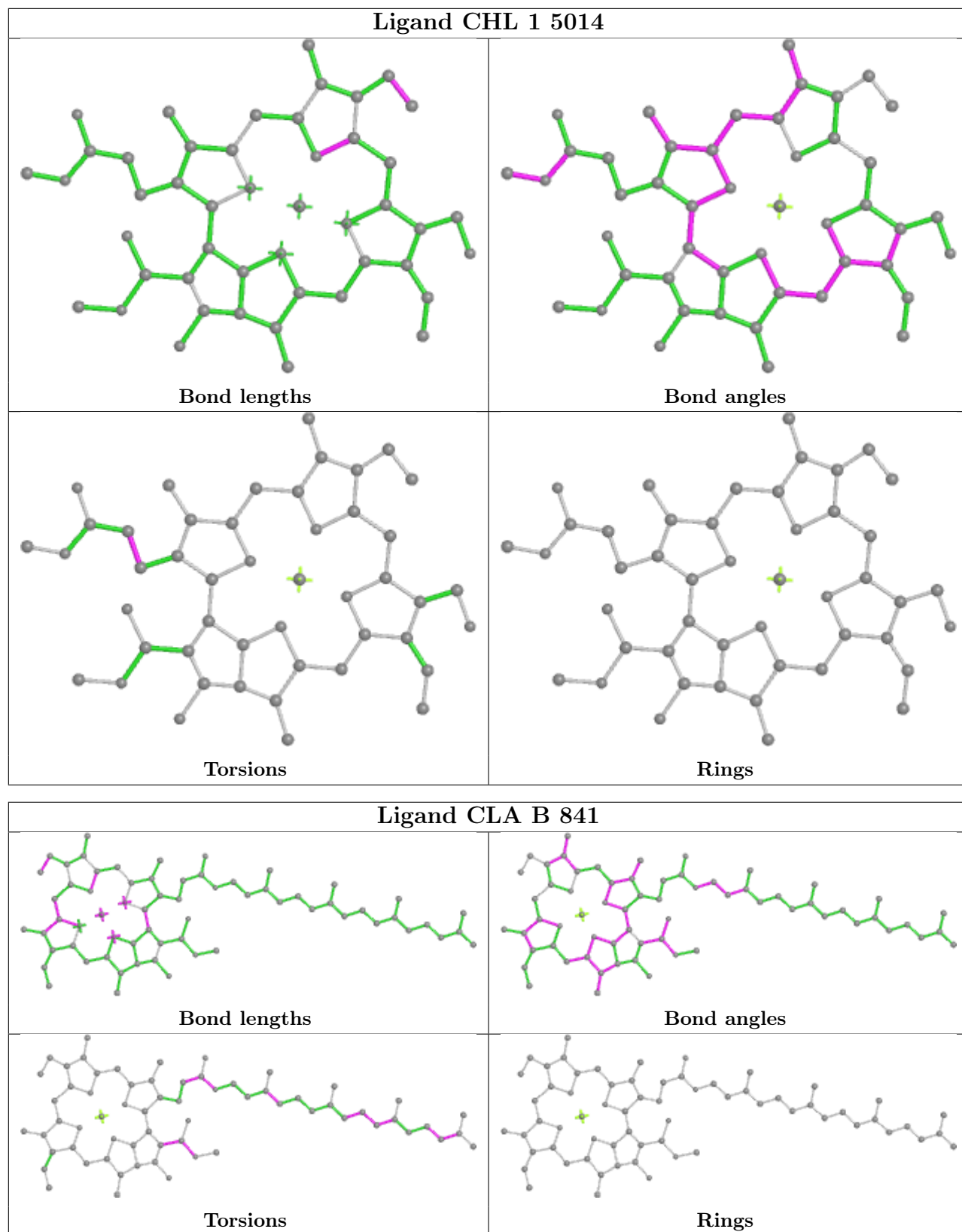


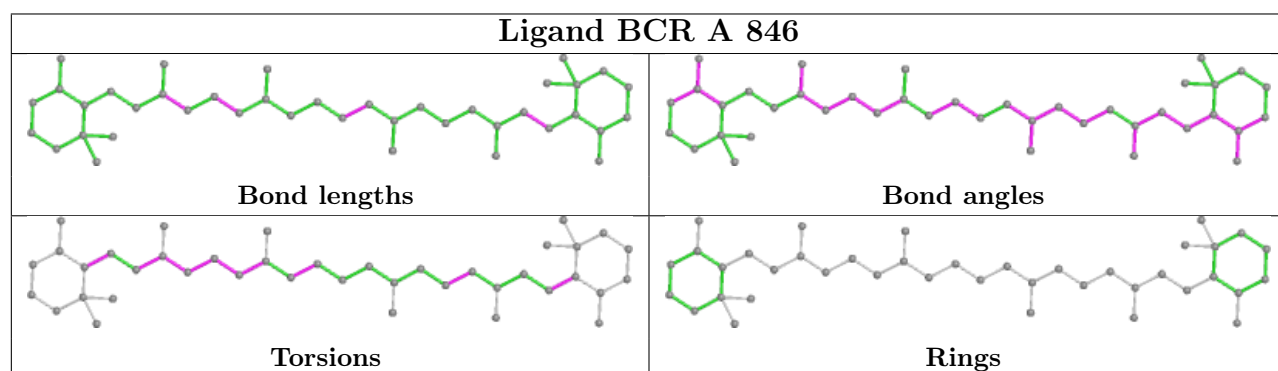
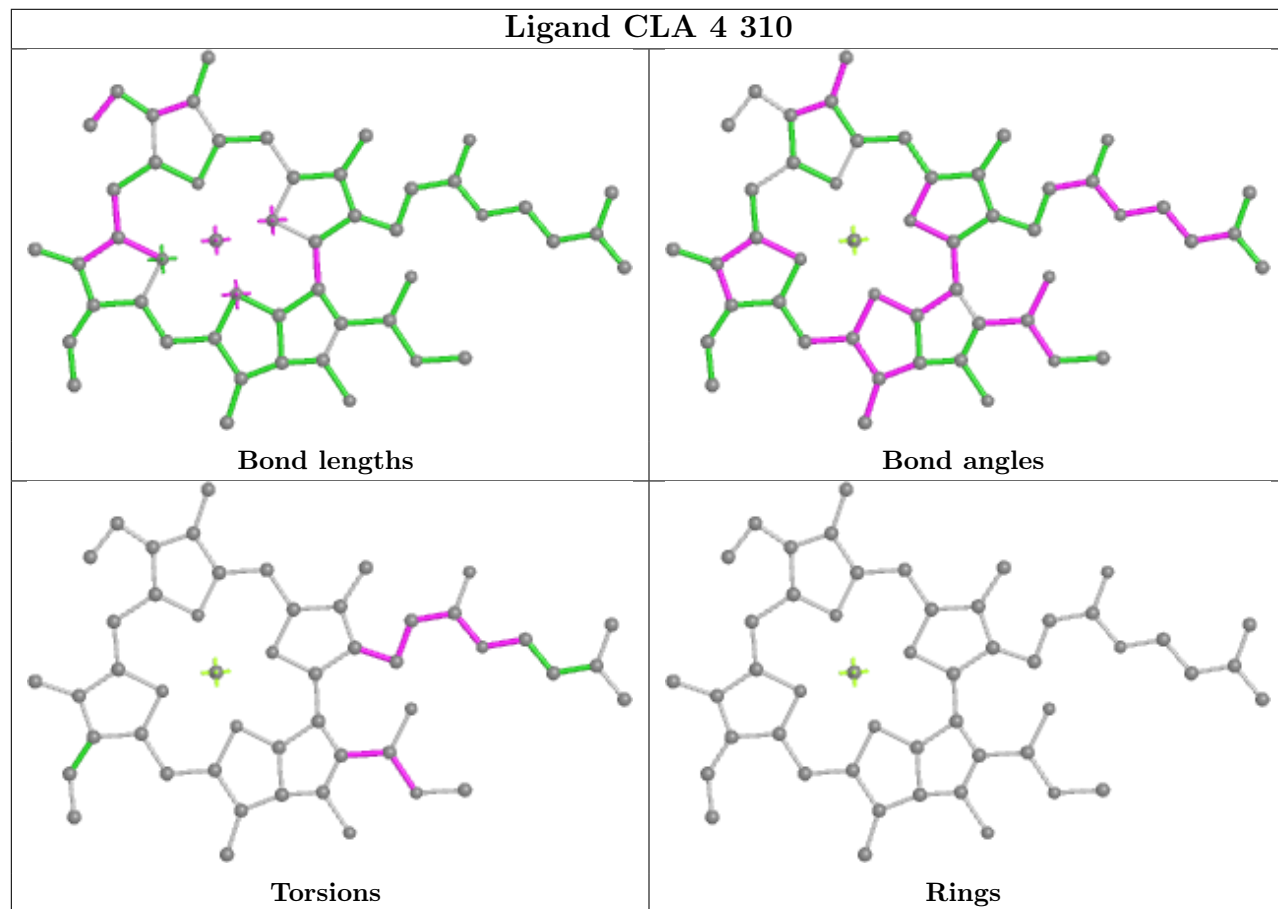
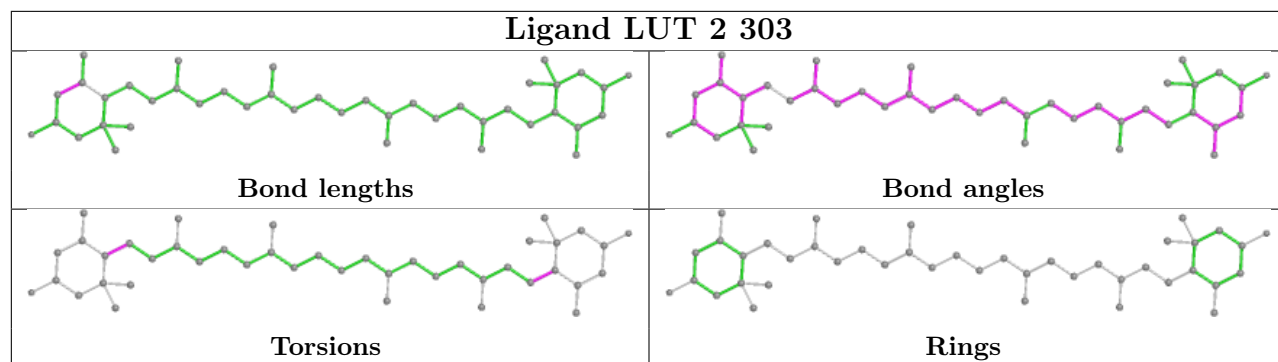


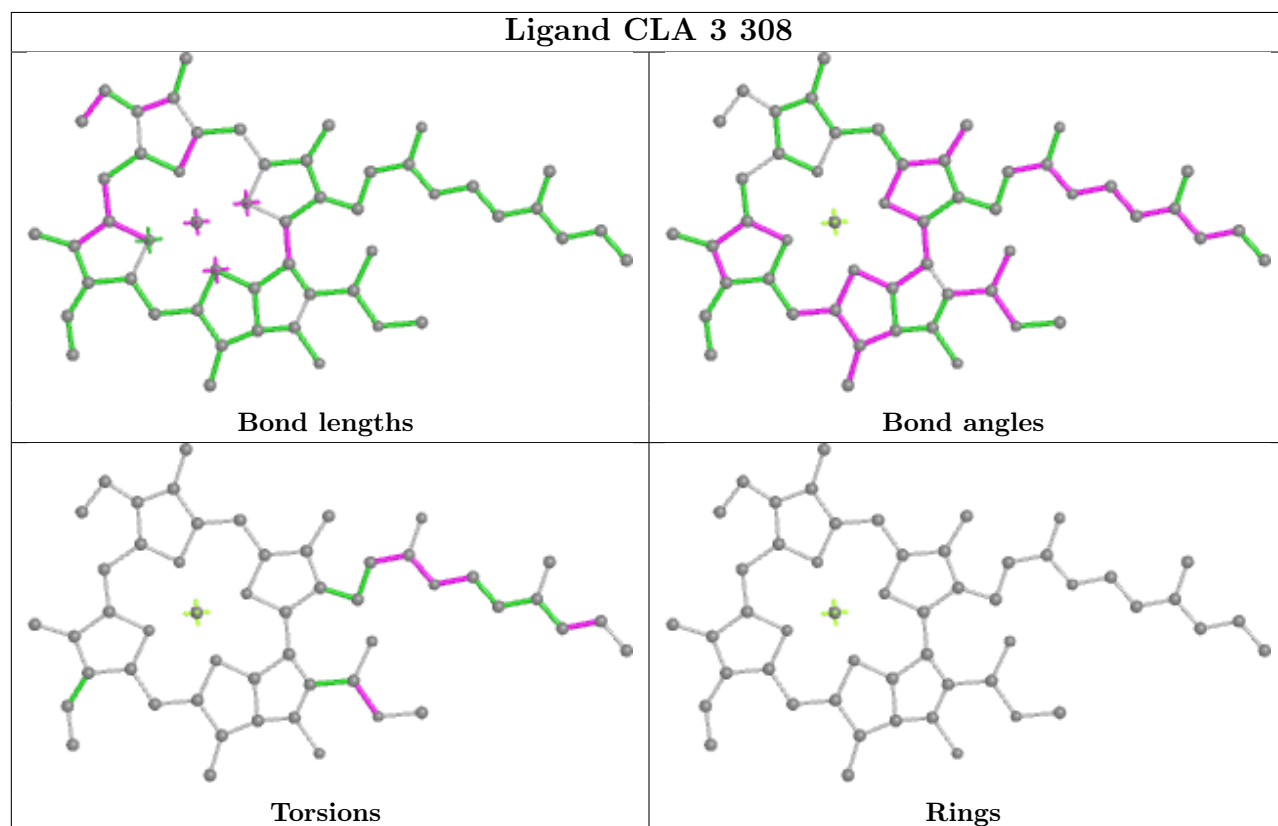
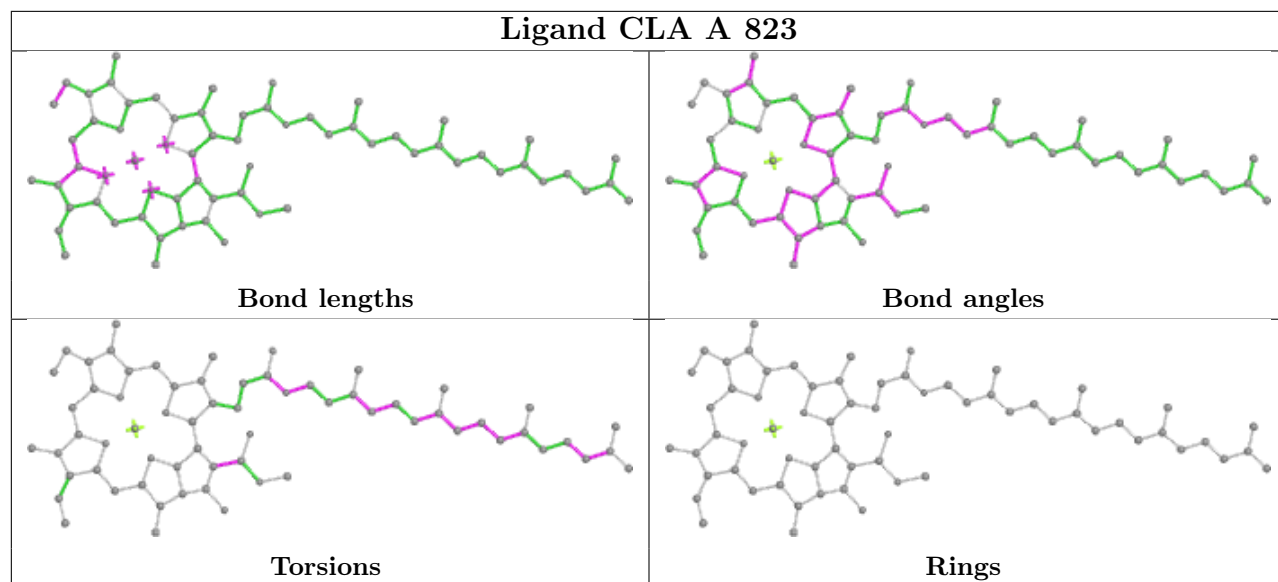


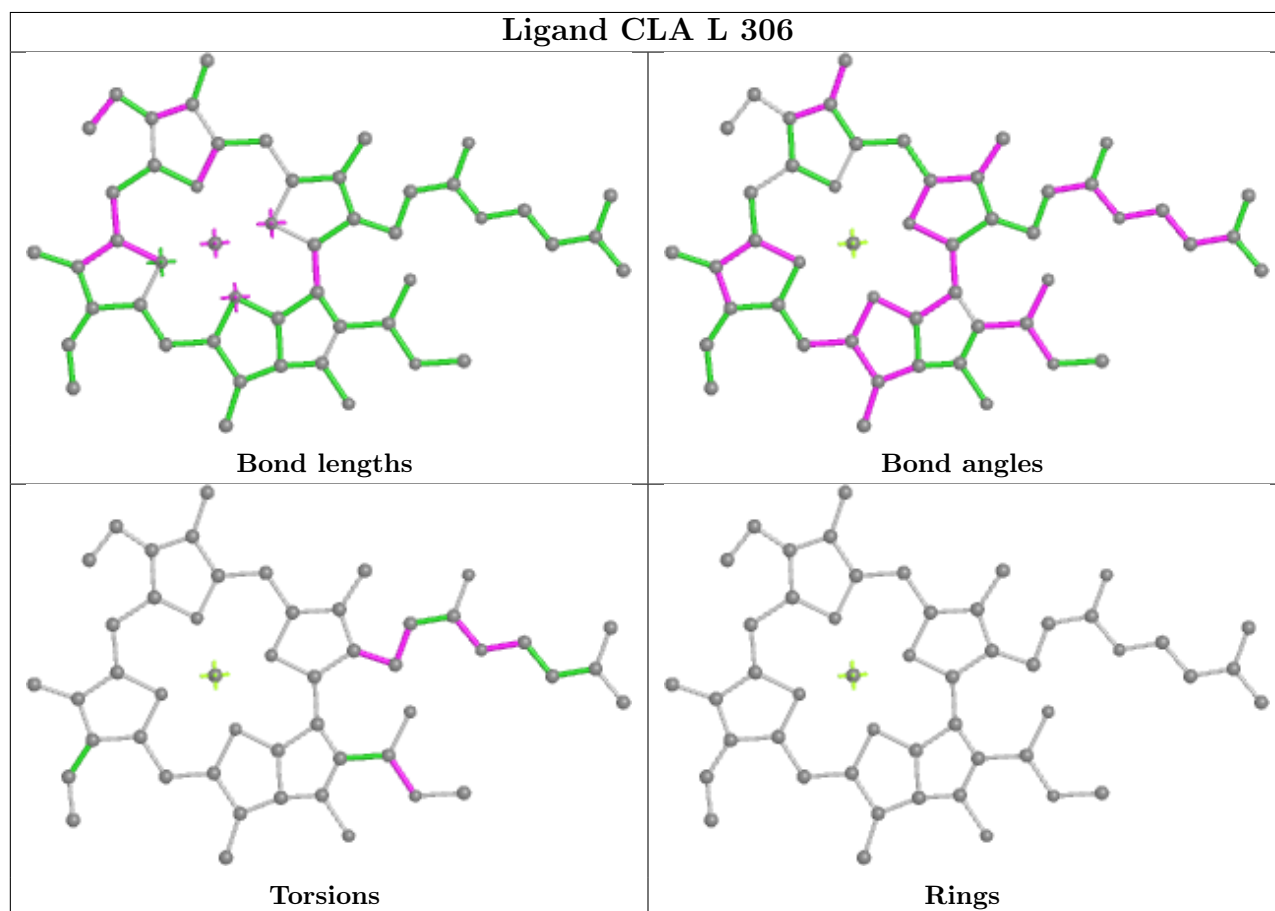
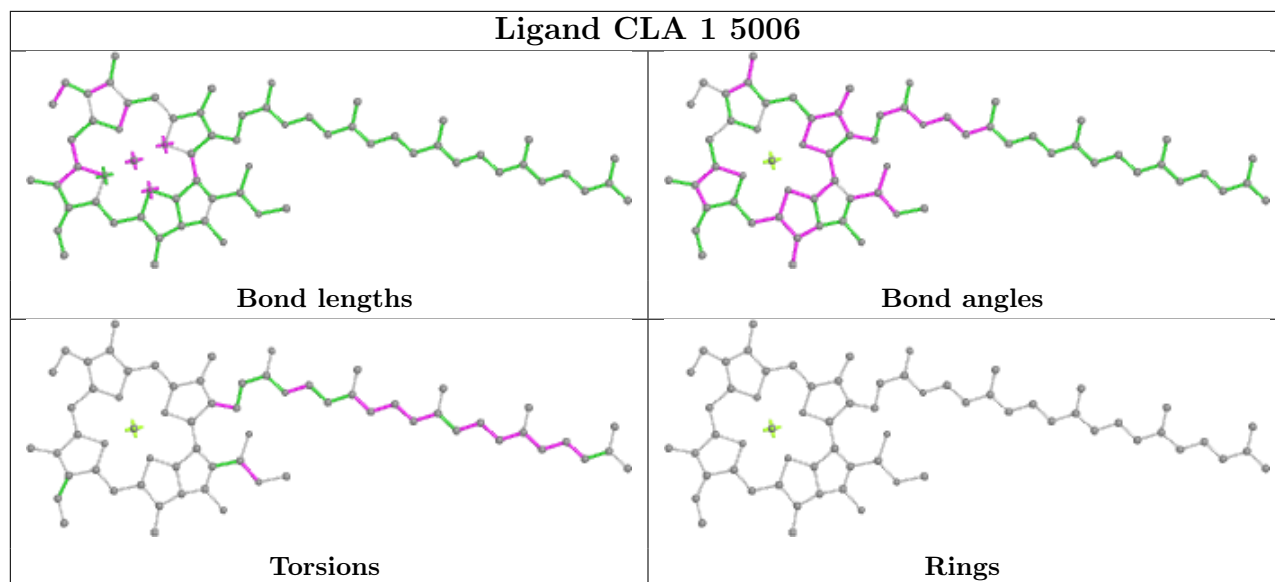


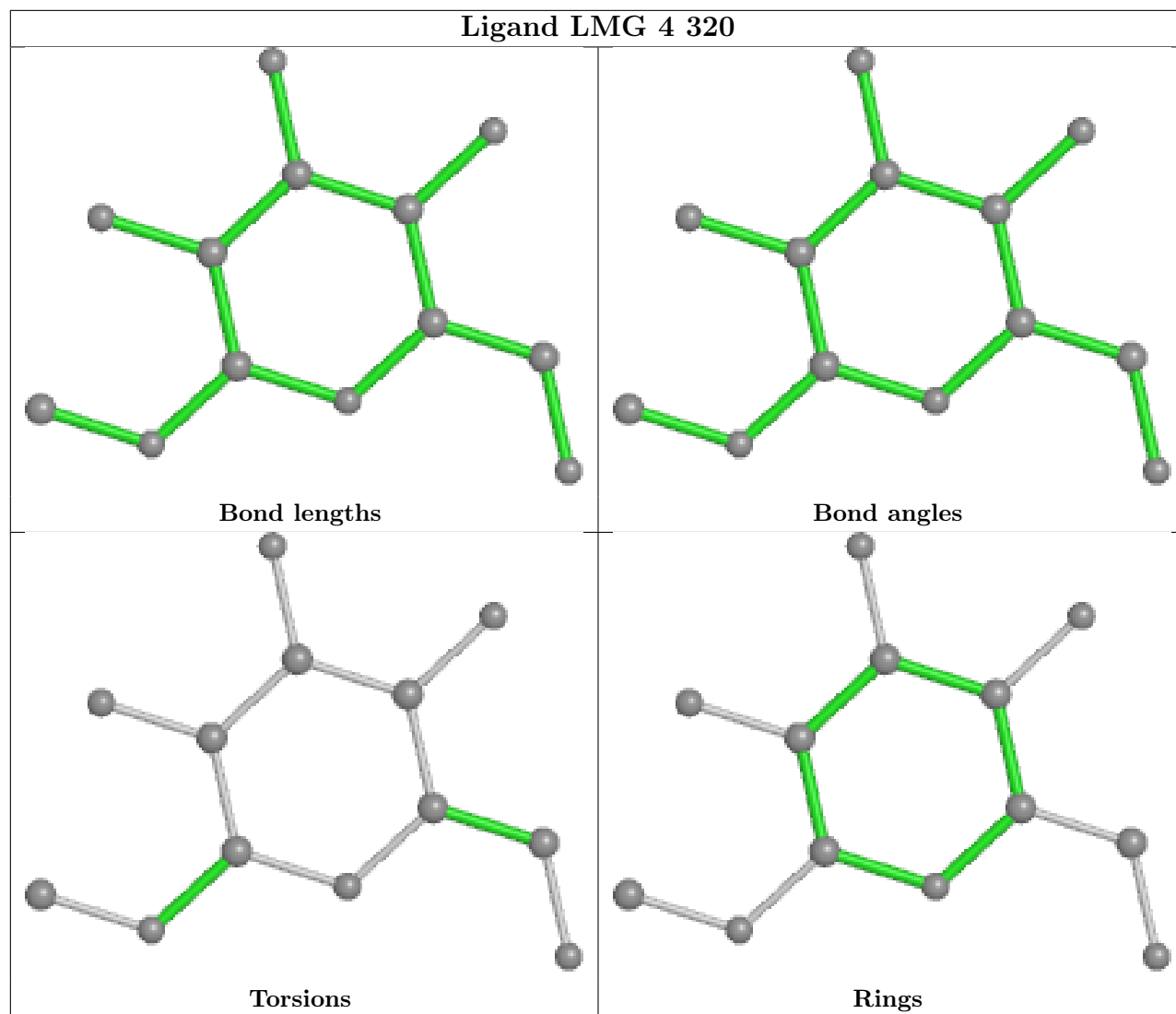




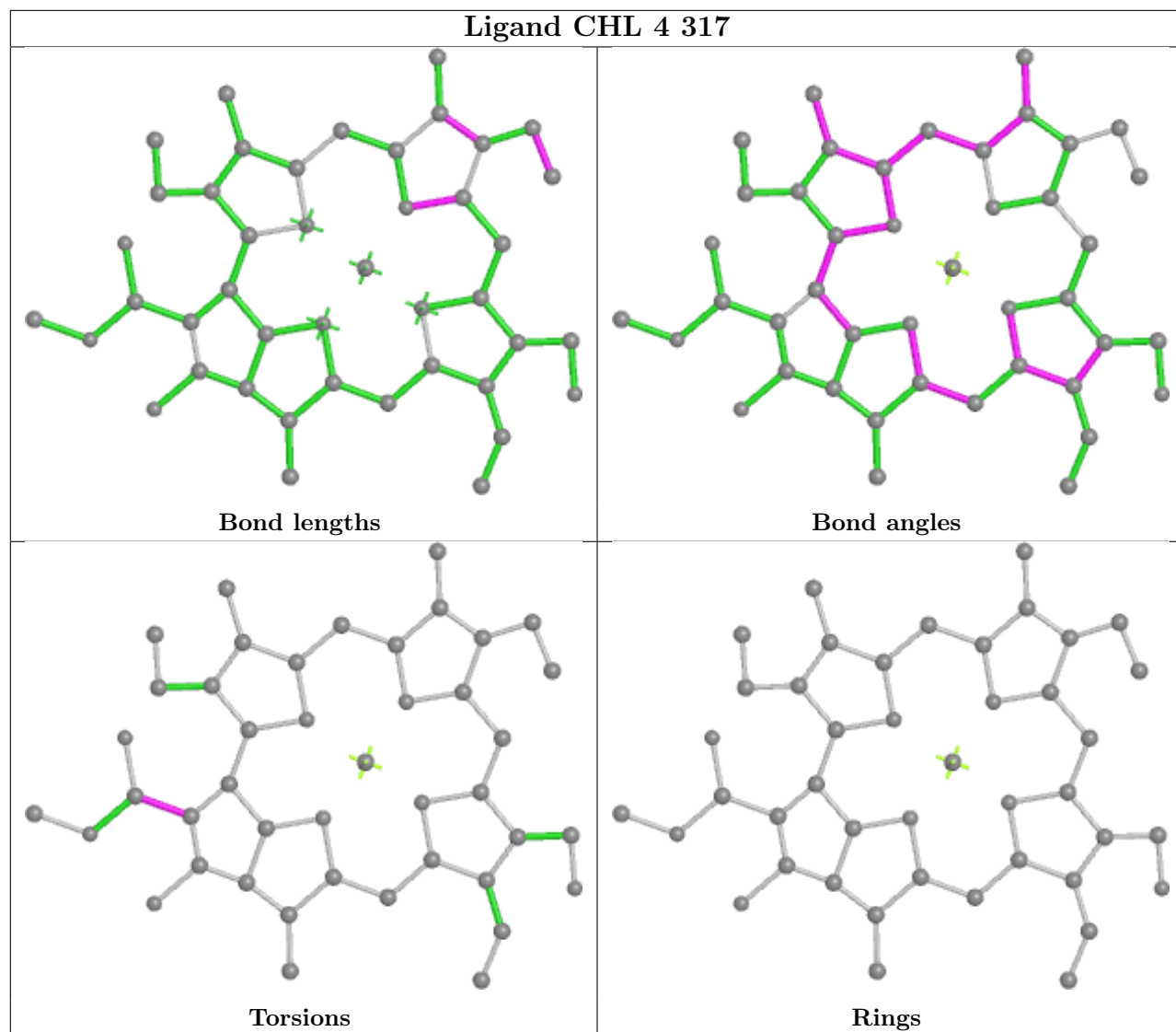


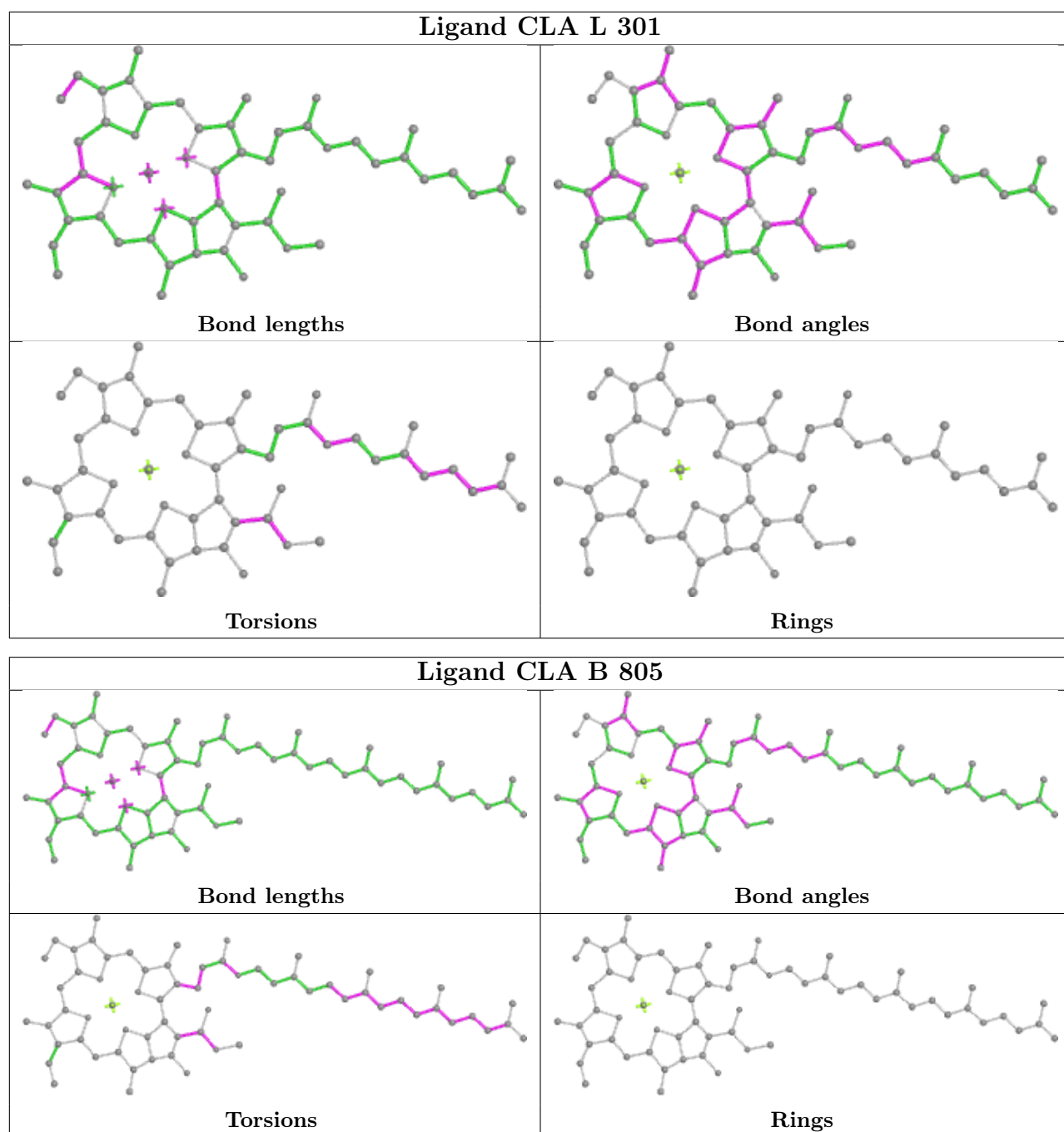


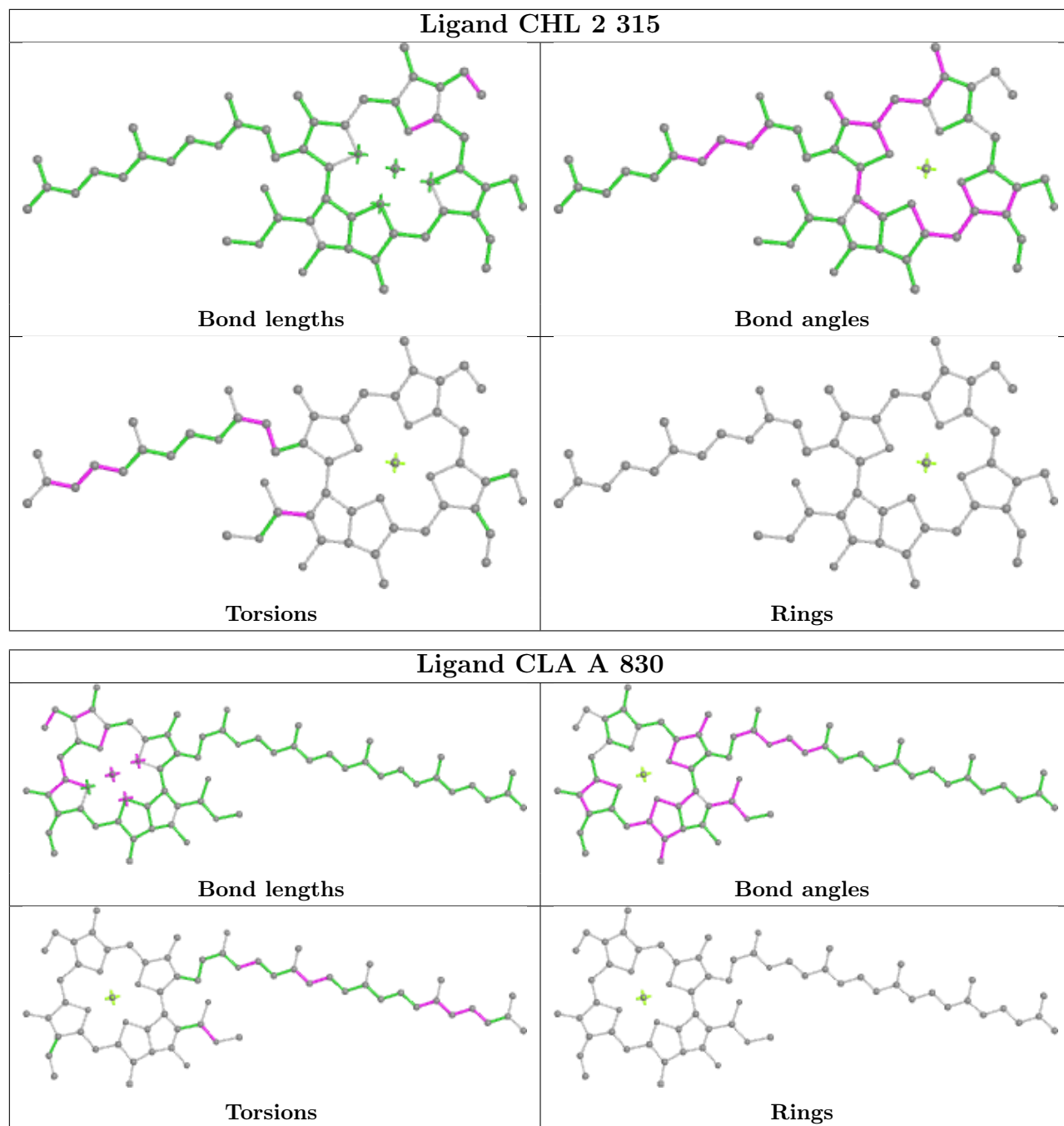


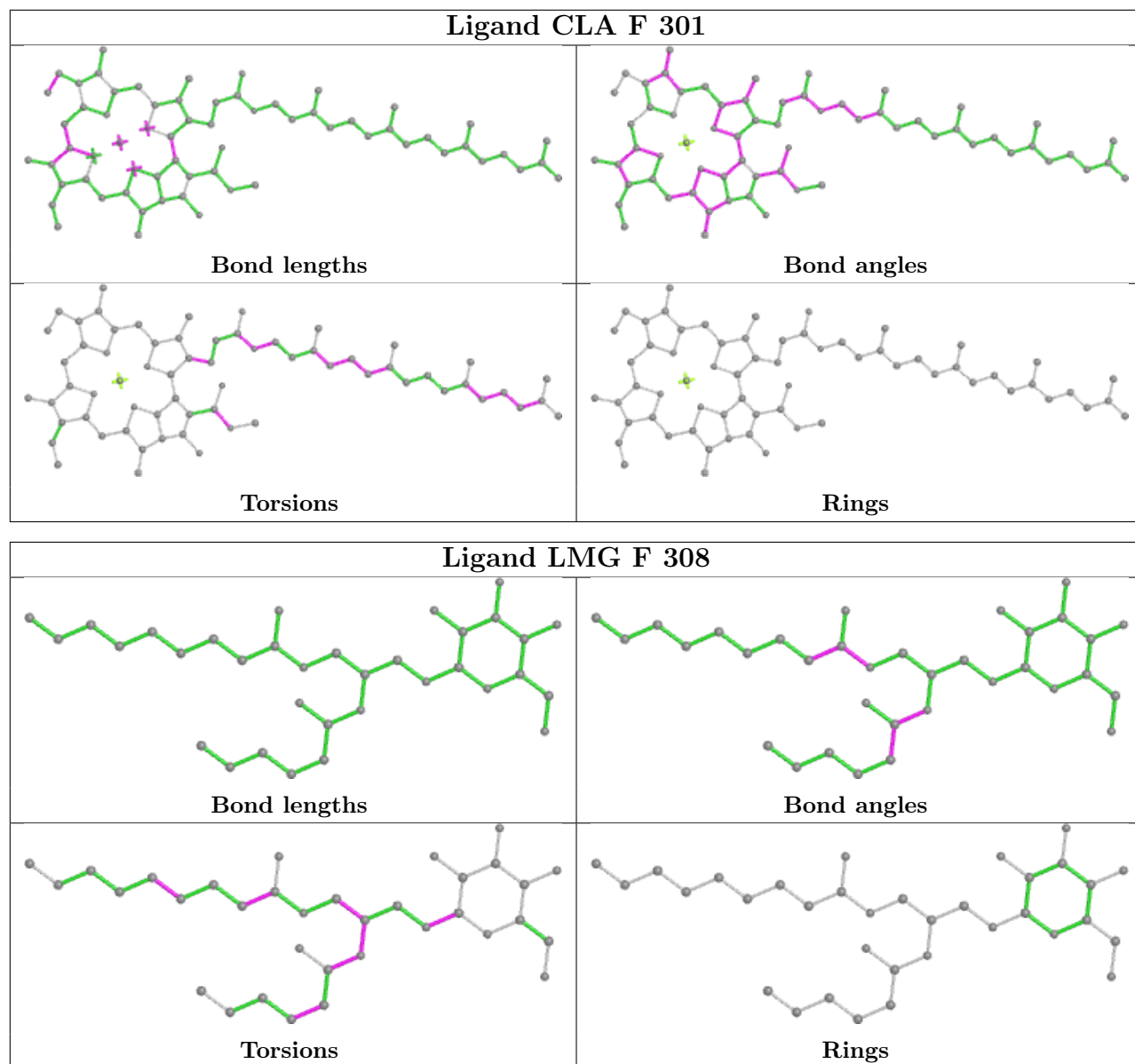


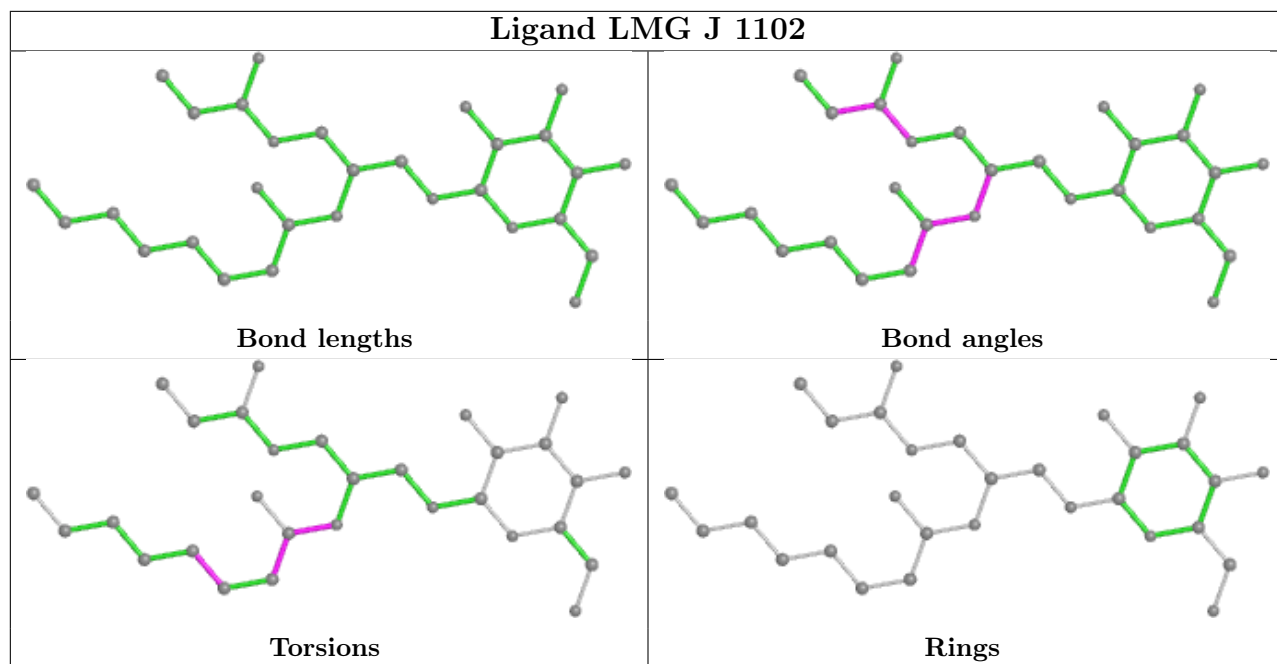


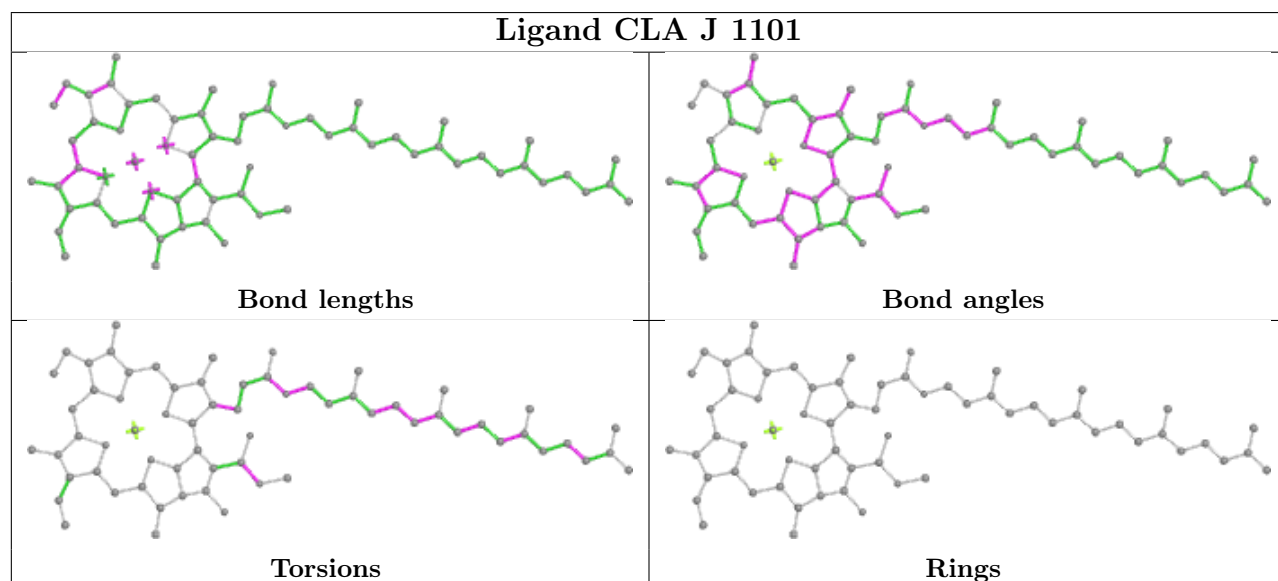
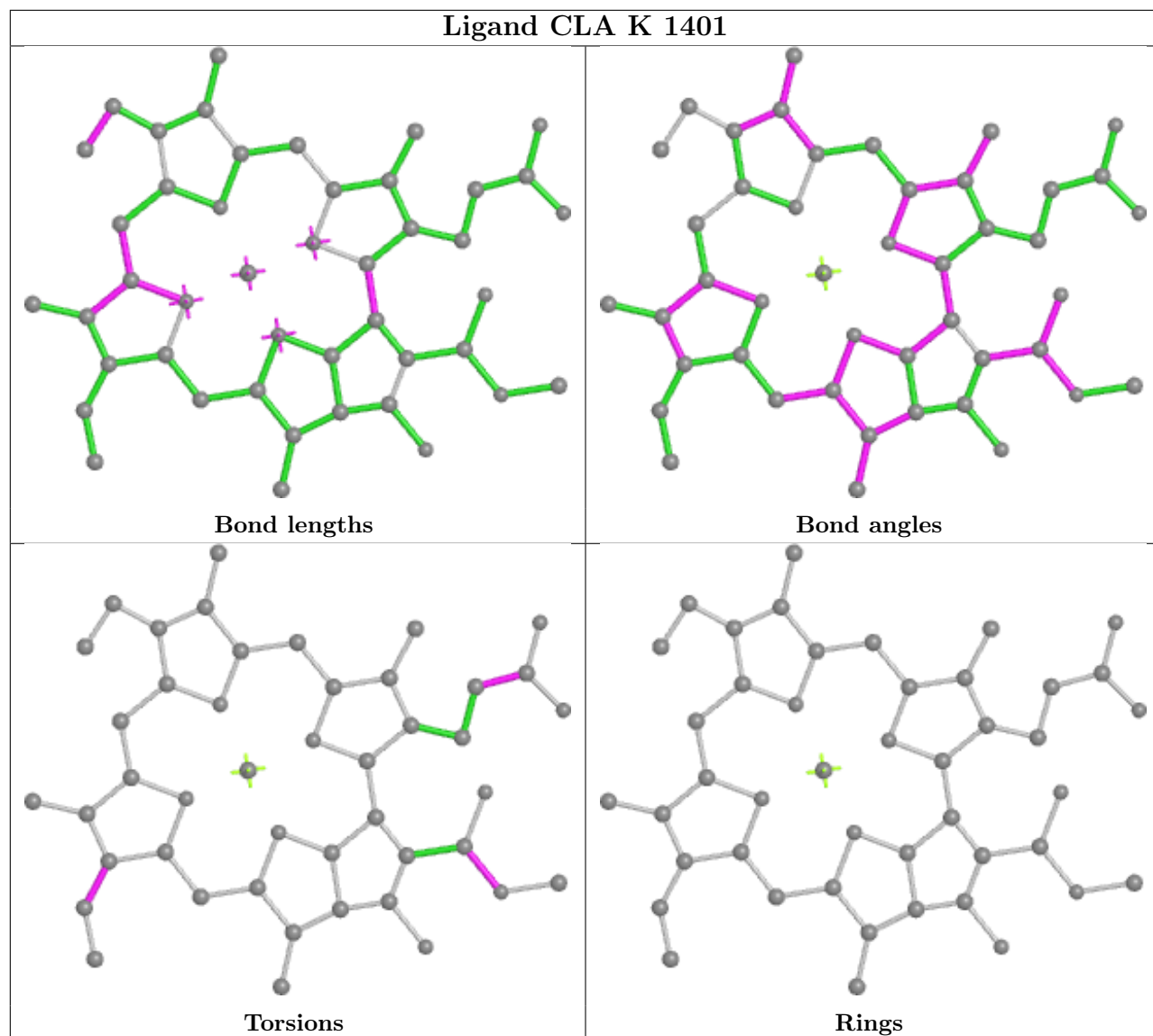


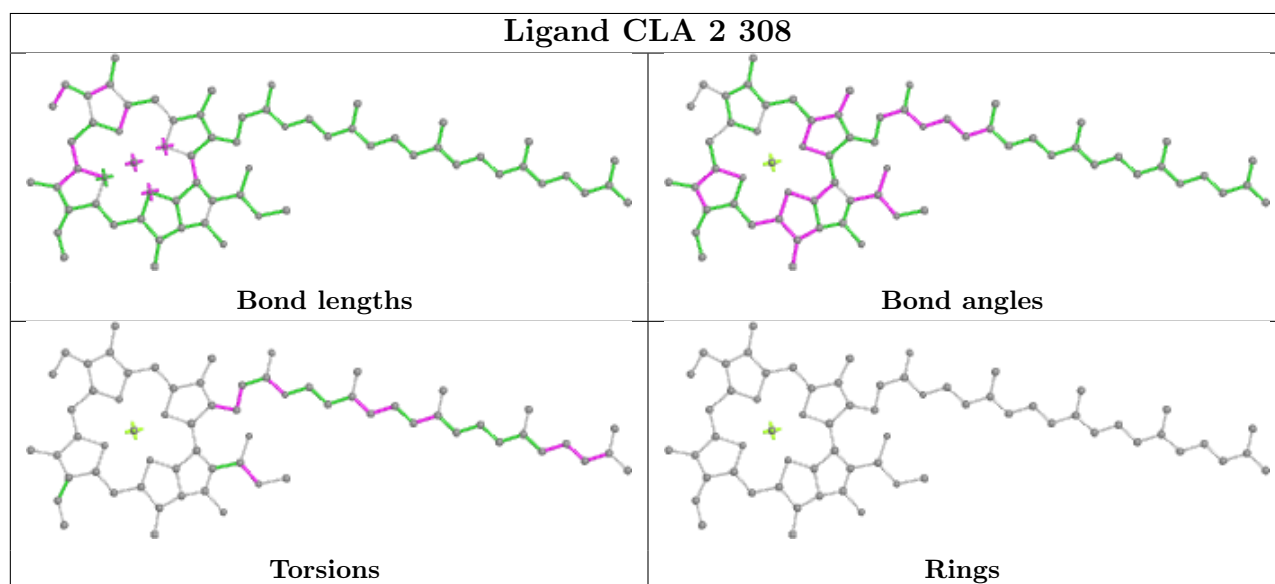
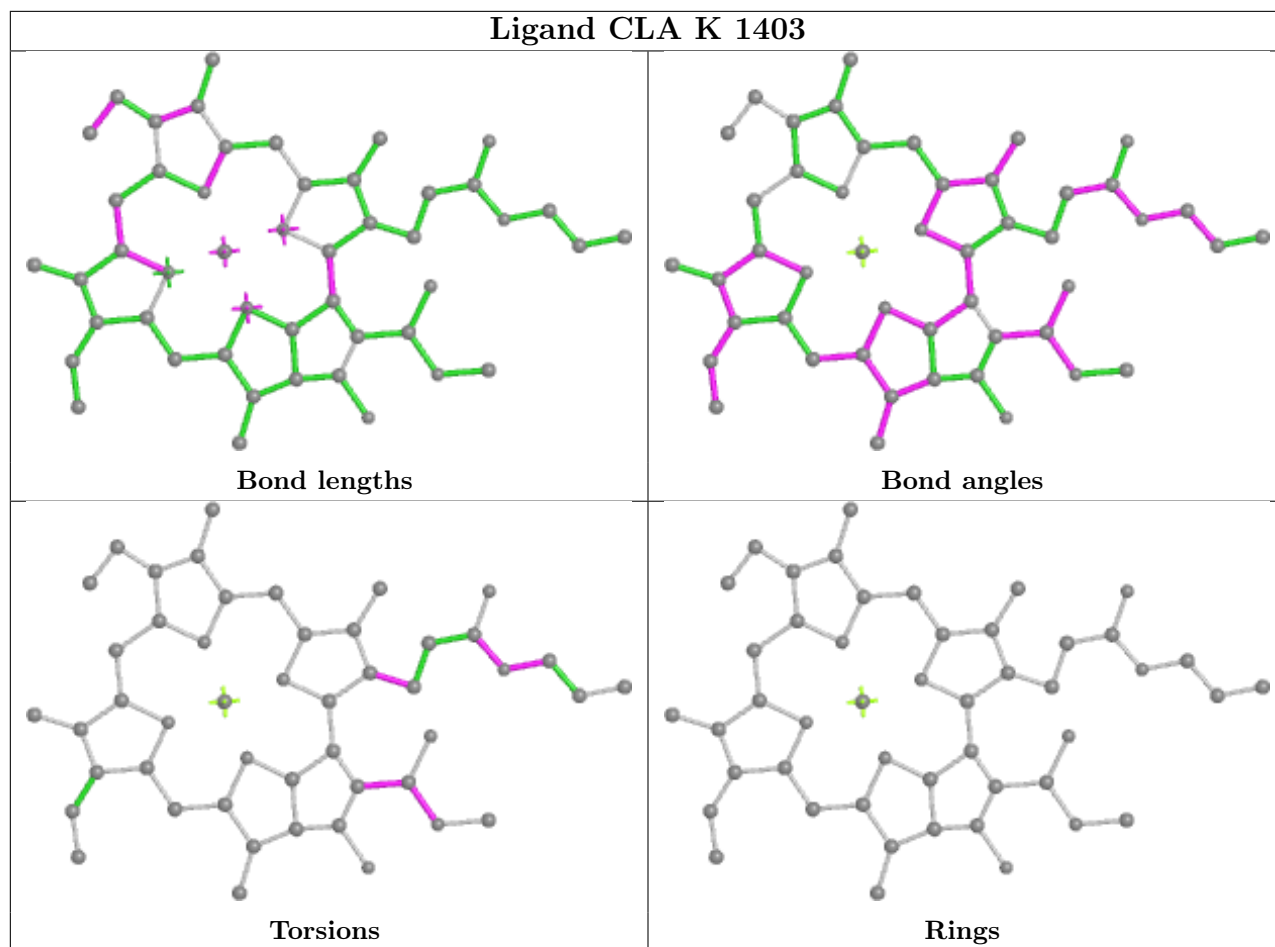


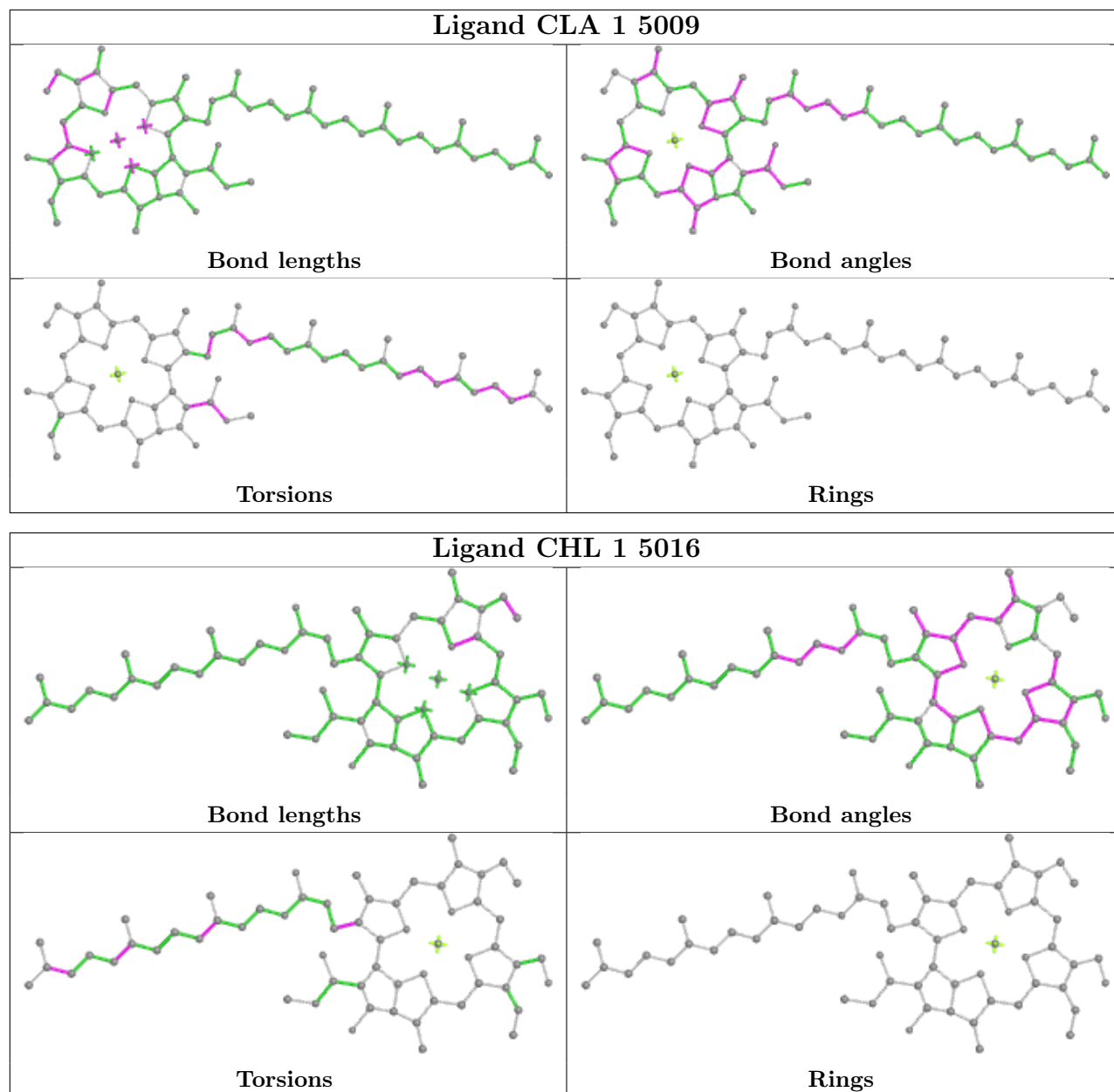




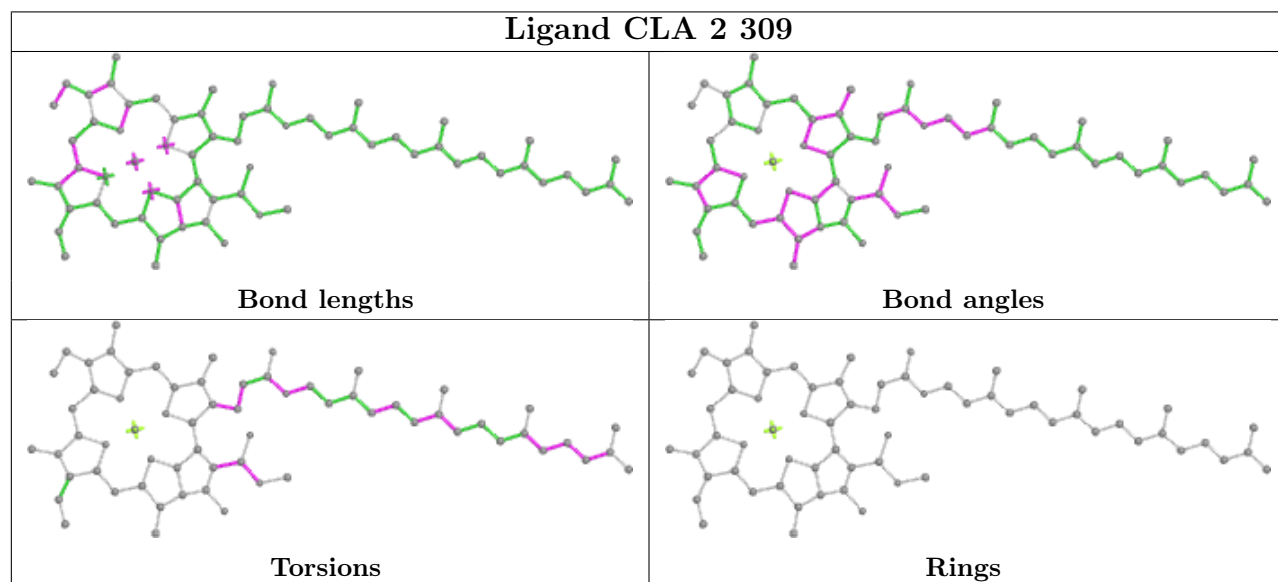
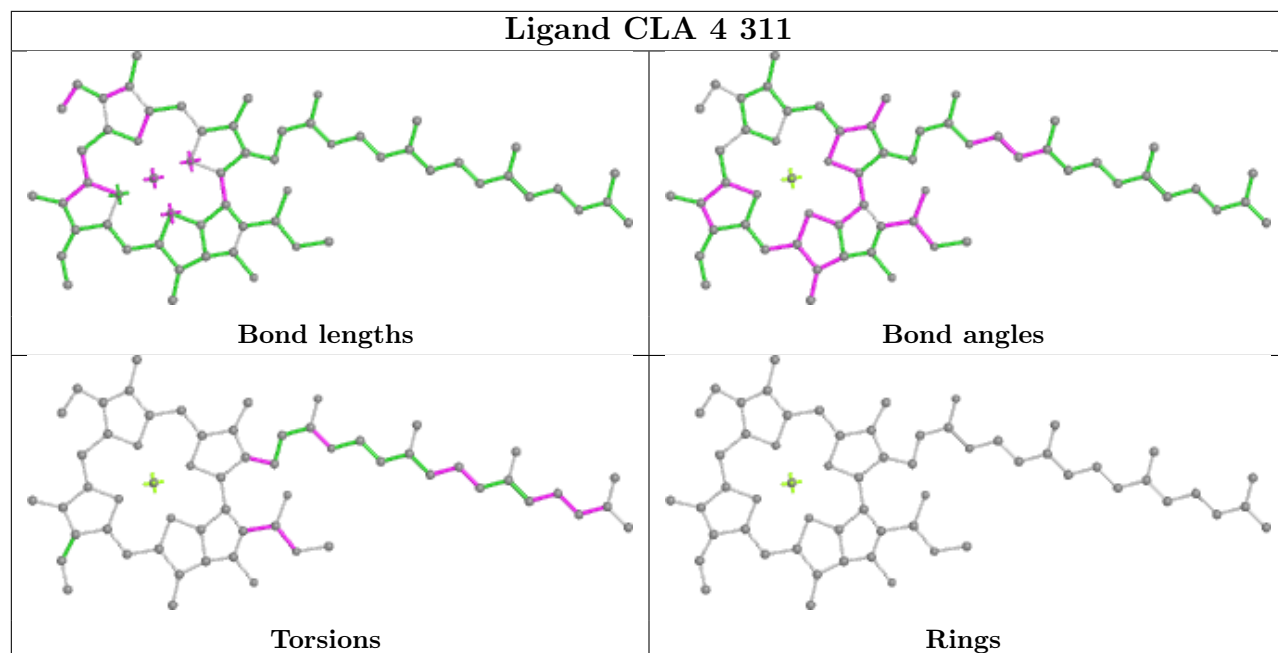


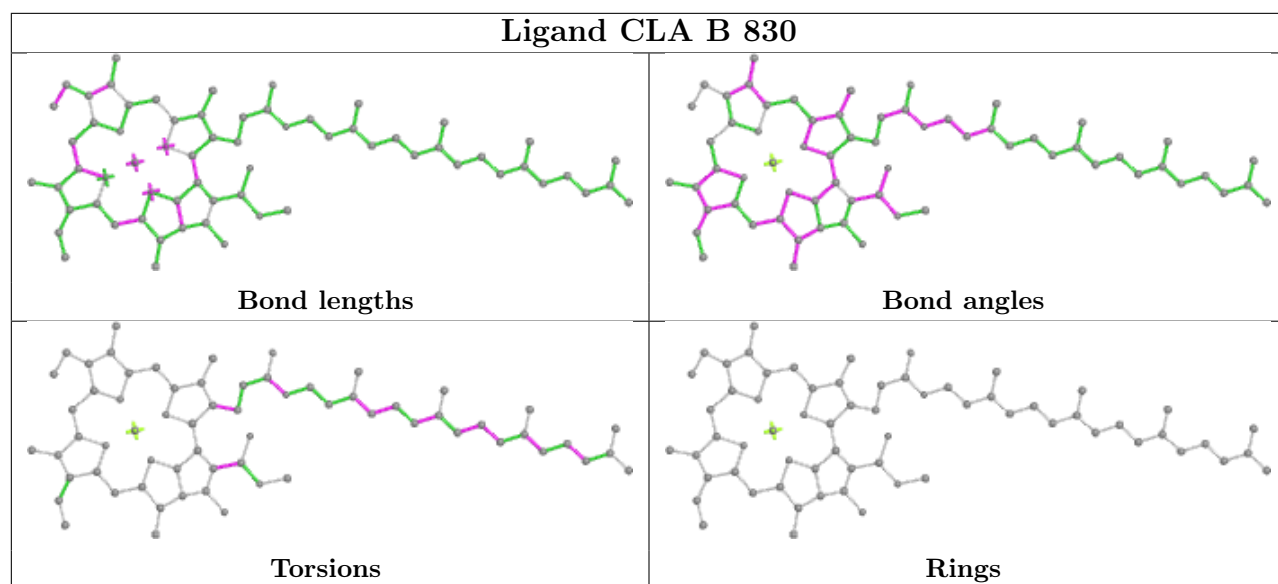
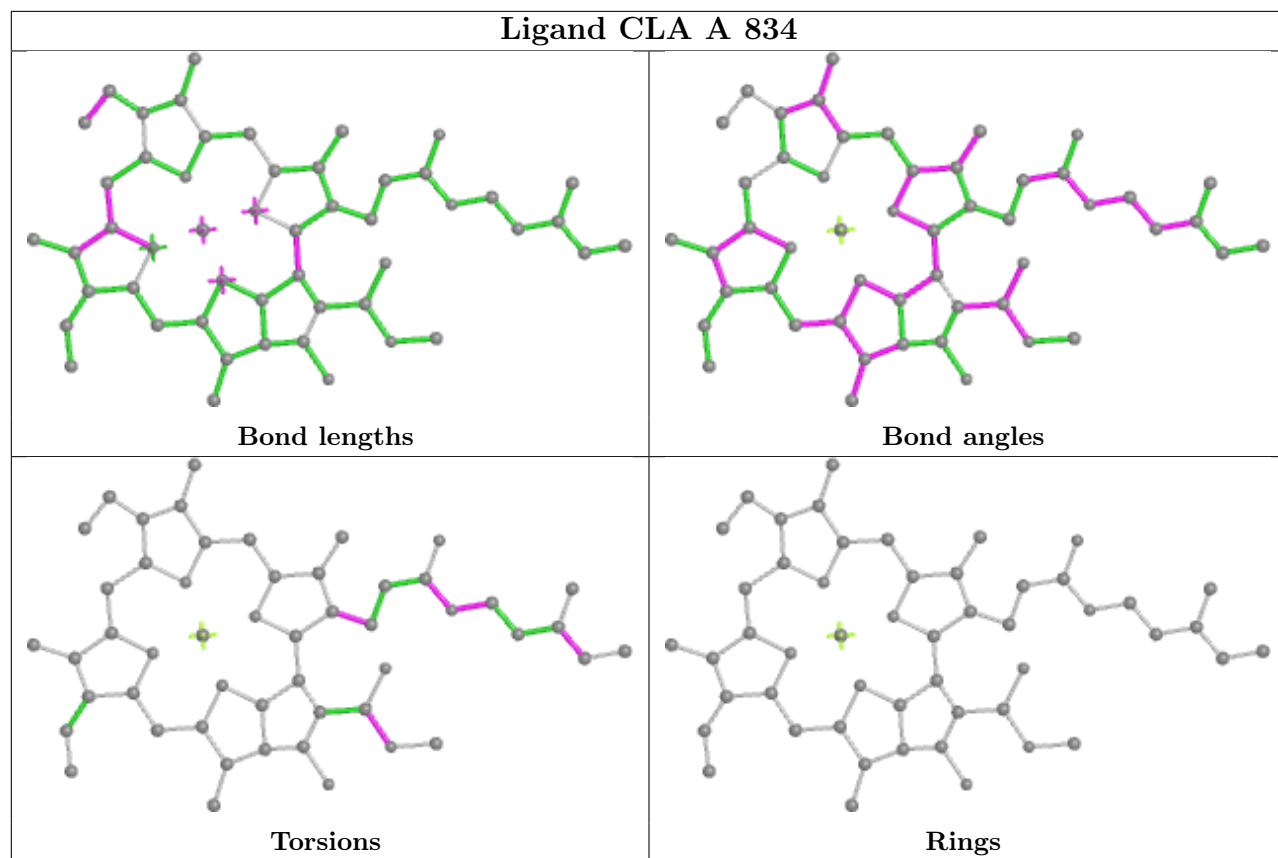


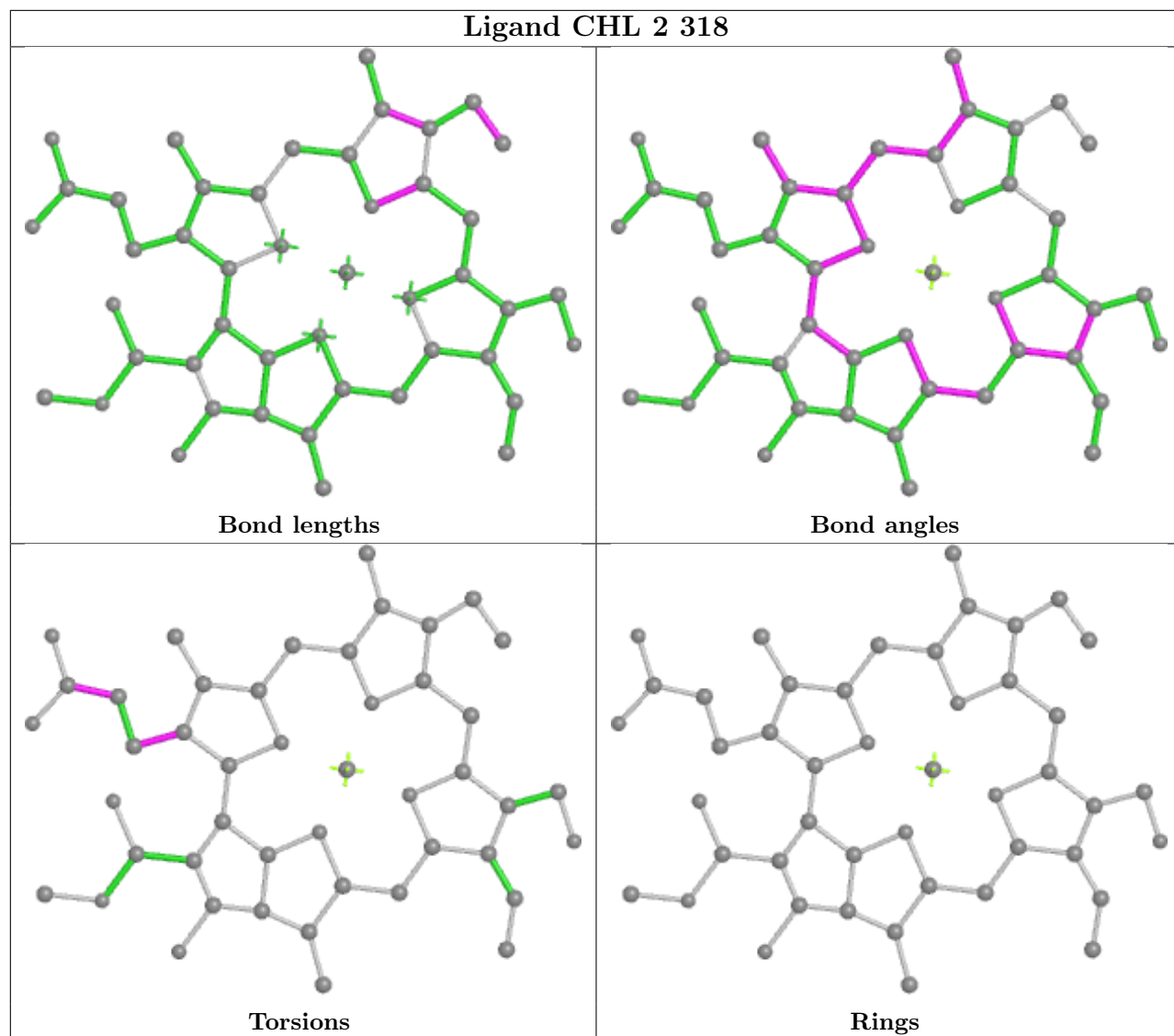
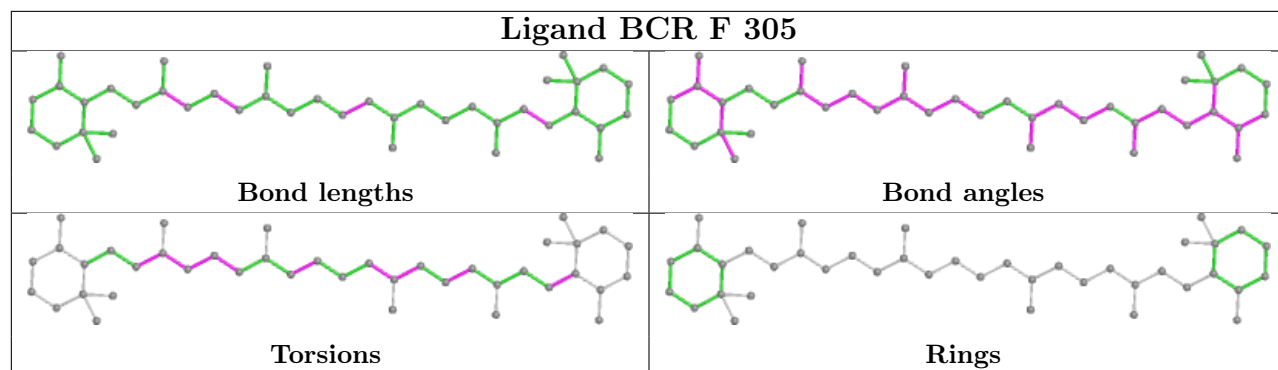


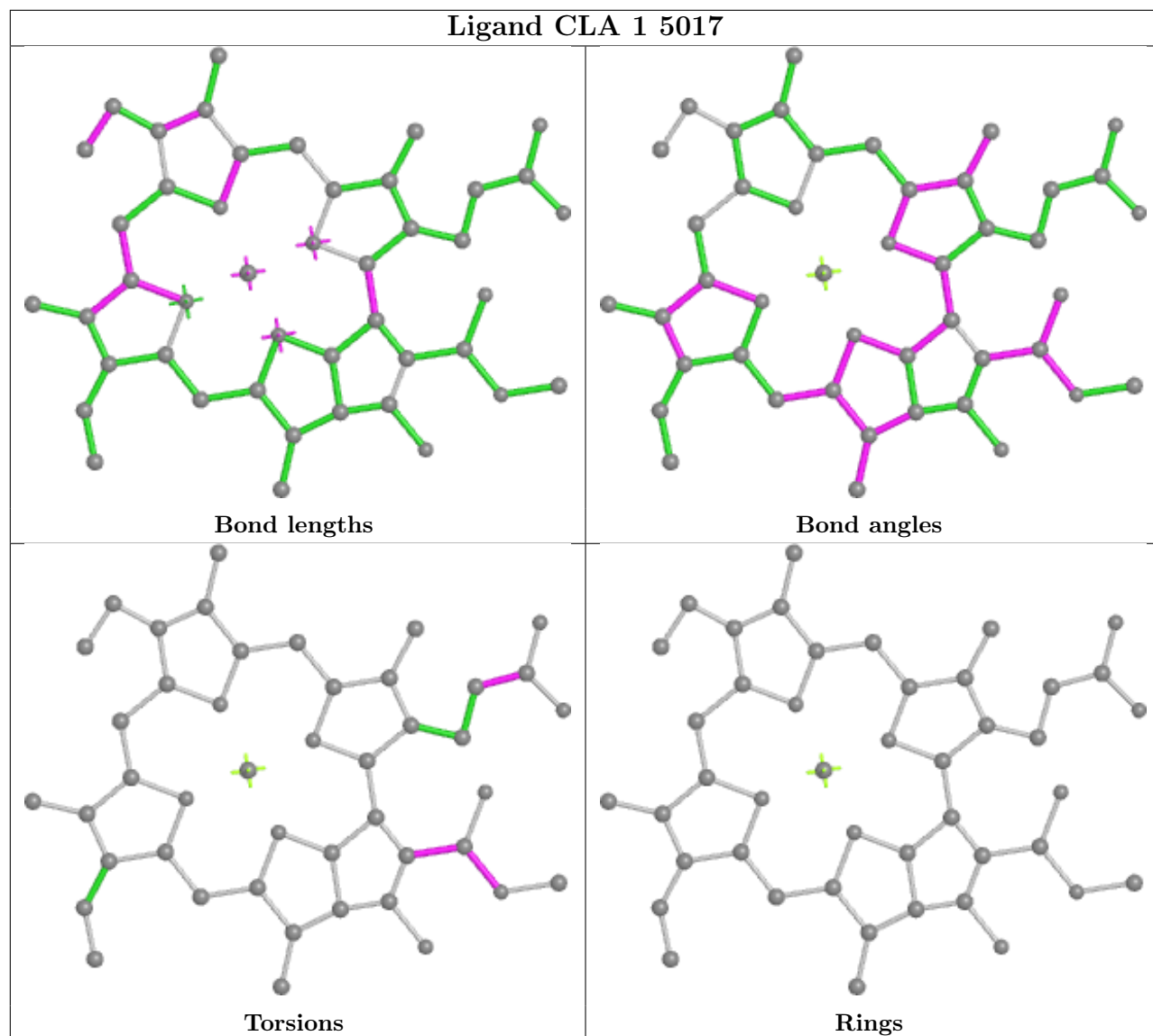


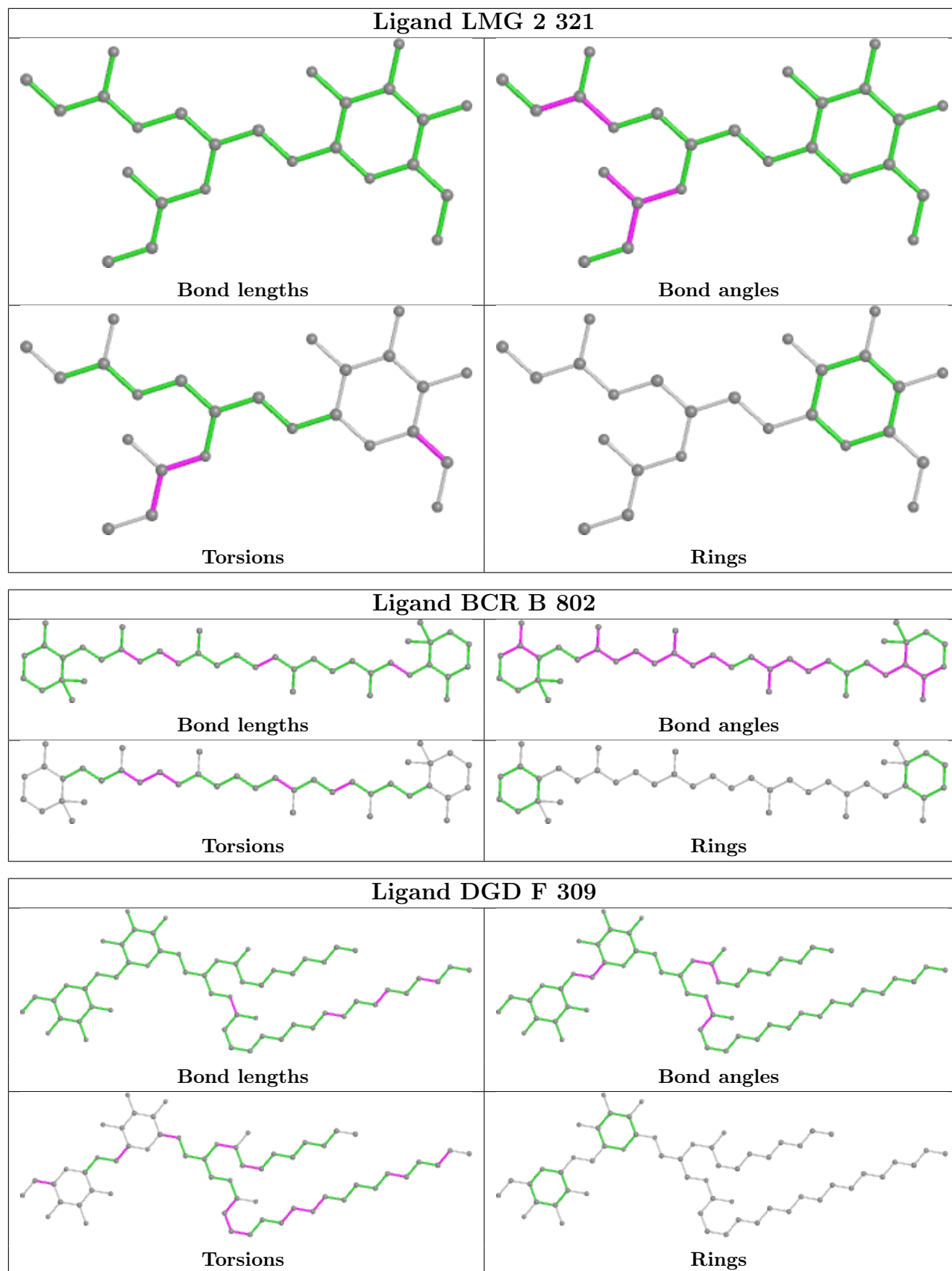


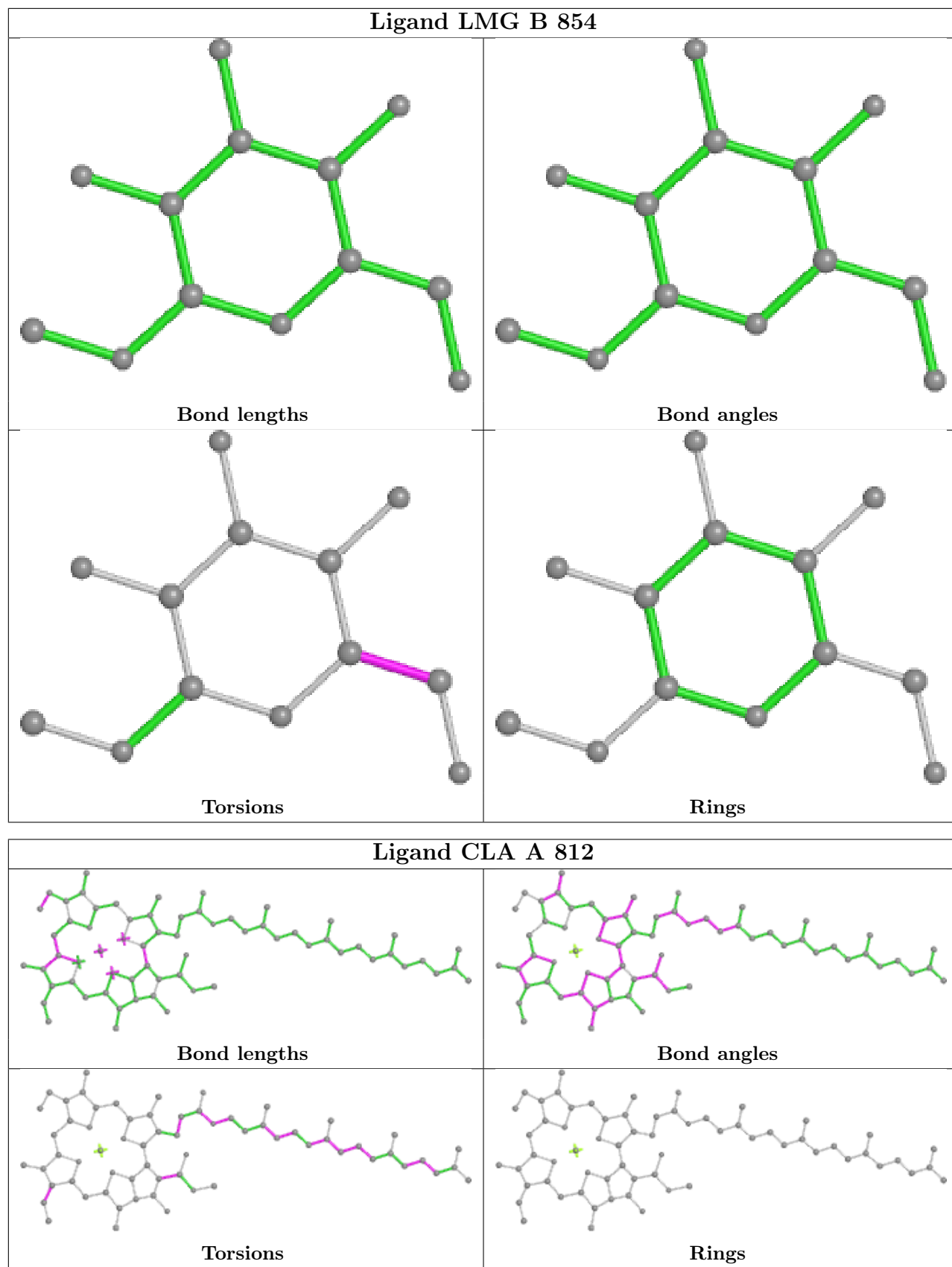


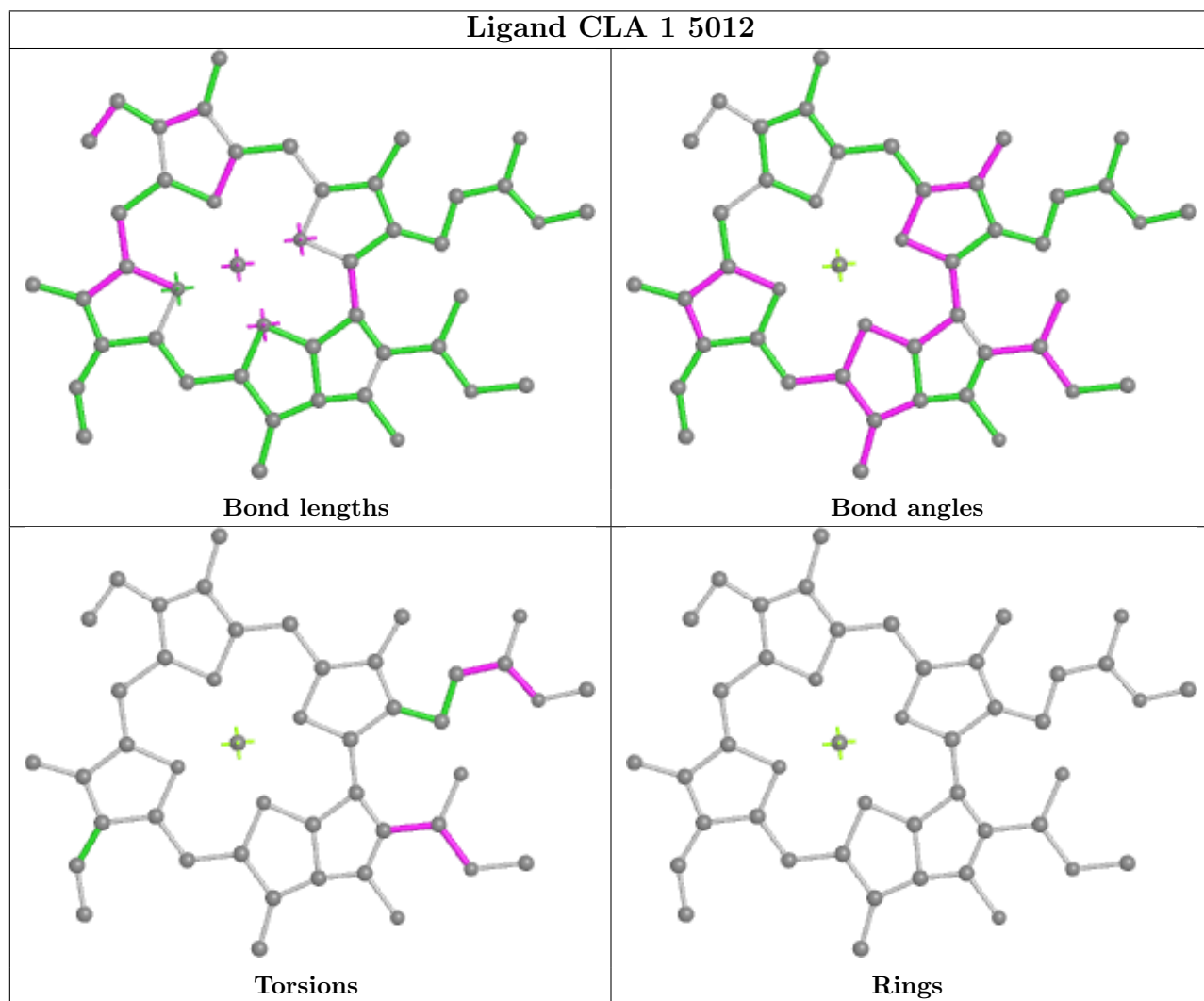
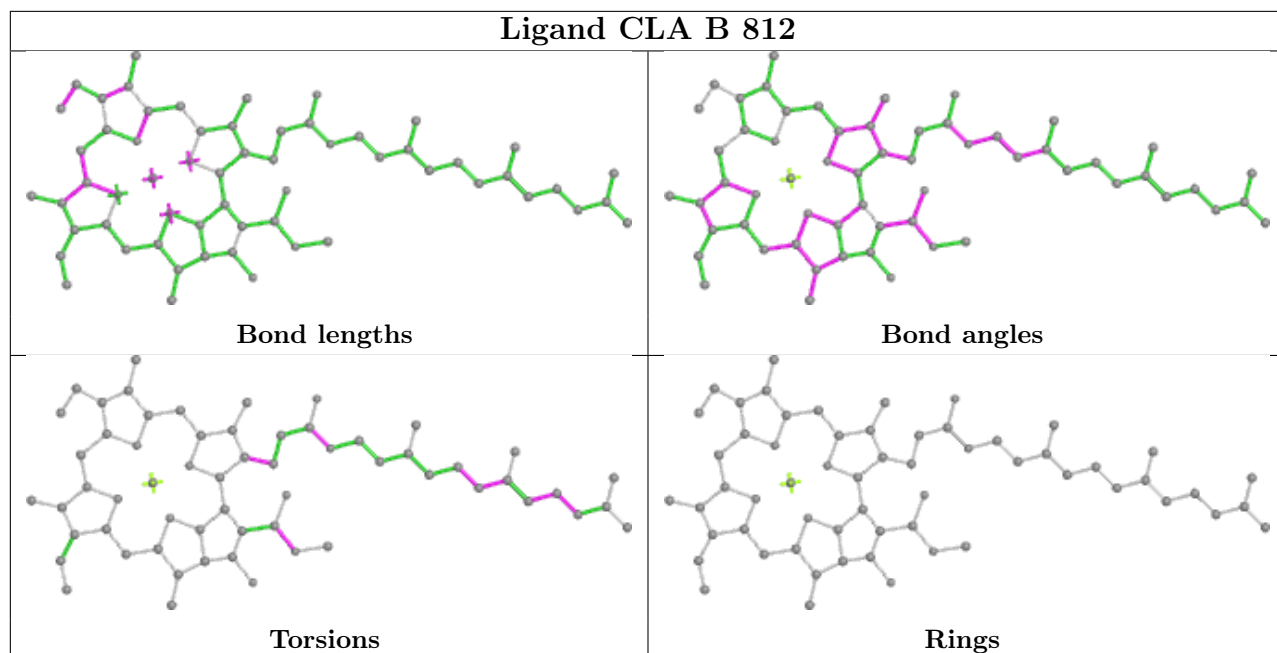


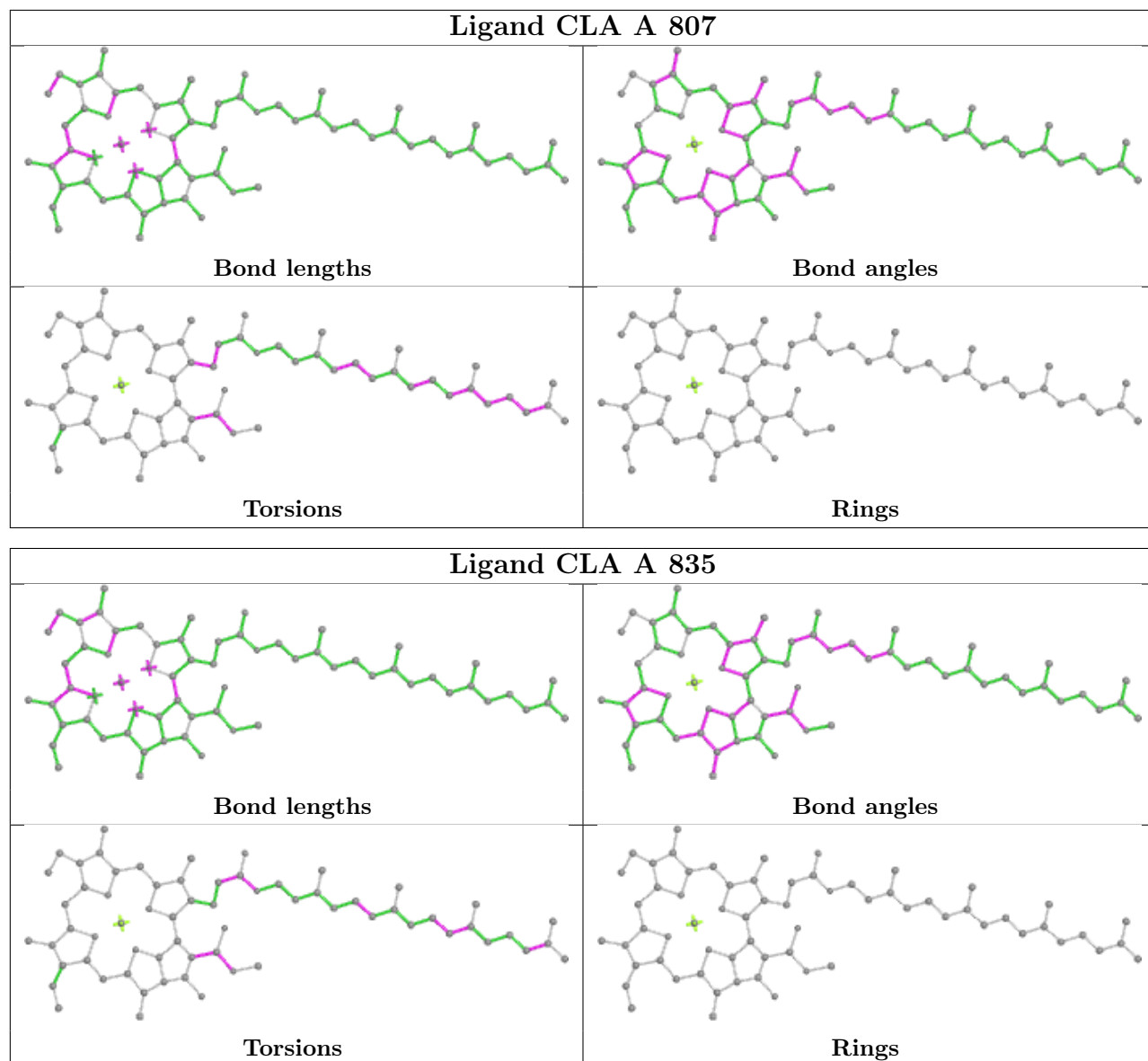






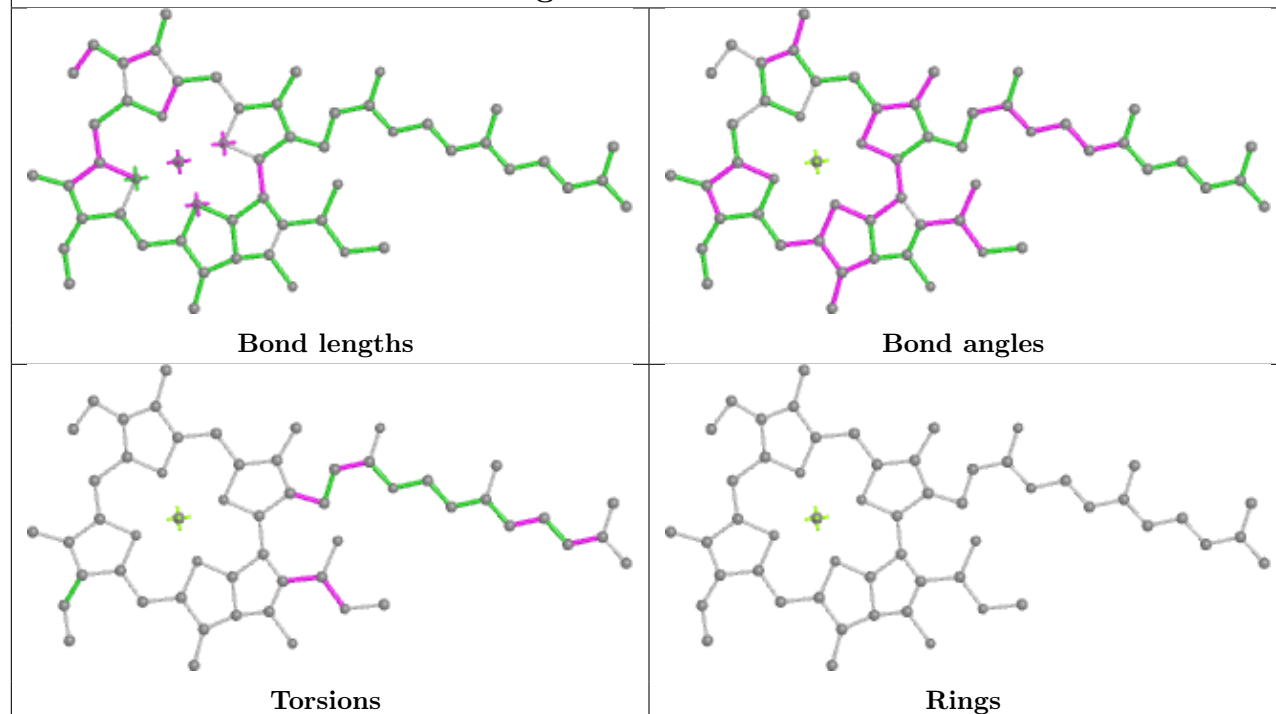




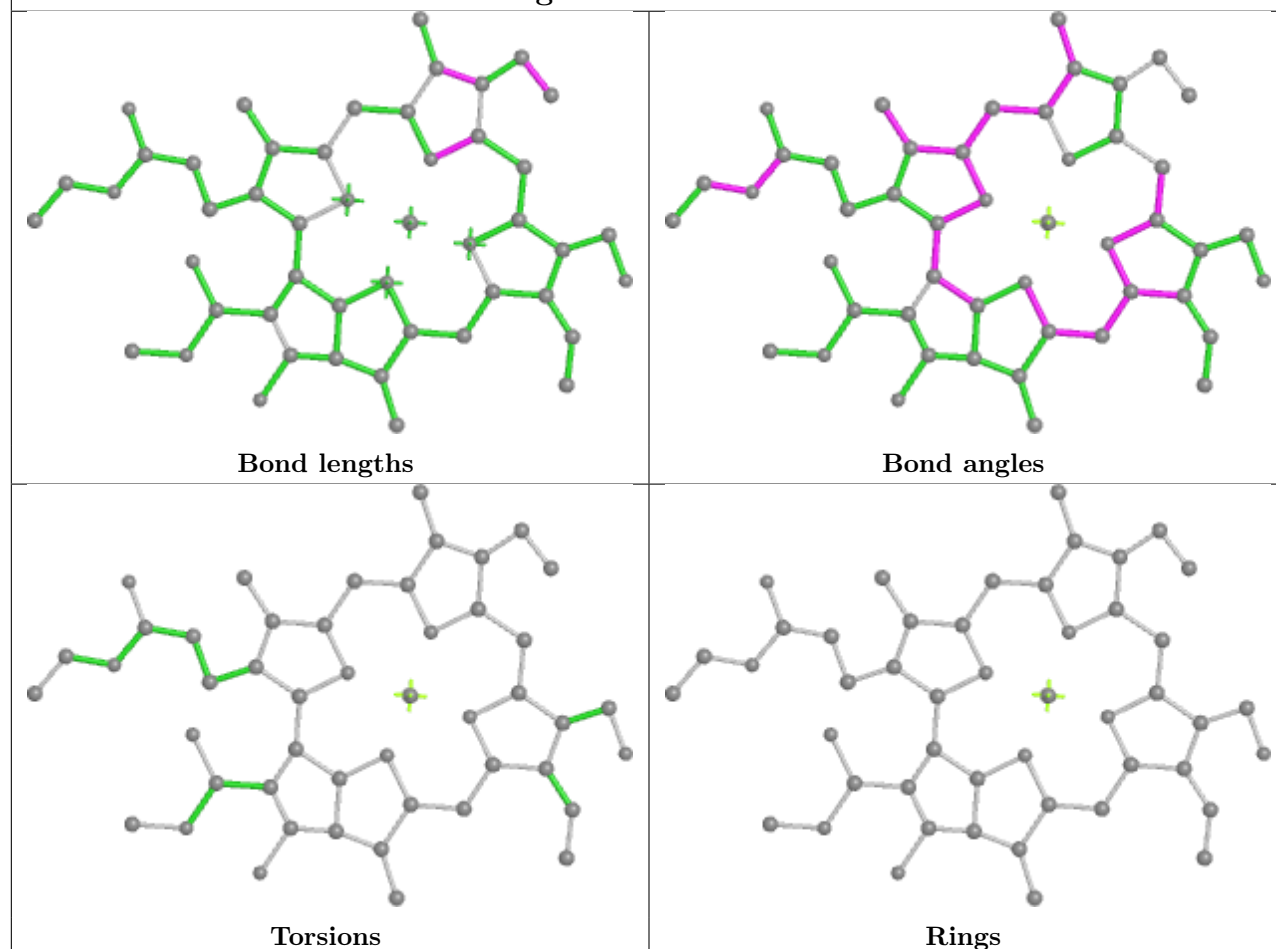


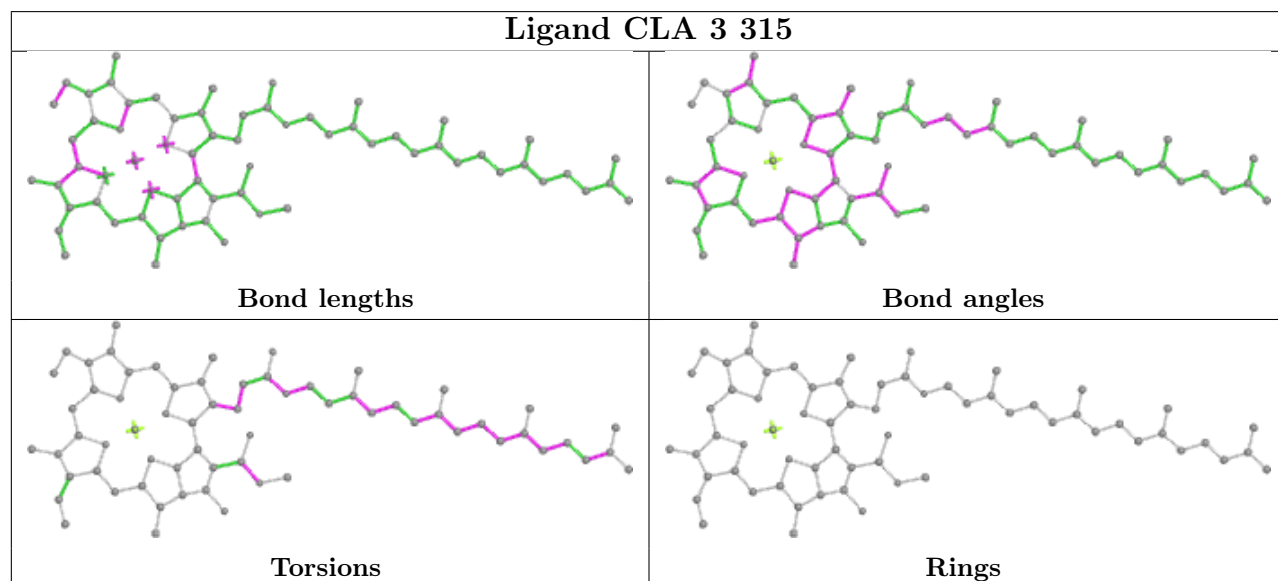
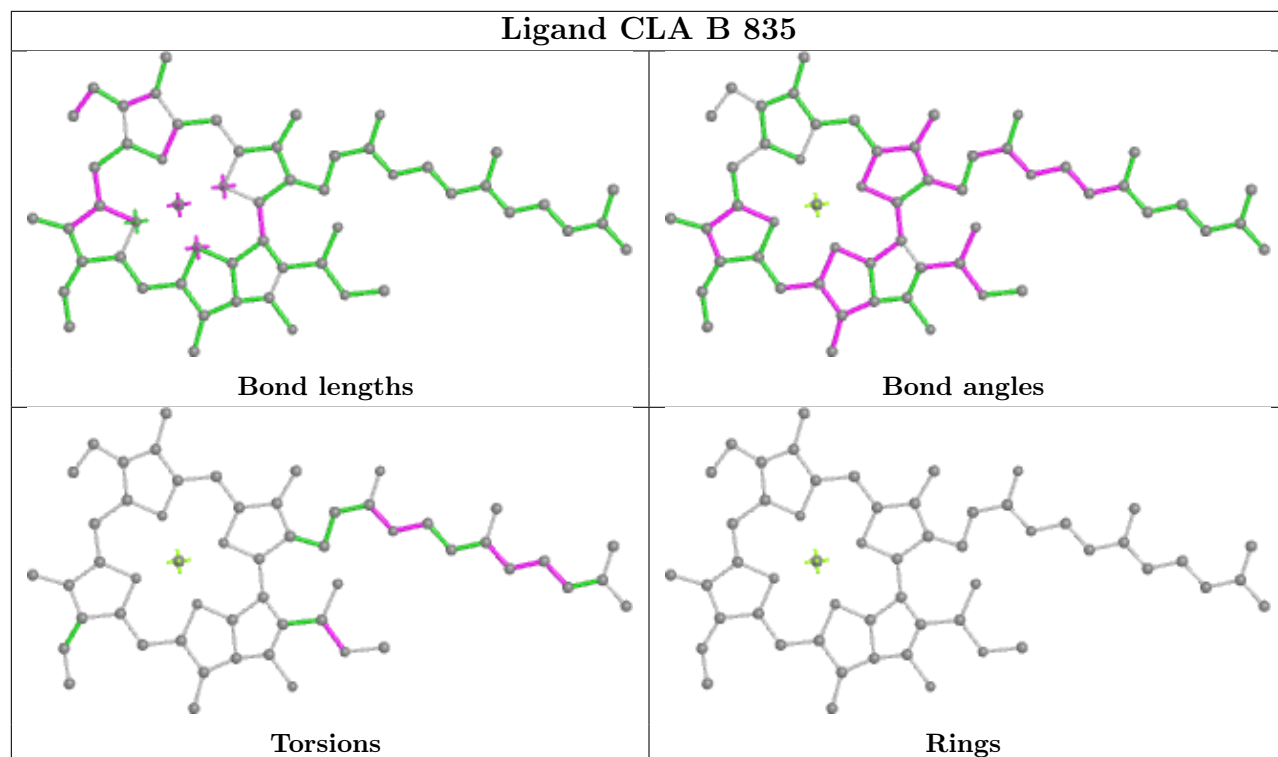
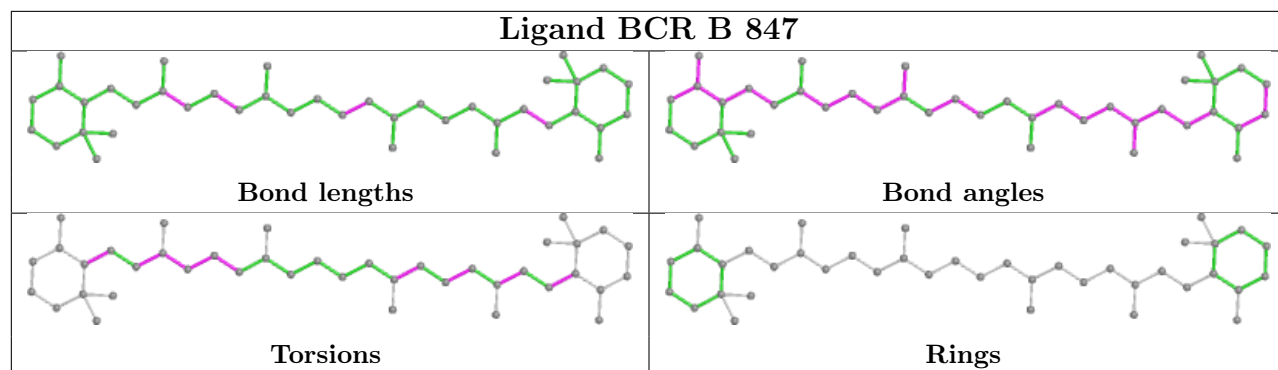


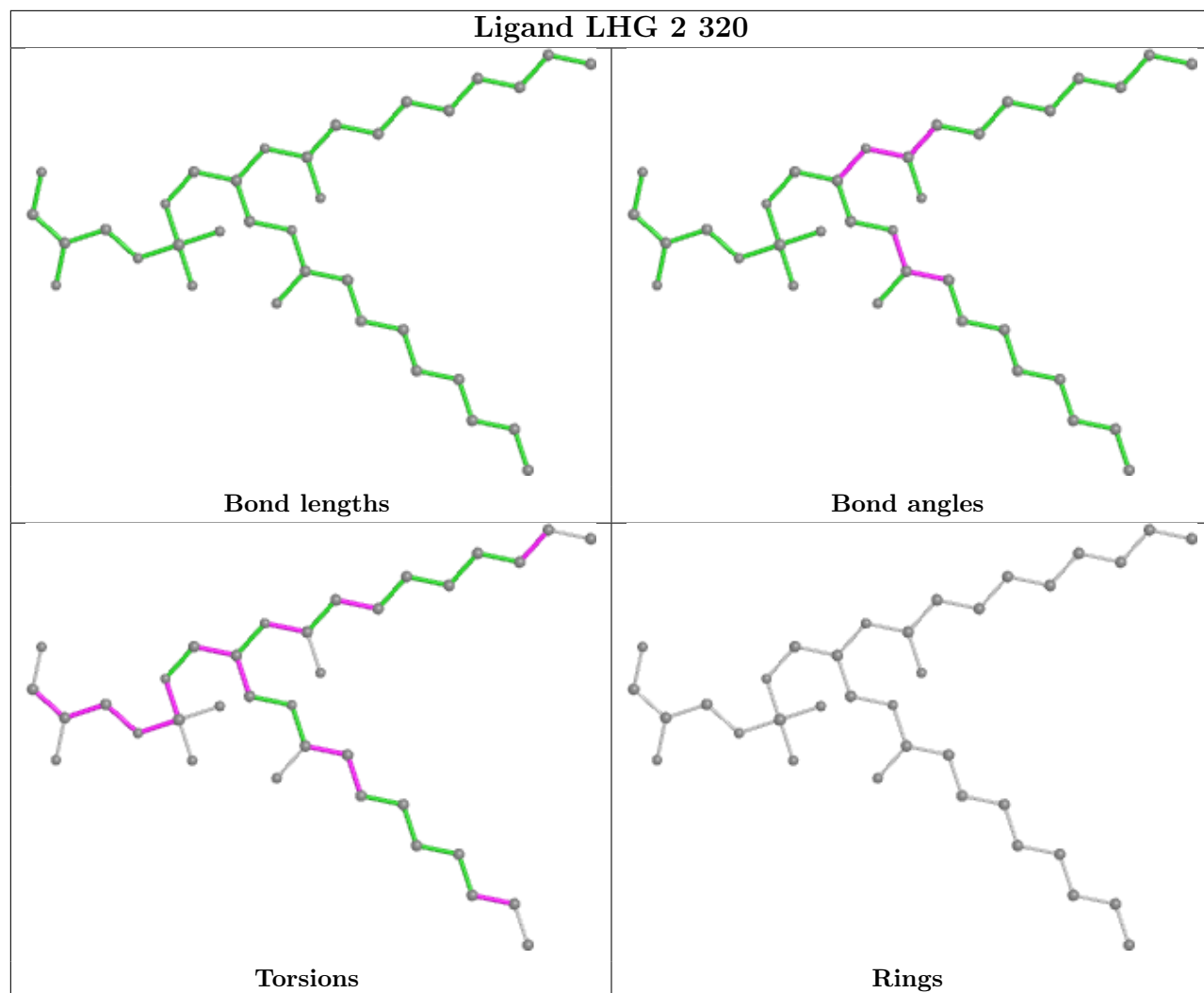
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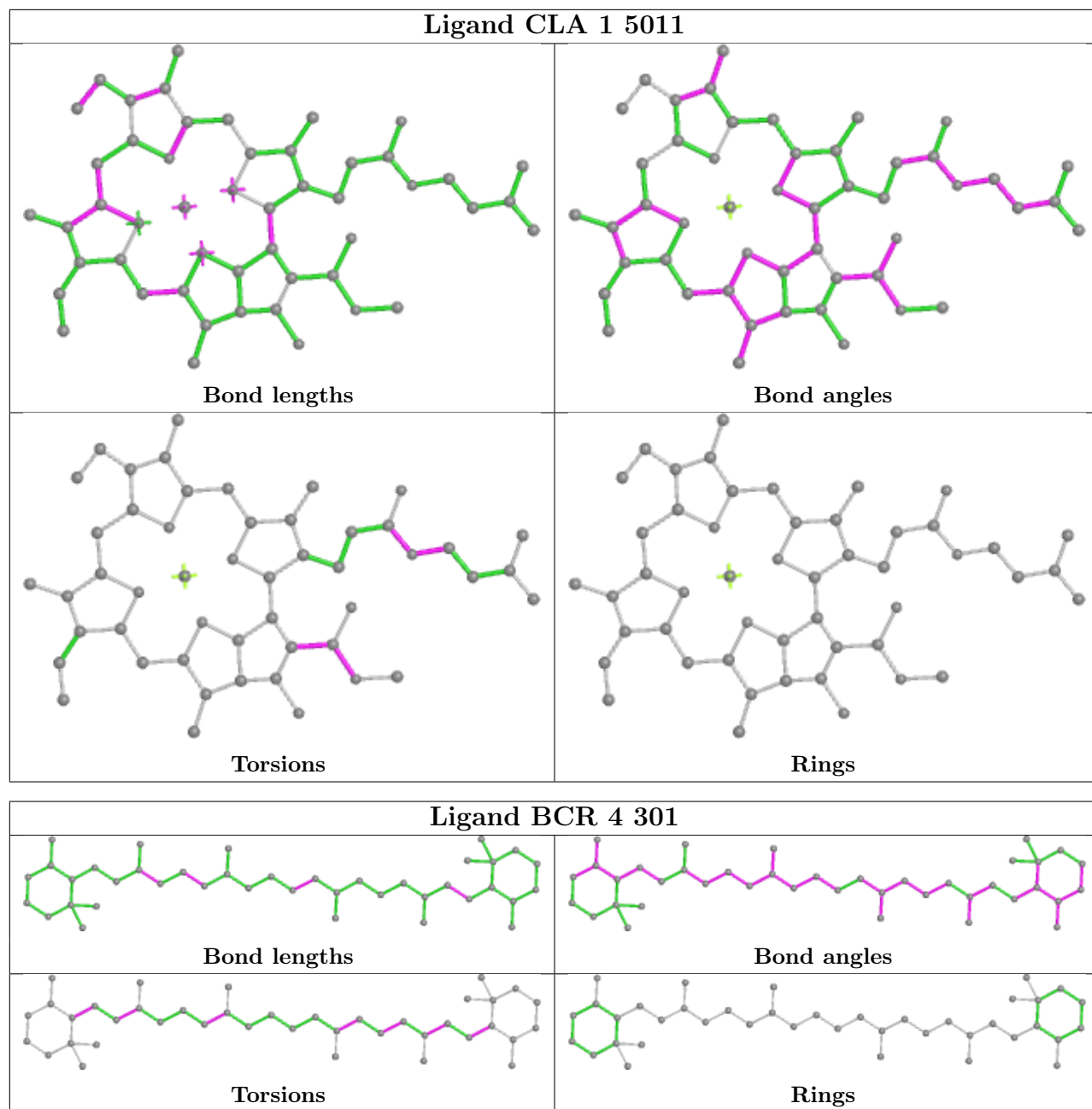


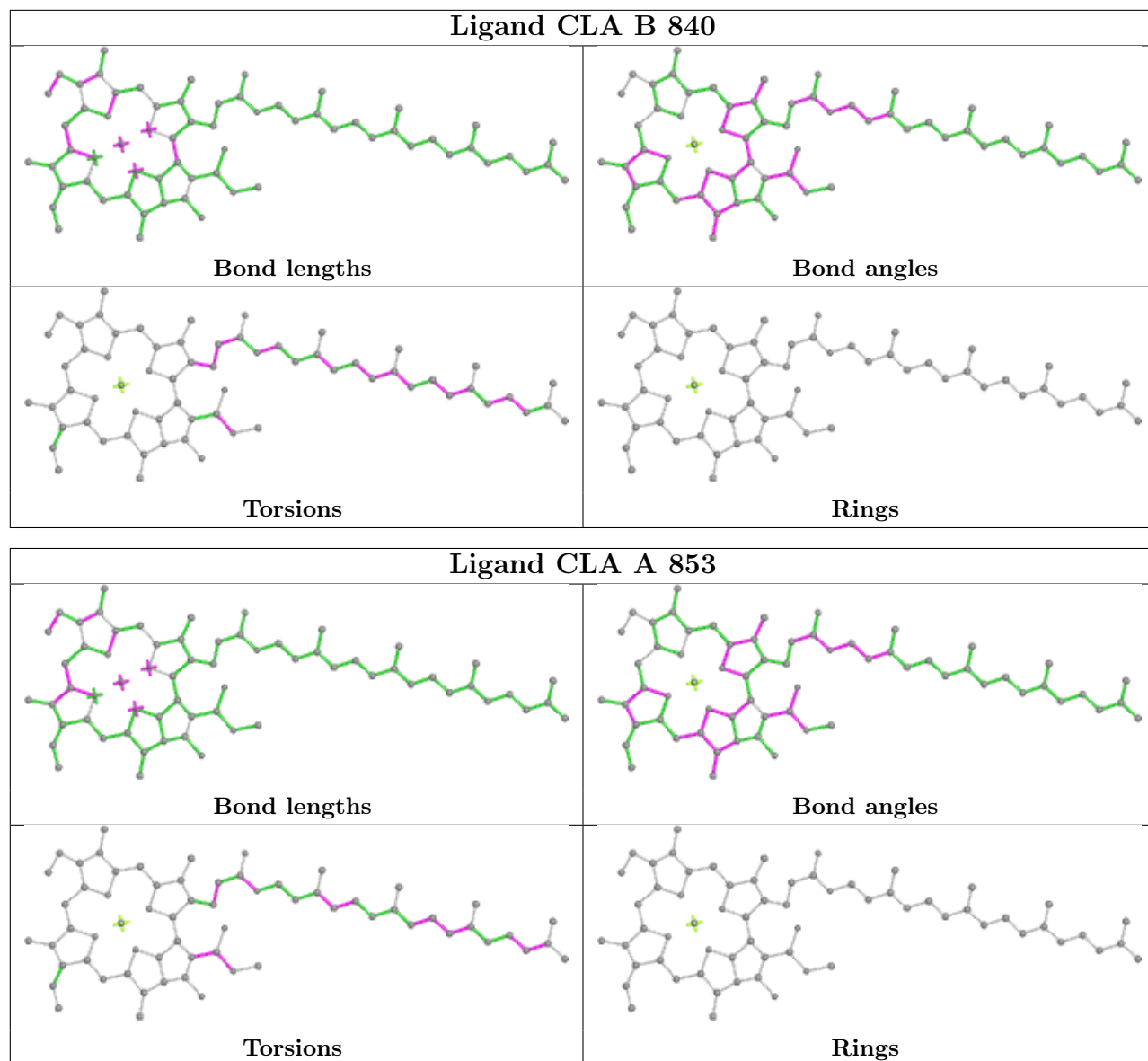
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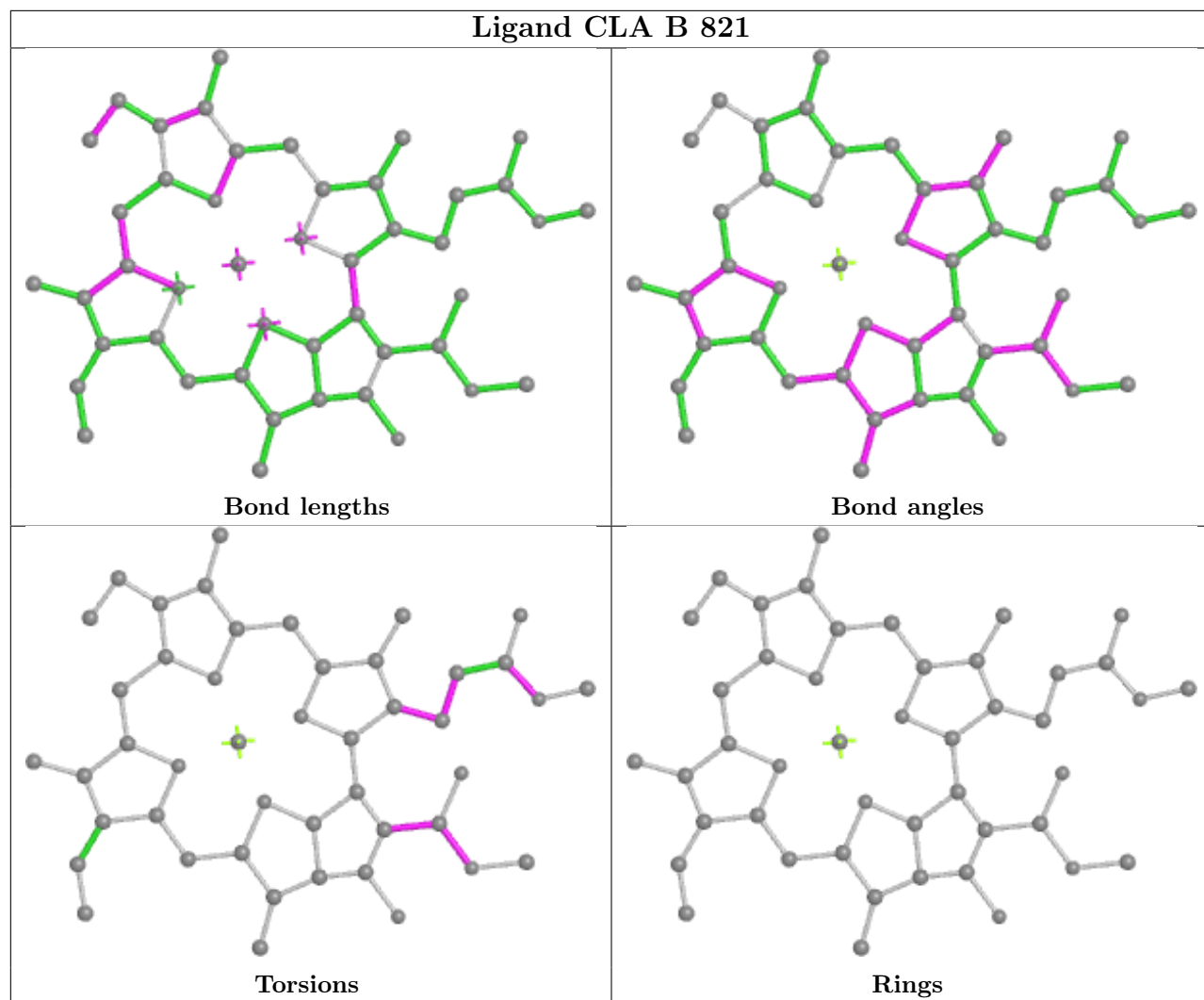


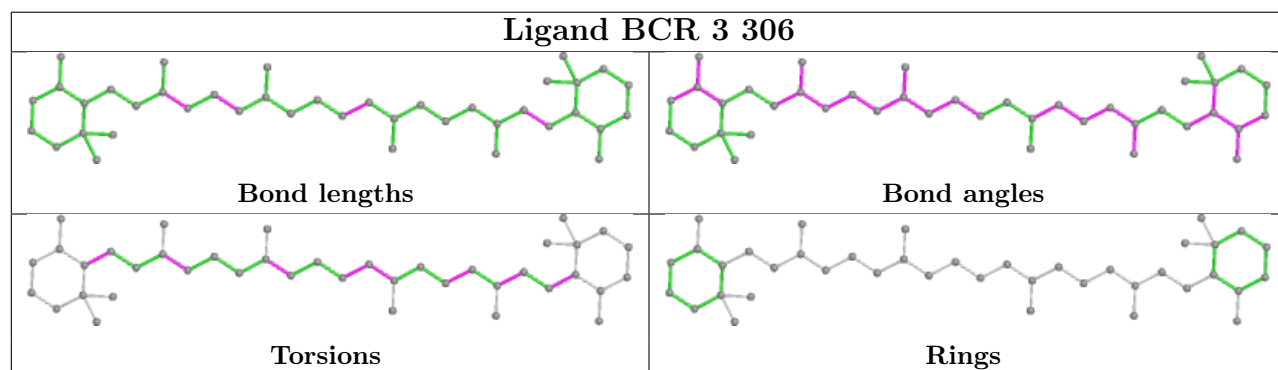
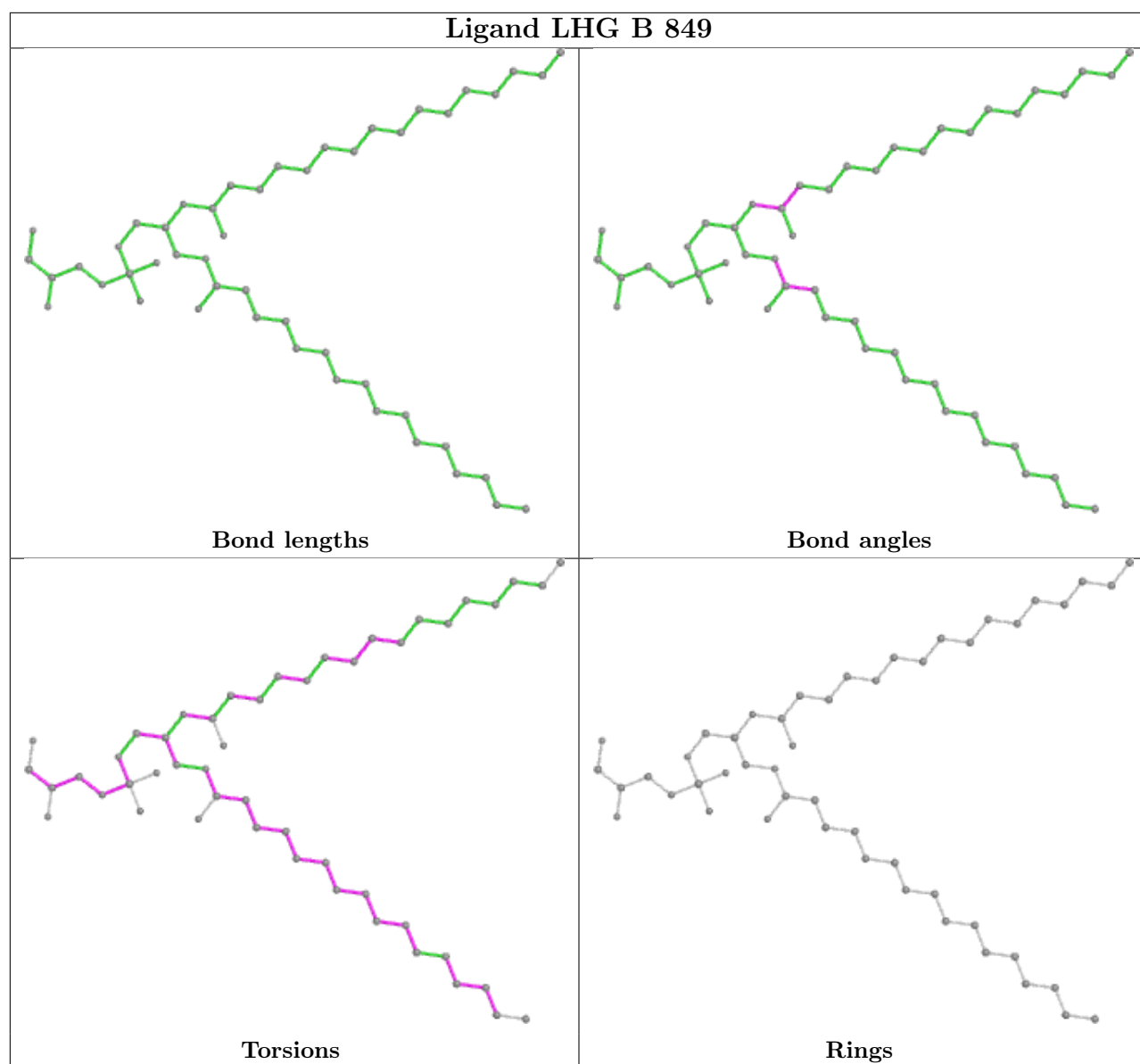


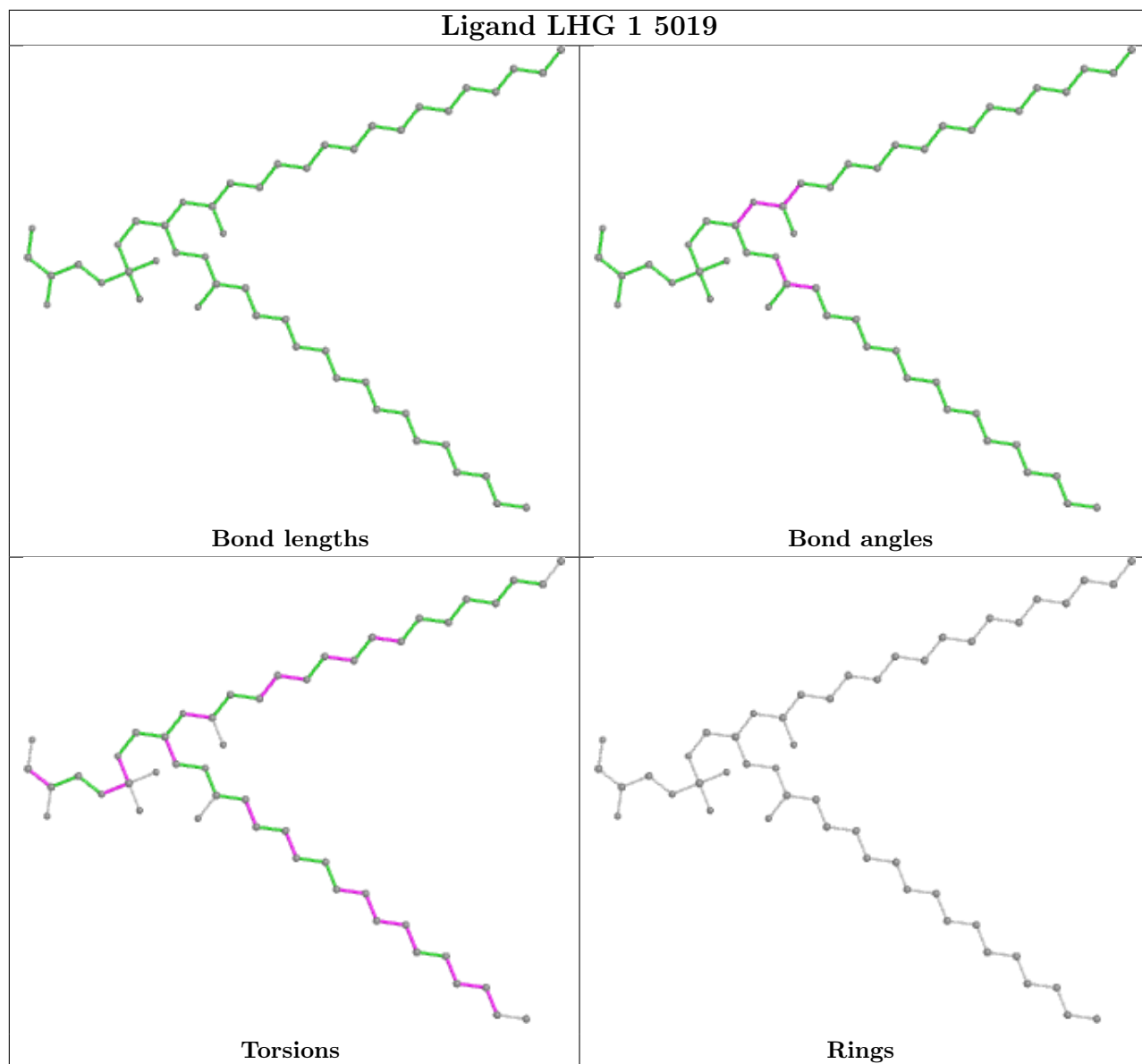




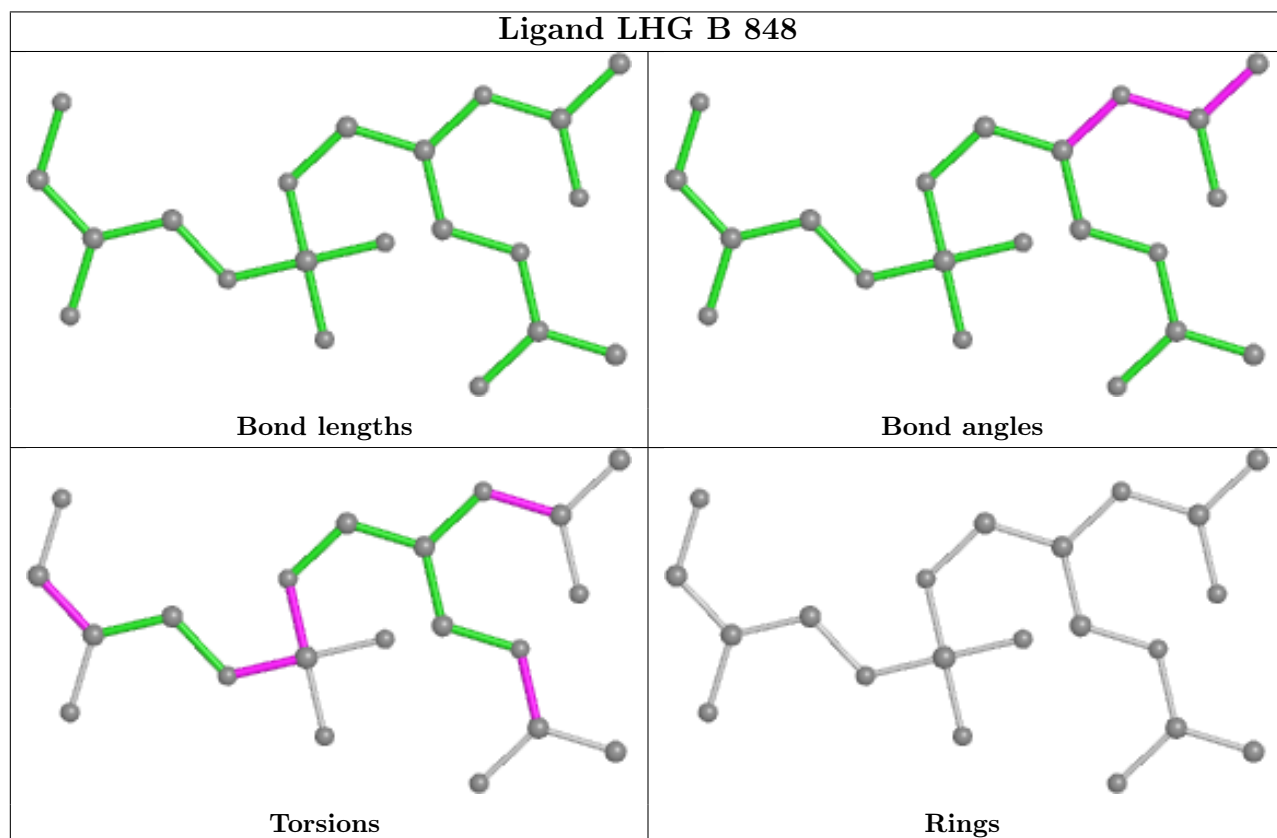
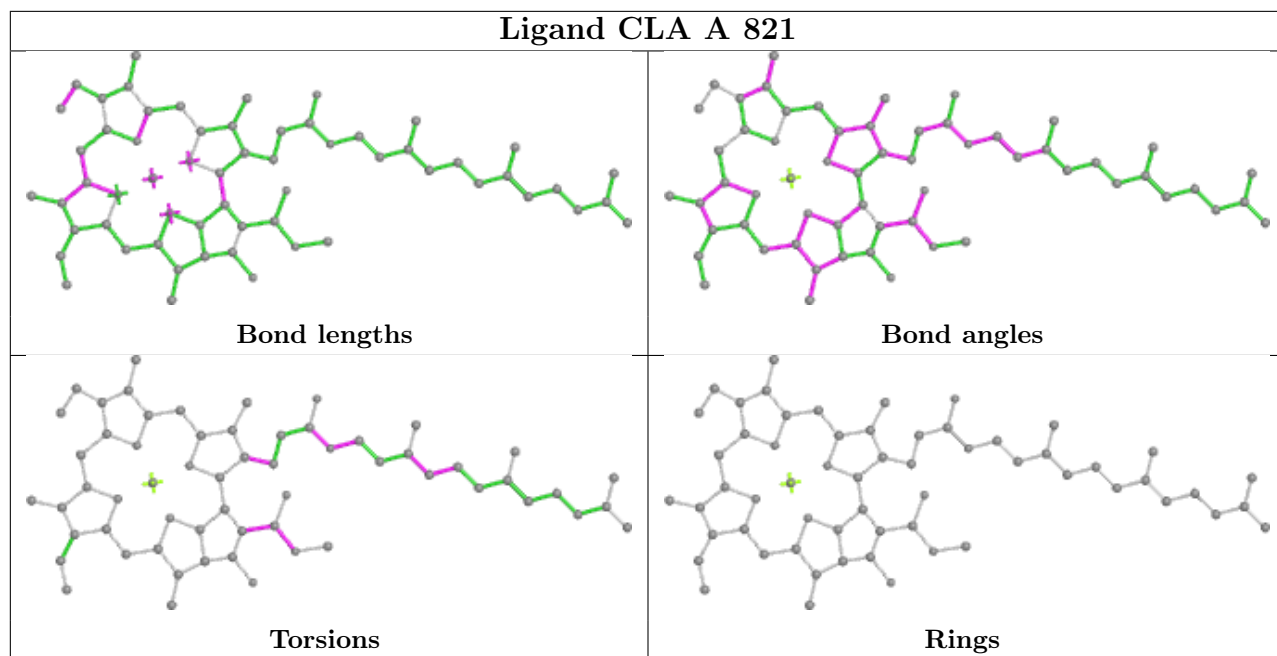


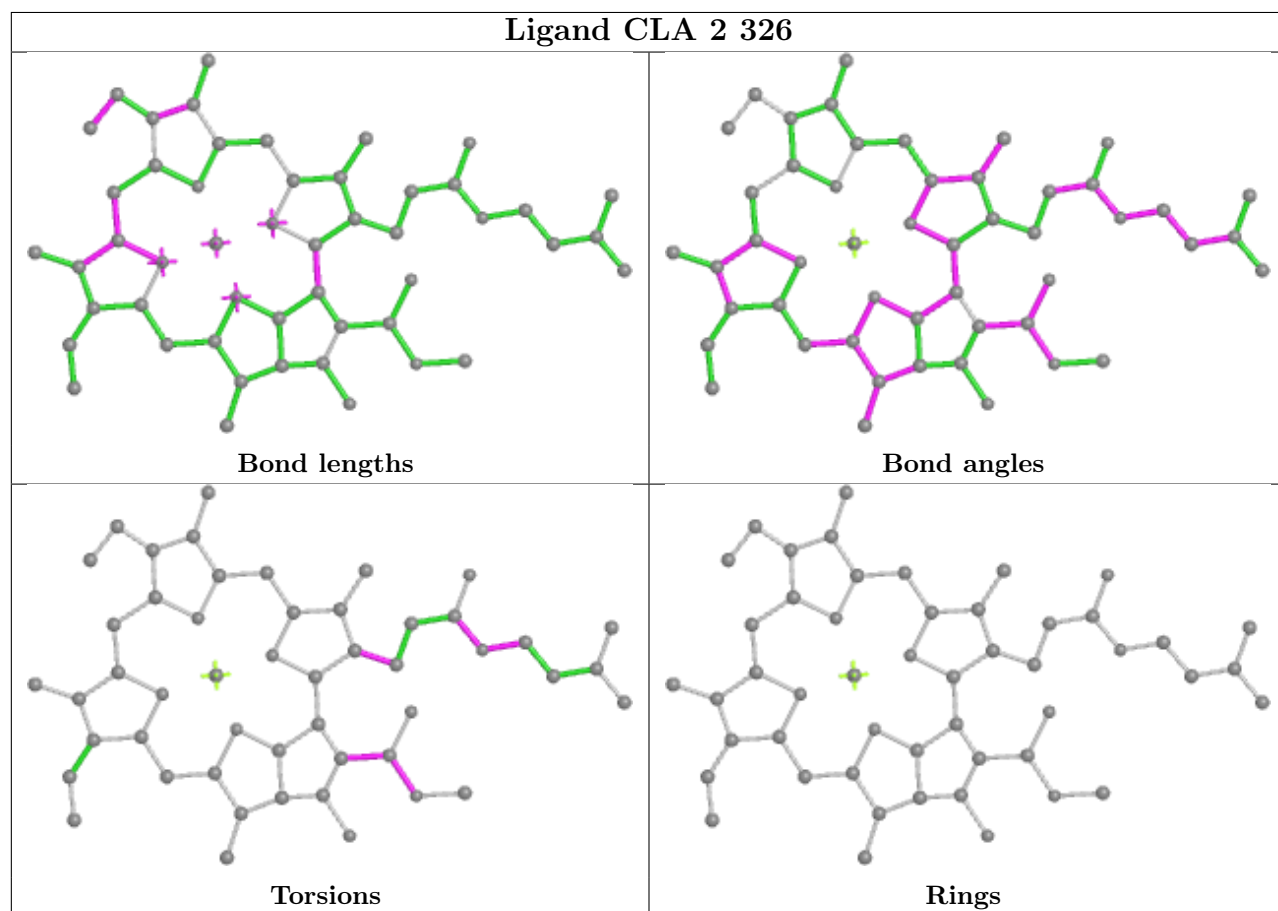
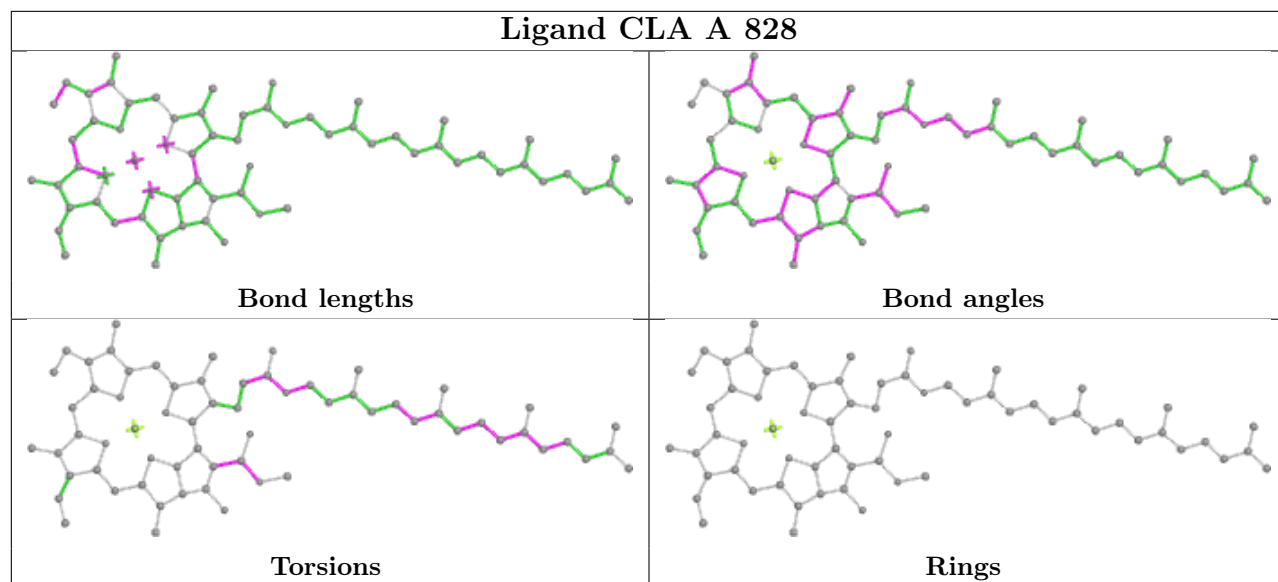


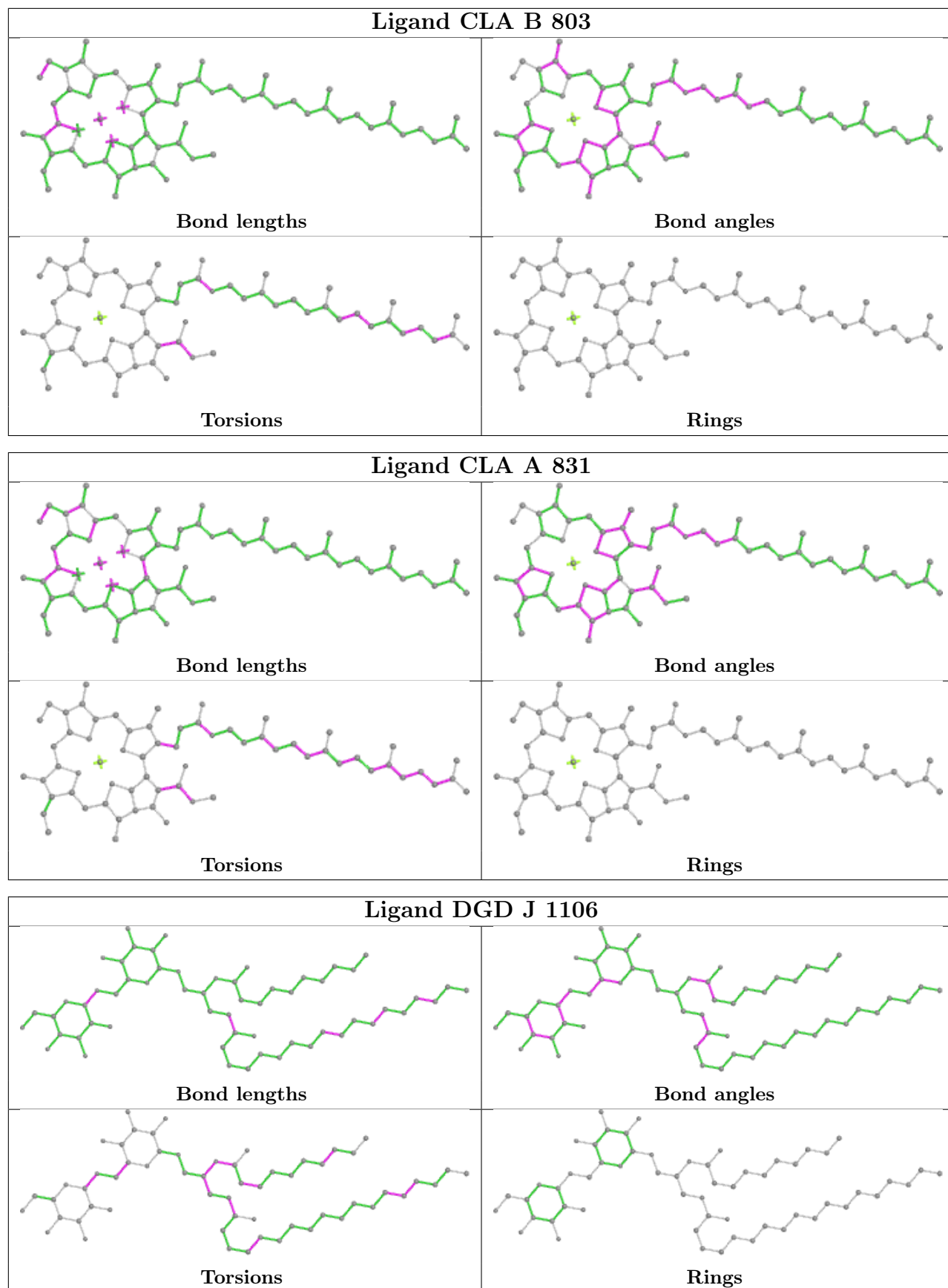


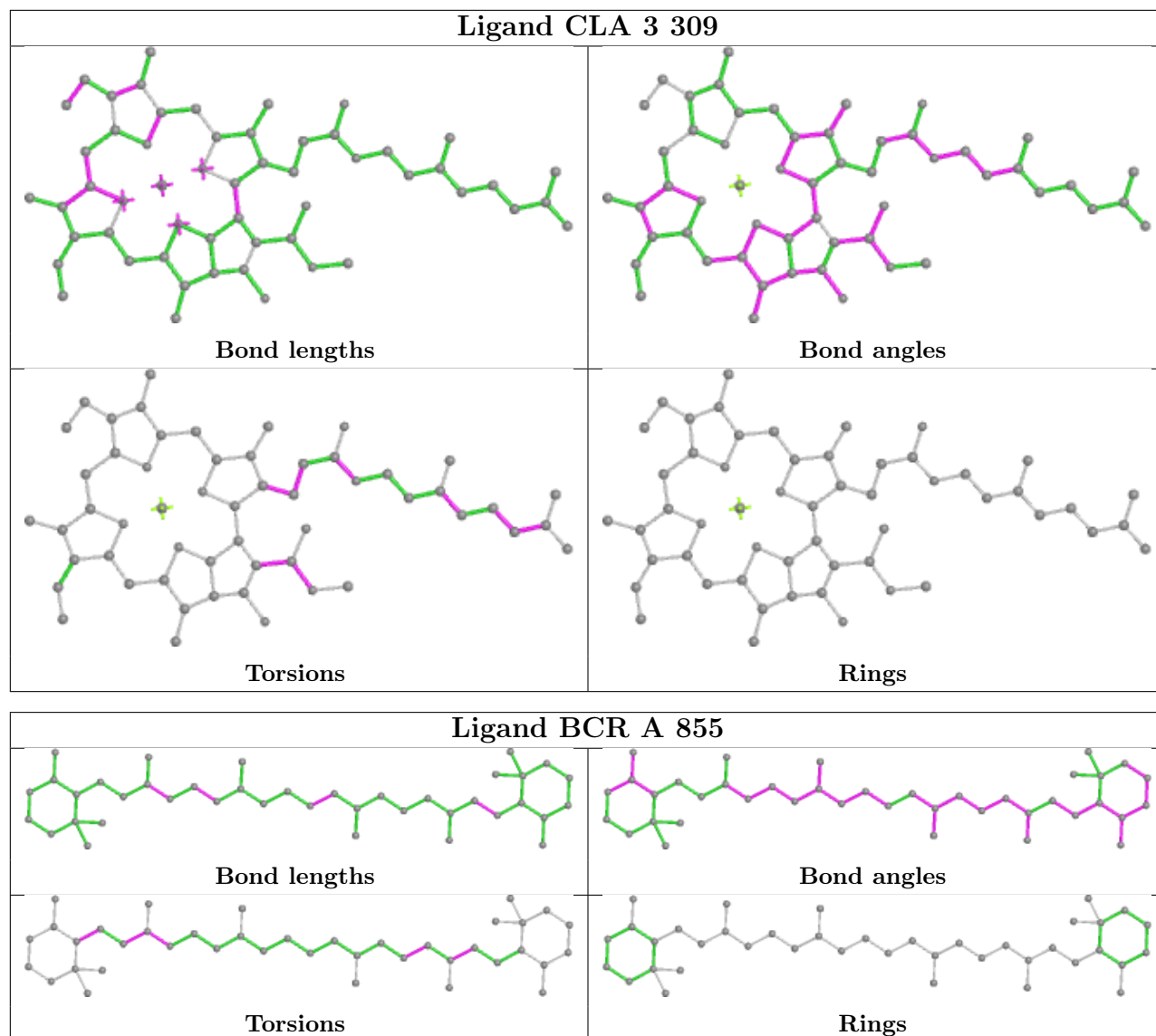


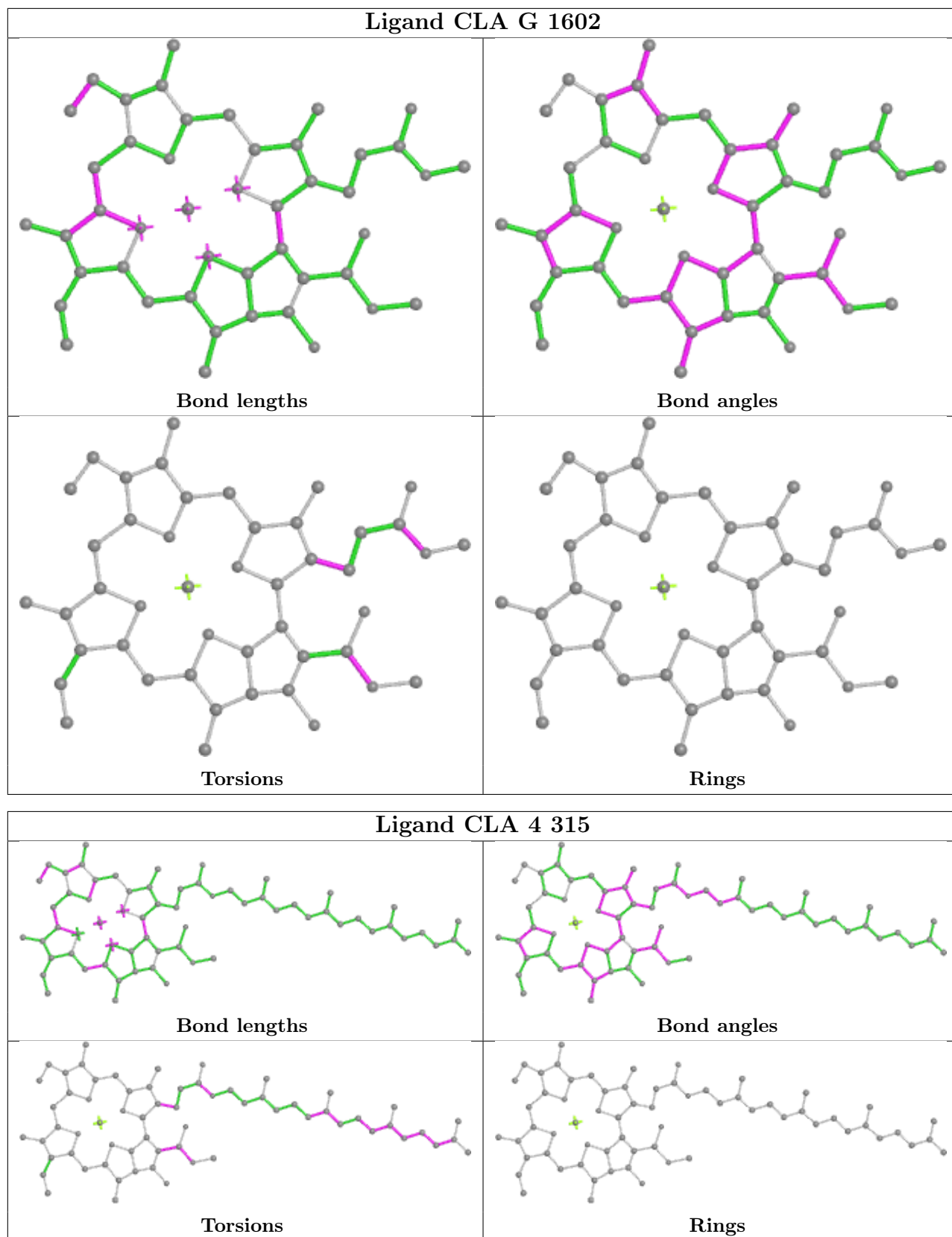


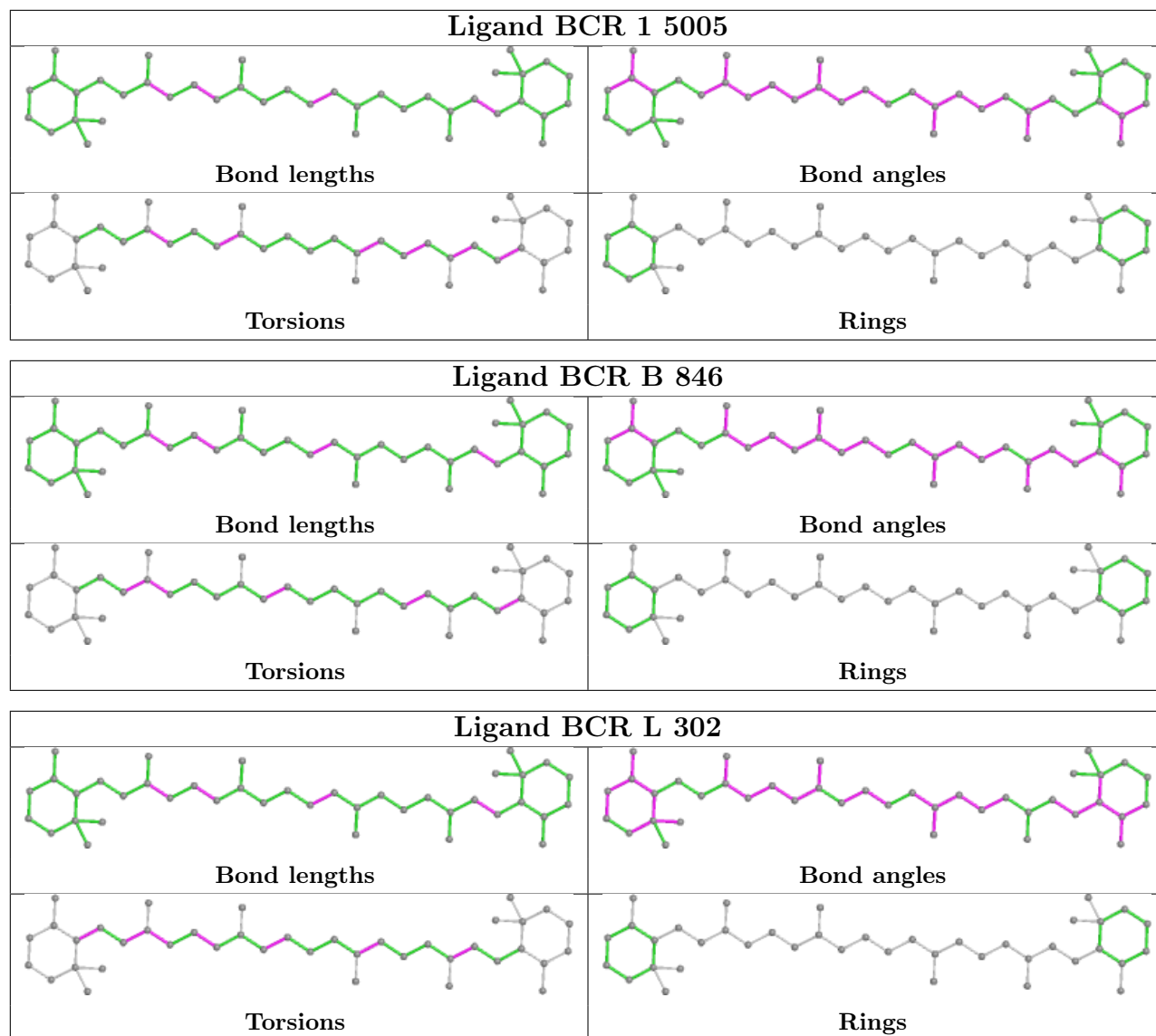


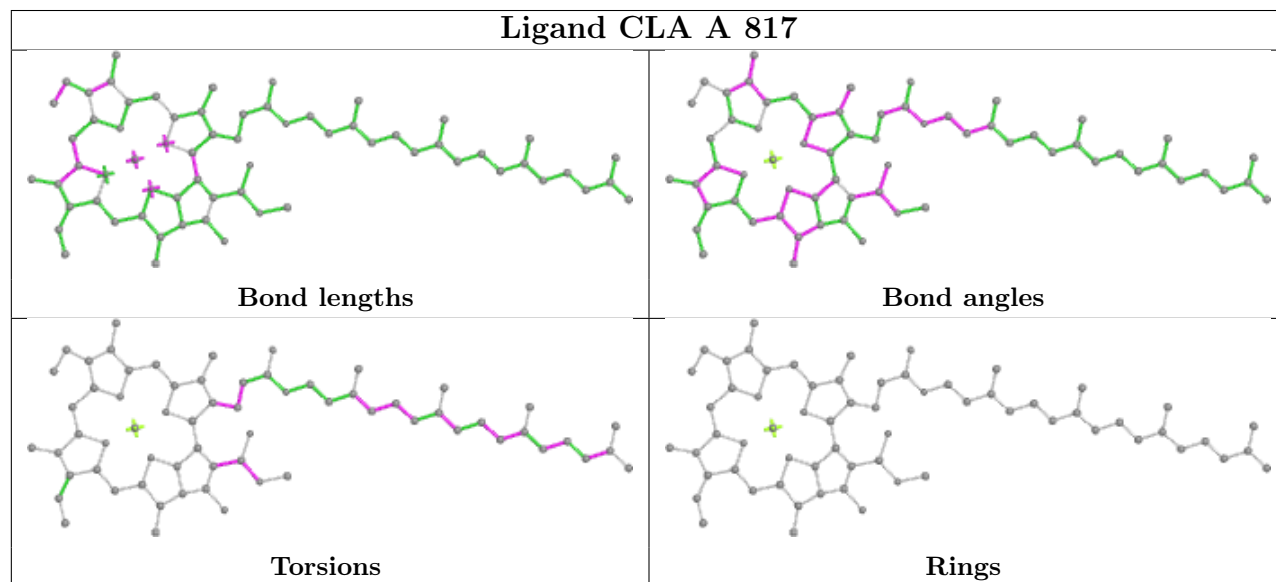
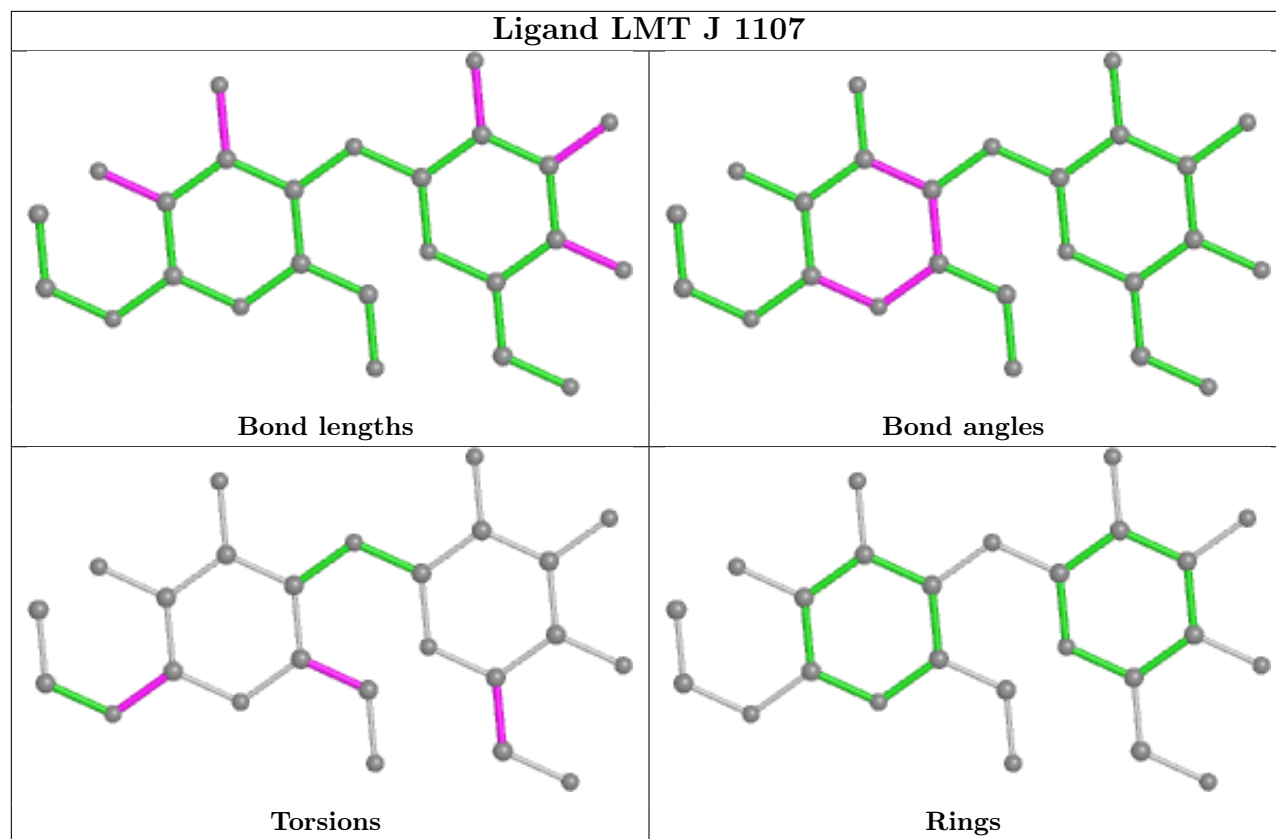


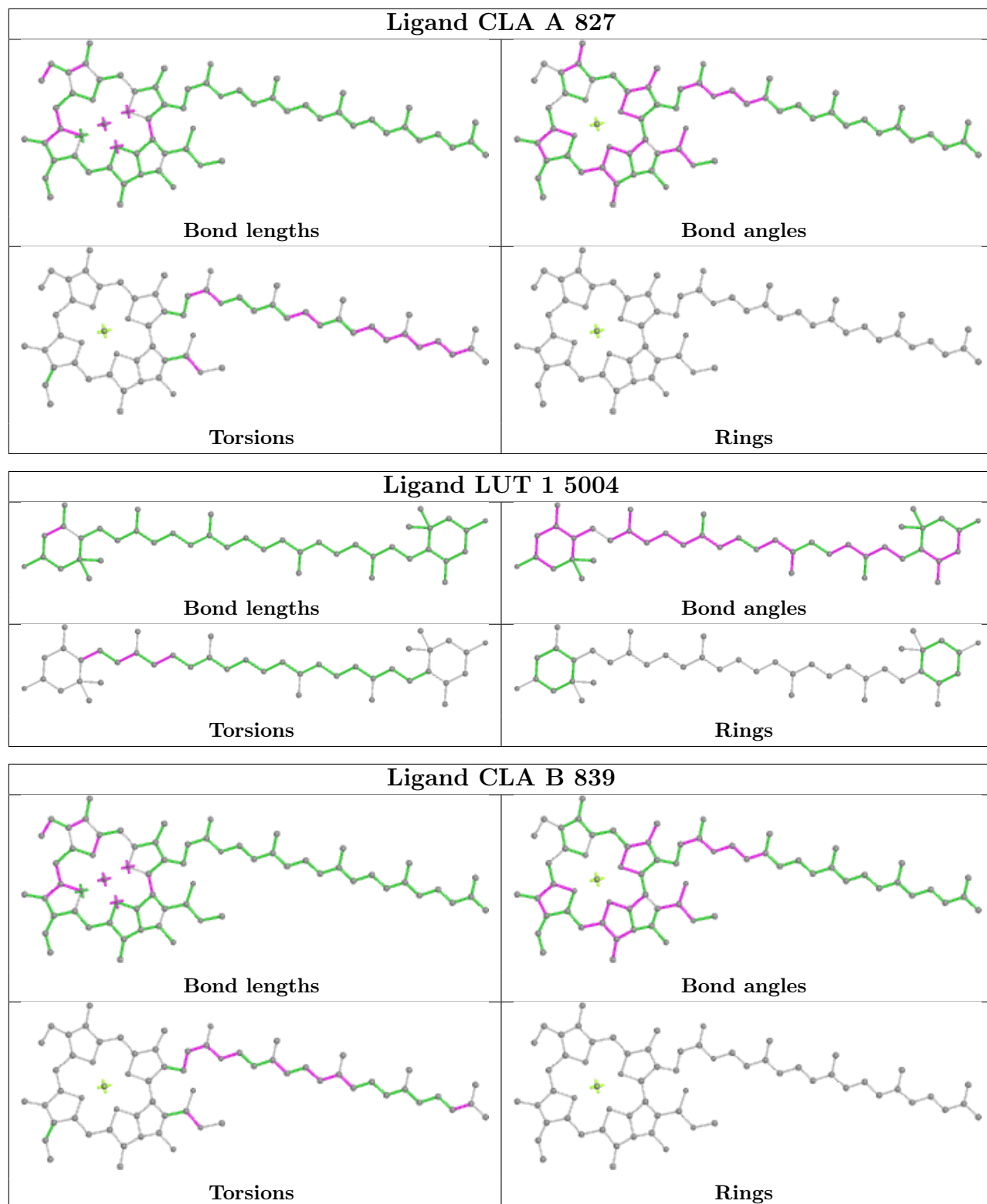




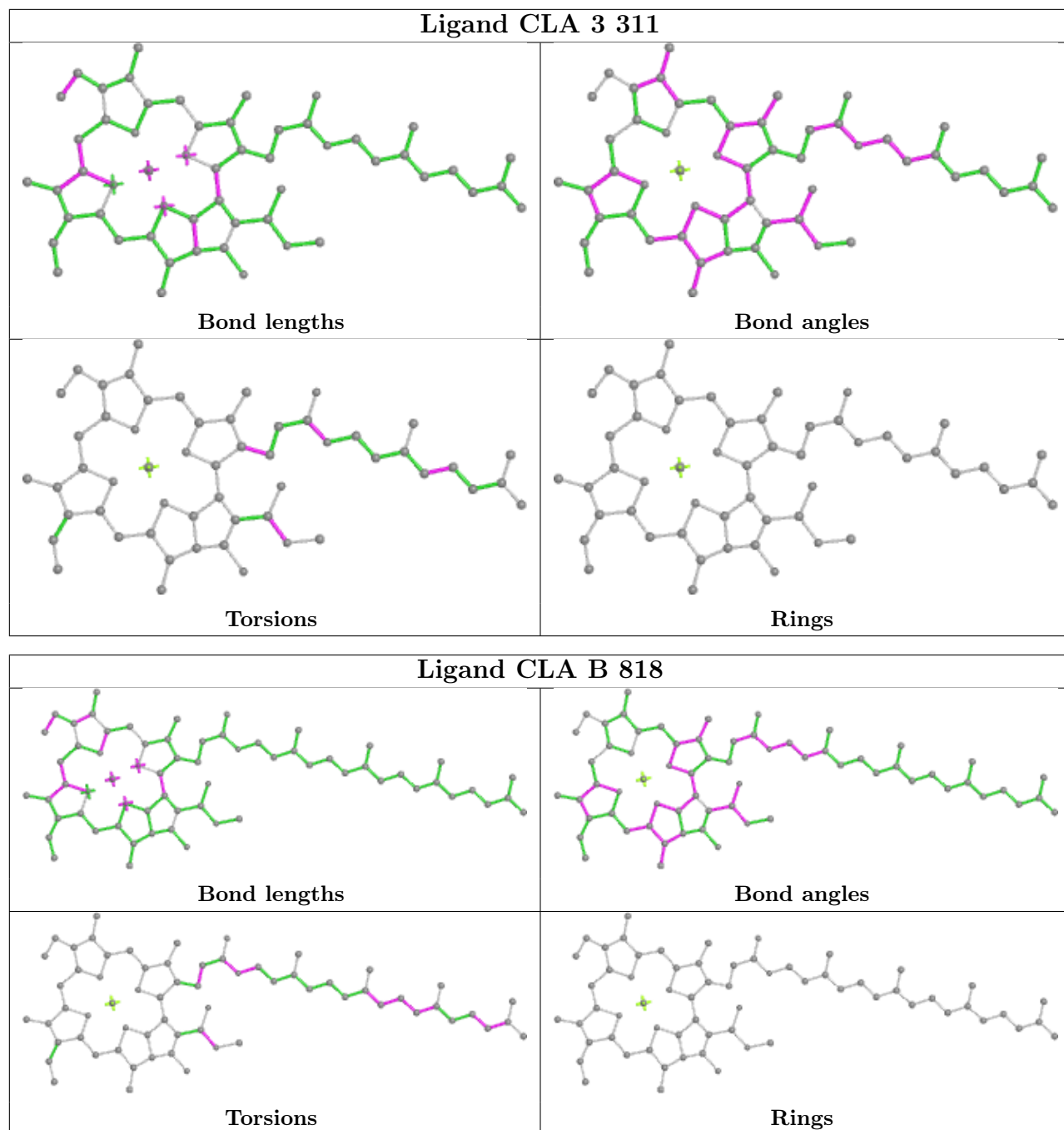


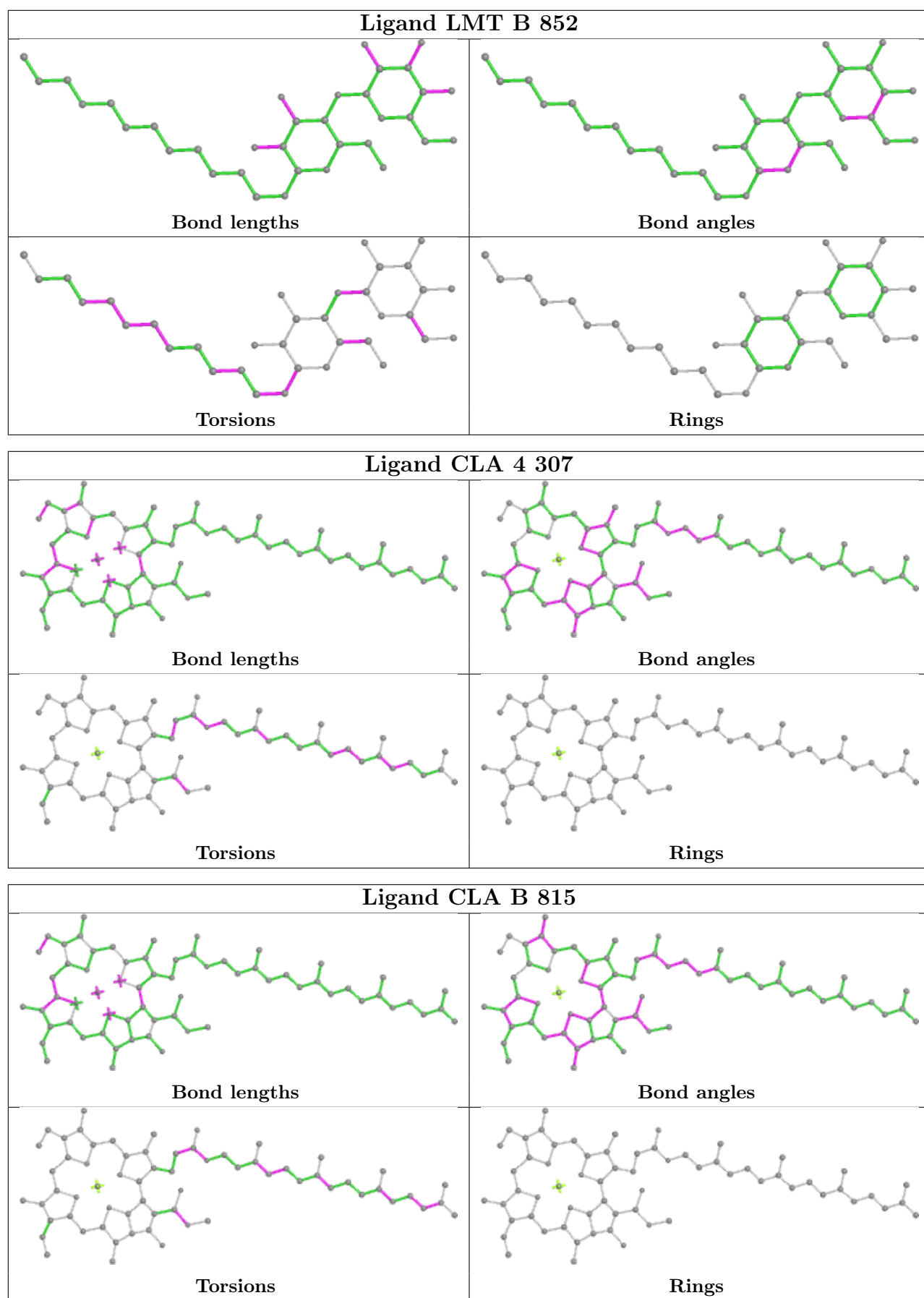


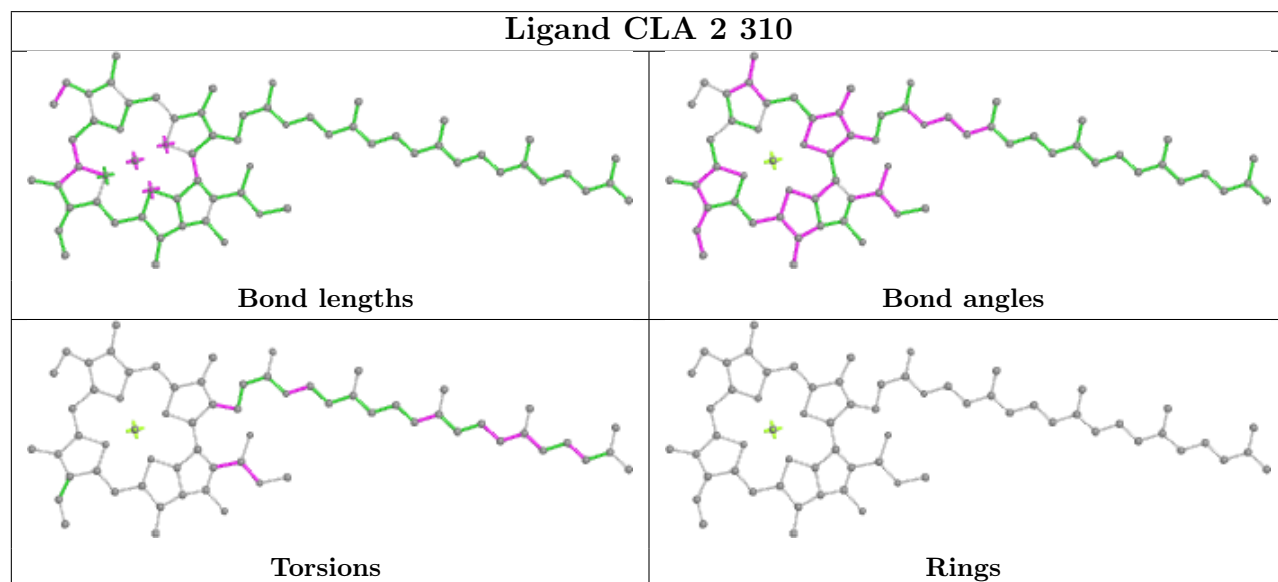
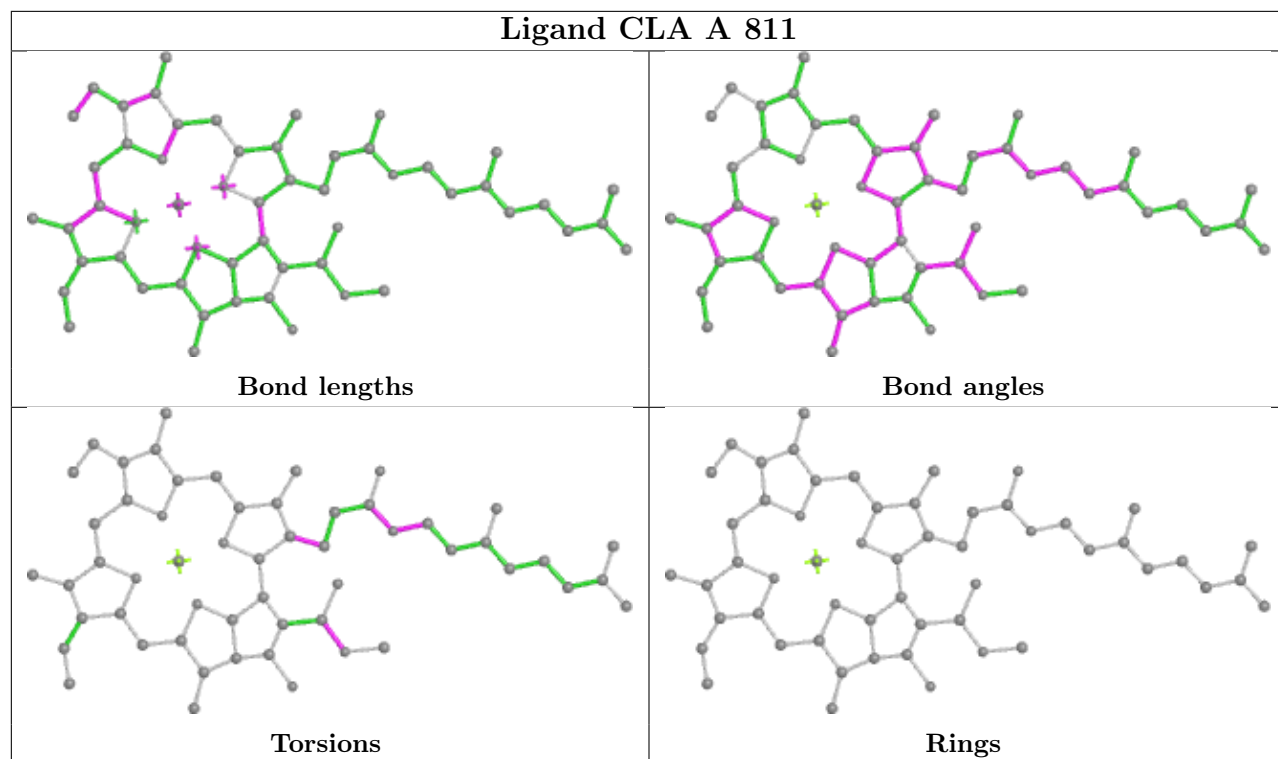


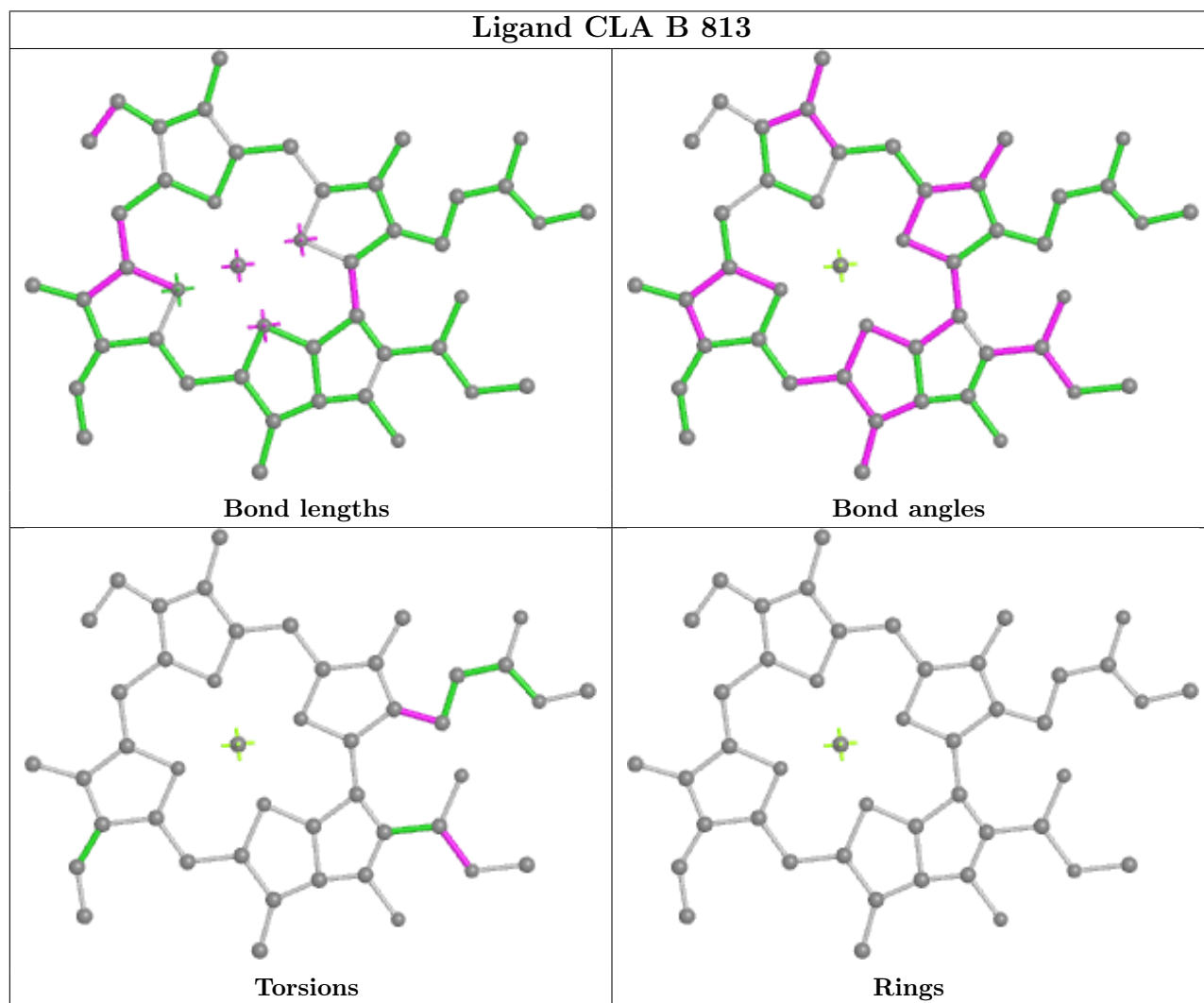
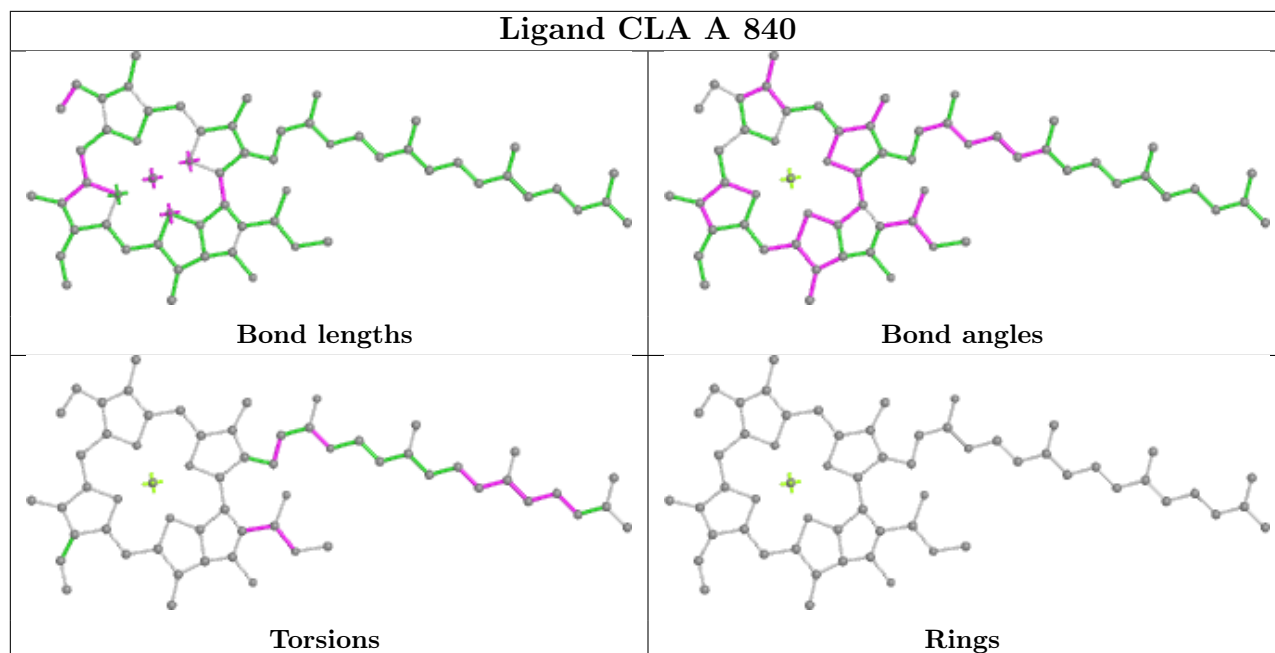


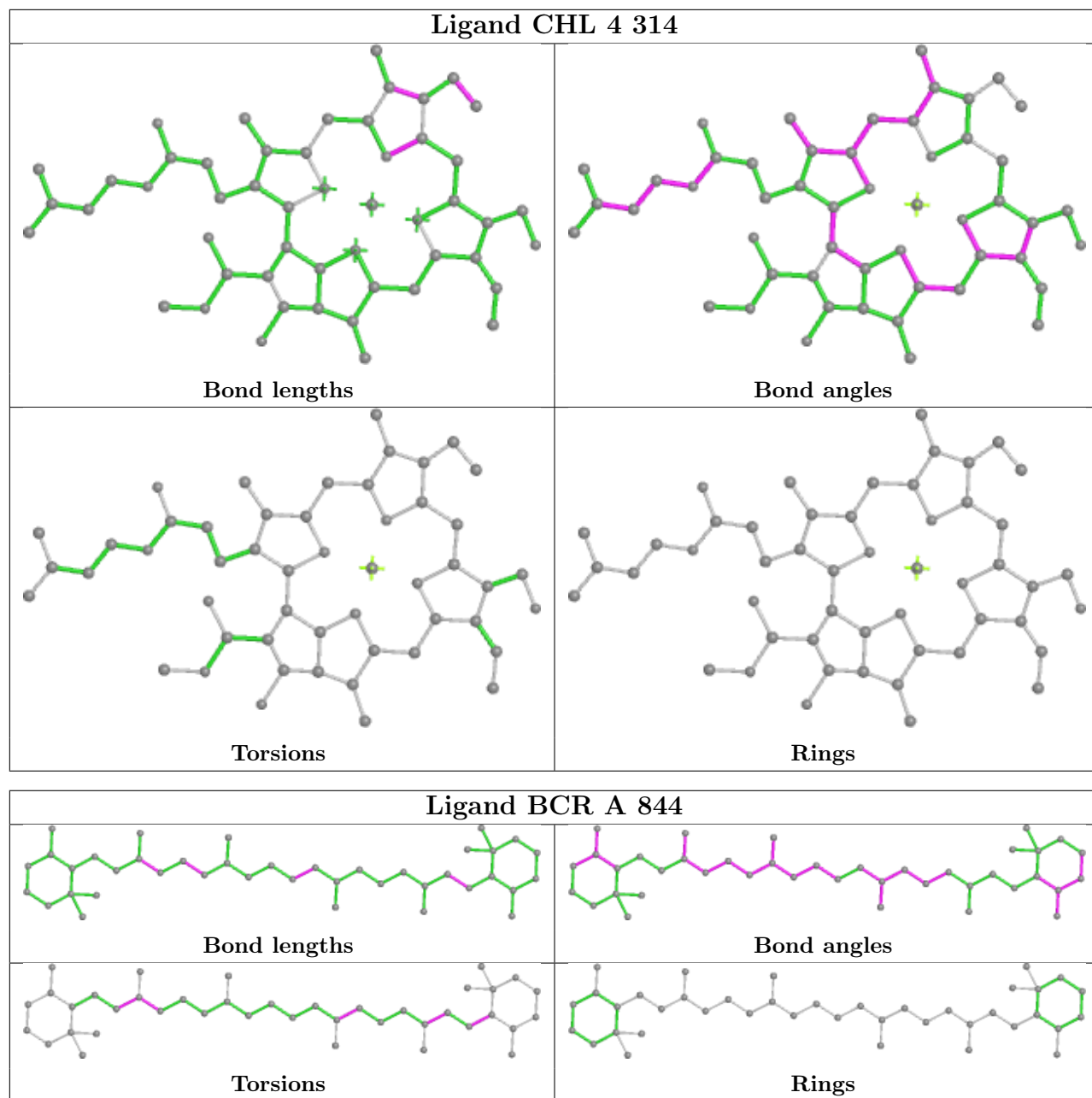


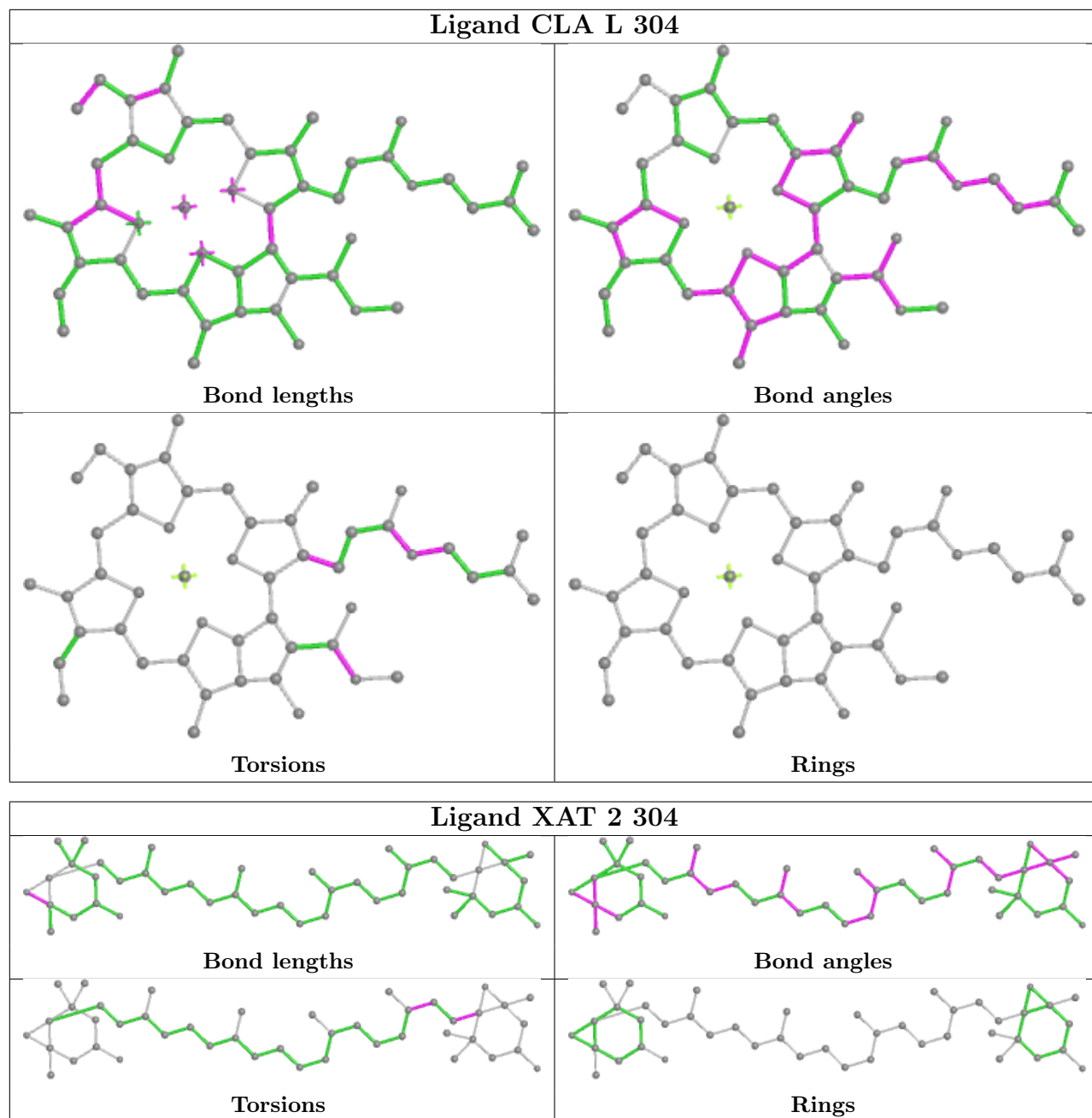


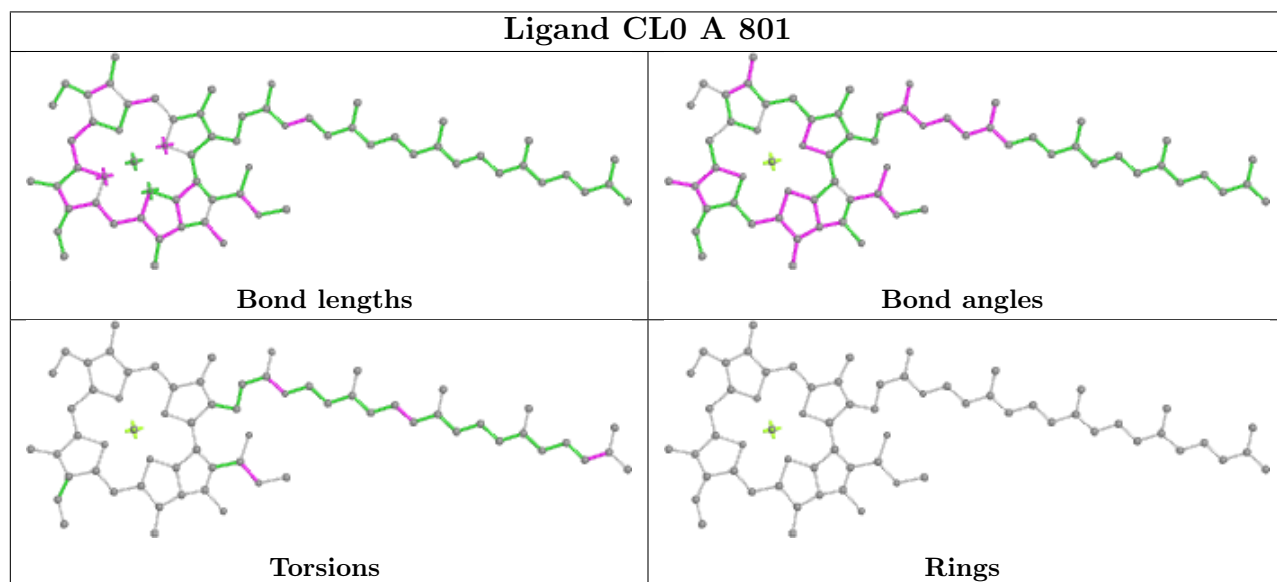
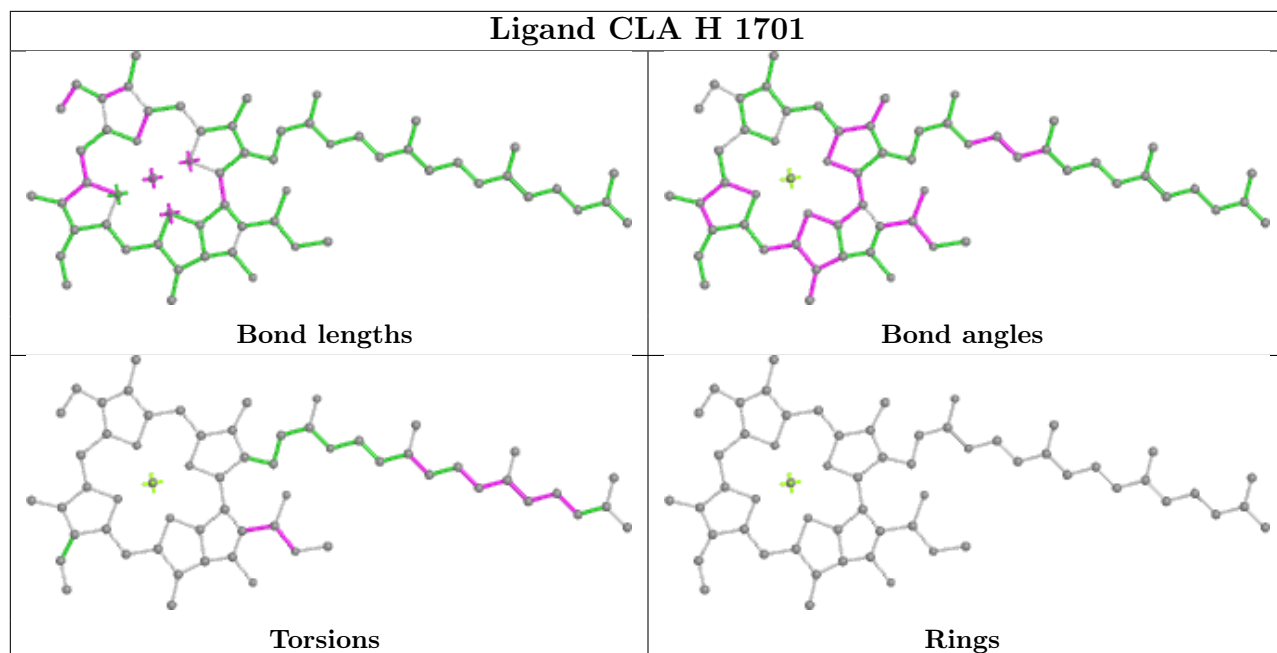


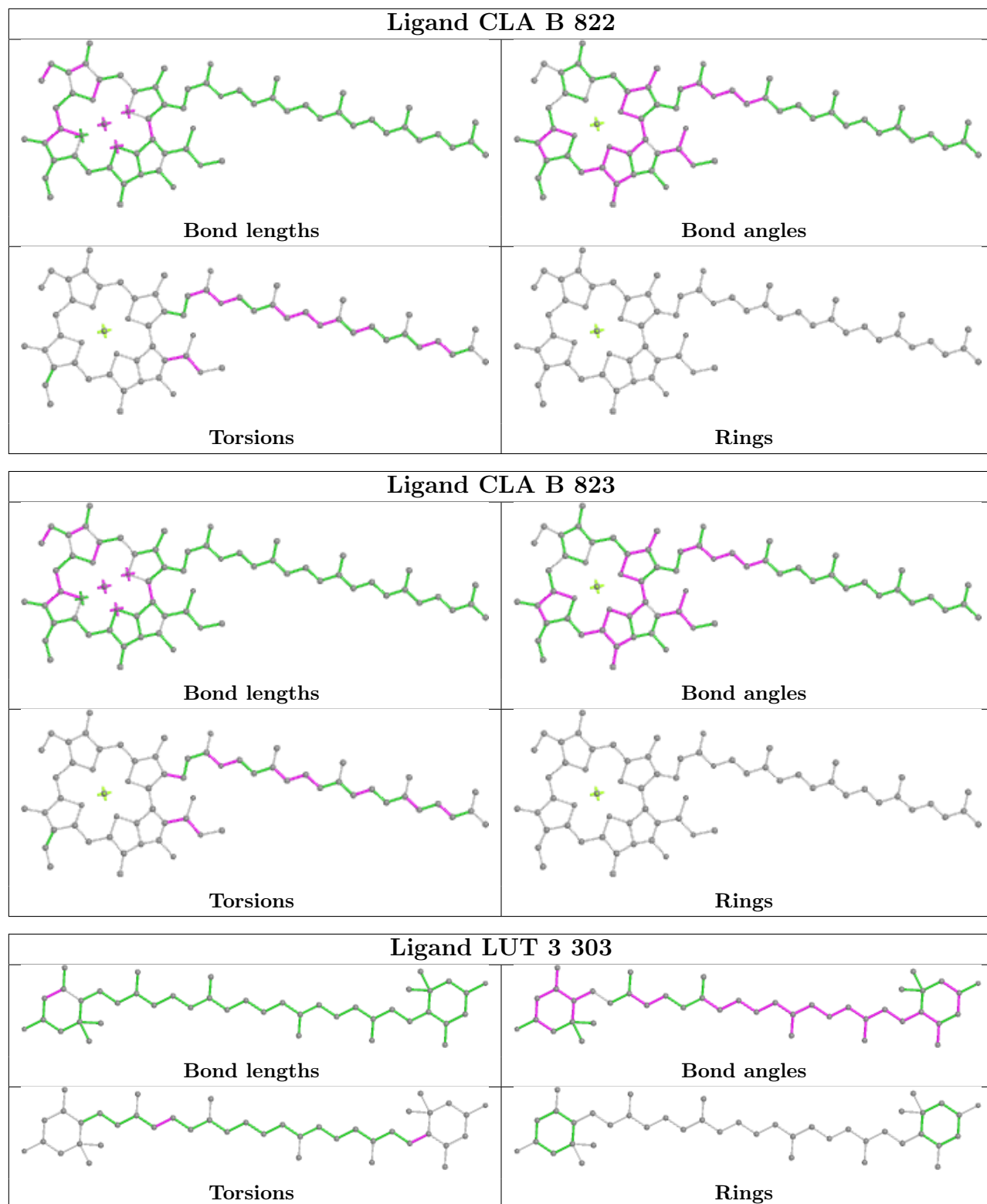




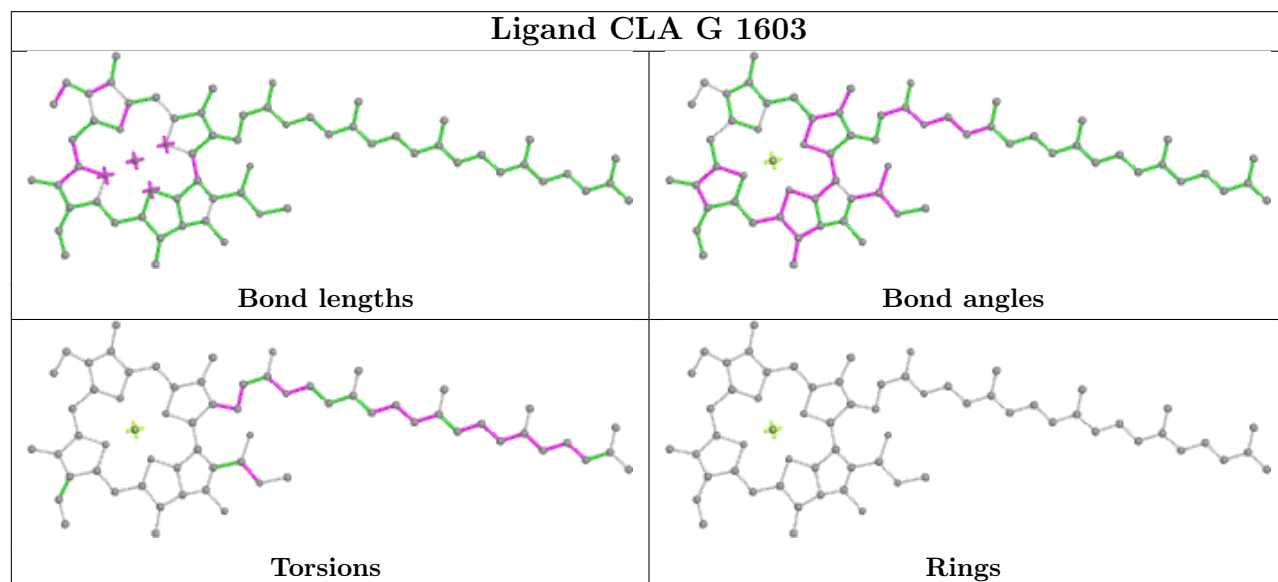
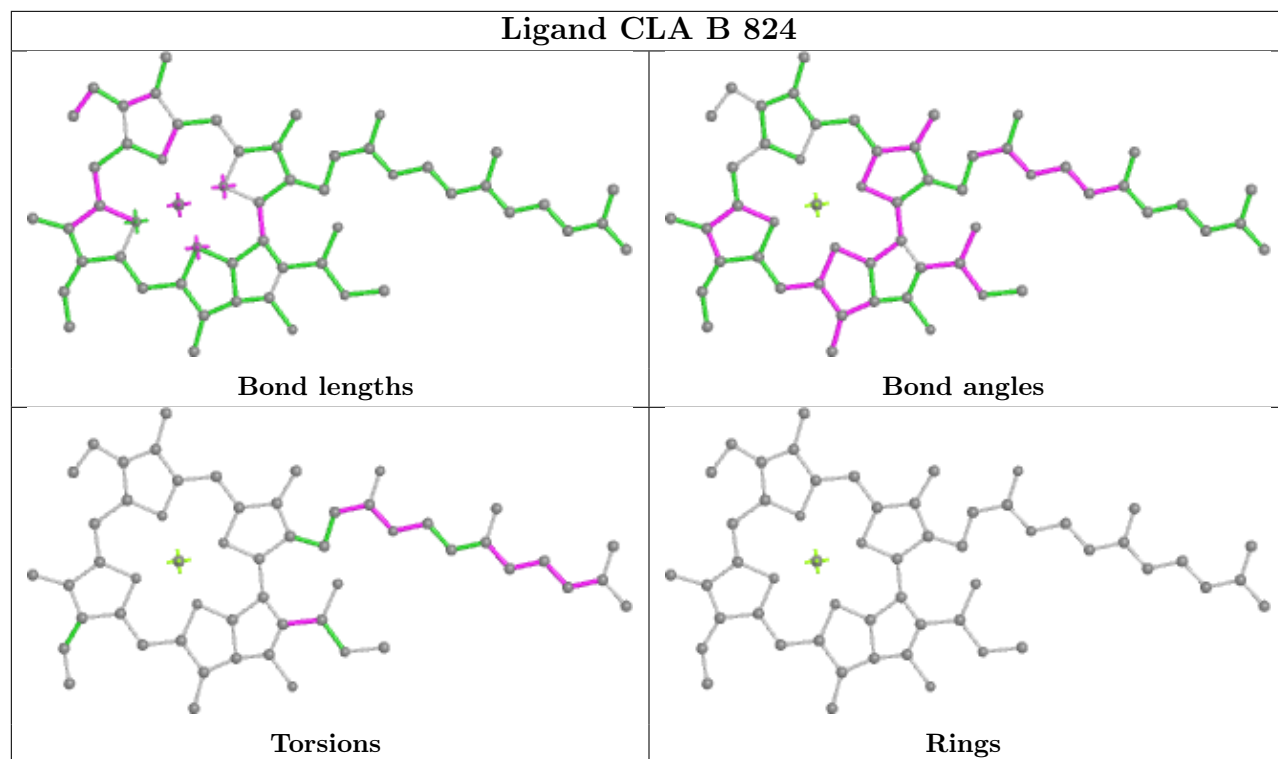


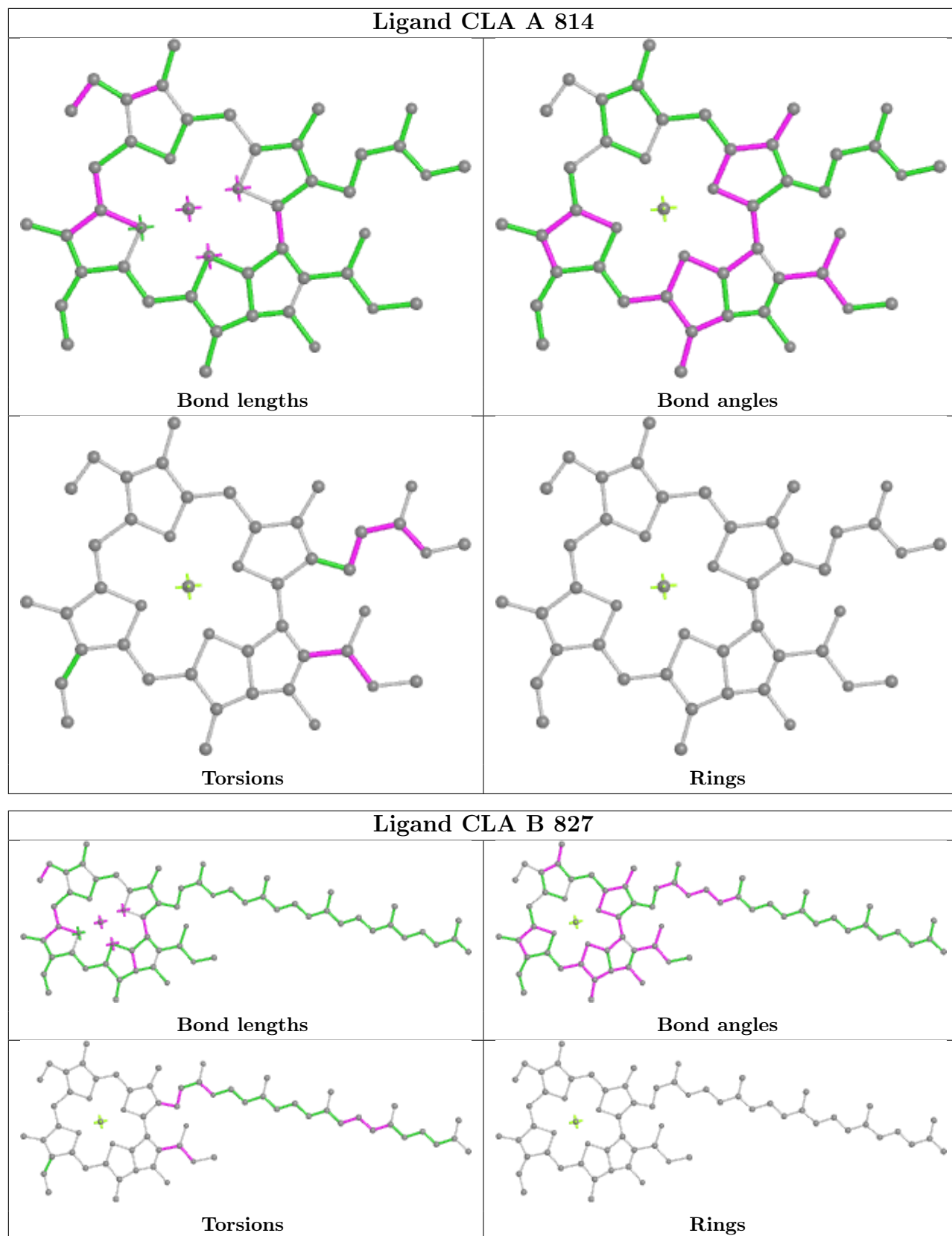


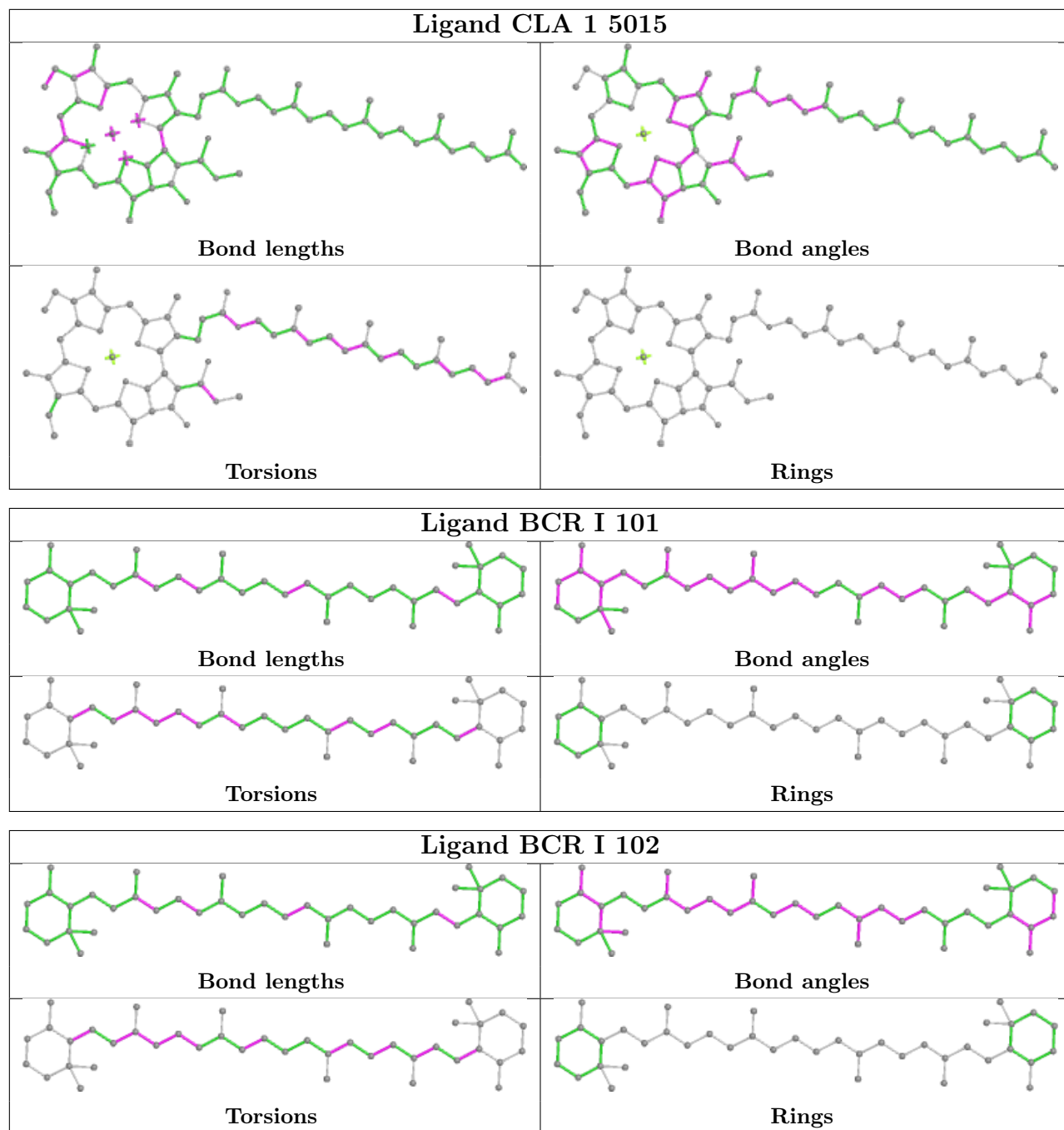


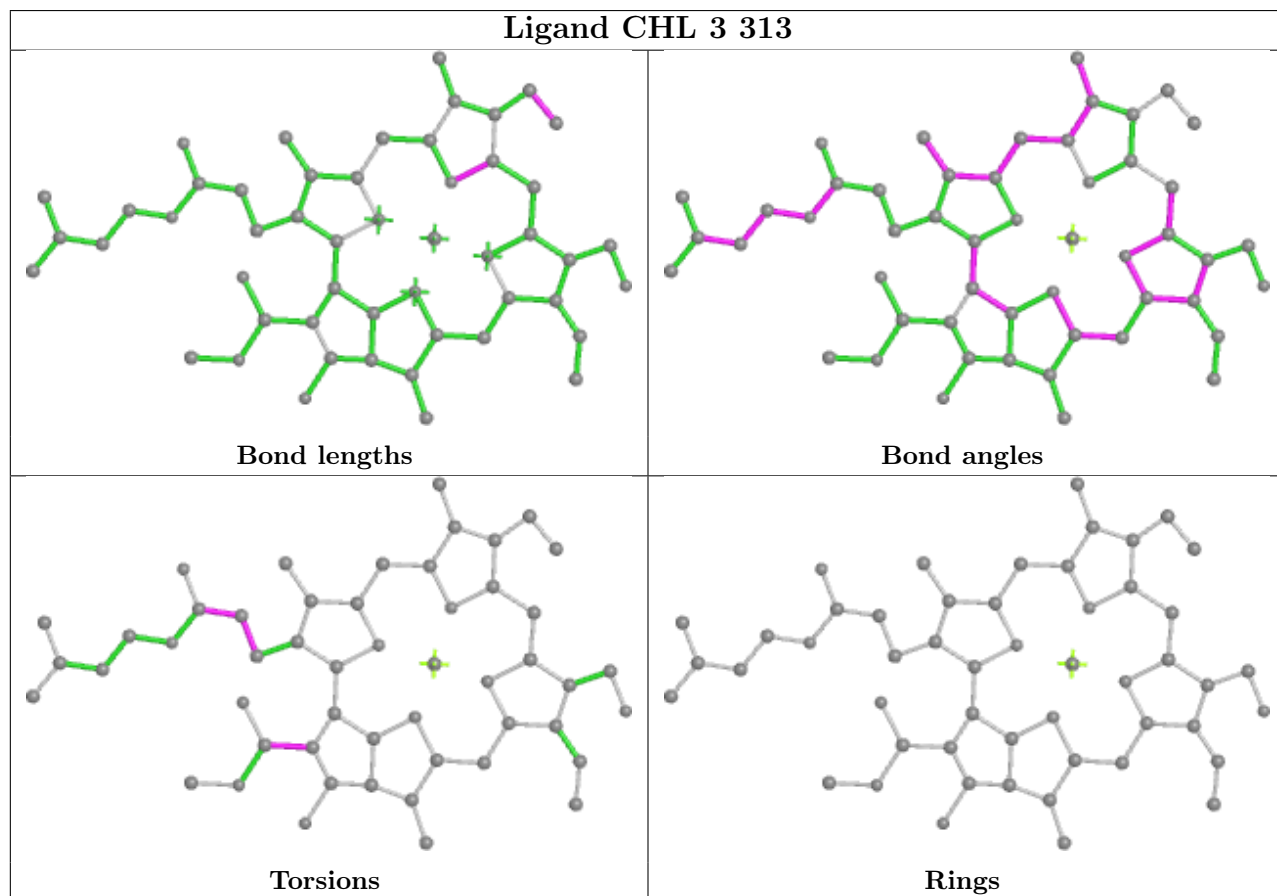
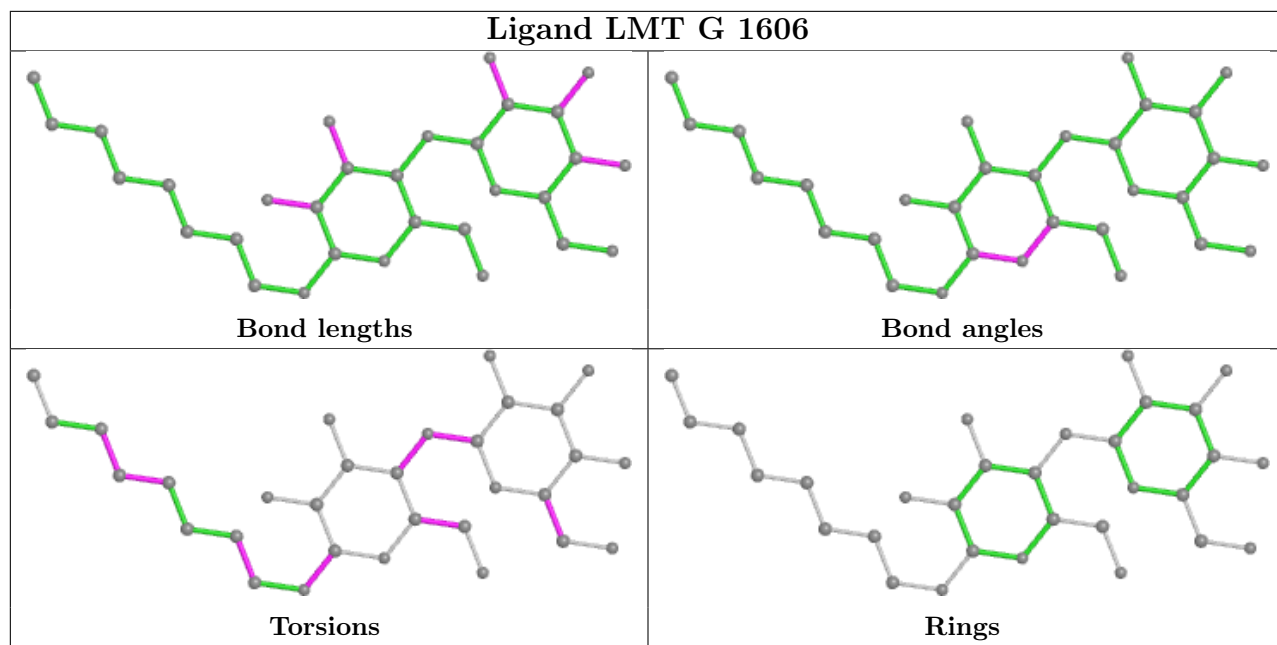


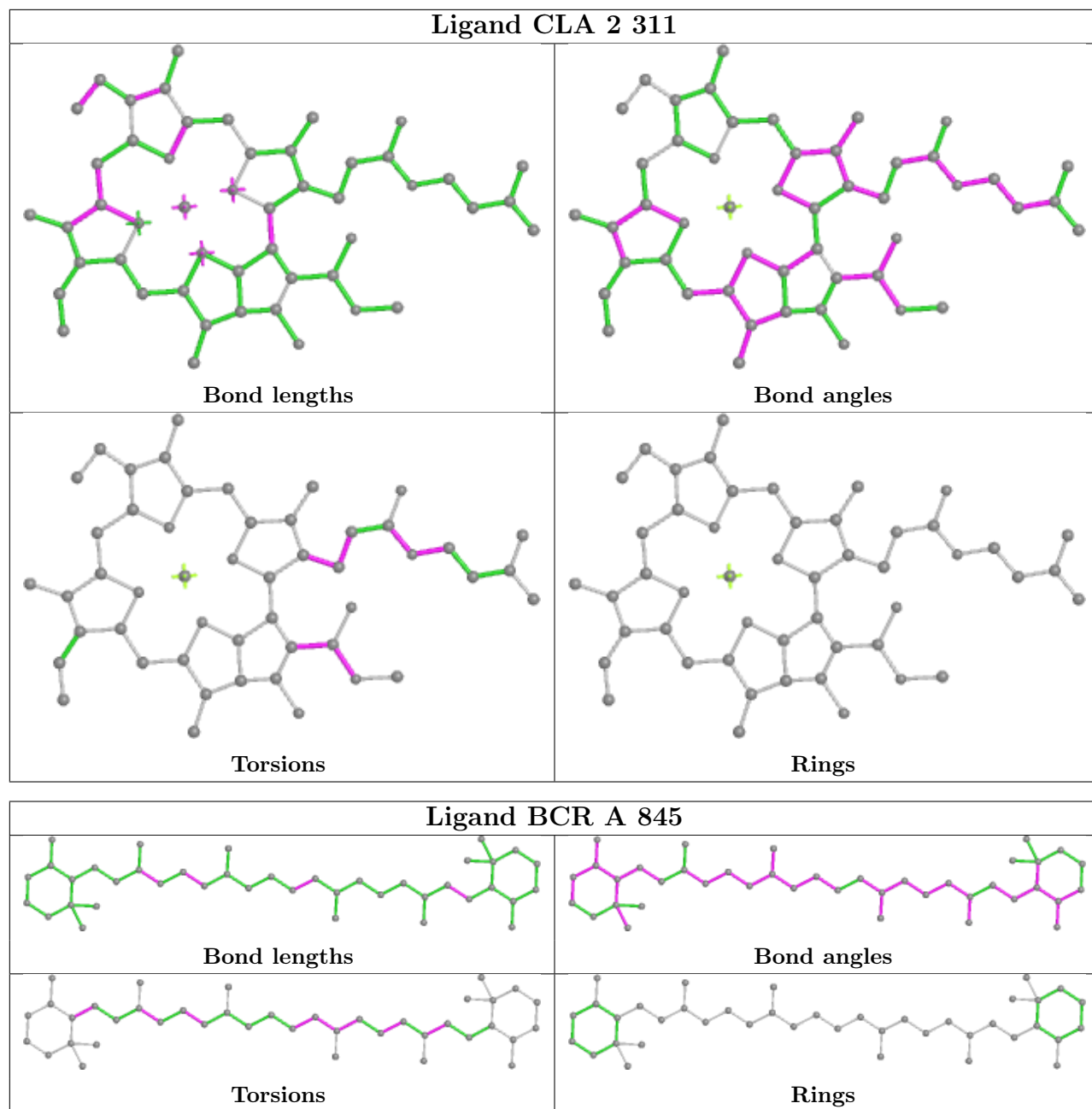


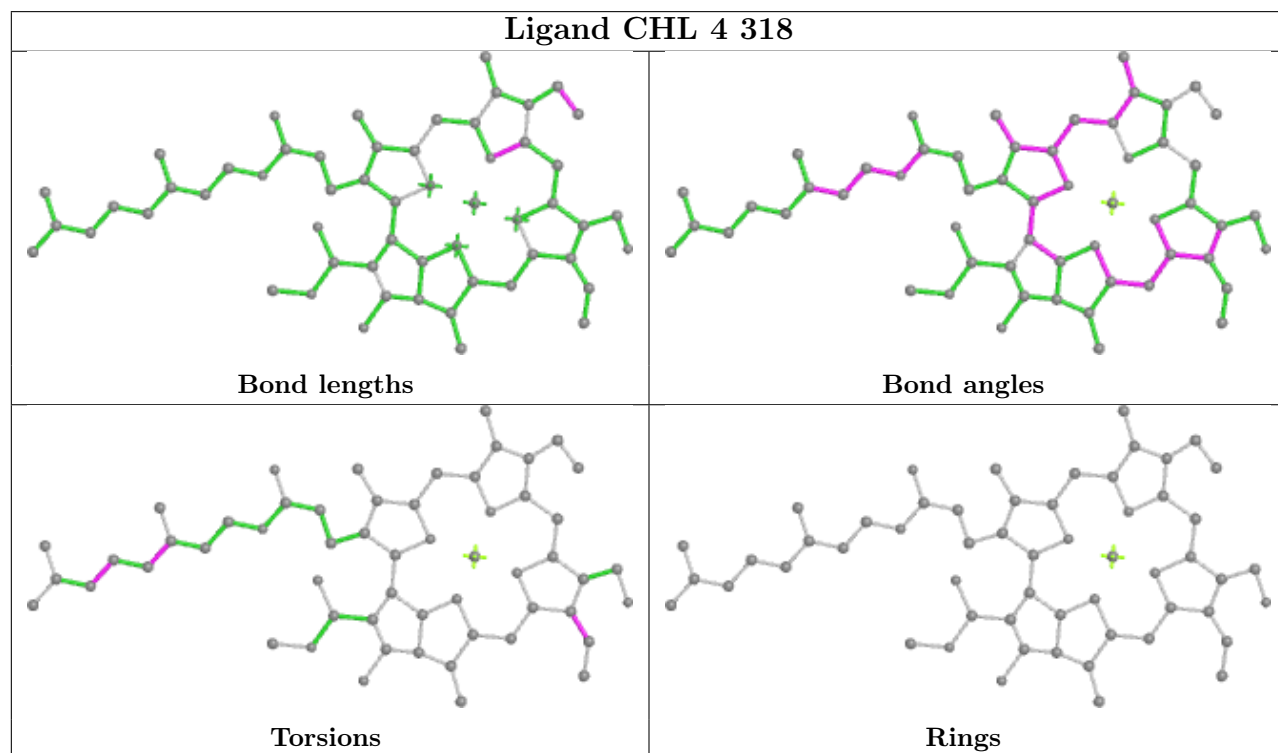
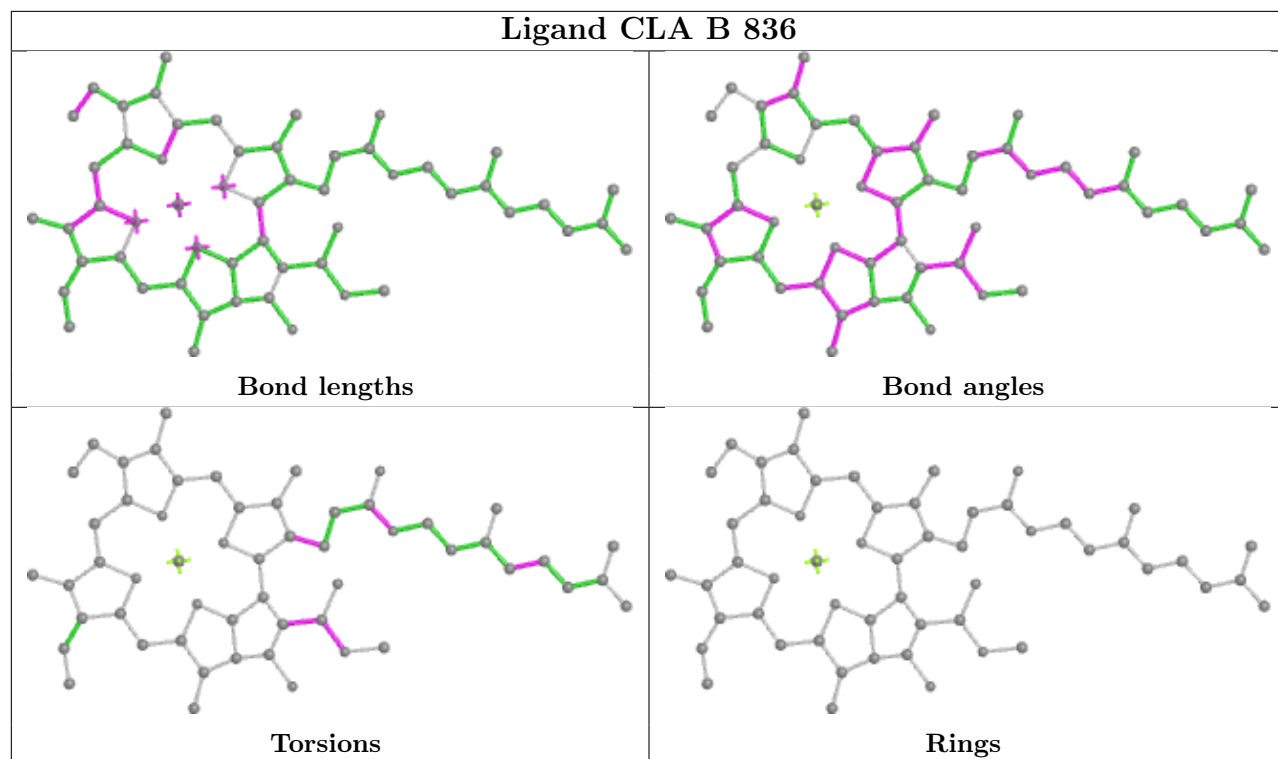


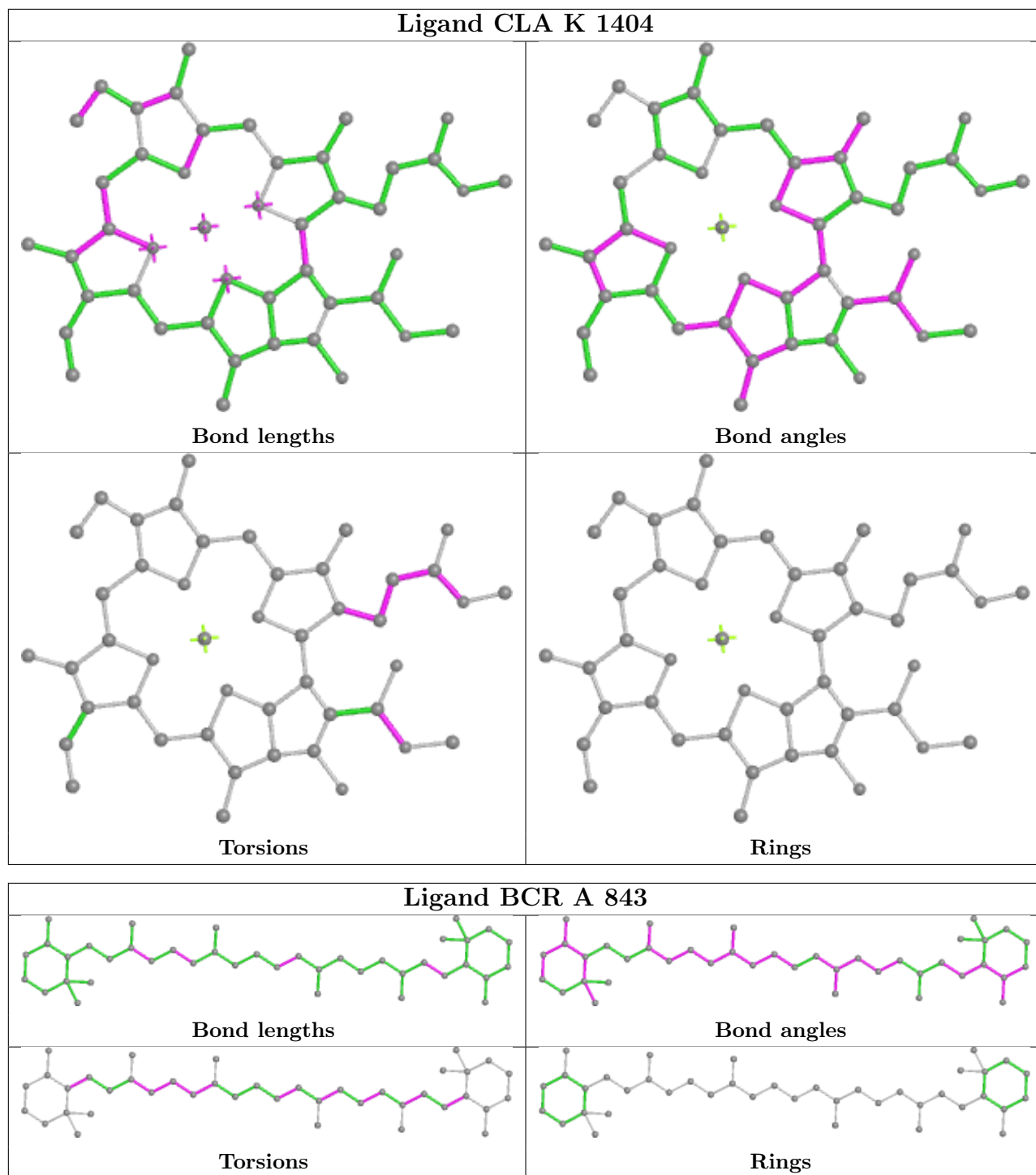


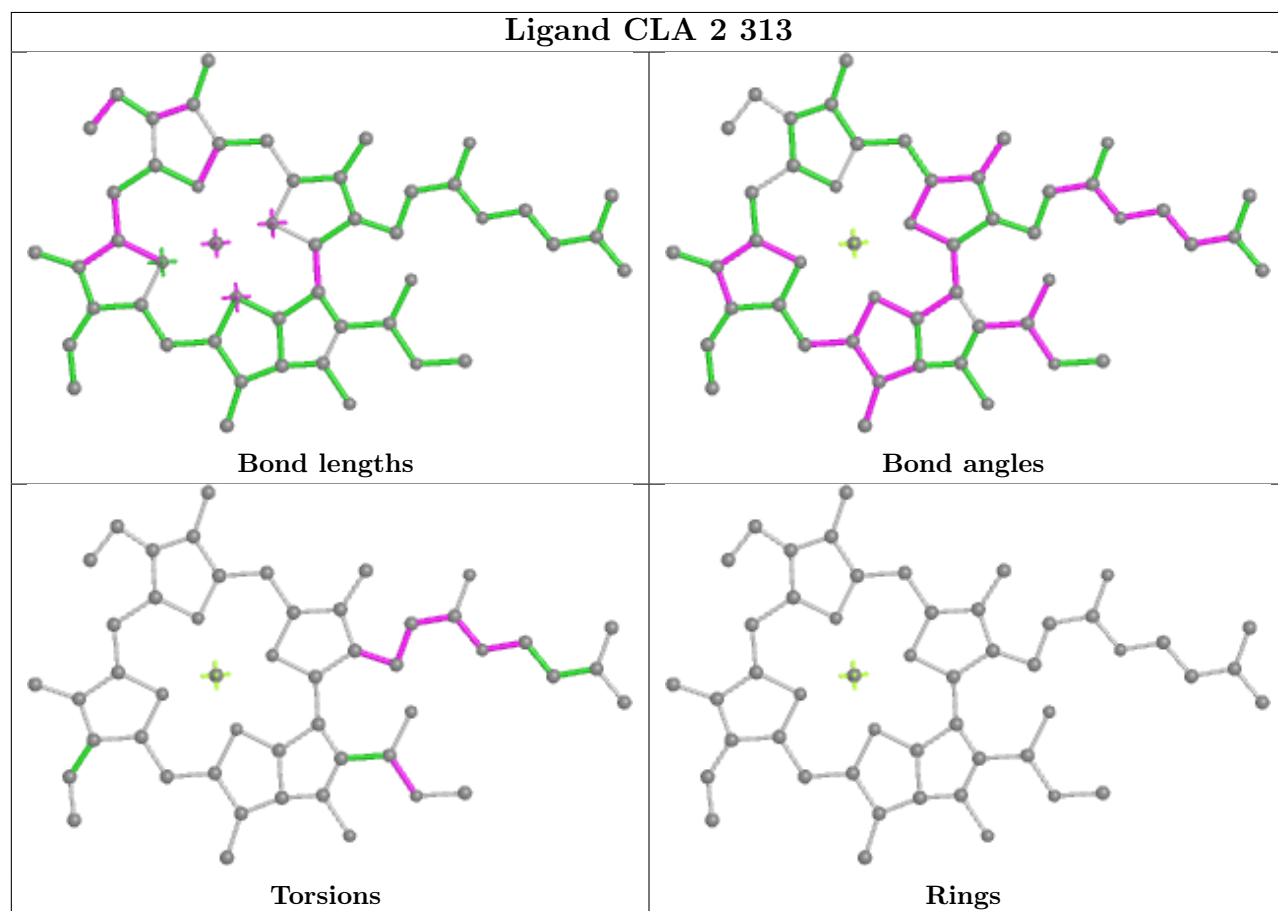
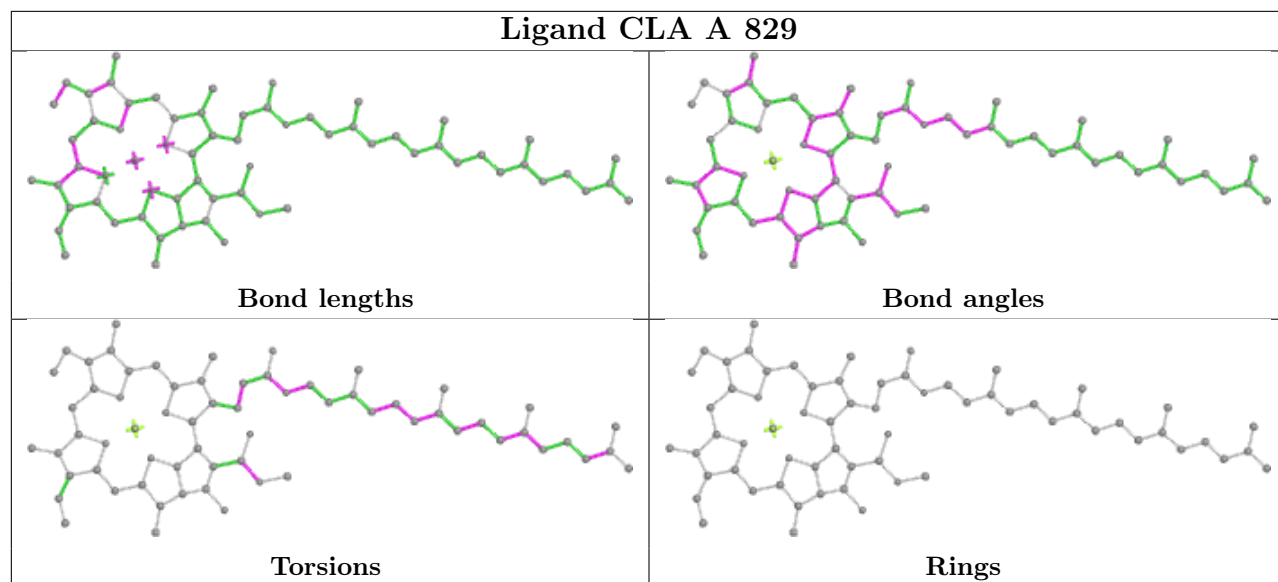




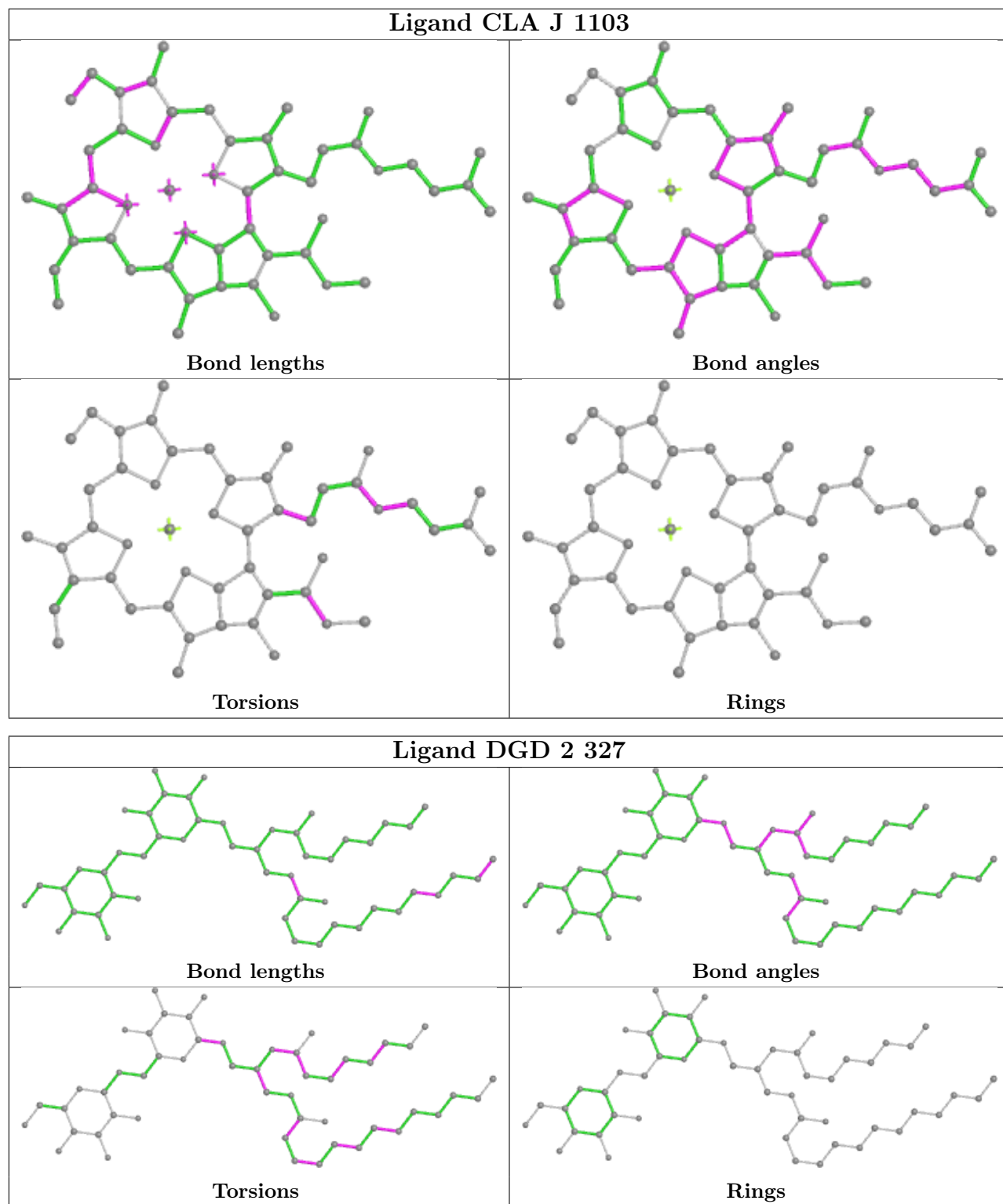


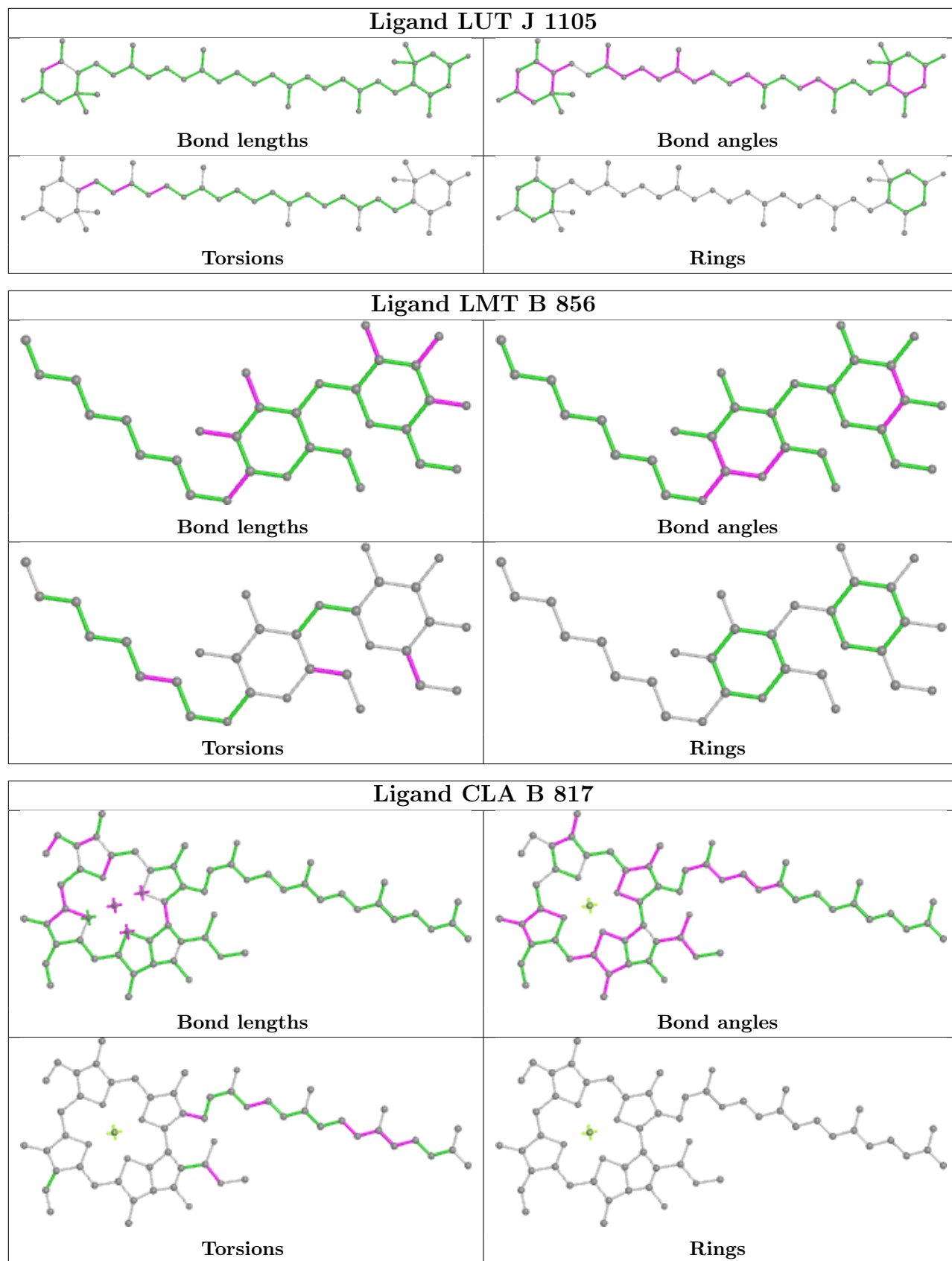


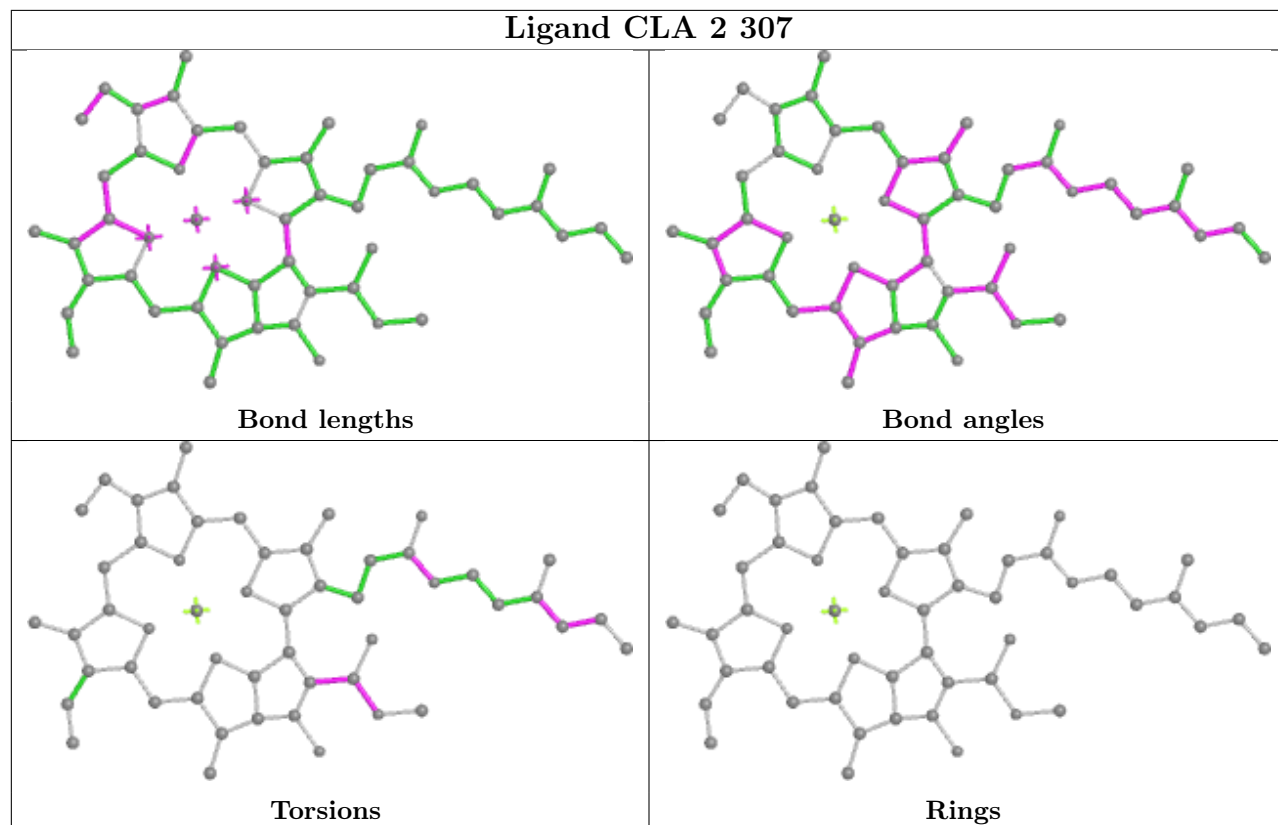
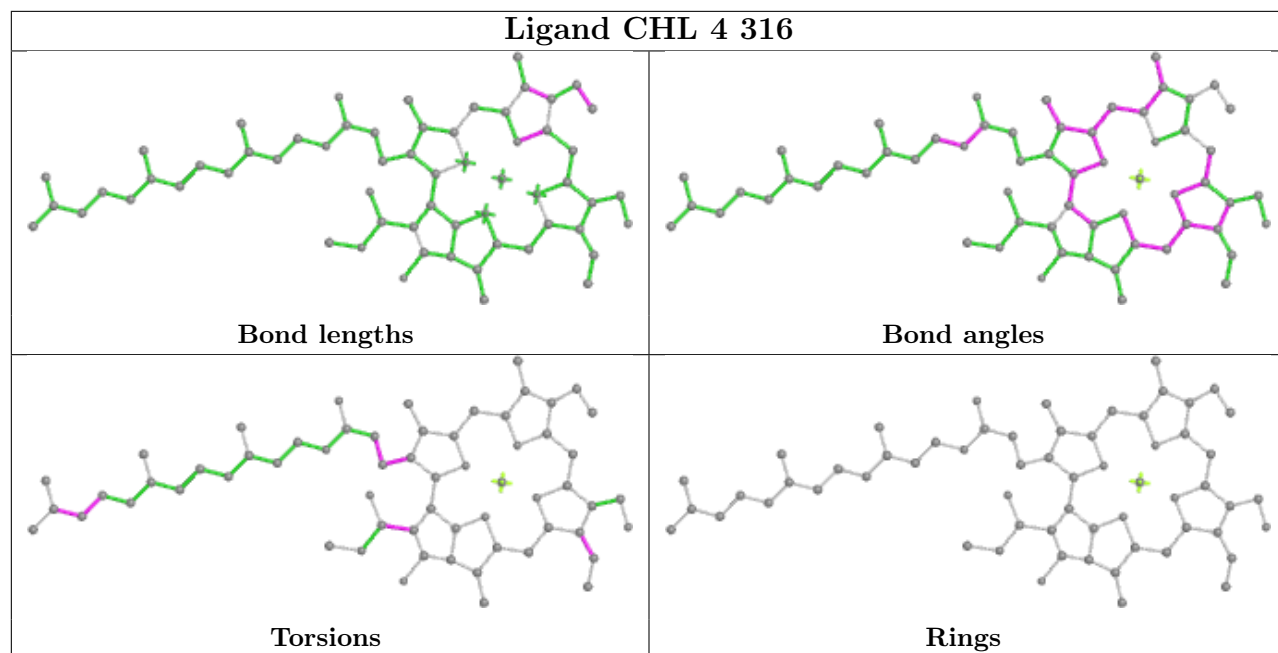


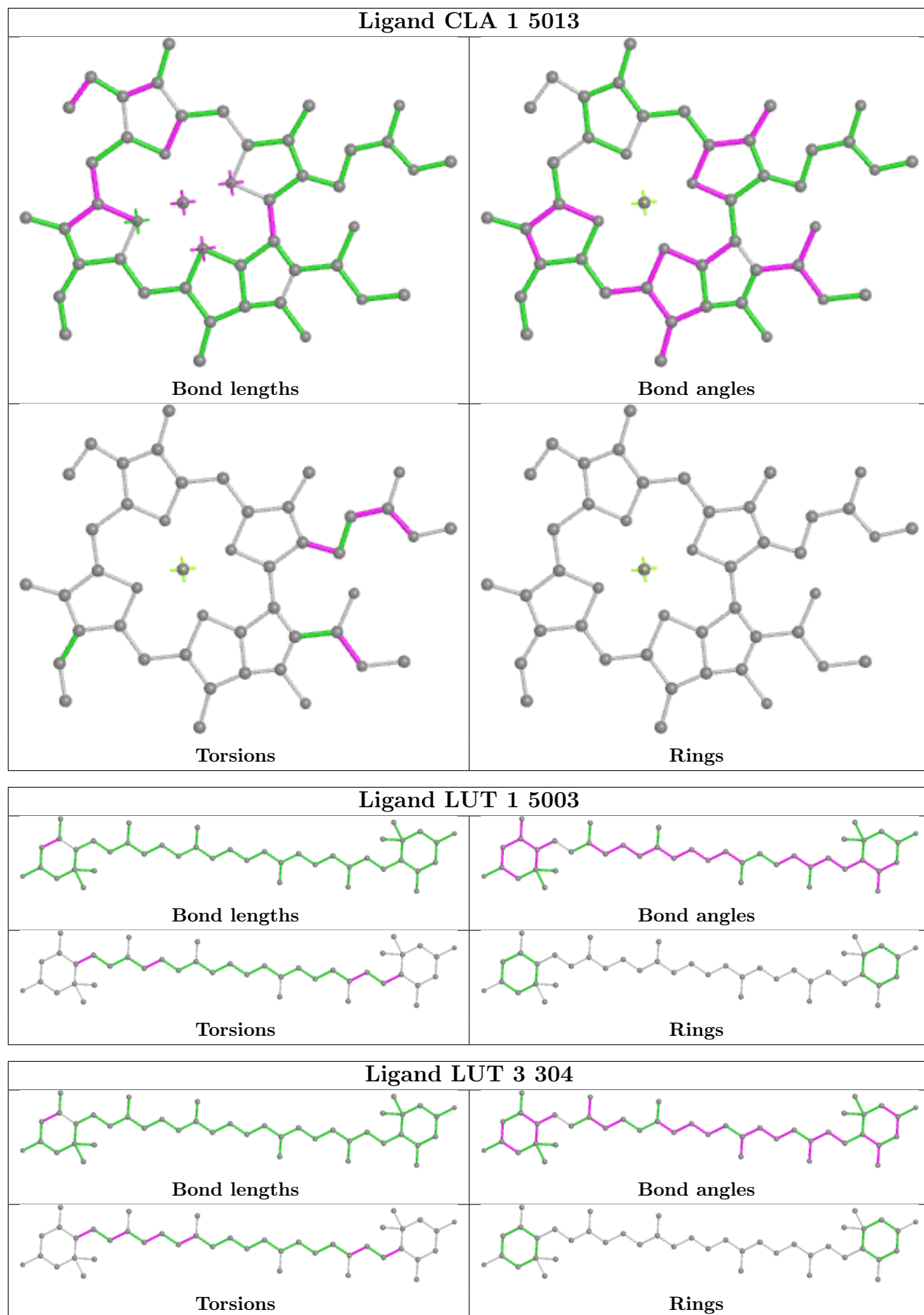


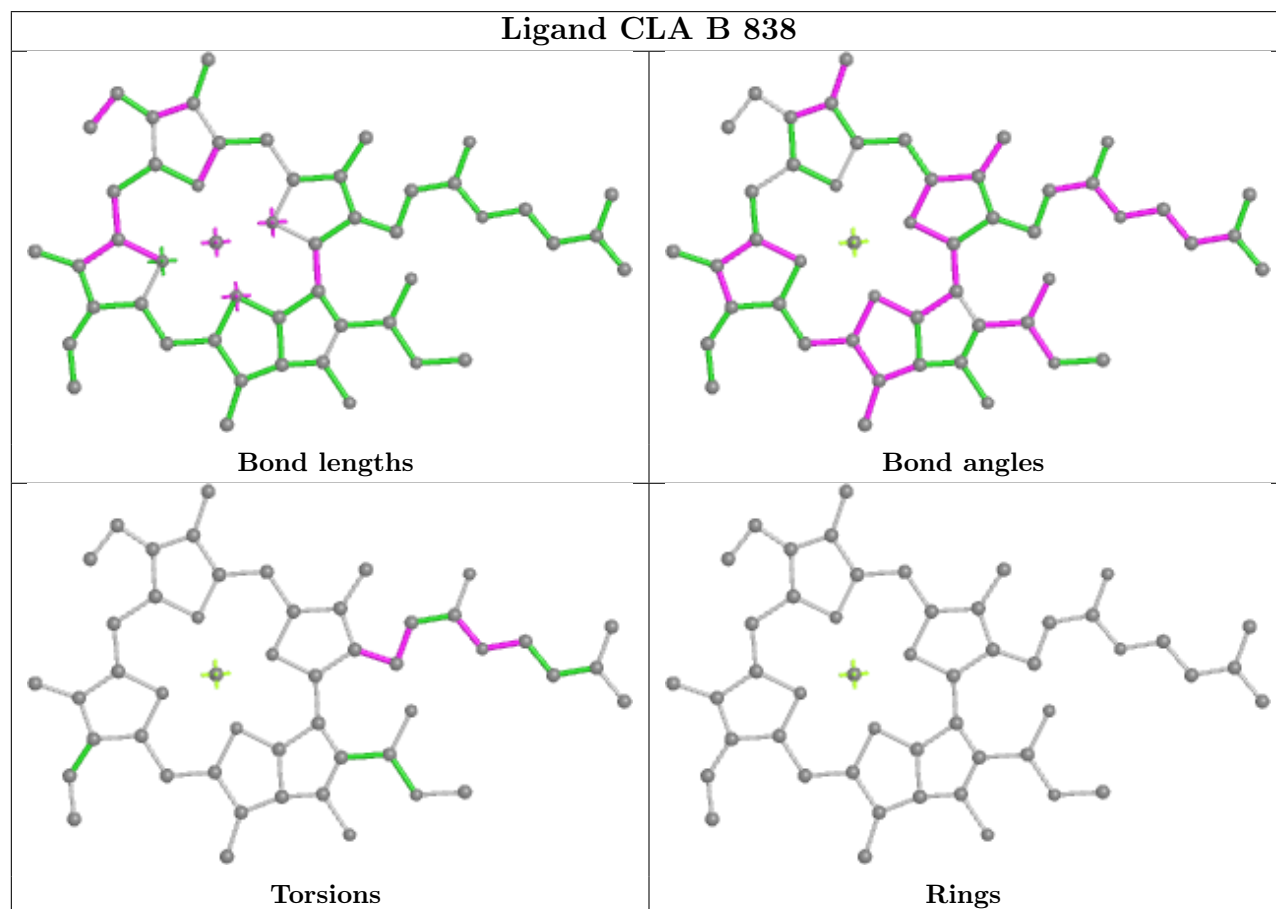
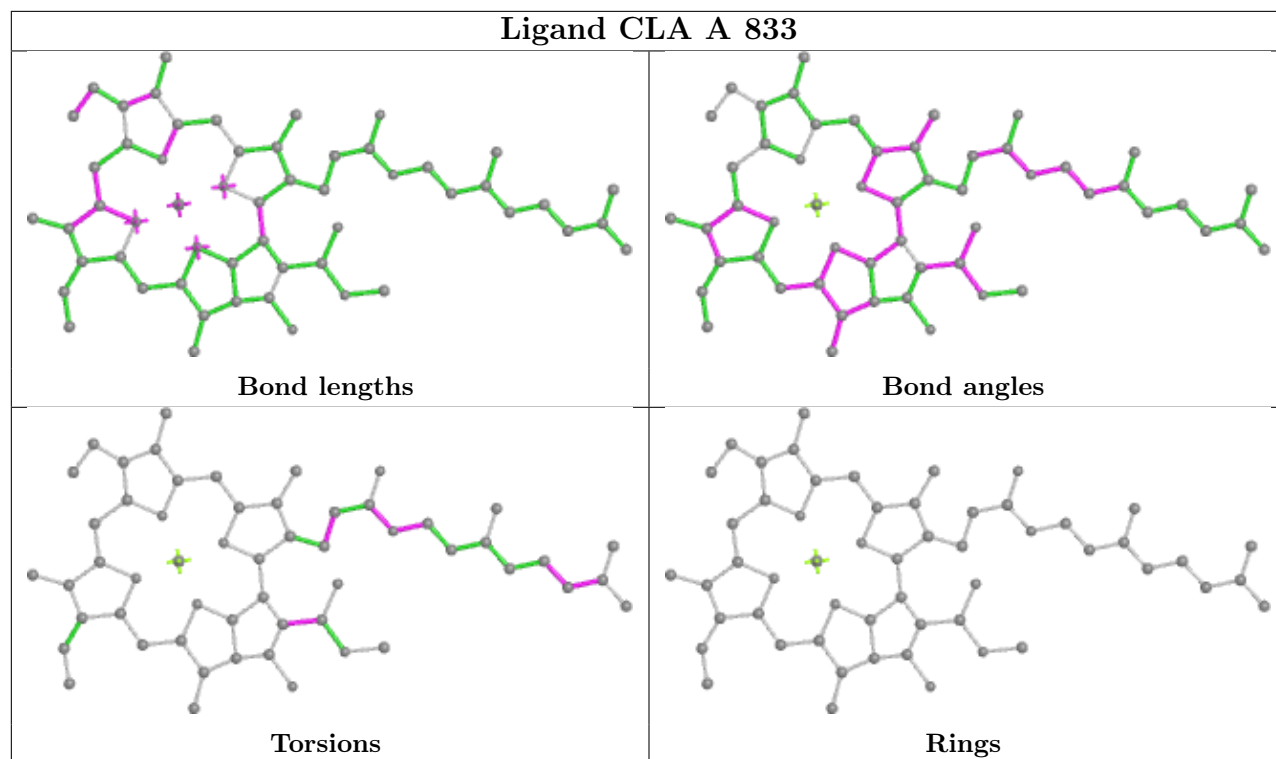


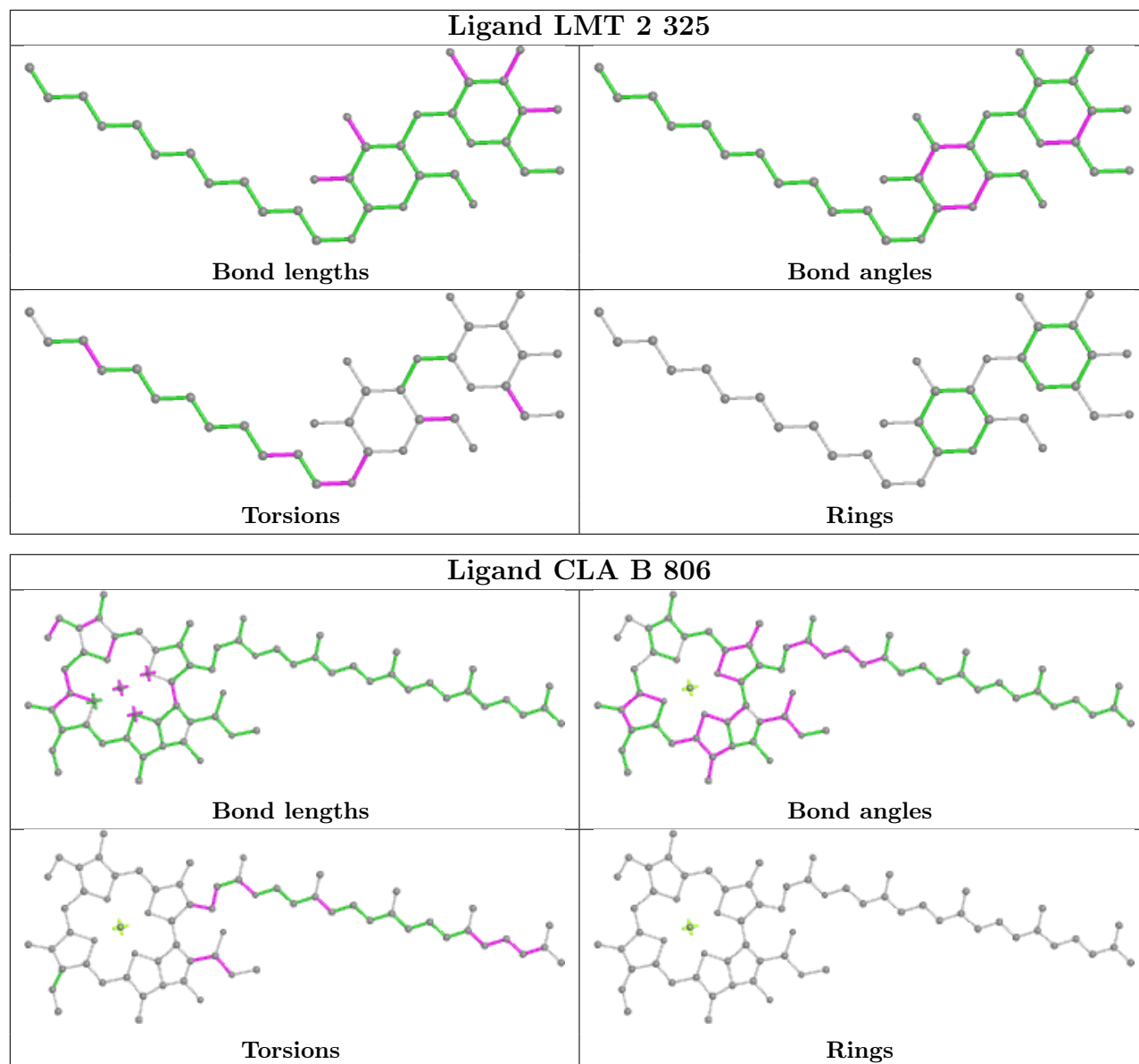


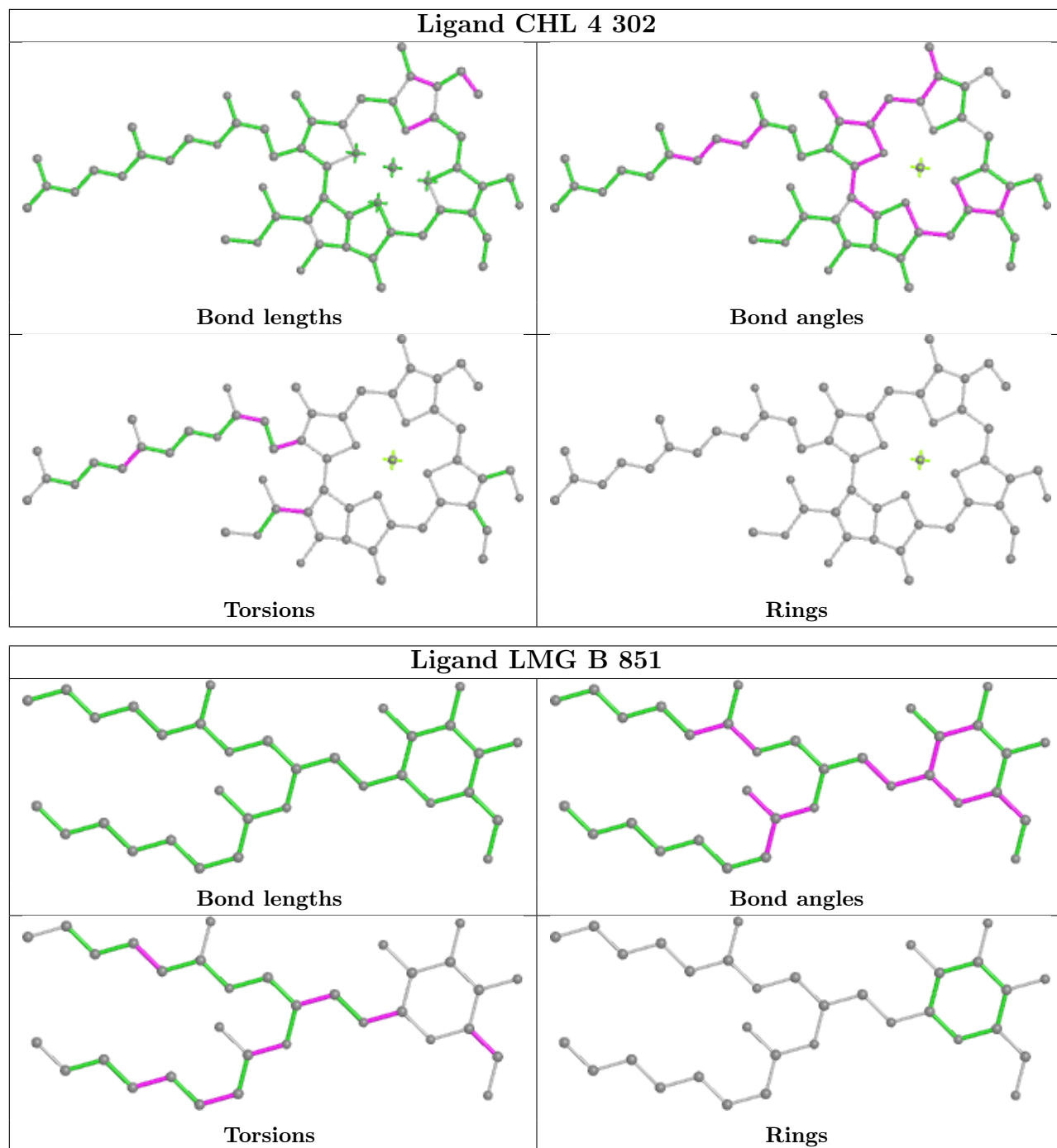


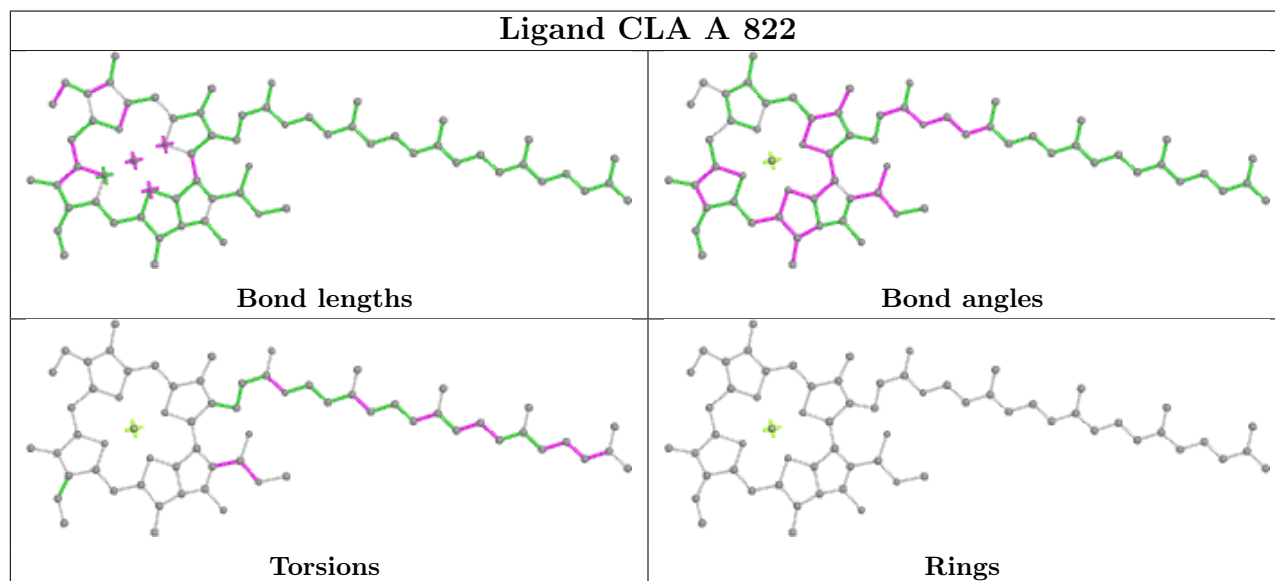
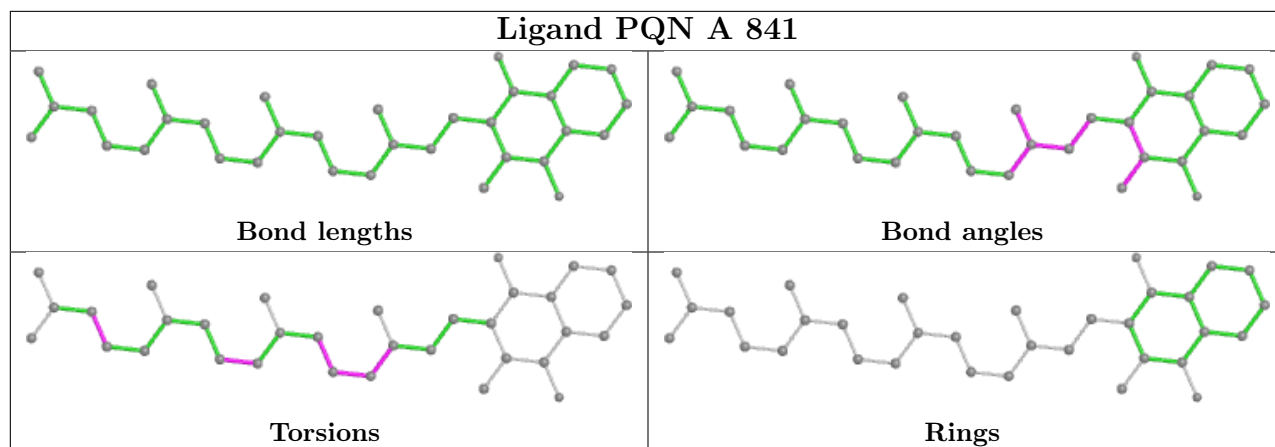




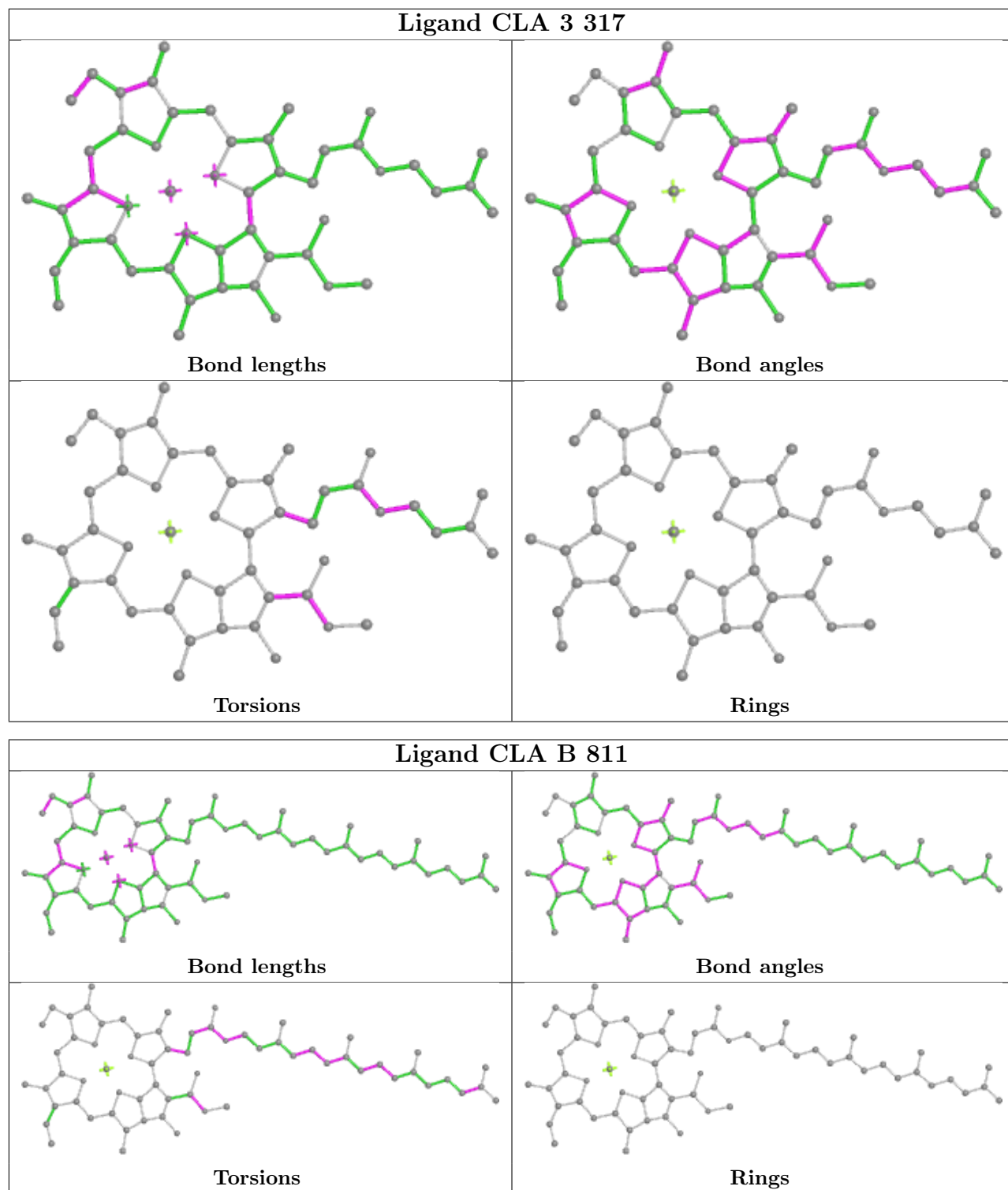


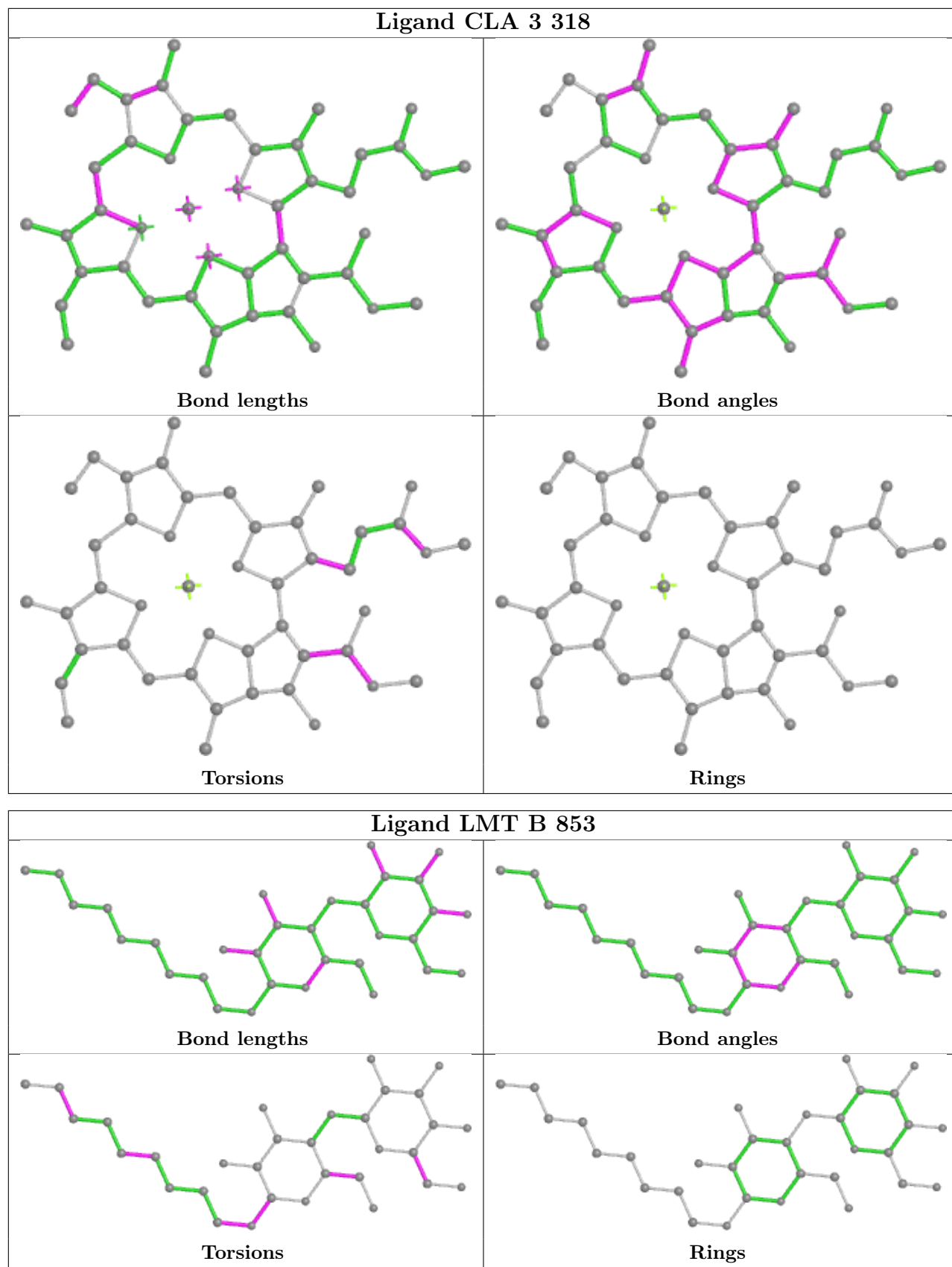


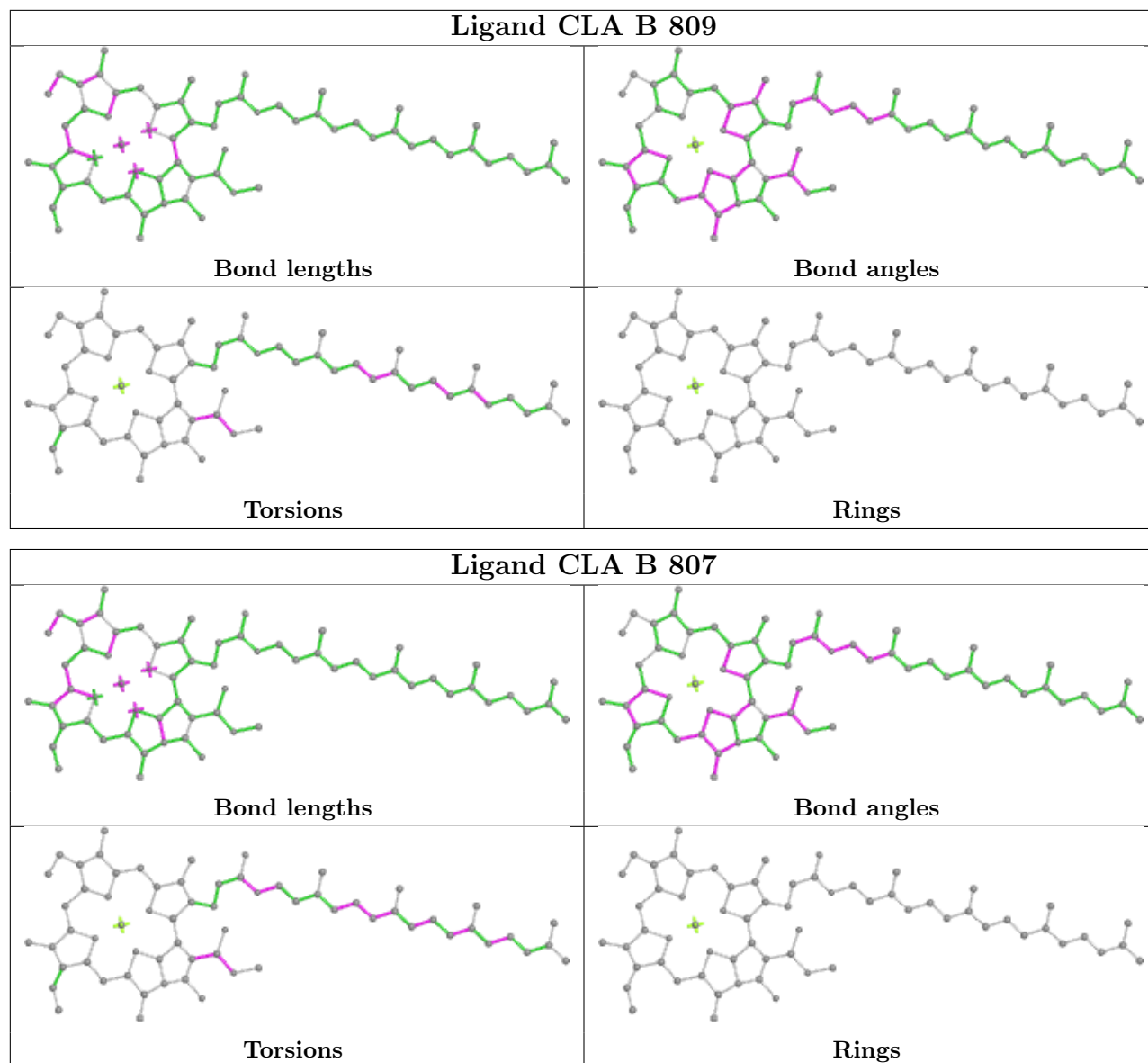


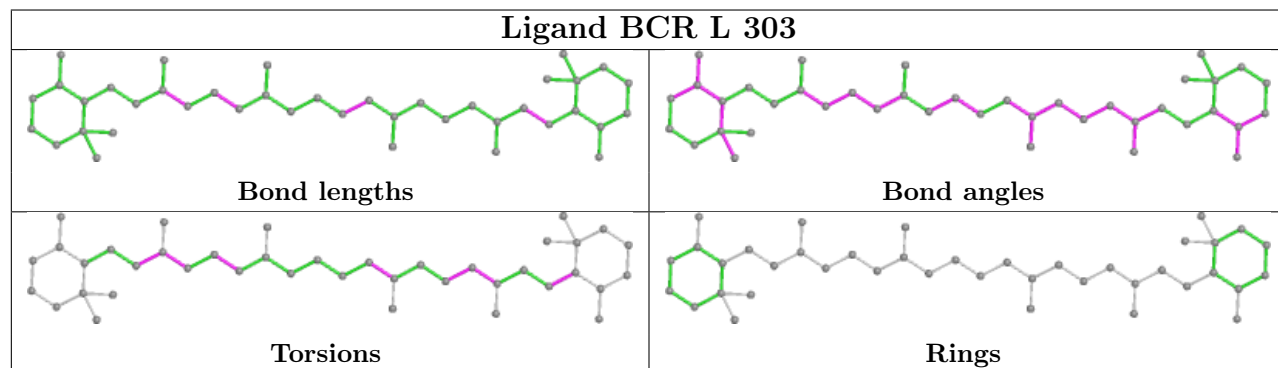
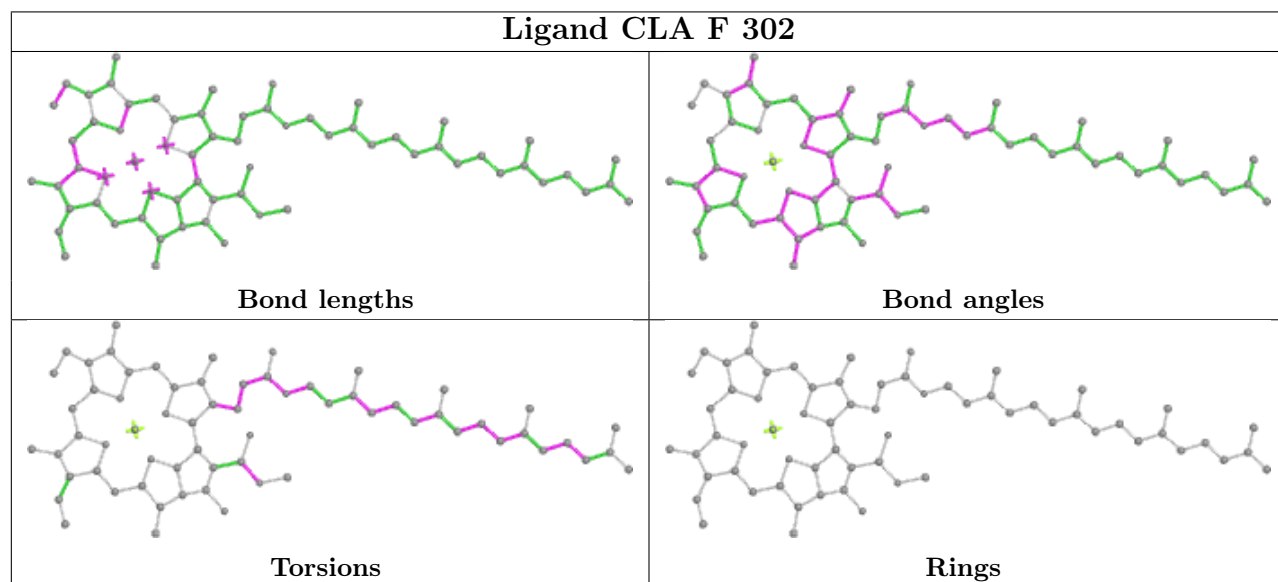
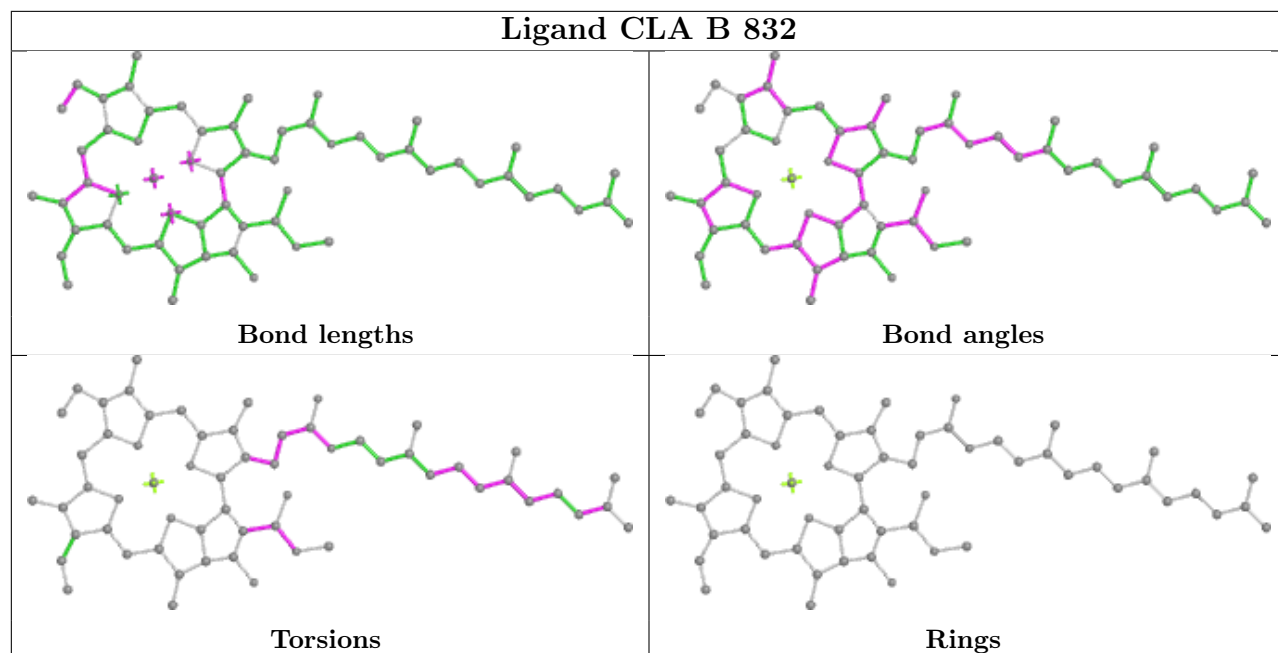


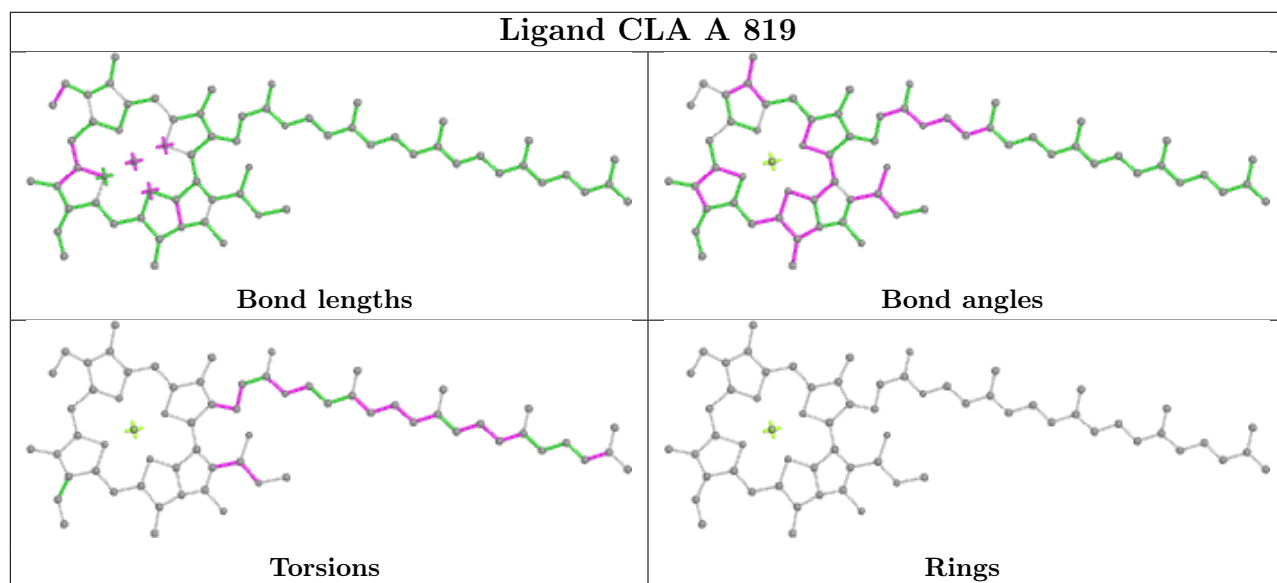
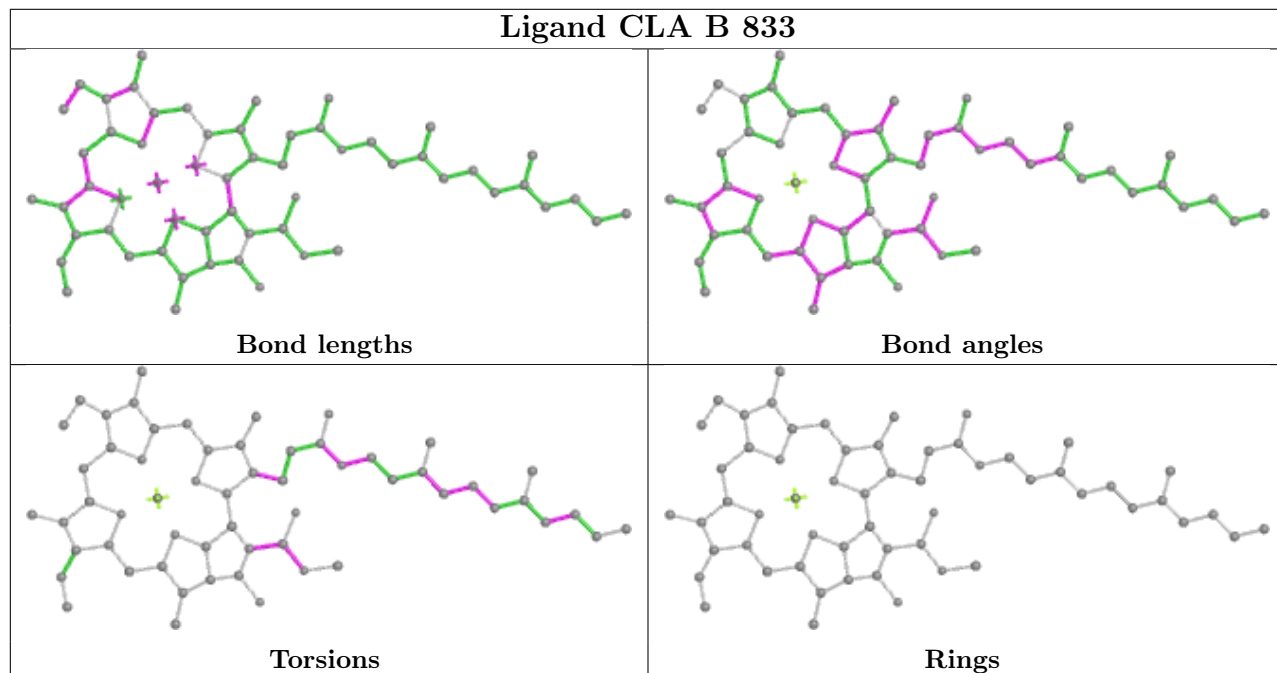
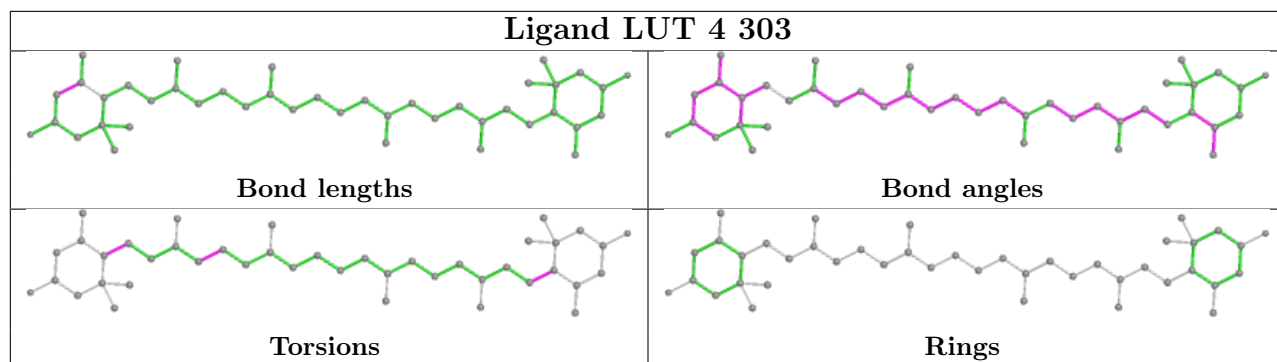


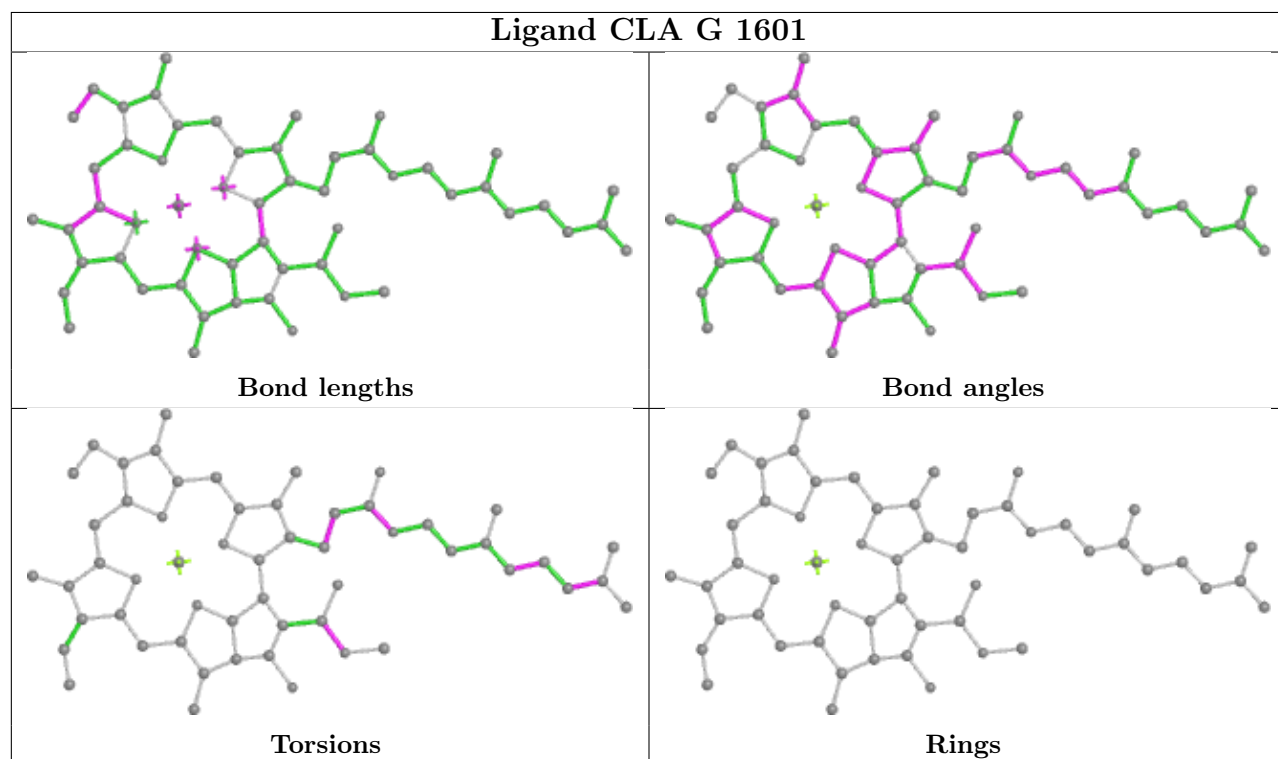
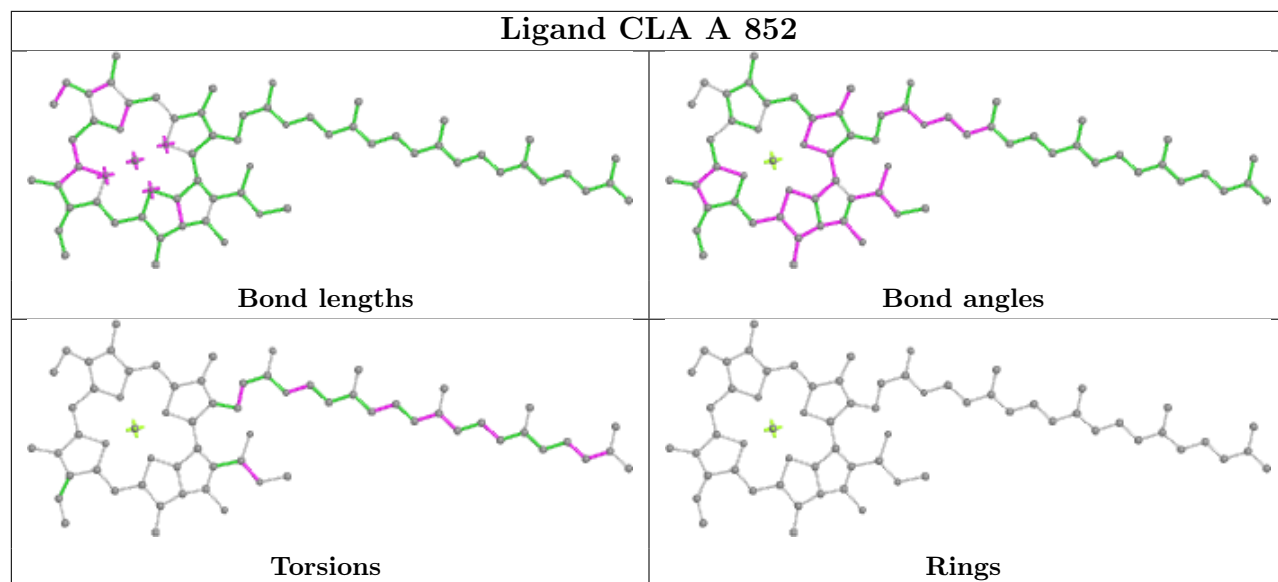


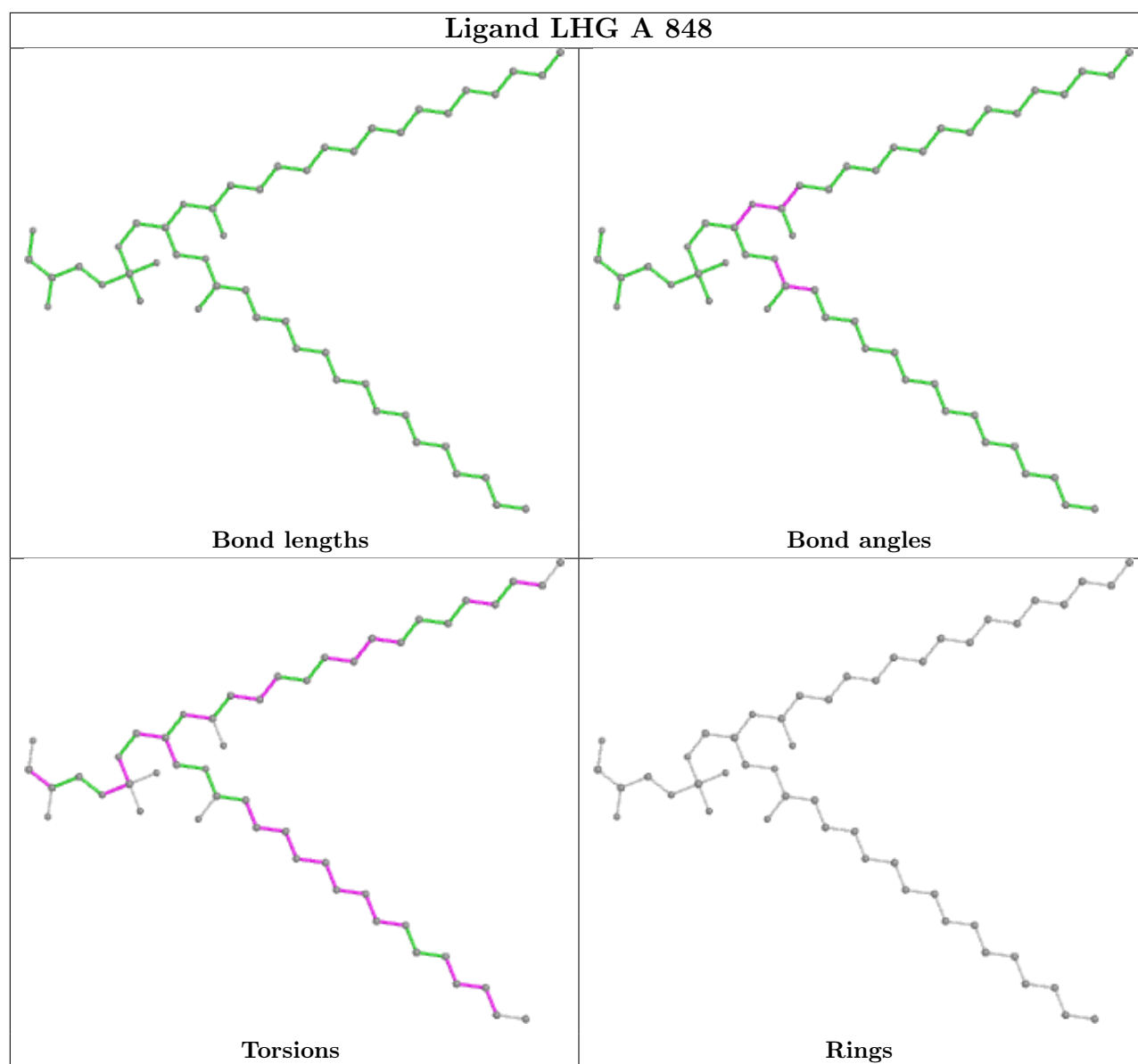


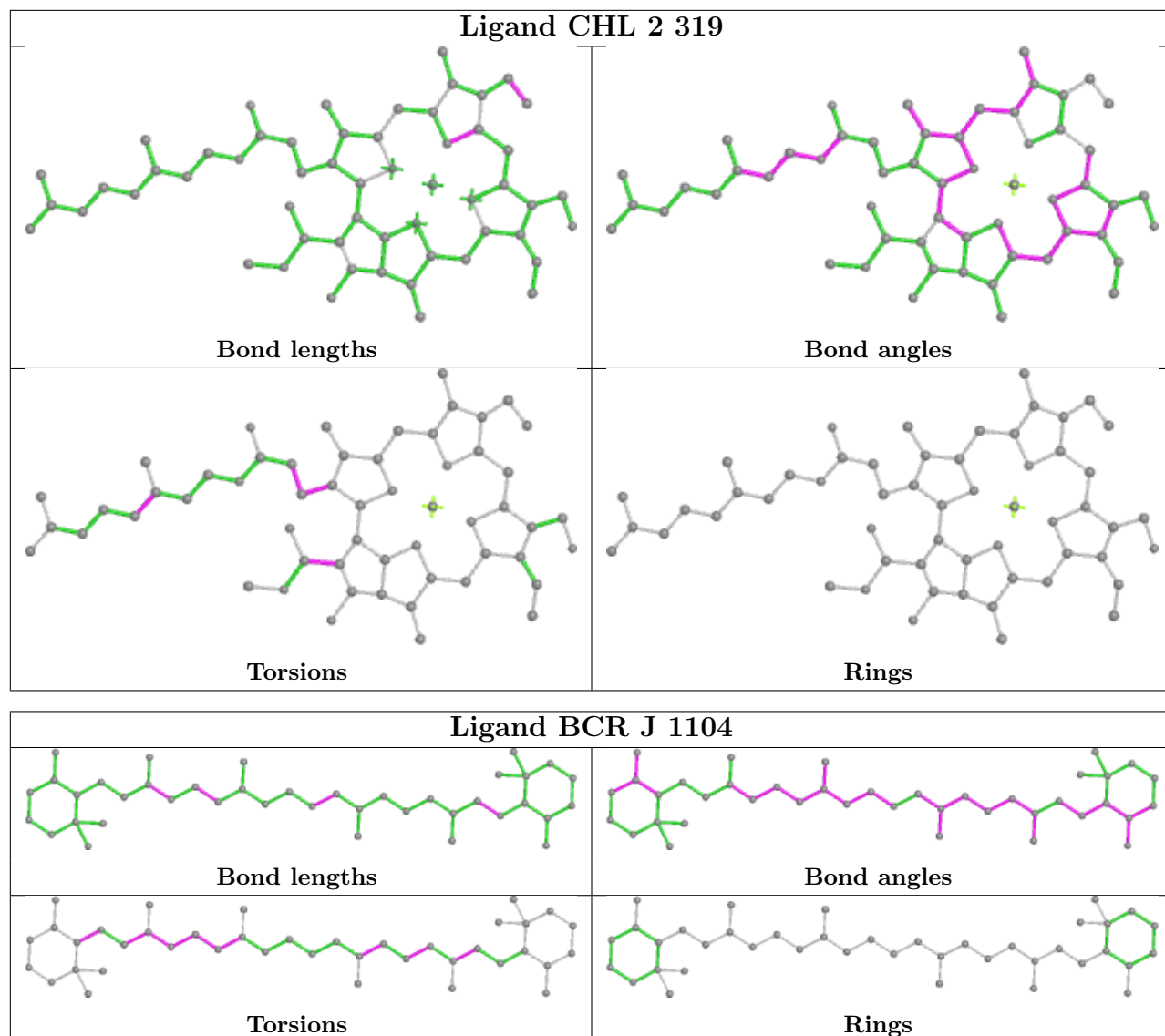




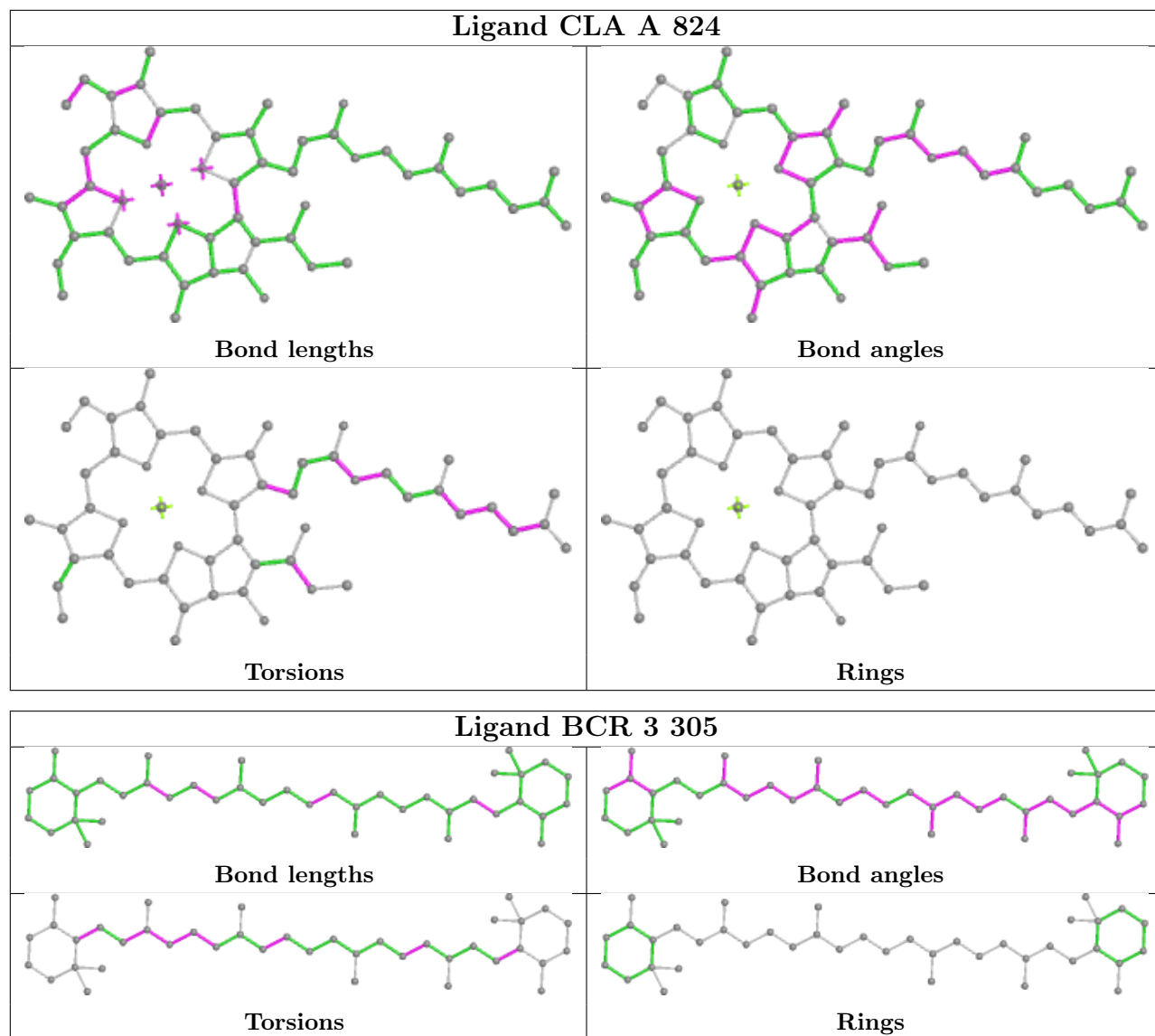












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	743/743 (100%)	-0.12	25 (3%) 45 19	68, 103, 151, 196	0
2	B	733/733 (100%)	-0.18	20 (2%) 54 26	67, 101, 138, 182	0
3	C	80/80 (100%)	-0.03	4 (5%) 28 10	77, 95, 158, 180	0
4	D	143/143 (100%)	0.00	12 (8%) 11 3	77, 105, 128, 151	0
5	E	66/66 (100%)	0.58	11 (16%) 1 0	85, 113, 168, 180	0
6	F	154/154 (100%)	-0.19	7 (4%) 33 12	82, 105, 141, 156	0
7	G	97/97 (100%)	-0.03	8 (8%) 11 3	109, 139, 165, 198	0
8	H	88/88 (100%)	-0.27	3 (3%) 45 19	100, 132, 160, 169	0
9	I	30/30 (100%)	-0.03	2 (6%) 17 5	97, 115, 132, 154	0
10	J	42/42 (100%)	-0.53	0 100 100	82, 96, 138, 171	0
11	K	80/80 (100%)	0.16	5 (6%) 20 6	142, 177, 208, 219	0
12	L	157/157 (100%)	-0.01	11 (7%) 16 5	96, 125, 173, 204	0
13	1	193/193 (100%)	0.59	32 (16%) 1 0	124, 156, 201, 228	0
14	2	208/208 (100%)	0.02	23 (11%) 5 1	106, 134, 168, 200	0
15	3	221/221 (100%)	0.29	25 (11%) 5 1	124, 161, 218, 248	0
16	4	198/198 (100%)	0.07	18 (9%) 9 3	110, 136, 174, 204	0
All	All	3233/3233 (100%)	-0.02	206 (6%) 19 6	67, 118, 178, 248	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	34	CYS	12.1
13	1	103	GLY	10.7
3	C	35	LYS	8.8
13	1	101	GLY	8.1
13	1	102	LEU	7.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
15	3	87	GLU	7.6
12	L	210	PRO	7.2
13	1	172	LYS	6.4
5	E	98	ASN	6.2
12	L	54	TYR	6.1
2	B	294	ASN	6.0
16	4	133	GLU	5.5
2	B	295	PHE	5.2
11	K	81	GLY	5.2
13	1	125	PRO	4.9
2	B	296	GLY	4.8
15	3	212	GLY	4.8
13	1	171	SER	4.7
7	G	114	LEU	4.7
12	L	111	VAL	4.6
13	1	123	GLY	4.6
5	E	129	LYS	4.5
13	1	219	ALA	4.5
3	C	33	GLY	4.5
13	1	100	LEU	4.4
13	1	155	PRO	4.4
12	L	128	GLN	4.4
8	H	78	TYR	4.4
4	D	71	THR	4.4
15	3	96	ARG	4.4
13	1	161	PRO	4.3
4	D	196	VAL	4.3
14	2	125	PHE	4.3
15	3	86	PRO	4.3
3	C	36	ALA	4.2
13	1	153	LYS	4.2
14	2	127	THR	4.1
7	G	111	TYR	3.9
15	3	121	TYR	3.9
13	1	59	PHE	3.9
11	K	97	ALA	3.9
1	A	46	LYS	3.8
13	1	127	PRO	3.8
14	2	124	GLU	3.8
4	D	208	PRO	3.7
16	4	53	LYS	3.7
12	L	209	LEU	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
15	3	211	LEU	3.7
14	2	130	GLY	3.6
13	1	99	ALA	3.6
16	4	122	ASN	3.6
14	2	128	LYS	3.6
16	4	64	GLY	3.6
16	4	52	LYS	3.6
6	F	78	ASP	3.6
4	D	206	LYS	3.5
2	B	214	SER	3.5
2	B	297	ILE	3.5
6	F	113	SER	3.4
6	F	189	LYS	3.4
8	H	115	SER	3.4
13	1	60	GLY	3.4
1	A	277	TYR	3.3
7	G	110	GLU	3.3
15	3	260	VAL	3.3
2	B	566	GLY	3.3
14	2	248	ASP	3.3
1	A	261	SER	3.3
1	A	262	PHE	3.3
2	B	215	VAL	3.2
2	B	299	HIS	3.2
15	3	97	TRP	3.2
14	2	131	ILE	3.1
1	A	209	GLY	3.1
16	4	196	PRO	3.1
13	1	173	ASP	3.1
2	B	213	LEU	3.1
12	L	110	LEU	3.0
15	3	213	PHE	3.0
13	1	151	MET	3.0
1	A	42	ARG	3.0
1	A	264	GLU	3.0
1	A	276	LYS	3.0
14	2	134	THR	3.0
12	L	115	VAL	2.9
11	K	92	GLN	2.9
13	1	176	LYS	2.9
14	2	132	LEU	2.9
4	D	72	PRO	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	E	66	ILE	2.9
4	D	211	LEU	2.9
1	A	215	SER	2.9
4	D	199	ILE	2.9
14	2	204	LEU	2.8
5	E	91	VAL	2.8
14	2	123	PRO	2.8
14	2	137	TRP	2.8
5	E	94	ASP	2.8
2	B	159	PRO	2.8
15	3	62	LYS	2.8
1	A	279	ASP	2.8
15	3	173	PHE	2.8
2	B	293	THR	2.8
15	3	92	PHE	2.8
13	1	152	GLU	2.7
6	F	112	ASP	2.7
5	E	106	ARG	2.7
14	2	187	LYS	2.7
1	A	257	GLN	2.7
2	B	211	ASN	2.7
14	2	251	PHE	2.7
14	2	133	ASN	2.7
12	L	124	GLU	2.7
7	G	153	LYS	2.6
6	F	109	TYR	2.6
14	2	135	PRO	2.6
2	B	212	PHE	2.6
1	A	214	GLY	2.6
12	L	201	PHE	2.6
14	2	136	SER	2.6
1	A	492	ILE	2.6
14	2	209	ALA	2.6
15	3	124	LYS	2.6
2	B	298	GLY	2.5
13	1	58	ASP	2.5
15	3	94	GLU	2.5
13	1	98	GLU	2.5
16	4	121	ILE	2.5
16	4	132	GLU	2.5
7	G	151	ASP	2.5
15	3	125	VAL	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
15	3	267	ASN	2.5
15	3	256	LEU	2.5
1	A	16	PRO	2.5
1	A	208	ALA	2.5
5	E	128	VAL	2.4
1	A	32	GLU	2.4
6	F	111	PRO	2.4
9	I	32	LEU	2.4
12	L	116	LYS	2.4
1	A	258	LEU	2.4
6	F	87	ASP	2.4
4	D	75	LEU	2.4
13	1	51	LEU	2.4
13	1	159	LYS	2.4
15	3	95	PRO	2.4
1	A	265	GLY	2.4
12	L	206	VAL	2.4
13	1	174	PRO	2.4
11	K	96	PRO	2.3
15	3	65	LEU	2.3
1	A	36	LYS	2.3
1	A	33	GLN	2.3
8	H	113	TYR	2.3
14	2	70	GLY	2.3
15	3	192	LYS	2.3
4	D	165	GLN	2.3
2	B	206	TYR	2.3
14	2	138	TYR	2.3
5	E	93	VAL	2.3
4	D	197	SER	2.3
14	2	129	LEU	2.3
13	1	150	SER	2.3
16	4	67	THR	2.3
13	1	49	SER	2.2
16	4	238	SER	2.2
13	1	61	PHE	2.2
13	1	177	PHE	2.2
7	G	113	SER	2.2
1	A	212	GLY	2.2
15	3	123	GLY	2.2
16	4	119	GLY	2.2
13	1	95	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	511	THR	2.2
15	3	89	THR	2.2
2	B	157	LEU	2.2
5	E	89	SER	2.2
7	G	109	LYS	2.2
5	E	68	PRO	2.2
4	D	156	TYR	2.2
14	2	208	SER	2.2
4	D	70	PHE	2.2
16	4	193	ASN	2.2
11	K	88	ASP	2.2
16	4	227	LYS	2.2
9	I	30	LYS	2.2
14	2	170	ASP	2.1
16	4	65	TYR	2.1
2	B	207	VAL	2.1
16	4	195	ALA	2.1
1	A	37	PRO	2.1
13	1	47	ARG	2.1
13	1	170	TYR	2.1
2	B	210	ASN	2.1
7	G	115	LEU	2.1
1	A	519	ASP	2.1
5	E	96	ASP	2.1
1	A	263	ALA	2.0
2	B	585	ASN	2.0
15	3	261	ALA	2.0
16	4	120	ILE	2.0
16	4	194	PHE	2.0
2	B	292	ARG	2.0
16	4	131	LYS	2.0
15	3	177	ALA	2.0
15	3	130	GLN	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
23	LMT	J	1107	25/35	0.45	0.46	151,182,201,206	0
26	DGD	1	5002	35/66	0.52	0.67	125,209,233,236	0
24	LMG	2	302	13/55	0.55	0.39	130,165,187,190	0
22	LHG	B	849	49/49	0.59	0.53	101,139,196,220	0
24	LMG	B	850	35/55	0.59	0.30	74,146,176,185	0
24	LMG	A	851	50/55	0.64	0.58	136,173,197,203	0
23	LMT	2	325	35/35	0.65	0.38	157,224,241,245	0
25	GOL	4	321	6/6	0.66	0.65	135,146,153,158	0
24	LMG	2	301	13/55	0.68	0.46	148,168,192,202	0
24	LMG	B	851	33/55	0.68	0.38	133,208,223,227	0
21	BCR	2	305	40/40	0.71	0.57	131,154,181,186	0
24	LMG	1	5020	46/55	0.71	0.60	88,157,201,209	0
23	LMT	A	850	35/35	0.71	0.46	79,146,165,174	0
21	BCR	1	5005	40/40	0.72	0.57	135,175,224,229	0
24	LMG	G	1607	25/55	0.72	0.37	130,194,215,220	0
24	LMG	1	5001	49/55	0.72	0.38	91,156,219,221	0
18	CLA	K	1404	46/65	0.72	0.41	170,208,235,242	0
21	BCR	K	1405	40/40	0.74	0.54	138,166,194,201	0
21	BCR	L	302	40/40	0.74	0.44	118,167,216,221	0
21	BCR	3	306	40/40	0.75	0.79	134,160,182,188	0
24	LMG	4	320	13/55	0.75	0.41	166,194,213,219	0
24	LMG	2	323	13/55	0.76	0.19	126,164,190,192	0
21	BCR	G	1604	40/40	0.77	0.30	106,133,171,173	0
18	CLA	K	1401	45/65	0.77	0.36	133,166,181,194	0
21	BCR	B	845	40/40	0.78	0.44	92,121,179,183	0
23	LMT	B	852	35/35	0.79	0.54	114,212,231,232	0
23	LMT	G	1606	31/35	0.79	0.44	144,198,232,237	0
18	CLA	A	823	65/65	0.81	0.37	82,110,130,137	0
21	BCR	A	855	40/40	0.81	0.43	128,148,176,177	0
18	CLA	K	1402	60/65	0.81	0.48	100,164,183,192	0
27	CA	3	302	1/1	0.81	0.23	129,129,129,129	0
29	LUT	J	1105	42/42	0.81	0.33	89,122,148,163	0
29	LUT	3	303	42/42	0.81	0.49	145,166,176,181	0
29	LUT	3	304	42/42	0.81	0.34	116,146,169,173	0
24	LMG	2	322	36/55	0.82	0.35	111,177,212,217	0
24	LMG	F	307	36/55	0.82	0.46	125,159,194,197	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	LMT	4	319	35/35	0.82	0.36	95,179,207,207	0
25	GOL	A	854	6/6	0.82	0.80	124,136,142,142	0
24	LMG	2	321	25/55	0.82	0.18	114,144,164,168	0
18	CLA	3	314	48/65	0.83	0.36	159,194,205,208	0
18	CLA	J	1103	50/65	0.83	0.22	92,155,195,209	0
18	CLA	H	1701	60/65	0.83	0.29	148,175,199,206	0
18	CLA	1	5013	46/65	0.83	0.25	118,159,175,202	0
29	LUT	4	303	42/42	0.83	0.37	106,128,148,160	0
26	DGD	B	855	61/66	0.84	0.29	70,100,132,155	0
26	DGD	F	309	57/66	0.84	0.39	105,158,186,192	0
21	BCR	A	845	40/40	0.84	0.39	79,99,155,162	0
24	LMG	J	1102	30/55	0.84	0.29	103,123,146,159	0
21	BCR	B	844	40/40	0.84	0.35	81,109,151,165	0
21	BCR	L	307	40/40	0.84	0.47	102,130,153,164	0
24	LMG	B	854	13/55	0.84	0.20	131,170,201,202	0
23	LMT	G	1605	35/35	0.84	0.31	116,177,214,218	0
18	CLA	G	1603	65/65	0.85	0.27	127,161,197,202	0
21	BCR	A	846	40/40	0.85	0.32	72,100,129,147	0
29	LUT	2	303	42/42	0.85	0.38	114,132,145,159	0
18	CLA	1	5017	45/65	0.85	0.23	159,182,206,210	0
18	CLA	B	816	55/65	0.85	0.27	107,133,154,171	0
26	DGD	2	327	51/66	0.85	0.20	99,129,165,174	0
21	BCR	B	846	40/40	0.86	0.33	73,106,123,130	0
21	BCR	B	847	40/40	0.86	0.31	73,99,115,120	0
24	LMG	F	308	34/55	0.86	0.39	102,163,181,202	0
18	CLA	A	803	65/65	0.86	0.28	67,91,146,172	0
24	LMG	2	324	13/55	0.86	0.13	159,183,205,212	0
18	CLA	B	818	65/65	0.86	0.31	82,102,119,128	0
18	CLA	4	311	60/65	0.86	0.30	117,134,155,167	0
21	BCR	L	303	40/40	0.86	0.30	90,108,127,135	0
18	CLA	B	810	65/65	0.86	0.28	87,116,141,161	0
31	XAT	2	304	44/44	0.86	0.30	106,124,144,150	0
18	CLA	1	5015	65/65	0.87	0.26	140,176,193,202	0
28	ZEX	F	310	42/42	0.87	0.24	104,141,157,167	0
22	LHG	1	5019	49/49	0.87	0.26	112,135,168,176	0
29	LUT	1	5003	42/42	0.87	0.43	117,157,181,193	0
30	CHL	3	310	66/66	0.87	0.23	107,148,166,194	0
30	CHL	3	313	51/66	0.87	0.21	185,220,249,260	0
29	LUT	1	5004	42/42	0.87	0.34	105,145,165,174	0
21	BCR	B	843	40/40	0.88	0.35	104,121,144,166	0
18	CLA	L	304	50/65	0.88	0.23	123,151,170,179	0
18	CLA	3	307	55/65	0.88	0.26	148,169,183,191	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
30	CHL	3	312	51/66	0.88	0.19	141,157,177,183	0
18	CLA	4	312	46/65	0.88	0.17	115,145,160,175	0
21	BCR	3	305	40/40	0.88	0.24	120,134,155,161	0
18	CLA	A	840	60/65	0.89	0.27	101,147,196,206	0
18	CLA	2	311	50/65	0.89	0.30	116,139,154,158	0
23	LMT	B	853	32/35	0.89	0.37	121,153,174,179	0
30	CHL	1	5014	47/66	0.89	0.23	139,168,192,198	0
30	CHL	2	318	46/66	0.89	0.18	117,142,157,175	0
18	CLA	L	306	50/65	0.89	0.42	101,134,155,170	0
18	CLA	K	1403	48/65	0.89	0.31	166,197,226,242	0
26	DGD	J	1106	58/66	0.89	0.32	67,115,186,193	0
30	CHL	4	316	61/66	0.89	0.33	121,144,165,172	0
18	CLA	A	833	55/65	0.89	0.34	113,137,165,171	0
18	CLA	A	824	55/65	0.90	0.31	82,99,124,135	0
18	CLA	B	834	60/65	0.90	0.22	82,106,129,140	0
18	CLA	B	841	65/65	0.90	0.22	72,107,126,133	0
18	CLA	3	309	55/65	0.90	0.22	132,175,204,219	0
18	CLA	B	805	65/65	0.90	0.23	89,123,175,194	0
18	CLA	4	310	50/65	0.90	0.23	125,146,176,189	0
18	CLA	B	808	65/65	0.90	0.26	87,100,144,165	0
21	BCR	I	102	40/40	0.90	0.28	83,115,133,139	0
18	CLA	1	5008	55/65	0.90	0.20	114,142,159,162	0
18	CLA	A	825	65/65	0.90	0.27	85,116,136,143	0
18	CLA	A	814	46/65	0.90	0.26	127,143,167,179	0
31	XAT	4	304	44/44	0.90	0.26	92,127,146,156	0
18	CLA	1	5006	65/65	0.91	0.20	137,169,186,193	0
21	BCR	4	301	40/40	0.91	0.24	120,140,157,165	0
18	CLA	3	319	60/65	0.91	0.28	118,140,186,194	0
18	CLA	4	306	50/65	0.91	0.23	118,145,159,169	0
18	CLA	A	810	65/65	0.91	0.30	70,97,115,128	0
18	CLA	1	5009	65/65	0.91	0.29	91,137,151,157	0
18	CLA	B	801	65/65	0.91	0.26	63,84,96,109	0
30	CHL	2	315	56/66	0.91	0.25	109,151,170,175	0
21	BCR	A	844	40/40	0.91	0.31	87,115,169,186	0
30	CHL	2	319	56/66	0.91	0.15	117,147,181,192	0
18	CLA	A	829	65/65	0.91	0.26	78,118,173,180	0
18	CLA	B	835	55/65	0.91	0.21	99,115,163,178	0
27	CA	B	857	1/1	0.91	0.06	123,123,123,123	0
30	CHL	4	302	56/66	0.91	0.20	109,129,143,148	0
18	CLA	A	816	56/65	0.91	0.26	93,129,143,150	0
18	CLA	A	836	65/65	0.91	0.29	80,107,169,181	0
18	CLA	B	811	65/65	0.91	0.28	82,109,139,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
18	CLA	A	813	65/65	0.92	0.23	104,133,165,180	0
18	CLA	A	809	50/65	0.92	0.23	97,128,146,159	0
18	CLA	A	831	65/65	0.92	0.24	81,104,128,146	0
21	BCR	A	843	40/40	0.92	0.24	86,116,155,162	0
18	CLA	B	812	60/65	0.92	0.21	94,128,153,169	0
18	CLA	B	814	65/65	0.92	0.23	84,107,122,131	0
18	CLA	A	832	65/65	0.92	0.30	92,120,139,165	0
18	CLA	L	305	60/65	0.92	0.24	93,121,133,146	0
18	CLA	B	817	60/65	0.92	0.19	110,133,148,156	0
18	CLA	A	815	65/65	0.92	0.24	135,149,171,179	0
18	CLA	B	822	65/65	0.92	0.23	95,114,160,165	0
18	CLA	B	826	65/65	0.92	0.25	67,88,122,124	0
24	LMG	F	306	47/55	0.92	0.23	96,131,158,169	0
18	CLA	1	5011	50/65	0.92	0.26	146,167,182,191	0
18	CLA	B	827	65/65	0.92	0.24	74,94,112,120	0
18	CLA	A	806	60/65	0.92	0.22	79,112,152,161	0
18	CLA	A	818	50/65	0.92	0.28	101,128,151,163	0
30	CHL	1	5016	61/66	0.92	0.25	114,154,166,171	0
18	CLA	B	839	65/65	0.92	0.27	82,101,124,130	0
18	CLA	2	317	55/65	0.92	0.26	91,126,157,174	0
18	CLA	A	852	65/65	0.92	0.24	70,91,105,112	0
18	CLA	3	308	52/65	0.92	0.20	165,202,217,224	0
18	CLA	F	303	65/65	0.92	0.21	83,116,145,166	0
18	CLA	A	811	55/65	0.92	0.31	102,127,140,151	0
18	CLA	3	317	50/65	0.92	0.27	111,145,156,171	0
30	CHL	4	313	47/66	0.92	0.19	104,133,160,176	0
18	CLA	A	812	65/65	0.92	0.28	92,113,130,139	0
18	CLA	4	305	60/65	0.92	0.32	119,141,161,167	0
18	CLA	J	1101	65/65	0.92	0.18	65,87,114,129	0
18	CLA	B	830	65/65	0.93	0.21	77,98,128,139	0
18	CLA	B	815	65/65	0.93	0.24	96,116,136,155	0
18	CLA	A	835	65/65	0.93	0.25	89,114,148,162	0
18	CLA	L	301	55/65	0.93	0.25	89,120,136,145	0
18	CLA	B	837	65/65	0.93	0.19	68,88,105,114	0
21	BCR	F	304	40/40	0.93	0.22	67,85,100,105	0
18	CLA	3	311	55/65	0.93	0.25	113,139,155,160	0
18	CLA	A	804	65/65	0.93	0.21	78,91,114,138	0
21	BCR	J	1104	40/40	0.93	0.22	67,92,114,125	0
18	CLA	A	819	65/65	0.93	0.23	78,111,133,145	0
18	CLA	F	302	65/65	0.93	0.31	73,107,198,210	0
18	CLA	B	821	46/65	0.93	0.28	110,126,143,155	0
17	CL0	A	801	65/65	0.93	0.27	65,86,99,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
18	CLA	1	5010	65/65	0.93	0.25	89,146,162,180	0
18	CLA	B	823	65/65	0.93	0.24	87,114,150,162	0
18	CLA	A	834	51/65	0.93	0.40	81,106,134,147	0
18	CLA	4	315	65/65	0.93	0.29	107,134,164,176	0
19	PQN	B	842	33/33	0.93	0.24	67,84,105,120	0
18	CLA	B	804	65/65	0.93	0.30	69,90,105,117	0
18	CLA	B	828	65/65	0.93	0.31	72,100,128,141	0
22	LHG	2	320	35/49	0.93	0.21	101,131,149,160	0
18	CLA	1	5018	60/65	0.93	0.16	88,137,192,196	0
18	CLA	2	307	52/65	0.93	0.14	120,144,157,159	0
30	CHL	4	314	51/66	0.93	0.24	120,144,159,172	0
18	CLA	2	310	65/65	0.93	0.25	107,128,155,166	0
30	CHL	4	317	43/66	0.93	0.13	125,162,177,190	0
23	LMT	B	856	31/35	0.93	0.20	138,156,173,179	0
21	BCR	B	802	40/40	0.93	0.26	72,100,119,128	0
18	CLA	B	831	65/65	0.94	0.21	69,88,115,121	0
18	CLA	B	832	60/65	0.94	0.24	70,99,137,153	0
18	CLA	A	828	65/65	0.94	0.22	64,79,99,118	0
18	CLA	A	817	65/65	0.94	0.41	84,115,134,143	0
18	CLA	B	836	55/65	0.94	0.21	74,92,108,115	0
18	CLA	3	318	46/65	0.94	0.17	140,158,170,172	0
18	CLA	B	806	65/65	0.94	0.22	76,92,112,121	0
18	CLA	B	838	50/65	0.94	0.30	69,91,103,126	0
18	CLA	1	5007	46/65	0.94	0.15	122,149,167,180	0
22	LHG	A	848	49/49	0.94	0.23	63,90,107,112	0
18	CLA	4	307	65/65	0.94	0.17	109,135,157,165	0
18	CLA	4	309	60/65	0.94	0.24	83,123,138,143	0
18	CLA	B	819	65/65	0.94	0.28	82,104,123,132	0
18	CLA	B	840	65/65	0.94	0.30	74,97,120,127	0
18	CLA	A	830	65/65	0.94	0.27	77,95,108,122	0
18	CLA	B	809	65/65	0.94	0.22	79,108,122,129	0
19	PQN	A	841	33/33	0.94	0.23	63,82,97,104	0
18	CLA	A	807	65/65	0.94	0.27	66,84,106,119	0
18	CLA	G	1601	55/65	0.94	0.19	120,147,172,177	0
18	CLA	G	1602	46/65	0.94	0.24	132,158,180,206	0
18	CLA	B	825	65/65	0.94	0.25	77,94,120,134	0
18	CLA	2	306	60/65	0.94	0.33	115,134,164,175	0
21	BCR	A	847	40/40	0.94	0.24	63,75,103,105	0
30	CHL	2	314	66/66	0.94	0.20	99,128,151,165	0
18	CLA	A	826	65/65	0.94	0.28	66,88,109,121	0
30	CHL	2	316	48/66	0.94	0.23	107,124,145,160	0
18	CLA	2	308	65/65	0.94	0.21	113,132,152,167	0

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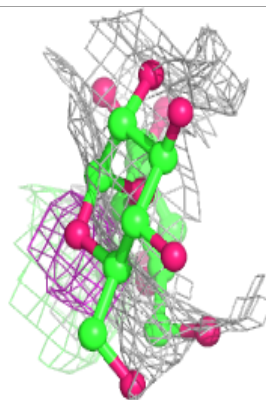
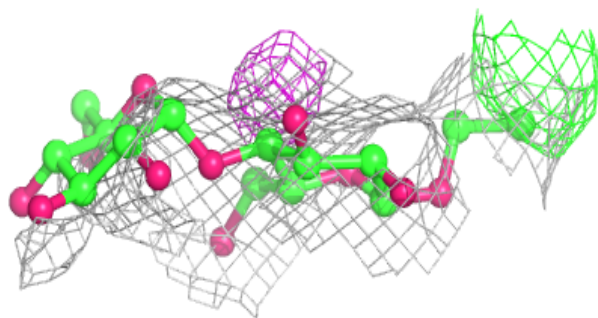
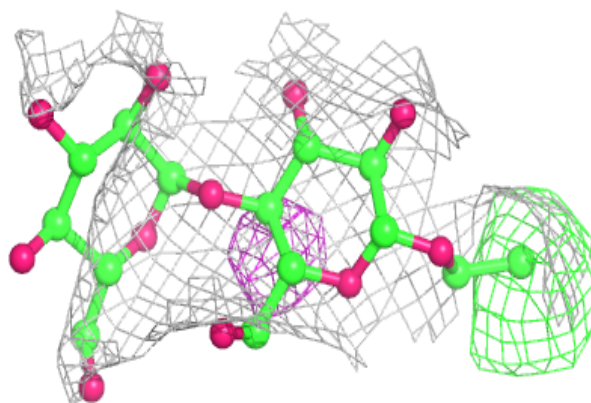
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
18	CLA	2	309	65/65	0.94	0.18	99,121,132,145	0
18	CLA	A	853	65/65	0.94	0.27	84,105,130,138	0
18	CLA	A	827	65/65	0.94	0.38	81,99,115,120	0
18	CLA	2	312	60/65	0.94	0.15	122,139,161,183	0
30	CHL	3	316	47/66	0.94	0.21	135,159,171,181	0
18	CLA	2	313	50/65	0.94	0.23	121,134,153,157	0
18	CLA	B	829	65/65	0.94	0.21	78,93,111,127	0
21	BCR	F	305	40/40	0.94	0.20	76,98,116,120	0
18	CLA	2	326	50/65	0.94	0.19	94,114,150,160	0
21	BCR	I	101	40/40	0.94	0.29	85,108,125,129	0
18	CLA	3	301	45/65	0.94	0.24	120,138,174,192	0
18	CLA	B	803	65/65	0.94	0.23	64,81,98,107	0
18	CLA	B	820	65/65	0.95	0.29	84,106,123,152	0
18	CLA	A	822	65/65	0.95	0.23	78,93,121,129	0
18	CLA	A	820	60/65	0.95	0.20	121,148,178,189	0
18	CLA	4	308	60/65	0.95	0.23	92,118,142,153	0
18	CLA	1	5012	46/65	0.95	0.12	117,149,168,183	0
18	CLA	A	821	60/65	0.95	0.22	122,149,190,193	0
22	LHG	A	849	40/49	0.95	0.23	88,125,152,155	0
18	CLA	B	824	55/65	0.95	0.21	82,105,123,133	0
18	CLA	3	315	65/65	0.95	0.22	115,153,164,191	0
18	CLA	A	838	65/65	0.95	0.18	64,84,119,134	0
30	CHL	4	318	56/66	0.95	0.26	109,134,178,182	0
18	CLA	B	807	65/65	0.95	0.23	73,93,108,115	0
18	CLA	B	813	46/65	0.95	0.23	107,126,142,166	0
18	CLA	A	802	65/65	0.96	0.27	62,77,96,111	0
18	CLA	B	833	58/65	0.96	0.20	65,87,107,117	0
18	CLA	A	837	65/65	0.96	0.19	63,77,94,114	0
22	LHG	B	848	21/49	0.96	0.15	88,113,140,155	0
18	CLA	A	805	65/65	0.96	0.23	65,86,103,115	0
18	CLA	A	808	65/65	0.96	0.20	67,85,132,144	0
18	CLA	F	301	65/65	0.96	0.22	65,87,105,109	0
18	CLA	A	839	65/65	0.97	0.23	61,82,97,106	0
20	SF4	A	842	8/8	0.98	0.21	70,71,119,144	0
20	SF4	C	102	8/8	0.98	0.16	79,89,122,145	0
20	SF4	C	101	8/8	0.99	0.19	69,86,120,124	0

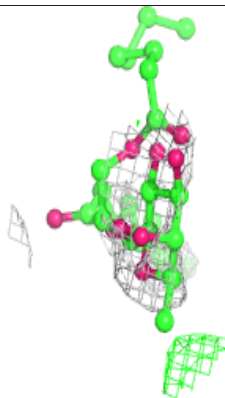
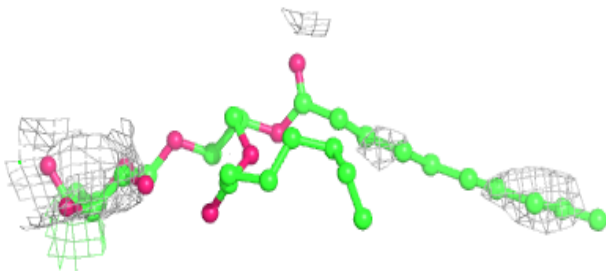
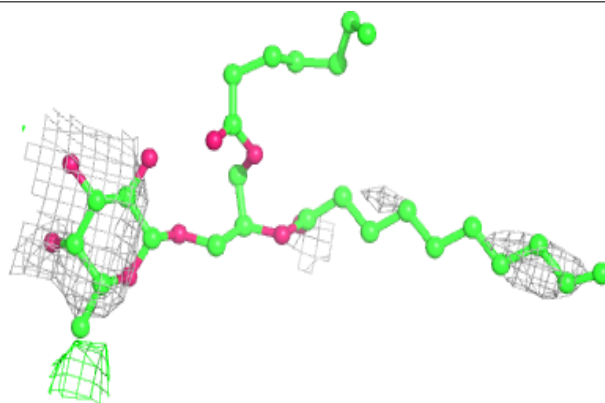
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around LMT 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)

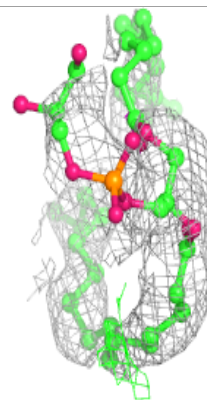
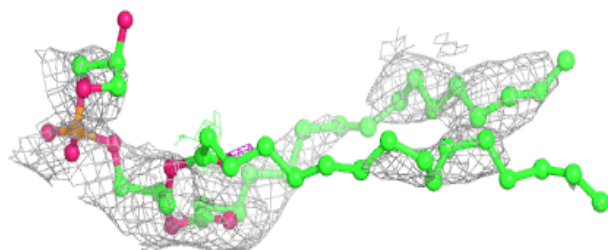
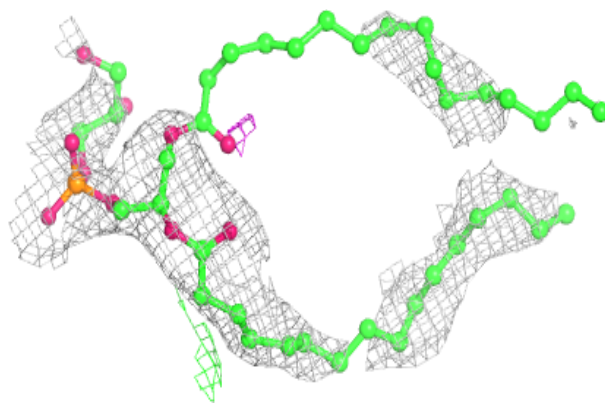
**Electron density around DGD 1 5002:**

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

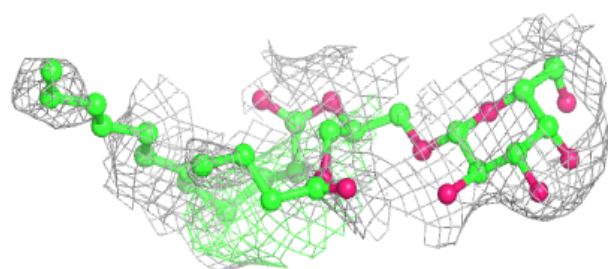
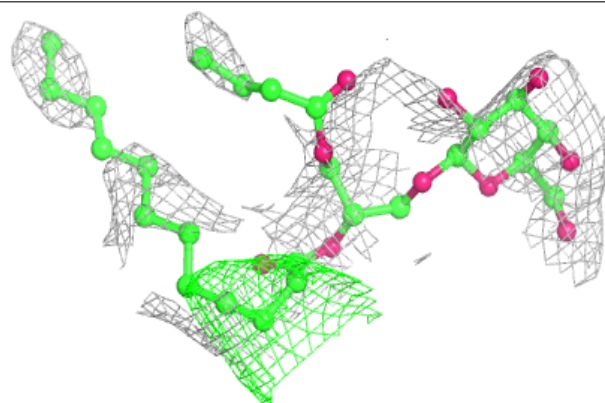


**Electron density around LHG B 849:**

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

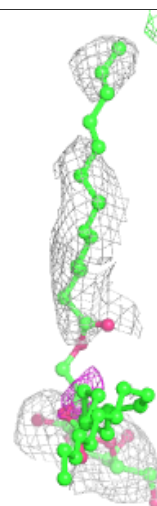
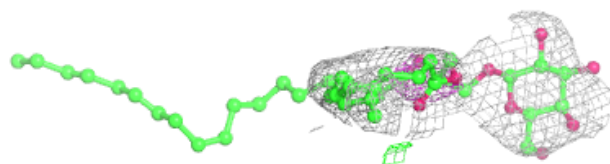
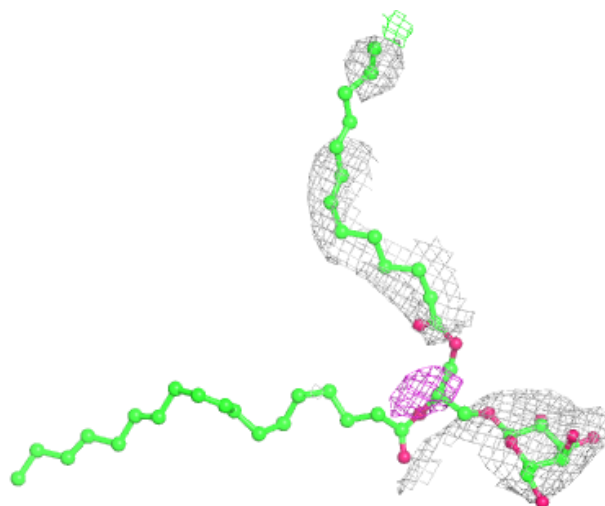
**Electron density around LMG B 850:**

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



**Electron density around LMG A 851:**

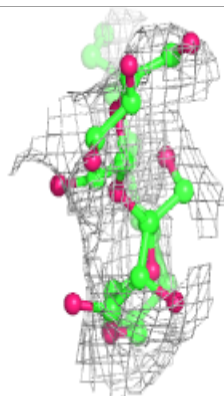
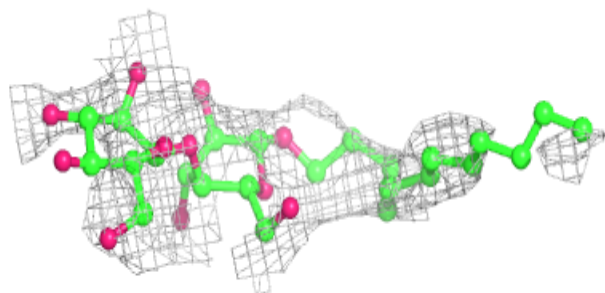
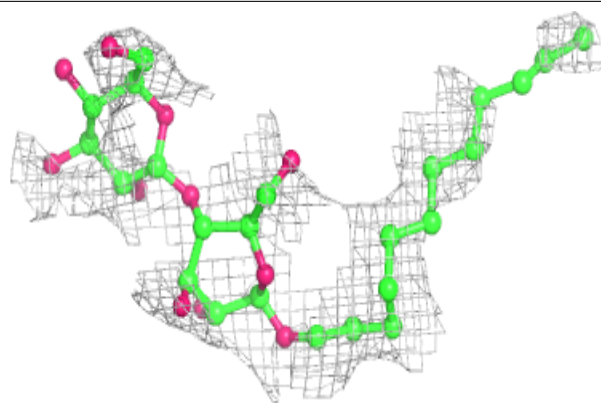
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





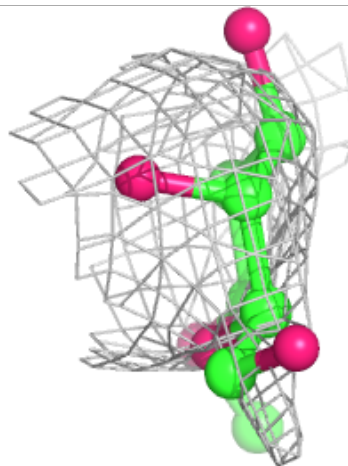
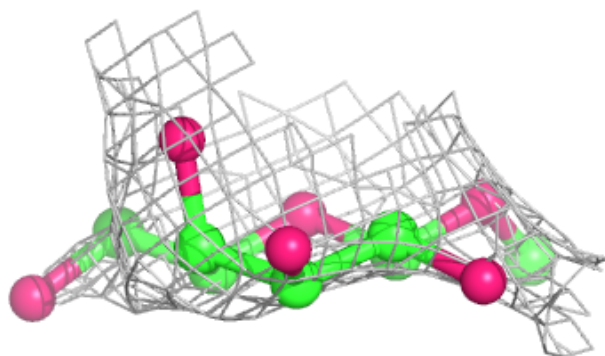
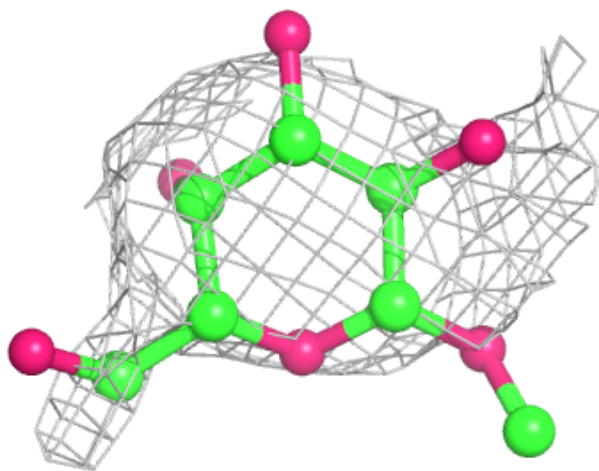
**Electron density around LMT 2 325:**

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



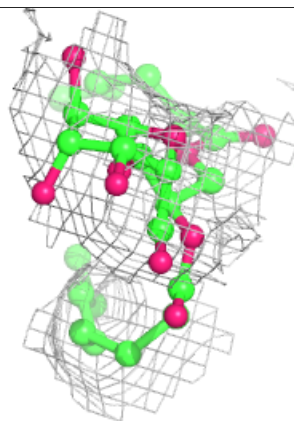
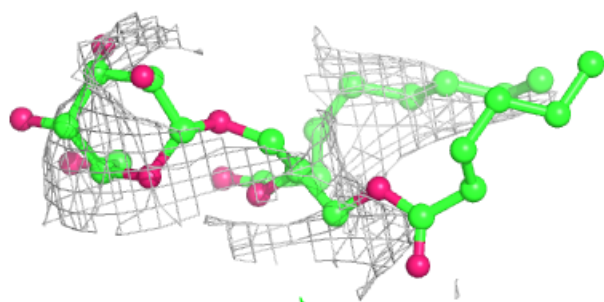
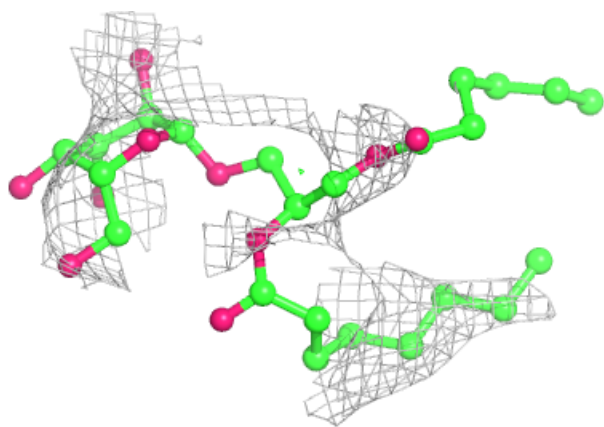
**Electron density around LMG 2 301:**

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

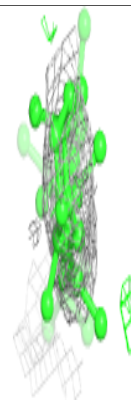
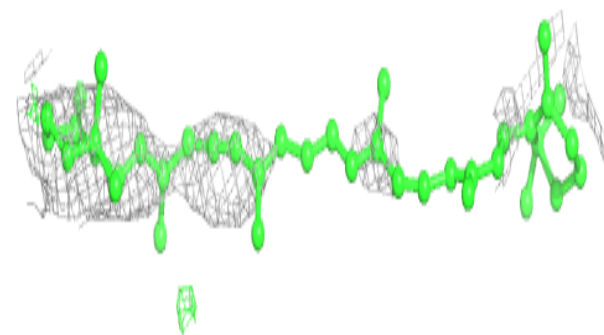
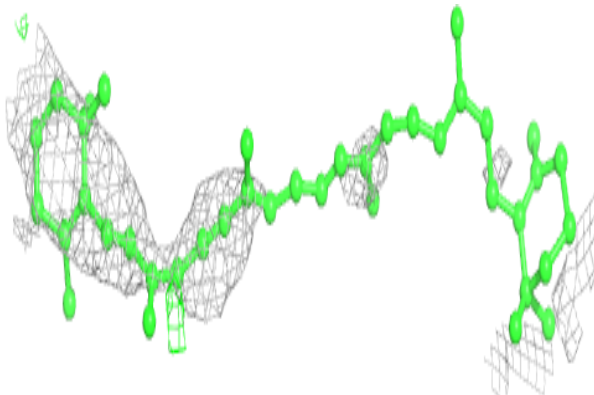


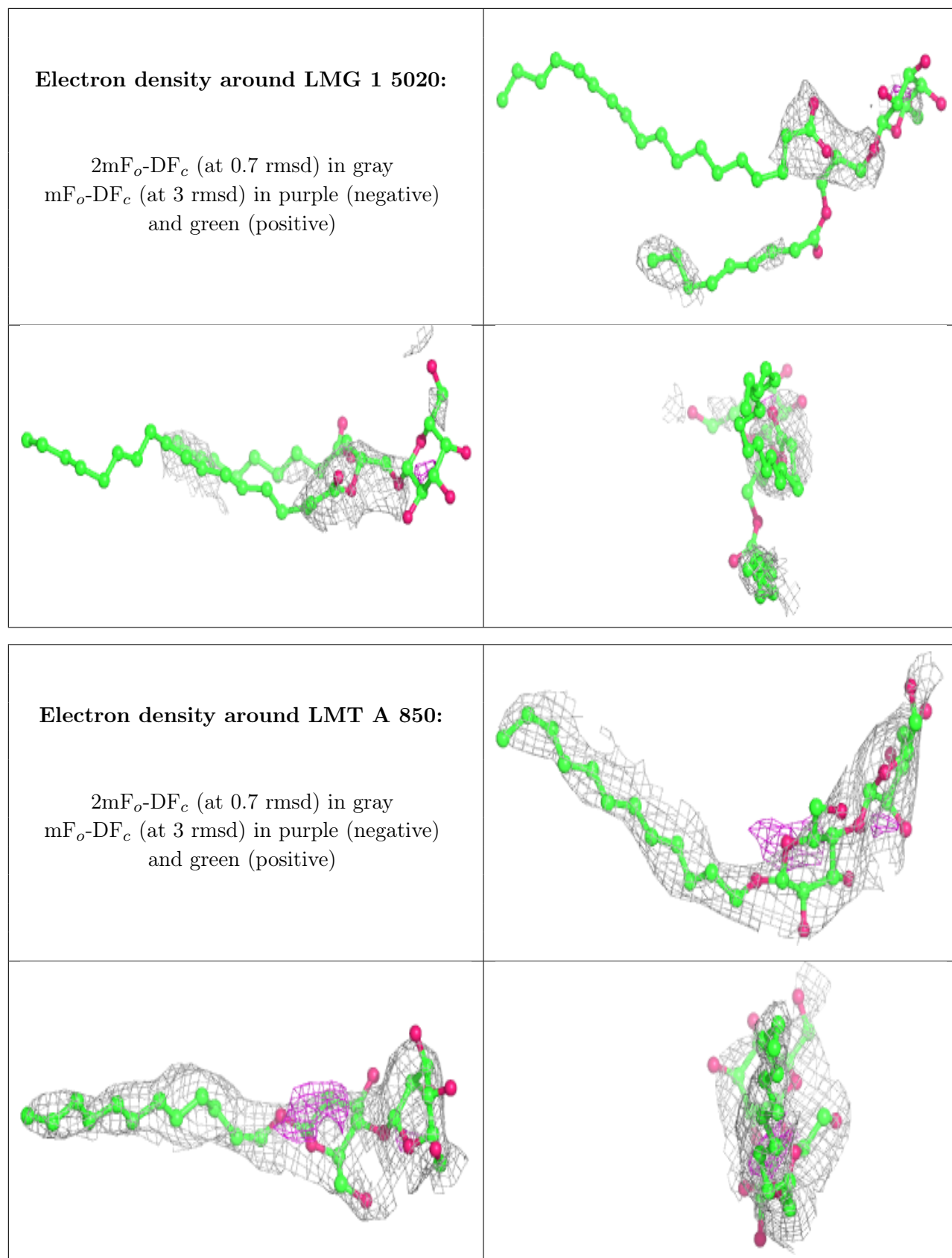
**Electron density around LMG B 851:**

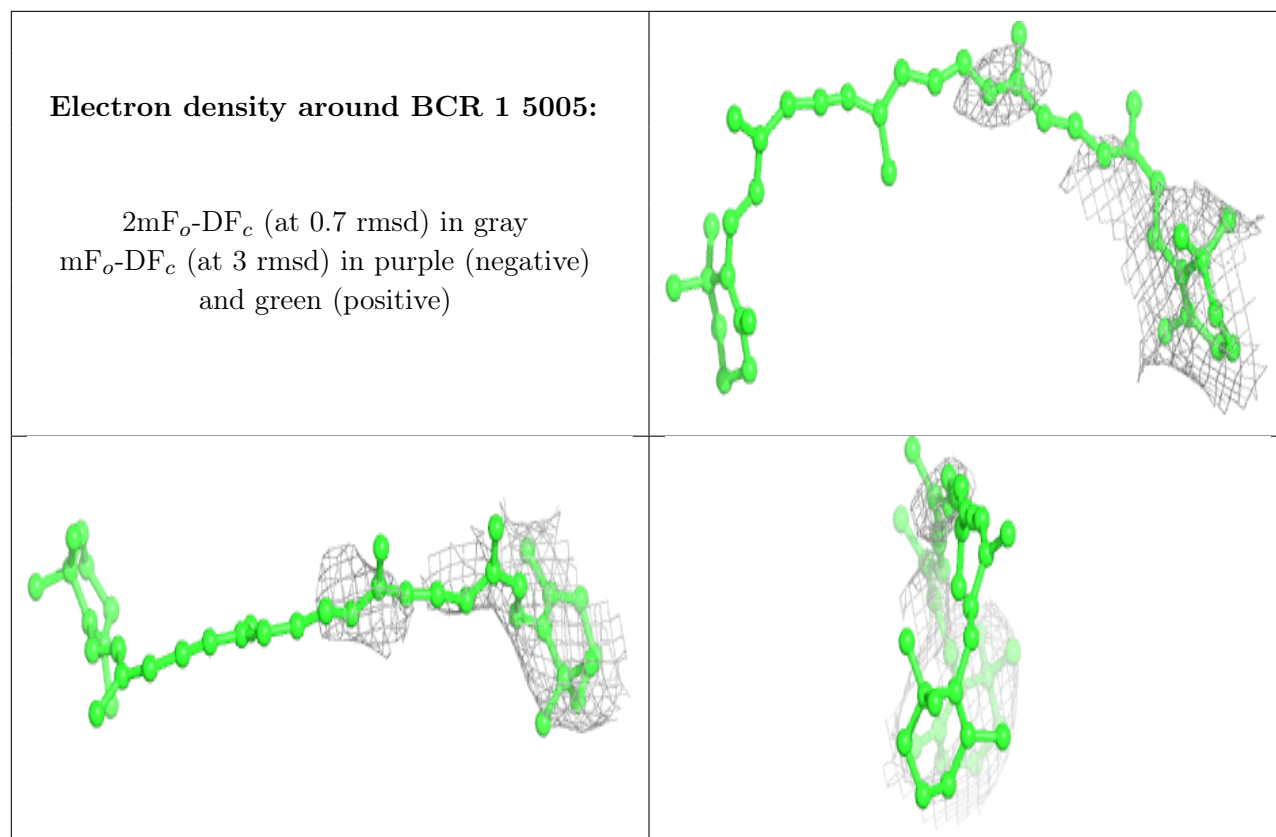
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCR 2 305:**

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

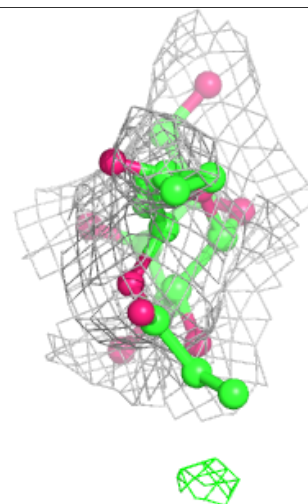
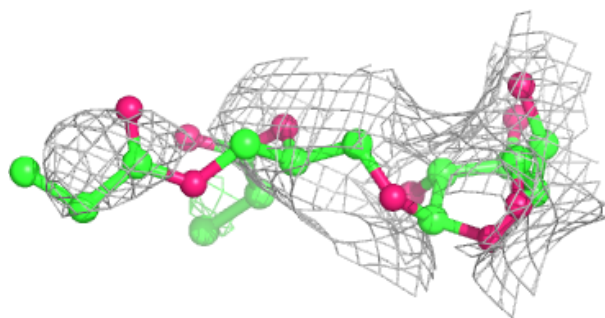
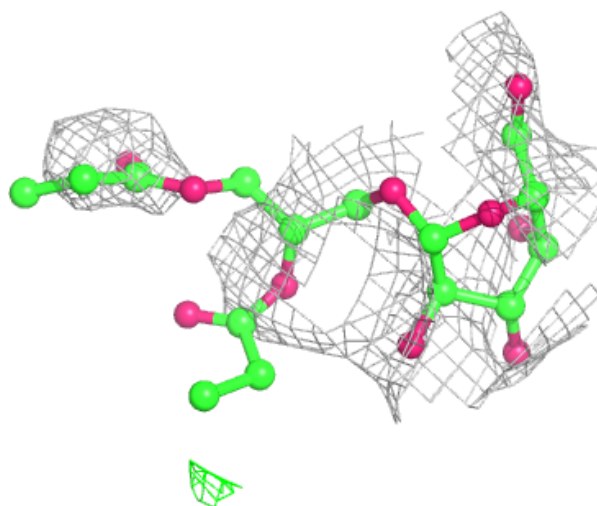






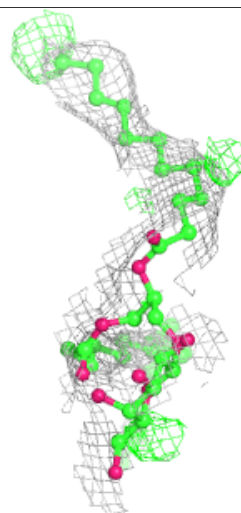
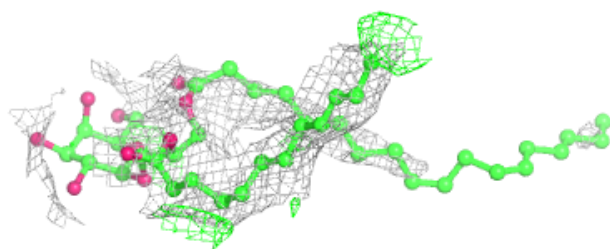
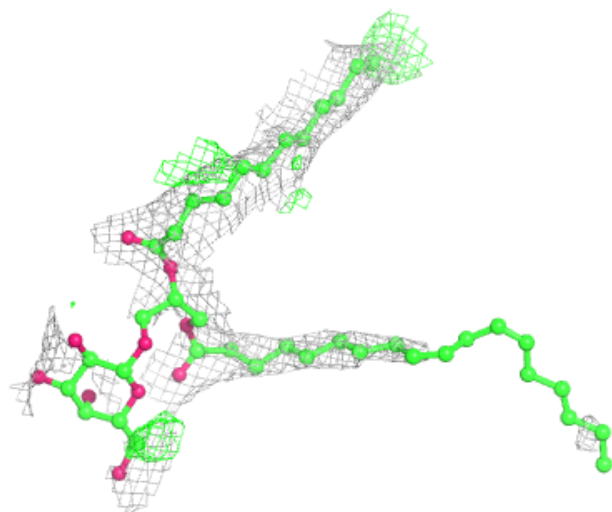
**Electron density around LMG G 1607:**

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



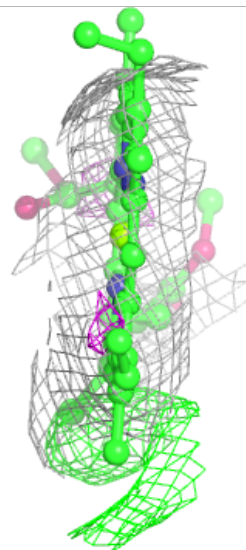
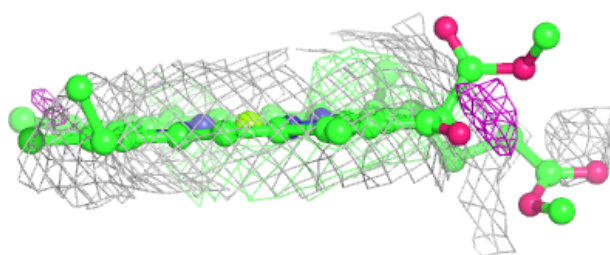
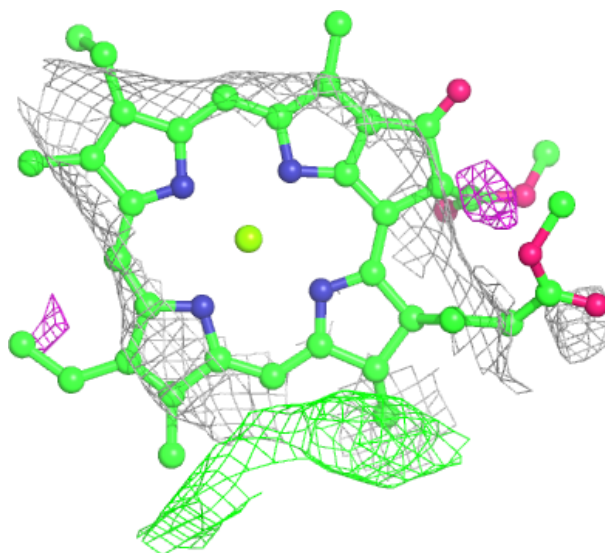
**Electron density around LMG 1 5001:**

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



**Electron density around CLA K 1404:**

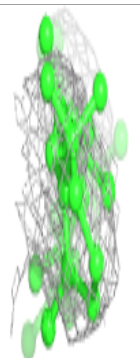
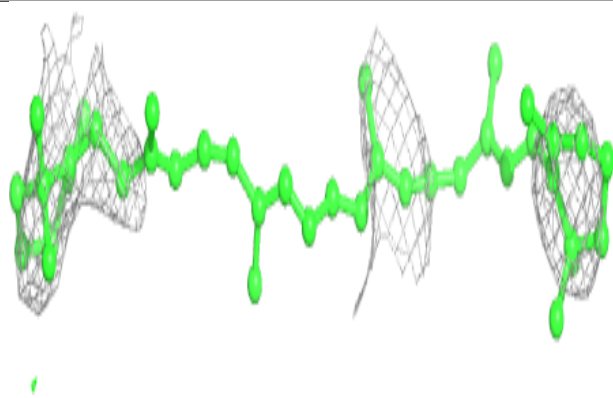
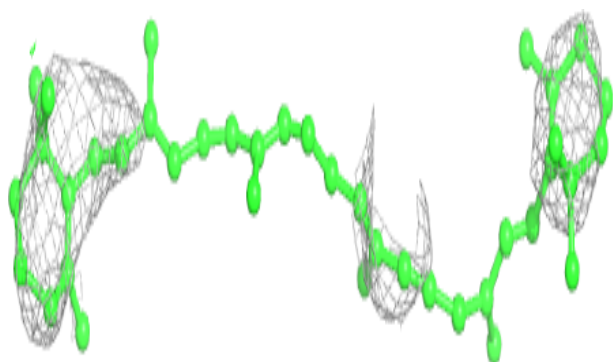
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



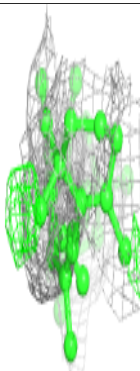
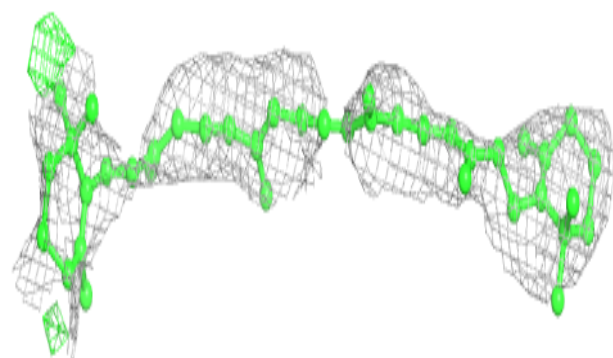
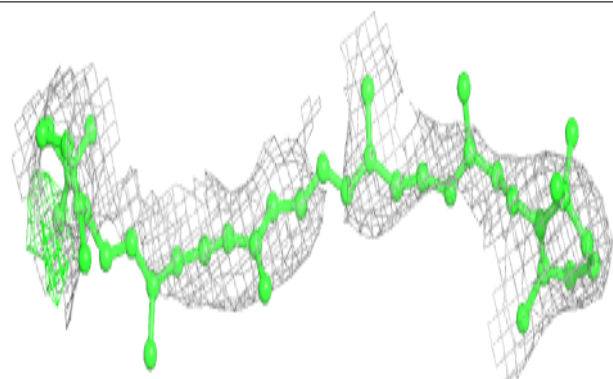


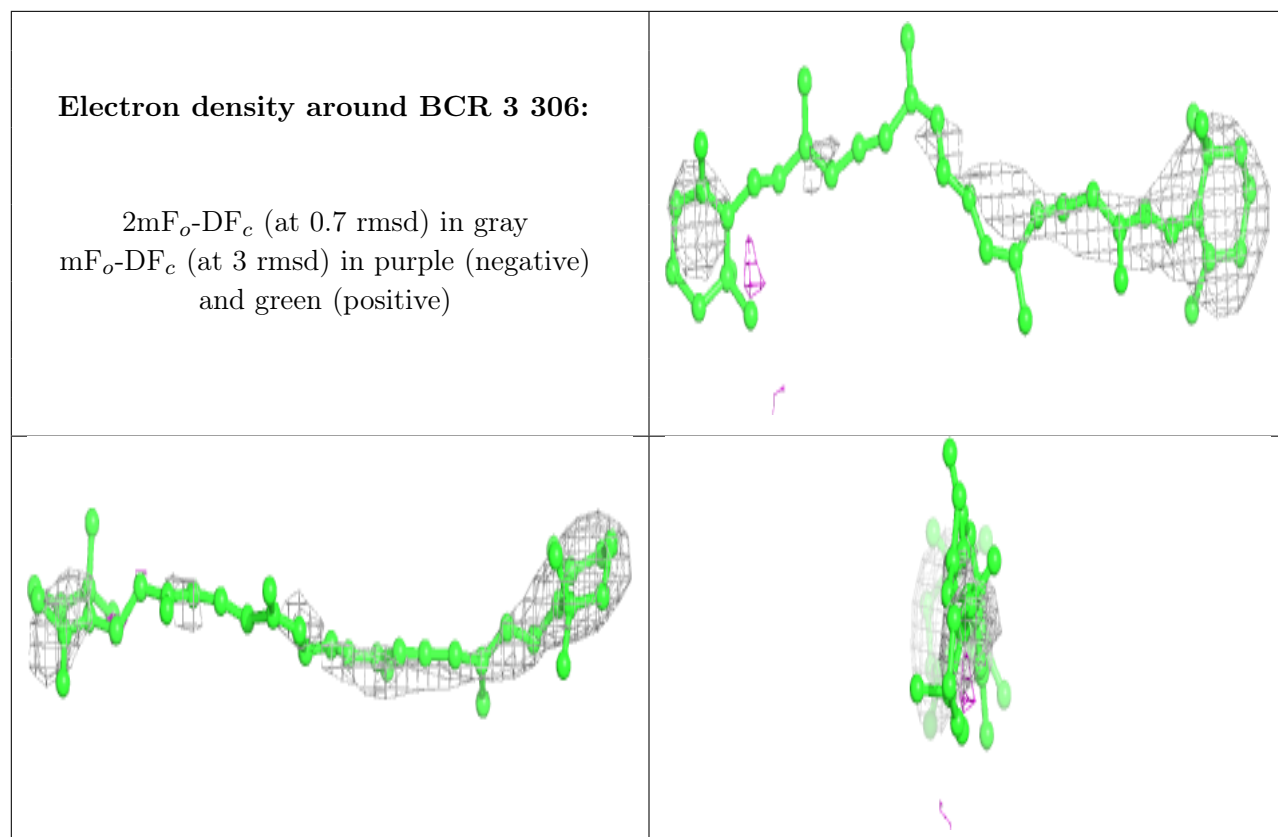
**Electron density around BCR K 1405:**

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

**Electron density around BCR L 302:**

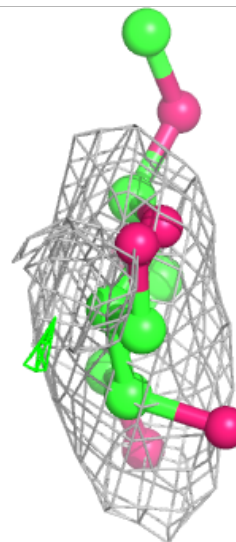
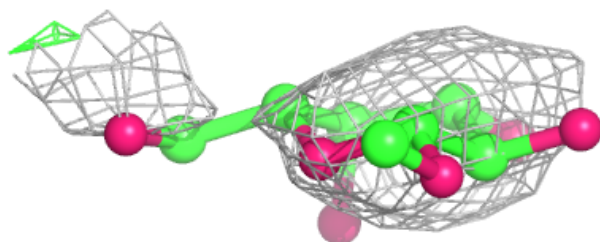
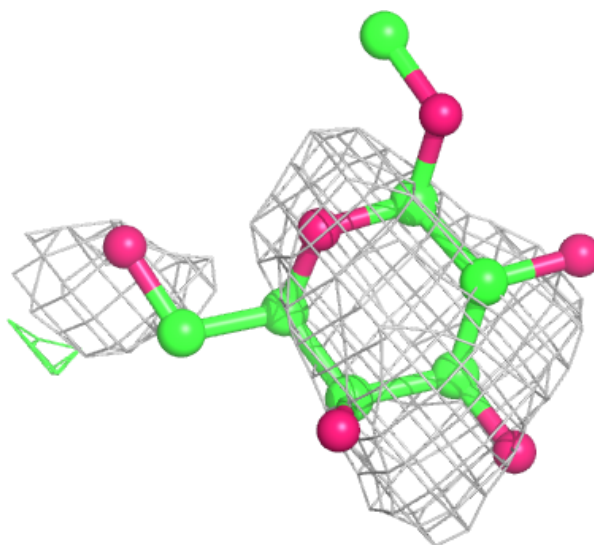
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





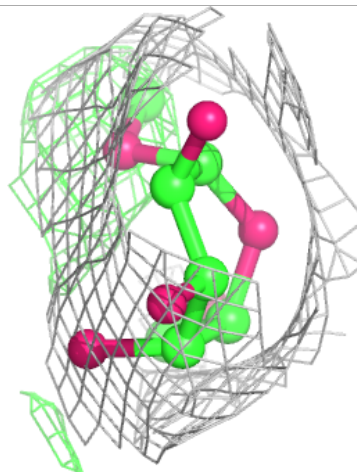
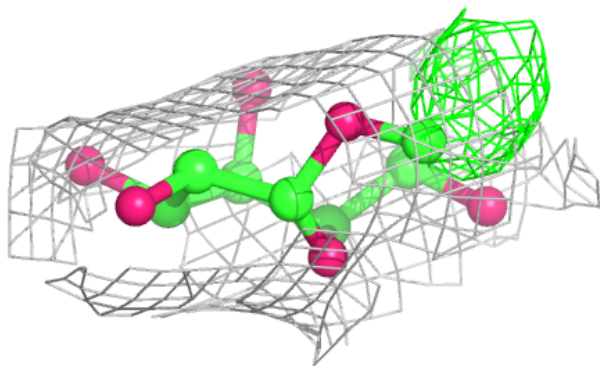
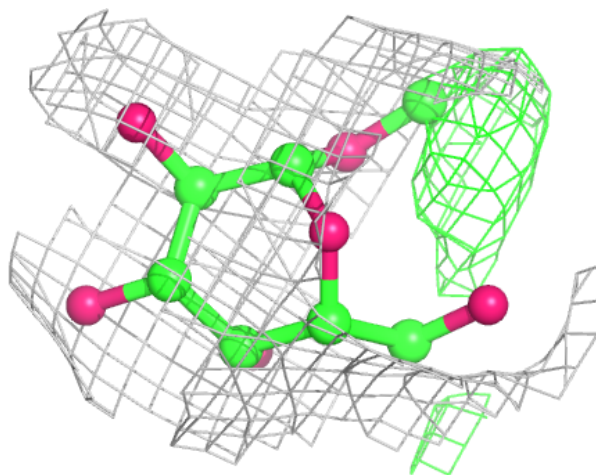
**Electron density around LMG 4 320:**

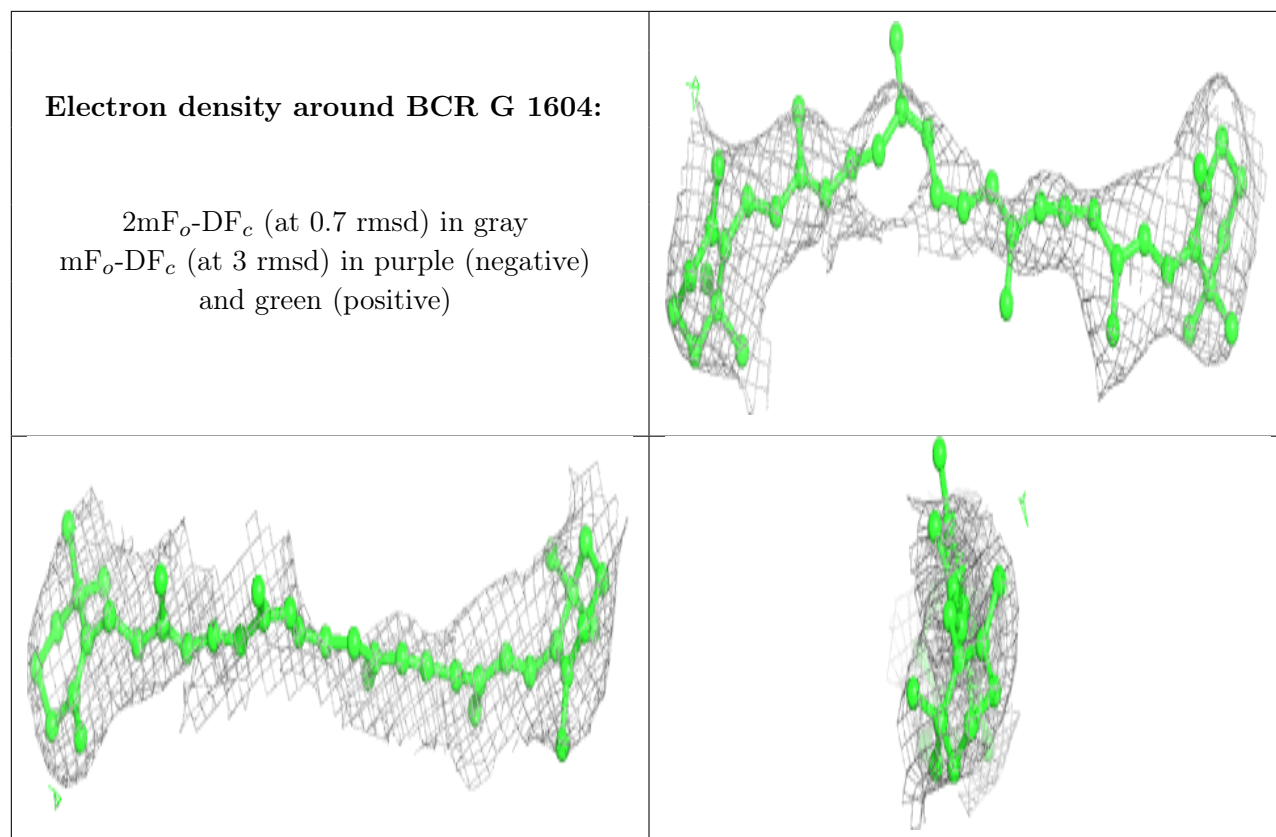
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around LMG 2 323:**

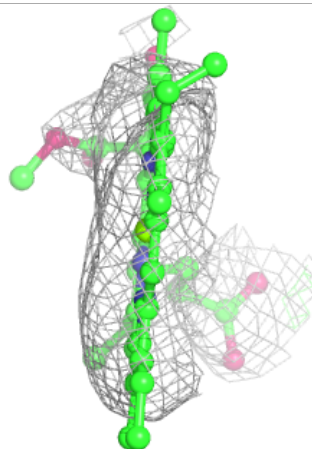
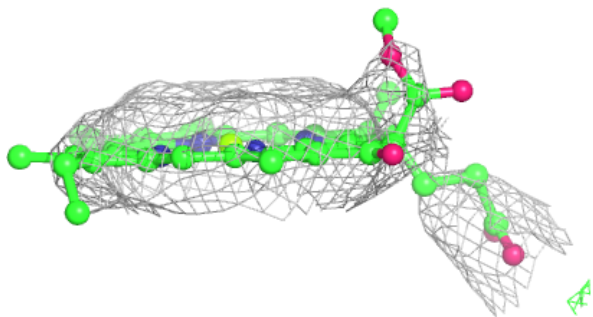
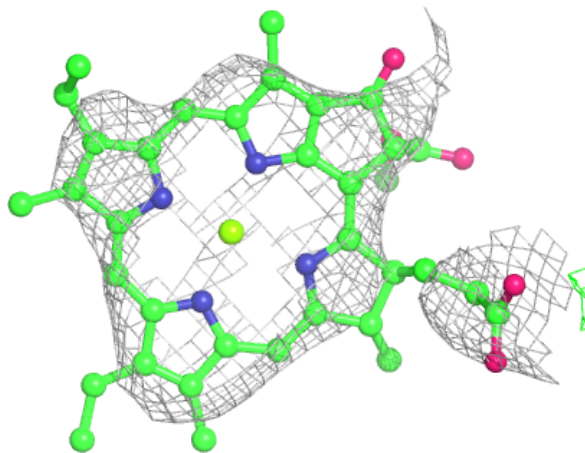
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

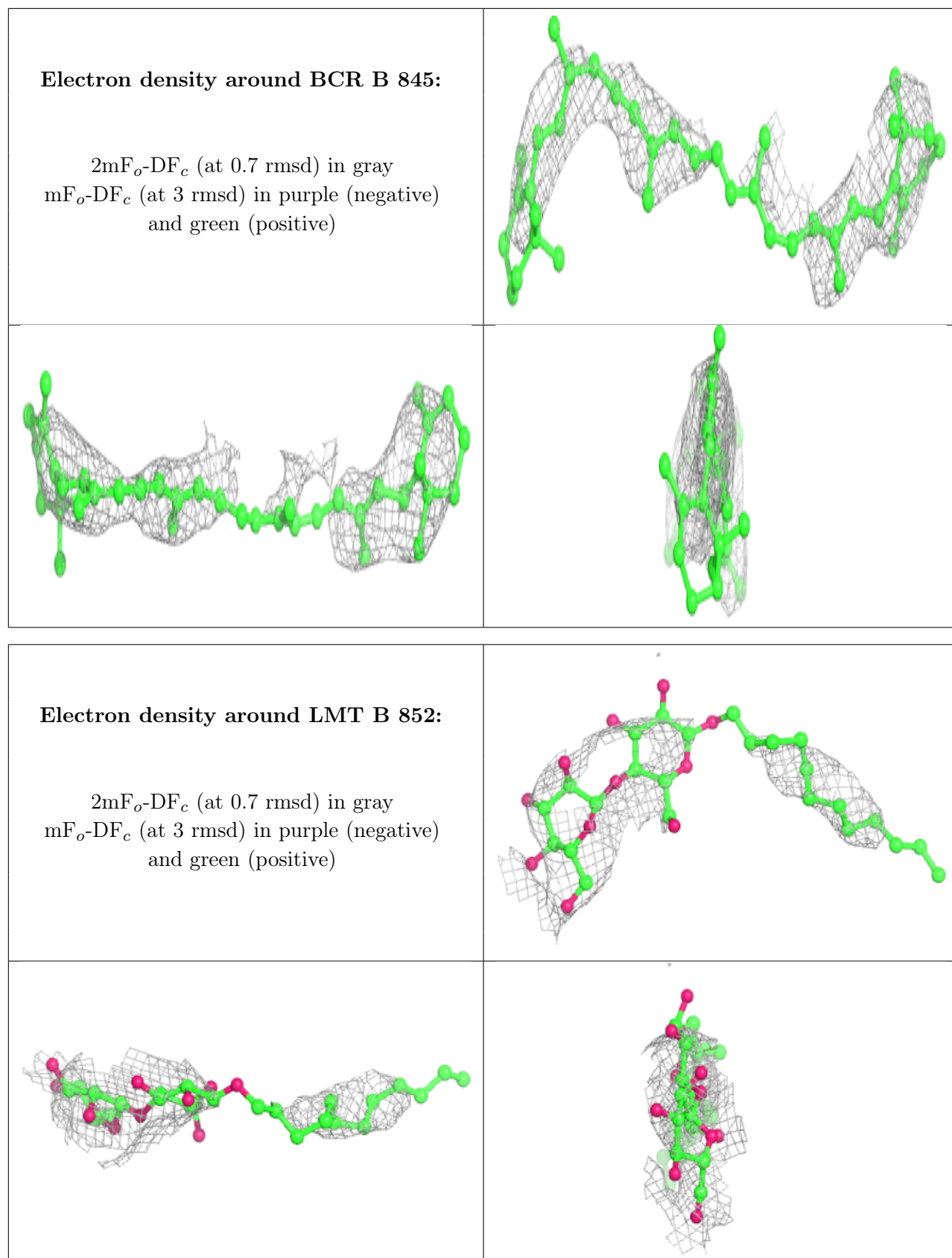


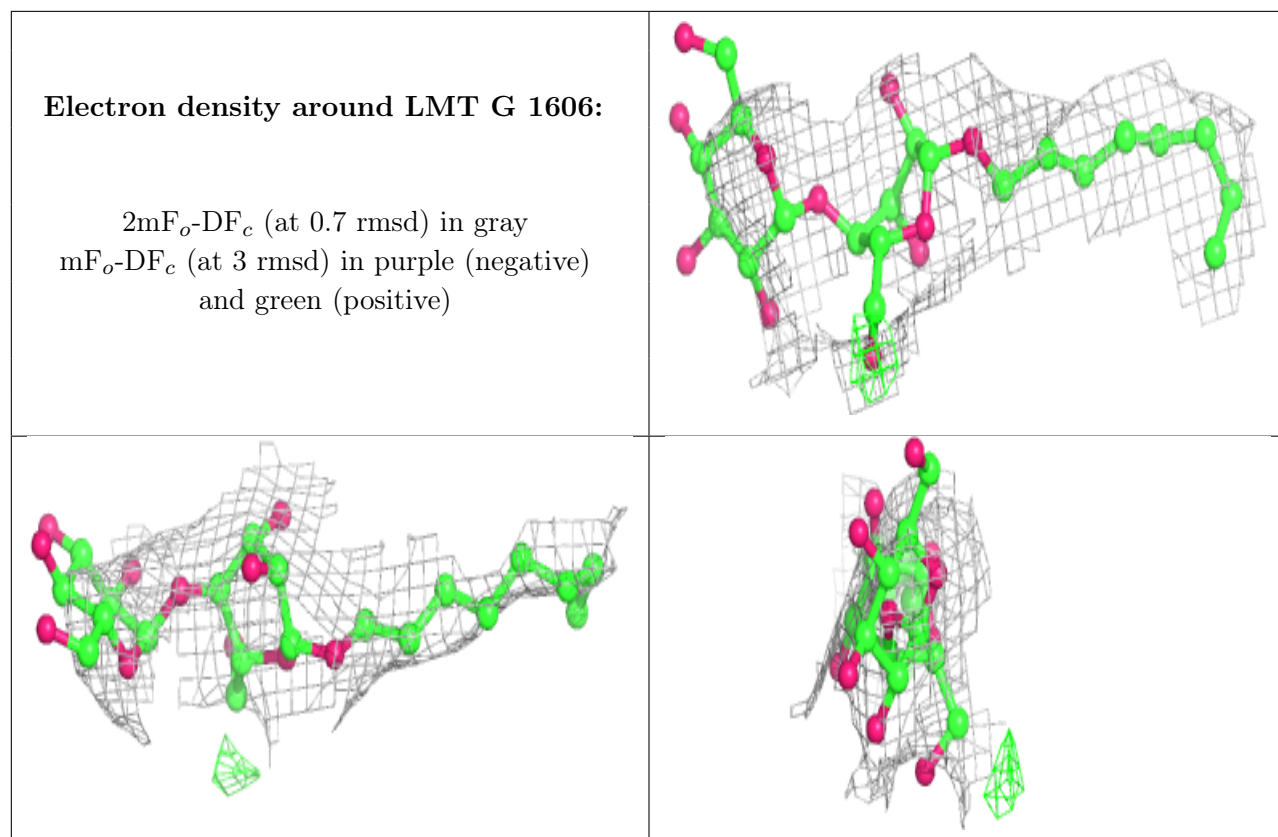


**Electron density around CLA K 1401:**

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



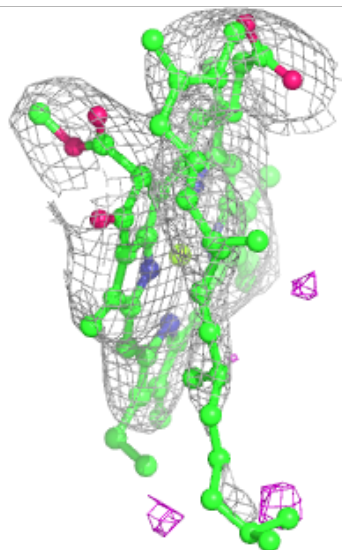
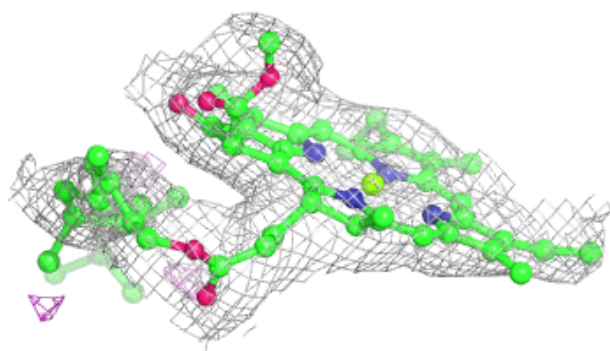
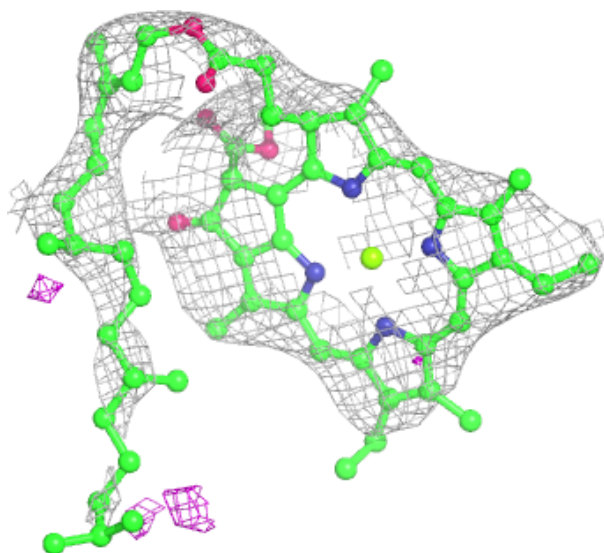


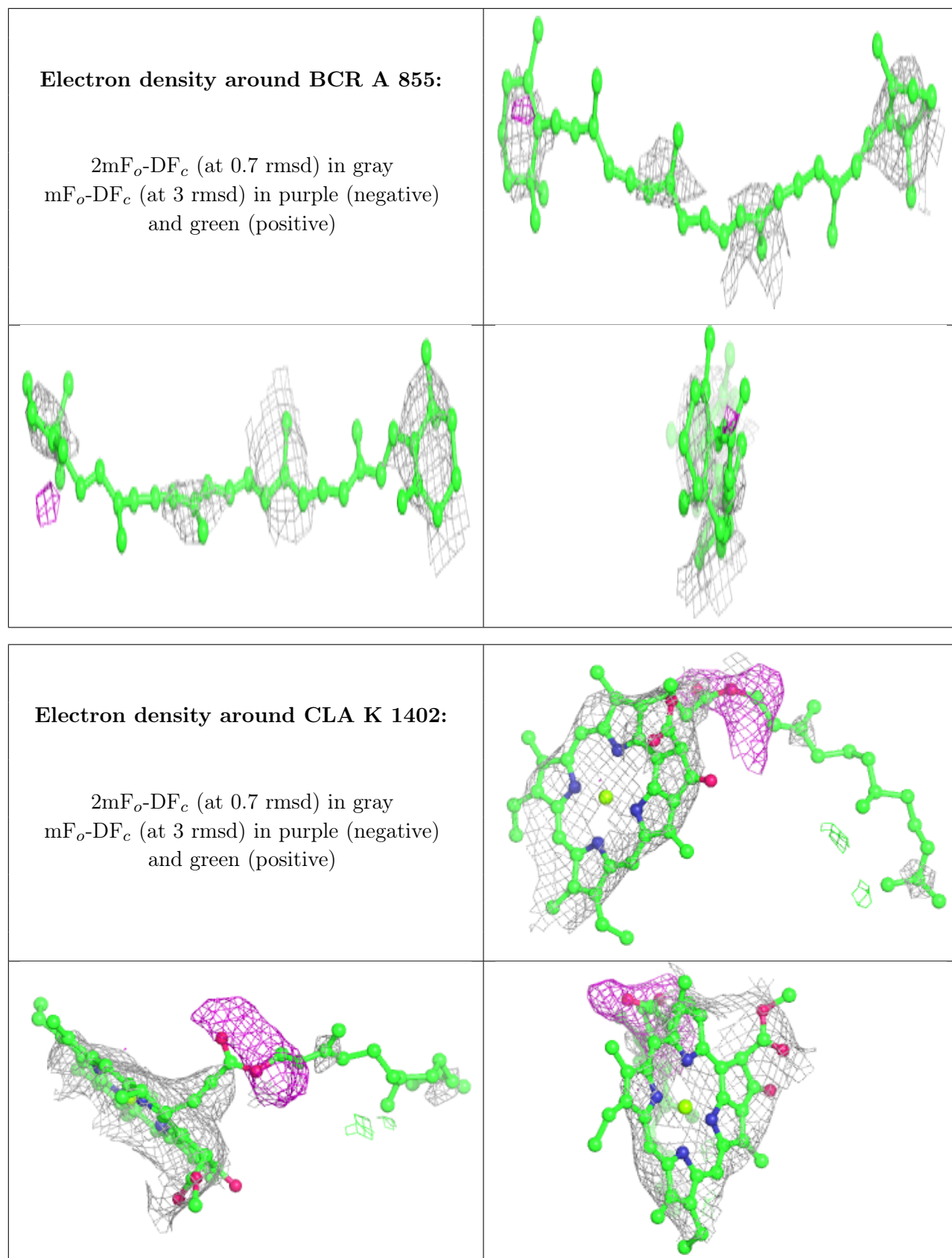




**Electron density around CLA A 823:**

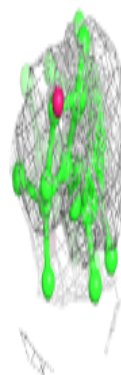
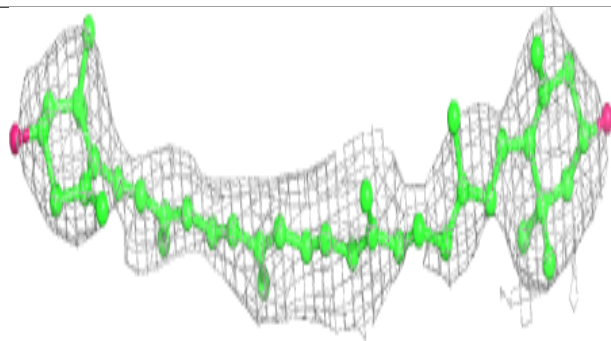
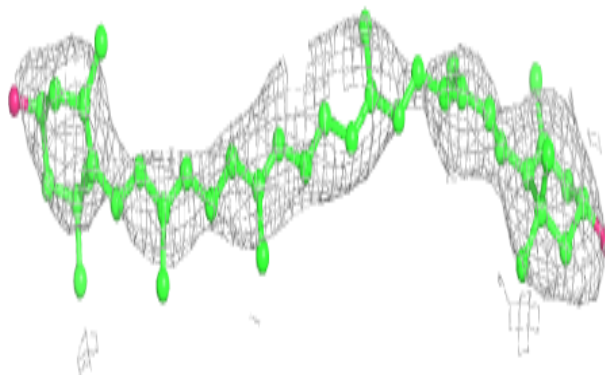
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



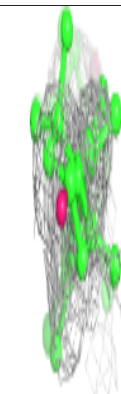
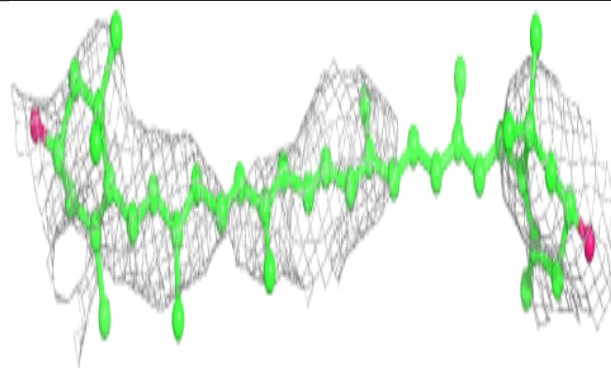
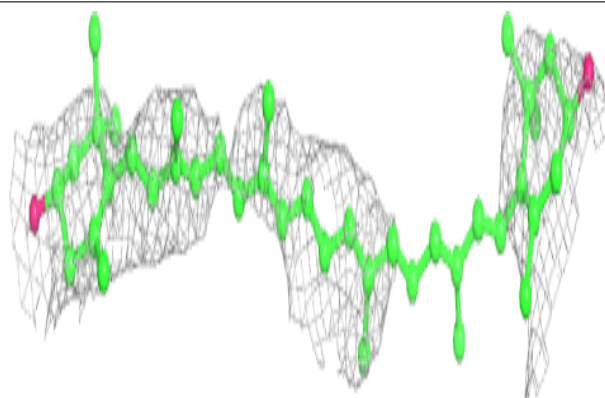


**Electron density around LUT J 1105:**

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

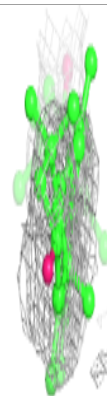
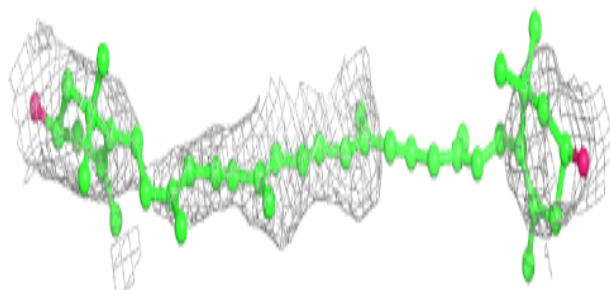
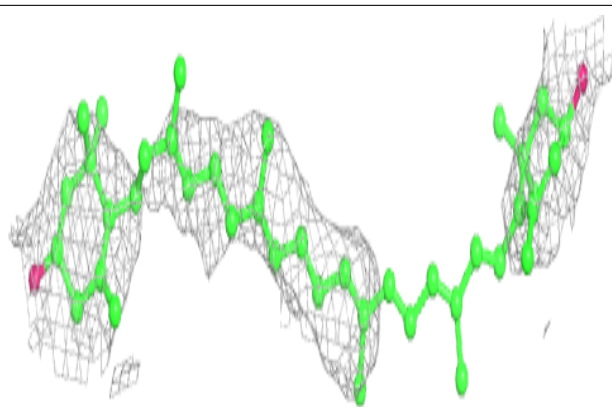
**Electron density around LUT 3 303:**

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

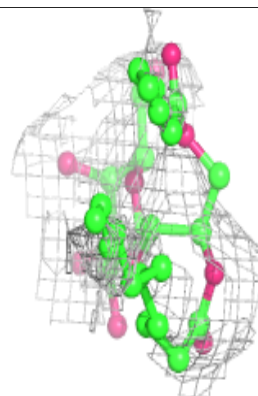
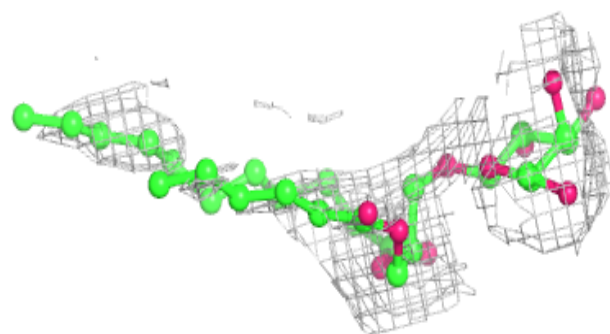
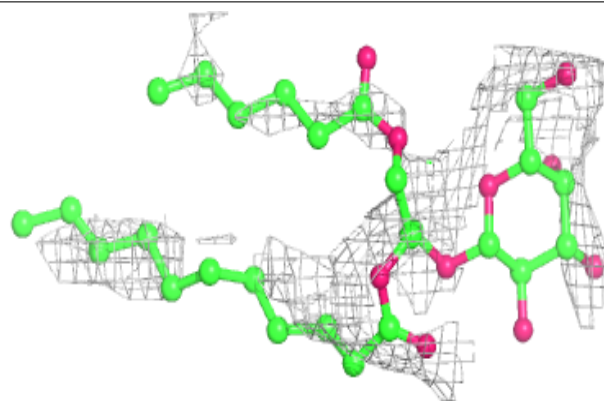


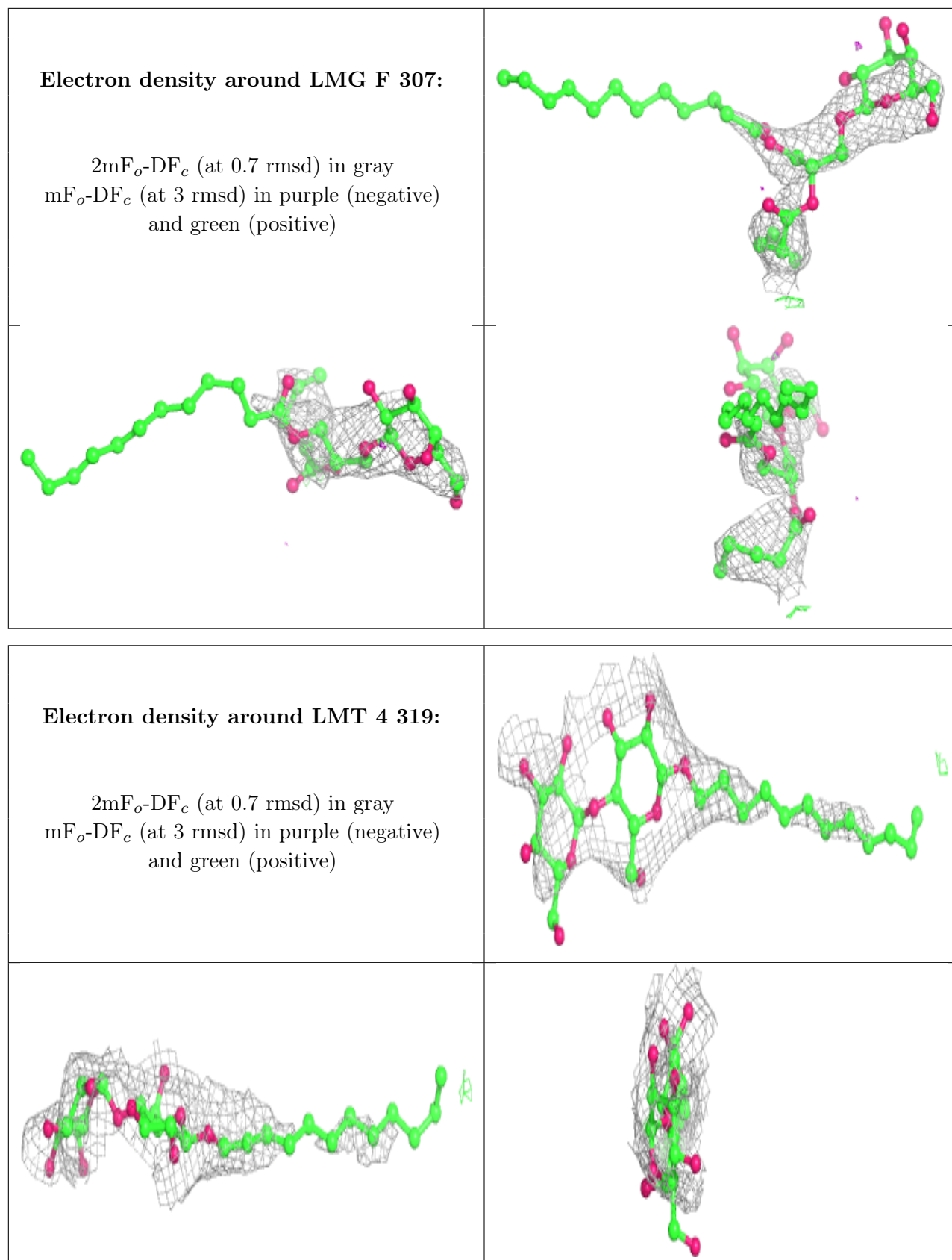
**Electron density around LUT 3 304:**

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

**Electron density around LMG 2 322:**

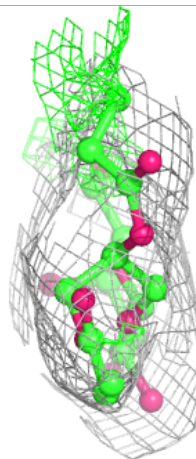
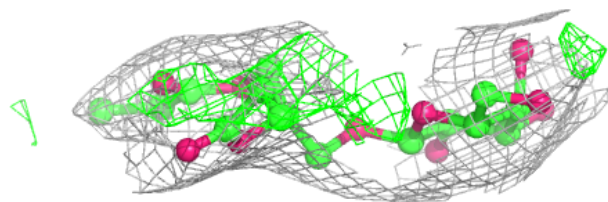
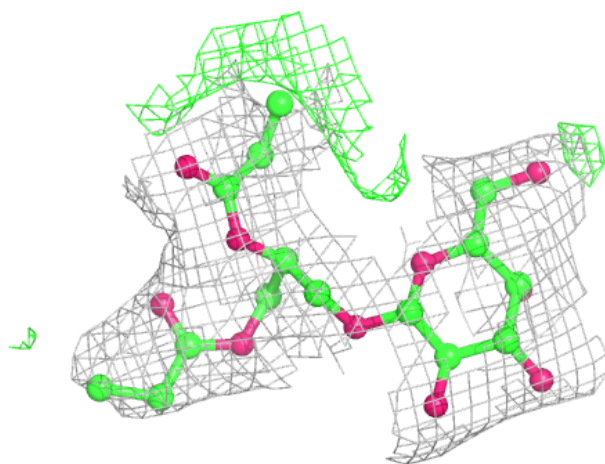
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





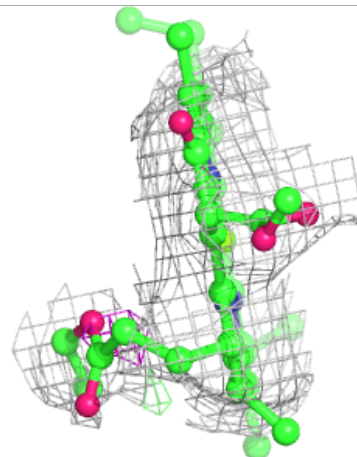
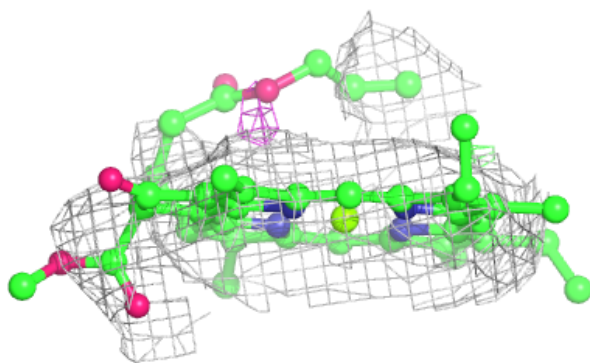
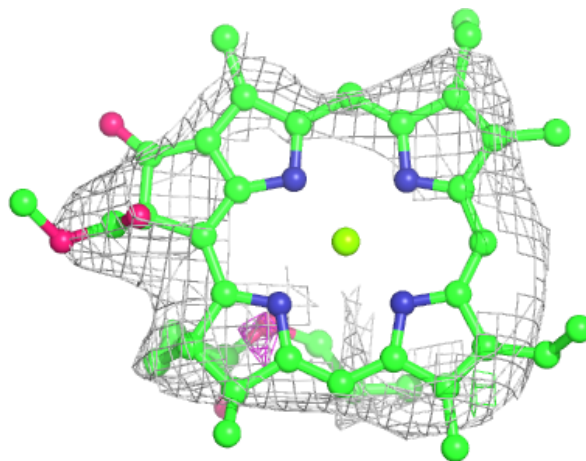
**Electron density around LMG 2 321:**

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



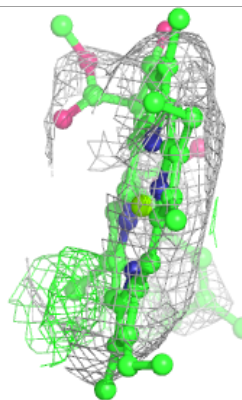
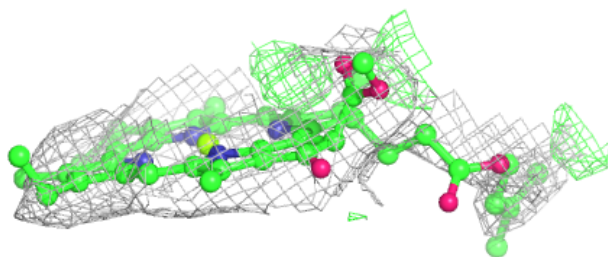
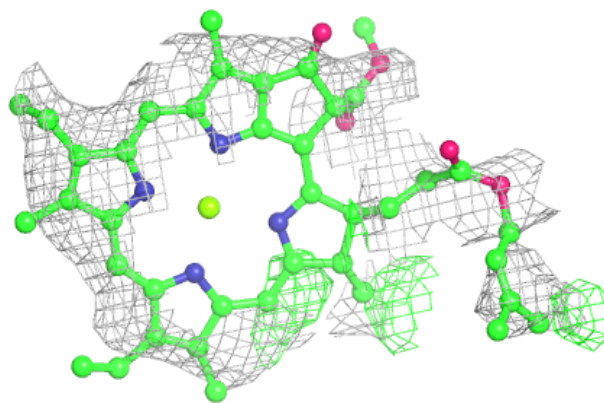
**Electron density around CLA 3 314:**

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

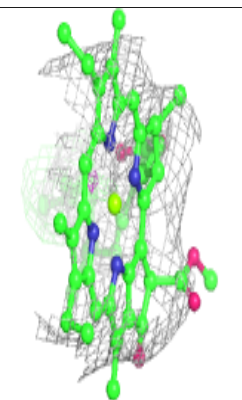
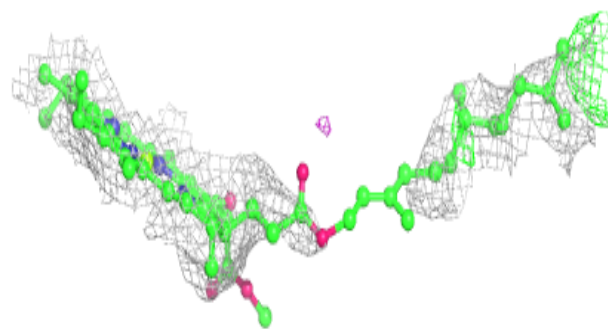
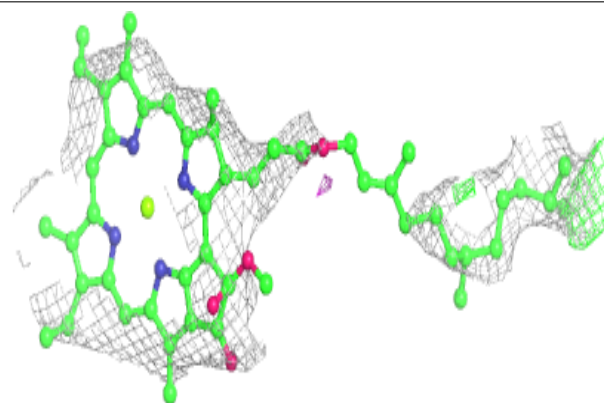


**Electron density around CLA J 1103:**

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

**Electron density around CLA H 1701:**

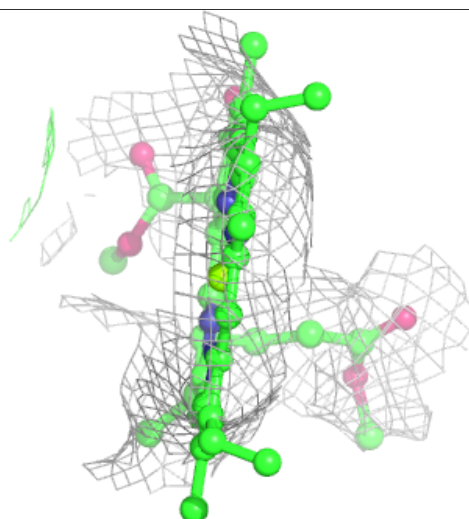
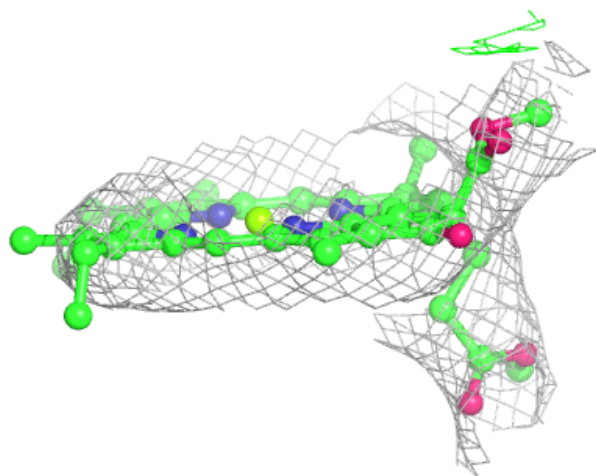
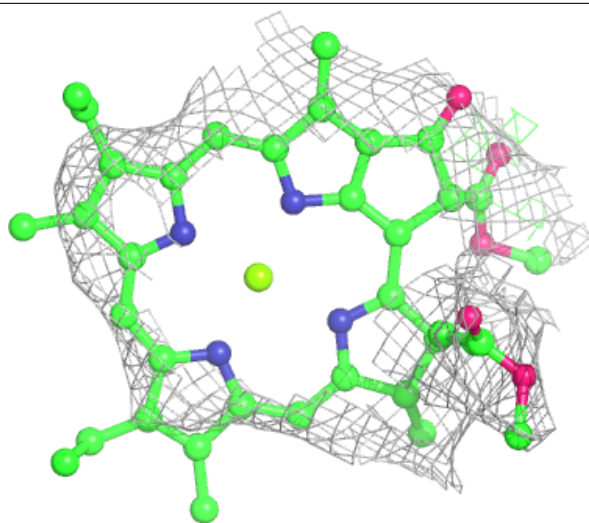
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





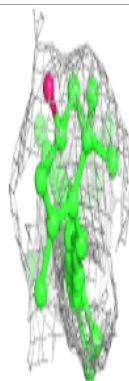
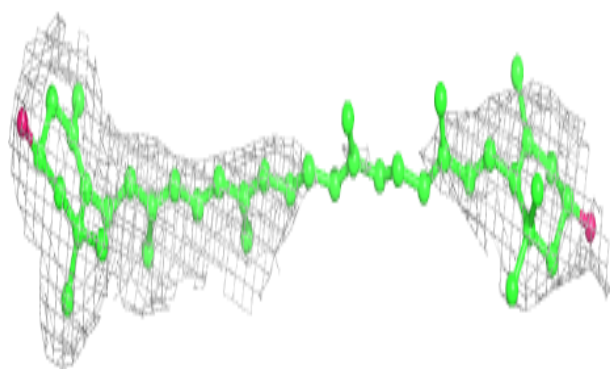
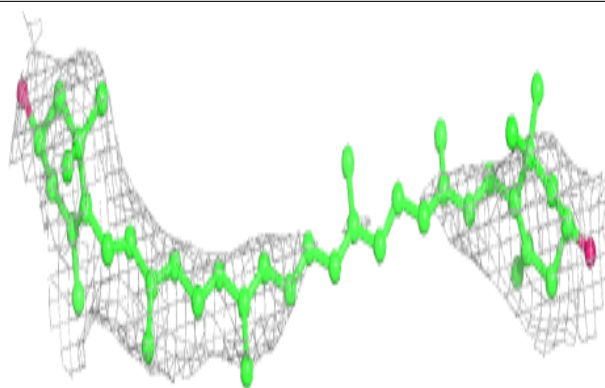
**Electron density around CLA 1 5013:**

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

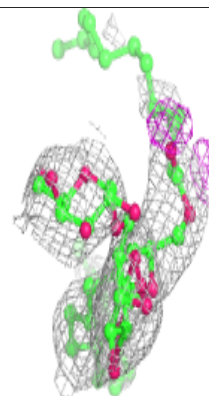
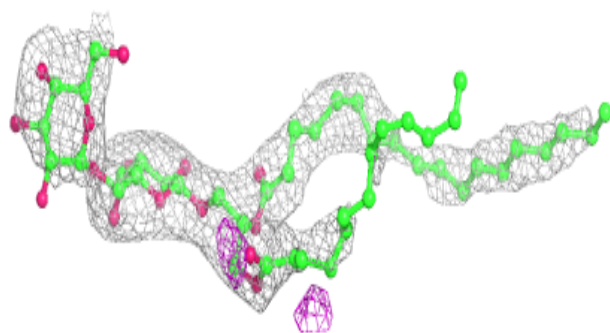
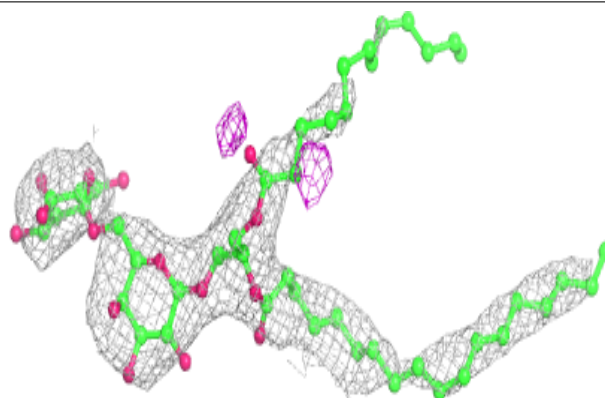


**Electron density around LUT 4 303:**

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

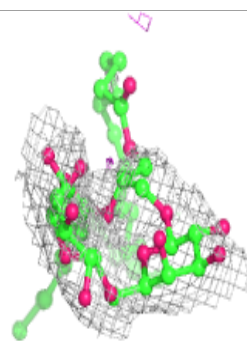
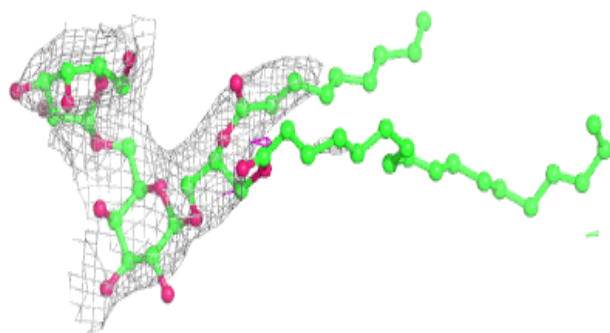
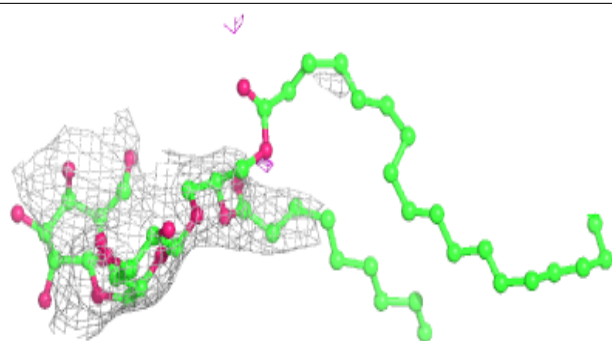
**Electron density around DGD B 855:**

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

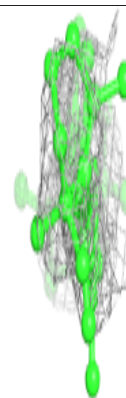
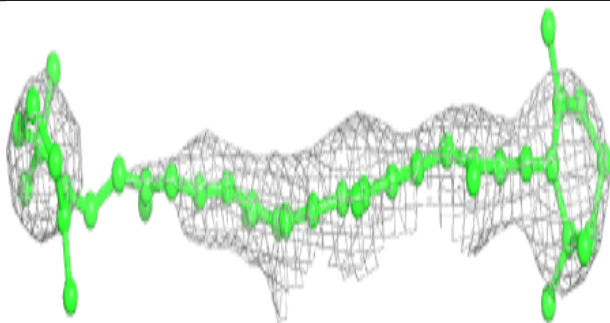
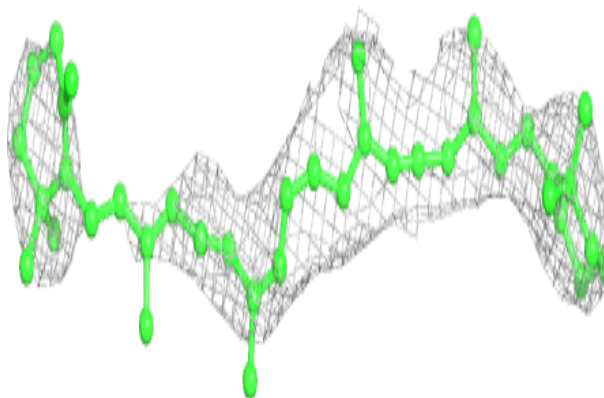


**Electron density around DGD F 309:**

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

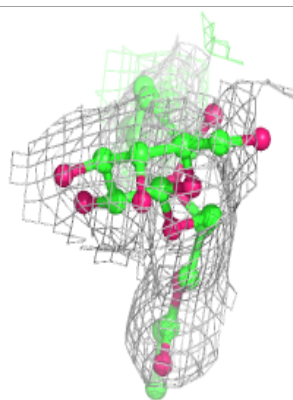
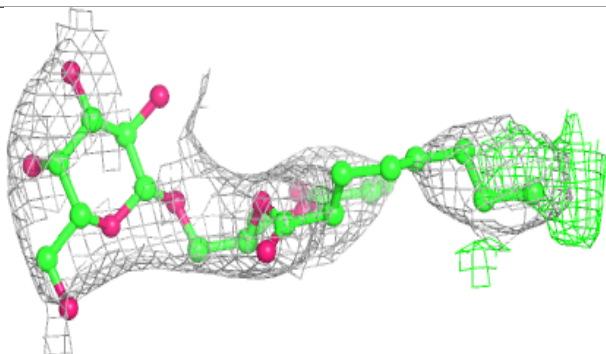
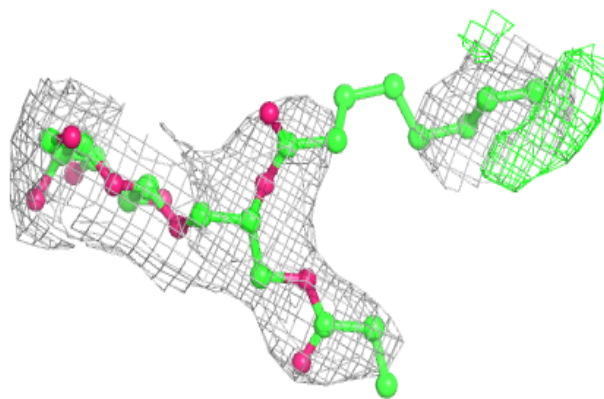
**Electron density around BCR A 845:**

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

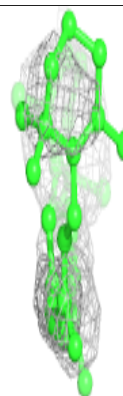
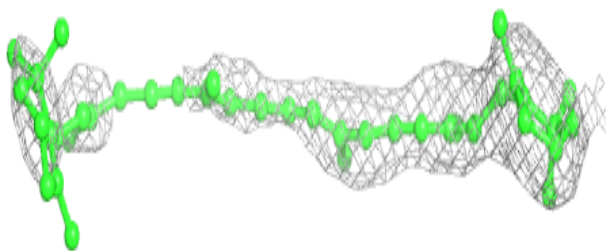
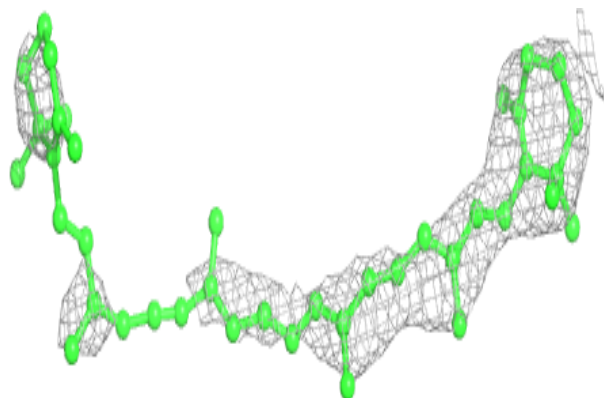


**Electron density around LMG J 1102:**

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

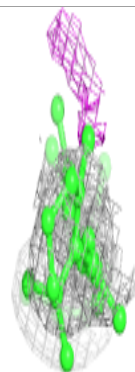
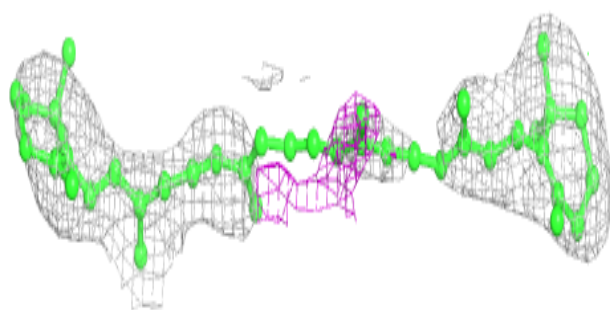
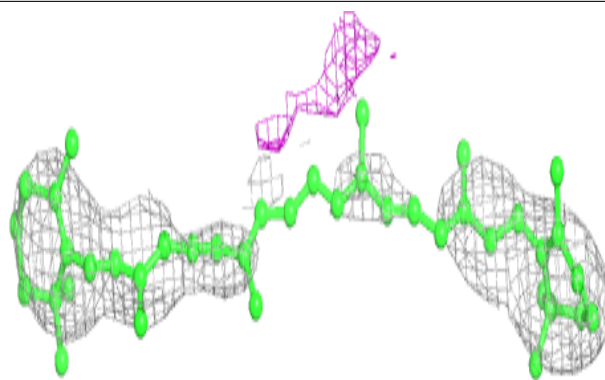
**Electron density around BCR B 844:**

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



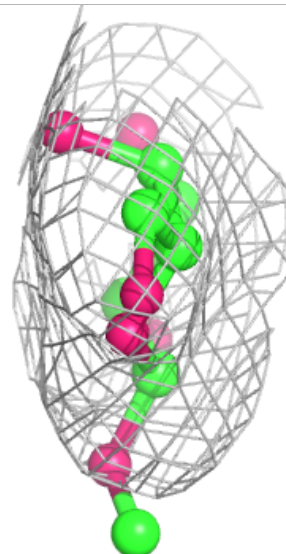
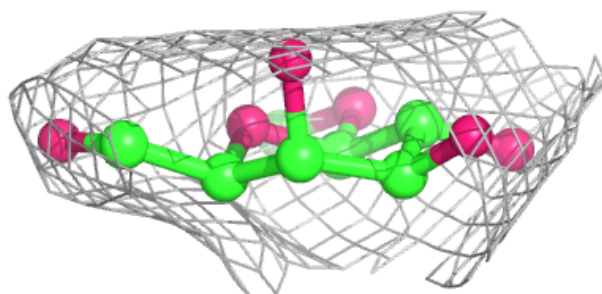
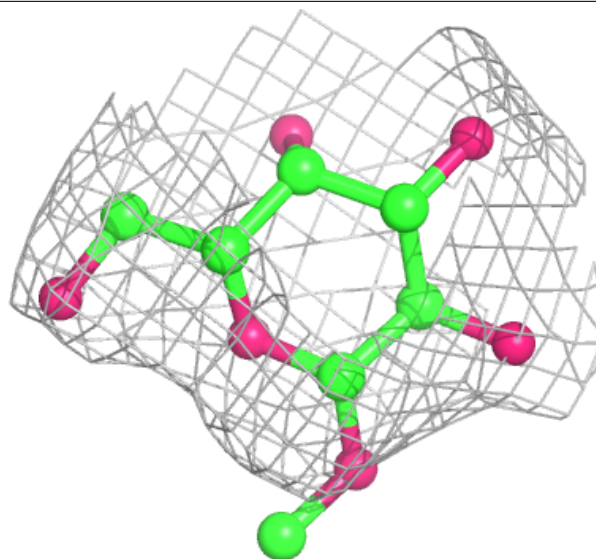
**Electron density around BCR L 307:**

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



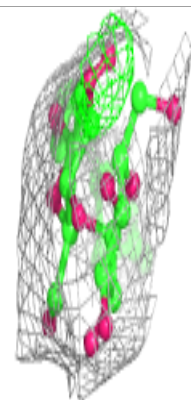
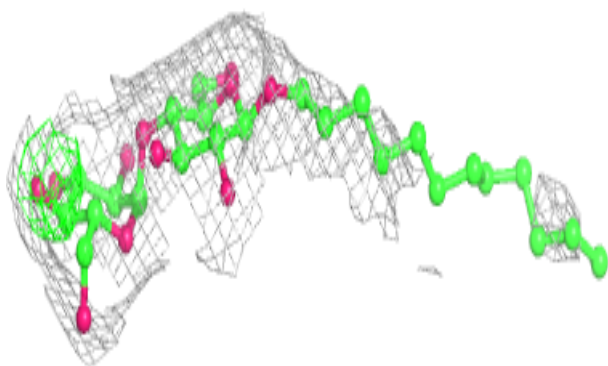
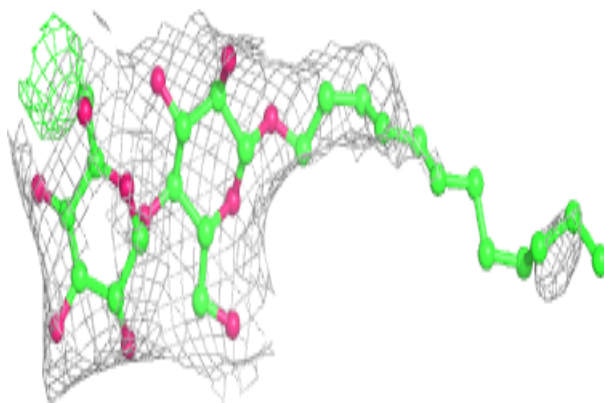
**Electron density around LMG B 854:**

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

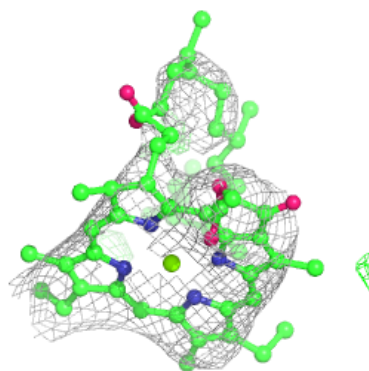
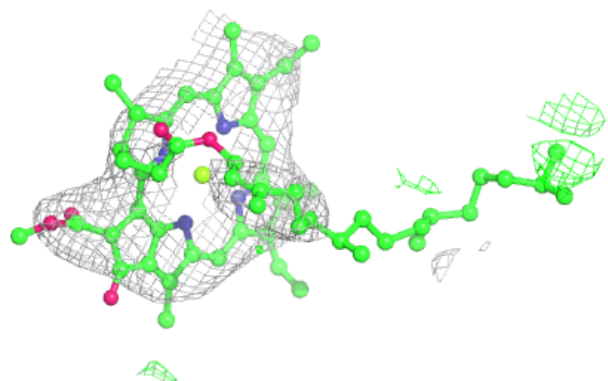
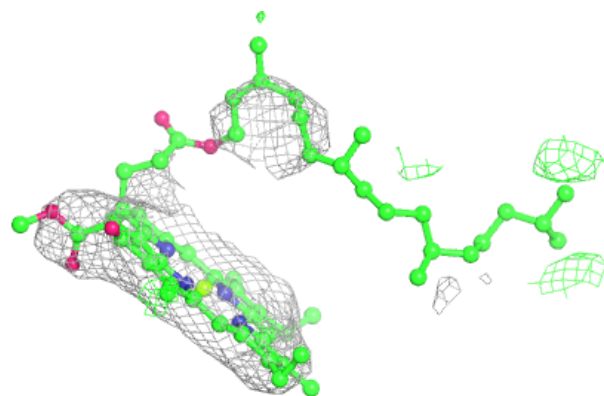


**Electron density around LMT G 1605:**

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

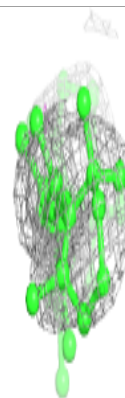
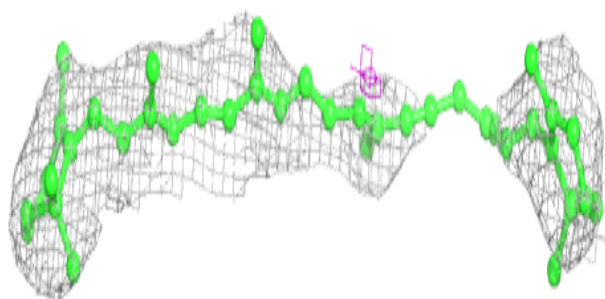
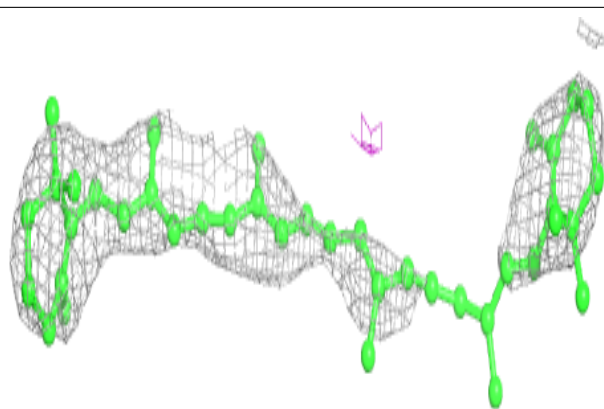
**Electron density around CLA G 1603:**

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

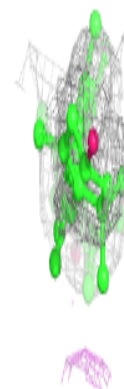
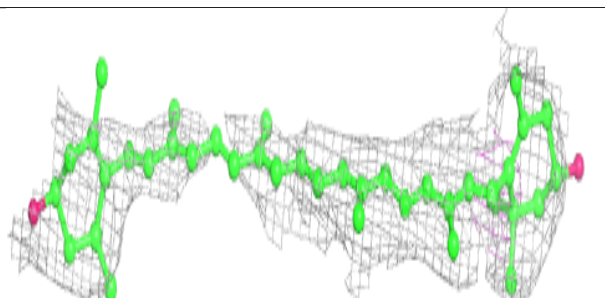
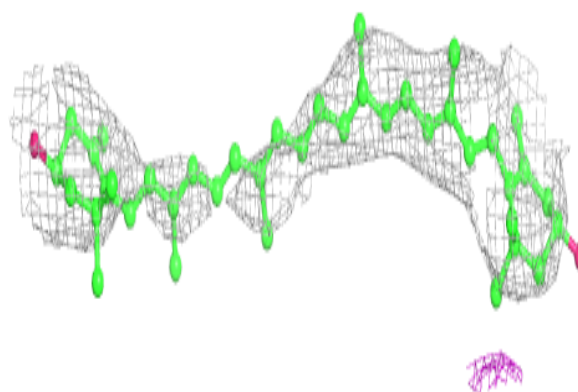


**Electron density around BCR A 846:**

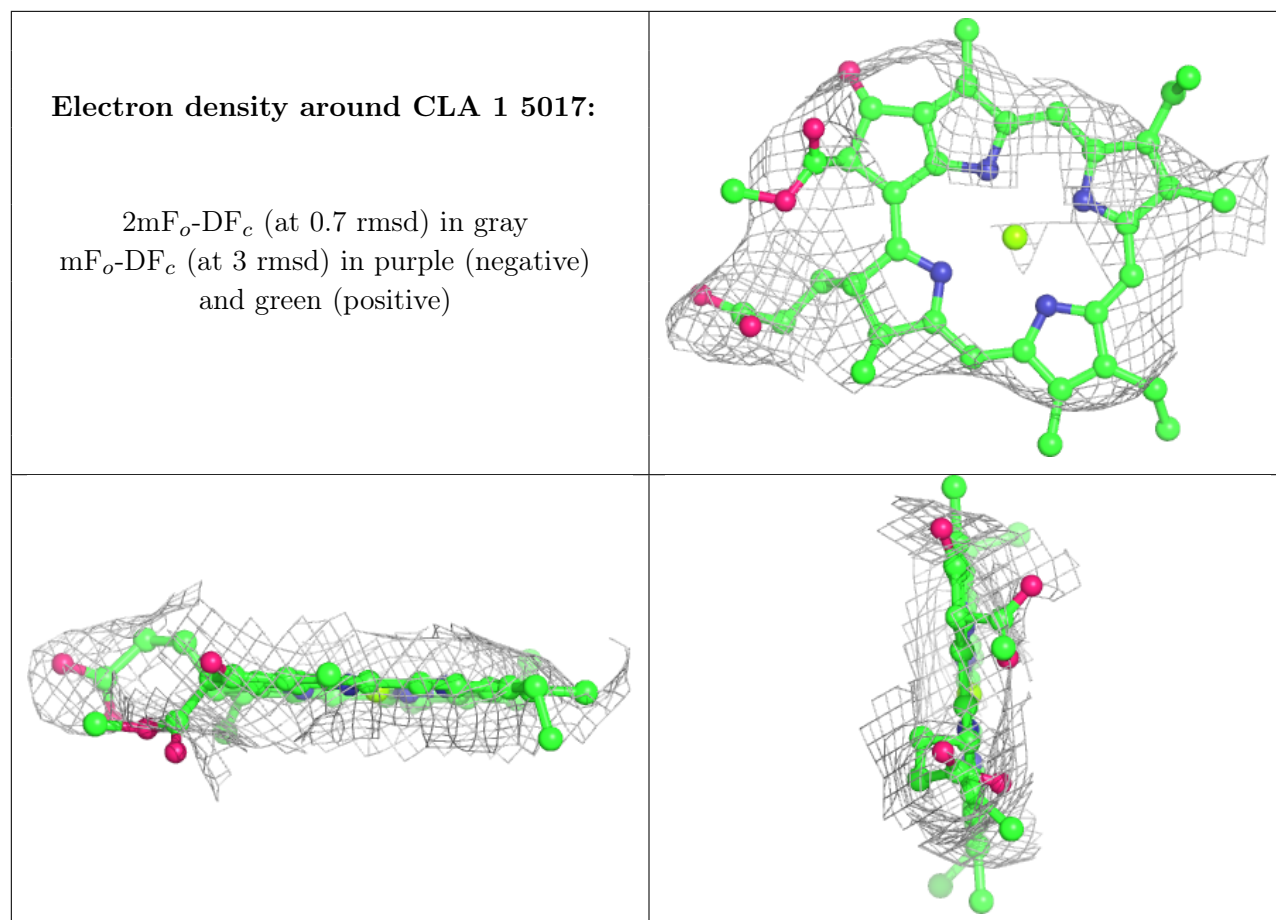
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LUT 2 303:**

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

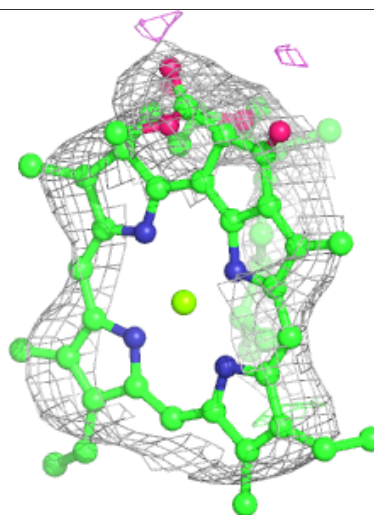
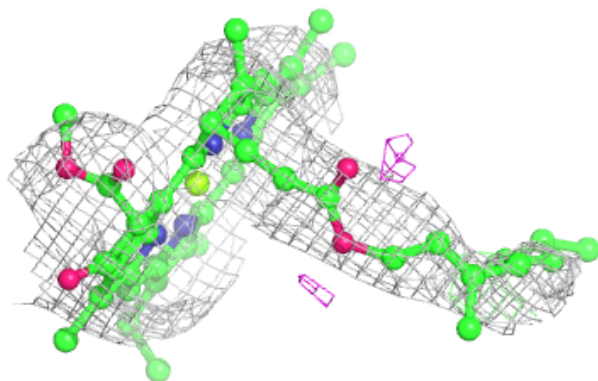
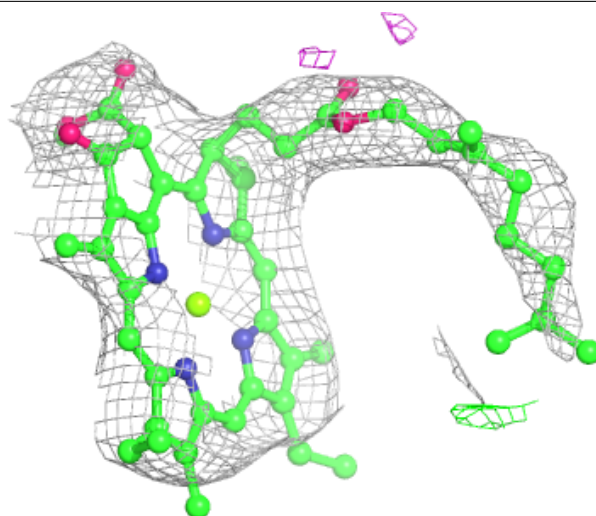






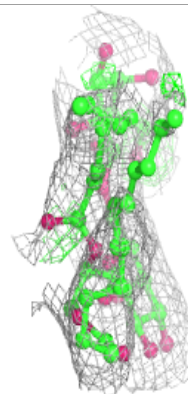
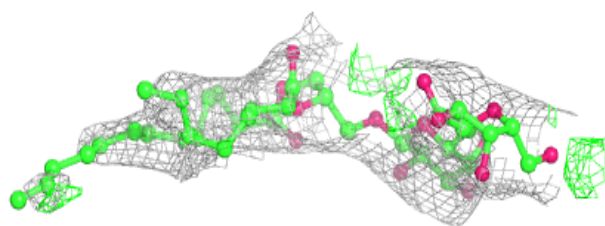
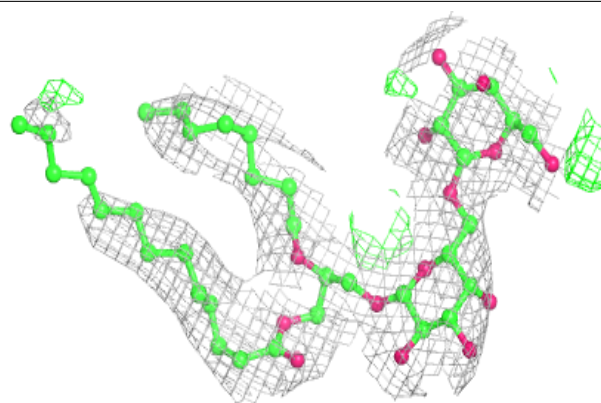
**Electron density around CLA B 816:**

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

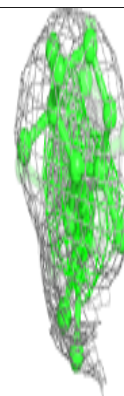
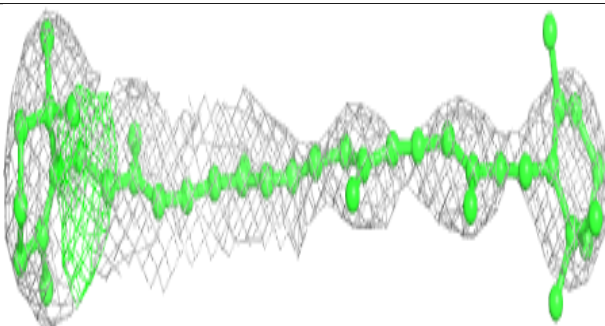
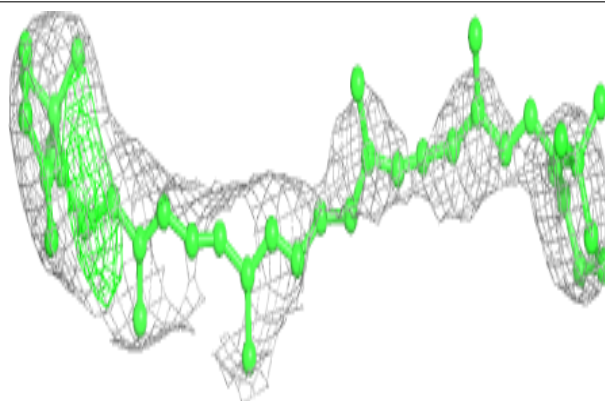


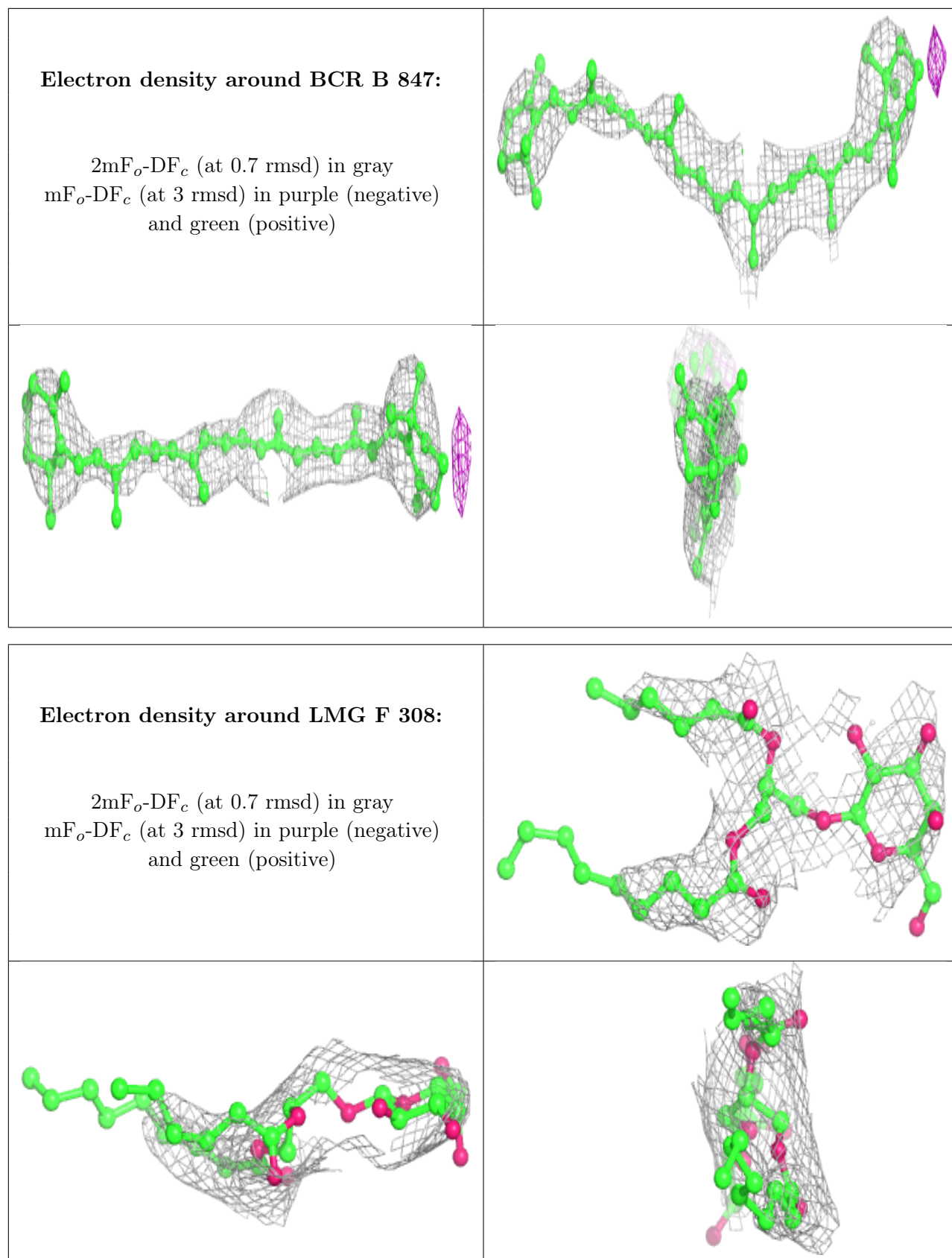
**Electron density around DGD 2 327:**

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

**Electron density around BCR B 846:**

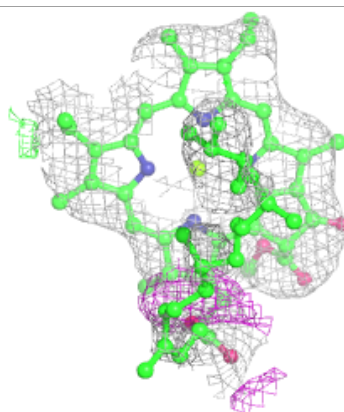
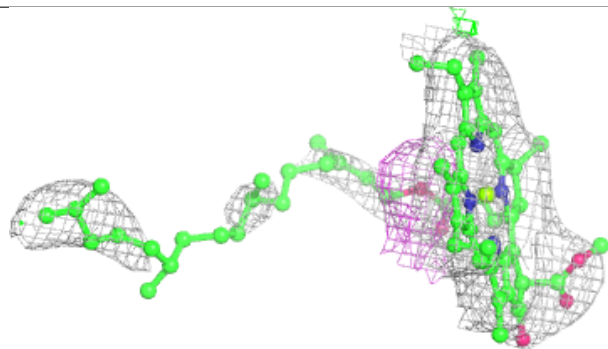
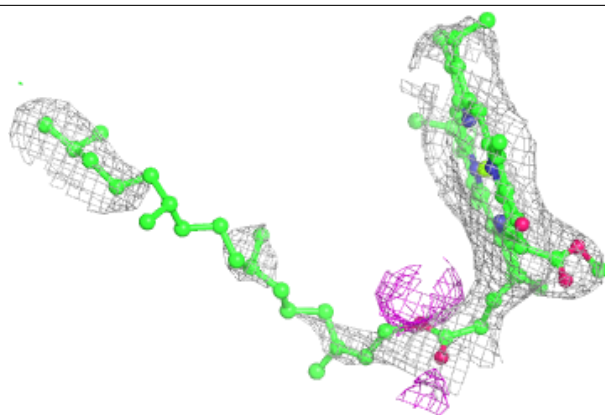
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



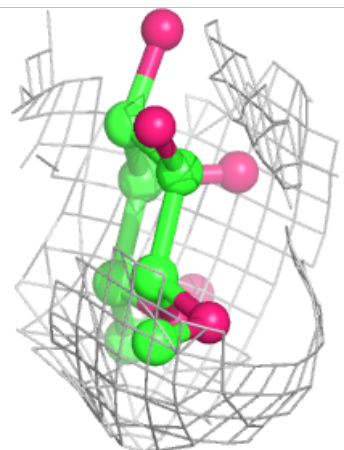
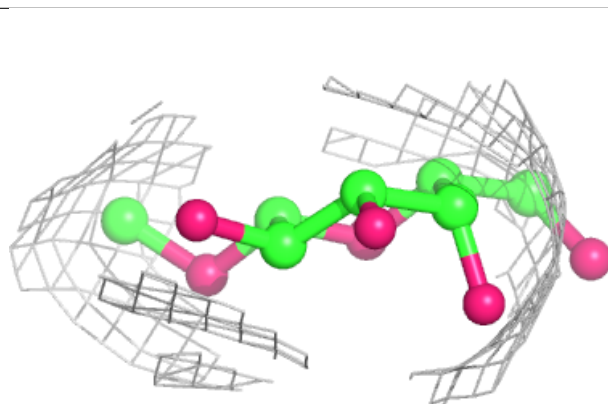
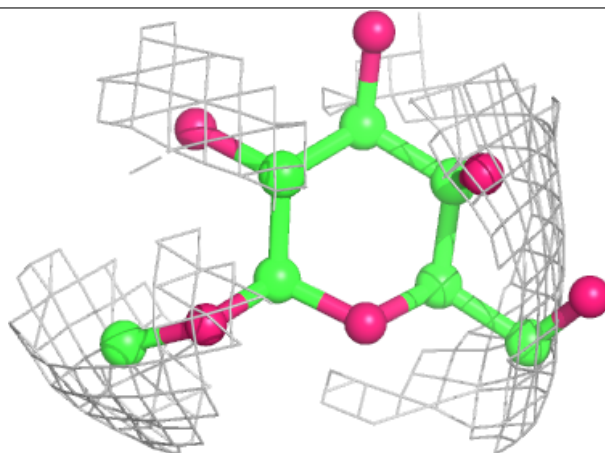


**Electron density around CLA A 803:**

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

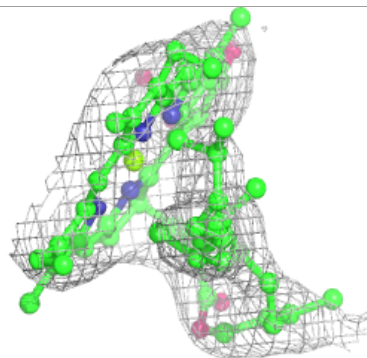
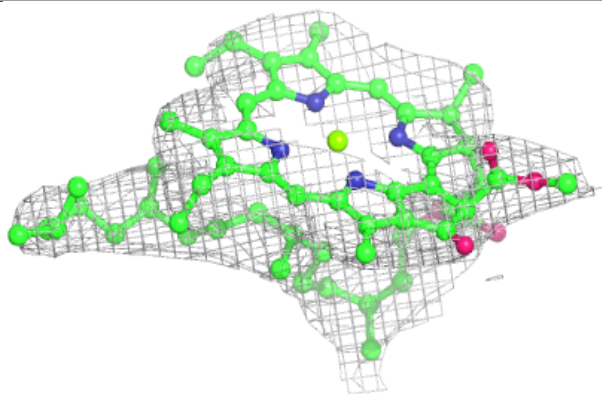
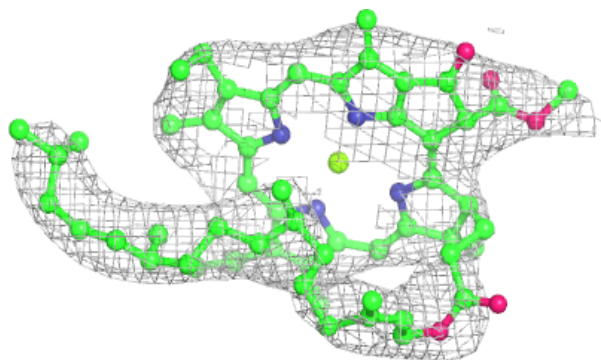
**Electron density around LMG 2 324:**

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

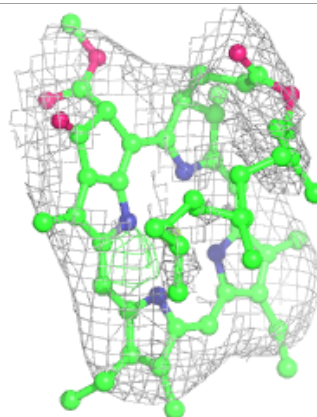
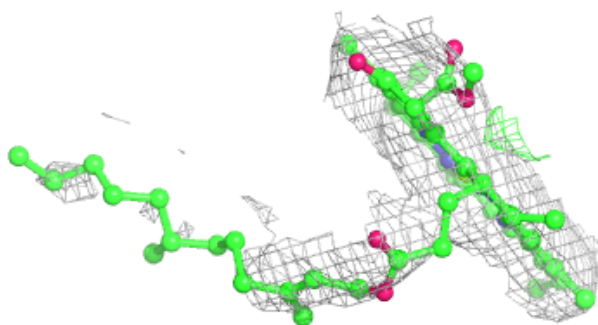
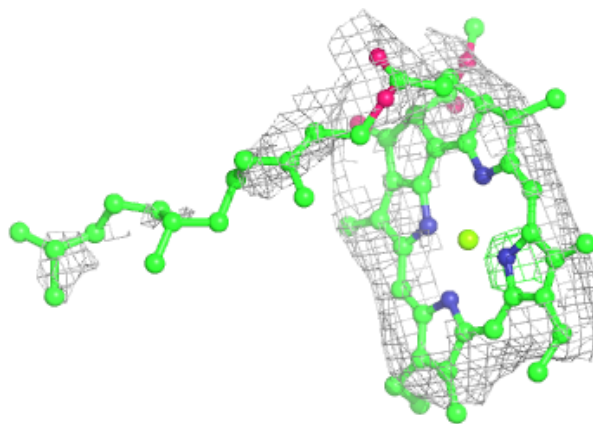


**Electron density around CLA B 818:**

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

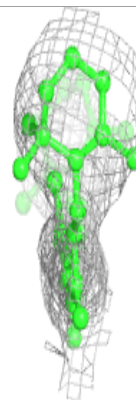
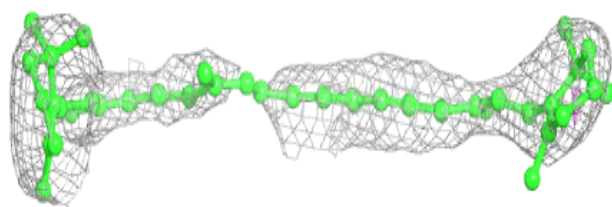
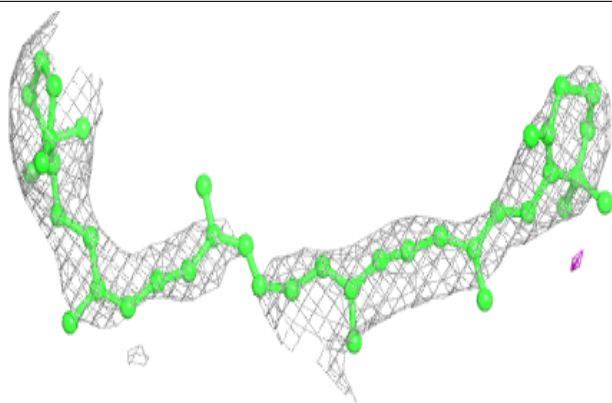
**Electron density around CLA 4 311:**

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

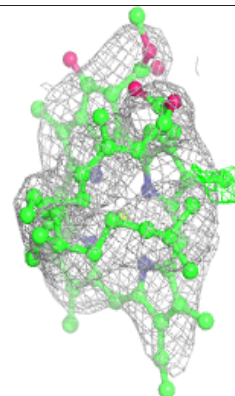
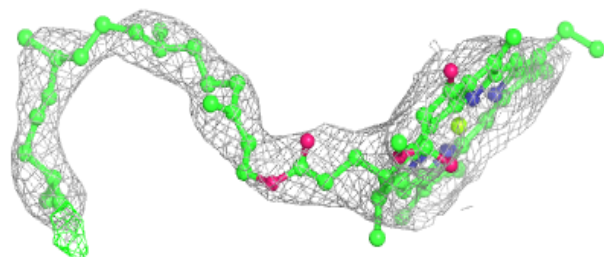
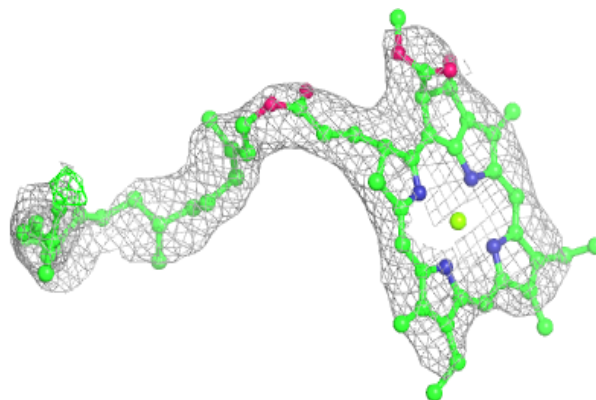


**Electron density around BCR L 303:**

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

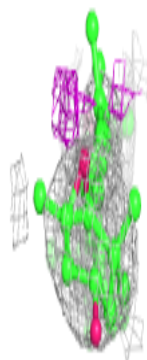
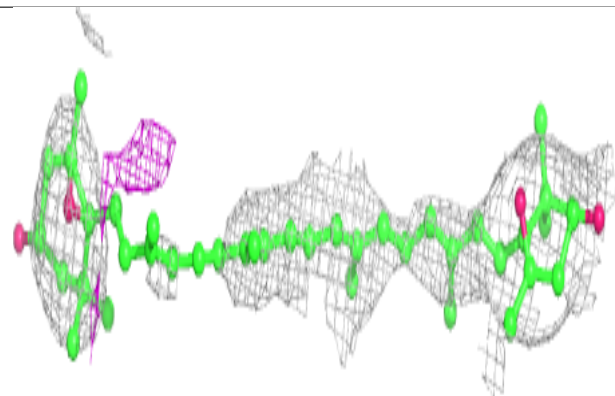
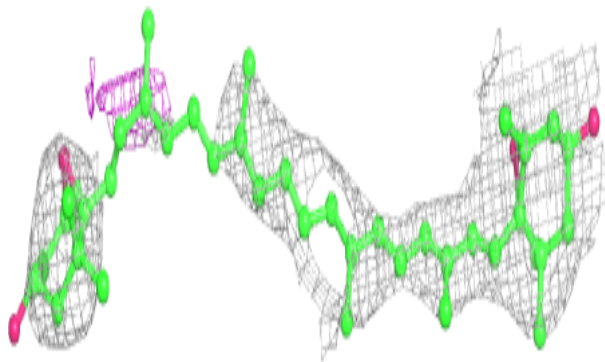
**Electron density around CLA B 810:**

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



**Electron density around XAT 2 304:**

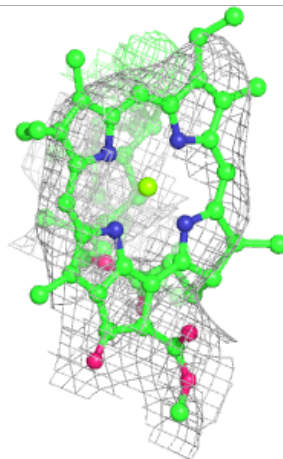
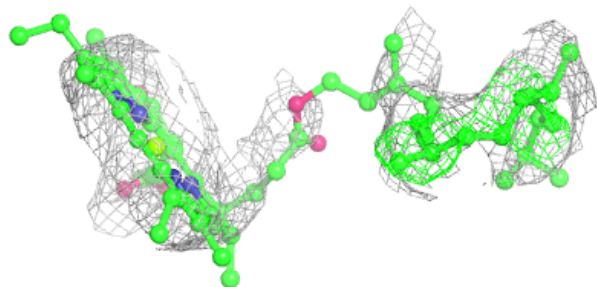
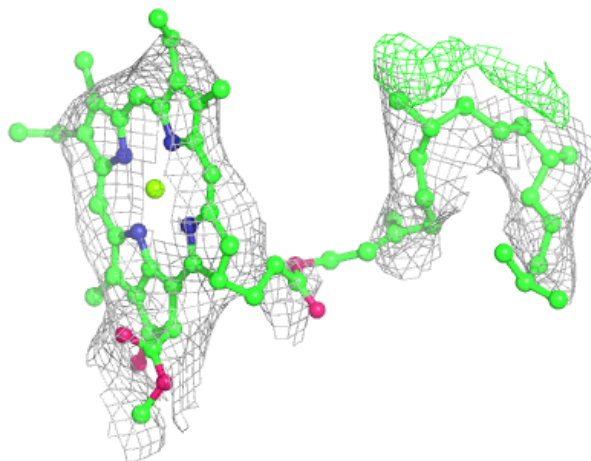
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





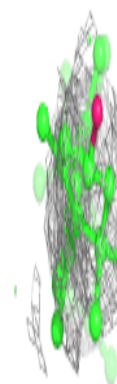
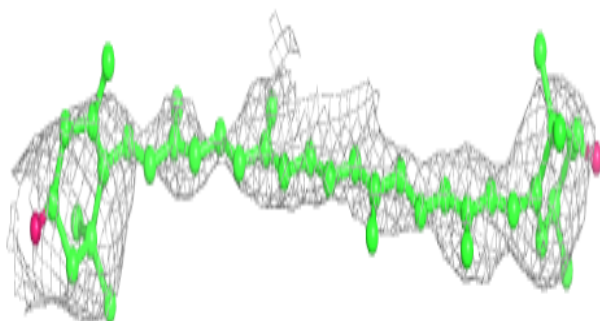
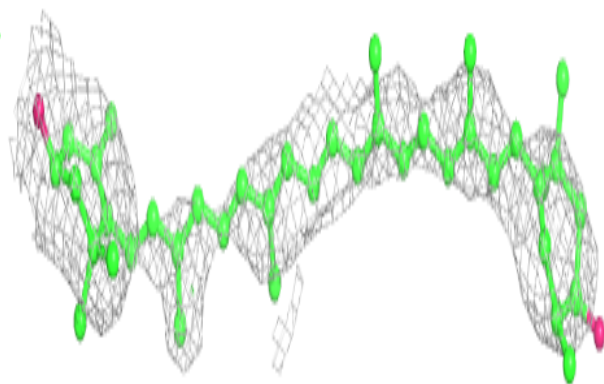
**Electron density around CLA 1 5015:**

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

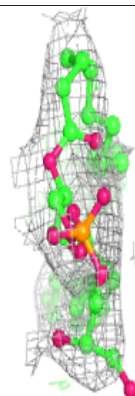
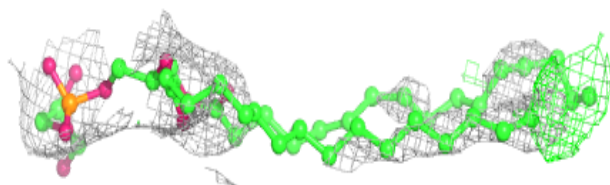
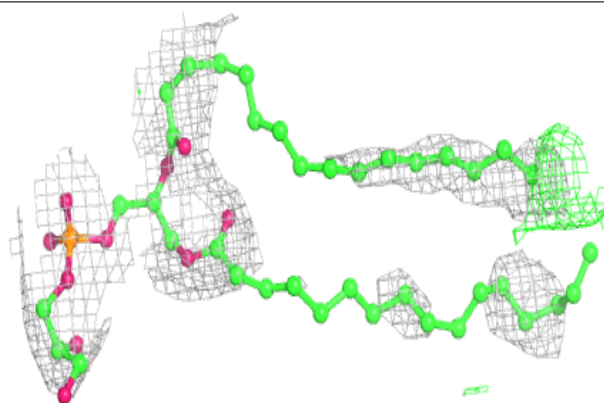


**Electron density around ZEX F 310:**

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

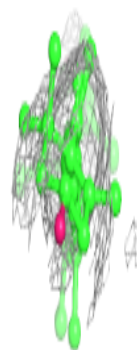
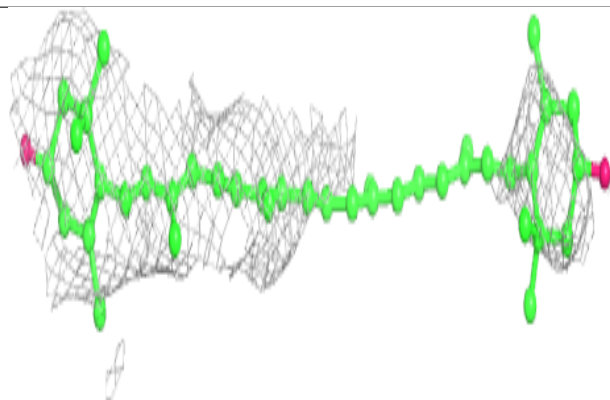
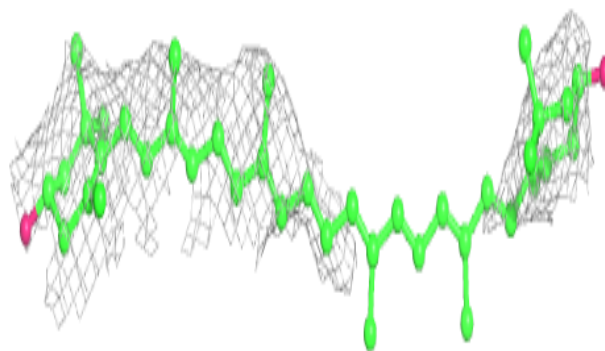
**Electron density around LHG 1 5019:**

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

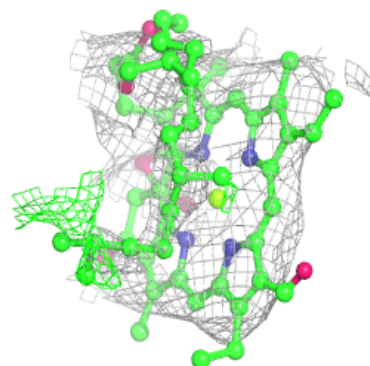
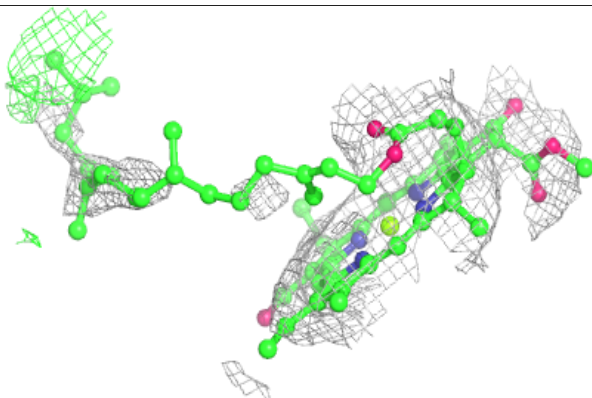
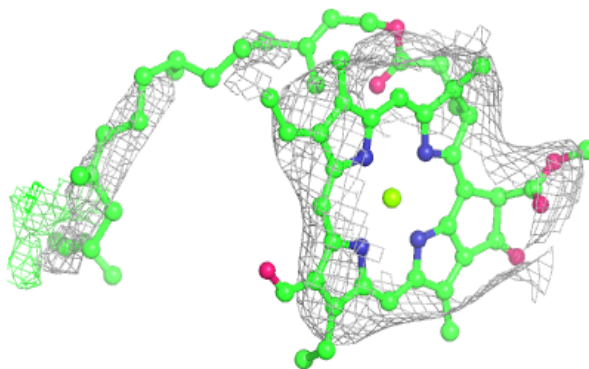


**Electron density around LUT 1 5003:**

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

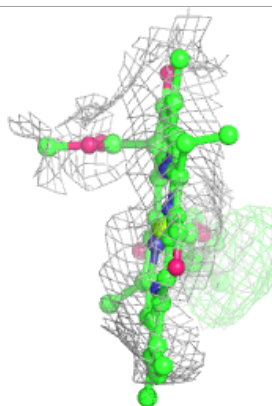
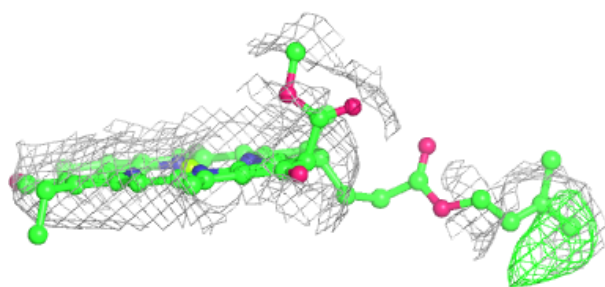
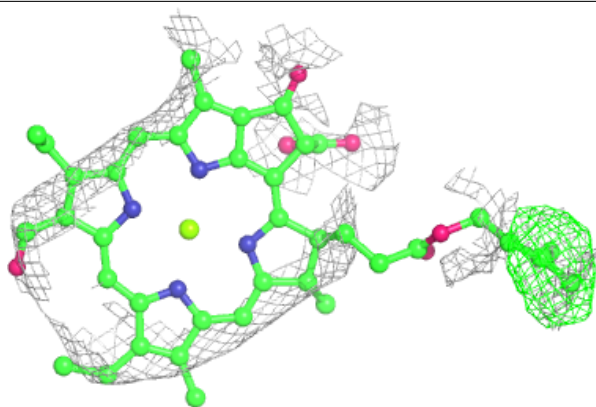
**Electron density around CHL 3 310:**

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

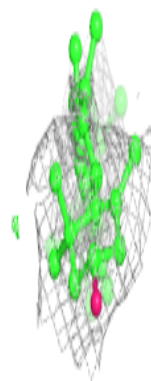
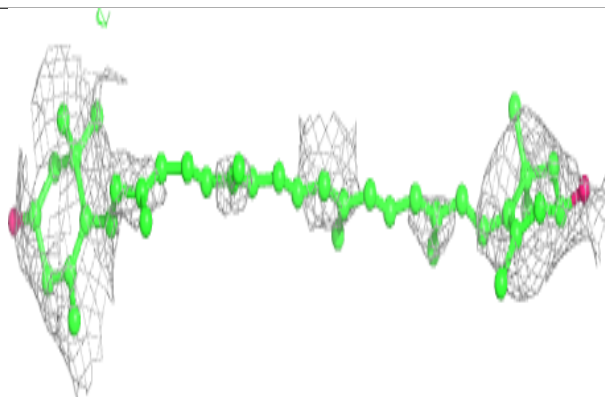
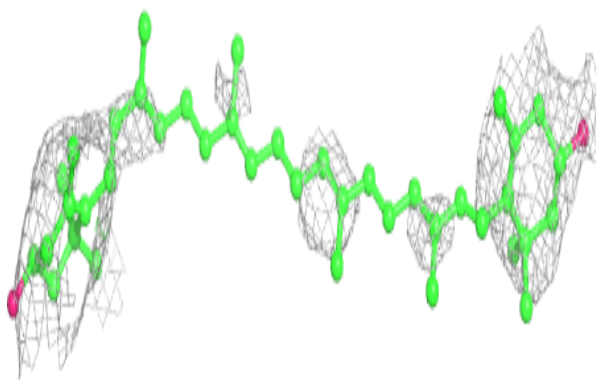


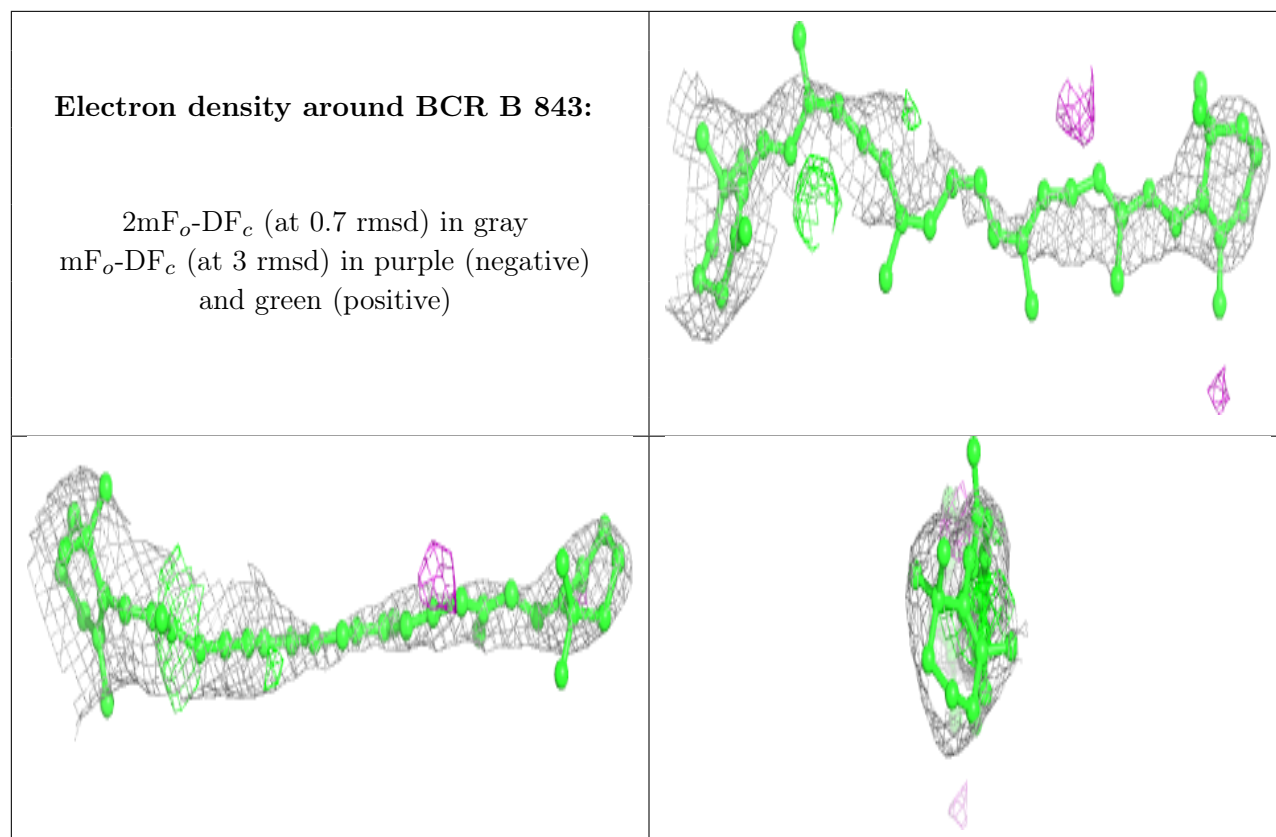
**Electron density around CHL 3 313:**

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

**Electron density around LUT 1 5004:**

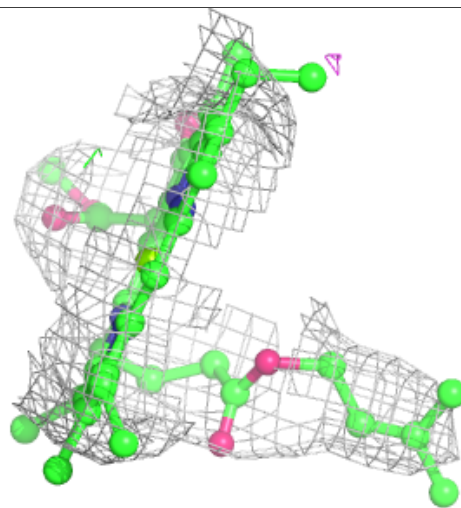
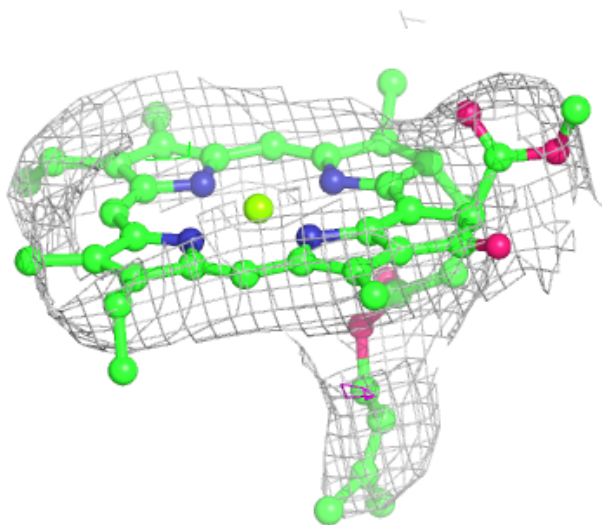
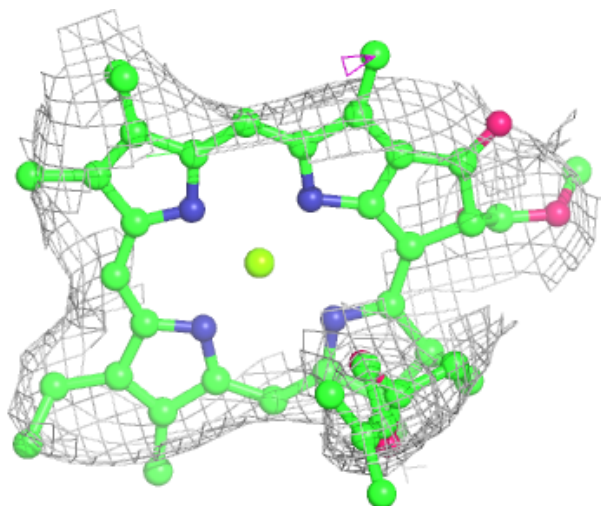
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





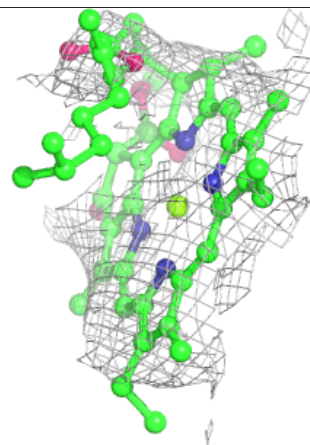
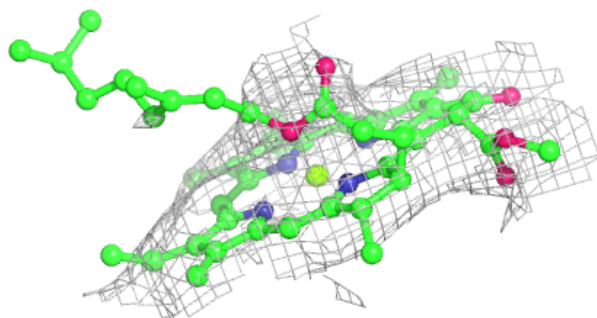
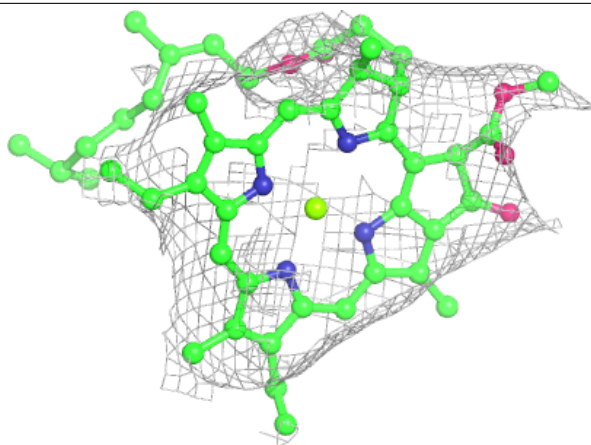
**Electron density around CLA L 304:**

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



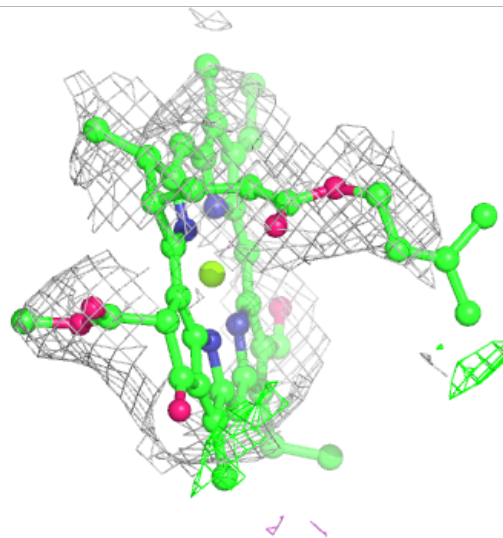
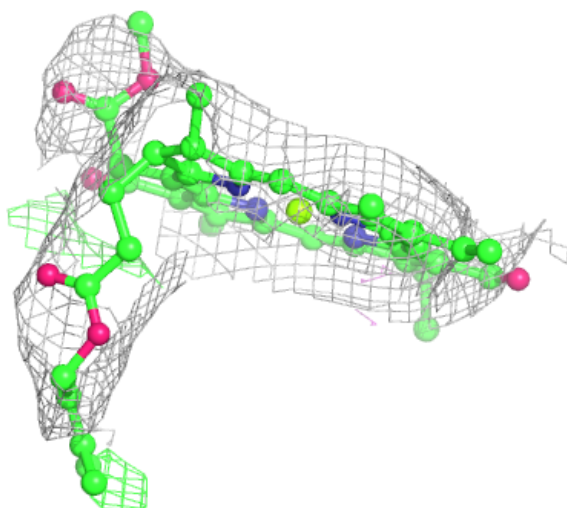
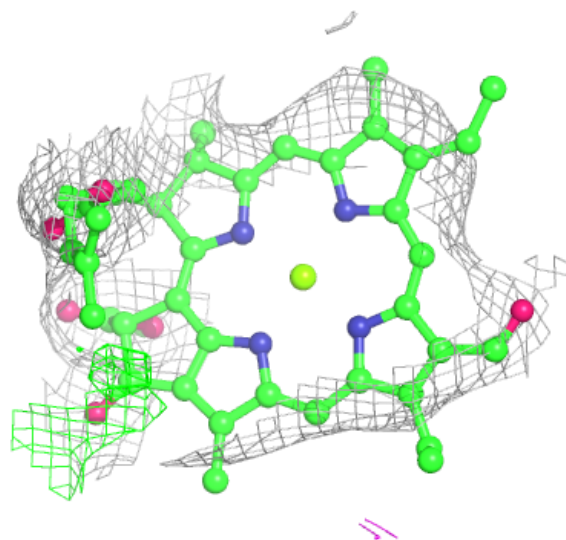
**Electron density around CLA 3 307:**

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



**Electron density around CHL 3 312:**

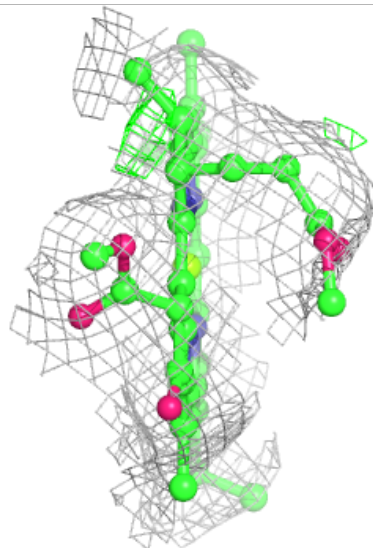
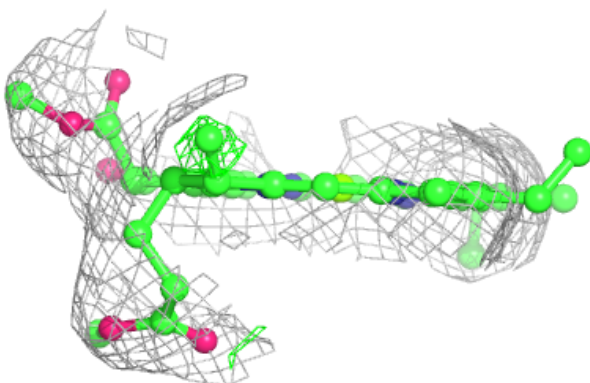
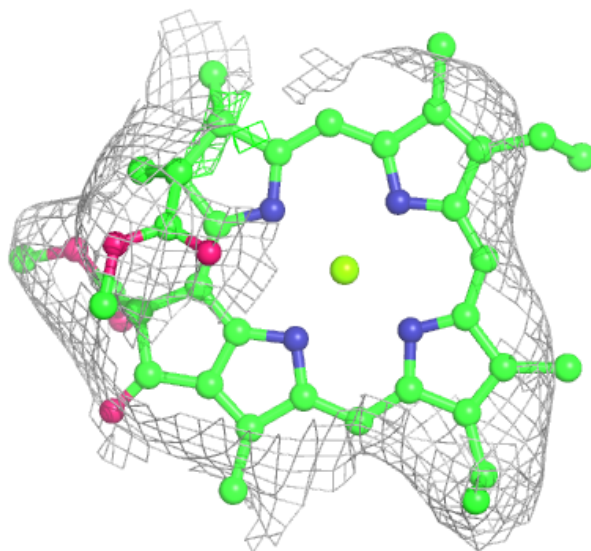
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





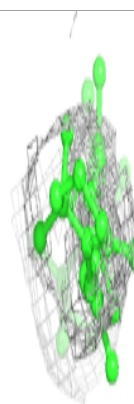
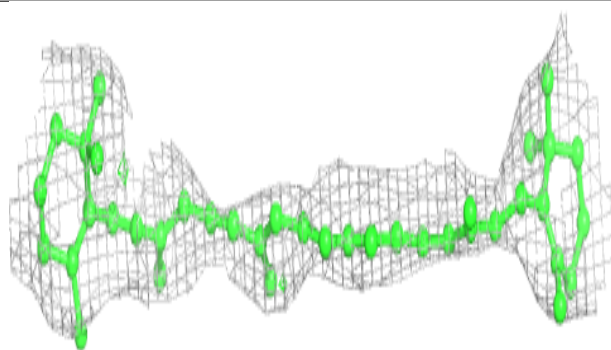
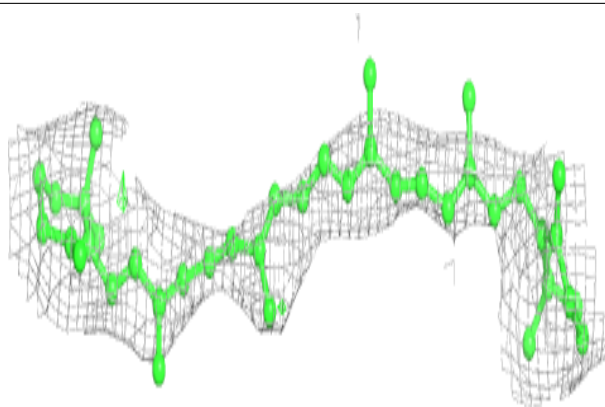
**Electron density around CLA 4 312:**

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

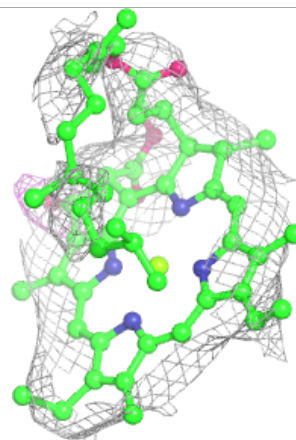
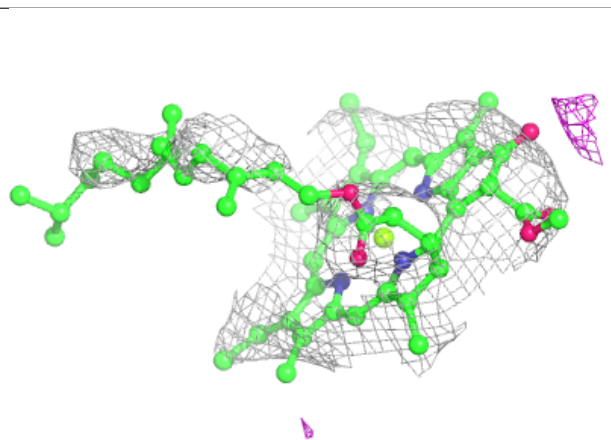
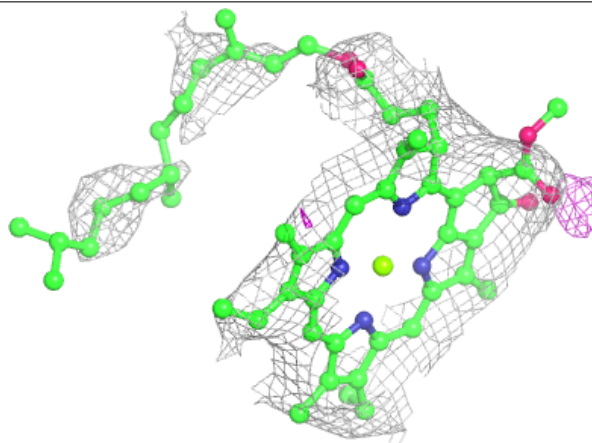


**Electron density around BCR 3 305:**

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

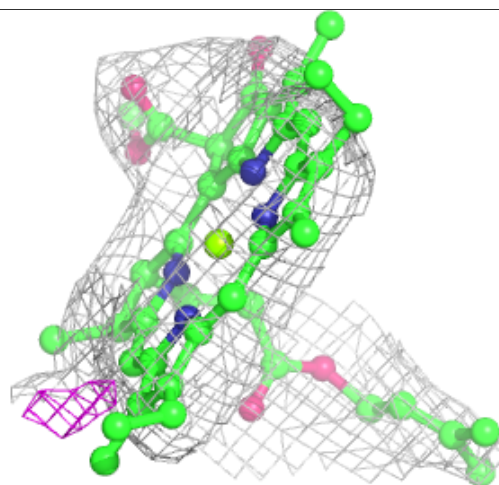
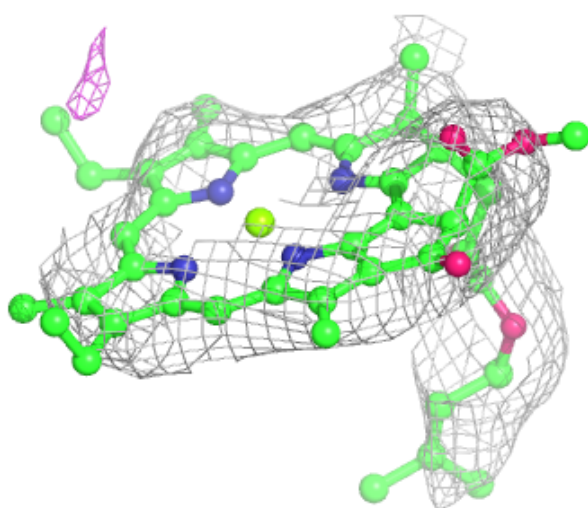
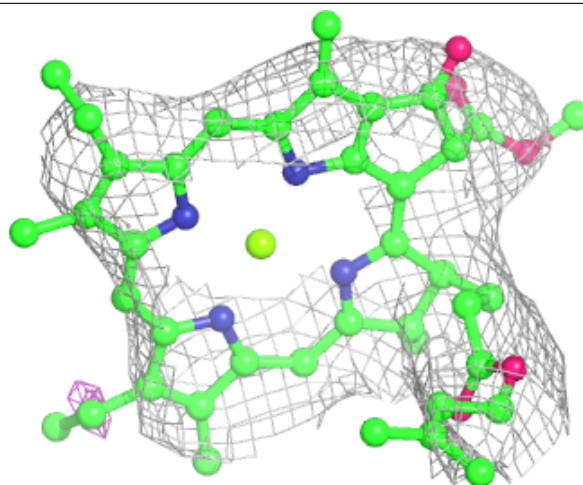
**Electron density around CLA A 840:**

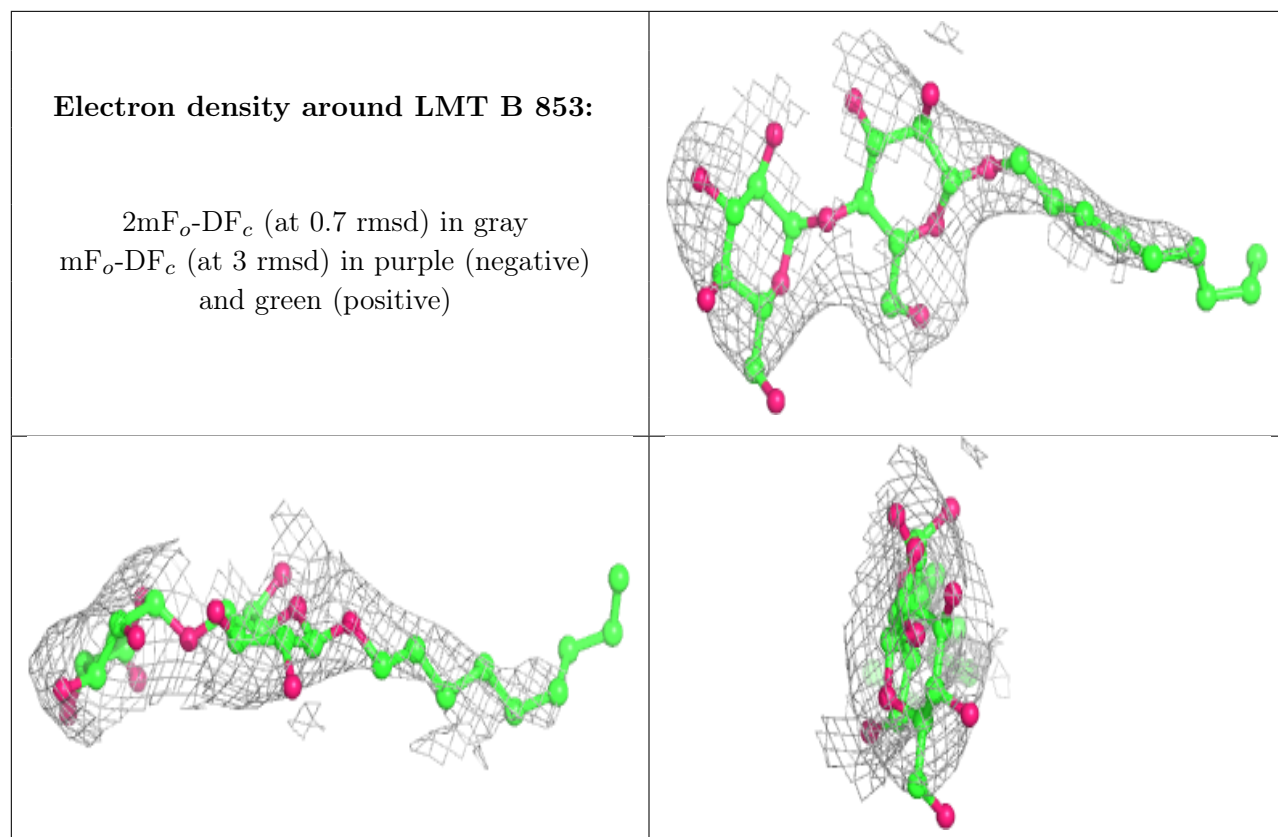
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 2 311:**

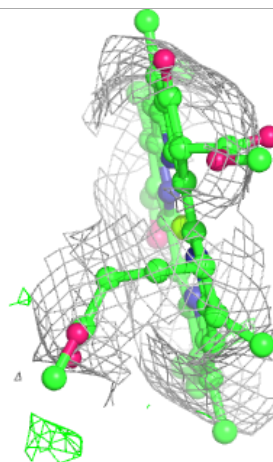
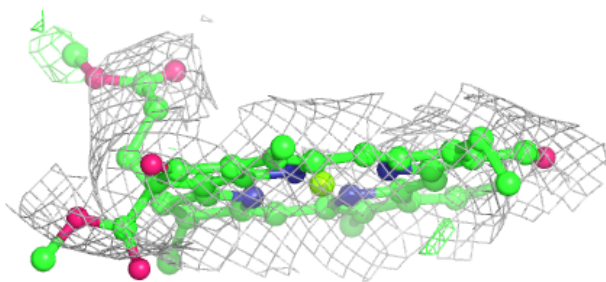
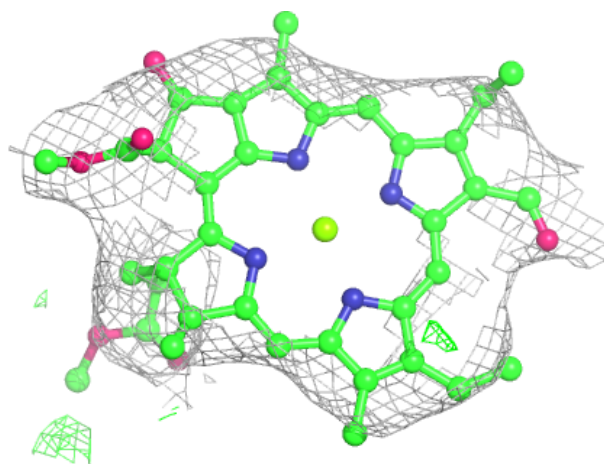
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





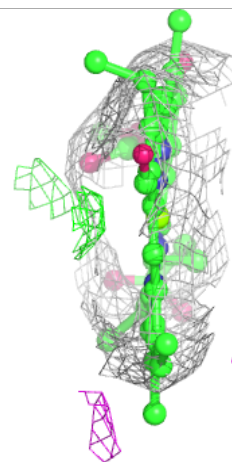
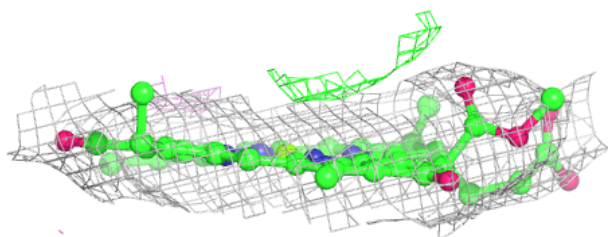
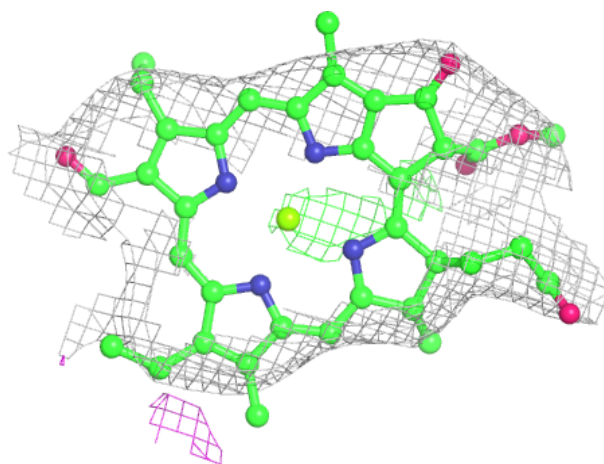
**Electron density around CHL 1 5014:**

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



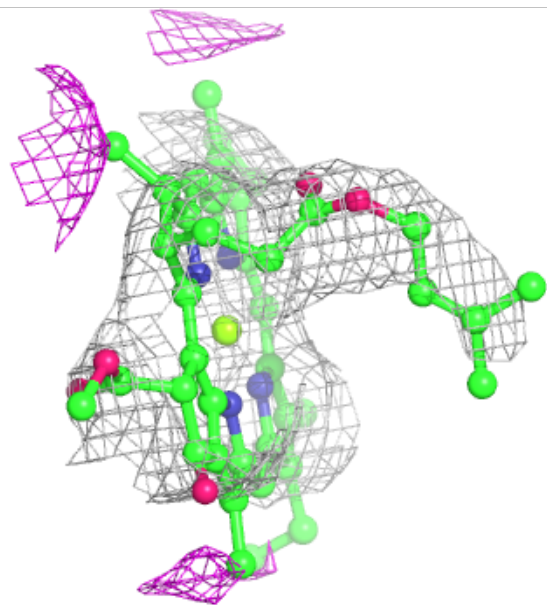
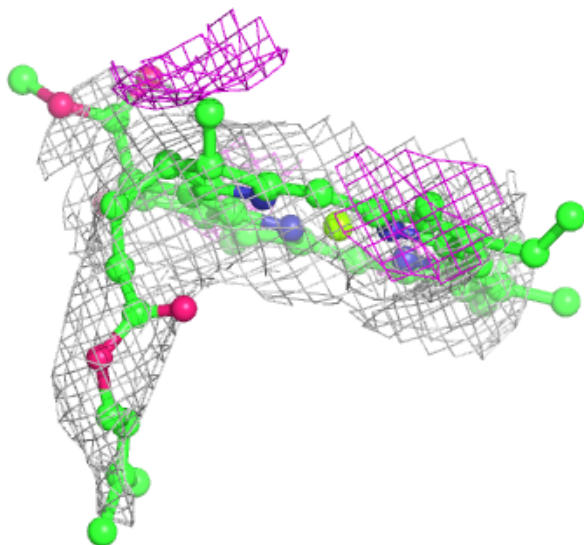
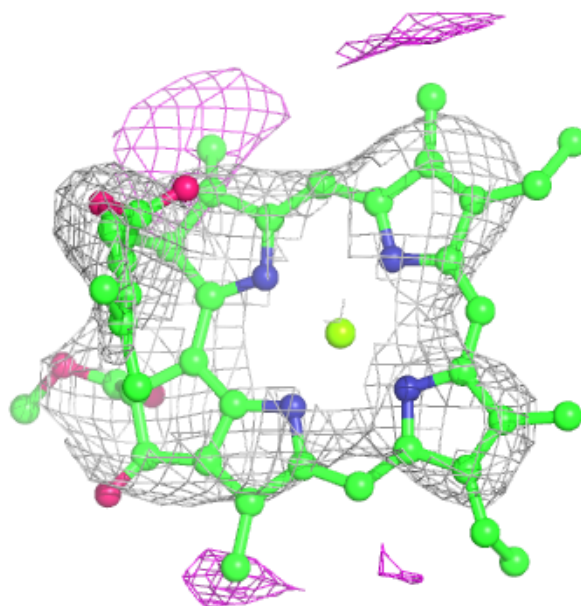
**Electron density around CHL 2 318:**

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



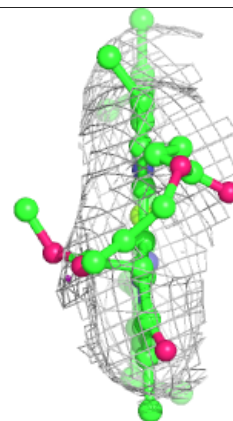
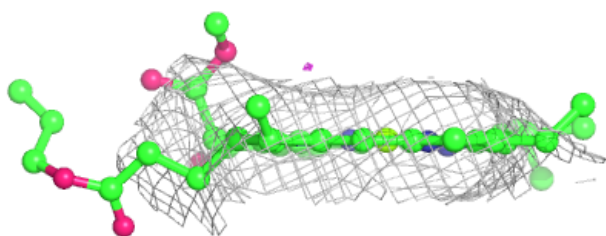
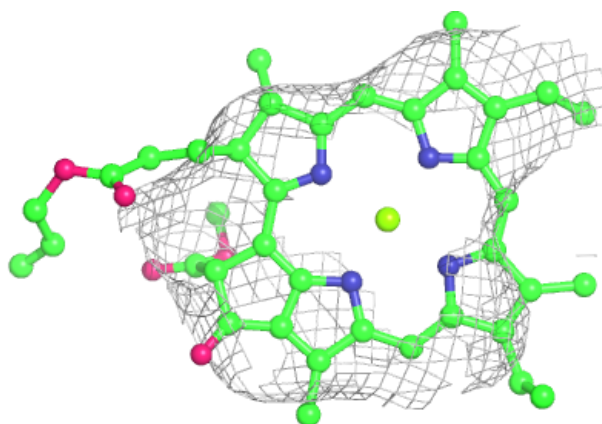
**Electron density around CLA L 306:**

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

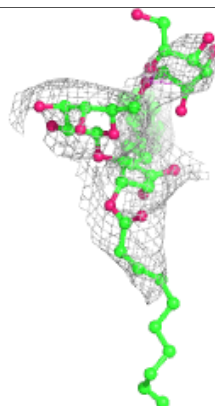
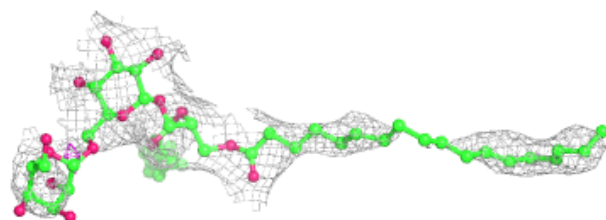
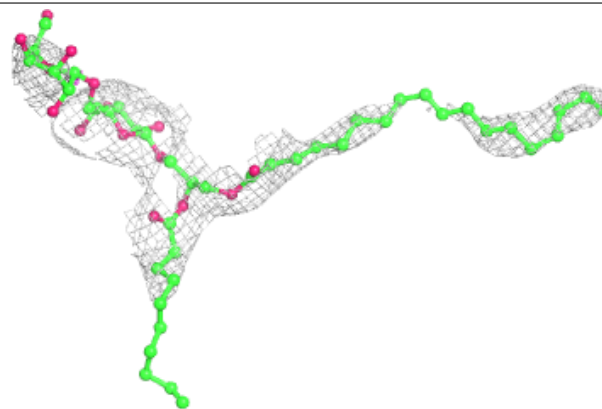


**Electron density around CLA K 1403:**

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

**Electron density around DGD J 1106:**

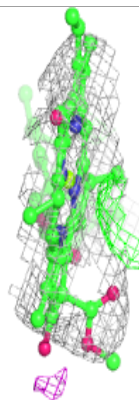
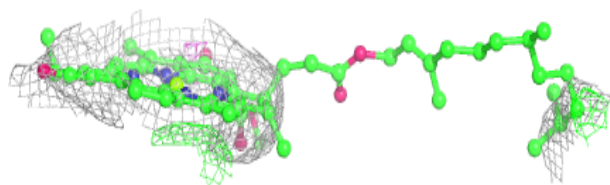
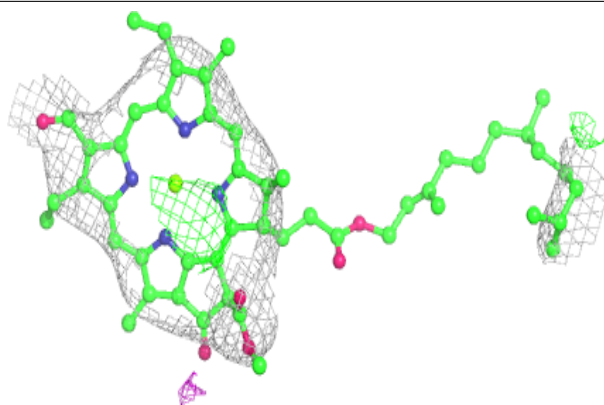
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





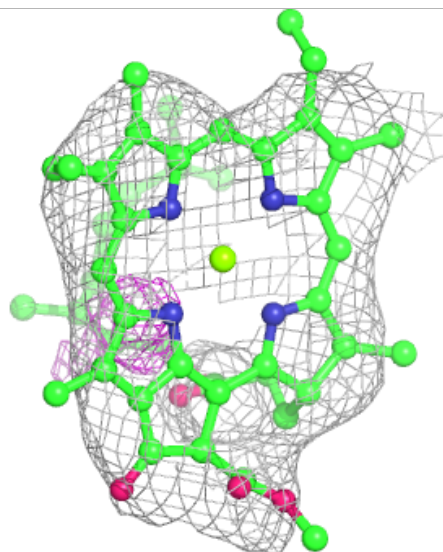
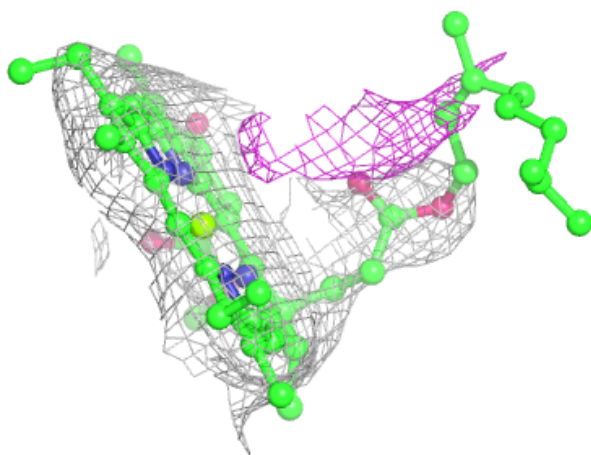
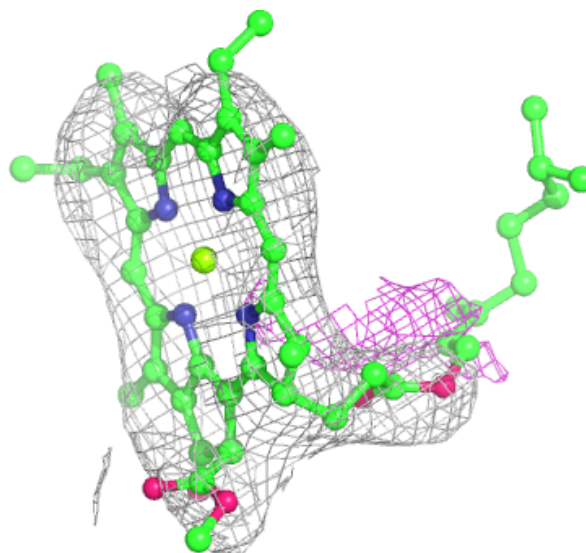
**Electron density around CHL 4 316:**

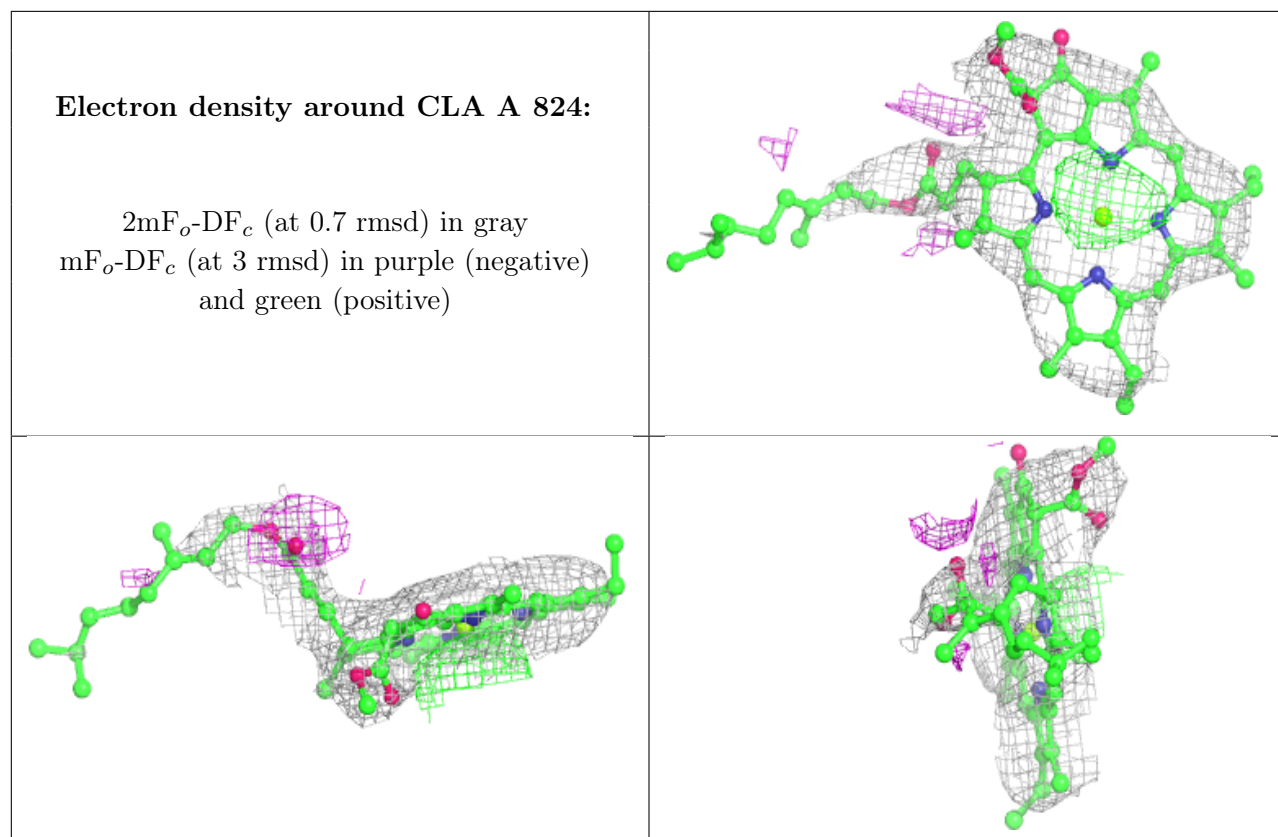
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA A 833:**

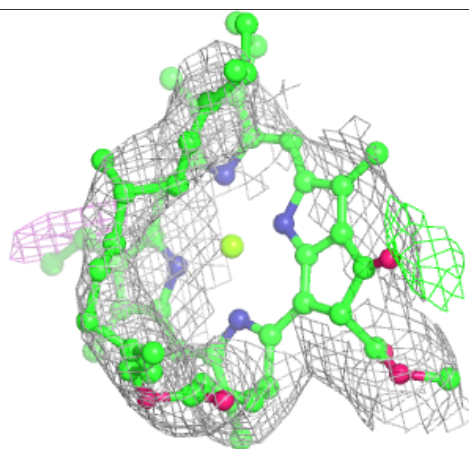
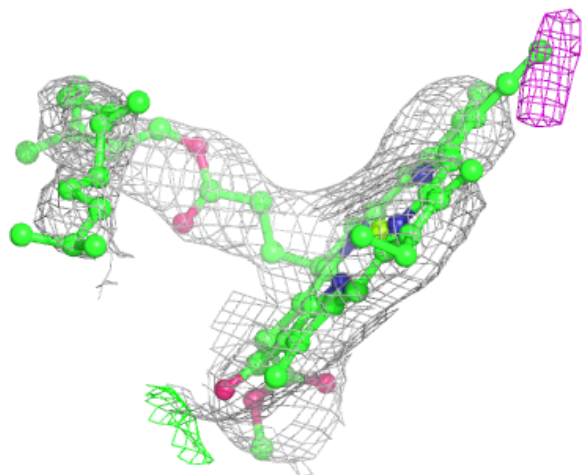
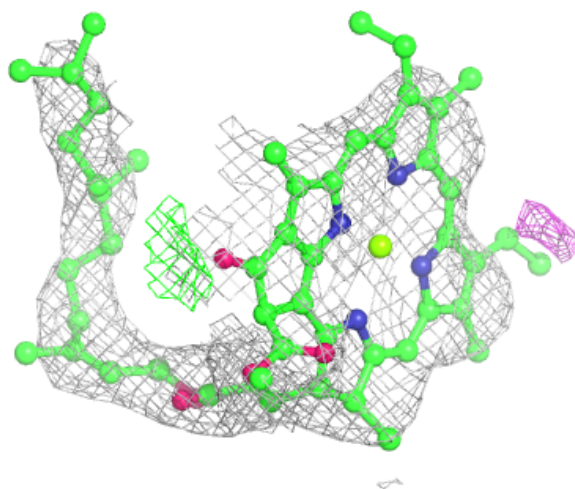
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





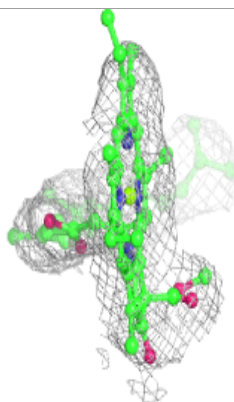
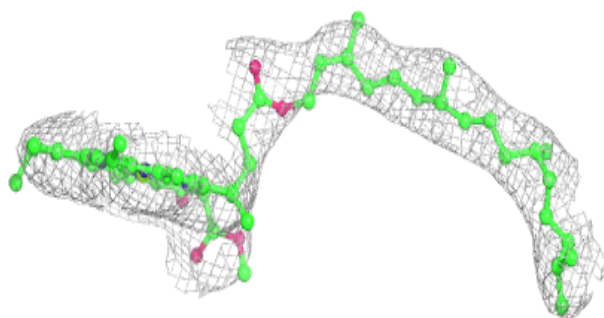
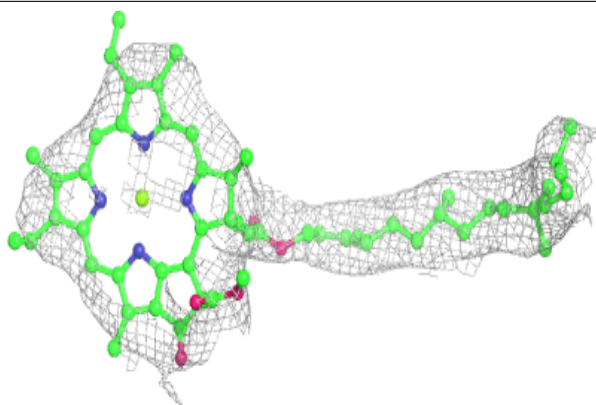
**Electron density around CLA B 834:**

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

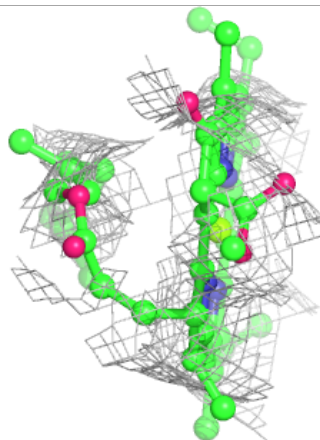
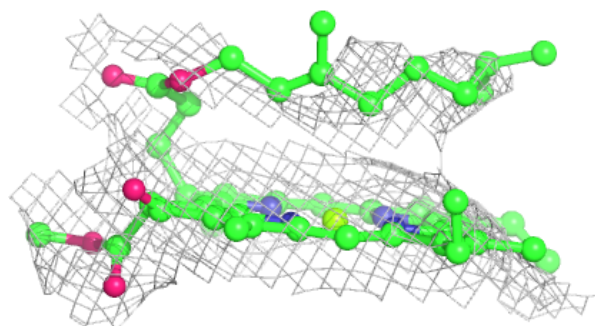
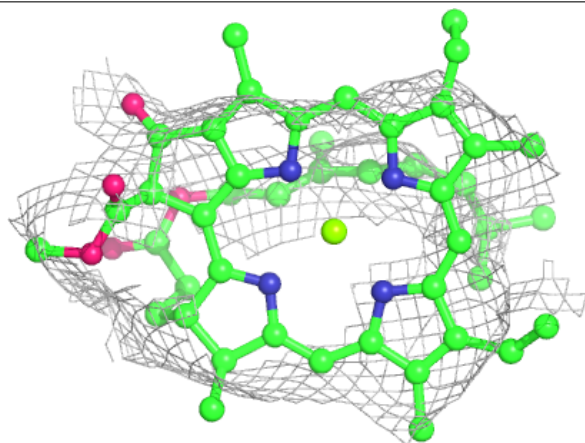


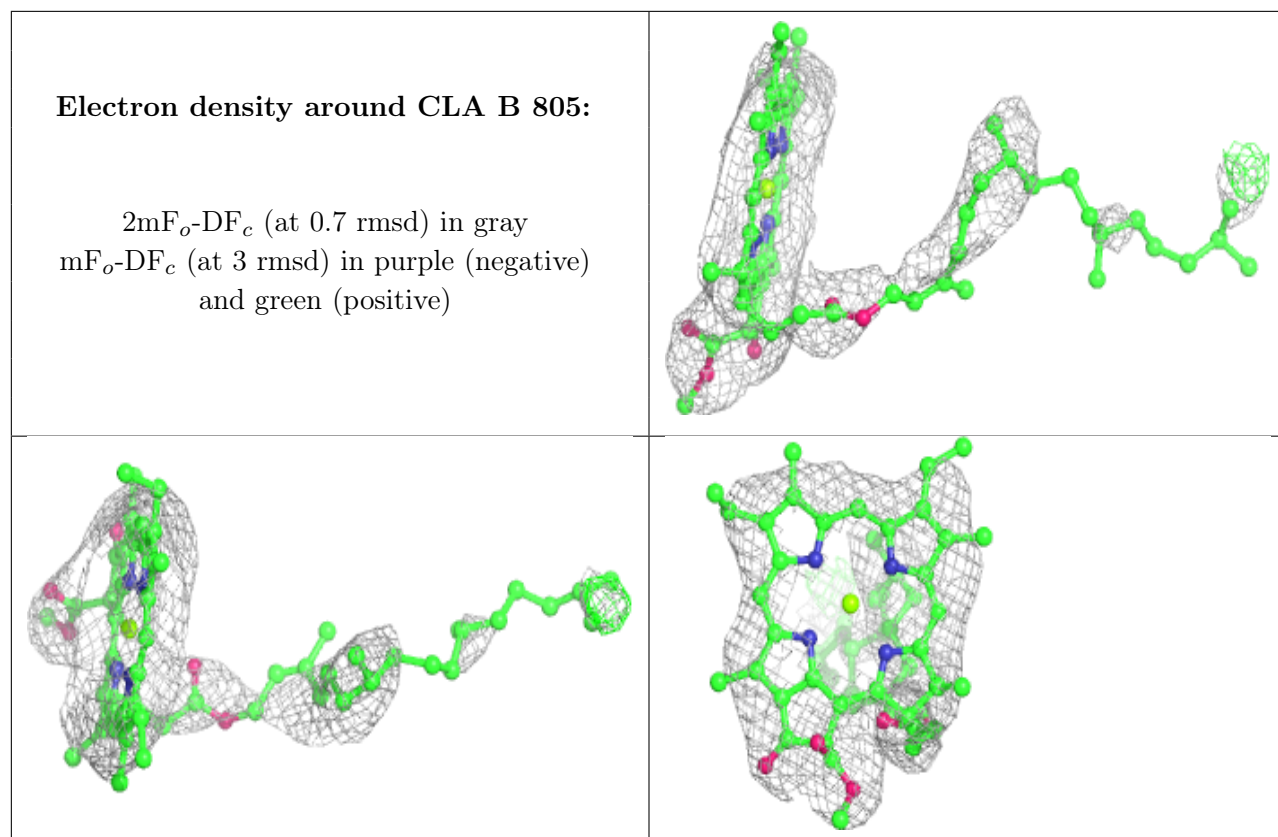
**Electron density around CLA B 841:**

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

**Electron density around CLA 3 309:**

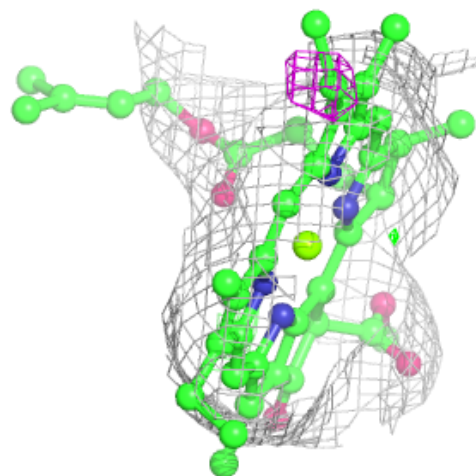
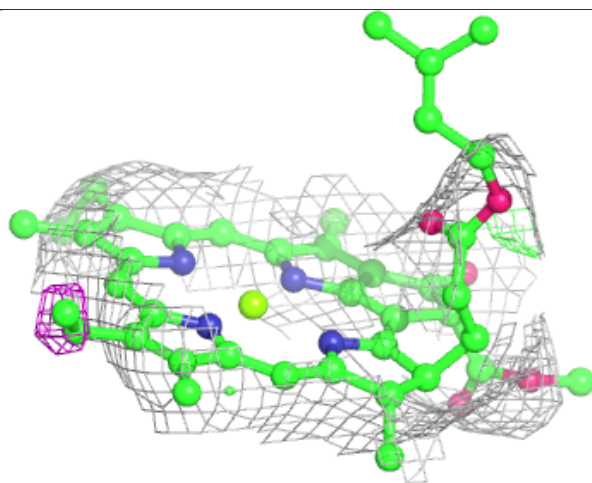
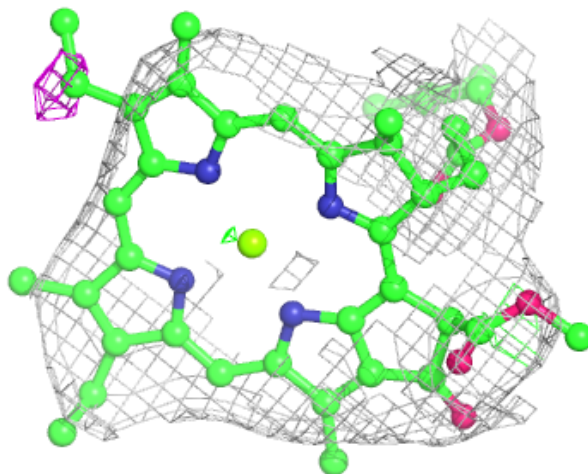
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





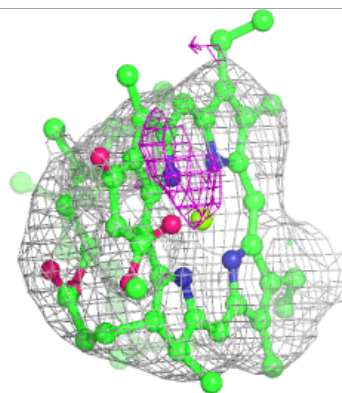
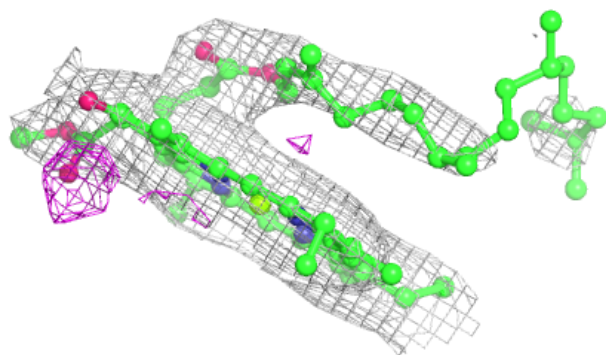
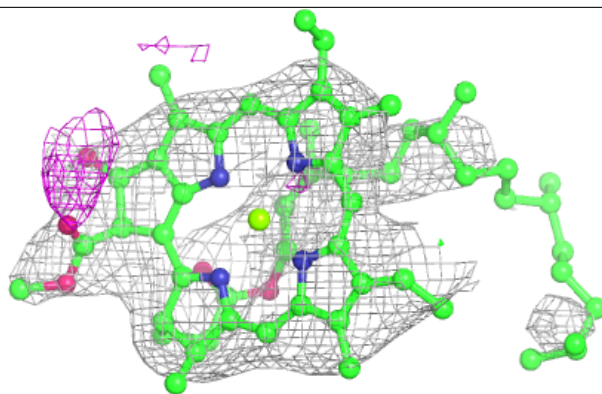
**Electron density around CLA 4 310:**

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

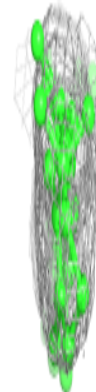
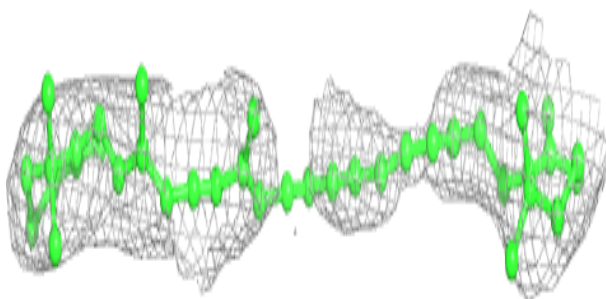
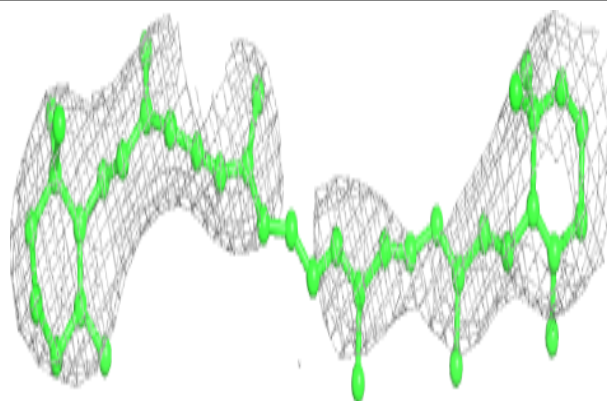


**Electron density around CLA B 808:**

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

**Electron density around BCR I 102:**

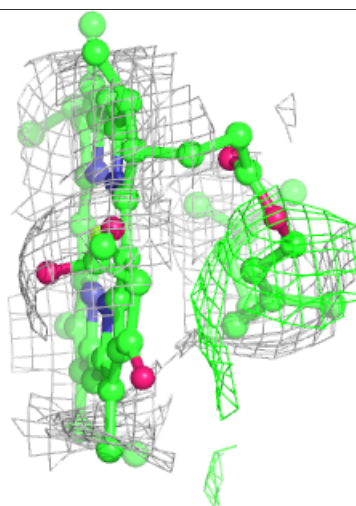
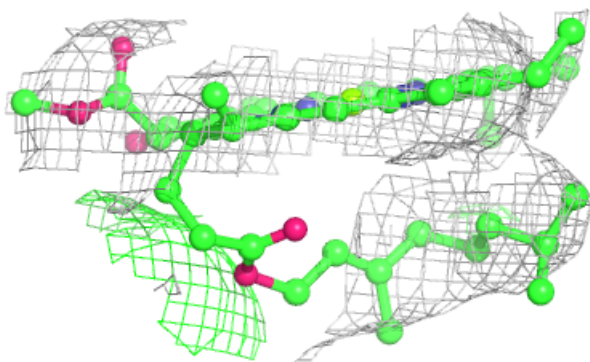
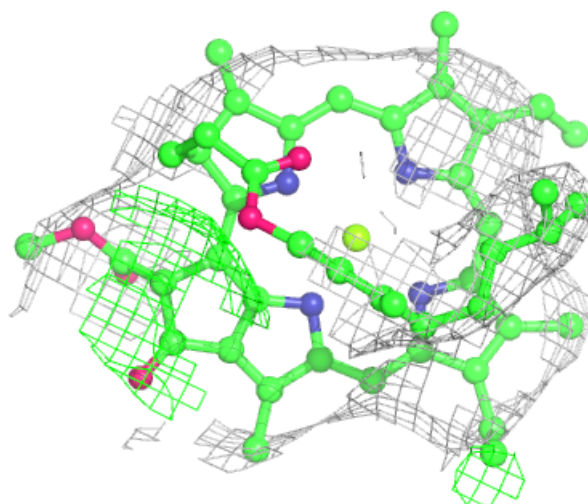
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

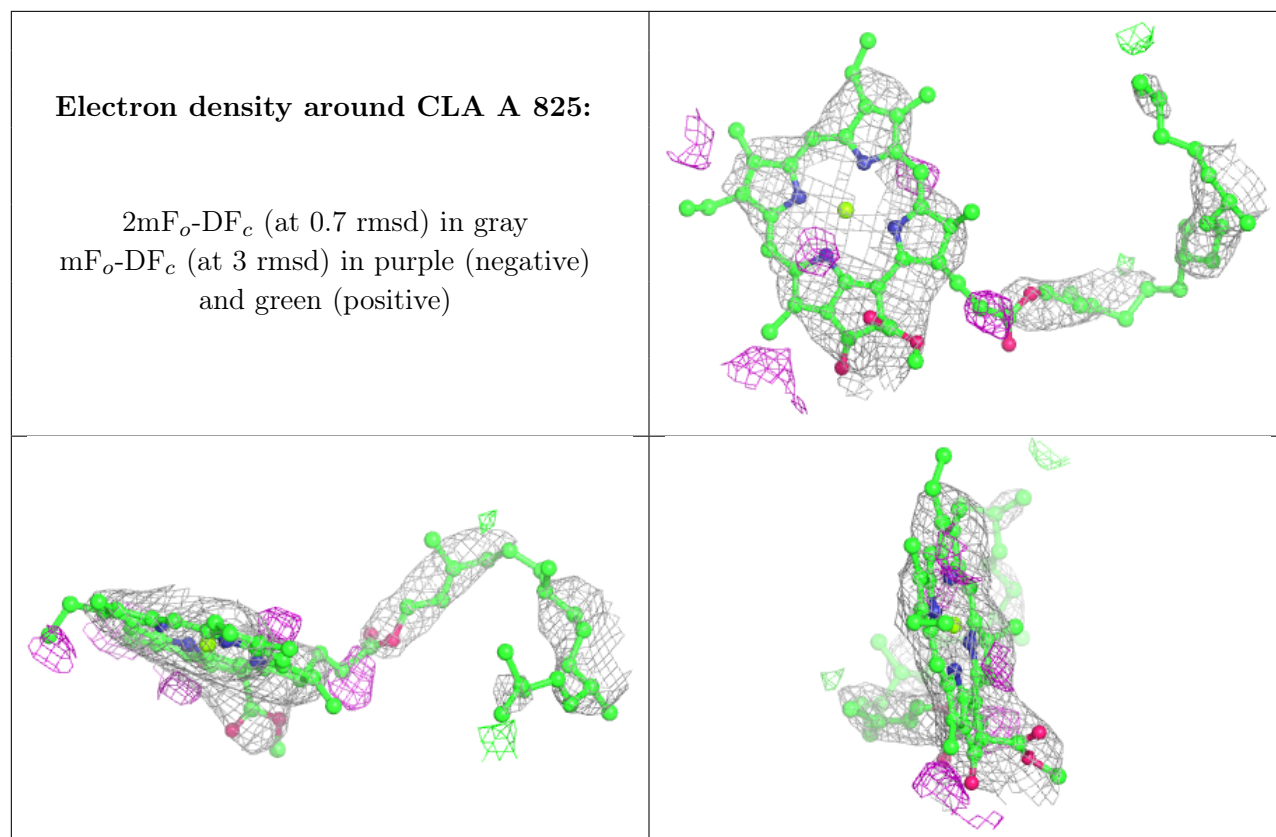


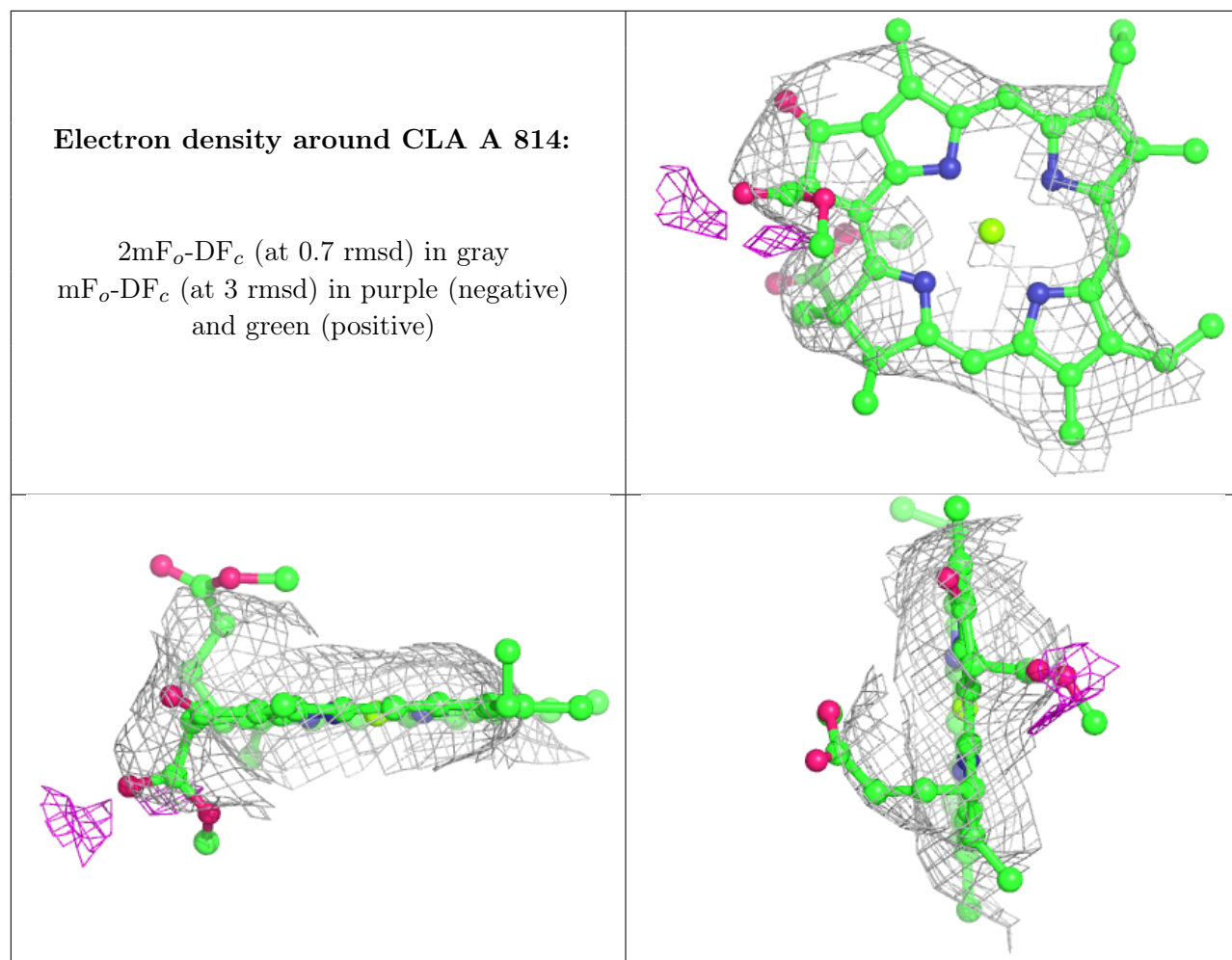


**Electron density around CLA 1 5008:**

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

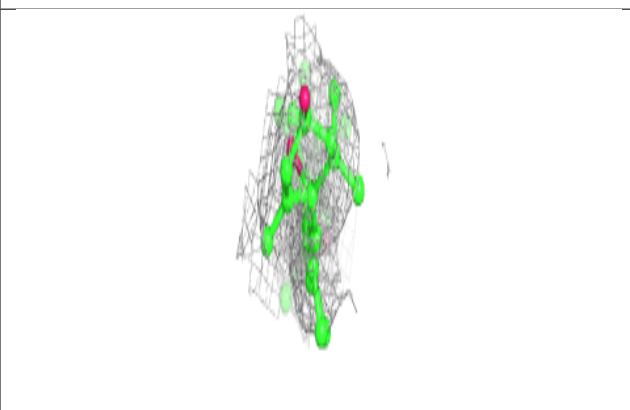
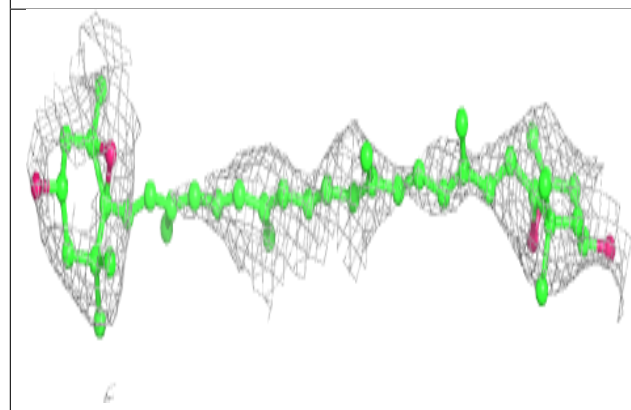
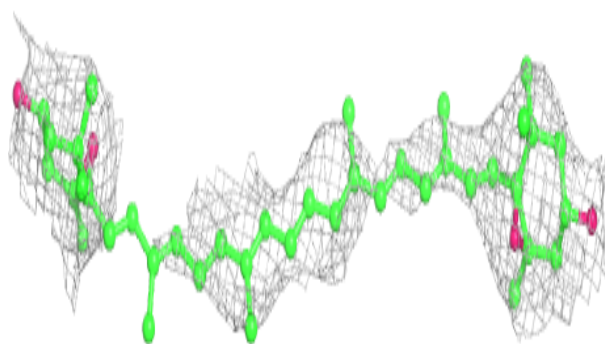




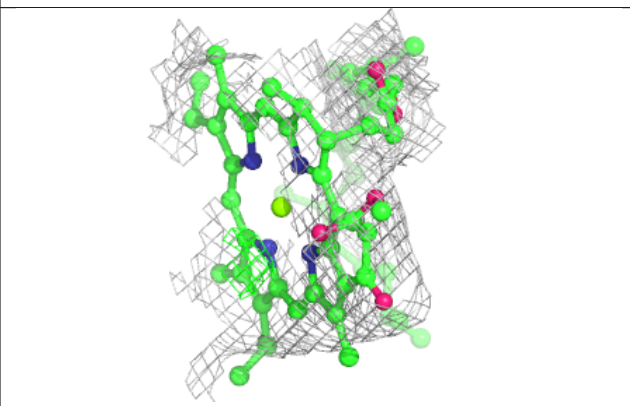
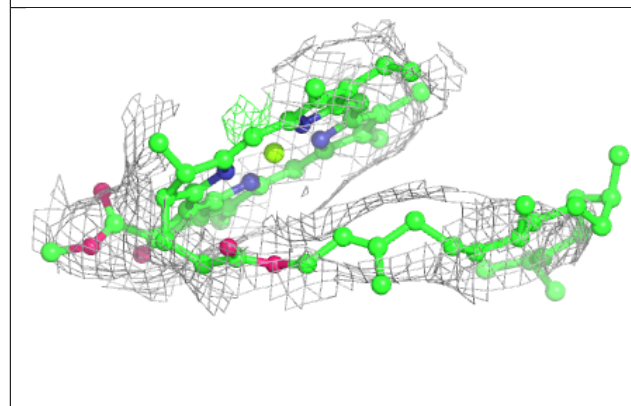
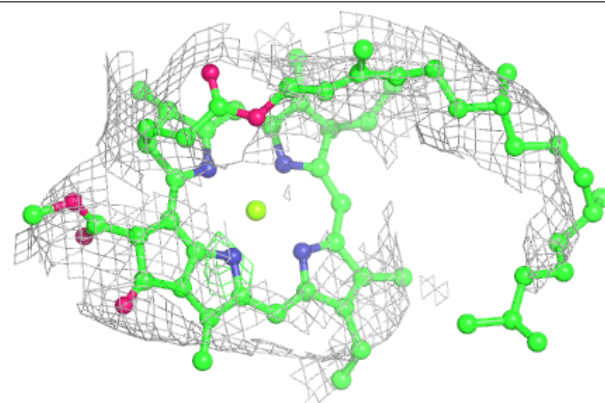


**Electron density around XAT 4 304:**

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

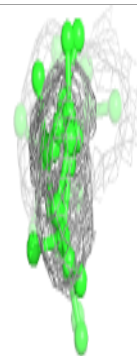
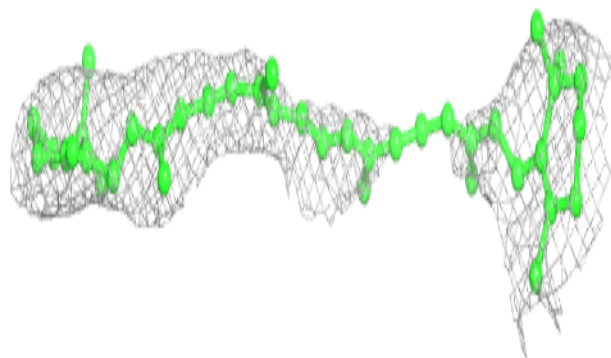
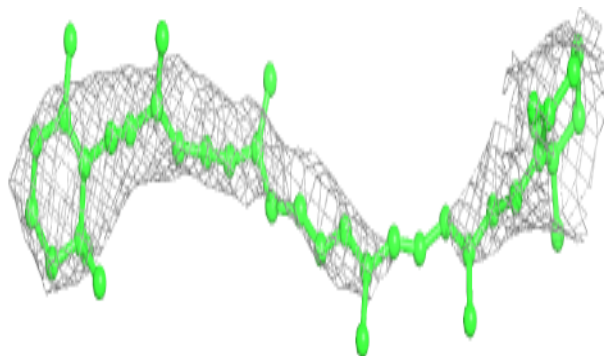
**Electron density around CLA 1 5006:**

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

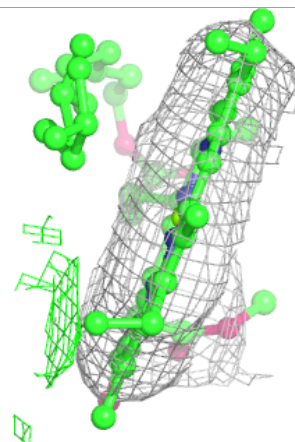
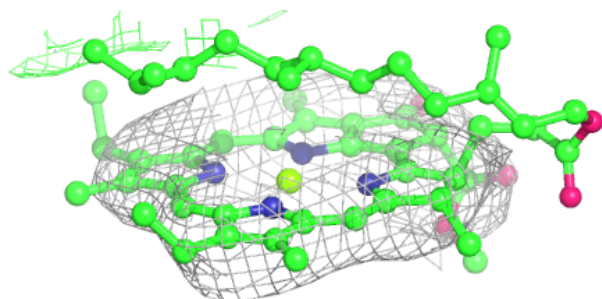
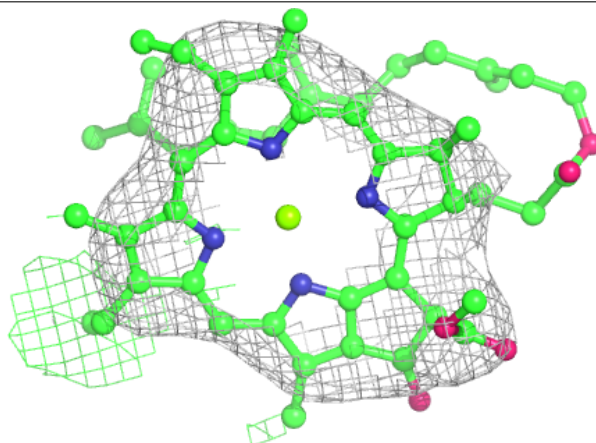


**Electron density around BCR 4 301:**

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

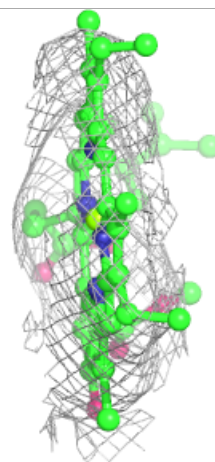
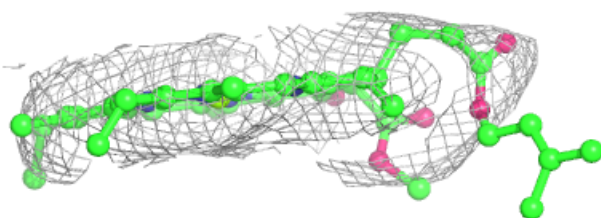
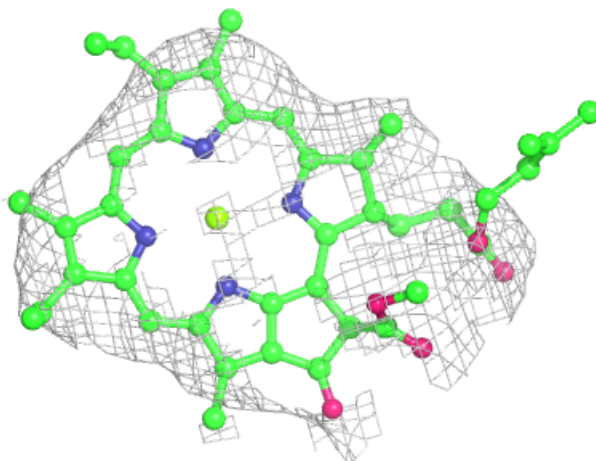
**Electron density around CLA 3 319:**

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



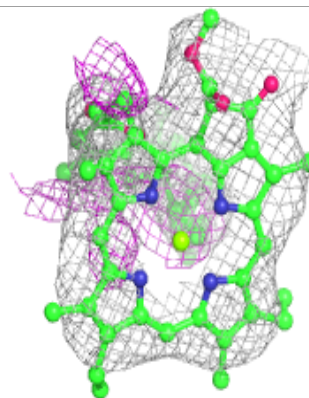
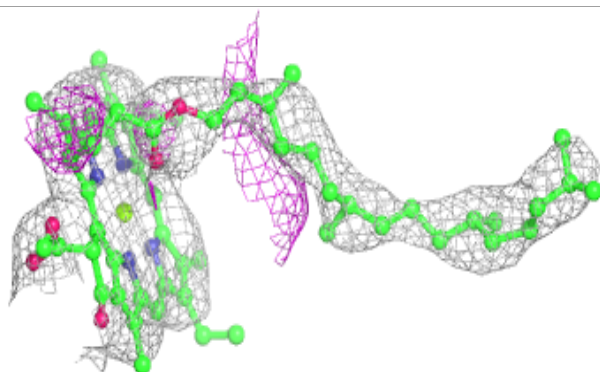
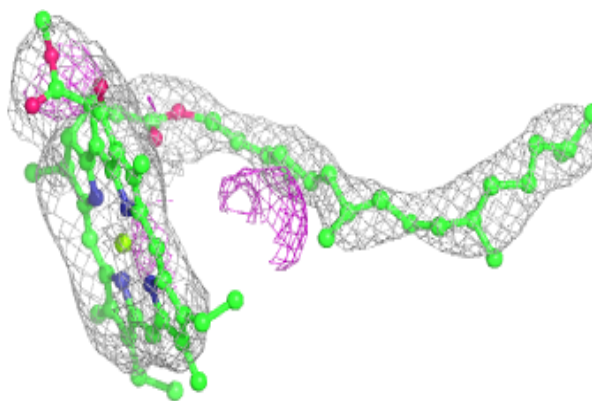
**Electron density around CLA 4 306:**

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

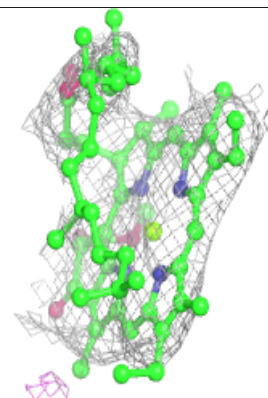
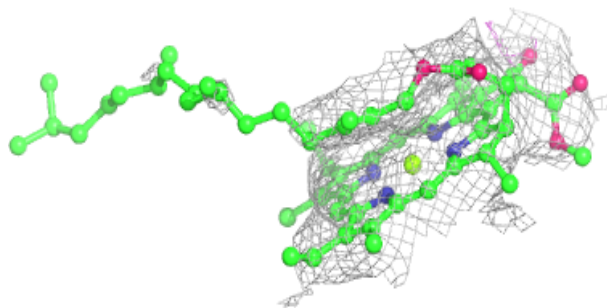
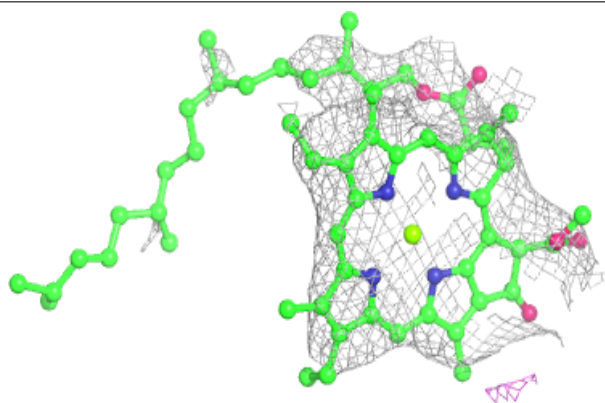


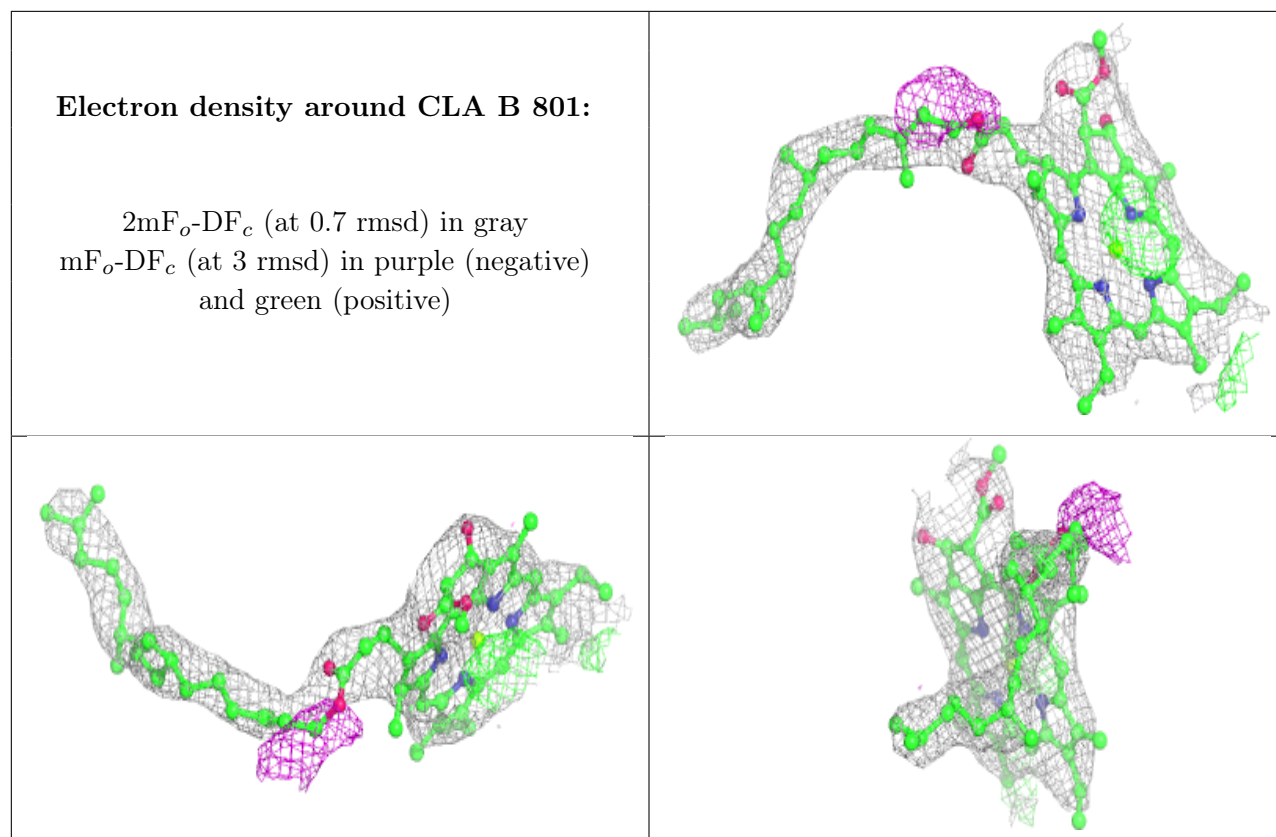
**Electron density around CLA A 810:**

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

**Electron density around CLA 1 5009:**

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

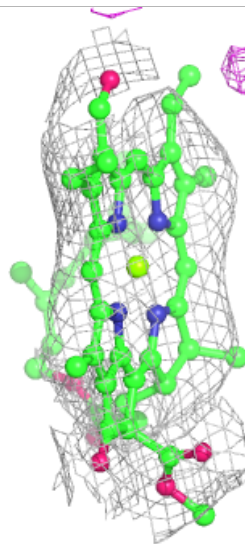
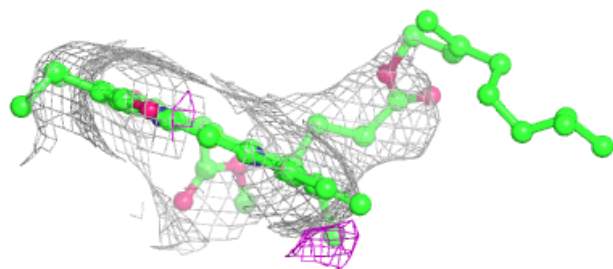
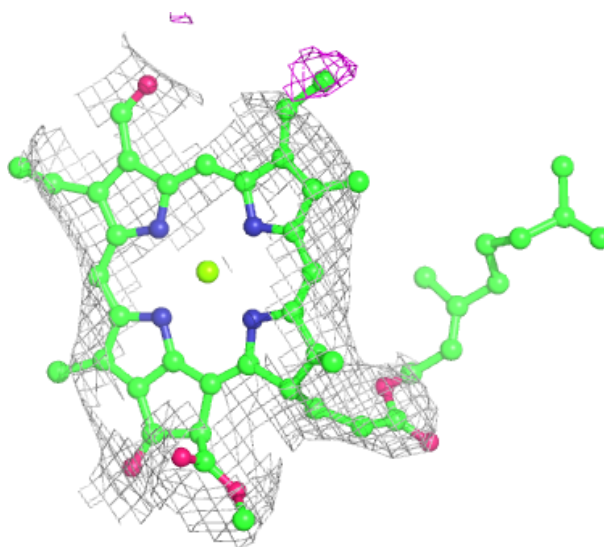


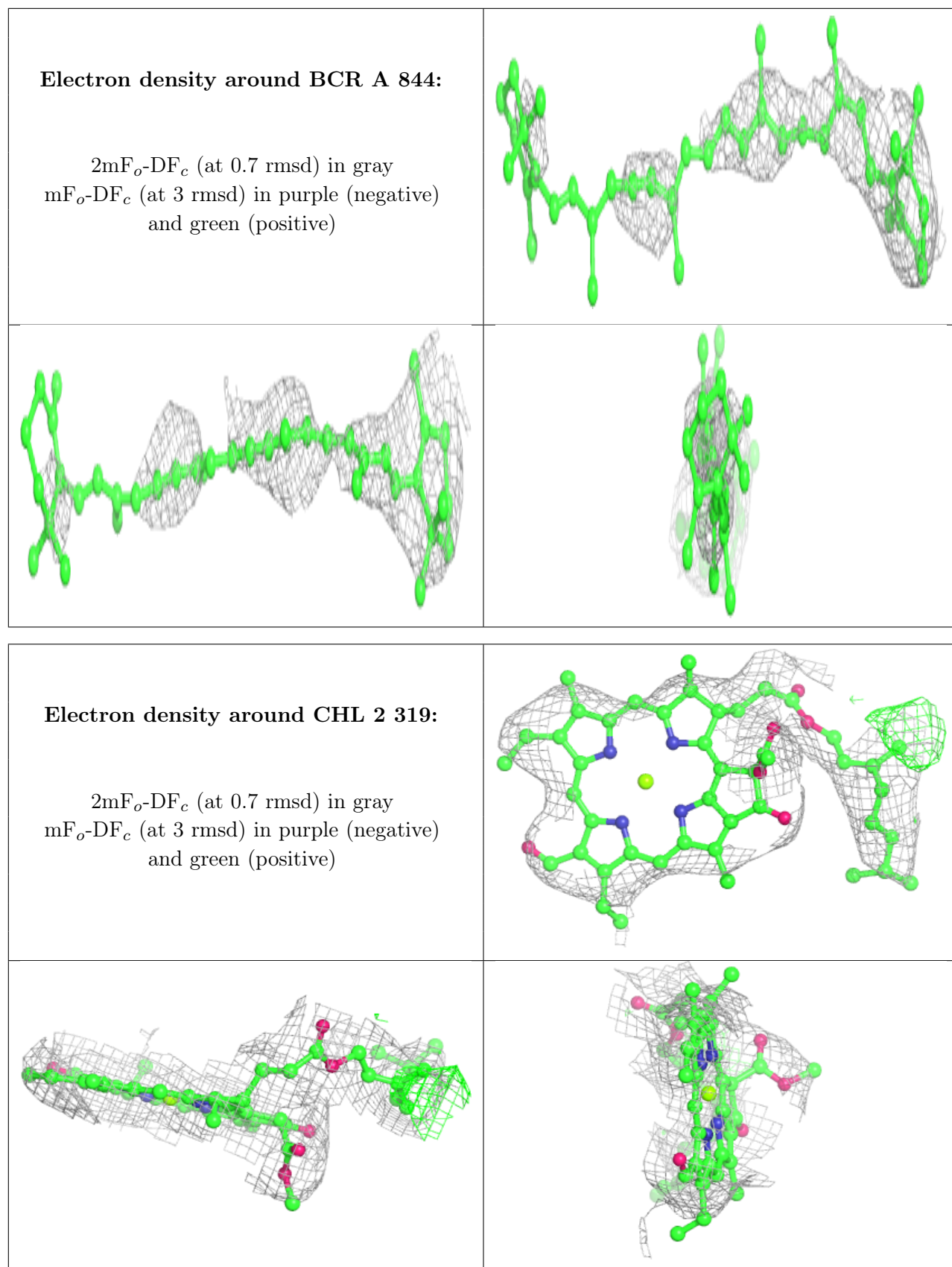


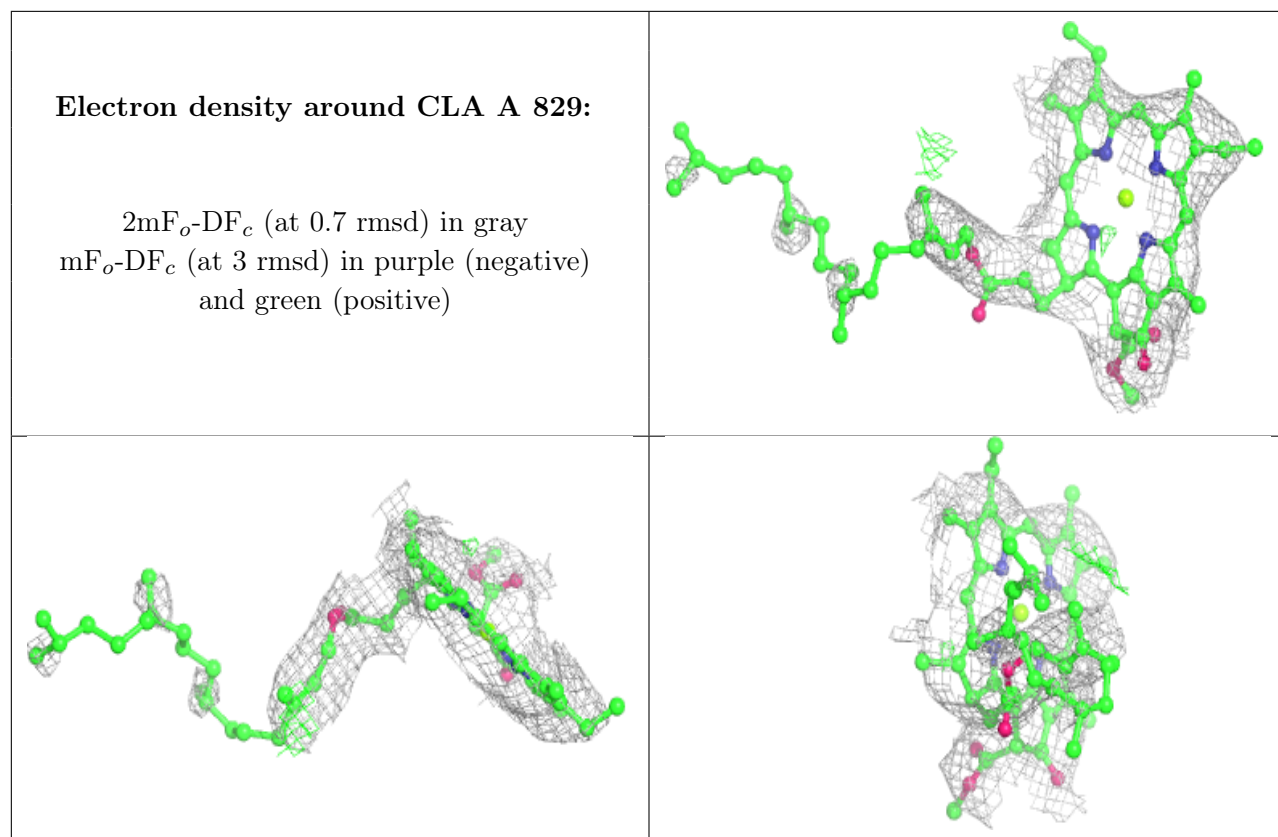


**Electron density around CHL 2 315:**

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

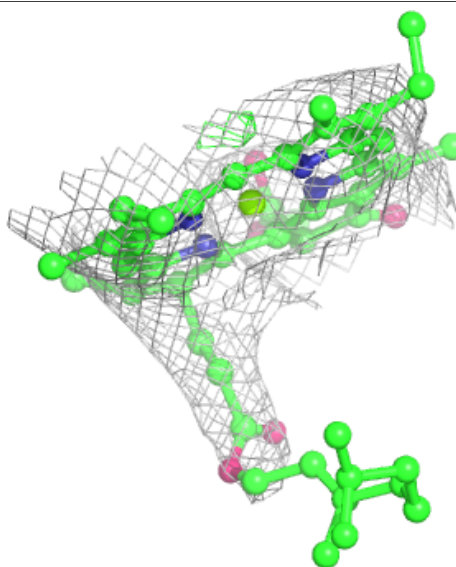
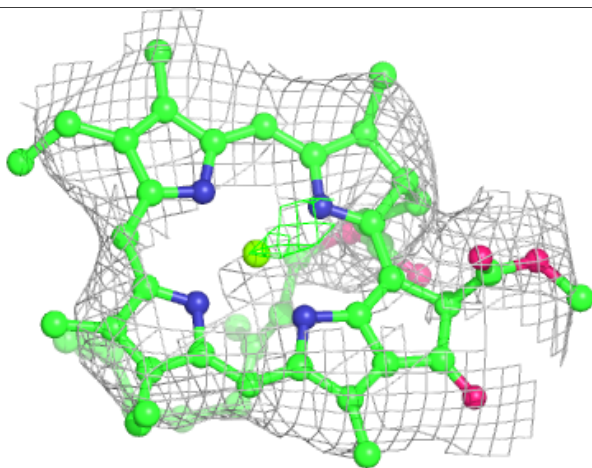
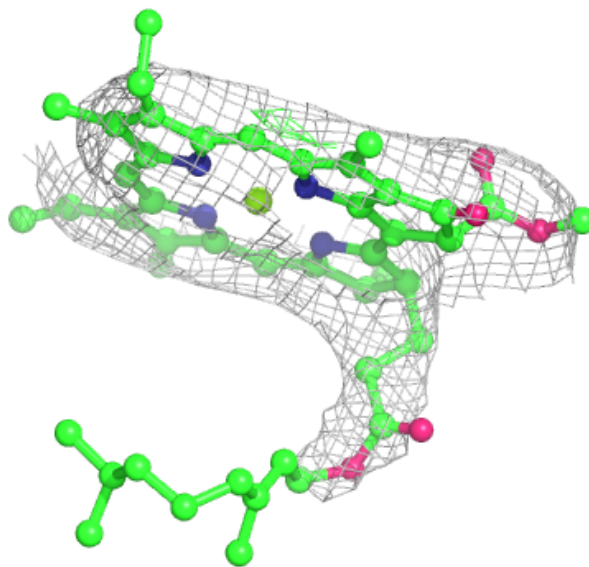






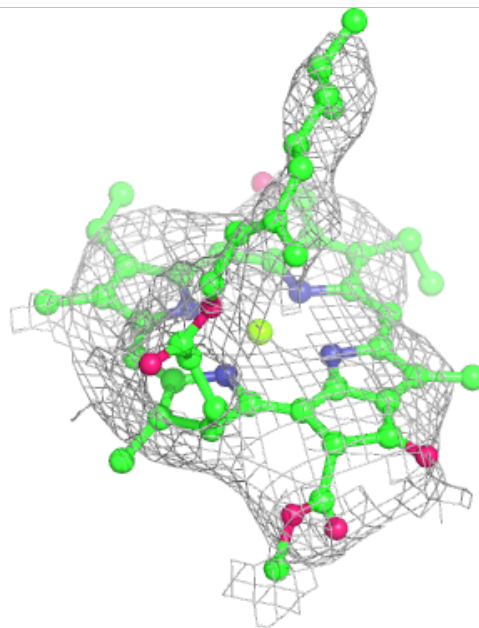
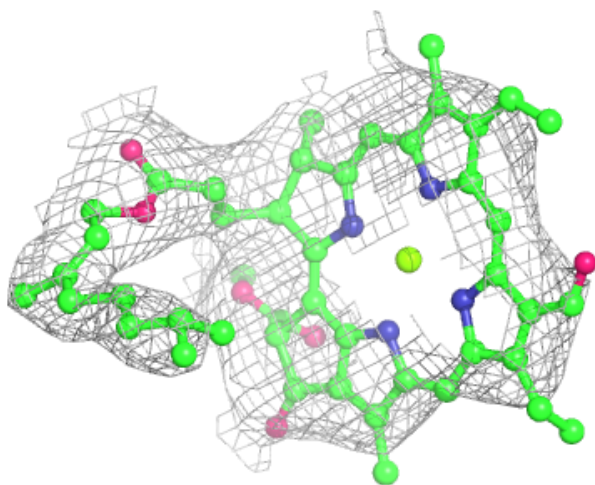
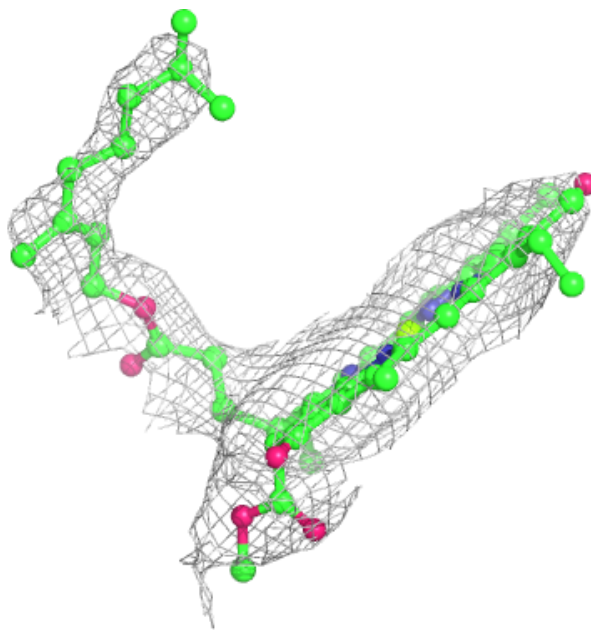
**Electron density around CLA B 835:**

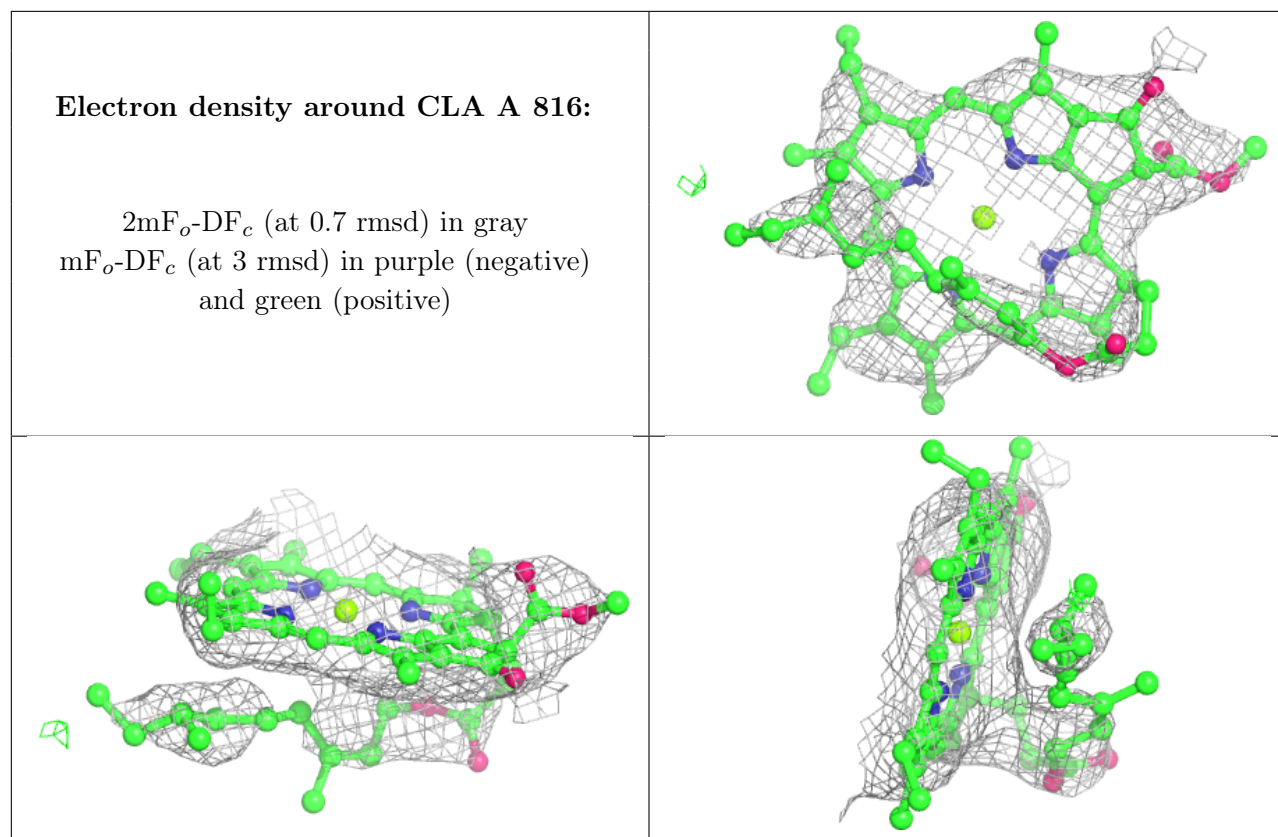
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

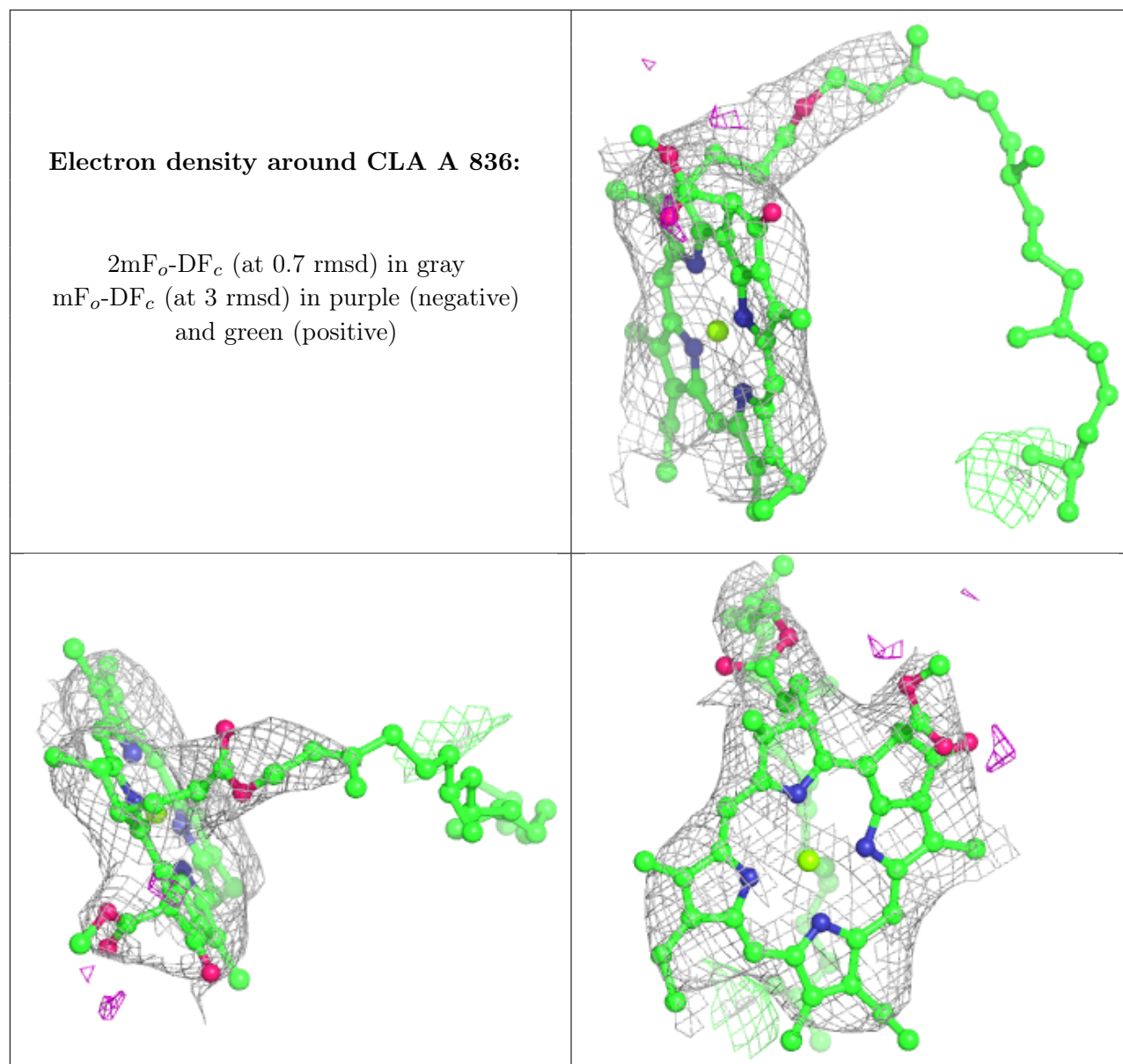


**Electron density around CHL 4 302:**

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

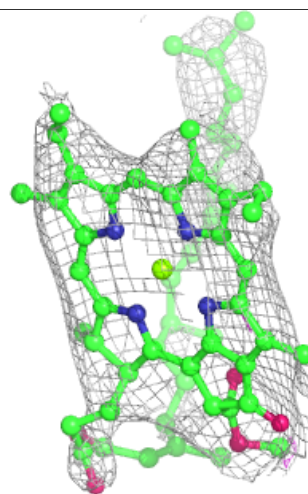
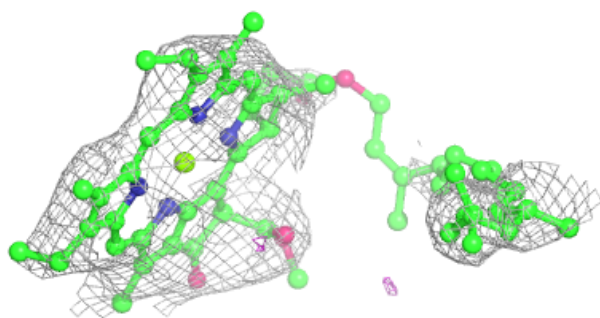
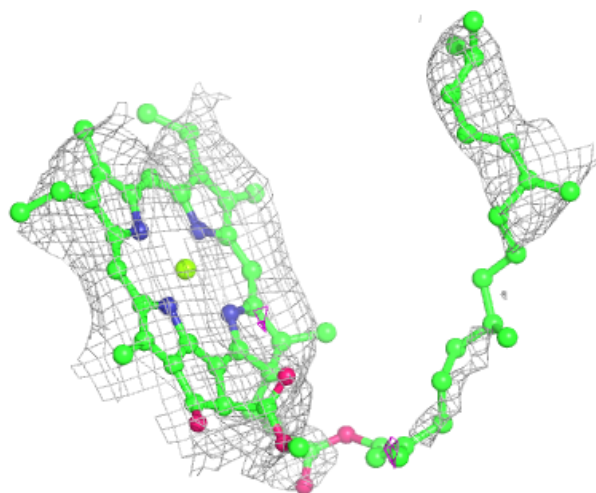




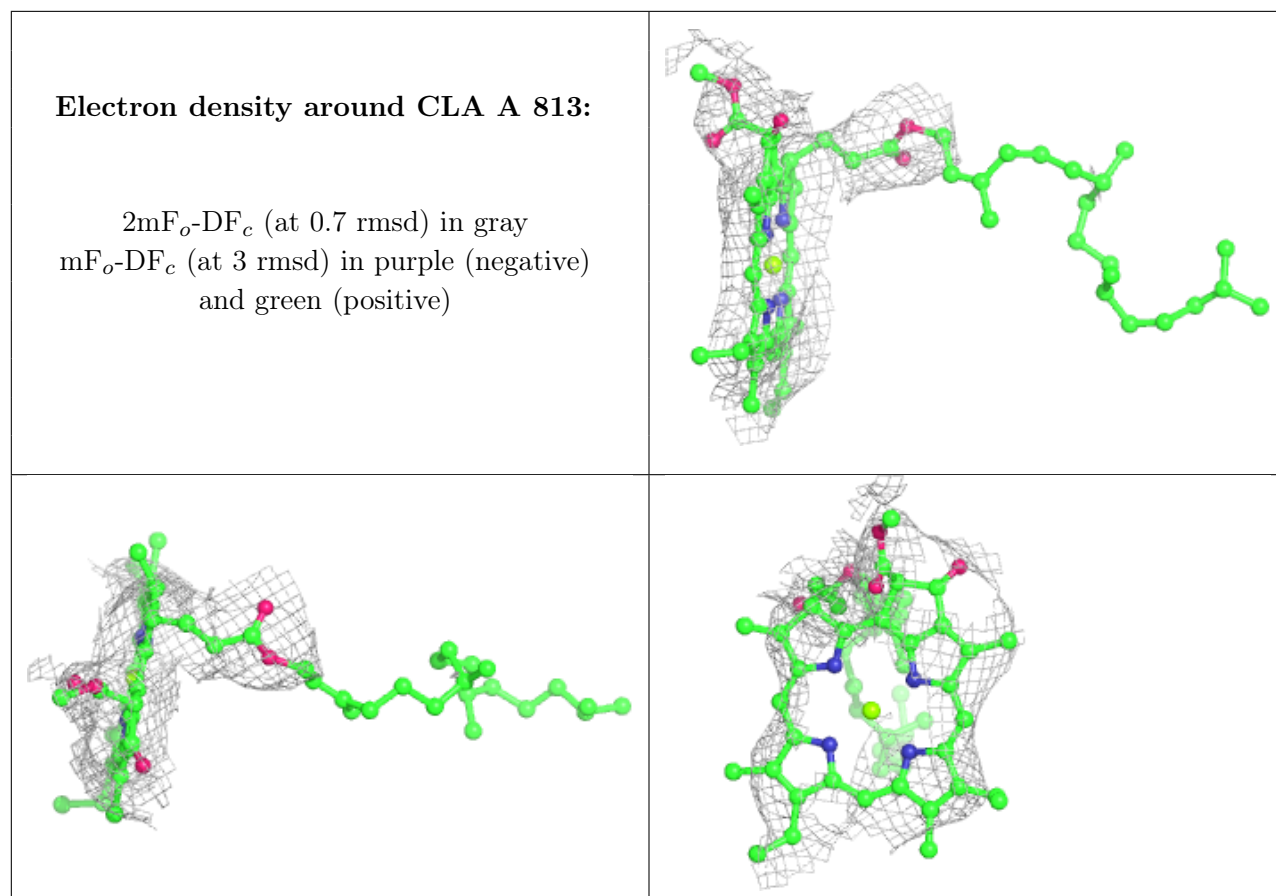


**Electron density around CLA B 811:**

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

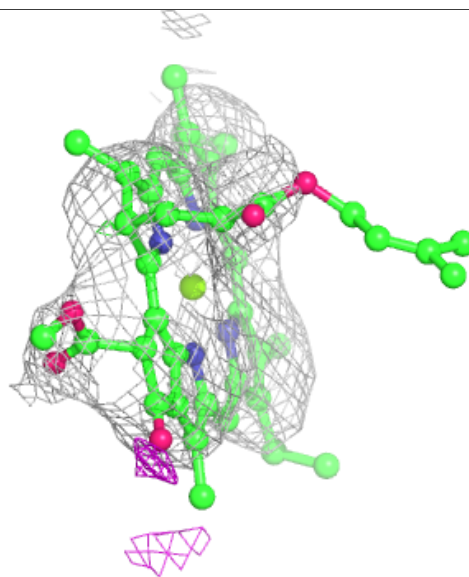
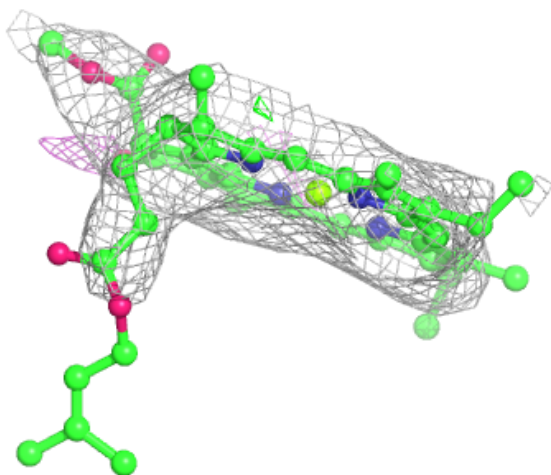
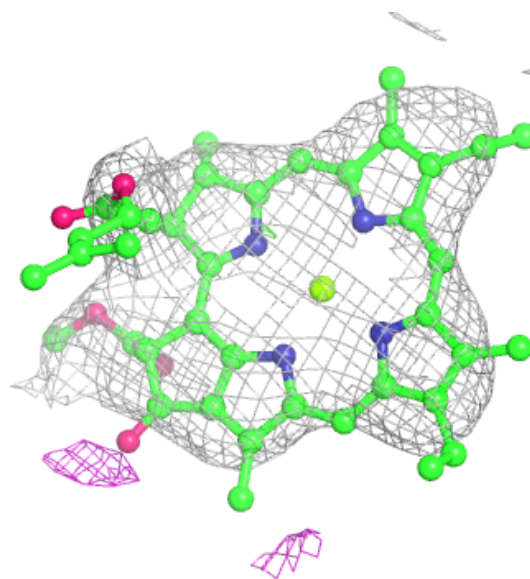






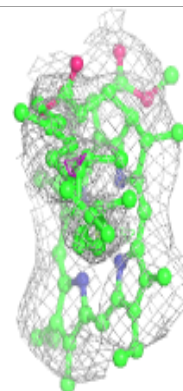
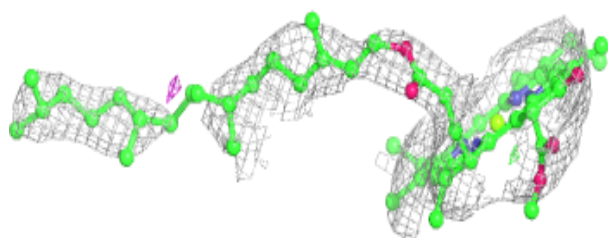
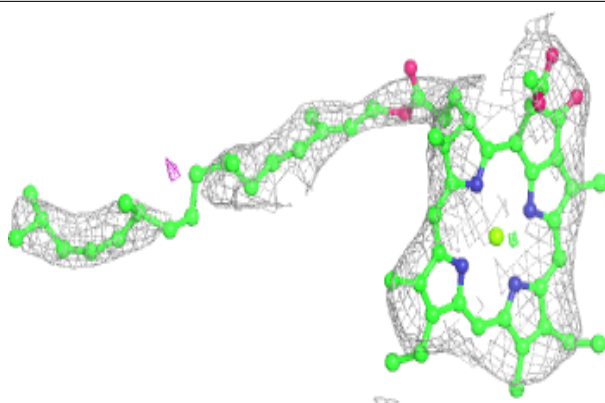
**Electron density around CLA A 809:**

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

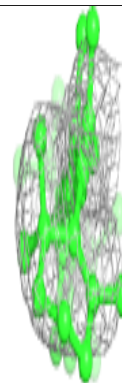
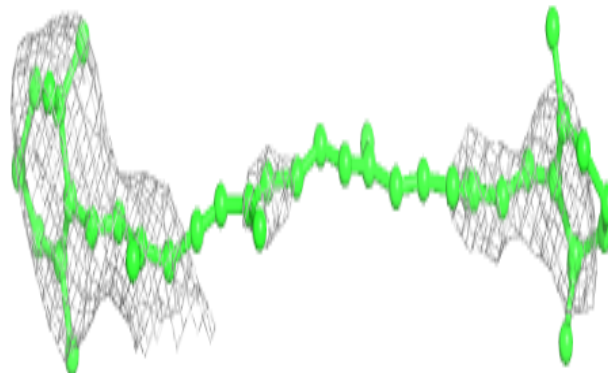
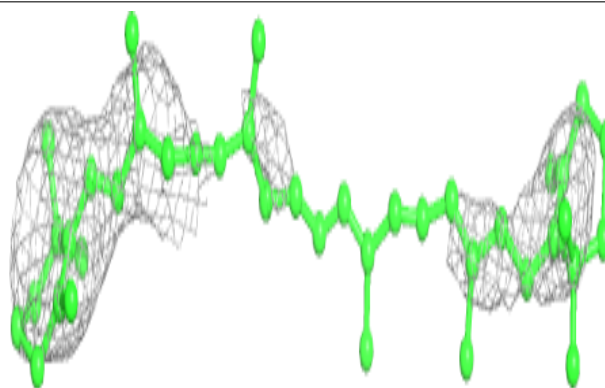


**Electron density around CLA A 831:**

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

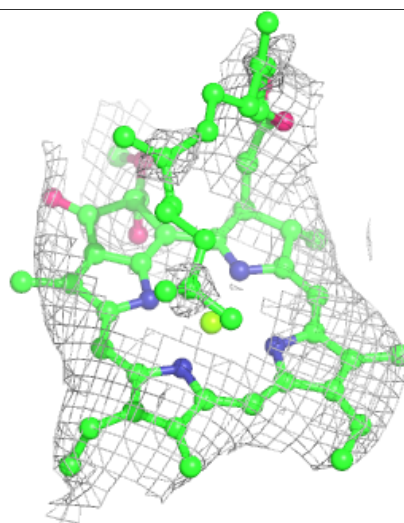
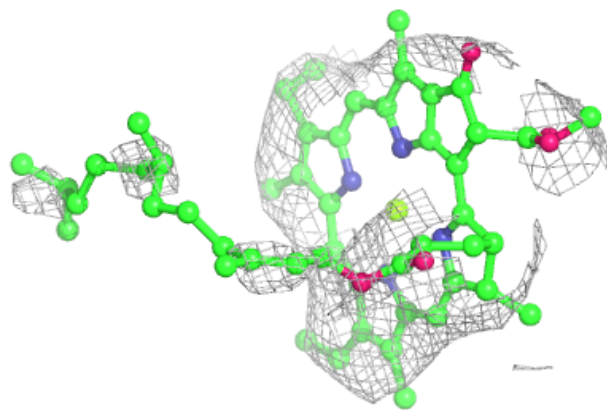
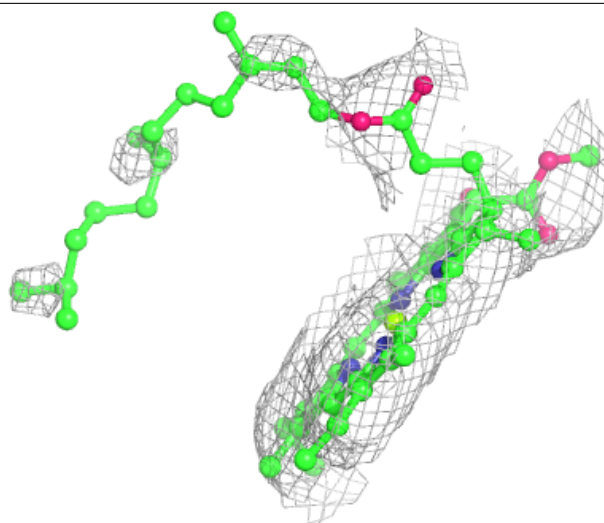
**Electron density around BCR A 843:**

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



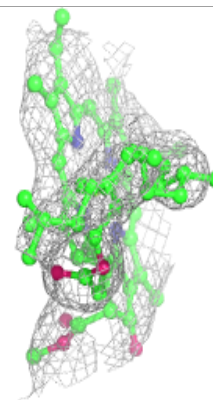
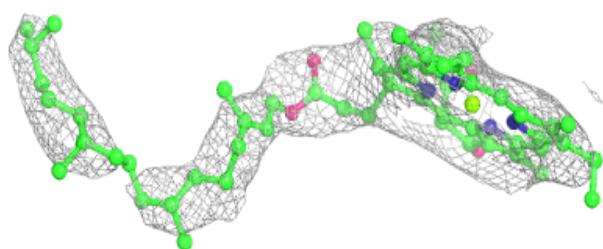
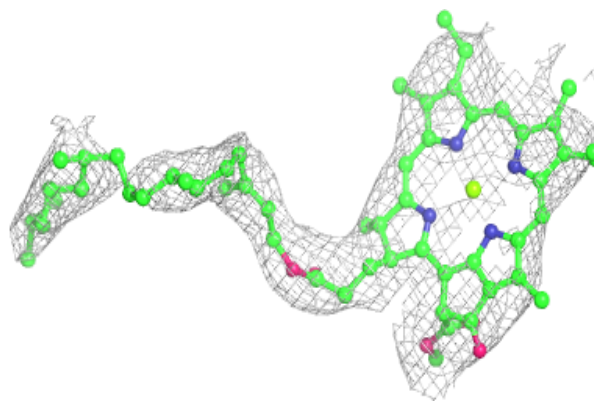
**Electron density around CLA B 812:**

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

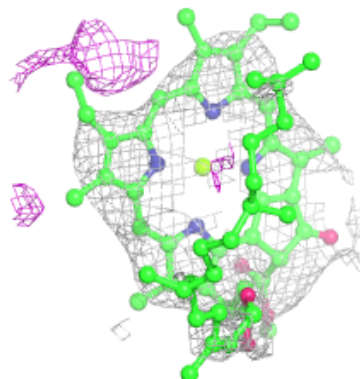
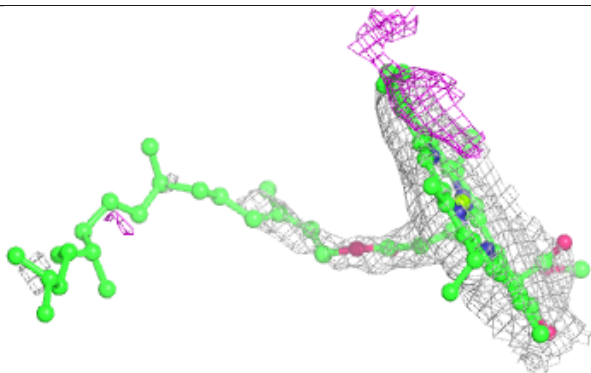
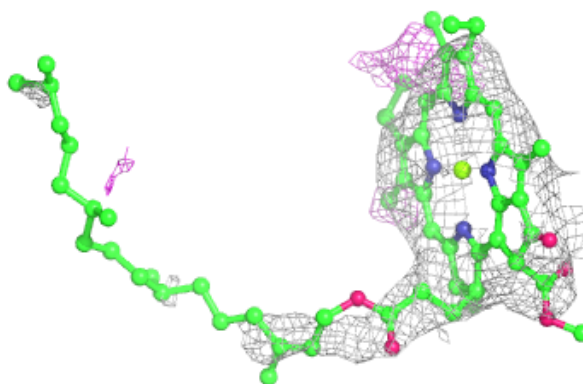


**Electron density around CLA B 814:**

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

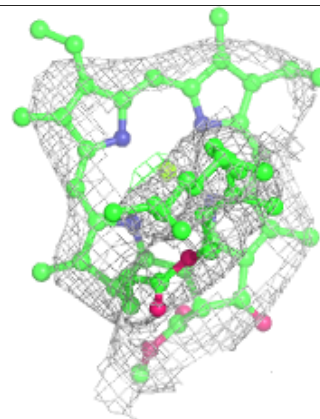
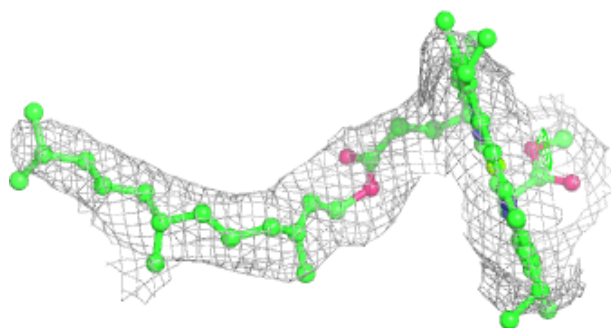
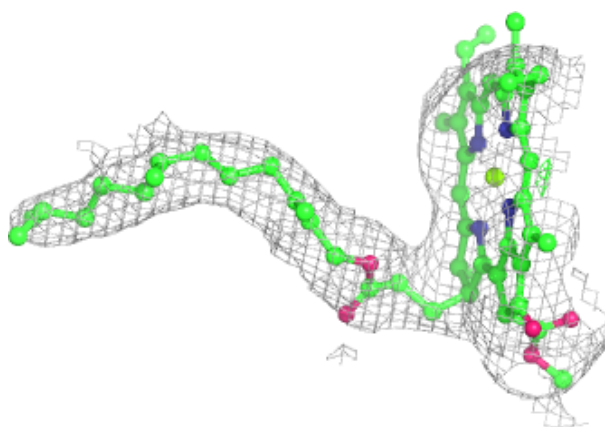
**Electron density around CLA A 832:**

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

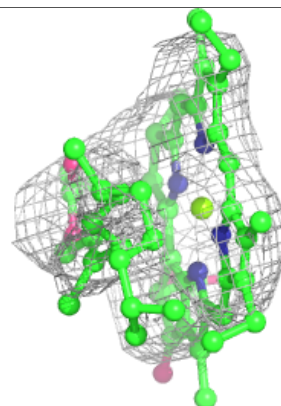
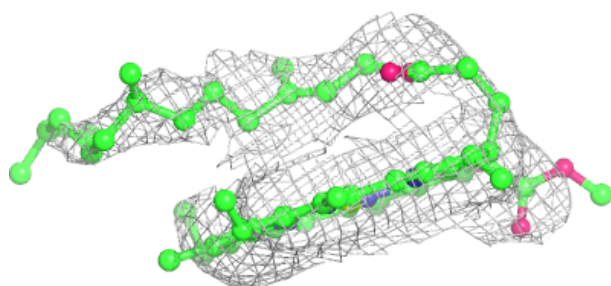
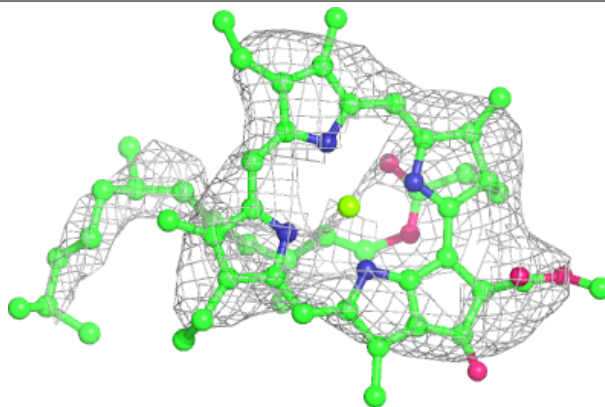


**Electron density around CLA L 305:**

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

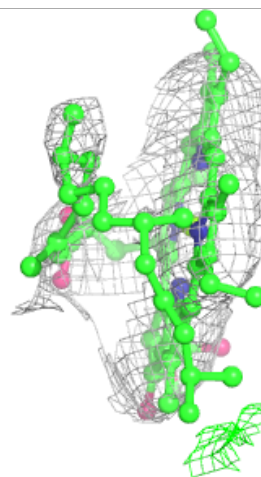
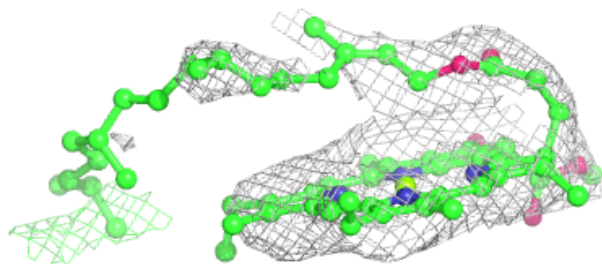
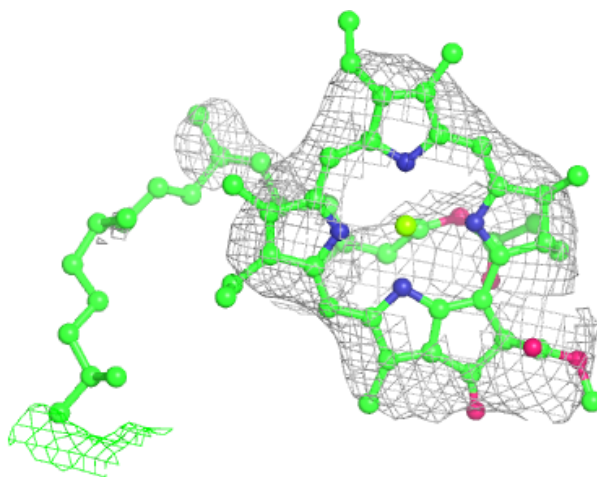
**Electron density around CLA B 817:**

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



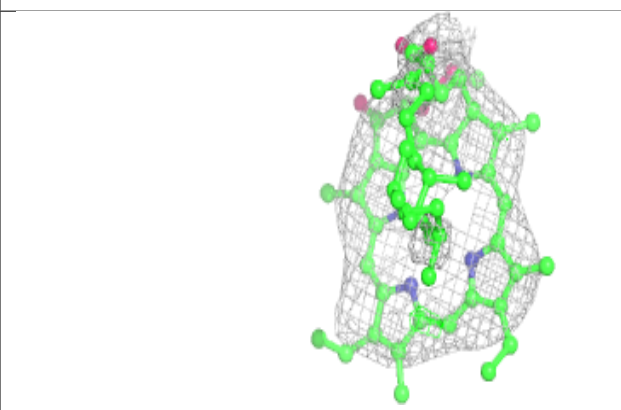
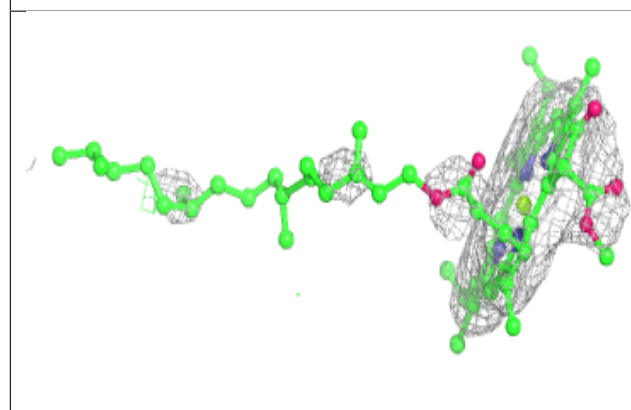
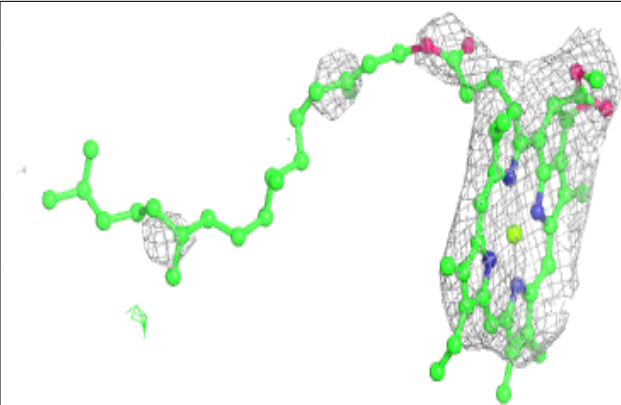
**Electron density around CLA A 815:**

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

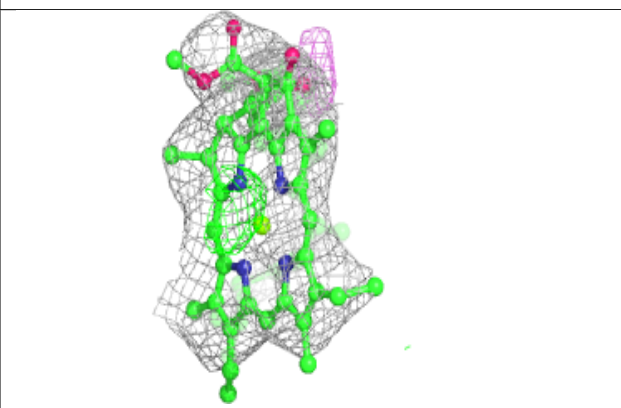
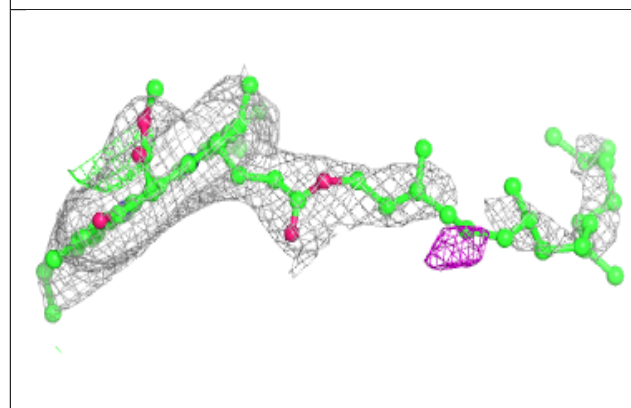
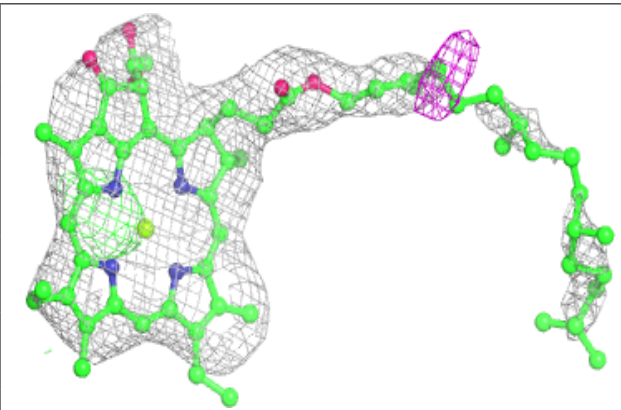


**Electron density around CLA B 822:**

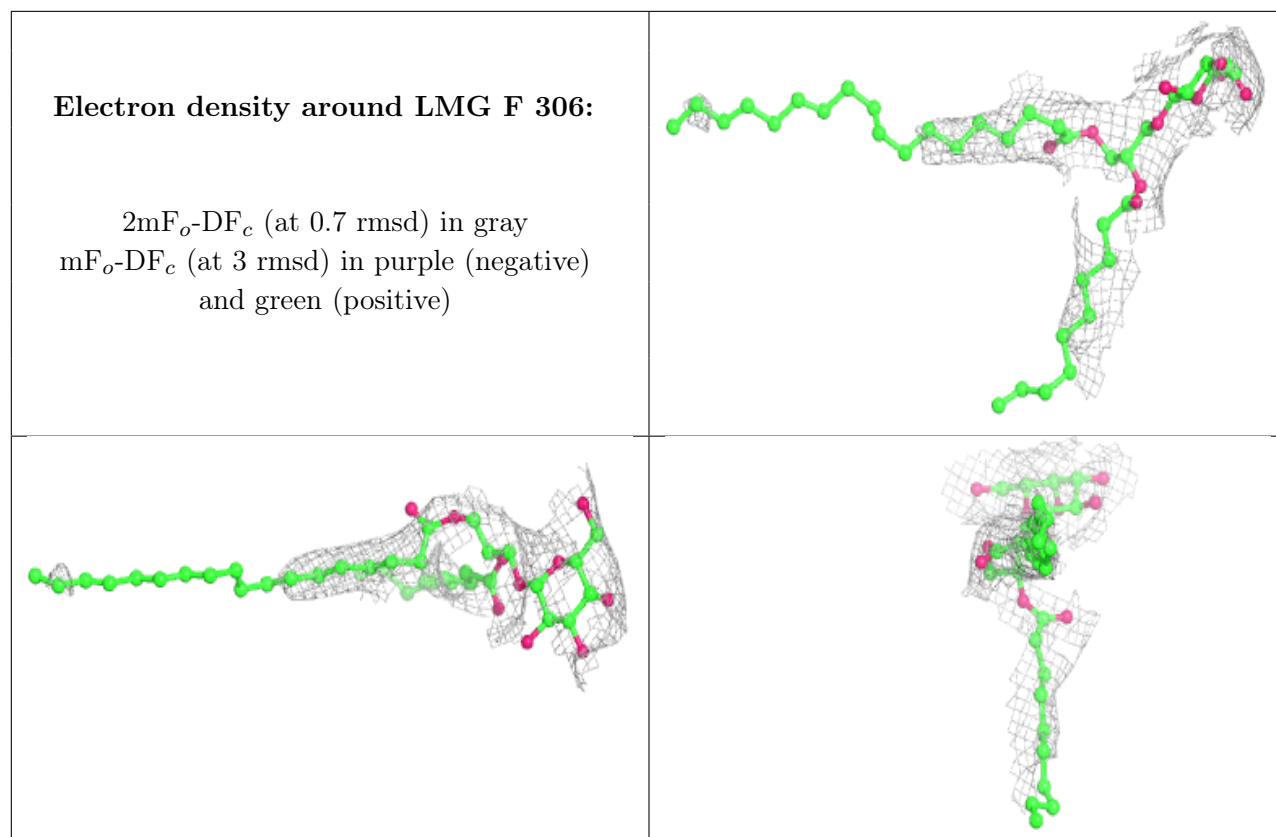
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 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)

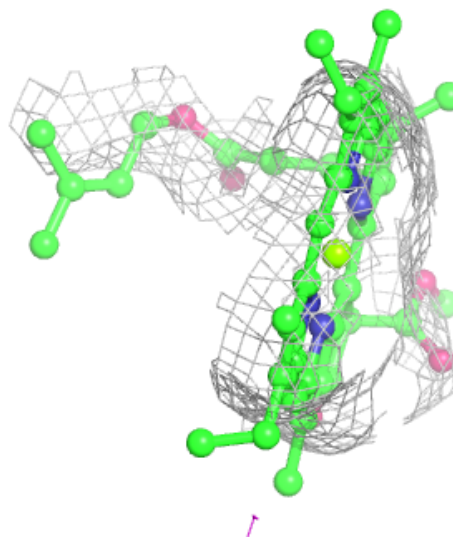
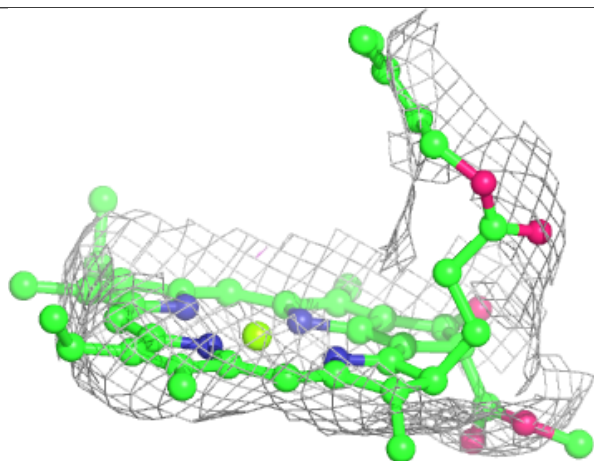
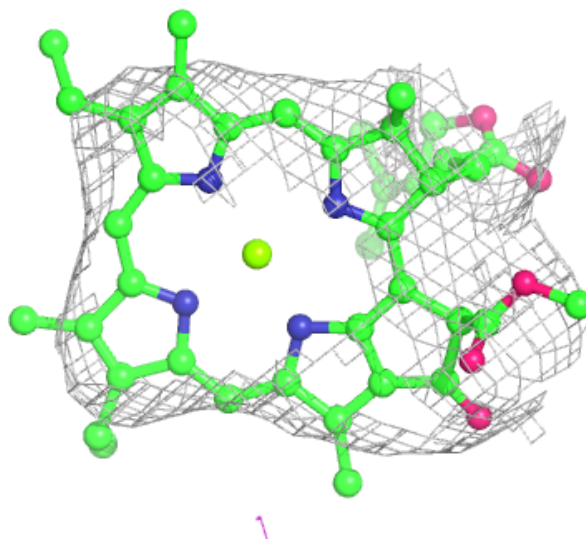






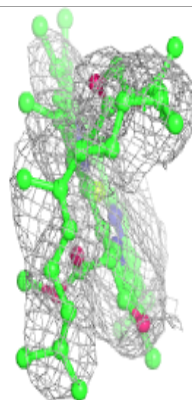
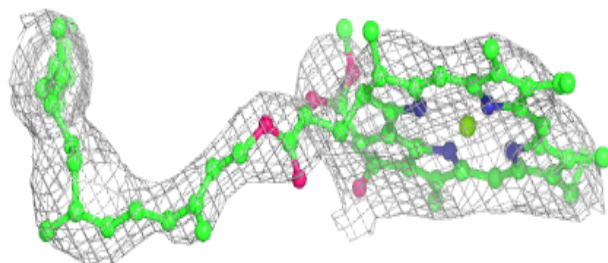
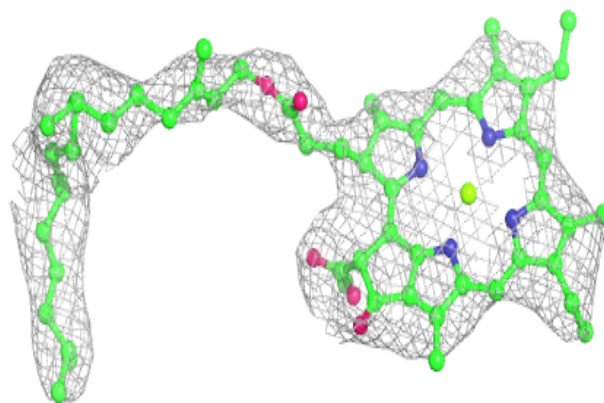
**Electron density around CLA 1 5011:**

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

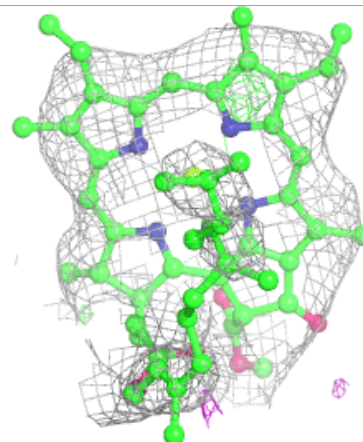
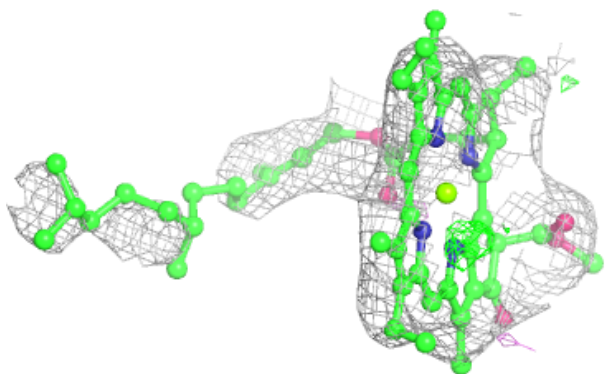
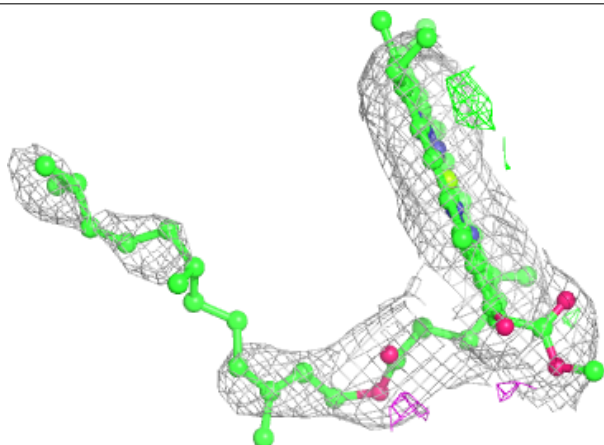


**Electron density around CLA B 827:**

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

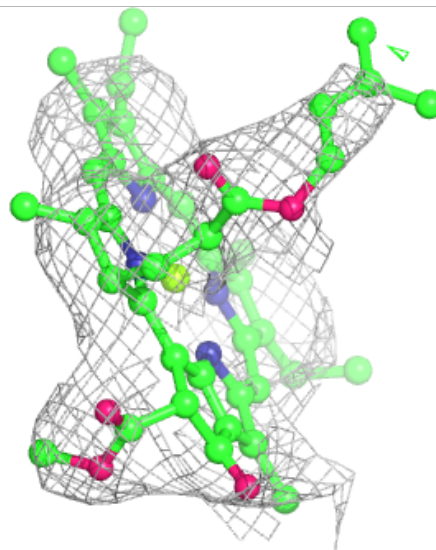
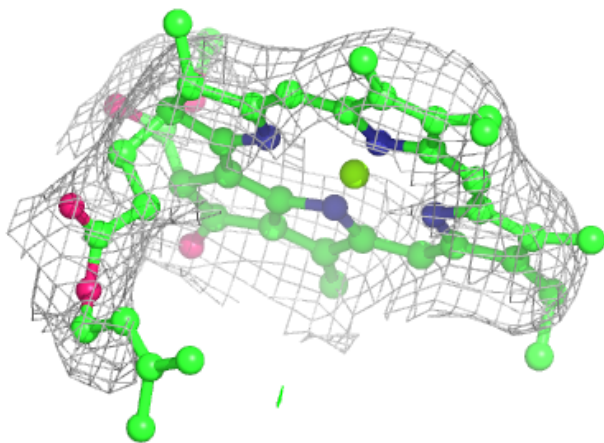
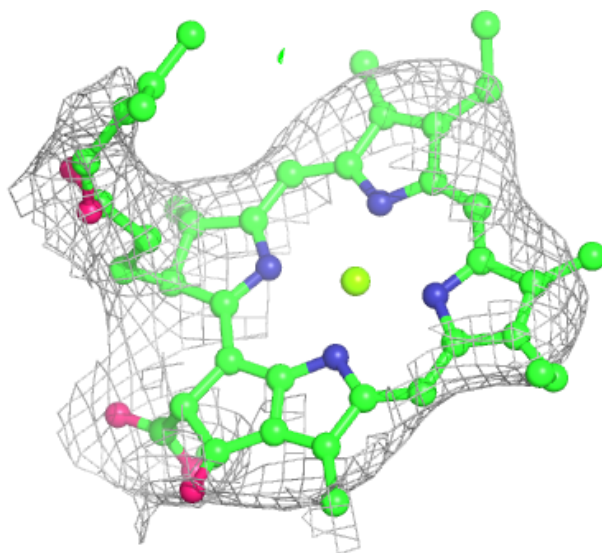
**Electron density around CLA A 806:**

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



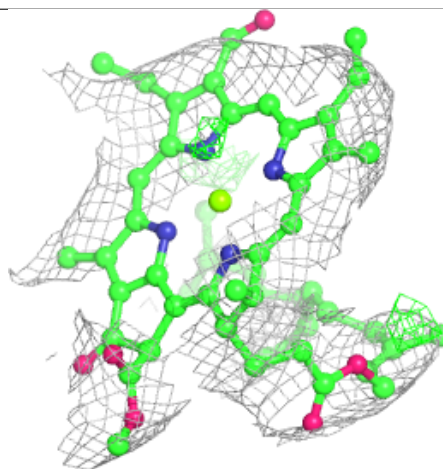
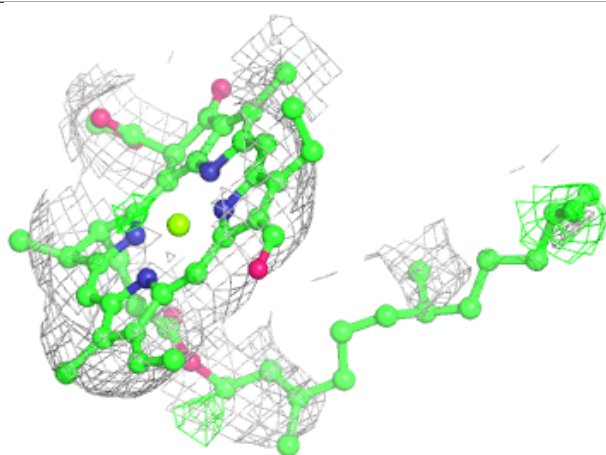
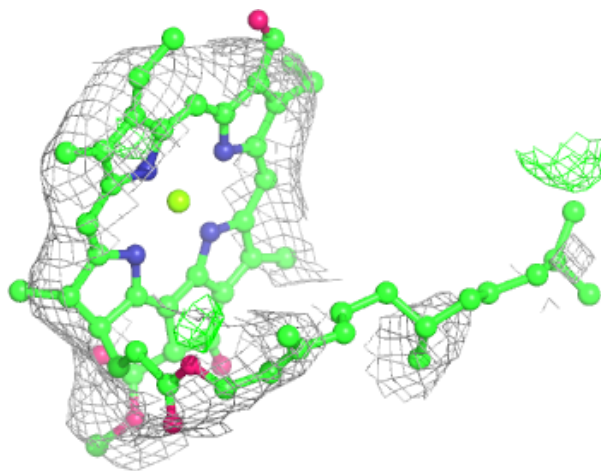
**Electron density around CLA A 818:**

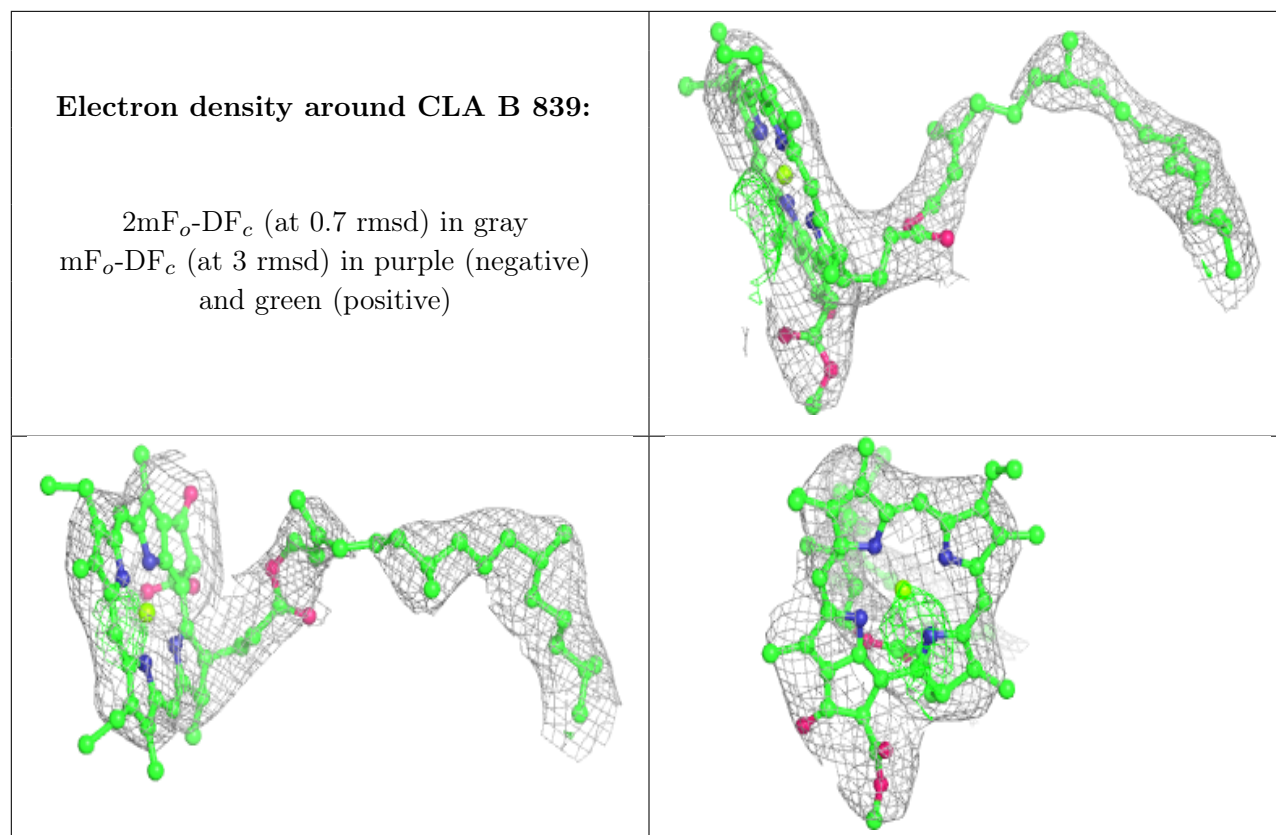
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CHL 1 5016:**

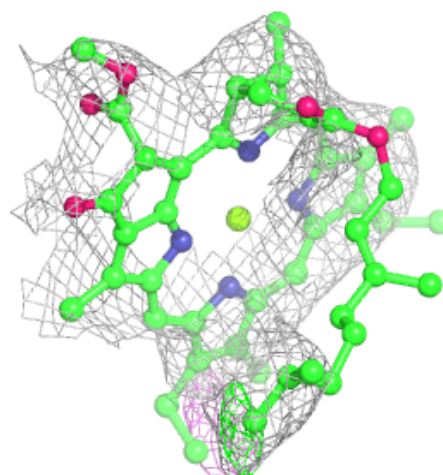
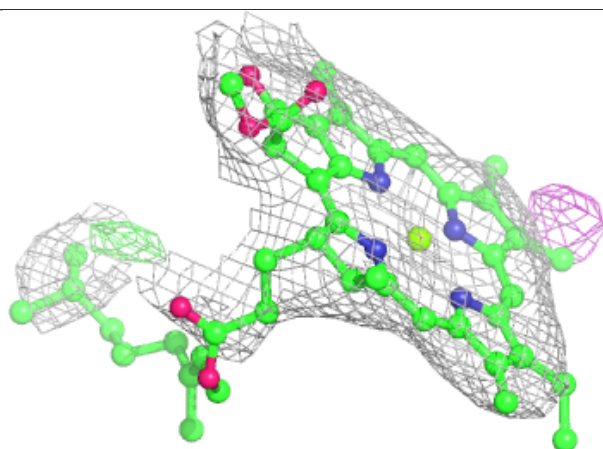
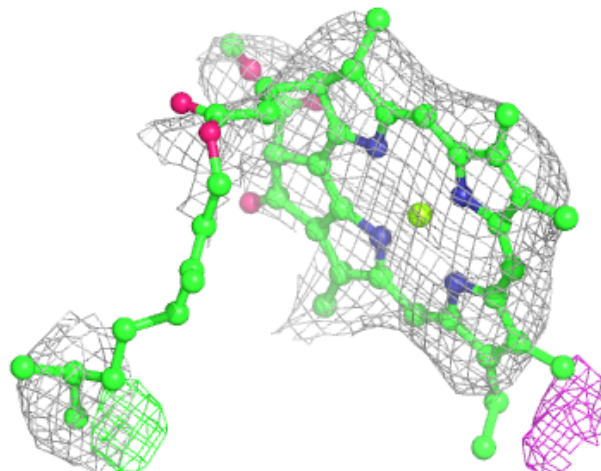
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





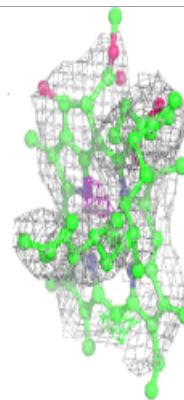
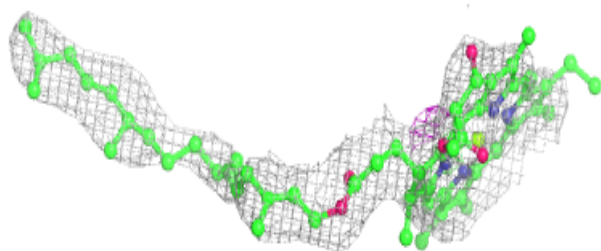
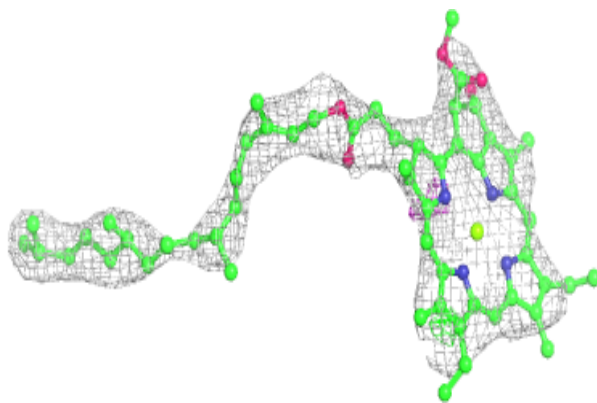
**Electron density around CLA 2 317:**

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

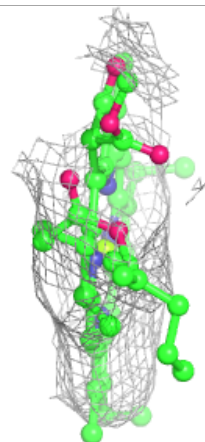
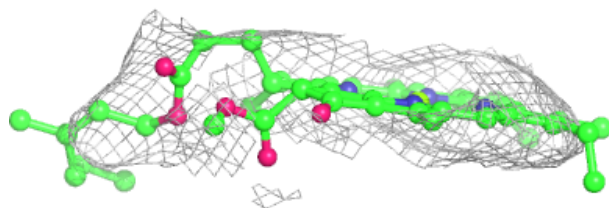
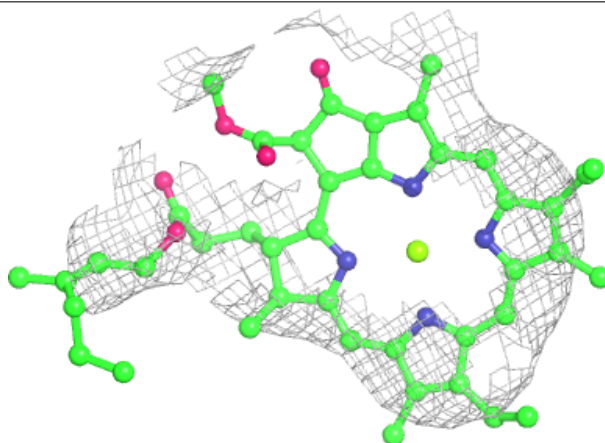


**Electron density around CLA A 852:**

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

**Electron density around CLA 3 308:**

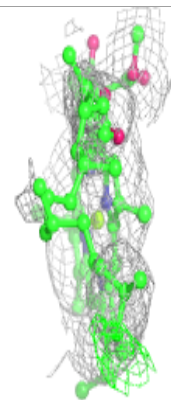
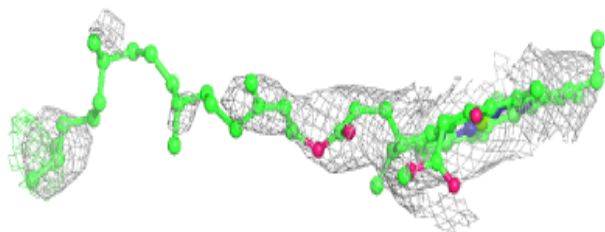
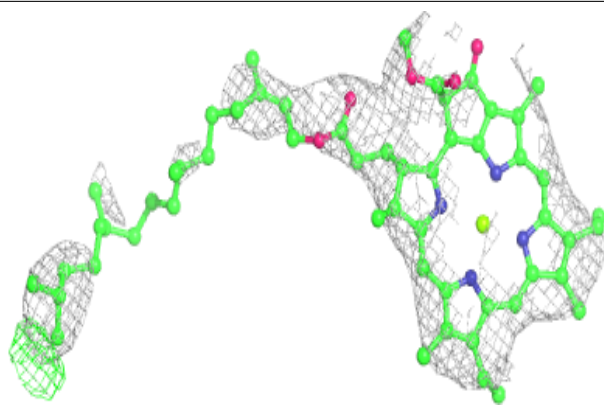
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



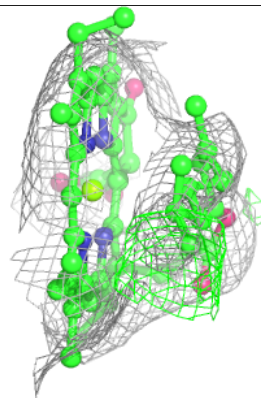
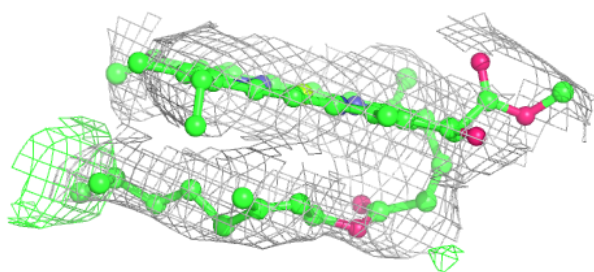
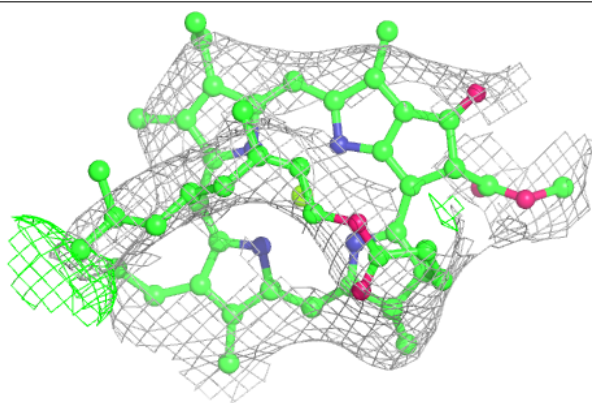


**Electron density around CLA F 303:**

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

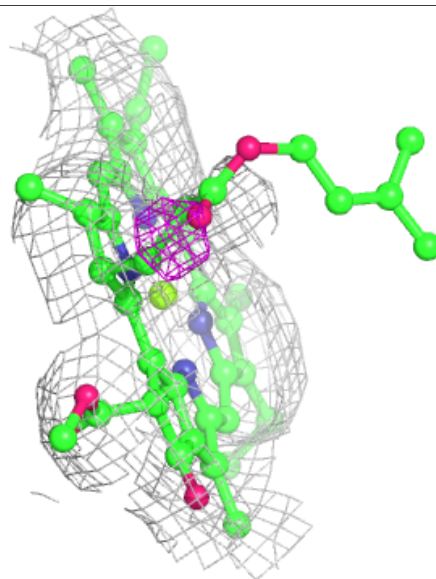
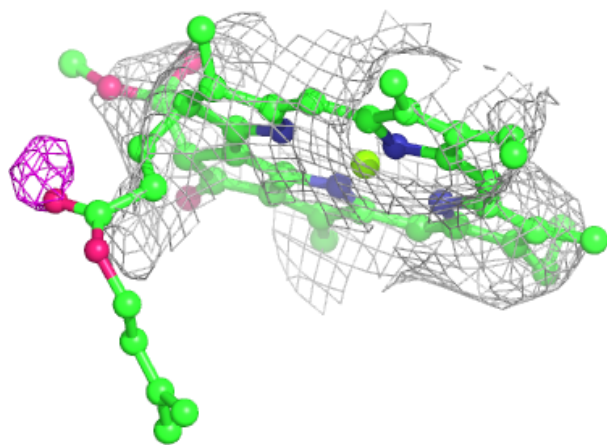
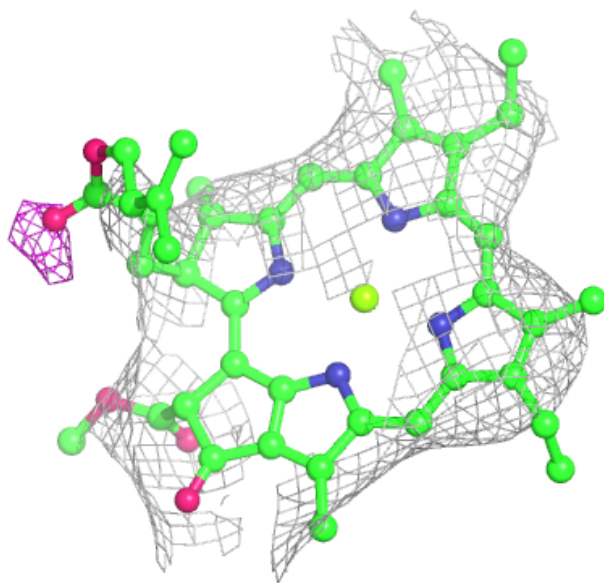
**Electron density around CLA A 811:**

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



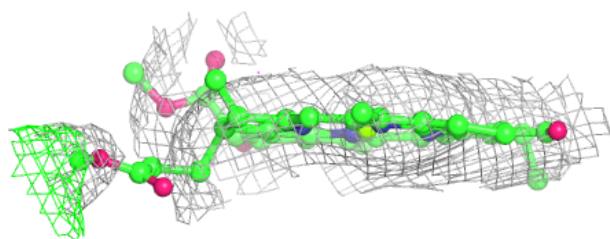
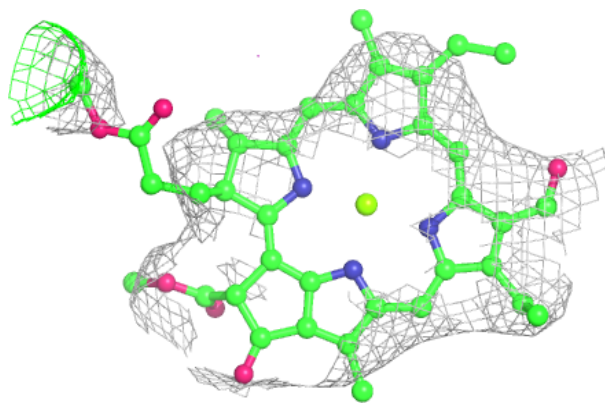
**Electron density around CLA 3 317:**

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



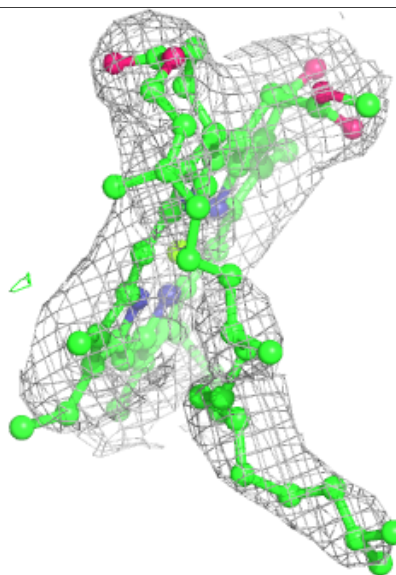
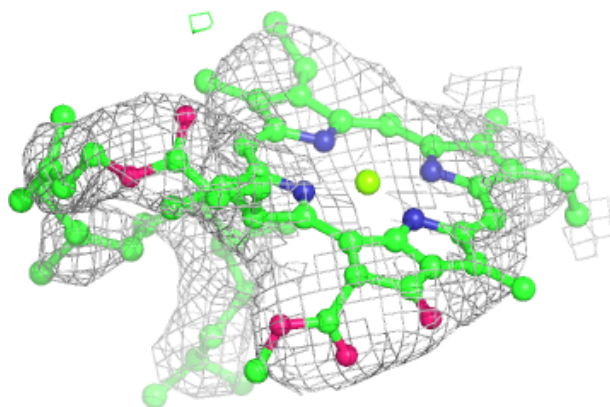
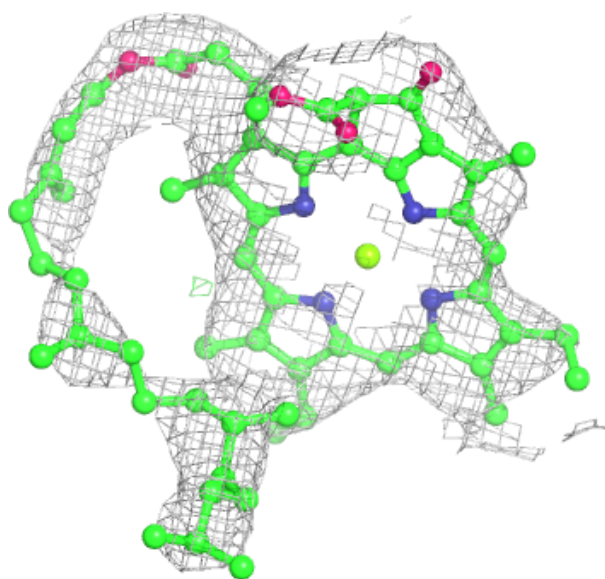
**Electron density around CHL 4 313:**

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



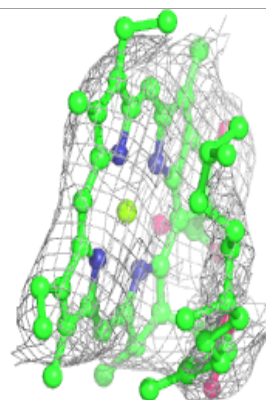
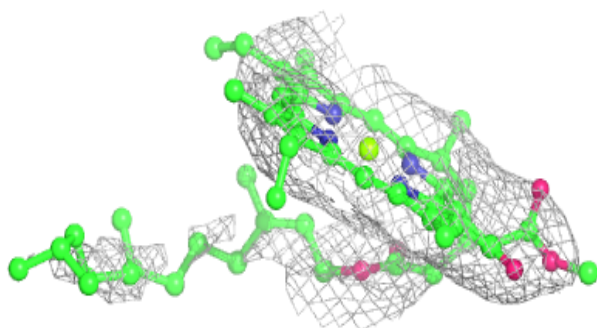
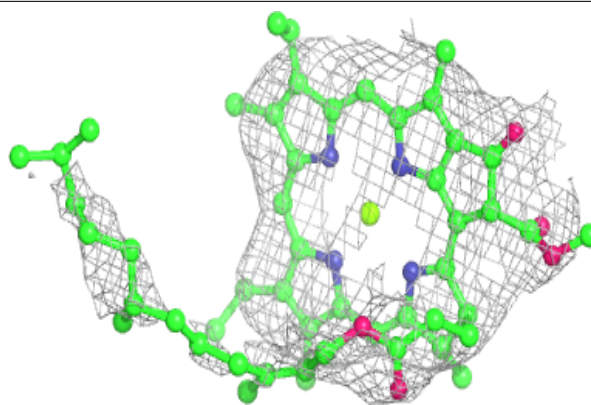
**Electron density around CLA A 812:**

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

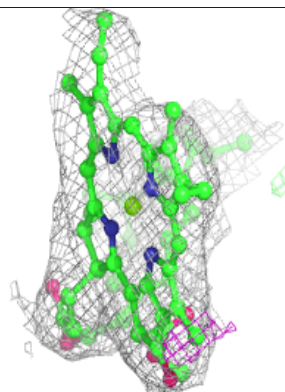
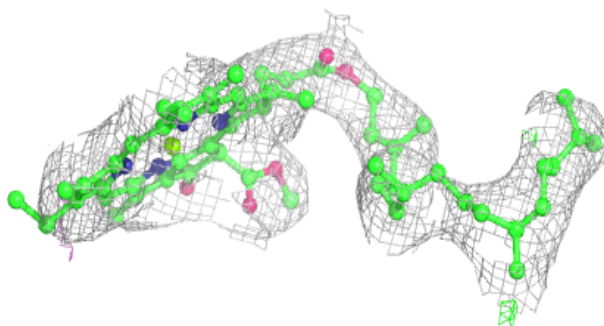
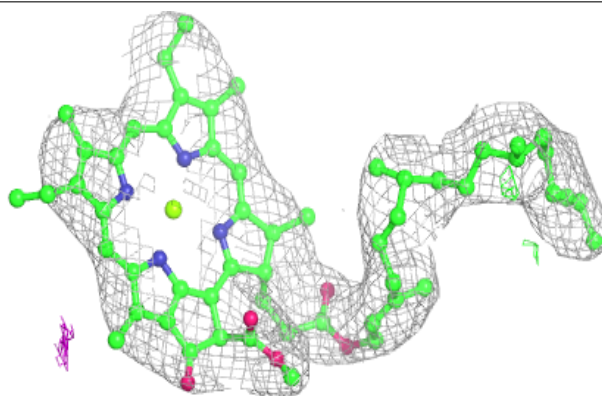


**Electron density around CLA 4 305:**

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

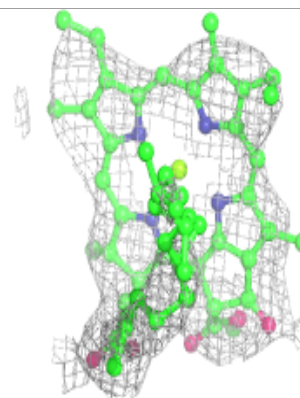
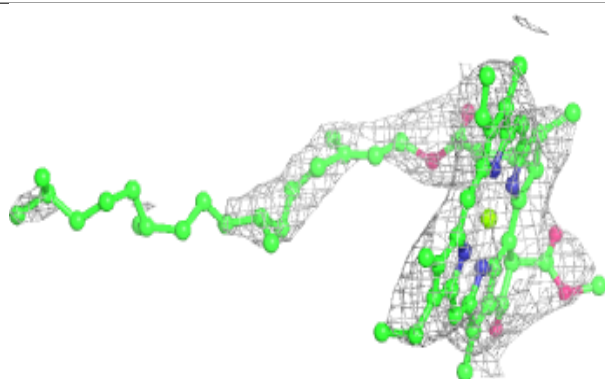
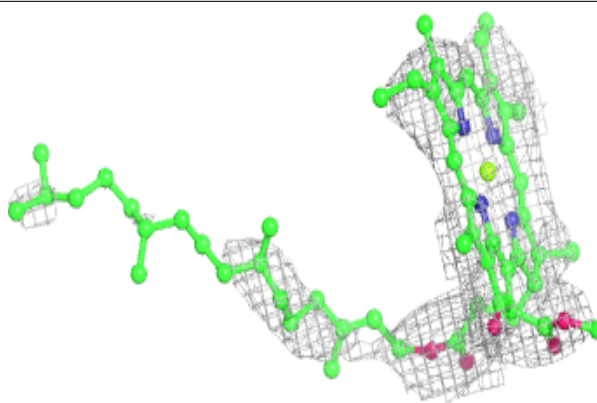
**Electron density around CLA J 1101:**

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

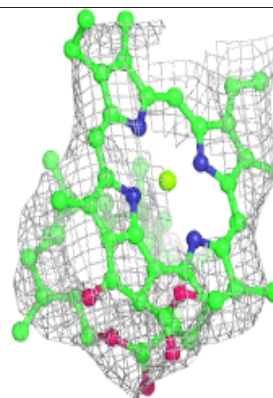
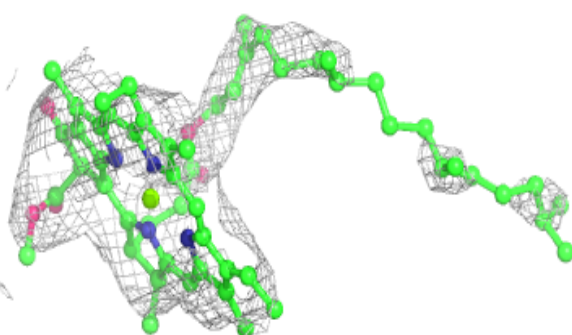
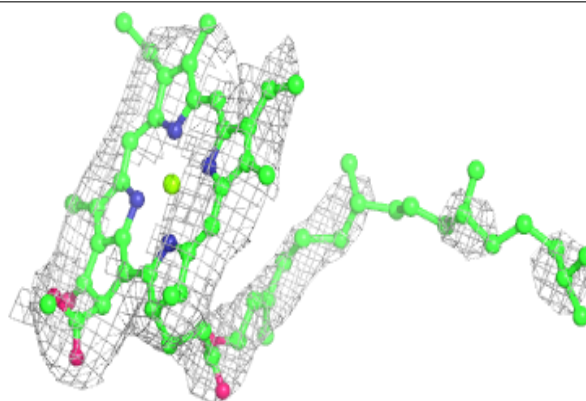


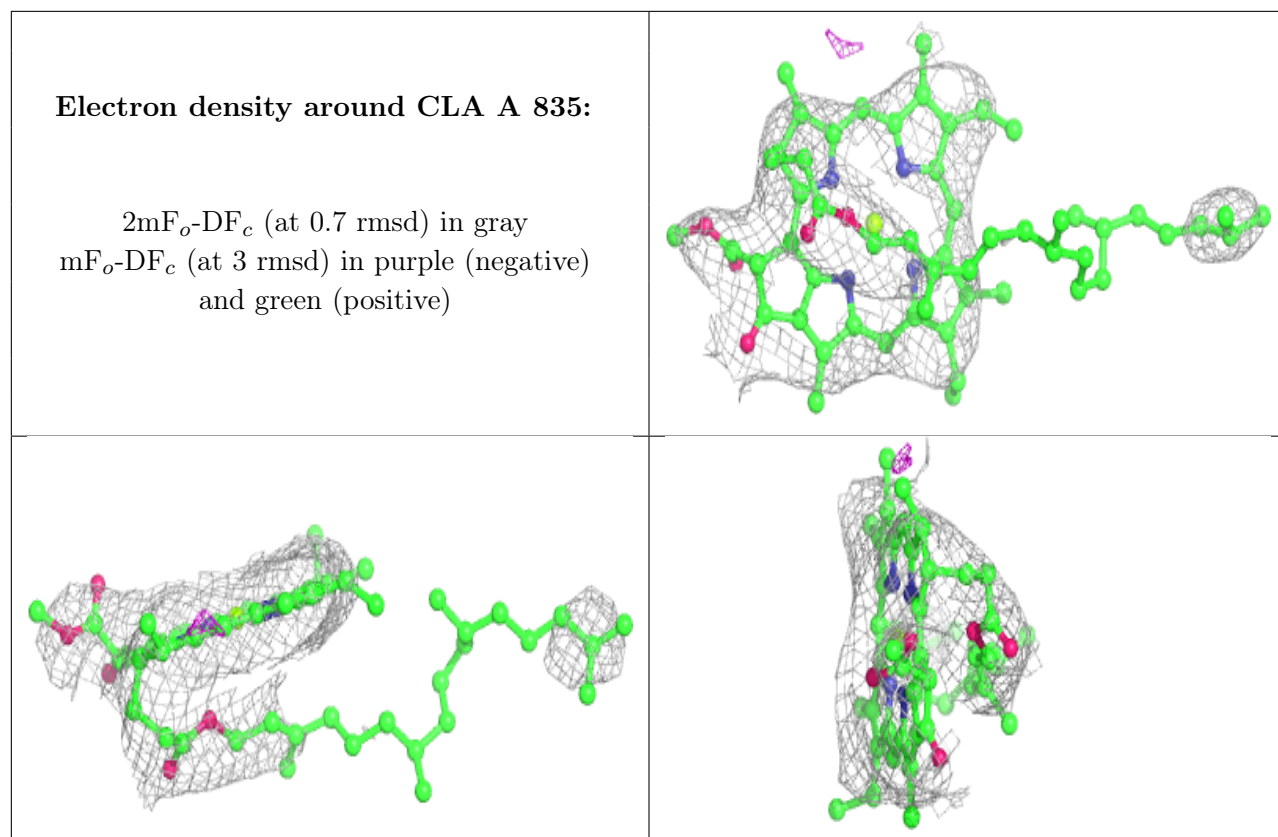
**Electron density around CLA B 830:**

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

**Electron density around CLA B 815:**

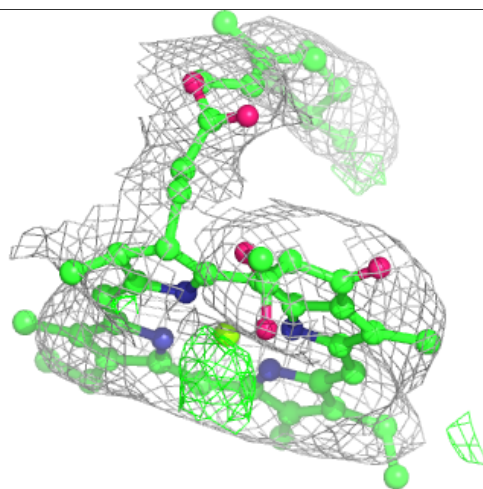
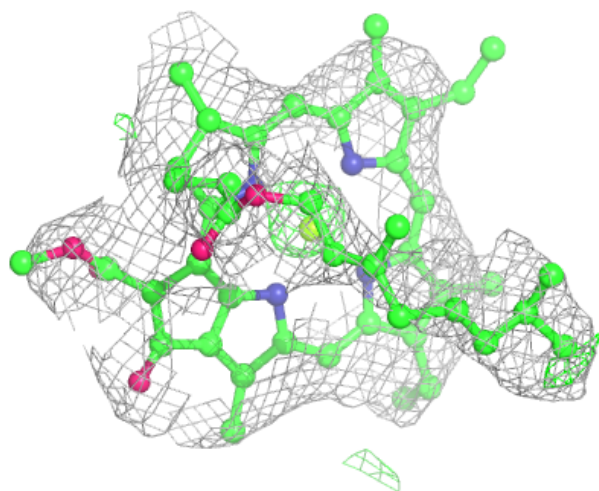
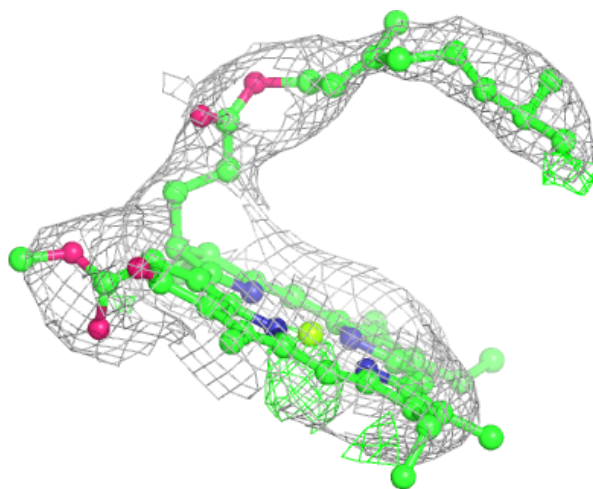
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA L 301:**

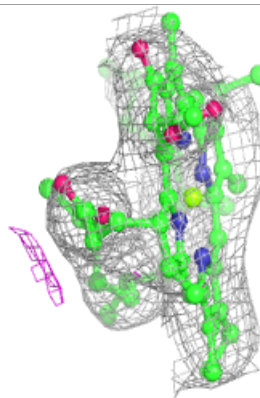
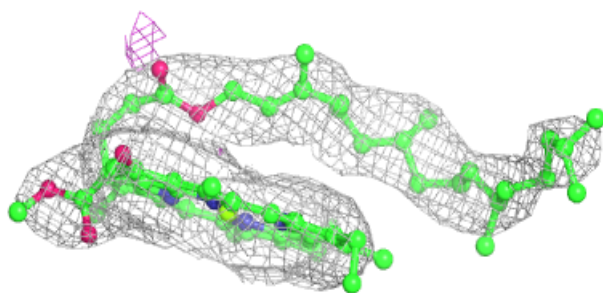
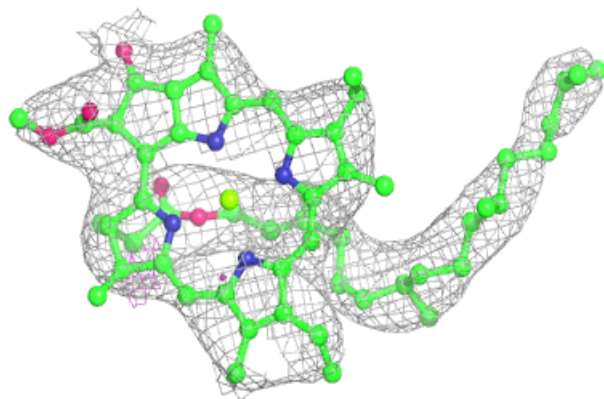
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



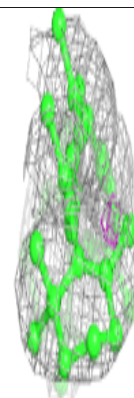
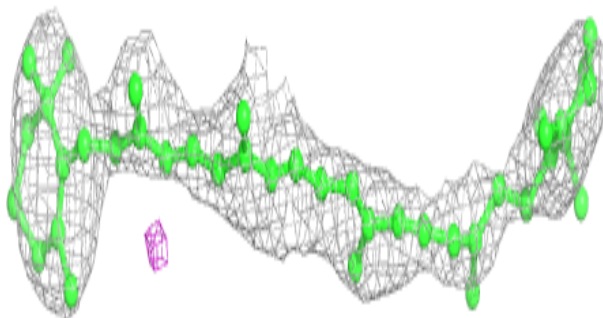
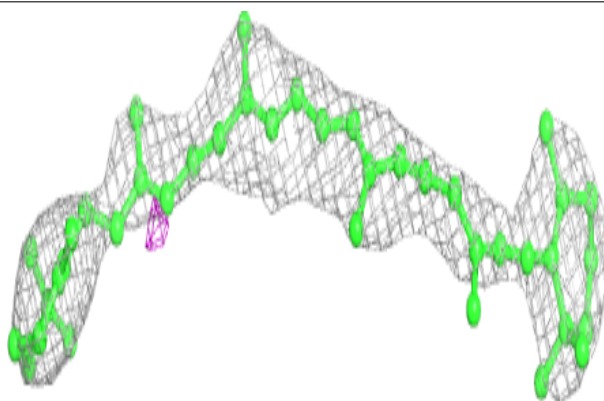


**Electron density around CLA B 837:**

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

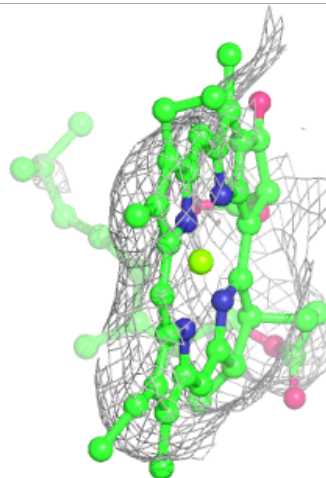
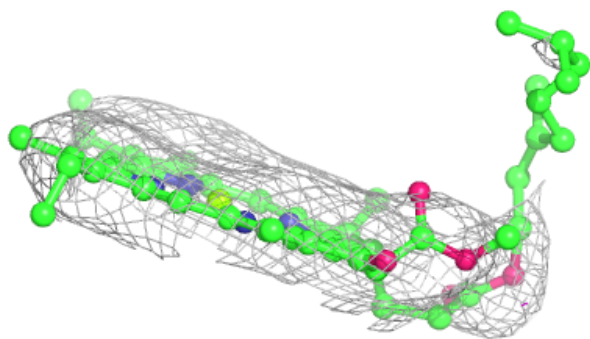
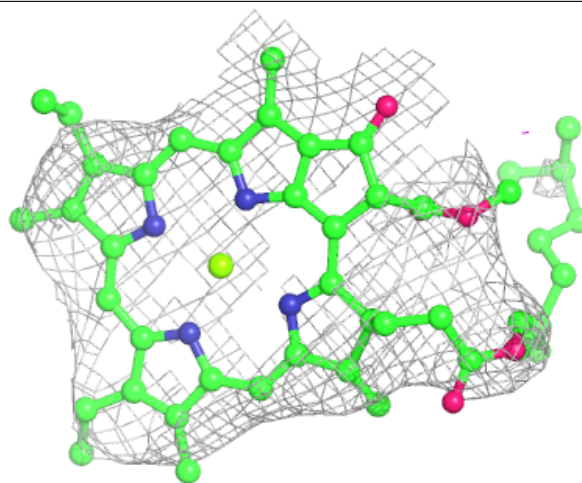
**Electron density around BCR F 304:**

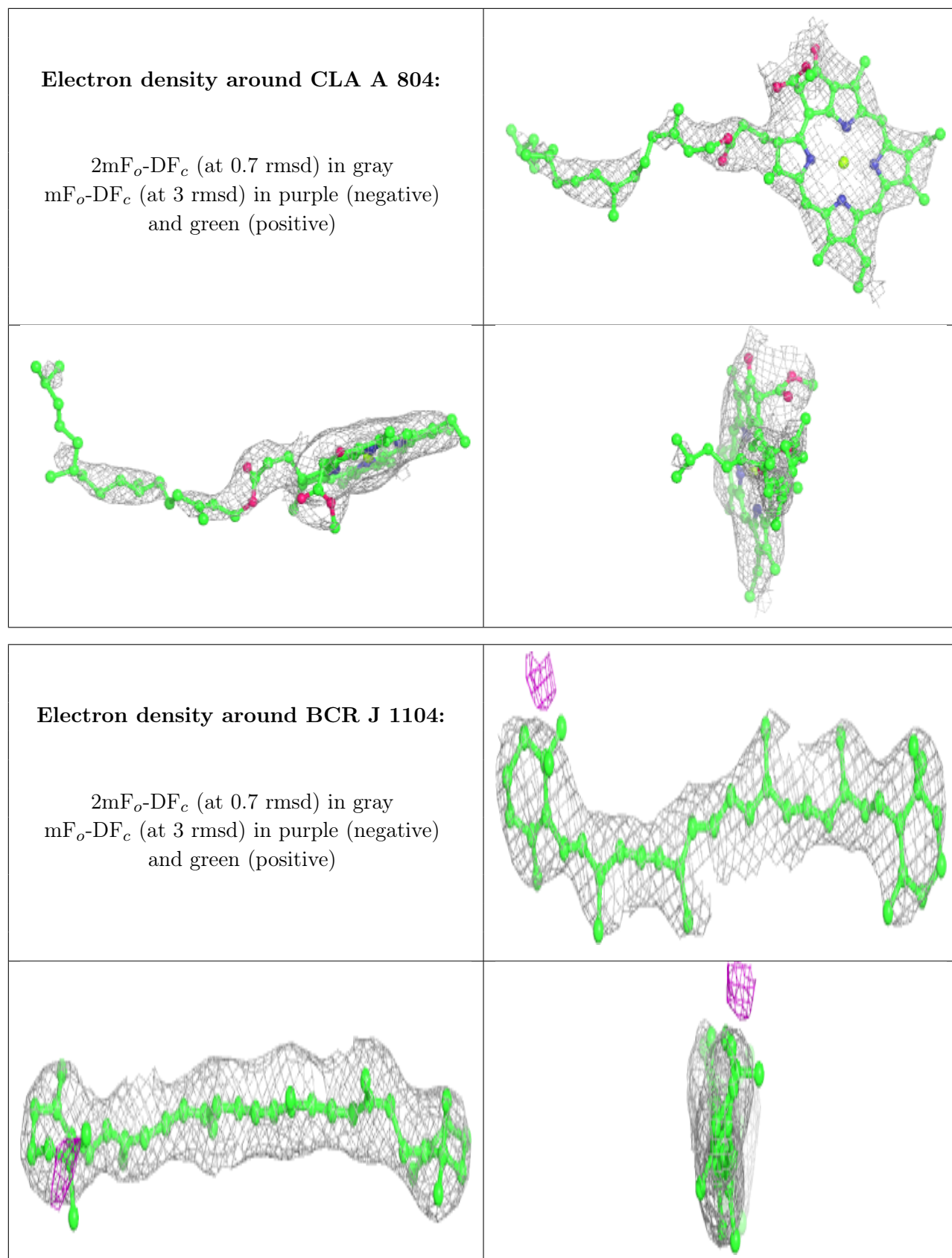
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 3 311:**

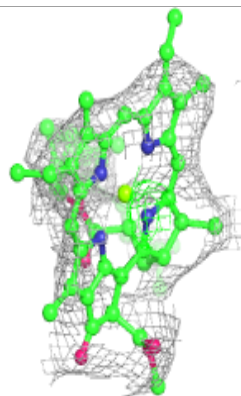
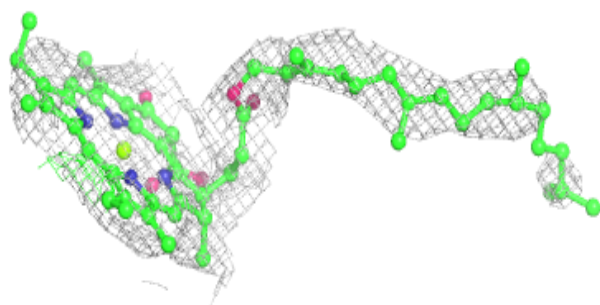
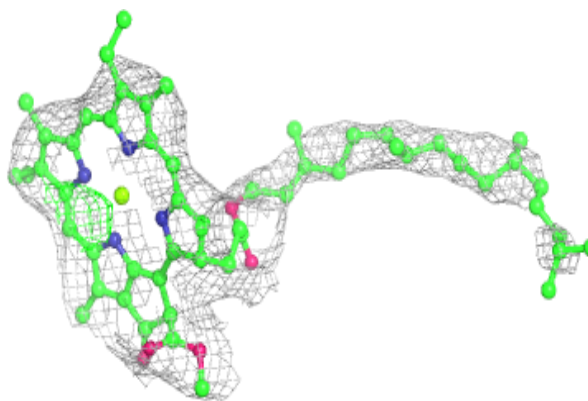
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



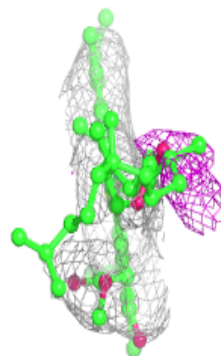
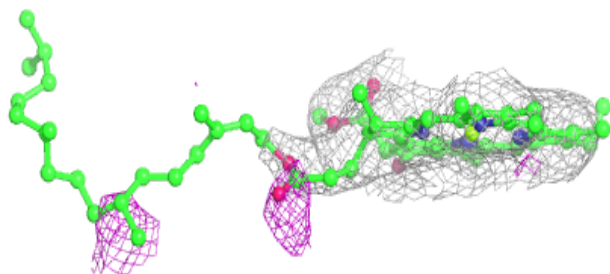
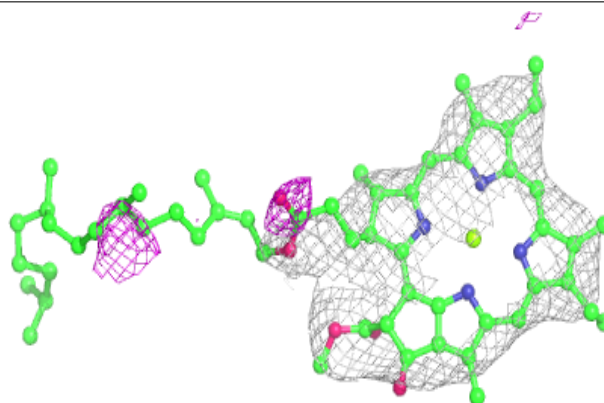


**Electron density around CLA A 819:**

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

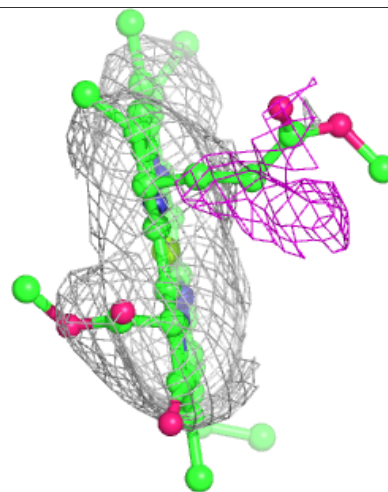
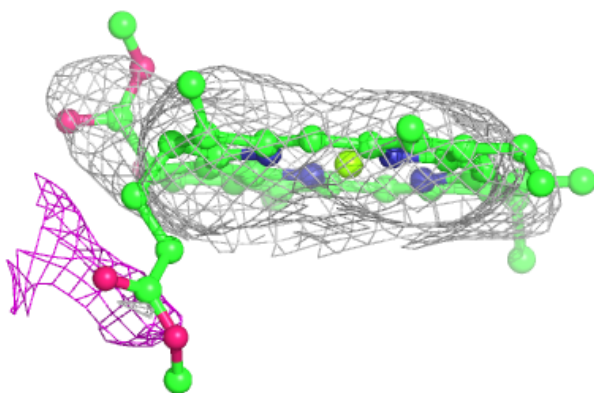
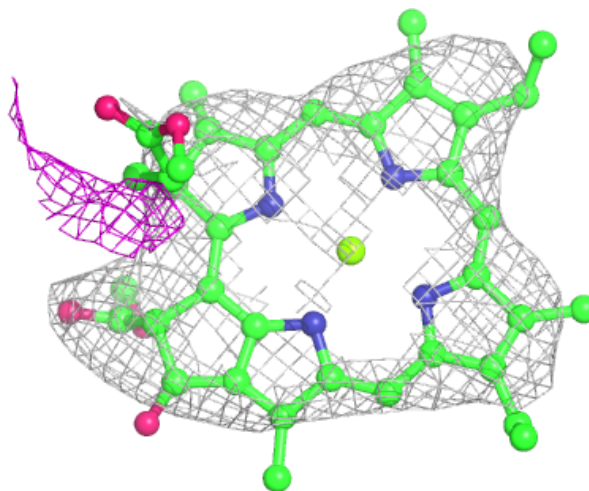
**Electron density around CLA F 302:**

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



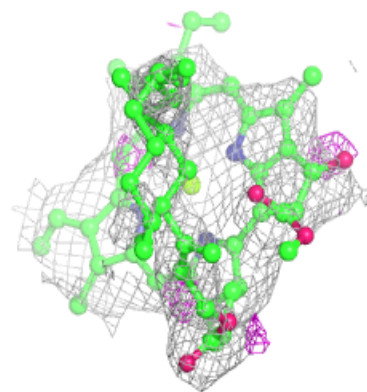
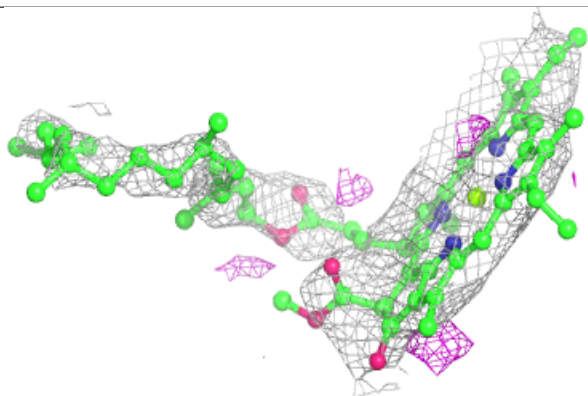
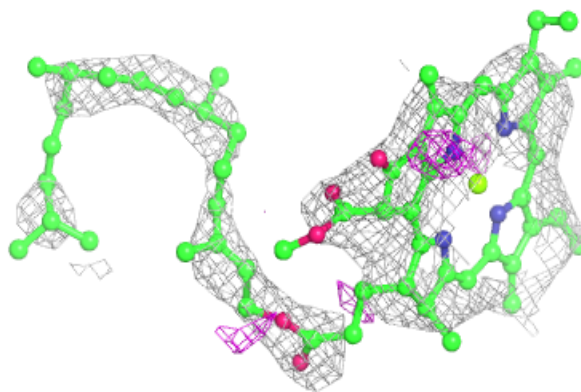
**Electron density around CLA B 821:**

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



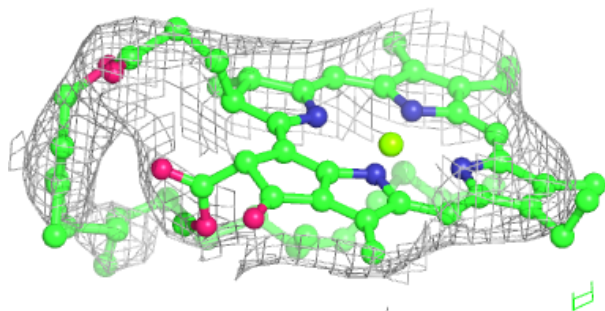
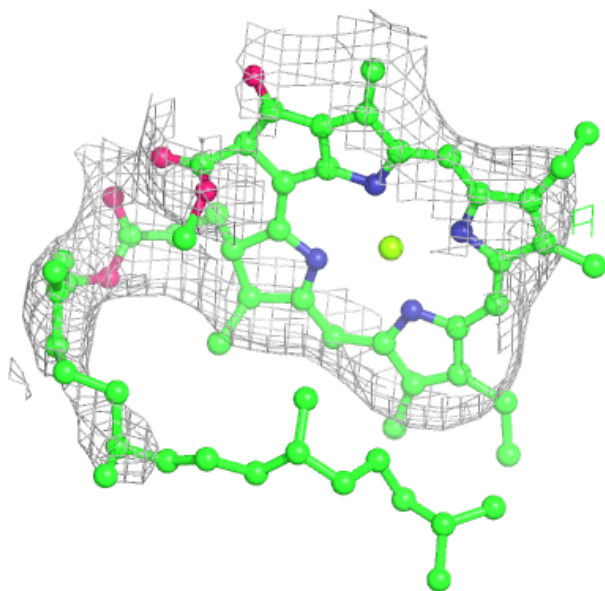
**Electron density around CL0 A 801:**

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



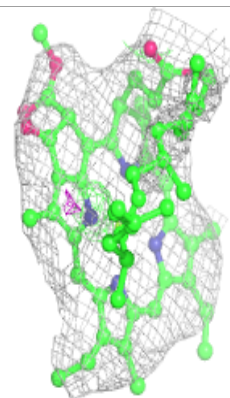
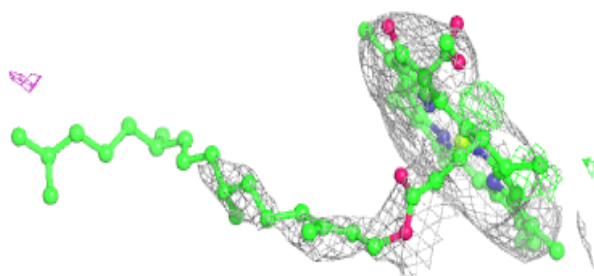
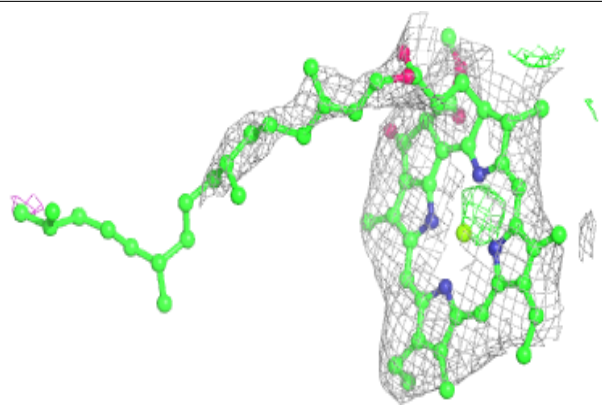
**Electron density around CLA 1 5010:**

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

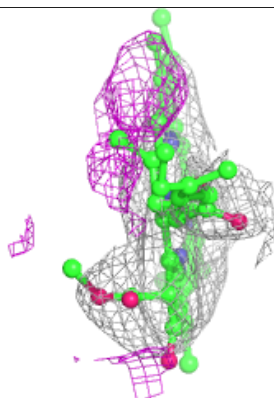
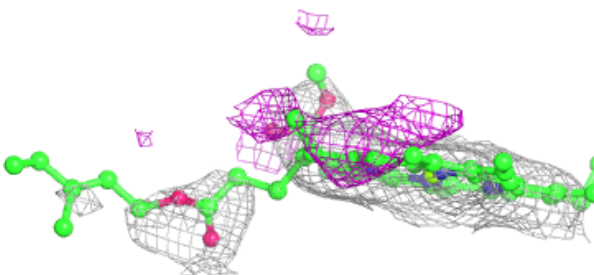
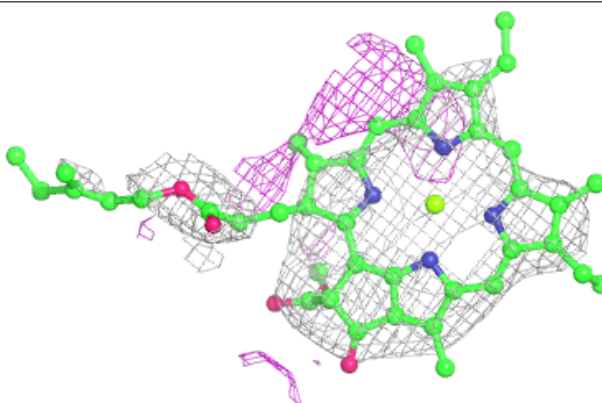


**Electron density around CLA B 823:**

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

**Electron density around CLA A 834:**

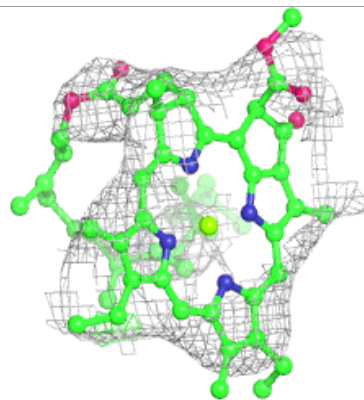
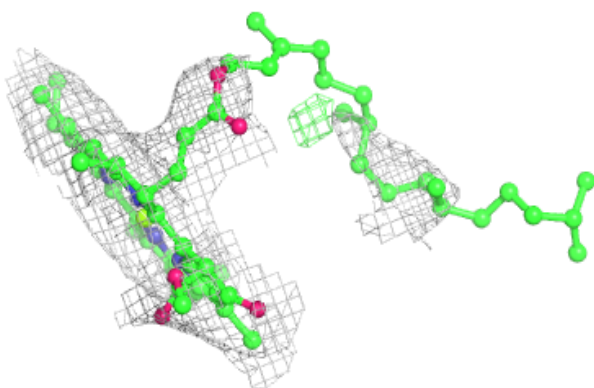
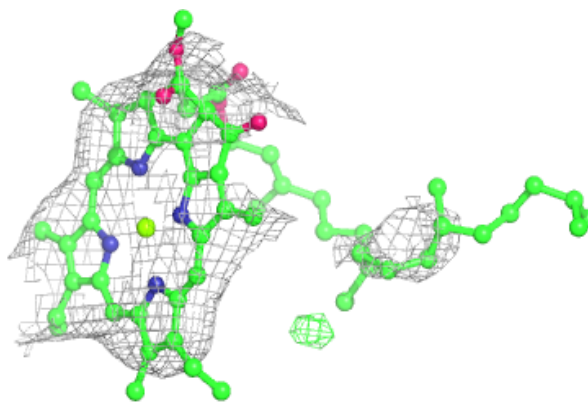
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



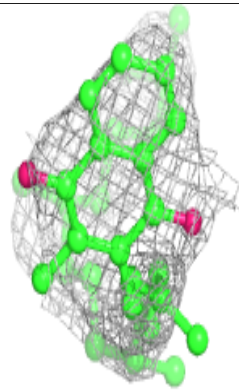
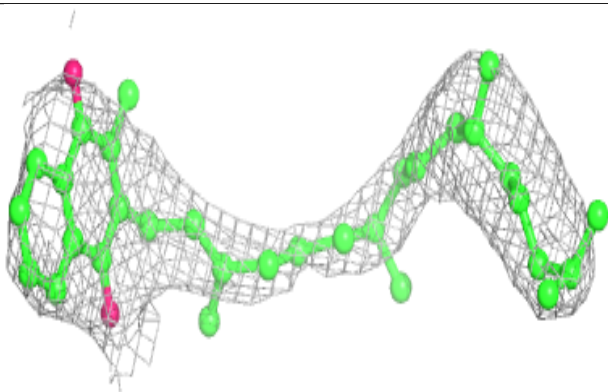
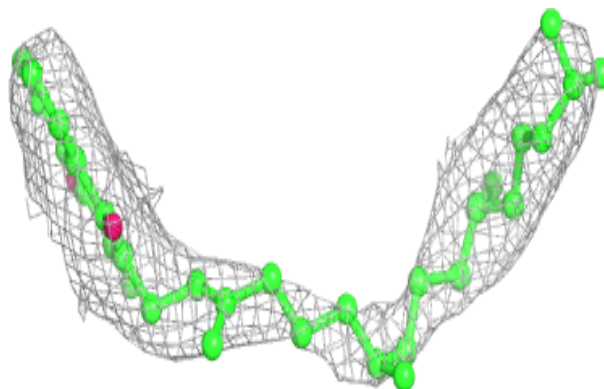


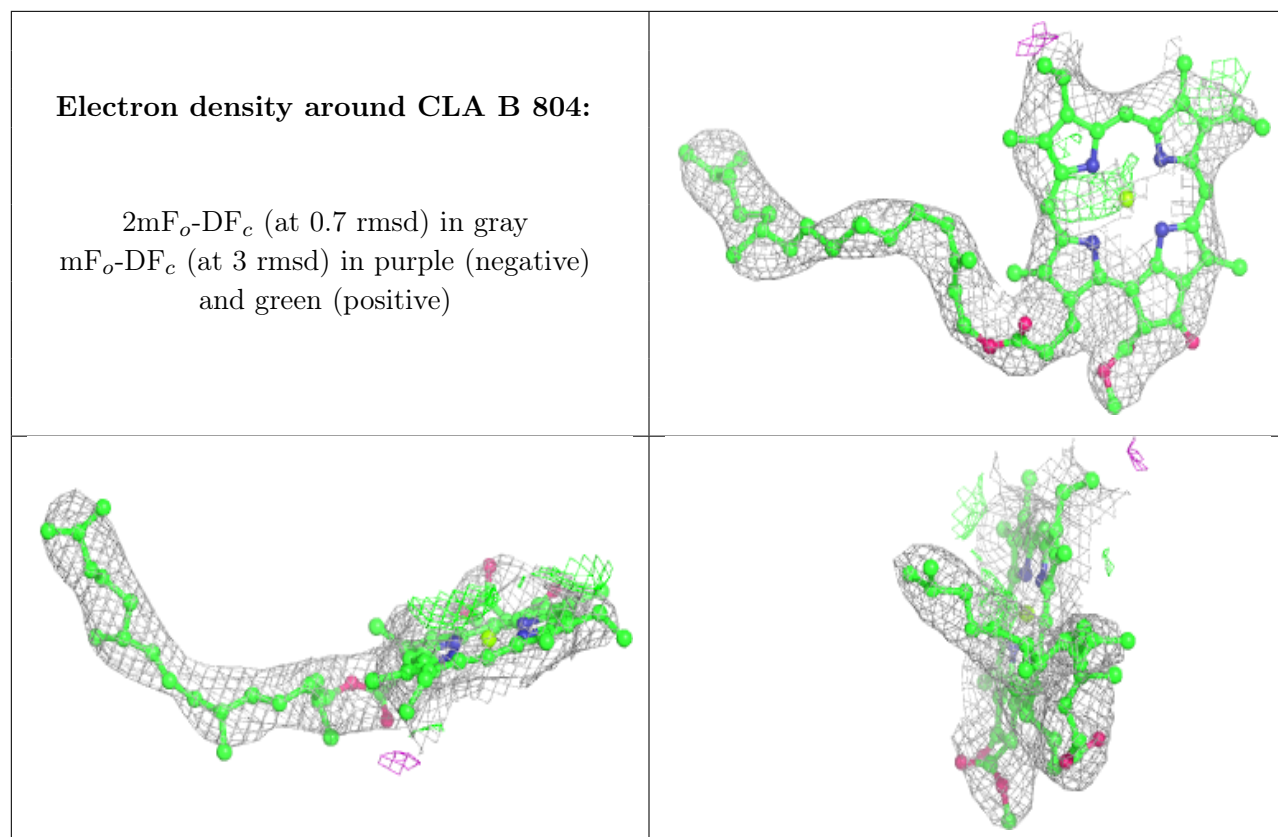
**Electron density around CLA 4 315:**

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

**Electron density around PQN B 842:**

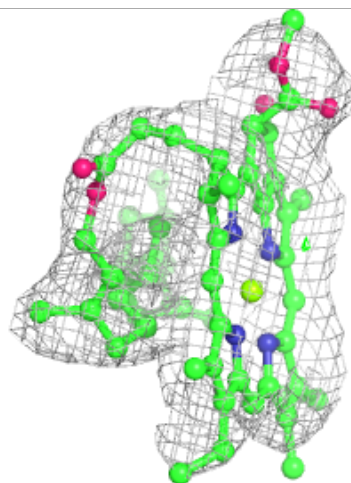
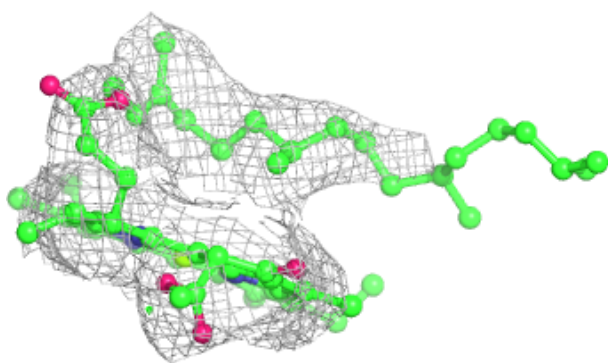
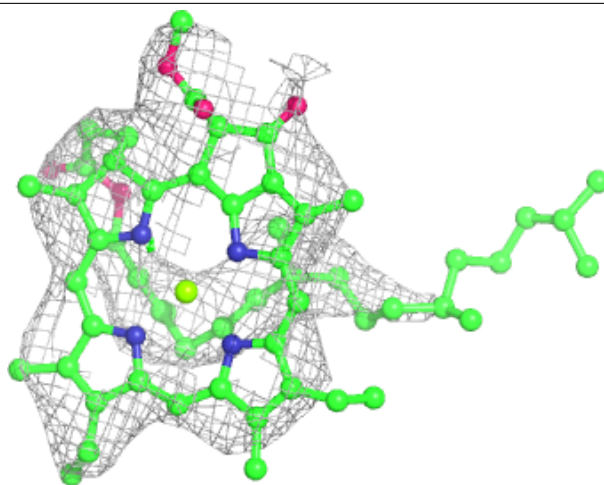
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





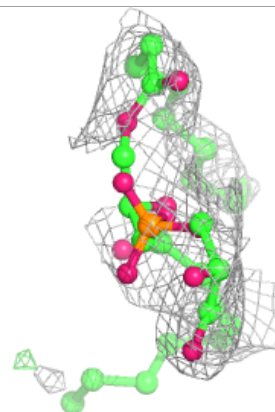
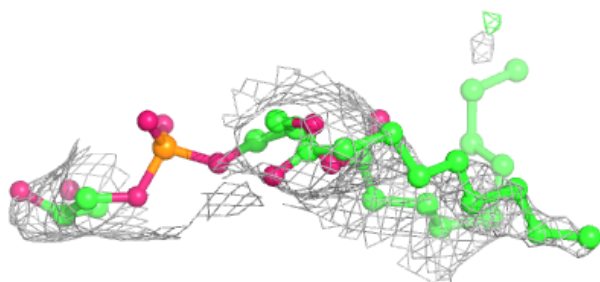
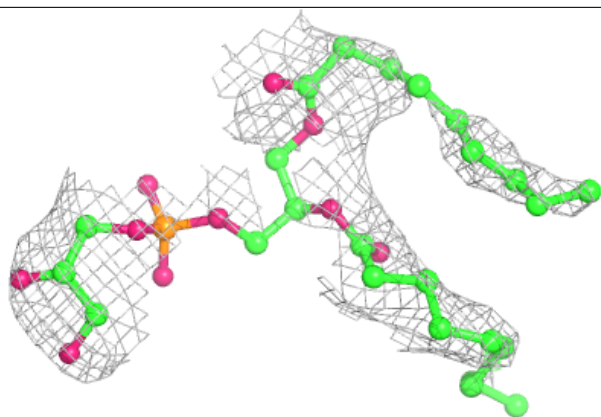
**Electron density around CLA B 828:**

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

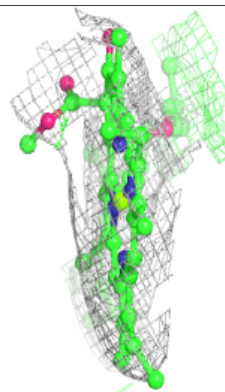
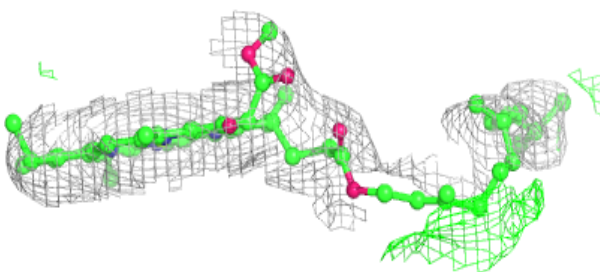
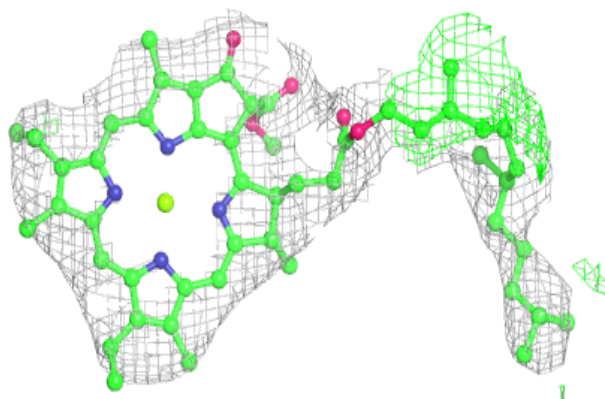


**Electron density around LHG 2 320:**

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

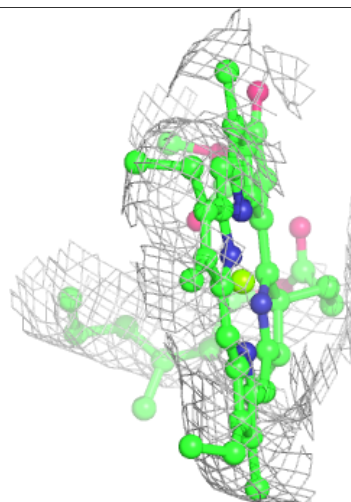
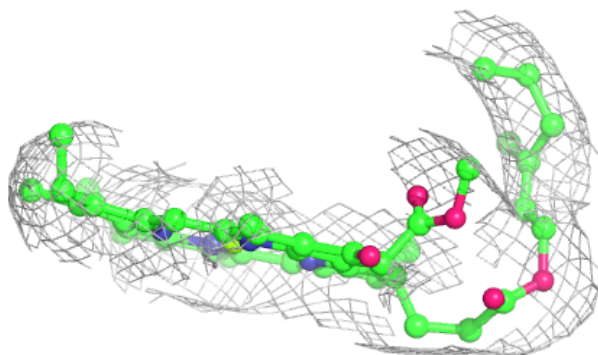
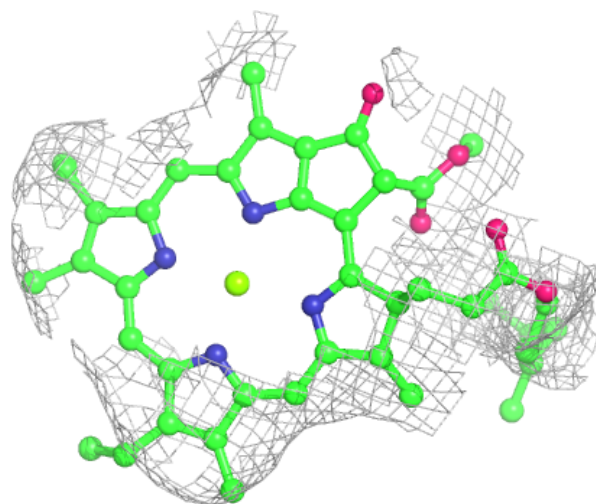
**Electron density around CLA 1 5018:**

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



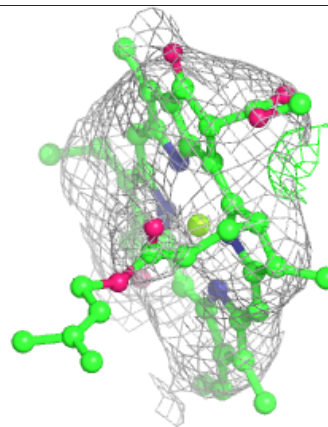
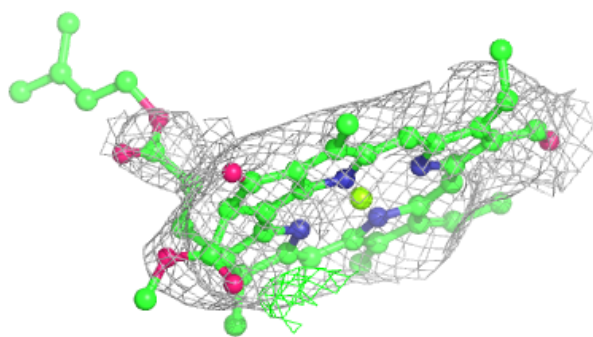
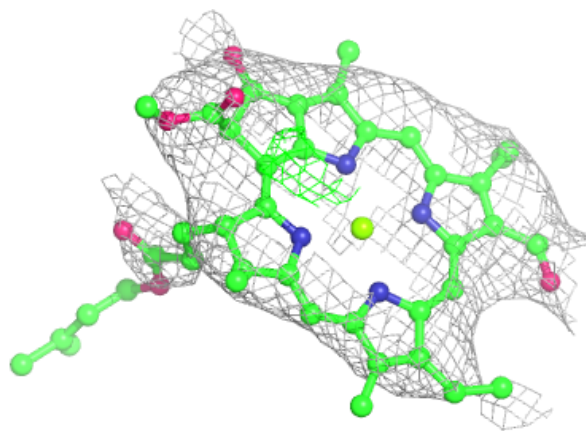
**Electron density around CLA 2 307:**

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



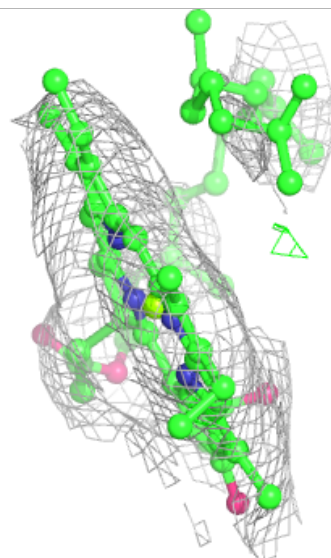
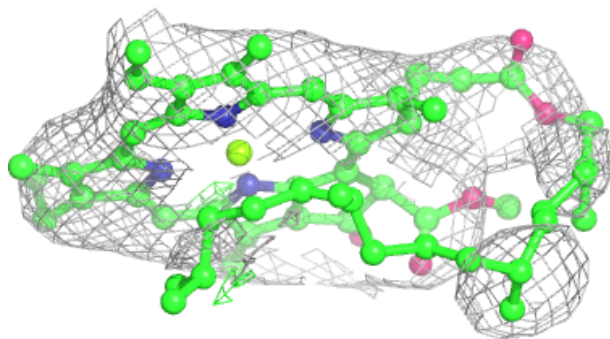
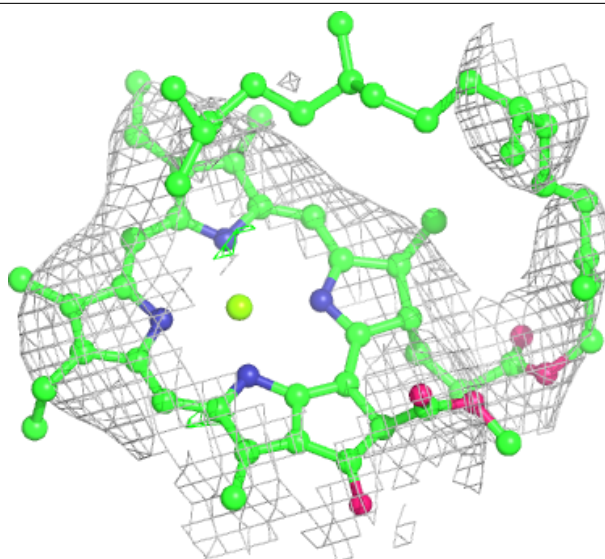
**Electron density around CHL 4 314:**

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



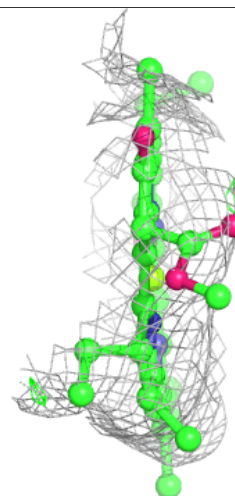
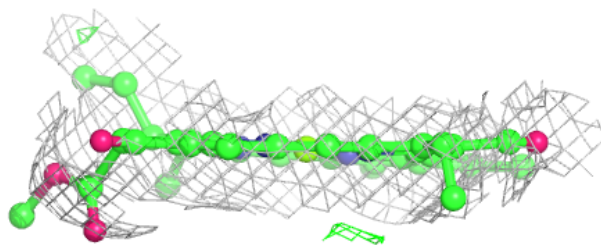
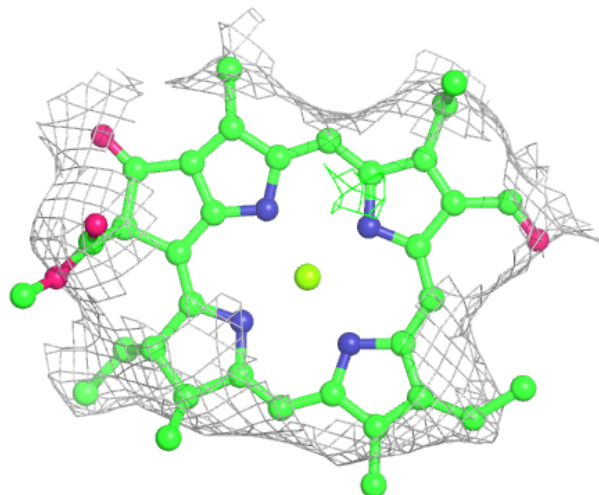
**Electron density around CLA 2 310:**

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



**Electron density around CHL 4 317:**

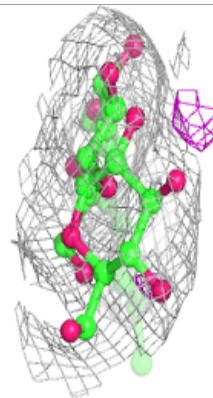
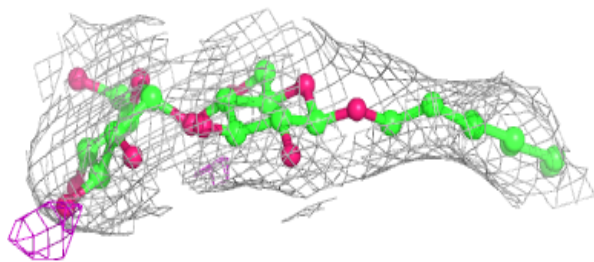
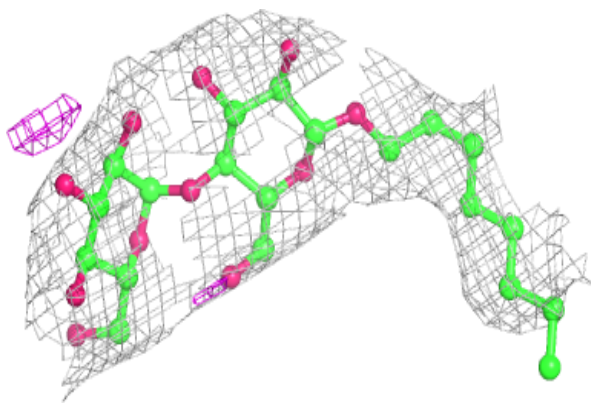
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



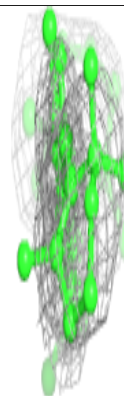
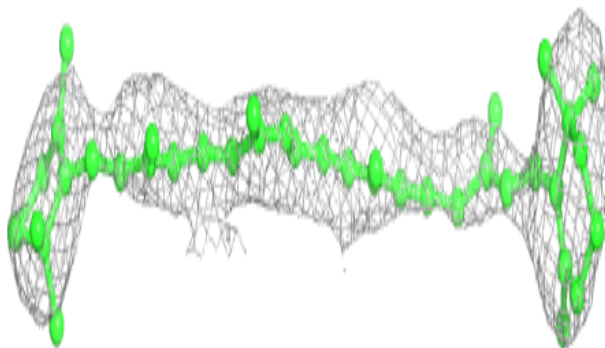
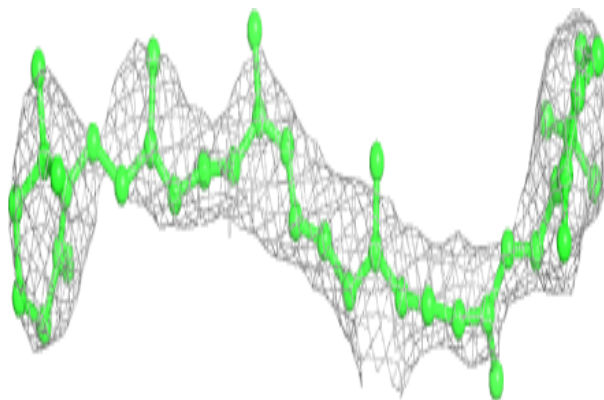


**Electron density around LMT B 856:**

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

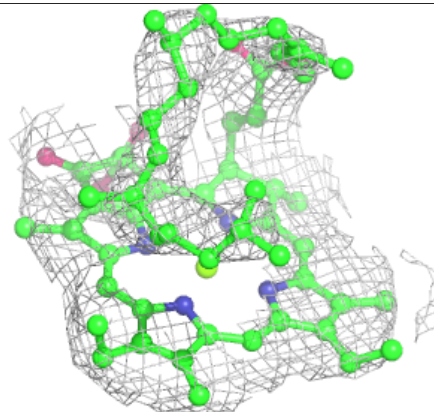
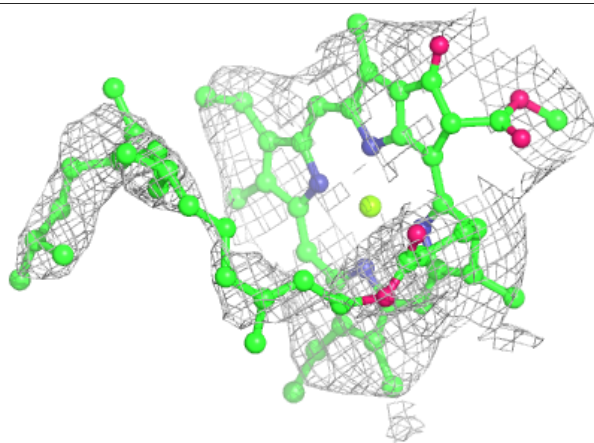
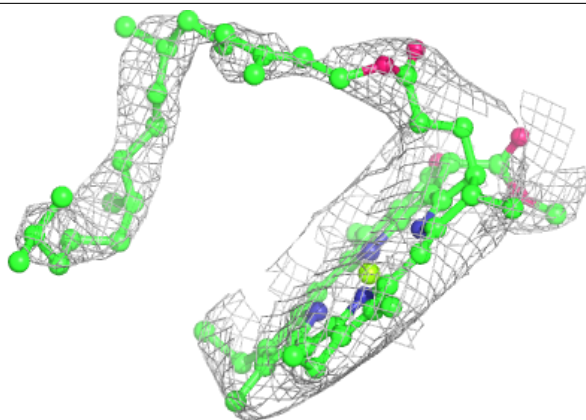
**Electron density around BCR B 802:**

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

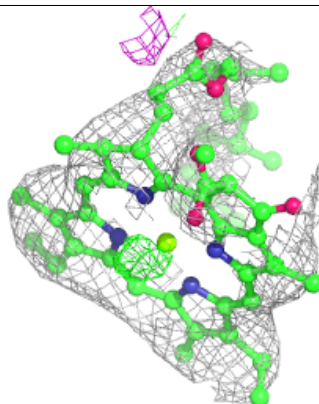
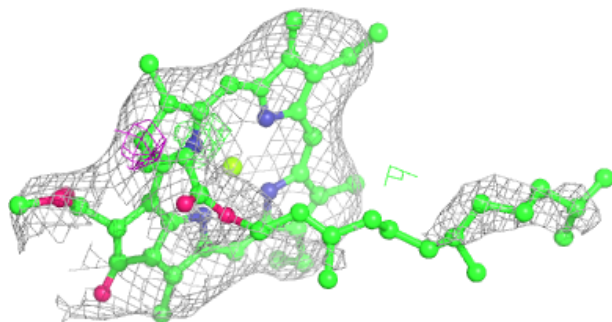
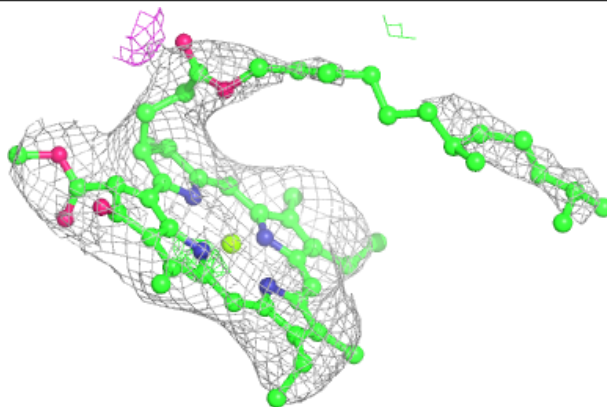


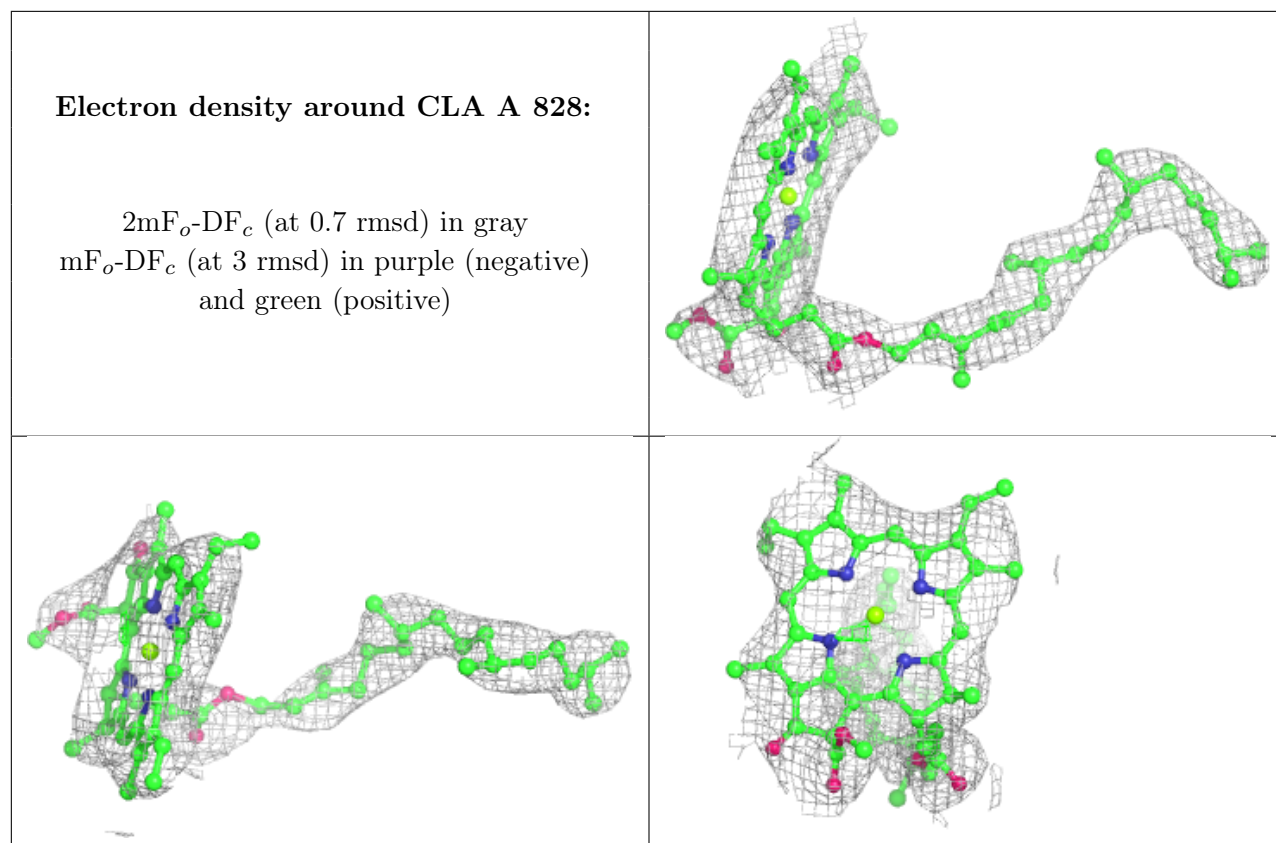
**Electron density around CLA B 831:**

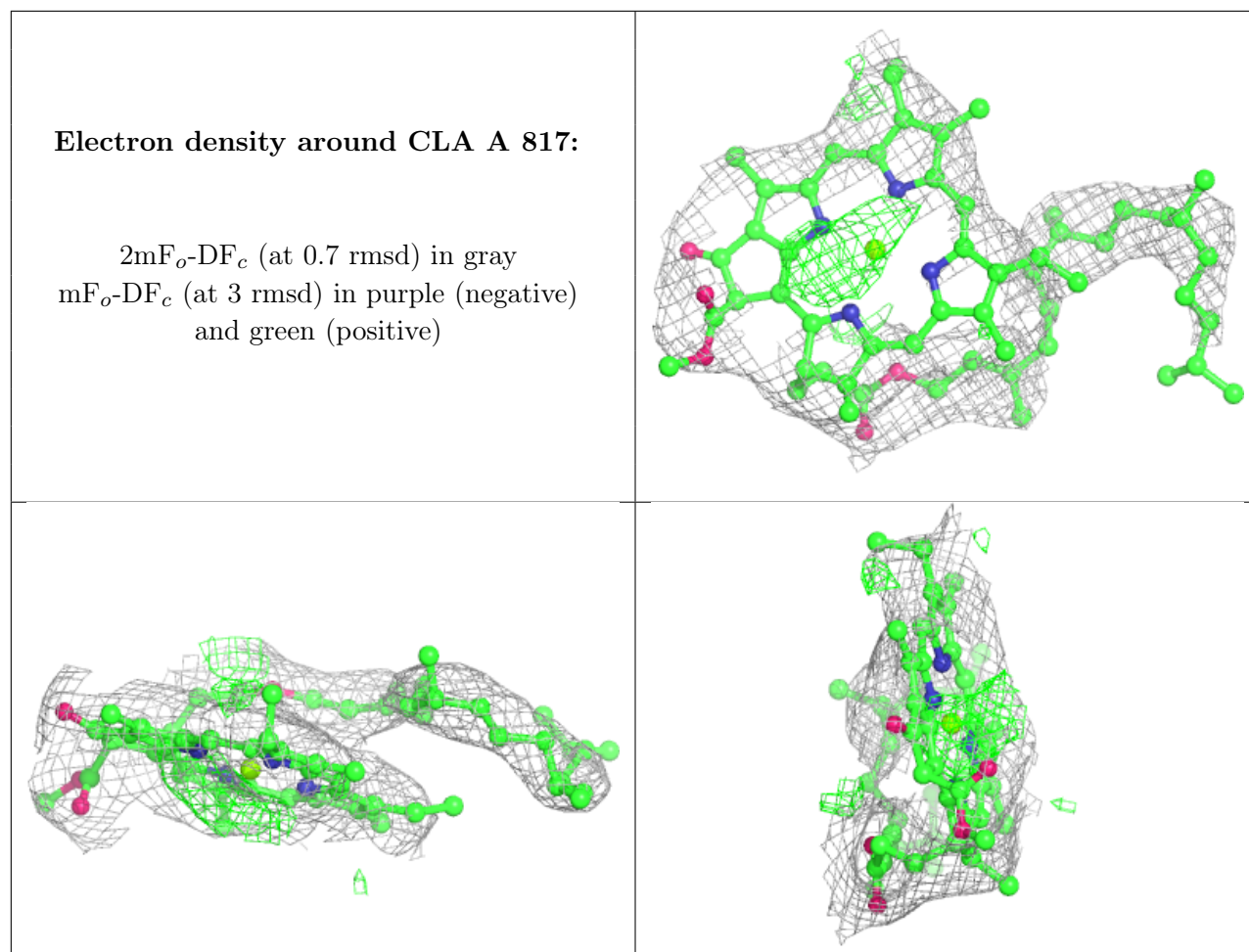
$2mF_o-DF_c$  (at 0.7 rnsd) in gray  
 $mF_o-DF_c$  (at 3 rnsd) in purple (negative)  
and green (positive)

**Electron density around CLA B 832:**

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

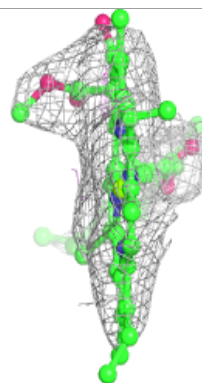
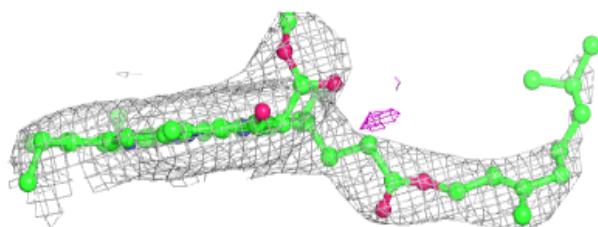
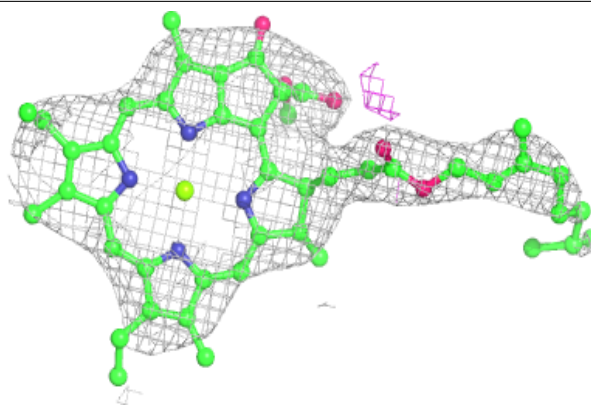




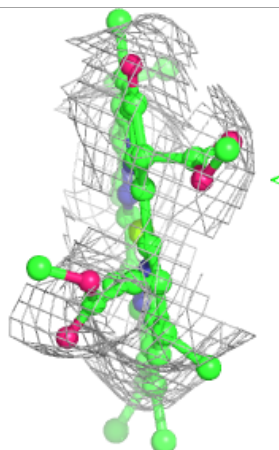
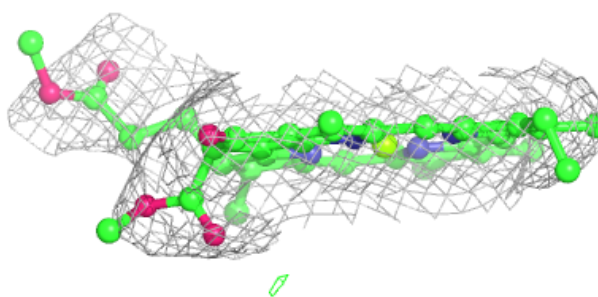
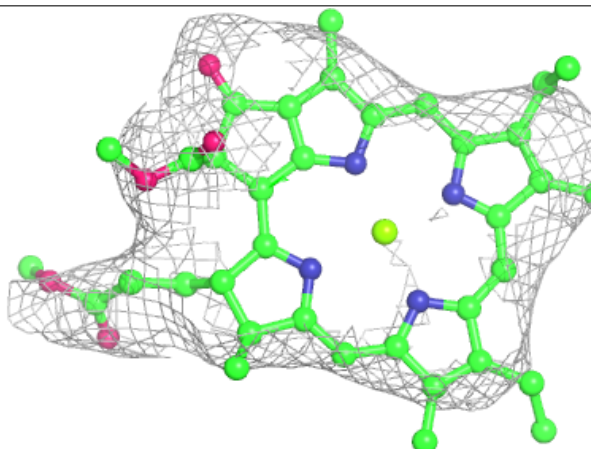


**Electron density around CLA B 836:**

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

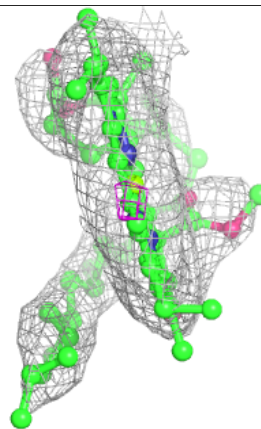
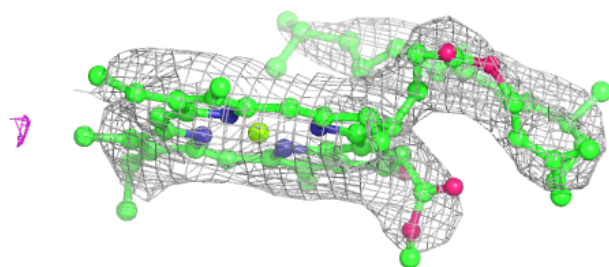
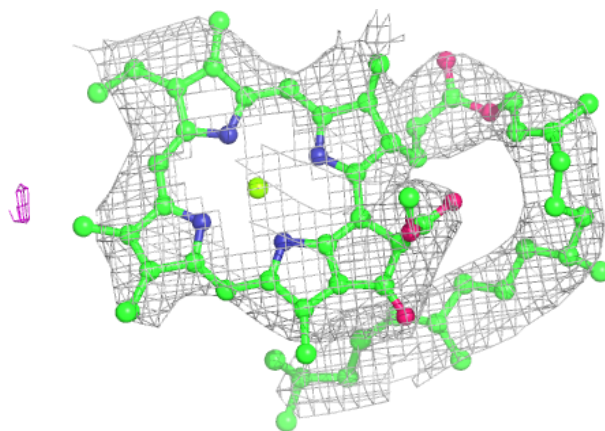
**Electron density around CLA 3 318:**

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



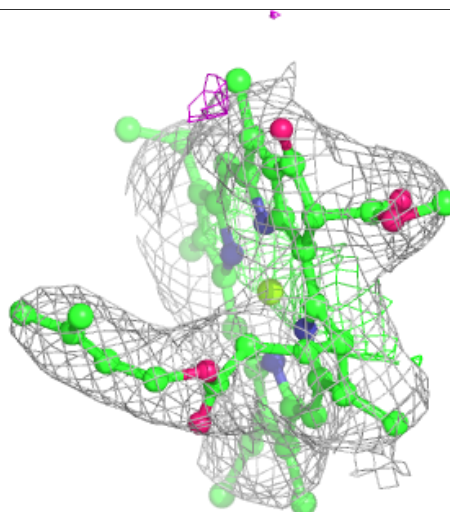
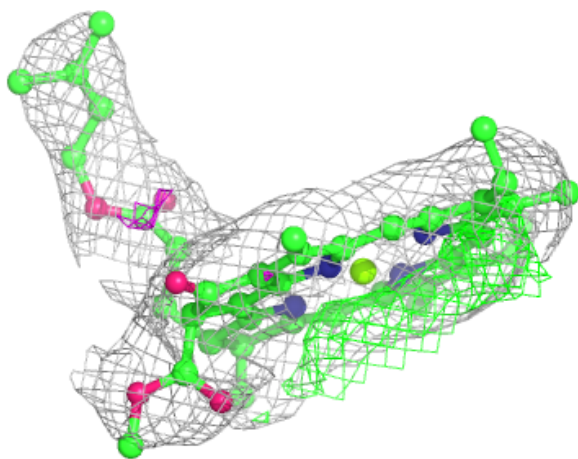
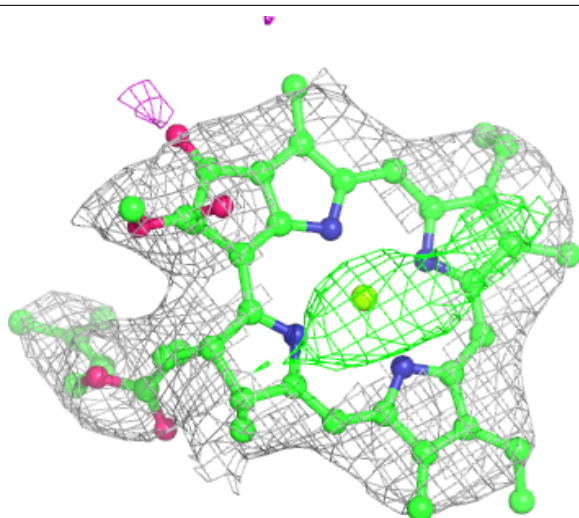
**Electron density around CLA B 806:**

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



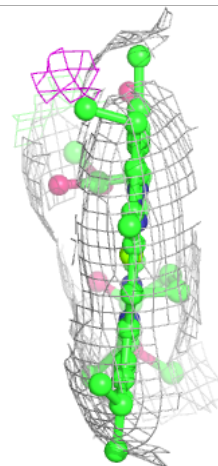
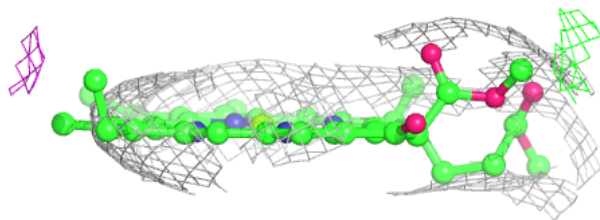
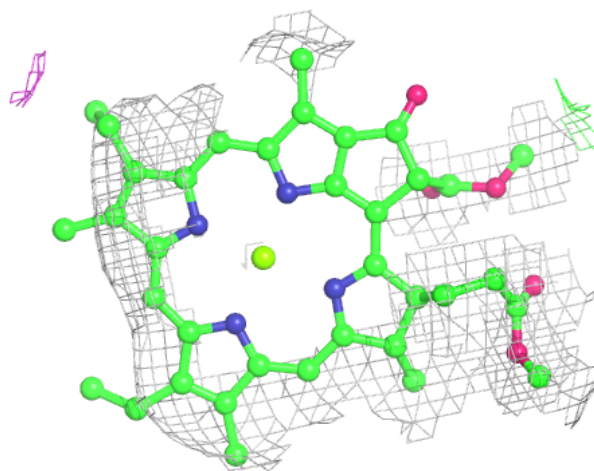
**Electron density around CLA B 838:**

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

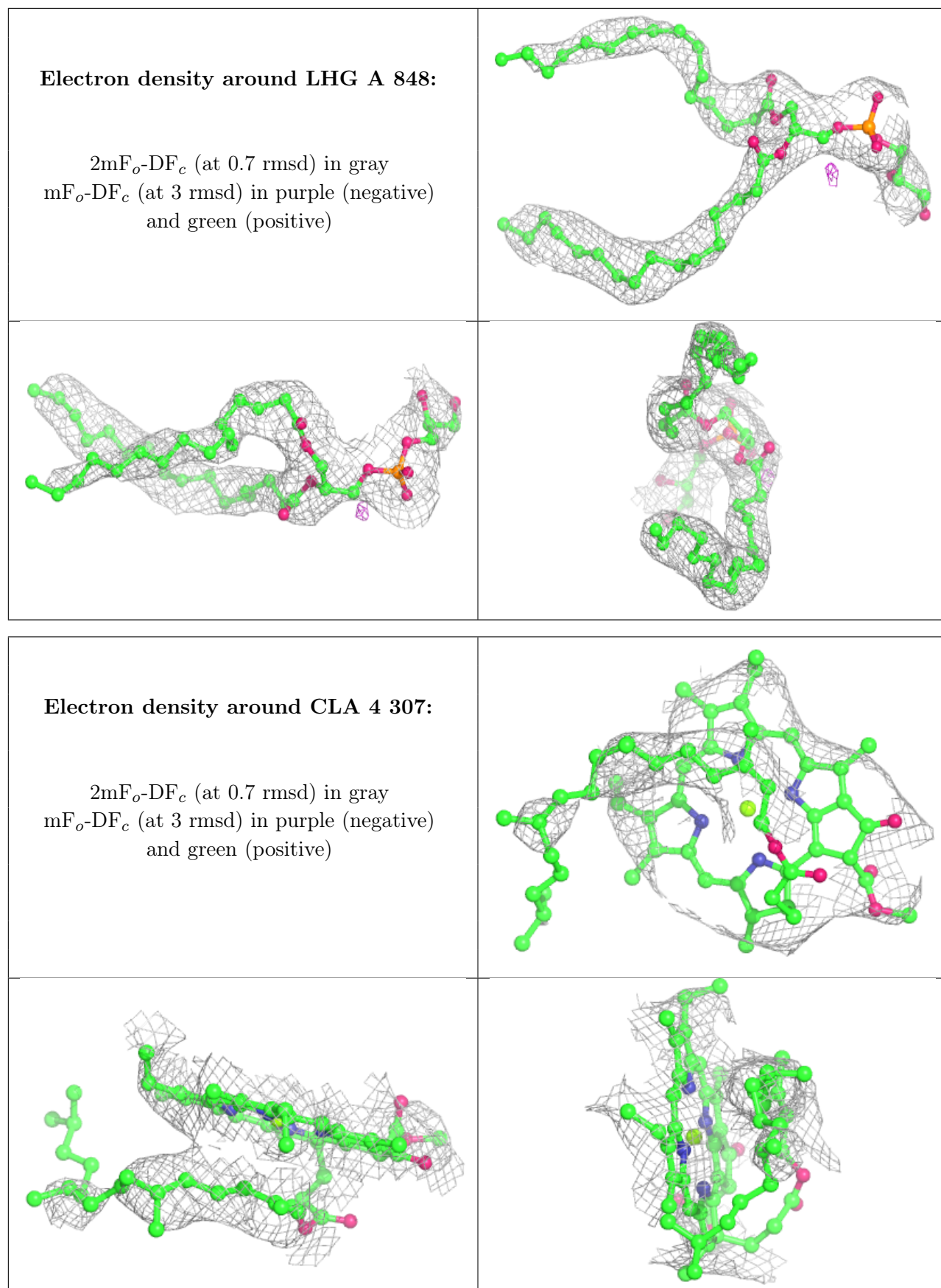


**Electron density around CLA 1 5007:**

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

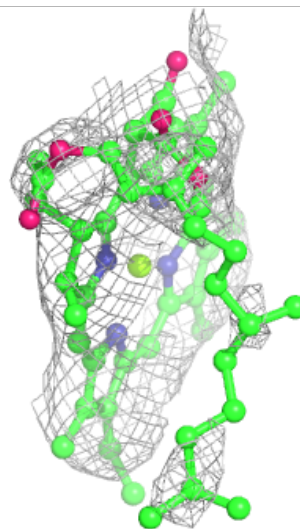
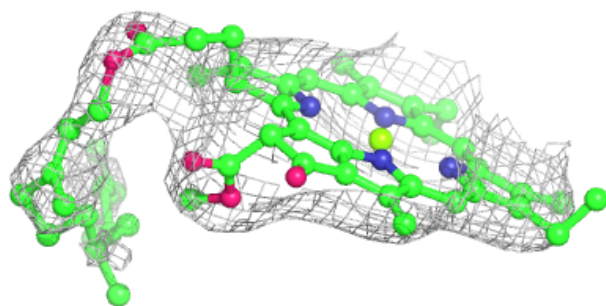
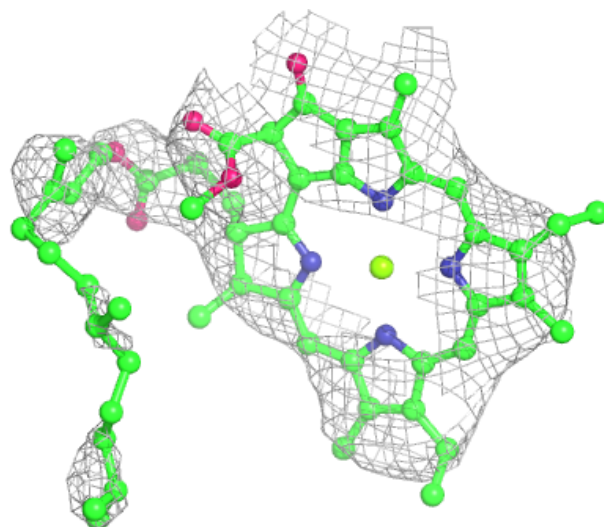






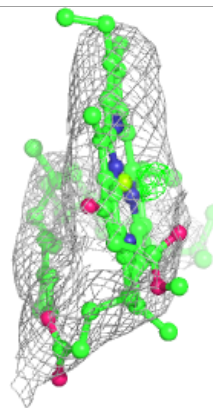
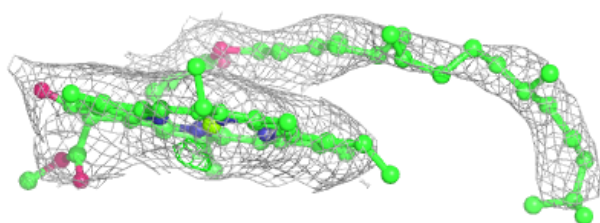
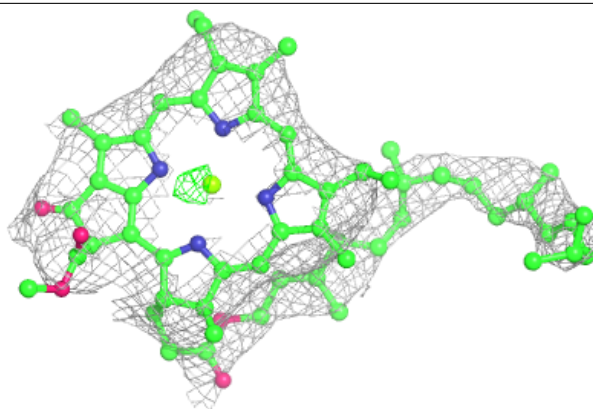
**Electron density around CLA 4 309:**

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

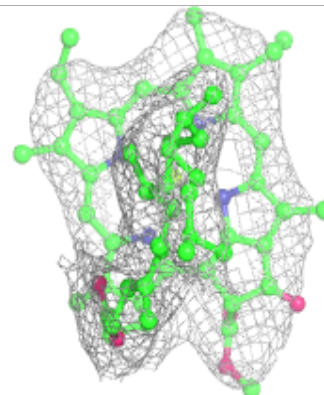
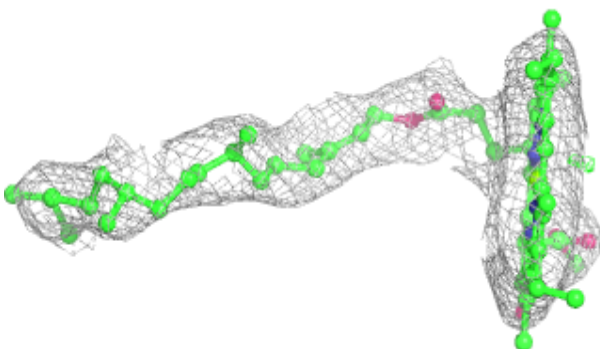
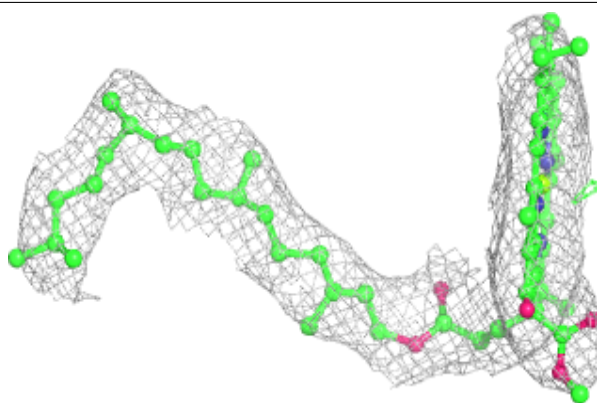


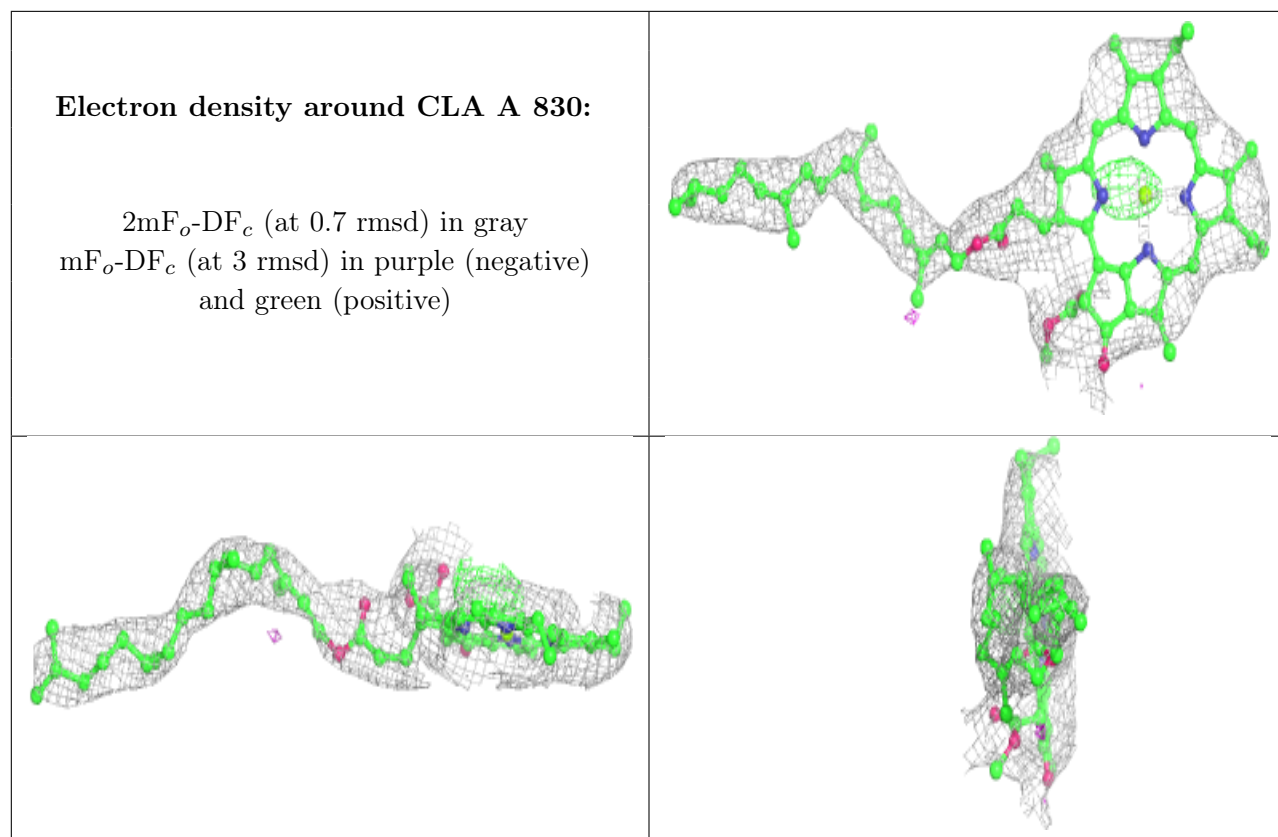
**Electron density around CLA B 819:**

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

**Electron density around CLA B 840:**

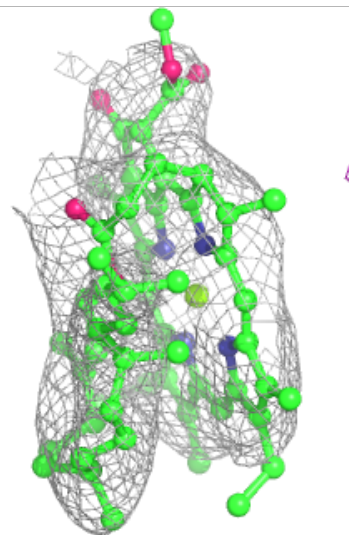
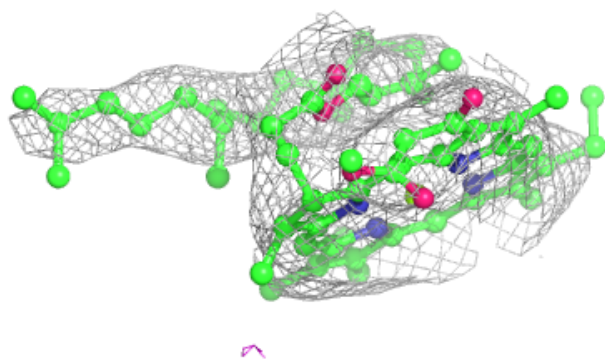
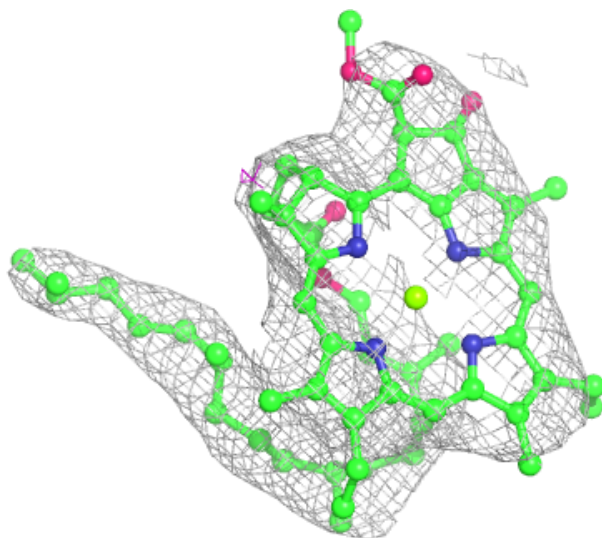
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





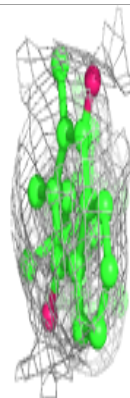
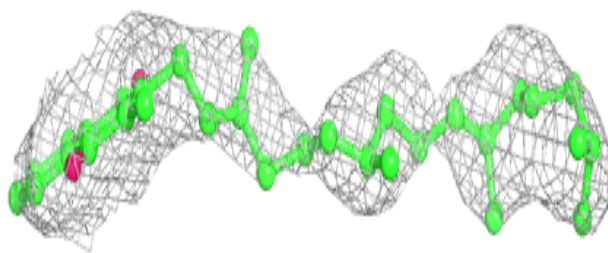
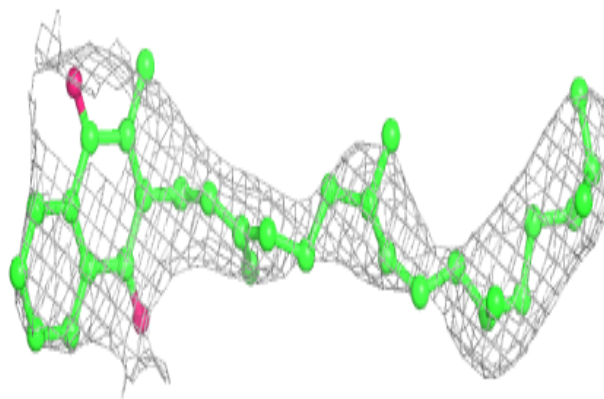
**Electron density around CLA B 809:**

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

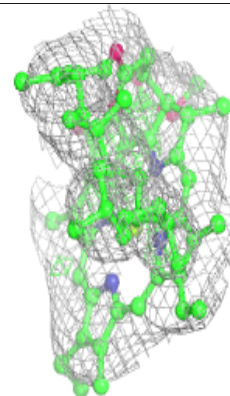
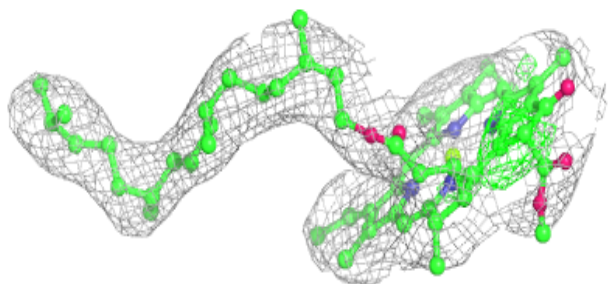
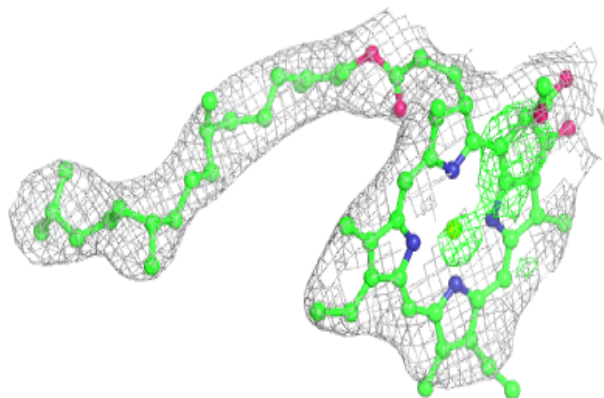


**Electron density around PQN A 841:**

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

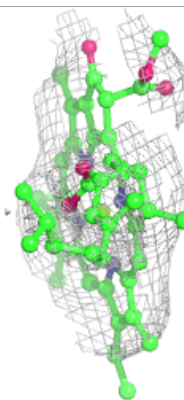
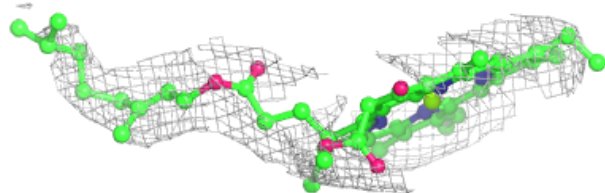
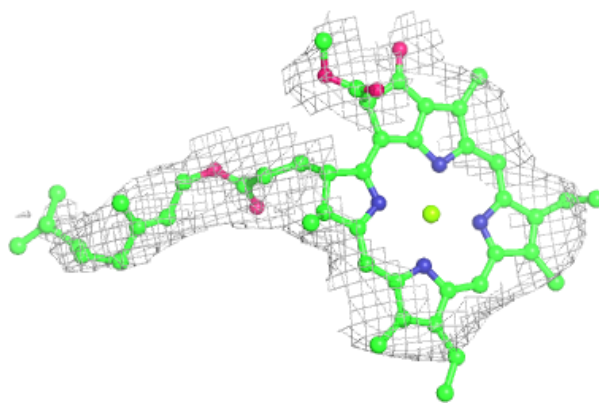
**Electron density around CLA A 807:**

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

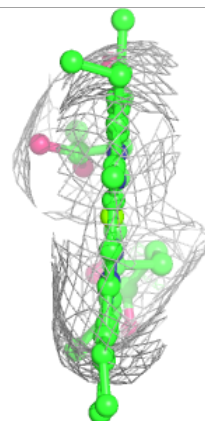
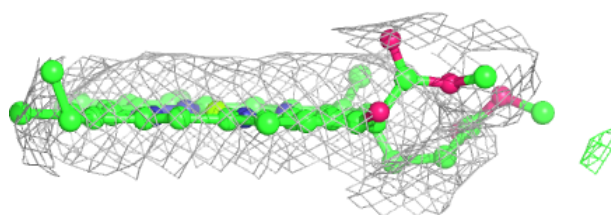
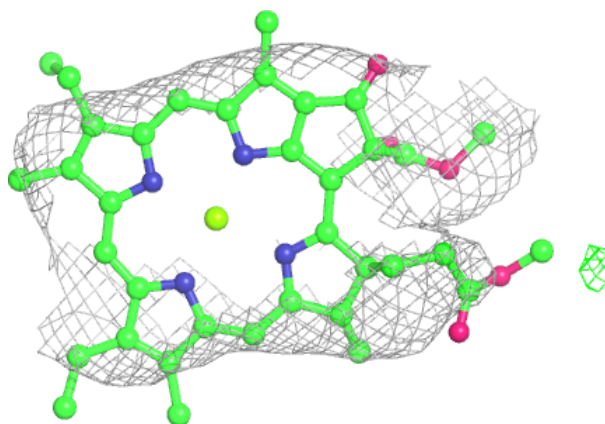


**Electron density around CLA G 1601:**

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

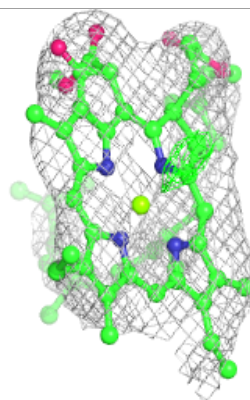
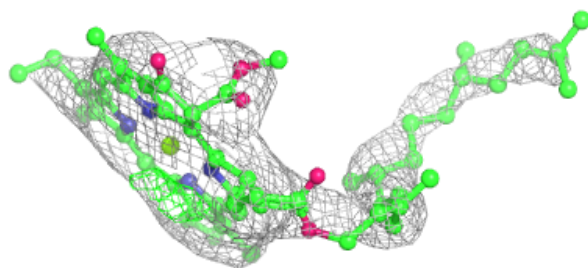
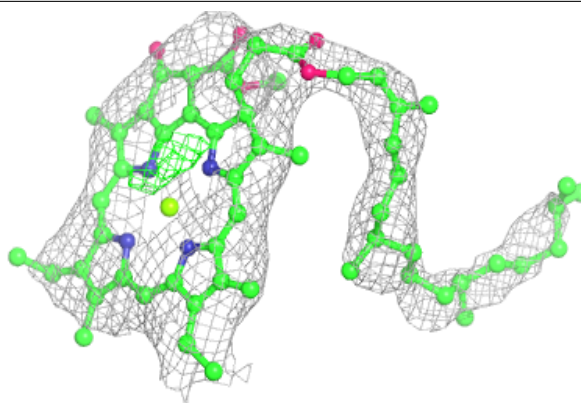
**Electron density around CLA G 1602:**

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

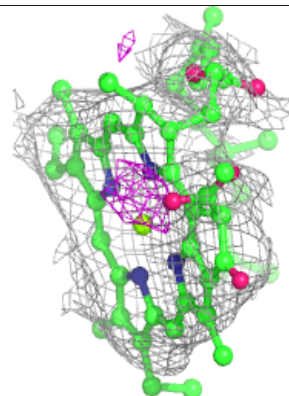
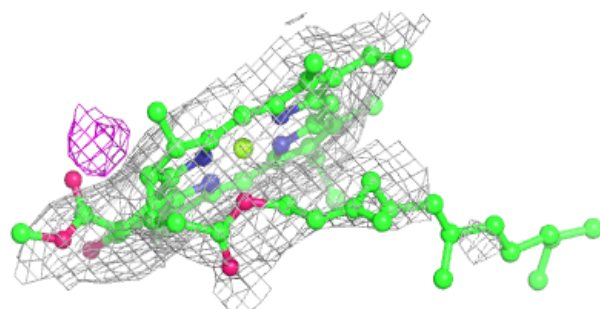
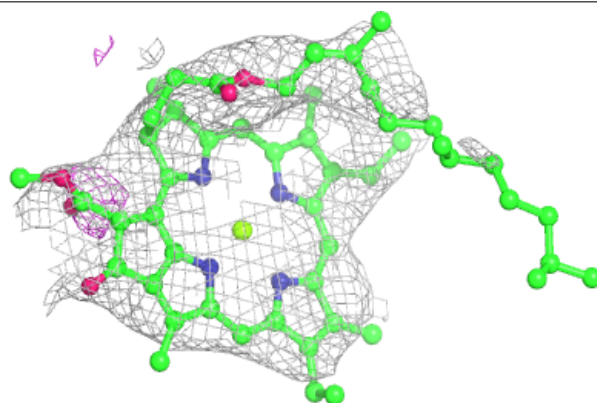


**Electron density around CLA B 825:**

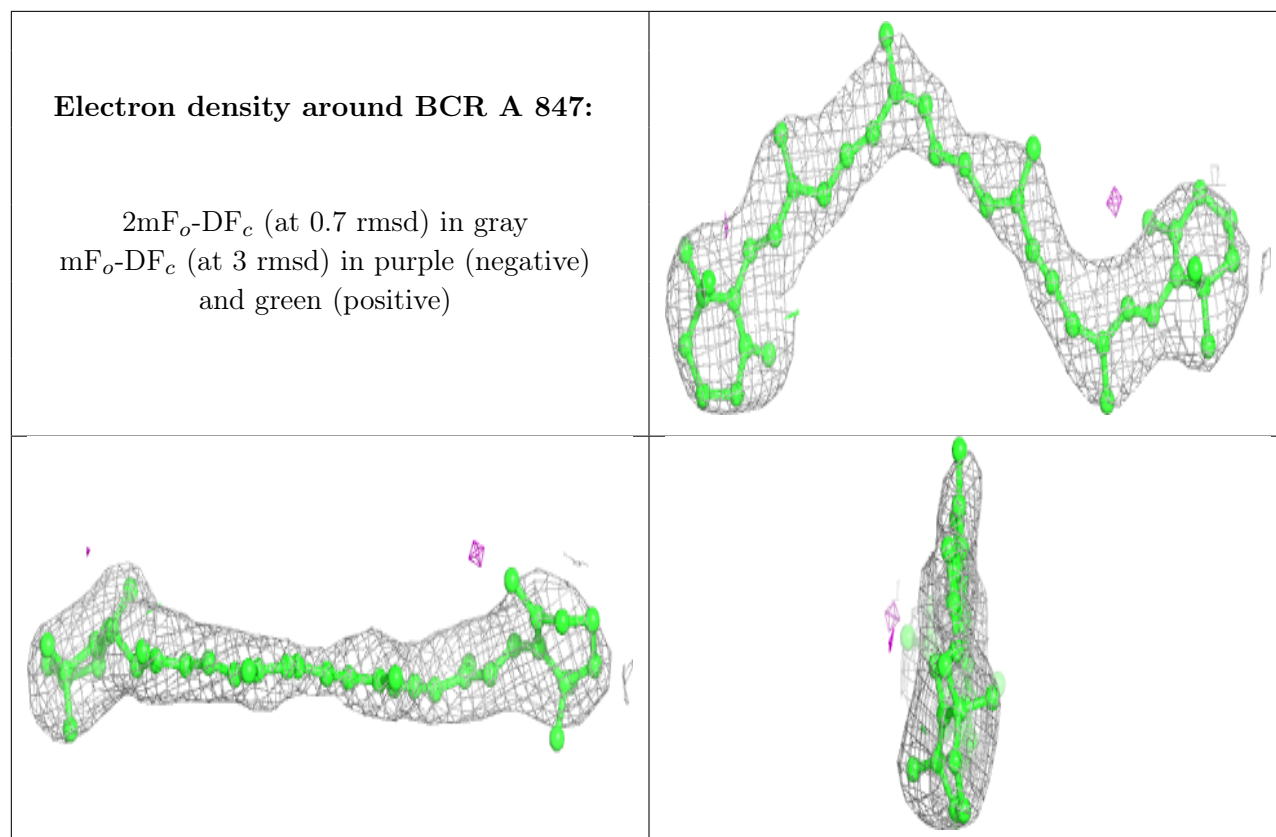
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA 2 306:**

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

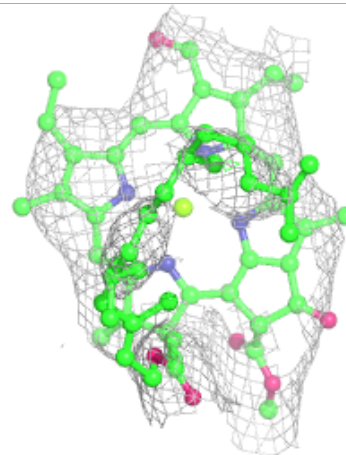
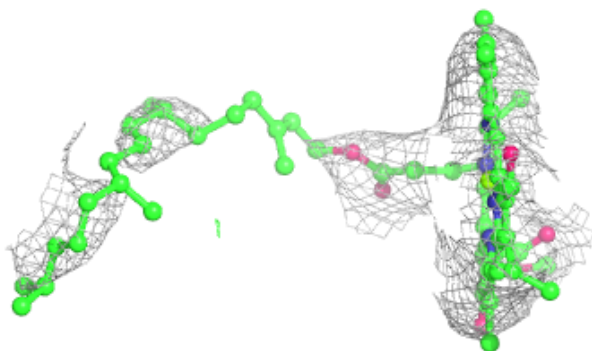
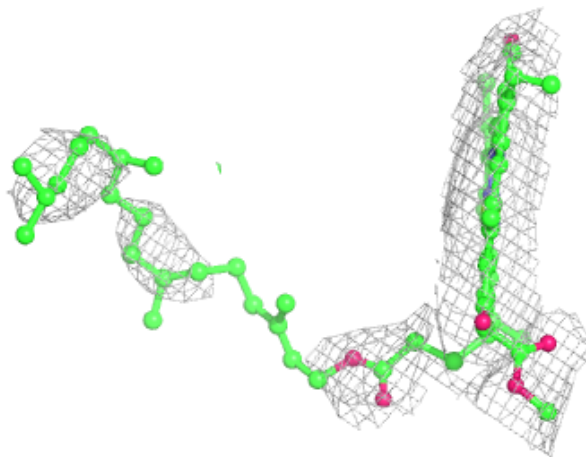






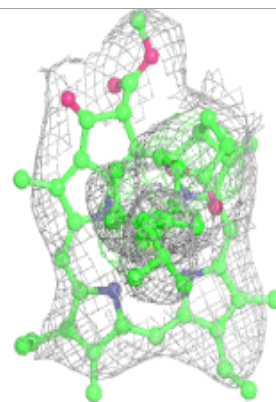
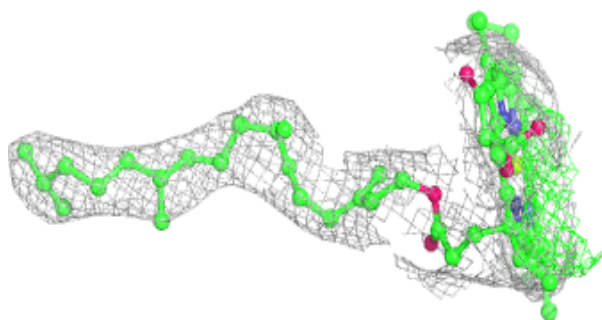
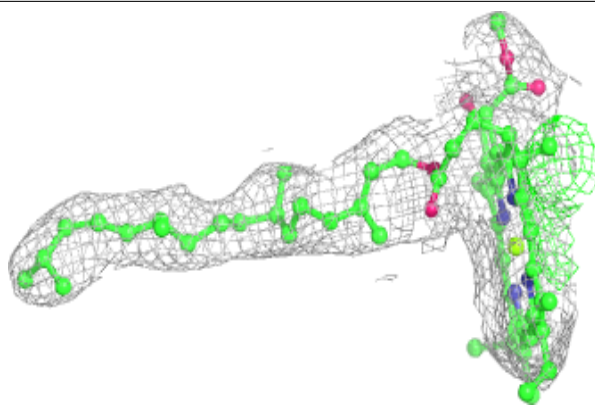
**Electron density around CHL 2 314:**

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

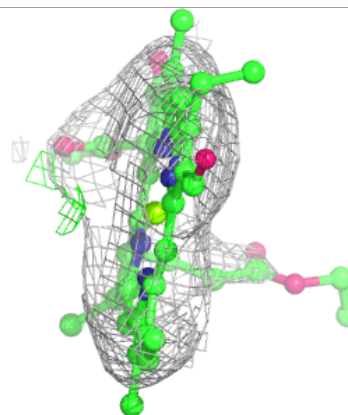
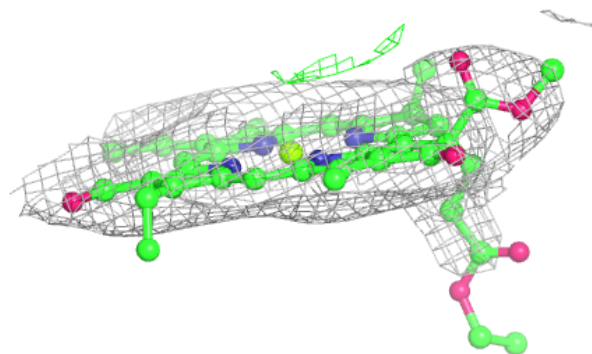
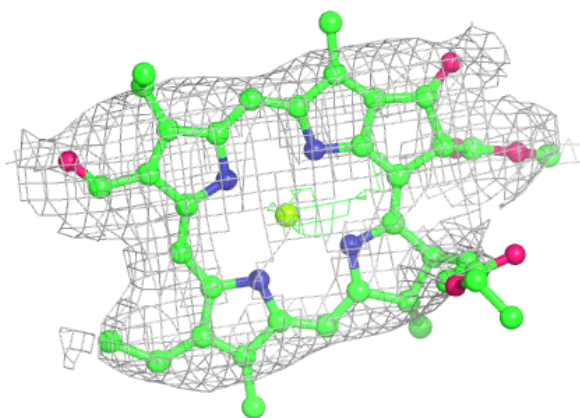


**Electron density around CLA A 826:**

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

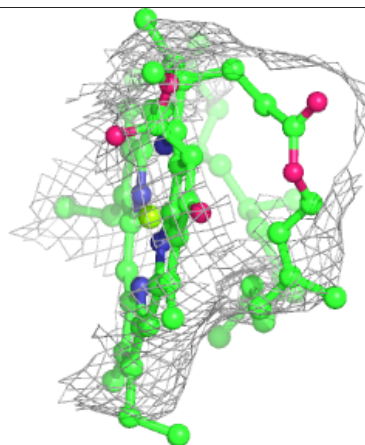
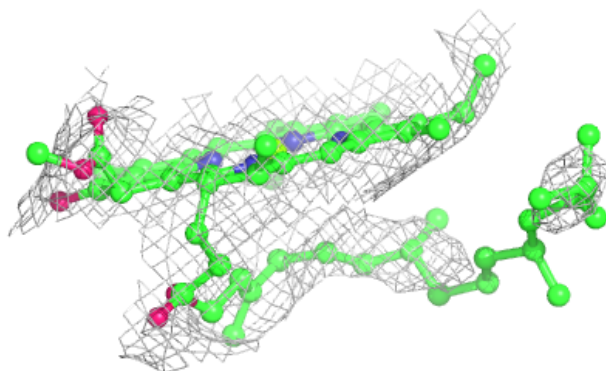
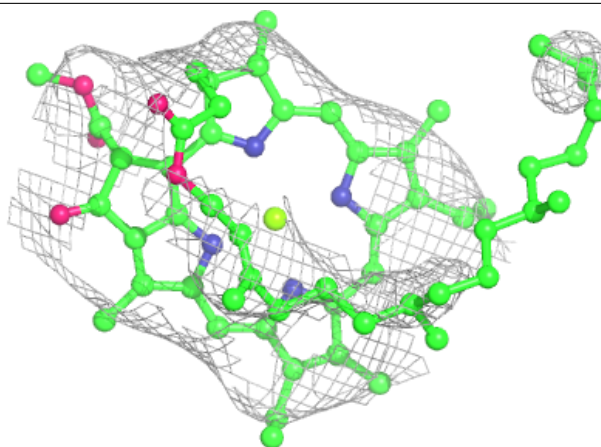
**Electron density around CHL 2 316:**

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

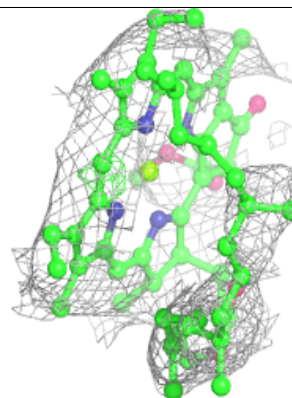
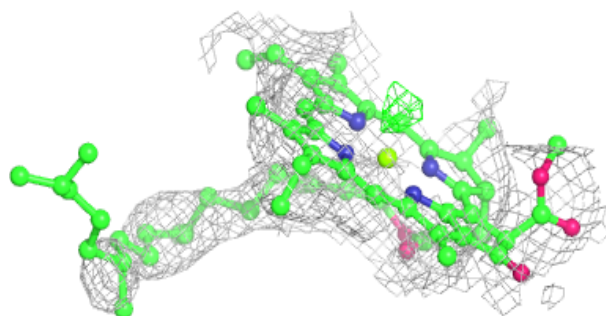
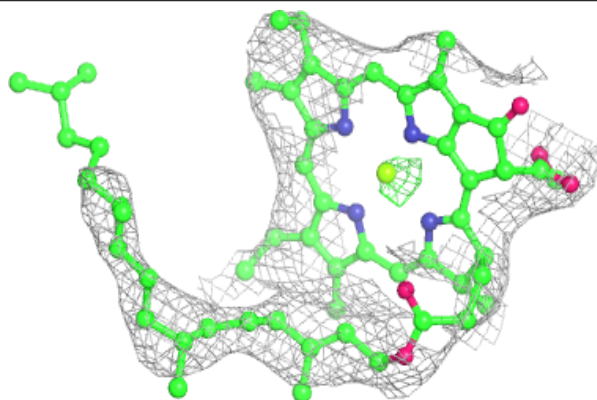


**Electron density around CLA 2 308:**

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

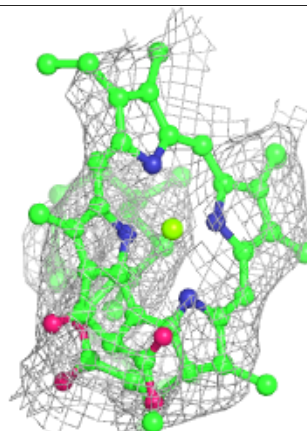
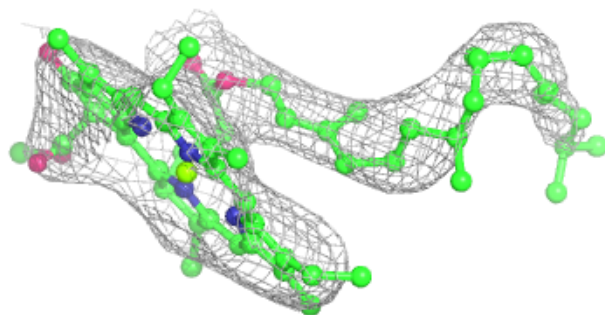
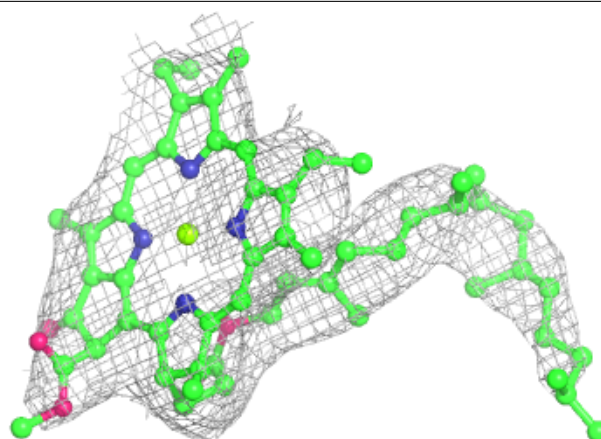
**Electron density around CLA 2 309:**

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



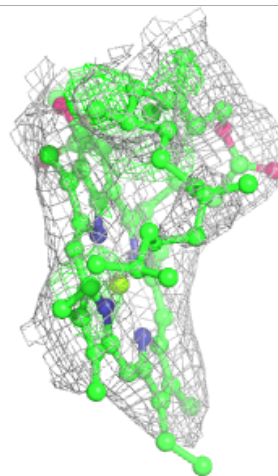
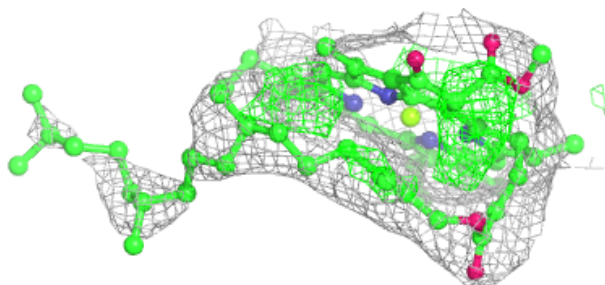
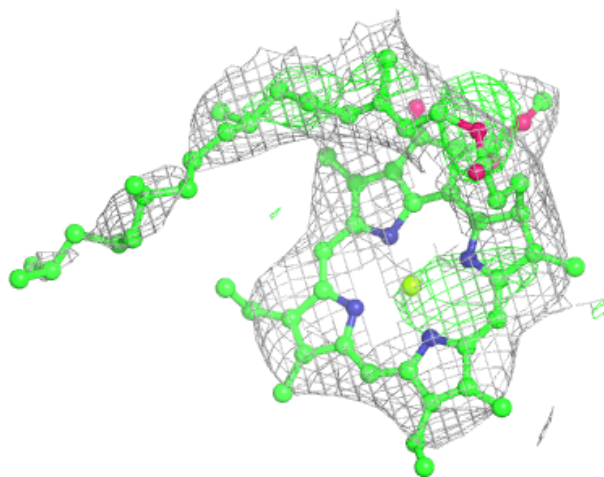
**Electron density around CLA A 853:**

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



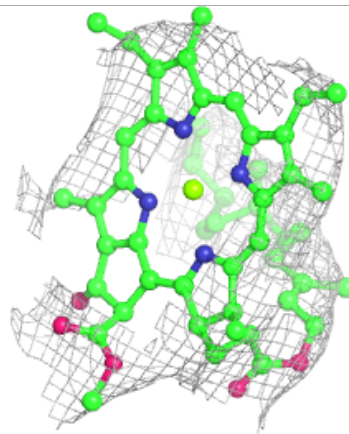
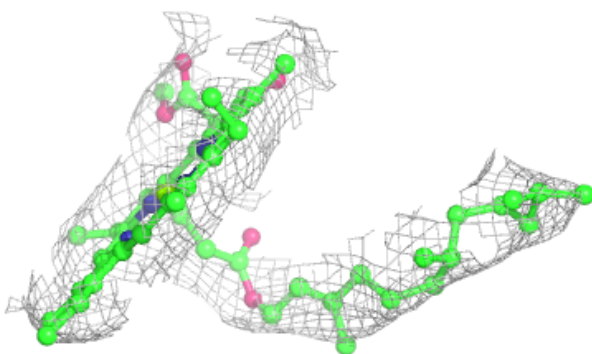
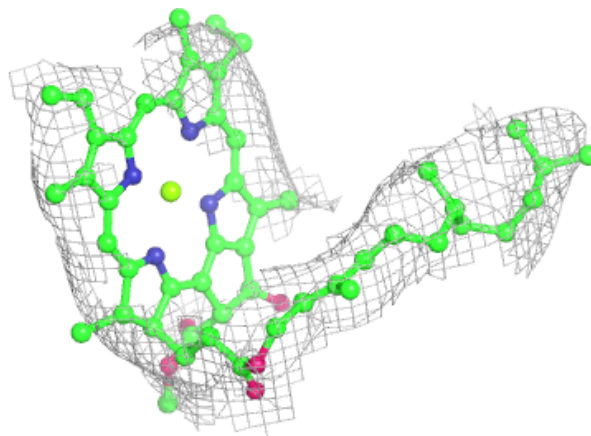
**Electron density around CLA A 827:**

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



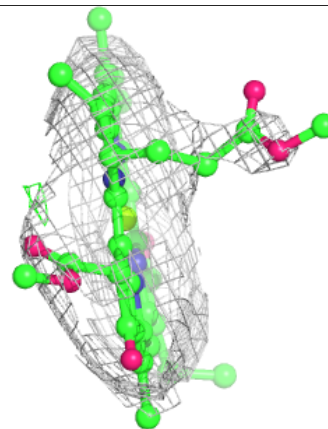
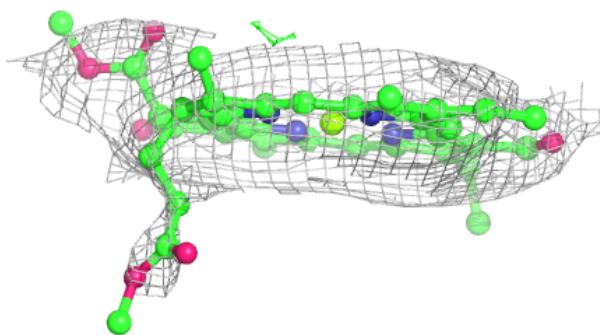
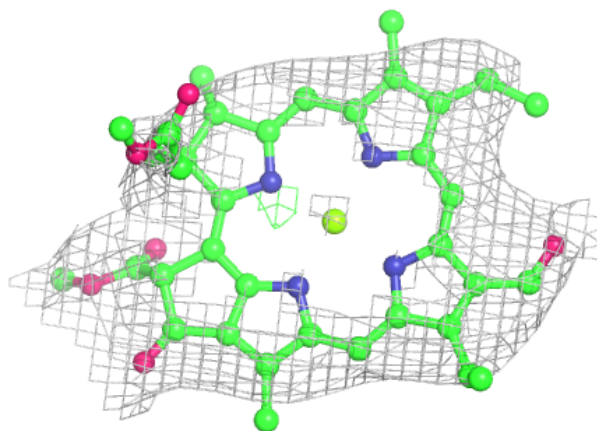
**Electron density around CLA 2 312:**

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



**Electron density around CHL 3 316:**

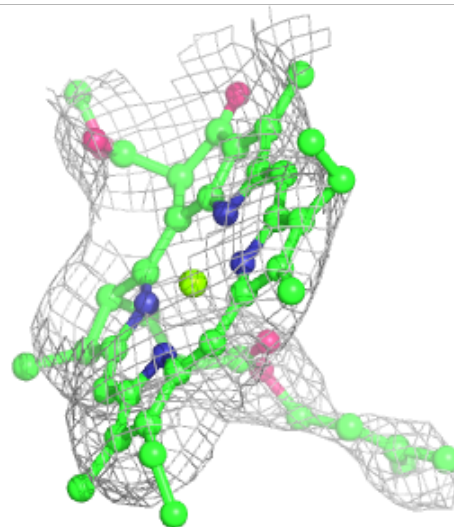
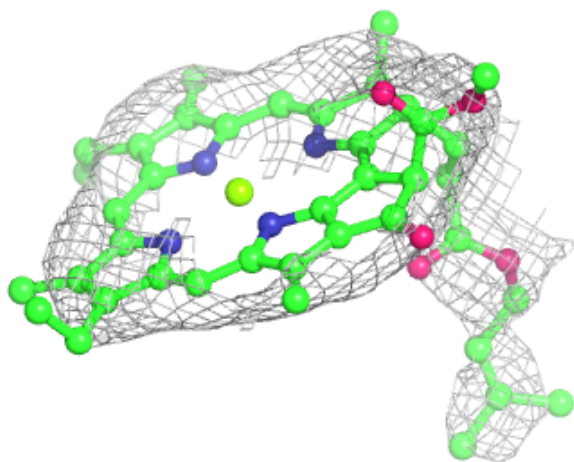
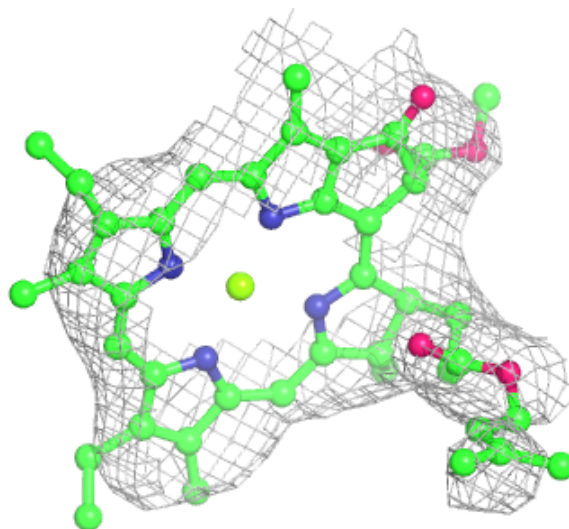
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





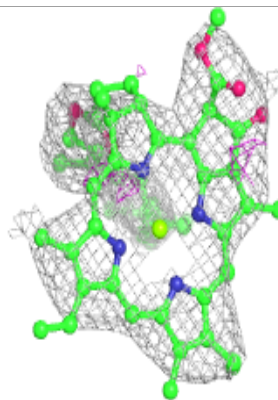
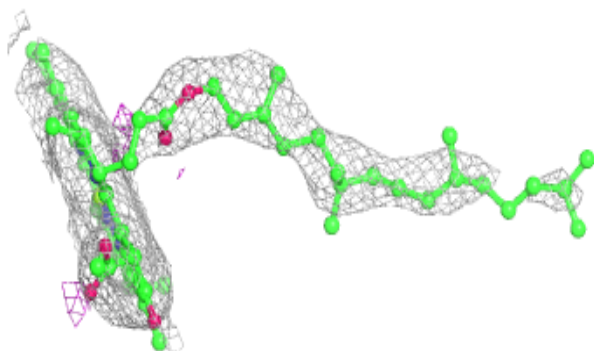
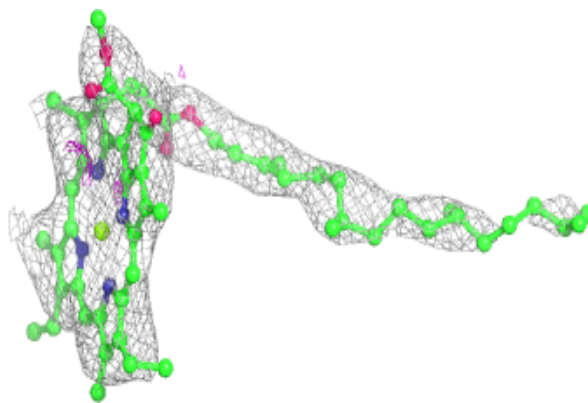
**Electron density around CLA 2 313:**

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

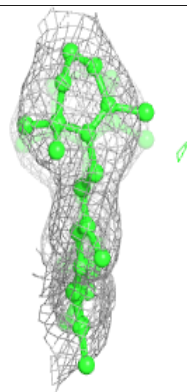
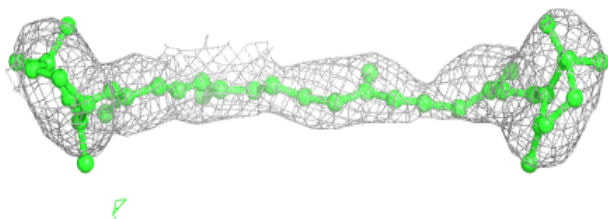
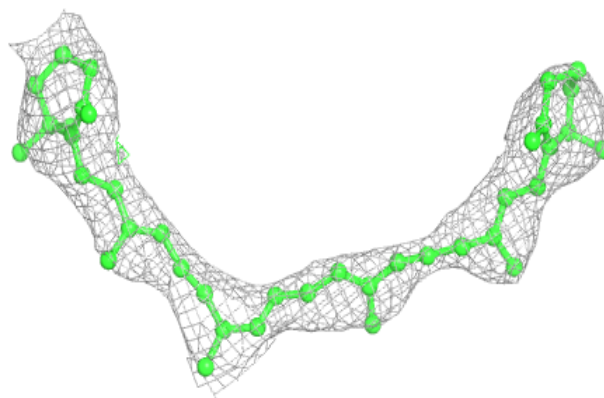


**Electron density around CLA B 829:**

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

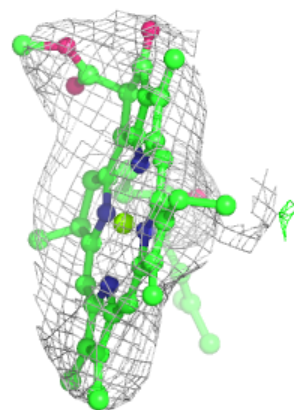
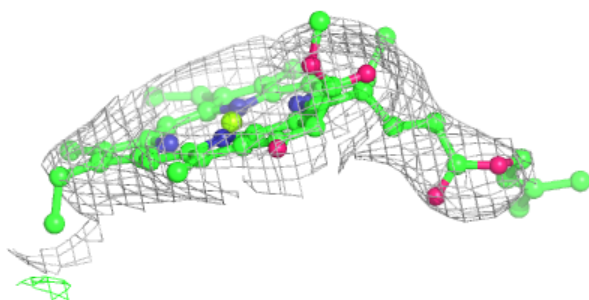
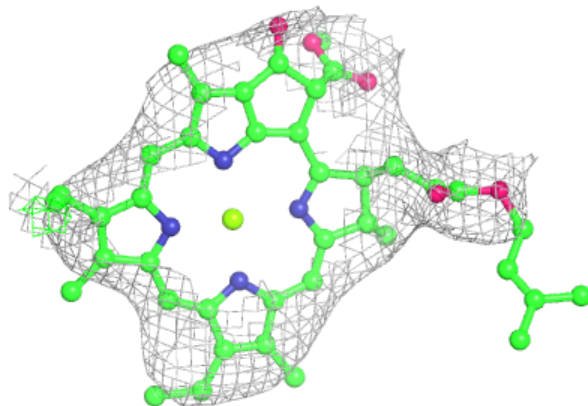
**Electron density around BCR F 305:**

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

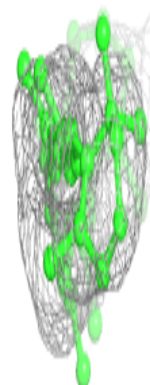
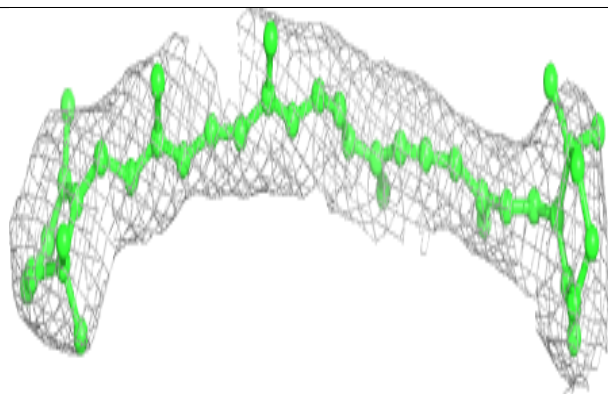
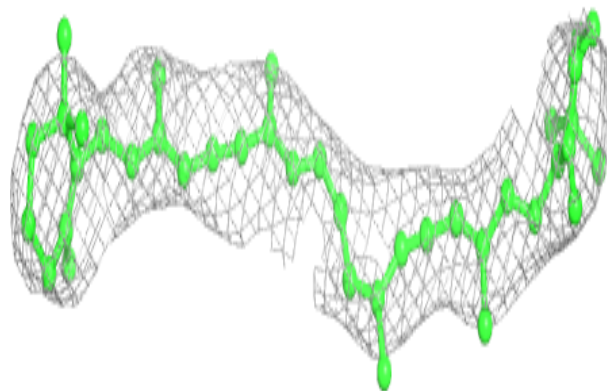


**Electron density around CLA 2 326:**

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

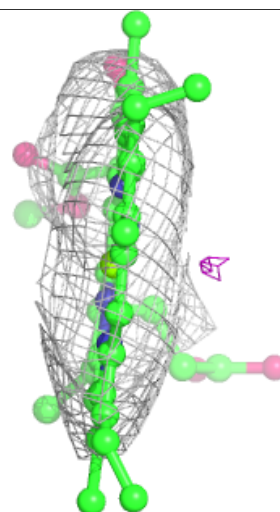
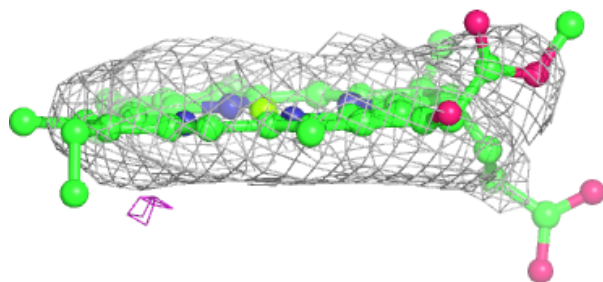
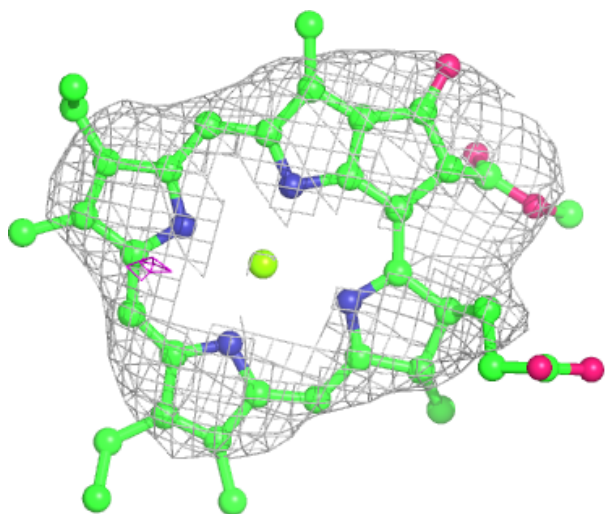
**Electron density around BCR I 101:**

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



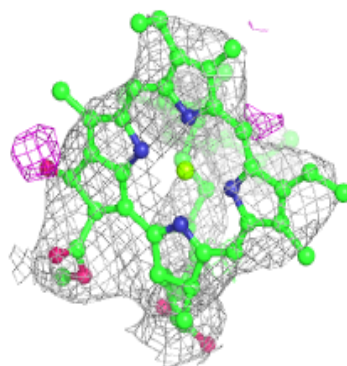
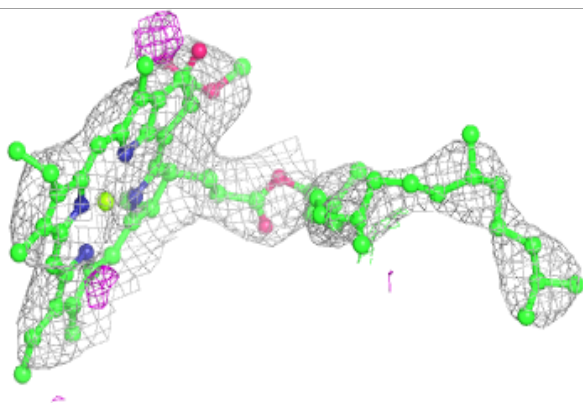
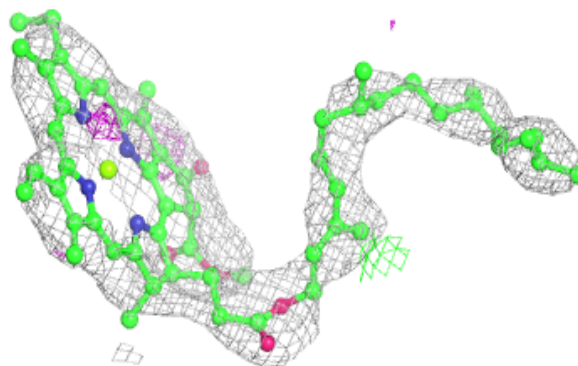
**Electron density around CLA 3 301:**

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



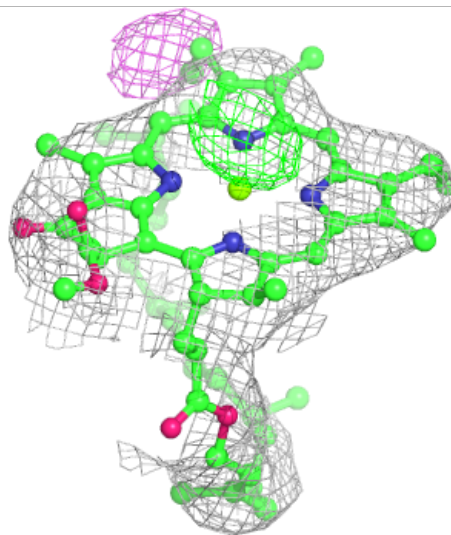
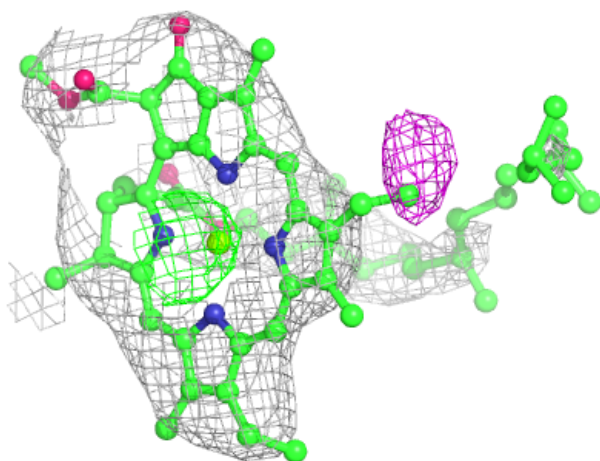
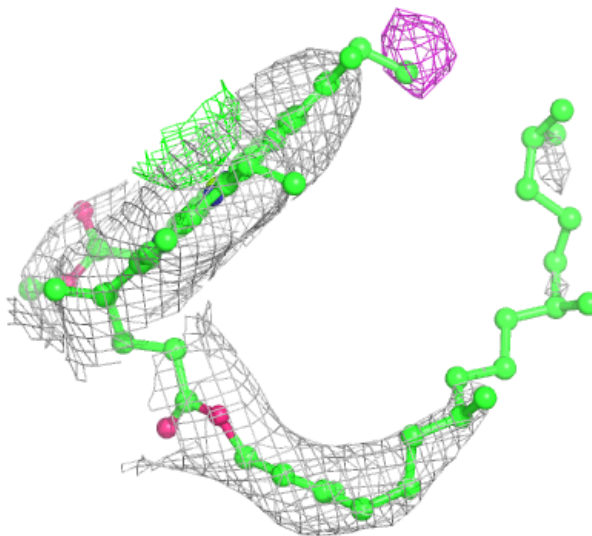
**Electron density around CLA B 803:**

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



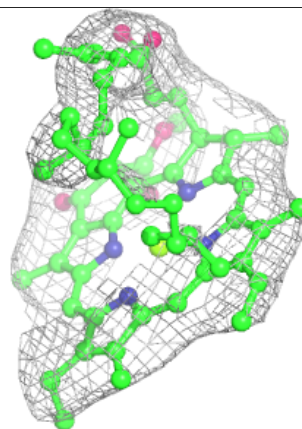
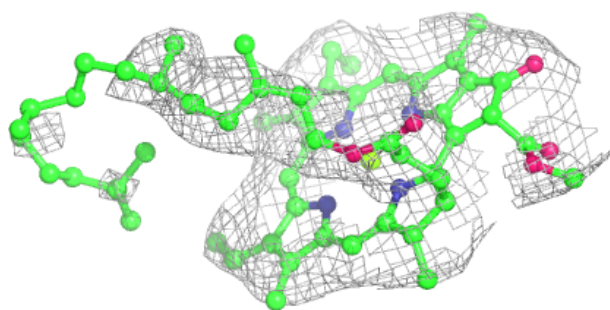
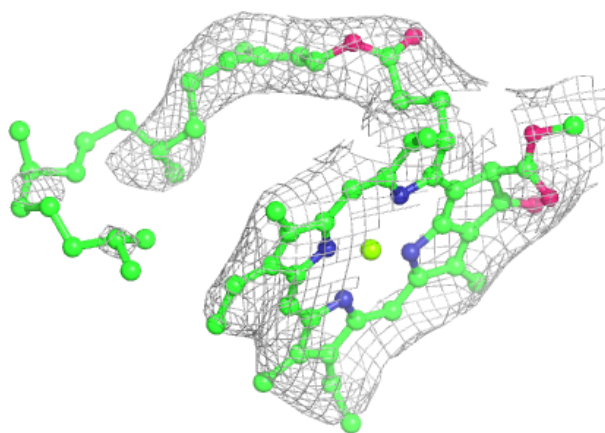
**Electron density around CLA B 820:**

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

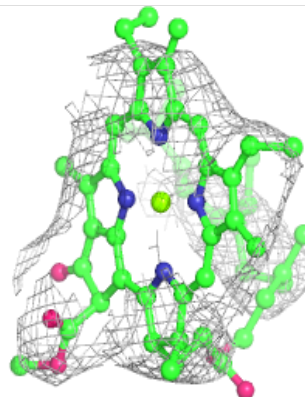
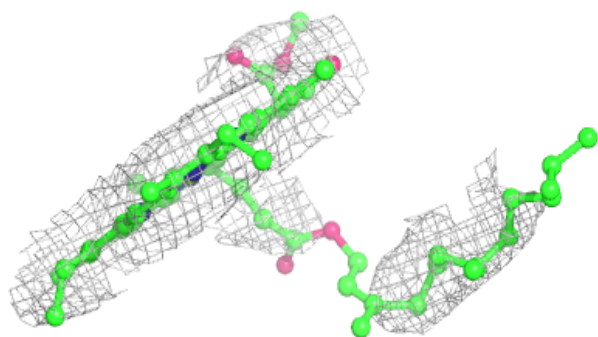
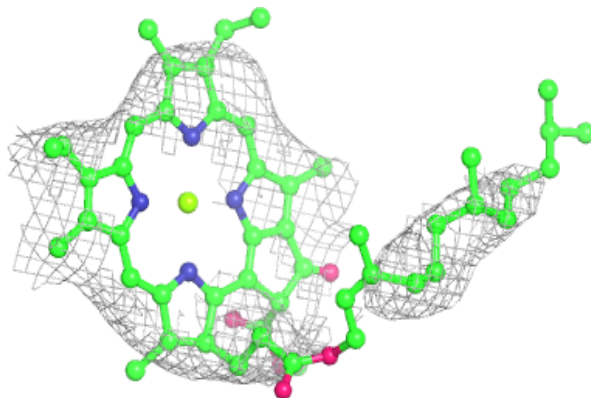


**Electron density around CLA A 822:**

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

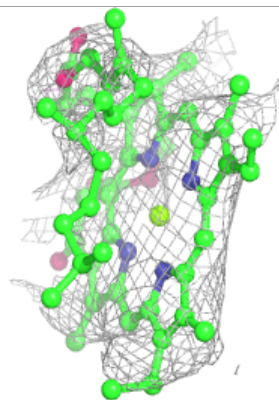
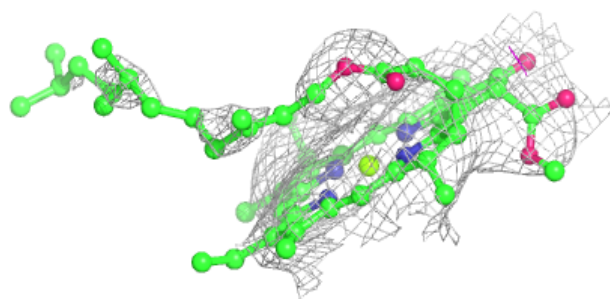
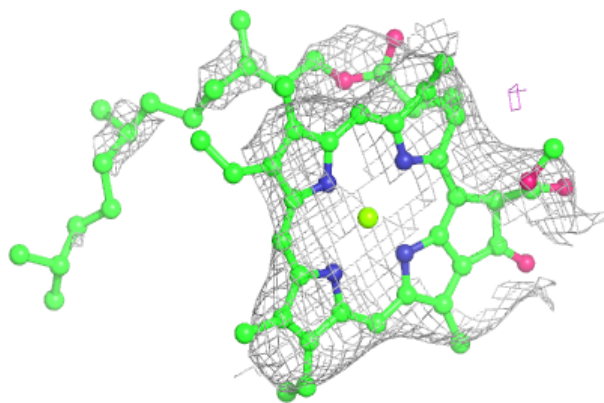
**Electron density around CLA A 820:**

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



**Electron density around CLA 4 308:**

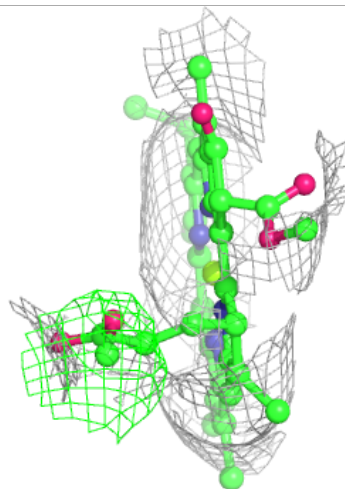
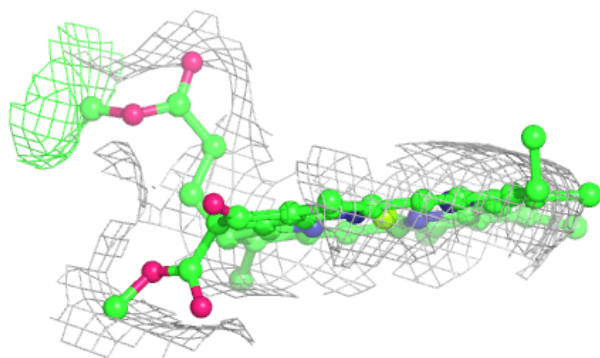
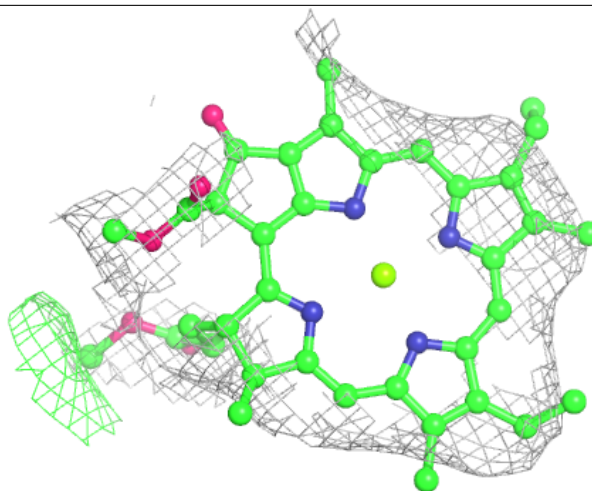
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





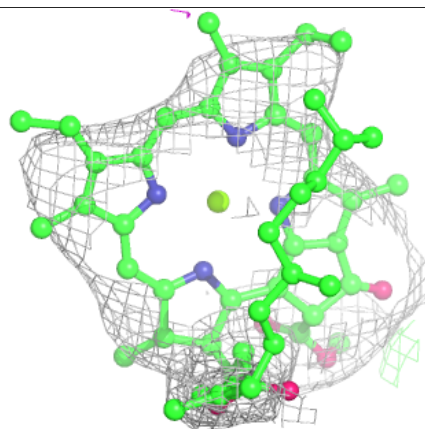
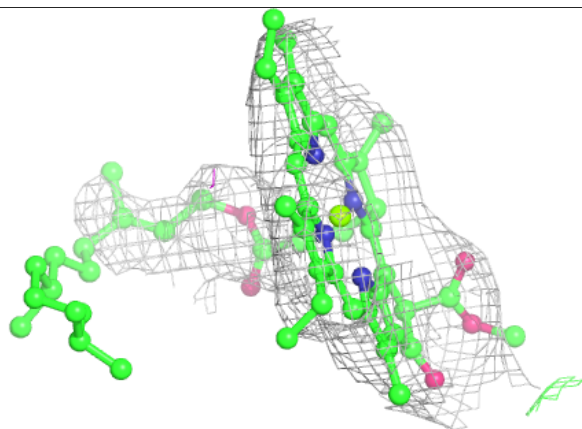
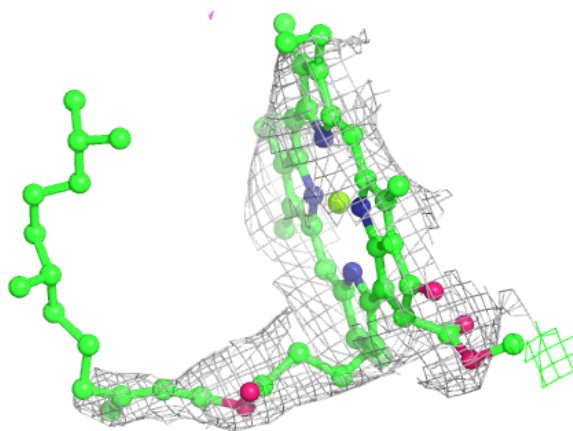
**Electron density around CLA 1 5012:**

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

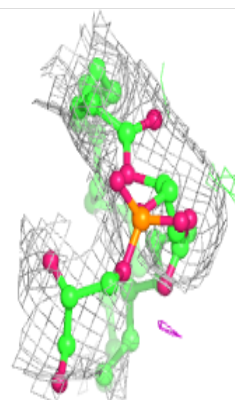
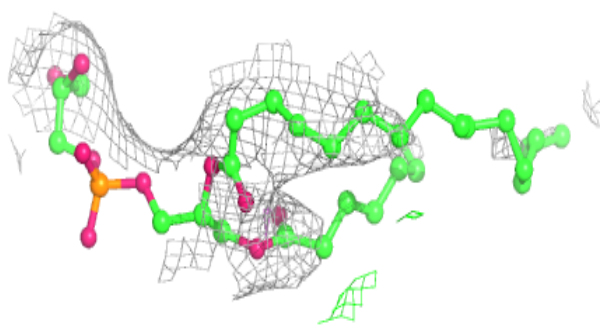
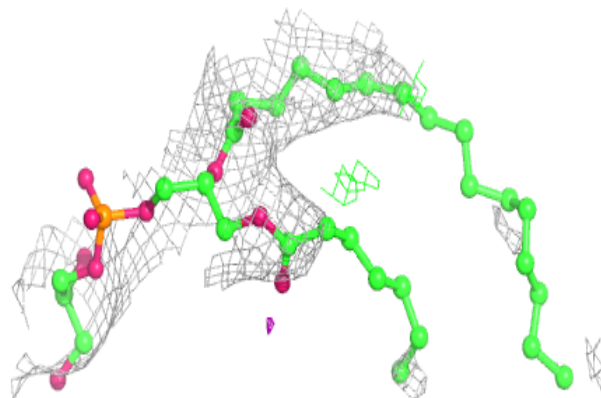


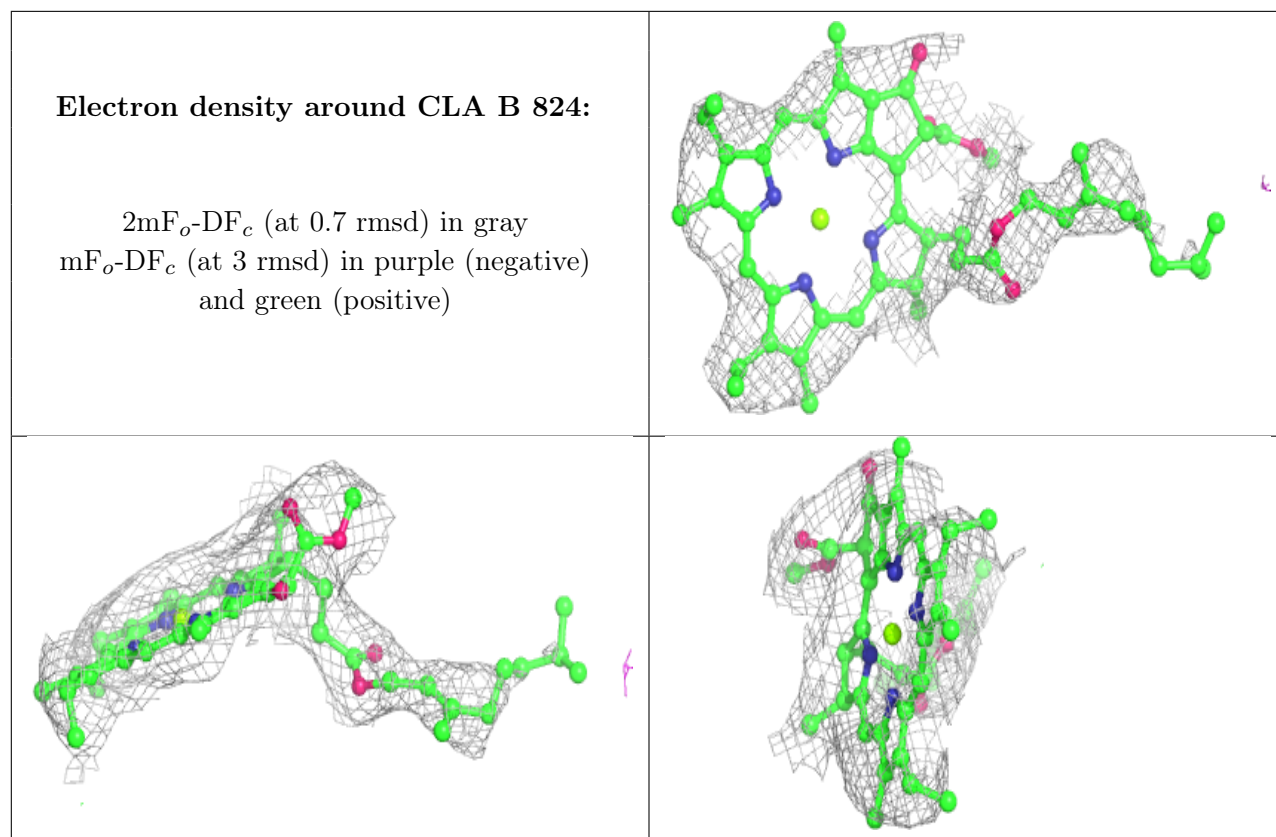
**Electron density around CLA A 821:**

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

**Electron density around LHG A 849:**

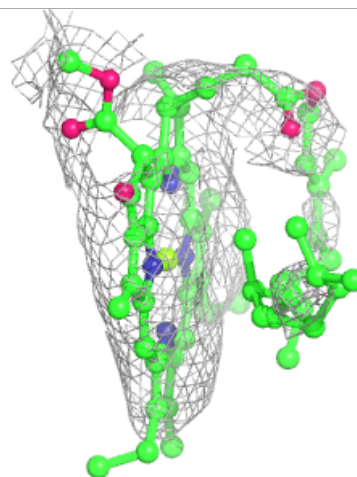
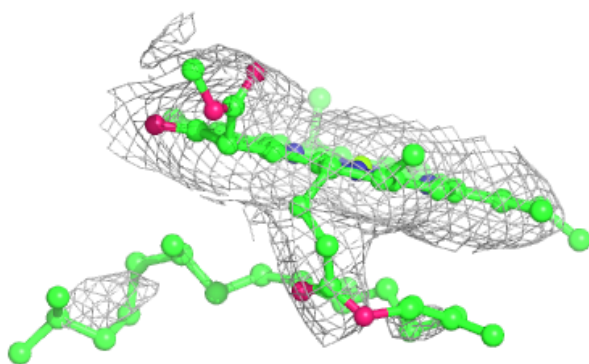
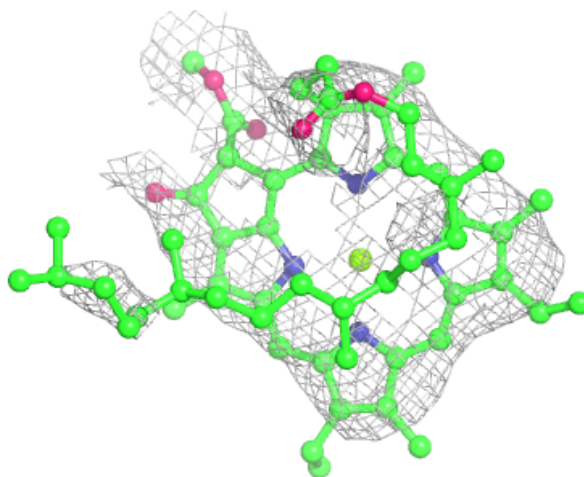
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





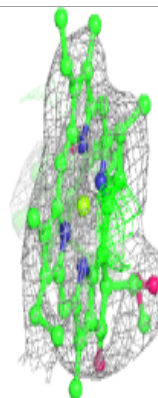
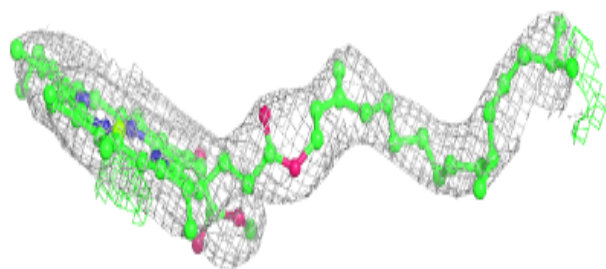
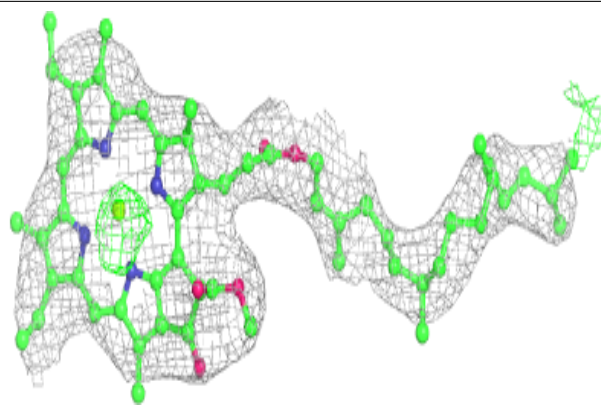
**Electron density around CLA 3 315:**

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

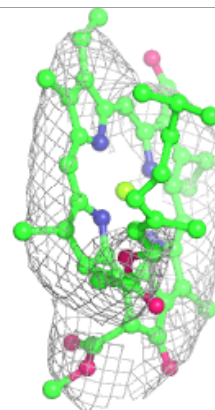
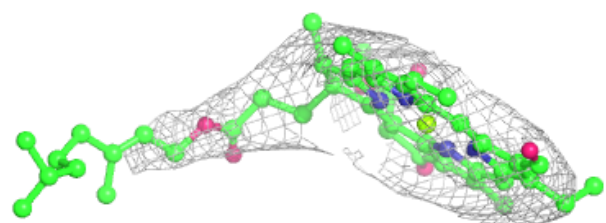
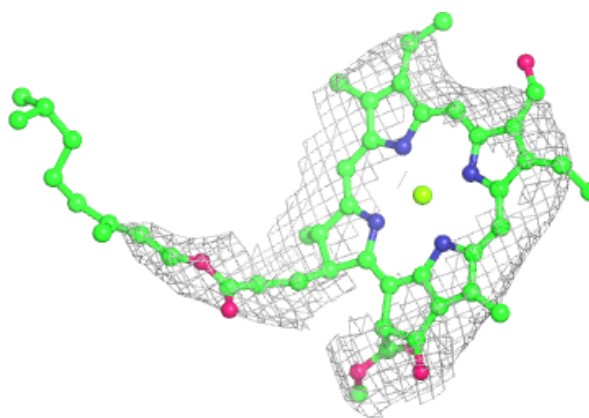


**Electron density around CLA A 838:**

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

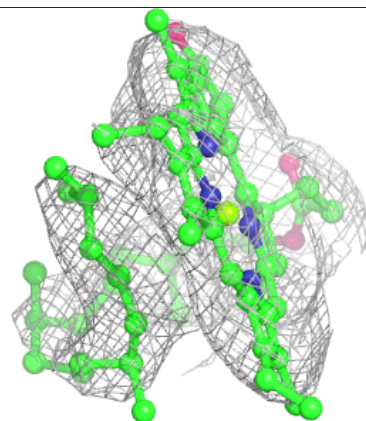
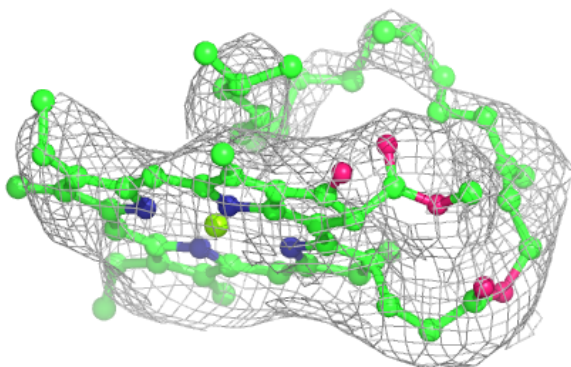
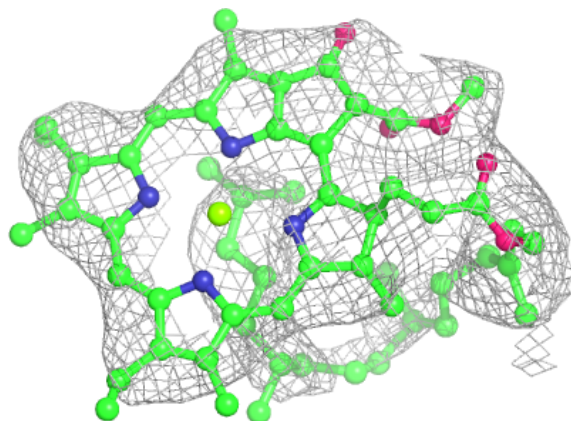
**Electron density around CHL 4 318:**

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



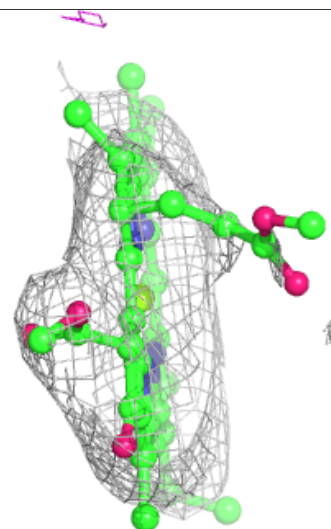
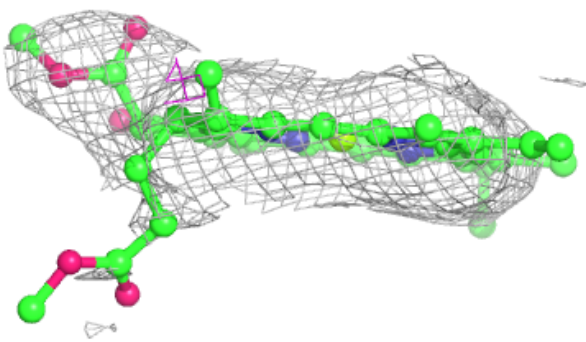
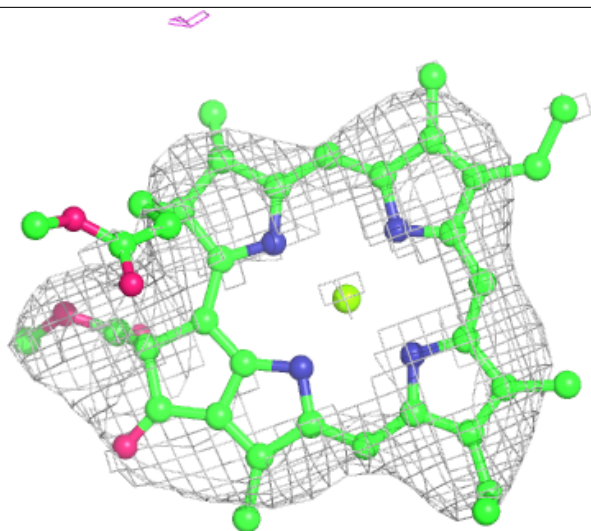
**Electron density around CLA B 807:**

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



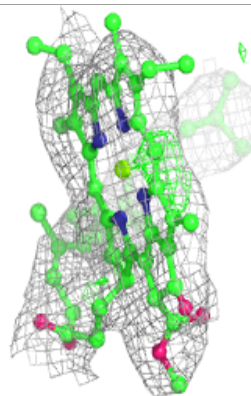
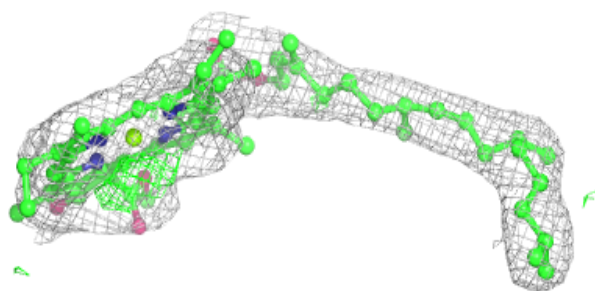
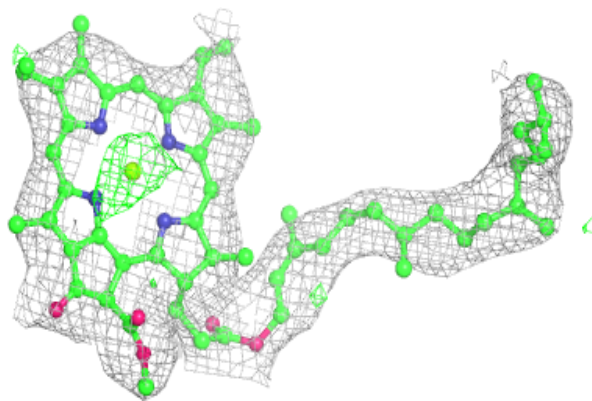
**Electron density around CLA B 813:**

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

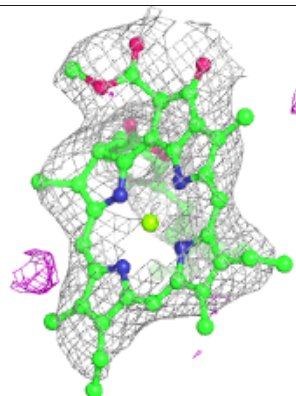
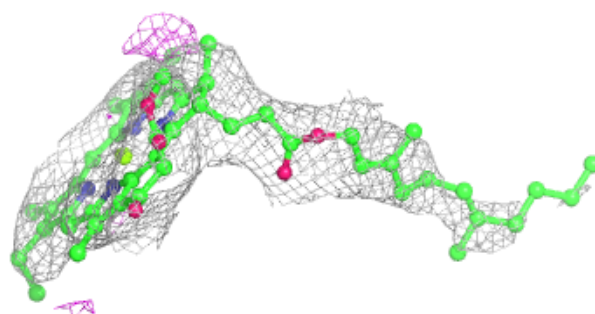
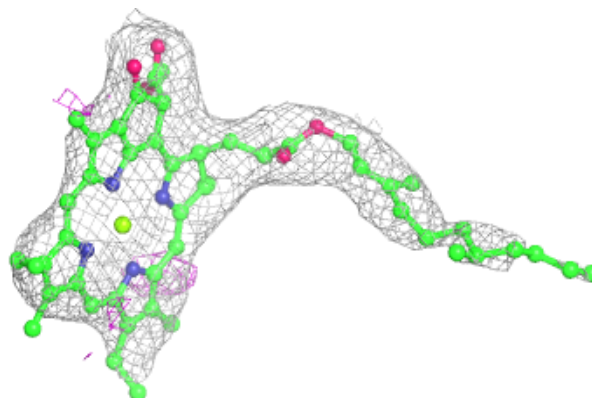


**Electron density around CLA A 802:**

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

**Electron density around CLA B 833:**

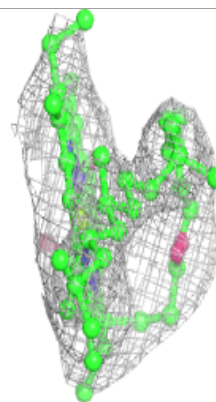
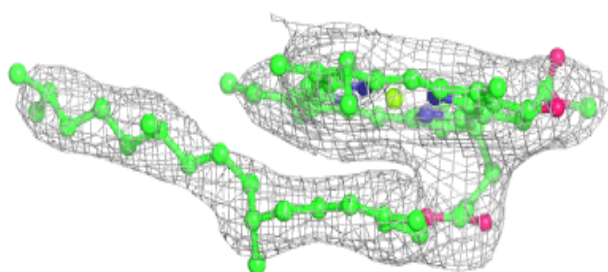
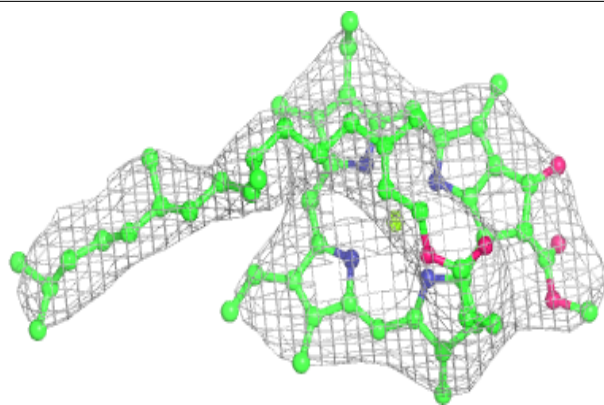
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



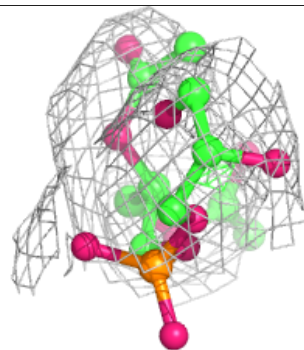
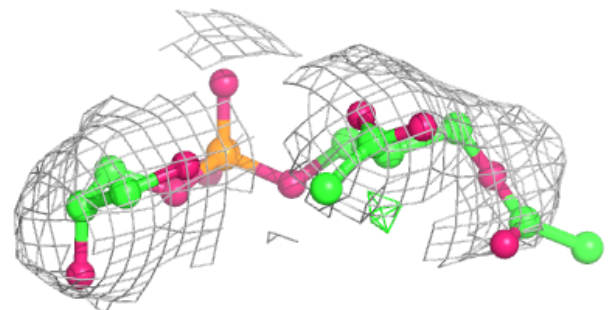
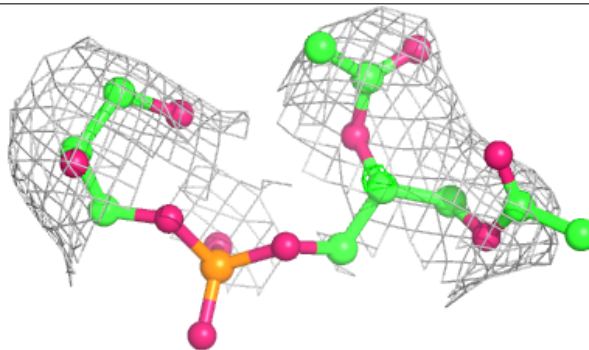


**Electron density around CLA A 837:**

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

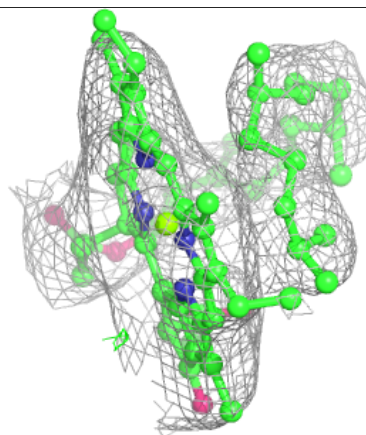
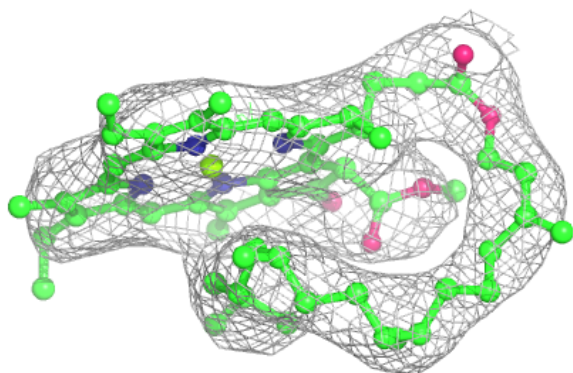
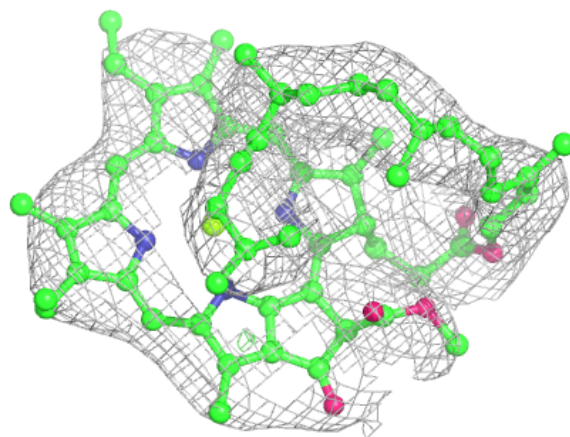
**Electron density around LHG B 848:**

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

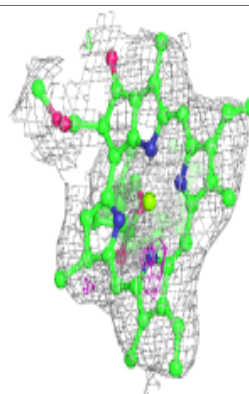
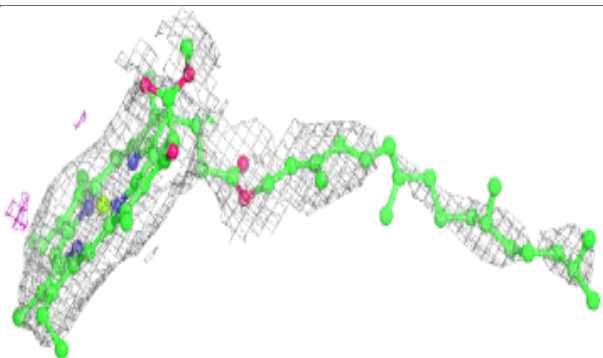
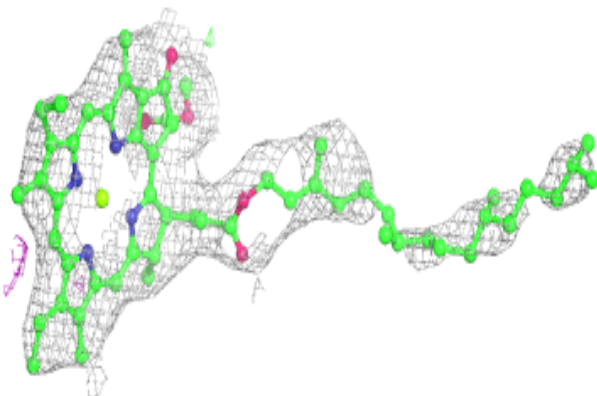


**Electron density around CLA A 805:**

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

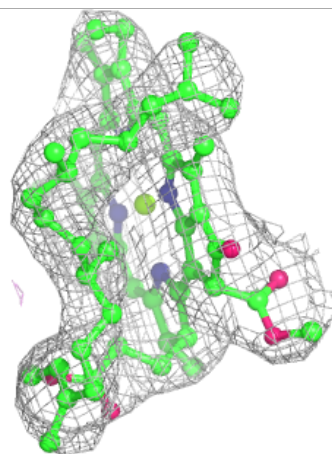
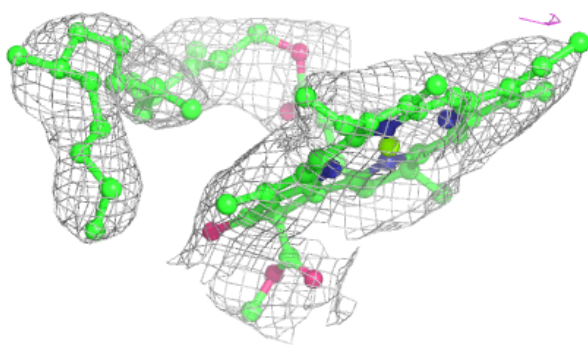
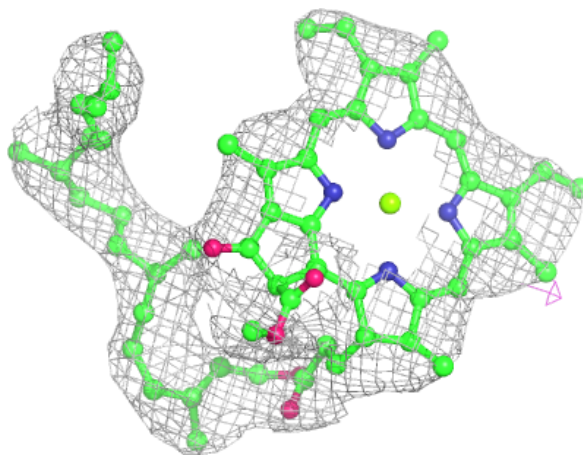
**Electron density around CLA A 808:**

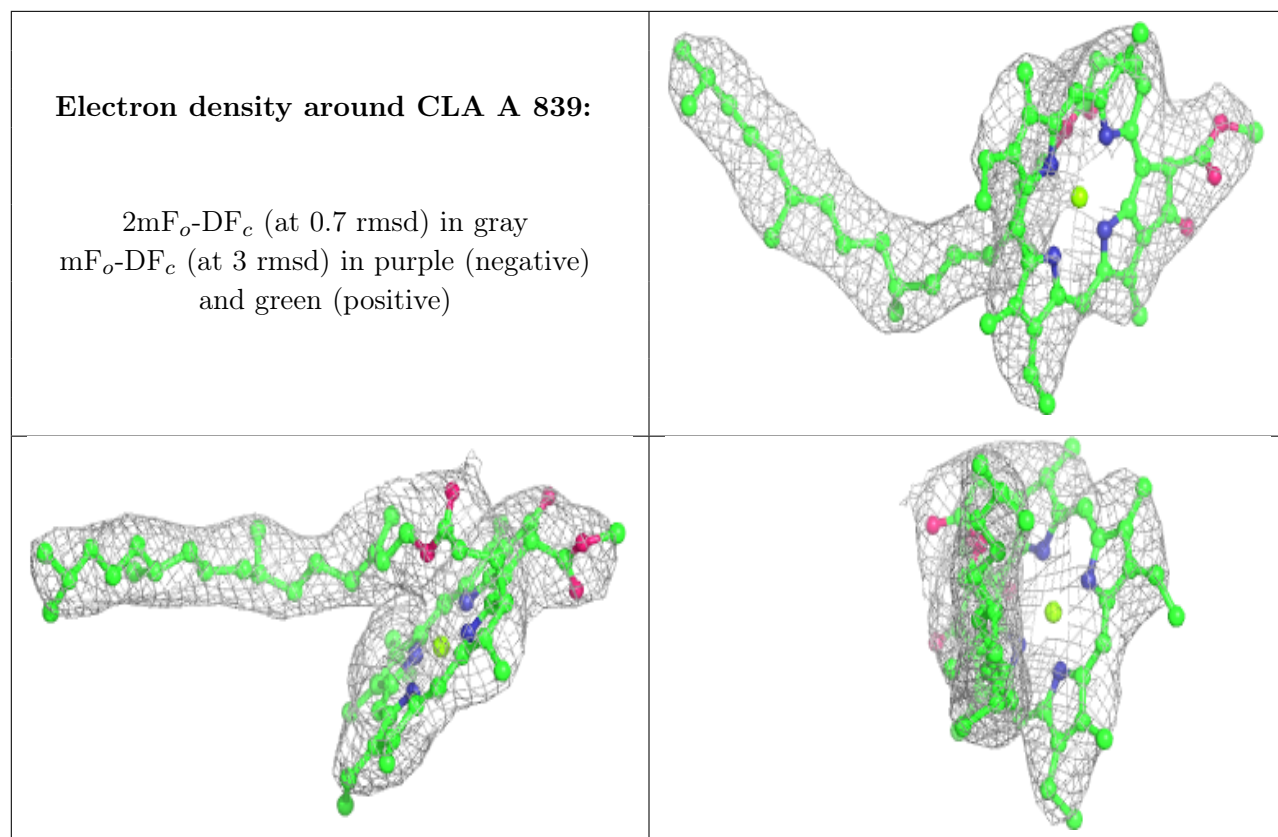
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.