



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2023 – 03:46 AM JST

PDB ID : 8GN0  
Title : Crystal structure of DCBQ-bound photosystem II complex  
Authors : Kamada, S.; Nakajima, Y.; Shen, J.-R.  
Deposited on : 2022-08-22  
Resolution : 2.15 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 : 1.8.5 (274361), 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

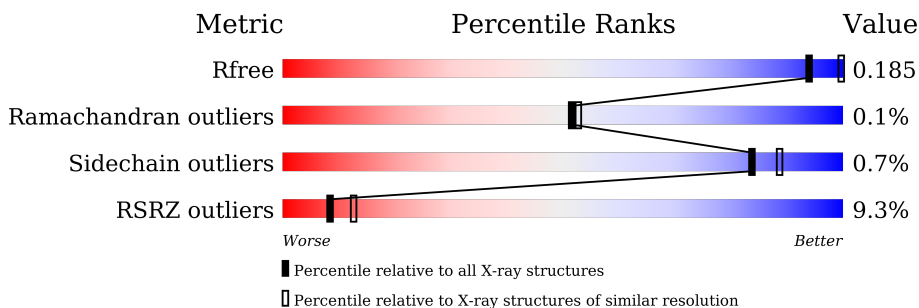
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	344	 3% 97%
1	a	344	 8% 96%
2	B	505	 10% 99%
2	b	505	 7% 95%
3	C	455	 6% 98%
3	c	455	 7% 99%
4	D	342	 2% 99%

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Mol	Chain	Length	Quality of chain
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	63	
7	h	63	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	
16	v	137	

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Mol	Chain	Length	Quality of chain
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	

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
23	CLA	A	405	X	-	-	-
23	CLA	A	410	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	B	617	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	513	X	-	-	-
23	CLA	D	2303	X	-	-	-
23	CLA	D	2304	X	-	-	-
23	CLA	a	2609	X	-	-	-
23	CLA	a	2613	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	-
23	CLA	b	620	X	-	-	-
23	CLA	b	621	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	c	514	X	-	-	-
23	CLA	c	515	X	-	-	-
23	CLA	c	516	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	408	X	-	-	-
23	CLA	d	409	X	-	-	-
28	LMT	f	101	-	-	-	X
29	GOL	v	204	-	-	-	X
30	UNL	B	629	-	-	-	X
30	UNL	T	101	-	-	-	X
30	UNL	a	2616	-	-	-	X
30	UNL	i	101	-	-	-	X
30	UNL	j	2702	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	JOX	a	2617	-	X	-	-
34	DMS	B	640	-	-	-	X
34	DMS	O	311	-	-	-	X
34	DMS	a	2620	-	-	-	X
34	DMS	c	541	-	-	-	X
34	DMS	c	547	-	-	-	X
34	DMS	o	309	-	-	-	X
36	HTG	B	625	-	-	-	X
36	HTG	C	522	-	-	-	X
36	HTG	c	524	-	-	-	X
36	HTG	d	407	-	-	-	X

## 2 Entry composition [i](#)

There are 43 unique types of molecules in this entry. The entry contains 53814 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 II protein D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	2614	1715	428	456	15	0	3	0
1	a	334	2629	1722	432	460	15	0	4	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	conflict	UNP P51765
a	279	PRO	ARG	conflict	UNP P51765

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	505	4005	2628	667	697	13	0	7	0
2	b	483	3833	2520	637	663	13	0	9	0

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	451	3494	2286	585	610	13	0	2	0
3	c	455	3518	2303	589	613	13	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	expression tag	UNP D0VWR7
C	20	SER	-	expression tag	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	expression tag	UNP D0VWR7
C	22	PHE	-	expression tag	UNP D0VWR7
c	19	ASN	-	expression tag	UNP D0VWR7
c	20	SER	-	expression tag	UNP D0VWR7
c	21	ILE	-	expression tag	UNP D0VWR7
c	22	PHE	-	expression tag	UNP D0VWR7

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	2	0
			2726	1809	443	462	12			
4	d	342	Total	C	N	O	S	0	3	0
			2738	1815	447	464	12			

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	80	Total	C	N	O	0	1	0
			643	422	101	120			
5	e	79	Total	C	N	O	0	1	0
			630	417	99	114			

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			271	184	45	41	1			
6	f	32	Total	C	N	O	S	0	0	0
			255	173	43	38	1			

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			
7	h	63	Total	C	N	O	S	0	1	0
			506	338	83	83	2			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	32	Total	C	N	O	S	0	0	0
			256	177	37	41	1			
8	i	32	Total	C	N	O	S	0	0	0
			259	178	37	43	1			

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	39	Total	C	N	O	S	0	0	0
			274	184	40	48	2			

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	1	0
			297	208	43	46			
10	k	37	Total	C	N	O	0	0	0
			289	201	42	46			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	conflict	UNP P19054
K	39	TRP	VAL	conflict	UNP P19054
k	33	LEU	PHE	conflict	UNP P19054
k	39	TRP	VAL	conflict	UNP P19054

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	1	0
			303	204	45	53	1			
11	l	36	Total	C	N	O		0	2	0
			305	206	47	52				

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	2	0
			267	180	38	48	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	1	0
			270	182	39	48	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	conflict	UNP P12312
m	8	LEU	PHE	conflict	UNP P12312

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	3	0
			1870	1171	314	380	5			
13	o	243	Total	C	N	O	S	0	4	0
			1874	1174	312	382	6			

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	1	0
			776	493	130	153			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	1	0
			1063	677	177	205	4			
16	v	137	Total	C	N	O	S	0	1	0
			1058	671	175	208	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	30	Total	C	N	O	S	0	0	0
			218	144	35	36	3			
17	y	30	Total	C	N	O	S	0	0	0
			216	139	38	36	3			

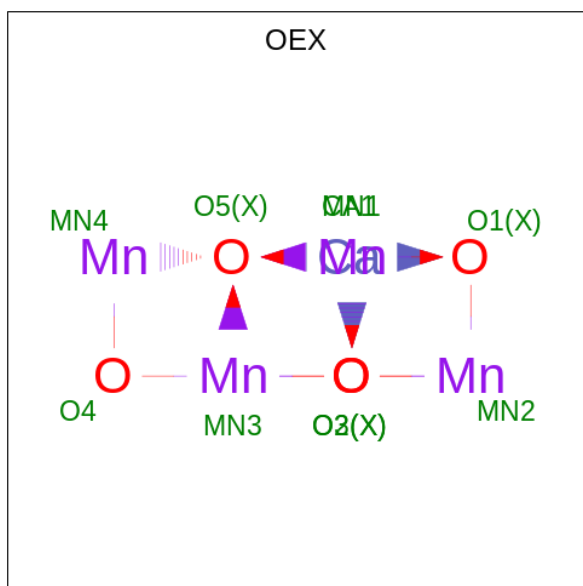
- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	S	0	0	0
			275	185	44	46				
18	x	35	Total	C	N	O	S	0	1	0
			257	176	38	43				

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			471	323	71	75	2			
19	z	61	Total	C	N	O	S	0	0	0
			456	312	70	72	2			

- Molecule 20 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
20	a	1	10	1	4	5	0	0

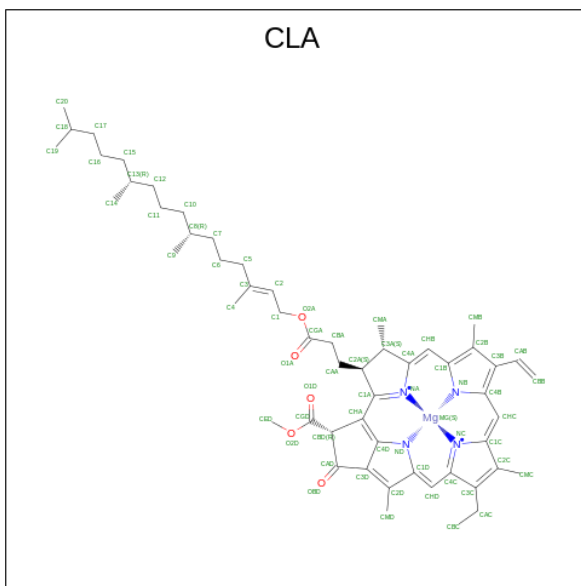
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
21	A	1	1	1	0	0
21	a	1	1	1	0	0

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
22	A	2	2	2	0	0
22	a	2	2	2	0	0

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (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
23	A	1	65	55	1	4	5	0	0
23	A	1	65	55	1	4	5	0	0

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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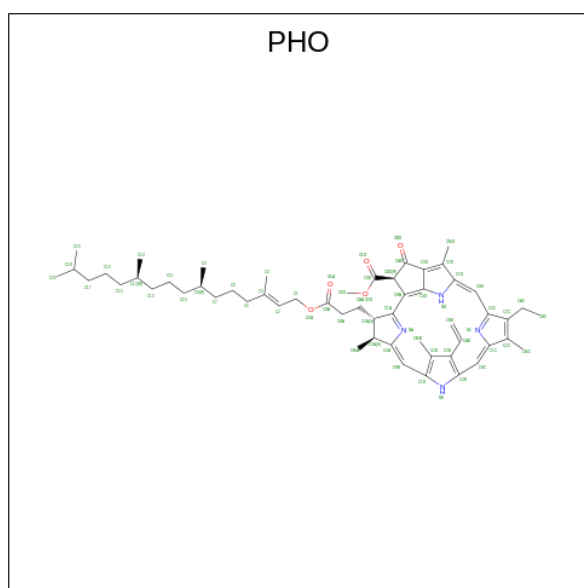
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

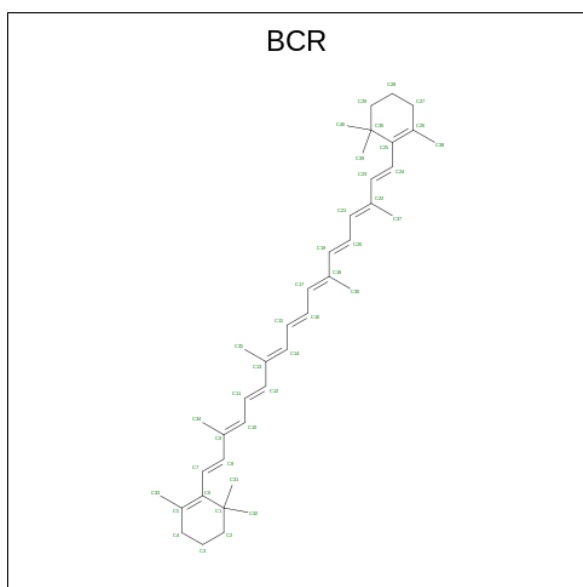
- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).





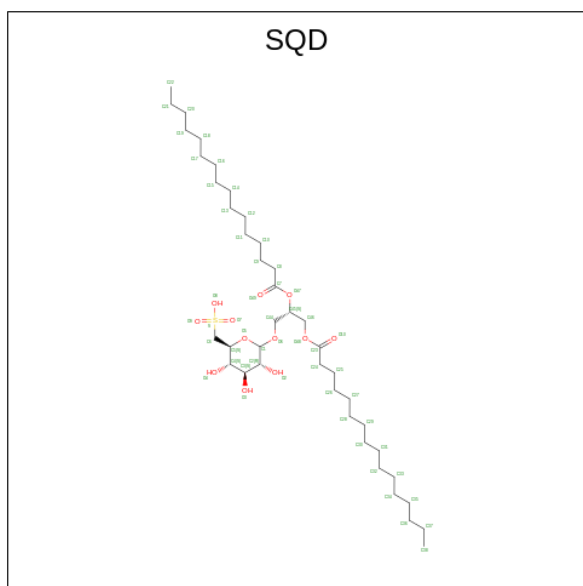
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total C 40 40	0	0
25	a	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	b	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	d	1	Total C 40 40	0	0
25	k	1	Total C 40 40	0	0
25	y	1	Total C 40 40	0	0
25	z	1	Total C 40 40	0	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



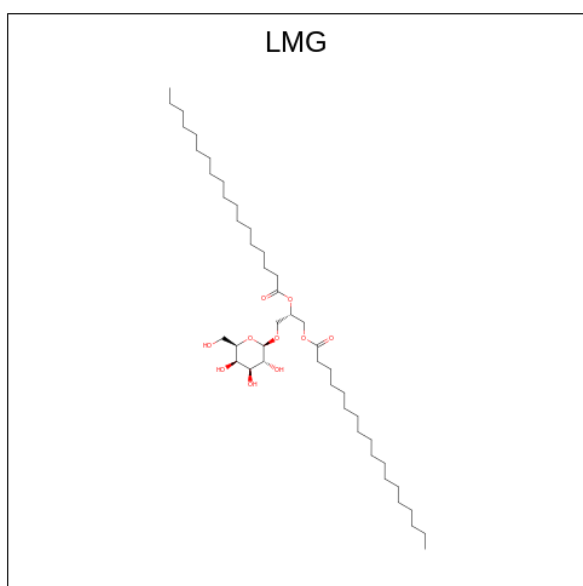
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 46 33 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0
26	D	1	Total C O S 54 41 12 1	0	0
26	D	1	Total C O S 45 32 12 1	0	0
26	a	1	Total C O S 54 41 12 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
26	a	1	48	35	12	1	0	0
26	b	1	48	35	12	1	0	0
26	d	1	33	23	9	1	0	0
26	l	1	54	41	12	1	0	0

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



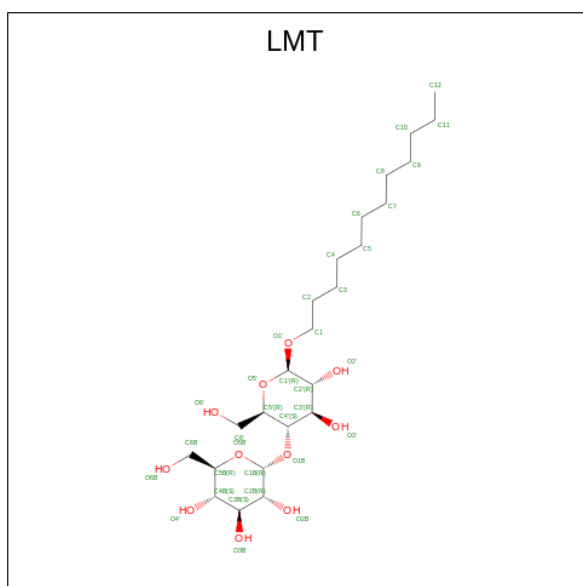
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
27	A	1	51	41	10	0	0
27	B	1	51	41	10	0	0
27	C	1	51	41	10	0	0
27	C	1	51	41	10	0	0
27	D	1	47	37	10	0	0
27	c	1	51	41	10	0	0
27	c	1	49	39	10	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	c	1	Total	C	O	0	0
			51	41	10		
27	d	1	Total	C	O	0	0
			51	41	10		
27	m	1	Total	C	O	0	0
			51	41	10		

- Molecule 28 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



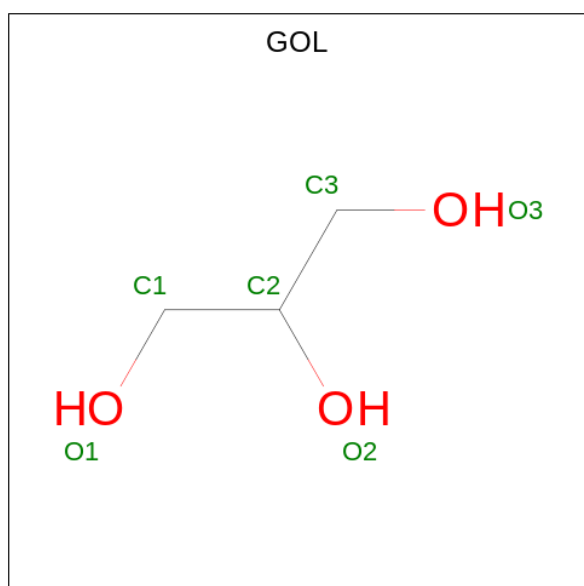
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			33	22	11		
28	A	1	Total	C	O	0	0
			24	18	6		
28	B	1	Total	C	O	0	0
			35	24	11		
28	B	1	Total	C	O	0	0
			35	24	11		
28	F	1	Total	C	O	0	0
			24	18	6		
28	J	1	Total	C	O	0	0
			24	18	6		
28	M	1	Total	C	O	0	0
			35	24	11		
28	M	1	Total	C	O	0	0
			35	24	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	T	1	Total	C	O	0	0
			24	18	6		
28	Z	1	Total	C	O	0	0
			35	24	11		
28	d	1	Total	C	O	0	0
			35	24	11		
28	d	1	Total	C	O	0	0
			25	19	6		
28	f	1	Total	C	O	0	0
			24	18	6		
28	i	1	Total	C	O	0	0
			24	18	6		
28	j	1	Total	C	O	0	0
			34	23	11		
28	m	1	Total	C	O	0	0
			35	24	11		
28	m	1	Total	C	O	0	0
			35	24	11		
28	z	1	Total	C	O	0	0
			33	22	11		

- Molecule 29 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
29	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
29	A	1	6	3	3	0	0
29	B	1	6	3	3	0	0
29	B	1	6	3	3	0	0
29	B	1	6	3	3	0	0
29	C	1	6	3	3	0	0
29	C	1	6	3	3	0	0
29	D	1	6	3	3	0	0
29	E	1	6	3	3	0	0
29	J	1	6	3	3	0	0
29	O	1	6	3	3	0	0
29	O	1	6	3	3	0	0
29	O	1	6	3	3	0	0
29	O	1	6	3	3	0	0
29	O	1	6	3	3	0	0
29	U	1	6	3	3	0	0
29	U	1	6	3	3	0	0
29	V	1	6	3	3	0	0
29	a	1	6	3	3	0	0
29	a	1	6	3	3	0	0
29	b	1	6	3	3	0	0
29	b	1	6	3	3	0	0
29	c	1	6	3	3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	c	1	Total C O 6 3 3	0	0
29	c	1	Total C O 6 3 3	0	0
29	d	1	Total C O 6 3 3	0	0
29	o	1	Total C O 6 3 3	0	0
29	u	1	Total C O 6 3 3	0	0
29	v	1	Total C O 6 3 3	0	0
29	v	1	Total C O 6 3 3	0	0
29	v	1	Total C O 6 3 3	0	0

- Molecule 30 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

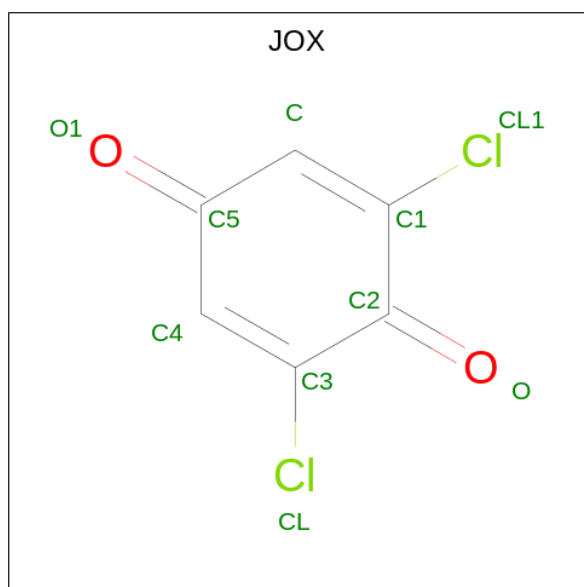
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	2	Total C O 37 32 5	0	0
30	B	3	Total C O 65 58 7	0	0
30	C	2	Total C O 50 45 5	0	0
30	D	3	Total C O 48 44 4	0	0
30	E	2	Total C 15 15	0	0
30	I	1	Total C O 40 35 5	0	0
30	J	1	Total C 5 5	0	0
30	T	1	Total C 13 13	0	0
30	Y	1	Total C 12 12	0	0
30	a	2	Total C O 42 37 5	0	0
30	b	5	Total C O 64 60 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	c	4	Total	C	O	0	0
			59	54	5		
30	d	2	Total	C	O	0	0
			55	48	7		
30	e	1	Total	C		0	0
			15	15			
30	i	1	Total	C	O	0	0
			19	15	4		
30	j	1	Total	C		0	0
			16	16			
30	k	1	Total	C		0	0
			16	16			
30	l	1	Total	C	O	0	0
			16	14	2		
30	m	1	Total	C	O	0	0
			15	13	2		
30	t	1	Total	C		0	0
			8	8			
30	x	1	Total	C	O	0	0
			18	16	2		

- Molecule 31 is 2,6-bis(chloranyl)cyclohexa-2,5-diene-1,4-dione (three-letter code: JOX) (formula: C<sub>6</sub>H<sub>2</sub>Cl<sub>2</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	Cl	O	0	0
			10	6	2	2		

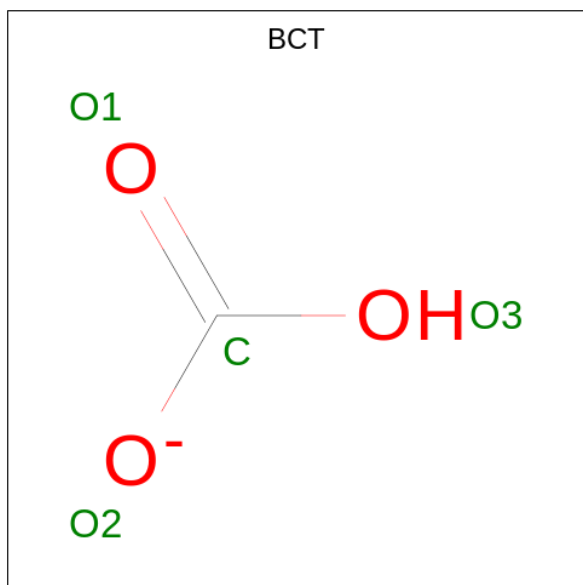
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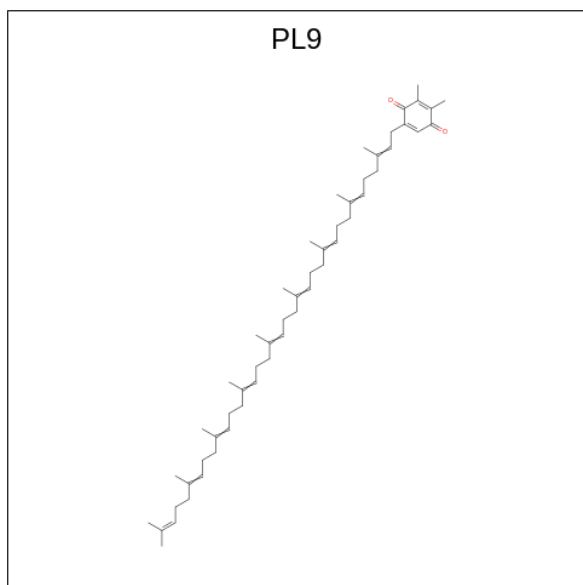
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	Cl	O	0	0
			10	6	2	2		
31	a	1	Total	C	Cl	O	0	0
			10	6	2	2		
31	a	1	Total	C	Cl	O	0	0
			10	6	2	2		

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



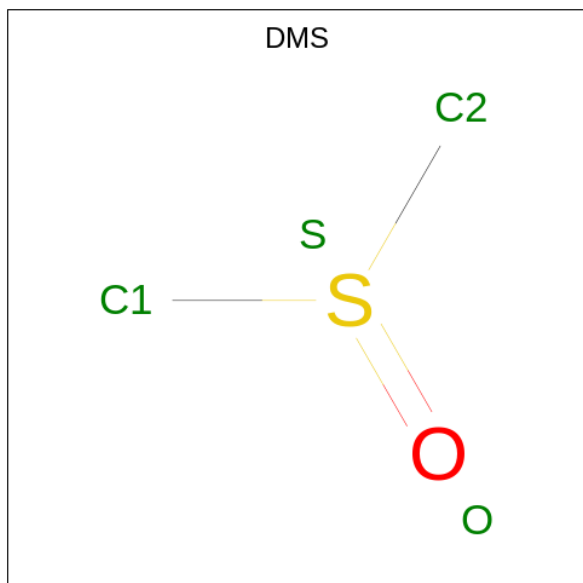
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			4	1	3		
32	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:  $\text{C}_{53}\text{H}_{80}\text{O}_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total C 39 39	0	0
33	D	1	Total C O 55 53 2	0	0
33	d	1	Total C O 55 53 2	0	0
33	x	1	Total C 39 39	0	0

- Molecule 34 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	A	1	Total 4	C 2	O 1	S 1	0	0
34	A	1	Total 4	C 2	O 1	S 1	0	0
34	A	1	Total 4	C 2	O 1	S 1	0	0
34	A	1	Total 4	C 2	O 1	S 1	0	0
34	A	1	Total 4	C 2	O 1	S 1	0	0
34	A	1	Total 4	C 2	O 1	S 1	0	0
34	A	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	D	1	Total 4	C 2	O 1	S 1	0	0
34	D	1	Total 4	C 2	O 1	S 1	0	0
34	D	1	Total 4	C 2	O 1	S 1	0	0
34	D	1	Total 4	C 2	O 1	S 1	0	0
34	D	1	Total 4	C 2	O 1	S 1	0	0
34	H	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	T	1	Total 4	C 2	O 1	S 1	0	0
34	T	1	Total 4	C 2	O 1	S 1	0	0
34	U	1	Total 4	C 2	O 1	S 1	0	0
34	U	1	Total 4	C 2	O 1	S 1	0	0
34	U	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	X	1	Total 4	C 2	O 1	S 1	0	0
34	a	1	Total 4	C 2	O 1	S 1	0	0
34	a	1	Total 4	C 2	O 1	S 1	0	0
34	a	1	Total 4	C 2	O 1	S 1	0	0
34	a	1	Total 4	C 2	O 1	S 1	0	0
34	a	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	d	1	Total 4	C 2	O 1	S 1	0	0
34	d	1	Total 4	C 2	O 1	S 1	0	0
34	d	1	Total 4	C 2	O 1	S 1	0	0
34	d	1	Total 4	C 2	O 1	S 1	0	0
34	d	1	Total 4	C 2	O 1	S 1	0	0
34	d	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	l	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	t	1	Total 4	C 2	O 1	S 1	0	0
34	u	1	Total 4	C 2	O 1	S 1	0	0
34	u	1	Total 4	C 2	O 1	S 1	0	0
34	u	1	Total 4	C 2	O 1	S 1	0	0
34	v	1	Total 4	C 2	O 1	S 1	0	0
34	v	1	Total 4	C 2	O 1	S 1	0	0
34	v	1	Total 4	C 2	O 1	S 1	0	0

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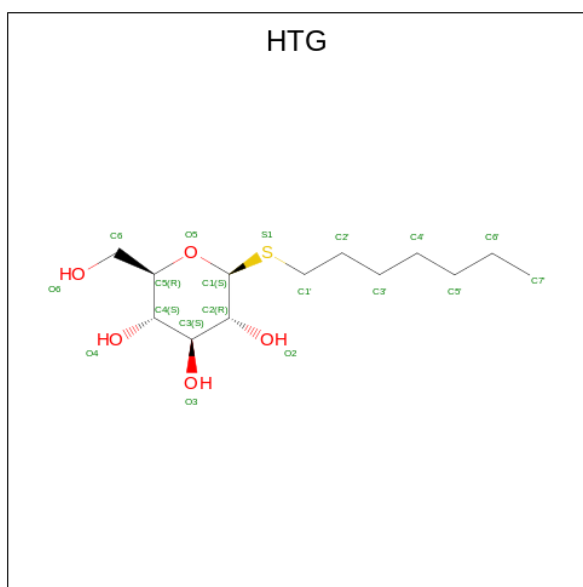
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	B	1	Total	Ca	0	0
			1	1		
35	O	1	Total	Ca	0	0
			1	1		
35	b	1	Total	Ca	0	0
			1	1		
35	c	1	Total	Ca	0	0
			1	1		
35	o	1	Total	Ca	0	0
			1	1		

- Molecule 36 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C<sub>13</sub>H<sub>26</sub>O<sub>5</sub>S).



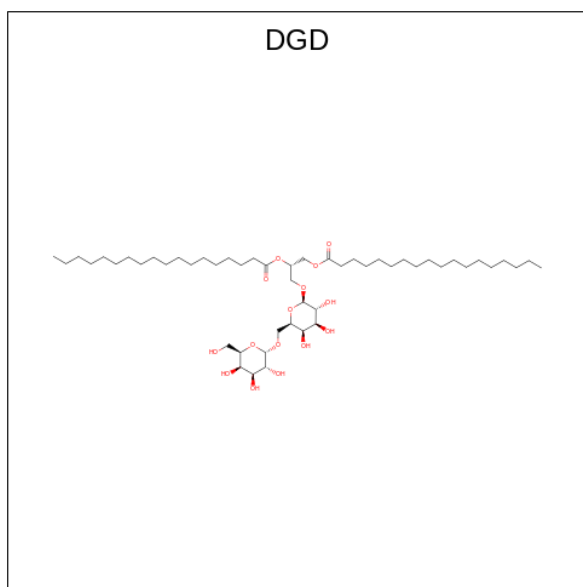
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	O			S
36	B	1	Total	C	O	S	0	1
			38	26	10	2		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	H	1	Total	C	O	S	0	0
			17	12	4	1		
36	I	1	Total	C	O	S	0	0
			19	13	5	1		
36	V	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	d	1	Total	C	O	S	0	0
			19	13	5	1		
36	d	1	Total	C	O	S	0	0
			19	13	5	1		
36	i	1	Total	C	O	S	0	0
			19	13	5	1		
36	o	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



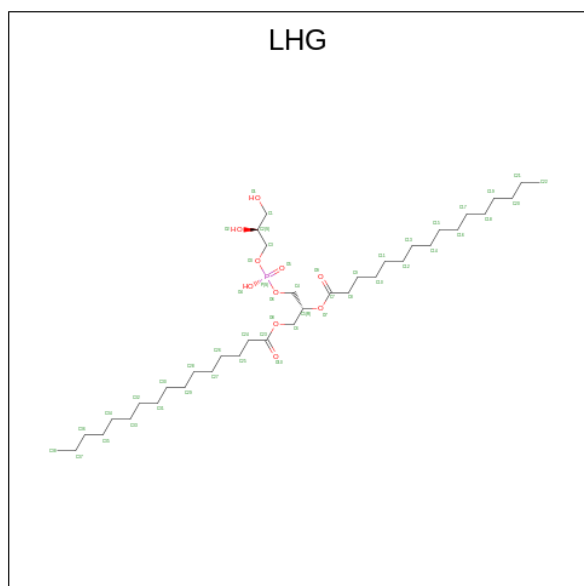
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			58	43	15		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	D	1	Total	C	O	0	0
			53	42	11		
37	H	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 38 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



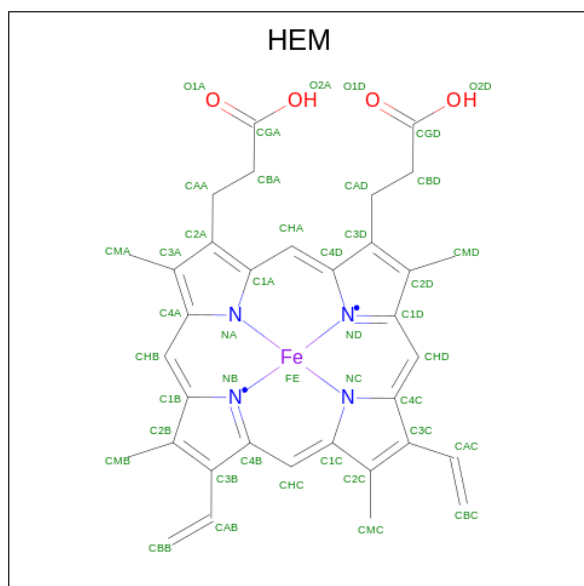
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	D	1	Total	C	O	P	0	0
			49	38	10	1		
38	D	1	Total	C	O	P	0	0
			49	38	10	1		
38	D	1	Total	C	O	P	0	0
			39	28	10	1		
38	E	1	Total	C	O	P	0	0
			40	29	10	1		
38	L	1	Total	C	O	P	0	0
			49	38	10	1		

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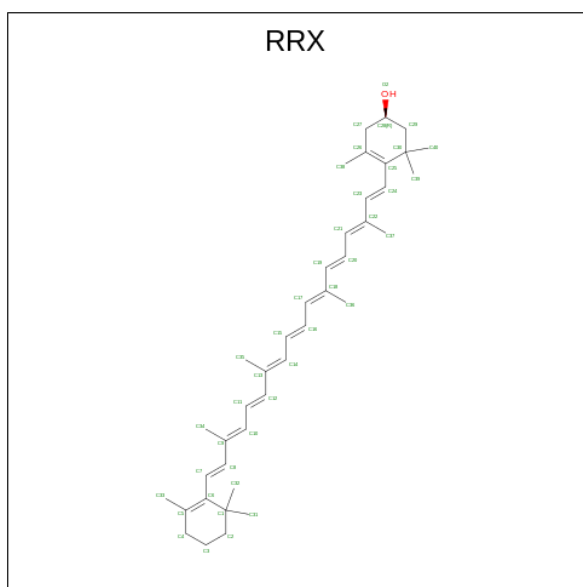
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	d	1	Total	C	O	P	0	0
			43	32	10	1		
38	d	1	Total	C	O	P	0	0
			49	38	10	1		
38	d	1	Total	C	O	P	0	0
			49	38	10	1		
38	e	1	Total	C	O	P	0	0
			40	29	10	1		
38	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
39	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
39	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 40 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula:  $C_{40}H_{56}O$ ).

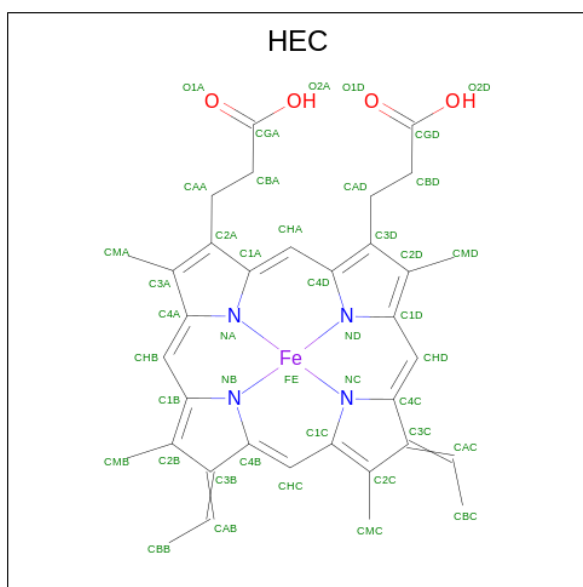


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	H	1	Total	C O	0	0
			41	40 1		
40	h	1	Total	C O	0	0
			41	40 1		

- Molecule 41 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	J	1	Total	Mg	0	0
			1	1		
41	K	1	Total	Mg	0	0
			1	1		
41	j	1	Total	Mg	0	0
			1	1		
41	k	1	Total	Mg	0	0
			1	1		

- Molecule 42 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
42	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
42	v	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 43 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
43	A	133	Total	O	0	0
			133	133		
43	B	302	Total	O	0	0
			302	302		
43	C	192	Total	O	0	0
			192	192		
43	D	146	Total	O	0	1
			147	147		
43	E	25	Total	O	0	0
			25	25		
43	F	9	Total	O	0	0
			9	9		
43	H	41	Total	O	0	0
			41	41		
43	I	8	Total	O	0	0
			8	8		
43	J	10	Total	O	0	0
			10	10		
43	K	10	Total	O	0	0
			10	10		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
43	L	15	Total O 15 15	0	0
43	M	12	Total O 12 12	0	0
43	O	144	Total O 145 145	0	1
43	T	12	Total O 12 12	0	0
43	U	79	Total O 79 79	0	0
43	V	113	Total O 113 113	0	0
43	Y	4	Total O 4 4	0	0
43	X	15	Total O 15 15	0	0
43	Z	8	Total O 8 8	0	0
43	a	122	Total O 122 122	0	0
43	b	250	Total O 251 251	0	1
43	c	211	Total O 211 211	0	0
43	d	146	Total O 147 147	0	1
43	e	19	Total O 19 19	0	0
43	f	7	Total O 7 7	0	0
43	h	27	Total O 27 27	0	0
43	i	8	Total O 8 8	0	0
43	j	10	Total O 10 10	0	0
43	k	5	Total O 5 5	0	0
43	l	20	Total O 20 20	0	0
43	m	11	Total O 11 11	0	0

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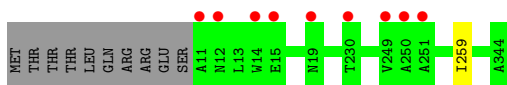
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
43	o	143	Total O 144 144	0	1
43	t	10	Total O 10 10	0	0
43	u	78	Total O 78 78	0	0
43	v	93	Total O 93 93	0	0
43	y	6	Total O 6 6	0	0
43	x	4	Total O 4 4	0	0
43	z	6	Total O 6 6	0	0

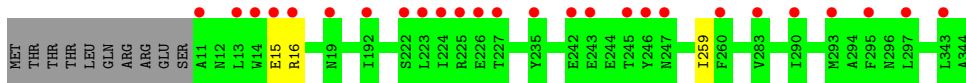
### 3 Residue-property plots

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

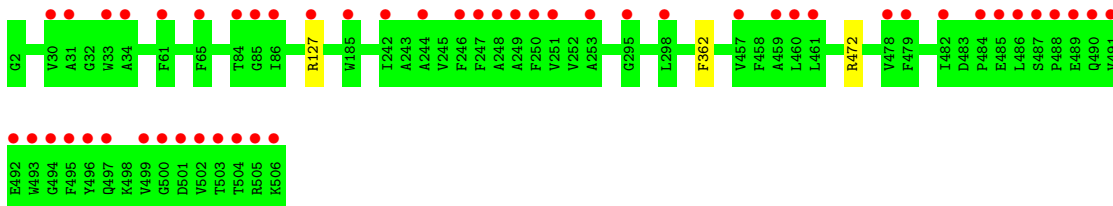
- Molecule 1: Photosystem II protein D1



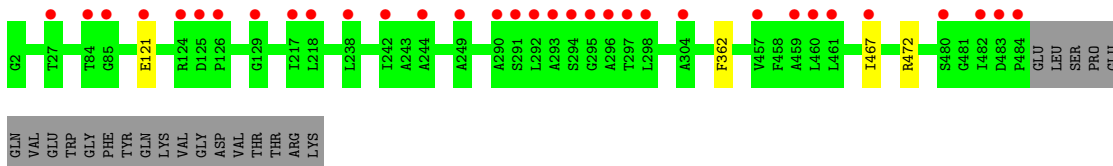
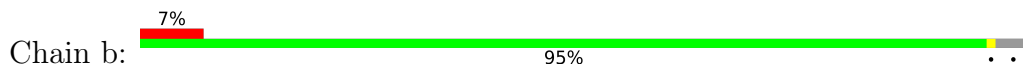
- Molecule 1: Photosystem II protein D1



- Molecule 2: Photosystem II CP47 reaction center protein

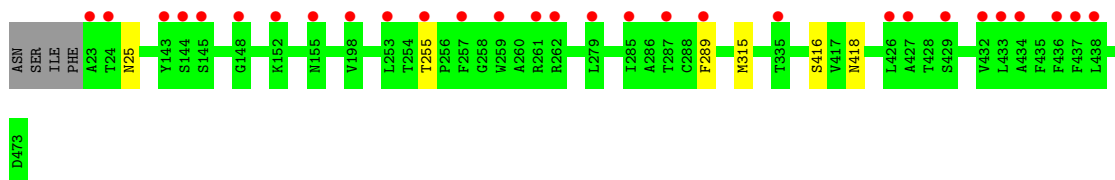


- Molecule 2: Photosystem II CP47 reaction center protein

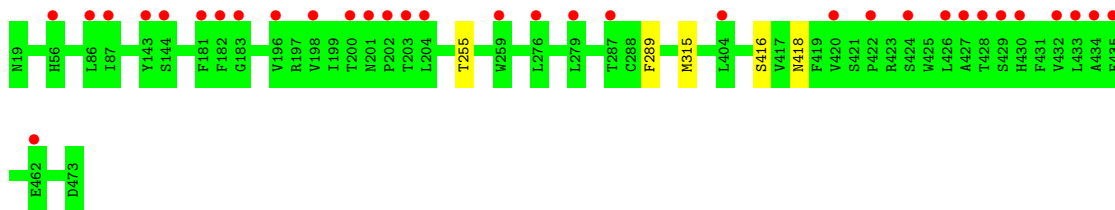


- Molecule 3: Photosystem II CP43 reaction center protein

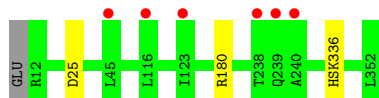




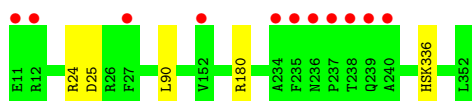
- Molecule 3: Photosystem II CP43 reaction center protein



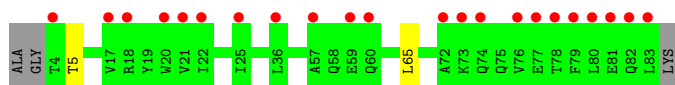
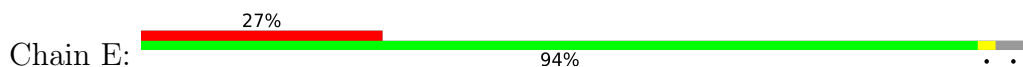
- Molecule 4: Photosystem II D2 protein



- Molecule 4: Photosystem II D2 protein



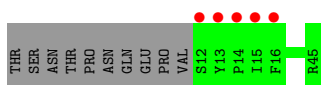
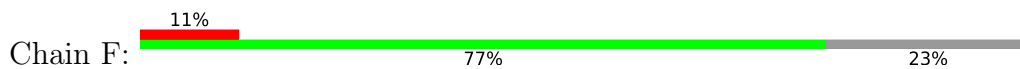
- Molecule 5: Cytochrome b559 subunit alpha



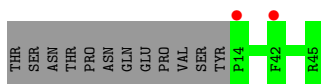
- Molecule 5: Cytochrome b559 subunit alpha



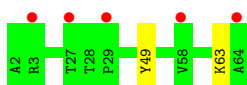
- Molecule 6: Cytochrome b559 subunit beta



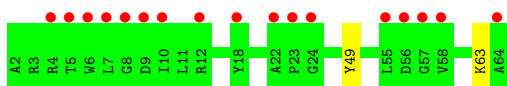
- Molecule 6: Cytochrome b559 subunit beta



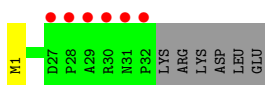
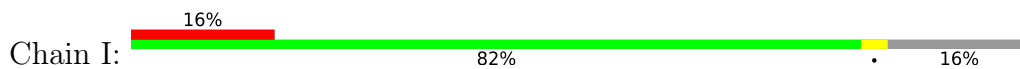
- Molecule 7: Photosystem II reaction center protein H



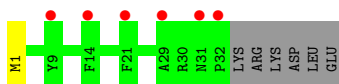
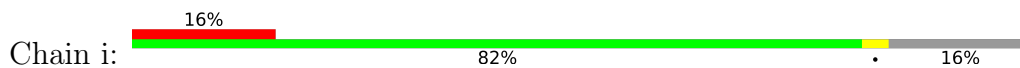
- Molecule 7: Photosystem II reaction center protein H



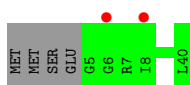
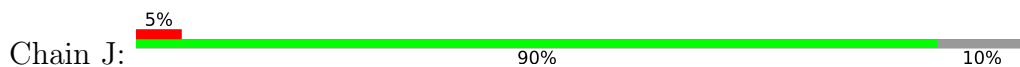
- Molecule 8: Photosystem II reaction center protein I



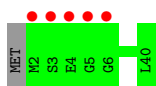
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



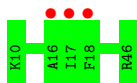
- Molecule 9: Photosystem II reaction center protein J



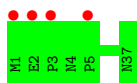
- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K



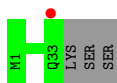
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L

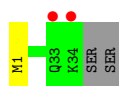


- Molecule 12: Photosystem II reaction center protein M

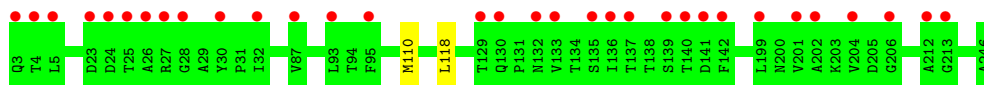


- Molecule 12: Photosystem II reaction center protein M

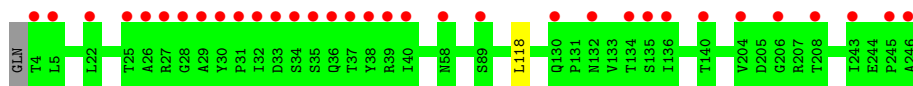




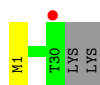
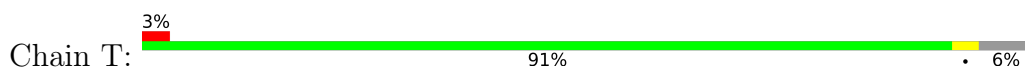
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



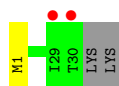
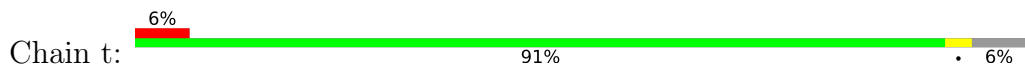
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



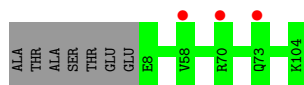
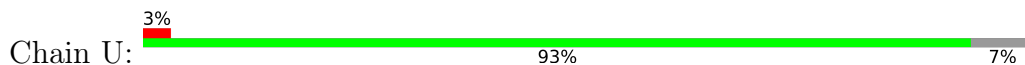
- Molecule 14: Photosystem II reaction center protein T



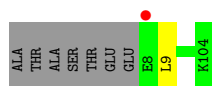
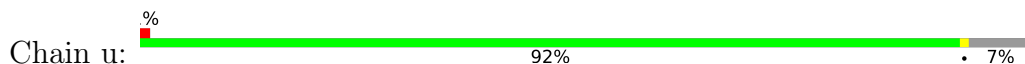
- Molecule 14: Photosystem II reaction center protein T



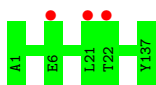
- Molecule 15: Photosystem II 12 kDa extrinsic protein



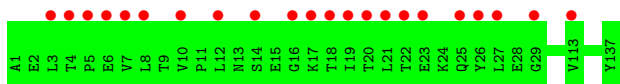
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Cytochrome c-550



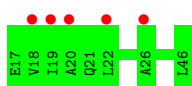
- Molecule 16: Cytochrome c-550



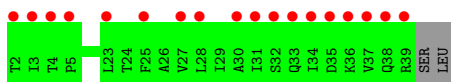
- Molecule 17: Photosystem II reaction center protein Ycf12



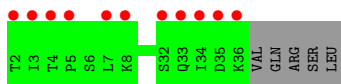
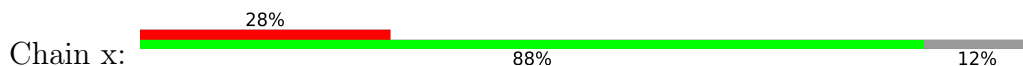
- Molecule 17: Photosystem II reaction center protein Ycf12



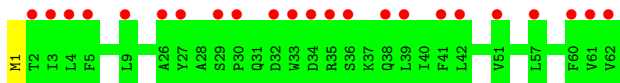
- Molecule 18: Photosystem II reaction center protein X



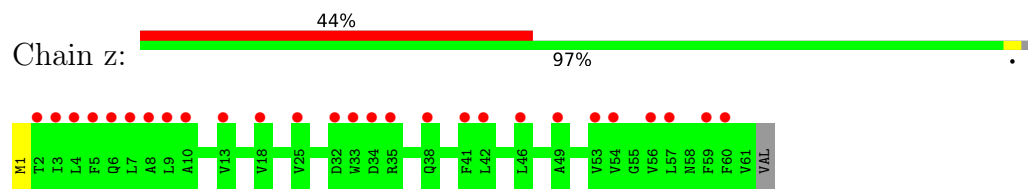
- Molecule 18: Photosystem II reaction center protein X



- Molecule 19: Photosystem II reaction center protein Z



## ● Molecule 19: Photosystem II reaction center protein Z





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.22Å 228.21Å 287.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 2.15 49.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.00-2.15) 83.7 (49.00-1.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.06 (at 1.90Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.151 , 0.185 0.151 , 0.185	Depositor DCC
$R_{free}$ test set	21442 reflections (3.47%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.3	Xtrriage
Anisotropy	0.401	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 77.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	53814	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% 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: UNL, LMG, CL, MG, CA, HEM, FME, JOX, GOL, CLA, LMT, LHG, HEC, SQD, BCR, HSK, DMS, FE2, OEX, RRX, DGD, BCT, PL9, PHO, HTG

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	0.45	0/2708	0.53	0/3695
1	a	0.42	0/2725	0.55	0/3716
2	B	0.42	0/4163	0.53	0/5672
2	b	0.41	0/3994	0.54	0/5442
3	C	0.38	0/3613	0.49	0/4919
3	c	0.38	0/3632	0.50	0/4945
4	D	0.47	0/2804	0.54	0/3820
4	d	0.44	0/2819	0.53	0/3840
5	E	0.33	0/665	0.47	0/911
5	e	0.32	0/652	0.46	0/893
6	F	0.33	0/280	0.47	0/382
6	f	0.35	0/262	0.46	0/356
7	H	0.33	0/511	0.49	0/697
7	h	0.32	0/522	0.47	0/711
8	I	0.31	0/253	0.42	0/345
8	i	0.33	0/256	0.43	0/349
9	J	0.37	0/257	0.48	0/349
9	j	0.35	0/280	0.48	0/379
10	K	0.31	0/310	0.44	0/426
10	k	0.36	0/299	0.46	0/412
11	L	0.48	0/313	0.47	0/426
11	l	0.45	0/318	0.48	0/433
12	M	0.39	0/266	0.59	0/364
12	m	0.41	0/266	0.49	0/363
13	O	0.38	0/1910	0.58	0/2592
13	o	0.37	0/1917	0.58	0/2599
14	T	0.44	0/257	0.46	0/349
14	t	0.42	0/257	0.46	0/349
15	U	0.42	0/790	0.54	0/1071
15	u	0.40	0/785	0.57	0/1064
16	V	0.37	0/1087	0.53	0/1475

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.33	0/1082	0.51	0/1472
17	Y	0.30	0/219	0.43	0/293
17	y	0.27	0/217	0.42	0/290
18	X	0.29	0/278	0.40	0/376
18	x	0.28	0/263	0.41	0/356
19	Z	0.29	0/472	0.42	0/646
19	z	0.30	0/457	0.41	0/626
All	All	0.40	0/42159	0.52	0/57403

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 [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	335/344 (97%)	331 (99%)	3 (1%)	1 (0%)	41	37
1	a	336/344 (98%)	332 (99%)	3 (1%)	1 (0%)	41	37
2	B	510/505 (101%)	501 (98%)	9 (2%)	0	100	100
2	b	490/505 (97%)	484 (99%)	6 (1%)	0	100	100
3	C	451/455 (99%)	441 (98%)	8 (2%)	2 (0%)	34	29
3	c	453/455 (100%)	444 (98%)	8 (2%)	1 (0%)	47	46
4	D	339/342 (99%)	332 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	341/342 (100%)	335 (98%)	6 (2%)	0	100	100
5	E	79/83 (95%)	79 (100%)	0	0	100	100
5	e	78/83 (94%)	78 (100%)	0	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	61/63 (97%)	58 (95%)	2 (3%)	1 (2%)	9	4
7	h	62/63 (98%)	59 (95%)	2 (3%)	1 (2%)	9	4
8	I	30/38 (79%)	29 (97%)	1 (3%)	0	100	100
8	i	30/38 (79%)	30 (100%)	0	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	37/40 (92%)	37 (100%)	0	0	100	100
10	K	36/37 (97%)	36 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	33/36 (92%)	33 (100%)	0	0	100	100
13	O	245/244 (100%)	240 (98%)	5 (2%)	0	100	100
13	o	245/244 (100%)	240 (98%)	5 (2%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	136/137 (99%)	133 (98%)	3 (2%)	0	100	100
16	v	136/137 (99%)	133 (98%)	3 (2%)	0	100	100
17	Y	28/30 (93%)	28 (100%)	0	0	100	100
17	y	28/30 (93%)	28 (100%)	0	0	100	100
18	X	36/40 (90%)	36 (100%)	0	0	100	100
18	x	34/40 (85%)	34 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5191/5346 (97%)	5103 (98%)	81 (2%)	7 (0%)	51	53

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	25	ASN
3	C	416	SER
3	c	416	SER
7	H	63	LYS
7	h	63	LYS
1	A	259	ILE
1	a	259	ILE

### 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	268/279 (96%)	268 (100%)	0	100	100
1	a	272/279 (98%)	270 (99%)	2 (1%)	84	89
2	B	406/403 (101%)	403 (99%)	3 (1%)	84	89
2	b	389/403 (96%)	385 (99%)	4 (1%)	76	81
3	C	354/356 (99%)	350 (99%)	4 (1%)	73	78
3	c	355/356 (100%)	351 (99%)	4 (1%)	73	78
4	D	275/276 (100%)	273 (99%)	2 (1%)	84	89
4	d	277/276 (100%)	273 (99%)	4 (1%)	67	72
5	E	69/72 (96%)	67 (97%)	2 (3%)	42	42
5	e	66/72 (92%)	66 (100%)	0	100	100
6	F	26/38 (68%)	26 (100%)	0	100	100
6	f	25/38 (66%)	25 (100%)	0	100	100
7	H	53/53 (100%)	52 (98%)	1 (2%)	57	61
7	h	54/53 (102%)	53 (98%)	1 (2%)	57	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	27/34 (79%)	27 (100%)	0	100	100
8	i	28/34 (82%)	28 (100%)	0	100	100
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	26/28 (93%)	26 (100%)	0	100	100
10	K	31/30 (103%)	31 (100%)	0	100	100
10	k	29/30 (97%)	29 (100%)	0	100	100
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	36/35 (103%)	36 (100%)	0	100	100
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	30/32 (94%)	30 (100%)	0	100	100
13	O	206/207 (100%)	204 (99%)	2 (1%)	76	81
13	o	208/207 (100%)	207 (100%)	1 (0%)	88	92
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	84/89 (94%)	84 (100%)	0	100	100
15	u	84/89 (94%)	83 (99%)	1 (1%)	71	76
16	V	116/117 (99%)	116 (100%)	0	100	100
16	v	115/117 (98%)	115 (100%)	0	100	100
17	Y	21/23 (91%)	21 (100%)	0	100	100
17	y	20/23 (87%)	20 (100%)	0	100	100
18	X	29/33 (88%)	29 (100%)	0	100	100
18	x	28/33 (85%)	28 (100%)	0	100	100
19	Z	48/51 (94%)	48 (100%)	0	100	100
19	z	44/51 (86%)	44 (100%)	0	100	100
All	All	4239/4368 (97%)	4208 (99%)	31 (1%)	84	89

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	127	ARG
2	B	362	PHE
2	B	472	ARG
3	C	255	THR
3	C	289	PHE

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Mol	Chain	Res	Type
3	C	315	MET
3	C	418	ASN
4	D	25	ASP
4	D	180	ARG
5	E	5	THR
5	E	65	LEU
7	H	49	TYR
13	O	110	MET
13	O	118	LEU
1	a	15	GLU
1	a	16	ARG
2	b	121	GLU
2	b	362	PHE
2	b	467	ILE
2	b	472	ARG
3	c	255	THR
3	c	289	PHE
3	c	315	MET
3	c	418	ASN
4	d	24	ARG
4	d	25	ASP
4	d	90	LEU
4	d	180	ARG
7	h	49	TYR
13	o	118	LEU
15	u	9	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	252	HIS
1	a	315	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	FME	m	1	12	8,9,10	0.53	0	7,9,11	1.36	1 (14%)
4	HSK	D	336[B]	-	7,11,12	1.23	1 (14%)	3,14,16	1.51	1 (33%)
4	HSK	d	336[A]	-	7,10,12	1.07	1 (14%)	3,12,16	1.19	0
14	FME	t	1	14	8,9,10	0.69	0	7,9,11	1.76	4 (57%)
12	FME	M	1	12	8,9,10	0.65	0	7,9,11	1.15	0
19	FME	Z	1	19	8,9,10	0.62	0	7,9,11	1.80	3 (42%)
14	FME	T	1	14	8,9,10	0.79	0	7,9,11	1.73	2 (28%)
8	FME	I	1	8	8,9,10	0.57	0	7,9,11	1.72	3 (42%)
4	HSK	d	336[B]	-	7,11,12	1.32	1 (14%)	3,14,16	1.47	1 (33%)
4	HSK	D	336[A]	-	7,10,12	0.98	1 (14%)	3,12,16	1.19	0
19	FME	z	1	19	8,9,10	0.58	0	7,9,11	1.70	3 (42%)
8	FME	i	1	8	8,9,10	0.64	0	7,9,11	1.69	3 (42%)

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
12	FME	m	1	12	-	0/7/9/11	-
4	HSK	D	336[B]	-	-	0/5/6/8	0/1/1/1
4	HSK	d	336[A]	-	-	0/5/6/8	0/1/1/1
14	FME	t	1	14	-	3/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-
19	FME	Z	1	19	-	3/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
4	HSK	d	336[B]	-	-	0/5/6/8	0/1/1/1
4	HSK	D	336[A]	-	-	0/5/6/8	0/1/1/1
19	FME	z	1	19	-	5/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-



All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	336[B]	HSK	CE1-ND1	-2.94	1.33	1.36
4	D	336[B]	HSK	CE1-ND1	-2.77	1.33	1.36
4	d	336[A]	HSK	CE1-ND1	-2.18	1.34	1.36
4	D	336[A]	HSK	CE1-ND1	-2.05	1.34	1.36

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	z	1	FME	CE-SD-CG	2.89	110.32	100.40
12	m	1	FME	CE-SD-CG	2.80	110.00	100.40
14	T	1	FME	CE-SD-CG	2.73	109.79	100.40
19	Z	1	FME	CE-SD-CG	2.68	109.61	100.40
8	i	1	FME	CA-N-CN	-2.51	118.97	122.82
14	t	1	FME	CE-SD-CG	2.48	108.93	100.40
19	Z	1	FME	CA-N-CN	-2.41	119.11	122.82
4	d	336[B]	HSK	CD2-NE2-CE1	2.39	109.51	105.78
19	z	1	FME	O-C-CA	-2.32	118.71	124.78
4	D	336[B]	HSK	CD2-NE2-CE1	2.26	109.31	105.78
14	t	1	FME	O-C-CA	-2.18	119.05	124.78
8	I	1	FME	CE-SD-CG	2.18	107.89	100.40
19	Z	1	FME	O1-CN-N	-2.14	119.64	125.27
14	t	1	FME	CA-N-CN	-2.12	119.56	122.82
14	t	1	FME	O1-CN-N	-2.11	119.71	125.27
8	I	1	FME	O-C-CA	-2.10	119.29	124.78
14	T	1	FME	O-C-CA	-2.09	119.31	124.78
8	i	1	FME	O1-CN-N	-2.05	119.88	125.27
19	z	1	FME	O1-CN-N	-2.04	119.90	125.27
8	i	1	FME	CE-SD-CG	2.02	107.34	100.40
8	I	1	FME	CA-N-CN	-2.01	119.72	122.82

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	N-CA-CB-CG
19	Z	1	FME	O-C-CA-CB
19	Z	1	FME	CA-CB-CG-SD
8	i	1	FME	O1-CN-N-CA
19	z	1	FME	O1-CN-N-CA
19	z	1	FME	CB-CA-N-CN
19	z	1	FME	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
14	T	1	FME	CB-CG-SD-CE
14	t	1	FME	CB-CG-SD-CE
14	t	1	FME	N-CA-CB-CG
19	Z	1	FME	CB-CG-SD-CE
14	T	1	FME	C-CA-CB-CG
14	t	1	FME	C-CA-CB-CG
8	I	1	FME	O1-CN-N-CA
12	M	1	FME	O1-CN-N-CA
19	z	1	FME	CB-CG-SD-CE
19	z	1	FME	C-CA-CB-CG
8	I	1	FME	CB-CA-N-CN
12	M	1	FME	CB-CA-N-CN
8	i	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 407 ligands modelled in this entry, 15 are monoatomic and 37 are unknown - leaving 355 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$
36	HTG	d	415	-	19,19,19	1.05	2 (10%)	23,24,24	1.52	1 (4%)
25	BCR	b	623	-	41,41,41	0.86	0	56,56,56	1.21	6 (10%)
23	CLA	C	511	-	65,73,73	2.60	20 (30%)	76,113,113	2.48	27 (35%)
36	HTG	b	626	-	19,19,19	1.14	2 (10%)	23,24,24	1.46	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DMS	u	502	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
36	HTG	c	526	-	19,19,19	1.00	2 (10%)	23,24,24	1.24	1 (4%)
23	CLA	B	608	43	65,73,73	2.44	18 (27%)	76,113,113	2.42	25 (32%)
34	DMS	C	536	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
23	CLA	C	509	-	65,73,73	2.49	18 (27%)	76,113,113	2.44	25 (32%)
26	SQD	a	2615	-	47,48,54	1.01	3 (6%)	56,59,65	1.79	12 (21%)
34	DMS	c	532	-	3,3,3	2.76	1 (33%)	3,3,3	0.80	0
26	SQD	D	2308	-	44,45,54	1.12	3 (6%)	53,56,65	1.31	8 (15%)
31	JOX	A	418	-	10,10,10	2.05	4 (40%)	14,14,14	3.36	10 (71%)
38	LHG	d	413	-	48,48,48	0.82	2 (4%)	51,54,54	0.99	3 (5%)
36	HTG	b	604	-	19,19,19	1.07	2 (10%)	23,24,24	1.66	4 (17%)
23	CLA	c	504	-	65,73,73	2.45	19 (29%)	76,113,113	2.63	22 (28%)
34	DMS	V	211	-	3,3,3	2.69	1 (33%)	3,3,3	0.55	0
34	DMS	c	549	-	3,3,3	2.72	1 (33%)	3,3,3	0.62	0
34	DMS	O	308	-	3,3,3	2.70	1 (33%)	3,3,3	0.55	0
34	DMS	b	633	-	3,3,3	2.50	1 (33%)	3,3,3	0.35	0
23	CLA	c	510	43	65,73,73	2.59	20 (30%)	76,113,113	2.53	29 (38%)
23	CLA	b	612	43	65,73,73	2.38	19 (29%)	76,113,113	2.44	26 (34%)
34	DMS	c	548	-	3,3,3	2.67	1 (33%)	3,3,3	0.55	0
24	PHO	a	2611	-	51,69,69	1.81	7 (13%)	47,99,99	1.75	12 (25%)
28	LMT	F	102	-	24,24,36	0.47	0	29,29,47	0.73	0
34	DMS	V	205	-	3,3,3	2.67	1 (33%)	3,3,3	0.55	0
34	DMS	A	426	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
34	DMS	V	206	-	3,3,3	2.71	1 (33%)	3,3,3	0.73	0
38	LHG	D	2309	-	48,48,48	0.90	2 (4%)	51,54,54	1.15	5 (9%)
34	DMS	o	310	-	3,3,3	2.67	1 (33%)	3,3,3	0.50	0
27	LMG	d	414	41	51,51,55	0.90	2 (3%)	59,59,63	0.86	1 (1%)
23	CLA	C	506	-	65,73,73	2.75	21 (32%)	76,113,113	2.21	24 (31%)
23	CLA	C	508	43	65,73,73	2.63	20 (30%)	76,113,113	2.46	23 (30%)
23	CLA	a	2613	-	65,73,73	2.29	18 (27%)	76,113,113	2.49	27 (35%)
34	DMS	b	635	-	3,3,3	2.70	1 (33%)	3,3,3	0.61	0
33	PL9	d	411	-	55,55,55	0.69	1 (1%)	68,69,69	1.60	15 (22%)
29	GOL	O	305	-	5,5,5	0.88	0	5,5,5	0.90	0
34	DMS	o	313	-	3,3,3	2.71	1 (33%)	3,3,3	0.60	0
23	CLA	B	602	43	65,73,73	2.70	22 (33%)	76,113,113	2.25	24 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	HTG	B	625	-	19,19,19	1.05	1 (5%)	23,24,24	2.09	4 (17%)
23	CLA	b	613	-	65,73,73	2.54	20 (30%)	76,113,113	2.47	29 (38%)
28	LMT	i	103	-	24,24,36	0.51	0	29,29,47	1.08	2 (6%)
29	GOL	c	529	-	5,5,5	0.91	0	5,5,5	0.98	0
34	DMS	b	642	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
38	LHG	D	2311	-	38,38,48	0.95	2 (5%)	41,44,54	1.11	3 (7%)
25	BCR	B	620	-	41,41,41	0.74	0	56,56,56	1.17	6 (10%)
23	CLA	b	608	-	65,73,73	2.55	21 (32%)	76,113,113	2.48	24 (31%)
27	LMG	c	501	-	51,51,55	0.95	2 (3%)	59,59,63	1.12	4 (6%)
20	OEX	A	401	3,43,1	0,15,15	-	-	-	-	-
25	BCR	b	622	-	41,41,41	0.78	0	56,56,56	1.39	9 (16%)
36	HTG	C	521	-	19,19,19	0.99	2 (10%)	23,24,24	1.04	1 (4%)
23	CLA	c	513	-	65,73,73	2.62	20 (30%)	76,113,113	2.32	27 (35%)
23	CLA	A	407	43	65,73,73	2.20	20 (30%)	76,113,113	2.50	28 (36%)
28	LMT	B	623	-	36,36,36	0.41	0	47,47,47	1.35	4 (8%)
23	CLA	C	510	-	65,73,73	2.61	21 (32%)	76,113,113	2.45	25 (32%)
29	GOL	B	630	-	5,5,5	0.98	0	5,5,5	0.93	0
23	CLA	D	2303	-	65,73,73	2.17	18 (27%)	76,113,113	2.67	24 (31%)
34	DMS	c	542	-	3,3,3	2.69	1 (33%)	3,3,3	0.53	0
34	DMS	O	317	-	3,3,3	2.68	1 (33%)	3,3,3	0.56	0
36	HTG	d	407	-	19,19,19	1.15	2 (10%)	23,24,24	1.64	5 (21%)
34	DMS	v	205	-	3,3,3	2.65	1 (33%)	3,3,3	0.51	0
34	DMS	B	645	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0
36	HTG	b	602	-	19,19,19	1.04	1 (5%)	23,24,24	1.04	2 (8%)
28	LMT	d	401	-	36,36,36	0.47	0	47,47,47	0.81	1 (2%)
24	PHO	a	2612	-	51,69,69	1.82	8 (15%)	47,99,99	1.95	10 (21%)
34	DMS	d	422	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0
34	DMS	D	2317	-	3,3,3	2.69	1 (33%)	3,3,3	0.55	0
23	CLA	B	615	-	65,73,73	2.31	19 (29%)	76,113,113	2.58	27 (35%)
34	DMS	v	213	-	3,3,3	2.66	1 (33%)	3,3,3	0.46	0
25	BCR	D	2305	-	41,41,41	0.82	1 (2%)	56,56,56	1.63	8 (14%)
34	DMS	B	637	-	3,3,3	2.68	1 (33%)	3,3,3	0.51	0
23	CLA	b	620	-	65,73,73	2.52	19 (29%)	76,113,113	2.23	28 (36%)
23	CLA	B	614	-	65,73,73	2.41	18 (27%)	76,113,113	2.53	26 (34%)
29	GOL	O	304	-	5,5,5	0.86	0	5,5,5	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DMS	O	315	-	3,3,3	2.69	1 (33%)	3,3,3	0.52	0
34	DMS	a	2621	-	3,3,3	2.66	1 (33%)	3,3,3	0.46	0
34	DMS	c	540	-	3,3,3	2.70	1 (33%)	3,3,3	0.55	0
23	CLA	B	606	-	65,73,73	2.39	19 (29%)	76,113,113	2.44	23 (30%)
23	CLA	b	614	-	65,73,73	2.64	20 (30%)	76,113,113	2.29	25 (32%)
34	DMS	d	419	-	3,3,3	2.66	1 (33%)	3,3,3	0.48	0
28	LMT	T	103	-	24,24,36	0.60	1 (4%)	29,29,47	0.94	2 (6%)
37	DGD	h	102	-	63,63,67	0.88	2 (3%)	77,77,81	1.03	5 (6%)
36	HTG	B	627	-	19,19,19	1.02	2 (10%)	23,24,24	1.37	2 (8%)
32	BCT	a	2608	21	2,3,3	0.67	0	2,3,3	1.05	0
23	CLA	b	607	-	65,73,73	2.56	20 (30%)	76,113,113	2.42	25 (32%)
29	GOL	c	531	-	5,5,5	0.95	0	5,5,5	0.86	0
27	LMG	C	527	-	51,51,55	0.96	2 (3%)	59,59,63	1.27	5 (8%)
34	DMS	B	642	-	3,3,3	2.64	1 (33%)	3,3,3	0.54	0
34	DMS	C	533	-	3,3,3	2.64	1 (33%)	3,3,3	0.35	0
34	DMS	b	636	-	3,3,3	2.68	1 (33%)	3,3,3	0.50	0
23	CLA	d	408	-	65,73,73	2.46	20 (30%)	76,113,113	2.53	24 (31%)
34	DMS	c	535	-	3,3,3	2.64	1 (33%)	3,3,3	0.47	0
23	CLA	C	503	-	65,73,73	2.65	20 (30%)	76,113,113	2.46	25 (32%)
29	GOL	O	302	-	5,5,5	0.92	0	5,5,5	1.03	0
34	DMS	U	503	-	3,3,3	2.70	1 (33%)	3,3,3	0.53	0
36	HTG	B	624[B]	-	19,19,19	0.96	1 (5%)	23,24,24	1.86	6 (26%)
39	HEM	F	101	6,5	41,50,50	1.94	6 (14%)	45,82,82	1.72	7 (15%)
23	CLA	c	515	-	65,73,73	2.63	20 (30%)	76,113,113	2.48	27 (35%)
23	CLA	b	621	-	65,73,73	2.63	19 (29%)	76,113,113	2.63	26 (34%)
34	DMS	u	504	-	3,3,3	2.67	1 (33%)	3,3,3	0.56	0
31	JOX	a	2617	-	10,10,10	1.85	4 (40%)	14,14,14	4.93	14 (100%)
23	CLA	B	617	-	65,73,73	2.61	19 (29%)	76,113,113	2.46	27 (35%)
34	DMS	O	311	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
27	LMG	B	622	-	51,51,55	0.94	2 (3%)	59,59,63	1.05	3 (5%)
23	CLA	B	609	-	65,73,73	2.47	20 (30%)	76,113,113	2.37	27 (35%)
25	BCR	T	102	-	41,41,41	0.69	0	56,56,56	1.85	14 (25%)
33	PL9	A	422	-	38,38,55	0.42	0	45,45,69	1.86	14 (31%)
34	DMS	V	209	-	3,3,3	2.64	1 (33%)	3,3,3	0.58	0
34	DMS	c	538	-	3,3,3	2.69	1 (33%)	3,3,3	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DMS	O	306	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
42	HEC	v	201	16	32,50,50	2.35	6 (18%)	24,82,82	1.84	6 (25%)
25	BCR	B	619	-	41,41,41	0.81	0	56,56,56	1.20	5 (8%)
23	CLA	c	516	-	65,73,73	2.54	20 (30%)	76,113,113	2.35	24 (31%)
34	DMS	b	634	-	3,3,3	2.62	1 (33%)	3,3,3	0.35	0
38	LHG	L	101	-	48,48,48	0.93	2 (4%)	51,54,54	1.06	5 (9%)
34	DMS	C	532	-	3,3,3	2.63	1 (33%)	3,3,3	0.72	0
39	HEM	e	103	6,5	41,50,50	1.93	6 (14%)	45,82,82	1.82	7 (15%)
36	HTG	c	524	-	19,19,19	1.05	2 (10%)	23,24,24	1.44	2 (8%)
28	LMT	M	102	-	36,36,36	0.41	0	47,47,47	0.81	0
34	DMS	d	418	-	3,3,3	2.65	1 (33%)	3,3,3	0.62	0
34	DMS	D	2318	-	3,3,3	2.57	1 (33%)	3,3,3	0.47	0
28	LMT	A	414	-	34,34,36	0.49	0	45,45,47	1.17	4 (8%)
23	CLA	b	611	-	65,73,73	2.69	18 (27%)	76,113,113	2.38	24 (31%)
23	CLA	c	514	3	65,73,73	2.49	19 (29%)	76,113,113	2.37	25 (32%)
23	CLA	C	507	-	65,73,73	2.61	19 (29%)	76,113,113	2.61	27 (35%)
34	DMS	c	547	-	3,3,3	2.70	1 (33%)	3,3,3	0.60	0
23	CLA	C	504	-	65,73,73	2.54	18 (27%)	76,113,113	2.37	24 (31%)
23	CLA	C	502	-	65,73,73	2.67	21 (32%)	76,113,113	2.26	21 (27%)
26	SQD	b	601	-	47,48,54	1.04	3 (6%)	56,59,65	1.46	9 (16%)
36	HTG	C	522	-	19,19,19	0.97	2 (10%)	23,24,24	2.32	4 (17%)
34	DMS	U	504	-	3,3,3	2.70	1 (33%)	3,3,3	0.64	0
34	DMS	B	638	-	3,3,3	2.54	1 (33%)	3,3,3	0.34	0
29	GOL	A	417	-	5,5,5	0.89	0	5,5,5	1.02	0
28	LMT	Z	101	-	36,36,36	0.45	0	47,47,47	0.91	2 (4%)
36	HTG	o	301	-	19,19,19	0.88	1 (5%)	23,24,24	1.15	2 (8%)
23	CLA	b	619	-	65,73,73	2.46	20 (30%)	76,113,113	2.58	30 (39%)
34	DMS	d	423	-	3,3,3	2.68	1 (33%)	3,3,3	0.51	0
34	DMS	c	541	-	3,3,3	2.68	1 (33%)	3,3,3	0.60	0
23	CLA	c	507	43	65,73,73	2.31	18 (27%)	76,113,113	2.62	22 (28%)
29	GOL	a	2602	-	5,5,5	0.85	0	5,5,5	1.03	0
28	LMT	m	2803	-	36,36,36	0.42	0	47,47,47	0.83	0
34	DMS	A	428	-	3,3,3	2.69	1 (33%)	3,3,3	0.53	0
28	LMT	J	303	-	24,24,36	0.54	0	29,29,47	0.94	1 (3%)
29	GOL	C	526	-	5,5,5	1.12	1 (20%)	5,5,5	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	HTG	I	101	-	19,19,19	1.10	2 (10%)	23,24,24	1.81	4 (17%)
26	SQD	l	101	-	53,54,54	1.05	4 (7%)	62,65,65	1.69	10 (16%)
23	CLA	b	609	-	65,73,73	2.83	19 (29%)	76,113,113	2.39	23 (30%)
28	LMT	m	2804	-	36,36,36	0.45	0	47,47,47	1.13	6 (12%)
34	DMS	c	536	-	3,3,3	2.65	1 (33%)	3,3,3	0.47	0
23	CLA	A	410	-	65,73,73	2.37	20 (30%)	76,113,113	2.53	26 (34%)
31	JOX	a	2619	1	10,10,10	1.91	6 (60%)	14,14,14	2.29	5 (35%)
23	CLA	B	603	-	65,73,73	2.57	19 (29%)	76,113,113	2.47	28 (36%)
34	DMS	B	646	-	3,3,3	2.69	1 (33%)	3,3,3	0.70	0
23	CLA	B	616	-	65,73,73	2.44	18 (27%)	76,113,113	2.58	28 (36%)
23	CLA	C	513	-	65,73,73	2.78	19 (29%)	76,113,113	2.40	25 (32%)
34	DMS	V	207	-	3,3,3	2.67	1 (33%)	3,3,3	0.55	0
26	SQD	a	2603	-	53,54,54	1.03	3 (5%)	62,65,65	1.14	3 (4%)
29	GOL	E	104	-	5,5,5	1.00	0	5,5,5	0.88	0
34	DMS	C	528	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
36	HTG	C	525	-	19,19,19	1.10	2 (10%)	23,24,24	1.69	4 (17%)
34	DMS	v	212	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
34	DMS	D	2320	-	3,3,3	2.66	1 (33%)	3,3,3	0.44	0
34	DMS	B	647	-	3,3,3	2.68	1 (33%)	3,3,3	0.59	0
34	DMS	d	421	-	3,3,3	2.66	1 (33%)	3,3,3	0.58	0
34	DMS	O	319	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
34	DMS	O	312	-	3,3,3	2.69	1 (33%)	3,3,3	0.56	0
23	CLA	B	607	-	65,73,73	2.54	19 (29%)	76,113,113	2.36	24 (31%)
36	HTG	b	603	-	19,19,19	0.95	2 (10%)	23,24,24	2.00	4 (17%)
25	BCR	B	633	-	41,41,41	0.69	0	56,56,56	1.72	12 (21%)
25	BCR	K	101	-	41,41,41	0.68	0	56,56,56	1.33	9 (16%)
40	RRX	H	102	-	42,42,42	0.69	0	57,58,58	1.47	9 (15%)
26	SQD	d	417	-	31,32,54	1.97	4 (12%)	34,36,65	1.57	4 (11%)
36	HTG	B	624[A]	-	19,19,19	0.90	1 (5%)	23,24,24	1.25	4 (17%)
34	DMS	a	2624	-	3,3,3	2.74	1 (33%)	3,3,3	0.70	0
25	BCR	d	410	-	41,41,41	0.80	0	56,56,56	1.65	5 (8%)
23	CLA	c	512	-	65,73,73	2.61	20 (30%)	76,113,113	2.45	23 (30%)
34	DMS	v	207	-	3,3,3	2.64	1 (33%)	3,3,3	0.46	0
28	LMT	B	634	-	36,36,36	0.53	1 (2%)	47,47,47	0.85	0
34	DMS	v	210	-	3,3,3	2.68	1 (33%)	3,3,3	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DMS	O	314	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
34	DMS	c	537	-	3,3,3	2.69	1 (33%)	3,3,3	0.56	0
34	DMS	o	316	-	3,3,3	2.72	1 (33%)	3,3,3	0.59	0
24	PHO	A	409	-	51,69,69	1.92	8 (15%)	47,99,99	1.95	9 (19%)
20	OEX	a	2604	3,43,1	0,15,15	-	-	-	-	-
34	DMS	T	105	-	3,3,3	2.69	1 (33%)	3,3,3	0.57	0
40	RRX	h	101	-	42,42,42	0.69	0	57,58,58	1.41	8 (14%)
36	HTG	b	625	-	19,19,19	0.89	1 (5%)	23,24,24	1.54	4 (17%)
34	DMS	D	2319	-	3,3,3	2.68	1 (33%)	3,3,3	0.52	0
34	DMS	O	309	-	3,3,3	2.68	1 (33%)	3,3,3	0.52	0
27	LMG	c	522	-	51,51,55	0.98	2 (3%)	59,59,63	1.34	6 (10%)
34	DMS	v	211	-	3,3,3	2.67	1 (33%)	3,3,3	0.54	0
32	BCT	A	421	21	2,3,3	0.65	0	2,3,3	1.06	0
37	DGD	D	2307	-	53,53,67	0.96	2 (3%)	60,61,81	1.20	5 (8%)
29	GOL	V	203	-	5,5,5	0.90	0	5,5,5	0.92	0
34	DMS	v	214	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0
23	CLA	b	606	43	65,73,73	2.72	22 (33%)	76,113,113	2.22	25 (32%)
36	HTG	H	101	-	17,17,19	1.23	2 (11%)	19,21,24	1.61	4 (21%)
34	DMS	c	533	-	3,3,3	2.61	1 (33%)	3,3,3	0.39	0
29	GOL	A	415	-	5,5,5	0.82	0	5,5,5	1.08	0
23	CLA	c	505	-	65,73,73	2.48	20 (30%)	76,113,113	2.34	22 (28%)
34	DMS	o	309	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0
36	HTG	V	204	-	19,19,19	0.96	1 (5%)	23,24,24	1.84	4 (17%)
34	DMS	T	104	-	3,3,3	2.67	1 (33%)	3,3,3	0.54	0
23	CLA	B	605	-	65,73,73	2.51	19 (29%)	76,113,113	2.42	25 (32%)
26	SQD	D	2302	-	53,54,54	1.05	4 (7%)	62,65,65	1.42	9 (14%)
34	DMS	A	427	-	3,3,3	2.67	1 (33%)	3,3,3	0.57	0
34	DMS	V	210	-	3,3,3	2.67	1 (33%)	3,3,3	0.57	0
34	DMS	o	307	-	3,3,3	2.63	1 (33%)	3,3,3	0.50	0
23	CLA	b	615	43	65,73,73	2.51	20 (30%)	76,113,113	2.42	27 (35%)
34	DMS	b	637	-	3,3,3	2.74	1 (33%)	3,3,3	0.67	0
28	LMT	z	102	-	33,33,36	0.54	0	43,43,47	1.06	4 (9%)
25	BCR	C	516	-	41,41,41	0.74	0	56,56,56	1.53	7 (12%)
38	LHG	e	101	-	39,39,48	1.08	2 (5%)	42,45,54	1.07	3 (7%)
28	LMT	j	2701	41	34,34,36	0.56	1 (2%)	44,44,47	1.05	3 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
38	LHG	d	412	-	48,48,48	0.93	2 (4%)	51,54,54	1.01	3 (5%)
29	GOL	o	303	-	5,5,5	0.97	0	5,5,5	0.94	0
36	HTG	B	626	-	19,19,19	1.01	2 (10%)	23,24,24	1.49	1 (4%)
34	DMS	B	641	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
34	DMS	V	202	-	3,3,3	2.65	1 (33%)	3,3,3	0.57	0
34	DMS	o	308	-	3,3,3	2.66	1 (33%)	3,3,3	0.46	0
24	PHO	A	408	-	51,69,69	1.85	7 (13%)	47,99,99	1.56	9 (19%)
29	GOL	B	648	-	5,5,5	0.89	0	5,5,5	0.94	0
29	GOL	d	416	-	5,5,5	0.89	0	5,5,5	0.99	0
23	CLA	c	506	-	65,73,73	2.58	20 (30%)	76,113,113	2.36	24 (31%)
29	GOL	a	2618	-	5,5,5	0.87	0	5,5,5	1.04	0
34	DMS	B	635	-	3,3,3	2.70	1 (33%)	3,3,3	0.52	0
34	DMS	b	641	-	3,3,3	2.68	1 (33%)	3,3,3	0.40	0
29	GOL	b	644	-	5,5,5	0.69	0	5,5,5	1.21	1 (20%)
34	DMS	O	313	-	3,3,3	2.70	1 (33%)	3,3,3	0.60	0
23	CLA	B	613	-	65,73,73	2.39	20 (30%)	76,113,113	2.53	24 (31%)
27	LMG	A	413	-	51,51,55	0.93	2 (3%)	59,59,63	1.24	6 (10%)
34	DMS	c	543	-	3,3,3	2.65	1 (33%)	3,3,3	0.50	0
23	CLA	c	511	-	65,73,73	2.74	20 (30%)	76,113,113	2.37	22 (28%)
38	LHG	l	103	-	48,48,48	0.87	2 (4%)	51,54,54	1.02	3 (5%)
34	DMS	t	102	-	3,3,3	2.69	1 (33%)	3,3,3	0.56	0
29	GOL	J	301	-	5,5,5	0.96	0	5,5,5	0.89	0
23	CLA	D	2304	-	65,73,73	2.24	17 (26%)	76,113,113	2.53	26 (34%)
23	CLA	c	509	-	65,73,73	2.68	21 (32%)	76,113,113	2.44	28 (36%)
34	DMS	v	208	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
34	DMS	b	643	-	3,3,3	2.69	1 (33%)	3,3,3	0.57	0
34	DMS	b	638	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
29	GOL	C	524	-	5,5,5	0.83	0	5,5,5	0.97	0
23	CLA	b	617	-	65,73,73	2.40	19 (29%)	76,113,113	2.57	25 (32%)
34	DMS	o	312	-	3,3,3	2.64	1 (33%)	3,3,3	0.49	0
37	DGD	C	518	-	63,63,67	0.87	2 (3%)	77,77,81	1.05	6 (7%)
34	DMS	B	640	-	3,3,3	2.66	1 (33%)	3,3,3	0.51	0
25	BCR	z	101	-	41,41,41	0.74	0	56,56,56	1.52	12 (21%)
25	BCR	a	2614	-	41,41,41	0.80	0	56,56,56	1.31	6 (10%)
34	DMS	o	304	-	3,3,3	2.54	1 (33%)	3,3,3	0.32	0
23	CLA	d	402	43	65,73,73	2.41	18 (27%)	76,113,113	2.55	25 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	b	610	-	65,73,73	2.40	19 (29%)	76,113,113	2.68	25 (32%)
25	BCR	C	515	-	41,41,41	0.76	0	56,56,56	1.49	8 (14%)
23	CLA	A	405	-	65,73,73	2.39	20 (30%)	76,113,113	2.51	28 (36%)
34	DMS	A	425	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
29	GOL	v	203	-	5,5,5	0.93	0	5,5,5	1.14	1 (20%)
34	DMS	A	424	-	3,3,3	2.61	1 (33%)	3,3,3	0.62	0
37	DGD	c	518	-	63,63,67	0.84	2 (3%)	77,77,81	1.04	4 (5%)
37	DGD	c	520	-	63,63,67	0.88	3 (4%)	77,77,81	0.86	5 (6%)
23	CLA	a	2610	43	65,73,73	2.36	18 (27%)	76,113,113	2.59	27 (35%)
23	CLA	c	508	-	65,73,73	2.60	21 (32%)	76,113,113	2.43	20 (26%)
28	LMT	d	404	-	25,25,36	0.52	0	30,30,47	0.90	2 (6%)
29	GOL	U	501	-	5,5,5	1.02	0	5,5,5	0.93	0
34	DMS	V	213	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
27	LMG	D	2312	41	47,47,55	0.90	2 (4%)	55,55,63	0.88	3 (5%)
25	BCR	Y	302	-	41,41,41	0.81	0	56,56,56	1.76	11 (19%)
28	LMT	A	420	-	24,24,36	0.42	0	29,29,47	0.96	0
42	HEC	V	201	16	32,50,50	2.18	6 (18%)	24,82,82	1.82	5 (20%)
34	DMS	A	429	-	3,3,3	2.69	1 (33%)	3,3,3	0.53	0
34	DMS	d	420	-	3,3,3	2.66	1 (33%)	3,3,3	0.48	0
36	HTG	i	102	-	19,19,19	1.13	2 (10%)	23,24,24	1.92	3 (13%)
29	GOL	u	501	-	5,5,5	1.25	0	5,5,5	0.83	0
23	CLA	B	612	-	65,73,73	2.58	17 (26%)	76,113,113	2.56	29 (38%)
25	BCR	k	302	-	41,41,41	0.69	0	56,56,56	1.47	12 (21%)
23	CLA	C	512	3	65,73,73	2.59	18 (27%)	76,113,113	2.37	25 (32%)
29	GOL	B	632	-	5,5,5	0.95	0	5,5,5	0.91	0
31	JOX	A	419	-	10,10,10	1.98	4 (40%)	14,14,14	4.85	11 (78%)
34	DMS	a	2620	-	3,3,3	2.68	1 (33%)	3,3,3	0.58	0
34	DMS	v	209	-	3,3,3	2.67	1 (33%)	3,3,3	0.64	0
29	GOL	v	202	-	5,5,5	1.01	0	5,5,5	0.89	0
34	DMS	l	104	-	3,3,3	2.69	1 (33%)	3,3,3	0.51	0
34	DMS	o	314	-	3,3,3	2.66	1 (33%)	3,3,3	0.50	0
34	DMS	B	636	-	3,3,3	2.57	1 (33%)	3,3,3	0.58	0
34	DMS	u	503	-	3,3,3	2.66	1 (33%)	3,3,3	0.59	0
34	DMS	C	537	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
29	GOL	b	631	-	5,5,5	1.07	0	5,5,5	0.60	0
28	LMT	f	101	-	24,24,36	0.46	0	29,29,47	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DMS	B	639	-	3,3,3	2.70	1 (33%)	3,3,3	0.59	0
34	DMS	c	544	-	3,3,3	2.73	1 (33%)	3,3,3	0.55	0
29	GOL	U	502	-	5,5,5	1.29	1 (20%)	5,5,5	0.80	0
28	LMT	M	101	-	36,36,36	0.47	0	47,47,47	1.27	7 (14%)
34	DMS	O	316	-	3,3,3	2.63	1 (33%)	3,3,3	0.51	0
34	DMS	b	640	-	3,3,3	2.66	1 (33%)	3,3,3	0.55	0
33	PL9	x	1301	-	38,38,55	0.44	0	45,45,69	1.72	11 (24%)
36	HTG	c	523	-	19,19,19	1.02	2 (10%)	23,24,24	1.49	2 (8%)
27	LMG	m	2802	-	51,51,55	0.95	2 (3%)	59,59,63	1.06	2 (3%)
26	SQD	A	412	-	45,46,54	1.05	3 (6%)	54,57,65	1.55	11 (20%)
29	GOL	c	530	-	5,5,5	0.92	0	5,5,5	0.80	0
25	BCR	A	411	-	41,41,41	0.75	0	56,56,56	1.39	8 (14%)
38	LHG	d	403	-	42,42,48	0.98	2 (4%)	45,48,54	0.91	3 (6%)
23	CLA	d	409	-	65,73,73	2.58	20 (30%)	76,113,113	2.42	25 (32%)
37	DGD	H	103	-	63,63,67	0.90	2 (3%)	77,77,81	1.09	7 (9%)
23	CLA	b	616	-	65,73,73	2.36	20 (30%)	76,113,113	2.47	29 (38%)
34	DMS	C	535	-	3,3,3	2.66	1 (33%)	3,3,3	0.56	0
23	CLA	C	514	-	65,73,73	2.49	20 (30%)	76,113,113	2.35	22 (28%)
26	SQD	B	621	-	53,54,54	1.05	4 (7%)	62,65,65	1.45	9 (14%)
34	DMS	O	310	-	3,3,3	2.65	1 (33%)	3,3,3	0.54	0
34	DMS	U	505	-	3,3,3	2.68	1 (33%)	3,3,3	0.62	0
23	CLA	B	611	43	65,73,73	2.33	21 (32%)	76,113,113	2.53	28 (36%)
23	CLA	A	406	43	65,73,73	2.35	18 (27%)	76,113,113	2.73	29 (38%)
34	DMS	B	644	-	3,3,3	2.68	1 (33%)	3,3,3	0.47	0
37	DGD	C	519	-	59,59,67	0.92	2 (3%)	73,73,81	1.28	6 (8%)
34	DMS	c	546	-	3,3,3	2.70	1 (33%)	3,3,3	0.57	0
34	DMS	H	104	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
25	BCR	B	618	-	41,41,41	0.76	0	56,56,56	1.28	5 (8%)
25	BCR	y	101	-	41,41,41	0.76	0	56,56,56	1.56	12 (21%)
34	DMS	C	534	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0
34	DMS	V	208	-	3,3,3	2.68	1 (33%)	3,3,3	0.59	0
34	DMS	O	318	-	3,3,3	2.67	1 (33%)	3,3,3	0.49	0
34	DMS	o	306	-	3,3,3	2.69	1 (33%)	3,3,3	0.64	0
34	DMS	o	305	-	3,3,3	2.68	1 (33%)	3,3,3	0.50	0
34	DMS	C	529	-	3,3,3	2.62	1 (33%)	3,3,3	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	DGD	C	517	-	63,63,67	0.84	2 (3%)	77,77,81	0.97	5 (6%)
34	DMS	o	315	-	3,3,3	2.68	1 (33%)	3,3,3	0.58	0
34	DMS	v	206	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
34	DMS	C	530	-	3,3,3	2.66	1 (33%)	3,3,3	0.46	0
34	DMS	X	101	-	3,3,3	2.67	1 (33%)	3,3,3	0.53	0
23	CLA	a	2609	-	65,73,73	2.53	19 (29%)	76,113,113	2.48	25 (32%)
34	DMS	c	534	-	3,3,3	2.64	1 (33%)	3,3,3	0.50	0
34	DMS	O	307	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
25	BCR	b	624	-	41,41,41	0.72	0	56,56,56	1.59	12 (21%)
34	DMS	b	639	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
29	GOL	D	2301	-	5,5,5	1.00	0	5,5,5	0.79	0
23	CLA	b	618	-	65,73,73	2.49	20 (30%)	76,113,113	2.39	23 (30%)
23	CLA	C	505	43	65,73,73	2.39	20 (30%)	76,113,113	2.45	24 (31%)
29	GOL	O	303	-	5,5,5	0.93	0	5,5,5	0.94	0
34	DMS	c	539	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
34	DMS	C	531	-	3,3,3	2.70	1 (33%)	3,3,3	0.51	0
34	DMS	V	212	-	3,3,3	2.68	1 (33%)	3,3,3	0.63	0
34	DMS	o	311	-	3,3,3	2.75	1 (33%)	3,3,3	0.60	0
27	LMG	c	521	-	49,49,55	0.91	2 (4%)	57,57,63	1.13	5 (8%)
34	DMS	A	430	-	3,3,3	2.72	1 (33%)	3,3,3	0.60	0
38	LHG	D	2310	-	48,48,48	0.87	2 (4%)	51,54,54	0.95	3 (5%)
23	CLA	B	604	-	65,73,73	2.57	20 (30%)	76,113,113	2.50	25 (32%)
23	CLA	B	610	-	65,73,73	2.69	20 (30%)	76,113,113	2.41	22 (28%)
33	PL9	D	2306	-	55,55,55	0.69	1 (1%)	68,69,69	1.60	18 (26%)
27	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.07	4 (6%)
34	DMS	c	545	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
34	DMS	B	643	-	3,3,3	2.72	1 (33%)	3,3,3	0.54	0
34	DMS	a	2622	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
38	LHG	E	101	-	39,39,48	1.06	2 (5%)	42,45,54	1.12	3 (7%)
37	DGD	c	519	-	63,63,67	0.86	2 (3%)	77,77,81	1.14	6 (7%)
34	DMS	a	2623	-	3,3,3	2.65	1 (33%)	3,3,3	0.52	0
29	GOL	v	204	-	5,5,5	0.88	0	5,5,5	0.96	0
34	DMS	D	2316	-	3,3,3	2.71	1 (33%)	3,3,3	0.52	0
25	BCR	c	517	-	41,41,41	0.75	0	56,56,56	1.57	9 (16%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	HTG	d	415	-	-	2/10/30/30	0/1/1/1
25	BCR	b	623	-	-	1/29/63/63	0/2/2/2
27	LMG	B	622	-	-	16/46/66/70	0/1/1/1
23	CLA	C	511	-	1/1/15/20	6/37/115/115	-
36	HTG	b	626	-	-	6/10/30/30	0/1/1/1
36	HTG	c	526	-	-	2/10/30/30	0/1/1/1
23	CLA	B	608	43	1/1/15/20	3/37/115/115	-
23	CLA	B	609	-	-	1/37/115/115	-
42	HEC	V	201	16	-	2/10/54/54	-
23	CLA	C	509	-	1/1/15/20	6/37/115/115	-
26	SQD	a	2615	-	-	8/43/63/69	0/1/1/1
25	BCR	T	102	-	-	3/29/63/63	0/2/2/2
36	HTG	i	102	-	-	6/10/30/30	0/1/1/1
29	GOL	u	501	-	-	1/4/4/4	-
33	PL9	A	422	-	-	10/42/42/73	-
26	SQD	D	2308	-	-	16/40/60/69	0/1/1/1
23	CLA	B	612	-	1/1/15/20	3/37/115/115	-
25	BCR	k	302	-	-	0/29/63/63	0/2/2/2
31	JOX	A	418	-	-	-	0/1/1/1
42	HEC	v	201	16	-	2/10/54/54	-
38	LHG	d	413	-	-	10/53/53/53	-
24	PHO	A	409	-	-	4/37/103/103	0/5/6/6
23	CLA	C	512	3	1/1/15/20	2/37/115/115	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
29	GOL	B	632	-	-	3/4/4/4	-
36	HTG	b	604	-	-	1/10/30/30	0/1/1/1
31	JOX	A	419	-	-	-	0/1/1/1
23	CLA	c	516	-	1/1/15/20	10/37/115/115	-
23	CLA	c	504	-	1/1/15/20	2/37/115/115	-
40	RRX	h	101	-	-	2/29/65/65	0/2/2/2
29	GOL	v	202	-	-	2/4/4/4	-
38	LHG	L	101	-	-	15/53/53/53	-
39	HEM	e	103	6,5	-	4/12/54/54	-
36	HTG	b	625	-	-	2/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	HTG	c	524	-	-	0/10/30/30	0/1/1/1
29	GOL	b	631	-	-	0/4/4/4	-
27	LMG	c	522	-	-	5/46/66/70	0/1/1/1
28	LMT	M	102	-	-	4/21/61/61	0/2/2/2
28	LMT	A	414	-	-	8/19/59/61	0/2/2/2
23	CLA	c	510	43	1/1/15/20	10/37/115/115	-
28	LMT	f	101	-	-	4/15/35/61	0/1/1/2
37	DGD	D	2307	-	-	23/47/68/95	0/1/1/2
23	CLA	b	611	-	1/1/15/20	9/37/115/115	-
23	CLA	c	514	3	1/1/15/20	1/37/115/115	-
23	CLA	C	507	-	1/1/15/20	14/37/115/115	-
29	GOL	V	203	-	-	0/4/4/4	-
23	CLA	b	612	43	1/1/15/20	1/37/115/115	-
24	PHO	a	2611	-	-	3/37/103/103	0/5/6/6
23	CLA	C	504	-	-	3/37/115/115	-
23	CLA	C	502	-	1/1/15/20	4/37/115/115	-
26	SQD	b	601	-	-	16/43/63/69	0/1/1/1
28	LMT	F	102	-	-	5/15/35/61	0/1/1/2
28	LMT	M	101	-	-	6/21/61/61	0/2/2/2
29	GOL	U	502	-	-	2/4/4/4	-
36	HTG	C	522	-	-	2/10/30/30	0/1/1/1
29	GOL	A	417	-	-	3/4/4/4	-
28	LMT	Z	101	-	-	7/21/61/61	0/2/2/2
23	CLA	b	606	43	1/1/15/20	8/37/115/115	-
36	HTG	o	301	-	-	6/10/30/30	0/1/1/1
36	HTG	H	101	-	-	2/8/25/30	0/1/1/1
33	PL9	x	1301	-	-	12/42/42/73	-
38	LHG	D	2309	-	-	13/53/53/53	-
36	HTG	c	523	-	-	2/10/30/30	0/1/1/1
23	CLA	b	619	-	1/1/15/20	8/37/115/115	-
29	GOL	A	415	-	-	2/4/4/4	-
23	CLA	c	505	-	1/1/15/20	4/37/115/115	-
27	LMG	d	414	41	-	11/46/66/70	0/1/1/1
23	CLA	C	506	-	1/1/15/20	8/37/115/115	-
27	LMG	m	2802	-	-	10/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	A	412	-	-	8/41/61/69	0/1/1/1
29	GOL	c	530	-	-	4/4/4/4	-
36	HTG	V	204	-	-	5/10/30/30	0/1/1/1
23	CLA	C	508	43	1/1/15/20	9/37/115/115	-
23	CLA	c	507	43	1/1/15/20	6/37/115/115	-
23	CLA	B	605	-	1/1/15/20	6/37/115/115	-
25	BCR	A	411	-	-	0/29/63/63	0/2/2/2
23	CLA	a	2613	-	1/1/15/20	7/37/115/115	-
26	SQD	D	2302	-	-	14/49/69/69	0/1/1/1
38	LHG	d	403	-	-	7/47/47/53	-
23	CLA	d	409	-	1/1/15/20	6/37/115/115	-
37	DGD	H	103	-	-	12/51/91/95	0/2/2/2
33	PL9	d	411	-	-	4/53/73/73	0/1/1/1
29	GOL	O	305	-	-	2/4/4/4	-
23	CLA	b	616	-	1/1/15/20	4/37/115/115	-
29	GOL	a	2602	-	-	4/4/4/4	-
23	CLA	B	602	43	1/1/15/20	10/37/115/115	-
36	HTG	B	625	-	-	1/10/30/30	0/1/1/1
23	CLA	C	514	-	-	6/37/115/115	-
23	CLA	b	613	-	-	1/37/115/115	-
23	CLA	b	615	43	1/1/15/20	6/37/115/115	-
26	SQD	B	621	-	-	22/49/69/69	0/1/1/1
28	LMT	m	2803	-	-	3/21/61/61	0/2/2/2
28	LMT	J	303	-	-	5/15/35/61	0/1/1/2
29	GOL	C	526	-	-	2/4/4/4	-
36	HTG	I	101	-	-	6/10/30/30	0/1/1/1
23	CLA	B	611	43	1/1/15/20	5/37/115/115	-
28	LMT	i	103	-	-	8/15/35/61	0/1/1/2
28	LMT	z	102	-	-	12/16/56/61	0/2/2/2
29	GOL	c	529	-	-	0/4/4/4	-
23	CLA	A	406	43	-	4/37/115/115	-
26	SQD	l	101	-	-	23/49/69/69	0/1/1/1
38	LHG	D	2311	-	-	9/43/43/53	-
37	DGD	C	519	-	-	14/47/87/95	0/2/2/2
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	C	516	-	-	3/29/63/63	0/2/2/2
38	LHG	e	101	-	-	14/44/44/53	-
25	BCR	B	618	-	-	2/29/63/63	0/2/2/2
23	CLA	b	608	-	1/1/15/20	3/37/115/115	-
23	CLA	b	609	-	1/1/15/20	2/37/115/115	-
27	LMG	c	501	-	-	12/46/66/70	0/1/1/1
25	BCR	b	622	-	-	2/29/63/63	0/2/2/2
25	BCR	y	101	-	-	6/29/63/63	0/2/2/2
28	LMT	j	2701	41	-	3/17/57/61	0/2/2/2
36	HTG	C	521	-	-	2/10/30/30	0/1/1/1
23	CLA	c	513	-	1/1/15/20	8/37/115/115	-
28	LMT	m	2804	-	-	10/21/61/61	0/2/2/2
38	LHG	d	412	-	-	13/53/53/53	-
29	GOL	o	303	-	-	0/4/4/4	-
36	HTG	B	626	-	-	3/10/30/30	0/1/1/1
23	CLA	A	407	43	-	6/37/115/115	-
28	LMT	B	623	-	-	12/21/61/61	0/2/2/2
23	CLA	A	410	-	1/1/15/20	10/37/115/115	-
23	CLA	C	510	-	1/1/15/20	6/37/115/115	-
29	GOL	B	630	-	-	0/4/4/4	-
24	PHO	A	408	-	-	4/37/103/103	0/5/6/6
29	GOL	B	648	-	-	0/4/4/4	-
29	GOL	d	416	-	-	2/4/4/4	-
23	CLA	c	506	-	-	3/37/115/115	-
23	CLA	D	2303	-	1/1/15/20	1/37/115/115	-
31	JOX	a	2619	1	-	-	0/1/1/1
29	GOL	a	2618	-	-	1/4/4/4	-
37	DGD	C	517	-	-	18/51/91/95	0/2/2/2
23	CLA	B	603	-	1/1/15/20	3/37/115/115	-
36	HTG	d	407	-	-	7/10/30/30	0/1/1/1
23	CLA	B	616	-	1/1/15/20	7/37/115/115	-
29	GOL	b	644	-	-	2/4/4/4	-
23	CLA	a	2609	-	1/1/15/20	4/37/115/115	-
28	LMT	d	401	-	-	8/21/61/61	0/2/2/2
23	CLA	C	513	-	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PHO	a	2612	-	-	1/37/103/103	0/5/6/6
26	SQD	a	2603	-	-	16/49/69/69	0/1/1/1
36	HTG	b	602	-	-	3/10/30/30	0/1/1/1
23	CLA	B	613	-	1/1/15/20	5/37/115/115	-
23	CLA	B	615	-	1/1/15/20	12/37/115/115	-
27	LMG	A	413	-	-	20/46/66/70	0/1/1/1
23	CLA	c	511	-	1/1/15/20	5/37/115/115	-
38	LHG	l	103	-	-	13/53/53/53	-
29	GOL	J	301	-	-	4/4/4/4	-
23	CLA	D	2304	-	1/1/15/20	6/37/115/115	-
23	CLA	c	509	-	1/1/15/20	11/37/115/115	-
25	BCR	b	624	-	-	4/29/63/63	0/2/2/2
29	GOL	E	104	-	-	0/4/4/4	-
25	BCR	D	2305	-	-	8/29/63/63	0/2/2/2
23	CLA	b	620	-	1/1/15/20	3/37/115/115	-
23	CLA	B	614	-	1/1/15/20	8/37/115/115	-
29	GOL	D	2301	-	-	2/4/4/4	-
29	GOL	O	304	-	-	2/4/4/4	-
23	CLA	b	618	-	1/1/15/20	6/37/115/115	-
23	CLA	C	505	43	1/1/15/20	6/37/115/115	-
29	GOL	C	524	-	-	2/4/4/4	-
36	HTG	C	525	-	-	0/10/30/30	0/1/1/1
23	CLA	b	617	-	1/1/15/20	2/37/115/115	-
37	DGD	C	518	-	-	17/51/91/95	0/2/2/2
29	GOL	O	303	-	-	0/4/4/4	-
23	CLA	B	606	-	1/1/15/20	7/37/115/115	-
25	BCR	z	101	-	-	0/29/63/63	0/2/2/2
25	BCR	Y	302	-	-	5/29/63/63	0/2/2/2
25	BCR	a	2614	-	-	3/29/63/63	0/2/2/2
23	CLA	b	614	-	1/1/15/20	5/37/115/115	-
28	LMT	T	103	-	-	9/15/35/61	0/1/1/2
27	LMG	c	521	-	-	14/44/64/70	0/1/1/1
37	DGD	h	102	-	-	12/51/91/95	0/2/2/2
23	CLA	d	402	43	1/1/15/20	5/37/115/115	-
36	HTG	B	627	-	-	3/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LHG	D	2310	-	-	8/53/53/53	-
23	CLA	B	604	-	1/1/15/20	5/37/115/115	-
23	CLA	B	610	-	1/1/15/20	3/37/115/115	-
23	CLA	B	607	-	1/1/15/20	4/37/115/115	-
23	CLA	b	610	-	1/1/15/20	3/37/115/115	-
36	HTG	b	603	-	-	0/10/30/30	0/1/1/1
23	CLA	b	607	-	1/1/15/20	3/37/115/115	-
25	BCR	C	515	-	-	7/29/63/63	0/2/2/2
33	PL9	D	2306	-	-	3/53/73/73	0/1/1/1
23	CLA	A	405	-	1/1/15/20	2/37/115/115	-
27	LMG	C	520	-	-	13/46/66/70	0/1/1/1
29	GOL	c	531	-	-	2/4/4/4	-
27	LMG	C	527	-	-	14/46/66/70	0/1/1/1
25	BCR	B	633	-	-	3/29/63/63	0/2/2/2
29	GOL	v	203	-	-	1/4/4/4	-
37	DGD	c	518	-	-	17/51/91/95	0/2/2/2
25	BCR	K	101	-	-	0/29/63/63	0/2/2/2
37	DGD	c	520	-	-	10/51/91/95	0/2/2/2
23	CLA	a	2610	43	-	11/37/115/115	-
40	RRX	H	102	-	-	1/29/65/65	0/2/2/2
23	CLA	d	408	-	1/1/15/20	1/37/115/115	-
26	SQD	d	417	-	-	13/33/33/69	-
36	HTG	B	624[A]	-	-	2/10/30/30	0/1/1/1
23	CLA	C	503	-	1/1/15/20	4/37/115/115	-
23	CLA	c	508	-	1/1/15/20	9/37/115/115	-
25	BCR	d	410	-	-	8/29/63/63	0/2/2/2
28	LMT	d	404	-	-	5/17/37/61	0/1/1/2
29	GOL	O	302	-	-	2/4/4/4	-
29	GOL	U	501	-	-	0/4/4/4	-
36	HTG	B	624[B]	-	-	4/10/30/30	0/1/1/1
38	LHG	E	101	-	-	13/44/44/53	-
37	DGD	c	519	-	-	18/51/91/95	0/2/2/2
23	CLA	c	512	-	1/1/15/20	5/37/115/115	-
23	CLA	c	515	-	1/1/15/20	6/37/115/115	-
23	CLA	b	621	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	GOL	v	204	-	-	1/4/4/4	-
27	LMG	D	2312	41	-	6/42/62/70	0/1/1/1
39	HEM	F	101	6,5	-	4/12/54/54	-
28	LMT	B	634	-	-	8/21/61/61	0/2/2/2
25	BCR	c	517	-	-	3/29/63/63	0/2/2/2
31	JOX	a	2617	-	-	-	0/1/1/1
23	CLA	B	617	-	1/1/15/20	9/37/115/115	-
28	LMT	A	420	-	-	6/15/35/61	0/1/1/2

All (1705) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	MG-NA	10.59	2.31	2.06
23	C	512	CLA	MG-NA	10.28	2.30	2.06
23	c	506	CLA	MG-NA	10.17	2.30	2.06
23	c	511	CLA	MG-ND	-9.74	1.86	2.05
23	b	609	CLA	MG-ND	-9.39	1.87	2.05
23	C	513	CLA	MG-NA	9.27	2.28	2.06
23	C	503	CLA	MG-NA	9.25	2.28	2.06
23	c	514	CLA	MG-NA	9.22	2.28	2.06
23	B	602	CLA	MG-NA	9.19	2.28	2.06
23	B	612	CLA	MG-NA	9.16	2.28	2.06
23	b	621	CLA	MG-NA	8.95	2.27	2.06
23	C	506	CLA	MG-NA	8.93	2.27	2.06
23	b	621	CLA	MG-ND	-8.84	1.88	2.05
23	b	614	CLA	MG-NA	8.78	2.27	2.06
23	B	616	CLA	MG-NA	8.69	2.26	2.06
23	C	513	CLA	MG-ND	-8.51	1.88	2.05
23	c	504	CLA	MG-NA	8.51	2.26	2.06
23	b	611	CLA	MG-ND	-8.51	1.88	2.05
23	b	609	CLA	MG-NA	8.37	2.26	2.06
23	c	515	CLA	MG-ND	-8.37	1.89	2.05
23	B	617	CLA	MG-NA	8.34	2.26	2.06
23	b	609	CLA	MG-NC	8.31	2.26	2.06
23	C	502	CLA	MG-NC	8.29	2.26	2.06
23	c	509	CLA	MG-ND	-8.25	1.89	2.05
23	B	608	CLA	MG-NA	8.23	2.25	2.06
23	C	504	CLA	MG-NA	8.19	2.25	2.06
23	b	606	CLA	MG-NC	7.96	2.25	2.06
23	C	511	CLA	MG-NA	7.96	2.25	2.06
23	C	510	CLA	MG-NA	7.96	2.25	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	2609	CLA	MG-ND	-7.95	1.90	2.05
23	b	620	CLA	MG-NA	7.92	2.25	2.06
23	c	511	CLA	MG-NC	7.87	2.25	2.06
39	F	101	HEM	C3D-C2D	7.86	1.53	1.36
23	B	610	CLA	MG-NC	7.84	2.24	2.06
23	b	608	CLA	MG-NA	7.84	2.24	2.06
39	e	103	HEM	C3D-C2D	7.80	1.53	1.36
23	B	610	CLA	MG-ND	-7.79	1.90	2.05
23	B	603	CLA	MG-ND	-7.73	1.90	2.05
23	c	508	CLA	MG-NA	7.70	2.24	2.06
23	B	607	CLA	MG-NA	7.68	2.24	2.06
23	C	507	CLA	MG-ND	-7.66	1.90	2.05
23	c	513	CLA	MG-ND	-7.66	1.90	2.05
23	c	510	CLA	MG-NA	7.64	2.24	2.06
23	B	604	CLA	MG-NA	7.63	2.24	2.06
23	C	504	CLA	MG-NC	7.54	2.24	2.06
23	c	508	CLA	MG-ND	-7.48	1.91	2.05
23	B	603	CLA	MG-NA	7.46	2.24	2.06
23	c	512	CLA	MG-NA	7.44	2.23	2.06
23	B	604	CLA	MG-NC	7.41	2.23	2.06
23	C	511	CLA	MG-ND	-7.37	1.91	2.05
23	B	617	CLA	MG-ND	-7.35	1.91	2.05
23	b	606	CLA	MG-NA	7.32	2.23	2.06
23	b	613	CLA	MG-ND	-7.31	1.91	2.05
23	c	510	CLA	MG-ND	-7.27	1.91	2.05
23	C	506	CLA	MG-ND	-7.26	1.91	2.05
23	b	611	CLA	MG-NC	7.24	2.23	2.06
23	C	514	CLA	MG-NC	7.22	2.23	2.06
23	B	609	CLA	MG-ND	-7.21	1.91	2.05
23	b	618	CLA	MG-NC	7.20	2.23	2.06
23	B	606	CLA	MG-NA	7.19	2.23	2.06
26	d	417	SQD	C6-S	-7.15	1.67	1.77
23	c	513	CLA	MG-NA	7.12	2.23	2.06
23	B	607	CLA	MG-NC	7.07	2.23	2.06
23	d	408	CLA	MG-NA	7.04	2.23	2.06
23	b	615	CLA	MG-NA	7.03	2.23	2.06
23	b	619	CLA	MG-ND	-7.02	1.91	2.05
23	c	515	CLA	MG-NA	7.01	2.22	2.06
23	b	611	CLA	MG-NA	6.97	2.22	2.06
23	B	605	CLA	MG-NA	6.97	2.22	2.06
23	d	402	CLA	MG-ND	-6.93	1.92	2.05
23	c	516	CLA	MG-NA	6.92	2.22	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	MG-ND	-6.90	1.92	2.05
23	b	612	CLA	MG-NA	6.86	2.22	2.06
23	c	509	CLA	MG-NA	6.76	2.22	2.06
23	B	610	CLA	MG-NA	6.76	2.22	2.06
23	b	613	CLA	MG-NA	6.75	2.22	2.06
23	c	507	CLA	MG-NA	6.73	2.22	2.06
24	A	409	PHO	C3B-C2B	6.71	1.49	1.40
23	b	614	CLA	MG-NC	6.70	2.22	2.06
23	B	612	CLA	MG-ND	-6.68	1.92	2.05
23	b	607	CLA	MG-NC	6.68	2.22	2.06
23	c	509	CLA	MG-NC	6.67	2.22	2.06
23	b	616	CLA	C3B-C2B	6.67	1.49	1.40
23	B	609	CLA	MG-NA	6.64	2.22	2.06
23	c	512	CLA	MG-ND	-6.63	1.92	2.05
23	b	610	CLA	MG-NA	6.63	2.22	2.06
23	b	618	CLA	C3B-C2B	6.61	1.49	1.40
23	B	610	CLA	C1D-ND	6.61	1.45	1.37
24	a	2611	PHO	C3B-C2B	6.59	1.49	1.40
23	C	507	CLA	MG-NA	6.57	2.21	2.06
23	c	511	CLA	C3B-C2B	6.56	1.49	1.40
23	A	406	CLA	C3B-C2B	6.54	1.49	1.40
23	C	506	CLA	MG-NC	6.52	2.21	2.06
23	A	406	CLA	MG-ND	-6.51	1.92	2.05
23	B	602	CLA	C3B-C2B	6.51	1.49	1.40
23	C	510	CLA	C3B-C2B	6.50	1.49	1.40
23	d	409	CLA	MG-NC	6.49	2.21	2.06
23	C	509	CLA	MG-ND	-6.48	1.92	2.05
23	B	617	CLA	C3B-C2B	6.47	1.49	1.40
23	B	613	CLA	MG-ND	-6.45	1.93	2.05
23	C	502	CLA	MG-NA	6.45	2.21	2.06
23	B	613	CLA	C3B-C2B	6.44	1.49	1.40
23	C	510	CLA	MG-ND	-6.43	1.93	2.05
23	b	616	CLA	MG-NA	6.42	2.21	2.06
23	b	615	CLA	MG-ND	-6.40	1.93	2.05
24	A	408	PHO	C3B-C2B	6.40	1.49	1.40
23	b	621	CLA	C3B-C2B	6.40	1.49	1.40
23	d	409	CLA	MG-NA	6.40	2.21	2.06
23	b	607	CLA	MG-NA	6.39	2.21	2.06
23	a	2609	CLA	C3B-C2B	6.38	1.49	1.40
23	c	506	CLA	MG-NC	6.38	2.21	2.06
23	b	617	CLA	C3B-C2B	6.38	1.49	1.40
23	b	610	CLA	C3B-C2B	6.38	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	MG-NC	6.36	2.21	2.06
23	c	512	CLA	C3B-C2B	6.34	1.49	1.40
23	C	503	CLA	C3B-C2B	6.34	1.49	1.40
23	c	510	CLA	C3B-C2B	6.34	1.49	1.40
23	C	512	CLA	C3B-C2B	6.34	1.49	1.40
23	d	409	CLA	MG-ND	-6.31	1.93	2.05
23	C	504	CLA	C3B-C2B	6.31	1.49	1.40
23	B	612	CLA	C3B-C2B	6.31	1.49	1.40
23	B	605	CLA	C3B-C2B	6.31	1.49	1.40
23	B	607	CLA	C3B-C2B	6.30	1.49	1.40
23	A	405	CLA	MG-NA	6.29	2.21	2.06
23	c	505	CLA	MG-NA	6.29	2.21	2.06
23	C	514	CLA	C1D-ND	6.28	1.45	1.37
23	C	509	CLA	C3B-C2B	6.27	1.49	1.40
23	B	605	CLA	MG-ND	-6.26	1.93	2.05
23	b	611	CLA	C3B-C2B	6.24	1.49	1.40
23	b	607	CLA	C3B-C2B	6.24	1.49	1.40
42	v	201	HEC	C3C-C2C	-6.23	1.34	1.40
23	c	513	CLA	C3B-C2B	6.23	1.49	1.40
23	D	2304	CLA	C3C-C2C	6.22	1.50	1.36
23	c	514	CLA	C3B-C2B	6.22	1.49	1.40
23	C	508	CLA	C3B-C2B	6.22	1.49	1.40
23	C	502	CLA	C1D-ND	6.21	1.45	1.37
23	a	2610	CLA	MG-NA	6.20	2.21	2.06
23	B	614	CLA	MG-NA	6.20	2.21	2.06
23	B	614	CLA	C3B-C2B	6.19	1.49	1.40
23	b	609	CLA	C3B-C2B	6.18	1.49	1.40
23	c	509	CLA	C1D-ND	6.18	1.45	1.37
23	b	611	CLA	C1D-ND	6.18	1.45	1.37
23	a	2609	CLA	MG-NC	6.17	2.20	2.06
23	D	2304	CLA	C3B-C2B	6.17	1.48	1.40
24	a	2612	PHO	C3B-C2B	6.17	1.48	1.40
23	c	515	CLA	C1D-ND	6.17	1.45	1.37
23	c	512	CLA	MG-NC	6.16	2.20	2.06
23	b	606	CLA	C3B-C2B	6.16	1.48	1.40
23	B	605	CLA	MG-NC	6.16	2.20	2.06
23	b	615	CLA	C1D-ND	6.16	1.45	1.37
23	b	606	CLA	C1D-ND	6.15	1.45	1.37
23	c	515	CLA	C3B-C2B	6.15	1.48	1.40
23	D	2303	CLA	C3B-C2B	6.14	1.48	1.40
23	c	505	CLA	C3B-C2B	6.13	1.48	1.40
23	c	504	CLA	MG-ND	-6.13	1.93	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	408	CLA	MG-NC	6.13	2.20	2.06
23	C	506	CLA	C3B-C2B	6.12	1.48	1.40
23	b	606	CLA	C3C-C2C	6.11	1.49	1.36
23	B	603	CLA	C3B-C2B	6.10	1.48	1.40
23	c	516	CLA	C3B-C2B	6.10	1.48	1.40
23	c	509	CLA	C3B-C2B	6.09	1.48	1.40
23	b	617	CLA	MG-ND	-6.08	1.93	2.05
23	b	608	CLA	MG-NC	6.08	2.20	2.06
23	d	408	CLA	C3B-C2B	6.08	1.48	1.40
23	A	405	CLA	C3B-C2B	6.07	1.48	1.40
23	d	409	CLA	C3B-C2B	6.07	1.48	1.40
23	c	510	CLA	MG-NC	6.07	2.20	2.06
23	c	508	CLA	C1D-ND	6.06	1.45	1.37
23	b	620	CLA	C3B-C2B	6.06	1.48	1.40
23	B	602	CLA	C3C-C2C	6.05	1.49	1.36
23	c	507	CLA	C3B-C2B	6.05	1.48	1.40
23	B	606	CLA	C3B-C2B	6.05	1.48	1.40
23	b	609	CLA	C1D-ND	6.03	1.45	1.37
23	C	513	CLA	MG-NC	6.03	2.20	2.06
23	c	513	CLA	C1D-ND	6.03	1.45	1.37
23	C	507	CLA	C1D-ND	6.01	1.45	1.37
23	B	602	CLA	MG-NC	6.00	2.20	2.06
23	B	609	CLA	C3B-C2B	6.00	1.48	1.40
23	b	610	CLA	MG-NC	5.99	2.20	2.06
23	c	511	CLA	C3C-C2C	5.99	1.49	1.36
23	c	516	CLA	C1D-ND	5.99	1.45	1.37
23	C	509	CLA	C3C-C2C	5.99	1.49	1.36
23	c	506	CLA	C3C-C2C	5.98	1.49	1.36
23	C	513	CLA	C3B-C2B	5.97	1.48	1.40
23	B	605	CLA	C1D-ND	5.97	1.45	1.37
23	c	516	CLA	MG-NC	5.97	2.20	2.06
42	v	201	HEC	C2B-C3B	-5.97	1.34	1.40
23	b	619	CLA	C1D-ND	5.96	1.45	1.37
23	B	610	CLA	C3C-C2C	5.96	1.49	1.36
23	d	409	CLA	C3C-C2C	5.96	1.49	1.36
23	B	604	CLA	C1D-ND	5.96	1.45	1.37
23	C	502	CLA	MG-ND	-5.95	1.94	2.05
23	C	506	CLA	C1D-ND	5.95	1.45	1.37
23	B	602	CLA	C1D-ND	5.94	1.45	1.37
23	C	511	CLA	C3B-C2B	5.94	1.48	1.40
23	b	614	CLA	C1D-ND	5.94	1.45	1.37
23	C	510	CLA	C1D-ND	5.94	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	615	CLA	C3B-C2B	5.92	1.48	1.40
23	C	511	CLA	C3C-C2C	5.92	1.49	1.36
23	a	2613	CLA	C3C-C2C	5.91	1.49	1.36
23	a	2613	CLA	C3B-C2B	5.91	1.48	1.40
23	b	607	CLA	C1D-ND	5.91	1.45	1.37
23	B	608	CLA	C3B-C2B	5.90	1.48	1.40
23	b	612	CLA	C3C-C2C	5.90	1.49	1.36
23	b	618	CLA	MG-NA	5.90	2.20	2.06
23	C	513	CLA	C3C-C2C	5.89	1.49	1.36
23	c	512	CLA	C1D-ND	5.89	1.45	1.37
23	c	504	CLA	C3B-C2B	5.89	1.48	1.40
23	C	503	CLA	C3C-C2C	5.88	1.49	1.36
23	C	505	CLA	MG-NC	5.87	2.20	2.06
23	C	509	CLA	MG-NC	5.87	2.20	2.06
23	b	614	CLA	C3C-C2C	5.87	1.49	1.36
23	c	505	CLA	C3C-C2C	5.86	1.49	1.36
23	C	514	CLA	C3B-C2B	5.86	1.48	1.40
23	B	614	CLA	C1D-ND	5.86	1.45	1.37
23	A	410	CLA	C3B-C2B	5.86	1.48	1.40
23	B	617	CLA	C1D-ND	5.86	1.45	1.37
23	B	611	CLA	C3C-C2C	5.86	1.49	1.36
23	B	616	CLA	MG-ND	-5.85	1.94	2.05
23	C	507	CLA	C3C-C2C	5.85	1.49	1.36
23	B	612	CLA	C1D-ND	5.85	1.45	1.37
23	b	613	CLA	C3B-C2B	5.85	1.48	1.40
23	b	619	CLA	C3B-C2B	5.84	1.48	1.40
23	B	611	CLA	C1D-ND	5.84	1.45	1.37
23	C	506	CLA	C3C-C2C	5.84	1.49	1.36
23	d	408	CLA	MG-ND	-5.83	1.94	2.05
23	C	505	CLA	C3B-C2B	5.83	1.48	1.40
23	c	515	CLA	C3C-C2C	5.83	1.49	1.36
23	b	608	CLA	C3C-C2C	5.83	1.49	1.36
23	D	2303	CLA	C3C-C2C	5.83	1.49	1.36
23	b	607	CLA	MG-ND	-5.82	1.94	2.05
23	c	508	CLA	C3B-C2B	5.82	1.48	1.40
23	B	607	CLA	C3C-C2C	5.82	1.49	1.36
23	b	618	CLA	C3C-C2C	5.82	1.49	1.36
23	a	2610	CLA	MG-ND	-5.81	1.94	2.05
23	c	516	CLA	MG-ND	-5.81	1.94	2.05
23	C	510	CLA	C3C-C2C	5.81	1.49	1.36
26	d	417	SQD	O47-C7	5.80	1.46	1.33
23	A	405	CLA	C3C-C2C	5.80	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	C3B-C2B	5.79	1.48	1.40
23	b	615	CLA	C3C-C2C	5.78	1.49	1.36
23	C	513	CLA	C1D-ND	5.78	1.44	1.37
23	a	2613	CLA	MG-NC	5.78	2.20	2.06
23	c	509	CLA	C3C-C2C	5.77	1.49	1.36
23	C	504	CLA	C3C-C2C	5.75	1.49	1.36
23	c	511	CLA	C1D-ND	5.74	1.44	1.37
23	d	409	CLA	C1D-ND	5.74	1.44	1.37
23	b	610	CLA	C3C-C2C	5.73	1.48	1.36
23	b	613	CLA	C1D-ND	5.73	1.44	1.37
23	b	620	CLA	C1D-ND	5.72	1.44	1.37
23	C	512	CLA	C3C-C2C	5.71	1.48	1.36
23	C	514	CLA	C3C-C2C	5.71	1.48	1.36
23	b	621	CLA	C1D-ND	5.71	1.44	1.37
23	b	607	CLA	C3C-C2C	5.69	1.48	1.36
23	c	508	CLA	MG-NC	5.68	2.19	2.06
23	B	615	CLA	MG-NA	5.68	2.19	2.06
23	C	513	CLA	CHC-C1C	5.68	1.49	1.35
23	B	607	CLA	C1D-ND	5.68	1.44	1.37
23	C	504	CLA	C1D-ND	5.68	1.44	1.37
23	b	620	CLA	MG-NC	5.67	2.19	2.06
23	a	2609	CLA	C3C-C2C	5.67	1.48	1.36
23	B	609	CLA	C1D-ND	5.67	1.44	1.37
23	B	603	CLA	C1D-ND	5.67	1.44	1.37
23	B	611	CLA	MG-NC	5.66	2.19	2.06
23	b	617	CLA	MG-NC	5.66	2.19	2.06
23	C	514	CLA	MG-ND	-5.66	1.94	2.05
23	B	615	CLA	C3C-C2C	5.66	1.48	1.36
23	c	505	CLA	MG-NC	5.66	2.19	2.06
23	d	402	CLA	MG-NA	5.65	2.19	2.06
23	B	616	CLA	C3B-C2B	5.64	1.48	1.40
23	b	611	CLA	C3C-C2C	5.64	1.48	1.36
24	A	408	PHO	C3D-C2D	5.64	1.49	1.39
23	B	603	CLA	C3C-C2C	5.63	1.48	1.36
23	C	502	CLA	C3C-C2C	5.63	1.48	1.36
23	B	604	CLA	C3C-C2C	5.62	1.48	1.36
23	a	2610	CLA	C1D-ND	5.62	1.44	1.37
23	B	602	CLA	CHC-C1C	5.62	1.49	1.35
23	b	617	CLA	C3C-C2C	5.61	1.48	1.36
23	C	502	CLA	CHC-C1C	5.60	1.49	1.35
23	c	506	CLA	C3B-C2B	5.60	1.48	1.40
23	a	2613	CLA	C1D-ND	5.60	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	C1D-ND	5.59	1.44	1.37
23	A	410	CLA	C1D-ND	5.59	1.44	1.37
23	d	402	CLA	C3C-C2C	5.59	1.48	1.36
42	V	201	HEC	C2B-C3B	-5.59	1.34	1.40
23	A	405	CLA	MG-ND	-5.58	1.94	2.05
23	B	609	CLA	C3C-C2C	5.57	1.48	1.36
23	b	609	CLA	C3C-C2C	5.57	1.48	1.36
23	b	608	CLA	C1D-ND	5.57	1.44	1.37
23	c	516	CLA	C3C-C2C	5.57	1.48	1.36
23	b	620	CLA	CHC-C1C	5.56	1.49	1.35
23	d	402	CLA	C3B-C2B	5.56	1.48	1.40
23	B	608	CLA	C3C-C2C	5.56	1.48	1.36
23	c	513	CLA	C3C-C2C	5.56	1.48	1.36
23	D	2304	CLA	CHC-C1C	5.55	1.49	1.35
23	C	505	CLA	C1D-ND	5.54	1.44	1.37
23	A	407	CLA	C3C-C2C	5.53	1.48	1.36
23	c	505	CLA	C1D-ND	5.53	1.44	1.37
23	b	608	CLA	MG-ND	-5.53	1.94	2.05
23	b	610	CLA	C1D-ND	5.53	1.44	1.37
23	c	508	CLA	C3C-C2C	5.52	1.48	1.36
23	c	512	CLA	C3C-C2C	5.52	1.48	1.36
23	b	620	CLA	C3C-C2C	5.51	1.48	1.36
23	B	606	CLA	C1D-ND	5.51	1.44	1.37
23	b	613	CLA	C3C-C2C	5.50	1.48	1.36
23	b	606	CLA	CHC-C1C	5.50	1.49	1.35
23	C	502	CLA	C3B-C2B	5.49	1.48	1.40
23	C	507	CLA	C3B-C2B	5.49	1.48	1.40
23	C	514	CLA	CHC-C1C	5.49	1.49	1.35
23	b	614	CLA	C3B-C2B	5.48	1.48	1.40
23	B	607	CLA	CHC-C1C	5.48	1.49	1.35
23	d	402	CLA	C1D-ND	5.48	1.44	1.37
23	c	514	CLA	C3C-C2C	5.48	1.48	1.36
23	C	505	CLA	C3C-C2C	5.47	1.48	1.36
23	c	516	CLA	CHC-C1C	5.47	1.49	1.35
23	b	616	CLA	C1D-ND	5.47	1.44	1.37
23	b	619	CLA	C3C-C2C	5.46	1.48	1.36
23	b	618	CLA	C1D-ND	5.46	1.44	1.37
23	b	608	CLA	C3B-C2B	5.46	1.47	1.40
23	B	613	CLA	MG-NA	5.45	2.19	2.06
23	B	604	CLA	CHC-C1C	5.44	1.48	1.35
23	c	515	CLA	MG-NC	5.44	2.19	2.06
23	a	2610	CLA	C3C-C2C	5.44	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	C1D-ND	5.44	1.44	1.37
23	c	513	CLA	MG-NC	5.43	2.19	2.06
23	B	615	CLA	C1D-ND	5.43	1.44	1.37
23	C	508	CLA	C3C-C2C	5.42	1.48	1.36
23	A	410	CLA	C3C-C2C	5.42	1.48	1.36
23	d	408	CLA	C3C-C2C	5.42	1.48	1.36
23	c	505	CLA	CHC-C1C	5.42	1.48	1.35
23	C	506	CLA	CHC-C1C	5.41	1.48	1.35
23	A	410	CLA	MG-NA	5.41	2.19	2.06
23	c	507	CLA	C3C-C2C	5.41	1.48	1.36
23	a	2609	CLA	MG-NA	5.40	2.19	2.06
23	b	615	CLA	CHC-C1C	5.40	1.48	1.35
23	c	506	CLA	C1D-ND	5.38	1.44	1.37
23	B	617	CLA	MG-NC	5.38	2.19	2.06
23	c	506	CLA	CHC-C1C	5.37	1.48	1.35
23	B	612	CLA	C3C-C2C	5.37	1.48	1.36
23	b	614	CLA	O2D-CGD	5.36	1.46	1.33
23	b	617	CLA	C1D-ND	5.35	1.44	1.37
23	c	510	CLA	C1D-ND	5.35	1.44	1.37
23	a	2610	CLA	C3B-C2B	5.35	1.47	1.40
23	c	504	CLA	C3C-C2C	5.34	1.48	1.36
23	B	609	CLA	CHC-C1C	5.34	1.48	1.35
23	c	514	CLA	C1D-ND	5.34	1.44	1.37
23	B	608	CLA	C1D-ND	5.34	1.44	1.37
23	b	614	CLA	CHC-C1C	5.34	1.48	1.35
23	c	510	CLA	C3C-C2C	5.34	1.48	1.36
23	C	506	CLA	CHD-C1D	5.33	1.48	1.38
23	C	509	CLA	CHC-C1C	5.33	1.48	1.35
23	c	515	CLA	CHC-C1C	5.33	1.48	1.35
23	c	511	CLA	CHC-C1C	5.32	1.48	1.35
23	B	615	CLA	CHC-C1C	5.32	1.48	1.35
23	C	507	CLA	CHC-C1C	5.32	1.48	1.35
23	B	617	CLA	C3C-C2C	5.31	1.48	1.36
23	b	610	CLA	MG-ND	-5.31	1.95	2.05
23	a	2609	CLA	C1D-ND	5.30	1.44	1.37
23	b	606	CLA	CHD-C1D	5.30	1.48	1.38
23	B	610	CLA	C3B-C2B	5.30	1.47	1.40
23	b	616	CLA	C3C-C2C	5.29	1.48	1.36
23	a	2610	CLA	CHC-C1C	5.29	1.48	1.35
23	C	503	CLA	CHC-C1C	5.28	1.48	1.35
42	v	201	HEC	C3D-C2D	5.28	1.53	1.37
23	d	409	CLA	CHC-C1C	5.28	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	C3C-C2C	5.28	1.47	1.36
23	B	604	CLA	C3B-C2B	5.28	1.47	1.40
23	B	614	CLA	C3C-C2C	5.27	1.47	1.36
23	C	504	CLA	CHC-C1C	5.27	1.48	1.35
23	C	505	CLA	MG-NA	5.27	2.18	2.06
23	c	514	CLA	CHC-C1C	5.27	1.48	1.35
23	A	407	CLA	CHC-C1C	5.26	1.48	1.35
23	B	614	CLA	O2D-CGD	5.26	1.46	1.33
23	b	619	CLA	MG-NA	5.26	2.18	2.06
23	C	511	CLA	C1D-ND	5.25	1.44	1.37
23	B	611	CLA	CHC-C1C	5.25	1.48	1.35
23	c	507	CLA	CHC-C1C	5.25	1.48	1.35
23	c	513	CLA	CHC-C1C	5.24	1.48	1.35
24	a	2611	PHO	C3D-C2D	5.24	1.48	1.39
23	B	610	CLA	O2D-CGD	5.24	1.46	1.33
23	A	410	CLA	CHC-C1C	5.24	1.48	1.35
23	B	616	CLA	C1D-ND	5.23	1.44	1.37
23	C	508	CLA	MG-NC	5.23	2.18	2.06
23	A	406	CLA	C3C-C2C	5.23	1.47	1.36
23	C	505	CLA	CHC-C1C	5.23	1.48	1.35
23	b	619	CLA	CHC-C1C	5.23	1.48	1.35
23	B	606	CLA	MG-NC	5.23	2.18	2.06
23	B	606	CLA	CHC-C1C	5.22	1.48	1.35
23	C	503	CLA	C1D-ND	5.22	1.44	1.37
23	C	512	CLA	C1D-ND	5.21	1.44	1.37
23	B	610	CLA	CHC-C1C	5.21	1.48	1.35
23	C	511	CLA	CHC-C1C	5.20	1.48	1.35
24	A	409	PHO	C3D-C2D	5.20	1.48	1.39
23	C	512	CLA	CHC-C1C	5.19	1.48	1.35
23	C	507	CLA	O2D-CGD	5.19	1.45	1.33
23	A	407	CLA	C1D-ND	5.19	1.44	1.37
23	B	616	CLA	C3C-C2C	5.19	1.47	1.36
23	a	2613	CLA	CHC-C1C	5.19	1.48	1.35
23	b	609	CLA	CHC-C1C	5.18	1.48	1.35
23	B	606	CLA	C3C-C2C	5.18	1.47	1.36
23	B	612	CLA	CHC-C1C	5.18	1.48	1.35
23	b	621	CLA	C3C-C2C	5.18	1.47	1.36
23	c	504	CLA	CHC-C1C	5.17	1.48	1.35
23	B	611	CLA	C3B-C2B	5.17	1.47	1.40
23	b	607	CLA	CHC-C1C	5.17	1.48	1.35
23	B	613	CLA	C3C-C2C	5.17	1.47	1.36
23	c	509	CLA	O2D-CGD	5.16	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	CHD-C1D	5.16	1.48	1.38
23	B	614	CLA	CHC-C1C	5.15	1.48	1.35
23	b	618	CLA	CHC-C1C	5.15	1.48	1.35
23	b	606	CLA	O2D-CGD	5.15	1.45	1.33
23	A	406	CLA	MG-NA	5.15	2.18	2.06
23	b	621	CLA	O2D-CGD	5.15	1.45	1.33
23	B	613	CLA	CHC-C1C	5.14	1.48	1.35
24	a	2612	PHO	C3D-C2D	5.14	1.48	1.39
23	B	603	CLA	CHC-C1C	5.13	1.48	1.35
23	b	608	CLA	CHC-C1C	5.13	1.48	1.35
23	A	405	CLA	C1D-ND	5.13	1.44	1.37
23	C	502	CLA	CHD-C1D	5.13	1.48	1.38
23	c	509	CLA	CHC-C1C	5.12	1.48	1.35
42	V	201	HEC	C3D-C2D	5.11	1.52	1.37
23	A	406	CLA	C1D-ND	5.10	1.44	1.37
23	D	2303	CLA	MG-NC	5.09	2.18	2.06
23	B	614	CLA	MG-ND	-5.09	1.95	2.05
23	c	507	CLA	O2D-CGD	5.09	1.45	1.33
23	A	410	CLA	MG-NC	5.08	2.18	2.06
23	b	611	CLA	CHC-C1C	5.08	1.48	1.35
23	d	408	CLA	CHC-C1C	5.08	1.48	1.35
23	b	613	CLA	MG-NC	5.08	2.18	2.06
23	b	613	CLA	CHC-C1C	5.07	1.48	1.35
23	B	615	CLA	C3B-C2B	5.07	1.47	1.40
23	C	510	CLA	CHC-C1C	5.07	1.48	1.35
23	B	602	CLA	O2D-CGD	5.06	1.45	1.33
23	b	613	CLA	O2D-CGD	5.06	1.45	1.33
23	B	608	CLA	CHC-C1C	5.06	1.47	1.35
23	c	512	CLA	CHC-C1C	5.04	1.47	1.35
23	b	614	CLA	CHD-C1D	5.04	1.48	1.38
23	c	508	CLA	CHC-C1C	5.03	1.47	1.35
23	B	616	CLA	CHC-C1C	5.03	1.47	1.35
23	b	619	CLA	O2D-CGD	5.03	1.45	1.33
23	b	606	CLA	MG-ND	-5.03	1.95	2.05
23	b	620	CLA	O2D-CGD	5.03	1.45	1.33
23	b	617	CLA	CHC-C1C	5.02	1.47	1.35
23	a	2609	CLA	CHC-C1C	5.02	1.47	1.35
23	b	607	CLA	O2D-CGD	5.02	1.45	1.33
23	d	402	CLA	CHC-C1C	5.01	1.47	1.35
23	b	616	CLA	CHC-C1C	5.00	1.47	1.35
23	B	617	CLA	CHC-C1C	5.00	1.47	1.35
42	V	201	HEC	C3C-C2C	-5.00	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	505	CLA	O2D-CGD	4.99	1.45	1.33
23	c	513	CLA	O2D-CGD	4.99	1.45	1.33
23	a	2613	CLA	O2D-CGD	4.99	1.45	1.33
23	C	505	CLA	O2D-CGD	4.98	1.45	1.33
23	b	619	CLA	MG-NC	4.98	2.18	2.06
23	B	613	CLA	O2D-CGD	4.96	1.45	1.33
24	A	409	PHO	O2D-CGD	4.95	1.45	1.33
23	c	514	CLA	CHD-C1D	4.95	1.48	1.38
23	C	508	CLA	CHC-C1C	4.95	1.47	1.35
24	a	2611	PHO	O2D-CGD	4.94	1.45	1.33
23	c	509	CLA	CHD-C1D	4.94	1.48	1.38
23	c	505	CLA	MG-ND	-4.94	1.96	2.05
23	d	409	CLA	O2D-CGD	4.93	1.45	1.33
23	B	616	CLA	O2D-CGD	4.93	1.45	1.33
23	c	507	CLA	MG-ND	-4.92	1.96	2.05
23	B	604	CLA	MG-ND	-4.92	1.96	2.05
23	b	612	CLA	CHC-C1C	4.91	1.47	1.35
23	d	402	CLA	O2D-CGD	4.91	1.45	1.33
23	b	612	CLA	MG-ND	-4.91	1.96	2.05
23	b	610	CLA	CHC-C1C	4.91	1.47	1.35
23	C	510	CLA	O2D-CGD	4.90	1.45	1.33
23	C	514	CLA	CHD-C1D	4.89	1.47	1.38
23	c	511	CLA	CHD-C1D	4.89	1.47	1.38
23	b	616	CLA	O2D-CGD	4.88	1.45	1.33
23	C	506	CLA	O2D-CGD	4.88	1.45	1.33
23	C	511	CLA	MG-NC	4.88	2.17	2.06
23	D	2303	CLA	CHC-C1C	4.88	1.47	1.35
23	C	514	CLA	O2D-CGD	4.88	1.45	1.33
24	a	2612	PHO	O2D-CGD	4.87	1.45	1.33
23	B	603	CLA	CHD-C1D	4.86	1.47	1.38
23	b	618	CLA	O2D-CGD	4.86	1.45	1.33
23	b	607	CLA	CHD-C1D	4.85	1.47	1.38
23	A	407	CLA	O2D-CGD	4.85	1.45	1.33
23	B	617	CLA	O2D-CGD	4.85	1.45	1.33
23	c	507	CLA	C1D-ND	4.85	1.43	1.37
23	B	607	CLA	CHD-C1D	4.83	1.47	1.38
23	A	410	CLA	CHD-C1D	4.82	1.47	1.38
23	C	508	CLA	O2D-CGD	4.82	1.45	1.33
23	c	516	CLA	CHD-C1D	4.82	1.47	1.38
24	A	408	PHO	O2D-CGD	4.81	1.44	1.33
23	D	2304	CLA	O2D-CGD	4.81	1.44	1.33
23	c	512	CLA	O2D-CGD	4.80	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	615	CLA	MG-NC	4.80	2.17	2.06
23	c	516	CLA	O2D-CGD	4.80	1.44	1.33
23	C	502	CLA	O2D-CGD	4.80	1.44	1.33
23	b	621	CLA	CHC-C1C	4.79	1.47	1.35
23	c	504	CLA	C1D-ND	4.79	1.43	1.37
23	C	513	CLA	O2D-CGD	4.79	1.44	1.33
23	b	617	CLA	O2D-CGD	4.79	1.44	1.33
23	b	611	CLA	O2D-CGD	4.79	1.44	1.33
23	b	616	CLA	CHD-C1D	4.78	1.47	1.38
23	b	612	CLA	MG-NC	4.78	2.17	2.06
23	B	606	CLA	CHD-C1D	4.77	1.47	1.38
23	C	512	CLA	CHD-C1D	4.77	1.47	1.38
23	A	405	CLA	CHC-C1C	4.77	1.47	1.35
23	A	407	CLA	C3B-C2B	4.77	1.47	1.40
23	C	503	CLA	O2D-CGD	4.76	1.44	1.33
23	C	509	CLA	O2D-CGD	4.76	1.44	1.33
23	B	614	CLA	MG-NC	4.76	2.17	2.06
23	b	608	CLA	O2D-CGD	4.75	1.44	1.33
23	C	513	CLA	CHD-C1D	4.75	1.47	1.38
23	b	612	CLA	O2D-CGD	4.74	1.44	1.33
23	c	508	CLA	O2D-CGD	4.74	1.44	1.33
23	C	503	CLA	CHD-C1D	4.73	1.47	1.38
23	A	410	CLA	MG-ND	-4.73	1.96	2.05
23	C	512	CLA	O2D-CGD	4.72	1.44	1.33
23	B	608	CLA	O2D-CGD	4.72	1.44	1.33
23	B	607	CLA	O2D-CGD	4.72	1.44	1.33
23	C	512	CLA	MG-ND	-4.71	1.96	2.05
23	b	608	CLA	CHD-C1D	4.71	1.47	1.38
23	b	610	CLA	O2D-CGD	4.70	1.44	1.33
23	B	610	CLA	CHD-C1D	4.70	1.47	1.38
23	B	605	CLA	CHC-C1C	4.70	1.47	1.35
23	c	510	CLA	O2D-CGD	4.69	1.44	1.33
23	C	505	CLA	CHD-C1D	4.68	1.47	1.38
23	B	606	CLA	O2D-CGD	4.68	1.44	1.33
23	c	513	CLA	CHD-C1D	4.68	1.47	1.38
23	b	609	CLA	O2D-CGD	4.67	1.44	1.33
23	A	405	CLA	O2D-CGD	4.67	1.44	1.33
23	c	504	CLA	O2D-CGD	4.67	1.44	1.33
23	c	510	CLA	CHC-C1C	4.66	1.46	1.35
23	c	515	CLA	O2D-CGD	4.66	1.44	1.33
23	B	603	CLA	O2D-CGD	4.64	1.44	1.33
23	B	604	CLA	O2D-CGD	4.64	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	O2D-CGD	4.63	1.44	1.33
23	C	509	CLA	MG-NA	4.63	2.17	2.06
23	c	511	CLA	MG-NA	4.63	2.17	2.06
23	b	613	CLA	CHD-C1D	4.62	1.47	1.38
23	d	402	CLA	CHD-C1D	4.62	1.47	1.38
34	c	532	DMS	O-S	4.62	1.81	1.50
34	o	311	DMS	O-S	4.61	1.81	1.50
23	A	410	CLA	O2D-CGD	4.61	1.44	1.33
23	B	608	CLA	MG-NC	4.60	2.17	2.06
23	A	407	CLA	CHD-C1D	4.60	1.47	1.38
23	a	2610	CLA	O2D-CGD	4.59	1.44	1.33
23	D	2304	CLA	C1D-ND	4.59	1.43	1.37
23	b	612	CLA	CHD-C1D	4.59	1.47	1.38
23	c	512	CLA	CHD-C1D	4.59	1.47	1.38
23	C	508	CLA	MG-ND	-4.59	1.96	2.05
34	b	637	DMS	O-S	4.59	1.81	1.50
23	B	611	CLA	CHD-C1D	4.59	1.47	1.38
34	c	544	DMS	O-S	4.58	1.81	1.50
23	B	611	CLA	MG-ND	-4.58	1.96	2.05
34	a	2624	DMS	O-S	4.58	1.81	1.50
23	b	612	CLA	C1D-ND	4.58	1.43	1.37
23	C	508	CLA	CHD-C1D	4.57	1.47	1.38
23	B	602	CLA	O2A-CGA	4.57	1.46	1.33
23	d	408	CLA	O2A-CGA	4.57	1.46	1.33
27	m	2802	LMG	O8-C28	4.57	1.46	1.33
23	B	612	CLA	O2D-CGD	4.56	1.44	1.33
34	A	430	DMS	O-S	4.56	1.81	1.50
23	b	620	CLA	MG-ND	-4.56	1.96	2.05
34	B	643	DMS	O-S	4.56	1.81	1.50
23	b	611	CLA	CHD-C1D	4.56	1.47	1.38
34	o	316	DMS	O-S	4.56	1.81	1.50
23	B	609	CLA	CHD-C1D	4.56	1.47	1.38
23	A	406	CLA	CHC-C1C	4.56	1.46	1.35
23	C	507	CLA	CHD-C1D	4.56	1.47	1.38
34	c	549	DMS	O-S	4.56	1.81	1.50
34	o	313	DMS	O-S	4.55	1.81	1.50
34	D	2316	DMS	O-S	4.55	1.81	1.50
23	A	406	CLA	O2D-CGD	4.55	1.44	1.33
23	b	620	CLA	CHD-C1D	4.55	1.47	1.38
34	V	206	DMS	O-S	4.54	1.80	1.50
23	B	603	CLA	MG-NC	4.54	2.17	2.06
34	C	531	DMS	O-S	4.54	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B	639	DMS	O-S	4.54	1.80	1.50
23	C	510	CLA	MG-NC	4.53	2.17	2.06
23	B	605	CLA	CHD-C1D	4.53	1.47	1.38
23	d	409	CLA	CHD-C1D	4.53	1.47	1.38
23	c	511	CLA	O2D-CGD	4.53	1.44	1.33
34	O	313	DMS	O-S	4.53	1.80	1.50
34	U	503	DMS	O-S	4.53	1.80	1.50
34	T	105	DMS	O-S	4.53	1.80	1.50
34	B	635	DMS	O-S	4.53	1.80	1.50
34	O	314	DMS	O-S	4.53	1.80	1.50
34	b	635	DMS	O-S	4.53	1.80	1.50
23	c	508	CLA	CHD-C1D	4.52	1.47	1.38
23	c	510	CLA	CHD-C1D	4.52	1.47	1.38
34	O	308	DMS	O-S	4.52	1.80	1.50
23	b	615	CLA	O2D-CGD	4.52	1.44	1.33
34	O	312	DMS	O-S	4.52	1.80	1.50
34	c	546	DMS	O-S	4.52	1.80	1.50
34	b	643	DMS	O-S	4.52	1.80	1.50
23	B	613	CLA	CHD-C1D	4.52	1.47	1.38
23	b	619	CLA	CHD-C1D	4.52	1.47	1.38
34	v	206	DMS	O-S	4.52	1.80	1.50
23	B	612	CLA	MG-NC	4.52	2.17	2.06
34	l	104	DMS	O-S	4.52	1.80	1.50
34	U	504	DMS	O-S	4.52	1.80	1.50
34	c	547	DMS	O-S	4.51	1.80	1.50
34	A	428	DMS	O-S	4.51	1.80	1.50
34	D	2317	DMS	O-S	4.51	1.80	1.50
34	O	315	DMS	O-S	4.51	1.80	1.50
34	C	528	DMS	O-S	4.51	1.80	1.50
34	V	205	DMS	O-S	4.51	1.80	1.50
34	b	641	DMS	O-S	4.51	1.80	1.50
23	B	611	CLA	O2D-CGD	4.51	1.44	1.33
34	c	542	DMS	O-S	4.51	1.80	1.50
34	B	644	DMS	O-S	4.51	1.80	1.50
34	t	102	DMS	O-S	4.51	1.80	1.50
34	c	537	DMS	O-S	4.51	1.80	1.50
34	B	646	DMS	O-S	4.51	1.80	1.50
34	c	540	DMS	O-S	4.51	1.80	1.50
34	A	426	DMS	O-S	4.51	1.80	1.50
34	o	309	DMS	O-S	4.50	1.80	1.50
34	B	637	DMS	O-S	4.50	1.80	1.50
34	c	538	DMS	O-S	4.50	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	A	429	DMS	O-S	4.50	1.80	1.50
34	B	641	DMS	O-S	4.50	1.80	1.50
34	B	645	DMS	O-S	4.50	1.80	1.50
34	b	636	DMS	O-S	4.50	1.80	1.50
34	V	208	DMS	O-S	4.50	1.80	1.50
26	l	101	SQD	O47-C7	4.50	1.47	1.34
34	c	545	DMS	O-S	4.50	1.80	1.50
23	b	618	CLA	CHD-C1D	4.50	1.47	1.38
34	o	306	DMS	O-S	4.50	1.80	1.50
34	V	211	DMS	O-S	4.50	1.80	1.50
34	o	305	DMS	O-S	4.49	1.80	1.50
34	D	2319	DMS	O-S	4.49	1.80	1.50
34	U	505	DMS	O-S	4.49	1.80	1.50
34	d	423	DMS	O-S	4.49	1.80	1.50
34	v	210	DMS	O-S	4.49	1.80	1.50
34	a	2620	DMS	O-S	4.49	1.80	1.50
23	C	509	CLA	CHD-C1D	4.49	1.47	1.38
34	C	537	DMS	O-S	4.49	1.80	1.50
27	c	522	LMG	O7-C10	4.49	1.47	1.34
34	B	647	DMS	O-S	4.49	1.80	1.50
34	O	317	DMS	O-S	4.49	1.80	1.50
34	v	214	DMS	O-S	4.49	1.80	1.50
23	b	615	CLA	CHD-C1D	4.49	1.47	1.38
34	O	311	DMS	O-S	4.49	1.80	1.50
34	V	210	DMS	O-S	4.49	1.80	1.50
34	O	309	DMS	O-S	4.49	1.80	1.50
34	T	104	DMS	O-S	4.49	1.80	1.50
23	c	506	CLA	O2D-CGD	4.48	1.44	1.33
34	o	315	DMS	O-S	4.48	1.80	1.50
34	X	101	DMS	O-S	4.48	1.80	1.50
34	v	208	DMS	O-S	4.48	1.80	1.50
34	v	211	DMS	O-S	4.48	1.80	1.50
34	V	212	DMS	O-S	4.48	1.80	1.50
34	v	212	DMS	O-S	4.48	1.80	1.50
34	O	319	DMS	O-S	4.48	1.80	1.50
34	H	104	DMS	O-S	4.48	1.80	1.50
34	c	541	DMS	O-S	4.48	1.80	1.50
34	b	639	DMS	O-S	4.48	1.80	1.50
34	c	539	DMS	O-S	4.48	1.80	1.50
23	B	605	CLA	O2D-CGD	4.48	1.44	1.33
23	c	505	CLA	CHD-C1D	4.48	1.47	1.38
34	c	548	DMS	O-S	4.48	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406	CLA	O2A-CGA	4.48	1.46	1.33
34	b	642	DMS	O-S	4.48	1.80	1.50
27	C	527	LMG	O7-C10	4.48	1.46	1.34
37	C	519	DGD	O1G-C1A	4.48	1.46	1.33
34	o	310	DMS	O-S	4.48	1.80	1.50
34	A	427	DMS	O-S	4.47	1.80	1.50
34	C	536	DMS	O-S	4.47	1.80	1.50
34	b	638	DMS	O-S	4.47	1.80	1.50
34	V	207	DMS	O-S	4.47	1.80	1.50
34	V	213	DMS	O-S	4.47	1.80	1.50
34	C	530	DMS	O-S	4.47	1.80	1.50
34	a	2621	DMS	O-S	4.47	1.80	1.50
26	a	2603	SQD	O47-C7	4.47	1.46	1.34
34	O	318	DMS	O-S	4.47	1.80	1.50
34	O	306	DMS	O-S	4.47	1.80	1.50
34	a	2622	DMS	O-S	4.46	1.80	1.50
34	d	419	DMS	O-S	4.46	1.80	1.50
34	D	2320	DMS	O-S	4.46	1.80	1.50
34	v	209	DMS	O-S	4.46	1.80	1.50
34	v	213	DMS	O-S	4.46	1.80	1.50
34	d	421	DMS	O-S	4.46	1.80	1.50
34	o	308	DMS	O-S	4.46	1.80	1.50
34	u	502	DMS	O-S	4.46	1.80	1.50
34	u	504	DMS	O-S	4.46	1.80	1.50
26	B	621	SQD	O47-C7	4.46	1.46	1.34
34	d	420	DMS	O-S	4.46	1.80	1.50
34	C	534	DMS	O-S	4.46	1.80	1.50
34	d	422	DMS	O-S	4.46	1.80	1.50
34	B	640	DMS	O-S	4.45	1.80	1.50
34	O	310	DMS	O-S	4.45	1.80	1.50
34	b	640	DMS	O-S	4.45	1.80	1.50
34	o	314	DMS	O-S	4.45	1.80	1.50
34	v	205	DMS	O-S	4.45	1.80	1.50
34	V	202	DMS	O-S	4.45	1.80	1.50
34	d	418	DMS	O-S	4.45	1.80	1.50
34	V	209	DMS	O-S	4.45	1.80	1.50
23	a	2609	CLA	CHD-C1D	4.45	1.47	1.38
34	c	543	DMS	O-S	4.45	1.80	1.50
38	e	101	LHG	O8-C23	4.45	1.46	1.33
34	A	425	DMS	O-S	4.45	1.80	1.50
34	C	535	DMS	O-S	4.45	1.80	1.50
34	c	536	DMS	O-S	4.45	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	2623	DMS	O-S	4.44	1.80	1.50
34	O	307	DMS	O-S	4.44	1.80	1.50
34	c	535	DMS	O-S	4.44	1.80	1.50
34	u	503	DMS	O-S	4.44	1.80	1.50
23	b	614	CLA	O2A-CGA	4.44	1.46	1.33
34	C	533	DMS	O-S	4.44	1.80	1.50
34	b	634	DMS	O-S	4.43	1.80	1.50
34	c	534	DMS	O-S	4.43	1.80	1.50
34	v	207	DMS	O-S	4.43	1.80	1.50
34	o	307	DMS	O-S	4.43	1.80	1.50
23	C	510	CLA	CHD-C1D	4.42	1.47	1.38
34	o	312	DMS	O-S	4.42	1.80	1.50
37	D	2307	DGD	O1G-C1A	4.42	1.46	1.33
23	B	615	CLA	MG-ND	-4.42	1.97	2.05
23	C	509	CLA	O2A-CGA	4.42	1.46	1.33
34	B	642	DMS	O-S	4.41	1.80	1.50
23	C	504	CLA	CHD-C1D	4.41	1.46	1.38
26	D	2302	SQD	O47-C7	4.41	1.46	1.34
34	O	316	DMS	O-S	4.41	1.80	1.50
34	C	529	DMS	O-S	4.40	1.80	1.50
23	c	516	CLA	O2A-CGA	4.39	1.46	1.33
23	B	617	CLA	CHD-C1D	4.39	1.46	1.38
27	C	520	LMG	O8-C28	4.38	1.46	1.33
34	A	424	DMS	O-S	4.38	1.79	1.50
34	C	532	DMS	O-S	4.37	1.79	1.50
23	C	510	CLA	O2A-CGA	4.37	1.46	1.33
23	B	615	CLA	O2A-CGA	4.37	1.46	1.33
34	c	533	DMS	O-S	4.37	1.79	1.50
23	B	602	CLA	CHD-C4C	4.37	1.49	1.39
38	E	101	LHG	O8-C23	4.37	1.46	1.33
23	B	608	CLA	O2A-CGA	4.37	1.46	1.33
26	d	417	SQD	O48-C23	4.36	1.46	1.33
23	c	514	CLA	O2D-CGD	4.36	1.43	1.33
23	B	613	CLA	C1D-ND	4.36	1.43	1.37
23	D	2303	CLA	O2D-CGD	4.36	1.43	1.33
23	d	408	CLA	O2D-CGD	4.36	1.43	1.33
23	B	609	CLA	O2D-CGD	4.36	1.43	1.33
26	D	2308	SQD	O47-C7	4.35	1.46	1.34
38	e	101	LHG	O7-C7	4.35	1.46	1.34
37	D	2307	DGD	O2G-C1B	4.35	1.46	1.34
27	c	501	LMG	O8-C28	4.34	1.46	1.33
23	C	511	CLA	CHD-C1D	4.34	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	409	PHO	CHA-CBD	-4.34	1.47	1.52
34	D	2318	DMS	O-S	4.34	1.79	1.50
23	b	606	CLA	O2A-CGA	4.33	1.46	1.33
23	B	610	CLA	O2A-CGA	4.33	1.46	1.33
23	C	502	CLA	CHD-C4C	4.33	1.49	1.39
23	d	402	CLA	OBD-CAD	4.32	1.29	1.22
23	B	604	CLA	CHD-C1D	4.32	1.46	1.38
23	d	408	CLA	C1D-ND	4.32	1.43	1.37
37	H	103	DGD	O1G-C1A	4.32	1.46	1.33
23	C	503	CLA	O2A-CGA	4.32	1.46	1.33
23	D	2303	CLA	O2A-CGA	4.31	1.45	1.33
23	B	614	CLA	CHD-C1D	4.31	1.46	1.38
34	B	636	DMS	O-S	4.31	1.79	1.50
23	C	504	CLA	O2D-CGD	4.30	1.43	1.33
23	b	606	CLA	CHD-C4C	4.30	1.49	1.39
23	B	615	CLA	CHD-C1D	4.30	1.46	1.38
23	B	608	CLA	CHD-C1D	4.29	1.46	1.38
23	c	510	CLA	OBD-CAD	4.29	1.29	1.22
26	D	2308	SQD	O48-C23	4.28	1.45	1.33
34	B	638	DMS	O-S	4.27	1.79	1.50
27	B	622	LMG	O8-C28	4.27	1.45	1.33
23	C	513	CLA	O2A-CGA	4.26	1.45	1.33
23	b	616	CLA	MG-NC	4.26	2.16	2.06
23	b	619	CLA	O2A-CGA	4.25	1.45	1.33
23	b	618	CLA	CHD-C4C	4.25	1.48	1.39
23	c	506	CLA	CHD-C1D	4.25	1.46	1.38
23	b	621	CLA	O2A-CGA	4.25	1.45	1.33
23	a	2613	CLA	CHD-C1D	4.25	1.46	1.38
38	E	101	LHG	O7-C7	4.25	1.46	1.34
23	b	617	CLA	CHD-C1D	4.25	1.46	1.38
23	b	609	CLA	CHD-C1D	4.24	1.46	1.38
23	A	405	CLA	OBD-CAD	4.24	1.29	1.22
34	o	304	DMS	O-S	4.23	1.78	1.50
23	b	620	CLA	C3D-C2D	4.23	1.50	1.39
23	C	506	CLA	O2A-CGA	4.23	1.45	1.33
23	a	2610	CLA	O2A-CGA	4.22	1.45	1.33
27	c	501	LMG	O7-C10	4.22	1.46	1.34
23	B	615	CLA	O2D-CGD	4.21	1.43	1.33
27	c	522	LMG	O8-C28	4.21	1.45	1.33
23	c	511	CLA	O2A-CGA	4.21	1.45	1.33
27	C	527	LMG	O8-C28	4.19	1.45	1.33
23	C	512	CLA	O2A-CGA	4.19	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	O2A-CGA	4.19	1.45	1.33
23	b	621	CLA	CHD-C1D	4.19	1.46	1.38
26	a	2603	SQD	O48-C23	4.19	1.45	1.33
23	b	611	CLA	O2A-CGA	4.19	1.45	1.33
34	b	633	DMS	O-S	4.19	1.78	1.50
23	b	613	CLA	O2A-CGA	4.18	1.45	1.33
24	A	409	PHO	OBD-CAD	4.18	1.28	1.22
23	B	604	CLA	O2A-CGA	4.18	1.45	1.33
23	b	618	CLA	MG-ND	-4.18	1.97	2.05
23	A	405	CLA	CHD-C1D	4.17	1.46	1.38
23	D	2304	CLA	MG-NC	4.17	2.16	2.06
23	c	514	CLA	O2A-CGA	4.17	1.45	1.33
23	B	609	CLA	O2A-CGA	4.17	1.45	1.33
23	c	515	CLA	O2A-CGA	4.17	1.45	1.33
23	b	617	CLA	O2A-CGA	4.17	1.45	1.33
23	C	508	CLA	O2A-CGA	4.17	1.45	1.33
27	c	521	LMG	O8-C28	4.16	1.45	1.33
23	B	612	CLA	CHD-C1D	4.16	1.46	1.38
24	A	408	PHO	O2A-CGA	4.16	1.45	1.33
23	c	504	CLA	CHD-C1D	4.16	1.46	1.38
23	C	505	CLA	CHD-C4C	4.16	1.48	1.39
23	B	614	CLA	O2A-CGA	4.16	1.45	1.33
23	a	2609	CLA	O2D-CGD	4.16	1.43	1.33
27	A	413	LMG	O8-C28	4.15	1.45	1.33
23	c	514	CLA	CHD-C4C	4.15	1.48	1.39
27	A	413	LMG	O7-C10	4.15	1.46	1.34
26	B	621	SQD	O48-C23	4.15	1.45	1.33
27	B	622	LMG	O7-C10	4.15	1.46	1.34
24	a	2611	PHO	OBD-CAD	4.15	1.28	1.22
23	D	2304	CLA	CHD-C4C	4.15	1.48	1.39
23	C	503	CLA	OBD-CAD	4.15	1.29	1.22
23	c	510	CLA	O2A-CGA	4.14	1.45	1.33
23	c	505	CLA	C3D-C2D	4.14	1.50	1.39
23	C	502	CLA	O2A-CGA	4.13	1.45	1.33
23	a	2610	CLA	CHD-C1D	4.13	1.46	1.38
23	c	507	CLA	CHD-C1D	4.12	1.46	1.38
27	m	2802	LMG	O7-C10	4.12	1.45	1.34
23	a	2613	CLA	O2A-CGA	4.11	1.45	1.33
36	d	407	HTG	C1'-S1	-4.11	1.76	1.81
38	d	412	LHG	O8-C23	4.11	1.45	1.33
26	D	2302	SQD	O48-C23	4.10	1.45	1.33
23	B	602	CLA	MG-ND	-4.10	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	509	CLA	O2A-CGA	4.10	1.45	1.33
23	c	513	CLA	OBD-CAD	4.10	1.29	1.22
38	L	101	LHG	O8-C23	4.10	1.45	1.33
23	c	515	CLA	CHD-C1D	4.10	1.46	1.38
23	B	611	CLA	MG-NA	4.10	2.16	2.06
37	c	520	DGD	O1G-C1A	4.10	1.45	1.33
23	b	607	CLA	O2A-CGA	4.10	1.45	1.33
23	c	512	CLA	O2A-CGA	4.09	1.45	1.33
23	d	402	CLA	C3D-C2D	4.08	1.50	1.39
27	d	414	LMG	O8-C28	4.08	1.45	1.33
36	i	102	HTG	C1'-S1	-4.08	1.76	1.81
23	C	502	CLA	OBD-CAD	4.08	1.29	1.22
23	B	613	CLA	MG-NC	4.07	2.15	2.06
23	B	613	CLA	OBD-CAD	4.07	1.29	1.22
36	H	101	HTG	C1'-S1	-4.07	1.76	1.81
23	D	2303	CLA	MG-NA	4.07	2.15	2.06
23	c	514	CLA	OBD-CAD	4.07	1.29	1.22
23	C	514	CLA	O2A-CGA	4.06	1.45	1.33
23	B	605	CLA	OBD-CAD	4.06	1.29	1.22
37	h	102	DGD	O2G-C1B	4.06	1.45	1.34
23	C	504	CLA	O2A-CGA	4.06	1.45	1.33
23	C	514	CLA	CHD-C4C	4.06	1.48	1.39
23	b	614	CLA	CHD-C4C	4.06	1.48	1.39
38	D	2309	LHG	O8-C23	4.06	1.45	1.33
23	D	2304	CLA	C3D-C2D	4.06	1.50	1.39
26	b	601	SQD	O48-C23	4.05	1.45	1.33
23	b	608	CLA	O2A-CGA	4.05	1.45	1.33
23	d	409	CLA	O2A-CGA	4.05	1.45	1.33
23	A	407	CLA	O2A-CGA	4.05	1.45	1.33
23	D	2303	CLA	C1D-ND	4.04	1.42	1.37
23	C	512	CLA	CHD-C4C	4.04	1.48	1.39
26	b	601	SQD	O47-C7	4.03	1.45	1.34
38	d	403	LHG	O7-C7	4.02	1.45	1.34
36	b	626	HTG	C1'-S1	-4.02	1.76	1.81
23	D	2304	CLA	O2A-CGA	4.01	1.45	1.33
37	C	519	DGD	O2G-C1B	4.01	1.45	1.34
23	a	2613	CLA	C3D-C2D	4.01	1.50	1.39
23	c	504	CLA	O2A-CGA	4.01	1.45	1.33
23	b	620	CLA	O2A-CGA	4.01	1.45	1.33
23	B	616	CLA	CHD-C1D	4.01	1.46	1.38
26	l	101	SQD	O48-C23	4.01	1.45	1.33
24	a	2612	PHO	OBD-CAD	4.00	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	2304	CLA	CHD-C1D	4.00	1.46	1.38
37	c	519	DGD	O2G-C1B	4.00	1.45	1.34
38	l	103	LHG	O8-C23	4.00	1.45	1.33
23	d	408	CLA	CHD-C1D	4.00	1.46	1.38
26	A	412	SQD	O47-C7	3.99	1.45	1.34
23	b	606	CLA	C3D-C2D	3.98	1.50	1.39
26	A	412	SQD	O48-C23	3.97	1.45	1.33
42	v	201	HEC	CBC-CAC	-3.97	1.34	1.49
23	c	515	CLA	CHD-C4C	3.97	1.48	1.39
37	h	102	DGD	O1G-C1A	3.97	1.44	1.33
26	a	2615	SQD	O48-C23	3.97	1.44	1.33
23	c	505	CLA	O2A-CGA	3.96	1.44	1.33
23	A	407	CLA	OBD-CAD	3.96	1.29	1.22
23	d	409	CLA	OBD-CAD	3.96	1.29	1.22
37	H	103	DGD	O2G-C1B	3.96	1.45	1.34
23	c	515	CLA	C3D-C2D	3.96	1.49	1.39
23	B	617	CLA	O2A-CGA	3.96	1.44	1.33
23	C	506	CLA	OBD-CAD	3.96	1.29	1.22
23	B	606	CLA	O2A-CGA	3.95	1.44	1.33
23	a	2610	CLA	CHD-C4C	3.95	1.48	1.39
23	a	2613	CLA	CHD-C4C	3.94	1.48	1.39
23	C	512	CLA	C3D-C2D	3.94	1.49	1.39
23	C	513	CLA	CHD-C4C	3.94	1.48	1.39
23	c	509	CLA	CHD-C4C	3.94	1.48	1.39
23	C	509	CLA	CHD-C4C	3.94	1.48	1.39
23	a	2609	CLA	OBD-CAD	3.94	1.29	1.22
27	D	2312	LMG	O8-C28	3.94	1.44	1.33
23	C	510	CLA	OBD-CAD	3.94	1.29	1.22
23	c	508	CLA	O2A-CGA	3.94	1.44	1.33
37	c	519	DGD	O1G-C1A	3.93	1.44	1.33
23	A	407	CLA	C3D-C2D	3.93	1.49	1.39
23	C	507	CLA	CHD-C4C	3.92	1.48	1.39
36	C	525	HTG	C1'-S1	-3.92	1.76	1.81
23	B	603	CLA	O2A-CGA	3.92	1.44	1.33
23	b	615	CLA	O2A-CGA	3.92	1.44	1.33
37	c	518	DGD	O1G-C1A	3.92	1.44	1.33
23	d	402	CLA	CHD-C4C	3.92	1.48	1.39
23	c	505	CLA	CHD-C4C	3.92	1.48	1.39
23	B	605	CLA	CHD-C4C	3.91	1.48	1.39
38	D	2310	LHG	O7-C7	3.91	1.45	1.34
36	I	101	HTG	C1'-S1	-3.91	1.76	1.81
24	A	408	PHO	OBD-CAD	3.90	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405	CLA	C3D-C2D	3.90	1.49	1.39
23	B	603	CLA	CHD-C4C	3.90	1.48	1.39
23	b	613	CLA	CHD-C4C	3.90	1.48	1.39
23	B	613	CLA	O2A-CGA	3.90	1.44	1.33
23	c	506	CLA	O2A-CGA	3.90	1.44	1.33
23	C	503	CLA	C3D-C2D	3.90	1.49	1.39
23	A	406	CLA	MG-NC	3.90	2.15	2.06
23	C	508	CLA	OBD-CAD	3.90	1.29	1.22
23	D	2304	CLA	MG-NA	3.90	2.15	2.06
23	A	407	CLA	CHD-C4C	3.89	1.48	1.39
37	c	520	DGD	O2G-C1B	3.89	1.45	1.34
23	B	609	CLA	C3D-C2D	3.89	1.49	1.39
42	V	201	HEC	CBC-CAC	-3.88	1.34	1.49
24	A	409	PHO	C3C-C2C	3.88	1.49	1.37
23	b	612	CLA	O2A-CGA	3.88	1.44	1.33
27	C	520	LMG	O7-C10	3.88	1.45	1.34
23	C	506	CLA	CHD-C4C	3.88	1.48	1.39
23	C	511	CLA	C3D-C2D	3.88	1.49	1.39
23	b	607	CLA	CHD-C4C	3.88	1.48	1.39
23	b	614	CLA	MG-ND	-3.88	1.98	2.05
23	b	616	CLA	CHD-C4C	3.87	1.48	1.39
23	A	410	CLA	O2A-CGA	3.87	1.44	1.33
23	b	614	CLA	OBD-CAD	3.87	1.29	1.22
23	B	607	CLA	O2A-CGA	3.87	1.44	1.33
23	b	608	CLA	OBD-CAD	3.86	1.29	1.22
23	A	407	CLA	MG-NC	3.86	2.15	2.06
23	d	409	CLA	CHD-C4C	3.86	1.48	1.39
38	d	403	LHG	O8-C23	3.86	1.44	1.33
23	A	410	CLA	OBD-CAD	3.86	1.29	1.22
23	c	513	CLA	O2A-CGA	3.86	1.44	1.33
23	c	512	CLA	OBD-CAD	3.86	1.29	1.22
23	B	610	CLA	OBD-CAD	3.86	1.29	1.22
37	C	518	DGD	O2G-C1B	3.86	1.45	1.34
23	a	2609	CLA	CHD-C4C	3.86	1.48	1.39
23	b	609	CLA	O2A-CGA	3.85	1.44	1.33
23	b	607	CLA	C3D-C2D	3.85	1.49	1.39
23	A	410	CLA	C3D-C2D	3.85	1.49	1.39
27	d	414	LMG	O7-C10	3.85	1.45	1.34
23	C	503	CLA	CHD-C4C	3.85	1.48	1.39
39	F	101	HEM	C3C-C2C	-3.84	1.35	1.40
23	c	512	CLA	CHD-C4C	3.84	1.48	1.39
37	C	518	DGD	O1G-C1A	3.84	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	C3D-C2D	3.84	1.49	1.39
23	B	616	CLA	OBD-CAD	3.84	1.29	1.22
23	B	608	CLA	CHD-C4C	3.84	1.48	1.39
23	b	620	CLA	CHD-C4C	3.84	1.48	1.39
23	C	510	CLA	CHD-C4C	3.84	1.48	1.39
23	B	602	CLA	C3D-C2D	3.84	1.49	1.39
26	a	2615	SQD	O47-C7	3.84	1.45	1.34
23	B	616	CLA	O2A-CGA	3.83	1.44	1.33
23	C	511	CLA	OBD-CAD	3.83	1.29	1.22
23	C	511	CLA	CHD-C4C	3.83	1.48	1.39
23	b	617	CLA	MG-NA	3.83	2.15	2.06
23	b	618	CLA	O2A-CGA	3.83	1.44	1.33
23	a	2610	CLA	C3D-C2D	3.83	1.49	1.39
23	C	505	CLA	MG-ND	-3.83	1.98	2.05
23	c	516	CLA	C3D-C2D	3.83	1.49	1.39
27	c	521	LMG	O7-C10	3.83	1.45	1.34
23	C	505	CLA	C3D-C2D	3.83	1.49	1.39
23	B	612	CLA	C3D-C2D	3.82	1.49	1.39
23	B	607	CLA	CHD-C4C	3.82	1.48	1.39
23	A	410	CLA	CHD-C4C	3.82	1.48	1.39
23	c	505	CLA	OBD-CAD	3.82	1.29	1.22
23	C	510	CLA	C3D-C2D	3.82	1.49	1.39
23	c	511	CLA	C3D-C2D	3.82	1.49	1.39
23	C	503	CLA	MG-NC	3.82	2.15	2.06
24	a	2612	PHO	O2A-CGA	3.81	1.44	1.33
23	b	614	CLA	C3D-C2D	3.81	1.49	1.39
23	C	505	CLA	O2A-CGA	3.81	1.44	1.33
23	B	606	CLA	MG-ND	-3.81	1.98	2.05
23	b	610	CLA	O2A-CGA	3.80	1.44	1.33
23	D	2303	CLA	CHD-C1D	3.80	1.45	1.38
23	B	615	CLA	CHD-C4C	3.80	1.47	1.39
36	b	602	HTG	C1'-S1	-3.79	1.76	1.81
23	b	606	CLA	OBD-CAD	3.79	1.29	1.22
23	d	409	CLA	C3D-C2D	3.79	1.49	1.39
23	c	507	CLA	CHD-C4C	3.78	1.47	1.39
23	B	617	CLA	C3D-C2D	3.78	1.49	1.39
38	D	2311	LHG	O8-C23	3.78	1.44	1.33
23	C	509	CLA	OBD-CAD	3.78	1.29	1.22
24	A	408	PHO	C3C-C2C	3.77	1.48	1.37
23	c	506	CLA	CHD-C4C	3.77	1.47	1.39
23	b	616	CLA	MG-ND	-3.77	1.98	2.05
39	e	103	HEM	C3C-CAC	3.77	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406	CLA	CHD-C1D	3.77	1.45	1.38
39	F	101	HEM	C3C-CAC	3.77	1.55	1.47
23	c	513	CLA	C3D-C2D	3.77	1.49	1.39
23	c	513	CLA	CHD-C4C	3.76	1.47	1.39
23	c	509	CLA	C3D-C2D	3.76	1.49	1.39
23	b	616	CLA	O2A-CGA	3.76	1.44	1.33
23	b	619	CLA	CHD-C4C	3.76	1.47	1.39
23	B	608	CLA	C3D-C2D	3.76	1.49	1.39
23	D	2303	CLA	CHD-C4C	3.76	1.47	1.39
24	A	409	PHO	O2A-CGA	3.75	1.44	1.33
42	v	201	HEC	CBB-CAB	-3.75	1.35	1.49
23	B	610	CLA	C3D-C2D	3.75	1.49	1.39
23	C	502	CLA	C3D-C2D	3.74	1.49	1.39
36	d	415	HTG	C1'-S1	-3.74	1.76	1.81
23	B	612	CLA	CHD-C4C	3.74	1.47	1.39
23	B	615	CLA	OBD-CAD	3.74	1.28	1.22
23	C	512	CLA	OBD-CAD	3.74	1.28	1.22
23	b	617	CLA	OBD-CAD	3.74	1.28	1.22
38	d	413	LHG	O7-C7	3.74	1.44	1.34
23	b	615	CLA	CHD-C4C	3.73	1.47	1.39
23	B	609	CLA	MG-NC	3.73	2.15	2.06
23	c	514	CLA	C3D-C2D	3.73	1.49	1.39
38	d	412	LHG	O7-C7	3.73	1.44	1.34
23	B	608	CLA	MG-ND	-3.72	1.98	2.05
37	C	517	DGD	O2G-C1B	3.72	1.44	1.34
23	C	513	CLA	C3D-C2D	3.71	1.49	1.39
23	b	611	CLA	C3D-C2D	3.71	1.49	1.39
23	B	614	CLA	CHD-C4C	3.71	1.47	1.39
23	c	504	CLA	OBD-CAD	3.71	1.28	1.22
23	c	507	CLA	O2A-CGA	3.71	1.44	1.33
23	b	609	CLA	C4D-CHA	3.70	1.51	1.38
23	b	610	CLA	CHD-C1D	3.70	1.45	1.38
36	B	625	HTG	C1'-S1	-3.70	1.76	1.81
23	c	515	CLA	OBD-CAD	3.70	1.28	1.22
23	c	516	CLA	CHD-C4C	3.70	1.47	1.39
23	B	616	CLA	C3D-C2D	3.70	1.49	1.39
23	b	616	CLA	C3D-C2D	3.70	1.49	1.39
23	A	405	CLA	CHD-C4C	3.70	1.47	1.39
36	c	524	HTG	C1'-S1	-3.70	1.76	1.81
23	A	406	CLA	OBD-CAD	3.69	1.28	1.22
23	B	604	CLA	CHD-C4C	3.69	1.47	1.39
23	B	614	CLA	OBD-CAD	3.69	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	OBD-CAD	3.69	1.28	1.22
36	b	604	HTG	C1'-S1	-3.68	1.76	1.81
23	b	611	CLA	CHD-C4C	3.68	1.47	1.39
23	d	408	CLA	C3D-C2D	3.68	1.49	1.39
23	B	603	CLA	C3D-C2D	3.68	1.49	1.39
23	c	508	CLA	CHD-C4C	3.68	1.47	1.39
23	B	612	CLA	O2A-CGA	3.67	1.44	1.33
38	L	101	LHG	O7-C7	3.67	1.44	1.34
23	b	612	CLA	C3D-C2D	3.67	1.49	1.39
23	B	603	CLA	OBD-CAD	3.67	1.28	1.22
24	a	2612	PHO	C3C-C2C	3.66	1.48	1.37
23	B	611	CLA	CHD-C4C	3.66	1.47	1.39
24	a	2611	PHO	O2A-CGA	3.66	1.44	1.33
23	C	513	CLA	OBD-CAD	3.65	1.28	1.22
23	B	608	CLA	OBD-CAD	3.65	1.28	1.22
23	C	514	CLA	OBD-CAD	3.65	1.28	1.22
23	b	609	CLA	OBD-CAD	3.64	1.28	1.22
23	c	511	CLA	CHD-C4C	3.64	1.47	1.39
23	b	615	CLA	OBD-CAD	3.64	1.28	1.22
23	B	611	CLA	C3D-C2D	3.64	1.49	1.39
23	b	609	CLA	CHD-C4C	3.64	1.47	1.39
23	C	508	CLA	CHD-C4C	3.64	1.47	1.39
39	e	103	HEM	C3C-C2C	-3.64	1.35	1.40
23	d	402	CLA	O2A-CGA	3.63	1.44	1.33
23	B	617	CLA	CHD-C4C	3.62	1.47	1.39
23	A	406	CLA	C3D-C2D	3.62	1.49	1.39
23	b	612	CLA	CHD-C4C	3.62	1.47	1.39
23	B	607	CLA	MG-ND	-3.61	1.98	2.05
37	C	517	DGD	O1G-C1A	3.61	1.43	1.33
23	b	617	CLA	C3D-C2D	3.61	1.49	1.39
23	B	609	CLA	CHD-C4C	3.61	1.47	1.39
23	C	511	CLA	O2A-CGA	3.60	1.43	1.33
23	b	613	CLA	OBD-CAD	3.60	1.28	1.22
23	B	615	CLA	C3D-C2D	3.60	1.49	1.39
23	b	609	CLA	C3D-C2D	3.60	1.48	1.39
23	C	504	CLA	C3D-C2D	3.60	1.48	1.39
23	B	606	CLA	C3D-C2D	3.60	1.48	1.39
23	a	2610	CLA	OBD-CAD	3.60	1.28	1.22
23	b	620	CLA	OBD-CAD	3.59	1.28	1.22
23	D	2304	CLA	OBD-CAD	3.59	1.28	1.22
37	c	518	DGD	O2G-C1B	3.58	1.44	1.34
23	B	611	CLA	O2A-CGA	3.58	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	606	CLA	CHD-C4C	3.57	1.47	1.39
23	c	514	CLA	MG-ND	-3.57	1.98	2.05
23	c	511	CLA	OBD-CAD	3.57	1.28	1.22
23	b	610	CLA	C3D-C2D	3.57	1.48	1.39
23	c	507	CLA	C3D-C2D	3.55	1.48	1.39
23	c	510	CLA	CHD-C4C	3.55	1.47	1.39
38	D	2310	LHG	O8-C23	3.55	1.43	1.33
23	B	607	CLA	C3D-C2D	3.54	1.48	1.39
23	a	2609	CLA	O2A-CGA	3.54	1.43	1.33
23	c	504	CLA	CHD-C4C	3.54	1.47	1.39
36	V	204	HTG	C1'-S1	-3.53	1.76	1.81
36	b	625	HTG	C1'-S1	-3.53	1.76	1.81
38	D	2311	LHG	O7-C7	3.53	1.44	1.34
36	B	627	HTG	C1'-S1	-3.52	1.76	1.81
23	A	405	CLA	MG-NC	3.52	2.14	2.06
23	C	514	CLA	C3D-C2D	3.52	1.48	1.39
23	b	612	CLA	OBD-CAD	3.52	1.28	1.22
31	A	418	JOX	C1-CL1	3.52	1.80	1.73
23	B	612	CLA	OBD-CAD	3.51	1.28	1.22
23	b	615	CLA	C3D-C2D	3.51	1.48	1.39
23	C	504	CLA	CHD-C4C	3.51	1.47	1.39
23	B	606	CLA	OBD-CAD	3.51	1.28	1.22
36	B	624[B]	HTG	C1'-S1	-3.51	1.76	1.81
23	b	619	CLA	OBD-CAD	3.51	1.28	1.22
23	B	607	CLA	OBD-CAD	3.50	1.28	1.22
23	b	608	CLA	CHD-C4C	3.50	1.47	1.39
23	c	512	CLA	C3D-C2D	3.50	1.48	1.39
23	B	616	CLA	CHD-C4C	3.50	1.47	1.39
23	B	604	CLA	C3D-C2D	3.50	1.48	1.39
23	D	2303	CLA	C3D-C2D	3.50	1.48	1.39
23	c	508	CLA	C3D-C2D	3.50	1.48	1.39
23	A	405	CLA	O2A-CGA	3.49	1.43	1.33
23	b	608	CLA	C3D-C2D	3.49	1.48	1.39
23	A	407	CLA	MG-NA	3.49	2.14	2.06
27	D	2312	LMG	O7-C10	3.49	1.44	1.34
23	c	510	CLA	C3D-C2D	3.48	1.48	1.39
36	c	526	HTG	C1'-S1	-3.48	1.77	1.81
23	b	618	CLA	OBD-CAD	3.48	1.28	1.22
42	V	201	HEC	CBB-CAB	-3.48	1.36	1.49
23	a	2613	CLA	OBD-CAD	3.47	1.28	1.22
23	b	611	CLA	OBD-CAD	3.47	1.28	1.22
31	A	418	JOX	C3-CL	3.46	1.79	1.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	C3D-C2D	3.46	1.48	1.39
23	c	508	CLA	OBD-CAD	3.45	1.28	1.22
23	d	408	CLA	CHD-C4C	3.44	1.47	1.39
23	b	613	CLA	C3D-C2D	3.44	1.48	1.39
23	B	605	CLA	C3D-C2D	3.44	1.48	1.39
36	c	523	HTG	C1'-S1	-3.44	1.77	1.81
23	B	613	CLA	CHD-C4C	3.44	1.47	1.39
38	D	2309	LHG	O7-C7	3.43	1.44	1.34
23	d	408	CLA	OBD-CAD	3.42	1.28	1.22
23	b	617	CLA	CHD-C4C	3.42	1.47	1.39
31	A	419	JOX	C1-CL1	3.41	1.79	1.73
23	B	614	CLA	C3D-C2D	3.41	1.48	1.39
23	b	607	CLA	OBD-CAD	3.41	1.28	1.22
23	b	618	CLA	C3D-C2D	3.40	1.48	1.39
23	B	605	CLA	O2A-CGA	3.40	1.43	1.33
23	c	506	CLA	C3D-C2D	3.40	1.48	1.39
23	B	611	CLA	OBD-CAD	3.40	1.28	1.22
36	B	626	HTG	C1'-S1	-3.40	1.77	1.81
23	c	507	CLA	OBD-CAD	3.40	1.28	1.22
23	a	2609	CLA	C3D-C2D	3.40	1.48	1.39
23	C	508	CLA	C3D-C2D	3.38	1.48	1.39
23	C	507	CLA	C3D-C2D	3.38	1.48	1.39
23	A	406	CLA	CHD-C4C	3.38	1.46	1.39
23	b	610	CLA	CHD-C4C	3.37	1.46	1.39
23	b	621	CLA	C3D-C2D	3.36	1.48	1.39
36	C	521	HTG	C1'-S1	-3.35	1.77	1.81
23	B	610	CLA	CHD-C4C	3.35	1.46	1.39
38	l	103	LHG	O7-C7	3.35	1.43	1.34
23	B	613	CLA	C3D-C2D	3.34	1.48	1.39
24	a	2611	PHO	C3C-C2C	3.33	1.47	1.37
23	B	613	CLA	C1B-CHB	3.33	1.50	1.41
23	C	507	CLA	OBD-CAD	3.32	1.28	1.22
23	c	506	CLA	OBD-CAD	3.32	1.28	1.22
23	b	621	CLA	MG-NC	3.32	2.14	2.06
23	a	2610	CLA	MG-NC	3.31	2.14	2.06
23	c	509	CLA	OBD-CAD	3.31	1.28	1.22
23	c	512	CLA	C1B-CHB	3.30	1.50	1.41
23	B	609	CLA	OBD-CAD	3.30	1.28	1.22
23	b	619	CLA	C3D-C2D	3.30	1.48	1.39
23	b	616	CLA	OBD-CAD	3.30	1.28	1.22
23	C	508	CLA	C4D-CHA	3.29	1.50	1.38
23	C	511	CLA	C1B-CHB	3.29	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	516	CLA	OBD-CAD	3.29	1.28	1.22
23	C	506	CLA	C3D-C2D	3.28	1.48	1.39
23	C	514	CLA	MG-NA	3.26	2.14	2.06
36	b	603	HTG	C1'-S1	-3.26	1.77	1.81
36	B	624[A]	HTG	C1'-S1	-3.25	1.77	1.81
23	B	612	CLA	C4D-CHA	3.25	1.49	1.38
23	B	617	CLA	C4D-CHA	3.24	1.49	1.38
36	C	522	HTG	C1'-S1	-3.24	1.77	1.81
23	c	506	CLA	C4D-CHA	3.23	1.49	1.38
23	B	607	CLA	C4B-CHC	3.22	1.49	1.41
23	B	604	CLA	C4B-CHC	3.21	1.49	1.41
23	c	506	CLA	C1B-CHB	3.20	1.49	1.41
23	C	502	CLA	C4B-CHC	3.20	1.49	1.41
23	a	2613	CLA	MG-ND	-3.19	1.99	2.05
23	C	504	CLA	OBD-CAD	3.19	1.28	1.22
23	B	615	CLA	MG-NC	3.19	2.13	2.06
23	B	608	CLA	C4D-CHA	3.19	1.49	1.38
23	b	621	CLA	CHD-C4C	3.18	1.46	1.39
23	C	505	CLA	OBD-CAD	3.18	1.28	1.22
23	b	615	CLA	C4D-CHA	3.18	1.49	1.38
23	C	511	CLA	C1C-C2C	3.15	1.50	1.44
23	C	504	CLA	C4B-CHC	3.15	1.49	1.41
23	b	620	CLA	C4D-CHA	3.15	1.49	1.38
38	d	413	LHG	O8-C23	3.14	1.42	1.33
26	d	417	SQD	O47-C45	-3.14	1.43	1.46
23	C	512	CLA	C4D-CHA	3.13	1.49	1.38
23	b	614	CLA	C1B-CHB	3.13	1.49	1.41
23	b	616	CLA	C1B-CHB	3.12	1.49	1.41
23	b	621	CLA	OBD-CAD	3.12	1.27	1.22
23	B	604	CLA	C1C-C2C	3.12	1.50	1.44
23	c	513	CLA	C1B-CHB	3.11	1.49	1.41
23	D	2303	CLA	OBD-CAD	3.11	1.27	1.22
23	d	408	CLA	C1C-NC	-3.10	1.33	1.37
23	B	604	CLA	OBD-CAD	3.10	1.27	1.22
23	B	615	CLA	C1B-CHB	3.10	1.49	1.41
23	B	602	CLA	C4D-CHA	3.10	1.49	1.38
23	c	510	CLA	C4D-CHA	3.10	1.49	1.38
23	C	512	CLA	C1B-CHB	3.09	1.49	1.41
23	C	504	CLA	C1B-CHB	3.09	1.49	1.41
23	B	604	CLA	C4D-CHA	3.09	1.49	1.38
23	B	610	CLA	C1B-CHB	3.07	1.49	1.41
23	c	514	CLA	MG-NC	3.07	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	MG-NC	3.06	2.13	2.06
23	C	510	CLA	C4D-CHA	3.06	1.49	1.38
24	a	2612	PHO	CHA-CBD	-3.06	1.48	1.52
23	C	503	CLA	C4D-CHA	3.04	1.49	1.38
23	B	602	CLA	C1B-CHB	3.03	1.49	1.41
23	C	502	CLA	C4D-CHA	3.03	1.49	1.38
23	B	615	CLA	C4D-CHA	3.03	1.49	1.38
23	A	410	CLA	C4D-CHA	3.03	1.49	1.38
23	c	515	CLA	C4D-CHA	3.02	1.49	1.38
39	e	103	HEM	CAB-C3B	3.02	1.55	1.47
23	b	606	CLA	C4B-CHC	3.02	1.49	1.41
23	b	621	CLA	C1B-CHB	3.02	1.49	1.41
23	B	605	CLA	C4D-CHA	3.01	1.49	1.38
23	b	606	CLA	C4D-CHA	3.01	1.49	1.38
36	o	301	HTG	C1'-S1	-3.01	1.77	1.81
23	B	603	CLA	C1B-CHB	3.01	1.49	1.41
23	c	512	CLA	C4D-CHA	3.01	1.49	1.38
23	B	607	CLA	C4D-CHA	3.01	1.49	1.38
23	C	513	CLA	C4D-CHA	3.00	1.49	1.38
23	b	611	CLA	C4D-CHA	3.00	1.49	1.38
23	C	514	CLA	C4B-CHC	3.00	1.49	1.41
23	C	503	CLA	C1B-CHB	3.00	1.49	1.41
23	C	513	CLA	C1B-CHB	3.00	1.49	1.41
23	b	617	CLA	C1B-CHB	2.99	1.49	1.41
23	C	506	CLA	C4D-CHA	2.99	1.49	1.38
23	b	612	CLA	C4D-CHA	2.99	1.49	1.38
23	C	502	CLA	C1B-CHB	2.99	1.49	1.41
23	b	621	CLA	C4D-CHA	2.98	1.49	1.38
23	b	621	CLA	C1C-NC	-2.98	1.33	1.37
23	B	602	CLA	C4B-CHC	2.97	1.49	1.41
23	a	2613	CLA	C1B-CHB	2.97	1.49	1.41
23	c	508	CLA	C4D-CHA	2.97	1.48	1.38
23	C	511	CLA	C4D-CHA	2.96	1.48	1.38
23	c	507	CLA	C4D-CHA	2.96	1.48	1.38
23	C	505	CLA	C4D-CHA	2.96	1.48	1.38
23	C	506	CLA	C1B-CHB	2.95	1.49	1.41
23	b	610	CLA	OBD-CAD	2.95	1.27	1.22
23	B	609	CLA	C1B-CHB	2.95	1.49	1.41
23	C	504	CLA	C1C-C2C	2.95	1.50	1.44
23	C	504	CLA	C4D-CHA	2.94	1.48	1.38
23	b	615	CLA	C4B-CHC	2.94	1.49	1.41
23	B	616	CLA	C1B-CHB	2.94	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	C4D-CHA	2.93	1.48	1.38
23	D	2304	CLA	C1B-CHB	2.93	1.49	1.41
23	c	505	CLA	C1B-CHB	2.93	1.49	1.41
23	A	407	CLA	MG-ND	-2.93	2.00	2.05
23	b	608	CLA	C1B-CHB	2.93	1.49	1.41
23	C	509	CLA	C1B-CHB	2.92	1.49	1.41
23	b	607	CLA	C4D-CHA	2.92	1.48	1.38
23	d	402	CLA	MG-NC	2.92	2.13	2.06
23	d	402	CLA	C1B-CHB	2.92	1.49	1.41
23	b	610	CLA	C4D-CHA	2.92	1.48	1.38
23	B	605	CLA	C1B-CHB	2.92	1.49	1.41
23	c	513	CLA	C4D-CHA	2.92	1.48	1.38
23	b	618	CLA	C4D-CHA	2.91	1.48	1.38
23	C	513	CLA	C4B-CHC	2.91	1.49	1.41
23	c	514	CLA	C4D-CHA	2.91	1.48	1.38
23	b	609	CLA	C1B-CHB	2.90	1.49	1.41
23	c	512	CLA	C1C-C2C	2.89	1.50	1.44
23	b	614	CLA	C4B-CHC	2.89	1.49	1.41
23	B	608	CLA	C4B-CHC	2.89	1.49	1.41
23	c	515	CLA	C1B-CHB	2.89	1.49	1.41
23	B	617	CLA	C1B-CHB	2.89	1.49	1.41
31	a	2619	JOX	C3-CL	2.89	1.78	1.73
23	c	508	CLA	C1C-NC	-2.89	1.33	1.37
23	B	611	CLA	C4D-CHA	2.89	1.48	1.38
23	B	608	CLA	C1B-CHB	2.88	1.49	1.41
39	F	101	HEM	CAB-C3B	2.88	1.55	1.47
23	C	507	CLA	C4D-CHA	2.87	1.48	1.38
23	B	614	CLA	C4D-CHA	2.87	1.48	1.38
23	d	408	CLA	C1B-CHB	2.87	1.49	1.41
23	C	508	CLA	C4B-CHC	2.87	1.49	1.41
23	b	618	CLA	C1B-CHB	2.87	1.49	1.41
23	c	516	CLA	C4D-CHA	2.86	1.48	1.38
23	C	510	CLA	C1B-CHB	2.86	1.48	1.41
23	C	514	CLA	C1B-CHB	2.85	1.48	1.41
23	b	611	CLA	C1B-CHB	2.85	1.48	1.41
23	B	615	CLA	C4B-CHC	2.85	1.48	1.41
23	b	616	CLA	C4D-CHA	2.85	1.48	1.38
23	B	617	CLA	OBD-CAD	2.85	1.27	1.22
23	a	2613	CLA	C4D-CHA	2.85	1.48	1.38
23	b	607	CLA	C1C-NC	-2.84	1.33	1.37
26	a	2603	SQD	C6-S	-2.84	1.66	1.77
23	b	614	CLA	C4D-CHA	2.84	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	C1B-CHB	2.84	1.48	1.41
23	b	609	CLA	C4B-CHC	2.84	1.48	1.41
23	a	2610	CLA	C1B-CHB	2.84	1.48	1.41
26	A	412	SQD	C6-S	-2.84	1.66	1.77
23	C	513	CLA	C1C-C2C	2.84	1.50	1.44
23	C	506	CLA	C4C-C3C	2.84	1.49	1.45
23	D	2303	CLA	C4B-CHC	2.84	1.48	1.41
23	A	406	CLA	C4D-CHA	2.84	1.48	1.38
23	C	503	CLA	C4B-CHC	2.84	1.48	1.41
23	b	613	CLA	C4D-CHA	2.83	1.48	1.38
23	c	504	CLA	C1B-CHB	2.83	1.48	1.41
23	B	603	CLA	C4D-CHA	2.83	1.48	1.38
23	b	615	CLA	C1B-CHB	2.83	1.48	1.41
23	B	617	CLA	C1C-NC	-2.83	1.33	1.37
23	B	614	CLA	C1B-CHB	2.82	1.48	1.41
23	C	508	CLA	C1B-CHB	2.81	1.48	1.41
23	b	617	CLA	C4D-CHA	2.81	1.48	1.38
39	F	101	HEM	FE-ND	2.81	2.10	1.96
23	c	514	CLA	C1B-CHB	2.80	1.48	1.41
23	A	405	CLA	C1B-CHB	2.80	1.48	1.41
23	D	2304	CLA	C4D-CHA	2.80	1.48	1.38
23	d	408	CLA	C4D-CHA	2.80	1.48	1.38
23	c	505	CLA	C4B-CHC	2.80	1.48	1.41
23	c	516	CLA	C1B-CHB	2.80	1.48	1.41
23	c	504	CLA	C4B-CHC	2.80	1.48	1.41
23	b	608	CLA	C4B-CHC	2.79	1.48	1.41
23	A	405	CLA	C4D-CHA	2.79	1.48	1.38
23	c	510	CLA	C1B-CHB	2.79	1.48	1.41
23	C	510	CLA	C1C-C2C	2.78	1.50	1.44
23	D	2303	CLA	C1B-CHB	2.78	1.48	1.41
23	C	507	CLA	C1B-CHB	2.78	1.48	1.41
31	a	2619	JOX	C1-CL1	2.78	1.78	1.73
23	c	507	CLA	C4B-CHC	2.78	1.48	1.41
23	b	610	CLA	C1C-NC	-2.78	1.33	1.37
23	c	504	CLA	C4D-CHA	2.78	1.48	1.38
23	B	609	CLA	C4D-CHA	2.78	1.48	1.38
23	A	407	CLA	C4D-CHA	2.78	1.48	1.38
39	e	103	HEM	FE-ND	2.78	2.10	1.96
23	B	616	CLA	MG-NC	2.77	2.12	2.06
23	d	409	CLA	C1B-CHB	2.77	1.48	1.41
23	c	505	CLA	C1C-C2C	2.77	1.49	1.44
23	b	607	CLA	C1B-CHB	2.76	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	611	CLA	C4B-CHC	2.76	1.48	1.41
23	b	620	CLA	C1B-CHB	2.75	1.48	1.41
23	c	506	CLA	C4B-CHC	2.75	1.48	1.41
23	B	603	CLA	C4B-CHC	2.75	1.48	1.41
23	b	608	CLA	C4D-CHA	2.75	1.48	1.38
23	b	613	CLA	C1B-CHB	2.75	1.48	1.41
23	a	2609	CLA	C1B-CHB	2.75	1.48	1.41
23	b	617	CLA	C1C-C2C	2.75	1.49	1.44
26	a	2615	SQD	C6-S	-2.75	1.67	1.77
23	B	606	CLA	C4D-CHA	2.75	1.48	1.38
23	C	509	CLA	C4B-CHC	2.75	1.48	1.41
23	D	2303	CLA	C4D-CHA	2.75	1.48	1.38
23	b	619	CLA	C4D-CHA	2.74	1.48	1.38
23	B	614	CLA	C4B-CHC	2.74	1.48	1.41
23	C	505	CLA	C1B-CHB	2.73	1.48	1.41
23	b	612	CLA	C1B-CHB	2.73	1.48	1.41
23	a	2613	CLA	MG-NA	2.73	2.12	2.06
23	c	508	CLA	C1B-CHB	2.73	1.48	1.41
23	c	511	CLA	C4B-CHC	2.73	1.48	1.41
23	C	509	CLA	C4D-CHA	2.73	1.48	1.38
23	C	507	CLA	C1C-NC	-2.72	1.33	1.37
23	c	505	CLA	C4D-CHA	2.72	1.48	1.38
23	B	606	CLA	C4B-CHC	2.72	1.48	1.41
26	b	601	SQD	C6-S	-2.71	1.67	1.77
23	B	610	CLA	C4D-CHA	2.71	1.48	1.38
23	c	509	CLA	C4D-CHA	2.71	1.48	1.38
23	c	513	CLA	C4B-CHC	2.71	1.48	1.41
26	D	2302	SQD	C6-S	-2.71	1.67	1.77
23	d	409	CLA	C4D-CHA	2.71	1.48	1.38
23	c	509	CLA	C1B-CHB	2.71	1.48	1.41
23	c	516	CLA	C4B-CHC	2.70	1.48	1.41
23	C	514	CLA	C1C-C2C	2.70	1.49	1.44
23	D	2304	CLA	C4B-CHC	2.70	1.48	1.41
23	C	506	CLA	C4B-CHC	2.69	1.48	1.41
23	B	612	CLA	C1B-CHB	2.69	1.48	1.41
23	B	611	CLA	C4B-CHC	2.69	1.48	1.41
24	a	2612	PHO	C3A-C2A	-2.69	1.52	1.54
26	D	2308	SQD	C6-S	-2.69	1.67	1.77
23	c	509	CLA	C1C-NC	-2.69	1.33	1.37
23	C	507	CLA	C4B-CHC	2.69	1.48	1.41
23	a	2609	CLA	C4B-CHC	2.68	1.48	1.41
23	C	508	CLA	C1C-NC	-2.68	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	C1C-C2C	2.68	1.49	1.44
23	d	409	CLA	C4C-C3C	2.67	1.49	1.45
23	d	402	CLA	C4D-CHA	2.67	1.47	1.38
23	a	2609	CLA	C4D-CHA	2.67	1.47	1.38
23	a	2610	CLA	C4D-CHA	2.67	1.47	1.38
23	b	613	CLA	C4B-CHC	2.67	1.48	1.41
23	c	510	CLA	C1C-NC	-2.67	1.33	1.37
23	c	506	CLA	MG-ND	-2.67	2.00	2.05
23	C	507	CLA	C1C-C2C	2.66	1.49	1.44
23	B	609	CLA	C4B-CHC	2.66	1.48	1.41
23	c	511	CLA	C1C-C2C	2.66	1.49	1.44
23	b	607	CLA	C4C-C3C	2.66	1.49	1.45
36	b	626	HTG	C1-S1	-2.66	1.76	1.80
23	c	504	CLA	C1C-NC	-2.65	1.33	1.37
23	c	508	CLA	C4B-CHC	2.65	1.48	1.41
23	c	512	CLA	C1C-NC	-2.65	1.33	1.37
23	b	619	CLA	C4B-CHC	2.65	1.48	1.41
39	e	103	HEM	FE-NB	2.65	2.09	1.96
23	c	507	CLA	C1B-CHB	2.65	1.48	1.41
26	B	621	SQD	C6-S	-2.64	1.67	1.77
33	D	2306	PL9	C6-C5	2.64	1.49	1.35
31	a	2617	JOX	C3-CL	2.64	1.78	1.73
23	d	409	CLA	C4B-CHC	2.64	1.48	1.41
23	c	511	CLA	C4D-CHA	2.63	1.47	1.38
23	c	508	CLA	C1C-C2C	2.63	1.49	1.44
23	C	503	CLA	C1C-C2C	2.62	1.49	1.44
23	A	405	CLA	C1C-C2C	2.62	1.49	1.44
23	B	605	CLA	C4B-CHC	2.62	1.48	1.41
31	A	419	JOX	C3-CL	2.61	1.78	1.73
23	b	609	CLA	C1C-C2C	2.61	1.49	1.44
23	c	516	CLA	C1C-C2C	2.61	1.49	1.44
23	A	406	CLA	C1B-CHB	2.61	1.48	1.41
23	b	617	CLA	C4B-CHC	2.61	1.48	1.41
23	B	614	CLA	C1C-C2C	2.60	1.49	1.44
23	B	604	CLA	C1B-CHB	2.60	1.48	1.41
26	l	101	SQD	C6-S	-2.60	1.67	1.77
23	b	614	CLA	C1C-C2C	2.60	1.49	1.44
23	C	512	CLA	C4C-C3C	2.60	1.49	1.45
23	B	606	CLA	C1B-CHB	2.60	1.48	1.41
23	B	616	CLA	C4B-CHC	2.60	1.48	1.41
23	B	617	CLA	C4B-CHC	2.60	1.48	1.41
23	c	512	CLA	C4C-C3C	2.59	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	C4C-C3C	2.59	1.49	1.45
23	B	603	CLA	C4C-C3C	2.59	1.49	1.45
23	C	510	CLA	C4C-C3C	2.59	1.49	1.45
23	B	611	CLA	C1B-CHB	2.59	1.48	1.41
23	c	512	CLA	C4B-CHC	2.59	1.48	1.41
23	b	610	CLA	C1B-CHB	2.58	1.48	1.41
23	A	405	CLA	C4B-CHC	2.58	1.48	1.41
23	b	608	CLA	C1C-C2C	2.58	1.49	1.44
23	C	514	CLA	C4D-CHA	2.58	1.47	1.38
23	d	409	CLA	C1C-C2C	2.58	1.49	1.44
23	b	618	CLA	C4B-CHC	2.57	1.48	1.41
23	C	504	CLA	C1C-NC	-2.57	1.34	1.37
23	b	618	CLA	C1C-NC	-2.56	1.34	1.37
23	B	610	CLA	C4B-CHC	2.56	1.48	1.41
24	a	2611	PHO	CHA-CBD	-2.56	1.49	1.52
23	C	511	CLA	C4B-CHC	2.56	1.48	1.41
23	A	406	CLA	C1C-NC	-2.56	1.34	1.37
23	C	502	CLA	C1C-C2C	2.56	1.49	1.44
23	A	410	CLA	C4B-CHC	2.56	1.48	1.41
23	B	602	CLA	C1C-C2C	2.56	1.49	1.44
23	C	505	CLA	C1C-C2C	2.55	1.49	1.44
23	c	510	CLA	C4B-CHC	2.55	1.48	1.41
23	C	505	CLA	C4B-CHC	2.55	1.48	1.41
23	b	607	CLA	C4B-CHC	2.55	1.48	1.41
23	b	610	CLA	C4B-CHC	2.55	1.48	1.41
23	c	507	CLA	MG-NC	2.55	2.12	2.06
23	c	504	CLA	C1C-C2C	2.55	1.49	1.44
23	c	506	CLA	C1C-NC	-2.55	1.34	1.37
23	b	607	CLA	C1C-C2C	2.54	1.49	1.44
23	C	506	CLA	C1C-NC	-2.54	1.34	1.37
23	B	607	CLA	C1B-CHB	2.54	1.48	1.41
23	A	410	CLA	C4C-C3C	2.54	1.49	1.45
23	b	606	CLA	C1C-C2C	2.54	1.49	1.44
23	c	515	CLA	C1C-C2C	2.54	1.49	1.44
23	B	612	CLA	C4B-CHC	2.54	1.48	1.41
23	c	514	CLA	C4B-CHC	2.53	1.48	1.41
23	b	617	CLA	C1C-NC	-2.53	1.34	1.37
23	b	612	CLA	C4B-CHC	2.53	1.48	1.41
23	d	408	CLA	C4C-C3C	2.53	1.49	1.45
23	B	613	CLA	C4D-CHA	2.52	1.47	1.38
23	B	613	CLA	C1C-NC	-2.52	1.34	1.37
23	D	2303	CLA	C1C-C2C	2.52	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	606	CLA	C1C-C2C	2.52	1.49	1.44
23	b	619	CLA	C4C-C3C	2.52	1.49	1.45
23	b	613	CLA	C1C-NC	-2.52	1.34	1.37
24	A	408	PHO	CHA-CBD	-2.51	1.49	1.52
23	C	502	CLA	C1C-NC	-2.51	1.34	1.37
29	U	502	GOL	O2-C2	-2.50	1.35	1.43
23	c	509	CLA	C4B-CHC	2.50	1.47	1.41
23	C	514	CLA	C3D-C4D	-2.50	1.38	1.44
23	B	607	CLA	C1C-C2C	2.49	1.49	1.44
23	a	2609	CLA	C1C-C2C	2.49	1.49	1.44
23	b	614	CLA	C1D-C2D	2.49	1.50	1.45
23	B	609	CLA	C1C-C2C	2.49	1.49	1.44
23	b	619	CLA	C1B-CHB	2.49	1.47	1.41
23	c	511	CLA	C1B-CHB	2.49	1.47	1.41
23	A	410	CLA	C1B-CHB	2.48	1.47	1.41
23	c	514	CLA	C1C-C2C	2.48	1.49	1.44
36	H	101	HTG	C1-S1	-2.48	1.76	1.80
23	b	620	CLA	C4B-CHC	2.48	1.47	1.41
23	C	510	CLA	C4B-CHC	2.48	1.47	1.41
23	A	407	CLA	C1B-NB	-2.48	1.33	1.35
23	B	615	CLA	C4B-NB	-2.48	1.33	1.35
23	C	506	CLA	C1C-C2C	2.47	1.49	1.44
23	c	515	CLA	C4B-CHC	2.47	1.47	1.41
23	b	619	CLA	C1C-C2C	2.46	1.49	1.44
23	b	608	CLA	C1C-NC	-2.46	1.34	1.37
23	A	406	CLA	C1C-C2C	2.45	1.49	1.44
23	B	615	CLA	C3D-C4D	-2.45	1.38	1.44
31	A	419	JOX	C-C1	2.45	1.40	1.35
23	B	613	CLA	C1C-C2C	2.45	1.49	1.44
23	c	509	CLA	C3D-C4D	-2.45	1.38	1.44
23	B	604	CLA	C1C-NC	-2.45	1.34	1.37
23	A	410	CLA	C1C-C2C	2.44	1.49	1.44
23	A	407	CLA	C3D-C4D	-2.44	1.38	1.44
36	d	407	HTG	C1-S1	-2.44	1.77	1.80
36	b	604	HTG	C1-S1	-2.44	1.77	1.80
23	B	611	CLA	C1C-NC	-2.44	1.34	1.37
23	b	609	CLA	C4C-C3C	2.44	1.49	1.45
23	A	407	CLA	C1B-CHB	2.43	1.47	1.41
23	C	512	CLA	C4B-CHC	2.43	1.47	1.41
23	C	511	CLA	C1C-NC	-2.43	1.34	1.37
36	c	524	HTG	C1-S1	-2.43	1.77	1.80
36	B	626	HTG	C1-S1	-2.43	1.77	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	d	411	PL9	C6-C5	2.43	1.48	1.35
23	B	614	CLA	C1C-NC	-2.43	1.34	1.37
23	C	509	CLA	C4C-C3C	2.42	1.49	1.45
31	a	2617	JOX	C1-CL1	2.42	1.77	1.73
23	d	408	CLA	C3D-C4D	-2.42	1.38	1.44
23	C	510	CLA	C1C-NC	-2.42	1.34	1.37
23	A	406	CLA	C4B-CHC	2.42	1.47	1.41
23	b	613	CLA	C1C-C2C	2.42	1.49	1.44
23	B	611	CLA	C4C-C3C	2.42	1.49	1.45
23	A	407	CLA	C4B-CHC	2.42	1.47	1.41
31	a	2617	JOX	C4-C3	2.41	1.40	1.35
23	d	402	CLA	C1B-NB	-2.41	1.33	1.35
23	a	2609	CLA	C1C-NC	-2.40	1.34	1.37
23	B	613	CLA	C3D-C4D	-2.40	1.38	1.44
23	C	511	CLA	C4C-C3C	2.40	1.49	1.45
31	a	2619	JOX	C4-C3	2.39	1.40	1.35
23	B	602	CLA	C4C-C3C	2.39	1.49	1.45
23	b	616	CLA	C3D-C4D	-2.39	1.38	1.44
23	B	617	CLA	C3D-C4D	-2.38	1.38	1.44
23	b	615	CLA	C1C-C2C	2.38	1.49	1.44
23	b	612	CLA	C1C-C2C	2.38	1.49	1.44
23	A	405	CLA	C4C-C3C	2.38	1.49	1.45
23	B	610	CLA	C4C-C3C	2.38	1.49	1.45
23	b	618	CLA	C1C-C2C	2.38	1.49	1.44
31	a	2617	JOX	C-C1	2.38	1.40	1.35
23	b	609	CLA	C1C-NC	-2.38	1.34	1.37
23	C	508	CLA	C1C-C2C	2.37	1.49	1.44
23	B	605	CLA	C4C-C3C	2.37	1.49	1.45
23	b	618	CLA	C4C-C3C	2.37	1.49	1.45
23	C	505	CLA	C3D-C4D	-2.37	1.38	1.44
23	A	410	CLA	C1C-NC	-2.37	1.34	1.37
23	a	2610	CLA	C1C-NC	-2.37	1.34	1.37
23	a	2613	CLA	C1C-NC	-2.37	1.34	1.37
28	j	2701	LMT	O1'-C1'	2.37	1.44	1.40
23	b	611	CLA	C1C-C2C	2.37	1.49	1.44
23	B	610	CLA	C1C-NC	-2.36	1.34	1.37
23	c	508	CLA	C4C-C3C	2.36	1.49	1.45
23	d	402	CLA	C4B-CHC	2.36	1.47	1.41
23	B	605	CLA	C1C-C2C	2.36	1.49	1.44
23	C	505	CLA	C1C-NC	-2.36	1.34	1.37
23	c	507	CLA	C1C-C2C	2.36	1.49	1.44
23	C	502	CLA	C3D-C4D	-2.35	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	2610	CLA	C4B-CHC	2.35	1.47	1.41
23	C	512	CLA	C1C-C2C	2.35	1.49	1.44
23	C	504	CLA	MG-ND	-2.35	2.01	2.05
23	b	614	CLA	C4C-C3C	2.34	1.49	1.45
23	C	507	CLA	C3D-C4D	-2.34	1.38	1.44
23	b	621	CLA	C4B-CHC	2.34	1.47	1.41
26	D	2302	SQD	O6-C1	2.33	1.44	1.40
31	A	418	JOX	C-C1	2.33	1.39	1.35
23	c	511	CLA	C1B-NB	-2.33	1.33	1.35
36	C	521	HTG	C1-S1	-2.32	1.77	1.80
23	B	613	CLA	C4B-CHC	2.32	1.47	1.41
23	c	511	CLA	C3D-C4D	-2.32	1.38	1.44
36	c	523	HTG	C1-S1	-2.32	1.77	1.80
23	B	606	CLA	C1C-NC	-2.32	1.34	1.37
23	B	611	CLA	C1C-C2C	2.32	1.49	1.44
23	c	509	CLA	C1C-C2C	2.32	1.49	1.44
23	c	510	CLA	C1C-C2C	2.32	1.49	1.44
23	b	614	CLA	C1C-NC	-2.31	1.34	1.37
28	B	634	LMT	O1'-C1'	2.30	1.44	1.40
23	C	510	CLA	C4D-ND	2.30	1.40	1.37
23	C	509	CLA	C1C-C2C	2.30	1.49	1.44
23	b	616	CLA	C4B-CHC	2.29	1.47	1.41
23	C	503	CLA	C4C-C3C	2.29	1.49	1.45
26	B	621	SQD	O6-C1	2.29	1.44	1.40
31	A	419	JOX	C4-C3	2.29	1.39	1.35
23	B	604	CLA	C4C-C3C	2.28	1.49	1.45
23	B	602	CLA	C1D-C2D	2.28	1.49	1.45
23	c	509	CLA	C4C-C3C	2.27	1.49	1.45
36	C	525	HTG	C1-S1	-2.27	1.77	1.80
23	c	507	CLA	C4C-C3C	2.27	1.49	1.45
23	b	620	CLA	C4D-ND	2.27	1.40	1.37
23	c	516	CLA	C4C-C3C	2.27	1.48	1.45
23	a	2609	CLA	C3D-C4D	-2.27	1.39	1.44
23	B	603	CLA	C1C-C2C	2.27	1.49	1.44
23	B	602	CLA	C1C-NC	-2.27	1.34	1.37
28	T	103	LMT	O1'-C1'	2.27	1.44	1.40
23	C	505	CLA	C4C-C3C	2.26	1.48	1.45
23	b	613	CLA	C3D-C4D	-2.26	1.39	1.44
23	b	621	CLA	C3D-C4D	-2.26	1.39	1.44
23	B	604	CLA	C3D-C4D	-2.26	1.39	1.44
23	b	606	CLA	C1C-NC	-2.25	1.34	1.37
36	d	415	HTG	C1-S1	-2.25	1.77	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	C1C-C2C	2.25	1.48	1.44
23	b	608	CLA	C4D-ND	2.25	1.40	1.37
23	A	410	CLA	C3D-C4D	-2.24	1.39	1.44
39	F	101	HEM	CMB-C2B	2.24	1.55	1.50
23	c	514	CLA	C4C-C3C	2.23	1.48	1.45
23	b	608	CLA	C3D-C4D	-2.23	1.39	1.44
23	a	2610	CLA	C1C-C2C	2.23	1.48	1.44
23	C	506	CLA	C4D-ND	2.23	1.40	1.37
23	B	608	CLA	C4C-C3C	2.23	1.48	1.45
23	C	513	CLA	C3D-C4D	-2.22	1.39	1.44
36	c	526	HTG	C1-S1	-2.22	1.77	1.80
23	B	617	CLA	C4D-ND	2.22	1.40	1.37
23	c	510	CLA	C4C-C3C	2.22	1.48	1.45
23	b	606	CLA	C3D-C4D	-2.22	1.39	1.44
23	D	2303	CLA	C4C-C3C	2.21	1.48	1.45
36	I	101	HTG	C1-S1	-2.21	1.77	1.80
23	b	619	CLA	C3D-C4D	-2.21	1.39	1.44
23	c	511	CLA	C1C-NC	-2.21	1.34	1.37
23	b	610	CLA	C1C-C2C	2.20	1.48	1.44
23	b	612	CLA	C3D-C4D	-2.20	1.39	1.44
23	B	613	CLA	C1B-NB	-2.20	1.33	1.35
23	c	506	CLA	C4C-C3C	2.20	1.48	1.45
23	B	612	CLA	C3D-C4D	-2.19	1.39	1.44
23	C	503	CLA	C1C-NC	-2.19	1.34	1.37
23	A	405	CLA	C1B-NB	-2.19	1.33	1.35
23	B	616	CLA	C1C-NC	-2.19	1.34	1.37
23	B	607	CLA	C4C-C3C	2.19	1.48	1.45
23	c	510	CLA	C4D-ND	2.18	1.40	1.37
42	V	201	HEC	C4B-C3B	2.18	1.47	1.43
23	b	613	CLA	C4C-C3C	2.18	1.48	1.45
23	B	615	CLA	C4C-C3C	2.18	1.48	1.45
23	C	503	CLA	C4D-ND	2.18	1.40	1.37
23	b	612	CLA	C1C-NC	-2.17	1.34	1.37
23	d	408	CLA	C4B-CHC	2.17	1.47	1.41
23	b	620	CLA	C1C-C2C	2.17	1.48	1.44
23	c	513	CLA	C1C-C2C	2.17	1.48	1.44
36	b	603	HTG	C1-S1	-2.17	1.77	1.80
23	C	506	CLA	C3D-C4D	-2.17	1.39	1.44
23	A	407	CLA	C1C-NC	-2.17	1.34	1.37
23	B	609	CLA	C1B-NB	-2.16	1.33	1.35
23	B	610	CLA	C3D-C4D	-2.16	1.39	1.44
23	b	619	CLA	C1C-NC	-2.16	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	615	CLA	C3D-C4D	-2.16	1.39	1.44
31	A	418	JOX	C4-C5	-2.16	1.40	1.45
23	C	502	CLA	C4D-ND	2.16	1.40	1.37
23	C	514	CLA	C4C-C3C	2.16	1.48	1.45
23	D	2303	CLA	C3D-C4D	-2.15	1.39	1.44
23	d	408	CLA	C1C-C2C	2.15	1.48	1.44
23	C	510	CLA	C3D-C4D	-2.15	1.39	1.44
36	B	627	HTG	C1-S1	-2.15	1.77	1.80
23	c	516	CLA	C1C-NC	-2.14	1.34	1.37
23	A	407	CLA	C1C-C2C	2.14	1.48	1.44
31	a	2619	JOX	C4-C5	-2.14	1.40	1.45
23	a	2613	CLA	C4B-CHC	2.13	1.46	1.41
23	C	511	CLA	C4D-ND	2.13	1.40	1.37
23	a	2613	CLA	C3D-C4D	-2.13	1.39	1.44
23	B	603	CLA	C3D-C4D	-2.13	1.39	1.44
23	B	606	CLA	C3D-C4D	-2.12	1.39	1.44
23	B	607	CLA	C3D-C4D	-2.12	1.39	1.44
23	c	508	CLA	C3D-C4D	-2.12	1.39	1.44
23	c	505	CLA	C3D-C4D	-2.12	1.39	1.44
23	b	617	CLA	C1B-NB	-2.12	1.33	1.35
23	b	618	CLA	C3D-C4D	-2.12	1.39	1.44
23	C	508	CLA	C4D-ND	2.11	1.40	1.37
23	c	514	CLA	C1C-NC	-2.11	1.34	1.37
23	b	620	CLA	C4C-C3C	2.11	1.48	1.45
23	b	615	CLA	C1C-NC	-2.11	1.34	1.37
23	d	409	CLA	C3D-C4D	-2.11	1.39	1.44
23	d	402	CLA	C1C-NC	-2.10	1.34	1.37
23	C	514	CLA	C1C-NC	-2.10	1.34	1.37
23	c	505	CLA	C4C-C3C	2.10	1.48	1.45
31	a	2619	JOX	C-C1	2.10	1.39	1.35
23	B	602	CLA	C4D-ND	2.10	1.40	1.37
23	b	611	CLA	C1C-NC	-2.09	1.34	1.37
37	c	520	DGD	O2G-C2G	-2.09	1.41	1.46
23	c	513	CLA	C3D-C4D	-2.09	1.39	1.44
36	i	102	HTG	C1-S1	-2.09	1.77	1.80
24	A	409	PHO	C3A-C2A	-2.08	1.52	1.54
23	C	513	CLA	C1C-NC	-2.08	1.34	1.37
36	C	522	HTG	C1-S1	-2.08	1.77	1.80
23	b	606	CLA	C1D-C2D	2.08	1.49	1.45
31	a	2619	JOX	C-C5	-2.08	1.40	1.45
23	b	606	CLA	C4D-ND	2.08	1.40	1.37
26	l	101	SQD	O6-C1	2.08	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	C3D-C4D	-2.08	1.39	1.44
23	b	616	CLA	C1C-C2C	2.08	1.48	1.44
23	A	405	CLA	C1C-NC	-2.07	1.34	1.37
23	D	2304	CLA	C1D-C2D	2.07	1.49	1.45
23	c	515	CLA	C3D-C4D	-2.07	1.39	1.44
23	D	2304	CLA	C3D-C4D	-2.07	1.39	1.44
23	b	616	CLA	C4C-C3C	2.07	1.48	1.45
23	c	513	CLA	C4D-ND	2.07	1.40	1.37
23	b	608	CLA	C4C-C3C	2.07	1.48	1.45
23	c	515	CLA	C1C-NC	-2.06	1.34	1.37
23	c	513	CLA	C1C-NC	-2.06	1.34	1.37
29	C	526	GOL	O2-C2	-2.06	1.37	1.43
23	B	609	CLA	C1C-NC	-2.06	1.34	1.37
23	c	516	CLA	C3D-C4D	-2.05	1.39	1.44
23	B	611	CLA	C3D-C4D	-2.05	1.39	1.44
23	c	508	CLA	C4D-ND	2.05	1.40	1.37
23	c	505	CLA	C1C-NC	-2.04	1.34	1.37
23	b	621	CLA	C1C-C2C	2.04	1.48	1.44
23	C	512	CLA	C1C-NC	-2.04	1.34	1.37
23	c	515	CLA	C4C-C3C	2.03	1.48	1.45
23	B	616	CLA	C3D-C4D	-2.03	1.39	1.44
23	B	605	CLA	C4D-ND	2.03	1.40	1.37
23	b	616	CLA	C1C-NC	-2.03	1.34	1.37
23	B	611	CLA	C1D-C2D	2.03	1.49	1.45
23	c	504	CLA	C4C-C3C	2.03	1.48	1.45
23	b	610	CLA	C3D-C4D	-2.03	1.39	1.44
23	B	609	CLA	C3D-C4D	-2.03	1.39	1.44
23	c	512	CLA	C3D-C4D	-2.03	1.39	1.44
23	c	509	CLA	C1D-C2D	2.02	1.49	1.45
25	D	2305	BCR	C30-C25	-2.02	1.51	1.53
23	b	607	CLA	C3D-C4D	-2.02	1.39	1.44
23	b	615	CLA	C4C-C3C	2.02	1.48	1.45
23	c	506	CLA	C3D-C4D	-2.01	1.39	1.44
23	d	409	CLA	C4D-ND	2.01	1.40	1.37
23	C	502	CLA	C1D-C2D	2.01	1.49	1.45
23	B	608	CLA	C1C-C2C	2.01	1.48	1.44
23	B	602	CLA	C3D-C4D	-2.00	1.39	1.44
42	v	201	HEC	C1D-ND	2.00	1.40	1.36

All (2435) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	504	CLA	C1D-ND-C4D	-10.80	98.66	106.33
23	b	617	CLA	C1D-ND-C4D	-10.14	99.13	106.33
23	B	613	CLA	C1D-ND-C4D	-10.14	99.14	106.33
23	a	2610	CLA	C1D-ND-C4D	-10.08	99.17	106.33
23	a	2609	CLA	C1D-ND-C4D	-9.95	99.27	106.33
31	A	419	JOX	C2-C3-CL	-9.95	107.56	115.84
23	A	406	CLA	C1D-ND-C4D	-9.93	99.28	106.33
23	c	507	CLA	C1D-ND-C4D	-9.88	99.32	106.33
23	b	610	CLA	C1D-ND-C4D	-9.88	99.32	106.33
23	D	2303	CLA	C1D-ND-C4D	-9.75	99.41	106.33
23	B	610	CLA	C1D-ND-C4D	-9.72	99.43	106.33
23	B	614	CLA	C1D-ND-C4D	-9.69	99.45	106.33
23	b	621	CLA	C1D-ND-C4D	-9.68	99.45	106.33
23	c	511	CLA	C1D-ND-C4D	-9.57	99.54	106.33
23	d	408	CLA	C1D-ND-C4D	-9.45	99.62	106.33
23	c	504	CLA	C2D-C1D-ND	9.38	117.01	110.10
23	C	514	CLA	C1D-ND-C4D	-9.33	99.71	106.33
23	A	406	CLA	C2D-C1D-ND	9.32	116.97	110.10
23	b	619	CLA	C1D-ND-C4D	-9.31	99.72	106.33
23	b	608	CLA	C1D-ND-C4D	-9.31	99.72	106.33
23	C	507	CLA	C1D-ND-C4D	-9.31	99.72	106.33
23	b	613	CLA	C1D-ND-C4D	-9.30	99.73	106.33
23	B	609	CLA	C1D-ND-C4D	-9.29	99.73	106.33
23	B	616	CLA	C1D-ND-C4D	-9.27	99.75	106.33
23	C	509	CLA	C1D-ND-C4D	-9.26	99.75	106.33
23	B	615	CLA	C1D-ND-C4D	-9.23	99.78	106.33
23	c	512	CLA	C1D-ND-C4D	-9.21	99.79	106.33
23	A	407	CLA	C1D-ND-C4D	-9.19	99.81	106.33
23	b	610	CLA	C2D-C1D-ND	9.15	116.85	110.10
23	C	511	CLA	C1D-ND-C4D	-9.15	99.83	106.33
23	c	505	CLA	C1D-ND-C4D	-9.14	99.84	106.33
23	B	612	CLA	C1D-ND-C4D	-9.12	99.86	106.33
23	b	618	CLA	C1D-ND-C4D	-9.05	99.91	106.33
23	A	410	CLA	C1D-ND-C4D	-9.02	99.93	106.33
23	d	409	CLA	C1D-ND-C4D	-9.00	99.94	106.33
23	B	606	CLA	C1D-ND-C4D	-9.00	99.94	106.33
31	a	2617	JOX	C2-C1-CL1	-8.99	108.36	115.84
23	D	2304	CLA	C1D-ND-C4D	-8.97	99.96	106.33
23	B	605	CLA	C1D-ND-C4D	-8.96	99.97	106.33
23	B	614	CLA	C2D-C1D-ND	8.94	116.69	110.10
23	a	2613	CLA	C1D-ND-C4D	-8.93	99.99	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	621	CLA	C2D-C1D-ND	8.93	116.68	110.10
23	A	405	CLA	C1D-ND-C4D	-8.92	100.00	106.33
23	c	508	CLA	C1D-ND-C4D	-8.91	100.01	106.33
23	D	2303	CLA	C2D-C1D-ND	8.91	116.67	110.10
23	B	616	CLA	C2D-C1D-ND	8.89	116.66	110.10
23	C	503	CLA	C1D-ND-C4D	-8.87	100.04	106.33
23	c	515	CLA	C1D-ND-C4D	-8.80	100.08	106.33
23	d	402	CLA	C1D-ND-C4D	-8.78	100.10	106.33
23	B	604	CLA	C1D-ND-C4D	-8.78	100.10	106.33
23	b	615	CLA	C1D-ND-C4D	-8.76	100.11	106.33
23	c	516	CLA	C1D-ND-C4D	-8.74	100.12	106.33
23	c	507	CLA	C2D-C1D-ND	8.73	116.53	110.10
23	c	509	CLA	C1D-ND-C4D	-8.70	100.15	106.33
23	a	2610	CLA	C2D-C1D-ND	8.69	116.51	110.10
23	b	611	CLA	C1D-ND-C4D	-8.69	100.16	106.33
36	C	522	HTG	C1'-S1-C1	8.67	116.30	100.09
23	c	510	CLA	C1D-ND-C4D	-8.66	100.18	106.33
23	B	612	CLA	C2D-C1D-ND	8.66	116.49	110.10
23	c	514	CLA	C1D-ND-C4D	-8.66	100.18	106.33
23	b	616	CLA	C1D-ND-C4D	-8.64	100.19	106.33
23	C	504	CLA	C1D-ND-C4D	-8.62	100.21	106.33
23	B	611	CLA	C1D-ND-C4D	-8.62	100.21	106.33
23	b	617	CLA	C2D-C1D-ND	8.60	116.44	110.10
23	b	614	CLA	C1D-ND-C4D	-8.59	100.23	106.33
23	B	603	CLA	C1D-ND-C4D	-8.58	100.24	106.33
23	B	608	CLA	C1D-ND-C4D	-8.55	100.26	106.33
23	B	617	CLA	C1D-ND-C4D	-8.52	100.28	106.33
23	c	513	CLA	C1D-ND-C4D	-8.51	100.29	106.33
23	C	508	CLA	C1D-ND-C4D	-8.46	100.33	106.33
23	C	513	CLA	C1D-ND-C4D	-8.45	100.33	106.33
23	B	613	CLA	C2D-C1D-ND	8.42	116.31	110.10
23	C	505	CLA	C1D-ND-C4D	-8.39	100.38	106.33
23	c	506	CLA	C1D-ND-C4D	-8.36	100.39	106.33
23	C	510	CLA	C1D-ND-C4D	-8.33	100.42	106.33
23	b	607	CLA	C1D-ND-C4D	-8.33	100.42	106.33
23	b	612	CLA	C1D-ND-C4D	-8.29	100.45	106.33
23	d	408	CLA	C2D-C1D-ND	8.26	116.19	110.10
23	B	607	CLA	C1D-ND-C4D	-8.20	100.51	106.33
23	B	608	CLA	C2D-C1D-ND	8.16	116.12	110.10
23	C	502	CLA	C1D-ND-C4D	-8.11	100.57	106.33
23	B	609	CLA	C2D-C1D-ND	8.06	116.05	110.10
23	c	515	CLA	C2D-C1D-ND	8.03	116.02	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	C2D-C1D-ND	8.00	116.00	110.10
23	C	512	CLA	C1D-ND-C4D	-7.99	100.66	106.33
23	c	512	CLA	C2D-C1D-ND	7.97	115.97	110.10
23	b	609	CLA	C1D-ND-C4D	-7.97	100.68	106.33
23	b	612	CLA	C2D-C1D-ND	7.95	115.97	110.10
23	C	508	CLA	C2D-C1D-ND	7.95	115.96	110.10
23	C	504	CLA	C2D-C1D-ND	7.93	115.95	110.10
23	C	503	CLA	C2D-C1D-ND	7.92	115.94	110.10
23	A	410	CLA	C2D-C1D-ND	7.87	115.91	110.10
23	c	506	CLA	C2D-C1D-ND	7.84	115.88	110.10
24	a	2611	PHO	O2D-CGD-CBD	7.83	120.91	111.00
23	D	2304	CLA	C2D-C1D-ND	7.82	115.87	110.10
23	d	402	CLA	C2D-C1D-ND	7.82	115.87	110.10
23	C	506	CLA	C1D-ND-C4D	-7.81	100.79	106.33
23	c	511	CLA	C2D-C1D-ND	7.81	115.86	110.10
23	C	509	CLA	C2D-C1D-ND	7.79	115.84	110.10
23	a	2609	CLA	C2D-C1D-ND	7.77	115.83	110.10
36	b	603	HTG	C1'-S1-C1	7.76	114.61	100.09
23	b	615	CLA	C2D-C1D-ND	7.76	115.82	110.10
23	a	2613	CLA	C2D-C1D-ND	7.75	115.82	110.10
23	b	620	CLA	C1D-ND-C4D	-7.75	100.83	106.33
31	a	2617	JOX	C2-C3-CL	-7.74	109.39	115.84
23	c	505	CLA	C2D-C1D-ND	7.68	115.77	110.10
23	B	610	CLA	C2D-C1D-ND	7.66	115.75	110.10
23	B	615	CLA	C2D-C1D-ND	7.65	115.74	110.10
23	A	405	CLA	C2D-C1D-ND	7.60	115.70	110.10
23	b	616	CLA	C2D-C1D-ND	7.59	115.70	110.10
23	C	511	CLA	C2D-C1D-ND	7.58	115.69	110.10
23	d	409	CLA	C2D-C1D-ND	7.55	115.67	110.10
23	b	606	CLA	C1D-ND-C4D	-7.55	100.97	106.33
23	b	611	CLA	C2D-C1D-ND	7.55	115.67	110.10
23	b	618	CLA	C2D-C1D-ND	7.52	115.65	110.10
23	B	617	CLA	C2D-C1D-ND	7.51	115.64	110.10
23	B	602	CLA	C1D-ND-C4D	-7.50	101.01	106.33
23	b	619	CLA	C2D-C1D-ND	7.47	115.61	110.10
23	b	613	CLA	C2D-C1D-ND	7.46	115.60	110.10
23	C	512	CLA	C2D-C1D-ND	7.41	115.57	110.10
23	c	510	CLA	C2D-C1D-ND	7.41	115.56	110.10
23	C	507	CLA	C1-C2-C3	-7.40	113.24	126.04
23	A	407	CLA	C2D-C1D-ND	7.40	115.56	110.10
23	B	607	CLA	C2D-C1D-ND	7.36	115.53	110.10
23	c	514	CLA	C2D-C1D-ND	7.34	115.51	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	C2D-C1D-ND	7.32	115.50	110.10
23	c	516	CLA	C2D-C1D-ND	7.32	115.50	110.10
23	C	513	CLA	C2D-C1D-ND	7.31	115.49	110.10
23	b	608	CLA	C2D-C1D-ND	7.29	115.48	110.10
23	C	507	CLA	C2D-C1D-ND	7.29	115.48	110.10
23	b	609	CLA	C2D-C1D-ND	7.27	115.46	110.10
23	b	619	CLA	CMD-C2D-C1D	7.25	137.50	124.71
23	B	603	CLA	C2D-C1D-ND	7.25	115.45	110.10
23	B	611	CLA	C2D-C1D-ND	7.22	115.43	110.10
23	C	507	CLA	CMD-C2D-C1D	7.21	137.41	124.71
23	B	604	CLA	C2D-C1D-ND	7.20	115.41	110.10
23	C	505	CLA	C2D-C1D-ND	7.19	115.41	110.10
23	C	510	CLA	C2D-C1D-ND	7.18	115.40	110.10
36	i	102	HTG	C1'-S1-C1	7.12	113.40	100.09
23	b	607	CLA	C2D-C1D-ND	7.08	115.32	110.10
23	c	508	CLA	C2D-C1D-ND	7.04	115.30	110.10
31	A	419	JOX	C3-C4-C5	-7.03	117.45	120.54
23	b	620	CLA	C2D-C1D-ND	6.96	115.23	110.10
23	B	604	CLA	O2D-CGD-CBD	6.96	123.63	111.27
23	b	614	CLA	C2D-C1D-ND	6.90	115.19	110.10
23	C	514	CLA	CMD-C2D-C1D	6.89	136.85	124.71
23	B	605	CLA	CMD-C2D-C1D	6.88	136.84	124.71
23	c	510	CLA	O2D-CGD-CBD	6.86	123.46	111.27
23	b	615	CLA	CMD-C2D-C1D	6.83	136.76	124.71
23	C	502	CLA	CMD-C2D-C1D	6.83	136.74	124.71
26	l	101	SQD	O6-C1-C2	6.82	118.95	108.30
24	A	409	PHO	C1-C2-C3	-6.79	114.30	126.04
24	A	409	PHO	O2D-CGD-CBD	6.75	119.55	111.00
23	b	614	CLA	CMD-C2D-C1D	6.71	136.54	124.71
36	B	625	HTG	C1'-S1-C1	6.64	112.52	100.09
23	B	602	CLA	CMD-C2D-C1D	6.64	136.41	124.71
23	C	514	CLA	C2D-C1D-ND	6.63	114.99	110.10
23	b	618	CLA	CMD-C2D-C1D	6.58	136.31	124.71
23	c	508	CLA	CMD-C2D-C1D	6.57	136.29	124.71
23	b	613	CLA	CMD-C2D-C1D	6.55	136.25	124.71
31	a	2617	JOX	C1-C-C5	-6.54	117.66	120.54
24	a	2612	PHO	O2D-CGD-CBD	6.54	119.29	111.00
23	C	506	CLA	CMD-C2D-C1D	6.53	136.23	124.71
23	c	509	CLA	CMD-C2D-C1D	6.51	136.19	124.71
23	c	513	CLA	C2D-C1D-ND	6.51	114.90	110.10
23	c	509	CLA	C2D-C1D-ND	6.46	114.86	110.10
23	C	505	CLA	CMD-C2D-C1D	6.43	136.05	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	604	CLA	CMD-C2D-C1D	6.43	136.04	124.71
31	A	419	JOX	C1-C2-C3	6.43	120.02	114.18
23	B	610	CLA	CMD-C2D-C1D	6.40	135.99	124.71
23	c	508	CLA	O2D-CGD-CBD	6.40	122.64	111.27
23	C	508	CLA	O2D-CGD-CBD	6.39	122.61	111.27
36	d	415	HTG	C1'-S1-C1	6.38	112.02	100.09
23	b	606	CLA	CMD-C2D-C1D	6.31	135.84	124.71
23	b	606	CLA	O2D-CGD-CBD	6.31	122.48	111.27
23	d	409	CLA	CMD-C2D-C1D	6.30	135.81	124.71
23	B	615	CLA	CMD-C2D-C1D	6.29	135.80	124.71
23	c	516	CLA	CMD-C2D-C1D	6.29	135.79	124.71
23	C	508	CLA	CMD-C2D-C1D	6.28	135.77	124.71
39	F	101	HEM	C4D-ND-C1D	6.27	111.55	105.07
23	b	608	CLA	CMD-C2D-C1D	6.26	135.75	124.71
23	C	510	CLA	O2D-CGD-CBD	6.25	122.38	111.27
23	d	408	CLA	CMD-C2D-C1D	6.25	135.72	124.71
39	e	103	HEM	C4D-ND-C1D	6.24	111.52	105.07
31	A	419	JOX	C-C1-C2	-6.24	118.17	123.18
23	C	504	CLA	CMD-C2D-C1D	6.23	135.70	124.71
23	c	506	CLA	CMD-C2D-C1D	6.23	135.69	124.71
23	B	614	CLA	CMD-C2D-C1D	6.22	135.68	124.71
23	b	621	CLA	CMD-C2D-C1D	6.21	135.66	124.71
23	D	2303	CLA	CMD-C2D-C1D	6.20	135.64	124.71
23	C	513	CLA	O2D-CGD-CBD	6.18	122.25	111.27
23	c	510	CLA	CMD-C2D-C1D	6.17	135.59	124.71
23	C	502	CLA	O2D-CGD-CBD	6.17	122.23	111.27
23	C	510	CLA	CMD-C2D-C1D	6.17	135.58	124.71
23	B	603	CLA	CMD-C2D-C1D	6.16	135.57	124.71
23	c	515	CLA	O2D-CGD-CBD	6.16	122.21	111.27
23	B	612	CLA	CMD-C2D-C1D	6.15	135.55	124.71
23	c	507	CLA	CMD-C2D-C1D	6.14	135.53	124.71
23	B	611	CLA	CMD-C2D-C1D	6.13	135.51	124.71
36	I	101	HTG	C1'-S1-C1	6.09	111.47	100.09
23	b	616	CLA	CMD-C2D-C1D	6.08	135.43	124.71
23	b	609	CLA	CMD-C2D-C1D	6.07	135.41	124.71
23	A	410	CLA	CMD-C2D-C1D	6.06	135.40	124.71
23	B	607	CLA	CMD-C2D-C1D	6.06	135.40	124.71
31	A	418	JOX	C1-C2-C3	6.05	119.68	114.18
23	B	617	CLA	O2D-CGD-CBD	6.04	122.00	111.27
23	c	513	CLA	CMD-C2D-C1D	6.03	135.34	124.71
23	C	513	CLA	CMD-C2D-C1D	6.02	135.33	124.71
23	b	611	CLA	CMD-C2D-C1D	6.01	135.31	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	502	CLA	C2D-C1D-ND	6.01	114.53	110.10
36	B	626	HTG	C1'-S1-C1	6.01	111.32	100.09
23	B	602	CLA	C2D-C1D-ND	6.00	114.53	110.10
23	a	2610	CLA	CMD-C2D-C1D	5.98	135.25	124.71
26	a	2615	SQD	O6-C1-C2	5.98	117.64	108.30
23	C	503	CLA	O2D-CGD-CBD	5.96	121.87	111.27
23	C	511	CLA	O2D-CGD-CBD	5.96	121.85	111.27
23	A	407	CLA	CMD-C2D-C1D	5.95	135.21	124.71
23	b	607	CLA	O2D-CGD-CBD	5.95	121.84	111.27
23	b	607	CLA	CMD-C2D-C1D	5.95	135.20	124.71
31	a	2617	JOX	C1-C2-C3	5.94	119.58	114.18
23	C	512	CLA	CMD-C2D-C1D	5.93	135.16	124.71
23	B	617	CLA	CMD-C2D-C1D	5.92	135.15	124.71
23	c	512	CLA	CMD-C2D-C1D	5.92	135.14	124.71
23	b	610	CLA	CMD-C2D-C1D	5.89	135.09	124.71
23	C	509	CLA	O2D-CGD-CBD	5.87	121.70	111.27
24	A	408	PHO	O2D-CGD-CBD	5.83	118.38	111.00
23	B	602	CLA	O2D-CGD-CBD	5.81	121.59	111.27
23	b	606	CLA	C2D-C1D-ND	5.81	114.39	110.10
23	D	2304	CLA	O2D-CGD-CBD	5.80	121.58	111.27
23	b	612	CLA	CMD-C2D-C1D	5.79	134.92	124.71
23	b	621	CLA	O2D-CGD-CBD	5.78	121.54	111.27
31	A	418	JOX	C4-C3-C2	-5.77	118.55	123.18
23	b	619	CLA	O2D-CGD-CBD	5.76	121.51	111.27
23	A	405	CLA	CMD-C2D-C1D	5.76	134.87	124.71
36	C	525	HTG	C1'-S1-C1	5.75	110.85	100.09
26	D	2302	SQD	O47-C7-C8	5.70	123.80	111.50
23	c	507	CLA	O2D-CGD-CBD	5.70	121.40	111.27
23	B	616	CLA	CMD-C2D-C1D	5.69	134.75	124.71
23	D	2304	CLA	CHD-C1D-ND	-5.68	119.24	124.45
31	A	418	JOX	C-C1-C2	-5.67	118.63	123.18
36	V	204	HTG	C1'-S1-C1	5.67	110.70	100.09
23	a	2609	CLA	CMD-C2D-C1D	5.67	134.70	124.71
23	B	615	CLA	O2D-CGD-CBD	5.65	121.31	111.27
23	b	610	CLA	O2D-CGD-CBD	5.64	121.28	111.27
23	C	506	CLA	O2D-CGD-CBD	5.59	121.21	111.27
23	b	609	CLA	C1-C2-C3	-5.59	116.37	126.04
23	c	504	CLA	CMD-C2D-C1D	5.59	134.56	124.71
25	d	410	BCR	C24-C23-C22	-5.59	117.80	126.23
36	c	524	HTG	C1'-S1-C1	5.58	110.53	100.09
23	D	2304	CLA	CMD-C2D-C1D	5.52	134.45	124.71
23	c	514	CLA	CMD-C2D-C1D	5.52	134.44	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	2610	CLA	CHD-C1D-ND	-5.51	119.39	124.45
24	a	2612	PHO	C1-C2-C3	-5.46	116.59	126.04
36	b	604	HTG	C1'-S1-C1	5.46	110.30	100.09
23	C	505	CLA	O2D-CGD-CBD	5.43	120.91	111.27
23	B	607	CLA	O2D-CGD-CBD	5.40	120.86	111.27
23	D	2303	CLA	O2D-CGD-CBD	5.40	120.86	111.27
23	B	606	CLA	CMD-C2D-C1D	5.39	134.20	124.71
23	B	613	CLA	CMD-C2D-C1D	5.39	134.20	124.71
36	d	407	HTG	C1'-S1-C1	5.38	110.15	100.09
36	b	626	HTG	C1'-S1-C1	5.37	110.14	100.09
23	A	406	CLA	CMD-C2D-C1D	5.34	134.13	124.71
23	C	503	CLA	CMD-C2D-C1D	5.34	134.12	124.71
36	c	523	HTG	C1'-S1-C1	5.33	110.07	100.09
42	V	201	HEC	CBD-CAD-C3D	-5.29	103.60	112.62
25	B	633	BCR	C33-C5-C6	-5.25	118.63	124.53
23	B	608	CLA	CMD-C2D-C1D	5.23	133.94	124.71
23	B	612	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
23	c	511	CLA	O2D-CGD-CBD	5.20	120.51	111.27
23	b	609	CLA	O2D-CGD-CBD	5.18	120.47	111.27
23	C	506	CLA	C2D-C1D-ND	5.16	113.91	110.10
23	A	406	CLA	C1C-C2C-C3C	-5.15	101.54	106.96
23	b	608	CLA	O2D-CGD-CBD	5.14	120.41	111.27
36	c	526	HTG	C1'-S1-C1	5.14	109.71	100.09
23	B	608	CLA	O2D-CGD-CBD	5.14	120.40	111.27
23	b	611	CLA	O2D-CGD-CBD	5.14	120.40	111.27
26	l	101	SQD	O47-C7-C8	5.13	122.55	111.50
36	B	625	HTG	O5-C1-C2	5.12	116.75	110.31
23	A	406	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
37	C	519	DGD	O2G-C1B-C2B	5.08	122.45	111.50
23	C	511	CLA	CMD-C2D-C1D	5.06	133.63	124.71
23	B	612	CLA	O2D-CGD-CBD	5.06	120.26	111.27
23	b	621	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
23	a	2613	CLA	CMD-C2D-C1D	5.03	133.58	124.71
26	B	621	SQD	O47-C7-C8	5.02	122.33	111.50
23	b	610	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
26	d	417	SQD	O47-C7-O49	-5.01	119.19	125.57
23	A	406	CLA	C2C-C1C-NC	5.01	114.67	109.97
23	B	611	CLA	O2D-CGD-CBD	4.99	120.14	111.27
36	B	627	HTG	C1'-S1-C1	4.99	109.42	100.09
23	d	408	CLA	C2C-C1C-NC	4.98	114.64	109.97
25	Y	302	BCR	C15-C14-C13	-4.98	120.21	127.31
36	H	101	HTG	C1'-S1-C1	4.97	109.39	100.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	527	LMG	O7-C10-C11	4.95	122.16	111.50
26	b	601	SQD	O8-S-C6	4.94	113.62	105.74
23	B	614	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
23	b	615	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
23	b	617	CLA	O2D-CGD-CBD	4.93	120.03	111.27
23	A	406	CLA	CBC-CAC-C3C	-4.92	98.85	112.43
23	d	402	CLA	CMD-C2D-C1D	4.91	133.37	124.71
23	c	515	CLA	CMD-C2D-C1D	4.91	133.36	124.71
23	b	620	CLA	CMD-C2D-C1D	4.87	133.30	124.71
27	A	413	LMG	O7-C10-C11	4.87	121.99	111.50
23	B	611	CLA	C1-C2-C3	-4.87	117.63	126.04
23	B	616	CLA	CHD-C4C-C3C	-4.86	117.69	124.84
23	c	504	CLA	CHD-C1D-ND	-4.86	119.98	124.45
23	D	2303	CLA	O2D-CGD-O1D	-4.86	114.33	123.84
23	D	2303	CLA	CHD-C4C-C3C	-4.85	117.72	124.84
23	c	512	CLA	O2D-CGD-CBD	4.84	119.87	111.27
23	B	613	CLA	O2D-CGD-CBD	4.84	119.87	111.27
23	c	506	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
23	B	603	CLA	O2D-CGD-CBD	4.82	119.83	111.27
31	a	2617	JOX	C3-C4-C5	-4.81	118.42	120.54
23	D	2304	CLA	CHD-C4C-C3C	-4.81	117.77	124.84
23	D	2303	CLA	C3D-C2D-C1D	-4.80	99.29	105.83
23	a	2610	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	C	509	CLA	CMD-C2D-C1D	4.79	133.16	124.71
23	D	2303	CLA	CHD-C1D-ND	-4.78	120.06	124.45
23	A	406	CLA	O2D-CGD-CBD	4.78	119.75	111.27
23	c	507	CLA	CHD-C1D-ND	-4.76	120.08	124.45
23	B	616	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
23	B	606	CLA	C3D-C2D-C1D	-4.75	99.34	105.83
23	b	617	CLA	CHD-C4C-C3C	-4.75	117.85	124.84
23	c	509	CLA	O2D-CGD-CBD	4.75	119.71	111.27
23	b	610	CLA	CHD-C4C-C3C	-4.75	117.85	124.84
23	c	505	CLA	CMD-C2D-C1D	4.75	133.09	124.71
23	b	612	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
23	c	510	CLA	C2C-C1C-NC	4.75	114.42	109.97
23	b	617	CLA	CMD-C2D-C1D	4.73	133.06	124.71
25	T	102	BCR	C33-C5-C6	-4.73	119.21	124.53
23	c	504	CLA	O2D-CGD-CBD	4.73	119.67	111.27
23	a	2613	CLA	O2D-CGD-CBD	4.72	119.66	111.27
23	B	615	CLA	CHD-C4C-C3C	-4.71	117.91	124.84
36	B	624[B]	HTG	C1'-S1-C1	4.70	108.87	100.09
23	C	504	CLA	CHD-C4C-C3C	-4.68	117.96	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	419	JOX	C4-C3-CL	4.66	131.29	120.02
23	b	612	CLA	O2D-CGD-CBD	4.66	119.54	111.27
23	d	409	CLA	O2D-CGD-CBD	4.65	119.53	111.27
37	D	2307	DGD	O2G-C1B-C2B	4.65	121.52	111.50
23	A	407	CLA	CHD-C4C-C3C	-4.63	118.03	124.84
23	a	2613	CLA	C1C-C2C-C3C	-4.62	102.10	106.96
23	b	616	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
23	B	614	CLA	CHD-C4C-C3C	-4.61	118.06	124.84
23	B	608	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
23	B	605	CLA	C2C-C1C-NC	4.60	114.28	109.97
23	c	505	CLA	O2D-CGD-CBD	4.59	119.43	111.27
25	C	516	BCR	C7-C8-C9	-4.59	119.29	126.23
23	C	508	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
23	D	2303	CLA	C2C-C1C-NC	4.59	114.27	109.97
25	D	2305	BCR	C24-C23-C22	-4.59	119.30	126.23
23	B	615	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
23	d	402	CLA	O2D-CGD-CBD	4.58	119.40	111.27
27	c	501	LMG	O7-C10-C11	4.57	121.34	111.50
23	C	504	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
23	A	410	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
23	B	609	CLA	CMD-C2D-C1D	4.54	132.71	124.71
23	d	402	CLA	C2C-C1C-NC	4.53	114.22	109.97
23	B	611	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
23	c	515	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
23	B	617	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
23	c	504	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
23	b	621	CLA	CHD-C4C-C3C	-4.53	118.19	124.84
23	B	606	CLA	CHD-C4C-C3C	-4.52	118.19	124.84
26	A	412	SQD	O47-C7-C8	4.52	121.23	111.50
25	D	2305	BCR	C38-C26-C25	-4.51	119.46	124.53
23	B	607	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
36	C	522	HTG	C1-O5-C5	4.51	120.90	112.58
31	a	2619	JOX	C-C1-C2	-4.51	119.56	123.18
25	D	2305	BCR	C7-C8-C9	-4.51	119.42	126.23
27	c	522	LMG	O7-C10-C11	4.51	121.21	111.50
23	b	619	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
23	c	507	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
23	a	2609	CLA	C3D-C4D-ND	4.48	117.49	110.24
23	b	611	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
31	a	2617	JOX	C-C1-CL1	4.48	130.84	120.02
23	C	503	CLA	O2D-CGD-O1D	-4.47	115.09	123.84
23	c	512	CLA	C3D-C2D-C1D	-4.47	99.73	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	CMD-C2D-C1D	4.46	132.58	124.71
23	b	614	CLA	CHD-C1D-ND	-4.46	120.35	124.45
39	e	103	HEM	CBA-CAA-C2A	-4.45	105.03	112.62
23	d	408	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
23	a	2613	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
23	b	621	CLA	C1D-CHD-C4C	-4.45	116.47	126.06
23	c	504	CLA	C3D-C4D-ND	4.45	117.43	110.24
23	A	410	CLA	C2C-C1C-NC	4.45	114.14	109.97
23	a	2610	CLA	C3D-C4D-ND	4.44	117.42	110.24
23	C	507	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
23	A	407	CLA	C3D-C4D-ND	4.44	117.42	110.24
23	d	402	CLA	C1C-C2C-C3C	-4.44	102.29	106.96
23	C	505	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
23	b	618	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
23	d	408	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
23	B	615	CLA	O2D-CGD-O1D	-4.43	115.18	123.84
25	Y	302	BCR	C38-C26-C25	-4.42	119.56	124.53
23	c	506	CLA	O2D-CGD-CBD	4.42	119.13	111.27
23	A	405	CLA	CHD-C1D-ND	-4.42	120.39	124.45
23	d	409	CLA	C3D-C2D-C1D	-4.42	99.81	105.83
23	C	505	CLA	C1C-C2C-C3C	-4.41	102.31	106.96
25	z	101	BCR	C15-C14-C13	-4.41	121.01	127.31
23	B	605	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
23	C	509	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
31	a	2617	JOX	C4-C3-CL	4.40	130.66	120.02
23	C	513	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
23	c	507	CLA	C2C-C1C-NC	4.39	114.08	109.97
26	a	2603	SQD	O47-C7-C8	4.39	120.96	111.50
23	c	514	CLA	CHD-C1D-ND	-4.39	120.42	124.45
26	a	2615	SQD	O47-C7-C8	4.38	120.95	111.50
23	c	504	CLA	CHD-C4C-C3C	-4.38	118.40	124.84
23	a	2613	CLA	C2C-C1C-NC	4.38	114.08	109.97
23	b	617	CLA	C3D-C4D-ND	4.38	117.32	110.24
25	c	517	BCR	C33-C5-C6	-4.38	119.61	124.53
23	b	616	CLA	CHD-C4C-C3C	-4.38	118.41	124.84
23	C	512	CLA	CHD-C1D-ND	-4.38	120.43	124.45
23	A	406	CLA	CHD-C4C-C3C	-4.37	118.42	124.84
25	d	410	BCR	C7-C8-C9	-4.37	119.64	126.23
23	b	610	CLA	C1C-C2C-C3C	-4.36	102.37	106.96
23	B	604	CLA	O2D-CGD-O1D	-4.36	115.31	123.84
23	d	402	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
25	d	410	BCR	C33-C5-C6	-4.35	119.64	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	514	CLA	C3D-C4D-ND	4.35	117.27	110.24
23	c	516	CLA	O2D-CGD-CBD	4.35	118.99	111.27
23	b	613	CLA	C3D-C2D-C1D	-4.34	99.90	105.83
23	B	615	CLA	CHD-C1D-ND	-4.34	120.46	124.45
31	A	419	JOX	O-C2-C3	-4.34	118.80	122.76
23	c	516	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
23	b	607	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
23	c	505	CLA	CHD-C4C-C3C	-4.33	118.48	124.84
25	T	102	BCR	C7-C8-C9	-4.33	119.69	126.23
23	c	508	CLA	C2C-C1C-NC	4.33	114.02	109.97
23	d	402	CLA	CHD-C4C-C3C	-4.32	118.48	124.84
23	B	603	CLA	C2C-C1C-NC	4.32	114.02	109.97
23	B	610	CLA	O2D-CGD-CBD	4.32	118.95	111.27
23	c	505	CLA	C3D-C4D-ND	4.32	117.23	110.24
23	B	613	CLA	C3D-C4D-ND	4.32	117.23	110.24
25	T	102	BCR	C15-C16-C17	-4.32	114.63	123.47
23	D	2304	CLA	C3D-C4D-ND	4.32	117.22	110.24
23	c	507	CLA	CHD-C4C-C3C	-4.31	118.50	124.84
23	c	510	CLA	C1C-C2C-C3C	-4.31	102.43	106.96
23	c	504	CLA	C1C-C2C-C3C	-4.31	102.43	106.96
23	B	603	CLA	C3D-C2D-C1D	-4.31	99.96	105.83
23	C	512	CLA	C3D-C2D-C1D	-4.30	99.97	105.83
25	B	618	BCR	C33-C5-C6	-4.29	119.70	124.53
23	B	610	CLA	C3D-C2D-C1D	-4.29	99.97	105.83
23	D	2304	CLA	C3D-C2D-C1D	-4.29	99.97	105.83
23	b	621	CLA	C3C-C4C-NC	4.29	115.38	110.57
23	c	507	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
23	c	511	CLA	C3D-C4D-ND	4.29	117.17	110.24
23	A	407	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
23	c	511	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
23	B	611	CLA	CAC-C3C-C4C	4.28	130.36	124.81
23	b	612	CLA	CHD-C4C-C3C	-4.28	118.55	124.84
23	b	610	CLA	O2D-CGD-O1D	-4.28	115.47	123.84
23	A	405	CLA	C2C-C1C-NC	4.28	113.98	109.97
23	C	510	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
23	A	407	CLA	O2D-CGD-CBD	4.27	118.86	111.27
23	c	513	CLA	O2D-CGD-CBD	4.27	118.86	111.27
23	D	2303	CLA	C3D-C4D-ND	4.27	117.14	110.24
23	d	409	CLA	C1C-C2C-C3C	-4.27	102.47	106.96
23	B	613	CLA	C3D-C2D-C1D	-4.27	100.01	105.83
25	T	102	BCR	C12-C13-C14	-4.26	112.40	118.94
28	M	101	LMT	O5'-C5'-C4'	4.26	118.74	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	O2D-CGD-CBD	4.26	118.84	111.27
25	Y	302	BCR	C33-C5-C6	-4.26	119.75	124.53
23	B	609	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
37	C	519	DGD	O1G-C1A-C2A	4.25	125.26	111.91
25	d	410	BCR	C38-C26-C25	-4.25	119.75	124.53
23	A	410	CLA	O2D-CGD-CBD	4.25	118.82	111.27
31	A	419	JOX	C2-C1-CL1	-4.25	112.30	115.84
23	d	402	CLA	CBC-CAC-C3C	-4.24	100.73	112.43
23	C	509	CLA	C3D-C4D-ND	4.24	117.10	110.24
25	b	624	BCR	C38-C26-C25	-4.24	119.77	124.53
23	b	620	CLA	O2D-CGD-CBD	4.24	118.80	111.27
23	C	503	CLA	C3D-C2D-C1D	-4.23	100.05	105.83
23	B	612	CLA	CAC-C3C-C4C	4.23	130.30	124.81
23	B	605	CLA	O2D-CGD-CBD	4.23	118.79	111.27
23	b	609	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
23	A	405	CLA	C3D-C4D-ND	4.22	117.07	110.24
23	b	617	CLA	C3D-C2D-C1D	-4.22	100.08	105.83
28	B	623	LMT	C1B-O5B-C5B	4.22	121.97	113.69
23	B	604	CLA	C3D-C2D-C1D	-4.22	100.08	105.83
25	y	101	BCR	C33-C5-C6	-4.21	119.80	124.53
26	b	601	SQD	O47-C7-C8	4.21	120.57	111.50
23	d	408	CLA	O2D-CGD-CBD	4.20	118.73	111.27
23	b	614	CLA	C3D-C2D-C1D	-4.20	100.10	105.83
26	D	2308	SQD	O47-C7-C8	4.20	120.55	111.50
23	d	409	CLA	C2C-C1C-NC	4.20	113.90	109.97
23	c	507	CLA	C3D-C4D-ND	4.19	117.01	110.24
23	B	608	CLA	C2C-C1C-NC	4.19	113.89	109.97
23	b	612	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
26	d	417	SQD	O8-S-C6	4.18	112.52	105.77
25	c	517	BCR	C7-C8-C9	-4.17	119.93	126.23
23	c	505	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
23	C	514	CLA	O2D-CGD-CBD	4.17	118.67	111.27
23	B	613	CLA	CHD-C4C-C3C	-4.16	118.72	124.84
24	a	2612	PHO	C4-C3-C5	4.16	122.28	115.27
23	c	509	CLA	C3D-C4D-ND	4.16	116.97	110.24
26	a	2615	SQD	O9-S-C6	4.16	111.89	106.94
23	C	510	CLA	C2C-C1C-NC	4.16	113.87	109.97
23	C	504	CLA	O2D-CGD-CBD	4.16	118.66	111.27
23	a	2613	CLA	CHD-C4C-C3C	-4.16	118.73	124.84
23	c	509	CLA	C3D-C2D-C1D	-4.16	100.16	105.83
23	b	618	CLA	C2C-C1C-NC	4.15	113.86	109.97
23	C	511	CLA	C3D-C4D-ND	4.15	116.95	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	408	CLA	C3D-C4D-ND	4.15	116.95	110.24
23	B	609	CLA	CHD-C4C-C3C	-4.15	118.74	124.84
23	C	505	CLA	C2C-C1C-NC	4.15	113.86	109.97
27	c	522	LMG	O6-C5-C4	4.15	117.23	109.69
23	b	616	CLA	O2D-CGD-CBD	4.15	118.63	111.27
23	A	406	CLA	C3D-C4D-ND	4.14	116.94	110.24
23	B	616	CLA	C2C-C1C-NC	4.14	113.85	109.97
23	b	610	CLA	C2C-C1C-NC	4.14	113.85	109.97
33	A	422	PL9	C27-C28-C29	-4.13	117.71	127.66
23	b	615	CLA	CHD-C4C-C3C	-4.13	118.77	124.84
23	B	605	CLA	C3D-C2D-C1D	-4.12	100.20	105.83
23	B	610	CLA	C3D-C4D-ND	4.12	116.90	110.24
23	d	408	CLA	C1-C2-C3	-4.12	118.92	126.04
38	E	101	LHG	O7-C7-C8	4.12	120.38	111.50
23	a	2609	CLA	C3D-C2D-C1D	-4.12	100.21	105.83
23	b	621	CLA	C2C-C1C-NC	4.11	113.83	109.97
23	b	619	CLA	C1-C2-C3	-4.11	118.93	126.04
37	c	518	DGD	O2G-C1B-C2B	4.11	120.36	111.50
23	b	614	CLA	C3D-C4D-ND	4.11	116.89	110.24
37	C	518	DGD	O2G-C1B-C2B	4.11	120.36	111.50
23	a	2613	CLA	C3D-C4D-ND	4.11	116.88	110.24
23	c	510	CLA	C3D-C2D-C1D	-4.10	100.23	105.83
23	A	407	CLA	CHD-C1D-ND	-4.10	120.69	124.45
23	C	514	CLA	C3D-C2D-C1D	-4.10	100.24	105.83
26	A	412	SQD	O6-C1-C2	4.09	114.69	108.30
26	a	2615	SQD	C1-O5-C5	-4.09	105.66	113.69
23	A	406	CLA	CHD-C1D-ND	-4.09	120.69	124.45
23	C	508	CLA	CHD-C4C-C3C	-4.09	118.83	124.84
40	H	102	RRX	C7-C8-C9	-4.09	120.06	126.23
23	b	616	CLA	CHD-C1D-ND	-4.08	120.70	124.45
23	C	505	CLA	CHD-C1D-ND	-4.08	120.70	124.45
23	B	615	CLA	C3D-C4D-ND	4.08	116.84	110.24
23	D	2303	CLA	C1C-C2C-C3C	-4.08	102.67	106.96
23	b	620	CLA	C3D-C2D-C1D	-4.08	100.27	105.83
23	b	613	CLA	O2D-CGD-CBD	4.07	118.51	111.27
23	A	405	CLA	C3D-C2D-C1D	-4.07	100.28	105.83
23	B	609	CLA	C3D-C4D-ND	4.07	116.82	110.24
23	c	504	CLA	O2D-CGD-O1D	-4.06	115.90	123.84
23	b	617	CLA	C3C-C4C-NC	4.05	115.12	110.57
23	C	508	CLA	C2C-C1C-NC	4.05	113.76	109.97
23	A	407	CLA	C1C-C2C-C3C	-4.04	102.70	106.96
23	B	616	CLA	C1D-CHD-C4C	-4.03	117.35	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	503	CLA	C1-C2-C3	-4.03	119.06	126.04
42	v	201	HEC	CBD-CAD-C3D	-4.03	105.74	112.62
23	b	613	CLA	C3D-C4D-ND	4.03	116.76	110.24
23	d	402	CLA	C3D-C4D-ND	4.03	116.76	110.24
31	a	2617	JOX	C4-C3-C2	-4.03	119.94	123.18
36	I	101	HTG	C1-O5-C5	4.03	120.01	112.58
27	m	2802	LMG	O7-C10-C11	4.02	120.17	111.50
23	b	612	CLA	CHD-C1D-ND	-4.02	120.76	124.45
23	b	619	CLA	O2D-CGD-O1D	-4.02	115.98	123.84
23	c	508	CLA	C3D-C2D-C1D	-4.02	100.34	105.83
23	C	512	CLA	C2C-C1C-NC	4.02	113.74	109.97
23	A	407	CLA	C1D-CHD-C4C	-4.02	117.39	126.06
23	b	619	CLA	C2C-C1C-NC	4.01	113.73	109.97
23	c	514	CLA	C3D-C2D-C1D	-4.01	100.36	105.83
23	D	2304	CLA	O2D-CGD-O1D	-4.01	116.01	123.84
40	h	101	RRX	C16-C17-C18	-4.00	121.60	127.31
23	A	410	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
23	B	603	CLA	CAA-C2A-C3A	-3.99	101.84	112.78
23	B	608	CLA	CAA-C2A-C3A	-3.99	101.84	112.78
25	k	302	BCR	C24-C23-C22	-3.99	120.21	126.23
23	b	608	CLA	C1C-C2C-C3C	-3.99	102.77	106.96
23	C	507	CLA	C1C-C2C-C3C	-3.98	102.77	106.96
37	c	519	DGD	O2G-C1B-C2B	3.98	120.08	111.50
23	C	507	CLA	C3D-C4D-ND	3.98	116.68	110.24
23	B	602	CLA	C3D-C2D-C1D	-3.98	100.41	105.83
23	c	514	CLA	CHD-C4C-C3C	-3.97	119.00	124.84
23	b	616	CLA	CBC-CAC-C3C	-3.97	101.48	112.43
23	b	618	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
23	B	609	CLA	O2D-CGD-CBD	3.97	118.32	111.27
27	c	522	LMG	C1-O6-C5	3.96	121.46	113.69
23	c	515	CLA	C1-O2A-CGA	3.96	126.84	116.44
23	b	616	CLA	C2C-C1C-NC	3.96	113.68	109.97
23	b	608	CLA	C3D-C4D-ND	3.96	116.64	110.24
23	B	606	CLA	O2A-CGA-O1A	-3.95	113.61	123.59
23	B	602	CLA	CHD-C1D-ND	-3.95	120.82	124.45
23	c	513	CLA	C3D-C4D-ND	3.95	116.63	110.24
23	B	603	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
23	B	614	CLA	C2C-C1C-NC	3.94	113.66	109.97
23	b	607	CLA	O2D-CGD-O1D	-3.94	116.14	123.84
31	A	419	JOX	C-C1-CL1	3.93	129.53	120.02
23	c	514	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
23	A	407	CLA	C2C-C1C-NC	3.93	113.65	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
23	d	409	CLA	C3D-C4D-ND	3.92	116.59	110.24
23	C	502	CLA	O2D-CGD-O1D	-3.92	116.17	123.84
23	C	510	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
23	B	606	CLA	C3D-C4D-ND	3.92	116.58	110.24
24	A	408	PHO	C1A-C2A-C3A	-3.92	99.11	102.84
23	b	608	CLA	C2C-C1C-NC	3.92	113.64	109.97
23	b	612	CLA	C2C-C1C-NC	3.92	113.64	109.97
23	b	609	CLA	C1C-C2C-C3C	-3.92	102.84	106.96
23	c	515	CLA	C1D-CHD-C4C	-3.91	117.61	126.06
23	a	2613	CLA	CBC-CAC-C3C	-3.91	101.64	112.43
23	a	2609	CLA	C2C-C1C-NC	3.91	113.64	109.97
23	B	611	CLA	CHD-C4C-C3C	-3.91	119.10	124.84
23	a	2610	CLA	CHD-C4C-C3C	-3.91	119.10	124.84
23	b	609	CLA	C2C-C1C-NC	3.90	113.63	109.97
23	b	616	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
26	D	2302	SQD	C1-O5-C5	3.90	121.34	113.69
39	F	101	HEM	CBD-CAD-C3D	-3.90	101.80	112.63
23	C	510	CLA	O2D-CGD-O1D	-3.90	116.22	123.84
23	B	611	CLA	C3D-C4D-ND	3.89	116.53	110.24
23	C	508	CLA	C1-C2-C3	-3.89	119.32	126.04
23	C	508	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
36	o	301	HTG	C1'-S1-C1	3.88	107.36	100.09
23	B	607	CLA	CHD-C4C-C3C	-3.88	119.13	124.84
33	x	1301	PL9	C27-C28-C29	-3.88	118.31	127.66
23	b	608	CLA	C3D-C2D-C1D	-3.88	100.54	105.83
23	c	514	CLA	C2C-C1C-NC	3.88	113.61	109.97
23	A	410	CLA	C3D-C4D-ND	3.88	116.51	110.24
23	C	502	CLA	C3D-C2D-C1D	-3.88	100.54	105.83
23	b	606	CLA	C3D-C2D-C1D	-3.88	100.54	105.83
23	c	508	CLA	C3C-C4C-NC	3.87	114.92	110.57
23	c	514	CLA	C3D-C4D-ND	3.87	116.50	110.24
25	C	515	BCR	C38-C26-C25	-3.87	120.18	124.53
23	B	608	CLA	C1C-C2C-C3C	-3.86	102.89	106.96
23	c	516	CLA	C3D-C4D-ND	3.86	116.48	110.24
23	C	512	CLA	C1-O2A-CGA	3.86	126.57	116.44
23	A	405	CLA	CHD-C4C-C3C	-3.86	119.17	124.84
23	c	512	CLA	C2C-C1C-NC	3.86	113.58	109.97
23	d	408	CLA	CHD-C1D-ND	-3.86	120.91	124.45
23	b	619	CLA	C3D-C4D-ND	3.86	116.47	110.24
33	A	422	PL9	C32-C33-C34	-3.85	118.39	127.66
23	b	611	CLA	CHD-C4C-C3C	-3.85	119.18	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	H	103	DGD	O2G-C1B-C2B	3.85	119.80	111.50
38	e	101	LHG	O7-C7-C8	3.85	119.80	111.50
27	C	520	LMG	O7-C10-C11	3.85	119.80	111.50
23	C	512	CLA	CHD-C4C-C3C	-3.85	119.18	124.84
23	B	615	CLA	C2C-C1C-NC	3.85	113.58	109.97
23	C	511	CLA	CBC-CAC-C3C	-3.85	101.82	112.43
23	B	617	CLA	C1D-CHD-C4C	-3.85	117.76	126.06
23	B	613	CLA	C3C-C4C-NC	3.84	114.88	110.57
39	F	101	HEM	CBA-CAA-C2A	-3.84	106.07	112.62
23	D	2304	CLA	C1-C2-C3	-3.84	119.41	126.04
23	c	509	CLA	C2C-C1C-NC	3.84	113.57	109.97
23	B	617	CLA	C2C-C1C-NC	3.84	113.57	109.97
23	A	410	CLA	CHD-C1D-ND	-3.83	120.93	124.45
23	d	402	CLA	C1D-CHD-C4C	-3.83	117.79	126.06
23	B	613	CLA	C2C-C1C-NC	3.83	113.56	109.97
39	e	103	HEM	CBD-CAD-C3D	-3.83	101.99	112.63
23	C	503	CLA	CHD-C4C-C3C	-3.83	119.21	124.84
23	a	2609	CLA	CAA-C2A-C3A	-3.83	102.30	112.78
23	C	511	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
28	B	623	LMT	C1-O1'-C1'	-3.82	107.50	113.84
23	c	505	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
23	b	618	CLA	C3D-C4D-ND	3.82	116.42	110.24
23	a	2613	CLA	C1-C2-C3	-3.82	119.44	126.04
25	C	516	BCR	C33-C5-C6	-3.81	120.25	124.53
23	C	503	CLA	C3D-C4D-ND	3.81	116.40	110.24
36	V	204	HTG	O5-C1-C2	-3.81	105.52	110.31
23	b	617	CLA	CMC-C2C-C1C	3.80	130.83	125.04
23	c	513	CLA	CBC-CAC-C3C	-3.80	101.95	112.43
23	C	507	CLA	O2D-CGD-CBD	3.80	118.02	111.27
23	b	616	CLA	C3D-C4D-ND	3.80	116.38	110.24
23	C	513	CLA	CHD-C4C-C3C	-3.80	119.26	124.84
23	c	515	CLA	CHD-C4C-C3C	-3.79	119.26	124.84
23	b	610	CLA	C3D-C4D-ND	3.79	116.38	110.24
23	d	402	CLA	CAA-C2A-C3A	-3.79	102.39	112.78
23	a	2609	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
23	C	502	CLA	C3D-C4D-ND	3.79	116.37	110.24
23	C	511	CLA	C3D-C2D-C1D	-3.78	100.67	105.83
23	b	608	CLA	CHD-C4C-C3C	-3.78	119.29	124.84
23	C	505	CLA	C3D-C4D-ND	3.78	116.35	110.24
23	C	509	CLA	C2C-C1C-NC	3.77	113.51	109.97
36	b	625	HTG	C1'-S1-C1	3.77	107.14	100.09
23	c	504	CLA	C2C-C1C-NC	3.77	113.50	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	514	CLA	CHD-C4C-C3C	-3.76	119.31	124.84
36	B	624[B]	HTG	C1-O5-C5	3.76	119.52	112.58
23	B	614	CLA	CHD-C1D-ND	-3.76	121.00	124.45
23	B	612	CLA	CHD-C1D-ND	-3.76	121.00	124.45
23	c	513	CLA	C3D-C2D-C1D	-3.76	100.70	105.83
23	B	607	CLA	O2D-CGD-O1D	-3.75	116.50	123.84
33	d	411	PL9	C7-C8-C9	-3.75	120.55	126.79
38	D	2309	LHG	O8-C23-C24	3.75	123.68	111.91
23	C	507	CLA	CHD-C4C-C3C	-3.75	119.33	124.84
23	c	511	CLA	O2D-CGD-O1D	-3.75	116.51	123.84
25	b	624	BCR	C24-C23-C22	-3.75	120.58	126.23
25	a	2614	BCR	C33-C5-C6	-3.74	120.32	124.53
23	C	507	CLA	C2C-C1C-NC	3.73	113.47	109.97
23	b	621	CLA	C4C-C3C-C2C	-3.73	101.46	106.90
28	B	623	LMT	O5B-C5B-C4B	3.73	116.47	109.69
23	c	508	CLA	C3D-C4D-ND	3.73	116.27	110.24
23	b	621	CLA	C3B-C4B-NB	3.73	114.03	109.21
23	a	2609	CLA	C1D-CHD-C4C	-3.73	118.02	126.06
23	B	605	CLA	C1-C2-C3	-3.73	119.60	126.04
23	B	615	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
23	b	607	CLA	C3D-C4D-ND	3.72	116.25	110.24
23	D	2303	CLA	C3C-C4C-NC	3.71	114.74	110.57
38	D	2309	LHG	O7-C7-C8	3.71	119.50	111.50
25	b	622	BCR	C24-C23-C22	-3.71	120.63	126.23
23	B	604	CLA	C3D-C4D-ND	3.71	116.23	110.24
23	c	513	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
23	c	507	CLA	CBC-CAC-C3C	-3.70	102.22	112.43
36	B	624[B]	HTG	O5-C1-C2	3.70	114.97	110.31
23	C	506	CLA	C2C-C1C-NC	3.70	113.44	109.97
23	A	410	CLA	C1-C2-C3	-3.70	119.65	126.04
23	A	410	CLA	CHD-C4C-C3C	-3.70	119.41	124.84
23	c	514	CLA	O2D-CGD-CBD	3.70	117.83	111.27
23	B	609	CLA	C1D-CHD-C4C	-3.69	118.09	126.06
23	a	2613	CLA	C1D-CHD-C4C	-3.69	118.09	126.06
23	c	506	CLA	C2C-C1C-NC	3.69	113.43	109.97
23	c	513	CLA	C2C-C1C-NC	3.69	113.43	109.97
23	c	512	CLA	C3D-C4D-ND	3.69	116.20	110.24
23	B	603	CLA	C3D-C4D-ND	3.69	116.20	110.24
23	B	605	CLA	C3D-C4D-ND	3.69	116.20	110.24
26	d	417	SQD	O9-S-C6	3.68	111.34	106.92
23	b	606	CLA	C3D-C4D-ND	3.68	116.18	110.24
23	B	608	CLA	CBC-CAC-C3C	-3.67	102.32	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	l	101	SQD	C1-C2-C3	-3.67	102.36	110.00
23	b	617	CLA	C2C-C1C-NC	3.67	113.41	109.97
26	a	2615	SQD	O8-S-C6	3.67	111.58	105.74
23	b	609	CLA	CAC-C3C-C4C	3.66	129.56	124.81
23	c	515	CLA	C3D-C4D-ND	3.66	116.16	110.24
23	c	508	CLA	CHD-C4C-C3C	-3.66	119.46	124.84
31	a	2619	JOX	C4-C3-C2	-3.66	120.24	123.18
25	b	622	BCR	C33-C5-C6	-3.66	120.42	124.53
26	a	2615	SQD	C1-C2-C3	-3.66	102.38	110.00
23	C	511	CLA	C4-C3-C5	3.66	121.42	115.27
23	B	606	CLA	C3C-C4C-NC	3.66	114.67	110.57
23	A	410	CLA	CMA-C3A-C4A	-3.65	101.96	111.77
23	B	614	CLA	C4-C3-C5	3.65	121.41	115.27
23	B	604	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
23	B	609	CLA	C3C-C4C-NC	3.65	114.66	110.57
23	A	405	CLA	CAA-C2A-C3A	-3.65	102.79	112.78
23	a	2610	CLA	O2D-CGD-CBD	3.64	117.74	111.27
23	A	405	CLA	C3C-C4C-NC	3.64	114.65	110.57
40	H	102	RRX	C24-C23-C22	-3.64	120.74	126.23
23	b	608	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
23	B	614	CLA	C3D-C4D-ND	3.63	116.12	110.24
23	B	604	CLA	C4-C3-C5	3.63	121.38	115.27
33	d	411	PL9	C42-C43-C44	-3.63	118.91	127.66
42	v	201	HEC	C1D-C2D-C3D	-3.63	104.47	107.00
23	d	402	CLA	C3B-C4B-NB	3.63	113.90	109.21
23	C	514	CLA	CHD-C1D-ND	-3.62	121.12	124.45
23	b	607	CLA	C2C-C1C-NC	3.62	113.37	109.97
23	C	502	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
23	C	506	CLA	C3D-C4D-ND	3.62	116.10	110.24
23	B	612	CLA	C2C-C1C-NC	3.62	113.36	109.97
23	c	505	CLA	CHD-C1D-ND	-3.62	121.13	124.45
23	b	613	CLA	C2C-C1C-NC	3.62	113.36	109.97
23	c	509	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
23	c	511	CLA	C3C-C4C-NC	3.61	114.62	110.57
23	c	515	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
27	c	521	LMG	O7-C10-C11	3.61	119.28	111.50
26	l	101	SQD	C3-C4-C5	3.61	116.68	110.24
39	e	103	HEM	C4B-CHC-C1C	3.61	127.32	122.56
23	c	514	CLA	CBC-CAC-C3C	-3.61	102.48	112.43
23	d	409	CLA	CHD-C1D-ND	-3.61	121.14	124.45
25	B	633	BCR	C15-C14-C13	3.60	132.45	127.31
25	B	633	BCR	C15-C16-C17	-3.60	116.11	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	O2D-CGD-O1D	-3.59	116.81	123.84
23	B	616	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
33	D	2306	PL9	C40-C39-C41	3.59	121.31	115.27
23	c	508	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
27	B	622	LMG	O7-C10-C11	3.59	119.23	111.50
23	b	613	CLA	C1C-C2C-C3C	-3.59	103.19	106.96
23	C	505	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
23	c	506	CLA	CHD-C4C-C3C	-3.58	119.57	124.84
23	b	610	CLA	C3C-C4C-NC	3.58	114.59	110.57
23	b	612	CLA	C3D-C4D-ND	3.58	116.03	110.24
23	C	513	CLA	C3D-C4D-ND	3.58	116.03	110.24
23	B	608	CLA	C3D-C4D-ND	3.58	116.02	110.24
23	A	405	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
23	B	617	CLA	C4-C3-C5	3.57	121.27	115.27
23	B	610	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
23	b	614	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
26	D	2308	SQD	O7-S-C6	3.56	111.17	106.94
23	C	504	CLA	C1-C2-C3	-3.56	119.88	126.04
23	c	506	CLA	CHD-C1D-ND	-3.56	121.18	124.45
23	B	602	CLA	C3D-C4D-ND	3.56	116.00	110.24
23	B	610	CLA	C2C-C1C-NC	3.56	113.31	109.97
23	A	405	CLA	O2D-CGD-CBD	3.56	117.59	111.27
23	c	511	CLA	CHD-C4C-C3C	-3.56	119.61	124.84
23	B	610	CLA	C1-C2-C3	-3.56	119.89	126.04
23	B	615	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
23	c	510	CLA	C3D-C4D-ND	3.55	115.99	110.24
23	B	611	CLA	C4C-C3C-C2C	-3.55	101.73	106.90
23	B	611	CLA	O2D-CGD-O1D	-3.54	116.92	123.84
23	b	611	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
25	T	102	BCR	C35-C13-C12	3.54	123.65	118.08
23	B	612	CLA	C3D-C4D-ND	3.53	115.95	110.24
23	b	613	CLA	CHD-C1D-ND	-3.53	121.21	124.45
38	L	101	LHG	O8-C23-C24	3.53	122.98	111.91
23	B	605	CLA	C1D-CHD-C4C	-3.53	118.45	126.06
23	c	507	CLA	C1D-CHD-C4C	-3.52	118.45	126.06
23	c	514	CLA	C1-O2A-CGA	3.52	125.69	116.44
31	a	2619	JOX	C1-C2-C3	3.52	117.38	114.18
23	c	512	CLA	C1-C2-C3	-3.52	119.95	126.04
23	C	511	CLA	CHD-C4C-C3C	-3.52	119.67	124.84
23	c	515	CLA	CBC-CAC-C3C	-3.52	102.73	112.43
23	b	620	CLA	C3D-C4D-ND	3.52	115.93	110.24
23	c	504	CLA	CBC-CAC-C3C	-3.52	102.74	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	C3D-C4D-ND	3.52	115.92	110.24
23	b	610	CLA	C1D-CHD-C4C	-3.52	118.47	126.06
23	d	402	CLA	CHD-C1D-ND	-3.51	121.22	124.45
23	C	514	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
23	C	509	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
23	C	512	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
23	B	606	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
23	b	606	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
23	B	616	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
26	B	621	SQD	C1-O5-C5	3.50	120.56	113.69
23	b	611	CLA	C3D-C4D-ND	3.50	115.90	110.24
23	B	616	CLA	C3D-C4D-ND	3.50	115.90	110.24
23	b	618	CLA	O2D-CGD-CBD	3.50	117.48	111.27
23	b	611	CLA	C1D-CHD-C4C	-3.50	118.52	126.06
23	b	608	CLA	C4-C3-C5	3.50	121.15	115.27
23	C	512	CLA	C3D-C4D-ND	3.50	115.89	110.24
23	B	603	CLA	C1D-CHD-C4C	-3.49	118.52	126.06
23	c	512	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
23	C	509	CLA	CHD-C1D-ND	-3.49	121.25	124.45
25	D	2305	BCR	C33-C5-C6	-3.49	120.61	124.53
23	B	617	CLA	CHD-C4C-C3C	-3.49	119.72	124.84
23	C	509	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
23	B	613	CLA	CHD-C1D-ND	-3.49	121.25	124.45
37	C	517	DGD	O2G-C1B-C2B	3.48	119.01	111.50
26	B	621	SQD	C3-C4-C5	3.48	116.45	110.24
23	B	602	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
23	a	2610	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
26	a	2603	SQD	O7-S-C6	3.48	111.07	106.94
23	B	617	CLA	CBC-CAC-C3C	-3.48	102.85	112.43
36	b	625	HTG	C6-C5-C4	-3.48	104.86	113.00
23	b	617	CLA	C1C-C2C-C3C	-3.47	103.30	106.96
23	d	408	CLA	C3C-C4C-NC	3.47	114.47	110.57
23	b	617	CLA	C1D-CHD-C4C	-3.47	118.57	126.06
23	c	509	CLA	C16-C15-C13	-3.47	104.70	115.92
23	C	506	CLA	C1D-CHD-C4C	-3.47	118.57	126.06
25	C	515	BCR	C33-C5-C6	-3.47	120.63	124.53
23	c	510	CLA	C4A-NA-C1A	3.47	108.27	106.71
23	c	506	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
23	B	611	CLA	CHD-C1D-ND	-3.47	121.27	124.45
23	B	603	CLA	O2D-CGD-O1D	-3.46	117.07	123.84
23	C	510	CLA	C1-C2-C3	-3.46	120.06	126.04
23	C	509	CLA	CHD-C4C-C3C	-3.46	119.75	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	615	CLA	C3D-C4D-ND	3.46	115.83	110.24
23	C	512	CLA	C4A-NA-C1A	3.46	108.26	106.71
36	C	521	HTG	C1'-S1-C1	3.46	106.56	100.09
23	a	2613	CLA	C3B-C4B-NB	3.46	113.68	109.21
23	B	613	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
23	C	510	CLA	C3D-C4D-ND	3.45	115.82	110.24
23	b	614	CLA	CBC-CAC-C3C	-3.45	102.92	112.43
23	b	619	CLA	C1D-CHD-C4C	-3.45	118.62	126.06
23	A	410	CLA	CBC-CAC-C3C	-3.45	102.93	112.43
23	b	619	CLA	CHD-C1D-ND	-3.45	121.29	124.45
23	B	612	CLA	O2D-CGD-O1D	-3.44	117.10	123.84
23	C	511	CLA	C1-C2-C3	-3.44	120.09	126.04
37	h	102	DGD	O2G-C1B-C2B	3.44	118.92	111.50
23	b	619	CLA	CAC-C3C-C4C	3.44	129.28	124.81
23	C	504	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
23	B	614	CLA	C3C-C4C-NC	3.44	114.43	110.57
36	i	102	HTG	C3-C4-C5	3.44	116.38	110.24
23	A	406	CLA	C3B-C4B-NB	3.44	113.66	109.21
23	b	613	CLA	C1-C2-C3	-3.44	120.09	126.04
23	b	620	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
23	c	512	CLA	CHD-C4C-C3C	-3.44	119.79	124.84
27	C	520	LMG	O8-C28-C29	3.44	122.70	111.91
23	c	512	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
23	C	510	CLA	CHD-C4C-C3C	-3.44	119.79	124.84
23	B	613	CLA	CMC-C2C-C1C	3.44	130.27	125.04
23	C	508	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
23	b	611	CLA	C3C-C4C-NC	3.43	114.42	110.57
37	D	2307	DGD	O1G-C1A-C2A	3.43	122.68	111.91
33	A	422	PL9	C32-C31-C29	-3.43	101.69	112.98
23	C	507	CLA	CHD-C1D-ND	-3.43	121.30	124.45
38	D	2309	LHG	O8-C23-O10	-3.43	114.94	123.59
23	b	615	CLA	C1D-CHD-C4C	-3.43	118.67	126.06
23	c	516	CLA	C1D-CHD-C4C	-3.42	118.67	126.06
23	B	604	CLA	CHD-C4C-C3C	-3.42	119.81	124.84
25	B	618	BCR	C7-C8-C9	-3.42	121.07	126.23
23	B	611	CLA	C2C-C1C-NC	3.42	113.17	109.97
23	a	2609	CLA	C3C-C4C-NC	3.42	114.41	110.57
23	c	516	CLA	CHD-C1D-ND	-3.42	121.31	124.45
23	A	406	CLA	C1D-CHD-C4C	-3.41	118.70	126.06
23	b	614	CLA	C2C-C1C-NC	3.41	113.17	109.97
25	c	517	BCR	C38-C26-C25	-3.41	120.70	124.53
25	C	515	BCR	C11-C10-C9	-3.40	122.45	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	621	CLA	C3D-C4D-ND	3.40	115.75	110.24
23	c	512	CLA	CAC-C3C-C4C	3.40	129.23	124.81
23	b	609	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
23	D	2304	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
23	c	513	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
23	b	612	CLA	C3C-C4C-NC	3.40	114.38	110.57
23	B	606	CLA	O2D-CGD-CBD	3.40	117.31	111.27
24	a	2612	PHO	O2D-CGD-O1D	-3.40	117.19	123.84
23	C	511	CLA	C2C-C1C-NC	3.40	113.16	109.97
23	b	615	CLA	CHD-C1D-ND	-3.40	121.33	124.45
23	b	614	CLA	CHD-C4C-C3C	-3.39	119.85	124.84
25	z	101	BCR	C16-C17-C18	-3.39	122.47	127.31
23	c	511	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
25	A	411	BCR	C33-C5-C6	-3.39	120.72	124.53
23	C	505	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
23	B	617	CLA	C3D-C4D-ND	3.39	115.72	110.24
23	B	617	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
38	d	412	LHG	O8-C23-C24	3.39	122.54	111.91
23	b	608	CLA	O2A-CGA-O1A	-3.39	115.04	123.59
23	B	611	CLA	C1D-CHD-C4C	-3.39	118.75	126.06
23	b	619	CLA	C1C-C2C-C3C	-3.39	103.40	106.96
23	b	610	CLA	C4-C3-C5	3.39	120.97	115.27
23	c	505	CLA	C2C-C1C-NC	3.39	113.14	109.97
28	z	102	LMT	O1B-C1B-C2B	3.39	116.87	108.10
23	B	613	CLA	C3B-C4B-NB	3.38	113.59	109.21
23	C	512	CLA	C3B-C4B-NB	3.38	113.59	109.21
24	a	2612	PHO	CMB-C2B-C3B	3.38	131.01	124.68
23	c	512	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
27	C	527	LMG	O8-C28-C29	3.38	122.52	111.91
23	B	612	CLA	C1C-C2C-C3C	-3.38	103.41	106.96
40	H	102	RRX	C10-C11-C12	-3.38	112.68	123.22
23	c	515	CLA	C2C-C1C-NC	3.38	113.14	109.97
23	c	508	CLA	C4C-C3C-C2C	-3.38	101.98	106.90
23	b	618	CLA	CHD-C1D-ND	-3.38	121.35	124.45
23	C	506	CLA	CAC-C3C-C4C	3.37	129.19	124.81
23	b	615	CLA	C3C-C4C-NC	3.37	114.35	110.57
23	B	617	CLA	C1C-C2C-C3C	-3.37	103.41	106.96
23	b	606	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
26	b	601	SQD	O5-C5-C4	3.37	115.81	109.69
23	C	503	CLA	C1C-C2C-C3C	-3.37	103.42	106.96
26	l	101	SQD	O7-S-C6	3.37	110.94	106.94
27	C	527	LMG	O6-C5-C4	3.36	115.80	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	CHD-C4C-C3C	-3.36	119.90	124.84
23	b	618	CLA	C1-C2-C3	-3.36	120.23	126.04
23	B	608	CLA	CAC-C3C-C4C	3.36	129.17	124.81
23	a	2610	CLA	C2C-C1C-NC	3.36	113.12	109.97
23	C	511	CLA	C3B-C4B-NB	3.36	113.55	109.21
23	b	619	CLA	CHD-C4C-C3C	-3.36	119.91	124.84
23	b	610	CLA	CHD-C1D-ND	-3.35	121.37	124.45
23	C	504	CLA	C4A-NA-C1A	3.35	108.21	106.71
23	c	515	CLA	CBA-CAA-C2A	-3.35	103.97	113.86
23	B	616	CLA	C3B-C4B-NB	3.35	113.54	109.21
23	C	507	CLA	C1D-CHD-C4C	-3.35	118.83	126.06
23	b	611	CLA	C2C-C1C-NC	3.35	113.11	109.97
23	c	508	CLA	C1D-CHD-C4C	-3.35	118.83	126.06
23	B	612	CLA	CHD-C4C-C3C	-3.35	119.92	124.84
23	b	607	CLA	C4C-C3C-C2C	-3.35	102.02	106.90
23	b	607	CLA	CAC-C3C-C4C	3.34	129.15	124.81
23	b	618	CLA	CHD-C4C-C3C	-3.34	119.93	124.84
23	C	504	CLA	C1D-CHD-C4C	-3.34	118.85	126.06
23	C	513	CLA	C1D-CHD-C4C	-3.34	118.85	126.06
23	B	606	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
23	a	2609	CLA	CHD-C4C-C3C	-3.34	119.93	124.84
23	C	505	CLA	CHD-C4C-C3C	-3.34	119.93	124.84
23	B	616	CLA	C3C-C4C-NC	3.34	114.31	110.57
23	b	616	CLA	C1D-CHD-C4C	-3.34	118.86	126.06
23	C	503	CLA	C2C-C1C-NC	3.33	113.09	109.97
23	B	611	CLA	C3C-C4C-NC	3.33	114.31	110.57
23	B	607	CLA	C3D-C4D-ND	3.33	115.62	110.24
23	C	512	CLA	C1D-CHD-C4C	-3.33	118.88	126.06
23	A	410	CLA	C4-C3-C5	3.33	120.87	115.27
23	c	509	CLA	CBC-CAC-C3C	-3.33	103.26	112.43
23	b	620	CLA	CHD-C4C-C3C	-3.32	119.96	124.84
23	B	606	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
23	c	505	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
23	c	511	CLA	C4C-C3C-C2C	-3.32	102.06	106.90
25	K	101	BCR	C24-C23-C22	-3.32	121.22	126.23
23	d	408	CLA	C3B-C4B-NB	3.32	113.50	109.21
24	A	409	PHO	C4-C3-C5	3.32	120.85	115.27
23	C	506	CLA	C4C-C3C-C2C	-3.32	102.06	106.90
25	B	633	BCR	C11-C10-C9	-3.31	122.58	127.31
28	M	101	LMT	C1'-O5'-C5'	3.31	120.19	113.69
23	c	516	CLA	C1-C2-C3	-3.31	120.32	126.04
23	b	608	CLA	C3C-C4C-NC	3.31	114.28	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	506	CLA	C3D-C4D-ND	3.31	115.59	110.24
23	c	512	CLA	C3C-C4C-NC	3.31	114.28	110.57
36	V	204	HTG	C1-C2-C3	-3.30	104.07	110.59
23	C	508	CLA	C1D-CHD-C4C	-3.30	118.94	126.06
23	c	516	CLA	CHD-C4C-C3C	-3.30	119.99	124.84
23	c	509	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
23	a	2609	CLA	CMB-C2B-C3B	3.30	130.85	124.68
23	a	2613	CLA	CMA-C3A-C2A	-3.30	100.53	113.83
23	A	407	CLA	CBC-CAC-C3C	-3.29	103.35	112.43
23	C	508	CLA	C3C-C4C-NC	3.29	114.26	110.57
23	C	509	CLA	C1-C2-C3	-3.29	120.35	126.04
23	c	514	CLA	C4-C3-C5	3.29	120.80	115.27
23	c	510	CLA	C3C-C4C-NC	3.29	114.26	110.57
23	C	514	CLA	C1D-CHD-C4C	-3.29	118.97	126.06
23	b	615	CLA	O2D-CGD-CBD	3.29	117.11	111.27
40	H	102	RRX	C38-C26-C25	-3.29	120.84	124.53
23	B	610	CLA	C4C-C3C-C2C	-3.28	102.11	106.90
23	d	409	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
23	a	2613	CLA	C4-C3-C5	3.28	120.79	115.27
23	C	507	CLA	CBC-CAC-C3C	-3.28	103.39	112.43
25	B	633	BCR	C12-C13-C14	-3.28	113.91	118.94
23	A	407	CLA	C4-C3-C5	3.27	120.78	115.27
23	c	506	CLA	C3C-C4C-NC	3.27	114.24	110.57
23	b	608	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
23	A	410	CLA	C1D-CHD-C4C	-3.27	119.01	126.06
23	B	604	CLA	C2C-C1C-NC	3.26	113.03	109.97
23	d	402	CLA	C3C-C4C-NC	3.26	114.23	110.57
23	B	607	CLA	C2C-C1C-NC	3.26	113.03	109.97
23	D	2303	CLA	O2A-CGA-CBA	3.26	122.14	111.91
23	c	509	CLA	C1D-CHD-C4C	-3.26	119.02	126.06
23	b	617	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
33	D	2306	PL9	C7-C8-C9	-3.26	121.37	126.79
23	c	513	CLA	CHD-C4C-C3C	-3.26	120.05	124.84
23	C	505	CLA	CBC-CAC-C3C	-3.25	103.46	112.43
23	c	516	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
33	d	411	PL9	C37-C38-C39	-3.25	119.84	127.66
33	A	422	PL9	C17-C18-C19	-3.25	119.84	127.66
23	A	407	CLA	CAA-C2A-C3A	-3.25	103.89	112.78
23	A	405	CLA	CAA-C2A-C1A	-3.25	101.33	111.97
23	B	607	CLA	C3C-C4C-NC	3.25	114.21	110.57
25	c	517	BCR	C15-C14-C13	-3.25	122.68	127.31
23	b	619	CLA	C3C-C4C-NC	3.24	114.21	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	409	CLA	C4-C3-C5	3.24	120.73	115.27
23	B	607	CLA	C1D-CHD-C4C	-3.24	119.06	126.06
25	y	101	BCR	C38-C26-C25	-3.24	120.89	124.53
23	B	606	CLA	O2A-CGA-CBA	3.24	122.08	111.91
23	C	504	CLA	CMC-C2C-C1C	3.24	129.97	125.04
38	d	412	LHG	O8-C23-O10	-3.24	115.43	123.59
23	b	615	CLA	C4C-C3C-C2C	-3.23	102.18	106.90
23	A	410	CLA	C3B-C4B-NB	3.23	113.39	109.21
23	b	612	CLA	CMC-C2C-C1C	3.23	129.96	125.04
23	B	609	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
23	B	606	CLA	CHD-C1D-ND	-3.23	121.49	124.45
23	C	510	CLA	C1D-CHD-C4C	-3.23	119.09	126.06
23	C	503	CLA	CHD-C1D-ND	-3.23	121.49	124.45
23	c	505	CLA	C1D-CHD-C4C	-3.23	119.09	126.06
23	B	610	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
23	B	606	CLA	CAC-C3C-C4C	3.23	129.00	124.81
23	B	604	CLA	C3C-C4C-NC	3.22	114.19	110.57
23	A	405	CLA	C3B-C4B-NB	3.22	113.37	109.21
23	a	2609	CLA	CAA-C2A-C1A	-3.22	101.44	111.97
31	A	418	JOX	O1-C5-C4	-3.21	116.81	121.41
23	b	615	CLA	C2C-C1C-NC	3.21	112.98	109.97
23	c	514	CLA	C1D-CHD-C4C	-3.21	119.13	126.06
23	C	510	CLA	C3B-C4B-NB	3.21	113.36	109.21
23	c	510	CLA	CHD-C4C-C3C	-3.21	120.12	124.84
23	b	608	CLA	O2A-CGA-CBA	3.21	121.97	111.91
23	B	614	CLA	C3B-C4B-NB	3.20	113.35	109.21
23	B	616	CLA	CBC-CAC-C3C	-3.20	103.60	112.43
27	c	521	LMG	O8-C28-C29	3.20	121.96	111.91
23	B	602	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
23	b	613	CLA	CHD-C4C-C3C	-3.20	120.14	124.84
23	C	503	CLA	C1D-CHD-C4C	-3.20	119.16	126.06
23	c	516	CLA	C2C-C1C-NC	3.20	112.97	109.97
23	B	608	CLA	C1D-CHD-C4C	-3.20	119.16	126.06
23	B	602	CLA	O2A-CGA-CBA	3.20	121.94	111.91
23	B	613	CLA	C4C-C3C-C2C	-3.20	102.24	106.90
23	B	610	CLA	C3C-C4C-NC	3.20	114.16	110.57
23	C	510	CLA	C3C-C4C-NC	3.19	114.15	110.57
33	A	422	PL9	C12-C13-C14	-3.19	119.97	127.66
25	B	633	BCR	C7-C8-C9	-3.19	121.41	126.23
23	b	612	CLA	C1D-CHD-C4C	-3.19	119.17	126.06
23	B	603	CLA	CHD-C1D-ND	-3.19	121.52	124.45
25	b	624	BCR	C15-C14-C13	-3.19	122.76	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	CLA	CAA-C2A-C3A	-3.19	104.05	112.78
23	B	607	CLA	CAC-C3C-C4C	3.19	128.94	124.81
23	b	610	CLA	CMC-C2C-C1C	3.19	129.89	125.04
25	A	411	BCR	C38-C26-C25	-3.18	120.95	124.53
23	c	510	CLA	C1-C2-C3	-3.18	120.54	126.04
23	B	605	CLA	C3B-C4B-NB	3.18	113.32	109.21
40	H	102	RRX	C16-C17-C18	-3.18	122.77	127.31
24	a	2612	PHO	C1A-C2A-C3A	-3.18	99.81	102.84
23	b	609	CLA	C3C-C4C-NC	3.18	114.14	110.57
23	c	506	CLA	C1D-CHD-C4C	-3.18	119.20	126.06
37	c	519	DGD	O1G-C1A-C2A	3.18	121.88	111.91
23	b	606	CLA	C2C-C1C-NC	3.18	112.95	109.97
23	b	613	CLA	O2A-CGA-CBA	3.18	121.88	111.91
23	c	512	CLA	C3B-C4B-NB	3.17	113.31	109.21
23	C	504	CLA	C3C-C4C-NC	3.17	114.13	110.57
23	C	511	CLA	CHD-C1D-ND	-3.17	121.54	124.45
33	d	411	PL9	C40-C39-C41	3.17	120.61	115.27
23	C	509	CLA	C3C-C4C-NC	3.16	114.12	110.57
25	b	622	BCR	C7-C8-C9	-3.16	121.45	126.23
33	x	1301	PL9	C12-C13-C14	-3.16	120.04	127.66
23	b	607	CLA	CHD-C1D-ND	-3.16	121.55	124.45
23	b	608	CLA	CAA-C2A-C3A	-3.16	104.12	112.78
23	A	405	CLA	CMA-C3A-C4A	-3.16	103.28	111.77
23	C	507	CLA	C3C-C4C-NC	3.16	114.11	110.57
25	C	515	BCR	C7-C8-C9	-3.16	121.47	126.23
23	C	513	CLA	C3C-C4C-NC	3.16	114.11	110.57
36	C	525	HTG	C1-O5-C5	3.16	118.40	112.58
23	b	616	CLA	CMC-C2C-C1C	3.15	129.84	125.04
23	C	513	CLA	C1C-C2C-C3C	-3.15	103.64	106.96
23	B	616	CLA	CHD-C1D-ND	-3.15	121.56	124.45
23	A	406	CLA	CMB-C2B-C3B	3.15	130.57	124.68
23	a	2610	CLA	C3C-C4C-NC	3.15	114.10	110.57
23	c	515	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
33	x	1301	PL9	C20-C19-C21	3.15	120.57	115.27
23	C	502	CLA	CHD-C1D-ND	-3.14	121.56	124.45
23	A	410	CLA	CMA-C3A-C2A	-3.14	101.15	113.83
23	B	603	CLA	CHD-C4C-C3C	-3.14	120.22	124.84
23	B	612	CLA	CMC-C2C-C1C	3.14	129.82	125.04
24	A	409	PHO	C1A-C2A-C3A	-3.14	99.85	102.84
23	c	513	CLA	C3B-C4B-NB	3.14	113.27	109.21
23	c	509	CLA	O2A-CGA-O1A	-3.14	115.67	123.59
23	c	511	CLA	C1C-C2C-C3C	-3.14	103.66	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	C4-C3-C5	3.14	120.55	115.27
23	c	512	CLA	CMC-C2C-C1C	3.13	129.81	125.04
23	c	508	CLA	CHA-C1A-NA	-3.13	119.22	126.40
23	B	606	CLA	CMC-C2C-C1C	3.13	129.81	125.04
23	b	620	CLA	CAC-C3C-C4C	3.13	128.88	124.81
23	B	608	CLA	CHD-C4C-C3C	-3.13	120.24	124.84
23	d	408	CLA	CHD-C4C-C3C	-3.13	120.24	124.84
23	B	604	CLA	C1D-CHD-C4C	-3.13	119.31	126.06
23	A	405	CLA	C1D-CHD-C4C	-3.13	119.31	126.06
23	B	613	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
23	C	506	CLA	CHA-C1A-NA	-3.12	119.25	126.40
23	B	609	CLA	C2C-C1C-NC	3.12	112.90	109.97
23	B	607	CLA	CHD-C1D-ND	-3.12	121.58	124.45
27	A	413	LMG	C8-O7-C10	-3.12	110.10	117.79
23	C	502	CLA	C1D-CHD-C4C	-3.12	119.32	126.06
24	a	2611	PHO	C1A-C2A-C3A	-3.12	99.87	102.84
27	c	521	LMG	C8-O7-C10	-3.12	110.11	117.79
23	c	506	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
23	B	603	CLA	CBC-CAC-C3C	-3.12	103.84	112.43
23	b	610	CLA	CMB-C2B-C3B	3.12	130.51	124.68
23	A	410	CLA	C3C-C4C-NC	3.12	114.07	110.57
23	C	513	CLA	CBA-CAA-C2A	-3.12	104.67	113.86
23	B	617	CLA	C3B-C4B-NB	3.11	113.23	109.21
33	d	411	PL9	C15-C14-C16	3.11	120.51	115.27
23	C	503	CLA	C3C-C4C-NC	3.11	114.06	110.57
23	b	607	CLA	C1D-CHD-C4C	-3.11	119.35	126.06
23	b	609	CLA	C3D-C4D-ND	3.11	115.27	110.24
38	e	101	LHG	O8-C23-C24	3.11	121.66	111.91
23	A	406	CLA	C3C-C4C-NC	3.11	114.06	110.57
23	c	512	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
23	C	509	CLA	CAC-C3C-C4C	3.11	128.84	124.81
23	b	607	CLA	C1C-C2C-C3C	-3.11	103.69	106.96
23	C	504	CLA	CBC-CAC-C3C	-3.11	103.87	112.43
23	A	405	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
23	B	615	CLA	C3B-C4B-NB	3.10	113.22	109.21
23	B	613	CLA	C1D-CHD-C4C	-3.10	119.36	126.06
23	c	510	CLA	CBC-CAC-C3C	-3.10	103.88	112.43
36	b	604	HTG	O5-C5-C4	3.10	115.33	109.69
23	D	2303	CLA	C1-C2-C3	-3.10	120.68	126.04
23	a	2610	CLA	O2A-CGA-O1A	-3.10	115.77	123.59
23	b	618	CLA	C3B-C4B-NB	3.10	113.22	109.21
23	B	614	CLA	C1D-CHD-C4C	-3.10	119.38	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	506	CLA	O2D-CGD-O1D	-3.10	117.79	123.84
23	C	511	CLA	C1D-CHD-C4C	-3.09	119.38	126.06
23	B	604	CLA	O2A-CGA-O1A	-3.09	115.78	123.59
23	b	607	CLA	C3C-C4C-NC	3.09	114.04	110.57
23	B	604	CLA	O2A-CGA-CBA	3.09	121.60	111.91
42	V	201	HEC	CMB-C2B-C1B	-3.09	123.72	128.46
23	B	612	CLA	C1D-CHD-C4C	-3.09	119.40	126.06
31	A	418	JOX	O-C2-C1	-3.09	119.95	122.76
23	b	615	CLA	C1-C2-C3	-3.09	120.71	126.04
23	B	616	CLA	C4-C3-C5	3.09	120.46	115.27
37	H	103	DGD	O1G-C1A-C2A	3.08	121.58	111.91
23	c	510	CLA	C1D-CHD-C4C	-3.08	119.41	126.06
23	c	507	CLA	C4-C3-C5	3.08	120.45	115.27
25	B	618	BCR	C24-C23-C22	-3.08	121.58	126.23
26	A	412	SQD	O8-S-C6	3.08	110.65	105.74
23	d	402	CLA	O2A-CGA-O1A	-3.08	115.82	123.59
42	v	201	HEC	CMB-C2B-C1B	-3.08	123.73	128.46
23	B	605	CLA	O2A-CGA-O1A	-3.08	115.83	123.59
23	C	506	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
28	m	2804	LMT	C1B-C2B-C3B	3.08	116.40	110.00
23	B	610	CLA	CHD-C4C-C3C	-3.07	120.32	124.84
37	h	102	DGD	O1G-C1A-O1A	-3.07	115.84	123.59
23	b	613	CLA	C3B-C4B-NB	3.07	113.18	109.21
23	C	511	CLA	C3C-C4C-NC	3.07	114.01	110.57
25	C	516	BCR	C38-C26-C25	-3.07	121.08	124.53
28	i	103	LMT	C1'-O5'-C5'	3.07	119.71	113.69
23	c	510	CLA	C4-C3-C5	3.07	120.43	115.27
23	b	613	CLA	CBC-CAC-C3C	-3.07	103.98	112.43
23	b	616	CLA	C1-C2-C3	-3.07	120.74	126.04
23	B	608	CLA	C3B-C4B-NB	3.06	113.17	109.21
23	d	402	CLA	C1-C2-C3	-3.06	120.75	126.04
23	B	608	CLA	CHD-C1D-ND	-3.06	121.64	124.45
23	b	610	CLA	C3B-C4B-NB	3.06	113.17	109.21
23	C	513	CLA	C1-C2-C3	-3.06	120.75	126.04
23	B	616	CLA	CMC-C2C-C1C	3.06	129.70	125.04
23	C	507	CLA	O2A-CGA-CBA	3.06	121.51	111.91
23	d	408	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
23	a	2610	CLA	C4-C3-C5	3.06	120.42	115.27
23	c	509	CLA	CAA-C2A-C3A	-3.06	104.40	112.78
23	b	608	CLA	CHD-C1D-ND	-3.06	121.64	124.45
23	c	514	CLA	C3B-C4B-NB	3.06	113.16	109.21
23	A	405	CLA	CMB-C2B-C3B	3.06	130.39	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	509	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
23	B	615	CLA	O2A-CGA-O1A	-3.05	115.89	123.59
23	b	612	CLA	CBC-CAC-C3C	-3.05	104.03	112.43
23	b	621	CLA	CBC-CAC-C3C	-3.05	104.03	112.43
23	C	502	CLA	C2C-C1C-NC	3.05	112.83	109.97
23	C	503	CLA	C4C-C3C-C2C	-3.04	102.46	106.90
23	C	513	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
25	b	623	BCR	C38-C26-C25	-3.04	121.11	124.53
33	x	1301	PL9	C32-C33-C34	-3.04	120.34	127.66
26	d	417	SQD	O48-C23-C24	3.04	121.45	111.91
23	B	604	CLA	CHD-C1D-ND	-3.04	121.66	124.45
23	D	2303	CLA	C1D-CHD-C4C	-3.03	119.51	126.06
27	A	413	LMG	C7-O1-C1	-3.03	107.81	113.74
23	c	504	CLA	C1D-CHD-C4C	-3.03	119.52	126.06
23	b	609	CLA	CHA-C1A-NA	-3.03	119.46	126.40
23	c	507	CLA	C3B-C4B-NB	3.03	113.13	109.21
23	C	513	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
23	B	605	CLA	CHD-C1D-ND	-3.03	121.67	124.45
23	B	617	CLA	C3C-C4C-NC	3.02	113.96	110.57
23	B	607	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
23	b	617	CLA	C1-C2-C3	-3.02	120.82	126.04
23	C	514	CLA	C2C-C1C-NC	3.02	112.80	109.97
23	c	504	CLA	C3C-C4C-NC	3.02	113.95	110.57
23	B	617	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
23	d	409	CLA	C3B-C4B-NB	3.01	113.11	109.21
23	b	613	CLA	C1D-CHD-C4C	-3.01	119.56	126.06
36	d	407	HTG	C1-O5-C5	3.01	118.13	112.58
23	B	605	CLA	C3C-C4C-NC	3.01	113.94	110.57
23	A	407	CLA	O2A-CGA-O1A	-3.01	116.00	123.59
23	B	608	CLA	C1-O2A-CGA	3.01	124.33	116.44
23	C	506	CLA	C3D-C2D-C1D	-3.01	101.73	105.83
23	B	609	CLA	C1C-C2C-C3C	-3.00	103.80	106.96
23	b	619	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
23	a	2609	CLA	CMC-C2C-C1C	3.00	129.61	125.04
23	B	605	CLA	CMC-C2C-C1C	3.00	129.61	125.04
23	B	602	CLA	C2C-C1C-NC	3.00	112.78	109.97
23	b	611	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
37	c	520	DGD	O1G-C1A-C2A	3.00	121.32	111.91
33	D	2306	PL9	C25-C24-C26	3.00	120.31	115.27
23	c	509	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
23	c	505	CLA	C3C-C4C-NC	3.00	113.93	110.57
23	b	607	CLA	CAA-CBA-CGA	-2.99	104.50	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	H	103	DGD	C2G-O2G-C1B	-2.99	110.42	117.79
23	b	620	CLA	C1C-C2C-C3C	-2.99	103.81	106.96
23	c	510	CLA	C3B-C4B-NB	2.99	113.08	109.21
23	c	511	CLA	C4-C3-C5	2.99	120.30	115.27
23	b	615	CLA	C1C-C2C-C3C	-2.99	103.81	106.96
23	c	509	CLA	CHD-C4C-C3C	-2.99	120.44	124.84
23	B	606	CLA	C2C-C1C-NC	2.99	112.77	109.97
23	b	620	CLA	C2C-C1C-NC	2.99	112.77	109.97
23	C	506	CLA	C3C-C4C-NC	2.99	113.92	110.57
23	B	615	CLA	CBC-CAC-C3C	-2.99	104.19	112.43
25	k	302	BCR	C38-C26-C25	-2.99	121.17	124.53
23	B	607	CLA	C4C-C3C-C2C	-2.99	102.55	106.90
23	B	613	CLA	CMB-C2B-C3B	2.98	130.26	124.68
23	c	505	CLA	O2A-CGA-O1A	-2.98	116.06	123.59
23	b	606	CLA	CHD-C1D-ND	-2.98	121.71	124.45
23	B	605	CLA	C4A-NA-C1A	2.98	108.05	106.71
23	B	602	CLA	C1D-CHD-C4C	-2.98	119.63	126.06
23	c	507	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
23	B	603	CLA	C3C-C4C-NC	2.98	113.91	110.57
36	C	522	HTG	O5-C1-C2	2.98	114.06	110.31
23	b	617	CLA	O2A-CGA-CBA	2.98	121.25	111.91
23	B	611	CLA	CMA-C3A-C4A	-2.98	103.77	111.77
23	b	610	CLA	O2A-CGA-O1A	-2.98	116.08	123.59
26	A	412	SQD	O9-S-C6	2.98	110.48	106.94
23	a	2610	CLA	O2A-CGA-CBA	2.98	121.25	111.91
37	H	103	DGD	C3G-O3G-C1D	-2.97	107.93	113.74
23	d	408	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
23	c	516	CLA	C3C-C4C-NC	2.97	113.90	110.57
23	b	620	CLA	CED-O2D-CGD	2.97	122.66	115.94
23	B	602	CLA	CHD-C4C-C3C	-2.97	120.47	124.84
23	a	2609	CLA	C3B-C4B-NB	2.97	113.05	109.21
25	T	102	BCR	C11-C10-C9	-2.97	123.07	127.31
31	a	2617	JOX	C-C1-C2	-2.97	120.80	123.18
33	d	411	PL9	O1-C4-C3	-2.97	117.45	120.72
23	c	509	CLA	C4-C3-C5	2.97	120.26	115.27
25	y	101	BCR	C16-C17-C18	-2.97	123.08	127.31
23	c	508	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
23	b	617	CLA	C3B-C4B-NB	2.96	113.04	109.21
23	b	611	CLA	CMC-C2C-C1C	2.96	129.55	125.04
26	A	412	SQD	C1-C2-C3	-2.96	103.83	110.00
23	B	612	CLA	C3C-C4C-NC	2.96	113.89	110.57
31	a	2617	JOX	C-C5-C4	2.96	123.59	117.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	C4A-NA-C1A	2.96	108.03	106.71
23	C	508	CLA	C3D-C4D-ND	2.95	115.02	110.24
23	b	612	CLA	C3B-C4B-NB	2.95	113.03	109.21
25	K	101	BCR	C7-C8-C9	-2.95	121.78	126.23
23	B	612	CLA	CHA-C1A-NA	-2.95	119.64	126.40
23	b	616	CLA	CAA-C2A-C3A	-2.95	104.70	112.78
23	C	514	CLA	C1-C2-C3	-2.95	120.94	126.04
23	d	408	CLA	CAA-C2A-C3A	-2.95	104.70	112.78
23	d	402	CLA	CHC-C1C-C2C	-2.95	118.57	126.72
23	c	509	CLA	O2A-CGA-CBA	2.95	121.16	111.91
23	b	618	CLA	C1D-CHD-C4C	-2.95	119.70	126.06
37	C	517	DGD	O3G-C3G-C2G	-2.95	103.79	110.90
23	C	512	CLA	O2D-CGD-CBD	2.94	116.50	111.27
23	b	615	CLA	O2A-CGA-CBA	2.94	121.14	111.91
23	c	509	CLA	C3C-C4C-NC	2.94	113.87	110.57
38	d	413	LHG	O8-C23-O10	-2.94	116.16	123.59
23	D	2304	CLA	C2C-C1C-NC	2.94	112.73	109.97
23	b	616	CLA	C3B-C4B-NB	2.94	113.01	109.21
23	b	619	CLA	CBC-CAC-C3C	-2.94	104.32	112.43
23	c	512	CLA	C4A-NA-C1A	2.94	108.03	106.71
23	c	511	CLA	C2C-C1C-NC	2.94	112.73	109.97
23	A	410	CLA	CMB-C2B-C3B	2.94	130.18	124.68
38	L	101	LHG	O8-C23-O10	-2.94	116.17	123.59
23	c	506	CLA	C1-C2-C3	-2.94	120.96	126.04
23	b	618	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
23	c	505	CLA	O2A-CGA-CBA	2.94	121.12	111.91
42	V	201	HEC	C1D-C2D-C3D	-2.94	104.95	107.00
36	B	624[B]	HTG	C6-C5-C4	-2.93	106.13	113.00
23	A	405	CLA	O2A-CGA-CBA	2.93	121.11	111.91
23	b	607	CLA	C1-C2-C3	-2.93	120.97	126.04
23	d	409	CLA	CHD-C4C-C3C	-2.93	120.53	124.84
23	C	511	CLA	C1-O2A-CGA	2.93	124.13	116.44
23	C	504	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
23	B	611	CLA	C1-O2A-CGA	2.93	124.13	116.44
23	c	508	CLA	C3B-C4B-NB	2.93	112.99	109.21
23	B	607	CLA	C1-O2A-CGA	2.93	124.12	116.44
23	C	510	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
23	B	603	CLA	C3B-C4B-NB	2.92	112.99	109.21
23	B	615	CLA	O2A-CGA-CBA	2.92	121.08	111.91
42	v	201	HEC	CBA-CAA-C2A	-2.92	107.68	112.60
23	C	503	CLA	CBC-CAC-C3C	-2.92	104.38	112.43
23	B	614	CLA	O2A-CGA-CBA	2.92	121.06	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	x	1301	PL9	C37-C38-C39	-2.91	120.64	127.66
37	c	518	DGD	O2G-C1B-O1B	-2.91	116.66	123.70
23	C	509	CLA	C1D-CHD-C4C	-2.91	119.78	126.06
23	a	2609	CLA	O2A-CGA-CBA	2.91	121.05	111.91
23	C	509	CLA	CAA-C2A-C3A	-2.91	104.80	112.78
23	c	515	CLA	C3C-C4C-NC	2.91	113.84	110.57
23	a	2609	CLA	O2A-CGA-O1A	-2.91	116.25	123.59
23	b	609	CLA	CMC-C2C-C1C	2.91	129.47	125.04
23	c	511	CLA	CMB-C2B-C3B	2.91	130.12	124.68
23	B	613	CLA	C4-C3-C5	2.91	120.16	115.27
23	C	514	CLA	C4-C3-C5	2.91	120.16	115.27
23	c	506	CLA	CAC-C3C-C4C	2.91	128.58	124.81
23	B	602	CLA	CBC-CAC-C3C	-2.91	104.42	112.43
23	c	507	CLA	C3C-C4C-NC	2.91	113.83	110.57
23	B	616	CLA	CAC-C3C-C4C	2.91	128.58	124.81
40	H	102	RRX	C20-C21-C22	-2.90	123.17	127.31
26	D	2308	SQD	O6-C1-C2	2.90	112.84	108.30
23	a	2610	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
23	A	405	CLA	C1-C2-C3	-2.90	121.02	126.04
23	c	516	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
23	a	2609	CLA	CHD-C1D-ND	-2.90	121.79	124.45
23	a	2609	CLA	C4C-C3C-C2C	-2.90	102.68	106.90
23	A	410	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
23	B	604	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
23	B	604	CLA	CBC-CAC-C3C	-2.89	104.45	112.43
23	b	608	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
23	b	618	CLA	C3C-C4C-NC	2.89	113.81	110.57
38	D	2311	LHG	O8-C23-C24	2.89	120.98	111.91
23	C	508	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
23	c	509	CLA	C3B-C4B-NB	2.89	112.94	109.21
23	b	621	CLA	C1-C2-C3	-2.89	121.05	126.04
23	C	504	CLA	C2C-C1C-NC	2.89	112.68	109.97
31	a	2617	JOX	O-C2-C1	-2.89	120.13	122.76
31	A	418	JOX	C2-C3-CL	2.88	118.24	115.84
23	b	620	CLA	C4C-C3C-C2C	-2.88	102.69	106.90
23	b	607	CLA	C3B-C4B-NB	2.88	112.94	109.21
23	b	609	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
26	A	412	SQD	O48-C23-C24	2.88	120.95	111.91
25	Y	302	BCR	C35-C13-C14	-2.88	118.89	122.92
28	J	303	LMT	C1'-O5'-C5'	2.88	119.34	113.69
37	h	102	DGD	O1G-C1A-C2A	2.88	120.94	111.91
23	d	408	CLA	O2A-CGA-CBA	2.88	120.94	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	410	CLA	CAA-C2A-C3A	-2.88	104.90	112.78
23	b	614	CLA	O2D-CGD-CBD	2.88	116.38	111.27
23	c	515	CLA	CMA-C3A-C4A	-2.88	104.04	111.77
23	c	516	CLA	CAC-C3C-C4C	2.87	128.54	124.81
23	B	611	CLA	CAA-C2A-C3A	-2.87	104.91	112.78
23	B	602	CLA	C4A-NA-C1A	2.87	108.00	106.71
23	b	606	CLA	C1D-CHD-C4C	-2.87	119.87	126.06
38	l	103	LHG	O7-C7-C8	2.87	117.68	111.50
23	b	609	CLA	CHD-C4C-C3C	-2.87	120.62	124.84
23	D	2303	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
28	j	2701	LMT	O1B-C4'-C3'	2.87	114.91	107.28
23	b	610	CLA	CBC-CAC-C3C	-2.87	104.53	112.43
26	a	2615	SQD	C45-O47-C7	-2.86	110.74	117.79
23	B	609	CLA	O2A-CGA-CBA	2.86	120.89	111.91
38	l	103	LHG	O8-C23-C24	2.86	120.89	111.91
26	b	601	SQD	C3-C4-C5	2.86	115.34	110.24
23	b	617	CLA	C4-C3-C5	2.86	120.08	115.27
23	C	510	CLA	CHD-C1D-ND	-2.86	121.83	124.45
23	b	621	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
31	A	418	JOX	C-C5-C4	2.85	123.36	117.15
31	A	419	JOX	O1-C5-C	-2.85	117.33	121.41
23	b	621	CLA	CAC-C3C-C4C	2.85	128.51	124.81
23	B	616	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
23	a	2610	CLA	CED-O2D-CGD	2.85	122.38	115.94
23	C	507	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
23	C	502	CLA	CBC-CAC-C3C	-2.85	104.58	112.43
23	C	511	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
23	b	611	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
33	A	422	PL9	C40-C39-C41	2.84	120.05	115.27
24	a	2611	PHO	O2D-CGD-O1D	-2.84	118.28	123.84
24	a	2611	PHO	C4-C3-C5	2.84	120.05	115.27
24	A	409	PHO	CMB-C2B-C3B	2.84	129.99	124.68
36	B	625	HTG	C1-C2-C3	2.84	116.19	110.59
23	b	613	CLA	O2A-CGA-O1A	-2.84	116.43	123.59
23	C	512	CLA	C3C-C4C-NC	2.84	113.75	110.57
23	C	512	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
24	A	408	PHO	CMB-C2B-C3B	2.83	129.98	124.68
38	D	2310	LHG	O8-C23-O10	-2.83	116.44	123.59
23	B	615	CLA	C4A-NA-C1A	2.83	107.98	106.71
26	l	101	SQD	C44-O6-C1	-2.83	108.21	113.74
23	c	513	CLA	C3C-C4C-NC	2.83	113.75	110.57
23	B	617	CLA	O2A-CGA-CBA	2.83	120.79	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	621	CLA	CHA-C1A-NA	-2.83	119.92	126.40
23	C	512	CLA	C4-C3-C5	2.83	120.03	115.27
23	A	407	CLA	C3B-C4B-NB	2.83	112.87	109.21
25	B	619	BCR	C38-C26-C25	-2.83	121.35	124.53
25	y	101	BCR	C15-C14-C13	-2.83	123.28	127.31
23	b	620	CLA	CHD-C1D-ND	-2.82	121.86	124.45
28	A	414	LMT	C1B-O5B-C5B	2.82	119.23	113.69
23	b	618	CLA	O2A-CGA-CBA	2.82	120.77	111.91
23	b	615	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
26	D	2308	SQD	O48-C23-C24	2.82	120.77	111.91
33	D	2306	PL9	C10-C9-C11	2.82	120.01	115.27
23	c	509	CLA	CHD-C1D-ND	-2.82	121.86	124.45
40	h	101	RRX	C38-C26-C25	-2.82	121.36	124.53
23	C	509	CLA	C3B-C4B-NB	2.82	112.85	109.21
23	B	606	CLA	C1-C2-C3	-2.82	121.17	126.04
23	b	618	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
23	b	607	CLA	CHD-C4C-C3C	-2.82	120.70	124.84
23	b	615	CLA	CMA-C3A-C4A	-2.81	104.21	111.77
23	b	608	CLA	C6-C7-C8	-2.81	106.83	115.92
23	b	609	CLA	C3B-C4B-NB	2.81	112.84	109.21
23	B	604	CLA	CMC-C2C-C1C	2.81	129.32	125.04
42	V	201	HEC	CBA-CAA-C2A	-2.81	107.87	112.60
23	D	2304	CLA	CAA-C2A-C3A	-2.81	105.09	112.78
26	D	2302	SQD	O9-S-C6	2.81	110.27	106.94
23	c	515	CLA	C3B-C4B-NB	2.80	112.83	109.21
23	b	610	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
36	i	102	HTG	O5-C5-C4	2.80	114.78	109.69
23	C	503	CLA	O2A-C1-C2	2.80	115.99	108.64
23	A	406	CLA	CMC-C2C-C1C	2.80	129.30	125.04
23	c	507	CLA	O2A-CGA-O1A	-2.80	116.53	123.59
23	a	2610	CLA	C3B-C4B-NB	2.80	112.82	109.21
25	b	624	BCR	C3-C4-C5	-2.80	109.09	114.08
23	C	513	CLA	CHA-C1A-NA	-2.79	120.00	126.40
28	j	2701	LMT	C3'-C4'-C5'	-2.79	104.52	110.93
23	C	514	CLA	CBC-CAC-C3C	-2.79	104.73	112.43
23	b	613	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
23	a	2613	CLA	CAA-C2A-C3A	-2.79	105.13	112.78
23	C	511	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
23	B	612	CLA	CMB-C2B-C3B	2.79	129.90	124.68
23	B	610	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
33	D	2306	PL9	C37-C38-C39	-2.79	120.94	127.66
23	b	621	CLA	O2A-CGA-CBA	2.79	120.66	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	2303	CLA	CBC-CAC-C3C	-2.79	104.74	112.43
23	b	608	CLA	C3B-C4B-NB	2.79	112.81	109.21
23	c	505	CLA	CMC-C2C-C1C	2.79	129.28	125.04
27	B	622	LMG	O8-C28-C29	2.79	120.65	111.91
23	b	613	CLA	C3C-C4C-NC	2.79	113.69	110.57
23	c	506	CLA	C4-C3-C5	2.78	119.95	115.27
23	B	608	CLA	C3C-C4C-NC	2.78	113.69	110.57
23	c	506	CLA	CHA-C1A-NA	-2.78	120.02	126.40
23	C	512	CLA	CBC-CAC-C3C	-2.78	104.76	112.43
23	a	2609	CLA	C7-C6-C5	-2.78	105.80	113.36
23	C	508	CLA	CHA-C1A-NA	-2.78	120.03	126.40
23	c	516	CLA	O2A-CGA-CBA	2.78	120.63	111.91
25	T	102	BCR	C7-C6-C5	-2.78	114.73	121.46
23	b	614	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
23	B	612	CLA	C1-O2A-CGA	2.78	123.73	116.44
23	D	2304	CLA	CHD-C4C-NC	2.78	128.58	124.20
23	b	614	CLA	CED-O2D-CGD	2.78	122.21	115.94
25	k	302	BCR	C31-C1-C6	-2.77	105.80	110.30
33	D	2306	PL9	C42-C43-C44	-2.77	120.98	127.66
23	C	513	CLA	CHD-C1D-ND	-2.77	121.91	124.45
23	B	607	CLA	C4-C3-C5	2.77	119.93	115.27
23	A	407	CLA	C1-C2-C3	-2.77	121.25	126.04
23	A	410	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
37	C	518	DGD	O1G-C1A-O1A	-2.77	116.61	123.59
27	m	2802	LMG	O8-C28-C29	2.77	120.59	111.91
23	B	615	CLA	CHC-C1C-C2C	-2.77	119.07	126.72
23	c	515	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
23	c	511	CLA	CAA-C2A-C3A	-2.76	105.21	112.78
40	h	101	RRX	C10-C11-C12	-2.76	114.59	123.22
38	d	403	LHG	O7-C7-C8	2.76	117.46	111.50
23	B	604	CLA	CAA-C2A-C3A	-2.76	105.21	112.78
23	B	611	CLA	C4-C3-C5	2.76	119.92	115.27
23	C	508	CLA	CBC-CAC-C3C	-2.76	104.81	112.43
23	c	504	CLA	C1-O2A-CGA	2.76	123.69	116.44
23	A	407	CLA	C4A-NA-C1A	-2.76	105.47	106.71
23	D	2304	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
38	L	101	LHG	O7-C7-C8	2.76	117.45	111.50
23	B	613	CLA	CAC-C3C-C4C	2.76	128.39	124.81
38	d	413	LHG	O7-C7-C8	2.76	117.44	111.50
37	c	518	DGD	C2G-O2G-C1B	-2.76	111.00	117.79
23	C	504	CLA	CHD-C1D-ND	-2.76	121.92	124.45
23	b	620	CLA	C3C-C4C-NC	2.76	113.66	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	613	CLA	CAC-C3C-C4C	2.76	128.39	124.81
23	b	611	CLA	C4-C3-C5	2.76	119.91	115.27
23	C	505	CLA	CAA-C2A-C3A	-2.75	105.23	112.78
23	b	615	CLA	CHA-C1A-NA	-2.75	120.09	126.40
23	b	607	CLA	C4-C3-C5	2.75	119.90	115.27
23	b	617	CLA	CHD-C1D-ND	-2.75	121.93	124.45
39	e	103	HEM	C1B-NB-C4B	2.75	107.91	105.07
23	D	2303	CLA	O2A-CGA-O1A	-2.75	116.65	123.59
23	B	610	CLA	C3B-C4B-NB	2.75	112.76	109.21
23	c	510	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
23	b	607	CLA	C1-O2A-CGA	2.75	123.65	116.44
23	b	616	CLA	CAC-C3C-C4C	2.75	128.38	124.81
23	B	616	CLA	CHA-C1A-NA	-2.75	120.11	126.40
23	c	516	CLA	CMB-C2B-C3B	2.75	129.82	124.68
23	D	2304	CLA	C3C-C4C-NC	2.75	113.65	110.57
23	C	510	CLA	O2A-CGA-CBA	2.74	120.51	111.91
23	d	409	CLA	C3C-C4C-NC	2.74	113.65	110.57
25	C	516	BCR	C2-C1-C6	2.74	114.70	110.48
24	a	2612	PHO	C4A-C3A-C2A	-2.74	100.23	102.84
23	b	606	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
23	b	606	CLA	C1-C2-C3	-2.74	121.31	126.04
25	C	516	BCR	C15-C14-C13	-2.74	123.40	127.31
23	C	506	CLA	O2A-CGA-CBA	2.74	120.50	111.91
23	c	513	CLA	CHD-C1D-ND	-2.74	121.94	124.45
23	B	614	CLA	CED-O2D-CGD	2.74	122.13	115.94
40	h	101	RRX	C24-C23-C22	-2.74	122.10	126.23
23	B	615	CLA	C3C-C4C-NC	2.73	113.64	110.57
23	a	2613	CLA	CHD-C1D-ND	-2.73	121.94	124.45
23	c	506	CLA	C4A-NA-C1A	2.73	107.93	106.71
38	D	2311	LHG	O7-C7-C8	2.73	117.39	111.50
23	c	505	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
23	C	513	CLA	C4A-NA-C1A	2.73	107.93	106.71
23	C	511	CLA	CMC-C2C-C1C	2.73	129.19	125.04
23	B	612	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
23	c	515	CLA	C4-C3-C5	2.73	119.86	115.27
39	F	101	HEM	CMC-C2C-C3C	2.73	129.78	124.68
25	T	102	BCR	C15-C14-C13	2.73	131.20	127.31
37	D	2307	DGD	O6D-C5D-C4D	2.73	114.65	109.69
23	D	2303	CLA	C3B-C4B-NB	2.73	112.73	109.21
23	B	617	CLA	CMB-C2B-C3B	2.73	129.78	124.68
26	B	621	SQD	O7-S-C6	2.73	110.18	106.94
23	b	606	CLA	C4-C3-C5	2.72	119.85	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	CBC-CAC-C3C	-2.72	104.92	112.43
23	c	504	CLA	C3B-C4B-NB	2.72	112.73	109.21
23	C	513	CLA	CBC-CAC-C3C	-2.72	104.93	112.43
23	C	512	CLA	CAC-C3C-C4C	2.72	128.34	124.81
33	A	422	PL9	C27-C26-C24	-2.72	104.03	112.98
23	b	613	CLA	CMB-C2B-C3B	2.72	129.76	124.68
25	B	633	BCR	C35-C13-C12	2.72	122.36	118.08
38	d	403	LHG	O8-C23-C24	2.72	120.44	111.91
23	a	2609	CLA	CAC-C3C-C4C	2.72	128.34	124.81
23	C	502	CLA	CHD-C4C-C3C	-2.72	120.85	124.84
23	b	619	CLA	C3B-C4B-NB	2.71	112.72	109.21
23	b	615	CLA	CAA-C2A-C3A	-2.71	105.35	112.78
25	k	302	BCR	C16-C17-C18	-2.71	123.44	127.31
23	c	511	CLA	C1-C2-C3	-2.71	121.35	126.04
25	b	624	BCR	C8-C7-C6	-2.71	119.59	127.20
23	C	505	CLA	C3B-C4B-NB	2.71	112.71	109.21
31	a	2617	JOX	O-C2-C3	-2.71	120.29	122.76
26	a	2615	SQD	O48-C23-C24	2.71	120.40	111.91
23	d	409	CLA	C1-C2-C3	-2.70	121.36	126.04
23	b	619	CLA	O2A-CGA-CBA	2.70	120.39	111.91
23	d	409	CLA	C1D-CHD-C4C	-2.70	120.22	126.06
23	C	506	CLA	C3B-C4B-NB	2.70	112.70	109.21
23	B	614	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
28	j	2701	LMT	C1'-O5'-C5'	2.70	118.99	113.69
23	d	409	CLA	CMB-C2B-C3B	2.70	129.72	124.68
23	c	514	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
23	c	508	CLA	O2A-CGA-CBA	2.70	120.37	111.91
23	B	603	CLA	C4-C3-C5	2.70	119.81	115.27
28	A	414	LMT	C3'-C4'-C5'	-2.70	104.75	110.93
26	b	601	SQD	O48-C23-C24	2.69	120.36	111.91
37	c	519	DGD	C5A-C4A-C3A	-2.69	100.75	114.42
23	b	607	CLA	CMB-C2B-C3B	2.69	129.72	124.68
23	a	2613	CLA	C3C-C4C-NC	2.69	113.59	110.57
23	C	514	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
26	A	412	SQD	C44-O6-C1	-2.69	108.48	113.74
23	a	2610	CLA	CBC-CAC-C3C	-2.69	105.02	112.43
38	D	2311	LHG	O8-C23-O10	-2.69	116.81	123.59
23	b	615	CLA	CMB-C2B-C3B	2.69	129.71	124.68
23	b	616	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
23	A	407	CLA	CHD-C4C-NC	2.69	128.44	124.20
37	c	519	DGD	C3A-C2A-C1A	-2.69	103.85	113.62
25	T	102	BCR	C3-C4-C5	-2.68	109.28	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	CLA	CMA-C3A-C2A	-2.68	103.02	113.83
37	C	518	DGD	O2G-C1B-O1B	-2.68	117.23	123.70
25	A	411	BCR	C15-C16-C17	-2.67	118.00	123.47
38	d	412	LHG	O7-C7-C8	2.67	117.26	111.50
24	A	409	PHO	O2D-CGD-O1D	-2.67	118.62	123.84
23	C	506	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
23	b	616	CLA	CMB-C2B-C3B	2.67	129.67	124.68
23	b	614	CLA	C3C-C4C-NC	2.67	113.56	110.57
36	B	625	HTG	C1-O5-C5	2.67	117.50	112.58
23	D	2304	CLA	C1D-CHD-C4C	-2.66	120.31	126.06
23	C	503	CLA	O2A-CGA-CBA	2.66	120.27	111.91
23	B	612	CLA	C4A-NA-C1A	2.66	107.90	106.71
23	b	614	CLA	C1-O2A-CGA	2.66	123.43	116.44
23	b	611	CLA	O2A-CGA-O1A	-2.66	116.88	123.59
24	A	408	PHO	CMC-C2C-C3C	2.66	129.95	124.94
23	a	2613	CLA	O2A-CGA-CBA	2.66	120.25	111.91
23	C	503	CLA	CHA-C1A-NA	-2.66	120.31	126.40
23	b	616	CLA	CMA-C3A-C4A	-2.66	104.63	111.77
25	k	302	BCR	C11-C10-C9	-2.66	123.52	127.31
25	z	101	BCR	C38-C26-C25	-2.66	121.55	124.53
23	B	609	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
23	c	504	CLA	CMC-C2C-C1C	2.65	129.08	125.04
23	C	512	CLA	CHA-C1A-NA	-2.65	120.33	126.40
23	A	406	CLA	CMA-C3A-C2A	-2.65	103.13	113.83
23	B	609	CLA	O2A-CGA-O1A	-2.65	116.90	123.59
23	c	513	CLA	CMB-C2B-C3B	2.65	129.64	124.68
26	B	621	SQD	O9-S-C6	2.65	110.09	106.94
23	c	515	CLA	CHA-C1A-NA	-2.65	120.33	126.40
37	h	102	DGD	C2G-O2G-C1B	-2.65	111.27	117.79
25	Y	302	BCR	C37-C22-C23	2.65	122.25	118.08
33	D	2306	PL9	C17-C18-C19	-2.65	121.29	127.66
23	B	610	CLA	CED-O2D-CGD	2.65	121.92	115.94
23	B	611	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
23	b	612	CLA	C4C-C3C-C2C	-2.65	103.04	106.90
23	b	618	CLA	O2A-CGA-O1A	-2.64	116.92	123.59
36	C	525	HTG	O5-C1-C2	2.64	113.64	110.31
23	B	614	CLA	CMC-C2C-C1C	2.64	129.07	125.04
25	B	633	BCR	C1-C6-C7	2.64	123.26	115.78
33	D	2306	PL9	C31-C32-C33	-2.64	103.19	111.88
23	B	603	CLA	O2A-CGA-CBA	2.64	120.20	111.91
36	H	101	HTG	O5-C5-C4	2.64	114.85	110.77
23	b	609	CLA	C6-C5-C3	-2.64	106.53	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	102	BCR	C1-C6-C7	2.64	123.25	115.78
37	C	517	DGD	O1G-C1A-O1A	-2.64	116.93	123.59
23	C	514	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
23	C	510	CLA	C4A-NA-C1A	2.64	107.89	106.71
23	C	505	CLA	O2A-CGA-O1A	-2.64	116.93	123.59
23	B	615	CLA	CHD-C4C-NC	2.64	128.36	124.20
23	B	603	CLA	CAC-C3C-C4C	2.64	128.23	124.81
23	A	405	CLA	CAA-CBA-CGA	-2.64	105.54	113.25
25	B	633	BCR	C3-C4-C5	-2.64	109.37	114.08
23	c	513	CLA	C4C-C3C-C2C	-2.64	103.06	106.90
23	C	509	CLA	O2A-CGA-CBA	2.64	120.18	111.91
23	B	612	CLA	C1-C2-C3	-2.64	121.48	126.04
23	A	407	CLA	C3C-C4C-NC	2.64	113.53	110.57
23	B	603	CLA	CMC-C2C-C1C	2.64	129.05	125.04
31	A	419	JOX	C-C5-C4	2.63	122.89	117.15
23	b	611	CLA	O2A-CGA-CBA	2.63	120.17	111.91
25	c	517	BCR	C21-C20-C19	-2.63	115.00	123.22
26	D	2302	SQD	O8-S-C6	2.63	109.93	105.74
23	b	611	CLA	CMB-C2B-C3B	2.63	129.60	124.68
33	x	1301	PL9	C15-C14-C16	2.63	119.70	115.27
23	a	2613	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
23	B	602	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
23	c	513	CLA	C1-O2A-CGA	2.63	123.34	116.44
23	c	511	CLA	C3B-C4B-NB	2.63	112.61	109.21
23	A	405	CLA	CMC-C2C-C1C	2.63	129.04	125.04
23	A	405	CLA	CAC-C3C-C4C	2.63	128.22	124.81
23	c	505	CLA	O2A-C1-C2	2.63	115.53	108.64
27	C	527	LMG	C3-C4-C5	2.62	114.92	110.24
25	y	101	BCR	C24-C23-C22	-2.62	122.27	126.23
23	B	606	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
23	c	510	CLA	CAC-C3C-C4C	2.62	128.21	124.81
26	A	412	SQD	O48-C23-O10	-2.62	116.98	123.59
31	A	418	JOX	O-C2-C3	-2.62	120.37	122.76
23	B	612	CLA	C3B-C4B-NB	2.62	112.59	109.21
23	D	2304	CLA	O2A-CGA-O1A	-2.61	117.00	123.59
23	b	611	CLA	CBC-CAC-C3C	-2.61	105.23	112.43
25	Y	302	BCR	C16-C17-C18	-2.61	123.58	127.31
23	B	609	CLA	CMA-C3A-C4A	-2.61	104.77	111.77
23	d	402	CLA	O2A-CGA-CBA	2.61	120.08	111.91
23	c	508	CLA	CHD-C1D-ND	-2.61	122.06	124.45
23	C	502	CLA	C4C-C3C-C2C	-2.60	103.10	106.90
23	C	504	CLA	C1-O2A-CGA	2.60	123.28	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	516	CLA	C3B-C4B-NB	2.60	112.57	109.21
38	l	103	LHG	O8-C23-O10	-2.60	117.03	123.59
25	B	633	BCR	C7-C6-C5	-2.60	115.16	121.46
23	C	508	CLA	CHD-C1D-ND	-2.60	122.06	124.45
23	c	504	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
36	H	101	HTG	C5-C4-C3	2.60	112.86	109.67
23	c	509	CLA	CHA-C1A-NA	-2.60	120.45	126.40
23	c	513	CLA	O2A-CGA-CBA	2.60	120.05	111.91
23	C	505	CLA	C1-O2A-CGA	2.59	123.25	116.44
23	C	507	CLA	CMC-C2C-C1C	2.59	128.99	125.04
23	b	620	CLA	C1-C2-C3	-2.59	121.56	126.04
33	x	1301	PL9	C35-C34-C36	2.59	119.63	115.27
23	b	621	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
33	d	411	PL9	C53-C6-C1	2.59	120.28	114.99
23	C	505	CLA	CMC-C2C-C1C	2.59	128.98	125.04
23	C	506	CLA	C1-C2-C3	-2.59	121.56	126.04
23	c	507	CLA	CHC-C1C-C2C	-2.59	119.56	126.72
25	y	101	BCR	C34-C9-C8	2.59	122.16	118.08
23	B	616	CLA	CED-O2D-CGD	2.59	121.79	115.94
33	D	2306	PL9	C53-C6-C1	2.59	120.28	114.99
23	B	617	CLA	CHA-C1A-NA	-2.59	120.48	126.40
23	b	619	CLA	O2A-CGA-O1A	-2.58	117.07	123.59
36	B	624[A]	HTG	C1-C2-C3	2.58	115.69	110.59
23	c	511	CLA	CHA-C1A-NA	-2.58	120.49	126.40
26	D	2302	SQD	O7-S-C6	2.58	110.00	106.94
25	C	515	BCR	C20-C21-C22	-2.58	123.63	127.31
23	B	603	CLA	CHA-C1A-NA	-2.58	120.49	126.40
23	b	616	CLA	C4A-NA-C1A	2.58	107.86	106.71
23	b	620	CLA	CHA-C1A-NA	-2.58	120.50	126.40
23	B	614	CLA	CMA-C3A-C4A	-2.58	104.85	111.77
23	B	603	CLA	C4C-C3C-C2C	-2.58	103.14	106.90
23	b	617	CLA	CMB-C2B-C3B	2.58	129.50	124.68
33	d	411	PL9	C27-C28-C29	-2.57	121.46	127.66
25	Y	302	BCR	C10-C11-C12	-2.57	115.19	123.22
23	b	614	CLA	C1D-CHD-C4C	-2.57	120.51	126.06
38	D	2309	LHG	O7-C7-O9	-2.57	117.49	123.70
23	B	613	CLA	O2A-CGA-CBA	2.57	119.98	111.91
23	C	506	CLA	CMA-C3A-C4A	-2.57	104.86	111.77
24	A	408	PHO	CMA-C3A-C4A	-2.57	108.75	114.38
23	C	514	CLA	C3C-C4C-NC	2.57	113.45	110.57
23	C	506	CLA	CHD-C4C-C3C	-2.57	121.07	124.84
23	c	508	CLA	O1D-CGD-CBD	-2.57	119.23	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	C7-C6-C5	-2.57	106.39	113.36
23	C	510	CLA	CMB-C2B-C3B	2.57	129.48	124.68
37	C	519	DGD	O6E-C1E-O5D	-2.57	103.90	109.97
36	b	603	HTG	C6-C5-C4	-2.56	107.00	113.00
23	B	605	CLA	O2A-CGA-CBA	2.56	119.95	111.91
23	c	510	CLA	CMC-C2C-C1C	2.56	128.94	125.04
23	B	611	CLA	CAA-CBA-CGA	-2.56	105.76	113.25
37	H	103	DGD	O1G-C1A-O1A	-2.56	117.13	123.59
25	k	302	BCR	C33-C5-C6	-2.56	121.65	124.53
24	a	2612	PHO	CMC-C2C-C3C	2.56	129.77	124.94
23	d	409	CLA	C4C-C3C-C2C	-2.56	103.17	106.90
23	b	606	CLA	CHD-C4C-C3C	-2.56	121.08	124.84
33	D	2306	PL9	C51-C49-C50	2.56	120.25	114.60
23	C	512	CLA	O2A-CGA-CBA	2.56	119.94	111.91
23	b	610	CLA	CMA-C3A-C4A	-2.56	104.90	111.77
25	z	101	BCR	C33-C5-C6	-2.56	121.66	124.53
28	M	101	LMT	C1-O1'-C1'	-2.56	109.60	113.84
23	b	610	CLA	CHA-C1A-NA	-2.56	120.54	126.40
33	x	1301	PL9	C46-C44-C45	2.56	120.25	114.60
38	D	2310	LHG	O7-C7-C8	2.56	117.01	111.50
23	b	614	CLA	CHA-C1A-NA	-2.56	120.55	126.40
39	F	101	HEM	C4B-CHC-C1C	2.56	125.93	122.56
37	C	517	DGD	O2G-C1B-O1B	-2.55	117.53	123.70
23	c	516	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
23	c	516	CLA	CMC-C2C-C1C	2.55	128.92	125.04
23	d	409	CLA	CMC-C2C-C1C	2.55	128.92	125.04
23	B	603	CLA	CMA-C3A-C2A	-2.55	103.55	113.83
33	d	411	PL9	C36-C37-C38	-2.55	103.50	111.88
23	D	2304	CLA	C3B-C4B-NB	2.55	112.50	109.21
23	a	2610	CLA	C11-C10-C8	-2.55	107.68	115.92
23	C	512	CLA	CHC-C1C-C2C	-2.55	119.68	126.72
23	B	606	CLA	C4-C3-C5	2.55	119.56	115.27
23	c	514	CLA	C3C-C4C-NC	2.55	113.43	110.57
23	b	621	CLA	CMB-C2B-C3B	2.55	129.44	124.68
23	C	502	CLA	C3C-C4C-NC	2.55	113.43	110.57
23	B	612	CLA	CBC-CAC-C3C	-2.55	105.41	112.43
23	b	608	CLA	CMC-C2C-C1C	2.54	128.91	125.04
23	B	617	CLA	CAC-C3C-C4C	2.54	128.11	124.81
24	A	408	PHO	C4-C3-C5	2.54	119.55	115.27
23	b	615	CLA	CAC-C3C-C4C	2.54	128.11	124.81
23	A	405	CLA	C4-C3-C5	2.54	119.54	115.27
23	A	406	CLA	O2A-CGA-O1A	-2.54	117.18	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	h	101	RRX	C15-C14-C13	-2.54	123.69	127.31
23	b	613	CLA	CMC-C2C-C1C	2.54	128.91	125.04
23	B	607	CLA	CMB-C2B-C3B	2.54	129.42	124.68
23	a	2609	CLA	CMA-C3A-C2A	-2.54	103.60	113.83
23	c	514	CLA	CMC-C2C-C1C	2.54	128.90	125.04
23	a	2610	CLA	C1D-CHD-C4C	-2.53	120.59	126.06
23	B	616	CLA	CBA-CAA-C2A	-2.53	106.38	113.86
23	a	2610	CLA	C1-C2-C3	-2.53	121.66	126.04
27	c	522	LMG	O8-C28-C29	2.53	119.86	111.91
23	C	506	CLA	C4-C3-C5	2.53	119.53	115.27
23	C	507	CLA	CAA-C2A-C3A	-2.53	105.85	112.78
28	d	401	LMT	C1B-O1B-C4'	-2.53	111.71	117.96
26	a	2615	SQD	O47-C7-O49	-2.53	117.59	123.70
23	A	405	CLA	O2A-CGA-O1A	-2.53	117.22	123.59
38	E	101	LHG	C5-O7-C7	-2.53	111.57	117.79
23	b	608	CLA	C5-C3-C2	-2.53	116.01	121.12
23	B	608	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
28	z	102	LMT	O5B-C5B-C4B	2.53	114.28	109.69
23	B	615	CLA	CMB-C2B-C3B	2.52	129.40	124.68
23	A	406	CLA	CHC-C1C-C2C	-2.52	119.75	126.72
31	A	419	JOX	C4-C3-C2	-2.52	121.16	123.18
25	B	620	BCR	C2-C3-C4	-2.52	105.75	111.38
28	m	2804	LMT	O5'-C5'-C4'	2.52	115.06	109.75
23	C	507	CLA	C3B-C4B-NB	2.52	112.47	109.21
24	a	2611	PHO	CMB-C2B-C3B	2.52	129.39	124.68
23	A	406	CLA	O2A-CGA-CBA	2.52	119.81	111.91
23	b	609	CLA	O2A-CGA-CBA	2.51	119.80	111.91
23	B	615	CLA	C4C-C3C-C2C	-2.51	103.23	106.90
23	B	608	CLA	C4C-C3C-C2C	-2.51	103.23	106.90
25	B	619	BCR	C31-C1-C6	-2.51	106.23	110.30
26	l	101	SQD	O48-C23-C24	2.51	119.78	111.91
36	b	604	HTG	C3-C4-C5	2.51	114.71	110.24
23	b	611	CLA	CHA-C1A-NA	-2.50	120.66	126.40
23	c	505	CLA	CED-O2D-CGD	2.50	121.60	115.94
23	D	2303	CLA	CAA-C2A-C3A	-2.50	105.92	112.78
26	B	621	SQD	O5-C1-C2	2.50	115.64	110.35
23	c	510	CLA	CHA-C1A-NA	-2.50	120.67	126.40
23	c	506	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
38	D	2310	LHG	O8-C23-C24	2.50	119.75	111.91
33	A	422	PL9	C22-C23-C24	-2.50	121.64	127.66
23	C	507	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
23	B	609	CLA	CHD-C1D-ND	-2.50	122.16	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	621	CLA	OBD-CAD-C3D	-2.49	122.52	128.52
23	B	609	CLA	CMA-C3A-C2A	-2.49	103.77	113.83
23	c	514	CLA	O2A-CGA-O1A	-2.49	117.30	123.59
23	D	2304	CLA	CMB-C2B-C3B	2.49	129.34	124.68
37	c	520	DGD	O1G-C1A-O1A	-2.49	117.31	123.59
23	B	603	CLA	CMB-C2B-C3B	2.49	129.34	124.68
25	b	624	BCR	C11-C10-C9	-2.49	123.76	127.31
23	b	620	CLA	C6-C5-C3	-2.49	106.93	113.45
23	b	613	CLA	CMA-C3A-C2A	-2.49	103.80	113.83
26	b	601	SQD	O48-C23-O10	-2.48	117.32	123.59
23	b	606	CLA	CMB-C2B-C3B	2.48	129.33	124.68
23	d	402	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
33	A	422	PL9	C37-C38-C39	-2.48	121.68	127.66
25	K	101	BCR	C38-C26-C25	-2.48	121.74	124.53
23	C	508	CLA	C3B-C4B-NB	2.48	112.42	109.21
23	C	510	CLA	CAC-C3C-C4C	2.48	128.03	124.81
23	b	620	CLA	C6-C7-C8	-2.48	107.90	115.92
23	d	408	CLA	CBC-CAC-C3C	-2.48	105.59	112.43
23	C	505	CLA	C3C-C4C-NC	2.48	113.35	110.57
23	C	503	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
23	b	611	CLA	C3B-C4B-NB	2.48	112.41	109.21
23	d	409	CLA	C6-C7-C8	-2.48	107.91	115.92
36	B	624[A]	HTG	C1'-S1-C1	2.48	104.72	100.09
23	b	620	CLA	C4-C3-C5	2.47	119.43	115.27
23	B	603	CLA	CMA-C3A-C4A	-2.47	105.12	111.77
23	b	612	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
26	D	2308	SQD	C44-O6-C1	-2.47	108.91	113.74
23	C	503	CLA	C3B-C4B-NB	2.47	112.41	109.21
37	c	519	DGD	O1G-C1A-O1A	-2.47	117.36	123.59
25	b	623	BCR	C8-C7-C6	-2.47	120.26	127.20
36	I	101	HTG	O5-C5-C4	2.47	114.18	109.69
23	c	514	CLA	O2A-CGA-CBA	2.47	119.65	111.91
23	C	507	CLA	CHA-C1A-NA	-2.46	120.75	126.40
23	c	509	CLA	O2A-C1-C2	2.46	115.11	108.64
23	C	512	CLA	CMB-C2B-C3B	2.46	129.29	124.68
23	B	608	CLA	CMC-C2C-C1C	2.46	128.79	125.04
37	D	2307	DGD	O1G-C1A-O1A	-2.46	117.38	123.59
23	C	513	CLA	C4-C3-C5	2.46	119.41	115.27
23	B	602	CLA	C4-C3-C5	2.46	119.41	115.27
25	A	411	BCR	C3-C4-C5	-2.46	109.68	114.08
23	B	604	CLA	C1-O2A-CGA	2.46	122.89	116.44
23	B	617	CLA	C1-C2-C3	-2.46	121.80	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	CMA-C3A-C4A	-2.46	105.17	111.77
23	B	614	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
24	a	2611	PHO	CMA-C3A-C4A	-2.45	109.00	114.38
25	y	101	BCR	C21-C20-C19	-2.45	115.57	123.22
23	C	511	CLA	C4A-NA-C1A	2.45	107.81	106.71
37	h	102	DGD	C3G-O3G-C1D	-2.45	108.95	113.74
23	b	612	CLA	CAA-C2A-C3A	-2.45	106.07	112.78
33	d	411	PL9	C25-C24-C26	2.45	119.39	115.27
25	C	516	BCR	C21-C20-C19	-2.45	115.58	123.22
23	a	2610	CLA	CAA-C2A-C3A	-2.45	106.07	112.78
33	d	411	PL9	C10-C9-C11	2.45	119.39	115.27
25	z	101	BCR	C20-C21-C22	-2.45	123.82	127.31
23	C	508	CLA	O2A-CGA-CBA	2.45	119.58	111.91
23	C	504	CLA	O2A-CGA-CBA	2.45	119.58	111.91
23	c	509	CLA	CMB-C2B-C3B	2.45	129.25	124.68
23	b	620	CLA	C3B-C4B-NB	2.45	112.37	109.21
33	A	422	PL9	C20-C19-C21	2.44	119.38	115.27
23	b	607	CLA	O2A-CGA-CBA	2.44	119.58	111.91
36	b	625	HTG	C1-C2-C3	2.44	115.42	110.59
26	A	412	SQD	C1-O5-C5	-2.44	108.89	113.69
23	d	402	CLA	CMA-C3A-C4A	-2.44	105.20	111.77
38	d	403	LHG	O8-C23-O10	-2.44	117.42	123.59
37	C	519	DGD	O2G-C1B-O1B	-2.44	117.80	123.70
27	C	520	LMG	O8-C28-O10	-2.44	117.43	123.59
37	c	519	DGD	O2G-C1B-O1B	-2.44	117.80	123.70
23	d	408	CLA	CMA-C3A-C2A	-2.44	103.99	113.83
23	C	508	CLA	C4-C3-C5	2.43	119.36	115.27
23	b	606	CLA	O2A-CGA-CBA	2.43	119.54	111.91
23	b	617	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
26	D	2308	SQD	O9-S-C6	2.43	109.83	106.94
23	C	502	CLA	CHA-C1A-NA	-2.43	120.83	126.40
33	D	2306	PL9	C40-C39-C38	-2.43	117.44	123.68
23	c	512	CLA	O2A-CGA-CBA	2.43	119.53	111.91
23	d	409	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
23	b	619	CLA	CMC-C2C-C1C	2.43	128.74	125.04
23	d	408	CLA	C1D-CHD-C4C	-2.43	120.82	126.06
23	c	508	CLA	CBC-CAC-C3C	-2.43	105.73	112.43
23	c	516	CLA	CBC-CAC-C3C	-2.43	105.74	112.43
33	D	2306	PL9	C15-C14-C16	2.43	119.35	115.27
25	T	102	BCR	C21-C20-C19	-2.43	115.64	123.22
23	B	607	CLA	CMC-C2C-C1C	2.42	128.73	125.04
23	c	504	CLA	C4-C3-C5	2.42	119.35	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	506	CLA	CMD-C2D-C3D	-2.42	122.04	127.61
25	K	101	BCR	C15-C14-C13	-2.42	123.86	127.31
23	b	607	CLA	CHA-C1A-NA	-2.42	120.86	126.40
23	b	616	CLA	CHC-C1C-C2C	-2.42	120.04	126.72
25	k	302	BCR	C3-C4-C5	-2.42	109.76	114.08
23	C	505	CLA	OBD-CAD-C3D	-2.42	122.71	128.52
25	a	2614	BCR	C11-C10-C9	-2.41	123.86	127.31
23	b	615	CLA	CMC-C2C-C1C	2.41	128.71	125.04
42	v	201	HEC	CMC-C2C-C1C	-2.41	124.76	128.46
23	c	512	CLA	CBC-CAC-C3C	-2.41	105.78	112.43
23	A	406	CLA	CED-O2D-CGD	2.41	121.39	115.94
23	a	2609	CLA	O2D-CGD-CBD	2.41	115.55	111.27
24	a	2611	PHO	C1-C2-C3	-2.41	121.88	126.04
23	d	402	CLA	C4C-C3C-C2C	-2.41	103.39	106.90
36	c	524	HTG	C1-O5-C5	2.41	117.02	112.58
25	B	633	BCR	C33-C5-C4	2.40	118.24	113.62
23	b	620	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
23	B	611	CLA	O2A-CGA-CBA	2.40	119.45	111.91
23	A	407	CLA	CMC-C2C-C1C	2.40	128.70	125.04
31	a	2617	JOX	O1-C5-C4	-2.40	117.97	121.41
26	a	2615	SQD	C44-O6-C1	-2.40	109.05	113.74
25	k	302	BCR	C8-C7-C6	-2.40	120.46	127.20
23	C	507	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
23	A	405	CLA	CMA-C3A-C2A	-2.40	104.14	113.83
23	A	406	CLA	CMA-C3A-C4A	-2.40	105.32	111.77
23	b	616	CLA	C3C-C4C-NC	2.40	113.26	110.57
23	B	609	CLA	C3B-C4B-NB	2.40	112.31	109.21
28	m	2804	LMT	C1-O1'-C1'	-2.40	109.86	113.84
23	d	408	CLA	CHA-C1A-NA	-2.40	120.91	126.40
23	C	507	CLA	CED-O2D-CGD	2.40	121.36	115.94
23	B	609	CLA	C4-C3-C5	2.40	119.31	115.27
42	V	201	HEC	CMC-C2C-C1C	-2.40	124.78	128.46
23	b	617	CLA	O2A-C1-C2	-2.40	102.33	108.64
23	c	506	CLA	O2A-CGA-CBA	2.40	119.43	111.91
23	d	409	CLA	CHA-C1A-NA	-2.40	120.91	126.40
24	A	409	PHO	C4-C3-C2	-2.40	117.53	123.68
23	c	513	CLA	CMC-C2C-C1C	2.40	128.69	125.04
23	b	621	CLA	C4-C3-C5	2.39	119.30	115.27
23	D	2304	CLA	C4-C3-C5	2.39	119.30	115.27
23	b	614	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
23	c	514	CLA	C4C-C3C-C2C	-2.39	103.41	106.90
24	a	2611	PHO	CBA-CAA-C2A	-2.39	106.82	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	407	CLA	O2A-CGA-CBA	2.39	119.41	111.91
23	b	620	CLA	CBC-CAC-C3C	-2.39	105.84	112.43
23	b	616	CLA	CHD-C4C-NC	2.39	127.97	124.20
23	B	603	CLA	CHC-C1C-C2C	-2.39	120.11	126.72
36	b	604	HTG	C1-O5-C5	2.39	116.99	112.58
23	B	605	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
36	B	624[A]	HTG	O5-C5-C6	2.39	112.37	106.44
28	d	404	LMT	C1'-O5'-C5'	2.39	118.37	113.69
23	b	606	CLA	CHA-C1A-NA	-2.39	120.93	126.40
24	a	2612	PHO	C4-C3-C2	-2.39	117.56	123.68
23	B	615	CLA	CAC-C3C-C4C	2.38	127.90	124.81
23	B	616	CLA	O2A-CGA-O1A	-2.38	117.57	123.59
23	B	616	CLA	CHC-C1C-C2C	-2.38	120.13	126.72
27	C	527	LMG	O8-C28-O10	-2.38	117.58	123.59
23	D	2303	CLA	CAC-C3C-C2C	2.38	131.60	127.53
37	c	520	DGD	O3G-C3G-C2G	-2.38	105.16	110.90
23	B	612	CLA	CHC-C1C-C2C	-2.38	120.14	126.72
23	b	618	CLA	CMA-C3A-C4A	-2.38	105.38	111.77
23	A	405	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
23	A	410	CLA	C7-C6-C5	-2.38	106.90	113.36
38	D	2309	LHG	C5-O7-C7	-2.38	111.93	117.79
26	D	2302	SQD	O47-C7-O49	-2.38	117.96	123.70
23	B	602	CLA	CMB-C2B-C3B	2.38	129.12	124.68
25	z	101	BCR	C11-C10-C9	-2.37	123.92	127.31
23	c	514	CLA	C4A-NA-C1A	2.37	107.77	106.71
23	B	611	CLA	CMC-C2C-C1C	2.37	128.65	125.04
38	E	101	LHG	O8-C23-C24	2.37	119.35	111.91
23	C	513	CLA	C2C-C1C-NC	2.37	112.19	109.97
26	a	2603	SQD	O48-C23-C24	2.37	119.35	111.91
23	C	511	CLA	CAA-CBA-CGA	-2.37	106.33	113.25
33	x	1301	PL9	C40-C39-C41	2.37	119.26	115.27
27	d	414	LMG	O7-C10-C11	2.37	116.60	111.50
23	b	612	CLA	C1-C2-C3	-2.37	121.95	126.04
23	c	509	CLA	CGD-CBD-CAD	-2.36	103.08	110.73
24	a	2611	PHO	O1D-CGD-CBD	-2.36	120.80	124.74
23	C	506	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
27	D	2312	LMG	O8-C28-O10	-2.36	117.63	123.59
25	K	101	BCR	C33-C5-C6	-2.36	121.88	124.53
25	a	2614	BCR	C38-C26-C25	-2.36	121.88	124.53
28	Z	101	LMT	C1B-O5B-C5B	2.36	118.32	113.69
28	T	103	LMT	C1-O1'-C1'	-2.36	109.93	113.84
23	b	621	CLA	CHC-C1C-C2C	-2.36	120.20	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	D	2306	PL9	C22-C23-C24	-2.36	121.98	127.66
25	b	624	BCR	C16-C17-C18	-2.36	123.95	127.31
33	D	2306	PL9	C30-C29-C31	2.36	119.24	115.27
23	c	515	CLA	CHB-C4A-NA	2.36	127.77	124.51
26	b	601	SQD	C45-O47-C7	-2.36	111.99	117.79
23	B	605	CLA	CHA-C1A-NA	-2.35	121.01	126.40
23	b	612	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
26	A	412	SQD	O47-C7-O49	-2.35	118.02	123.70
25	B	620	BCR	C3-C4-C5	-2.35	109.88	114.08
25	b	624	BCR	C21-C20-C19	-2.35	115.88	123.22
23	b	606	CLA	CBC-CAC-C3C	-2.35	105.95	112.43
23	b	613	CLA	CMA-C3A-C4A	-2.35	105.45	111.77
23	C	505	CLA	CMA-C3A-C4A	-2.35	105.45	111.77
23	B	607	CLA	CHA-C1A-NA	-2.35	121.02	126.40
25	k	302	BCR	C7-C8-C9	-2.35	122.69	126.23
23	b	621	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
25	B	633	BCR	C21-C20-C19	-2.35	115.89	123.22
25	b	622	BCR	C38-C26-C25	-2.35	121.89	124.53
23	B	615	CLA	CMC-C2C-C1C	2.35	128.61	125.04
23	C	509	CLA	CHC-C1C-C2C	-2.34	120.24	126.72
26	a	2615	SQD	O48-C23-O10	-2.34	117.68	123.59
23	b	618	CLA	CHA-C1A-NA	-2.34	121.03	126.40
23	c	507	CLA	C4C-C3C-C2C	-2.34	103.49	106.90
23	b	609	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
23	d	408	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
23	c	513	CLA	CHA-C1A-NA	-2.34	121.05	126.40
25	b	624	BCR	C2-C1-C6	2.34	114.08	110.48
23	c	512	CLA	CHA-C1A-NA	-2.34	121.05	126.40
36	I	101	HTG	O5-C1-C2	2.34	113.25	110.31
23	B	603	CLA	O2A-CGA-O1A	-2.34	117.70	123.59
23	b	614	CLA	C4-C3-C5	2.34	119.20	115.27
25	z	101	BCR	C35-C13-C14	-2.33	119.65	122.92
27	A	413	LMG	O7-C10-O9	-2.33	118.06	123.70
25	z	101	BCR	C8-C7-C6	-2.33	120.65	127.20
23	C	510	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
23	d	402	CLA	CHB-C4A-NA	2.33	127.73	124.51
23	c	509	CLA	CAC-C3C-C4C	2.33	127.83	124.81
25	K	101	BCR	C10-C11-C12	-2.33	115.95	123.22
23	c	506	CLA	CMC-C2C-C1C	2.33	128.59	125.04
23	c	515	CLA	C4A-NA-C1A	2.33	107.75	106.71
37	D	2307	DGD	C1D-O6D-C5D	2.33	118.26	113.69
23	A	406	CLA	C1-O2A-CGA	2.33	122.55	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	101	BCR	C34-C9-C10	-2.33	119.66	122.92
23	c	510	CLA	O1D-CGD-CBD	-2.33	119.72	124.48
23	B	606	CLA	C3B-C4B-NB	2.32	112.21	109.21
23	B	609	CLA	CAA-C2A-C3A	-2.32	106.42	112.78
23	B	615	CLA	OBD-CAD-C3D	-2.32	122.93	128.52
23	b	612	CLA	CMB-C2B-C3B	2.32	129.02	124.68
23	d	402	CLA	CMB-C2B-C3B	2.32	129.02	124.68
25	Y	302	BCR	C1-C6-C7	2.32	122.34	115.78
23	b	616	CLA	C4C-C3C-C2C	-2.32	103.52	106.90
23	C	511	CLA	CMA-C3A-C4A	-2.32	105.54	111.77
23	b	613	CLA	C11-C12-C13	-2.32	108.43	115.92
28	Z	101	LMT	C1-O1'-C1'	-2.32	110.00	113.84
28	d	404	LMT	O5'-C5'-C4'	2.32	114.64	109.75
23	C	510	CLA	CMC-C2C-C1C	2.32	128.57	125.04
23	b	613	CLA	C11-C10-C8	-2.31	108.44	115.92
23	C	511	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
23	b	618	CLA	C4-C3-C5	2.31	119.16	115.27
25	b	624	BCR	C33-C5-C6	-2.31	121.93	124.53
23	B	607	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
23	C	508	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
23	B	605	CLA	C4C-C3C-C2C	-2.31	103.53	106.90
23	B	602	CLA	CHA-C1A-NA	-2.31	121.11	126.40
23	A	406	CLA	C4-C3-C5	2.31	119.16	115.27
23	a	2613	CLA	CMA-C3A-C4A	-2.31	105.57	111.77
28	M	101	LMT	C1'-C2'-C3'	-2.31	105.19	110.00
23	C	513	CLA	CMC-C2C-C1C	2.31	128.55	125.04
23	c	508	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
23	a	2613	CLA	C4C-C3C-C2C	-2.31	103.54	106.90
23	b	621	CLA	CHD-C1D-C2D	-2.30	120.65	125.48
23	C	502	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
37	c	520	DGD	O3G-C1D-C2D	-2.30	104.71	108.30
25	c	517	BCR	C16-C17-C18	-2.30	124.02	127.31
23	a	2613	CLA	CMC-C2C-C1C	2.30	128.55	125.04
26	B	621	SQD	O47-C7-O49	-2.30	118.14	123.70
23	b	619	CLA	CHC-C1C-C2C	-2.30	120.35	126.72
25	B	619	BCR	C20-C21-C22	-2.30	124.03	127.31
28	T	103	LMT	O1'-C1'-C2'	2.30	111.90	108.30
33	A	422	PL9	C46-C44-C45	2.30	119.68	114.60
25	K	101	BCR	C3-C4-C5	-2.30	109.98	114.08
33	d	411	PL9	C22-C23-C24	-2.29	122.14	127.66
26	l	101	SQD	O47-C7-O49	-2.29	118.16	123.70
23	C	511	CLA	C4-C3-C2	-2.29	117.80	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	407	CLA	C4C-C3C-C2C	-2.29	103.56	106.90
25	B	620	BCR	C7-C8-C9	-2.29	122.77	126.23
23	D	2304	CLA	O2A-CGA-CBA	2.29	119.10	111.91
23	b	615	CLA	C3B-C4B-NB	2.29	112.17	109.21
25	D	2305	BCR	C15-C14-C13	-2.29	124.04	127.31
25	b	622	BCR	C15-C14-C13	-2.29	124.04	127.31
25	b	624	BCR	C10-C11-C12	-2.29	116.07	123.22
23	B	604	CLA	C3B-C4B-NB	2.29	112.17	109.21
25	z	101	BCR	C2-C1-C6	2.29	114.01	110.48
23	b	617	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
23	B	611	CLA	CHA-C1A-NA	-2.29	121.16	126.40
33	d	411	PL9	C40-C39-C38	-2.29	117.81	123.68
23	C	507	CLA	CMB-C2B-C3B	2.29	128.96	124.68
25	b	624	BCR	C32-C1-C6	-2.29	106.59	110.30
23	B	616	CLA	C1-C2-C3	-2.29	122.09	126.04
25	c	517	BCR	C3-C4-C5	-2.29	110.00	114.08
37	C	518	DGD	O1G-C1A-C2A	2.28	119.08	111.91
33	D	2306	PL9	C36-C37-C38	-2.28	104.37	111.88
24	A	408	PHO	O1D-CGD-CBD	-2.28	120.94	124.74
23	c	514	CLA	CHC-C1C-C2C	-2.28	120.41	126.72
23	B	612	CLA	C7-C6-C5	-2.28	107.16	113.36
23	B	617	CLA	CMA-C3A-C4A	-2.28	105.64	111.77
23	c	510	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
23	c	513	CLA	C4-C3-C5	2.28	119.11	115.27
23	B	607	CLA	C3B-C4B-NB	2.28	112.16	109.21
23	B	612	CLA	O2A-CGA-CBA	2.28	119.06	111.91
23	C	503	CLA	C4A-NA-C1A	2.28	107.73	106.71
23	B	607	CLA	O2A-CGA-CBA	2.28	119.05	111.91
23	a	2613	CLA	CHC-C1C-C2C	-2.28	120.43	126.72
25	Y	302	BCR	C36-C18-C17	-2.28	119.73	122.92
23	c	513	CLA	O2A-CGA-O1A	-2.27	117.85	123.59
36	b	625	HTG	O6-C6-C5	-2.27	103.49	111.29
23	B	614	CLA	C1-C2-C3	-2.27	122.11	126.04
23	C	510	CLA	CHA-C1A-NA	-2.27	121.19	126.40
23	D	2304	CLA	CMC-C2C-C1C	2.27	128.50	125.04
23	B	609	CLA	CBC-CAC-C3C	-2.27	106.17	112.43
23	C	513	CLA	CMA-C3A-C4A	-2.27	105.67	111.77
33	A	422	PL9	C25-C24-C26	2.27	119.08	115.27
23	b	613	CLA	CAA-C2A-C3A	-2.27	106.57	112.78
23	d	409	CLA	CBC-CAC-C3C	-2.27	106.19	112.43
27	B	622	LMG	C9-C8-C7	-2.26	106.43	111.79
23	A	410	CLA	CMC-C2C-C1C	2.26	128.49	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	x	1301	PL9	C42-C43-C44	-2.26	120.02	127.75
33	A	422	PL9	C15-C14-C16	2.26	119.08	115.27
23	B	617	CLA	CHD-C1D-ND	-2.26	122.38	124.45
31	a	2619	JOX	C2-C1-CL1	2.26	117.72	115.84
25	c	517	BCR	C31-C1-C6	-2.26	106.64	110.30
23	C	513	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
23	b	621	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
23	C	502	CLA	C4-C3-C5	2.26	119.07	115.27
26	D	2302	SQD	O48-C23-C24	2.26	118.99	111.91
23	b	614	CLA	O2A-CGA-CBA	2.25	118.98	111.91
33	x	1301	PL9	C25-C24-C23	-2.25	117.89	123.68
23	B	613	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
23	b	613	CLA	CHA-C1A-NA	-2.25	121.24	126.40
23	c	515	CLA	CHC-C1C-C2C	-2.25	120.49	126.72
23	b	617	CLA	CHB-C4A-NA	2.25	127.62	124.51
23	C	502	CLA	O2A-CGA-CBA	2.25	118.97	111.91
23	A	406	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
23	c	513	CLA	CAC-C3C-C4C	2.25	127.73	124.81
25	b	622	BCR	C21-C20-C19	-2.25	116.20	123.22
23	B	617	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
23	b	619	CLA	OBD-CAD-C3D	-2.25	123.11	128.52
23	C	505	CLA	C4C-C3C-C2C	-2.25	103.62	106.90
23	b	614	CLA	C3B-C4B-NB	2.25	112.11	109.21
23	b	614	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
26	l	101	SQD	O8-S-C6	2.24	109.32	105.74
23	b	617	CLA	CMA-C3A-C4A	-2.24	105.75	111.77
23	b	606	CLA	C3C-C4C-NC	2.24	113.08	110.57
23	B	610	CLA	CHA-C1A-NA	-2.24	121.27	126.40
25	b	623	BCR	C37-C22-C21	-2.24	119.79	122.92
27	C	520	LMG	O7-C10-O9	-2.24	118.29	123.70
23	B	602	CLA	CMC-C2C-C1C	2.24	128.44	125.04
29	b	644	GOL	C3-C2-C1	-2.24	103.01	111.70
23	b	609	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
23	C	511	CLA	CHA-C1A-NA	-2.23	121.29	126.40
36	b	602	HTG	O5-C1-C2	2.23	113.12	110.31
25	B	620	BCR	C15-C16-C17	-2.23	118.90	123.47
23	C	505	CLA	C7-C6-C5	-2.23	107.30	113.36
23	B	609	CLA	CMC-C2C-C1C	2.23	128.44	125.04
23	C	504	CLA	CHD-C4C-NC	2.23	127.72	124.20
33	A	422	PL9	C42-C43-C44	-2.23	120.12	127.75
23	b	609	CLA	CHD-C1D-C2D	-2.23	120.80	125.48
25	b	622	BCR	C3-C4-C5	-2.23	110.10	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	620	CLA	C11-C10-C8	-2.23	108.72	115.92
25	C	515	BCR	C8-C7-C6	-2.23	120.94	127.20
25	y	101	BCR	C1-C6-C7	2.23	122.08	115.78
37	c	518	DGD	C6D-O5D-C1E	2.23	118.09	113.74
23	B	605	CLA	CHC-C1C-C2C	-2.23	120.57	126.72
23	c	516	CLA	CHA-C1A-NA	-2.23	121.30	126.40
33	D	2306	PL9	C35-C34-C36	2.22	119.01	115.27
23	c	511	CLA	C6-C7-C8	-2.22	108.73	115.92
23	B	614	CLA	CMB-C2B-C3B	2.22	128.84	124.68
33	d	411	PL9	C35-C34-C36	2.22	119.01	115.27
26	B	621	SQD	O48-C23-C24	2.22	118.88	111.91
28	m	2804	LMT	C1B-O5B-C5B	2.22	118.05	113.69
23	B	616	CLA	CHD-C4C-NC	2.22	127.70	124.20
23	c	505	CLA	CHA-C1A-NA	-2.22	121.32	126.40
38	d	413	LHG	O8-C23-C24	2.22	118.87	111.91
27	c	522	LMG	C8-O7-C10	-2.22	112.33	117.79
24	a	2611	PHO	CMC-C2C-C3C	2.22	129.12	124.94
25	T	102	BCR	C33-C5-C4	2.22	117.87	113.62
31	A	418	JOX	C1-C-C5	-2.21	119.57	120.54
28	M	101	LMT	O1B-C1B-C2B	2.21	113.83	108.10
23	B	612	CLA	OBD-CAD-C3D	-2.21	123.19	128.52
23	B	602	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
28	B	623	LMT	O1B-C4'-C5'	-2.21	103.39	109.45
23	B	614	CLA	OBD-CAD-C3D	-2.21	123.20	128.52
36	d	407	HTG	O5-C5-C4	2.21	113.71	109.69
23	B	608	CLA	CHA-C1A-NA	-2.21	121.34	126.40
25	k	302	BCR	C20-C21-C22	-2.21	124.16	127.31
23	b	615	CLA	CAA-CBA-CGA	-2.21	106.81	113.25
23	b	610	CLA	C1-C2-C3	-2.21	122.23	126.04
25	y	101	BCR	C10-C11-C12	-2.21	116.33	123.22
23	b	606	CLA	CAC-C3C-C4C	2.21	127.67	124.81
23	B	610	CLA	C7-C6-C5	-2.20	107.37	113.36
23	B	617	CLA	CHC-C1C-C2C	-2.20	120.62	126.72
23	c	514	CLA	CHA-C1A-NA	-2.20	121.35	126.40
23	c	513	CLA	C1-C2-C3	-2.20	122.23	126.04
25	C	516	BCR	C11-C10-C9	-2.20	124.17	127.31
25	D	2305	BCR	C16-C17-C18	-2.20	124.17	127.31
23	C	504	CLA	CHA-C1A-NA	-2.20	121.36	126.40
25	A	411	BCR	C7-C8-C9	-2.20	122.91	126.23
23	B	614	CLA	CBC-CAC-C3C	-2.20	106.37	112.43
23	B	608	CLA	CHC-C1C-C2C	-2.20	120.64	126.72
23	B	609	CLA	C1-C2-C3	-2.20	122.24	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	2613	CLA	CHD-C4C-NC	2.20	127.67	124.20
23	C	508	CLA	CMC-C2C-C1C	2.20	128.38	125.04
23	A	406	CLA	C4C-C3C-C2C	-2.20	103.70	106.90
23	A	405	CLA	CHC-C1C-C2C	-2.19	120.66	126.72
23	B	602	CLA	CAC-C3C-C4C	2.19	127.65	124.81
23	D	2303	CLA	CMC-C2C-C1C	2.19	128.38	125.04
23	b	615	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
25	A	411	BCR	C31-C1-C6	-2.19	106.75	110.30
23	B	608	CLA	O2A-CGA-CBA	2.19	118.78	111.91
23	A	407	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
25	Y	302	BCR	C35-C13-C12	2.19	121.52	118.08
23	b	612	CLA	CAA-C2A-C1A	-2.19	104.81	111.97
37	C	518	DGD	O6E-C5E-C6E	2.19	111.87	106.44
23	c	505	CLA	C3B-C4B-NB	2.19	112.04	109.21
23	c	513	CLA	C6-C7-C8	-2.19	108.85	115.92
23	B	605	CLA	CAC-C3C-C4C	2.19	127.65	124.81
37	c	520	DGD	O2G-C1B-C2B	2.19	116.21	111.50
40	H	102	RRX	C29-C28-C27	-2.18	107.31	110.30
36	C	522	HTG	O5-C5-C4	2.18	113.66	109.69
23	B	609	CLA	CHA-C1A-NA	-2.18	121.40	126.40
23	A	407	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
23	a	2613	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
23	B	604	CLA	CMA-C3A-C2A	-2.18	105.03	113.83
23	B	611	CLA	C3B-C4B-NB	2.18	112.03	109.21
33	D	2306	PL9	C12-C13-C14	-2.18	122.41	127.66
23	b	620	CLA	CMC-C2C-C1C	2.18	128.36	125.04
25	A	411	BCR	C8-C7-C6	-2.18	121.09	127.20
23	c	509	CLA	CHC-C1C-C2C	-2.18	120.70	126.72
23	C	504	CLA	C3B-C4B-NB	2.18	112.02	109.21
36	d	407	HTG	C4-C3-C2	-2.17	107.03	110.82
23	C	508	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
26	D	2308	SQD	O8-S-C6	2.17	109.20	105.74
23	c	513	CLA	CHC-C1C-C2C	-2.17	120.71	126.72
36	b	603	HTG	O5-C5-C4	2.17	113.64	109.69
23	d	409	CLA	CAC-C3C-C4C	2.17	127.63	124.81
23	B	612	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
23	c	516	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
23	C	507	CLA	C4-C3-C2	-2.17	118.12	123.68
39	F	101	HEM	C4C-CHD-C1D	2.17	125.42	122.56
40	h	101	RRX	C7-C8-C9	-2.16	122.96	126.23
23	D	2304	CLA	CAC-C3C-C2C	2.16	131.23	127.53
23	B	613	CLA	C1-C2-C3	-2.16	122.30	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	C4D-CHA-C1A	2.16	123.88	121.25
26	B	621	SQD	O8-S-C6	2.16	109.18	105.74
23	a	2610	CLA	CMC-C2C-C1C	2.16	128.33	125.04
23	C	509	CLA	C11-C12-C13	-2.16	108.94	115.92
23	B	612	CLA	CAA-C2A-C3A	-2.16	106.87	112.78
39	e	103	HEM	CMA-C3A-C4A	-2.16	125.15	128.46
23	a	2609	CLA	CMA-C3A-C4A	-2.16	105.97	111.77
23	C	509	CLA	CMB-C2B-C3B	2.16	128.72	124.68
23	B	611	CLA	CHC-C1C-C2C	-2.16	120.75	126.72
23	C	514	CLA	O2A-CGA-CBA	2.16	118.68	111.91
23	b	610	CLA	O2A-CGA-CBA	2.16	118.68	111.91
25	y	101	BCR	C32-C1-C6	-2.16	106.80	110.30
23	A	407	CLA	CMA-C3A-C2A	-2.16	105.13	113.83
23	C	504	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
23	c	506	CLA	C3B-C4B-NB	2.15	112.00	109.21
25	Y	302	BCR	C34-C9-C8	2.15	121.47	118.08
27	c	501	LMG	C30-C29-C28	-2.15	105.79	113.62
33	D	2306	PL9	C47-C48-C49	-2.15	120.39	127.75
25	a	2614	BCR	C34-C9-C10	-2.15	119.91	122.92
36	c	523	HTG	C6-C5-C4	-2.15	107.96	113.00
23	b	611	CLA	CAC-C3C-C4C	2.15	127.60	124.81
23	B	608	CLA	C4A-NA-C1A	2.15	107.67	106.71
23	C	503	CLA	CMB-C2B-C3B	2.15	128.70	124.68
25	K	101	BCR	C20-C21-C22	-2.15	124.24	127.31
23	B	611	CLA	O2A-C1-C2	2.15	114.28	108.64
26	D	2302	SQD	O5-C1-C2	2.15	114.90	110.35
27	D	2312	LMG	C7-O1-C1	-2.15	109.54	113.74
25	z	101	BCR	C37-C22-C23	2.15	121.46	118.08
23	B	604	CLA	CAA-C2A-C1A	-2.15	104.94	111.97
24	A	408	PHO	C1-O2A-CGA	2.14	122.07	116.44
26	b	601	SQD	C46-C45-C44	-2.14	106.72	111.79
23	d	408	CLA	CAC-C3C-C4C	2.14	127.59	124.81
23	b	607	CLA	CAA-C2A-C3A	-2.14	106.91	112.78
25	B	618	BCR	C21-C20-C19	-2.14	116.53	123.22
23	c	515	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
25	T	102	BCR	C16-C17-C18	-2.14	124.25	127.31
25	K	101	BCR	C2-C3-C4	-2.14	106.59	111.38
23	C	510	CLA	CHC-C1C-C2C	-2.14	120.81	126.72
25	B	619	BCR	C29-C28-C27	-2.14	106.60	111.38
23	C	503	CLA	CHC-C1C-C2C	-2.14	120.81	126.72
23	b	606	CLA	C3B-C4B-NB	2.14	111.97	109.21
23	b	612	CLA	C4A-NA-C1A	2.14	107.67	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	407	CLA	CAA-CBA-CGA	2.14	119.49	113.25
23	c	507	CLA	CHD-C4C-NC	2.13	127.57	124.20
36	d	407	HTG	C6-C5-C4	-2.13	108.00	113.00
23	B	606	CLA	C12-C11-C10	-2.13	103.43	113.24
25	y	101	BCR	C23-C24-C25	-2.13	121.21	127.20
23	b	620	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
23	B	602	CLA	C3C-C4C-NC	2.13	112.96	110.57
23	b	618	CLA	CBC-CAC-C3C	-2.13	106.55	112.43
28	A	414	LMT	C3B-C4B-C5B	2.13	114.04	110.24
23	B	607	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
23	C	502	CLA	C1-C2-C3	-2.13	122.36	126.04
23	c	510	CLA	C6-C7-C8	-2.13	109.03	115.92
23	b	614	CLA	CMC-C2C-C1C	2.13	128.28	125.04
23	C	502	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
37	H	103	DGD	O2G-C1B-O1B	-2.13	118.56	123.70
23	b	617	CLA	OBD-CAD-C3D	-2.13	123.40	128.52
25	a	2614	BCR	C8-C7-C6	-2.13	121.23	127.20
23	b	616	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
23	c	504	CLA	CHD-C4C-NC	2.13	127.55	124.20
23	b	620	CLA	C1-O2A-CGA	2.13	122.02	116.44
23	b	606	CLA	CAA-C2A-C3A	-2.12	106.96	112.78
29	v	203	GOL	C3-C2-C1	-2.12	103.45	111.70
23	B	605	CLA	CMB-C2B-C3B	2.12	128.65	124.68
25	b	623	BCR	C40-C30-C25	-2.12	106.86	110.30
23	B	609	CLA	CMB-C2B-C3B	2.12	128.65	124.68
36	b	626	HTG	O5-C1-C2	2.12	112.98	110.31
25	k	302	BCR	C15-C14-C13	-2.12	124.29	127.31
23	C	505	CLA	CHC-C1C-C2C	-2.12	120.86	126.72
23	B	608	CLA	C4-C3-C5	2.12	118.83	115.27
23	C	511	CLA	C11-C10-C8	-2.12	109.07	115.92
25	k	302	BCR	C21-C20-C19	-2.12	116.61	123.22
23	D	2303	CLA	CHD-C4C-NC	2.12	127.54	124.20
36	B	624[A]	HTG	O5-C1-C2	2.12	112.98	110.31
23	B	613	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
23	B	615	CLA	C4-C3-C5	2.12	118.83	115.27
23	b	608	CLA	CHA-C1A-NA	-2.12	121.55	126.40
23	b	612	CLA	CAA-CBA-CGA	2.12	119.44	113.25
23	b	611	CLA	C11-C10-C8	-2.12	109.08	115.92
40	h	101	RRX	C20-C21-C22	-2.12	124.29	127.31
25	z	101	BCR	C37-C22-C21	-2.12	119.96	122.92
23	c	516	CLA	C4-C3-C5	2.12	118.83	115.27
23	b	619	CLA	CAA-C2A-C3A	-2.11	106.99	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	CHD-C4C-NC	2.11	127.53	124.20
23	b	606	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
24	A	409	PHO	CMC-C2C-C3C	2.11	128.93	124.94
23	b	614	CLA	CAC-C3C-C4C	2.11	127.55	124.81
23	D	2304	CLA	CHB-C4A-NA	2.11	127.43	124.51
23	c	514	CLA	CHD-C4C-NC	2.11	127.53	124.20
26	l	101	SQD	O9-S-C6	2.11	109.44	106.94
25	T	102	BCR	C36-C18-C19	2.11	121.40	118.08
23	B	609	CLA	CHC-C1C-C2C	-2.11	120.89	126.72
23	b	620	CLA	CHC-C1C-C2C	-2.11	120.89	126.72
23	D	2304	CLA	C11-C10-C8	-2.11	109.11	115.92
23	a	2610	CLA	CMB-C2B-C3B	2.11	128.62	124.68
23	C	506	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
37	H	103	DGD	C3E-C4E-C5E	-2.11	106.48	110.24
23	C	503	CLA	C1-O2A-CGA	2.11	121.97	116.44
23	A	406	CLA	CHD-C4C-NC	2.10	127.52	124.20
23	C	512	CLA	CMC-C2C-C1C	2.10	128.24	125.04
25	B	618	BCR	C15-C14-C13	-2.10	124.31	127.31
23	B	616	CLA	C4A-NA-C1A	2.10	107.65	106.71
23	A	406	CLA	CAA-CBA-CGA	2.10	119.39	113.25
23	b	616	CLA	CHA-C1A-NA	-2.10	121.59	126.40
23	A	407	CLA	CHA-C1A-NA	-2.10	121.59	126.40
23	B	616	CLA	CMB-C2B-C3B	2.10	128.60	124.68
25	C	515	BCR	C16-C17-C18	-2.10	124.31	127.31
23	C	509	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
25	c	517	BCR	C33-C5-C4	2.10	117.65	113.62
23	B	603	CLA	CAA-CBA-CGA	-2.10	107.13	113.25
23	B	614	CLA	CHA-C1A-NA	-2.10	121.60	126.40
23	b	618	CLA	CHC-C1C-C2C	-2.10	120.93	126.72
26	D	2308	SQD	O48-C23-O10	-2.10	118.30	123.59
23	C	504	CLA	C4-C3-C5	2.09	118.80	115.27
25	D	2305	BCR	C10-C11-C12	-2.09	116.68	123.22
24	A	409	PHO	C4A-C3A-C2A	-2.09	100.85	102.84
23	c	510	CLA	O2A-CGA-CBA	2.09	118.48	111.91
23	c	510	CLA	CHD-C1D-ND	-2.09	122.53	124.45
23	B	614	CLA	CHD-C4C-NC	2.09	127.50	124.20
23	c	510	CLA	CMB-C2B-C3B	2.09	128.59	124.68
27	A	413	LMG	O8-C28-C29	2.09	118.47	111.91
23	C	506	CLA	C4A-NA-C1A	2.09	107.65	106.71
23	c	506	CLA	CMB-C2B-C1B	2.09	131.68	128.46
23	b	619	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
23	b	613	CLA	OBD-CAD-C3D	-2.09	123.49	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	m	2804	LMT	O5B-C1B-C2B	2.09	114.77	110.35
25	z	101	BCR	C3-C4-C5	-2.09	110.35	114.08
23	b	619	CLA	CHA-C1A-NA	-2.09	121.61	126.40
38	L	101	LHG	O4-P-O5	2.09	122.56	112.24
33	d	411	PL9	C47-C48-C49	-2.09	120.61	127.75
28	z	102	LMT	C1B-O5B-C5B	2.09	117.79	113.69
23	b	619	CLA	CMB-C2B-C3B	2.09	128.58	124.68
23	C	507	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
23	b	612	CLA	C4-C3-C5	2.08	118.78	115.27
23	B	617	CLA	OBD-CAD-C3D	-2.08	123.50	128.52
23	a	2609	CLA	C4-C3-C5	2.08	118.78	115.27
37	C	519	DGD	O1G-C1A-O1A	-2.08	118.34	123.59
23	B	611	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
28	i	103	LMT	C3'-C4'-C5'	2.08	113.95	110.24
23	c	515	CLA	C1-C2-C3	-2.08	122.45	126.04
31	a	2617	JOX	O1-C5-C	-2.08	118.44	121.41
23	C	514	CLA	CMC-C2C-C1C	2.08	128.20	125.04
23	b	619	CLA	CMA-C3A-C4A	-2.08	106.19	111.77
23	B	615	CLA	CHC-C1C-NC	2.08	127.35	124.20
38	L	101	LHG	O7-C7-O9	-2.07	118.69	123.70
23	c	507	CLA	O2A-CGA-CBA	2.07	118.42	111.91
23	C	512	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
26	D	2302	SQD	C9-C8-C7	-2.07	106.09	113.62
25	d	410	BCR	C21-C20-C19	-2.07	116.75	123.22
23	c	511	CLA	CHD-C1D-C2D	-2.07	121.14	125.48
23	B	604	CLA	CHA-C1A-NA	-2.07	121.66	126.40
23	b	615	CLA	C4-C3-C5	2.07	118.75	115.27
36	b	602	HTG	C1'-S1-C1	2.07	103.96	100.09
23	c	513	CLA	C11-C10-C8	-2.07	109.23	115.92
23	B	610	CLA	CAC-C3C-C4C	2.07	127.49	124.81
23	c	512	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
23	B	602	CLA	C3B-C4B-NB	2.07	111.88	109.21
38	e	101	LHG	O8-C23-O10	-2.07	118.38	123.59
24	A	408	PHO	CBA-CAA-C2A	-2.07	107.77	113.81
25	D	2305	BCR	C15-C16-C17	-2.07	119.24	123.47
23	C	514	CLA	CED-O2D-CGD	2.07	120.61	115.94
23	A	410	CLA	CHC-C1C-C2C	-2.07	121.01	126.72
39	e	103	HEM	CMC-C2C-C3C	2.07	128.54	124.68
23	c	510	CLA	OBD-CAD-C3D	-2.07	123.55	128.52
23	b	612	CLA	CAC-C3C-C2C	2.07	131.06	127.53
25	b	623	BCR	C29-C28-C27	-2.06	106.76	111.38
23	a	2610	CLA	CHA-C1A-NA	-2.06	121.67	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	z	102	LMT	C1'-O5'-C5'	2.06	117.73	113.69
23	d	408	CLA	C4-C3-C5	2.06	118.74	115.27
40	h	101	RRX	C11-C10-C9	-2.06	124.37	127.31
24	a	2611	PHO	C1-O2A-CGA	2.06	121.85	116.44
25	A	411	BCR	C2-C3-C4	-2.06	106.77	111.38
40	H	102	RRX	C37-C22-C21	-2.06	120.04	122.92
23	c	512	CLA	CHD-C1D-ND	-2.06	122.56	124.45
36	V	204	HTG	O5-C5-C4	2.06	113.43	109.69
37	C	519	DGD	O4D-C4D-C3D	-2.06	105.59	110.35
23	b	619	CLA	C4-C3-C2	-2.06	118.40	123.68
25	C	515	BCR	C23-C24-C25	-2.06	121.43	127.20
25	B	620	BCR	C38-C26-C25	-2.06	122.22	124.53
36	C	525	HTG	C4-C3-C2	-2.06	107.23	110.82
25	B	620	BCR	C10-C11-C12	-2.06	116.80	123.22
24	a	2612	PHO	CMA-C3A-C4A	-2.05	109.88	114.38
23	a	2613	CLA	CMB-C2B-C3B	2.05	128.52	124.68
27	c	521	LMG	O8-C28-O10	-2.05	118.41	123.59
28	A	414	LMT	O1B-C1B-O5B	-2.05	104.94	110.67
26	A	412	SQD	C45-O47-C7	-2.05	112.74	117.79
36	B	624[B]	HTG	O5-C5-C4	2.05	113.42	109.69
23	b	615	CLA	C11-C12-C13	-2.05	109.28	115.92
36	o	301	HTG	O5-C5-C6	2.05	111.54	106.44
26	b	601	SQD	O47-C7-O49	-2.05	118.74	123.70
28	M	101	LMT	C1B-O1B-C4'	-2.05	112.89	117.96
27	D	2312	LMG	C9-C8-C7	-2.05	106.94	111.79
23	B	605	CLA	CMD-C2D-C3D	-2.05	122.90	127.61
23	b	616	CLA	CHB-C4A-NA	2.05	127.34	124.51
23	a	2610	CLA	CHC-C1C-C2C	-2.05	121.06	126.72
25	b	623	BCR	C28-C27-C26	-2.05	110.42	114.08
37	C	518	DGD	C6D-O5D-C1E	2.05	117.74	113.74
23	C	514	CLA	CMD-C2D-C3D	-2.05	122.91	127.61
23	c	515	CLA	CMC-C2C-C1C	2.05	128.15	125.04
27	c	501	LMG	O8-C28-C29	2.04	118.33	111.91
23	C	509	CLA	CMC-C2C-C1C	2.04	128.15	125.04
23	D	2303	CLA	CHC-C1C-C2C	-2.04	121.07	126.72
27	c	521	LMG	O7-C10-O9	-2.04	118.77	123.70
23	B	610	CLA	O2A-CGA-CBA	2.04	118.31	111.91
23	C	513	CLA	C1-O2A-CGA	2.04	121.80	116.44
26	a	2615	SQD	O5-C1-C2	-2.04	106.03	110.35
36	H	101	HTG	O5-C1-C2	2.04	112.85	110.25
42	v	201	HEC	CMB-C2B-C3B	2.04	128.22	125.82
23	c	507	CLA	CMC-C2C-C1C	2.04	128.14	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	2619	JOX	C-C5-C4	2.04	121.58	117.15
23	b	619	CLA	CHB-C4A-NA	2.03	127.33	124.51
23	b	606	CLA	C4-C3-C2	-2.03	118.46	123.68
23	b	608	CLA	CAA-C2A-C1A	-2.03	105.31	111.97
23	b	613	CLA	CHC-C1C-C2C	-2.03	121.10	126.72
36	B	624[B]	HTG	C1-C2-C3	2.03	114.60	110.59
23	C	509	CLA	CHB-C4A-NA	2.03	127.32	124.51
23	c	504	CLA	CMB-C2B-C3B	2.03	128.47	124.68
23	B	610	CLA	CMA-C3A-C4A	-2.03	106.32	111.77
36	B	627	HTG	C1-O5-C5	2.03	116.32	112.58
23	b	611	CLA	CHC-C1C-C2C	-2.03	121.11	126.72
28	M	101	LMT	C1B-O5B-C5B	2.03	117.67	113.69
23	c	504	CLA	CHC-C1C-C2C	-2.03	121.12	126.72
27	A	413	LMG	O6-C5-C4	2.03	113.37	109.69
23	a	2610	CLA	O2D-CGD-O1D	-2.03	119.88	123.84
31	A	418	JOX	C-C1-CL1	2.02	124.91	120.02
23	B	606	CLA	CHA-C1A-NA	-2.02	121.76	126.40
36	b	603	HTG	C2'-C1'-S1	-2.02	105.87	112.40
23	c	505	CLA	CHD-C4C-NC	2.02	127.39	124.20
23	C	510	CLA	OBD-CAD-C3D	-2.02	123.66	128.52
27	c	522	LMG	C4-C3-C2	-2.02	107.30	110.82
23	c	509	CLA	C1-C2-C3	-2.02	122.55	126.04
23	c	515	CLA	CHD-C1D-C2D	-2.02	121.25	125.48
25	b	622	BCR	C35-C13-C14	-2.02	120.10	122.92
39	F	101	HEM	C1B-NB-C4B	2.02	107.16	105.07
23	c	511	CLA	CHC-C1C-C2C	-2.01	121.15	126.72
25	B	619	BCR	C11-C10-C9	-2.01	124.44	127.31
23	A	410	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
23	B	617	CLA	C5-C3-C2	-2.01	117.04	121.12
25	a	2614	BCR	C15-C14-C13	-2.01	124.44	127.31
40	H	102	RRX	C21-C20-C19	-2.01	116.94	123.22
23	B	614	CLA	C5-C3-C2	-2.01	117.05	121.12
28	m	2804	LMT	C4B-C3B-C2B	2.01	114.33	110.82
23	d	409	CLA	O2A-CGA-CBA	2.01	118.22	111.91
23	C	513	CLA	CAC-C3C-C2C	2.01	130.96	127.53
23	c	510	CLA	CHC-C1C-C2C	-2.01	121.17	126.72
24	a	2611	PHO	C4A-C3A-C2A	-2.01	100.93	102.84
23	B	613	CLA	C2A-C1A-CHA	-2.00	120.35	123.86
25	b	622	BCR	C16-C17-C18	-2.00	124.45	127.31
23	C	514	CLA	CHC-C1C-C2C	-2.00	121.18	126.72
37	C	517	DGD	C2G-O2G-C1B	-2.00	112.86	117.79
27	c	501	LMG	C8-O7-C10	-2.00	112.87	117.79

All (62) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	405	CLA	ND
23	A	410	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND
23	B	607	CLA	ND
23	B	608	CLA	ND
23	B	610	CLA	ND
23	B	611	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	B	617	CLA	ND
23	C	502	CLA	ND
23	C	503	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	508	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	D	2303	CLA	ND
23	D	2304	CLA	ND
23	a	2609	CLA	ND
23	a	2613	CLA	ND
23	b	606	CLA	ND
23	b	607	CLA	ND
23	b	608	CLA	ND
23	b	609	CLA	ND
23	b	610	CLA	ND
23	b	611	CLA	ND
23	b	612	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	b	616	CLA	ND

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Mol	Chain	Res	Type	Atom
23	b	617	CLA	ND
23	b	618	CLA	ND
23	b	619	CLA	ND
23	b	620	CLA	ND
23	b	621	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	507	CLA	ND
23	c	508	CLA	ND
23	c	509	CLA	ND
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND
23	c	513	CLA	ND
23	c	514	CLA	ND
23	c	515	CLA	ND
23	c	516	CLA	ND
23	d	402	CLA	ND
23	d	408	CLA	ND
23	d	409	CLA	ND

All (1254) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	603	CLA	CHA-CBD-CGD-O1D
23	B	607	CLA	CHA-CBD-CGD-O1D
23	B	607	CLA	CHA-CBD-CGD-O2D
23	B	611	CLA	C14-C13-C15-C16
23	B	615	CLA	CHA-CBD-CGD-O2D
23	B	615	CLA	CAD-CBD-CGD-O2D
23	C	507	CLA	C2-C3-C5-C6
23	C	507	CLA	C4-C3-C5-C6
23	D	2304	CLA	C2-C3-C5-C6
23	D	2304	CLA	C4-C3-C5-C6
23	b	607	CLA	CHA-CBD-CGD-O1D
23	b	608	CLA	C4-C3-C5-C6
23	b	610	CLA	C2-C3-C5-C6
23	b	610	CLA	C4-C3-C5-C6
23	b	611	CLA	CHA-CBD-CGD-O1D
23	b	611	CLA	CHA-CBD-CGD-O2D
23	b	619	CLA	CHA-CBD-CGD-O1D
23	b	619	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	b	619	CLA	CAD-CBD-CGD-O1D
23	b	619	CLA	CAD-CBD-CGD-O2D
23	c	510	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	C4-C3-C5-C6
25	B	618	BCR	C1-C6-C7-C8
25	B	633	BCR	C11-C12-C13-C14
25	B	633	BCR	C11-C12-C13-C35
25	B	633	BCR	C13-C14-C15-C16
25	C	516	BCR	C1-C6-C7-C8
25	D	2305	BCR	C7-C8-C9-C10
25	D	2305	BCR	C7-C8-C9-C34
25	D	2305	BCR	C21-C22-C23-C24
25	D	2305	BCR	C37-C22-C23-C24
25	D	2305	BCR	C23-C24-C25-C30
25	T	102	BCR	C11-C12-C13-C14
25	T	102	BCR	C11-C12-C13-C35
25	Y	302	BCR	C21-C22-C23-C24
25	Y	302	BCR	C37-C22-C23-C24
25	b	622	BCR	C1-C6-C7-C8
25	b	624	BCR	C37-C22-C23-C24
25	d	410	BCR	C7-C8-C9-C10
25	d	410	BCR	C7-C8-C9-C34
25	d	410	BCR	C21-C22-C23-C24
25	d	410	BCR	C37-C22-C23-C24
25	y	101	BCR	C21-C22-C23-C24
25	y	101	BCR	C37-C22-C23-C24
26	B	621	SQD	O5-C1-O6-C44
26	B	621	SQD	O49-C7-O47-C45
26	B	621	SQD	C8-C7-O47-C45
26	B	621	SQD	C5-C6-S-O7
26	B	621	SQD	C5-C6-S-O8
26	B	621	SQD	C5-C6-S-O9
26	D	2302	SQD	O49-C7-O47-C45
26	D	2308	SQD	C8-C7-O47-C45
26	D	2308	SQD	C5-C6-S-O7
26	a	2603	SQD	O6-C44-C45-O47
26	a	2603	SQD	C5-C6-S-O7
26	a	2603	SQD	C5-C6-S-O8
26	a	2603	SQD	C5-C6-S-O9
26	b	601	SQD	C5-C6-S-O7
26	b	601	SQD	C5-C6-S-O8
26	b	601	SQD	C5-C6-S-O9

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Mol	Chain	Res	Type	Atoms
26	d	417	SQD	C44-C45-O47-C7
26	d	417	SQD	C46-C45-O47-C7
26	d	417	SQD	O49-C7-O47-C45
26	l	101	SQD	O5-C1-O6-C44
26	l	101	SQD	O49-C7-O47-C45
26	l	101	SQD	C8-C7-O47-C45
26	l	101	SQD	C5-C6-S-O7
27	C	527	LMG	O9-C10-O7-C8
27	C	527	LMG	C11-C10-O7-C8
27	c	501	LMG	O9-C10-O7-C8
28	A	414	LMT	C2'-C1'-O1'-C1
28	A	414	LMT	O5'-C1'-O1'-C1
28	A	414	LMT	C2-C1-O1'-C1'
28	A	420	LMT	O5'-C1'-O1'-C1
28	B	623	LMT	C2-C1-O1'-C1'
28	F	102	LMT	C2'-C1'-O1'-C1
28	F	102	LMT	O5'-C1'-O1'-C1
28	J	303	LMT	C2'-C1'-O1'-C1
28	T	103	LMT	C2'-C1'-O1'-C1
28	T	103	LMT	O5'-C1'-O1'-C1
28	Z	101	LMT	C2-C1-O1'-C1'
28	d	401	LMT	C2'-C1'-O1'-C1
28	d	401	LMT	O5'-C1'-O1'-C1
28	d	404	LMT	C2'-C1'-O1'-C1
28	d	404	LMT	O5'-C1'-O1'-C1
28	f	101	LMT	C2'-C1'-O1'-C1
28	f	101	LMT	O5'-C1'-O1'-C1
28	i	103	LMT	C2'-C1'-O1'-C1
28	i	103	LMT	O5'-C1'-O1'-C1
28	z	102	LMT	C2'-C1'-O1'-C1
28	z	102	LMT	O5'-C1'-O1'-C1
29	B	632	GOL	O1-C1-C2-C3
29	C	524	GOL	O1-C1-C2-O2
29	C	524	GOL	O1-C1-C2-C3
29	C	526	GOL	O1-C1-C2-C3
29	J	301	GOL	O1-C1-C2-C3
29	J	301	GOL	C1-C2-C3-O3
29	J	301	GOL	O2-C2-C3-O3
29	O	302	GOL	C1-C2-C3-O3
29	O	304	GOL	O1-C1-C2-C3
29	U	502	GOL	C1-C2-C3-O3
29	b	644	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
33	x	1301	PL9	C18-C19-C21-C22
33	x	1301	PL9	C20-C19-C21-C22
36	C	521	HTG	C2'-C1'-S1-C1
36	I	101	HTG	C2-C1-S1-C1'
36	I	101	HTG	O5-C1-S1-C1'
36	V	204	HTG	C2-C1-S1-C1'
36	V	204	HTG	O5-C1-S1-C1'
36	b	602	HTG	C2'-C1'-S1-C1
36	b	625	HTG	C2'-C1'-S1-C1
36	b	626	HTG	O5-C1-S1-C1'
36	d	407	HTG	C2-C1-S1-C1'
36	d	407	HTG	O5-C1-S1-C1'
36	d	407	HTG	C2'-C1'-S1-C1
36	d	415	HTG	O5-C1-S1-C1'
36	i	102	HTG	C2-C1-S1-C1'
36	i	102	HTG	O5-C1-S1-C1'
36	o	301	HTG	C2'-C1'-S1-C1
37	D	2307	DGD	C2B-C1B-O2G-C2G
37	D	2307	DGD	C2D-C1D-O3G-C3G
37	D	2307	DGD	O6D-C1D-O3G-C3G
38	D	2310	LHG	C4-O6-P-O4
38	E	101	LHG	C4-O6-P-O5
38	L	101	LHG	C4-O6-P-O4
38	d	412	LHG	O2-C2-C3-O3
38	d	413	LHG	O1-C1-C2-C3
38	e	101	LHG	O10-C23-O8-C6
38	e	101	LHG	C24-C23-O8-C6
38	l	103	LHG	C4-O6-P-O4
23	C	507	CLA	C15-C16-C17-C18
23	b	611	CLA	C10-C11-C12-C13
26	D	2308	SQD	O49-C7-O47-C45
37	D	2307	DGD	O1B-C1B-O2G-C2G
26	D	2308	SQD	O10-C23-O48-C46
26	D	2302	SQD	C8-C7-O47-C45
27	c	501	LMG	C11-C10-O7-C8
23	B	606	CLA	C4-C3-C5-C6
23	B	615	CLA	C4-C3-C5-C6
23	b	608	CLA	C2-C3-C5-C6
23	D	2304	CLA	C3-C5-C6-C7
23	b	606	CLA	C3-C5-C6-C7
23	b	621	CLA	C3-C5-C6-C7
26	D	2308	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
36	I	101	HTG	S1-C1'-C2'-C3'
25	T	102	BCR	C13-C14-C15-C16
36	b	626	HTG	O5-C5-C6-O6
23	B	605	CLA	C3-C5-C6-C7
23	c	516	CLA	C3-C5-C6-C7
23	d	409	CLA	C3-C5-C6-C7
38	E	101	LHG	C24-C23-O8-C6
28	T	103	LMT	O5'-C5'-C6'-O6'
28	z	102	LMT	O5B-C5B-C6B-O6B
28	A	414	LMT	C2-C3-C4-C5
37	C	517	DGD	CCB-CDB-CEB-CFB
36	B	624[A]	HTG	S1-C1'-C2'-C3'
36	b	602	HTG	S1-C1'-C2'-C3'
38	E	101	LHG	O10-C23-O8-C6
28	Z	101	LMT	O5B-C5B-C6B-O6B
23	b	619	CLA	C4-C3-C5-C6
36	B	626	HTG	C4-C5-C6-O6
23	B	606	CLA	C2-C3-C5-C6
23	B	615	CLA	C2-C3-C5-C6
23	b	619	CLA	C2-C3-C5-C6
23	c	510	CLA	C2-C3-C5-C6
28	B	634	LMT	O5'-C5'-C6'-O6'
36	i	102	HTG	O5-C5-C6-O6
28	J	303	LMT	O5'-C1'-O1'-C1
33	A	422	PL9	C9-C11-C12-C13
33	A	422	PL9	C14-C16-C17-C18
33	x	1301	PL9	C9-C11-C12-C13
33	x	1301	PL9	C14-C16-C17-C18
37	C	518	DGD	C8A-C9A-CAA-CBA
28	Z	101	LMT	O5B-C1B-O1B-C4'
37	c	518	DGD	C8A-C9A-CAA-CBA
28	z	102	LMT	C4B-C5B-C6B-O6B
37	h	102	DGD	C9A-CAA-CBA-CCA
28	B	634	LMT	C4'-C5'-C6'-O6'
37	H	103	DGD	C9A-CAA-CBA-CCA
27	B	622	LMG	C15-C16-C17-C18
23	a	2609	CLA	C15-C16-C17-C18
28	i	103	LMT	O5'-C5'-C6'-O6'
23	B	616	CLA	C13-C15-C16-C17
27	C	520	LMG	C10-C11-C12-C13
26	B	621	SQD	C2-C1-O6-C44
38	d	403	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
23	d	409	CLA	C4-C3-C5-C6
23	A	410	CLA	C14-C13-C15-C16
23	B	602	CLA	C6-C7-C8-C9
23	B	616	CLA	C11-C10-C8-C9
23	C	505	CLA	C11-C12-C13-C14
23	C	507	CLA	C14-C13-C15-C16
23	a	2610	CLA	C11-C12-C13-C14
23	c	507	CLA	C11-C12-C13-C14
25	C	515	BCR	C37-C22-C23-C24
36	d	407	HTG	O5-C5-C6-O6
36	V	204	HTG	C4-C5-C6-O6
26	D	2302	SQD	C23-C24-C25-C26
23	C	514	CLA	C10-C11-C12-C13
28	Z	101	LMT	C2B-C1B-O1B-C4'
27	m	2802	LMG	C30-C31-C32-C33
28	J	303	LMT	O5'-C5'-C6'-O6'
28	Z	101	LMT	C4B-C5B-C6B-O6B
36	i	102	HTG	C4-C5-C6-O6
23	a	2613	CLA	C5-C6-C7-C8
23	b	606	CLA	C10-C11-C12-C13
37	c	519	DGD	C1B-C2B-C3B-C4B
23	B	614	CLA	C10-C11-C12-C13
23	b	616	CLA	C13-C15-C16-C17
23	c	515	CLA	C10-C11-C12-C13
23	c	516	CLA	C10-C11-C12-C13
29	J	301	GOL	O1-C1-C2-O2
29	v	202	GOL	O2-C2-C3-O3
37	C	517	DGD	C1B-C2B-C3B-C4B
36	B	626	HTG	O5-C5-C6-O6
23	D	2304	CLA	C8-C10-C11-C12
28	z	102	LMT	O5'-C5'-C6'-O6'
28	B	623	LMT	O1'-C1-C2-C3
28	d	401	LMT	O1'-C1-C2-C3
23	d	409	CLA	C8-C10-C11-C12
26	B	621	SQD	C7-C8-C9-C10
27	m	2802	LMG	C10-C11-C12-C13
37	C	518	DGD	C1B-C2B-C3B-C4B
23	A	410	CLA	C11-C12-C13-C15
23	B	614	CLA	C12-C13-C15-C16
23	B	617	CLA	C12-C13-C15-C16
23	b	611	CLA	C12-C13-C15-C16
23	b	618	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
23	d	409	CLA	C6-C7-C8-C10
23	C	508	CLA	C15-C16-C17-C18
33	A	422	PL9	C19-C21-C22-C23
33	x	1301	PL9	C24-C26-C27-C28
33	x	1301	PL9	C34-C36-C37-C38
28	T	103	LMT	C4'-C5'-C6'-O6'
23	B	604	CLA	C5-C6-C7-C8
23	C	510	CLA	C13-C15-C16-C17
27	B	622	LMG	C10-C11-C12-C13
36	b	626	HTG	C4-C5-C6-O6
23	b	621	CLA	C13-C15-C16-C17
36	o	301	HTG	C4-C5-C6-O6
23	B	617	CLA	C5-C6-C7-C8
23	B	617	CLA	C10-C11-C12-C13
23	b	621	CLA	C5-C6-C7-C8
38	E	101	LHG	C4-O6-P-O3
38	l	103	LHG	C4-O6-P-O3
23	B	615	CLA	C3-C5-C6-C7
28	F	102	LMT	C1-C2-C3-C4
23	C	504	CLA	CBD-CGD-O2D-CED
38	d	412	LHG	C1-C2-C3-O3
23	d	409	CLA	C2-C3-C5-C6
23	C	511	CLA	C8-C10-C11-C12
23	b	620	CLA	C10-C11-C12-C13
23	B	607	CLA	C2A-CAA-CBA-CGA
37	D	2307	DGD	O6D-C5D-C6D-O5D
28	B	623	LMT	O5B-C1B-O1B-C4'
23	c	509	CLA	C15-C16-C17-C18
26	l	101	SQD	C31-C32-C33-C34
38	l	103	LHG	C33-C34-C35-C36
23	c	516	CLA	CBD-CGD-O2D-CED
27	c	521	LMG	C11-C10-O7-C8
23	c	512	CLA	C8-C10-C11-C12
26	D	2302	SQD	C24-C23-O48-C46
37	D	2307	DGD	C3B-C4B-C5B-C6B
38	L	101	LHG	C33-C34-C35-C36
27	c	521	LMG	O9-C10-O7-C8
37	c	519	DGD	C1A-C2A-C3A-C4A
28	d	401	LMT	C5-C6-C7-C8
27	C	520	LMG	C16-C17-C18-C19
28	j	2701	LMT	C2'-C1'-O1'-C1
27	A	413	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
37	C	518	DGD	C4B-C5B-C6B-C7B
23	C	502	CLA	C16-C17-C18-C19
23	C	507	CLA	C16-C17-C18-C20
23	b	621	CLA	C4-C3-C5-C6
33	D	2306	PL9	C15-C14-C16-C17
26	a	2603	SQD	C34-C35-C36-C37
36	H	101	HTG	C3'-C4'-C5'-C6'
33	D	2306	PL9	C13-C14-C16-C17
23	B	604	CLA	C6-C7-C8-C9
23	a	2610	CLA	C6-C7-C8-C9
23	c	509	CLA	C11-C10-C8-C9
23	c	509	CLA	C14-C13-C15-C16
26	a	2603	SQD	C31-C32-C33-C34
27	A	413	LMG	C38-C39-C40-C41
27	d	414	LMG	C19-C20-C21-C22
28	z	102	LMT	C7-C8-C9-C10
37	C	517	DGD	C5B-C6B-C7B-C8B
29	A	415	GOL	O1-C1-C2-C3
29	A	417	GOL	C1-C2-C3-O3
29	D	2301	GOL	O1-C1-C2-C3
29	a	2602	GOL	O1-C1-C2-C3
29	c	530	GOL	O1-C1-C2-C3
29	c	530	GOL	C1-C2-C3-O3
29	c	531	GOL	C1-C2-C3-O3
29	d	416	GOL	C1-C2-C3-O3
29	v	202	GOL	C1-C2-C3-O3
38	D	2310	LHG	O1-C1-C2-C3
38	D	2311	LHG	O1-C1-C2-C3
38	d	412	LHG	O1-C1-C2-C3
27	d	414	LMG	O6-C5-C6-O5
23	B	606	CLA	C10-C11-C12-C13
23	c	513	CLA	C8-C10-C11-C12
26	D	2302	SQD	C17-C18-C19-C20
27	B	622	LMG	C37-C38-C39-C40
27	C	527	LMG	C33-C34-C35-C36
27	C	527	LMG	C34-C35-C36-C37
37	C	518	DGD	CBB-CCB-CDB-CEB
37	c	518	DGD	C4B-C5B-C6B-C7B
37	c	519	DGD	C4B-C5B-C6B-C7B
36	B	627	HTG	C4-C5-C6-O6
37	D	2307	DGD	C1B-C2B-C3B-C4B
27	C	520	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
27	c	521	LMG	C36-C37-C38-C39
27	C	527	LMG	O6-C5-C6-O5
26	l	101	SQD	C29-C30-C31-C32
37	C	518	DGD	C5A-C6A-C7A-C8A
28	A	420	LMT	C1-C2-C3-C4
37	c	518	DGD	CBB-CCB-CDB-CEB
27	c	501	LMG	C11-C12-C13-C14
37	C	518	DGD	C3B-C4B-C5B-C6B
38	D	2309	LHG	C32-C33-C34-C35
28	M	101	LMT	O5B-C5B-C6B-O6B
23	B	602	CLA	CBA-CGA-O2A-C1
26	l	101	SQD	C11-C10-C9-C8
23	C	513	CLA	C3A-C2A-CAA-CBA
23	C	514	CLA	C3A-C2A-CAA-CBA
28	i	103	LMT	C1-C2-C3-C4
28	M	101	LMT	C2-C1-O1'-C1'
28	T	103	LMT	C6-C7-C8-C9
37	C	517	DGD	C4A-C5A-C6A-C7A
28	A	414	LMT	C1-C2-C3-C4
26	a	2615	SQD	C23-C24-C25-C26
28	i	103	LMT	C6-C7-C8-C9
23	C	511	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
23	B	612	CLA	C2-C3-C5-C6
23	C	506	CLA	C2-C3-C5-C6
23	C	511	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
33	d	411	PL9	C13-C14-C16-C17
37	c	519	DGD	CCA-CDA-CEA-CFA
38	D	2309	LHG	C24-C25-C26-C27
29	A	417	GOL	O2-C2-C3-O3
29	O	302	GOL	O2-C2-C3-O3
29	U	502	GOL	O2-C2-C3-O3
29	b	644	GOL	O1-C1-C2-O2
29	c	530	GOL	O2-C2-C3-O3
38	d	413	LHG	O1-C1-C2-O2
26	B	621	SQD	C27-C28-C29-C30
26	a	2603	SQD	C24-C25-C26-C27
38	l	103	LHG	C13-C14-C15-C16
23	b	618	CLA	C8-C10-C11-C12
36	I	101	HTG	O5-C5-C6-O6
26	b	601	SQD	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
26	D	2302	SQD	O10-C23-O48-C46
28	B	623	LMT	C7-C8-C9-C10
37	c	518	DGD	C3B-C4B-C5B-C6B
38	D	2311	LHG	C27-C28-C29-C30
38	L	101	LHG	C13-C14-C15-C16
23	B	602	CLA	C2-C1-O2A-CGA
26	B	621	SQD	C28-C29-C30-C31
27	B	622	LMG	C30-C31-C32-C33
28	B	634	LMT	C11-C10-C9-C8
28	z	102	LMT	C6-C7-C8-C9
23	B	602	CLA	O1A-CGA-O2A-C1
38	E	101	LHG	C7-C8-C9-C10
25	B	618	BCR	C5-C6-C7-C8
25	C	516	BCR	C5-C6-C7-C8
25	D	2305	BCR	C23-C24-C25-C26
25	Y	302	BCR	C1-C6-C7-C8
25	Y	302	BCR	C5-C6-C7-C8
25	b	622	BCR	C5-C6-C7-C8
25	c	517	BCR	C1-C6-C7-C8
25	c	517	BCR	C5-C6-C7-C8
25	d	410	BCR	C23-C24-C25-C26
25	d	410	BCR	C23-C24-C25-C30
25	y	101	BCR	C1-C6-C7-C8
25	y	101	BCR	C5-C6-C7-C8
36	V	204	HTG	O5-C5-C6-O6
26	l	101	SQD	C15-C16-C17-C18
28	B	634	LMT	C9-C10-C11-C12
38	d	403	LHG	C32-C33-C34-C35
27	D	2312	LMG	C35-C36-C37-C38
28	T	103	LMT	C9-C10-C11-C12
37	D	2307	DGD	CCB-CDB-CEB-CFB
27	A	413	LMG	C35-C36-C37-C38
36	V	204	HTG	C2'-C3'-C4'-C5'
23	B	617	CLA	C4-C3-C5-C6
33	d	411	PL9	C15-C14-C16-C17
23	A	410	CLA	C12-C13-C15-C16
23	B	604	CLA	C6-C7-C8-C10
23	B	605	CLA	C6-C7-C8-C10
23	B	617	CLA	C2-C3-C5-C6
23	C	505	CLA	C11-C12-C13-C15
23	C	507	CLA	C12-C13-C15-C16
23	a	2610	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	b	621	CLA	C2-C3-C5-C6
23	c	507	CLA	C11-C12-C13-C15
23	c	511	CLA	C11-C10-C8-C7
24	a	2611	PHO	C2-C3-C5-C6
23	A	410	CLA	C3-C5-C6-C7
27	B	622	LMG	C36-C37-C38-C39
27	c	501	LMG	C36-C37-C38-C39
28	Z	101	LMT	C2-C3-C4-C5
38	L	101	LHG	C30-C31-C32-C33
23	c	508	CLA	C16-C17-C18-C20
27	c	521	LMG	C10-C11-C12-C13
23	b	611	CLA	C2A-CAA-CBA-CGA
23	a	2613	CLA	C10-C11-C12-C13
26	l	101	SQD	C28-C29-C30-C31
28	A	414	LMT	O1'-C1-C2-C3
26	D	2308	SQD	C23-C24-C25-C26
27	c	522	LMG	O6-C5-C6-O5
28	M	101	LMT	C11-C10-C9-C8
28	i	103	LMT	C2-C3-C4-C5
28	f	101	LMT	C1-C2-C3-C4
26	D	2302	SQD	C24-C25-C26-C27
36	o	301	HTG	O5-C5-C6-O6
37	D	2307	DGD	C4D-C5D-C6D-O5D
23	A	407	CLA	C16-C17-C18-C20
23	b	611	CLA	C16-C17-C18-C20
23	c	516	CLA	C16-C17-C18-C19
26	a	2603	SQD	O5-C1-O6-C44
28	B	634	LMT	O5'-C1'-O1'-C1
28	j	2701	LMT	O5'-C1'-O1'-C1
27	A	413	LMG	C37-C38-C39-C40
27	A	413	LMG	C11-C10-O7-C8
27	m	2802	LMG	C11-C10-O7-C8
38	E	101	LHG	O6-C4-C5-O7
38	d	412	LHG	C25-C26-C27-C28
38	L	101	LHG	C11-C10-C9-C8
26	D	2302	SQD	C2-C1-O6-C44
26	a	2603	SQD	C2-C1-O6-C44
28	B	634	LMT	C2'-C1'-O1'-C1
28	j	2701	LMT	O5B-C5B-C6B-O6B
37	h	102	DGD	C7A-C8A-C9A-CAA
38	D	2309	LHG	C25-C26-C27-C28
27	D	2312	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
37	c	520	DGD	CBA-CCA-CDA-CEA
38	D	2311	LHG	C25-C26-C27-C28
38	l	103	LHG	C30-C31-C32-C33
23	c	507	CLA	C4-C3-C5-C6
24	a	2611	PHO	C4-C3-C5-C6
26	b	601	SQD	C23-C24-C25-C26
37	H	103	DGD	C7A-C8A-C9A-CAA
23	B	614	CLA	C11-C12-C13-C14
23	C	506	CLA	C11-C12-C13-C14
23	b	611	CLA	C14-C13-C15-C16
23	d	409	CLA	C6-C7-C8-C9
27	A	413	LMG	C36-C37-C38-C39
26	A	412	SQD	C30-C31-C32-C33
26	l	101	SQD	C32-C33-C34-C35
37	c	520	DGD	C7B-C8B-C9B-CAB
36	B	625	HTG	O5-C5-C6-O6
28	B	623	LMT	C4B-C5B-C6B-O6B
37	C	519	DGD	C5B-C6B-C7B-C8B
23	C	513	CLA	C1A-C2A-CAA-CBA
23	C	514	CLA	C1A-C2A-CAA-CBA
23	b	616	CLA	C1A-C2A-CAA-CBA
23	c	509	CLA	C1A-C2A-CAA-CBA
23	c	511	CLA	C1A-C2A-CAA-CBA
23	C	502	CLA	C16-C17-C18-C20
23	c	508	CLA	C16-C17-C18-C19
27	A	413	LMG	O9-C10-O7-C8
27	B	622	LMG	C29-C30-C31-C32
27	m	2802	LMG	C13-C14-C15-C16
38	d	412	LHG	C26-C27-C28-C29
38	l	103	LHG	C11-C10-C9-C8
38	L	101	LHG	C4-O6-P-O3
38	D	2309	LHG	C23-C24-C25-C26
38	d	412	LHG	C29-C30-C31-C32
37	c	520	DGD	C9B-CAB-CBB-CCB
27	C	520	LMG	C32-C33-C34-C35
37	c	518	DGD	CDB-CEB-CFB-CGB
23	c	510	CLA	C5-C6-C7-C8
26	D	2302	SQD	C34-C35-C36-C37
37	C	517	DGD	O6E-C5E-C6E-O5E
38	L	101	LHG	C12-C13-C14-C15
23	C	506	CLA	C4-C3-C5-C6
26	d	417	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
23	C	509	CLA	C5-C6-C7-C8
26	l	101	SQD	C12-C13-C14-C15
38	d	403	LHG	C28-C29-C30-C31
38	l	103	LHG	C7-C8-C9-C10
26	b	601	SQD	C11-C12-C13-C14
27	A	413	LMG	C21-C22-C23-C24
36	c	526	HTG	C2'-C3'-C4'-C5'
23	B	611	CLA	C2A-CAA-CBA-CGA
23	C	507	CLA	C16-C17-C18-C19
28	F	102	LMT	O5'-C5'-C6'-O6'
26	d	417	SQD	C44-C45-C46-O48
26	l	101	SQD	C44-C45-C46-O48
27	A	413	LMG	C7-C8-C9-O8
27	c	521	LMG	C7-C8-C9-O8
37	c	518	DGD	C9A-CAA-CBA-CCA
38	D	2309	LHG	C11-C10-C9-C8
23	A	410	CLA	C8-C10-C11-C12
37	c	519	DGD	C2G-C3G-O3G-C1D
37	c	519	DGD	C5D-C6D-O5D-C1E
27	c	501	LMG	C40-C41-C42-C43
23	c	512	CLA	C13-C15-C16-C17
28	m	2804	LMT	C3'-C4'-O1B-C1B
26	l	101	SQD	C23-C24-C25-C26
36	b	625	HTG	C4'-C5'-C6'-C7'
28	B	623	LMT	C1-C2-C3-C4
23	a	2610	CLA	C8-C10-C11-C12
29	a	2602	GOL	O1-C1-C2-O2
38	D	2310	LHG	O1-C1-C2-O2
26	B	621	SQD	C29-C30-C31-C32
27	B	622	LMG	C32-C33-C34-C35
38	E	101	LHG	C26-C27-C28-C29
23	B	615	CLA	C5-C6-C7-C8
28	m	2804	LMT	O5B-C5B-C6B-O6B
37	c	518	DGD	O6E-C5E-C6E-O5E
33	A	422	PL9	C15-C14-C16-C17
28	m	2804	LMT	C5'-C4'-O1B-C1B
23	C	507	CLA	C5-C6-C7-C8
38	E	101	LHG	C13-C14-C15-C16
26	B	621	SQD	C46-C45-O47-C7
26	l	101	SQD	C46-C45-O47-C7
27	D	2312	LMG	O6-C5-C6-O5
23	c	509	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
37	C	517	DGD	O6D-C5D-C6D-O5D
26	A	412	SQD	C11-C12-C13-C14
23	c	516	CLA	CBA-CGA-O2A-C1
23	A	407	CLA	C16-C17-C18-C19
23	b	611	CLA	C16-C17-C18-C19
26	b	601	SQD	C25-C26-C27-C28
27	B	622	LMG	C17-C18-C19-C20
27	C	520	LMG	C39-C40-C41-C42
36	b	626	HTG	C1'-C2'-C3'-C4'
28	A	420	LMT	C2'-C1'-O1'-C1
26	l	101	SQD	C27-C28-C29-C30
27	m	2802	LMG	O9-C10-O7-C8
23	c	516	CLA	C16-C17-C18-C20
26	a	2615	SQD	C30-C31-C32-C33
38	l	103	LHG	C12-C13-C14-C15
26	D	2302	SQD	C7-C8-C9-C10
36	d	407	HTG	C3'-C4'-C5'-C6'
37	D	2307	DGD	CDB-CEB-CFB-CGB
23	B	611	CLA	C12-C13-C15-C16
23	B	616	CLA	C11-C12-C13-C15
23	B	616	CLA	C12-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C15
23	A	410	CLA	C11-C12-C13-C14
23	B	605	CLA	C6-C7-C8-C9
23	C	508	CLA	C11-C10-C8-C9
23	C	510	CLA	C11-C10-C8-C9
23	b	616	CLA	C14-C13-C15-C16
23	c	508	CLA	C11-C12-C13-C14
23	c	512	CLA	C6-C7-C8-C9
37	C	517	DGD	CAA-CBA-CCA-CDA
37	C	517	DGD	C2B-C3B-C4B-C5B
38	e	101	LHG	C15-C16-C17-C18
26	B	621	SQD	C24-C23-O48-C46
25	b	624	BCR	C21-C22-C23-C24
38	e	101	LHG	C1-C2-C3-O3
37	h	102	DGD	CDA-CEA-CFA-CGA
23	a	2613	CLA	CBA-CGA-O2A-C1
28	d	401	LMT	C9-C10-C11-C12
36	d	407	HTG	C4'-C5'-C6'-C7'
37	H	103	DGD	CDA-CEA-CFA-CGA
37	c	519	DGD	C8A-C9A-CAA-CBA
38	D	2309	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
38	E	101	LHG	O6-C4-C5-C6
38	e	101	LHG	O6-C4-C5-C6
38	L	101	LHG	C7-C8-C9-C10
27	m	2802	LMG	C31-C32-C33-C34
37	C	518	DGD	C9A-CAA-CBA-CCA
37	C	519	DGD	C6A-C7A-C8A-C9A
38	D	2309	LHG	C9-C10-C11-C12
33	A	422	PL9	C13-C14-C16-C17
37	c	519	DGD	C6A-C7A-C8A-C9A
37	c	519	DGD	C5B-C6B-C7B-C8B
23	c	516	CLA	O1D-CGD-O2D-CED
26	A	412	SQD	C33-C34-C35-C36
37	C	518	DGD	C6A-C7A-C8A-C9A
37	c	519	DGD	CBB-CCB-CDB-CEB
23	B	607	CLA	C10-C11-C12-C13
23	C	512	CLA	CBA-CGA-O2A-C1
37	c	520	DGD	C2A-C1A-O1G-C1G
23	B	610	CLA	C3A-C2A-CAA-CBA
23	C	507	CLA	C3A-C2A-CAA-CBA
28	i	103	LMT	C2-C1-O1'-C1'
37	D	2307	DGD	C4A-C5A-C6A-C7A
38	D	2309	LHG	C17-C18-C19-C20
23	C	513	CLA	C10-C11-C12-C13
27	C	520	LMG	C37-C38-C39-C40
36	d	415	HTG	S1-C1'-C2'-C3'
26	B	621	SQD	C44-C45-C46-O48
26	a	2603	SQD	O6-C44-C45-C46
27	c	501	LMG	C7-C8-C9-O8
23	d	402	CLA	C2C-C3C-CAC-CBC
28	B	623	LMT	C3'-C4'-O1B-C1B
28	M	101	LMT	C1-C2-C3-C4
23	c	516	CLA	O1A-CGA-O2A-C1
23	B	617	CLA	C3-C5-C6-C7
29	B	632	GOL	O1-C1-C2-O2
38	d	412	LHG	O1-C1-C2-O2
36	B	626	HTG	C2'-C3'-C4'-C5'
37	h	102	DGD	C6B-C7B-C8B-C9B
27	d	414	LMG	C36-C37-C38-C39
28	F	102	LMT	O1'-C1-C2-C3
28	d	404	LMT	C6-C7-C8-C9
23	C	512	CLA	O1A-CGA-O2A-C1
38	e	101	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
37	H	103	DGD	C7B-C8B-C9B-CAB
37	C	517	DGD	C4D-C5D-C6D-O5D
26	d	417	SQD	O47-C45-C46-O48
37	C	518	DGD	CDB-CEB-CFB-CGB
28	Z	101	LMT	O1'-C1-C2-C3
37	H	103	DGD	C6B-C7B-C8B-C9B
37	c	518	DGD	C6B-C7B-C8B-C9B
23	B	614	CLA	C13-C15-C16-C17
23	b	615	CLA	C5-C6-C7-C8
33	D	2306	PL9	C39-C41-C42-C43
33	d	411	PL9	C39-C41-C42-C43
26	B	621	SQD	C11-C10-C9-C8
26	d	417	SQD	C26-C27-C28-C29
27	m	2802	LMG	C33-C34-C35-C36
23	B	615	CLA	C11-C12-C13-C14
23	B	616	CLA	C14-C13-C15-C16
23	C	505	CLA	C6-C7-C8-C9
23	c	510	CLA	C14-C13-C15-C16
37	c	518	DGD	C6A-C7A-C8A-C9A
26	A	412	SQD	C34-C35-C36-C37
26	a	2615	SQD	C32-C33-C34-C35
28	B	623	LMT	C5'-C4'-O1B-C1B
38	D	2311	LHG	C2-C3-O3-P
23	a	2613	CLA	O1A-CGA-O2A-C1
36	d	407	HTG	C4-C5-C6-O6
38	L	101	LHG	C10-C11-C12-C13
23	b	607	CLA	C2A-CAA-CBA-CGA
25	C	515	BCR	C1-C6-C7-C8
25	C	515	BCR	C5-C6-C7-C8
25	C	515	BCR	C23-C24-C25-C30
25	D	2305	BCR	C1-C6-C7-C8
25	D	2305	BCR	C5-C6-C7-C8
25	d	410	BCR	C1-C6-C7-C8
23	B	615	CLA	C8-C10-C11-C12
27	m	2802	LMG	C20-C21-C22-C23
37	h	102	DGD	O2G-C1B-C2B-C3B
26	d	417	SQD	C30-C31-C32-C33
25	C	515	BCR	C21-C22-C23-C24
38	D	2310	LHG	C34-C35-C36-C37
28	m	2804	LMT	C6-C7-C8-C9
27	c	522	LMG	C37-C38-C39-C40
28	f	101	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
37	C	517	DGD	C2A-C3A-C4A-C5A
36	B	627	HTG	O5-C5-C6-O6
38	e	101	LHG	O2-C2-C3-O3
23	A	407	CLA	C11-C10-C8-C7
23	A	410	CLA	C6-C7-C8-C10
23	B	615	CLA	C11-C12-C13-C15
23	C	505	CLA	C6-C7-C8-C10
23	C	508	CLA	C11-C10-C8-C7
23	C	509	CLA	C11-C10-C8-C7
23	b	616	CLA	C12-C13-C15-C16
23	b	621	CLA	C11-C10-C8-C7
23	c	508	CLA	C11-C12-C13-C15
23	c	508	CLA	C12-C13-C15-C16
26	B	621	SQD	O10-C23-O48-C46
23	b	621	CLA	CBA-CGA-O2A-C1
37	D	2307	DGD	C6A-C7A-C8A-C9A
26	d	417	SQD	C34-C35-C36-C37
36	C	522	HTG	O5-C1-S1-C1'
36	b	626	HTG	C2'-C1'-S1-C1
36	B	624[B]	HTG	C1'-C2'-C3'-C4'
23	c	513	CLA	CBA-CGA-O2A-C1
26	D	2308	SQD	C33-C34-C35-C36
23	B	603	CLA	C13-C15-C16-C17
23	b	613	CLA	C13-C15-C16-C17
26	l	101	SQD	C34-C35-C36-C37
28	d	401	LMT	C11-C10-C9-C8
23	B	611	CLA	CAD-CBD-CGD-O2D
23	B	617	CLA	CAD-CBD-CGD-O2D
23	C	511	CLA	CAD-CBD-CGD-O2D
23	b	621	CLA	CAD-CBD-CGD-O2D
23	c	504	CLA	CAD-CBD-CGD-O2D
23	c	509	CLA	CAD-CBD-CGD-O2D
23	c	515	CLA	CAD-CBD-CGD-O2D
24	A	408	PHO	CAD-CBD-CGD-O2D
26	D	2308	SQD	C46-C45-O47-C7
26	B	621	SQD	C31-C32-C33-C34
38	d	412	LHG	C15-C16-C17-C18
37	D	2307	DGD	C7A-C8A-C9A-CAA
37	h	102	DGD	C7B-C8B-C9B-CAB
26	b	601	SQD	C28-C29-C30-C31
23	a	2613	CLA	C2-C3-C5-C6
24	A	408	PHO	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
26	D	2302	SQD	O6-C44-C45-C46
37	H	103	DGD	O1G-C1G-C2G-C3G
37	h	102	DGD	O1G-C1G-C2G-C3G
38	d	403	LHG	C2-C3-O3-P
37	C	517	DGD	C6B-C7B-C8B-C9B
38	e	101	LHG	O6-C4-C5-O7
38	l	103	LHG	C11-C12-C13-C14
36	c	526	HTG	S1-C1'-C2'-C3'
38	D	2309	LHG	C33-C34-C35-C36
37	c	518	DGD	C5B-C6B-C7B-C8B
23	B	602	CLA	CHA-CBD-CGD-O1D
23	B	602	CLA	CHA-CBD-CGD-O2D
23	B	603	CLA	CHA-CBD-CGD-O2D
23	B	615	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O2D
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	C	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	b	606	CLA	CHA-CBD-CGD-O1D
23	b	606	CLA	CHA-CBD-CGD-O2D
23	c	505	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	CHA-CBD-CGD-O1D
23	c	511	CLA	CHA-CBD-CGD-O1D
23	c	511	CLA	CHA-CBD-CGD-O2D
26	B	621	SQD	O47-C45-C46-O48
26	D	2302	SQD	O6-C44-C45-O47
26	D	2308	SQD	O47-C45-C46-O48
27	C	527	LMG	O7-C8-C9-O8
37	D	2307	DGD	O1G-C1G-C2G-O2G
26	a	2615	SQD	C26-C27-C28-C29
37	H	103	DGD	O2G-C1B-C2B-C3B
37	h	102	DGD	C8A-C9A-CAA-CBA
29	A	415	GOL	O1-C1-C2-O2
29	C	526	GOL	O1-C1-C2-O2
29	O	305	GOL	O2-C2-C3-O3
29	a	2602	GOL	O2-C2-C3-O3
29	a	2618	GOL	O1-C1-C2-O2
29	v	203	GOL	O2-C2-C3-O3
36	B	624[B]	HTG	C2'-C3'-C4'-C5'
23	a	2613	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	d	404	LMT	O1'-C1-C2-C3
23	c	513	CLA	O1A-CGA-O2A-C1
37	c	520	DGD	O1A-C1A-O1G-C1G
28	z	102	LMT	C2B-C1B-O1B-C4'
38	d	412	LHG	C13-C14-C15-C16
23	b	621	CLA	C11-C10-C8-C9
23	c	508	CLA	C14-C13-C15-C16
27	A	413	LMG	C12-C13-C14-C15
23	b	621	CLA	O1A-CGA-O2A-C1
38	l	103	LHG	C10-C11-C12-C13
26	D	2308	SQD	C5-C6-S-O8
26	l	101	SQD	C5-C6-S-O8
23	A	406	CLA	C2C-C3C-CAC-CBC
38	D	2309	LHG	O1-C1-C2-C3
36	C	521	HTG	S1-C1'-C2'-C3'
36	b	604	HTG	O5-C5-C6-O6
27	C	520	LMG	C11-C12-C13-C14
23	B	605	CLA	C1A-C2A-CAA-CBA
27	A	413	LMG	C22-C23-C24-C25
23	B	611	CLA	C2-C1-O2A-CGA
38	L	101	LHG	C11-C12-C13-C14
40	H	102	RRX	C9-C10-C11-C12
40	h	101	RRX	C9-C10-C11-C12
38	e	101	LHG	C4-O6-P-O3
37	h	102	DGD	C5B-C6B-C7B-C8B
27	D	2312	LMG	C12-C13-C14-C15
27	C	527	LMG	C31-C32-C33-C34
27	d	414	LMG	C30-C31-C32-C33
38	D	2309	LHG	C26-C27-C28-C29
38	E	101	LHG	C4-O6-P-O4
38	L	101	LHG	C4-O6-P-O5
38	l	103	LHG	C4-O6-P-O5
26	b	601	SQD	O5-C1-O6-C44
27	A	413	LMG	C29-C28-O8-C9
28	z	102	LMT	C4-C5-C6-C7
37	H	103	DGD	C5B-C6B-C7B-C8B
38	d	412	LHG	C30-C31-C32-C33
26	a	2603	SQD	C32-C33-C34-C35
38	e	101	LHG	C13-C14-C15-C16
37	H	103	DGD	C8A-C9A-CAA-CBA
23	B	602	CLA	CAD-CBD-CGD-O1D
23	B	606	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	B	615	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CAD-CBD-CGD-O1D
23	b	606	CLA	CAD-CBD-CGD-O1D
23	b	610	CLA	CAD-CBD-CGD-O1D
23	c	505	CLA	CAD-CBD-CGD-O1D
26	D	2308	SQD	C5-C6-S-O9
26	a	2603	SQD	O5-C5-C6-S
26	l	101	SQD	C5-C6-S-O9
37	C	519	DGD	C8A-C9A-CAA-CBA
26	B	621	SQD	C23-C24-C25-C26
26	a	2603	SQD	C35-C36-C37-C38
26	D	2302	SQD	C9-C10-C11-C12
26	l	101	SQD	C17-C18-C19-C20
23	A	410	CLA	C11-C10-C8-C7
23	B	604	CLA	C11-C10-C8-C7
23	C	507	CLA	C11-C12-C13-C15
23	C	514	CLA	C12-C13-C15-C16
23	a	2610	CLA	C11-C10-C8-C7
23	a	2610	CLA	C12-C13-C15-C16
23	c	510	CLA	C11-C10-C8-C7
23	c	515	CLA	C12-C13-C15-C16
36	C	522	HTG	C2-C1-S1-C1'
36	c	523	HTG	C2-C1-S1-C1'
26	d	417	SQD	C32-C33-C34-C35
37	c	519	DGD	C6B-C7B-C8B-C9B
27	d	414	LMG	C29-C30-C31-C32
37	c	518	DGD	O6D-C5D-C6D-O5D
23	b	606	CLA	CAA-CBA-CGA-O2A
38	D	2310	LHG	C32-C33-C34-C35
38	e	101	LHG	C19-C20-C21-C22
26	D	2308	SQD	C44-C45-C46-O48
26	b	601	SQD	C2-C1-O6-C44
37	D	2307	DGD	O1G-C1G-C2G-C3G
26	A	412	SQD	O6-C44-C45-O47
27	A	413	LMG	O7-C8-C9-O8
27	c	521	LMG	O7-C8-C9-O8
37	H	103	DGD	O1G-C1G-C2G-O2G
27	c	521	LMG	C19-C20-C21-C22
23	a	2609	CLA	C2C-C3C-CAC-CBC
27	A	413	LMG	O10-C28-O8-C9
27	c	521	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
27	d	414	LMG	C12-C13-C14-C15
27	c	522	LMG	C8-C7-O1-C1
37	C	518	DGD	C2G-C3G-O3G-C1D
37	C	518	DGD	C5D-C6D-O5D-C1E
38	e	101	LHG	C9-C10-C11-C12
27	C	520	LMG	C33-C34-C35-C36
23	C	505	CLA	C15-C16-C17-C18
23	b	615	CLA	C8-C10-C11-C12
37	D	2307	DGD	C9A-CAA-CBA-CCA
23	A	407	CLA	C11-C10-C8-C9
23	C	507	CLA	C11-C12-C13-C14
23	C	509	CLA	C11-C10-C8-C9
38	D	2311	LHG	O10-C23-O8-C6
26	a	2603	SQD	C33-C34-C35-C36
23	b	617	CLA	C8-C10-C11-C12
27	c	522	LMG	C10-C11-C12-C13
28	T	103	LMT	C11-C10-C9-C8
26	B	621	SQD	C26-C27-C28-C29
28	J	303	LMT	C7-C8-C9-C10
37	C	518	DGD	C5B-C6B-C7B-C8B
37	H	103	DGD	C9B-CAB-CBB-CCB
23	a	2610	CLA	C16-C17-C18-C20
26	B	621	SQD	C12-C13-C14-C15
36	b	602	HTG	C2'-C3'-C4'-C5'
37	c	519	DGD	C2A-C3A-C4A-C5A
23	c	506	CLA	C15-C16-C17-C18
37	c	518	DGD	C4D-C5D-C6D-O5D
23	b	615	CLA	C2A-CAA-CBA-CGA
23	C	510	CLA	C2-C1-O2A-CGA
23	b	619	CLA	C2-C1-O2A-CGA
23	c	510	CLA	C2-C1-O2A-CGA
28	M	101	LMT	C7-C8-C9-C10
37	c	520	DGD	C2A-C3A-C4A-C5A
28	m	2803	LMT	O5'-C5'-C6'-O6'
36	I	101	HTG	C1'-C2'-C3'-C4'
38	L	101	LHG	C14-C15-C16-C17
23	C	507	CLA	O1A-CGA-O2A-C1
26	l	101	SQD	C13-C14-C15-C16
28	A	420	LMT	C5-C6-C7-C8
23	c	506	CLA	C10-C11-C12-C13
25	C	515	BCR	C23-C24-C25-C26
25	a	2614	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	d	410	BCR	C5-C6-C7-C8
37	C	517	DGD	C7A-C8A-C9A-CAA
36	o	301	HTG	C2'-C3'-C4'-C5'
37	C	519	DGD	C6B-C7B-C8B-C9B
36	H	101	HTG	C2'-C3'-C4'-C5'
37	C	519	DGD	C2A-C3A-C4A-C5A
38	e	101	LHG	C11-C10-C9-C8
33	A	422	PL9	C12-C11-C9-C10
27	C	520	LMG	C11-C10-O7-C8
28	m	2804	LMT	O5'-C1'-O1'-C1
37	C	517	DGD	O6E-C1E-O5D-C6D
37	C	518	DGD	O6E-C1E-O5D-C6D
37	c	519	DGD	O6E-C1E-O5D-C6D
27	B	622	LMG	C28-C29-C30-C31
23	c	510	CLA	C2A-CAA-CBA-CGA
37	c	519	DGD	C2E-C1E-O5D-C6D
36	B	624[B]	HTG	S1-C1'-C2'-C3'
26	l	101	SQD	O47-C45-C46-O48
27	c	501	LMG	O7-C8-C9-O8
37	h	102	DGD	O1G-C1G-C2G-O2G
27	B	622	LMG	C16-C17-C18-C19
27	m	2802	LMG	C19-C20-C21-C22
38	D	2310	LHG	C3-O3-P-O6
38	d	413	LHG	C3-O3-P-O6
27	C	527	LMG	C28-C29-C30-C31
23	a	2609	CLA	C16-C17-C18-C20
28	m	2804	LMT	C2B-C1B-O1B-C4'
26	A	412	SQD	O6-C44-C45-C46
27	C	527	LMG	C7-C8-C9-O8
37	C	519	DGD	O1G-C1G-C2G-C3G
28	m	2804	LMT	C5-C6-C7-C8
37	C	517	DGD	CBA-CCA-CDA-CEA
23	c	513	CLA	C2-C3-C5-C6
24	A	408	PHO	C2-C3-C5-C6
23	A	410	CLA	C11-C10-C8-C9
23	B	617	CLA	C14-C13-C15-C16
23	b	618	CLA	C11-C12-C13-C14
23	c	510	CLA	C11-C10-C8-C9
27	B	622	LMG	O6-C5-C6-O5
23	c	507	CLA	C16-C17-C18-C20
38	d	403	LHG	O1-C1-C2-C3
38	E	101	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
38	E	101	LHG	C19-C20-C21-C22
27	C	520	LMG	O9-C10-O7-C8
24	A	408	PHO	C4-C3-C5-C6
29	D	2301	GOL	O1-C1-C2-O2
29	c	531	GOL	O2-C2-C3-O3
29	d	416	GOL	O2-C2-C3-O3
23	B	602	CLA	C2-C3-C5-C6
38	D	2311	LHG	C24-C23-O8-C6
23	B	609	CLA	C13-C15-C16-C17
28	M	102	LMT	O5'-C5'-C6'-O6'
28	z	102	LMT	O5B-C1B-O1B-C4'
27	C	527	LMG	C39-C40-C41-C42
37	C	517	DGD	CAB-CBB-CCB-CDB
37	C	519	DGD	C4B-C5B-C6B-C7B
23	a	2610	CLA	C16-C17-C18-C19
37	c	518	DGD	O6E-C1E-O5D-C6D
23	b	619	CLA	C10-C11-C12-C13
23	b	615	CLA	C16-C17-C18-C19
23	B	602	CLA	C4-C3-C5-C6
23	c	513	CLA	C4-C3-C5-C6
27	c	521	LMG	C30-C31-C32-C33
38	D	2311	LHG	C31-C32-C33-C34
36	i	102	HTG	C1'-C2'-C3'-C4'
37	h	102	DGD	C9B-CAB-CBB-CCB
23	b	621	CLA	C15-C16-C17-C18
23	b	618	CLA	C2-C1-O2A-CGA
23	d	408	CLA	C2-C1-O2A-CGA
28	B	623	LMT	C6-C7-C8-C9
28	m	2804	LMT	O5'-C5'-C6'-O6'
37	C	517	DGD	C2E-C1E-O5D-C6D
37	C	518	DGD	C2E-C1E-O5D-C6D
27	C	527	LMG	C11-C12-C13-C14
23	c	504	CLA	C2A-CAA-CBA-CGA
37	c	519	DGD	C9B-CAB-CBB-CCB
36	B	624[A]	HTG	C2'-C3'-C4'-C5'
38	d	412	LHG	C11-C10-C9-C8
28	A	414	LMT	C2B-C1B-O1B-C4'
23	b	614	CLA	C3A-C2A-CAA-CBA
23	a	2609	CLA	C4C-C3C-CAC-CBC
38	d	413	LHG	C34-C35-C36-C37
26	A	412	SQD	C11-C10-C9-C8
38	d	413	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
38	l	103	LHG	C14-C15-C16-C17
26	b	601	SQD	C16-C17-C18-C19
27	A	413	LMG	C20-C21-C22-C23
23	B	612	CLA	C4-C3-C5-C6
33	x	1301	PL9	C40-C39-C41-C42
23	b	611	CLA	C11-C10-C8-C9
23	b	621	CLA	C6-C7-C8-C9
26	D	2308	SQD	C25-C26-C27-C28
39	F	101	HEM	CAD-CBD-CGD-O1D
37	D	2307	DGD	C2B-C3B-C4B-C5B
23	b	615	CLA	C16-C17-C18-C20
38	d	413	LHG	O2-C2-C3-O3
28	M	102	LMT	O5'-C1'-O1'-C1
28	m	2803	LMT	O5'-C1'-O1'-C1
38	d	413	LHG	C32-C33-C34-C35
38	e	101	LHG	C26-C27-C28-C29
28	A	420	LMT	C3-C4-C5-C6
28	A	414	LMT	O5B-C1B-O1B-C4'
26	D	2308	SQD	C28-C29-C30-C31
23	C	513	CLA	O1A-CGA-O2A-C1
23	c	509	CLA	C5-C6-C7-C8
23	B	614	CLA	C11-C12-C13-C15
23	b	620	CLA	C12-C13-C15-C16
23	c	509	CLA	C12-C13-C15-C16
23	c	514	CLA	C11-C12-C13-C15
37	C	519	DGD	C8B-C9B-CAB-CBB
27	c	501	LMG	C21-C22-C23-C24
23	B	606	CLA	O1A-CGA-O2A-C1
27	A	413	LMG	C11-C12-C13-C14
37	C	519	DGD	C1A-C2A-C3A-C4A
26	D	2308	SQD	C31-C32-C33-C34
26	D	2308	SQD	C34-C35-C36-C37
26	a	2603	SQD	C13-C14-C15-C16
23	B	608	CLA	C16-C17-C18-C19
27	c	521	LMG	C14-C15-C16-C17
28	B	623	LMT	C3-C4-C5-C6
23	C	503	CLA	C16-C17-C18-C20
27	C	527	LMG	C30-C31-C32-C33
23	B	615	CLA	C15-C16-C17-C18
23	C	504	CLA	C10-C11-C12-C13
38	d	413	LHG	C1-C2-C3-O3
33	A	422	PL9	C35-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
33	x	1301	PL9	C25-C24-C26-C27
33	x	1301	PL9	C38-C39-C41-C42
27	C	520	LMG	O10-C28-O8-C9
39	F	101	HEM	CAA-CBA-CGA-O2A
39	e	103	HEM	CAA-CBA-CGA-O2A
36	i	102	HTG	C2'-C3'-C4'-C5'
27	c	501	LMG	O8-C28-C29-C30
23	A	410	CLA	C6-C7-C8-C9
36	I	101	HTG	C4'-C5'-C6'-C7'
28	d	401	LMT	C1-C2-C3-C4
37	C	518	DGD	CBA-CCA-CDA-CEA
37	H	103	DGD	CDB-CEB-CFB-CGB
23	b	609	CLA	C13-C15-C16-C17
23	C	506	CLA	C16-C17-C18-C19
25	C	516	BCR	C23-C24-C25-C30
25	Y	302	BCR	C23-C24-C25-C30
25	b	623	BCR	C23-C24-C25-C30
25	b	624	BCR	C23-C24-C25-C30
25	y	101	BCR	C23-C24-C25-C30
40	h	101	RRX	C23-C24-C25-C30
23	C	509	CLA	C10-C11-C12-C13
23	B	602	CLA	CAA-CBA-CGA-O2A
27	d	414	LMG	C37-C38-C39-C40
29	v	204	GOL	O1-C1-C2-C3
27	d	414	LMG	C35-C36-C37-C38
25	a	2614	BCR	C19-C20-C21-C22
23	C	507	CLA	CBA-CGA-O2A-C1
37	D	2307	DGD	C5D-C6D-O5D-C1E
23	c	516	CLA	C2-C3-C5-C6
26	l	101	SQD	C9-C10-C11-C12
23	c	511	CLA	C15-C16-C17-C18
26	a	2603	SQD	C45-C44-O6-C1
37	c	518	DGD	C5D-C6D-O5D-C1E
28	T	103	LMT	C4-C5-C6-C7
37	D	2307	DGD	C6B-C7B-C8B-C9B
37	D	2307	DGD	O2G-C1B-C2B-C3B
26	D	2302	SQD	C16-C17-C18-C19
28	B	634	LMT	C6-C7-C8-C9
23	d	402	CLA	C4C-C3C-CAC-CBC
28	B	634	LMT	C4-C5-C6-C7
27	m	2802	LMG	C18-C19-C20-C21
37	h	102	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
23	c	507	CLA	C2-C3-C5-C6
23	c	509	CLA	C11-C12-C13-C15
27	C	520	LMG	C29-C28-O8-C9
23	B	612	CLA	C15-C16-C17-C18
37	D	2307	DGD	C5A-C6A-C7A-C8A
29	O	304	GOL	O1-C1-C2-O2
23	C	510	CLA	C15-C16-C17-C18
37	C	519	DGD	O1G-C1A-C2A-C3A
39	e	103	HEM	CAD-CBD-CGD-O1D
27	A	413	LMG	O1-C7-C8-O7
26	b	601	SQD	O49-C7-O47-C45
28	M	101	LMT	C5-C6-C7-C8
27	D	2312	LMG	C30-C31-C32-C33
38	D	2311	LHG	C30-C31-C32-C33
39	e	103	HEM	CAA-CBA-CGA-O1A
26	a	2615	SQD	C28-C29-C30-C31
27	C	527	LMG	C35-C36-C37-C38
23	B	605	CLA	C13-C15-C16-C17
26	d	417	SQD	C5-C6-S-O7
36	B	624[B]	HTG	C2'-C1'-S1-C1
36	c	523	HTG	O5-C1-S1-C1'
23	B	614	CLA	C15-C16-C17-C18
23	B	608	CLA	C16-C17-C18-C20
24	a	2611	PHO	C8-C10-C11-C12
37	C	517	DGD	O2G-C1B-C2B-C3B
23	B	604	CLA	C11-C10-C8-C9
23	C	514	CLA	C14-C13-C15-C16
23	a	2610	CLA	C11-C10-C8-C9
23	a	2610	CLA	C14-C13-C15-C16
23	b	614	CLA	C11-C10-C8-C9
23	b	620	CLA	C14-C13-C15-C16
23	c	515	CLA	C14-C13-C15-C16
27	D	2312	LMG	C17-C18-C19-C20
38	D	2309	LHG	C30-C31-C32-C33
23	c	508	CLA	C3A-C2A-CAA-CBA
28	J	303	LMT	C4'-C5'-C6'-O6'
39	F	101	HEM	CAD-CBD-CGD-O2D
42	V	201	HEC	CAD-CBD-CGD-O2D
23	B	605	CLA	CAD-CBD-CGD-O2D
23	B	613	CLA	CAD-CBD-CGD-O2D
23	C	502	CLA	CAD-CBD-CGD-O2D
23	C	506	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	b	608	CLA	CAD-CBD-CGD-O2D
23	b	609	CLA	CAD-CBD-CGD-O2D
23	c	512	CLA	CAD-CBD-CGD-O2D
23	c	513	CLA	CAD-CBD-CGD-O2D
24	A	409	PHO	CAD-CBD-CGD-O2D
23	A	405	CLA	C2C-C3C-CAC-CBC
26	b	601	SQD	C14-C15-C16-C17
23	C	508	CLA	C2A-CAA-CBA-CGA
23	c	509	CLA	C13-C15-C16-C17
23	D	2303	CLA	C2-C1-O2A-CGA
42	v	201	HEC	CAD-CBD-CGD-O2D
27	d	414	LMG	C13-C14-C15-C16
36	b	626	HTG	C3'-C4'-C5'-C6'
33	A	422	PL9	C40-C39-C41-C42
33	x	1301	PL9	C15-C14-C16-C17
36	o	301	HTG	S1-C1'-C2'-C3'
38	d	413	LHG	C31-C32-C33-C34
26	b	601	SQD	C15-C16-C17-C18
24	A	409	PHO	C2C-C3C-CAC-CBC
24	a	2612	PHO	C2C-C3C-CAC-CBC
23	A	407	CLA	C13-C15-C16-C17
37	C	518	DGD	O2G-C1B-C2B-C3B
28	M	102	LMT	C4B-C5B-C6B-O6B
42	v	201	HEC	CAD-CBD-CGD-O1D
23	B	614	CLA	O2A-C1-C2-C3
23	C	510	CLA	O2A-C1-C2-C3
23	C	514	CLA	O2A-C1-C2-C3
23	c	515	CLA	O2A-C1-C2-C3
23	C	502	CLA	C2A-CAA-CBA-CGA
38	d	412	LHG	O8-C23-C24-C25
28	T	103	LMT	C1-C2-C3-C4
23	A	406	CLA	CHA-CBD-CGD-O1D
23	A	406	CLA	CHA-CBD-CGD-O2D
23	B	606	CLA	CHA-CBD-CGD-O1D
23	C	510	CLA	CHA-CBD-CGD-O1D
23	b	607	CLA	CHA-CBD-CGD-O2D
23	c	505	CLA	CHA-CBD-CGD-O1D
23	c	506	CLA	CHA-CBD-CGD-O2D
23	d	402	CLA	CHA-CBD-CGD-O1D
23	d	402	CLA	CHA-CBD-CGD-O2D
42	V	201	HEC	CAD-CBD-CGD-O1D
28	i	103	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
23	D	2304	CLA	C16-C17-C18-C19
37	D	2307	DGD	C8B-C9B-CAB-CBB
26	a	2615	SQD	O6-C44-C45-O47
27	c	522	LMG	O7-C8-C9-O8
38	E	101	LHG	O7-C5-C6-O8
23	A	405	CLA	C4C-C3C-CAC-CBC
27	c	521	LMG	O7-C10-C11-C12
39	e	103	HEM	CAD-CBD-CGD-O2D
24	A	409	PHO	CHA-CBD-CGD-O1D
24	A	409	PHO	CHA-CBD-CGD-O2D
29	c	530	GOL	O1-C1-C2-O2
26	B	621	SQD	C30-C31-C32-C33
28	m	2804	LMT	C2-C3-C4-C5
36	B	627	HTG	C4'-C5'-C6'-C7'
38	L	101	LHG	C16-C17-C18-C19
23	c	513	CLA	CAA-CBA-CGA-O2A
23	C	508	CLA	C12-C13-C15-C16
33	x	1301	PL9	C13-C14-C16-C17
23	C	511	CLA	CAA-CBA-CGA-O2A
23	B	613	CLA	C3-C5-C6-C7
23	C	508	CLA	C14-C13-C15-C16
23	c	512	CLA	C14-C13-C15-C16
23	B	613	CLA	C8-C10-C11-C12
27	B	622	LMG	O8-C28-C29-C30
37	c	518	DGD	O2G-C1B-C2B-C3B
26	a	2615	SQD	C5-C6-S-O8
33	A	422	PL9	C12-C11-C9-C8
23	c	505	CLA	C16-C17-C18-C20
26	b	601	SQD	C8-C7-O47-C45
28	B	623	LMT	C5-C6-C7-C8
28	A	420	LMT	C11-C10-C9-C8
23	b	606	CLA	CBA-CGA-O2A-C1
37	C	519	DGD	O1A-C1A-C2A-C3A
23	a	2613	CLA	C16-C17-C18-C19
37	c	520	DGD	CAB-CBB-CCB-CDB
29	B	632	GOL	C1-C2-C3-O3
29	O	305	GOL	C1-C2-C3-O3
29	a	2602	GOL	C1-C2-C3-O3
29	u	501	GOL	C1-C2-C3-O3
23	B	613	CLA	CAA-CBA-CGA-O2A
23	C	513	CLA	CAA-CBA-CGA-O2A
26	d	417	SQD	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
23	B	610	CLA	C1A-C2A-CAA-CBA
26	l	101	SQD	C11-C12-C13-C14
39	F	101	HEM	CAA-CBA-CGA-O1A
27	c	501	LMG	C30-C31-C32-C33
23	B	606	CLA	CBA-CGA-O2A-C1
23	C	513	CLA	CBA-CGA-O2A-C1
37	C	517	DGD	O1B-C1B-C2B-C3B
28	B	623	LMT	C2B-C1B-O1B-C4'
27	A	413	LMG	O1-C7-C8-C9
27	c	521	LMG	O1-C7-C8-C9
37	C	519	DGD	O6E-C5E-C6E-O5E
23	C	508	CLA	C5-C6-C7-C8
23	b	618	CLA	CAA-CBA-CGA-O2A
23	C	513	CLA	CAA-CBA-CGA-O1A
37	c	518	DGD	C2E-C1E-O5D-C6D
23	d	402	CLA	C15-C16-C17-C18
26	d	417	SQD	O5-C5-C6-S
38	D	2310	LHG	C4-O6-P-O5
38	d	413	LHG	C3-O3-P-O5
28	m	2804	LMT	O5B-C1B-O1B-C4'
27	B	622	LMG	O10-C28-C29-C30
38	d	412	LHG	O10-C23-C24-C25
28	z	102	LMT	C4'-C5'-C6'-O6'
27	d	414	LMG	O7-C10-C11-C12
37	c	520	DGD	O1G-C1A-C2A-C3A
25	a	2614	BCR	C5-C6-C7-C8
25	b	624	BCR	C23-C24-C25-C26
25	y	101	BCR	C23-C24-C25-C26
27	B	622	LMG	O10-C28-O8-C9
28	d	401	LMT	O5B-C5B-C6B-O6B
38	L	101	LHG	O7-C7-C8-C9
38	l	103	LHG	O7-C7-C8-C9
38	D	2310	LHG	C16-C17-C18-C19
37	C	519	DGD	C9B-CAB-CBB-CCB
37	C	518	DGD	O1B-C1B-C2B-C3B
23	D	2304	CLA	O1A-CGA-O2A-C1
27	c	521	LMG	C12-C13-C14-C15
38	L	101	LHG	C17-C18-C19-C20
23	B	616	CLA	C5-C6-C7-C8
27	A	413	LMG	C29-C30-C31-C32
23	B	608	CLA	CAD-CBD-CGD-O1D
23	B	610	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	C	505	CLA	CAD-CBD-CGD-O1D
23	b	612	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	615	CLA	CAD-CBD-CGD-O1D
23	c	507	CLA	CAD-CBD-CGD-O1D
23	c	508	CLA	CAD-CBD-CGD-O1D
23	C	511	CLA	CAA-CBA-CGA-O1A
27	c	521	LMG	O9-C10-C11-C12
38	D	2309	LHG	C28-C29-C30-C31
23	b	617	CLA	CAA-CBA-CGA-O2A
37	c	520	DGD	O6D-C5D-C6D-O5D
23	A	407	CLA	C6-C7-C8-C9
23	B	614	CLA	C14-C13-C15-C16
23	c	509	CLA	C11-C12-C13-C14
29	A	417	GOL	O1-C1-C2-O2
27	C	527	LMG	C40-C41-C42-C43
23	C	506	CLA	CAA-CBA-CGA-O2A
23	c	508	CLA	CAA-CBA-CGA-O2A
27	c	501	LMG	C14-C15-C16-C17
37	D	2307	DGD	C9B-CAB-CBB-CCB
38	d	403	LHG	C29-C30-C31-C32
23	A	406	CLA	C15-C16-C17-C18
37	c	519	DGD	C8B-C9B-CAB-CBB
27	B	622	LMG	C33-C34-C35-C36
37	C	519	DGD	CBA-CCA-CDA-CEA
36	o	301	HTG	C1'-C2'-C3'-C4'
37	c	519	DGD	O2G-C1B-C2B-C3B
33	A	422	PL9	C16-C17-C18-C19
23	c	516	CLA	C4-C3-C5-C6
33	d	411	PL9	C30-C29-C31-C32
23	B	616	CLA	C11-C10-C8-C7
23	a	2610	CLA	C11-C12-C13-C15
33	x	1301	PL9	C23-C24-C26-C27
27	c	501	LMG	C22-C23-C24-C25
23	C	504	CLA	C15-C16-C17-C18
23	b	606	CLA	O1A-CGA-O2A-C1
28	z	102	LMT	C11-C10-C9-C8
26	A	412	SQD	C7-C8-C9-C10
25	C	515	BCR	C7-C8-C9-C10
25	c	517	BCR	C7-C8-C9-C10
23	C	506	CLA	CAA-CBA-CGA-O1A
37	c	518	DGD	O1B-C1B-C2B-C3B

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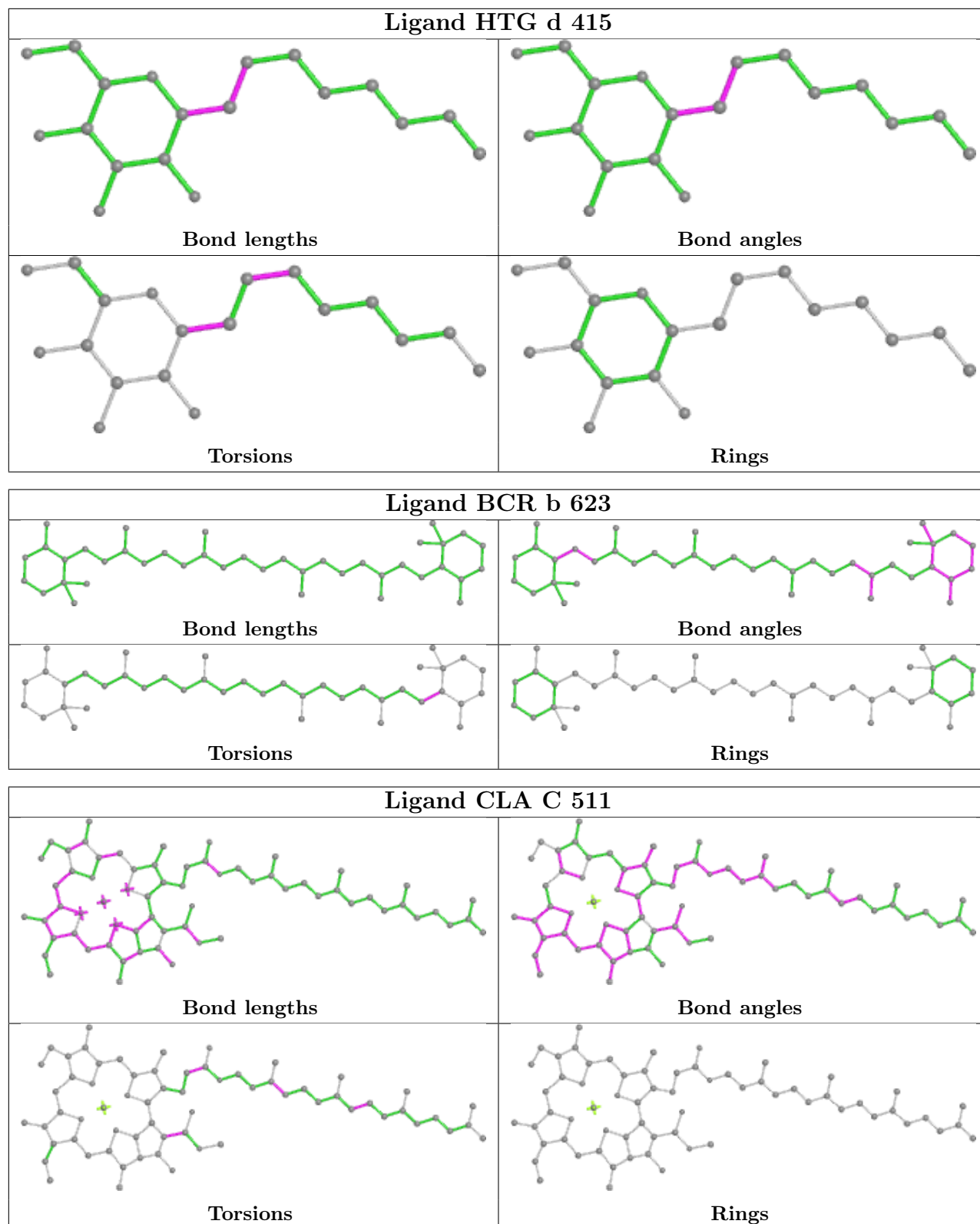
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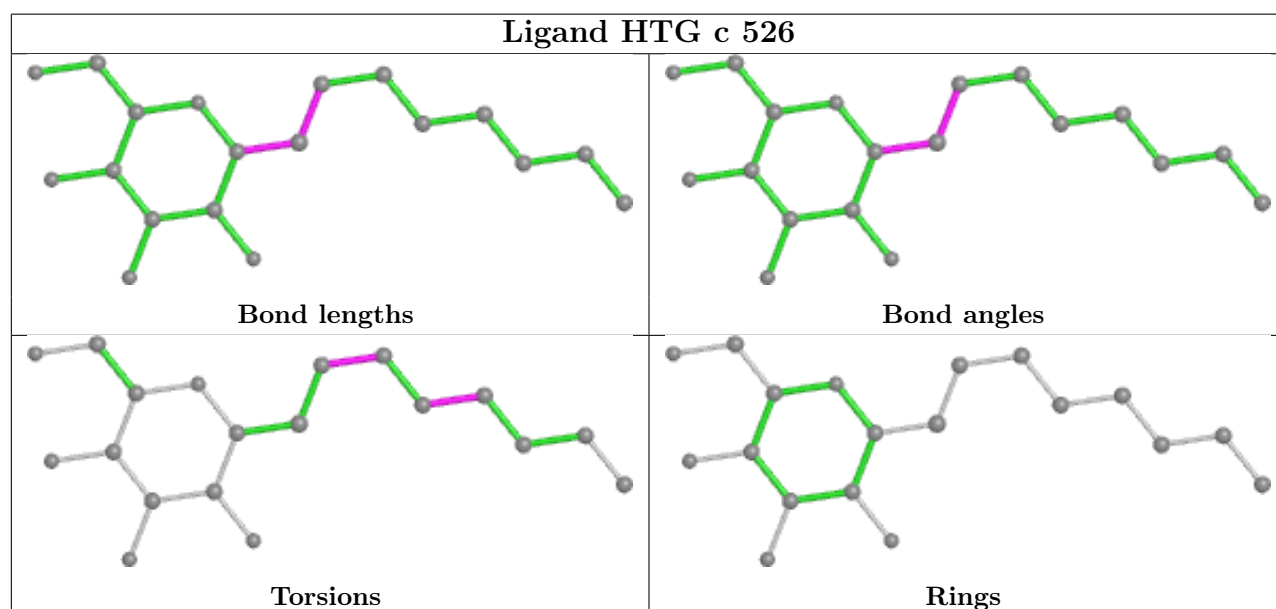
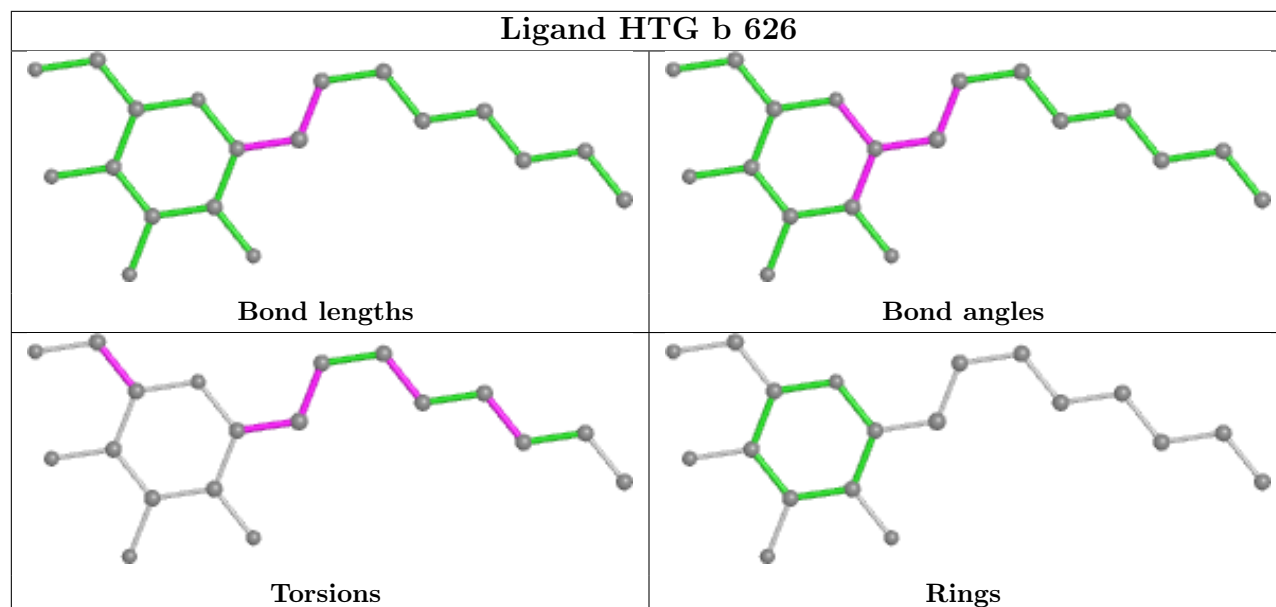
Mol	Chain	Res	Type	Atoms
37	c	519	DGD	O1B-C1B-C2B-C3B
27	C	520	LMG	C40-C41-C42-C43
28	M	102	LMT	C2-C1-O1'-C1'
28	m	2803	LMT	C2-C1-O1'-C1'
23	B	617	CLA	C13-C15-C16-C17
23	c	515	CLA	C15-C16-C17-C18
27	A	413	LMG	O8-C28-C29-C30
38	D	2311	LHG	O8-C23-C24-C25
38	d	403	LHG	O8-C23-C24-C25
26	b	601	SQD	C26-C27-C28-C29
23	b	618	CLA	CAA-CBA-CGA-O1A
23	c	513	CLA	CAA-CBA-CGA-O1A
37	c	520	DGD	O1A-C1A-C2A-C3A
27	B	622	LMG	C29-C28-O8-C9
23	B	613	CLA	CAA-CBA-CGA-O1A
26	a	2615	SQD	C31-C32-C33-C34
27	d	414	LMG	C20-C21-C22-C23
28	d	404	LMT	C3'-C4'-O1B-C1B

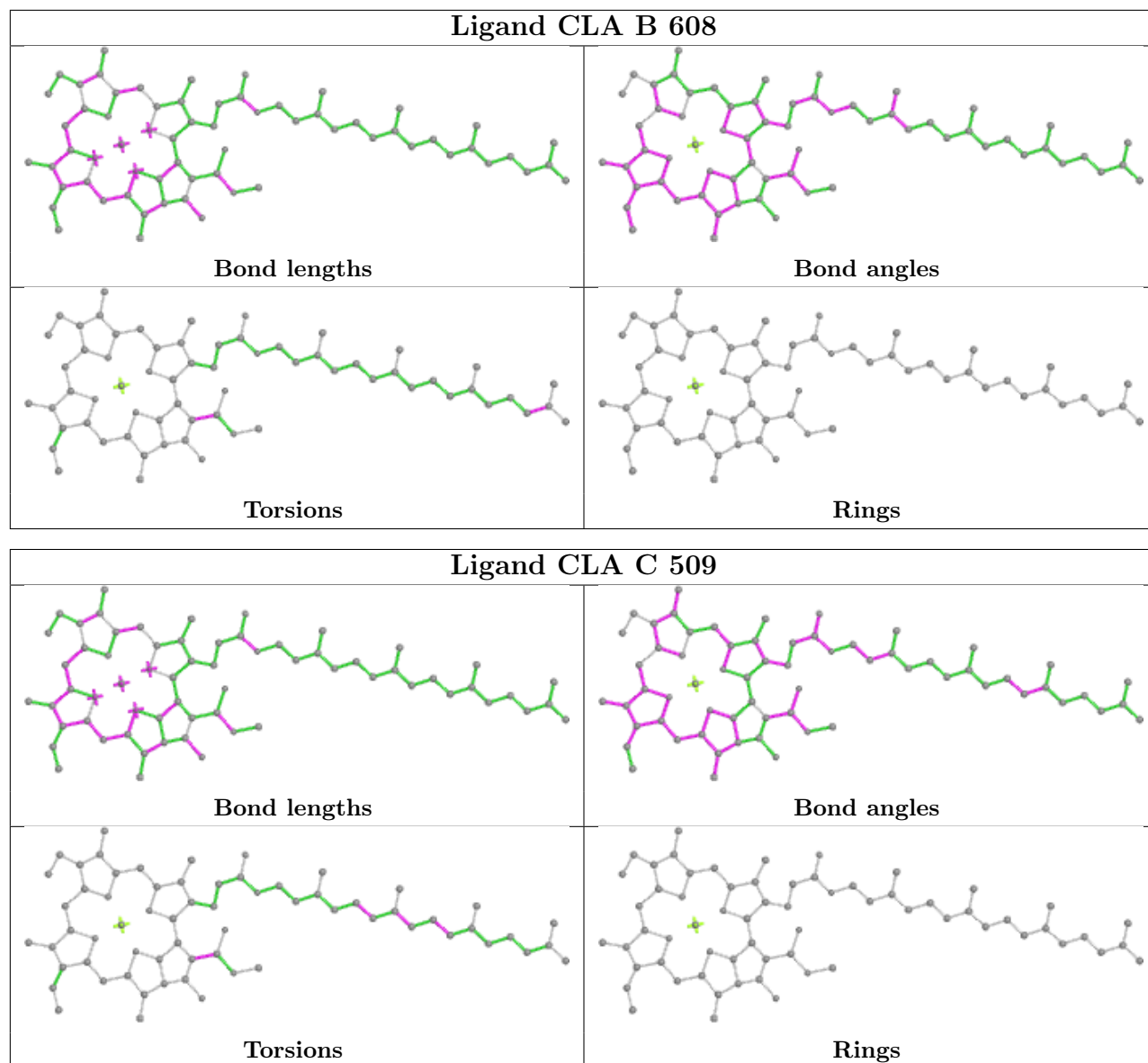
There are no ring outliers.

No monomer is involved in short contacts.

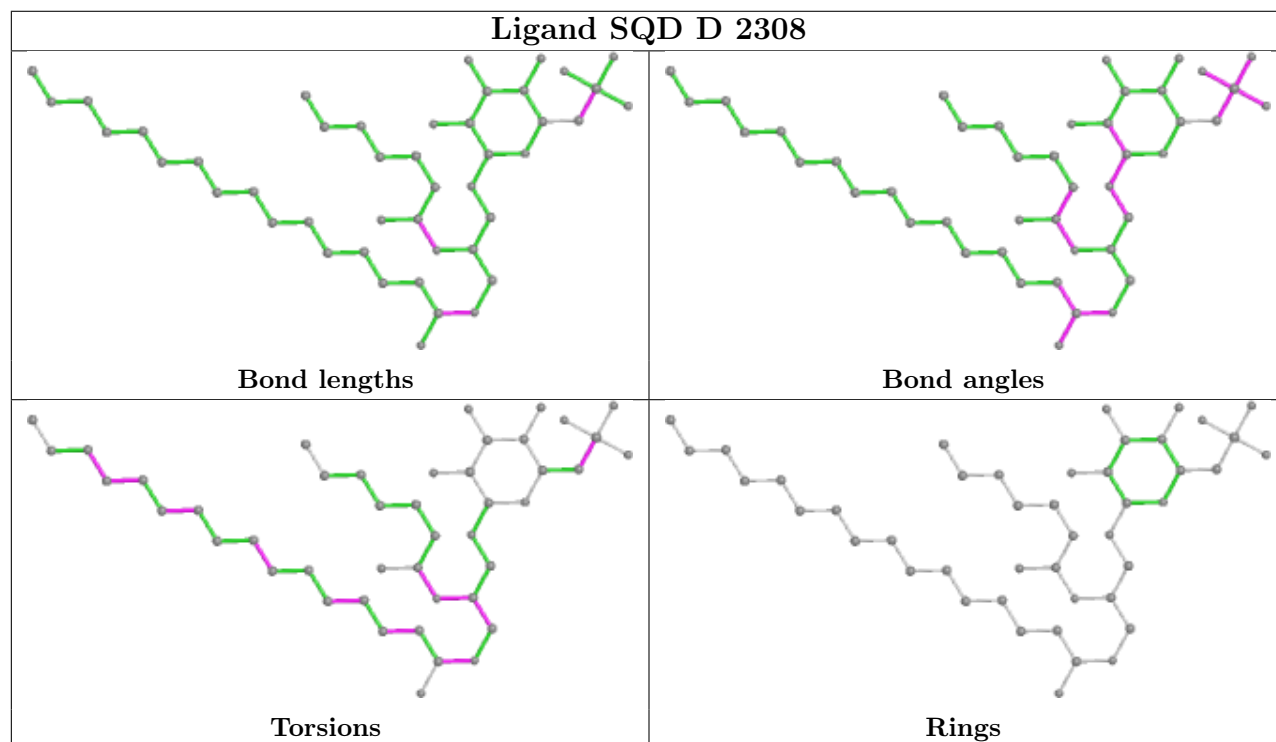
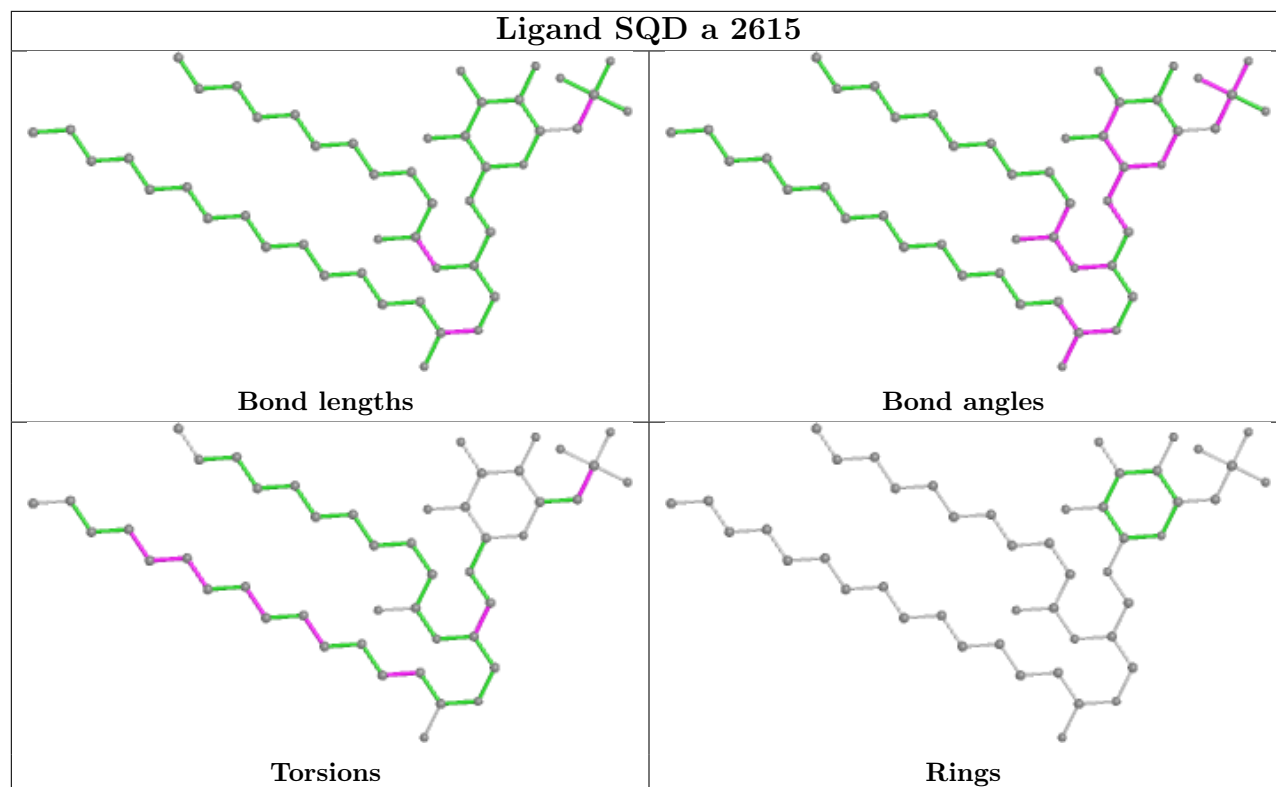
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

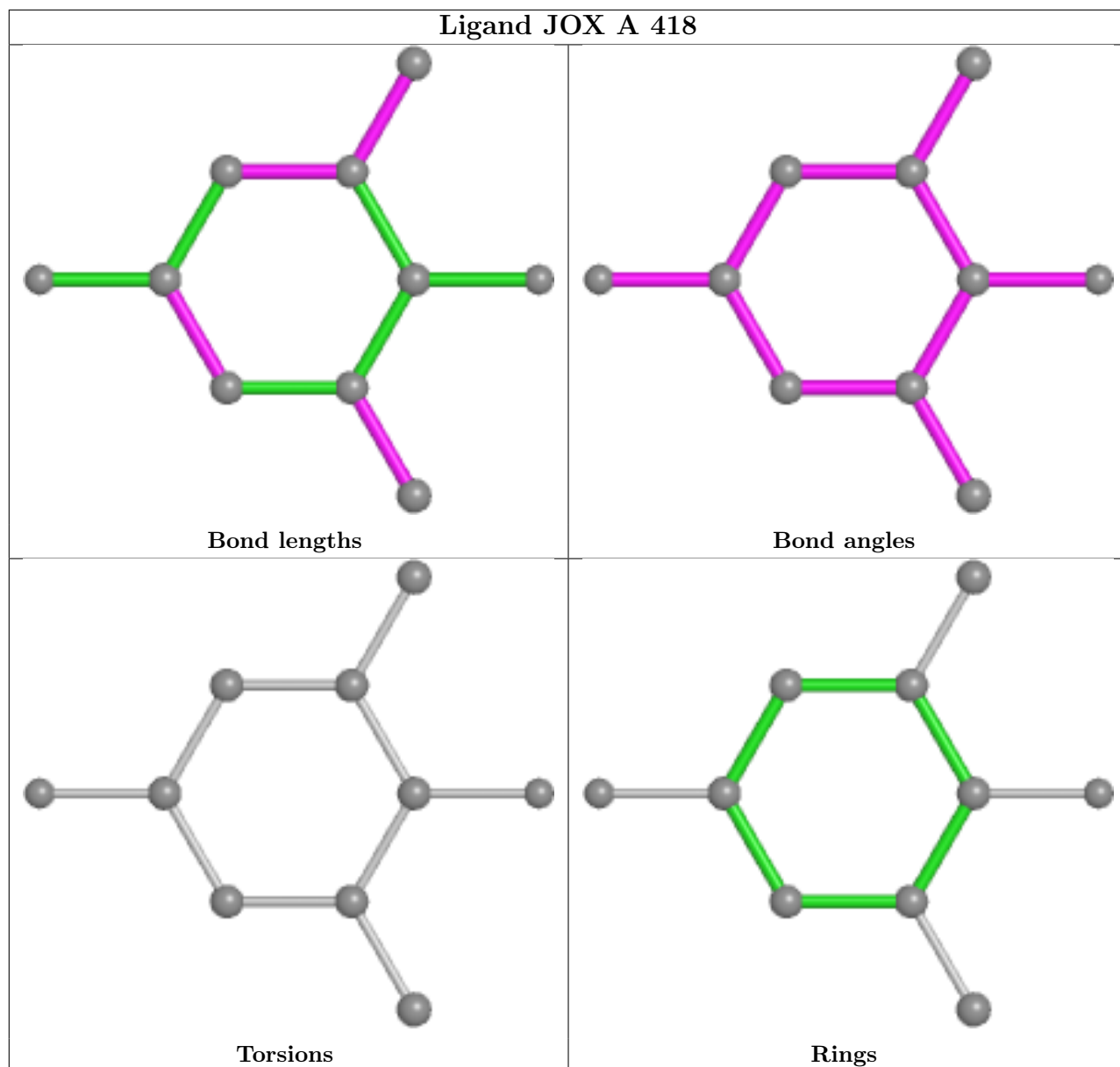


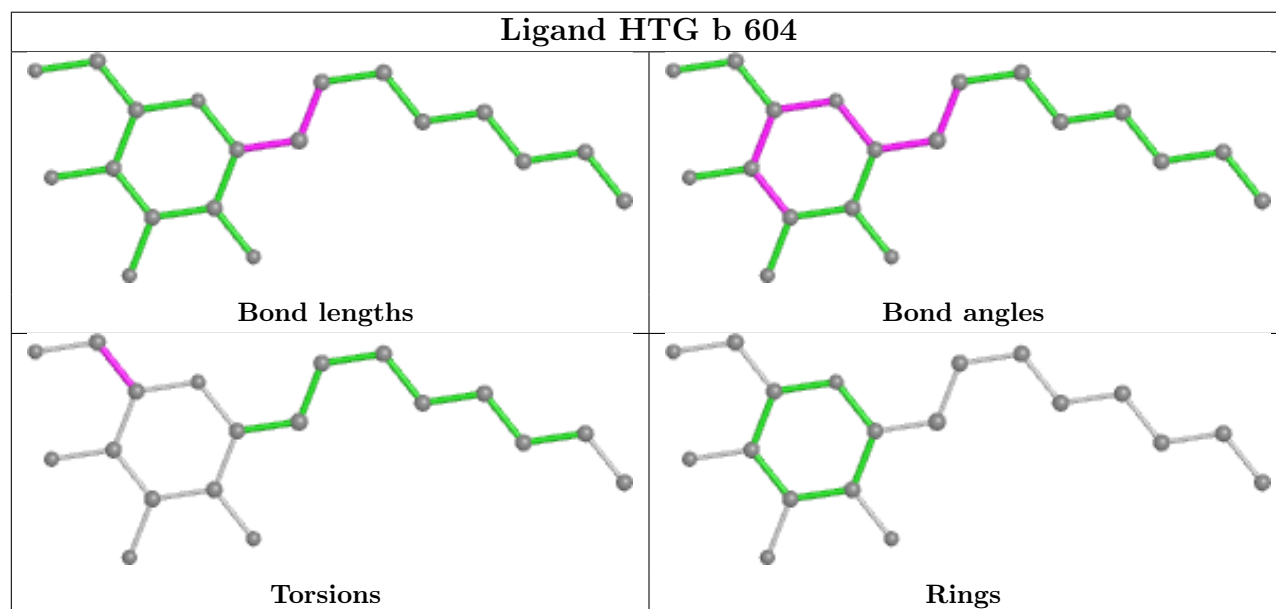
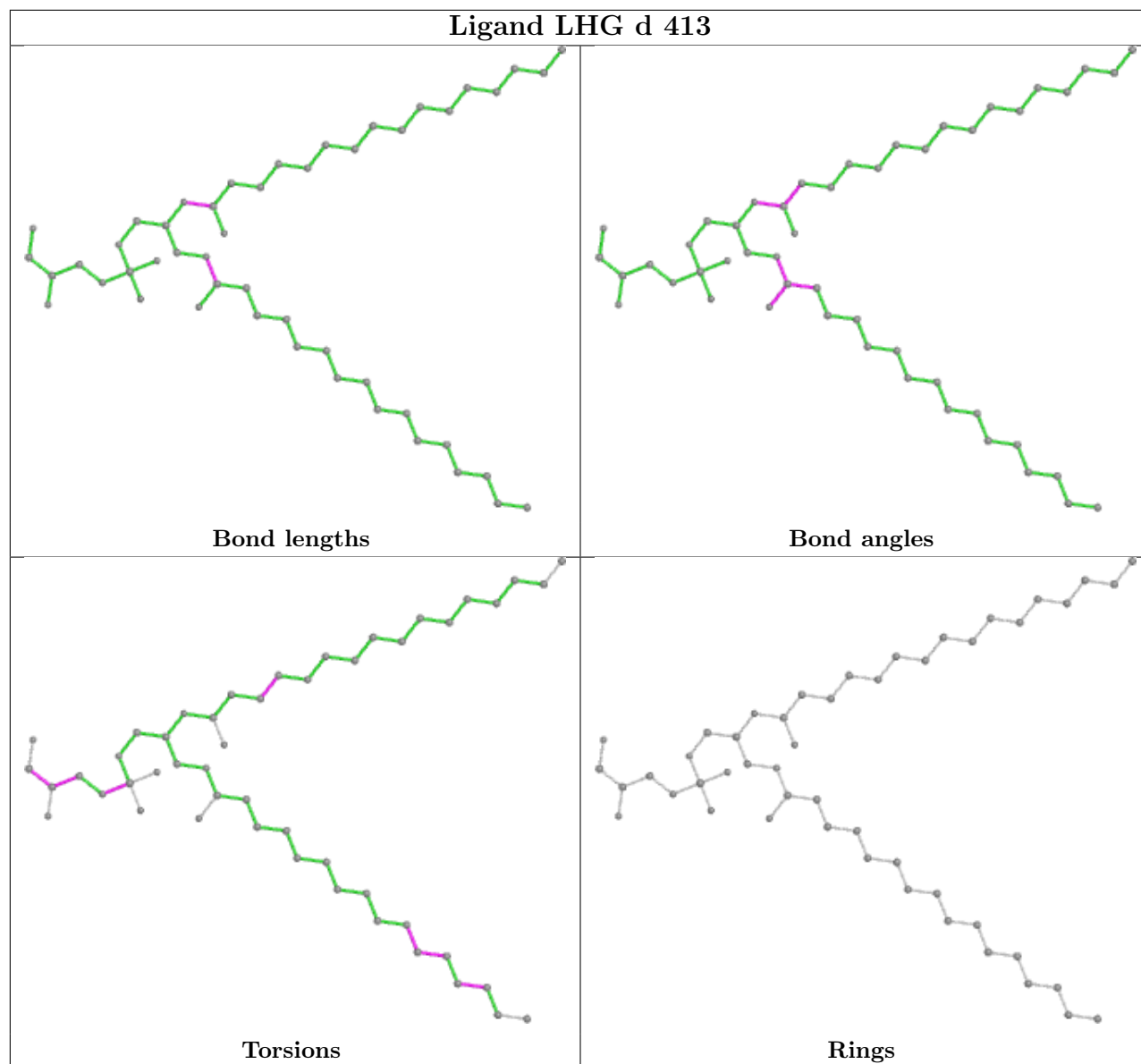


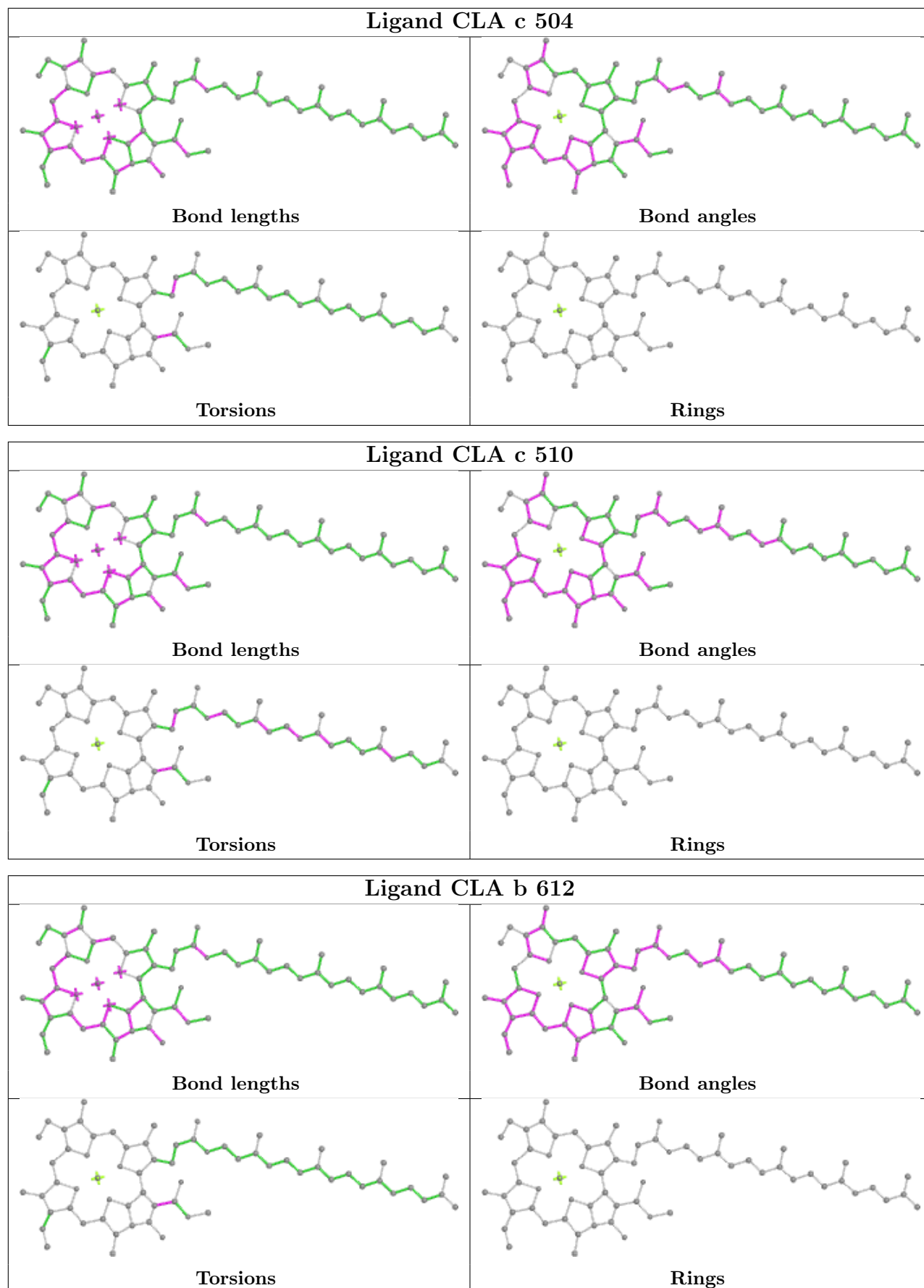


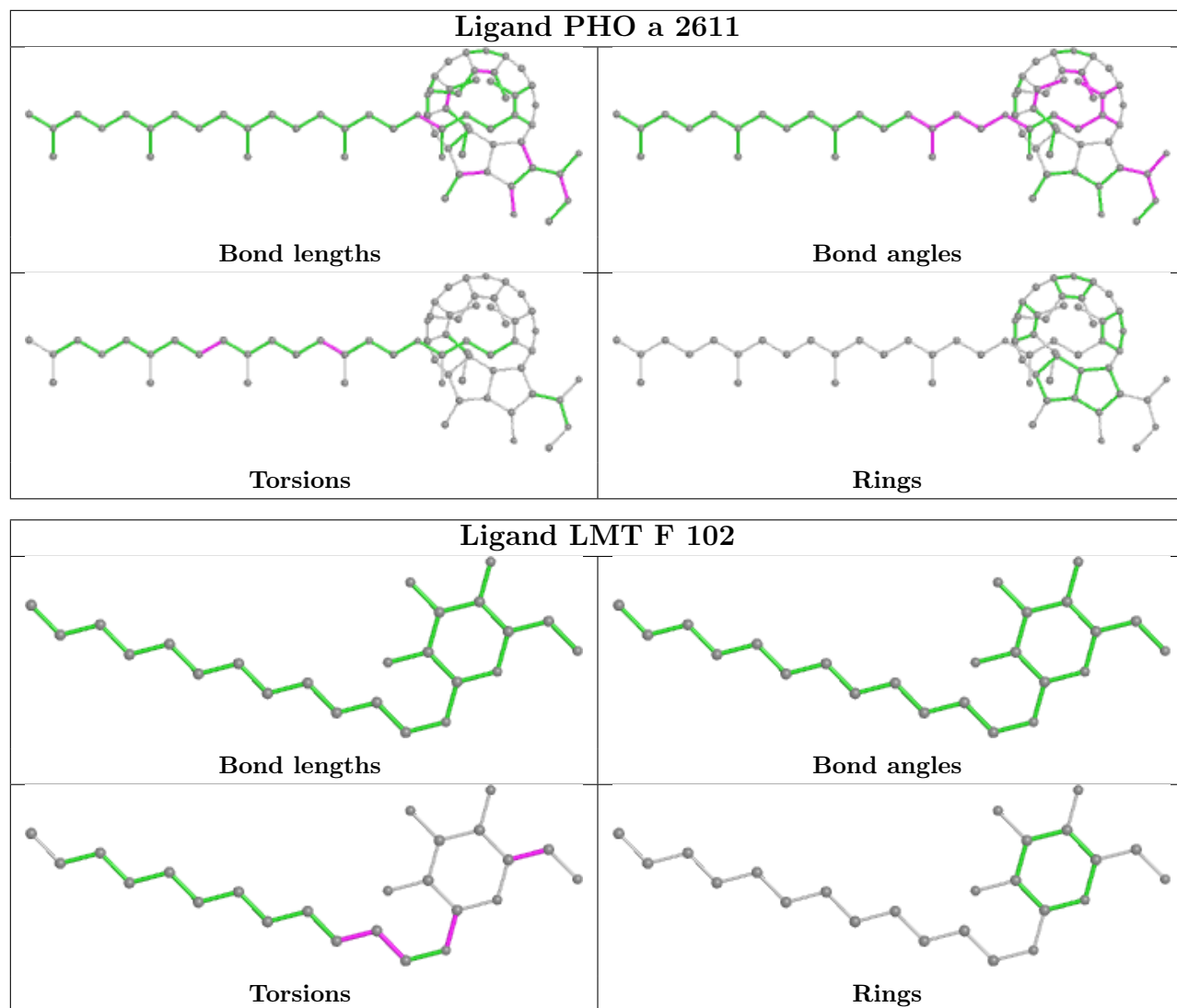


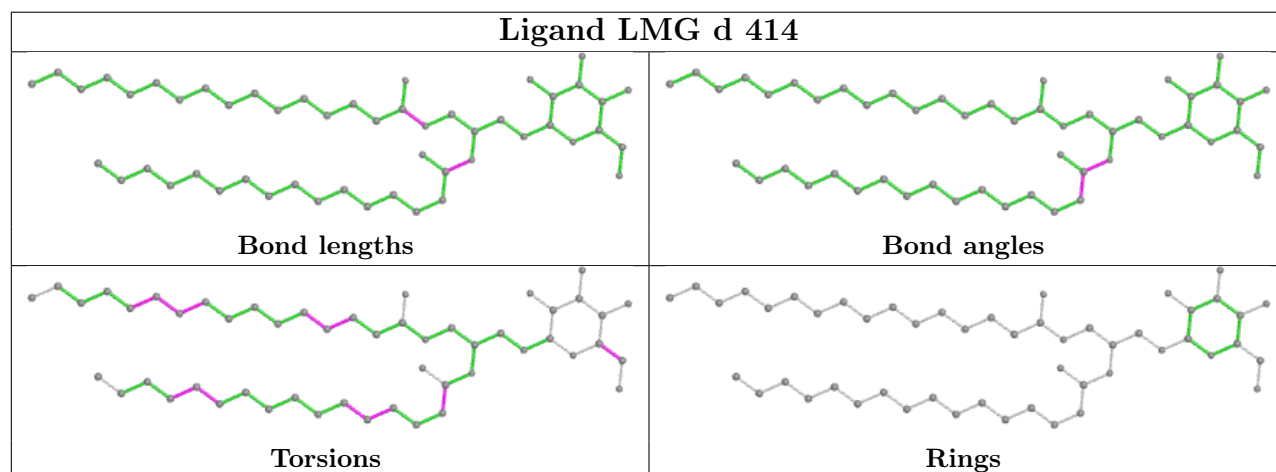
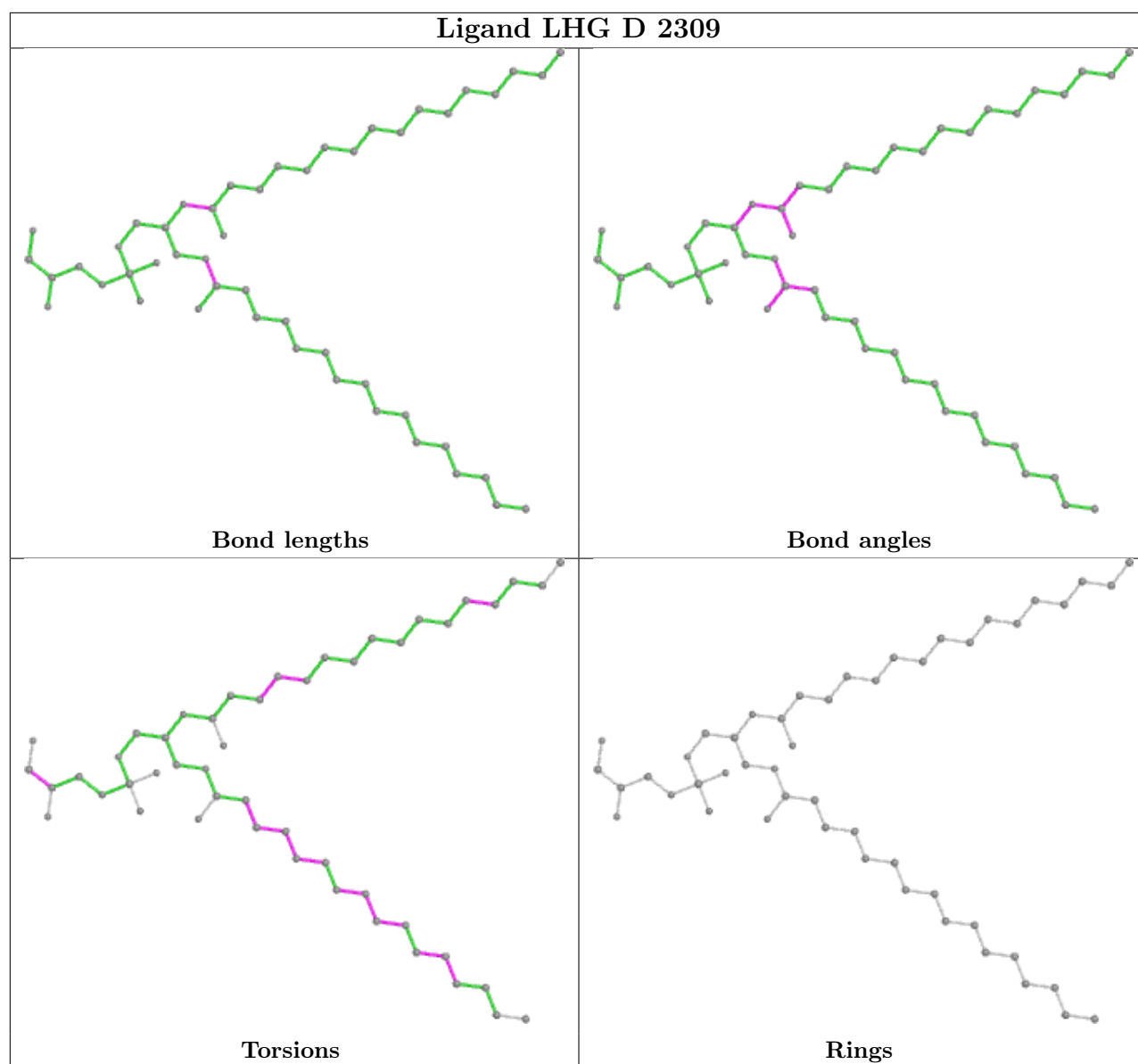


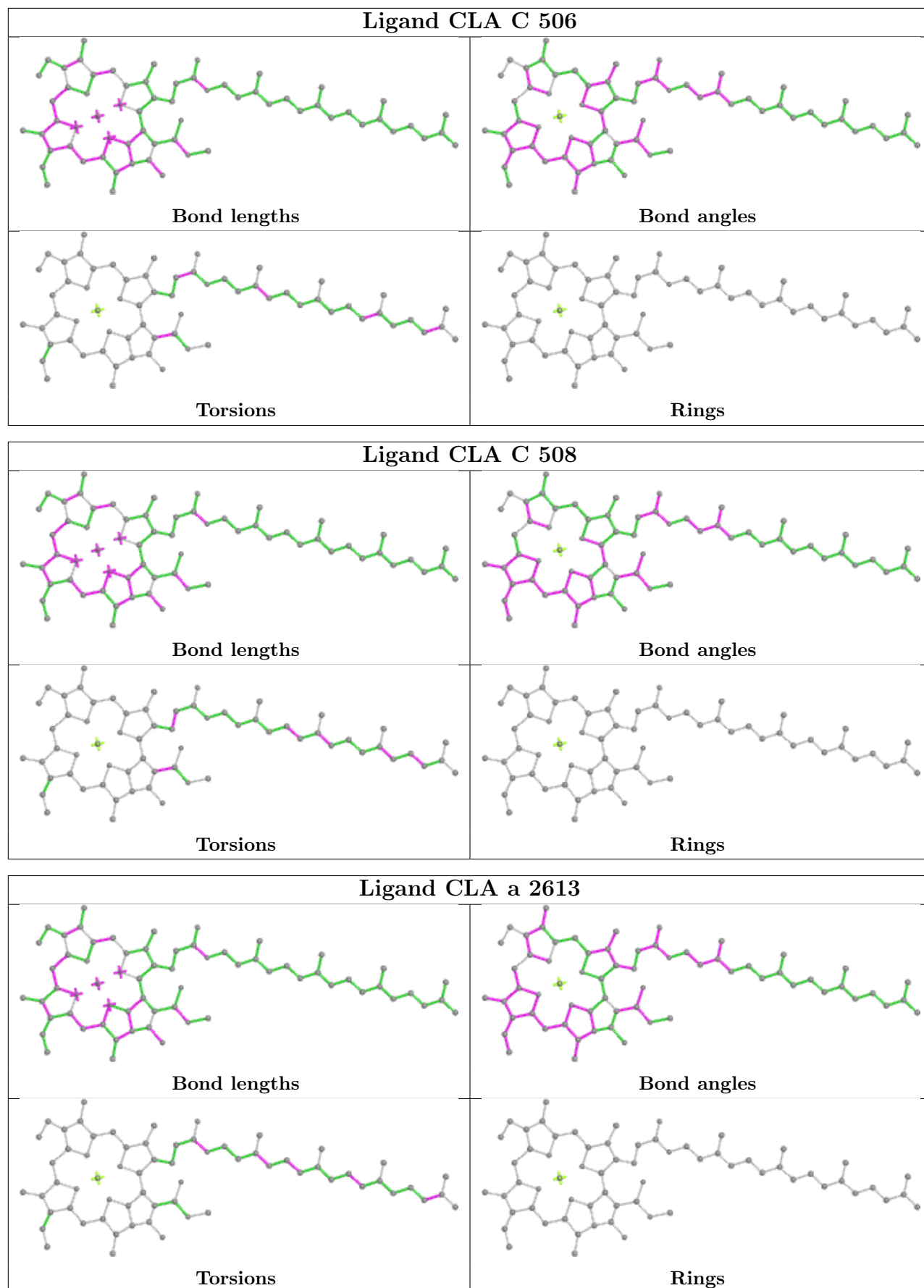


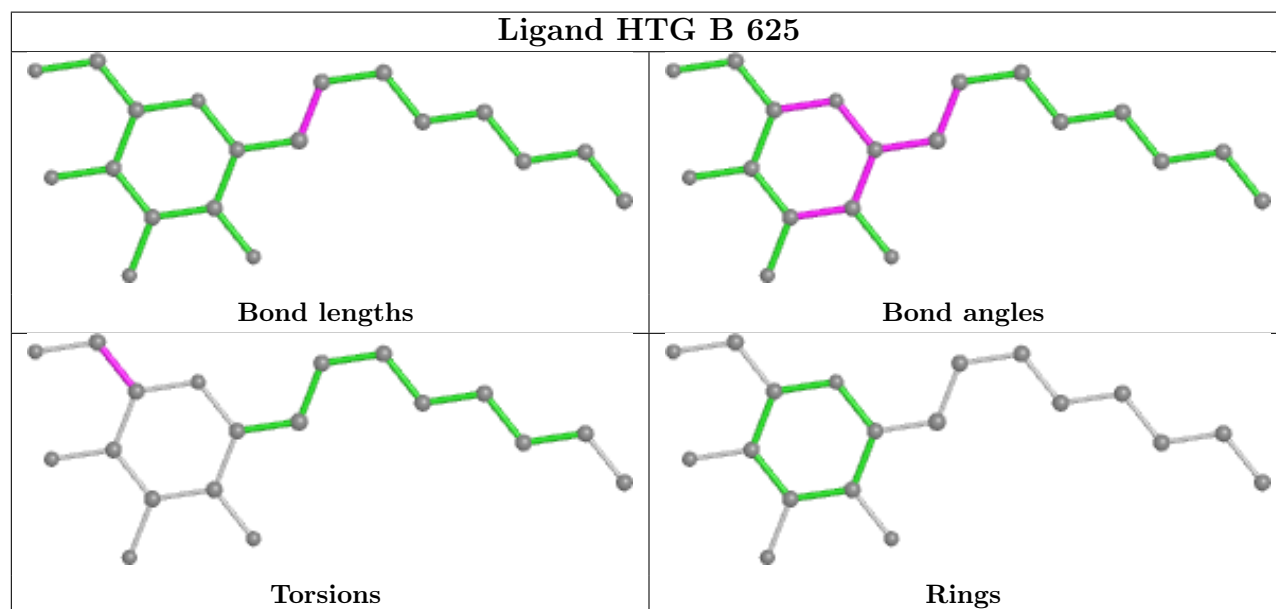
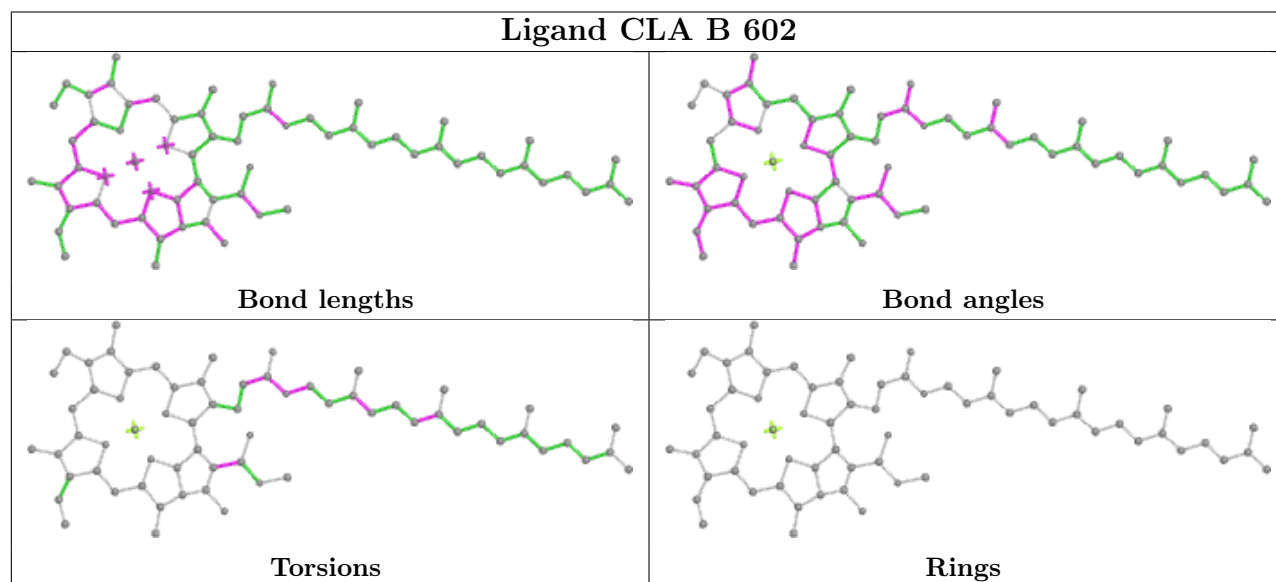
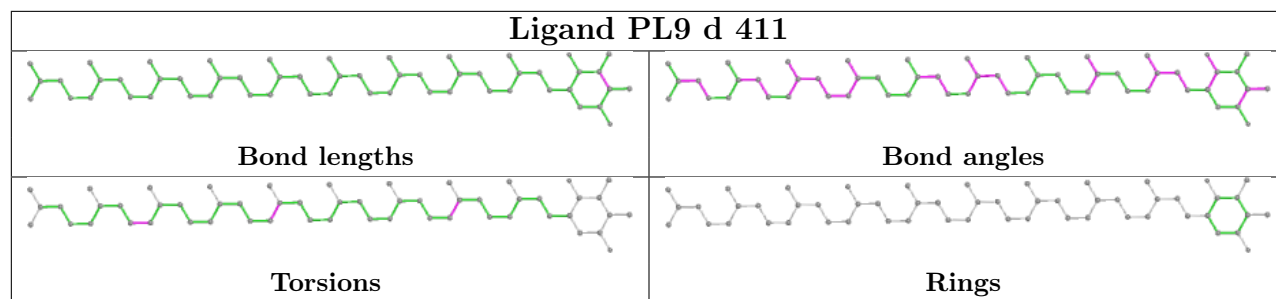




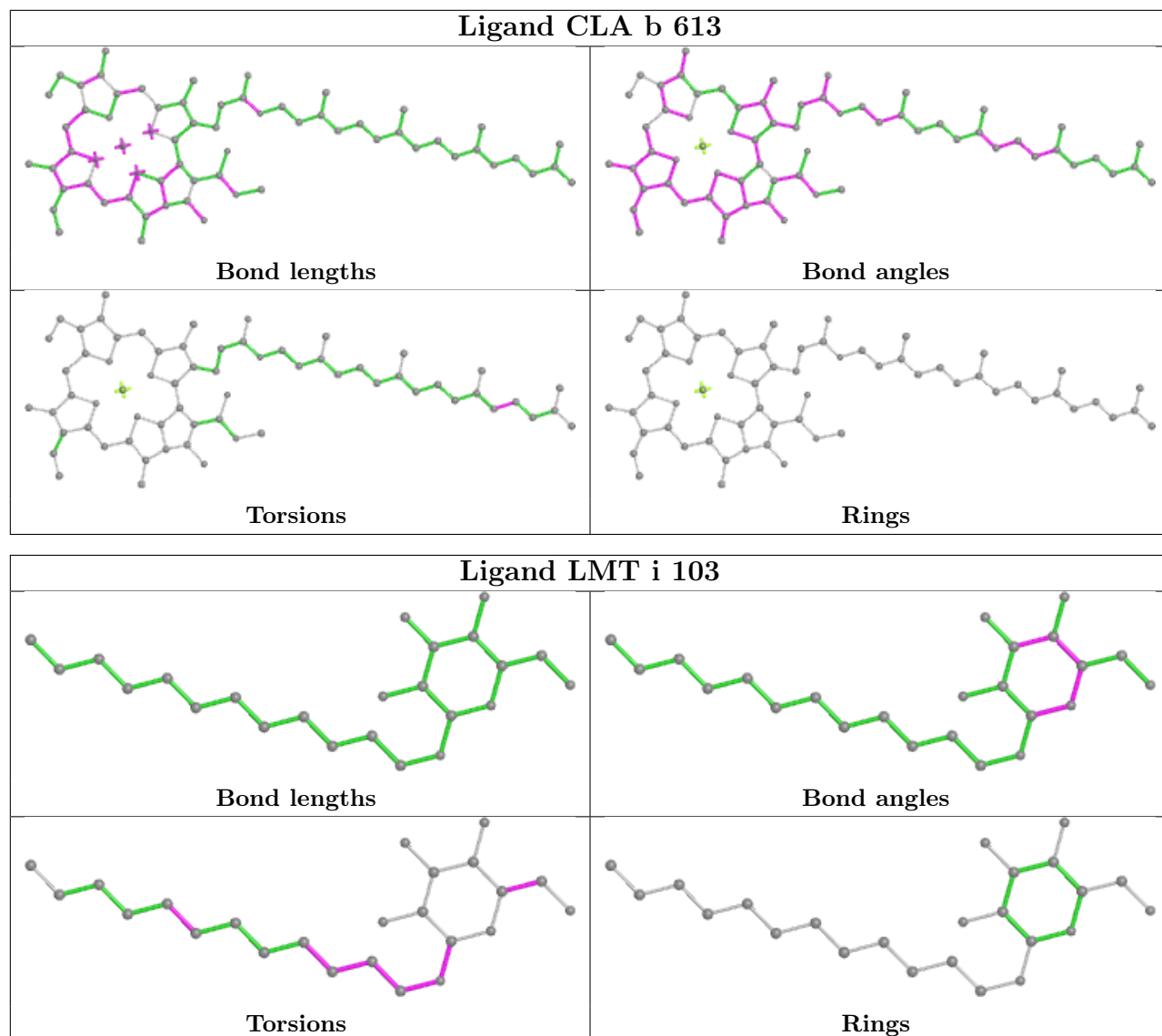


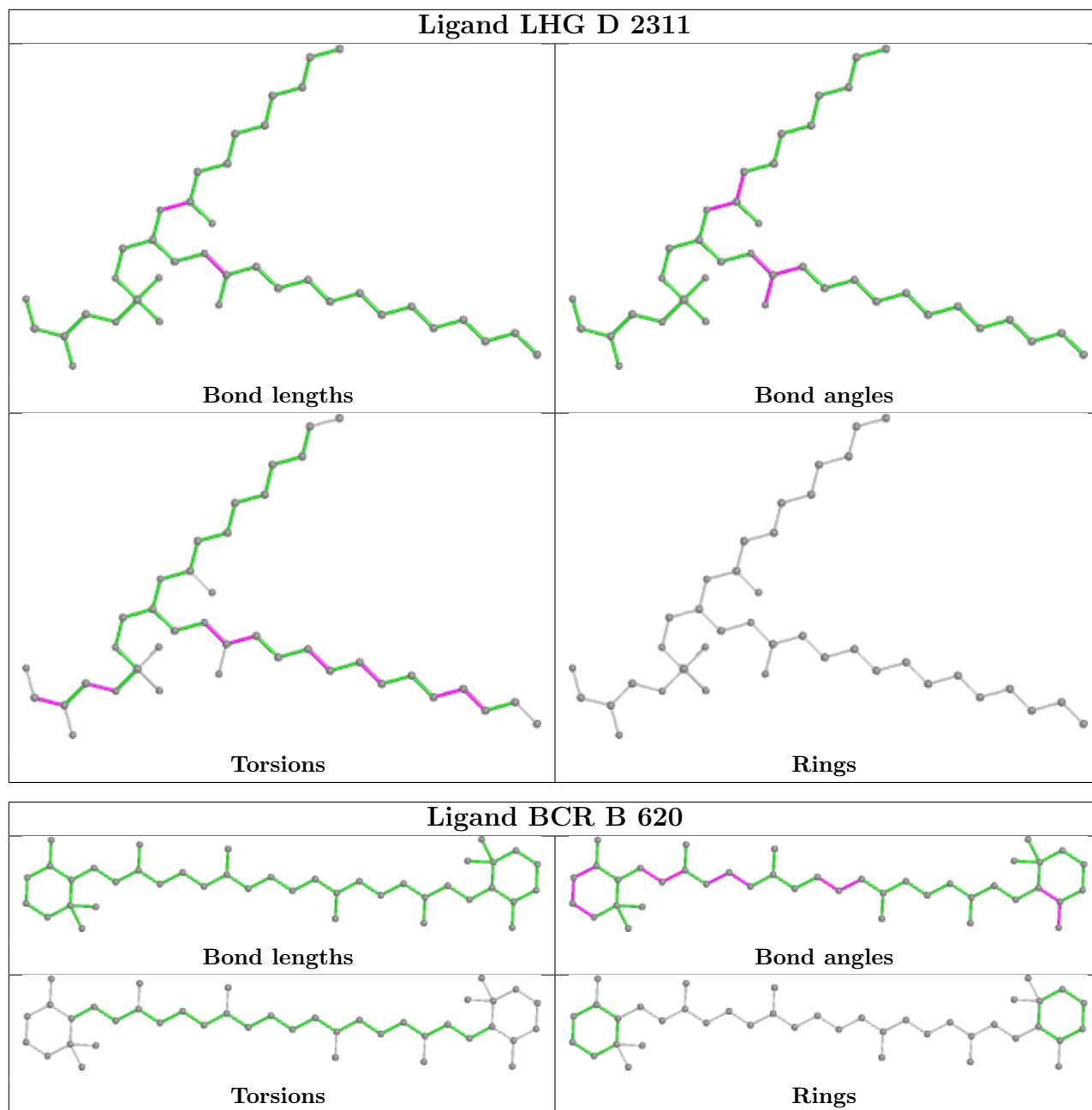


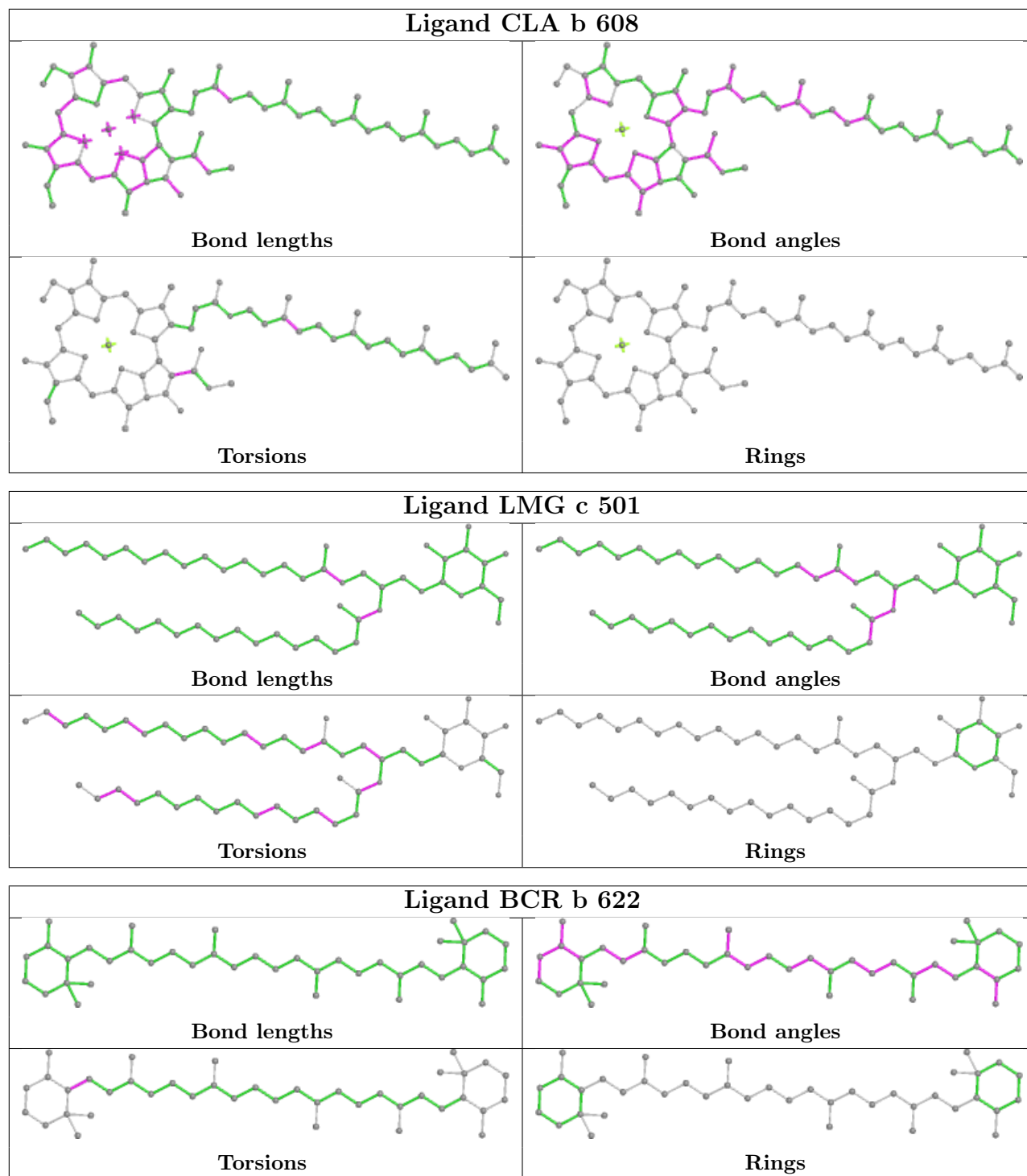


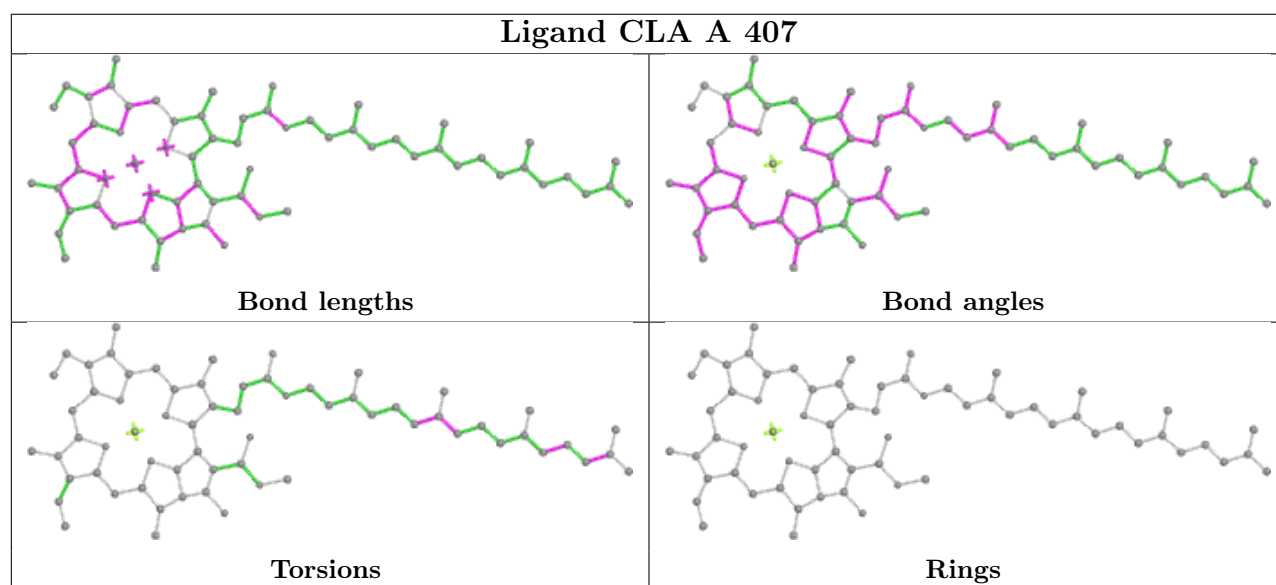
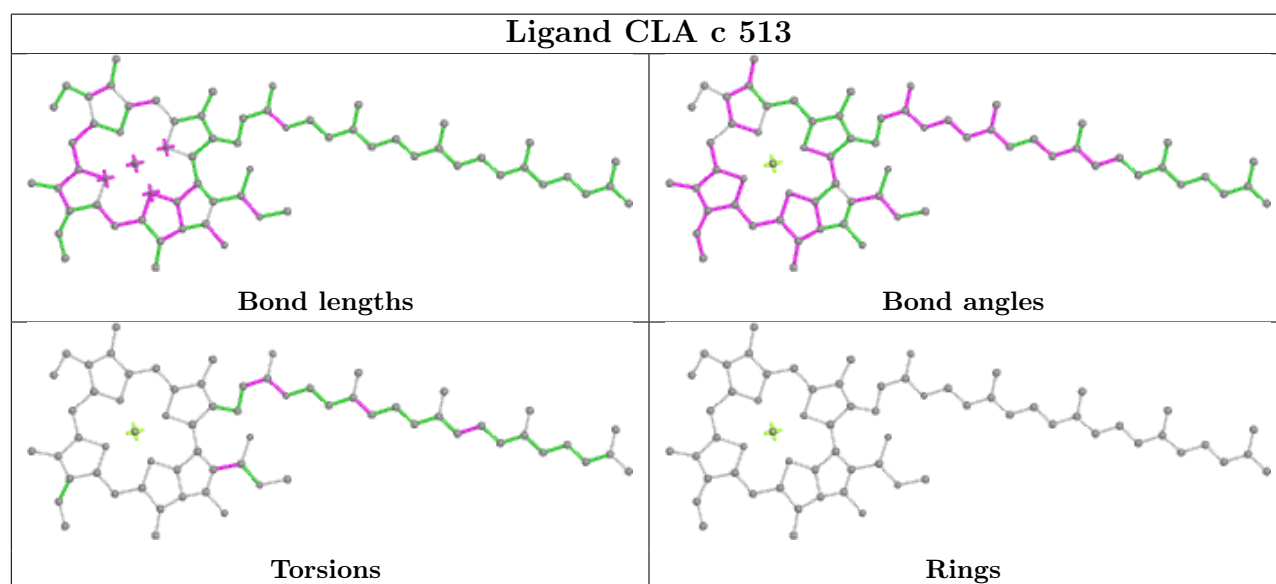
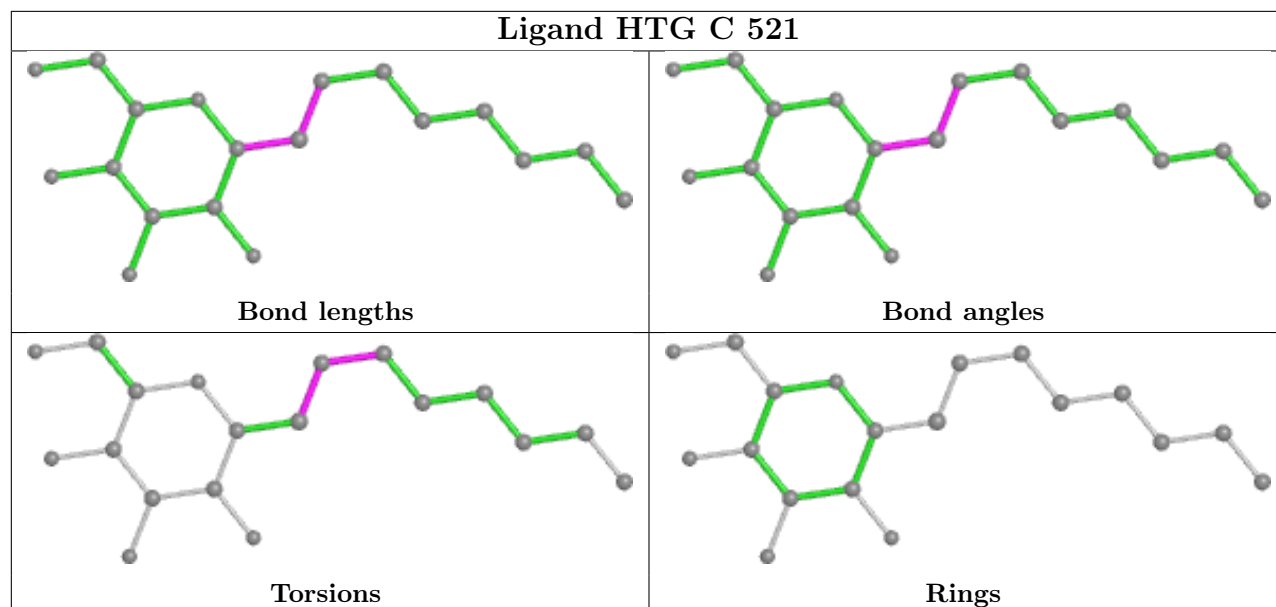


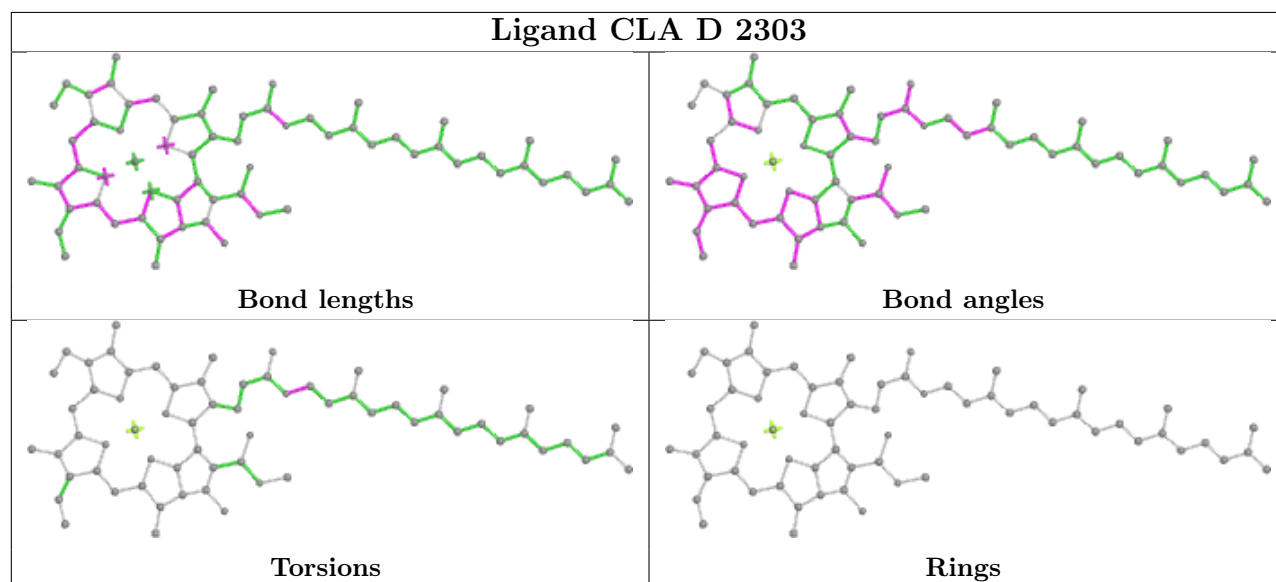
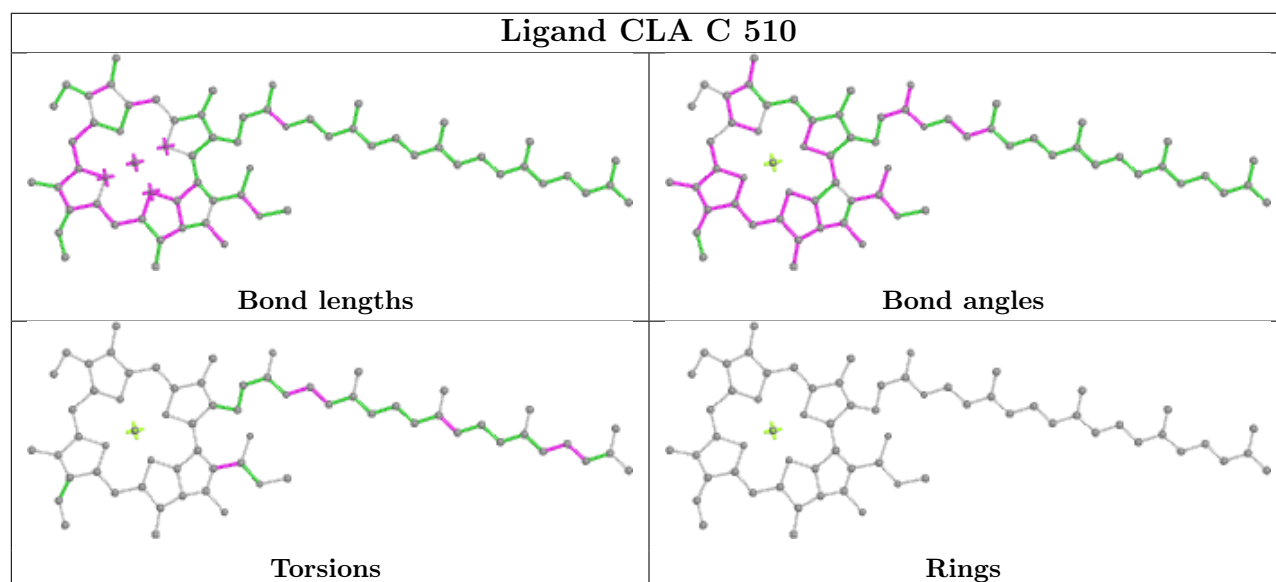
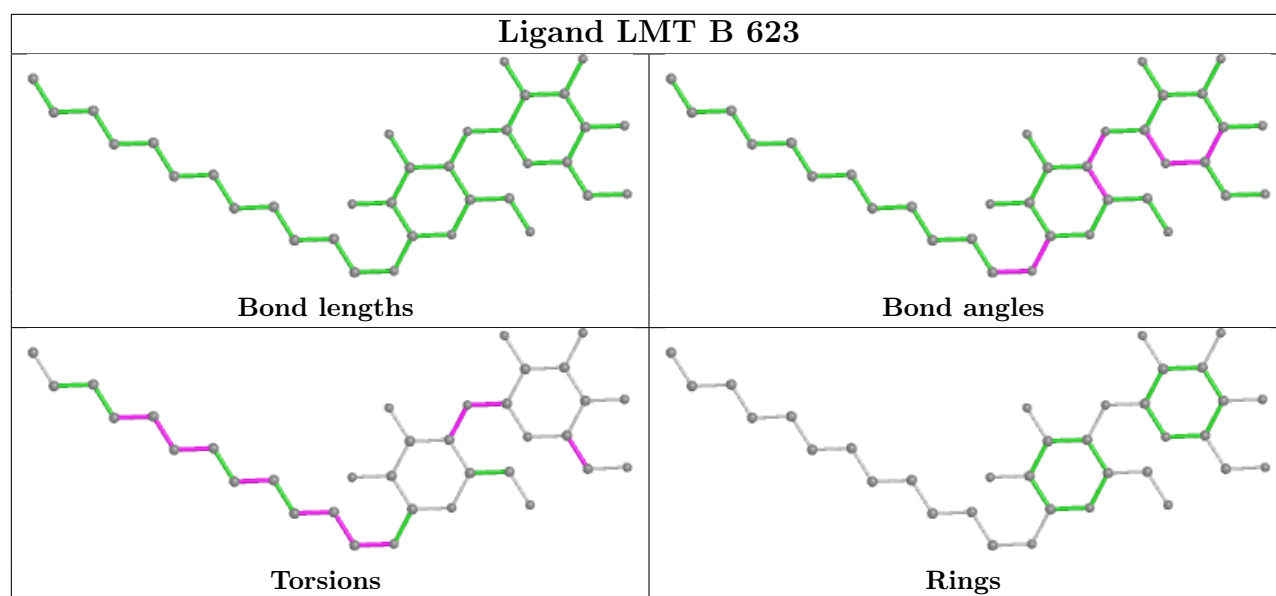


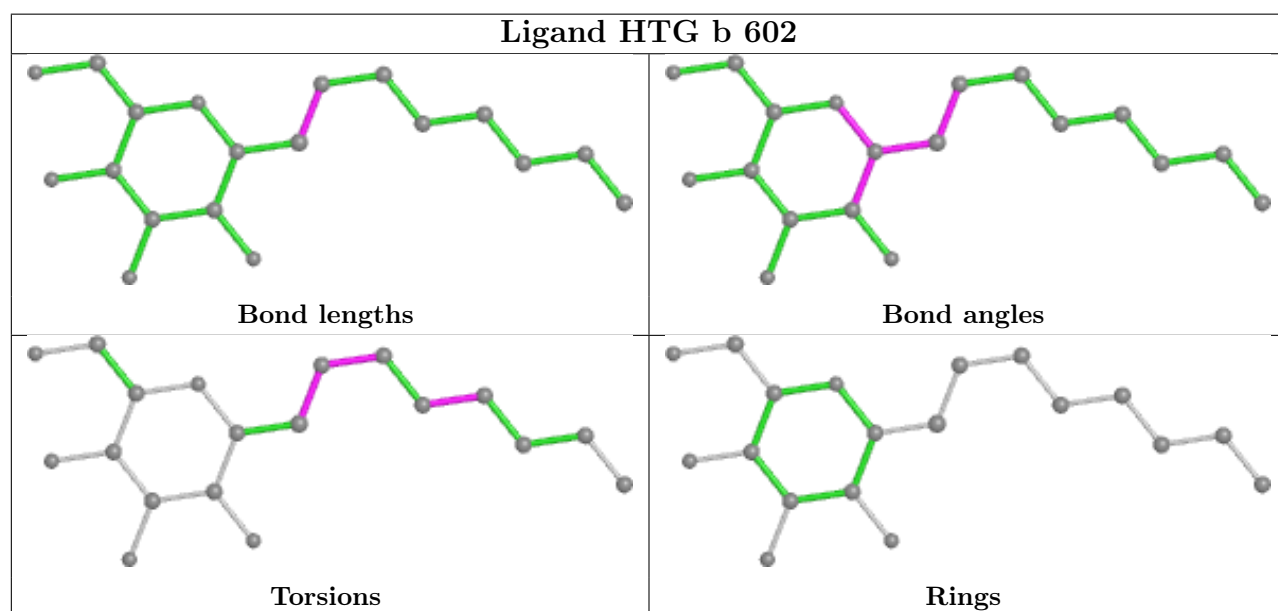
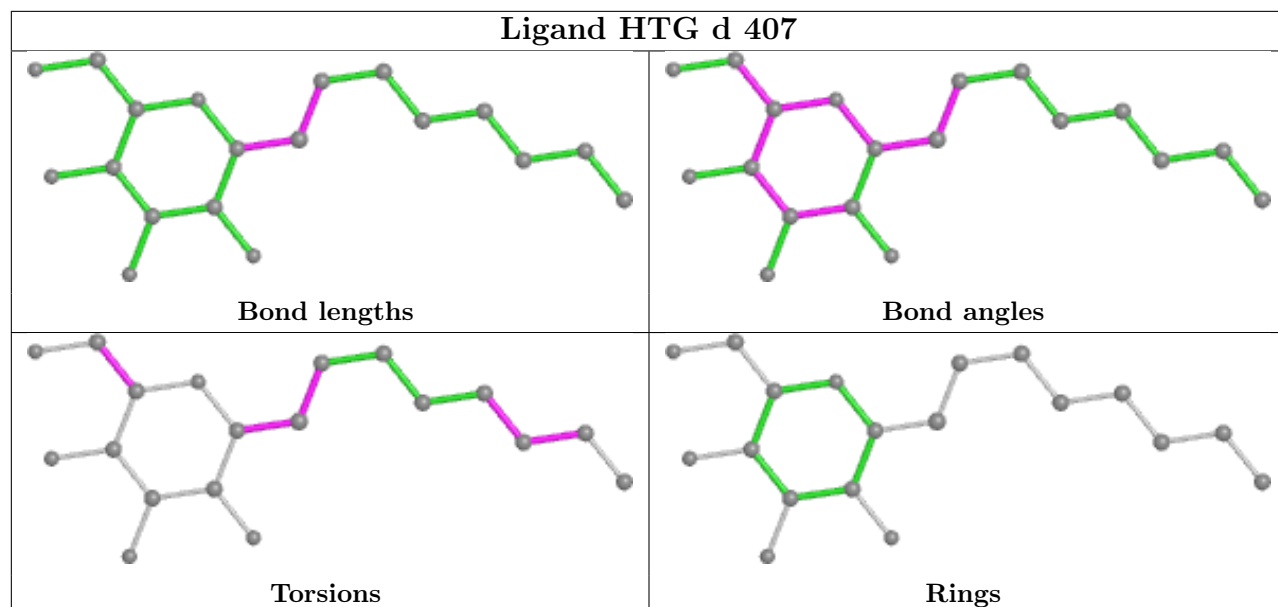


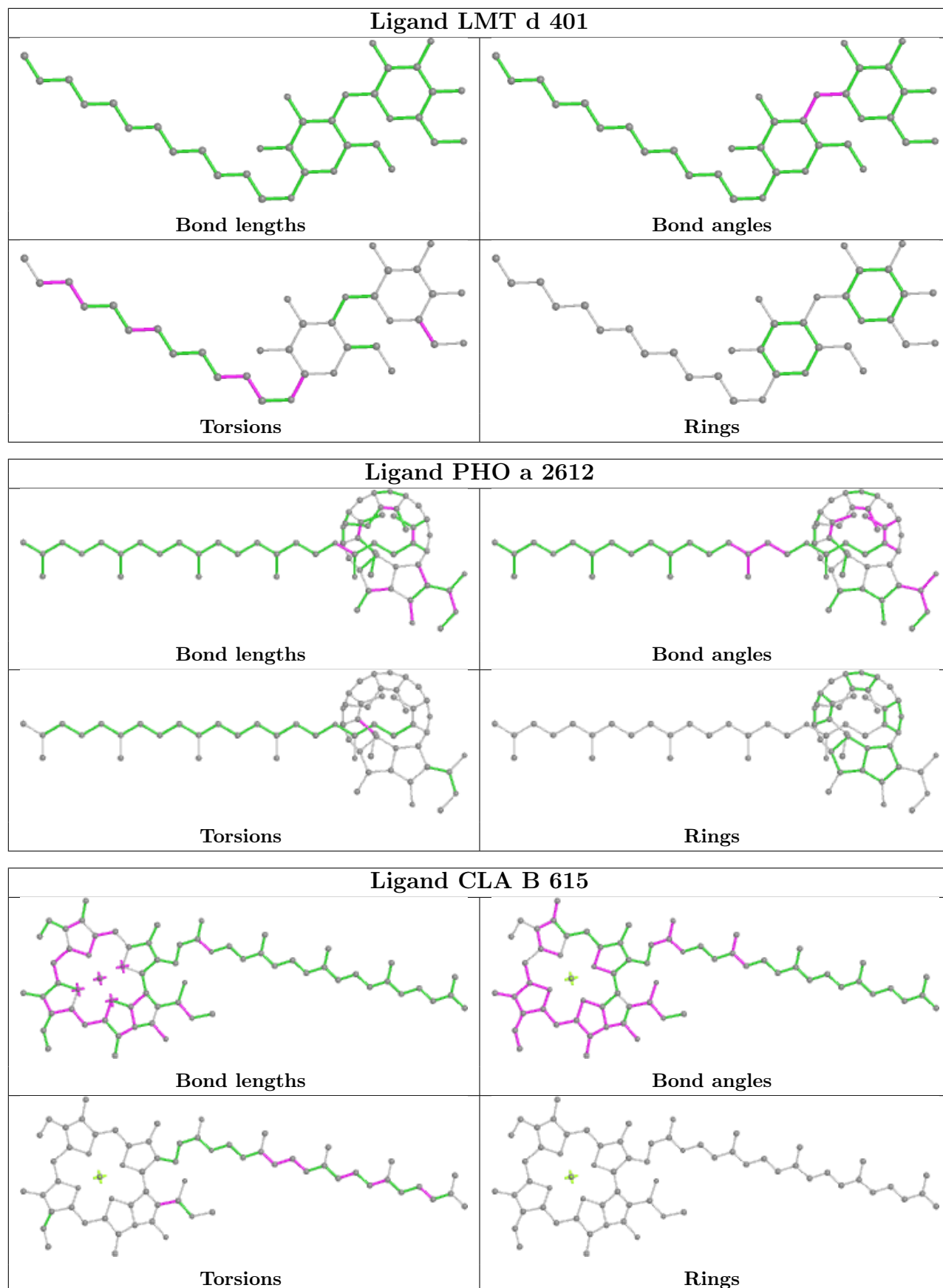


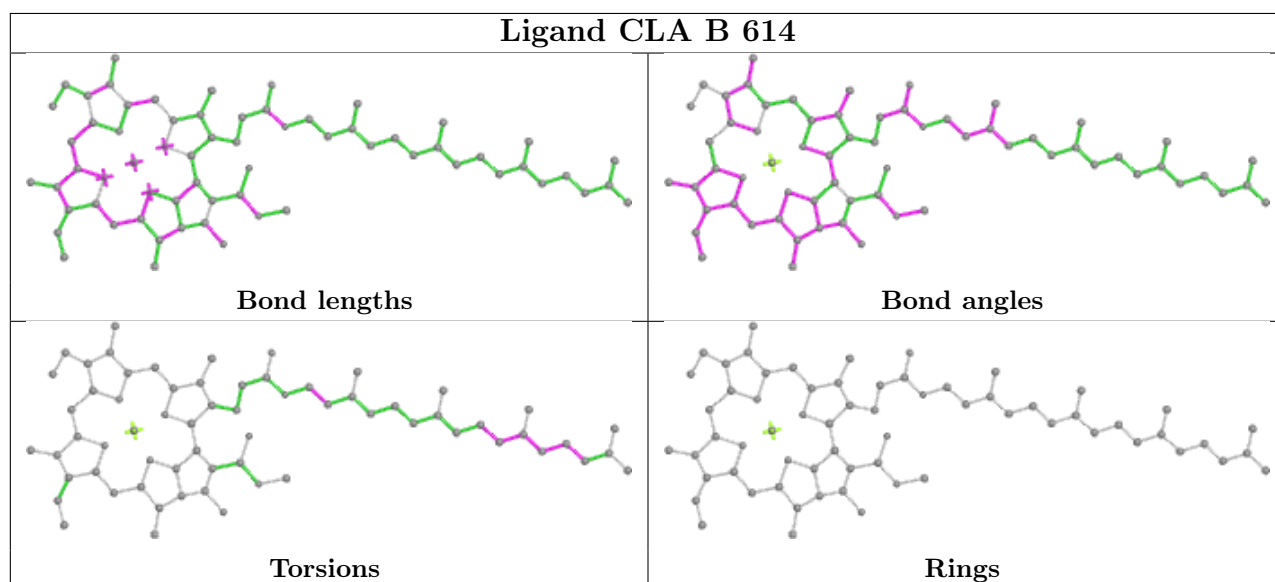
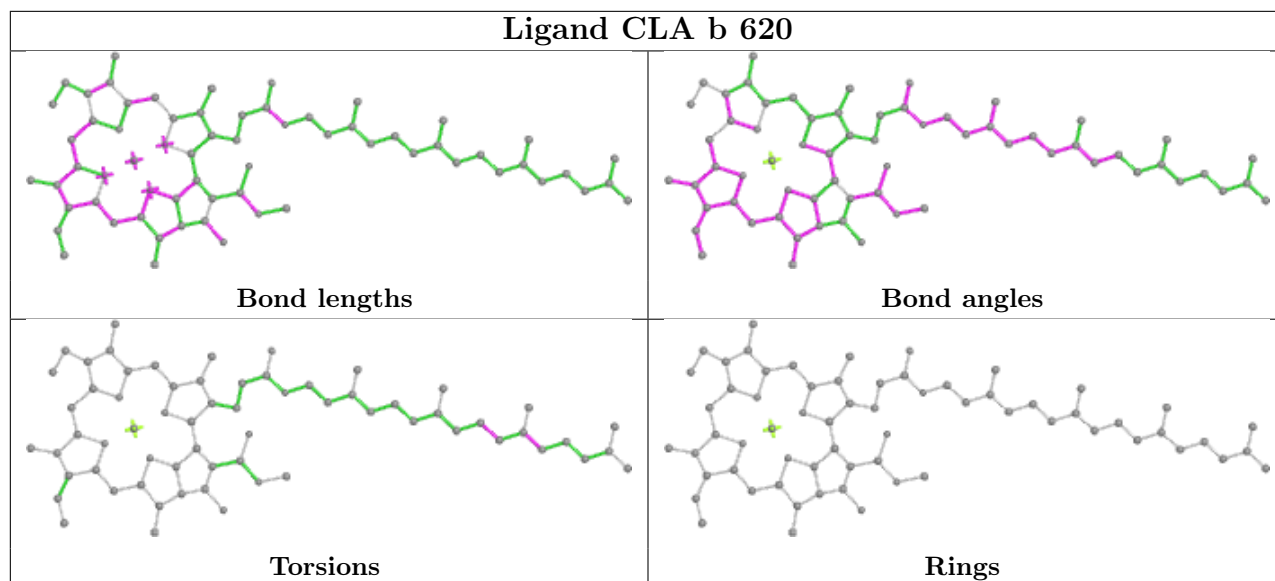
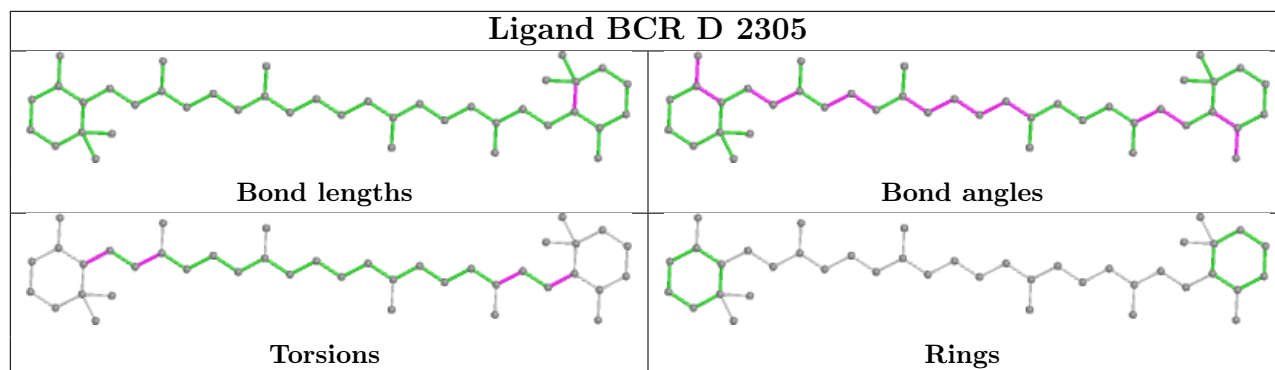




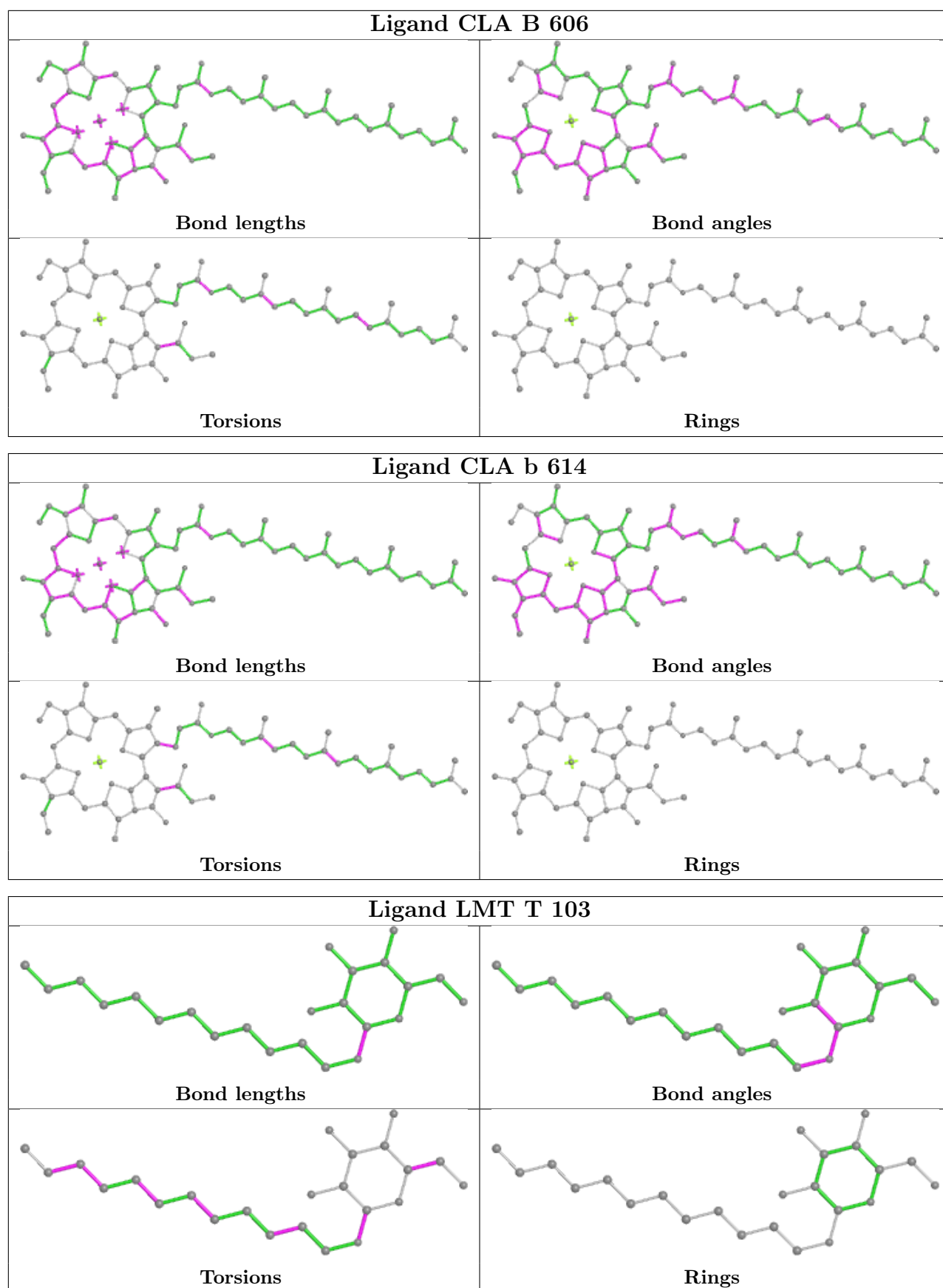


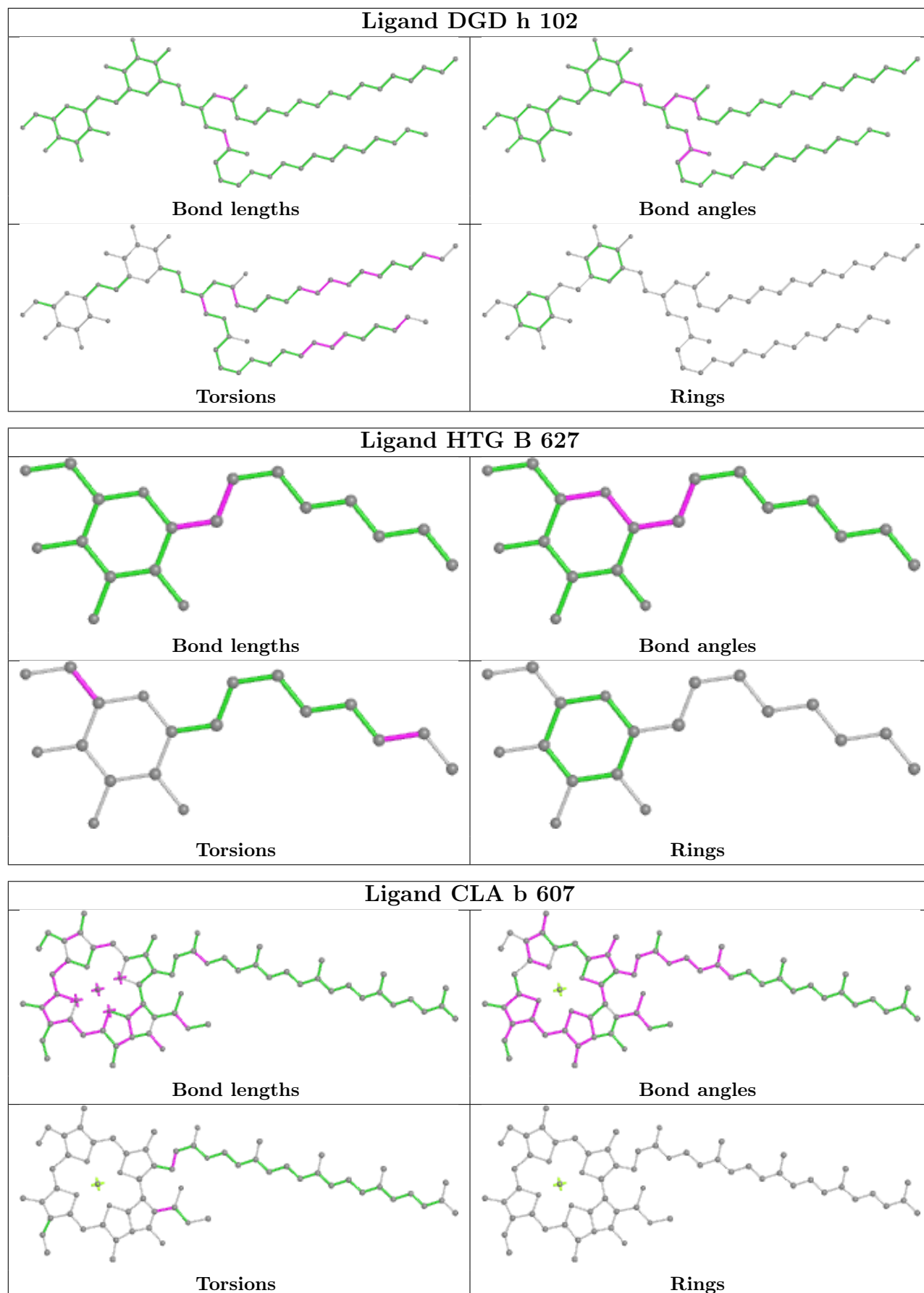


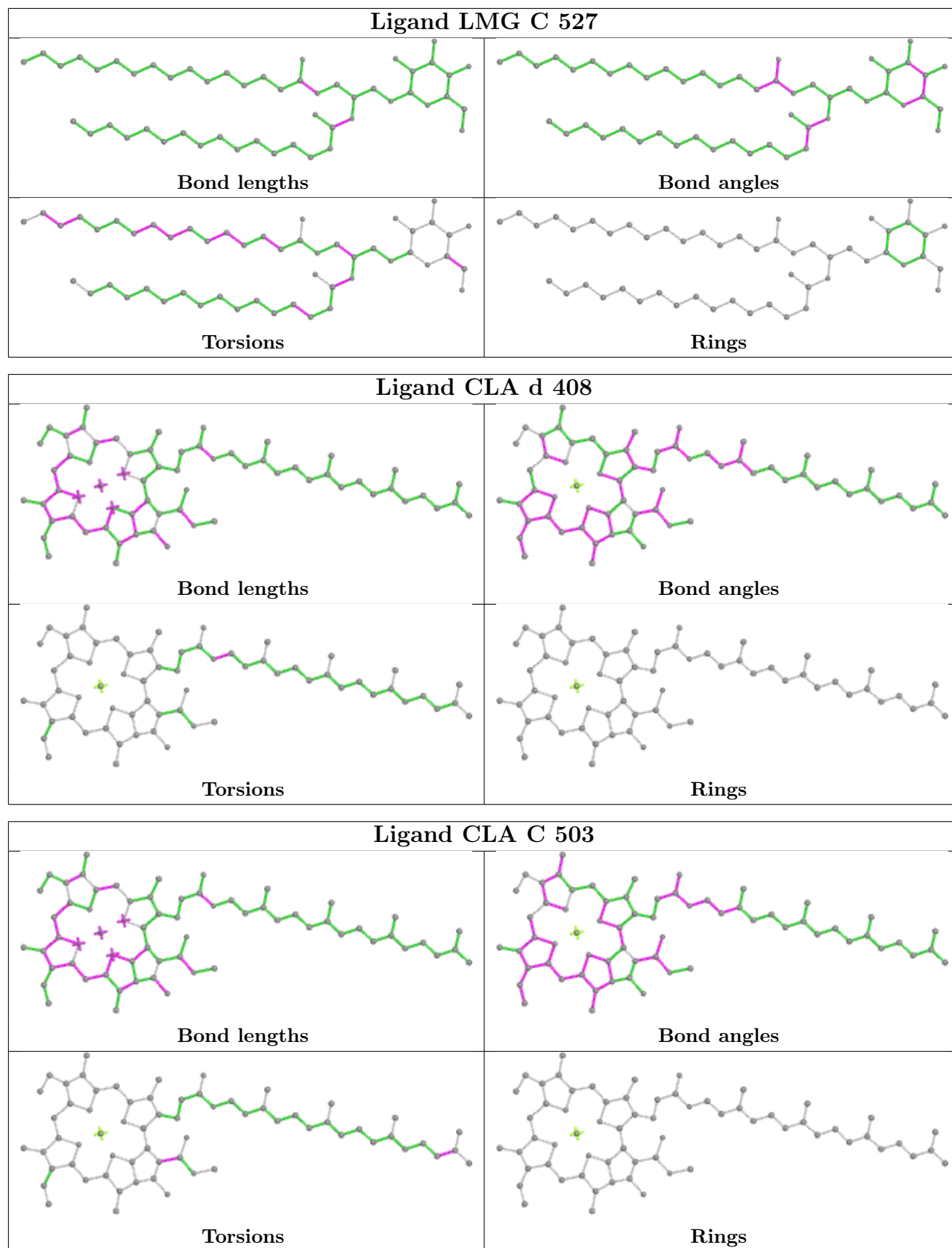


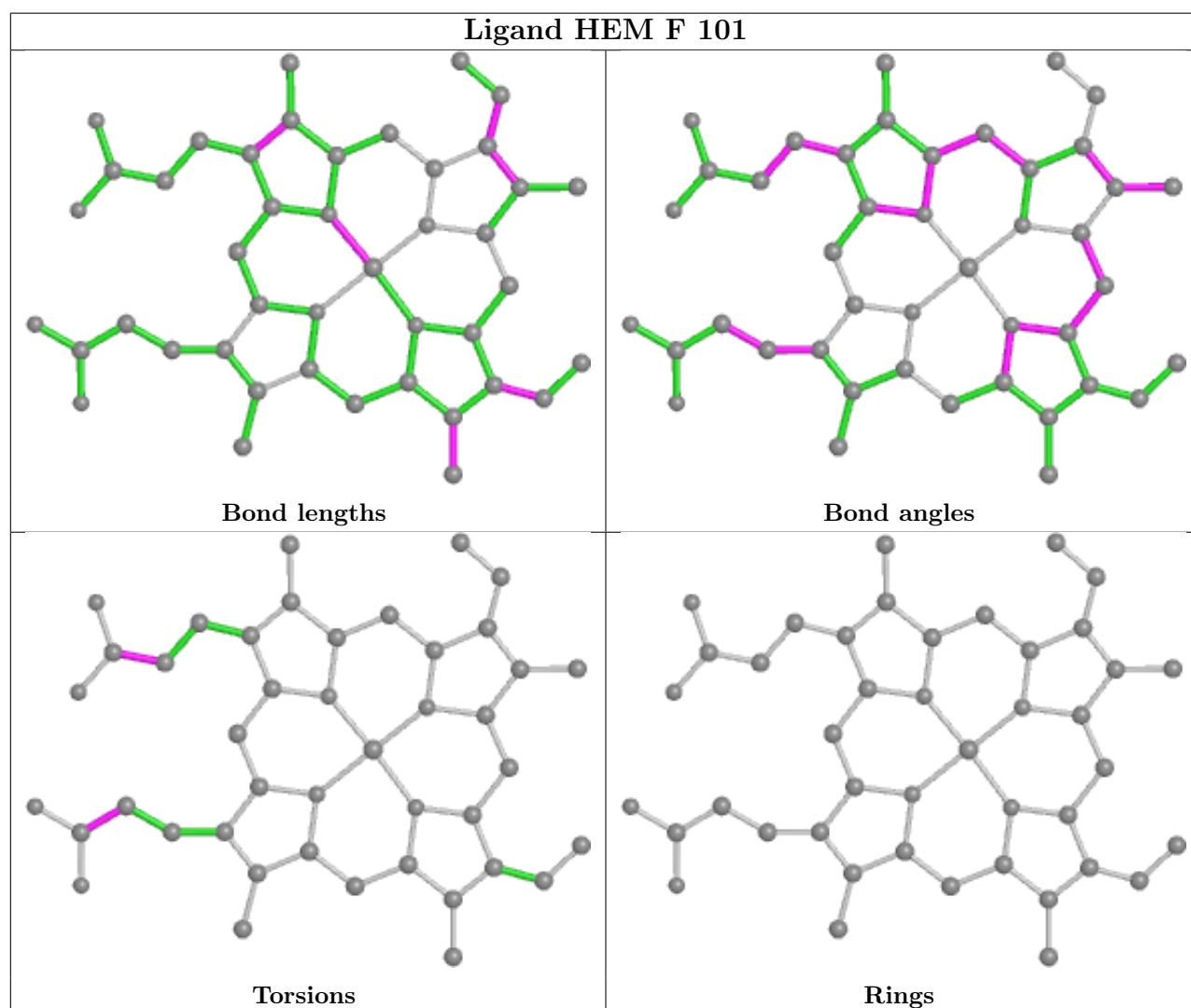
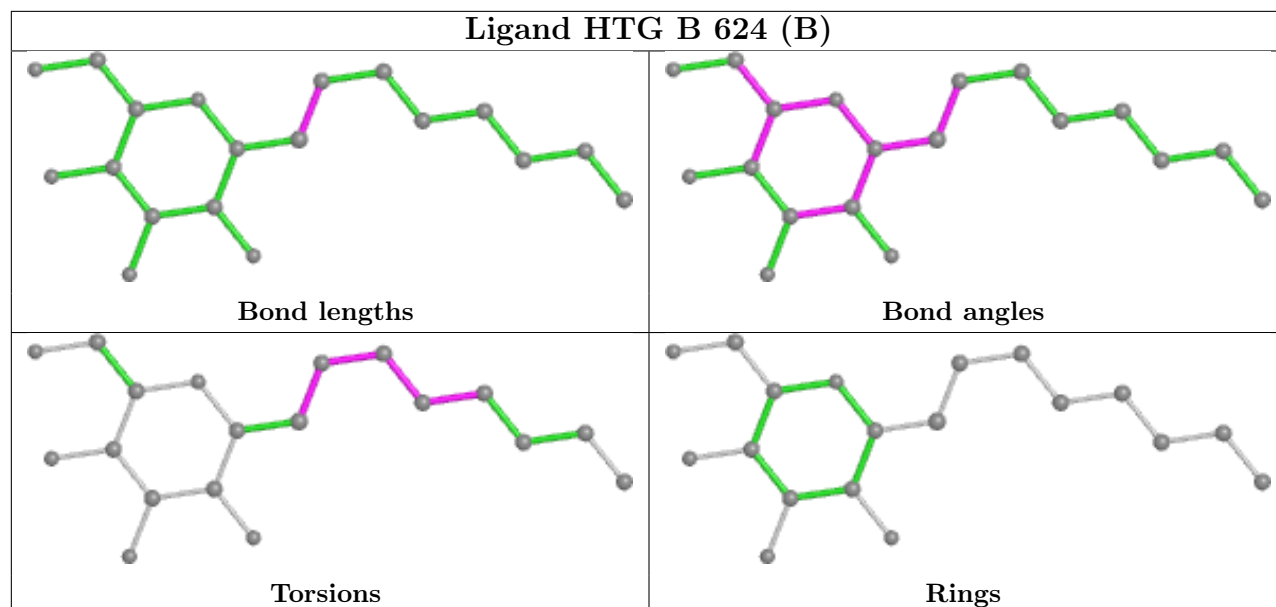


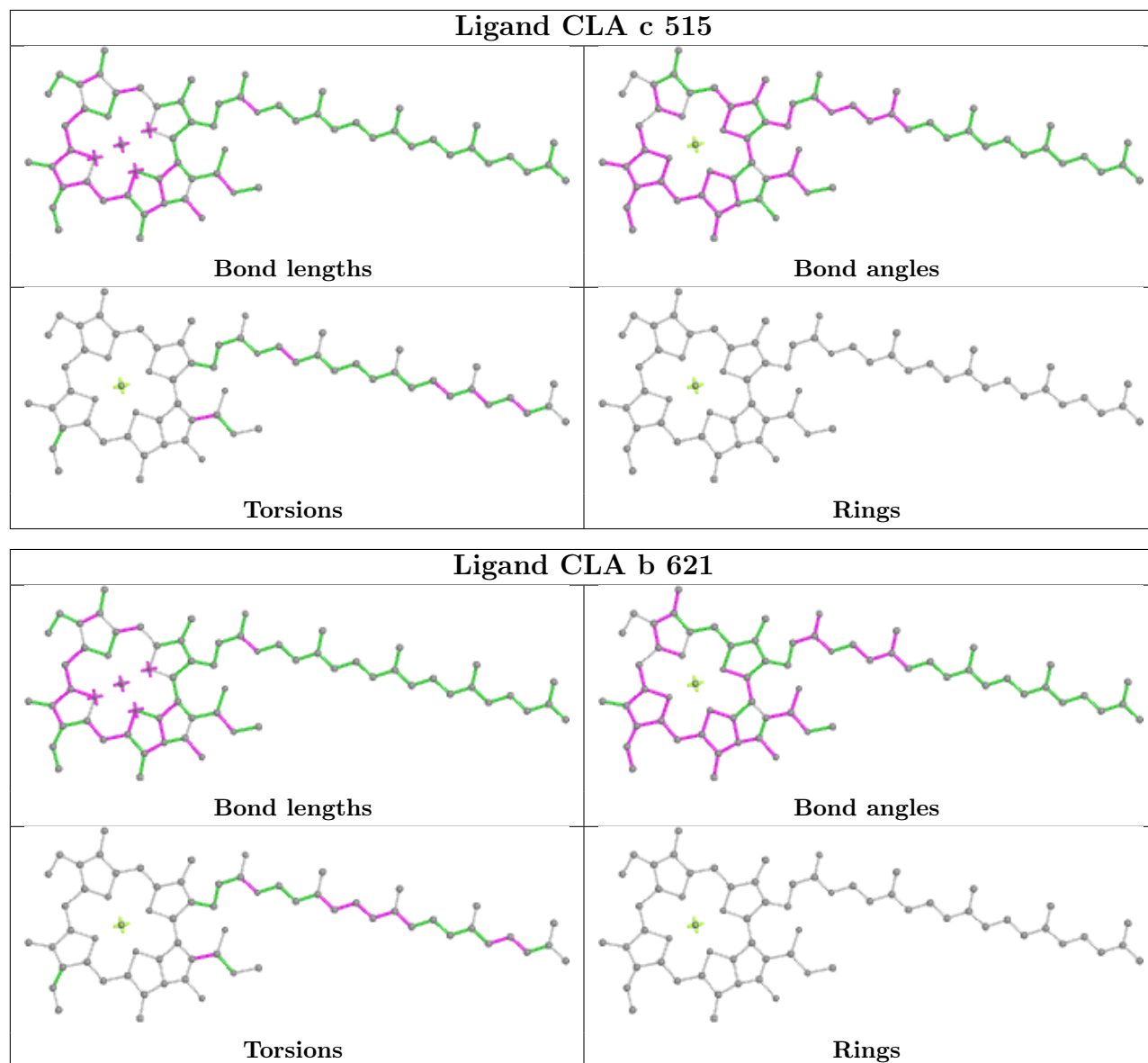


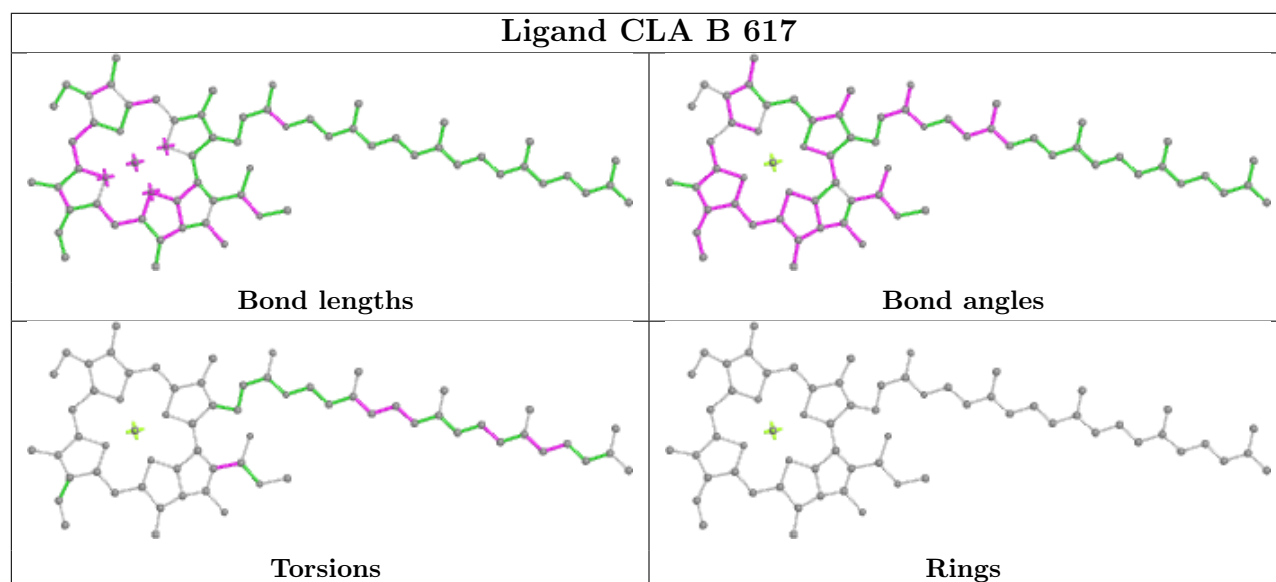
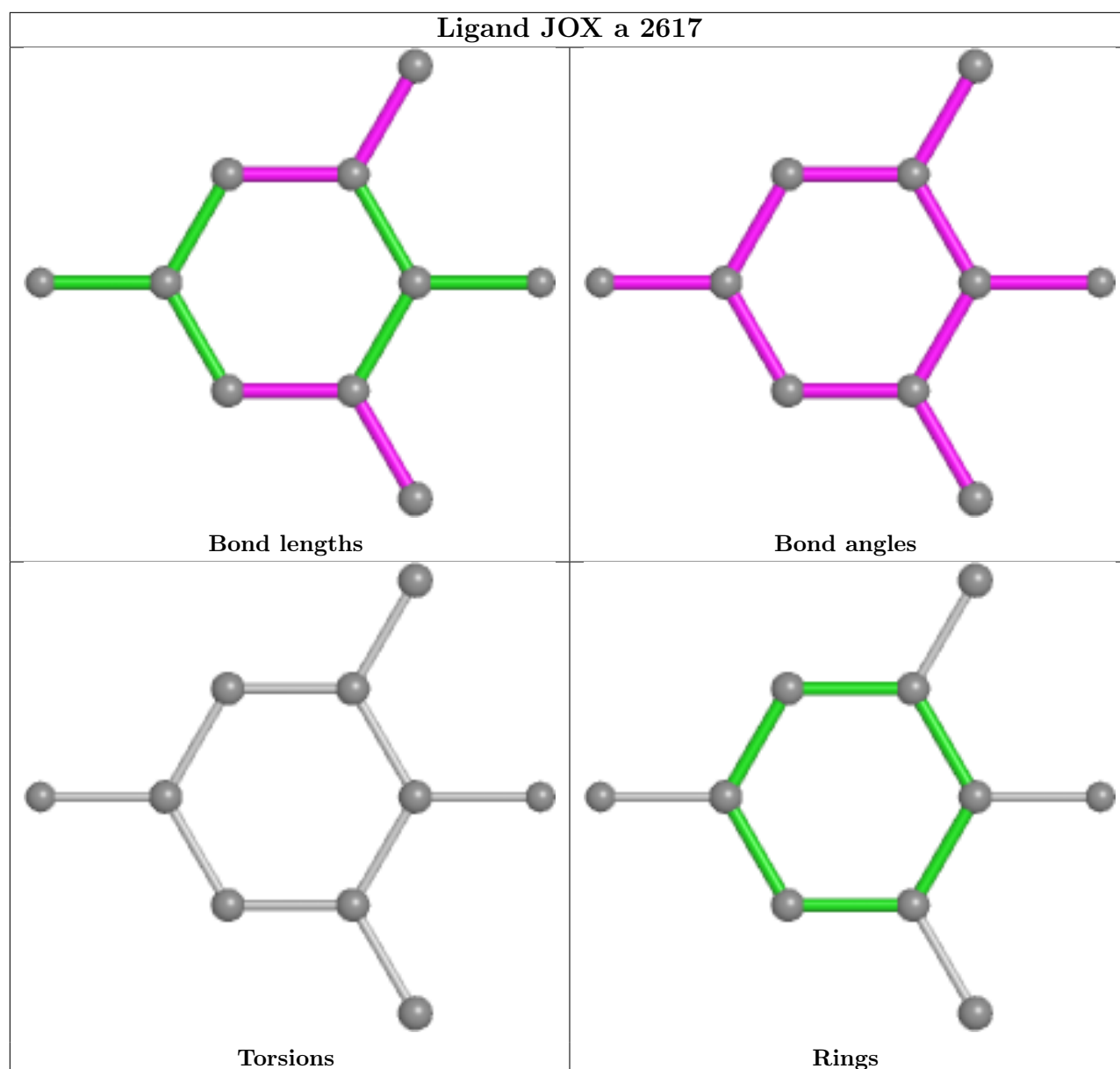


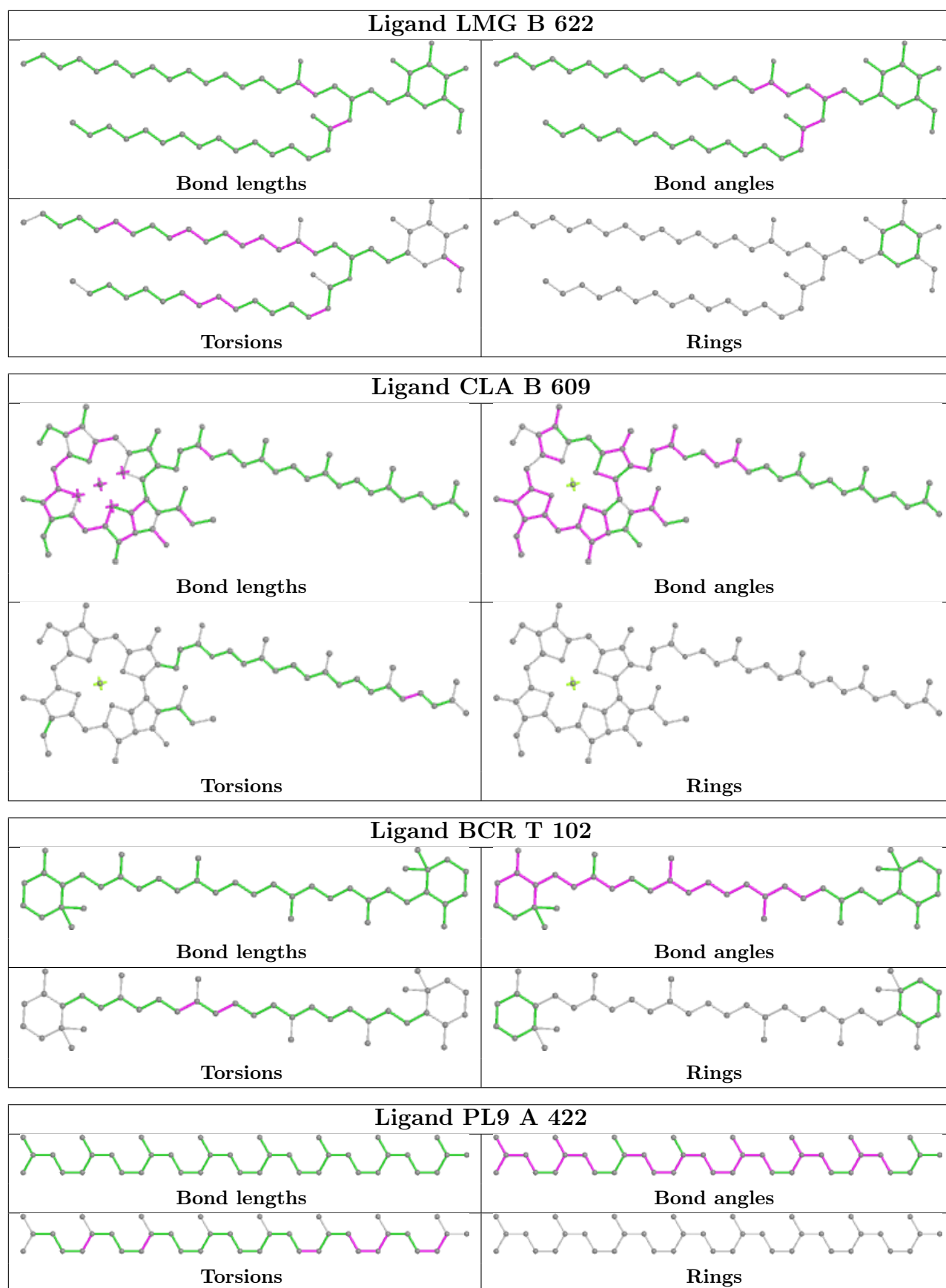


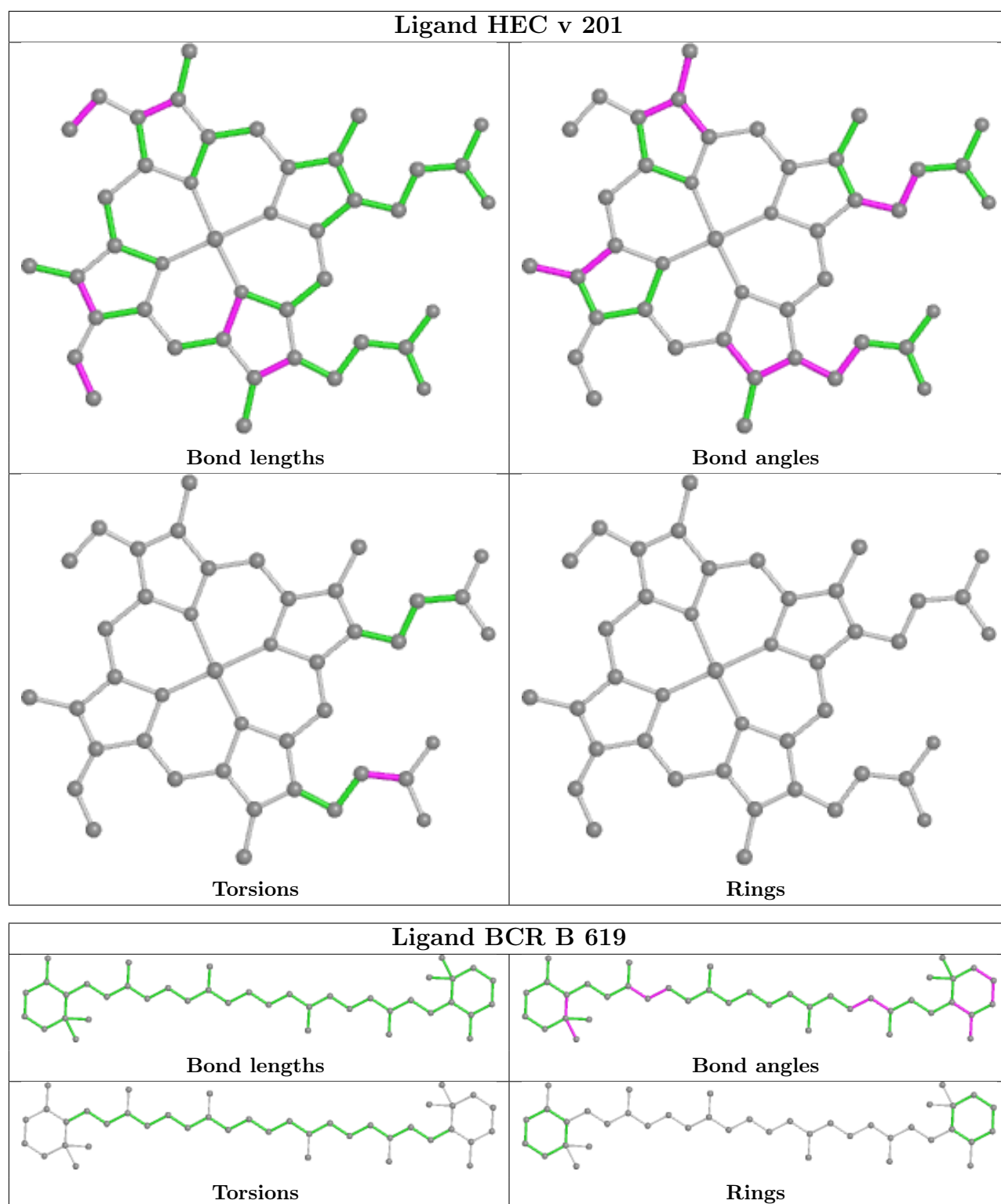




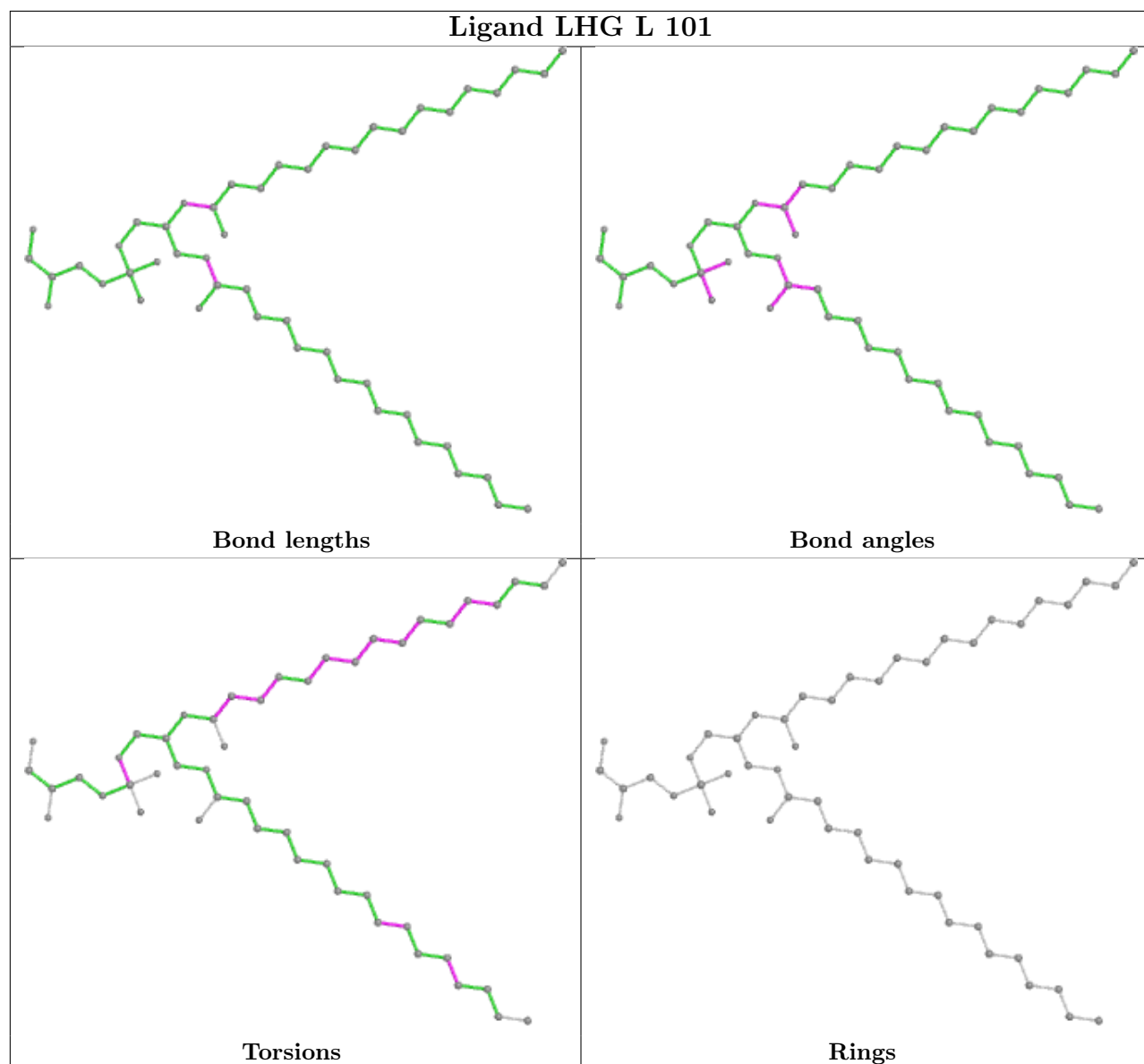
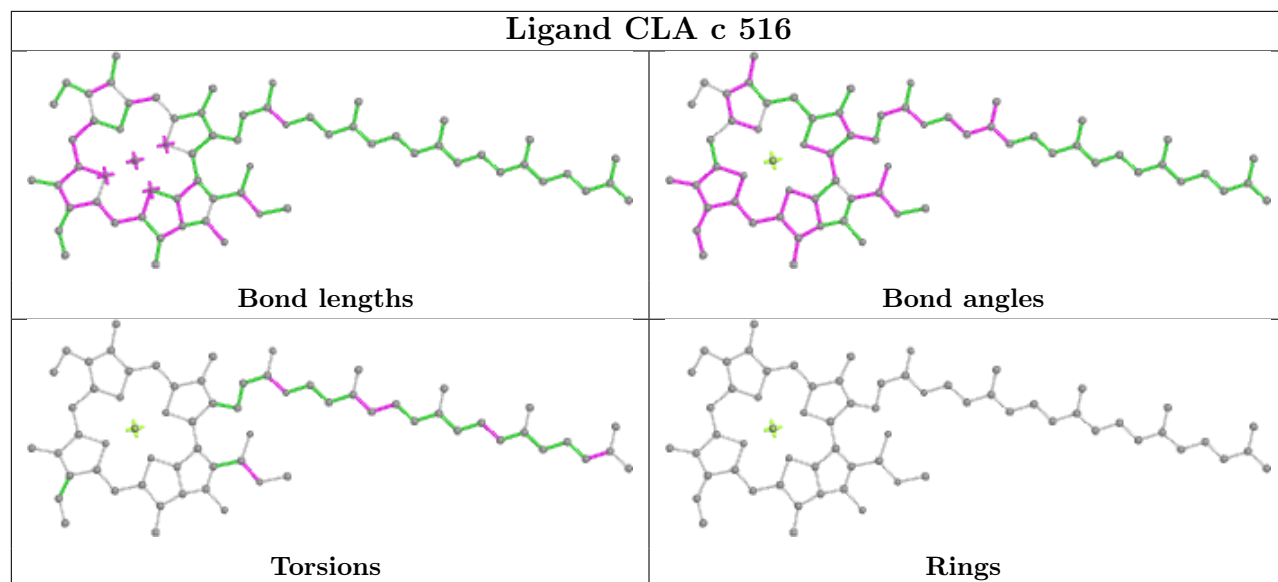


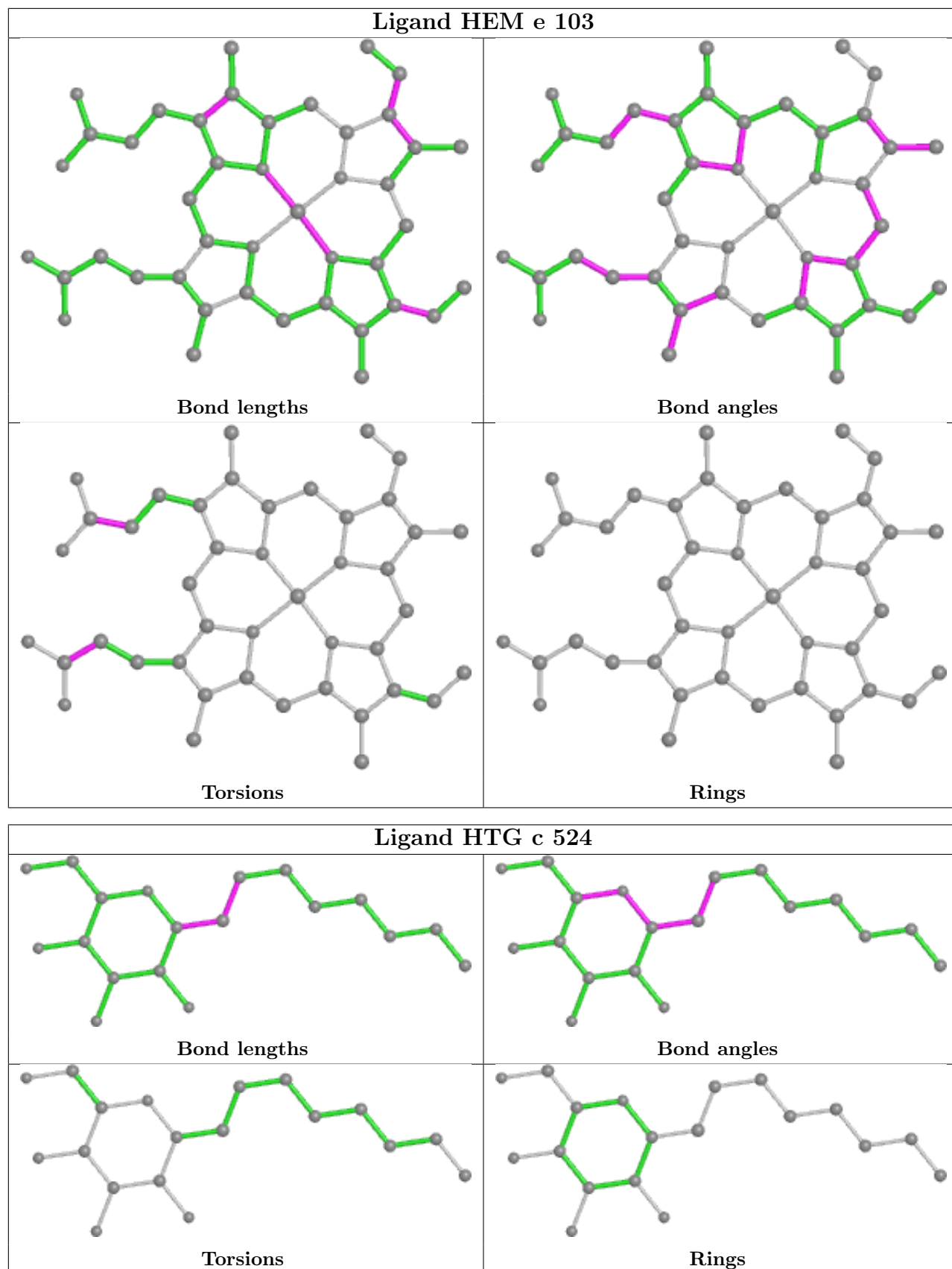


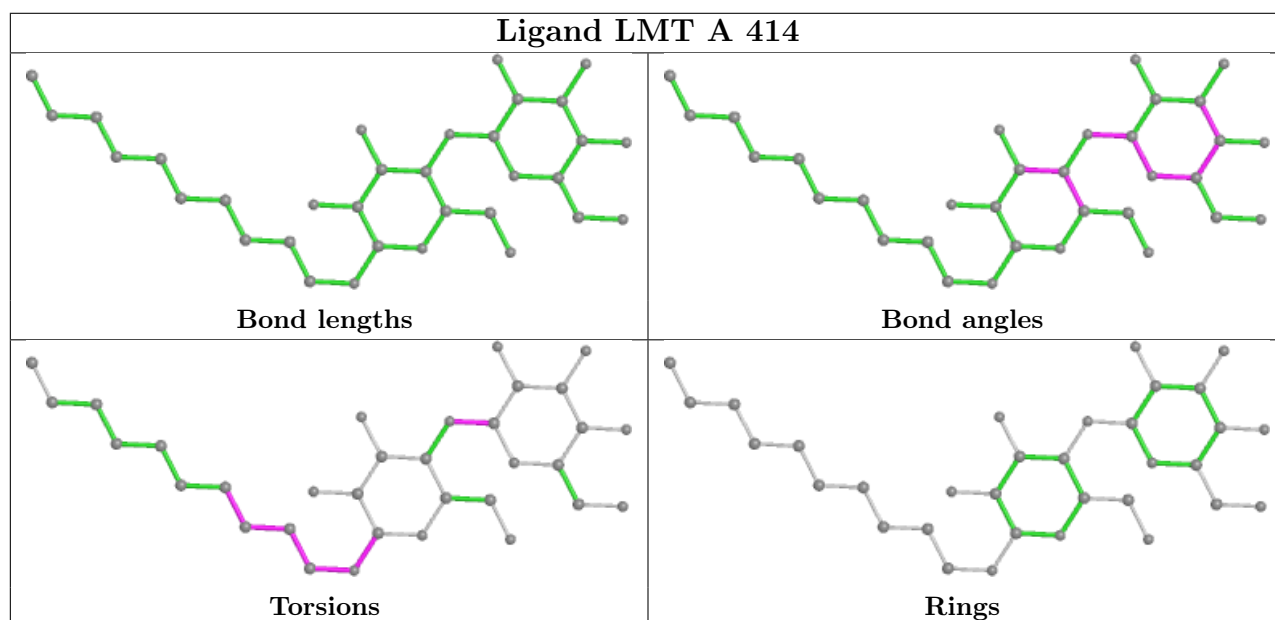
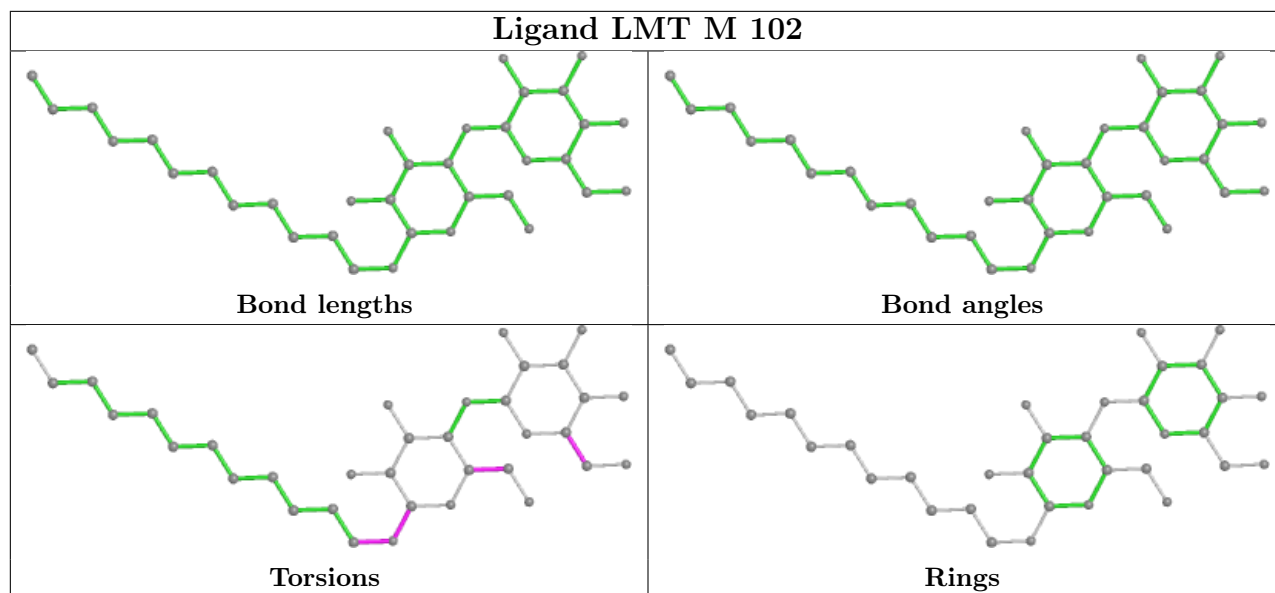


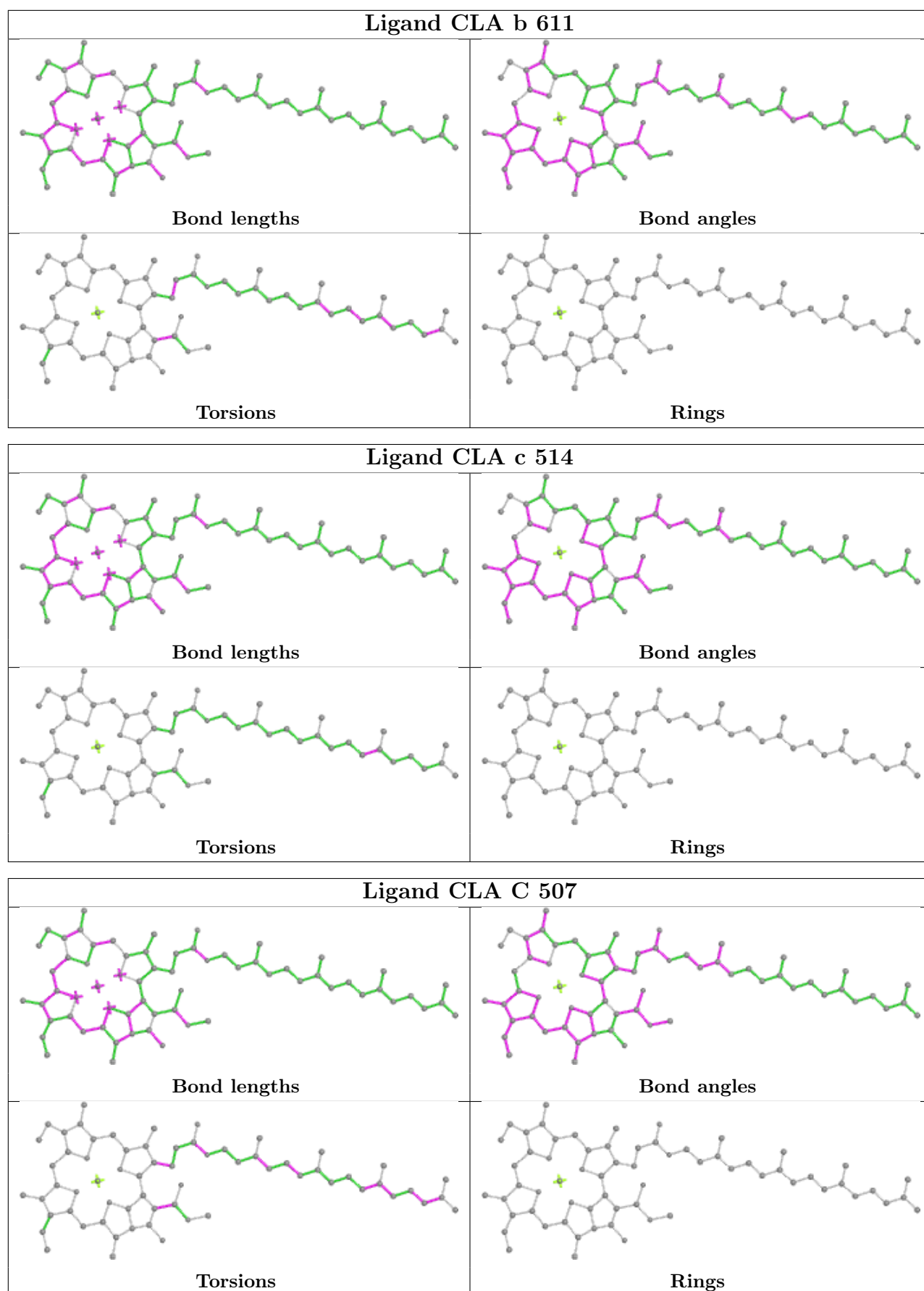


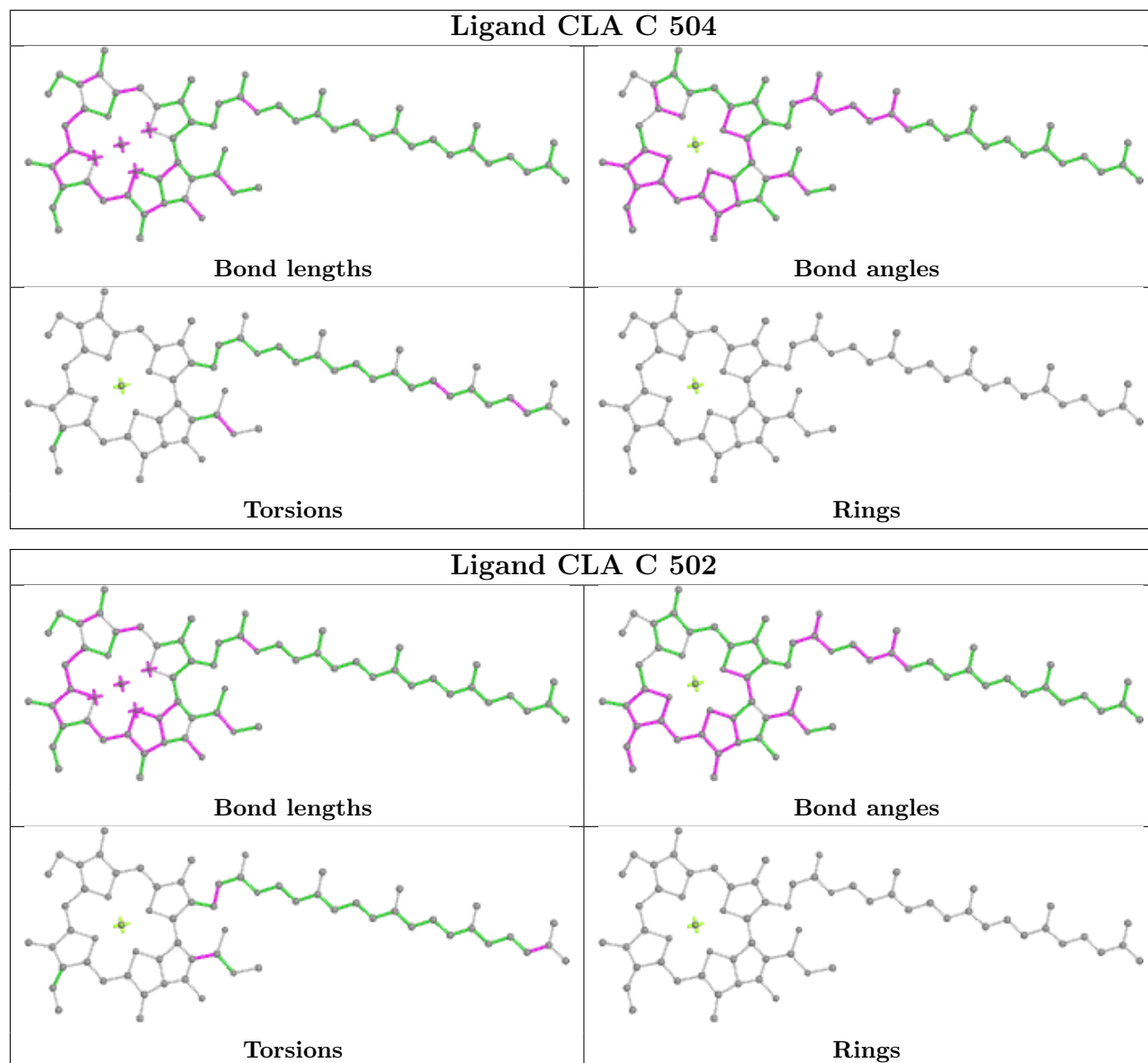


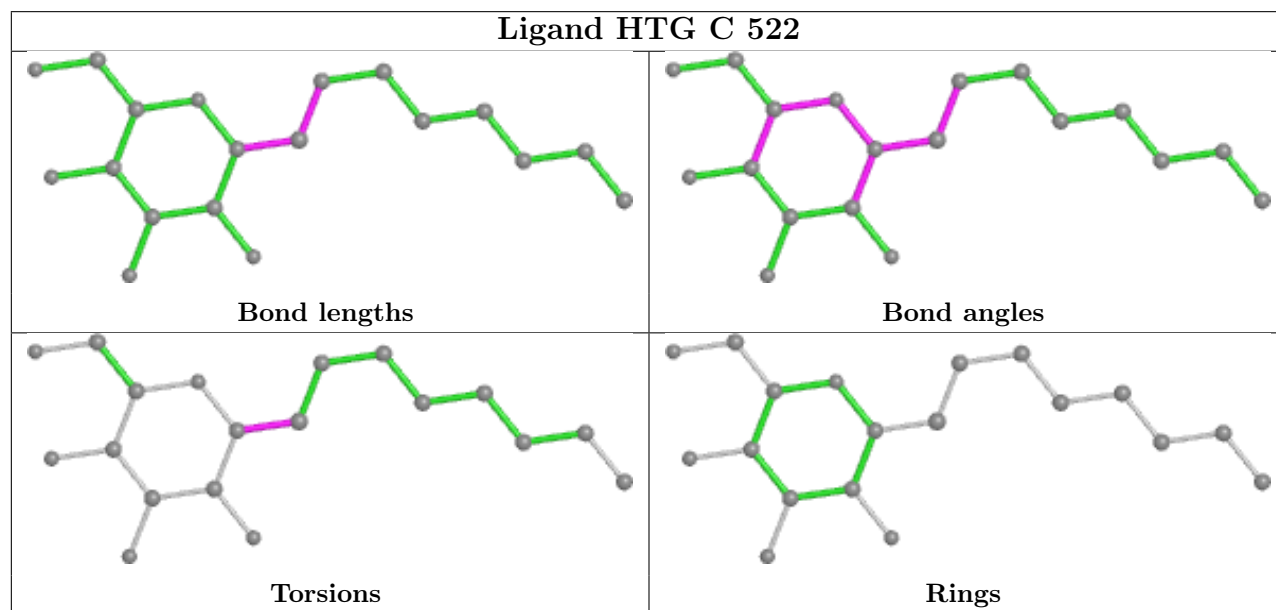
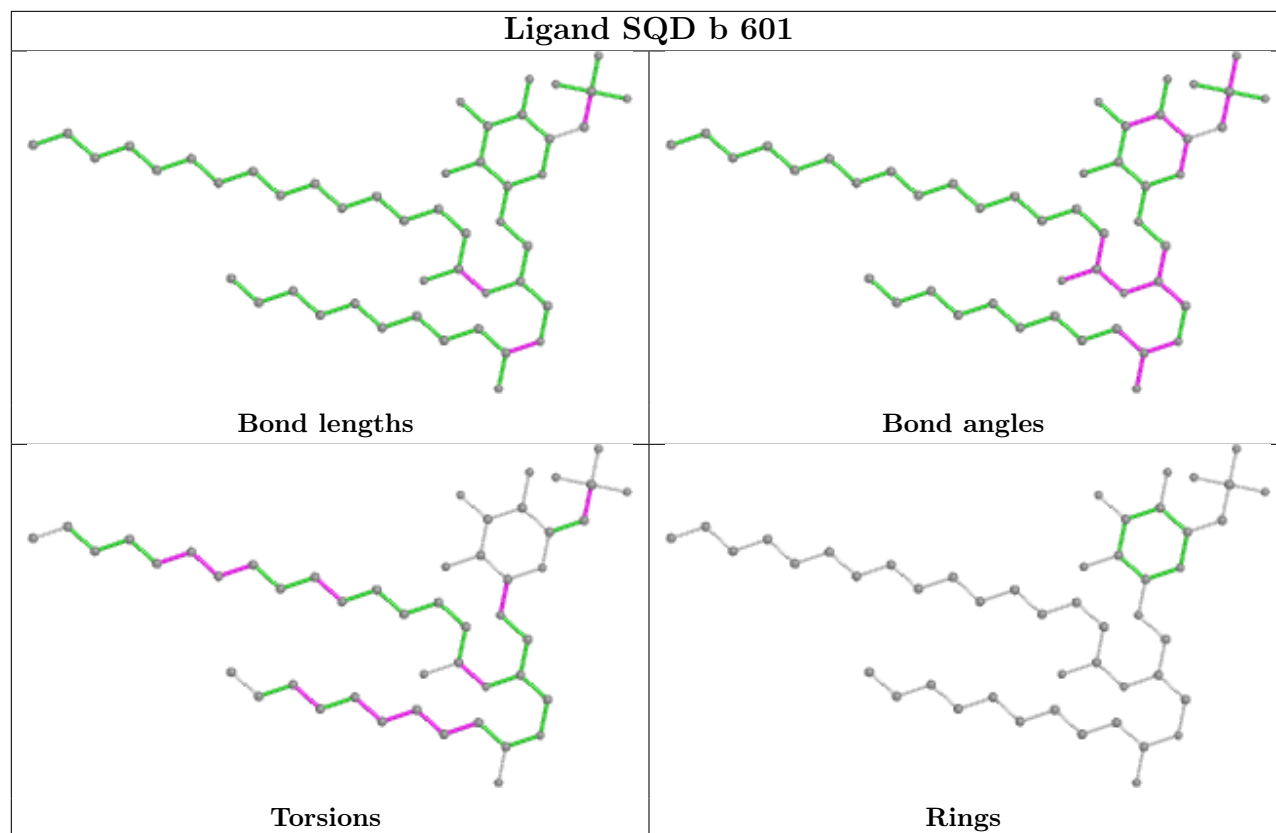


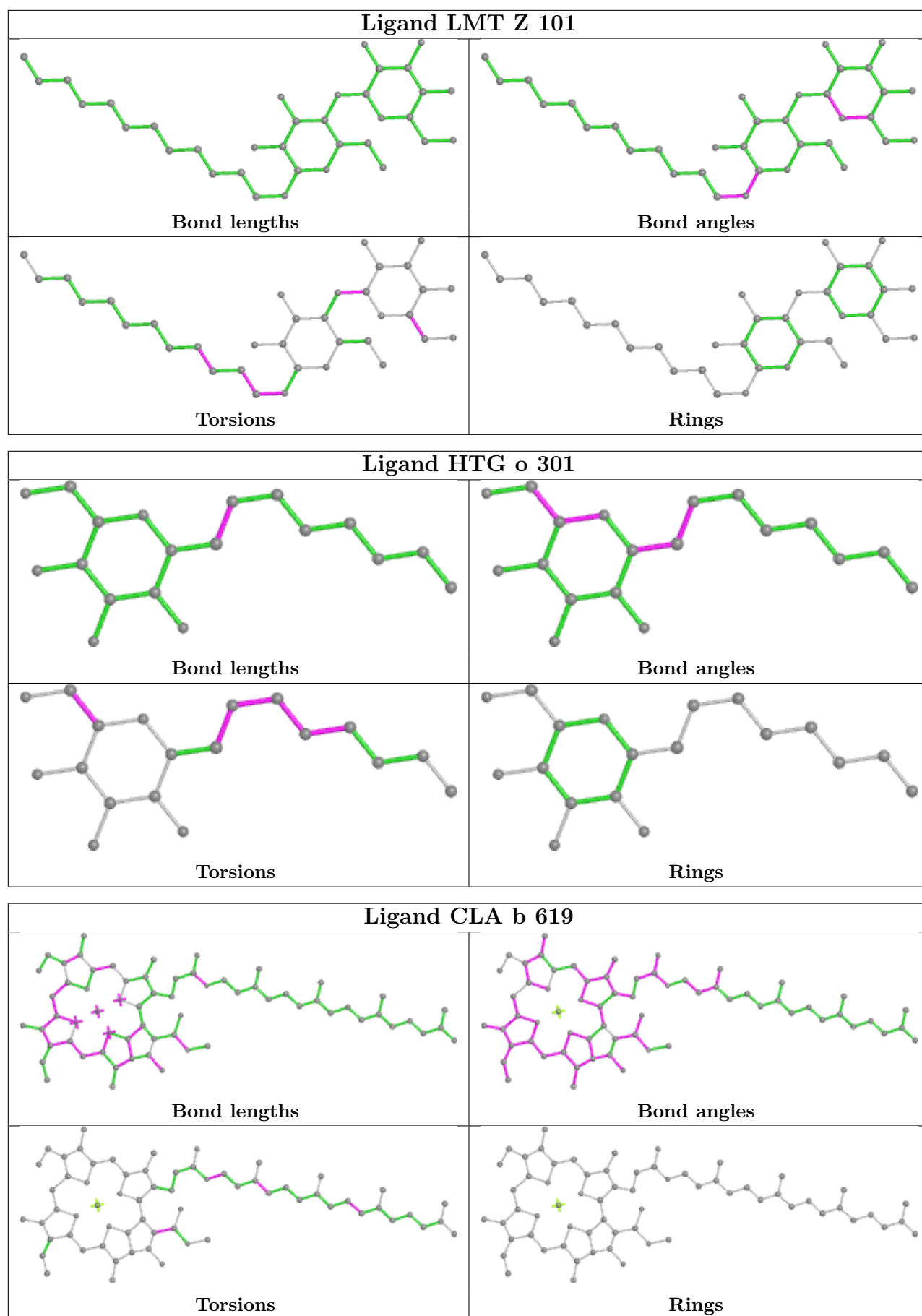


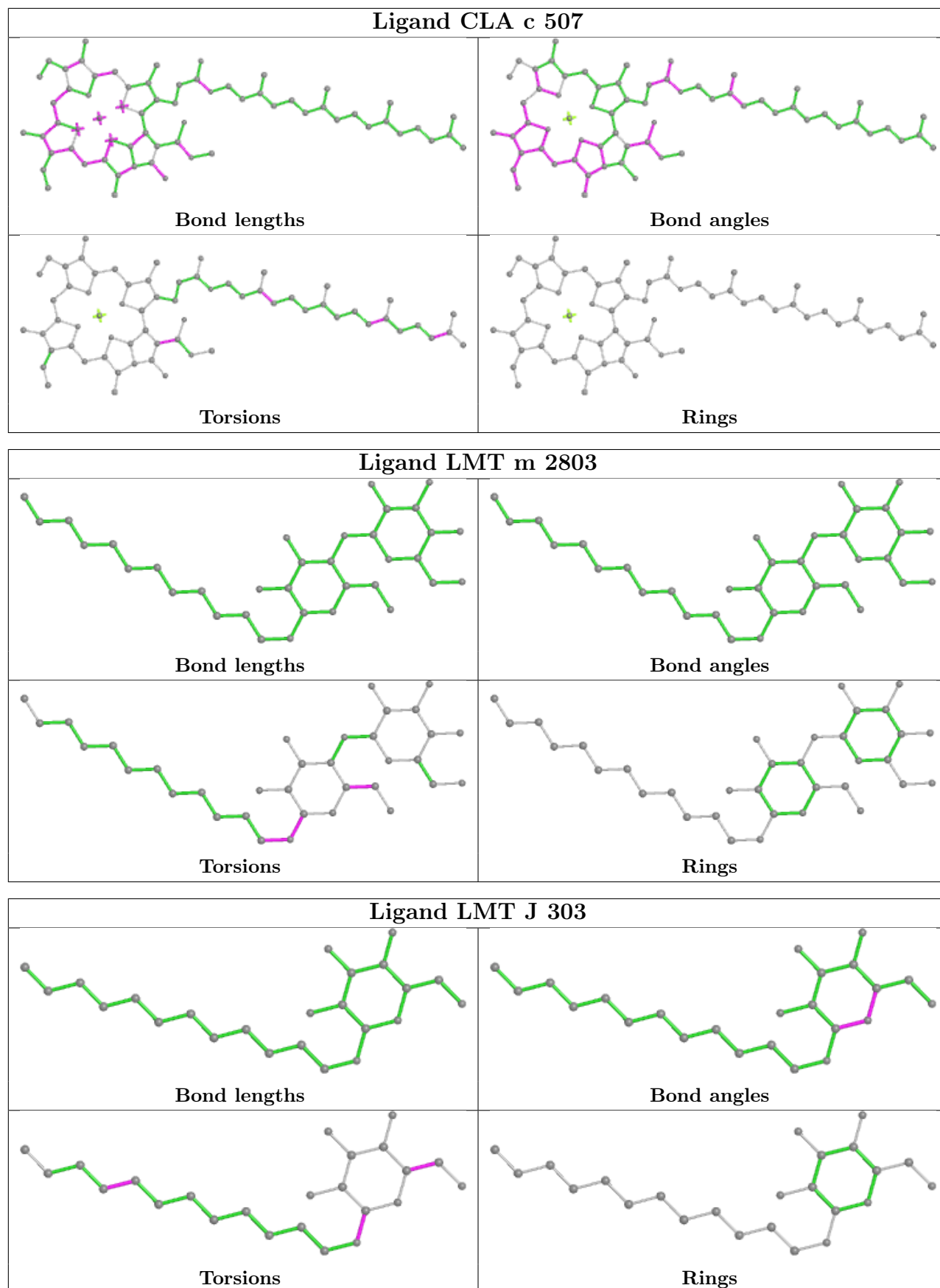




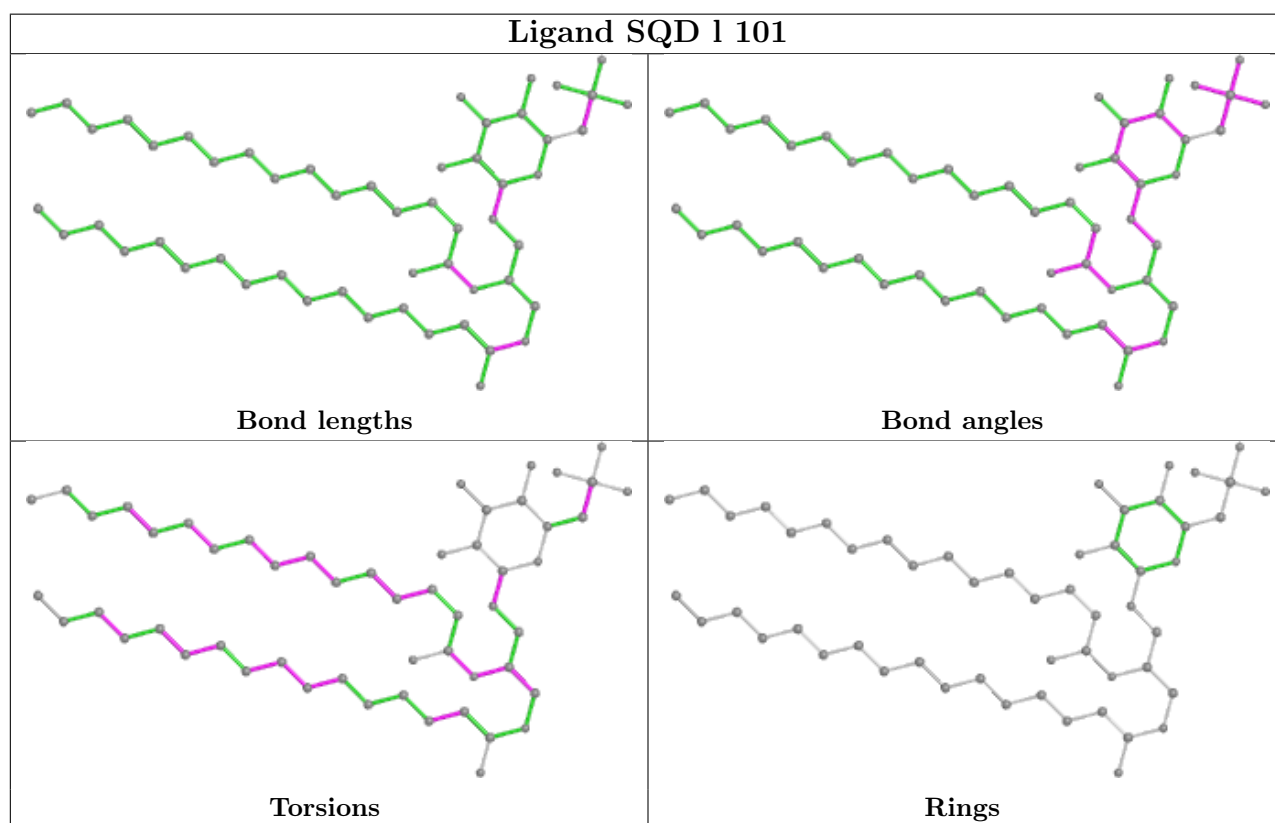
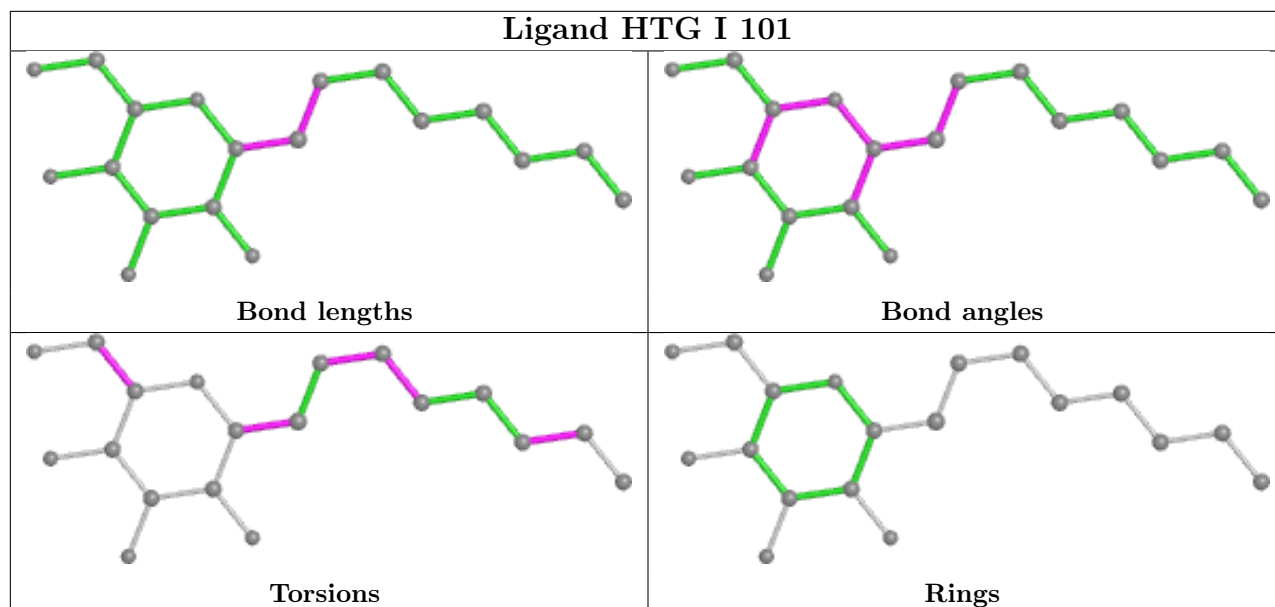


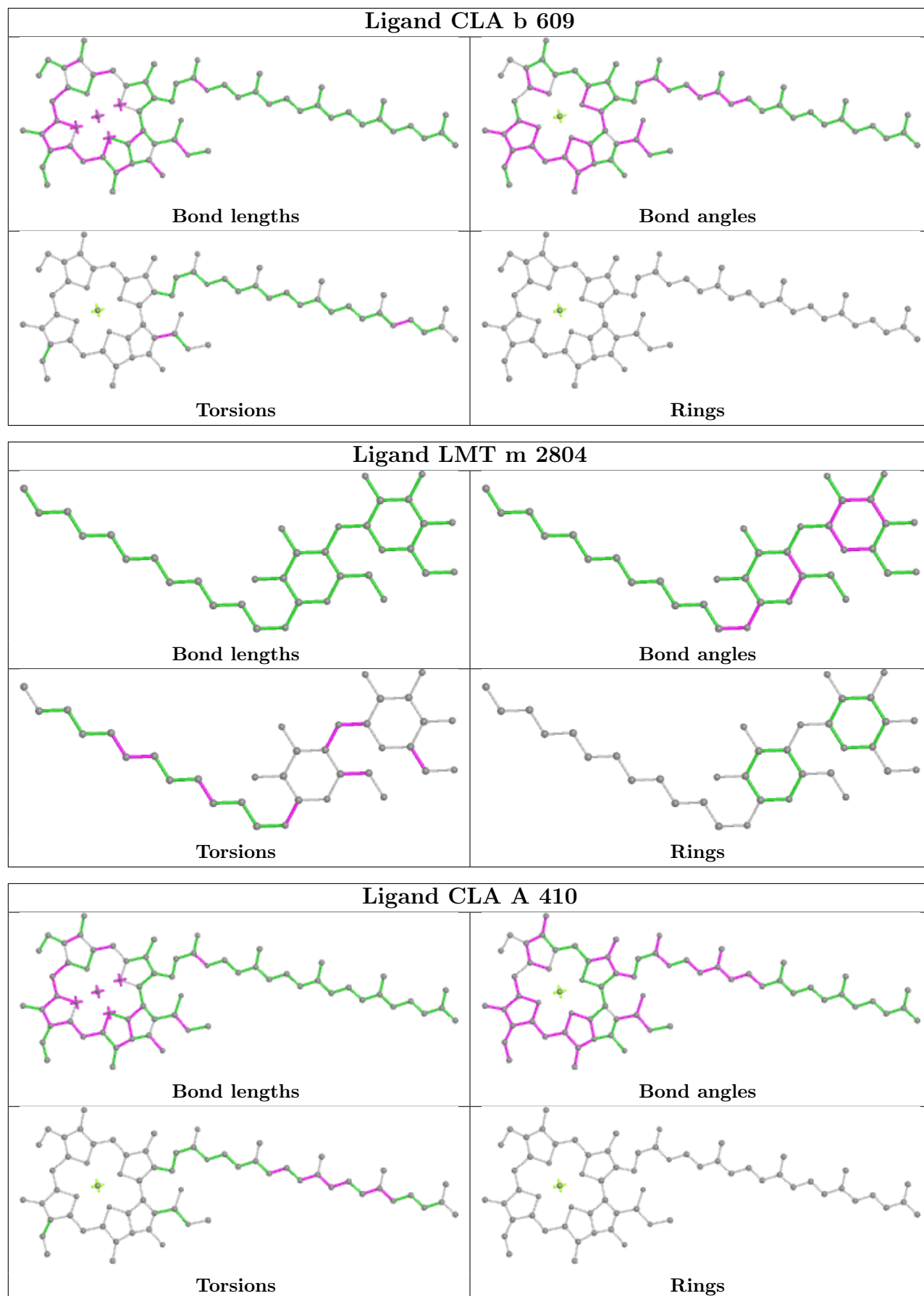


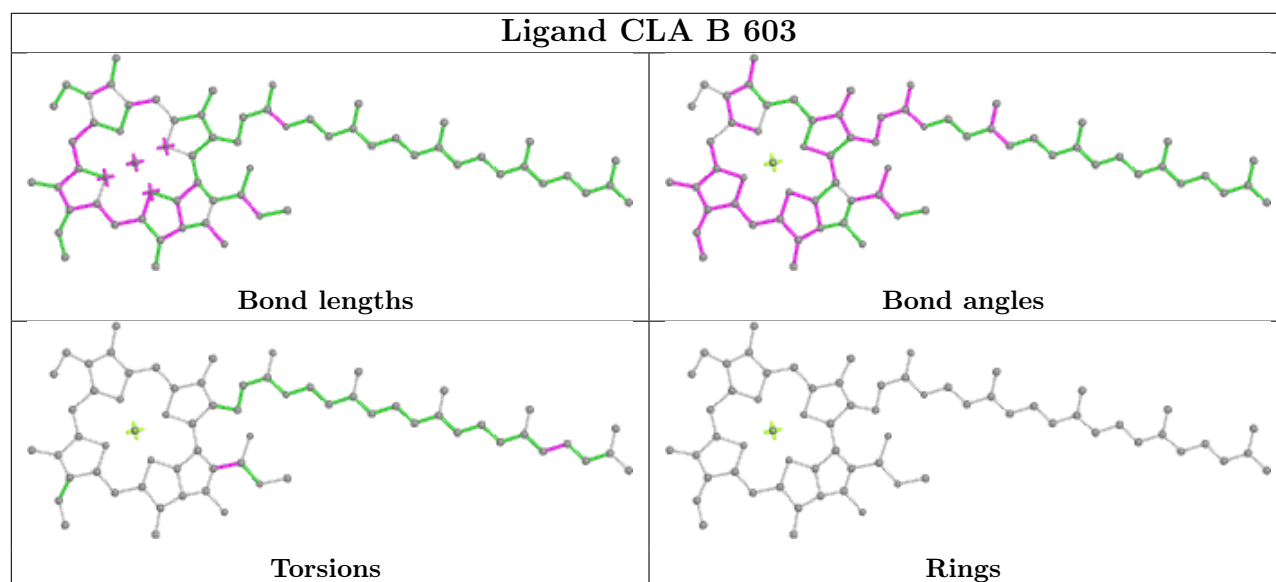
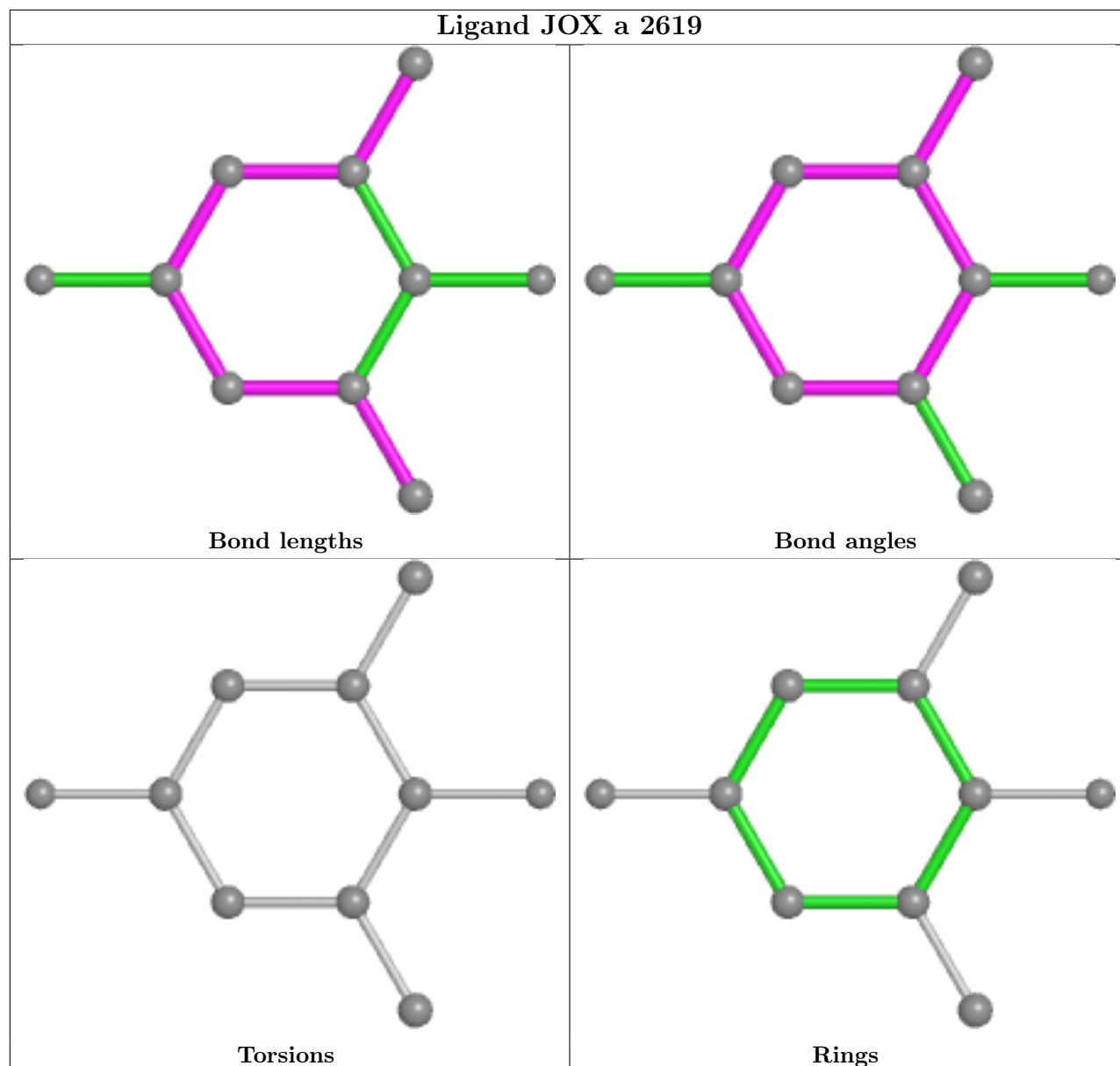


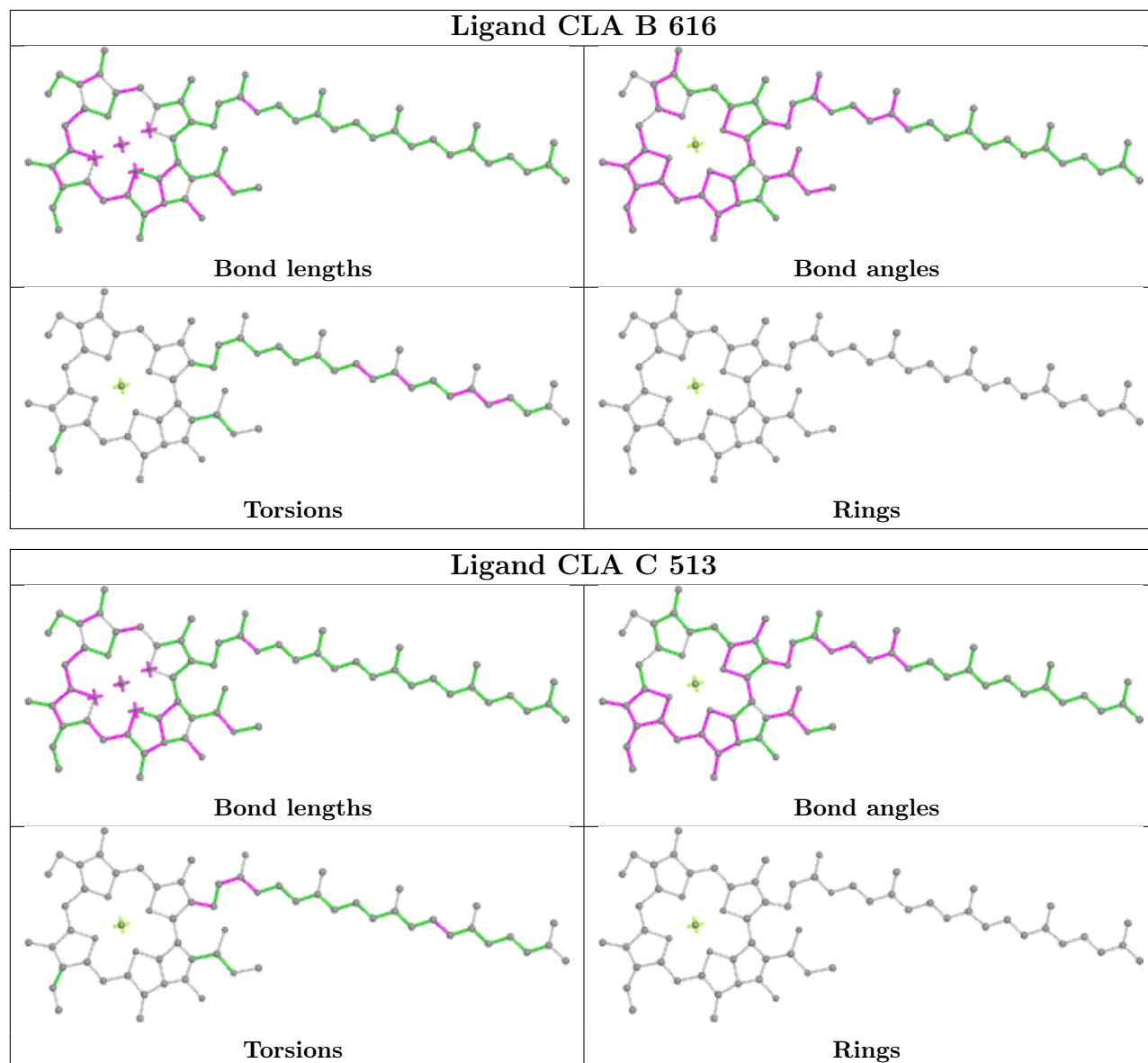


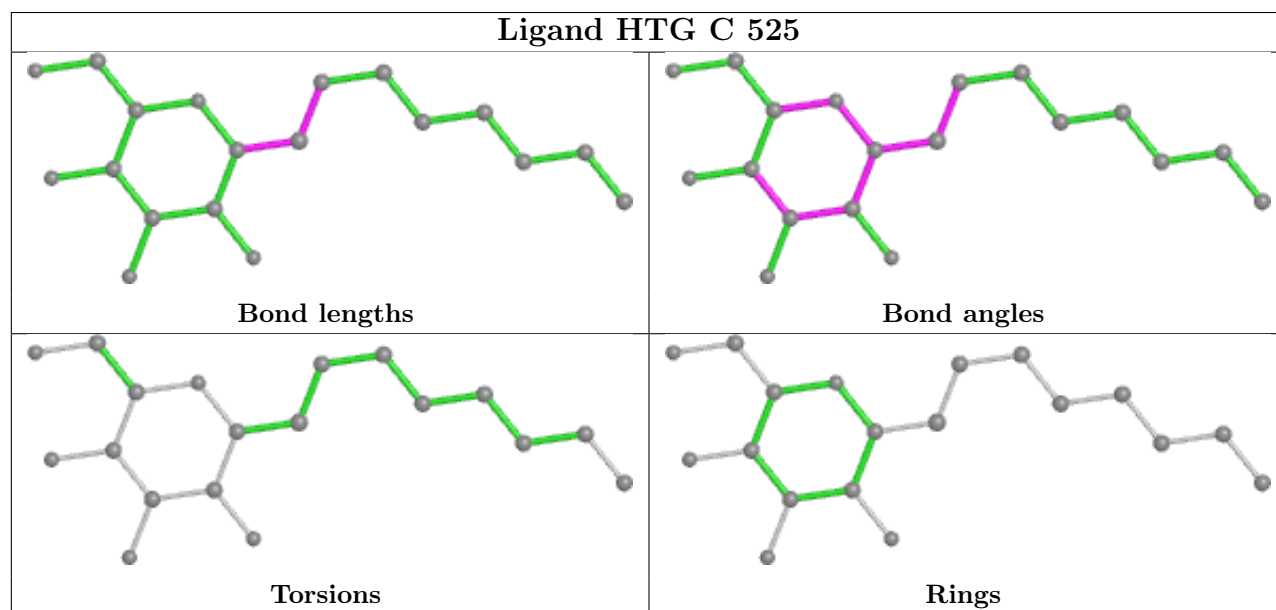
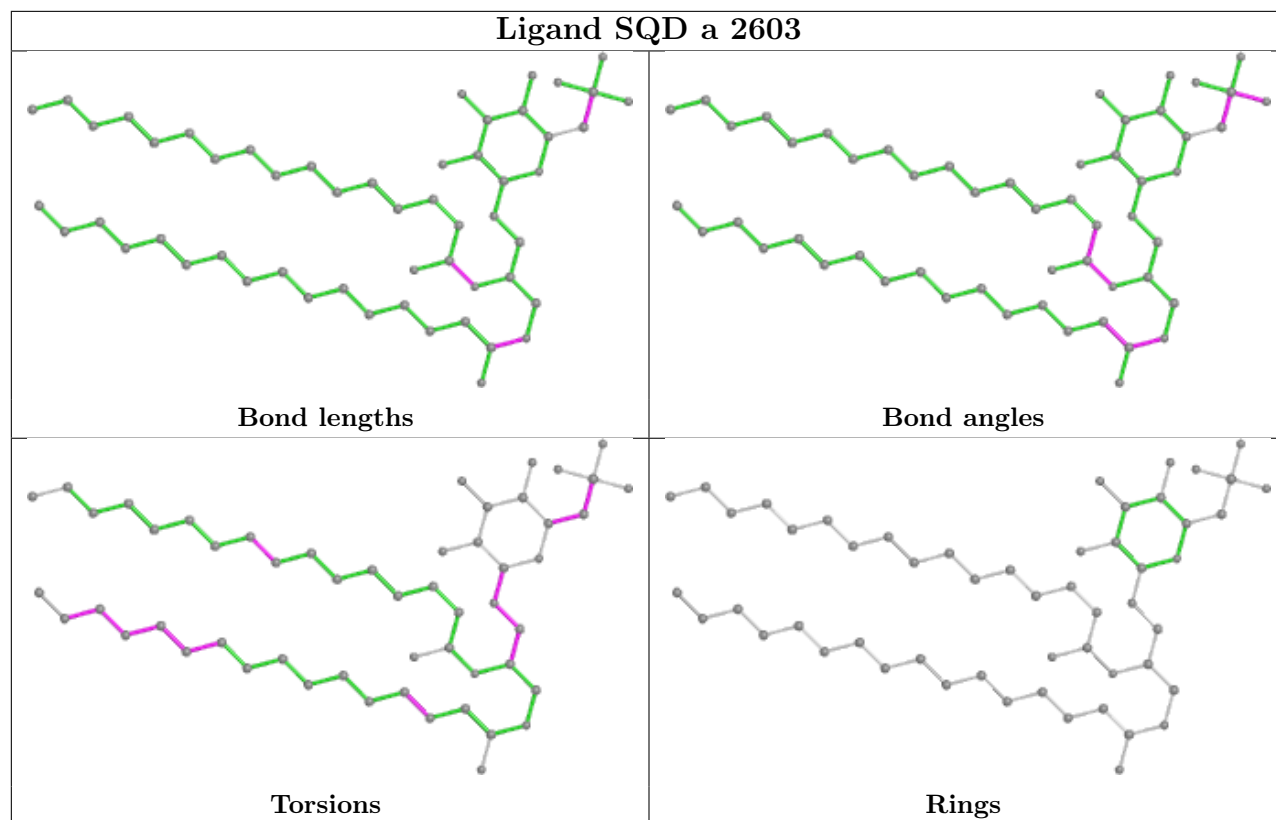


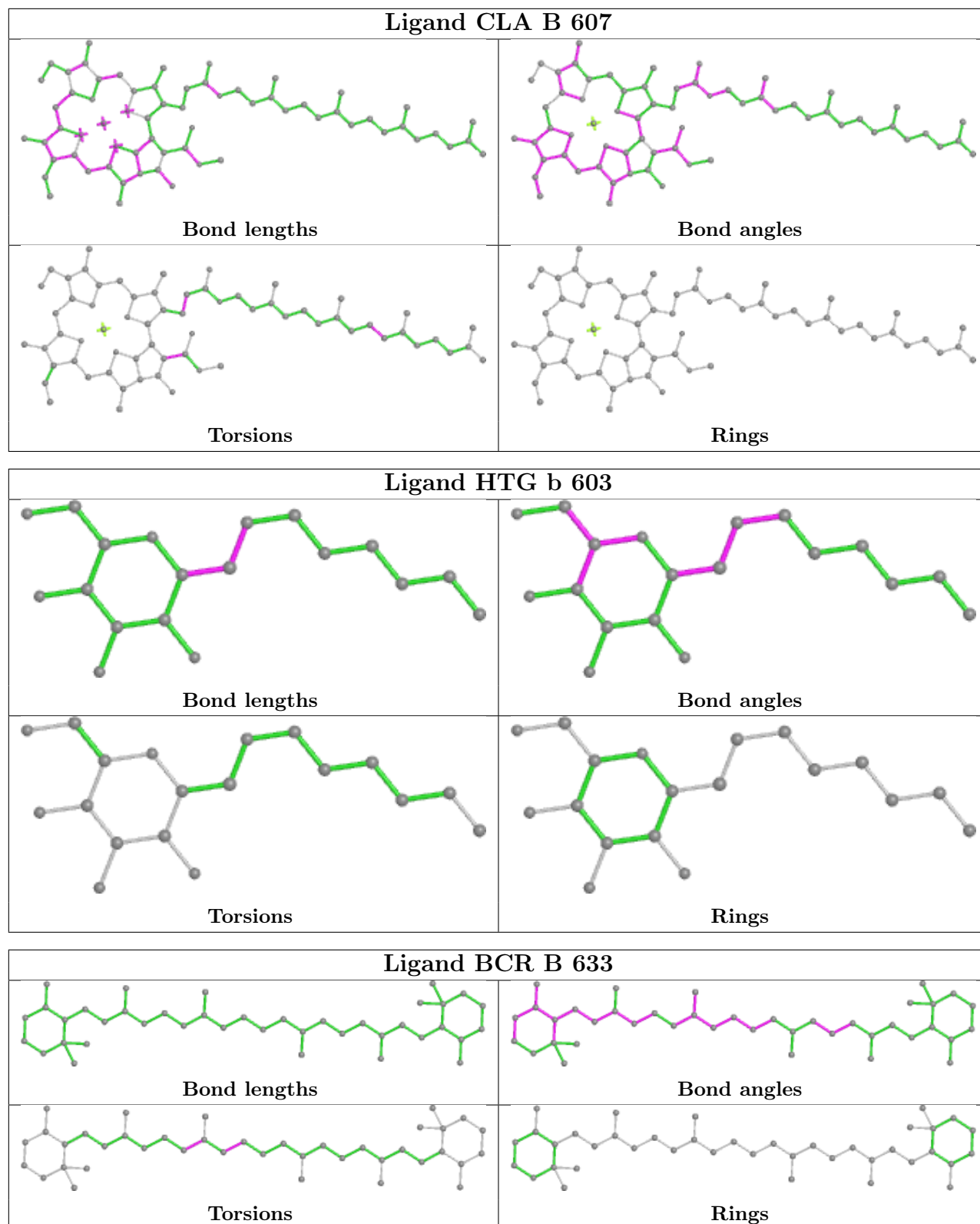


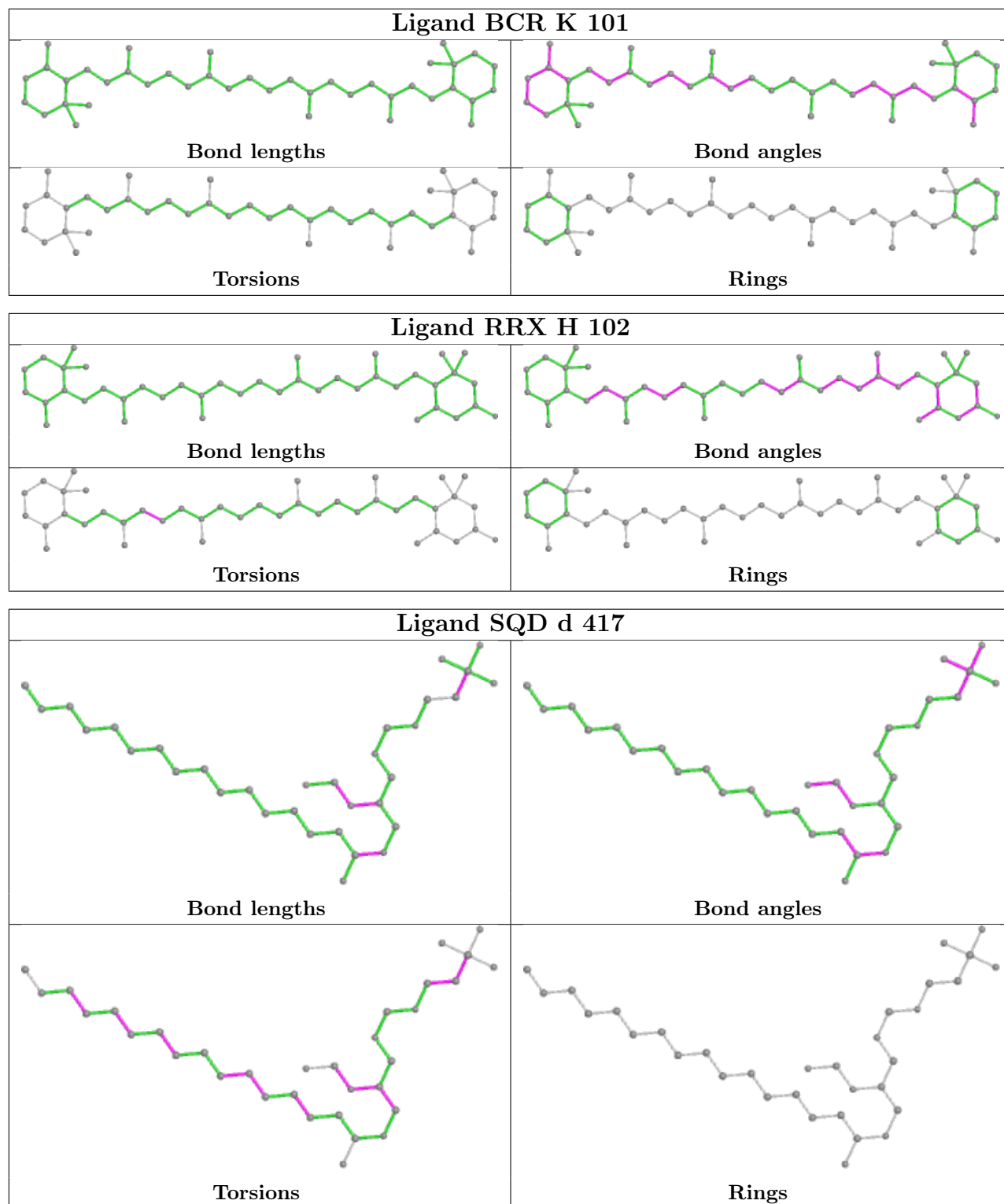


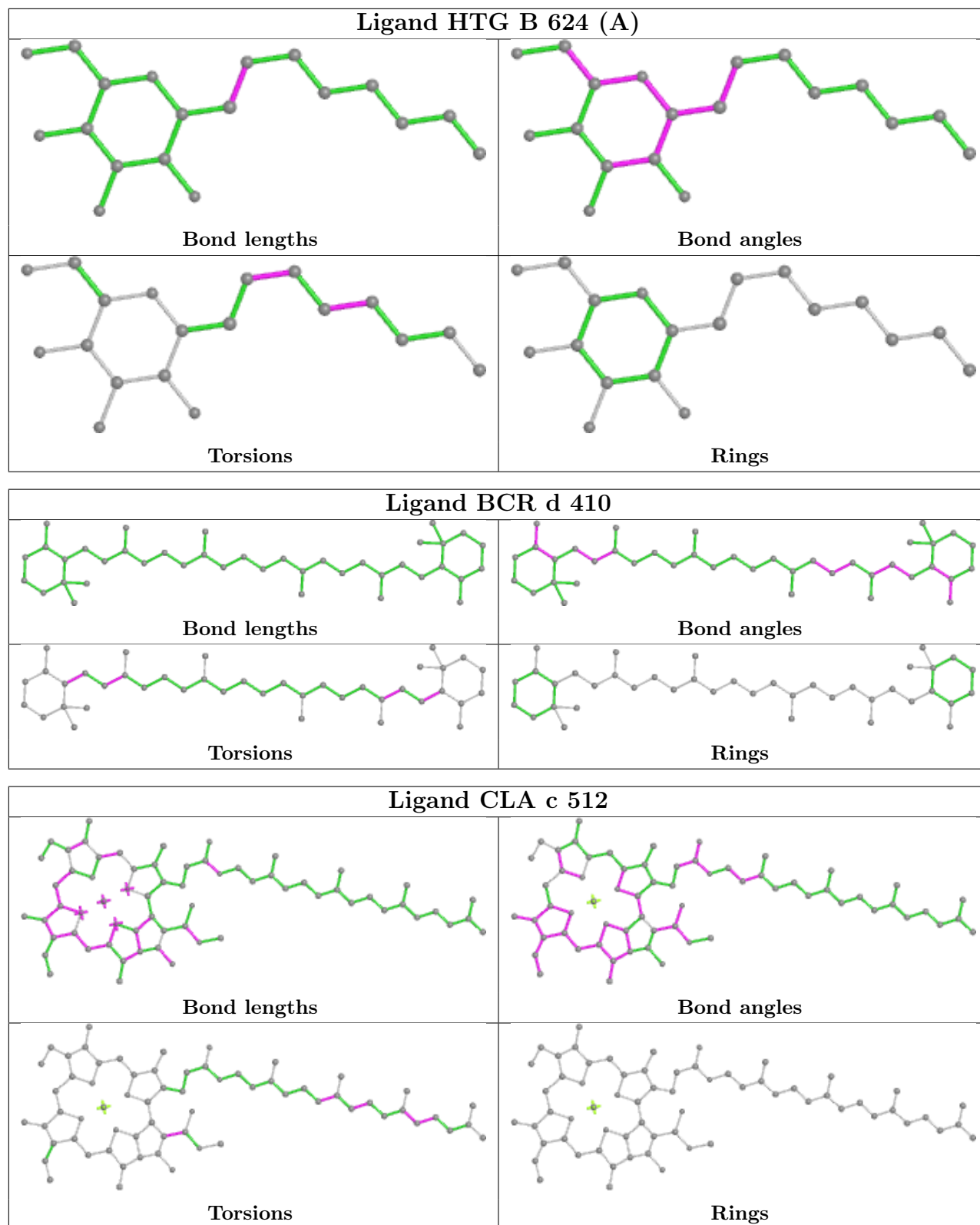




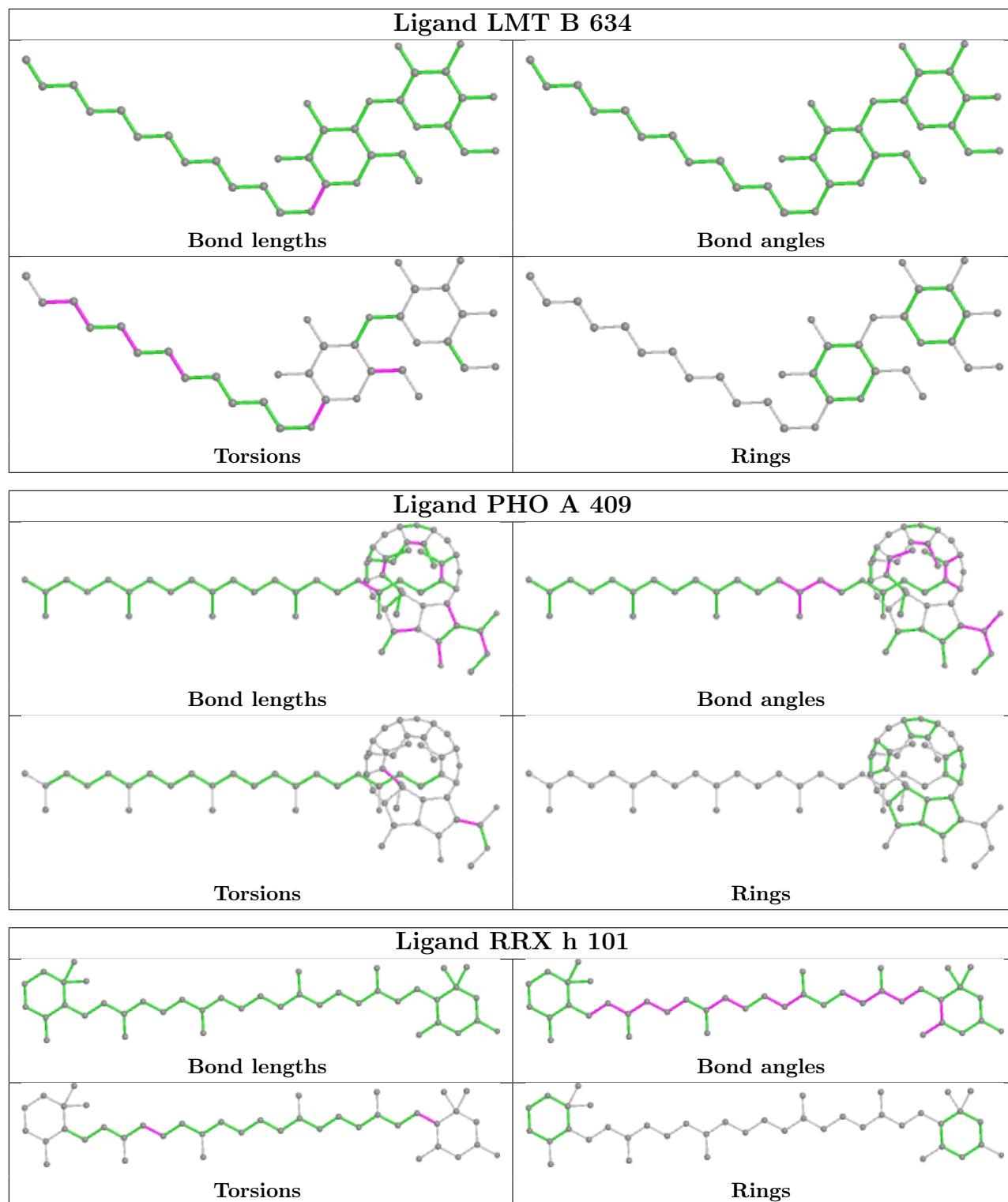


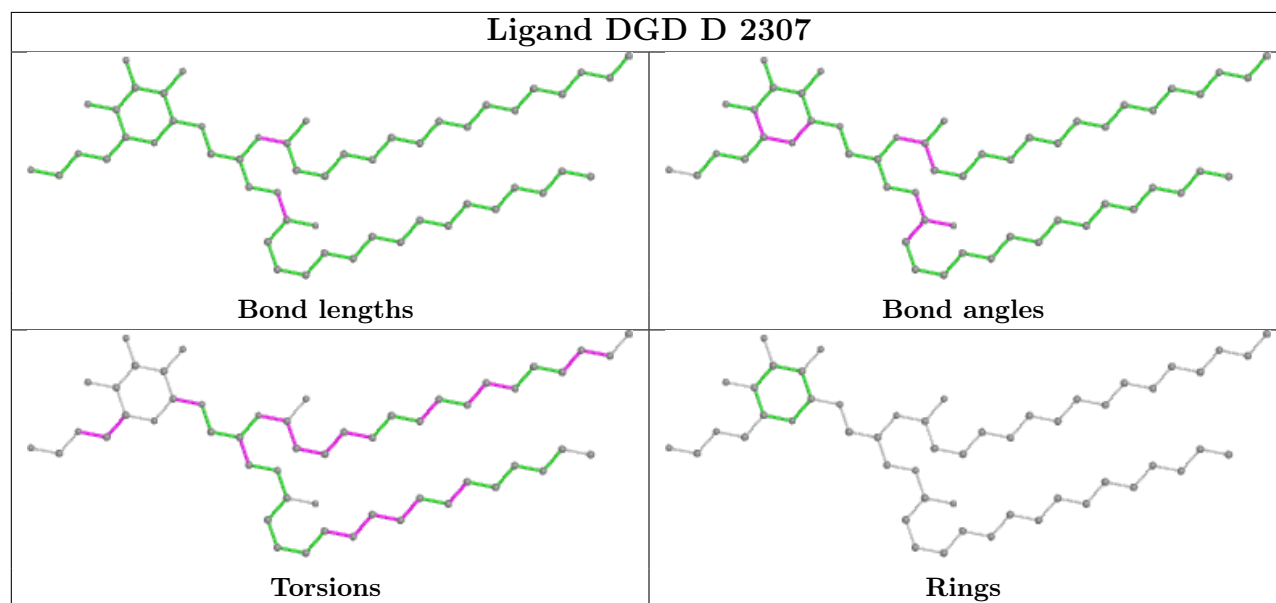
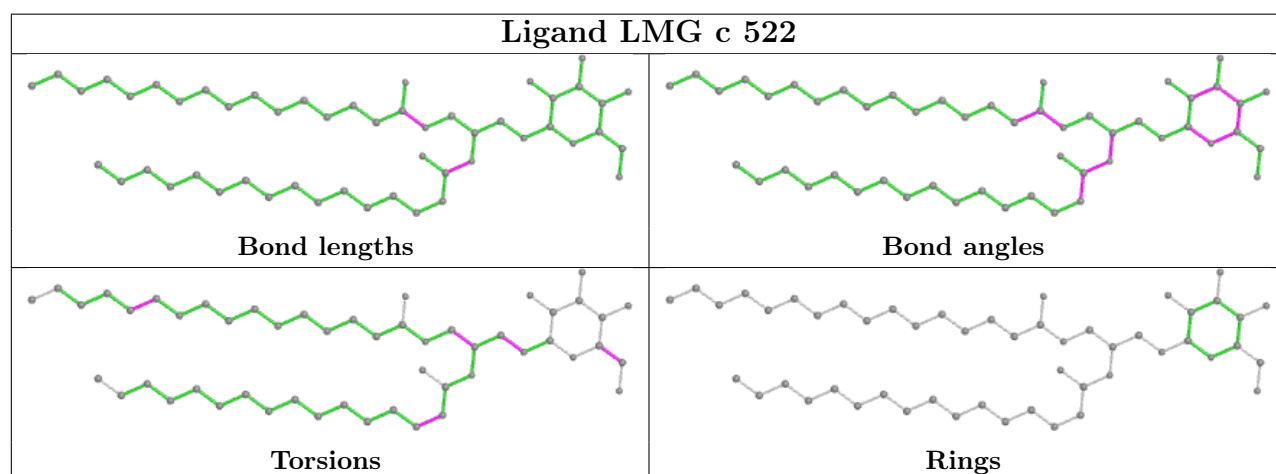
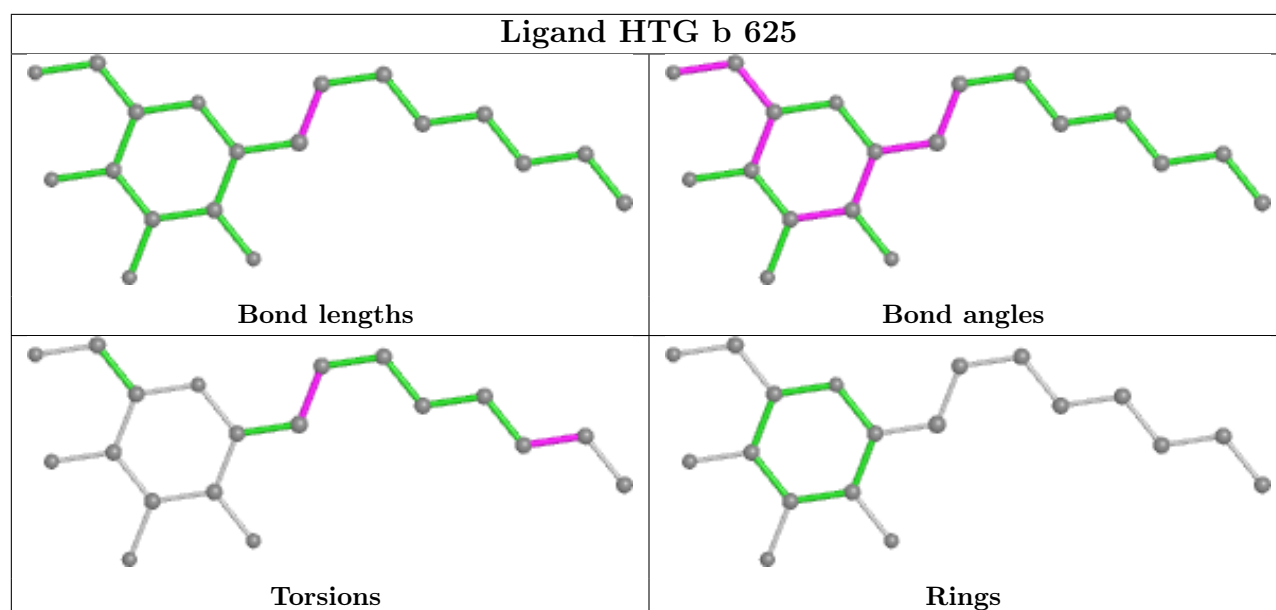


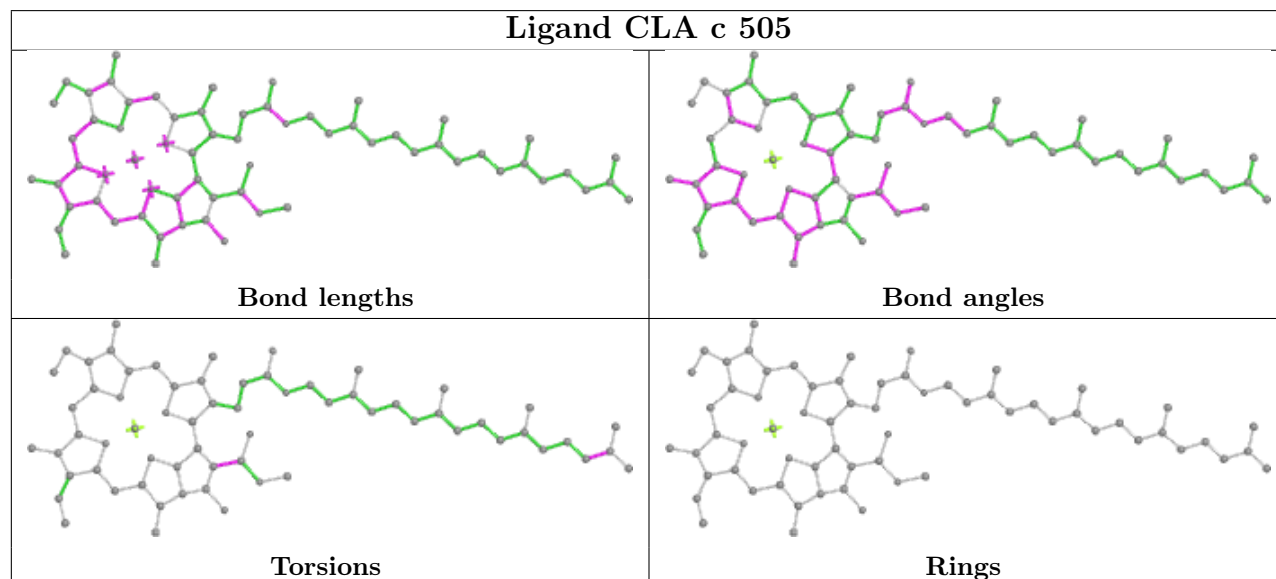
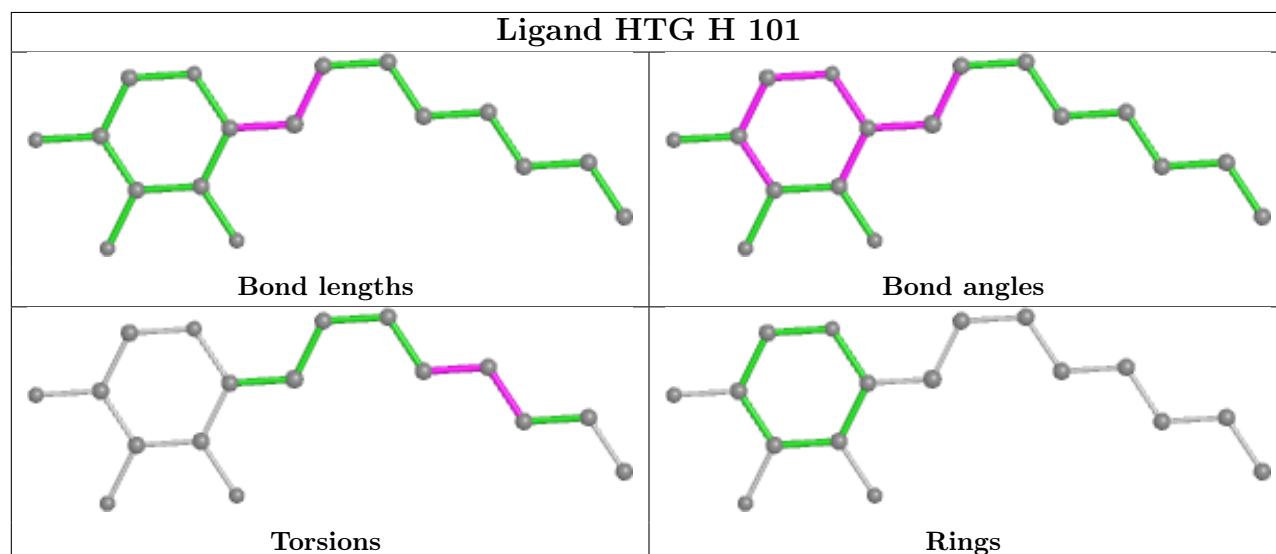
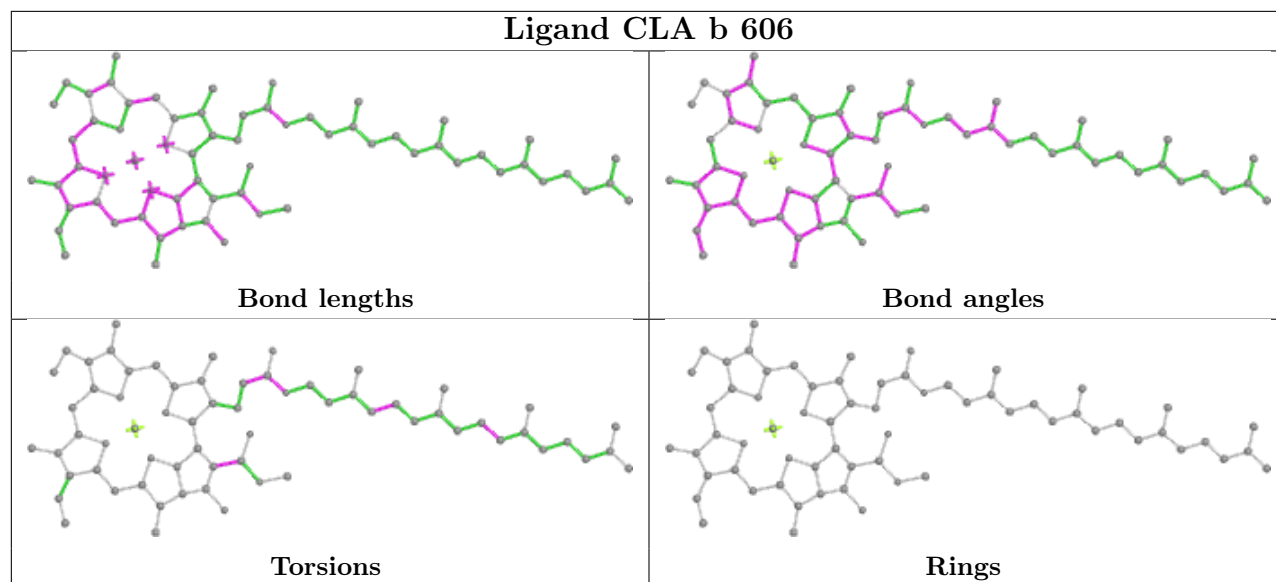


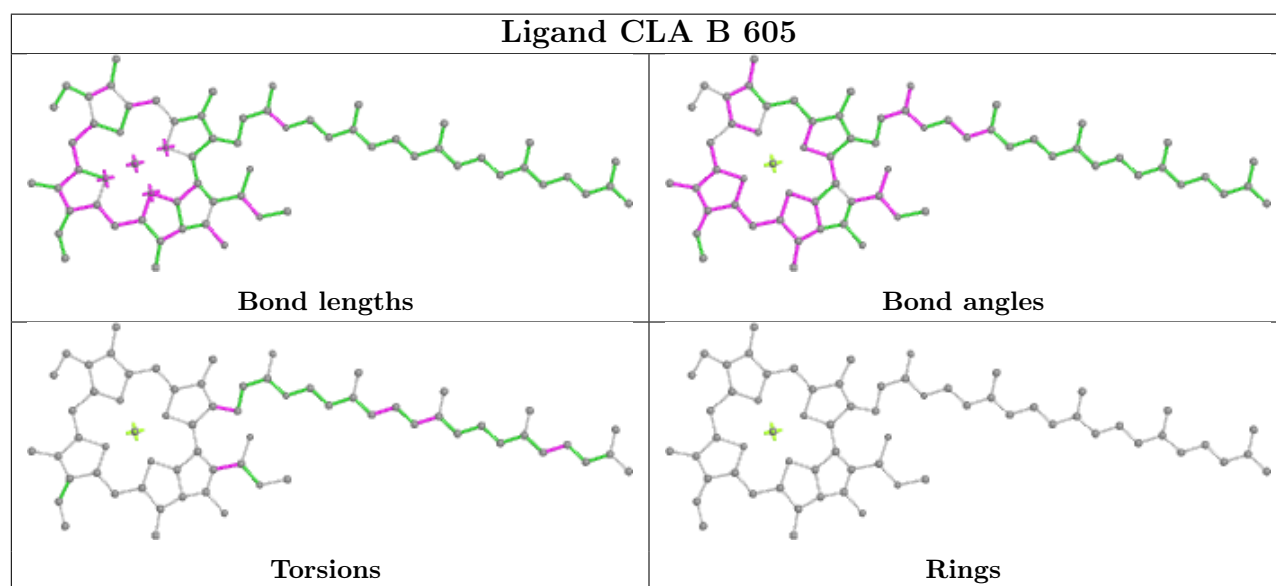
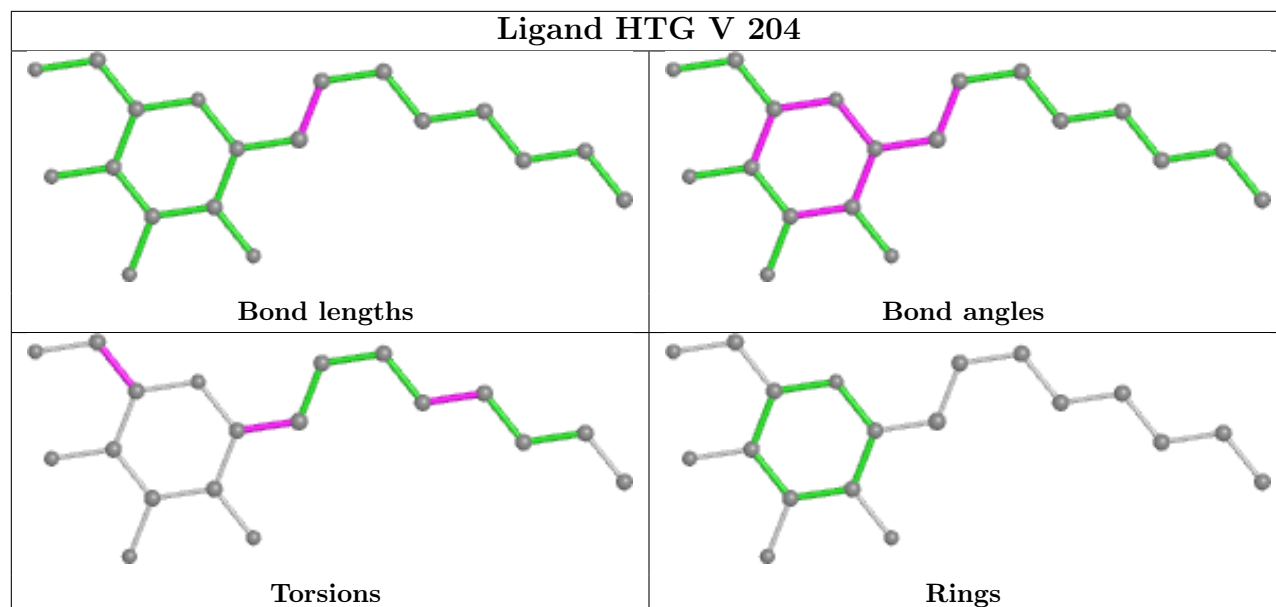


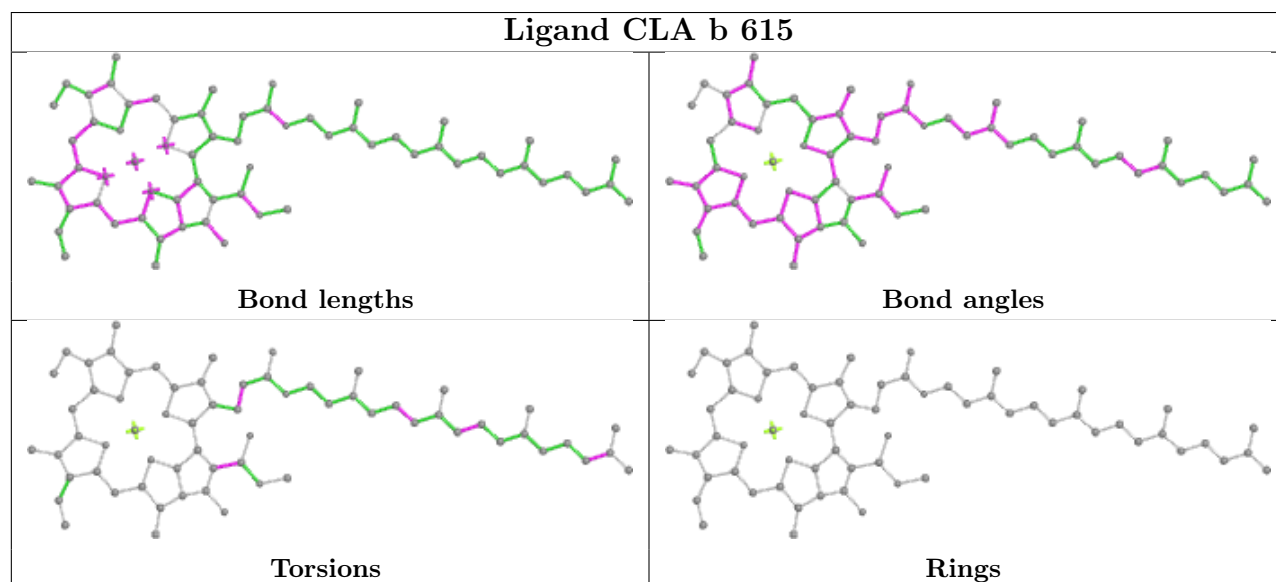
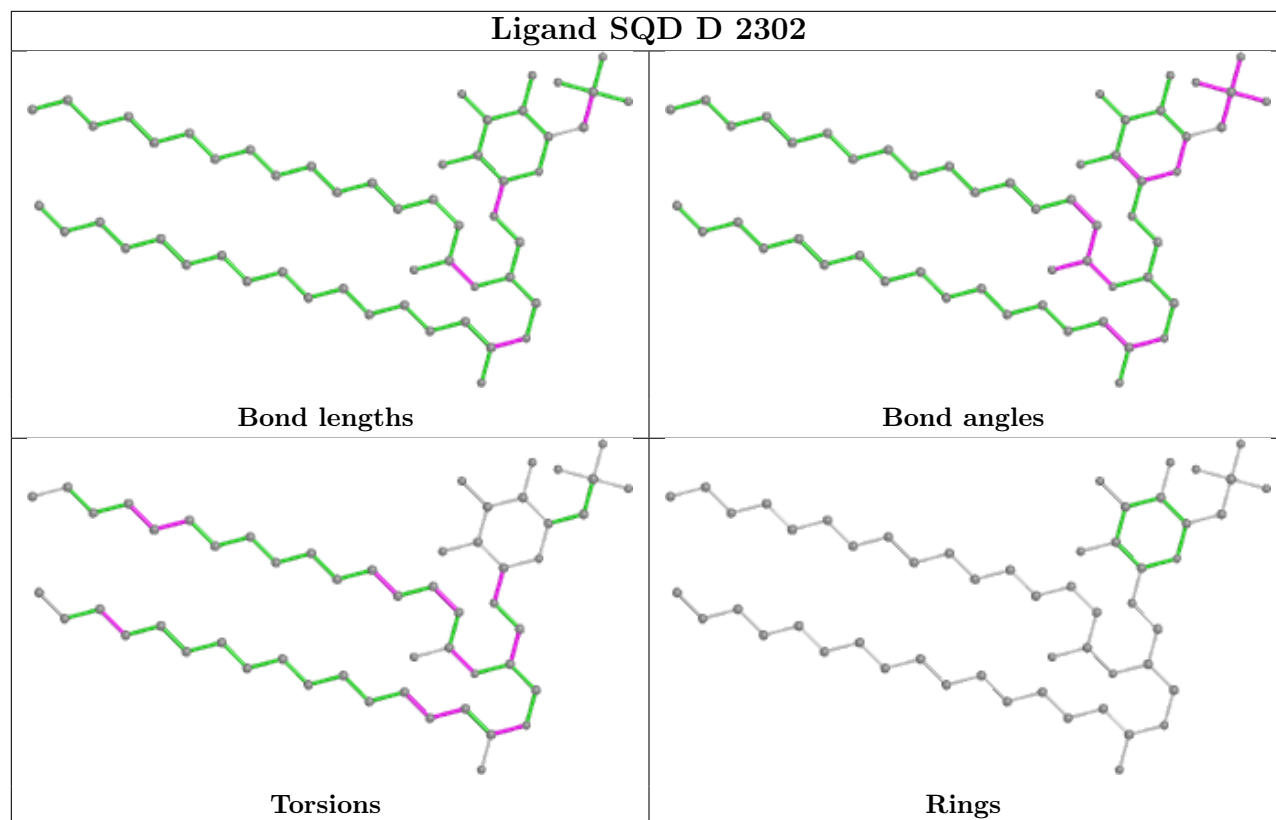


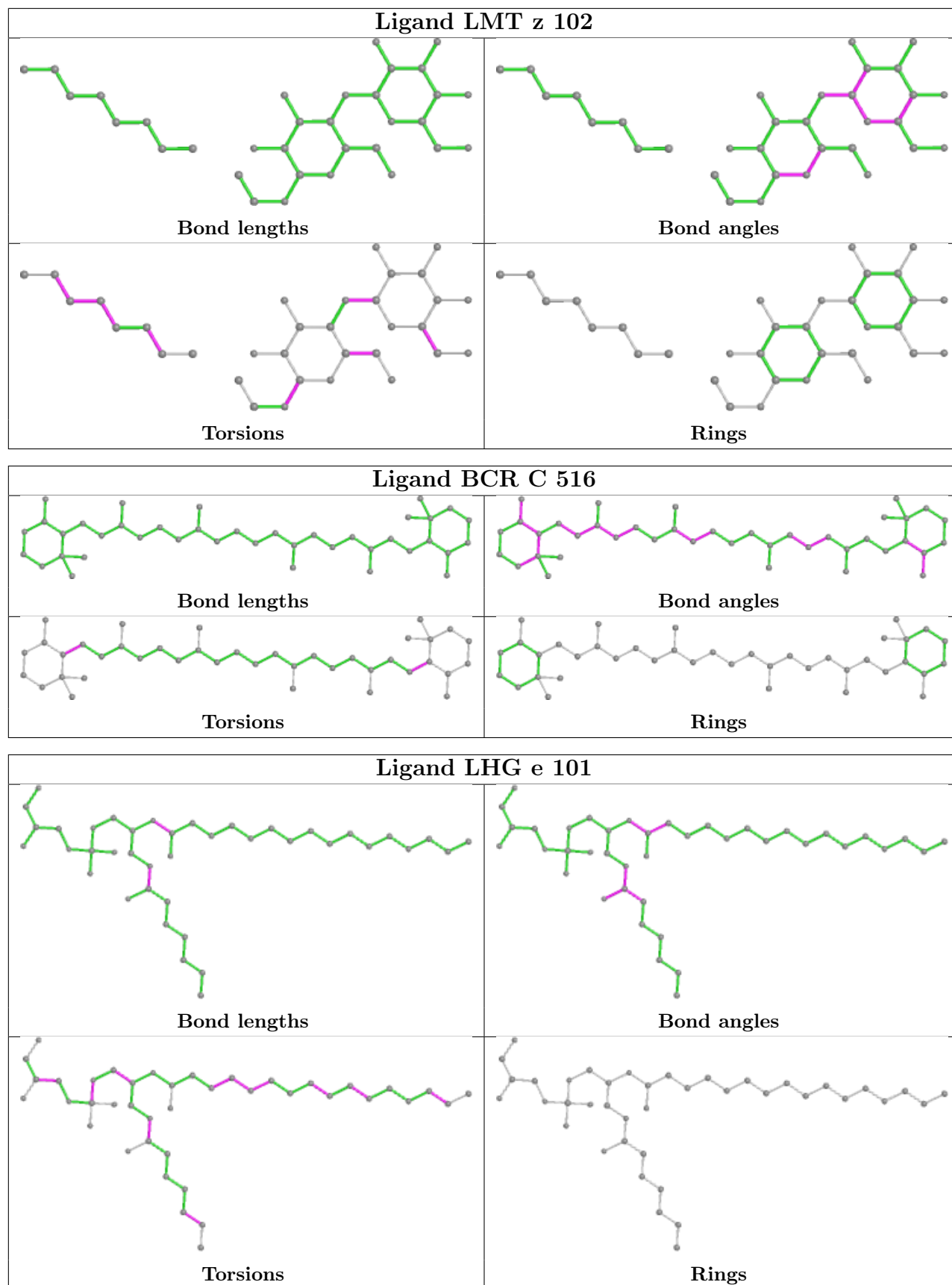


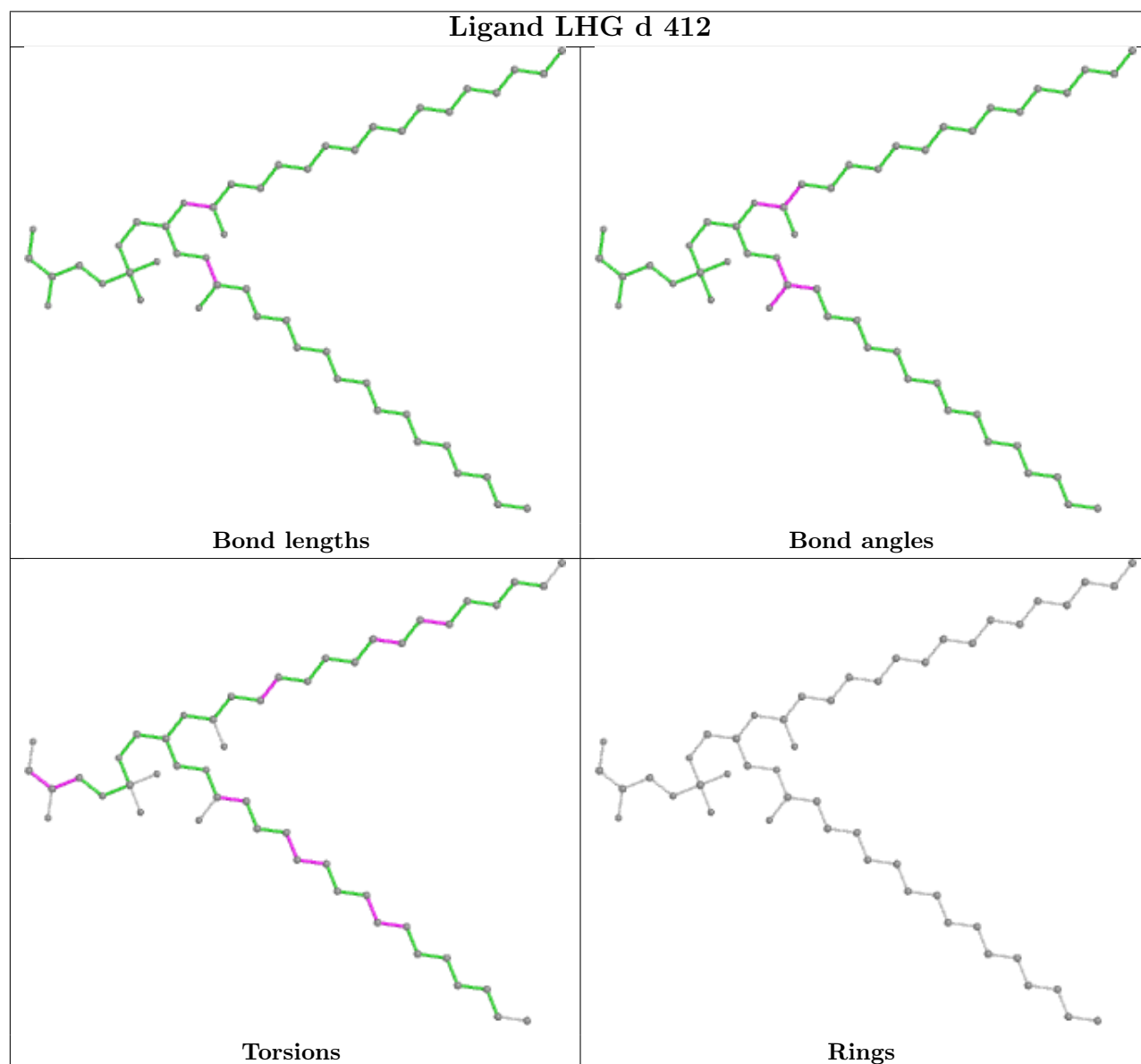
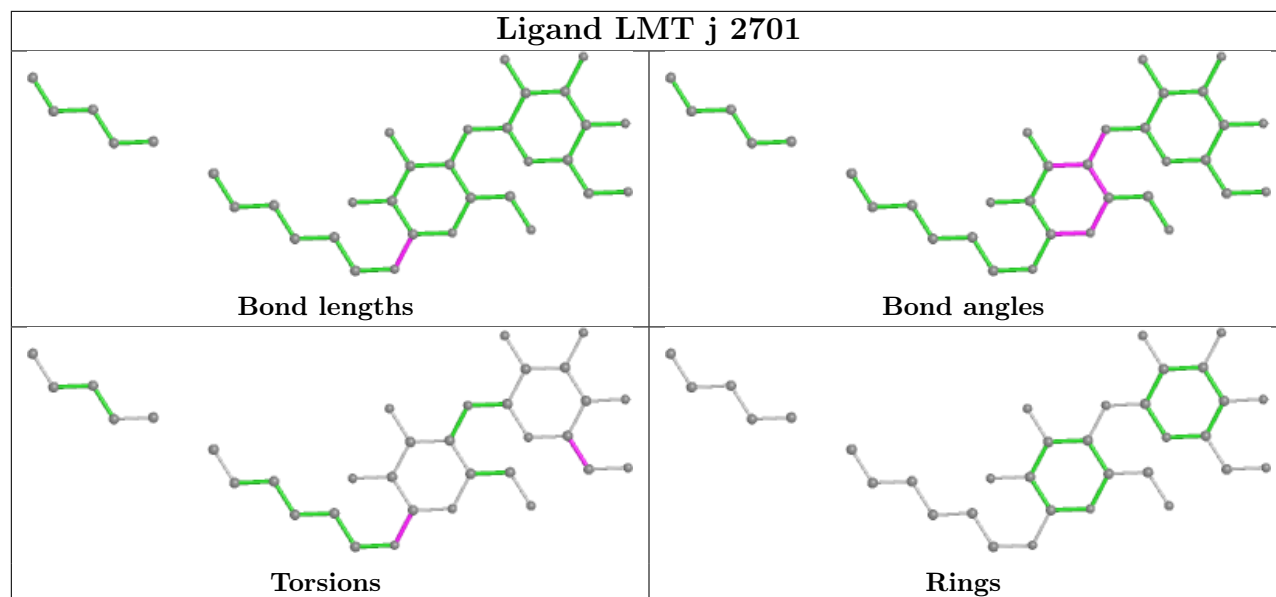


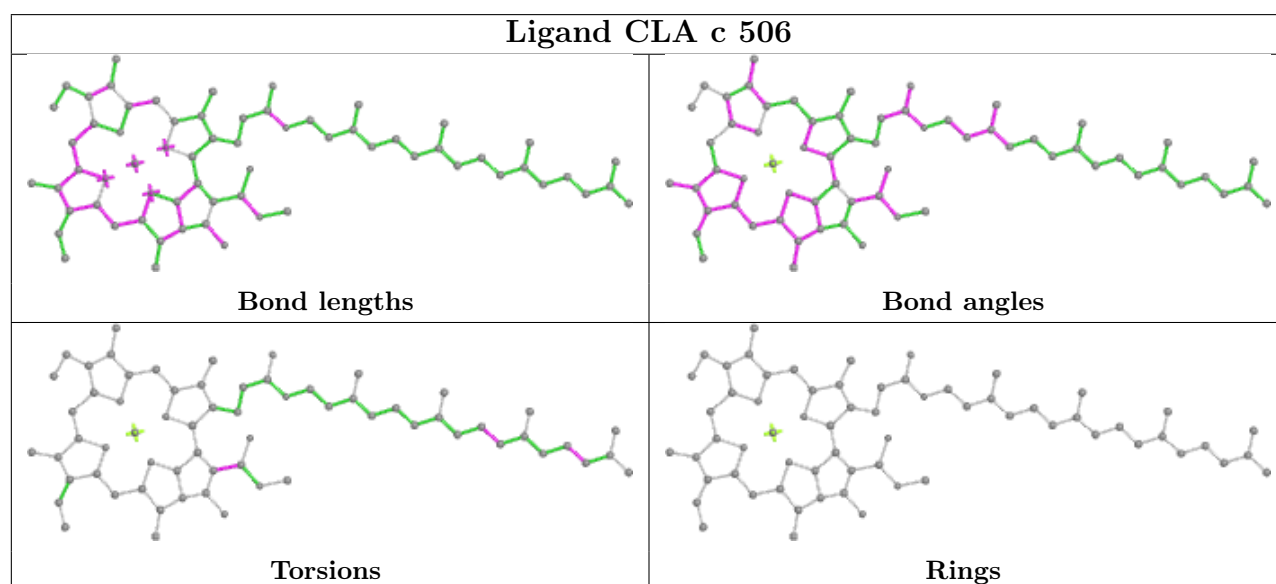
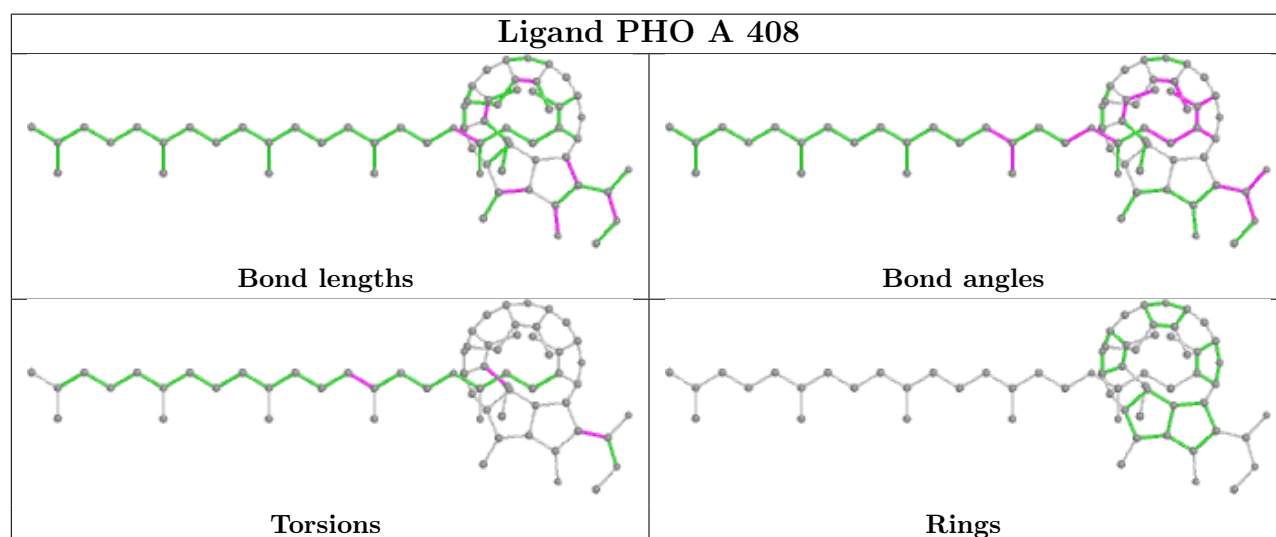
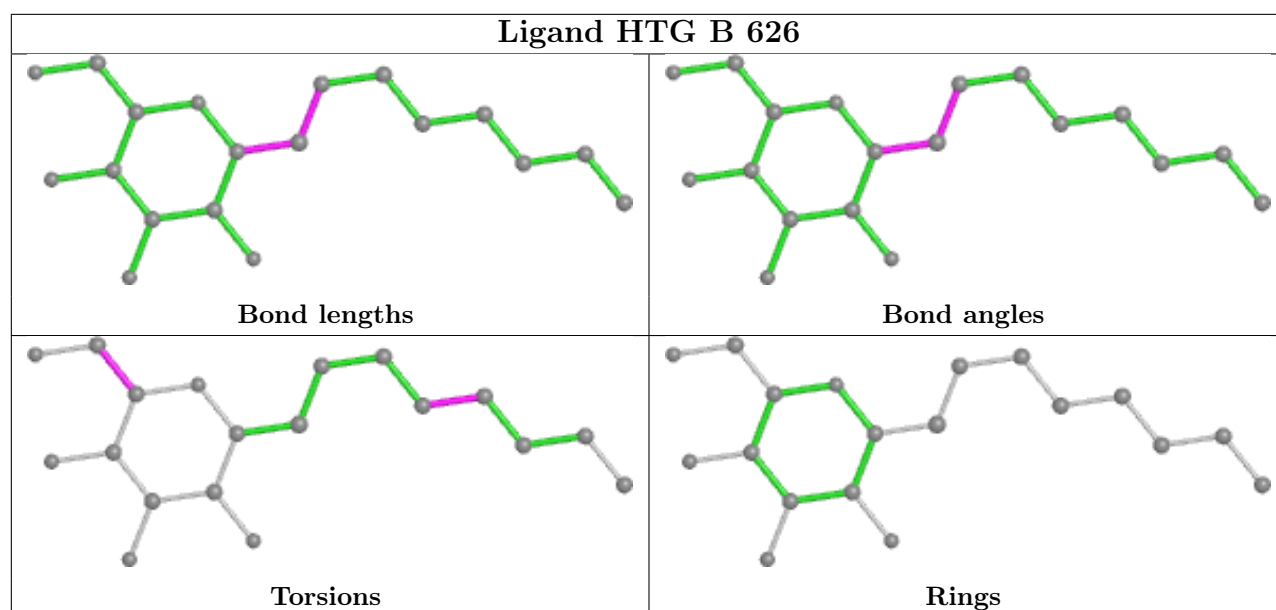




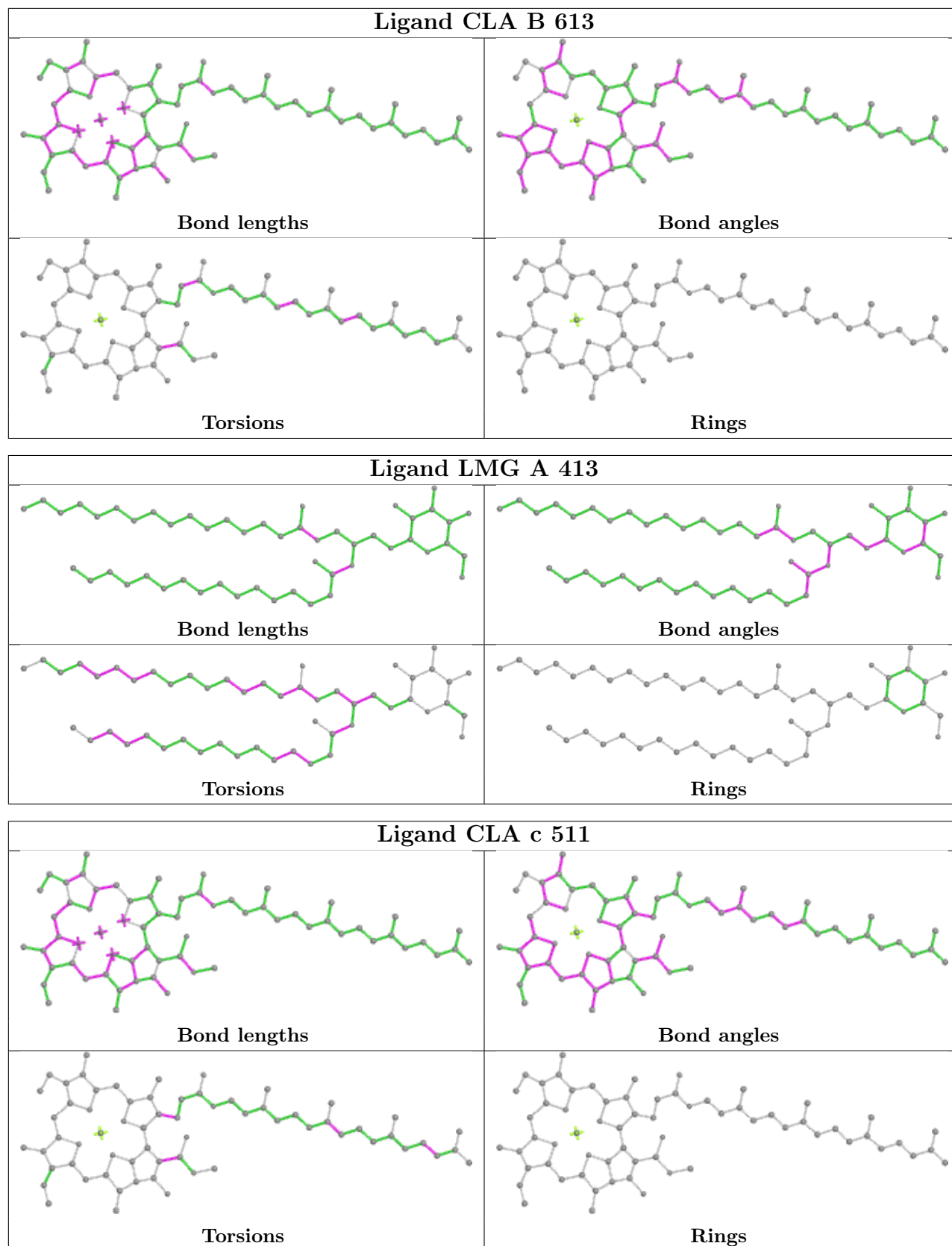


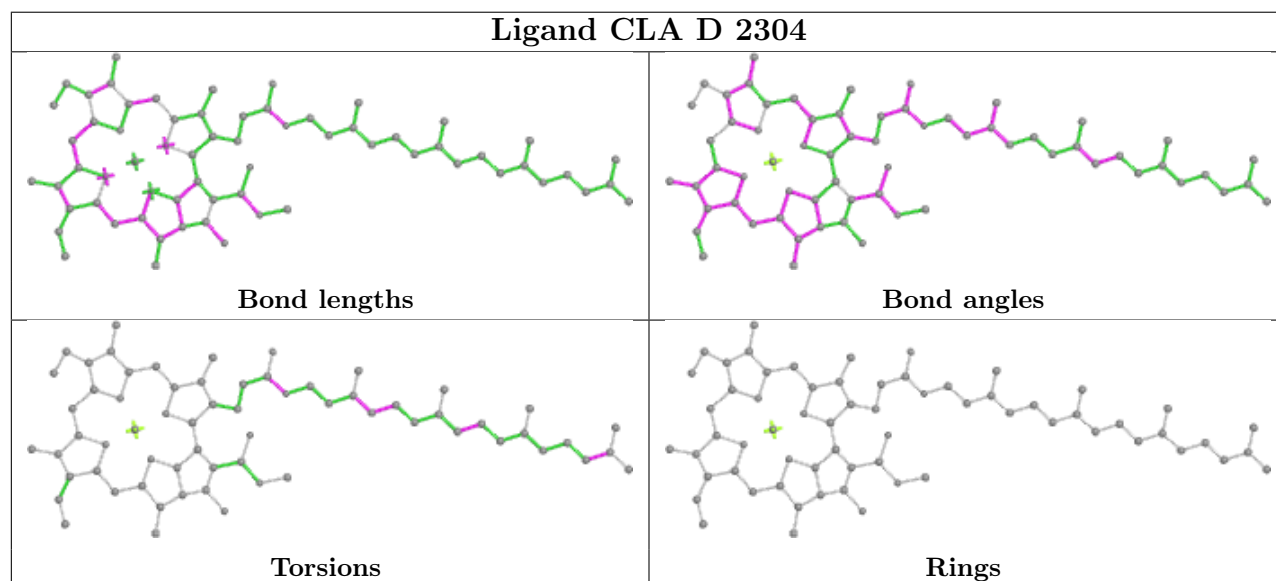
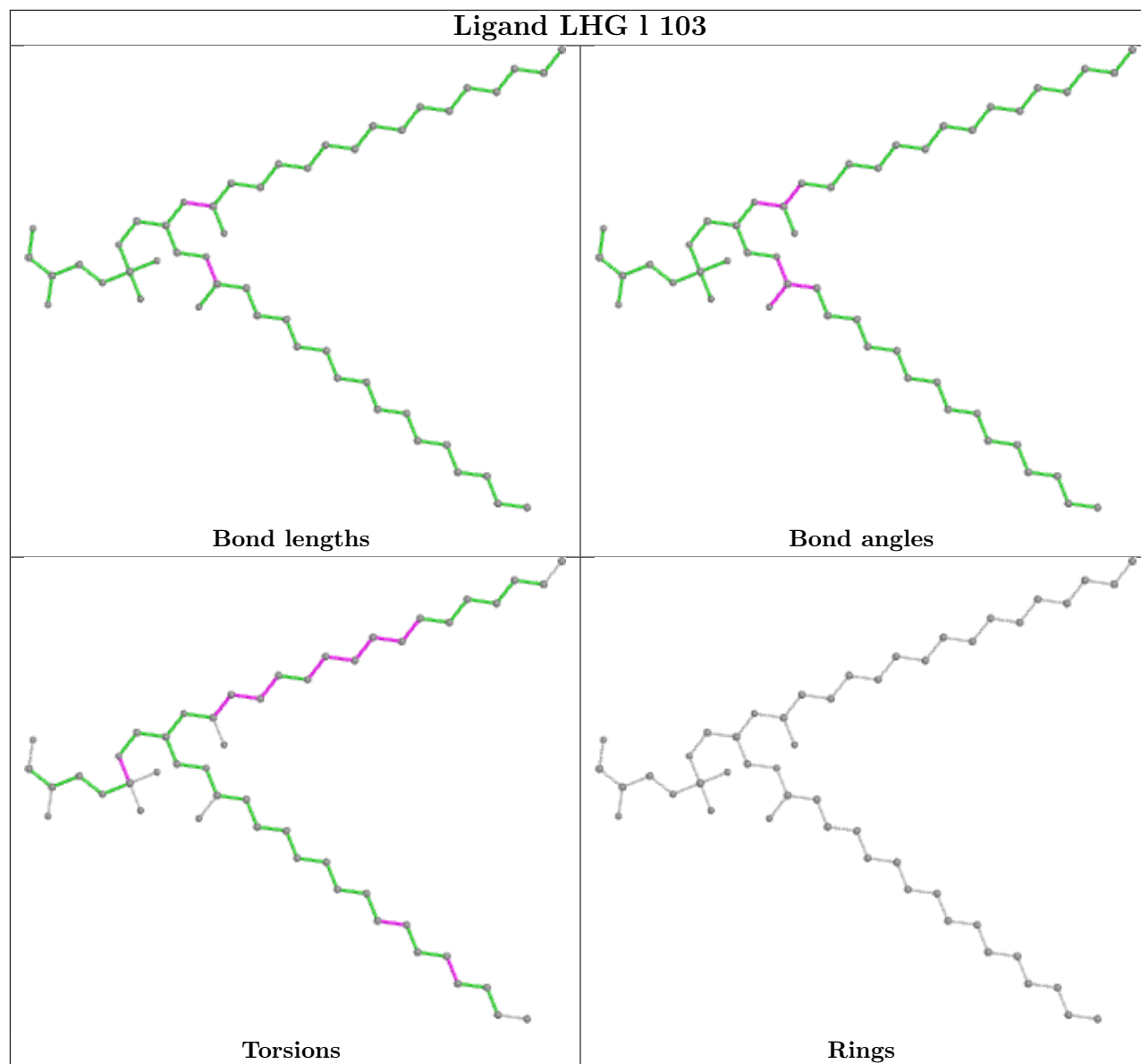


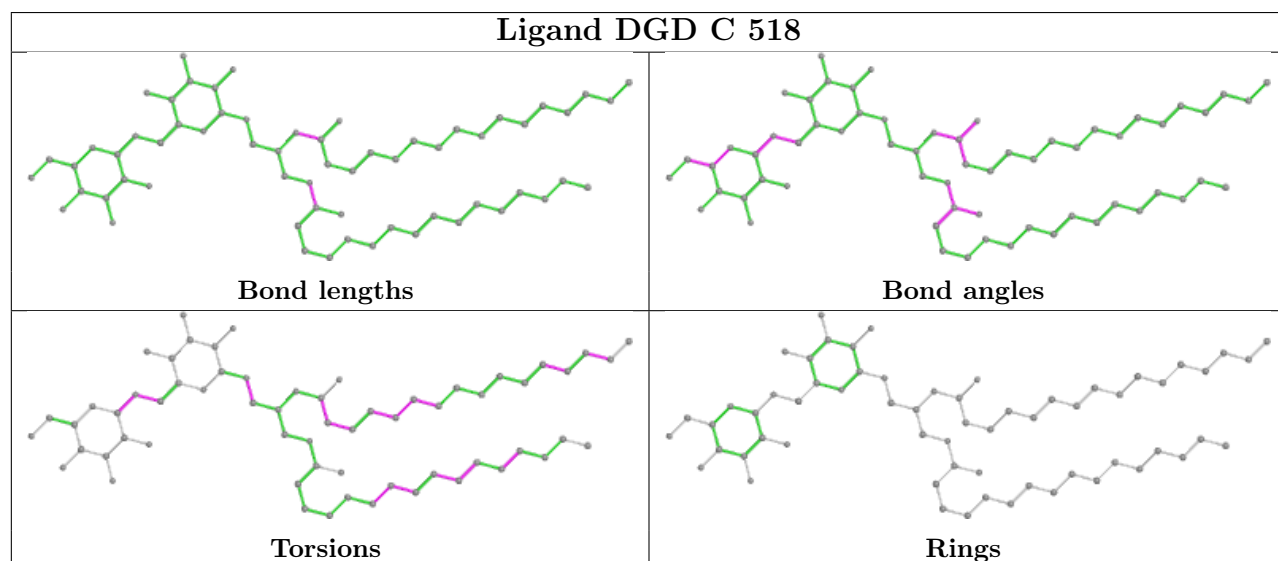
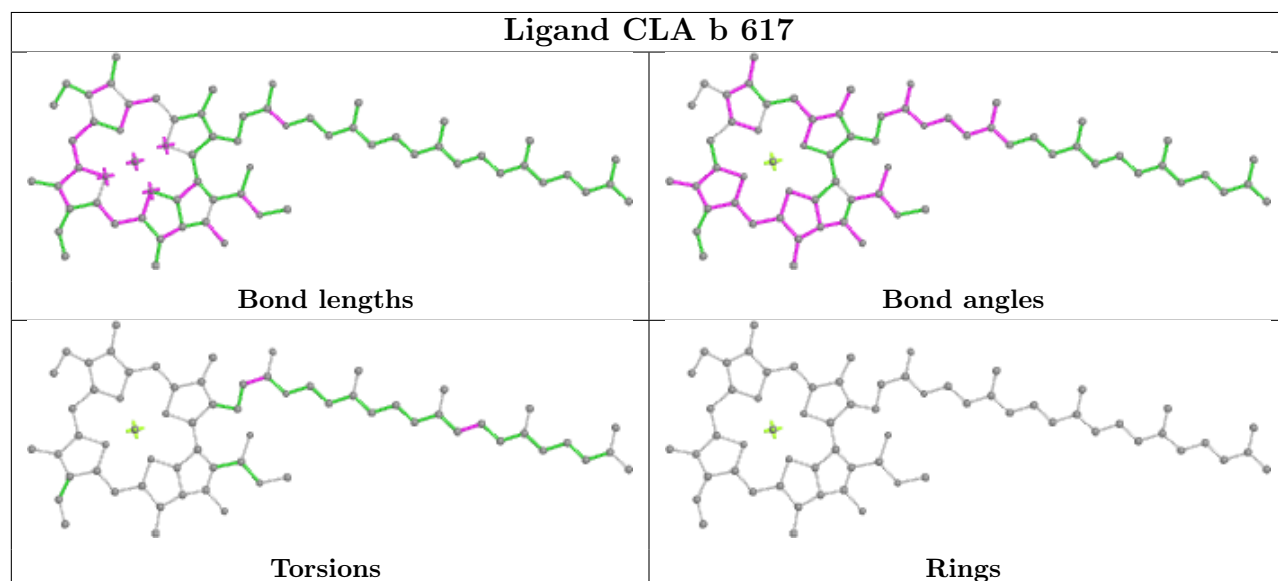
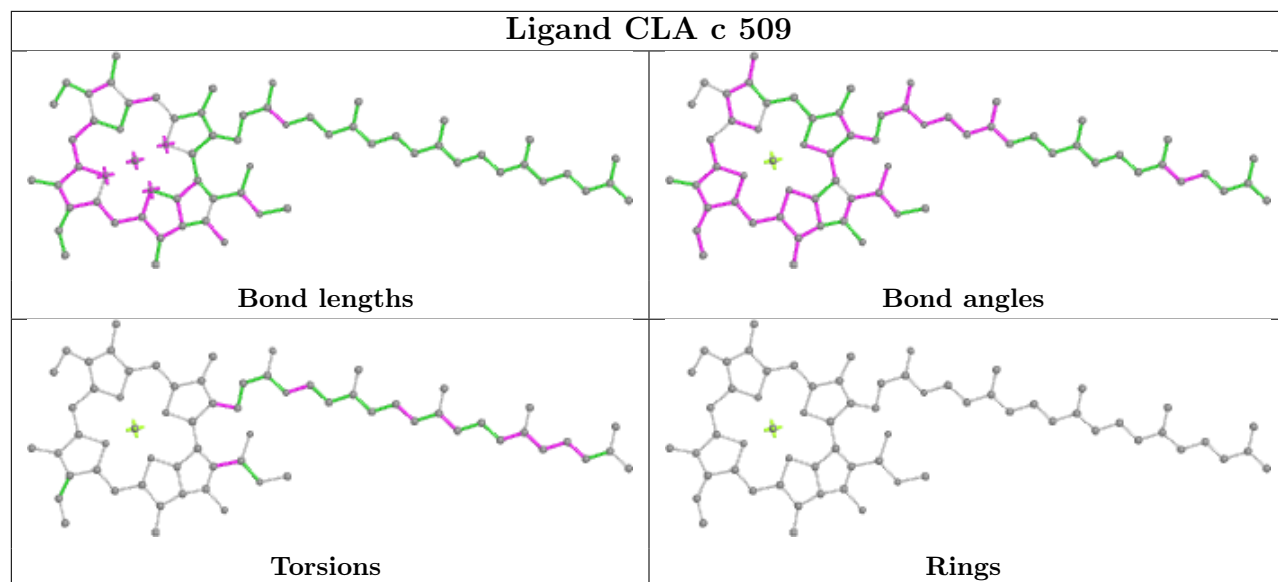


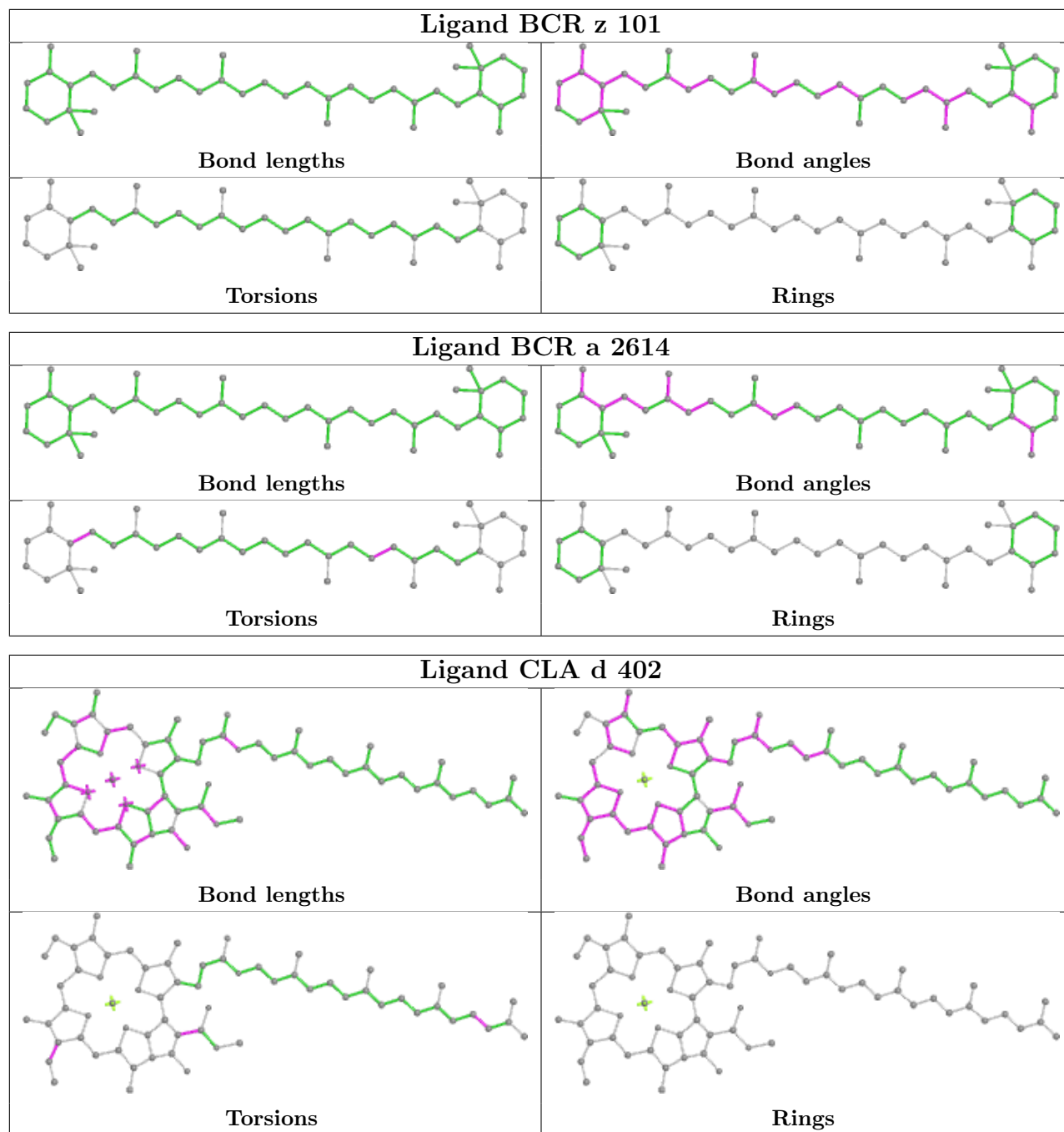


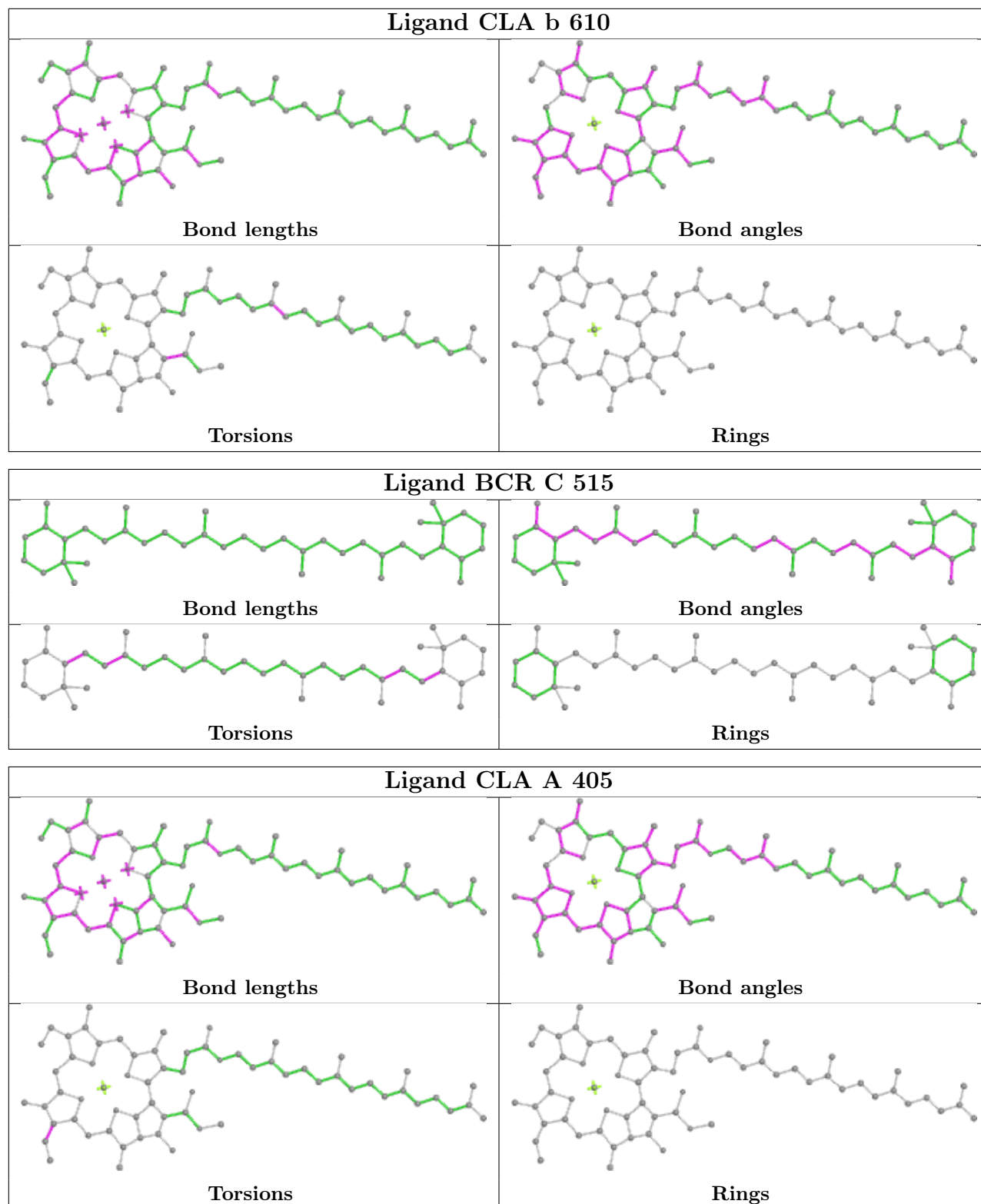


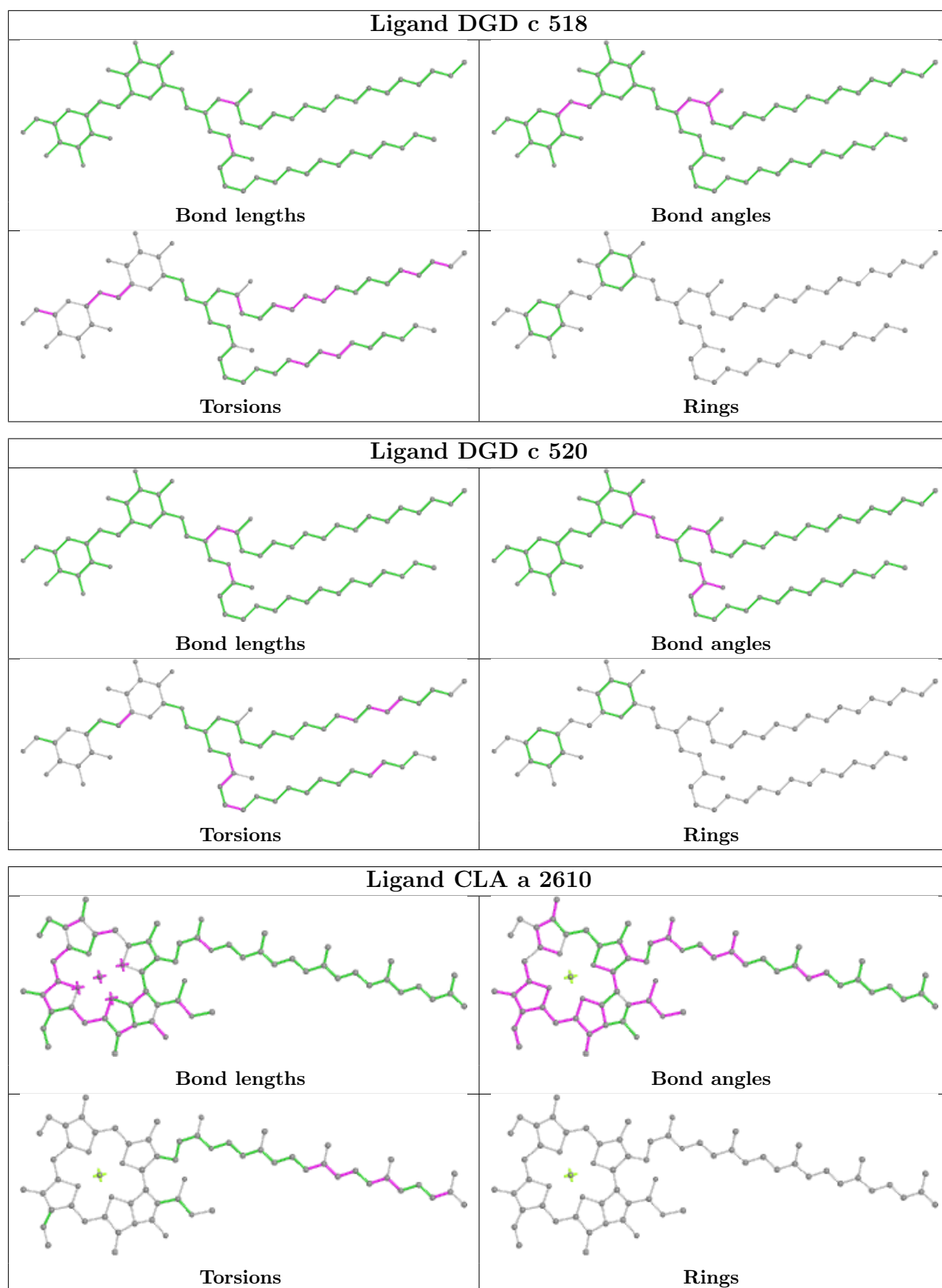


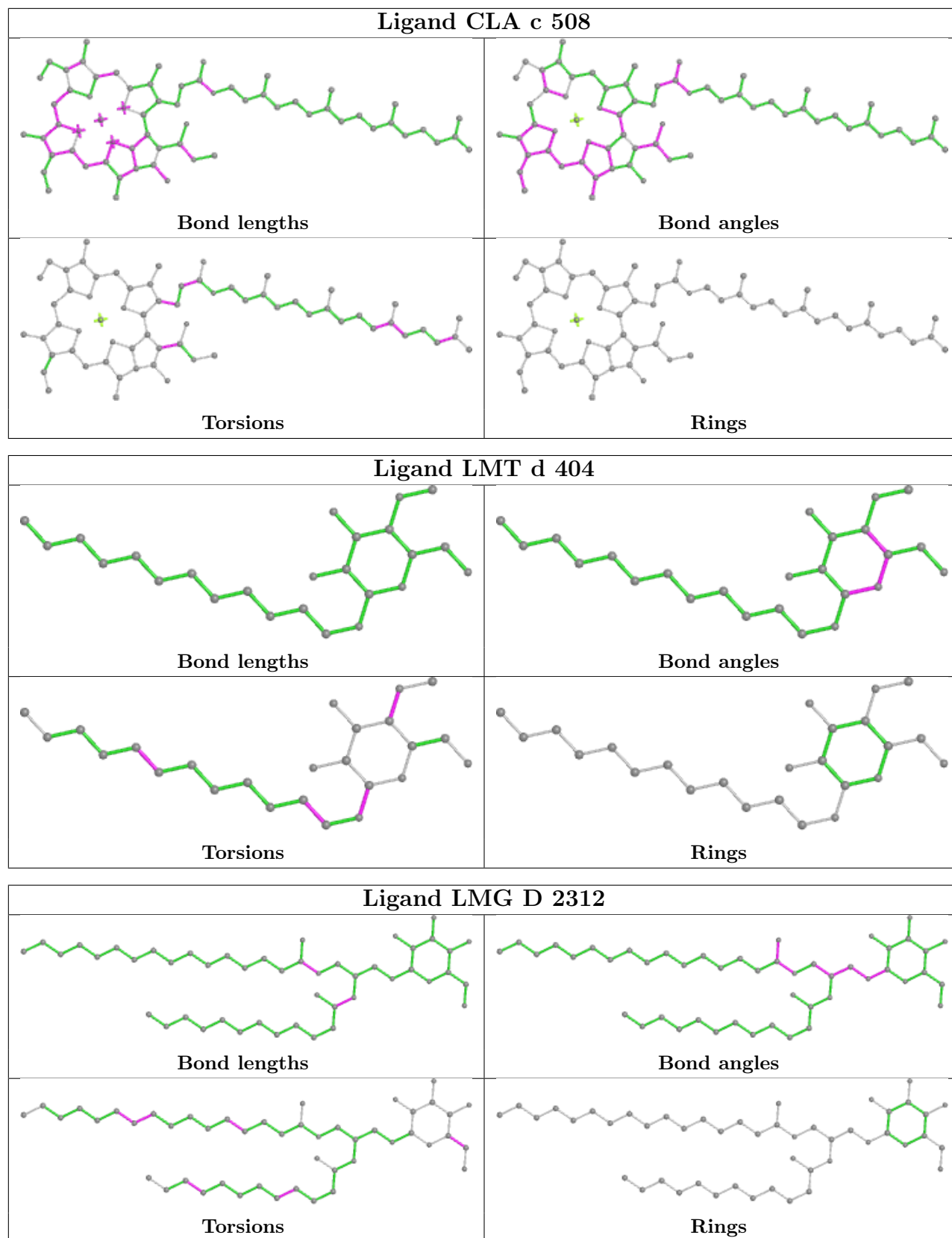


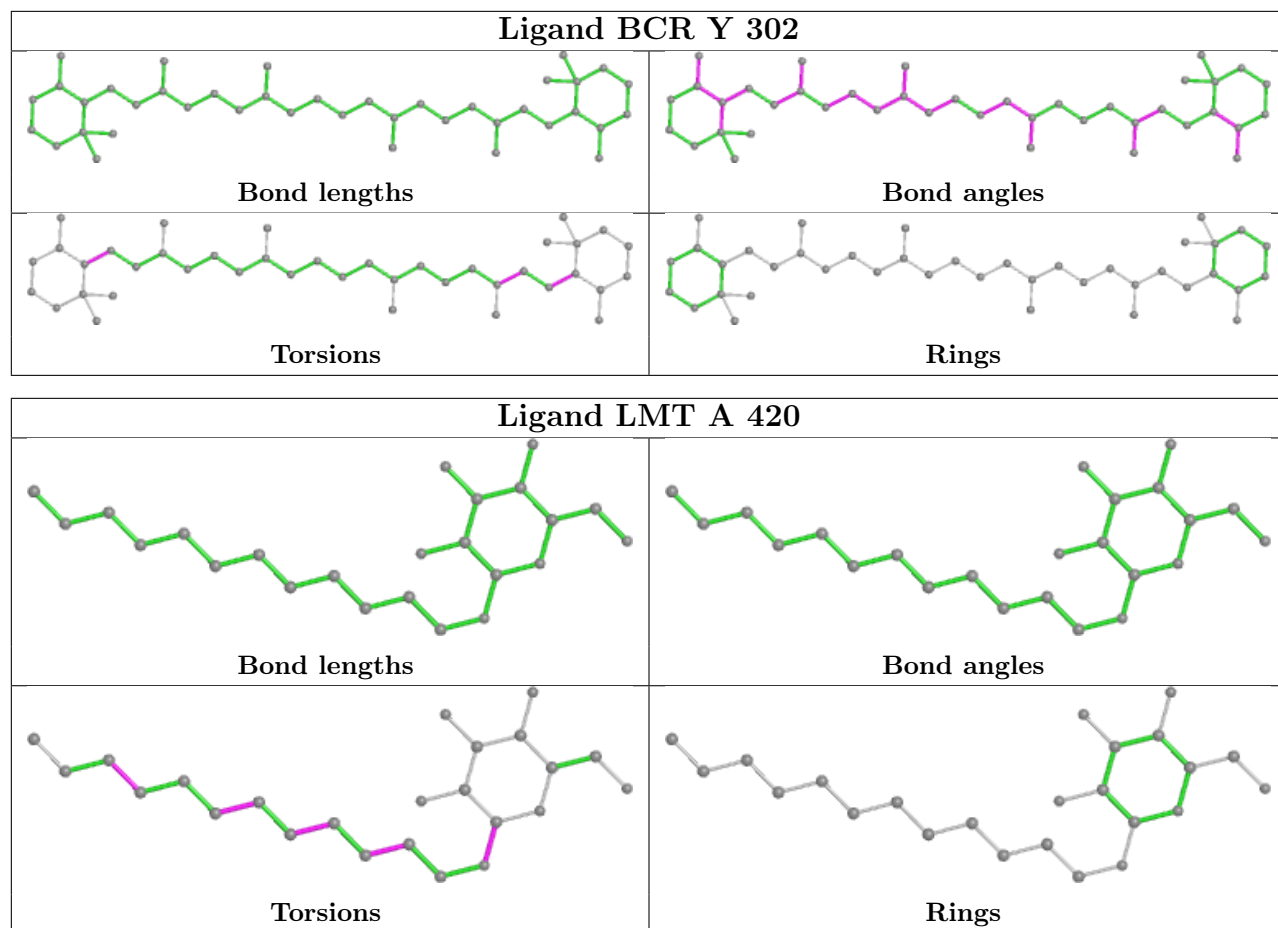




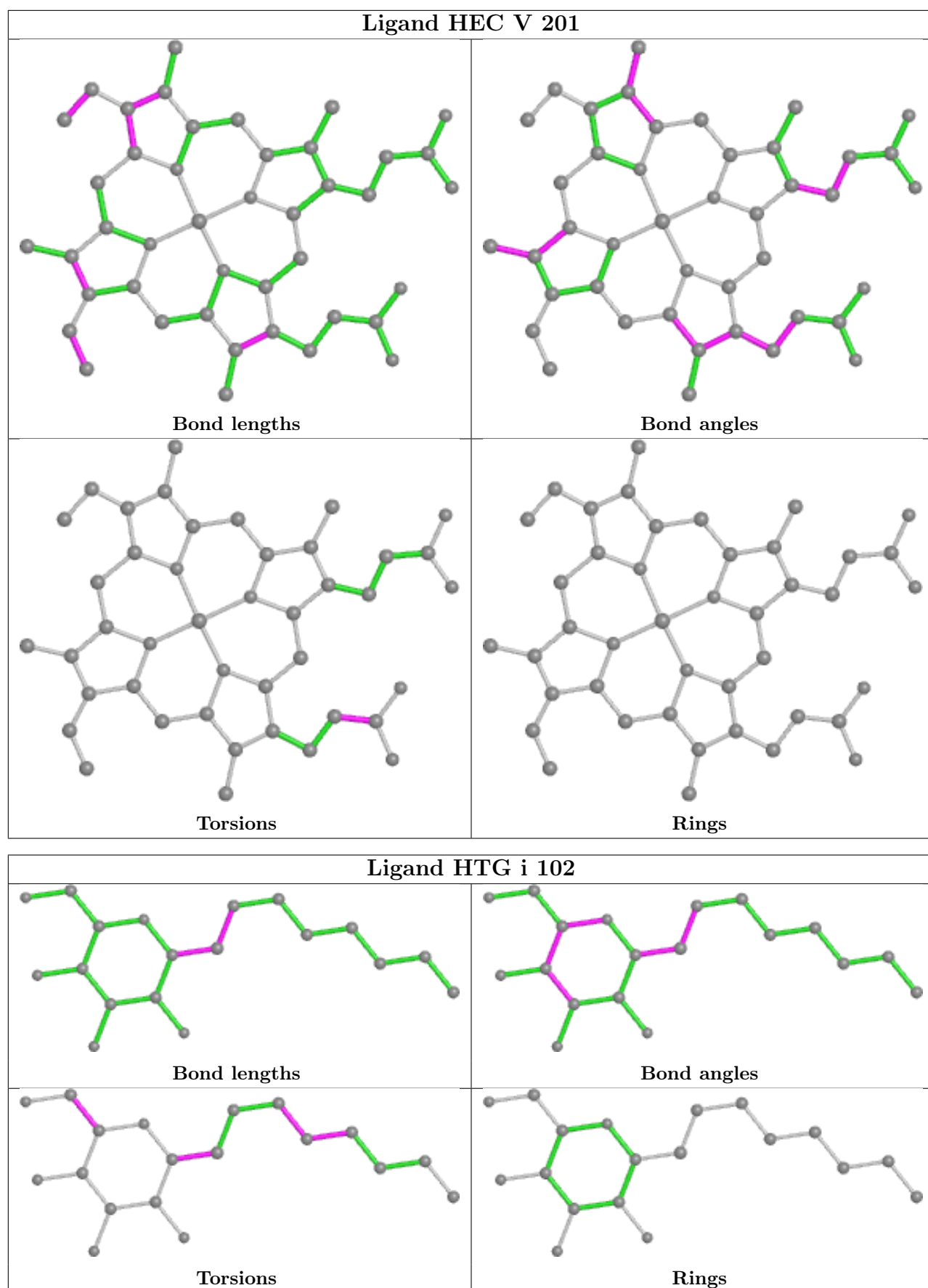


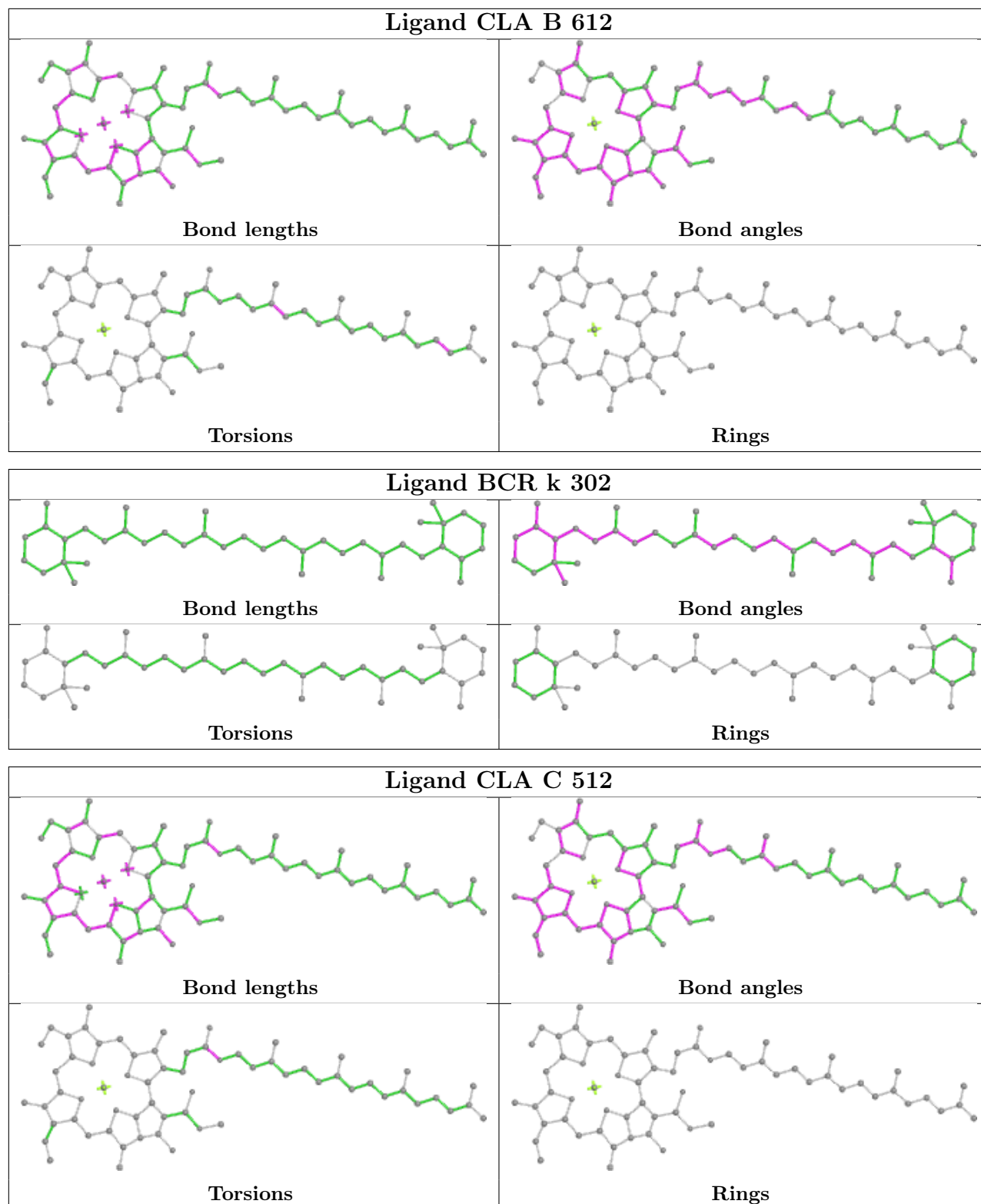


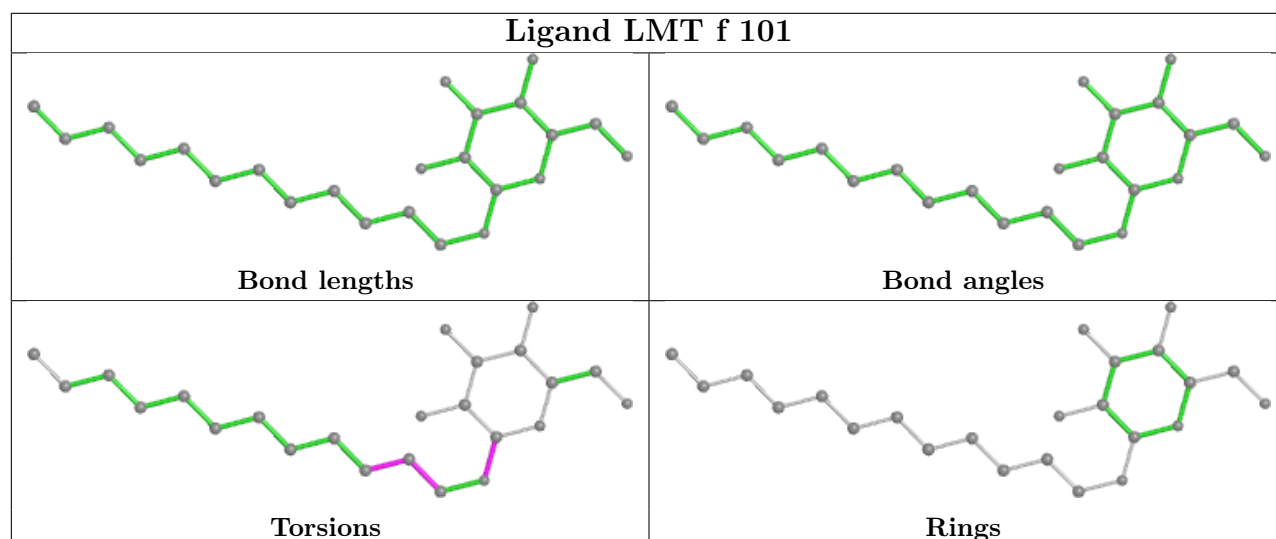
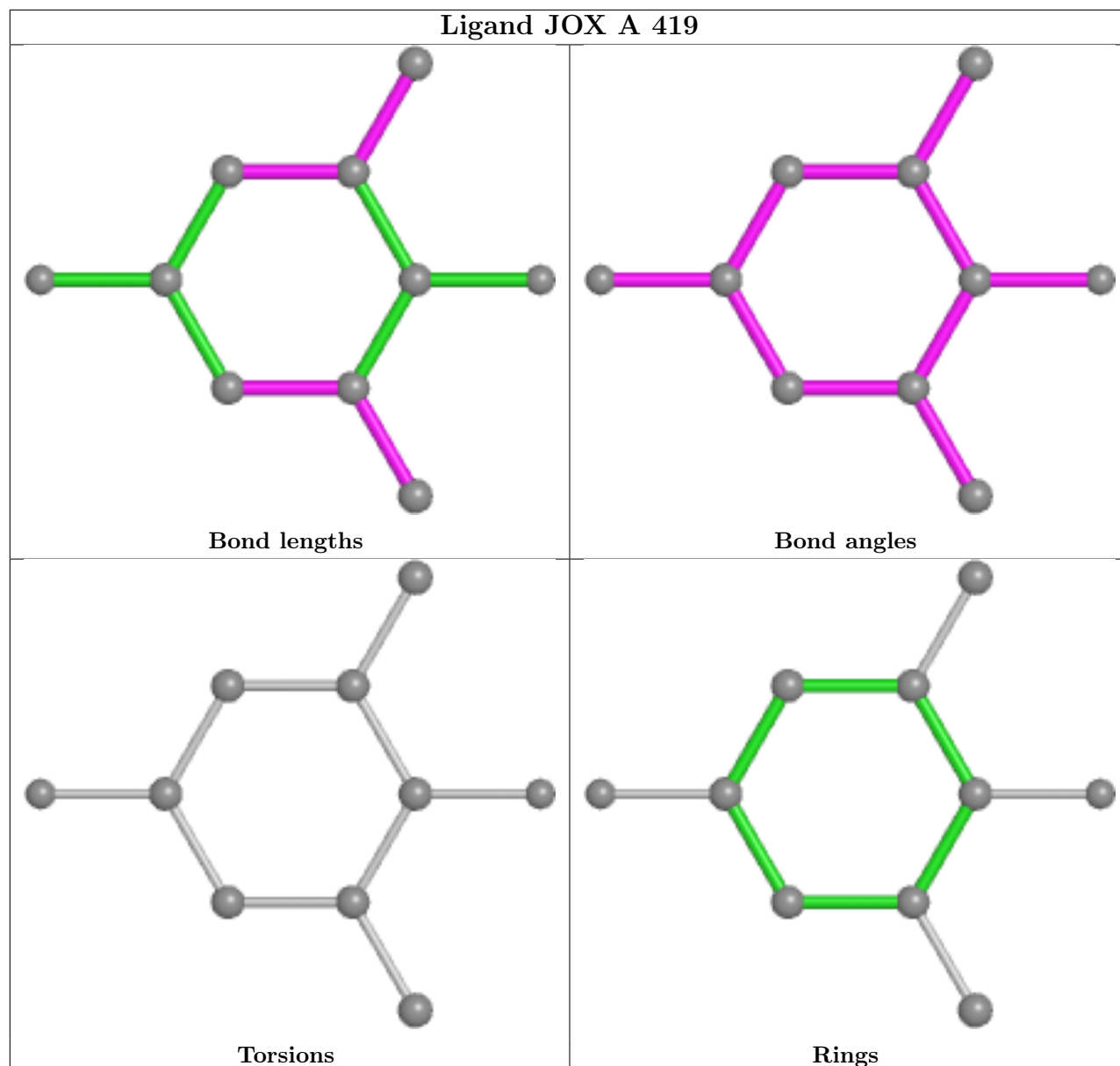


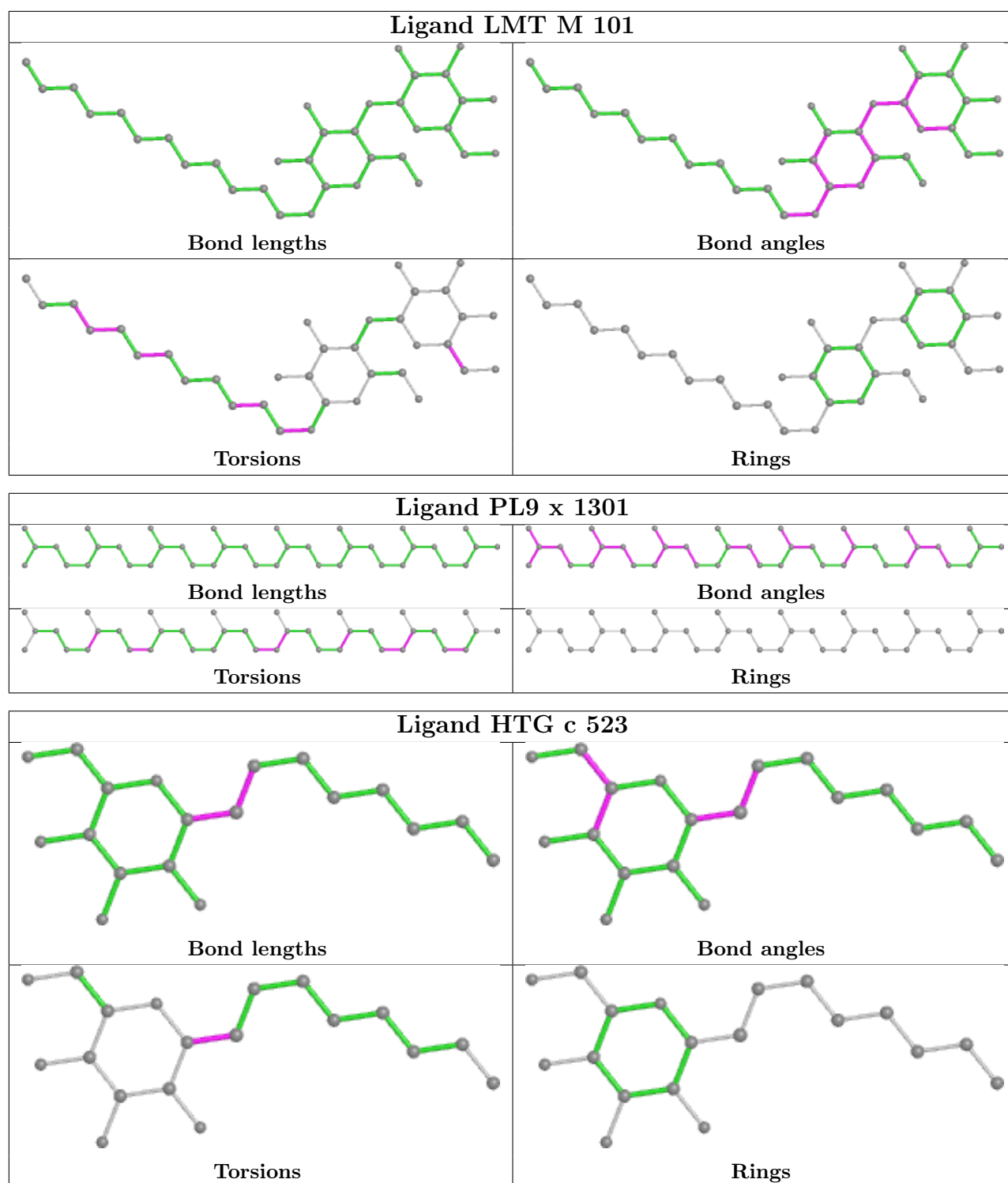


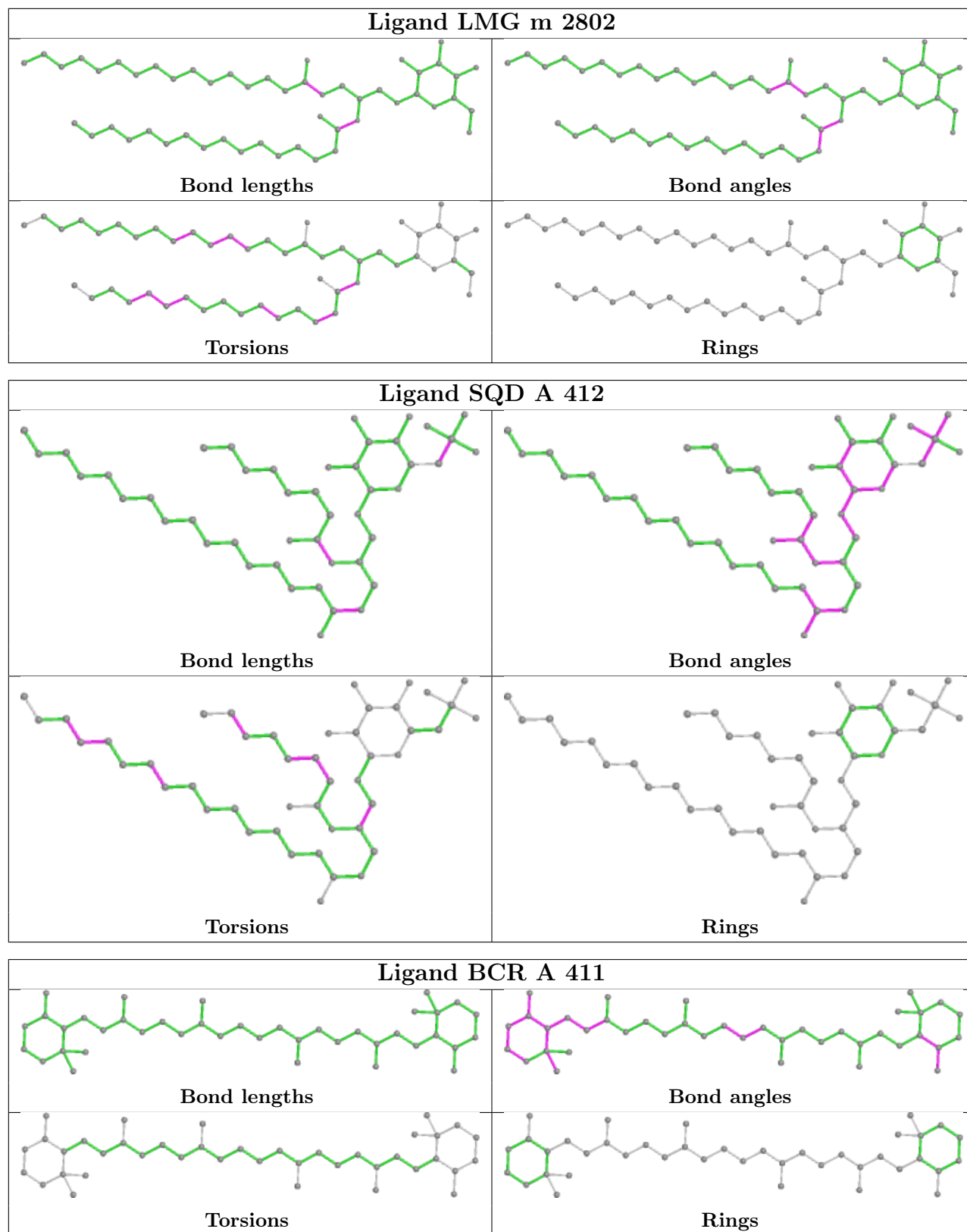


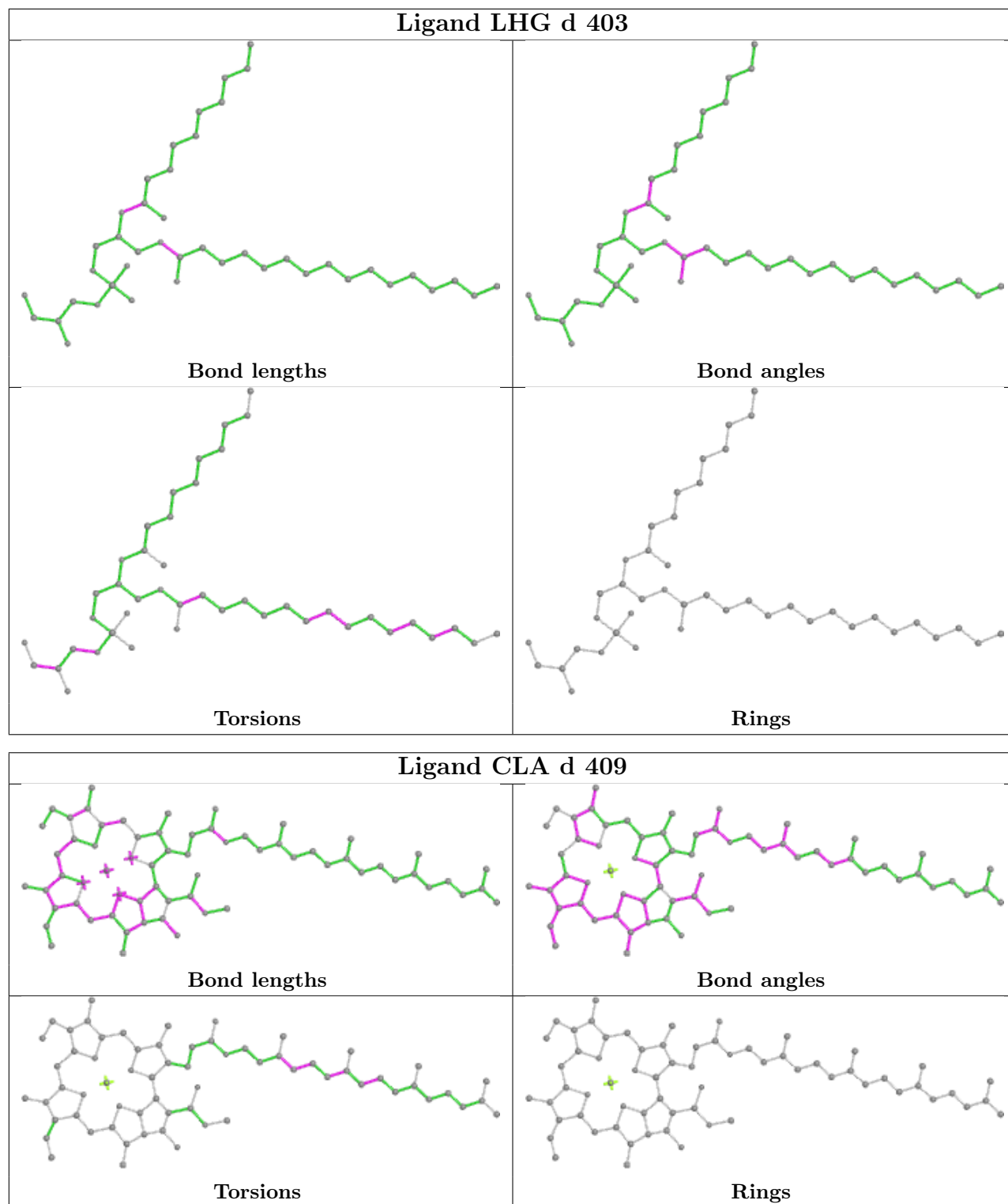


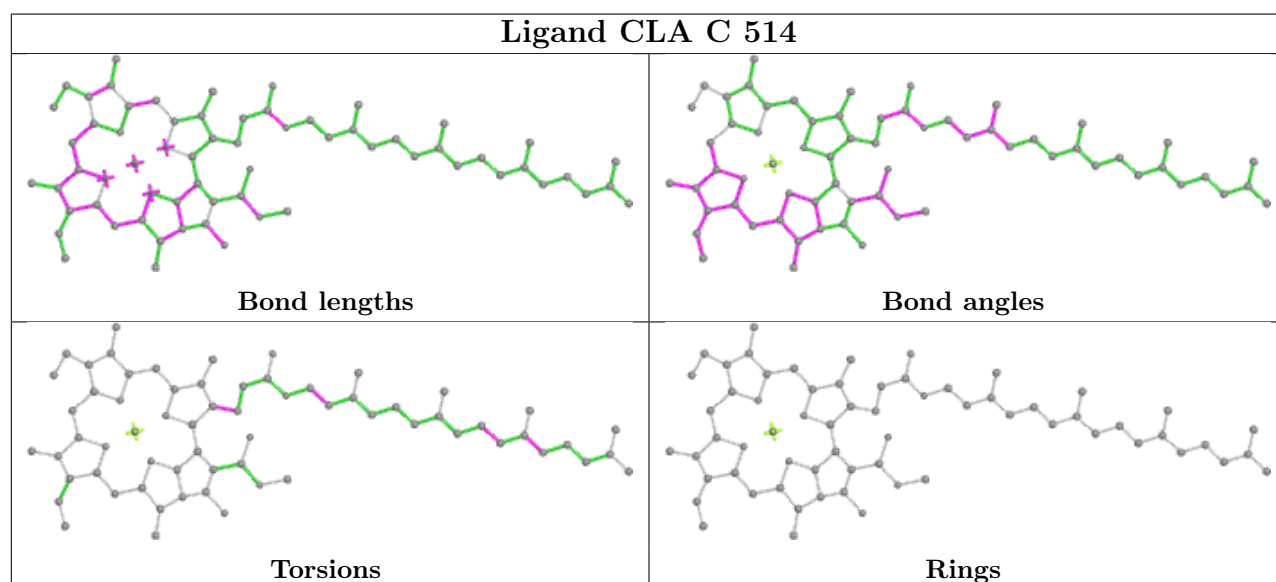
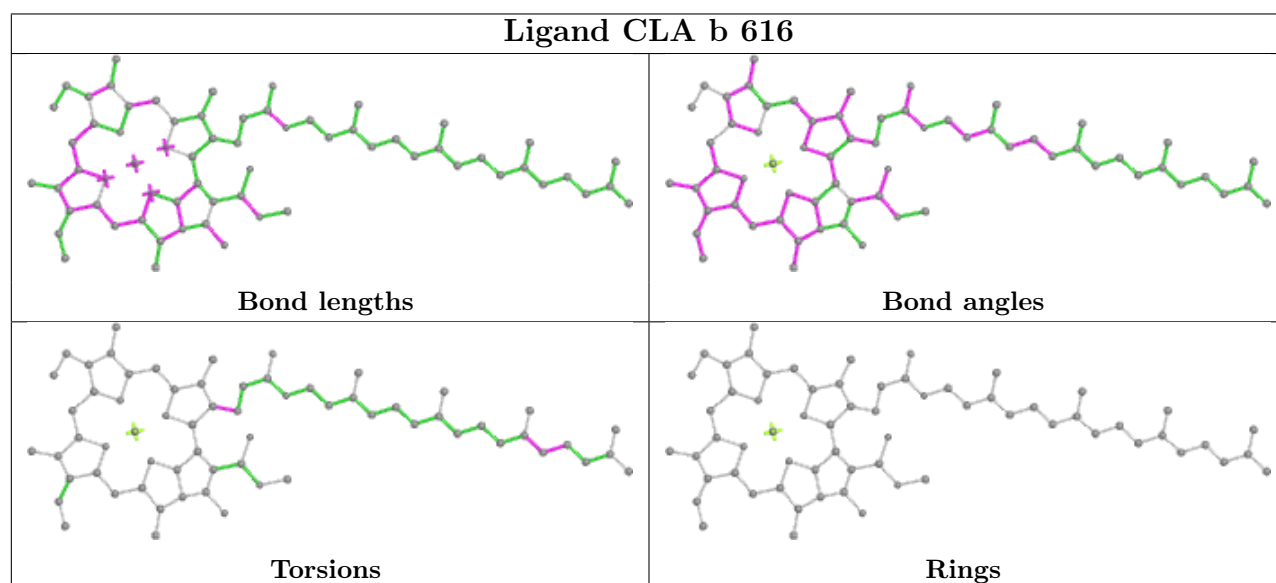
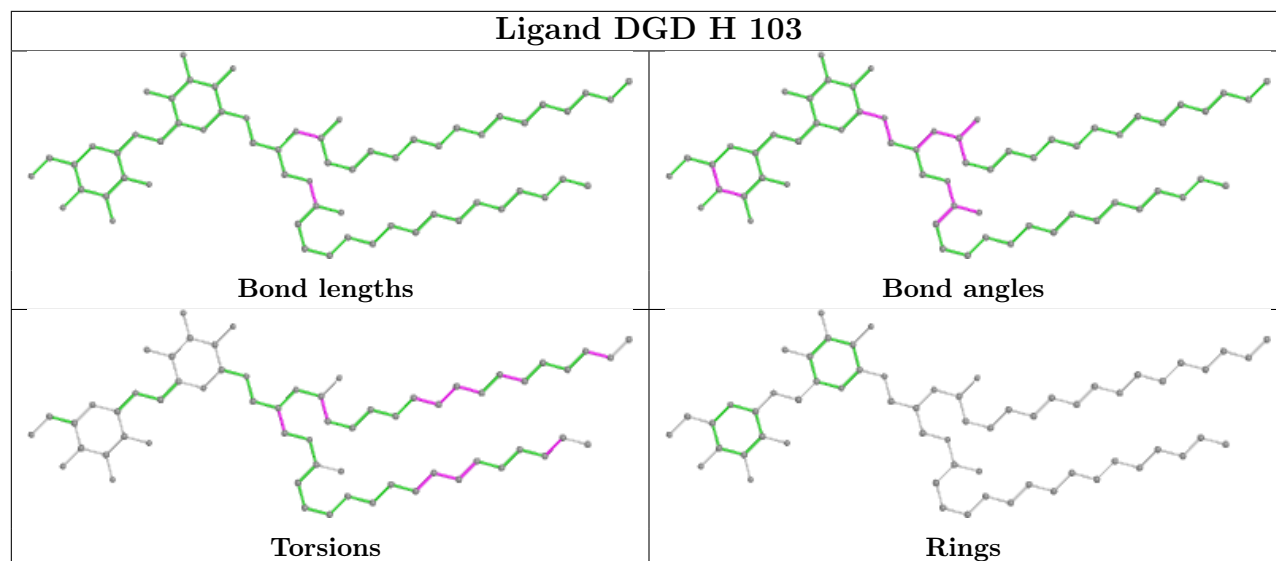


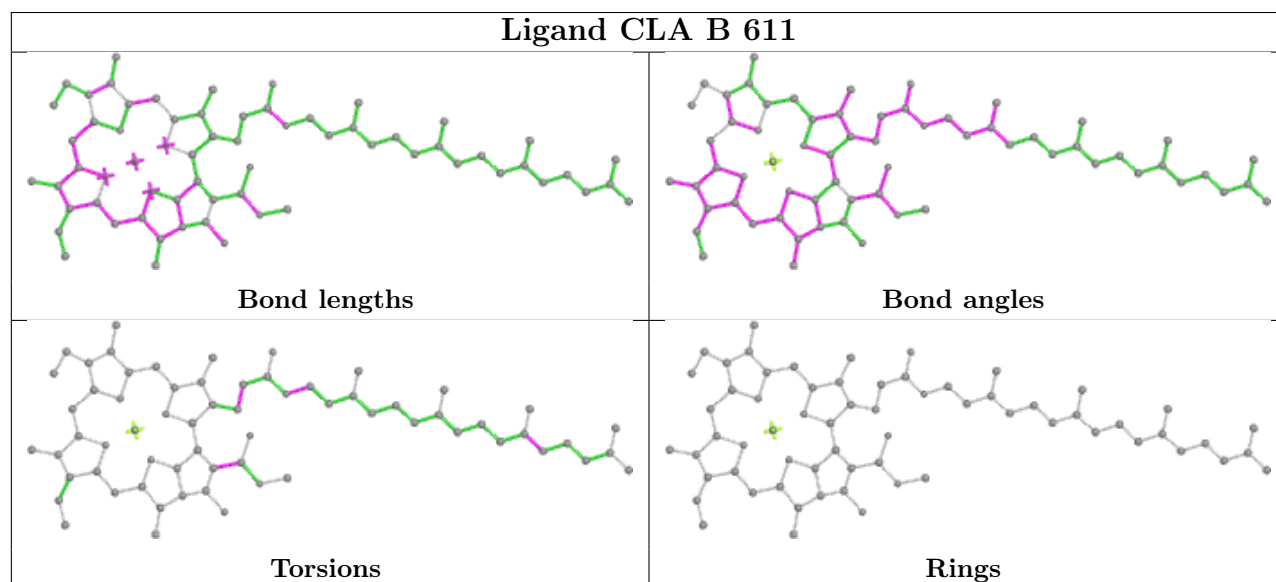
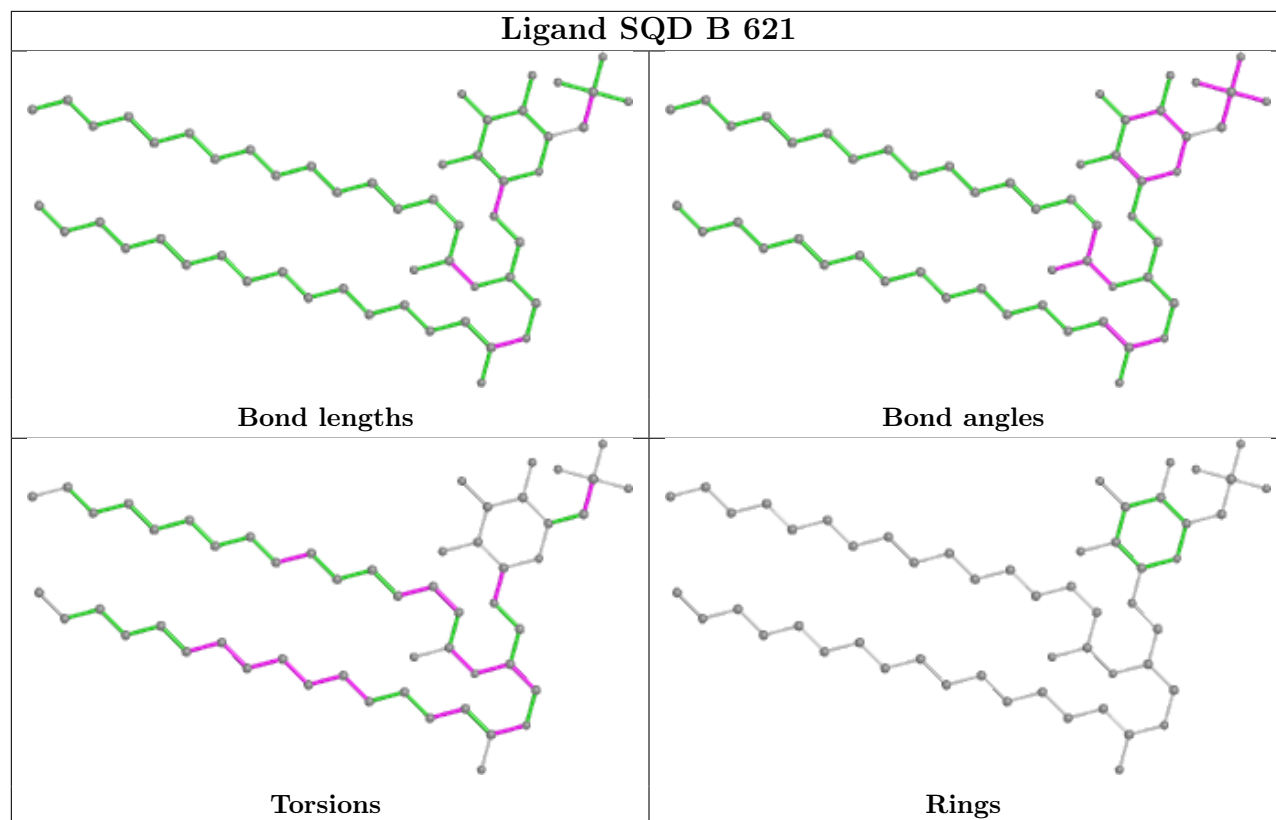




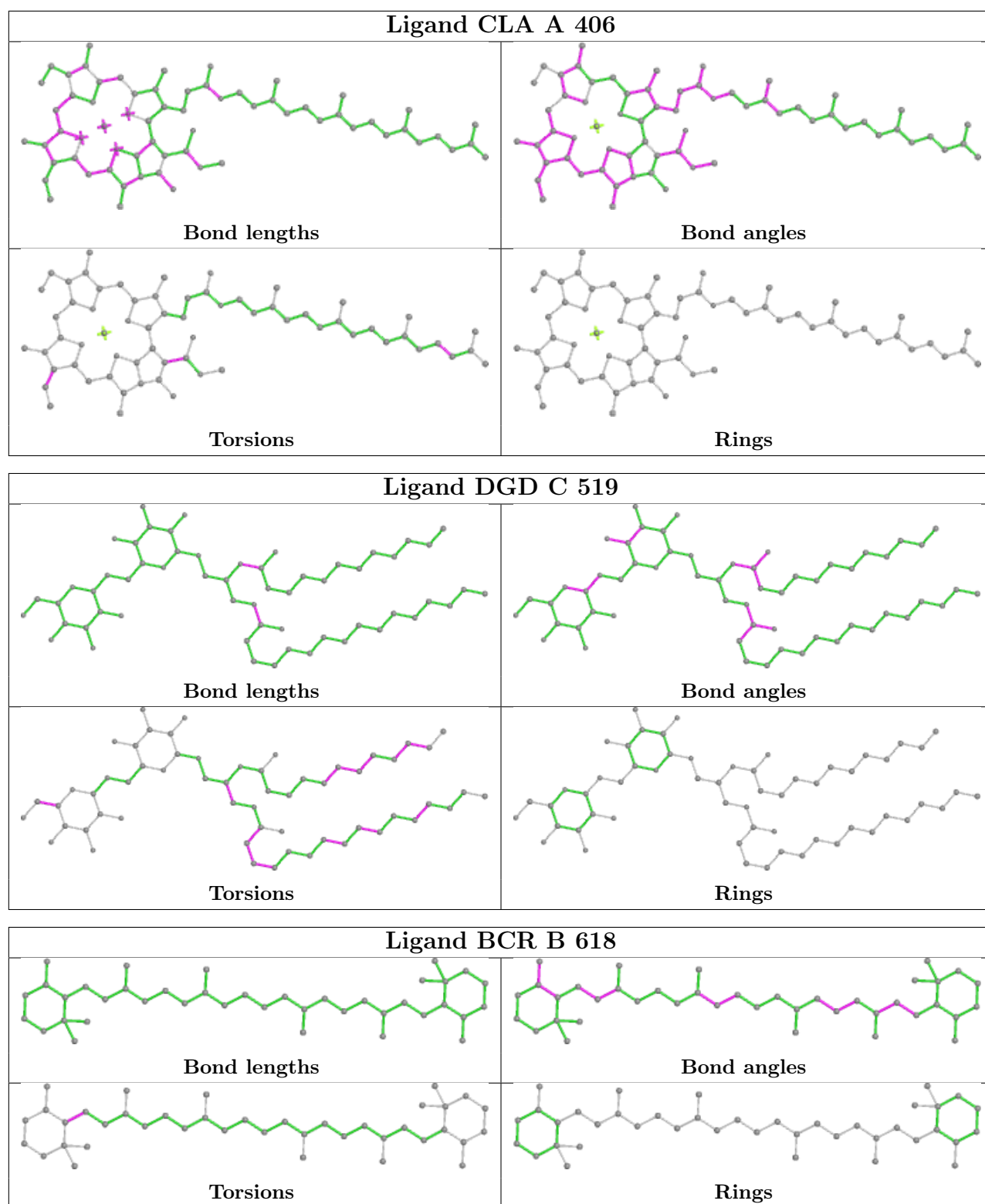


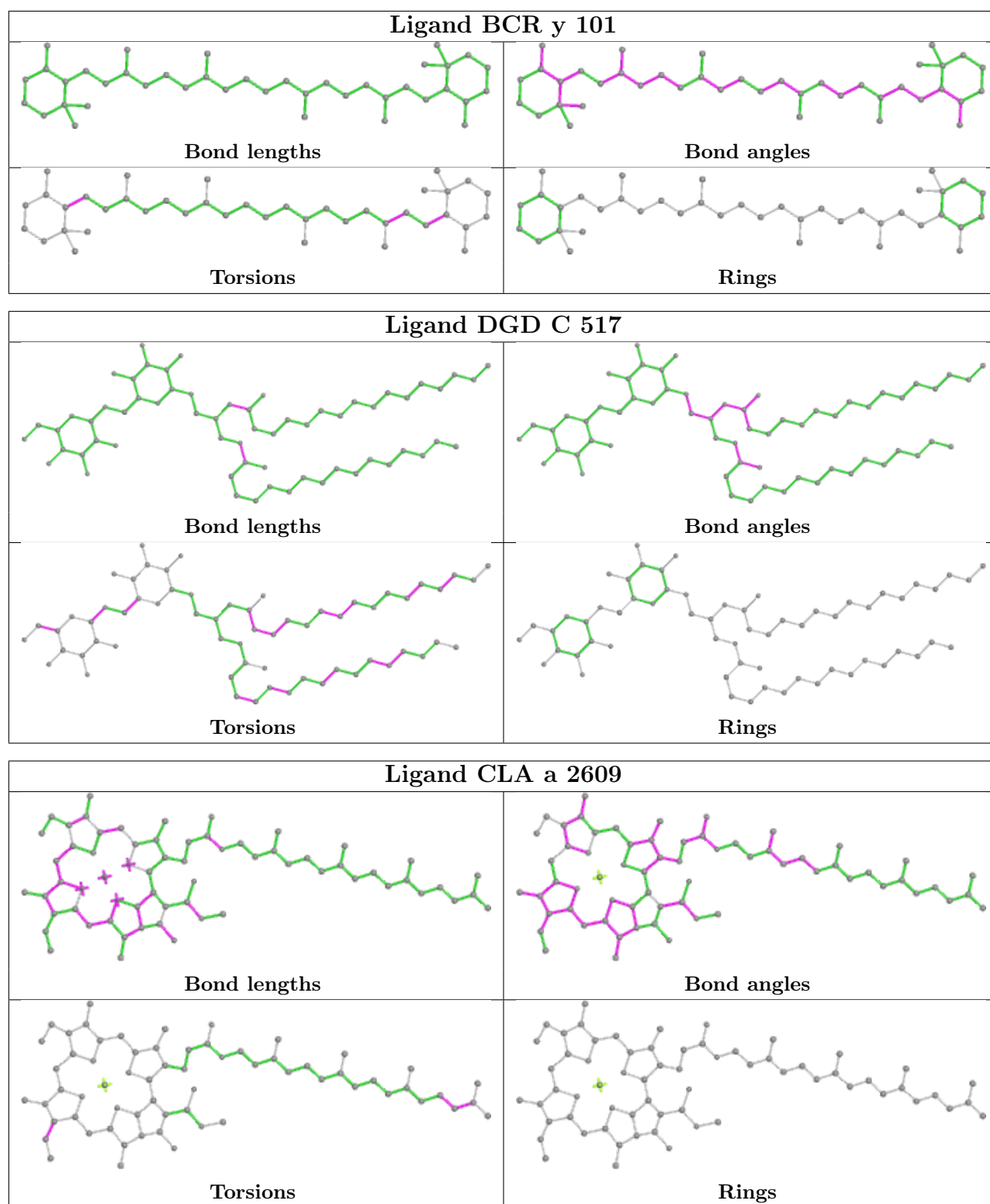


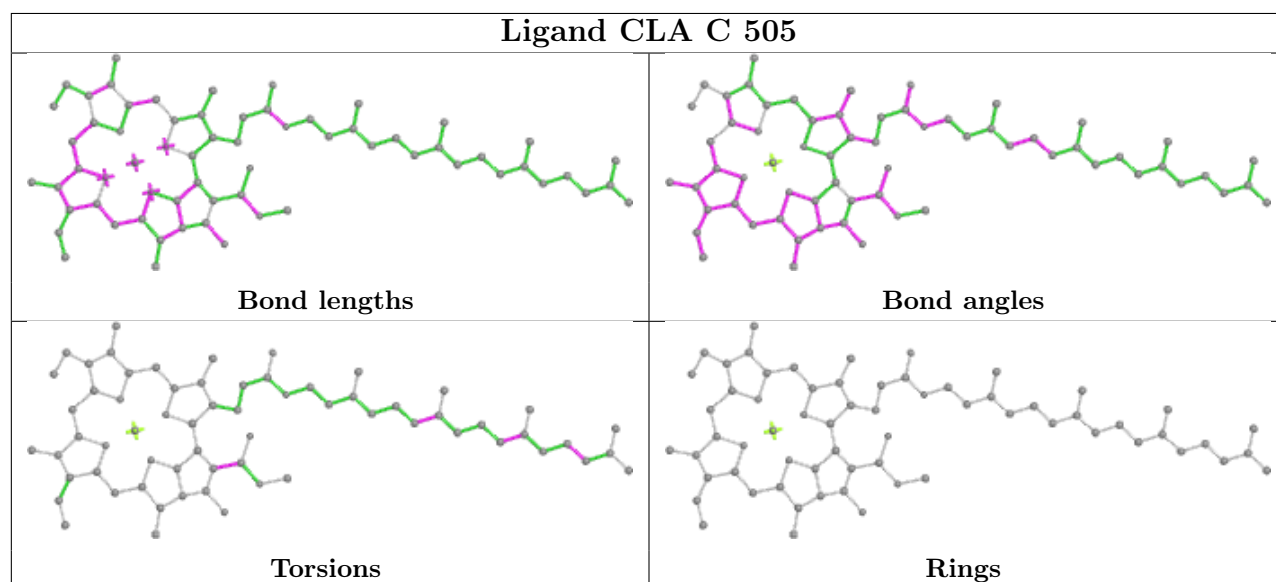
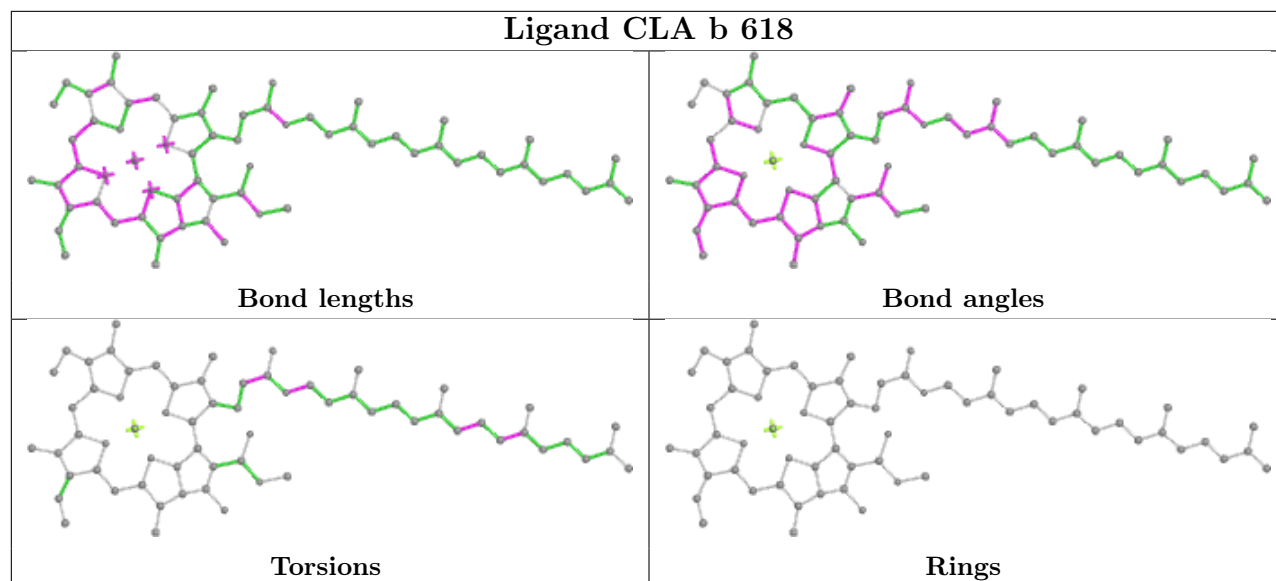
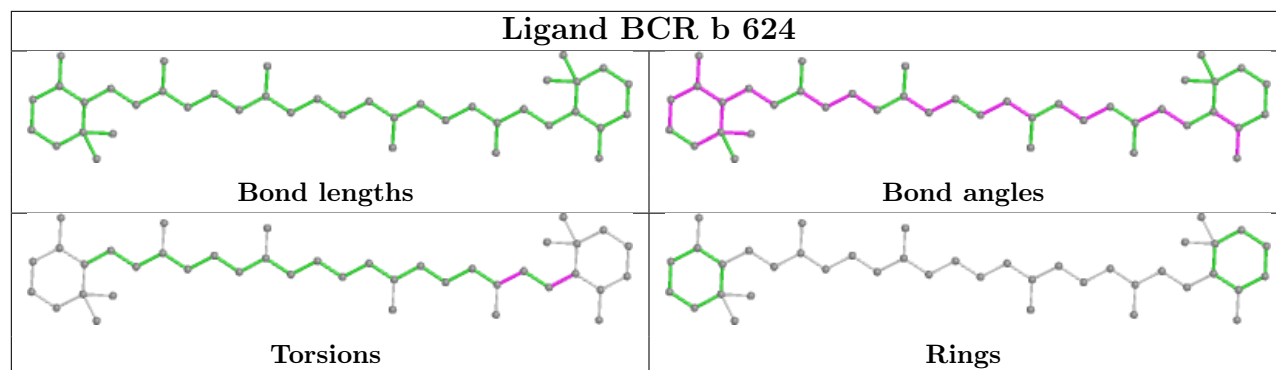


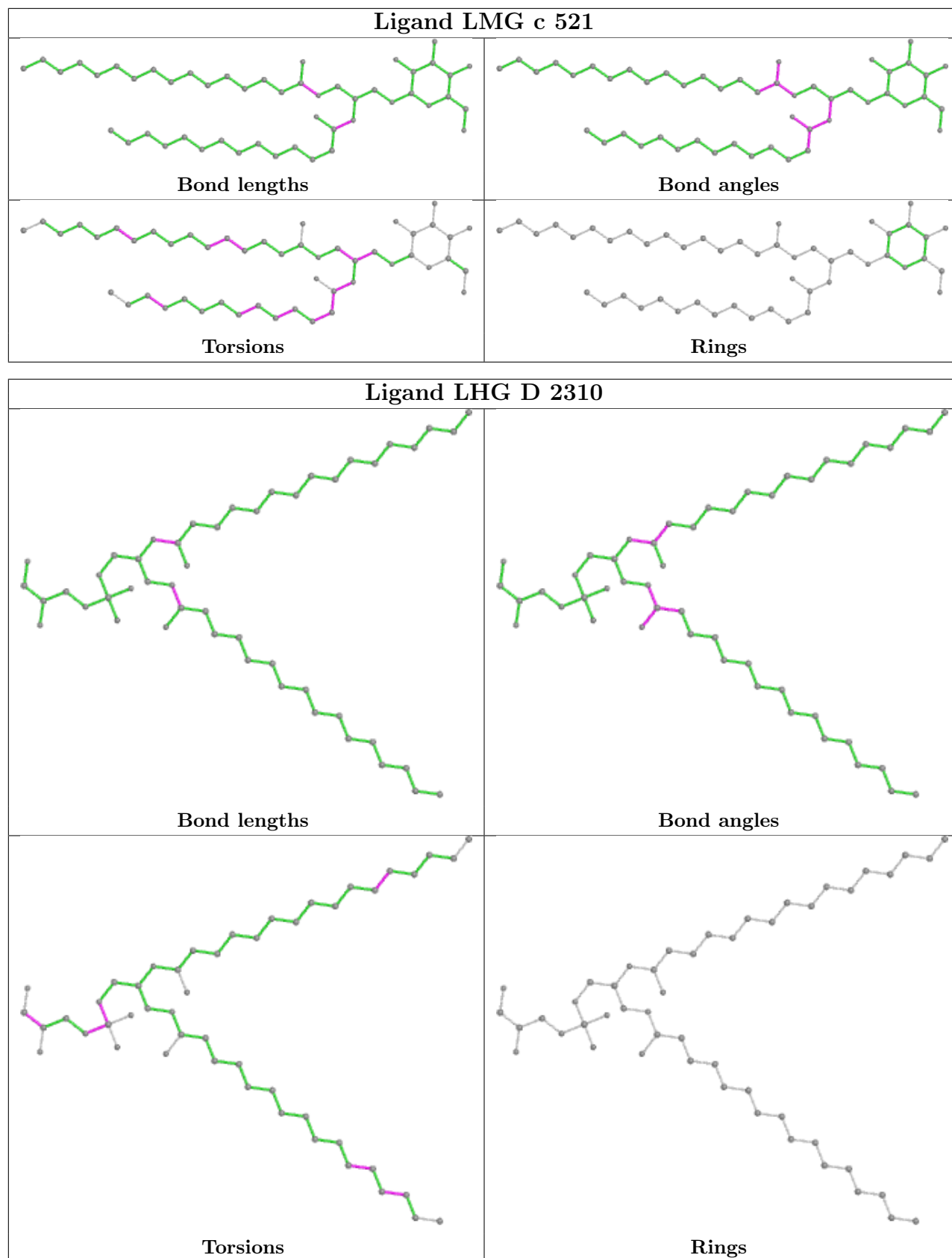


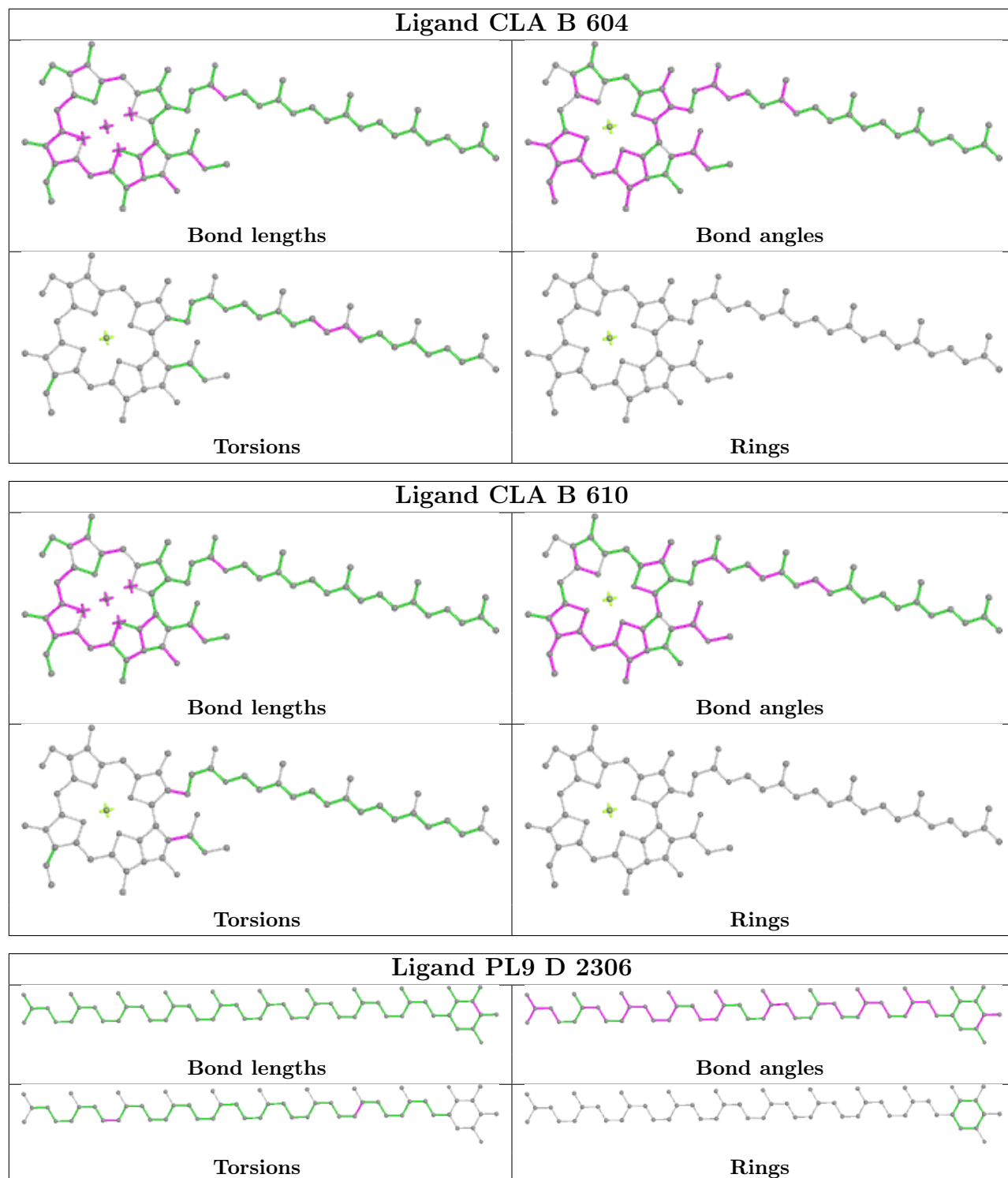


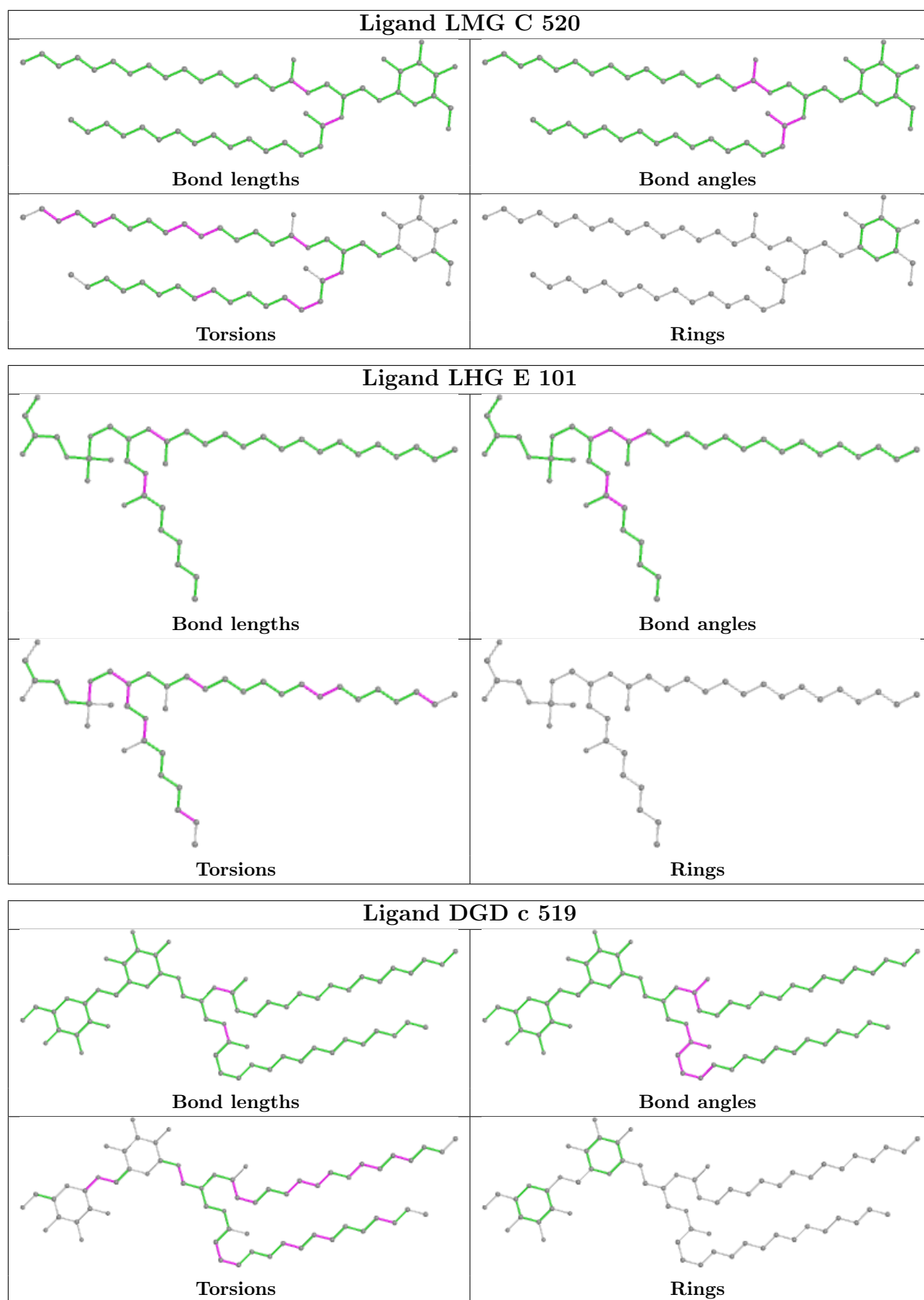


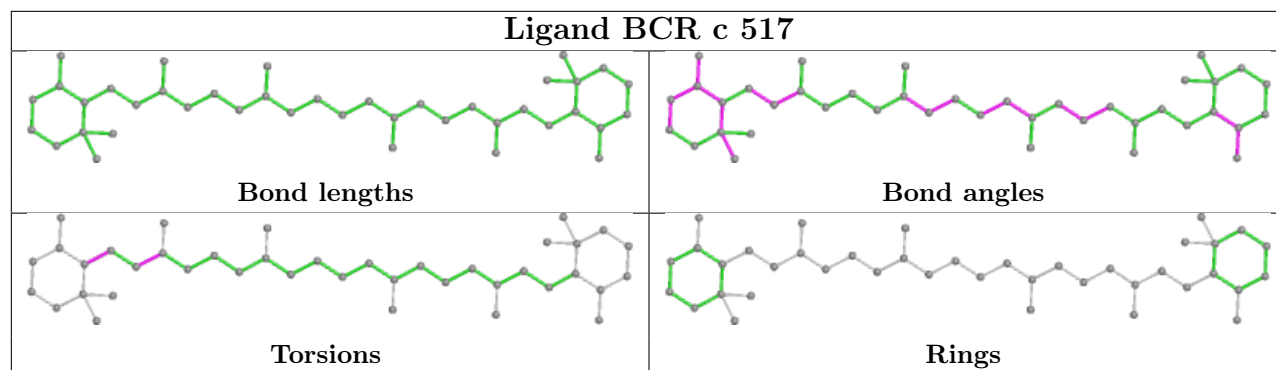












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	334/344 (97%)	-0.07	9 (2%) 54 63	38, 46, 86, 139	0
1	a	334/344 (97%)	0.25	26 (7%) 13 18	39, 47, 88, 143	1 (0%)
2	B	505/505 (100%)	0.12	51 (10%) 7 10	39, 52, 92, 138	0
2	b	483/505 (95%)	-0.06	33 (6%) 17 24	40, 53, 83, 143	0
3	C	451/455 (99%)	-0.00	29 (6%) 19 26	41, 59, 83, 164	0
3	c	455/455 (100%)	0.20	33 (7%) 15 21	45, 61, 81, 136	0
4	D	340/342 (99%)	-0.22	6 (1%) 68 75	37, 49, 75, 113	0
4	d	341/342 (99%)	-0.15	11 (3%) 47 56	38, 50, 77, 138	0
5	E	80/83 (96%)	0.90	22 (27%) 0 0	50, 77, 128, 144	0
5	e	79/83 (95%)	0.96	14 (17%) 1 1	56, 78, 124, 137	0
6	F	34/44 (77%)	0.04	5 (14%) 2 3	52, 64, 114, 124	0
6	f	32/44 (72%)	0.05	2 (6%) 20 27	53, 66, 119, 132	0
7	H	63/63 (100%)	0.23	5 (7%) 12 17	53, 69, 85, 111	0
7	h	63/63 (100%)	0.76	17 (26%) 0 0	56, 72, 89, 117	0
8	I	31/38 (81%)	0.35	6 (19%) 1 1	53, 71, 146, 152	0
8	i	31/38 (81%)	0.94	6 (19%) 1 1	51, 67, 129, 137	0
9	J	36/40 (90%)	-0.27	2 (5%) 24 33	48, 67, 111, 135	0
9	j	39/40 (97%)	0.14	5 (12%) 3 5	55, 68, 131, 162	0
10	K	37/37 (100%)	-0.37	1 (2%) 54 63	59, 68, 84, 92	0
10	k	37/37 (100%)	0.07	3 (8%) 12 16	58, 69, 95, 114	0
11	L	37/37 (100%)	-0.24	4 (10%) 5 8	38, 45, 88, 153	0
11	l	36/37 (97%)	0.00	1 (2%) 53 62	40, 46, 102, 158	0
12	M	32/36 (88%)	-0.50	1 (3%) 49 58	43, 48, 72, 106	0
12	m	33/36 (91%)	0.15	2 (6%) 21 28	41, 49, 100, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	244/244 (100%)	0.34	32 (13%) 3 4	38, 60, 104, 154	0
13	o	243/244 (99%)	0.21	33 (13%) 3 3	41, 60, 108, 162	0
14	T	29/32 (90%)	-0.20	1 (3%) 45 53	39, 46, 82, 150	0
14	t	29/32 (90%)	0.27	2 (6%) 16 23	40, 46, 80, 129	0
15	U	97/104 (93%)	-0.17	3 (3%) 49 58	46, 55, 86, 105	0
15	u	97/104 (93%)	-0.45	1 (1%) 82 86	49, 58, 80, 136	0
16	V	137/137 (100%)	-0.21	3 (2%) 62 69	45, 54, 80, 100	0
16	v	137/137 (100%)	0.43	22 (16%) 1 2	50, 66, 91, 110	0
17	Y	30/30 (100%)	1.18	7 (23%) 0 0	70, 83, 113, 124	0
17	y	30/30 (100%)	0.93	5 (16%) 1 2	75, 88, 105, 136	0
18	X	38/40 (95%)	1.56	18 (47%) 0 0	66, 79, 111, 122	0
18	x	35/40 (87%)	1.17	11 (31%) 0 0	71, 80, 122, 134	0
19	Z	61/62 (98%)	1.53	23 (37%) 0 0	66, 81, 124, 140	0
19	z	60/62 (96%)	1.89	27 (45%) 0 0	75, 88, 132, 159	0
All	All	5210/5346 (97%)	0.14	482 (9%) 8 13	37, 56, 98, 164	1 (0%)

All (482) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	O	3	GLN	9.7
2	B	486	LEU	7.9
1	A	11	ALA	7.7
18	x	2	THR	7.1
19	z	4	LEU	6.2
2	B	487	SER	6.1
19	z	5	PHE	5.9
1	a	224	ILE	5.9
16	v	21	LEU	5.7
6	f	14	PRO	5.7
19	z	3	ILE	5.6
13	o	246	ALA	5.5
2	B	495	PHE	5.5
1	a	14	TRP	5.5
16	v	26	TYR	5.4
1	A	14	TRP	5.4
8	I	32	PRO	5.4
13	o	36	GLN	5.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
9	j	2	MET	5.3
6	F	12	SER	5.2
8	I	29	ALA	5.2
1	A	12	ASN	5.1
18	X	34	ILE	5.1
2	b	292	LEU	5.0
19	z	2	THR	4.9
2	B	504	THR	4.9
9	j	4	GLU	4.8
17	y	22	LEU	4.8
1	a	235	TYR	4.8
19	Z	33	TRP	4.8
18	X	31	ILE	4.8
5	E	79	PHE	4.7
2	B	502	VAL	4.7
13	O	136	ILE	4.7
18	x	3	ILE	4.7
2	B	496	TYR	4.7
12	m	34	LYS	4.7
2	b	293	ALA	4.6
7	H	64	ALA	4.6
17	Y	19	ILE	4.6
3	c	433	LEU	4.6
19	Z	29	SER	4.5
17	Y	18	VAL	4.5
7	h	10	ILE	4.5
5	E	21	VAL	4.5
7	h	57	GLY	4.5
7	h	6	TRP	4.5
2	B	84	THR	4.5
5	E	76	VAL	4.4
7	h	64	ALA	4.4
2	B	503	THR	4.4
4	d	11	GLU	4.4
13	O	27	ARG	4.3
18	x	34	ILE	4.3
5	E	83	LEU	4.2
14	t	29	ILE	4.2
5	E	77	GLU	4.2
2	B	479	PHE	4.2
19	z	60	PHE	4.2
2	b	484	PRO	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
13	o	30	TYR	4.2
2	b	483	ASP	4.2
2	b	295	GLY	4.2
13	O	87	VAL	4.1
16	v	27	LEU	4.1
19	z	42	LEU	4.1
13	O	24	ASP	4.1
19	z	57	LEU	4.1
5	E	17	VAL	4.1
5	e	10	PHE	4.0
2	B	494	GLY	4.0
4	d	238	THR	4.0
13	o	136	ILE	4.0
19	z	9	LEU	4.0
13	O	137	THR	4.0
3	C	143	TYR	4.0
19	Z	26	ALA	4.0
2	B	501	ASP	3.9
2	B	490	GLN	3.9
5	E	74	GLN	3.9
4	d	240	ALA	3.9
18	x	8	LYS	3.9
13	o	135	SER	3.9
14	t	30	THR	3.9
18	X	2	THR	3.9
18	X	39	ARG	3.9
17	y	20	ALA	3.9
2	B	506	LYS	3.9
13	o	26	ALA	3.9
6	F	13	TYR	3.8
3	c	183	GLY	3.8
19	z	33	TRP	3.8
8	I	31	ASN	3.8
5	E	18	ARG	3.8
2	B	489	GLU	3.8
7	h	7	LEU	3.8
18	X	37	VAL	3.8
1	a	15	GLU	3.8
2	b	124	ARG	3.8
12	M	33	GLN	3.7
14	T	30	THR	3.7
19	z	7	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	485	GLU	3.7
1	a	260	PHE	3.7
16	v	10	VAL	3.6
18	X	3	ILE	3.6
18	x	32	SER	3.6
5	E	82	GLN	3.6
19	Z	61	VAL	3.6
1	a	246	TYR	3.6
2	b	297	THR	3.6
7	h	5	THR	3.6
17	y	18	VAL	3.6
16	v	20	THR	3.6
1	a	225	ARG	3.5
18	X	4	THR	3.5
1	a	297	LEU	3.5
5	e	59	GLU	3.5
5	E	78	THR	3.5
16	v	19	ILE	3.5
2	b	129	GLY	3.5
13	o	35	SER	3.5
8	i	32	PRO	3.5
19	Z	30	PRO	3.5
1	a	19	ASN	3.4
3	c	201	ASN	3.4
13	o	58	ASN	3.4
3	C	257	PHE	3.4
13	o	27	ARG	3.4
1	a	242	GLU	3.4
3	C	145	SER	3.4
3	C	433	LEU	3.4
4	D	238	THR	3.4
3	c	424	SER	3.4
15	U	73[A]	GLN	3.4
13	o	38	TYR	3.4
5	E	72	ALA	3.4
19	Z	35	ARG	3.4
2	B	488	PRO	3.4
5	e	25	ILE	3.4
3	C	24	THR	3.4
1	a	226	GLU	3.4
2	b	85	GLY	3.4
5	e	58	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
3	c	87	ILE	3.3
13	O	26	ALA	3.3
13	O	25	THR	3.3
13	o	37	THR	3.3
16	v	8	LEU	3.3
11	L	1	MET	3.3
2	b	296	ALA	3.3
10	K	14	ALA	3.3
3	C	255	THR	3.3
3	c	203	THR	3.3
19	Z	36	SER	3.3
1	a	11	ALA	3.3
13	O	130[A]	GLN	3.2
3	C	262	ARG	3.2
2	B	484	PRO	3.2
3	C	253	LEU	3.2
3	c	434	ALA	3.2
10	k	18	PHE	3.2
3	c	200	THR	3.2
3	c	143	TYR	3.2
6	F	16	PHE	3.2
7	h	9	ASP	3.2
7	h	8	GLY	3.2
4	D	240	ALA	3.2
13	o	204	VAL	3.2
16	v	4	THR	3.2
16	v	18	THR	3.1
2	b	126	PRO	3.1
19	Z	62	VAL	3.1
3	c	426	LEU	3.1
19	Z	3	ILE	3.1
2	b	298	LEU	3.1
13	o	243	ILE	3.1
17	y	19	ILE	3.1
19	z	53	VAL	3.1
3	C	259	TRP	3.1
2	B	127	ARG	3.1
16	v	3	LEU	3.1
3	c	182	PHE	3.1
5	E	81	GLU	3.1
3	C	23	ALA	3.1
2	b	460	LEU	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
13	o	28	GLY	3.0
3	c	198	VAL	3.0
5	E	73	LYS	3.0
1	A	15	GLU	3.0
5	E	80	LEU	3.0
3	c	432	VAL	3.0
4	d	27	PHE	3.0
16	v	5	PRO	3.0
19	Z	32	ASP	3.0
1	a	295	PHE	3.0
9	j	3	SER	3.0
18	X	32	SER	3.0
7	h	56	ASP	3.0
13	o	22	LEU	3.0
2	b	291	SER	3.0
3	c	429	SER	3.0
5	e	57	ALA	3.0
3	c	259	TRP	3.0
8	i	21	PHE	2.9
4	d	237	PRO	2.9
1	a	13	LEU	2.9
18	X	23	LEU	2.9
5	e	76	VAL	2.9
2	B	86	ILE	2.9
18	X	35	ASP	2.9
2	B	253	ALA	2.9
13	O	4	THR	2.9
11	L	2	GLU	2.9
4	d	235	PHE	2.9
5	e	72	ALA	2.9
2	B	492	GLU	2.9
3	c	276	LEU	2.9
19	Z	42	LEU	2.9
8	I	27	ASP	2.9
17	Y	20	ALA	2.9
3	c	287	THR	2.9
13	o	34	SER	2.9
19	z	46	LEU	2.9
5	e	21	VAL	2.8
18	X	33	GLN	2.8
2	B	500	GLY	2.8
8	I	30	ARG	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
9	j	5	GLY	2.8
13	O	30	TYR	2.8
13	o	33	ASP	2.8
2	b	461	LEU	2.8
17	Y	22	LEU	2.8
2	B	85	GLY	2.8
5	e	61	ARG	2.8
8	I	28	PRO	2.8
13	o	39	ARG	2.8
19	z	32	ASP	2.8
7	H	29	PRO	2.8
2	b	125	ASP	2.8
2	b	218	LEU	2.8
19	Z	34	ASP	2.8
19	Z	9	LEU	2.8
15	U	70	ARG	2.8
2	B	478	VAL	2.8
13	o	32	ILE	2.8
3	c	181	PHE	2.8
13	O	141	ASP	2.8
2	B	497	GLN	2.8
16	v	12	LEU	2.8
19	z	56	VAL	2.7
11	L	3	PRO	2.7
2	b	217	ILE	2.7
2	B	460	LEU	2.7
13	O	202	ALA	2.7
2	B	251	VAL	2.7
7	H	58	VAL	2.7
9	J	6	GLY	2.7
3	C	144	SER	2.7
1	a	223	LEU	2.7
2	B	459	ALA	2.7
13	O	199	LEU	2.7
18	X	38	GLN	2.7
3	C	261	ARG	2.7
3	c	202	PRO	2.7
18	x	5	PRO	2.7
2	B	244	ALA	2.7
8	i	29	ALA	2.7
5	e	20	TRP	2.7
19	Z	38	GLN	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	491	VAL	2.7
2	b	457	VAL	2.7
7	h	23	PRO	2.7
13	O	206	GLY	2.7
18	X	25	PHE	2.7
19	Z	5	PHE	2.7
12	m	33	GLN	2.7
19	z	35	ARG	2.7
16	v	7	VAL	2.6
17	Y	40	ALA	2.6
18	X	5	PRO	2.6
9	J	8	ILE	2.6
1	A	230	THR	2.6
4	D	45	LEU	2.6
13	o	5	LEU	2.6
1	a	243	GLU	2.6
19	z	54	VAL	2.6
2	B	34	ALA	2.6
3	C	427	ALA	2.6
19	z	49	ALA	2.6
3	C	289	PHE	2.6
6	f	42	PHE	2.6
13	o	4	THR	2.6
7	H	3	ARG	2.6
3	C	438	LEU	2.6
6	F	14	PRO	2.6
13	o	31	PRO	2.6
13	O	212	ALA	2.6
2	B	246	PHE	2.6
1	a	343	LEU	2.6
4	d	12	ARG	2.6
18	x	35	ASP	2.6
5	E	4	THR	2.6
16	v	22	THR	2.6
5	E	20	TRP	2.6
19	z	34	ASP	2.5
13	o	245	PRO	2.5
13	O	135	SER	2.5
2	b	84	THR	2.5
3	c	428	THR	2.5
19	z	38	GLN	2.5
2	B	242	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
15	u	8	GLU	2.5
3	c	56	HIS	2.5
19	Z	60	PHE	2.5
13	O	5	LEU	2.5
13	O	93	LEU	2.5
2	B	248	ALA	2.5
13	o	140	THR	2.5
2	b	242	ILE	2.5
5	E	25	ILE	2.5
8	i	14	PHE	2.5
4	d	234	ALA	2.5
2	B	499	VAL	2.5
13	O	32	ILE	2.5
18	x	33	GLN	2.4
2	B	250	PHE	2.4
13	O	142	PHE	2.4
19	Z	2	THR	2.4
13	o	89	SER	2.4
3	C	279	LEU	2.4
13	O	201	VAL	2.4
4	D	239	GLN	2.4
1	a	290	ILE	2.4
19	Z	27	TYR	2.4
13	o	134	THR	2.4
2	B	247	PHE	2.4
19	z	25	VAL	2.4
4	d	236	ASN	2.4
5	e	43	ALA	2.4
1	a	222[A]	SER	2.4
5	E	22	ILE	2.4
16	v	16	GLY	2.4
13	O	23	ASP	2.4
3	C	432	VAL	2.4
2	b	467	ILE	2.4
2	b	482	ILE	2.4
2	B	33	TRP	2.4
3	C	437	PHE	2.3
1	a	16	ARG	2.3
16	v	25	GLN	2.3
19	z	8	ALA	2.3
2	B	482	ILE	2.3
2	B	461	LEU	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
18	X	28	LEU	2.3
1	a	283	VAL	2.3
3	c	427	ALA	2.3
16	v	17	LYS	2.3
4	D	116	LEU	2.3
16	v	6	GLU	2.3
19	Z	41	PHE	2.3
7	h	58	VAL	2.3
19	z	13	VAL	2.3
1	A	251	ALA	2.3
3	C	434	ALA	2.3
18	x	36	LYS	2.3
2	b	27	THR	2.3
2	b	294	SER	2.3
13	O	213	GLY	2.3
8	i	31	ASN	2.3
2	B	249	ALA	2.3
4	d	152	VAL	2.3
2	b	121	GLU	2.3
1	a	192	ILE	2.3
3	C	285	ILE	2.3
1	A	19	ASN	2.3
2	B	505	ARG	2.3
19	Z	57	LEU	2.3
3	c	435	PHE	2.3
3	c	462	GLU	2.3
18	X	30	ALA	2.3
7	H	27	THR	2.3
13	o	208	THR	2.3
17	Y	41	VAL	2.3
7	h	18	TYR	2.2
18	x	7	LEU	2.2
19	z	59	PHE	2.2
3	C	198	VAL	2.2
18	X	27	VAL	2.2
1	a	247	ASN	2.2
13	O	132	ASN	2.2
19	z	6	GLN	2.2
16	v	29	GLY	2.2
2	b	244	ALA	2.2
13	o	130	GLN	2.2
19	Z	51	VAL	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	31	ALA	2.2
1	a	227	THR	2.2
3	c	279	LEU	2.2
19	Z	4	LEU	2.2
13	o	132	ASN	2.2
3	c	196	VAL	2.2
11	l	3	PRO	2.2
13	O	133	VAL	2.2
7	h	12	ARG	2.2
3	c	430	HIS	2.2
13	O	140	THR	2.2
13	O	204	VAL	2.2
5	E	57	ALA	2.2
19	z	10	ALA	2.2
2	B	185	TRP	2.2
9	j	6	GLY	2.2
13	o	206	GLY	2.2
2	B	298	LEU	2.2
3	c	404	LEU	2.2
2	B	30	VAL	2.2
16	v	113	VAL	2.2
7	h	4	ARG	2.2
19	Z	39	LEU	2.1
3	C	436	PHE	2.1
3	c	420	VAL	2.1
19	z	41	PHE	2.1
16	V	22	THR	2.1
16	v	14	SER	2.1
6	F	15	ILE	2.1
3	C	426	LEU	2.1
3	c	204	LEU	2.1
2	B	457	VAL	2.1
19	z	18	VAL	2.1
13	O	95	PHE	2.1
7	h	24	GLY	2.1
8	i	9	TYR	2.1
13	O	28	GLY	2.1
16	v	23	GLU	2.1
11	L	5	PRO	2.1
3	C	155	ASN	2.1
18	X	36	LYS	2.1
5	E	60	GLN	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
13	O	139	SER	2.1
1	A	250	ALA	2.1
2	b	249	ALA	2.1
2	b	459	ALA	2.1
13	O	129	THR	2.1
5	E	59	GLU	2.1
3	c	422	PRO	2.1
13	o	25	THR	2.1
17	y	26	ALA	2.1
2	B	493	TRP	2.1
3	C	429	SER	2.1
10	k	17	ILE	2.1
16	V	21	LEU	2.1
2	b	290	ALA	2.1
2	b	304	ALA	2.1
10	k	16	ALA	2.1
13	o	29	ALA	2.1
18	x	4	THR	2.1
5	e	19	TYR	2.1
2	b	480	SER	2.0
3	c	144	SER	2.0
2	b	238	LEU	2.0
5	e	14	ILE	2.0
4	d	239	GLN	2.0
1	A	249	VAL	2.0
1	a	245	THR	2.0
3	C	152	LYS	2.0
3	C	287	THR	2.0
2	B	61	PHE	2.0
17	Y	37	PHE	2.0
3	c	86	LEU	2.0
4	D	123	ILE	2.0
7	h	55	LEU	2.0
13	o	40	ILE	2.0
3	C	335	THR	2.0
15	U	58	VAL	2.0
16	V	6	GLU	2.0
2	B	65	PHE	2.0
2	B	295	GLY	2.0
1	a	293	MET	2.0
5	E	36	LEU	2.0
5	e	32	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
7	h	22	ALA	2.0
3	C	148	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
19	FME	Z	1	10/11	0.91	0.25	96,112,117,118	0
19	FME	z	1	10/11	0.91	0.34	114,129,141,143	0
8	FME	I	1	10/11	0.96	0.10	49,59,63,64	0
4	HSK	d	336[A]	10/12	0.96	0.12	51,56,59,60	7
4	HSK	d	336[B]	11/12	0.96	0.12	51,56,59,62	8
12	FME	M	1	10/11	0.96	0.11	48,56,80,81	0
12	FME	m	1	10/11	0.97	0.08	43,57,81,84	0
14	FME	t	1	10/11	0.97	0.07	46,51,77,79	0
14	FME	T	1	10/11	0.97	0.06	48,54,84,88	0
4	HSK	D	336[A]	10/12	0.98	0.10	49,51,51,51	7
4	HSK	D	336[B]	11/12	0.98	0.10	50,51,51,51	8
8	FME	i	1	10/11	0.98	0.11	52,60,62,64	0

## 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
41	MG	K	102	1/1	0.33	0.15	85,85,85,85	0
37	DGD	D	2307	53/66	0.37	0.36	96,121,171,177	0
38	LHG	e	101	40/49	0.40	0.38	93,156,201,202	0
34	DMS	c	546	4/4	0.44	0.23	151,153,154,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
29	GOL	E	104	6/6	0.47	0.23	124,126,128,129	0
30	UNL	j	2702	16/-	0.47	0.47	89,96,108,111	0
30	UNL	k	301	16/-	0.49	0.25	89,109,125,126	0
29	GOL	c	529	6/6	0.50	0.17	124,131,132,133	0
28	LMT	m	2804	35/35	0.51	0.31	79,146,162,166	0
34	DMS	c	547	4/4	0.53	0.46	132,138,140,141	0
29	GOL	b	631	6/6	0.53	0.26	84,100,106,106	0
29	GOL	v	204	6/6	0.53	0.41	92,115,115,123	0
30	UNL	A	416	28/-	0.53	0.29	93,104,133,143	0
28	LMT	j	2701	34/35	0.54	0.24	79,145,158,159	0
28	LMT	d	404	25/35	0.54	0.30	91,129,162,164	0
28	LMT	M	101	35/35	0.55	0.31	84,157,181,181	0
30	UNL	D	2313	12/-	0.57	0.40	93,112,114,115	0
34	DMS	b	638	4/4	0.58	0.36	159,163,163,165	0
28	LMT	M	102	35/35	0.59	0.26	59,106,136,139	0
30	UNL	I	102	40/-	0.59	0.35	101,119,151,152	0
30	UNL	c	527	12/-	0.59	0.38	104,113,125,126	0
30	UNL	i	101	19/-	0.59	0.41	88,112,144,146	0
29	GOL	d	416	6/6	0.59	0.15	129,131,132,133	0
30	UNL	B	629	15/-	0.59	0.57	90,105,111,112	0
28	LMT	B	634	35/35	0.60	0.32	55,133,160,162	0
38	LHG	E	101	40/49	0.60	0.35	94,137,163,165	0
29	GOL	B	630	6/6	0.61	0.20	94,104,109,117	0
34	DMS	c	549	4/4	0.62	0.27	124,126,128,128	0
29	GOL	O	305	6/6	0.63	0.26	70,91,97,105	0
30	UNL	Y	301	12/-	0.63	0.22	114,116,120,121	0
29	GOL	o	303	6/6	0.63	0.17	71,83,104,109	0
34	DMS	O	311	4/4	0.63	0.42	130,135,136,138	0
34	DMS	B	640	4/4	0.64	0.43	154,155,156,157	0
27	LMG	C	527	51/55	0.65	0.31	71,123,148,152	0
34	DMS	a	2620	4/4	0.65	0.45	142,146,149,151	0
29	GOL	u	501	6/6	0.66	0.21	84,92,98,102	0
36	HTG	i	102	19/19	0.66	0.23	68,143,157,158	0
30	UNL	a	2616	27/-	0.66	0.42	86,103,140,149	0
28	LMT	m	2803	35/35	0.67	0.27	61,101,118,121	0
34	DMS	T	104	4/4	0.67	0.33	156,160,160,161	0
26	SQD	D	2302	54/54	0.67	0.25	75,106,174,176	0
36	HTG	b	626	19/19	0.68	0.18	98,151,158,158	0
29	GOL	O	304	6/6	0.68	0.25	86,101,103,106	0
30	UNL	b	627	15/-	0.68	0.36	90,97,113,114	0
30	UNL	b	628	10/-	0.68	0.34	94,111,114,116	0
28	LMT	d	401	35/35	0.68	0.26	63,106,125,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
29	GOL	c	530	6/6	0.68	0.18	79,107,118,124	0
28	LMT	J	303	24/35	0.69	0.25	80,95,144,147	0
34	DMS	o	309	4/4	0.69	0.44	131,139,139,141	0
40	RRX	h	101	41/41	0.69	0.23	56,81,103,119	0
36	HTG	B	627	19/19	0.69	0.25	67,130,145,148	0
30	UNL	x	1302	18/-	0.70	0.20	76,86,120,124	0
29	GOL	c	531	6/6	0.70	0.16	116,118,119,120	0
30	UNL	C	501	40/-	0.70	0.37	102,120,136,139	0
29	GOL	B	632	6/6	0.71	0.26	87,96,98,101	0
36	HTG	c	526	19/19	0.71	0.27	120,165,175,175	0
34	DMS	X	101	4/4	0.71	0.25	172,174,175,175	0
28	LMT	F	102	24/35	0.71	0.35	114,127,159,161	0
34	DMS	b	643	4/4	0.72	0.35	125,131,133,136	0
36	HTG	B	625	19/19	0.72	0.42	77,130,138,140	19
30	UNL	b	632	10/-	0.72	0.26	83,93,104,105	0
30	UNL	D	2314	18/-	0.72	0.21	67,79,113,117	0
28	LMT	Z	101	35/35	0.72	0.27	68,142,184,187	0
36	HTG	d	407	19/19	0.72	0.41	102,133,146,148	0
29	GOL	V	203	6/6	0.73	0.14	98,111,118,123	0
36	HTG	B	624[A]	19/19	0.73	0.32	56,72,85,87	19
36	HTG	c	524	19/19	0.73	0.45	62,108,119,121	19
36	HTG	B	624[B]	19/19	0.73	0.32	57,72,86,88	19
33	PL9	A	422	39/55	0.73	0.38	88,101,124,127	0
36	HTG	d	415	19/19	0.73	0.23	80,117,124,125	19
36	HTG	C	522	19/19	0.74	0.46	88,124,137,140	0
34	DMS	c	542	4/4	0.74	0.25	148,149,150,151	0
34	DMS	b	642	4/4	0.74	0.32	153,154,156,159	0
30	UNL	C	523	10/-	0.74	0.24	99,101,107,112	0
29	GOL	U	501	6/6	0.75	0.25	105,111,113,115	0
29	GOL	O	302	6/6	0.75	0.12	78,82,87,91	0
26	SQD	a	2603	54/54	0.75	0.21	55,89,136,138	0
30	UNL	B	628	18/-	0.75	0.26	85,96,116,117	0
28	LMT	A	414	33/35	0.75	0.26	72,117,128,135	0
30	UNL	T	101	13/-	0.75	0.67	93,100,107,107	0
36	HTG	C	525	19/19	0.75	0.33	91,137,156,156	0
34	DMS	U	504	4/4	0.75	0.18	119,124,127,129	0
30	UNL	B	631	32/-	0.75	0.18	66,97,116,117	0
28	LMT	f	101	24/35	0.76	0.43	102,124,156,160	0
27	LMG	c	522	51/55	0.76	0.29	65,117,127,130	0
28	LMT	A	420	24/35	0.76	0.19	63,104,142,148	0
36	HTG	I	101	19/19	0.76	0.22	83,126,141,145	0
34	DMS	H	104	4/4	0.76	0.31	129,131,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
34	DMS	B	637	4/4	0.77	0.17	121,124,125,126	0
34	DMS	c	541	4/4	0.77	0.48	121,128,129,132	0
36	HTG	b	625	19/19	0.77	0.31	58,83,106,108	0
28	LMT	T	103	24/35	0.77	0.24	58,91,129,132	0
28	LMT	i	103	24/35	0.77	0.18	67,119,153,155	0
27	LMG	m	2802	51/55	0.77	0.26	56,81,98,107	0
30	UNL	J	304	5/-	0.77	0.34	97,98,103,104	0
33	PL9	x	1301	39/55	0.78	0.22	94,113,131,132	0
34	DMS	A	429	4/4	0.78	0.37	128,129,130,132	0
34	DMS	V	207	4/4	0.78	0.30	137,139,141,141	0
36	HTG	b	604	19/19	0.78	0.17	79,131,144,147	0
26	SQD	b	601	48/54	0.79	0.22	66,96,152,156	0
29	GOL	v	202	6/6	0.79	0.14	113,114,116,118	0
28	LMT	B	623	35/35	0.79	0.23	89,122,148,149	0
34	DMS	A	430	4/4	0.79	0.22	115,127,127,130	0
30	UNL	a	2601	15/-	0.79	0.33	79,86,93,96	0
30	UNL	c	502	36/-	0.79	0.25	91,115,128,130	0
31	JOX	A	419	10/10	0.80	0.19	60,69,76,78	0
30	UNL	d	405	37/-	0.80	0.20	74,101,137,137	0
28	LMT	z	102	33/35	0.80	0.22	80,141,156,157	0
34	DMS	o	310	4/4	0.80	0.34	144,147,149,149	0
30	UNL	A	423	9/-	0.80	0.47	84,89,93,94	0
27	LMG	c	501	51/55	0.80	0.23	67,90,101,105	0
40	RRX	H	102	41/41	0.80	0.20	48,75,95,100	0
34	DMS	B	635	4/4	0.80	0.20	130,132,133,133	0
26	SQD	B	621	54/54	0.80	0.21	60,92,128,131	0
29	GOL	D	2301	6/6	0.81	0.22	87,93,100,104	0
26	SQD	l	101	54/54	0.81	0.22	59,88,126,130	0
29	GOL	J	301	6/6	0.81	0.49	100,103,110,111	0
30	UNL	E	103	9/-	0.81	0.37	75,83,107,110	0
36	HTG	H	101	17/19	0.81	0.33	109,127,151,151	0
34	DMS	C	537	4/4	0.81	0.30	143,143,144,146	0
34	DMS	a	2624	4/4	0.81	0.47	79,105,106,109	0
29	GOL	U	502	6/6	0.81	0.24	73,82,89,97	0
27	LMG	B	622	51/55	0.81	0.22	57,81,98,100	0
34	DMS	O	319	4/4	0.81	0.34	131,134,135,136	0
37	DGD	h	102	62/66	0.82	0.21	52,71,117,119	0
30	UNL	b	630	21/-	0.82	0.16	56,79,122,124	0
34	DMS	B	646	4/4	0.82	0.30	94,96,102,107	0
34	DMS	b	637	4/4	0.82	0.25	89,107,109,112	0
34	DMS	O	314	4/4	0.82	0.51	117,121,126,133	0
27	LMG	C	520	51/55	0.82	0.21	59,91,107,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
29	GOL	C	524	6/6	0.83	0.14	101,110,113,118	0
30	UNL	c	528	5/-	0.83	0.30	87,89,97,97	0
34	DMS	O	306	4/4	0.83	0.32	146,150,150,153	0
29	GOL	a	2602	6/6	0.83	0.25	64,79,91,91	0
34	DMS	c	538	4/4	0.83	0.35	136,137,139,141	0
34	DMS	B	645	4/4	0.83	0.37	124,125,125,127	0
30	UNL	E	102	6/-	0.83	0.18	83,87,87,89	0
30	UNL	t	101	8/-	0.84	0.54	75,84,103,103	0
34	DMS	v	214	4/4	0.84	0.50	131,135,135,136	0
30	UNL	e	102	15/-	0.84	0.30	74,93,101,101	0
30	UNL	b	629	8/-	0.84	0.31	72,94,106,108	0
34	DMS	O	309	4/4	0.84	0.38	117,118,118,120	0
34	DMS	O	318	4/4	0.85	0.23	115,117,119,126	0
34	DMS	o	306	4/4	0.85	0.23	118,119,124,125	0
34	DMS	c	532	4/4	0.86	0.13	87,89,96,102	0
34	DMS	O	308	4/4	0.86	0.43	124,127,127,132	0
34	DMS	c	540	4/4	0.86	0.20	111,115,116,117	0
36	HTG	B	626	19/19	0.86	0.14	64,93,111,116	0
34	DMS	B	643	4/4	0.86	0.35	99,101,107,111	0
34	DMS	A	425	4/4	0.86	0.50	152,153,153,155	0
34	DMS	v	212	4/4	0.86	0.19	133,135,138,138	0
30	UNL	c	525	6/-	0.86	0.14	95,97,98,101	0
34	DMS	B	642	4/4	0.87	0.31	95,106,108,114	0
30	UNL	m	2801	15/-	0.87	0.21	68,85,119,123	0
29	GOL	v	203	6/6	0.87	0.15	81,87,91,92	0
25	BCR	k	302	40/40	0.87	0.15	53,64,78,79	0
26	SQD	D	2308	45/54	0.87	0.38	92,119,145,154	0
34	DMS	D	2317	4/4	0.88	0.21	99,105,106,109	0
34	DMS	d	420	4/4	0.88	0.46	121,122,123,124	0
34	DMS	d	422	4/4	0.88	0.43	118,121,124,128	0
34	DMS	b	640	4/4	0.88	0.33	110,112,115,117	0
34	DMS	D	2320	4/4	0.88	0.23	144,144,144,147	0
27	LMG	A	413	51/55	0.88	0.20	64,82,106,110	0
34	DMS	v	210	4/4	0.88	0.28	137,140,140,143	0
34	DMS	v	211	4/4	0.88	0.15	120,122,123,123	0
31	JOX	A	418	10/10	0.88	0.10	65,87,88,94	0
34	DMS	c	537	4/4	0.88	0.23	116,122,123,125	0
27	LMG	c	521	49/55	0.88	0.18	60,94,118,121	0
37	DGD	H	103	62/66	0.88	0.25	51,69,100,104	0
34	DMS	V	212	4/4	0.88	0.20	98,111,112,115	0
34	DMS	B	647	4/4	0.88	0.18	105,106,112,112	0
34	DMS	C	534	4/4	0.88	0.16	141,141,143,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
34	DMS	c	544	4/4	0.88	0.16	105,110,113,115	0
34	DMS	O	313	4/4	0.88	0.33	103,110,110,111	0
23	CLA	B	610	65/65	0.88	0.14	47,58,69,73	0
36	HTG	b	603	19/19	0.89	0.15	70,89,107,110	0
34	DMS	o	316	4/4	0.89	0.48	85,101,104,108	0
34	DMS	t	102	4/4	0.89	0.23	129,132,137,137	0
34	DMS	u	502	4/4	0.89	0.24	127,129,129,131	0
36	HTG	c	523	19/19	0.89	0.25	99,121,130,133	0
34	DMS	C	535	4/4	0.89	0.18	109,109,110,112	0
34	DMS	C	536	4/4	0.89	0.16	134,137,138,140	0
34	DMS	V	202	4/4	0.89	0.18	115,124,124,124	0
23	CLA	c	515	65/65	0.89	0.17	60,71,101,105	0
34	DMS	c	548	4/4	0.89	0.20	123,130,130,130	0
34	DMS	V	211	4/4	0.89	0.59	109,112,114,114	0
25	BCR	a	2614	40/40	0.89	0.14	38,48,55,57	0
34	DMS	V	213	4/4	0.89	0.20	115,118,119,120	0
34	DMS	d	423	4/4	0.89	0.25	133,137,137,140	0
30	UNL	l	102	16/-	0.89	0.25	67,90,115,121	0
34	DMS	A	428	4/4	0.89	0.18	118,118,118,120	0
23	CLA	C	514	65/65	0.89	0.23	66,78,111,115	0
34	DMS	o	315	4/4	0.89	0.29	135,137,138,138	0
37	DGD	C	518	62/66	0.90	0.16	48,63,101,111	0
34	DMS	c	545	4/4	0.90	0.22	123,124,125,127	0
34	DMS	O	315	4/4	0.90	0.35	107,114,115,121	0
34	DMS	o	308	4/4	0.90	0.34	127,131,133,135	0
38	LHG	D	2309	49/49	0.90	0.21	50,63,78,81	0
34	DMS	O	317	4/4	0.90	0.23	114,115,117,120	0
34	DMS	b	641	4/4	0.90	0.20	75,76,78,84	4
29	GOL	A	417	6/6	0.90	0.12	110,113,118,126	0
34	DMS	C	531	4/4	0.90	0.16	98,102,103,107	0
29	GOL	A	415	6/6	0.90	0.27	72,80,92,93	0
34	DMS	l	104	4/4	0.91	0.15	134,136,139,140	0
34	DMS	b	635	4/4	0.91	0.20	98,102,105,109	0
34	DMS	T	105	4/4	0.91	0.34	124,129,130,130	0
30	UNL	D	2315	18/-	0.91	0.24	65,90,111,113	0
34	DMS	A	426	4/4	0.91	0.19	94,103,103,114	0
34	DMS	o	311	4/4	0.91	0.28	86,101,102,104	0
30	UNL	d	406	18/-	0.91	0.23	70,93,104,106	0
23	CLA	B	602	65/65	0.91	0.30	58,83,121,131	0
34	DMS	O	316	4/4	0.91	0.21	107,108,109,110	0
29	GOL	b	644	6/6	0.91	0.39	75,97,105,105	0
34	DMS	v	208	4/4	0.91	0.18	125,126,127,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
23	CLA	c	506	65/65	0.91	0.21	47,60,66,82	0
38	LHG	l	103	49/49	0.91	0.20	46,57,79,86	0
26	SQD	d	417	33/54	0.91	0.18	100,120,146,151	0
29	GOL	a	2618	6/6	0.91	0.11	107,112,115,116	0
34	DMS	v	213	4/4	0.91	0.20	119,119,119,123	0
23	CLA	b	606	65/65	0.92	0.31	66,88,129,133	0
23	CLA	b	620	65/65	0.92	0.12	47,57,88,90	0
38	LHG	d	412	49/49	0.92	0.28	55,66,79,85	0
23	CLA	C	504	65/65	0.92	0.15	47,58,66,80	0
34	DMS	V	206	4/4	0.92	0.42	81,98,100,101	0
34	DMS	o	314	4/4	0.92	0.21	112,113,117,118	0
23	CLA	B	603	65/65	0.92	0.17	41,54,70,76	0
36	HTG	V	204	19/19	0.92	0.21	71,95,125,126	0
34	DMS	V	208	4/4	0.93	0.34	99,108,109,113	0
25	BCR	T	102	40/40	0.93	0.16	44,56,82,85	0
23	CLA	b	615	65/65	0.93	0.13	49,56,63,67	0
23	CLA	C	507	65/65	0.93	0.14	57,81,109,112	0
34	DMS	c	539	4/4	0.93	0.21	110,112,114,119	0
34	DMS	o	307	4/4	0.93	0.23	104,107,109,111	0
31	JOX	a	2617	10/10	0.93	0.11	64,69,89,91	0
36	HTG	o	301	19/19	0.93	0.13	62,70,85,87	0
31	JOX	a	2619	10/10	0.93	0.18	46,49,54,56	10
23	CLA	c	505	65/65	0.93	0.24	45,54,70,78	0
23	CLA	D	2304	65/65	0.93	0.14	49,58,128,136	0
37	DGD	c	519	62/66	0.93	0.19	52,65,112,125	0
36	HTG	C	521	19/19	0.93	0.24	108,112,121,121	0
34	DMS	O	307	4/4	0.93	0.15	98,107,107,110	0
23	CLA	C	510	65/65	0.93	0.15	53,63,84,88	0
25	BCR	B	619	40/40	0.93	0.20	45,55,76,79	0
25	BCR	B	633	40/40	0.93	0.17	46,62,78,79	0
25	BCR	C	515	40/40	0.93	0.13	55,78,88,89	0
34	DMS	u	504	4/4	0.93	0.31	74,90,95,98	0
34	DMS	d	418	4/4	0.93	0.30	98,99,100,111	0
34	DMS	v	209	4/4	0.93	0.46	82,93,96,102	0
41	MG	k	303	1/1	0.93	0.07	91,91,91,91	0
34	DMS	B	641	4/4	0.94	0.21	93,102,102,104	0
34	DMS	o	305	4/4	0.94	0.33	117,117,119,120	0
23	CLA	b	614	65/65	0.94	0.11	52,63,74,86	0
23	CLA	C	508	65/65	0.94	0.12	51,64,83,84	0
23	CLA	b	619	65/65	0.94	0.19	41,49,109,113	0
36	HTG	b	602	19/19	0.94	0.11	56,64,79,79	0
25	BCR	C	516	40/40	0.94	0.12	54,66,87,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	B	615	65/65	0.94	0.16	40,49,105,113	0
34	DMS	C	530	4/4	0.94	0.15	115,117,118,123	0
34	DMS	o	313	4/4	0.94	0.37	100,102,103,111	0
23	CLA	B	617	65/65	0.94	0.15	49,59,122,126	0
34	DMS	c	534	4/4	0.94	0.16	142,143,143,144	0
25	BCR	b	623	40/40	0.94	0.21	43,57,74,79	0
34	DMS	U	503	4/4	0.94	0.38	118,119,119,120	0
33	PL9	d	411	55/55	0.94	0.16	37,46,56,65	0
34	DMS	u	503	4/4	0.94	0.14	81,101,102,103	0
34	DMS	U	505	4/4	0.94	0.13	66,72,89,105	0
25	BCR	d	410	40/40	0.94	0.11	54,61,83,86	0
23	CLA	B	607	65/65	0.94	0.11	40,52,83,91	0
34	DMS	c	543	4/4	0.94	0.20	116,121,122,123	0
37	DGD	c	518	62/66	0.94	0.18	43,57,106,110	0
25	BCR	y	101	40/40	0.94	0.10	53,65,71,74	0
34	DMS	A	427	4/4	0.94	0.33	103,106,107,108	0
34	DMS	V	209	4/4	0.94	0.26	81,89,95,100	0
29	GOL	O	303	6/6	0.94	0.19	96,106,114,114	0
35	CA	b	605	1/1	0.94	0.06	72,72,72,72	0
26	SQD	A	412	46/54	0.94	0.16	76,88,106,108	0
27	LMG	d	414	51/55	0.94	0.12	54,69,105,109	0
23	CLA	c	510	65/65	0.94	0.12	48,62,75,83	0
23	CLA	B	611	65/65	0.94	0.21	47,55,67,72	0
34	DMS	a	2621	4/4	0.94	0.14	115,115,116,118	0
24	PHO	A	409	64/64	0.94	0.17	41,49,58,61	0
34	DMS	C	528	4/4	0.95	0.12	110,114,115,117	0
23	CLA	b	612	65/65	0.95	0.14	34,44,63,67	0
23	CLA	c	516	65/65	0.95	0.18	61,79,103,108	0
23	CLA	d	409	65/65	0.95	0.11	54,61,126,133	0
24	PHO	A	408	64/64	0.95	0.12	35,43,49,52	0
26	SQD	a	2615	48/54	0.95	0.13	66,86,112,114	0
23	CLA	C	513	65/65	0.95	0.11	62,75,115,122	0
25	BCR	B	618	40/40	0.95	0.17	43,51,57,60	0
34	DMS	D	2319	4/4	0.95	0.27	104,105,107,118	0
23	CLA	B	616	65/65	0.95	0.12	43,55,83,95	0
33	PL9	D	2306	55/55	0.95	0.10	38,47,55,64	0
34	DMS	b	636	4/4	0.95	0.24	101,102,104,106	0
23	CLA	b	616	65/65	0.95	0.22	40,47,68,73	0
23	CLA	D	2303	65/65	0.95	0.14	33,42,62,72	0
23	CLA	C	509	65/65	0.95	0.14	46,56,115,132	0
25	BCR	K	101	40/40	0.95	0.10	57,64,69,70	0
34	DMS	O	310	4/4	0.95	0.18	103,103,103,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
27	LMG	D	2312	47/55	0.95	0.18	48,59,97,100	0
34	DMS	O	312	4/4	0.95	0.31	108,109,110,113	0
23	CLA	b	621	65/65	0.95	0.15	48,61,128,132	0
25	BCR	Y	302	40/40	0.95	0.09	55,64,70,71	0
23	CLA	c	504	65/65	0.95	0.12	45,59,72,83	0
25	BCR	b	622	40/40	0.95	0.20	44,54,66,68	0
29	GOL	C	526	6/6	0.95	0.18	65,81,89,93	0
34	DMS	B	639	4/4	0.95	0.12	84,84,91,92	0
23	CLA	B	612	65/65	0.95	0.20	39,47,66,70	0
38	LHG	d	403	43/49	0.95	0.16	46,59,91,96	0
25	BCR	b	624	40/40	0.95	0.11	48,61,76,76	0
38	LHG	d	413	49/49	0.95	0.17	40,49,71,73	0
25	BCR	c	517	40/40	0.95	0.10	52,66,87,89	0
23	CLA	b	609	65/65	0.95	0.23	37,46,85,92	0
34	DMS	B	644	4/4	0.95	0.26	82,82,86,88	0
23	CLA	c	509	65/65	0.95	0.11	57,76,111,115	0
23	CLA	b	611	65/65	0.95	0.10	47,53,90,96	0
41	MG	j	2703	1/1	0.95	0.19	60,60,60,60	0
23	CLA	c	514	65/65	0.95	0.12	55,65,73,75	0
34	DMS	C	529	4/4	0.96	0.19	94,101,101,102	0
34	DMS	a	2623	4/4	0.96	0.15	100,107,108,111	0
34	DMS	v	206	4/4	0.96	0.09	84,102,103,104	0
34	DMS	v	207	4/4	0.96	0.20	107,110,111,114	0
23	CLA	C	512	65/65	0.96	0.08	55,63,74,81	0
23	CLA	C	502	65/65	0.96	0.17	48,58,75,83	0
23	CLA	b	617	65/65	0.96	0.21	41,49,56,58	0
25	BCR	z	101	40/40	0.96	0.17	68,78,93,97	0
23	CLA	C	503	65/65	0.96	0.19	41,53,70,76	0
34	DMS	b	639	4/4	0.96	0.09	93,96,97,98	0
37	DGD	C	519	58/66	0.96	0.14	43,53,79,93	0
23	CLA	A	410	65/65	0.96	0.11	41,50,123,127	0
25	BCR	B	620	40/40	0.96	0.09	50,56,67,71	0
35	CA	o	302	1/1	0.96	0.07	74,74,74,74	0
23	CLA	C	505	65/65	0.96	0.14	45,54,89,93	0
37	DGD	c	520	62/66	0.96	0.15	47,59,86,95	0
23	CLA	a	2613	65/65	0.96	0.13	39,48,130,137	0
23	CLA	B	613	65/65	0.96	0.21	39,46,56,61	0
38	LHG	D	2310	49/49	0.96	0.13	45,52,69,85	0
25	BCR	D	2305	40/40	0.96	0.19	50,60,85,86	0
38	LHG	L	101	49/49	0.96	0.12	46,57,73,76	0
34	DMS	c	536	4/4	0.96	0.26	64,74,76,78	0
23	CLA	b	607	65/65	0.96	0.12	48,57,69,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
23	CLA	c	508	65/65	0.96	0.12	49,57,80,86	0
34	DMS	o	312	4/4	0.96	0.23	95,98,101,105	0
23	CLA	b	608	65/65	0.96	0.14	40,52,71,75	0
23	CLA	B	608	65/65	0.96	0.15	34,44,61,73	0
23	CLA	c	511	65/65	0.96	0.23	46,56,114,137	0
23	CLA	B	604	65/65	0.96	0.21	42,51,66,72	0
23	CLA	B	605	65/65	0.96	0.26	37,44,85,94	0
23	CLA	C	511	65/65	0.96	0.16	47,56,68,78	0
24	PHO	a	2611	64/64	0.97	0.14	38,42,49,57	0
24	PHO	a	2612	64/64	0.97	0.15	39,49,59,65	0
25	BCR	A	411	40/40	0.97	0.13	38,48,58,62	0
23	CLA	A	407	65/65	0.97	0.15	36,47,109,115	0
23	CLA	C	506	65/65	0.97	0.14	51,59,80,81	0
23	CLA	b	618	65/65	0.97	0.26	40,46,93,96	0
23	CLA	b	610	65/65	0.97	0.15	39,49,60,63	0
34	DMS	d	419	4/4	0.97	0.18	92,94,98,106	0
23	CLA	c	512	65/65	0.97	0.24	51,59,89,100	0
34	DMS	d	421	4/4	0.97	0.13	75,89,94,98	0
38	LHG	D	2311	39/49	0.97	0.11	51,59,92,97	0
23	CLA	c	513	65/65	0.97	0.26	46,57,68,79	0
23	CLA	a	2610	65/65	0.97	0.19	38,46,116,121	0
23	CLA	B	614	65/65	0.97	0.21	37,45,91,99	0
23	CLA	b	613	65/65	0.97	0.13	41,53,72,77	0
23	CLA	d	402	65/65	0.97	0.15	35,41,50,62	0
23	CLA	B	606	65/65	0.97	0.23	37,47,62,64	0
34	DMS	D	2316	4/4	0.97	0.12	65,77,86,90	0
39	HEM	F	101	43/43	0.97	0.13	61,71,100,119	0
34	DMS	a	2622	4/4	0.97	0.46	105,107,110,115	0
23	CLA	B	609	65/65	0.97	0.19	45,54,73,79	0
23	CLA	c	507	65/65	0.97	0.20	46,56,91,95	0
34	DMS	b	634	4/4	0.97	0.21	81,86,88,92	0
37	DGD	C	517	62/66	0.97	0.20	42,55,109,112	0
23	CLA	d	408	65/65	0.98	0.18	31,42,60,71	0
35	CA	c	503	1/1	0.98	0.03	73,73,73,73	0
34	DMS	D	2318	4/4	0.98	0.25	82,85,90,92	0
23	CLA	a	2609	65/65	0.98	0.18	35,41,55,69	0
23	CLA	A	406	65/65	0.98	0.09	34,41,51,63	0
34	DMS	C	532	4/4	0.98	0.11	67,68,73,74	0
34	DMS	V	205	4/4	0.98	0.15	67,74,74,77	0
29	GOL	B	648	6/6	0.98	0.08	54,74,84,89	0
34	DMS	c	533	4/4	0.98	0.12	59,63,63,65	0
23	CLA	A	405	65/65	0.98	0.12	33,41,55,77	0

*Continued on next page...*

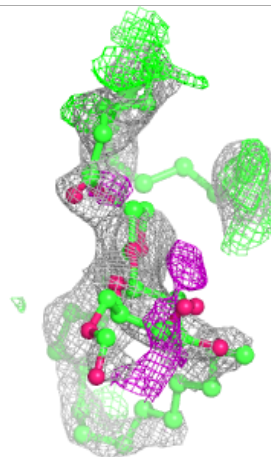
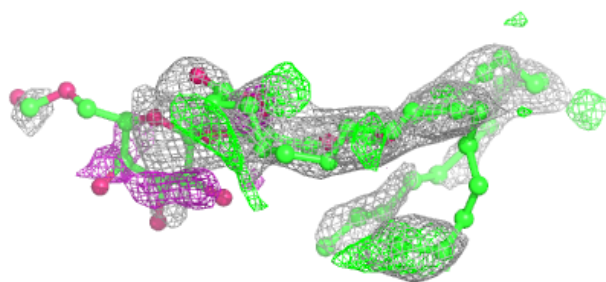
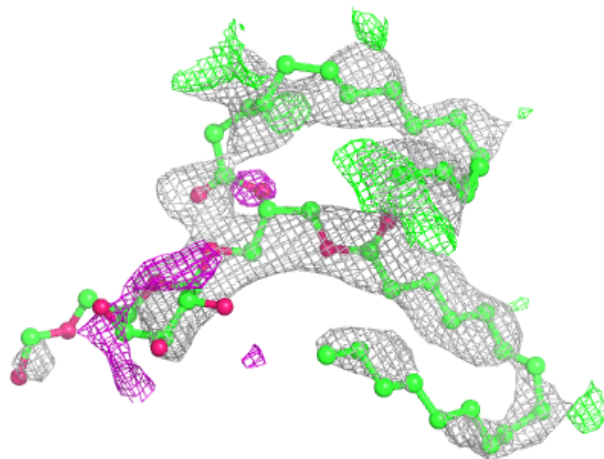
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
34	DMS	c	535	4/4	0.98	0.25	108,108,110,114	0
34	DMS	B	638	4/4	0.98	0.16	61,68,73,82	0
39	HEM	e	103	43/43	0.98	0.13	65,76,109,133	0
32	BCT	A	421	4/4	0.98	0.07	59,60,65,75	0
34	DMS	V	210	4/4	0.98	0.41	101,105,108,111	0
41	MG	J	302	1/1	0.98	0.10	58,58,58,58	0
32	BCT	a	2608	4/4	0.98	0.16	56,61,66,74	0
35	CA	B	601	1/1	0.98	0.04	68,68,68,68	0
35	CA	O	301	1/1	0.98	0.14	77,77,77,77	0
42	HEC	V	201	43/43	0.98	0.07	41,46,52,56	0
42	HEC	v	201	43/43	0.98	0.11	49,56,62,69	0
22	CL	A	403	1/1	0.99	0.05	46,46,46,46	0
34	DMS	A	424	4/4	0.99	0.12	48,50,52,59	0
34	DMS	B	636	4/4	0.99	0.13	43,47,47,59	0
34	DMS	C	533	4/4	0.99	0.09	61,64,65,66	0
34	DMS	b	633	4/4	0.99	0.12	45,50,52,61	0
34	DMS	v	205	4/4	0.99	0.14	75,77,83,86	0
22	CL	A	404	1/1	0.99	0.10	43,43,43,43	0
22	CL	a	2606	1/1	0.99	0.04	48,48,48,48	0
20	OEX	A	401	10/10	0.99	0.12	41,46,50,52	0
20	OEX	a	2604	10/10	0.99	0.10	41,46,51,52	0
21	FE2	A	402	1/1	0.99	0.05	54,54,54,54	0
34	DMS	o	304	4/4	0.99	0.11	43,53,55,59	0
22	CL	a	2607	1/1	1.00	0.16	46,46,46,46	0
21	FE2	a	2605	1/1	1.00	0.07	52,52,52,52	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 DGD D 2307:**

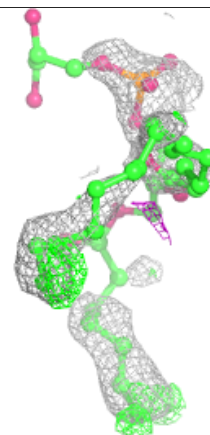
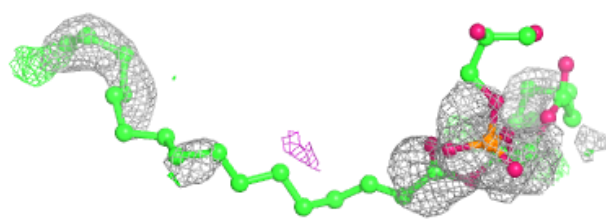
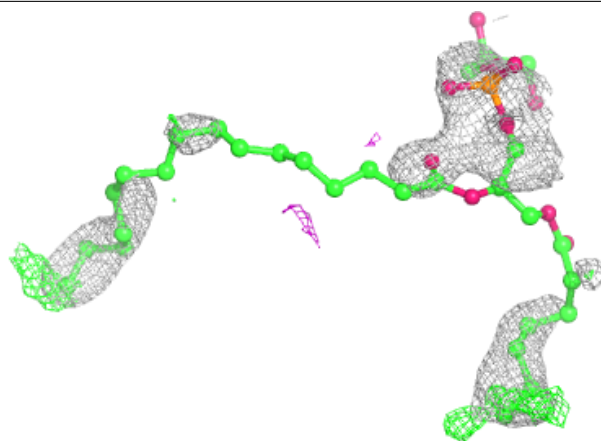
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



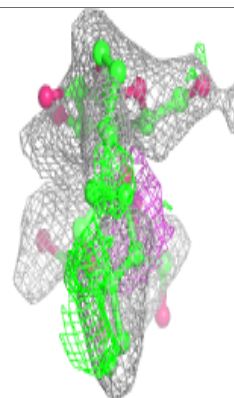
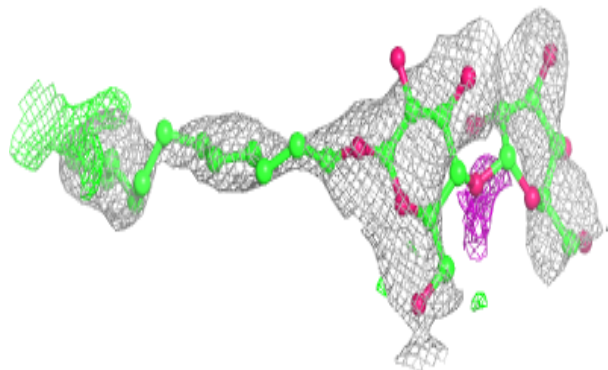
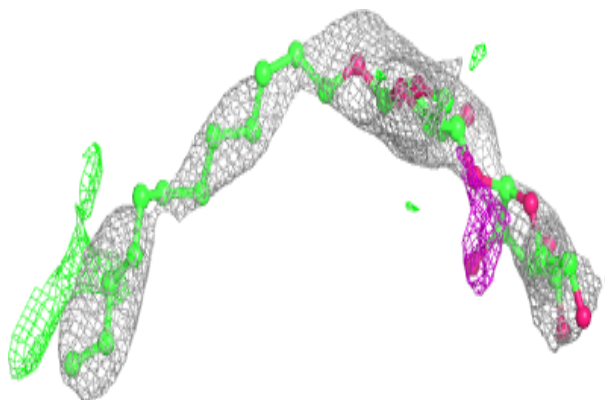


**Electron density around LHG e 101:**

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

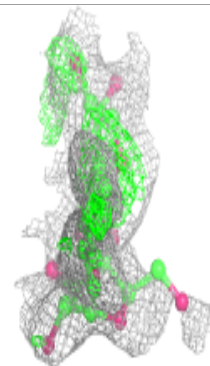
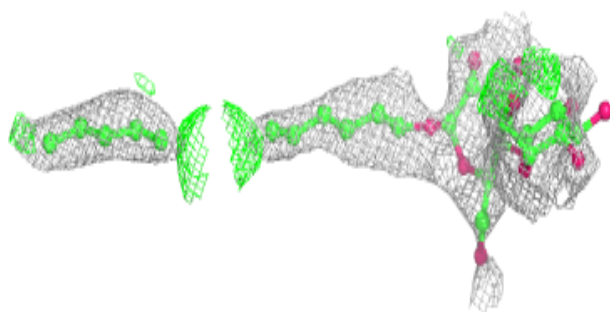
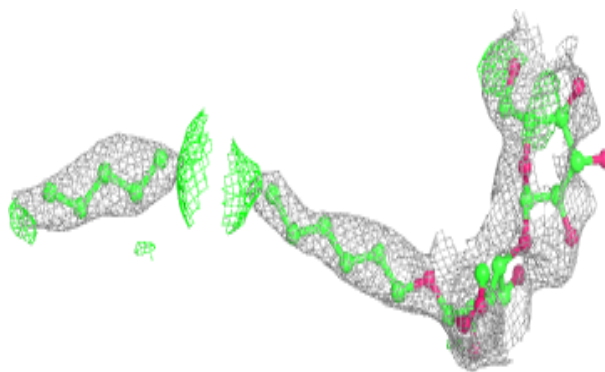
**Electron density around LMT m 2804:**

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

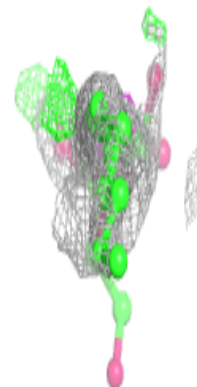
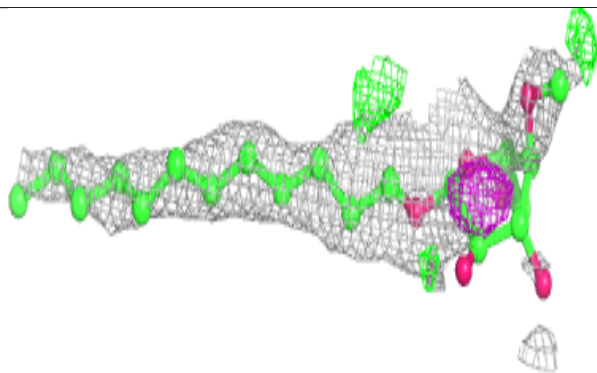
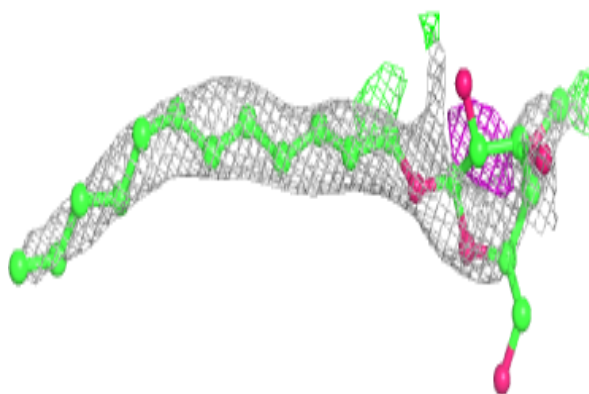


**Electron density around LMT j 2701:**

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

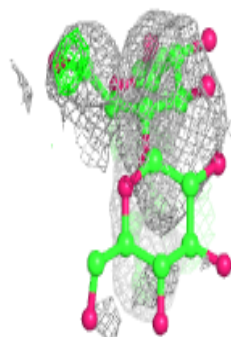
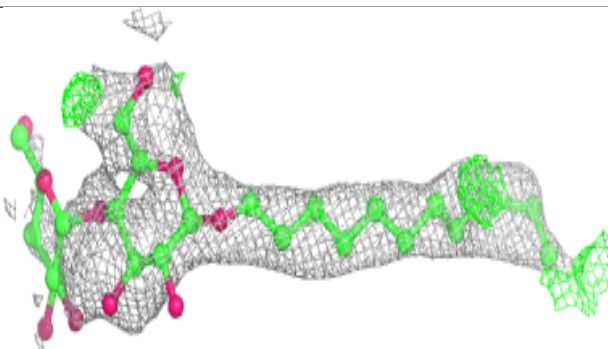
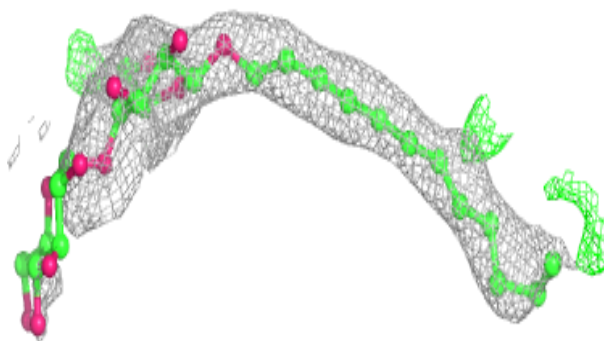
**Electron density around LMT d 404:**

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

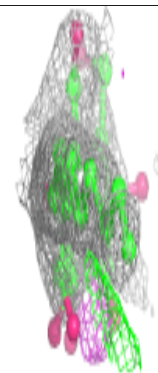
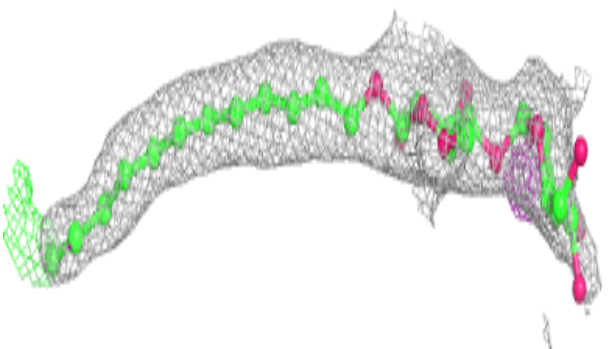
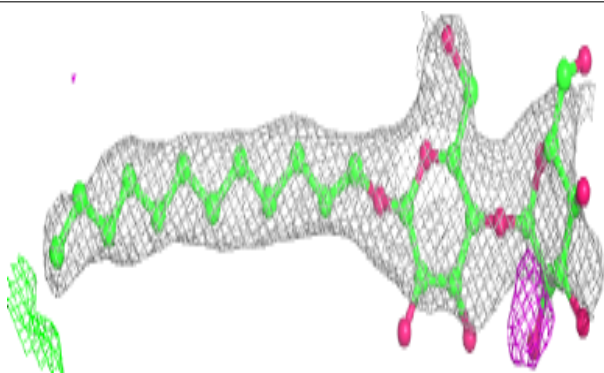


**Electron density around LMT M 101:**

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

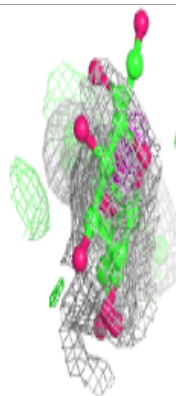
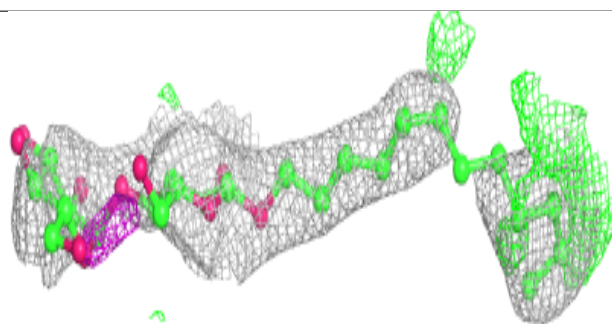
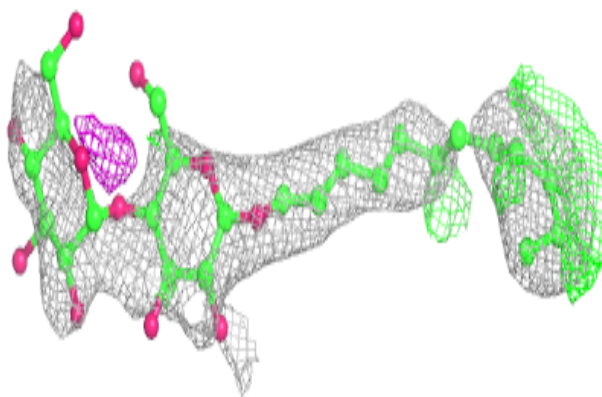
**Electron density around LMT M 102:**

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

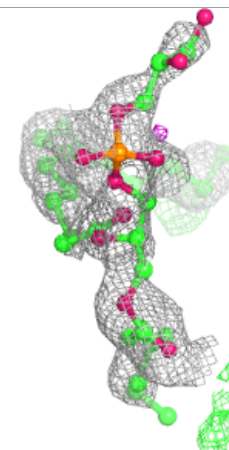
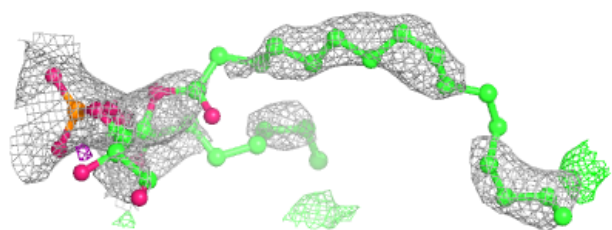
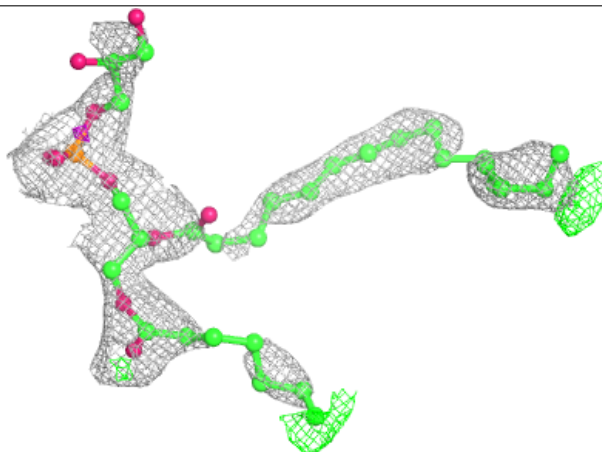


**Electron density around LMT B 634:**

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

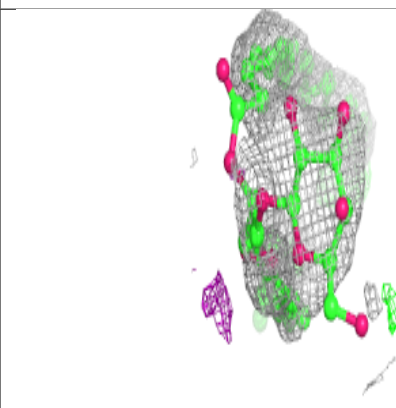
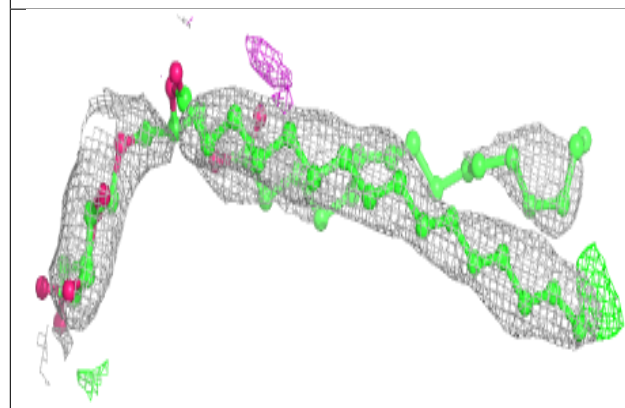
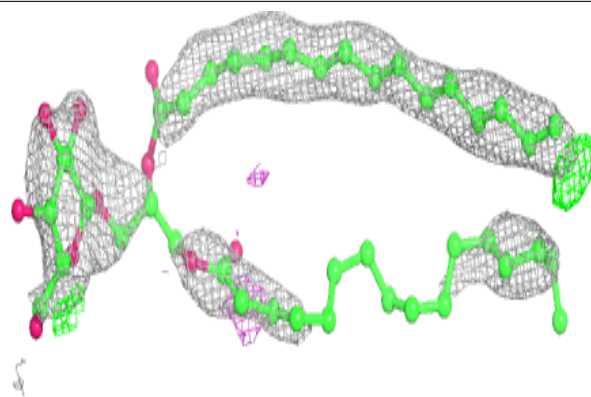
**Electron density around LHG E 101:**

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

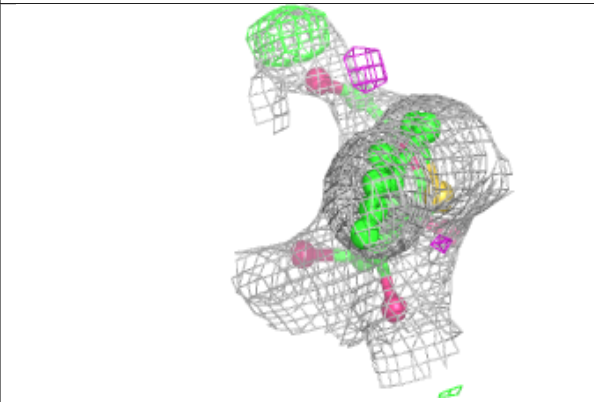
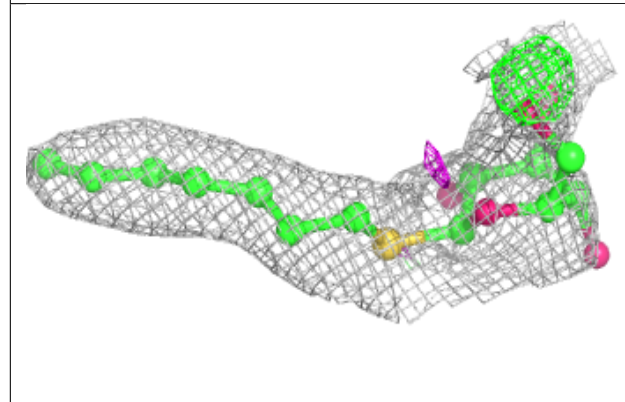
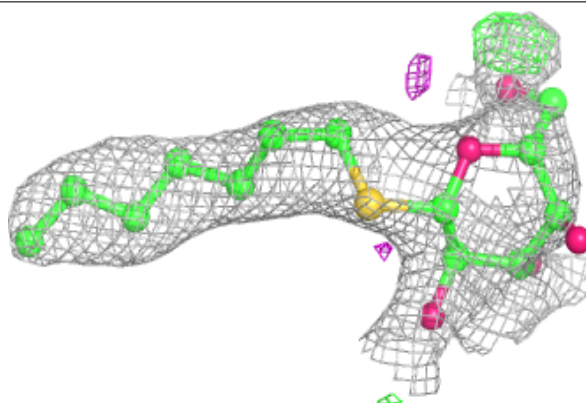


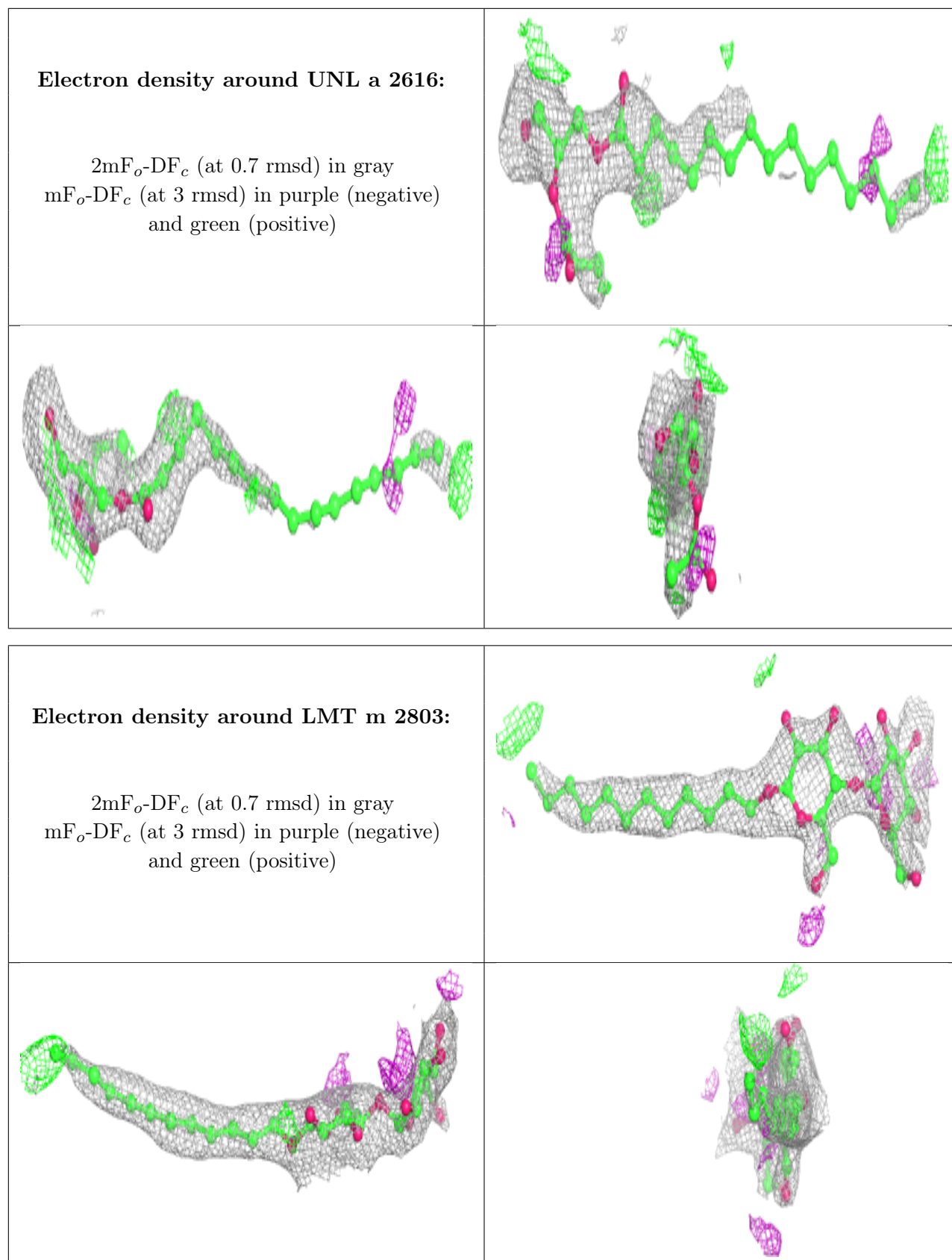
**Electron density around LMG C 527:**

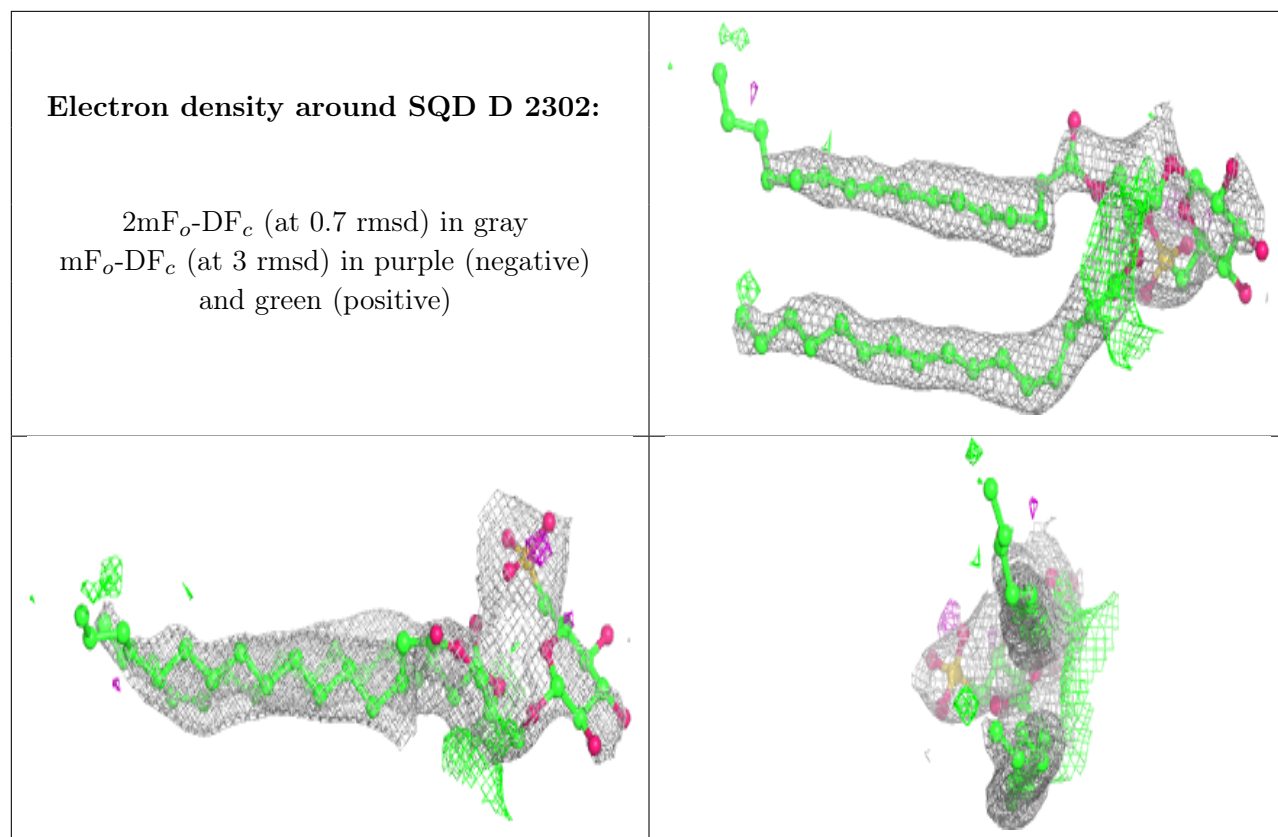
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around HTG 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)

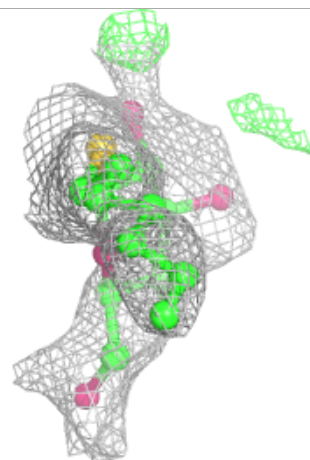
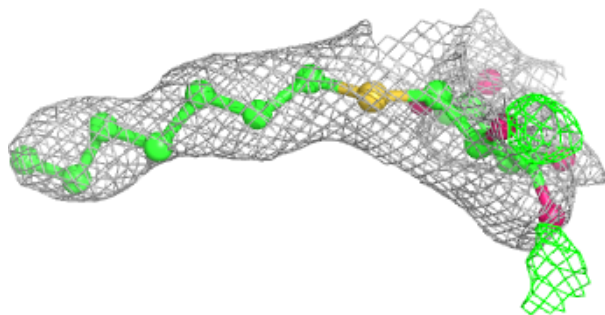
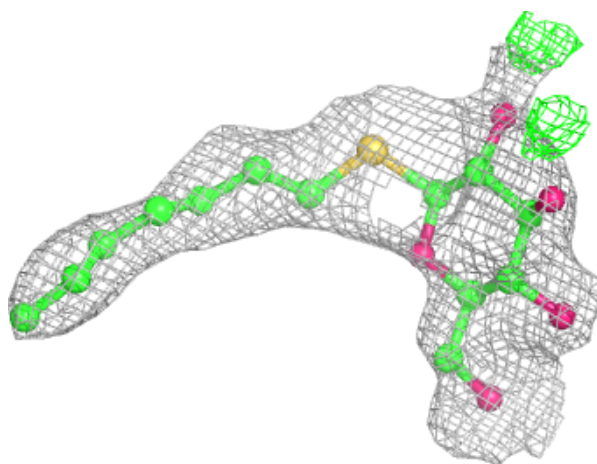






**Electron density around HTG b 626:**

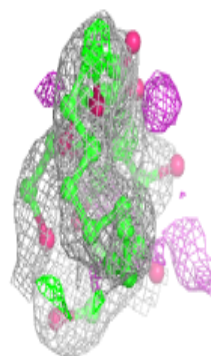
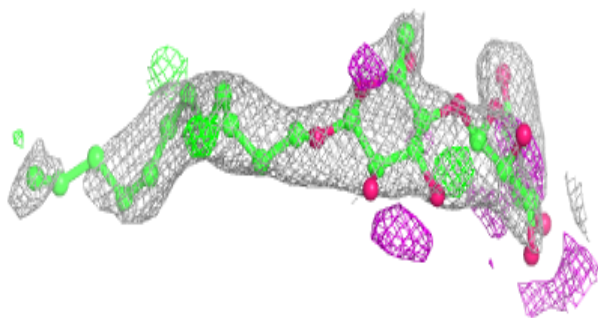
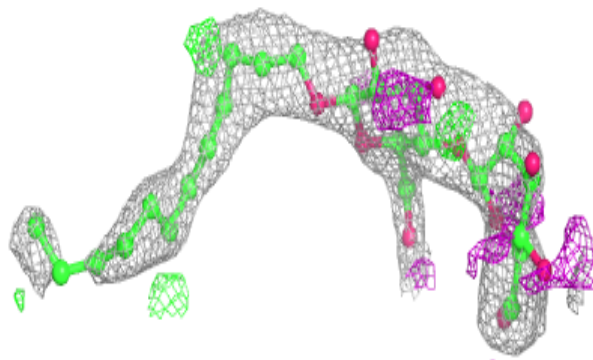
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
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and green (positive)



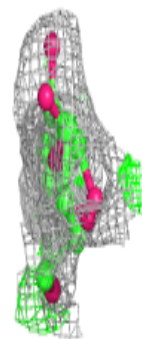
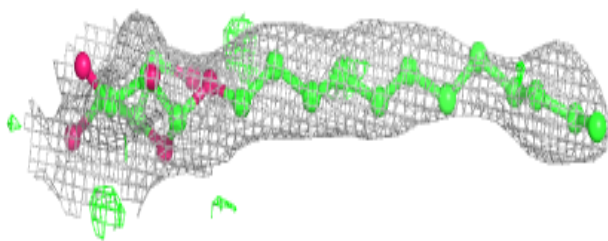
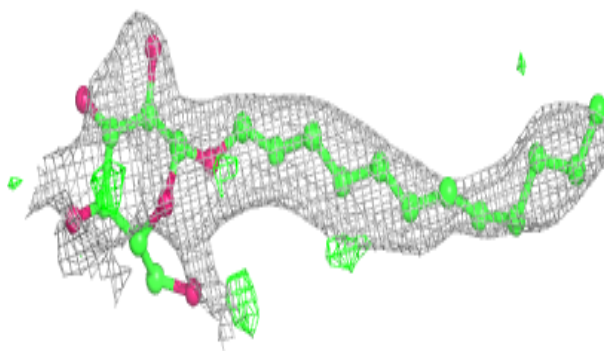


**Electron density around LMT d 401:**

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

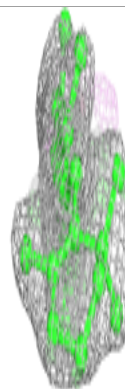
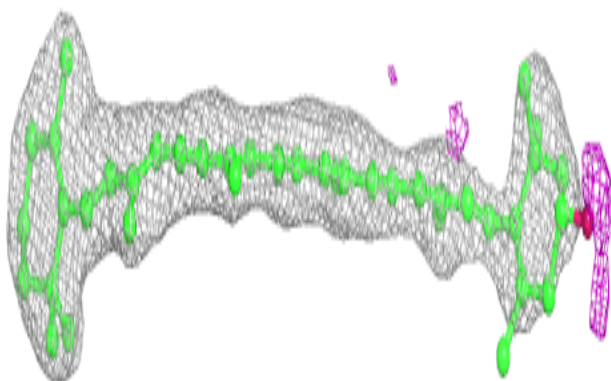
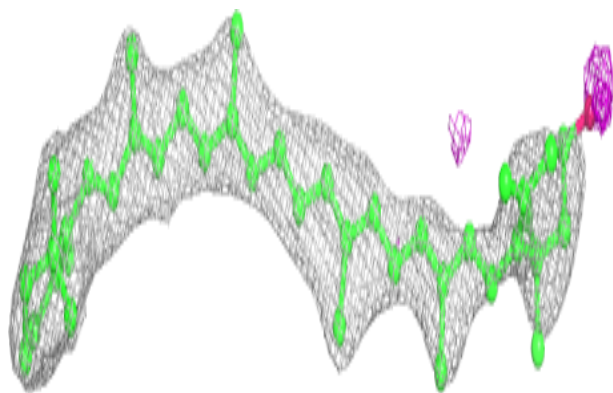
**Electron density around LMT J 303:**

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

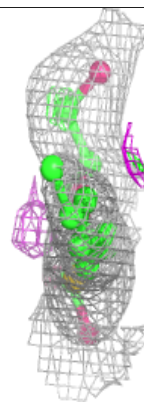
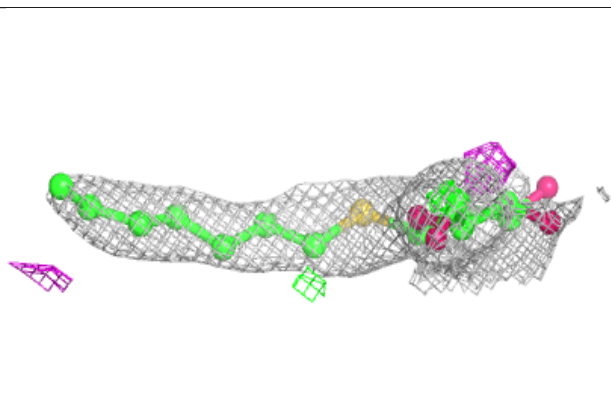
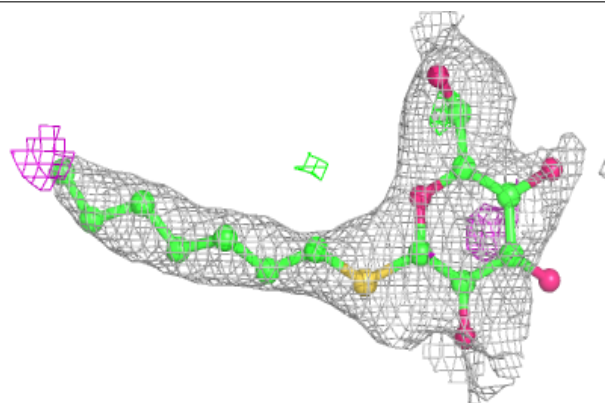


**Electron density around RRX h 101:**

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

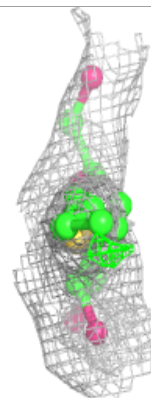
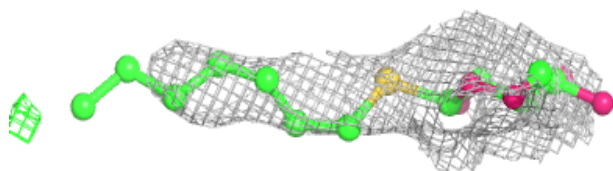
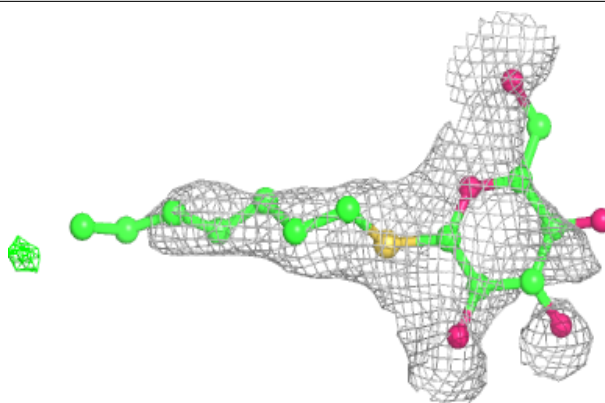
**Electron density around HTG B 627:**

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

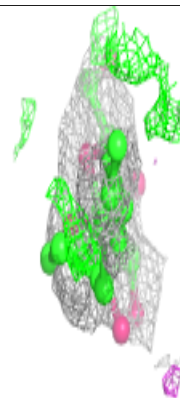
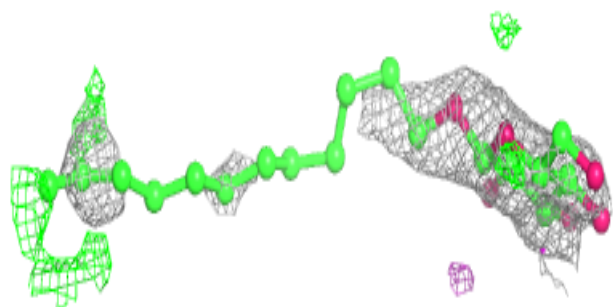
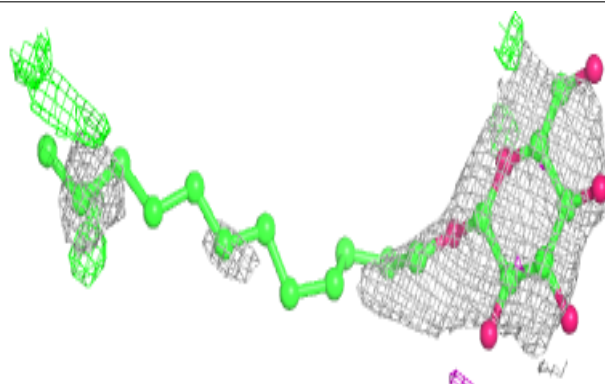


**Electron density around HTG c 526:**

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

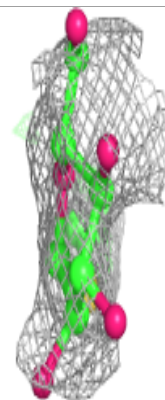
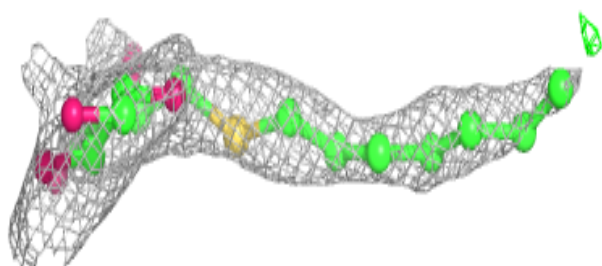
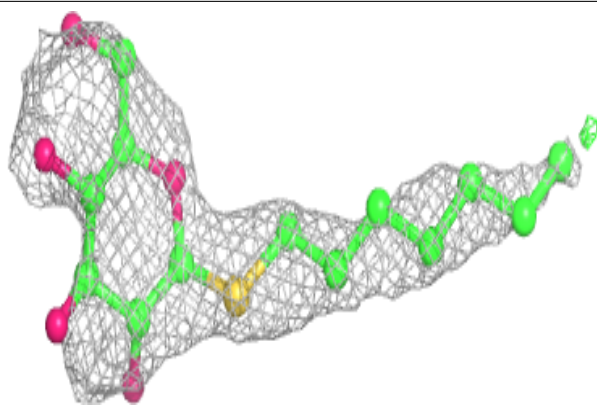
**Electron density around LMT F 102:**

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

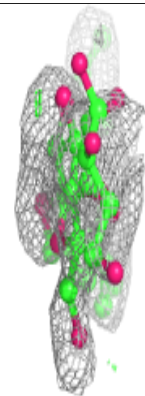
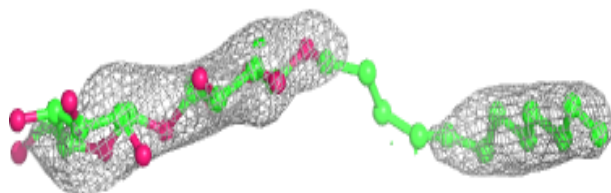
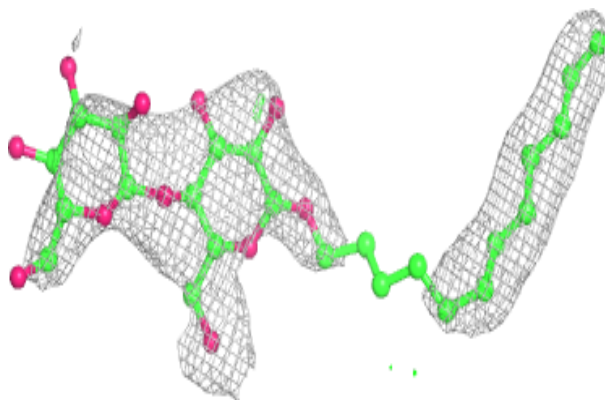


**Electron density around HTG B 625:**

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

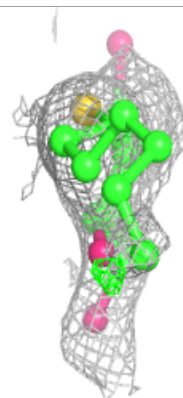
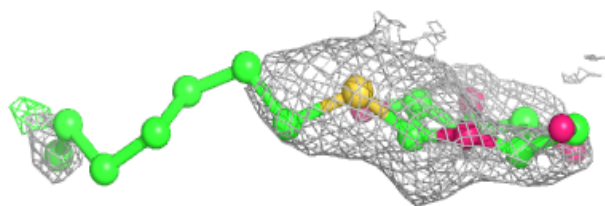
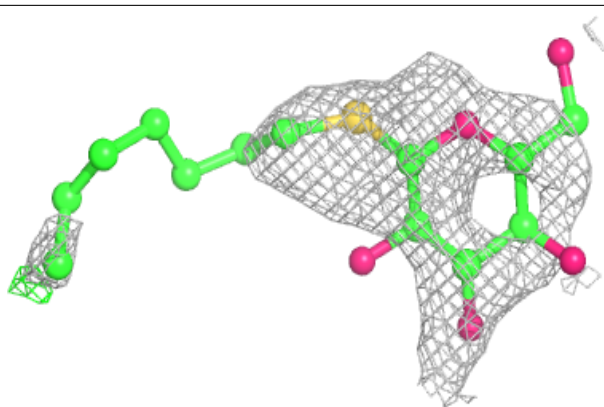
**Electron density around LMT Z 101:**

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

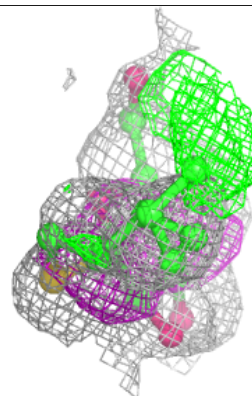
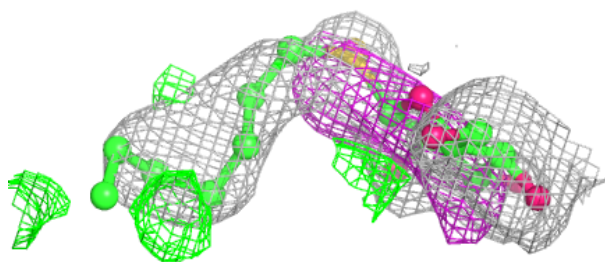
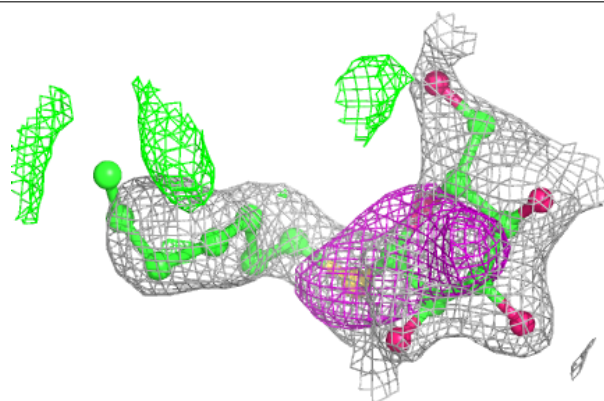


**Electron density around HTG d 407:**

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

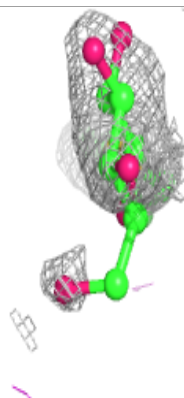
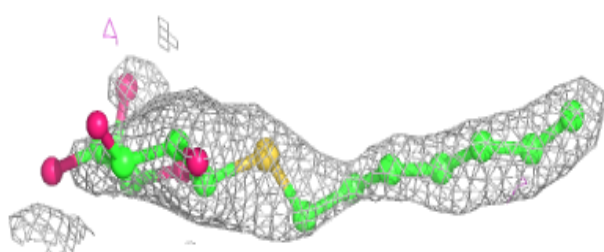
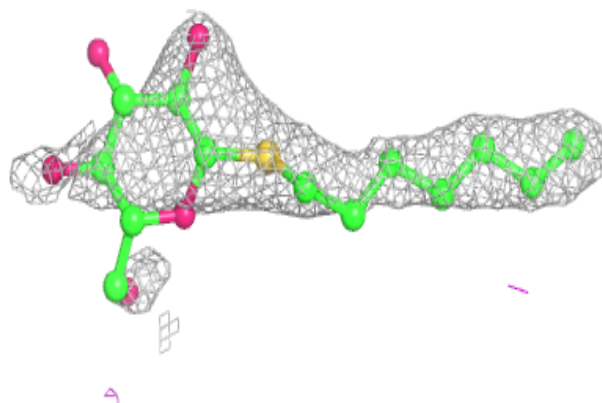
**Electron density around HTG B 624 (A):**

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

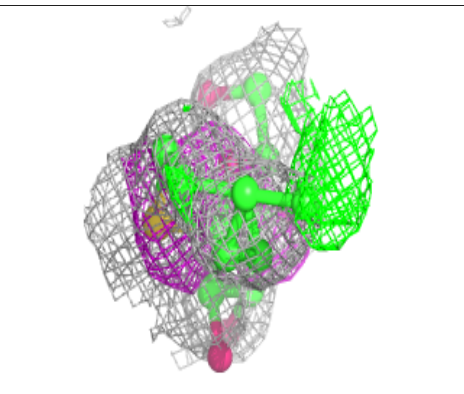
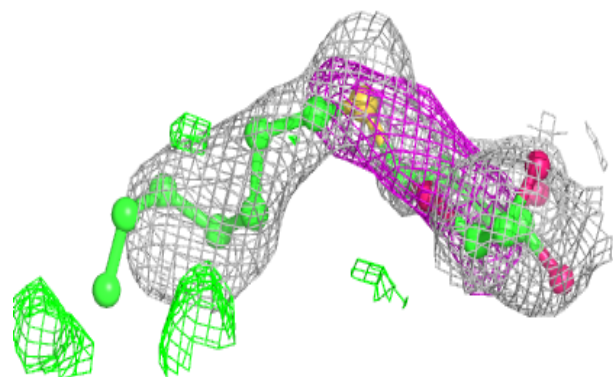
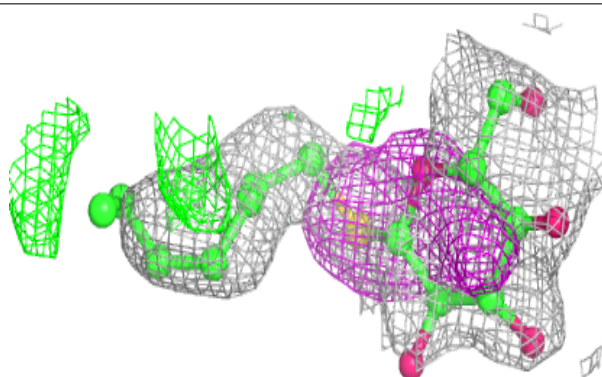


**Electron density around HTG c 524:**

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

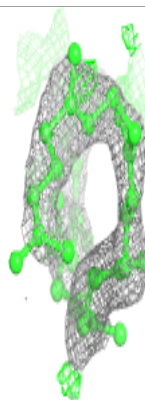
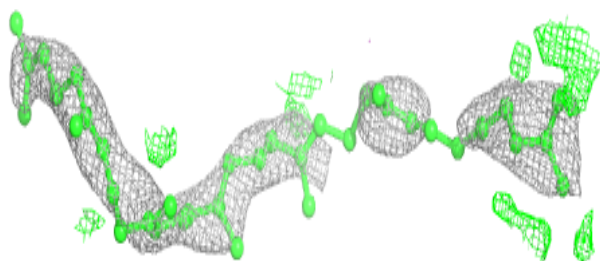
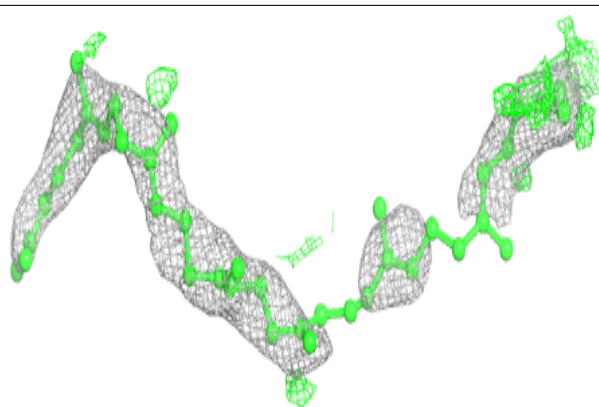
**Electron density around HTG B 624 (B):**

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

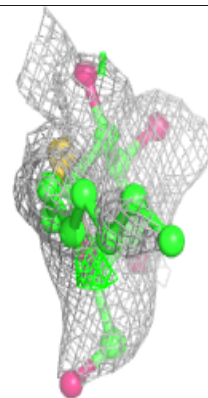
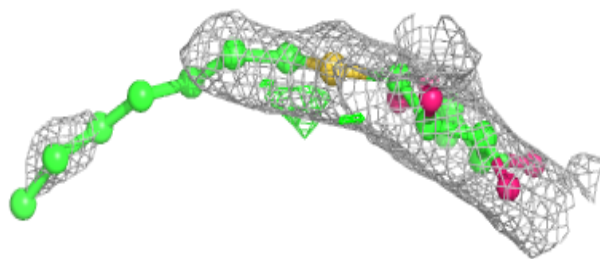
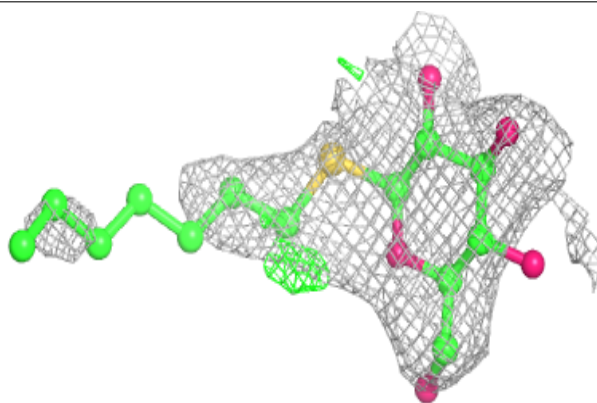


**Electron density around PL9 A 422:**

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

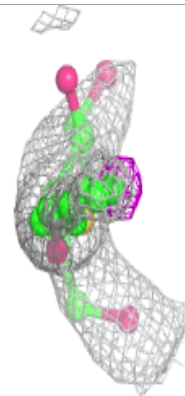
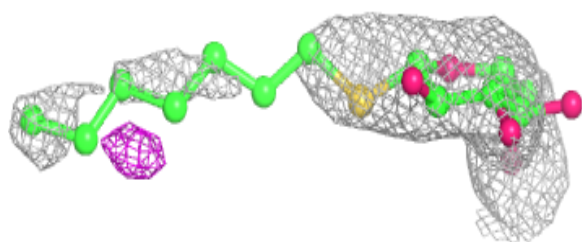
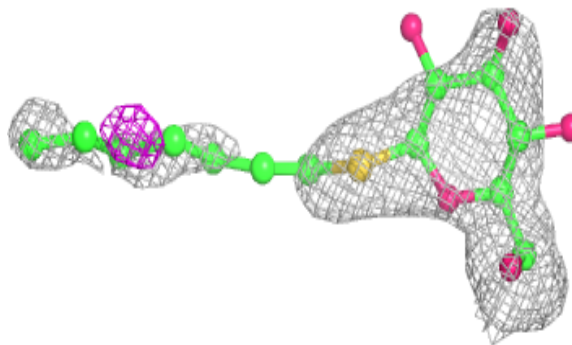
**Electron density around HTG d 415:**

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

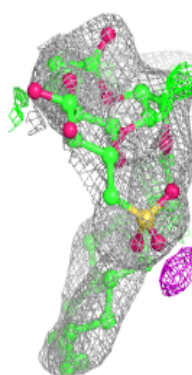
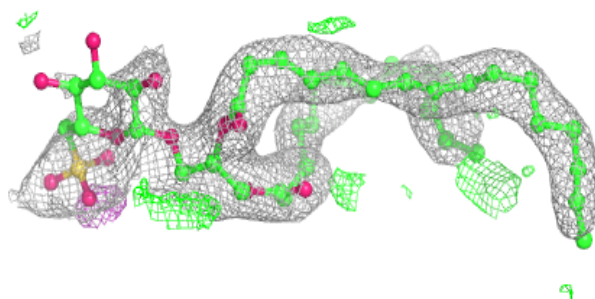
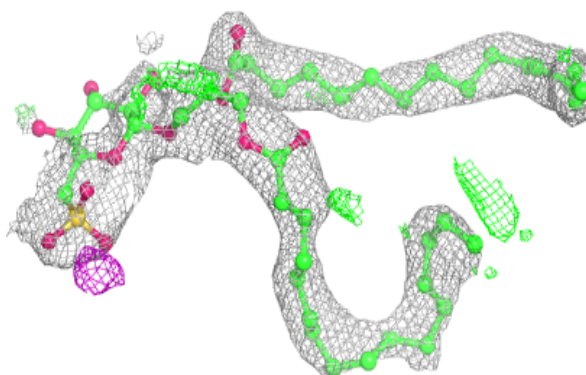


**Electron density around HTG C 522:**

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

**Electron density around SQD a 2603:**

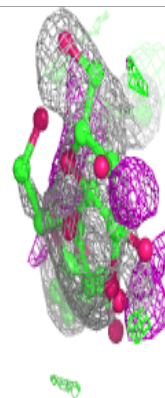
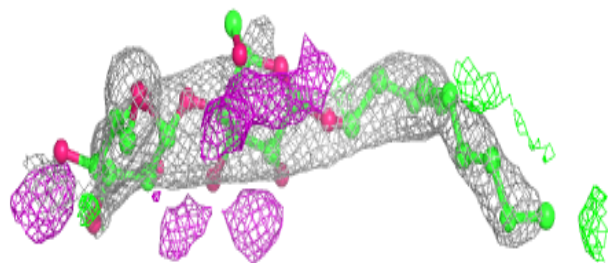
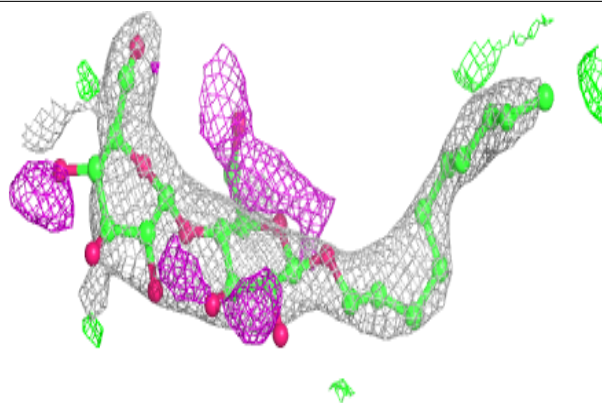
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



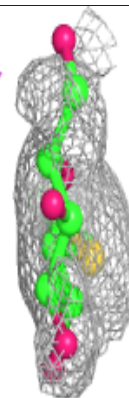
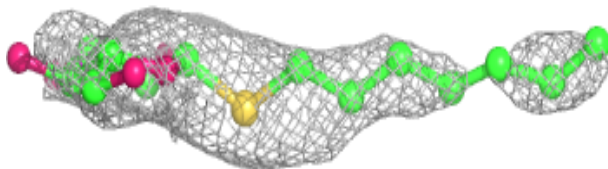
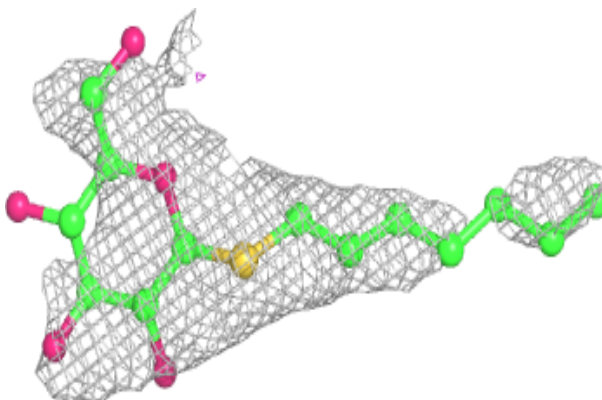


**Electron density around LMT A 414:**

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

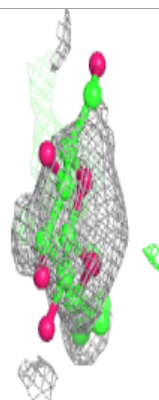
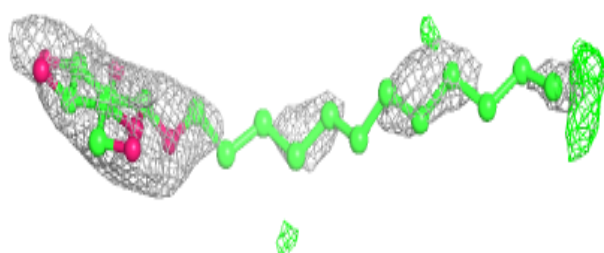
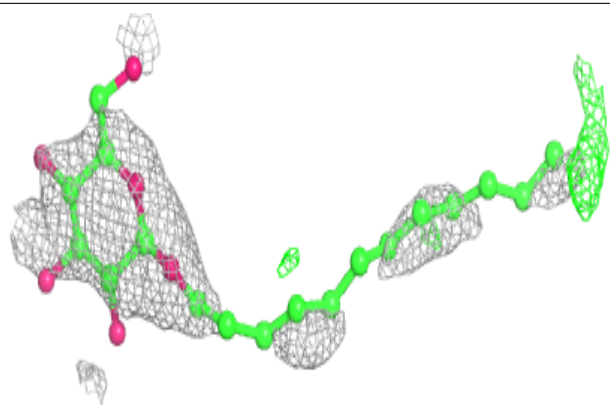
**Electron density around HTG C 525:**

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

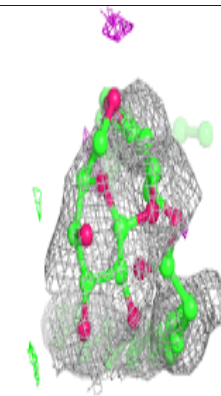
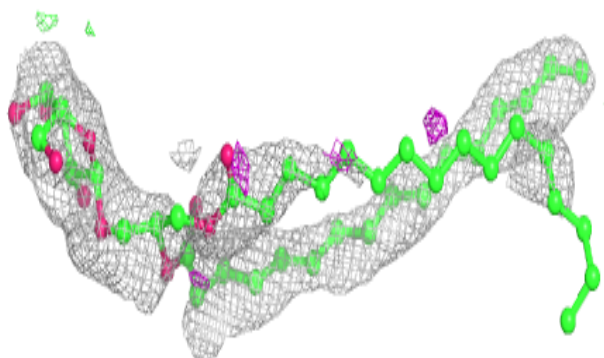
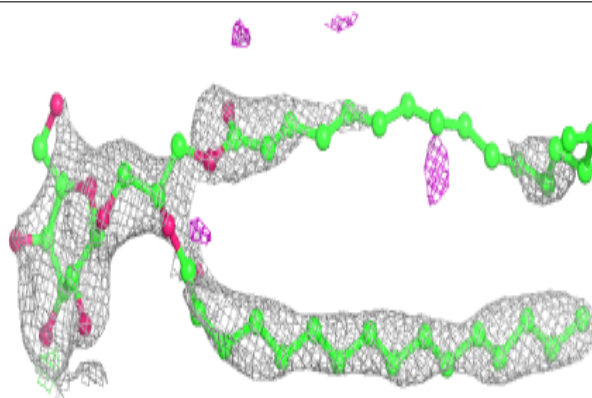


**Electron density around LMT f 101:**

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

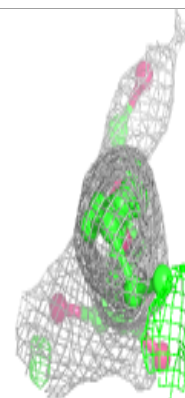
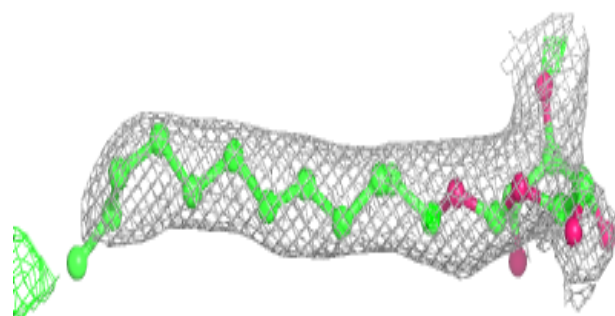
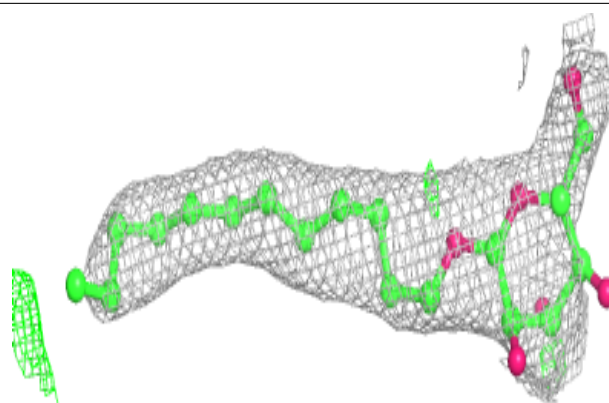
**Electron density around LMG c 522:**

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

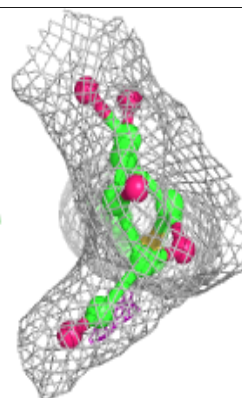
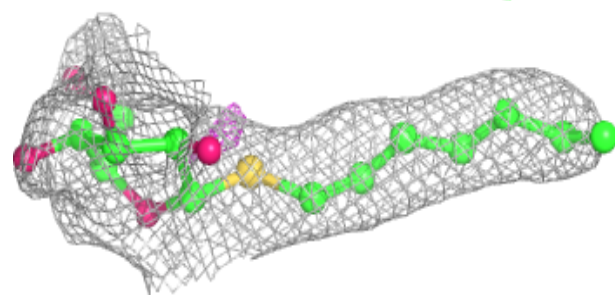
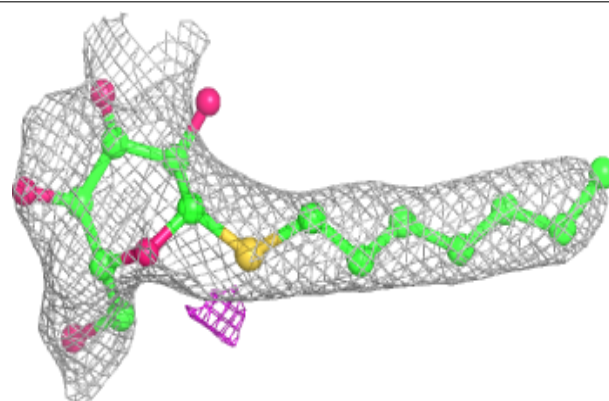


**Electron density around LMT A 420:**

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

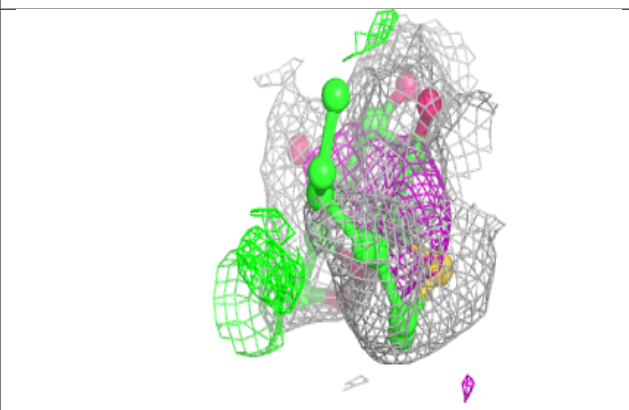
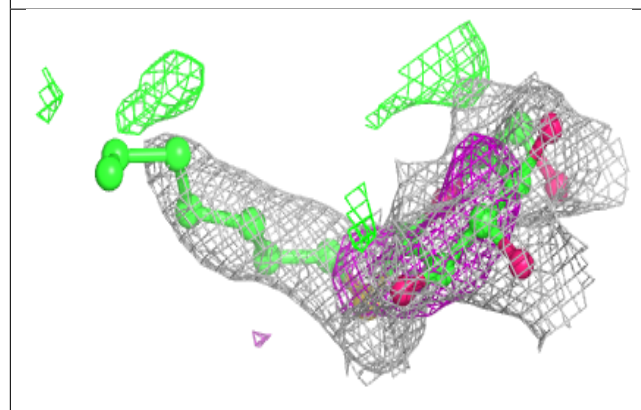
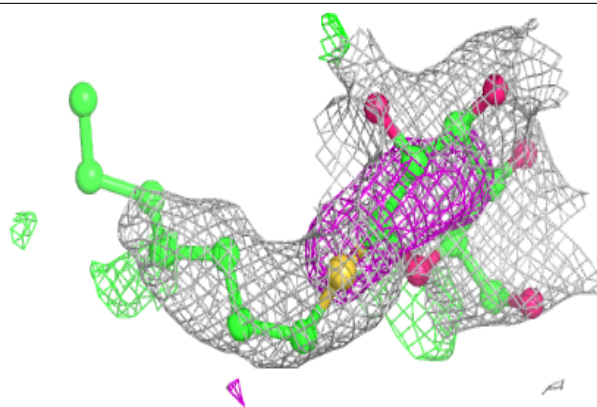
**Electron density around HTG I 101:**

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

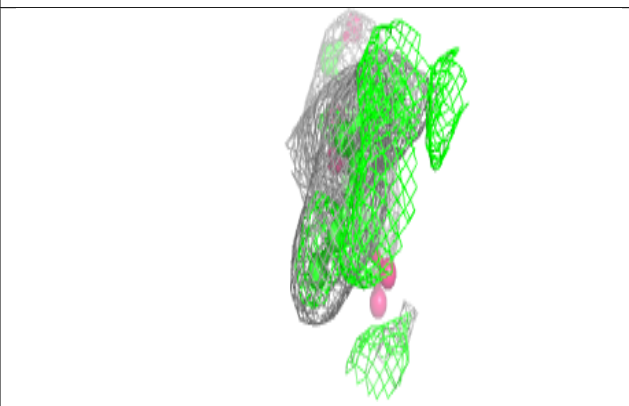
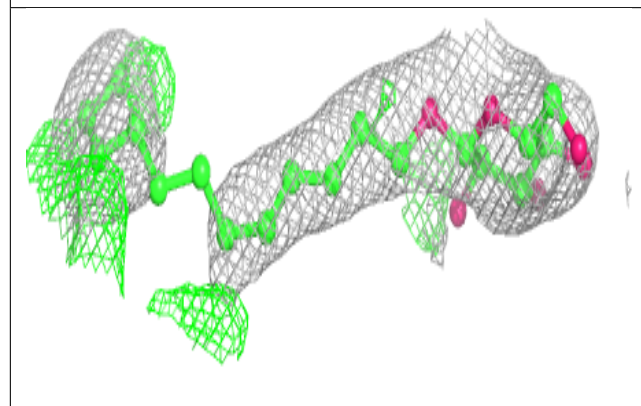
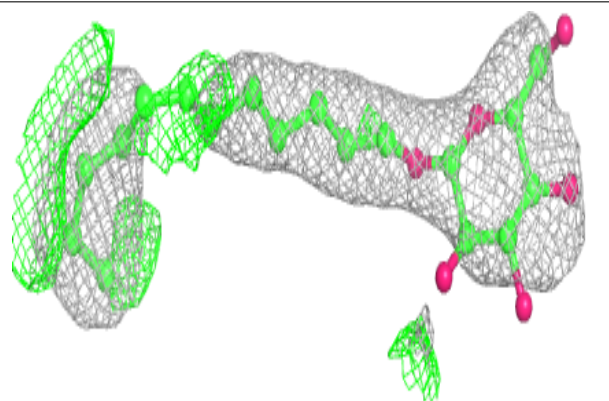


**Electron density around HTG b 625:**

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

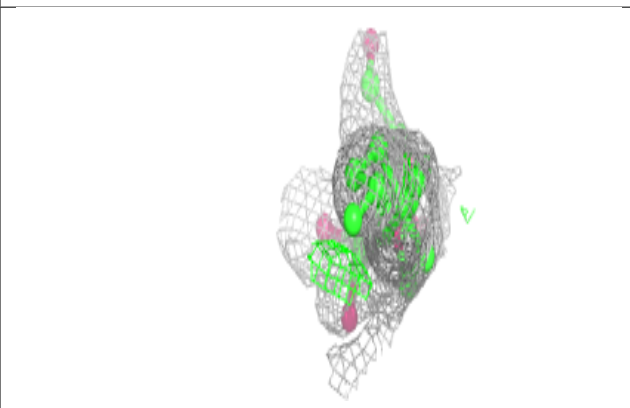
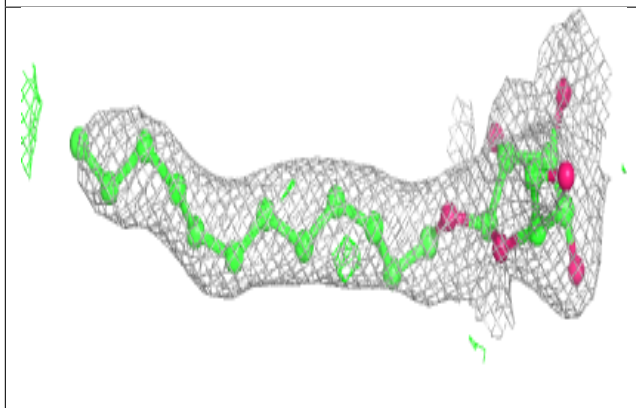
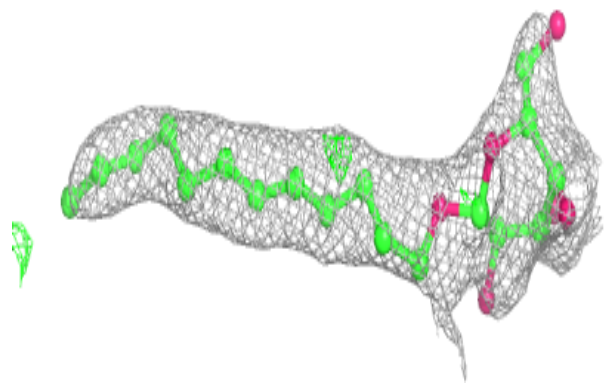
**Electron density around LMT T 103:**

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

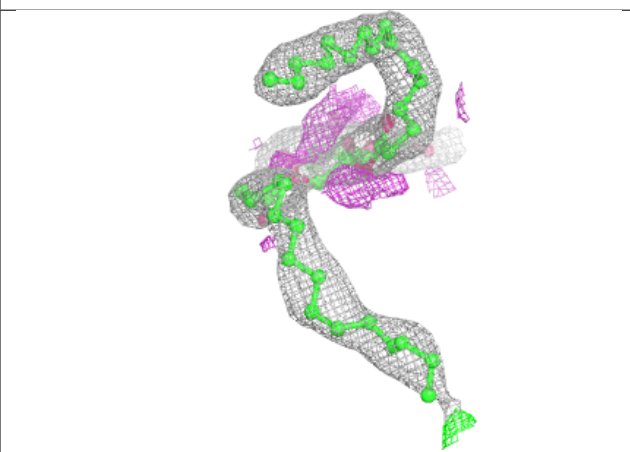
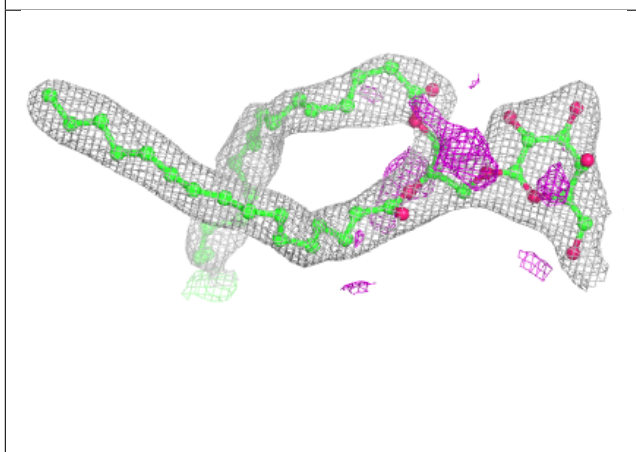
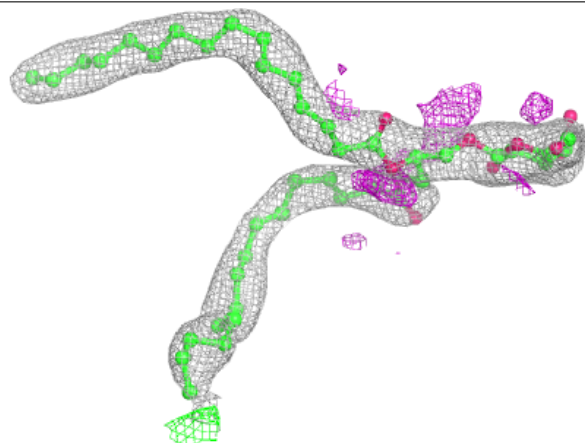


**Electron density around LMT i 103:**

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

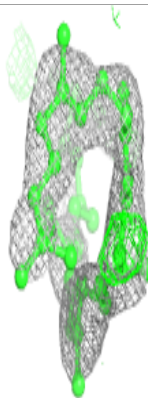
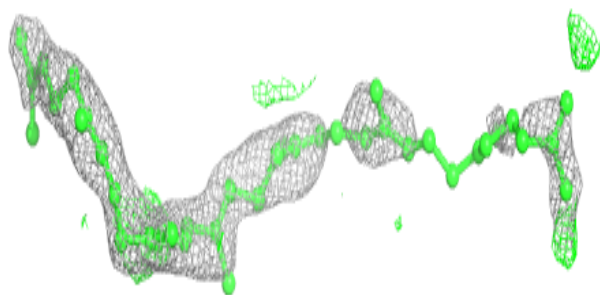
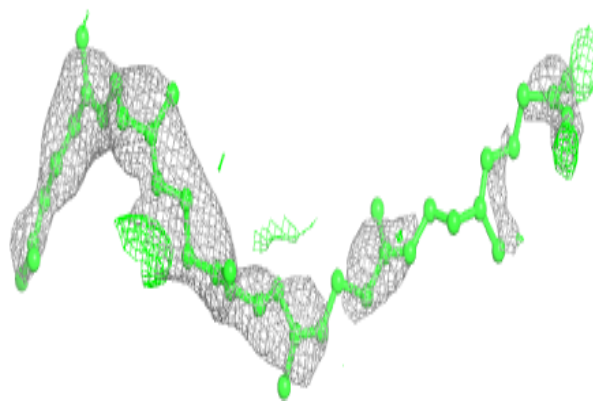
**Electron density around LMG m 2802:**

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

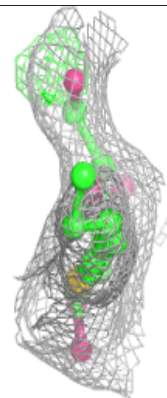
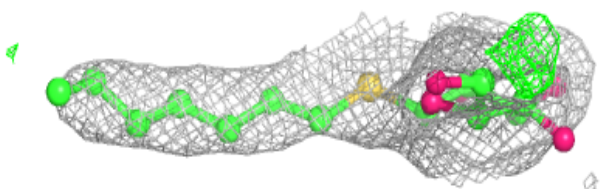
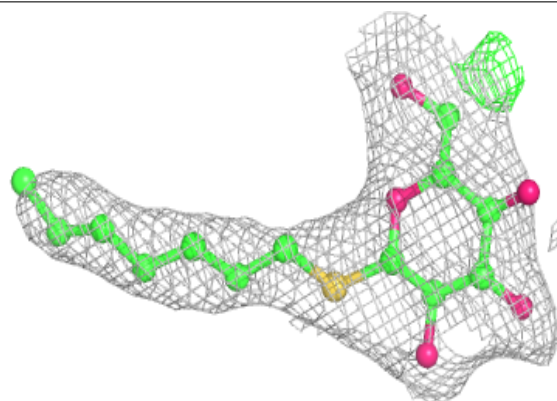


**Electron density around PL9 x 1301:**

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

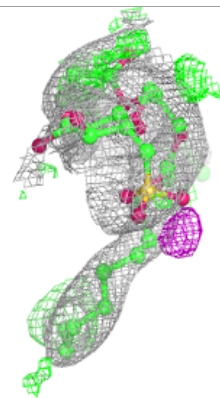
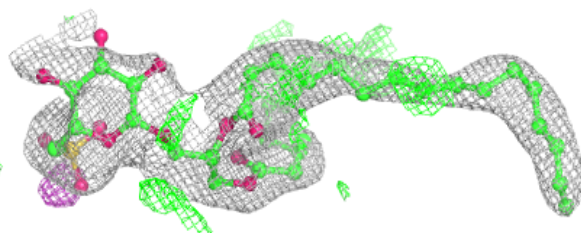
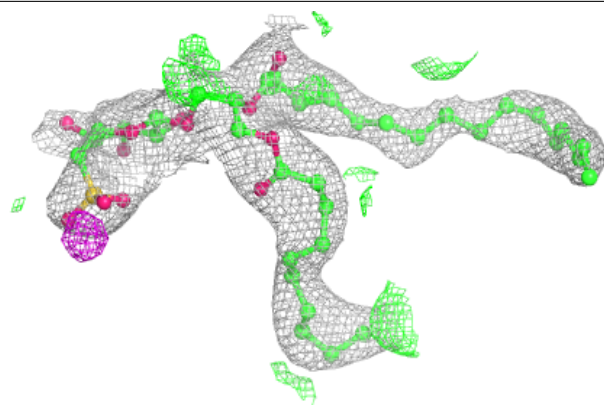
**Electron density around HTG b 604:**

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

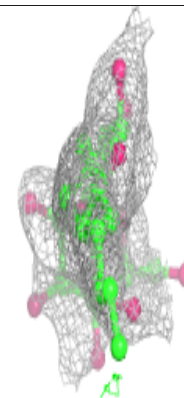
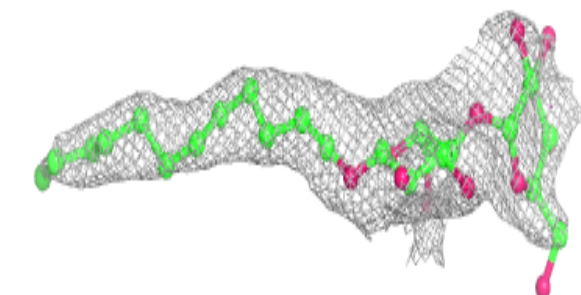
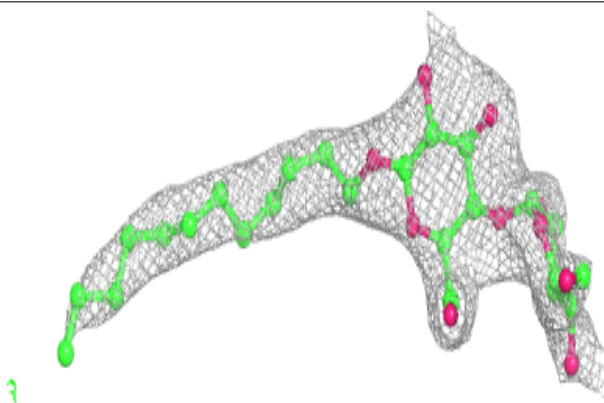


**Electron density around SQD b 601:**

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

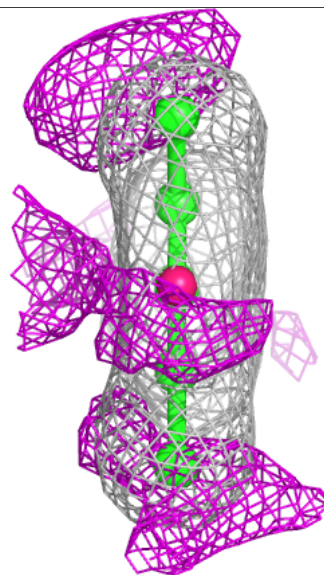
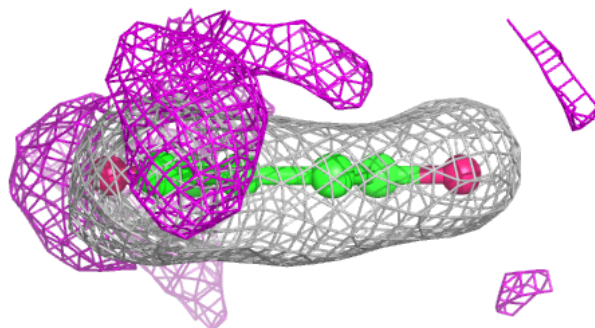
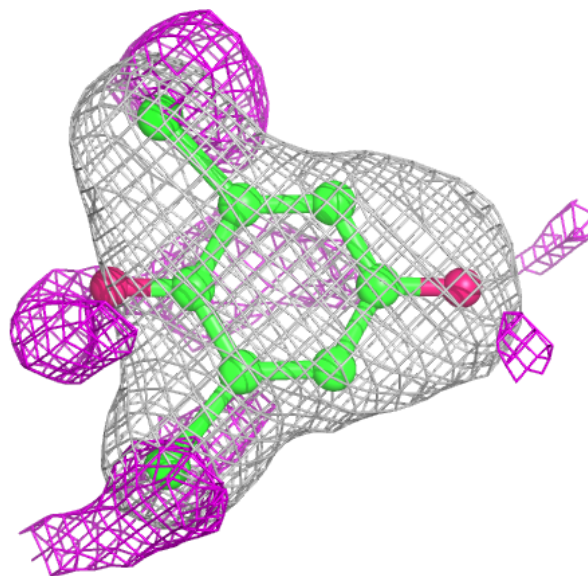
**Electron density around LMT B 623:**

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



**Electron density around JOX A 419:**

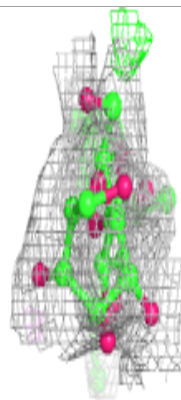
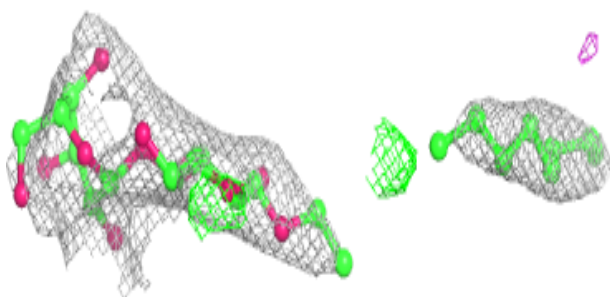
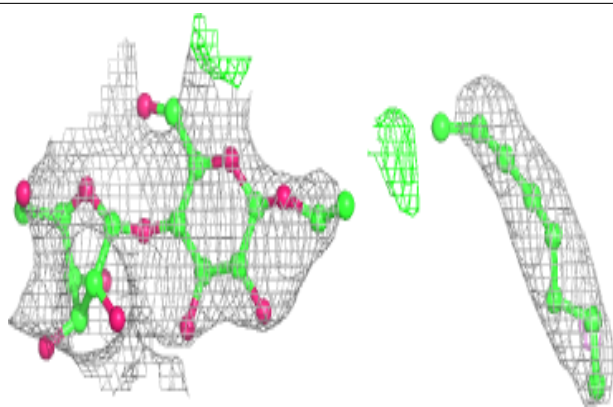
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



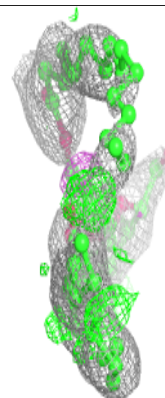
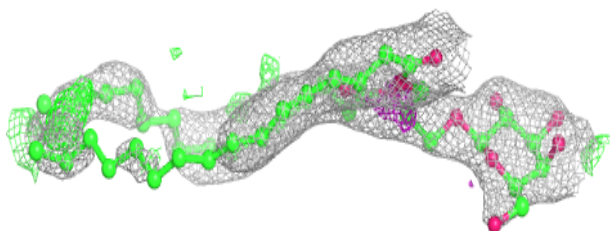
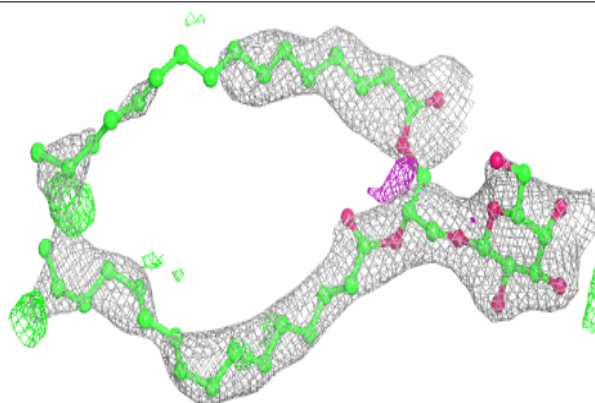


**Electron density around LMT z 102:**

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

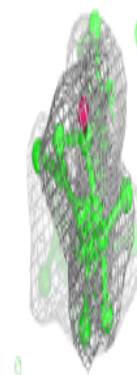
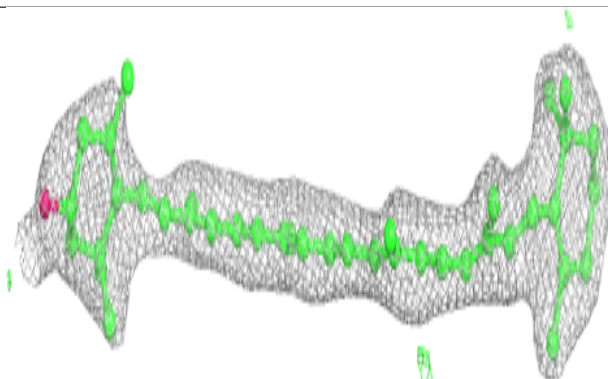
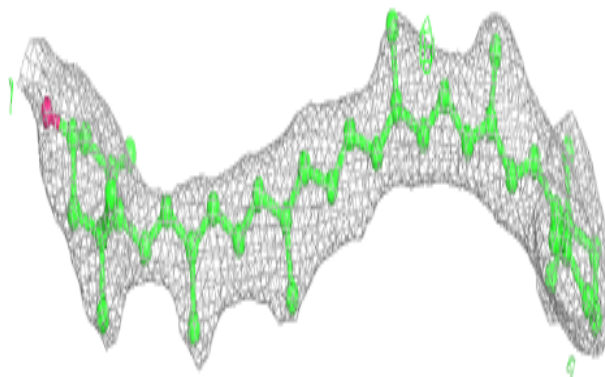
**Electron density around LMG c 501:**

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

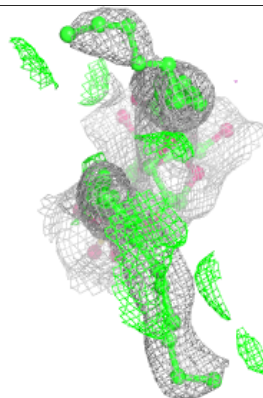
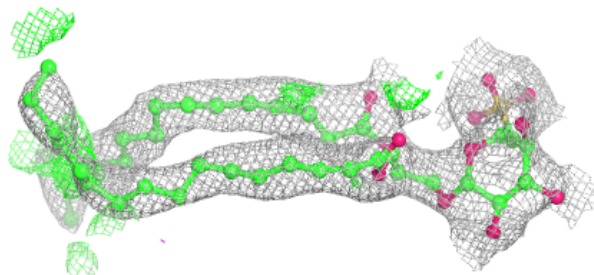
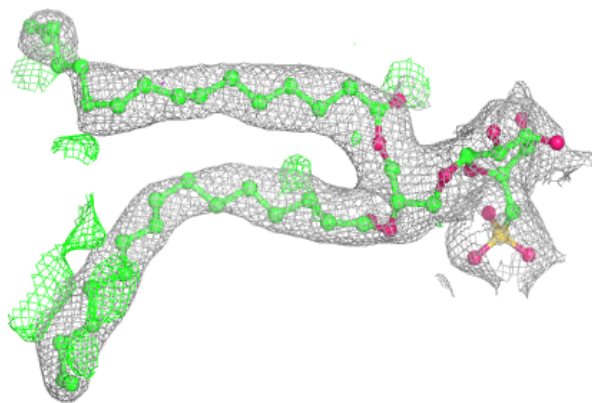


**Electron density around RRX H 102:**

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

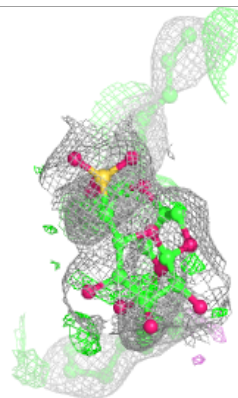
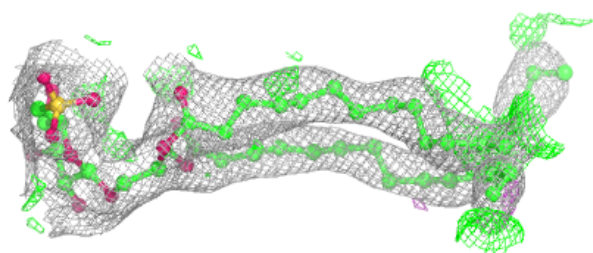
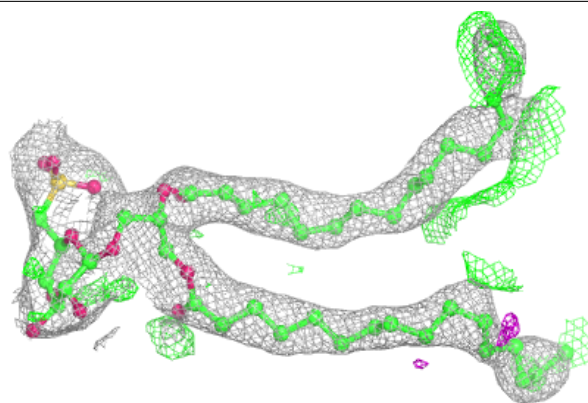
**Electron density around SQD B 621:**

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

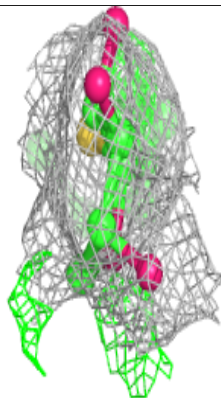
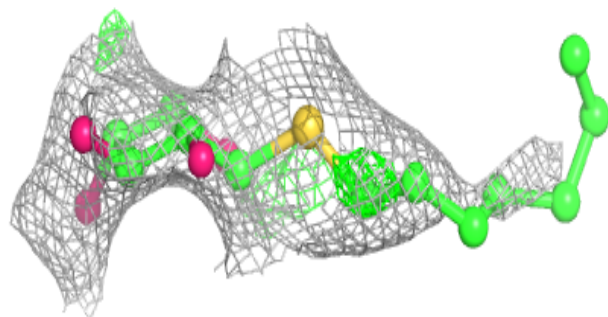
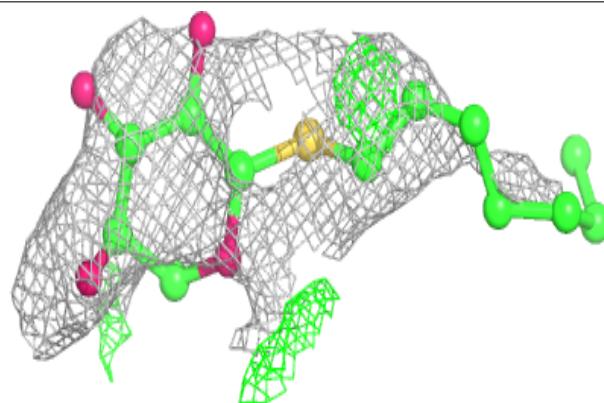


**Electron density around SQD I 101:**

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

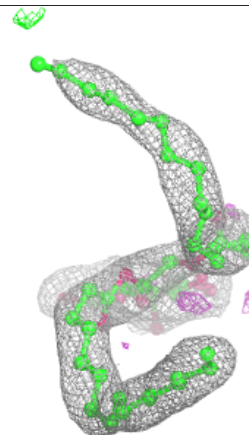
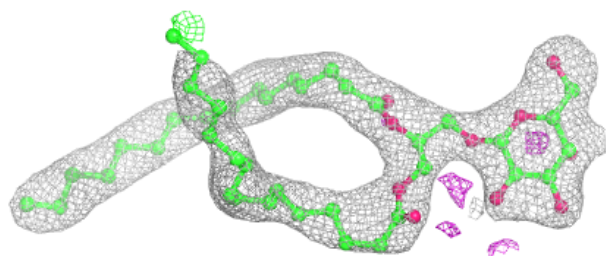
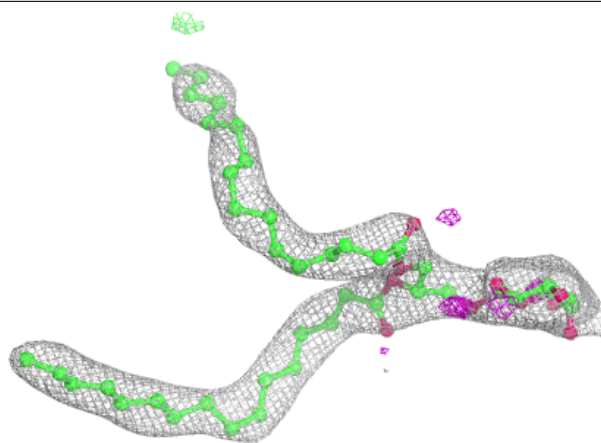
**Electron density around HTG H 101:**

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

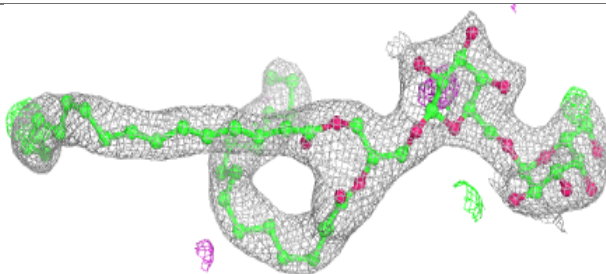
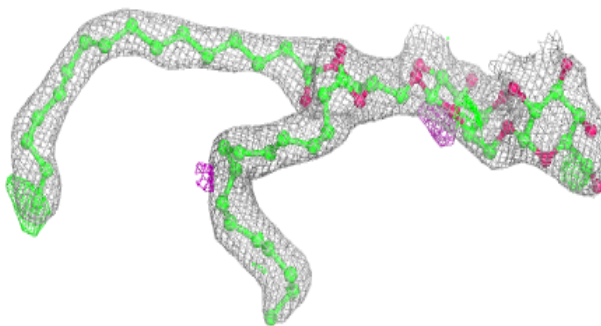


**Electron density around LMG B 622:**

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

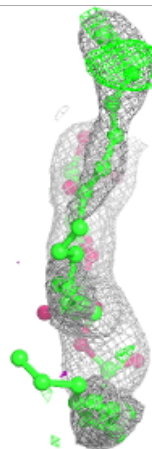
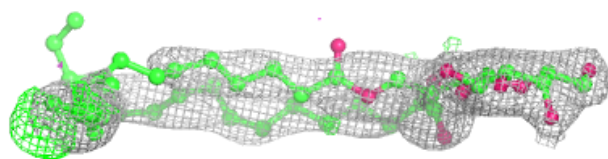
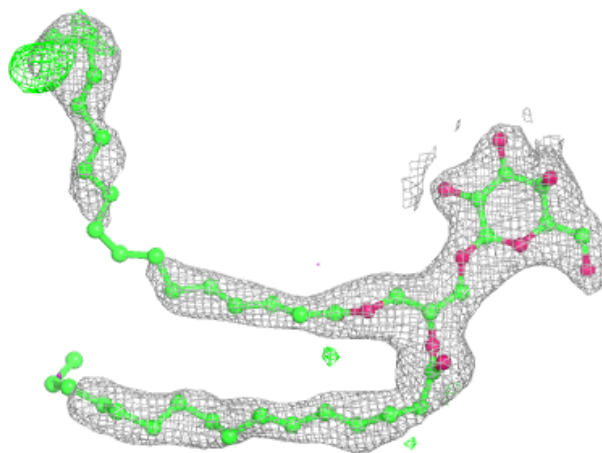
**Electron density around DGD h 102:**

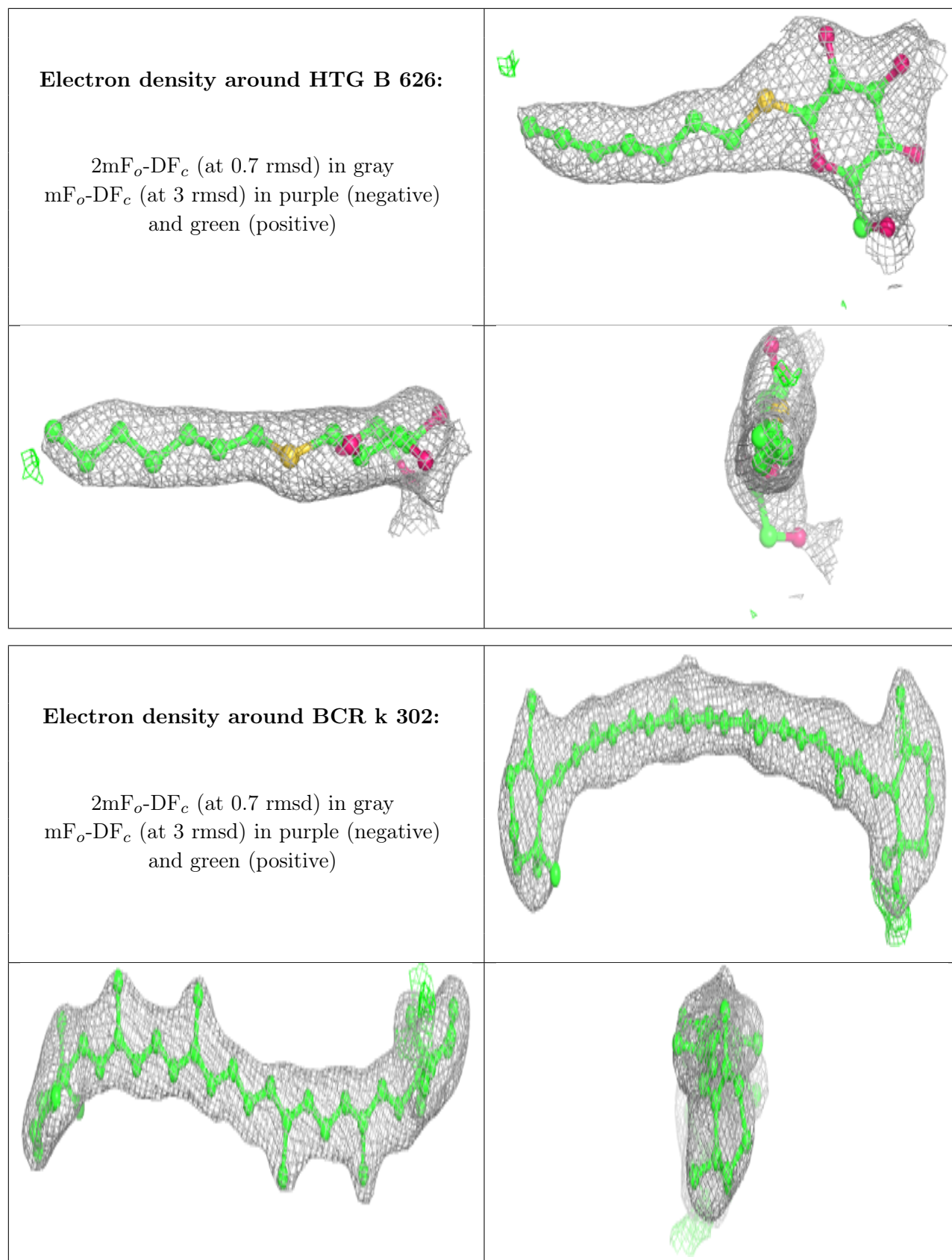
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around LMG C 520:**

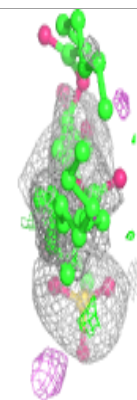
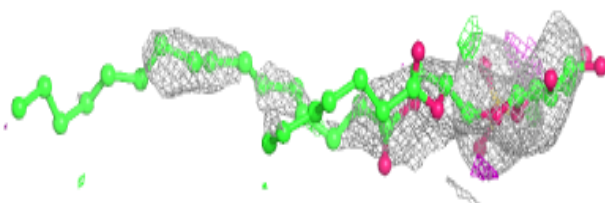
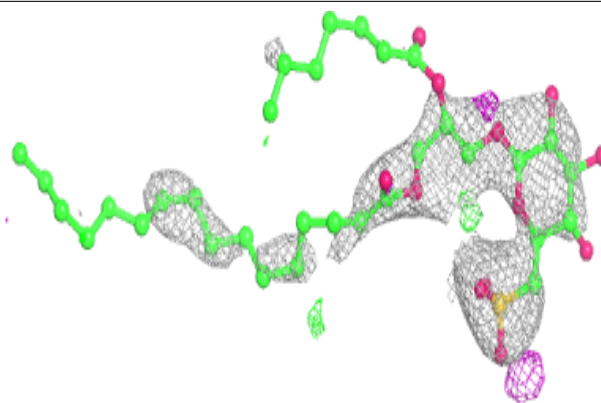
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



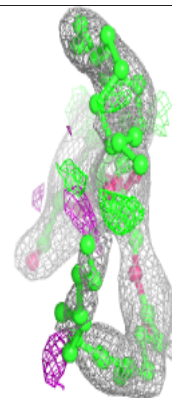
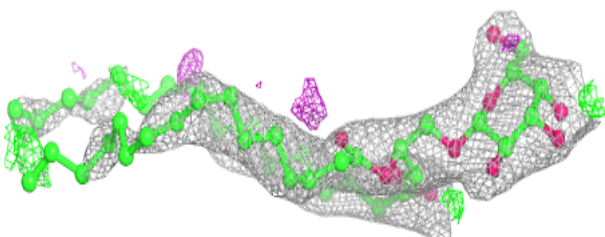
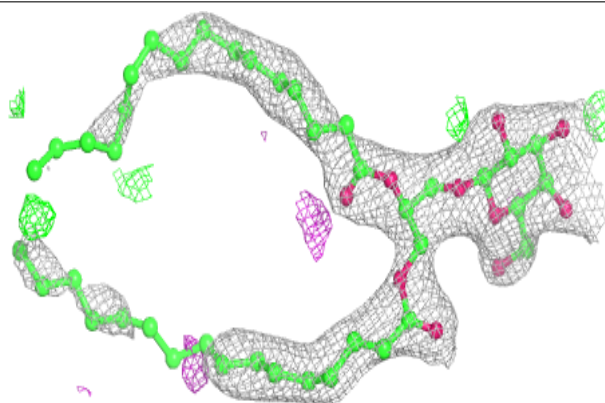


**Electron density around SQD D 2308:**

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

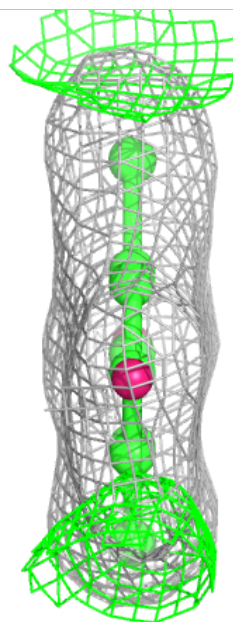
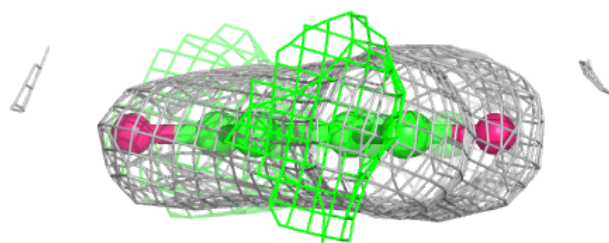
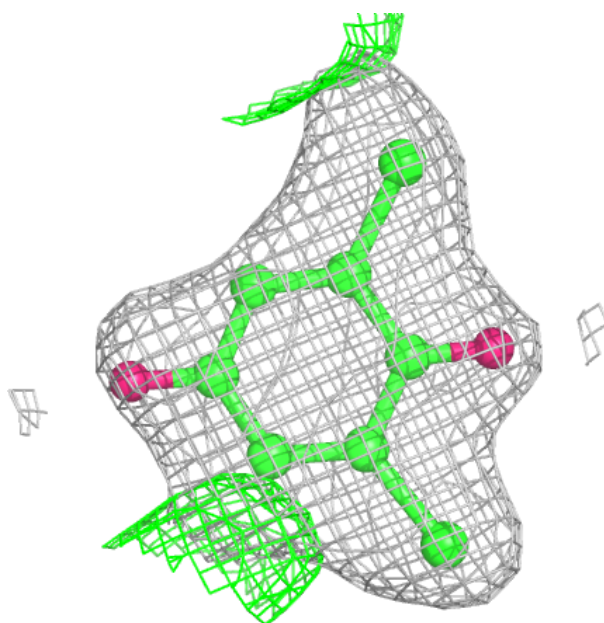
**Electron density around LMG A 413:**

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



**Electron density around JOX A 418:**

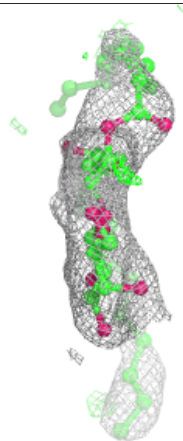
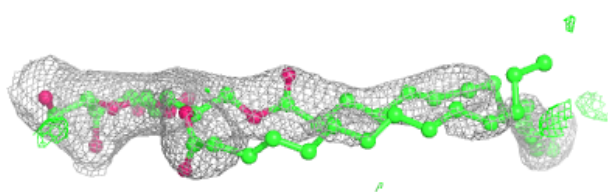
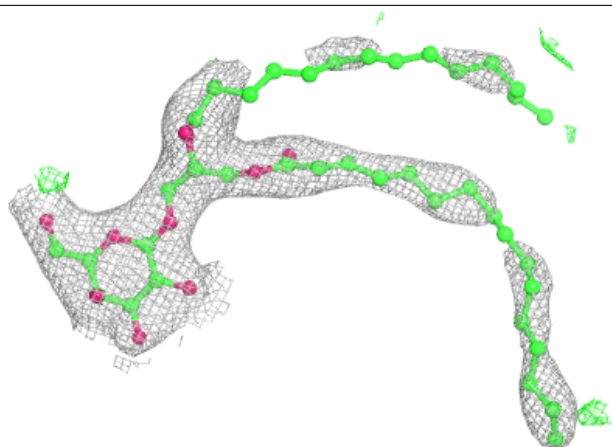
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



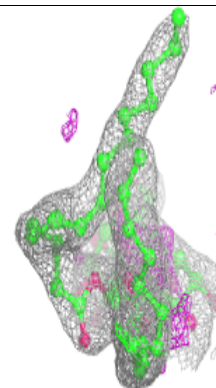
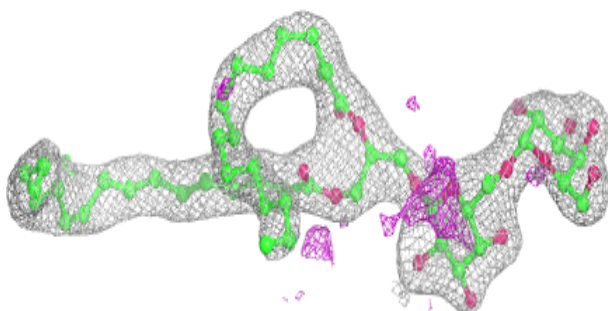
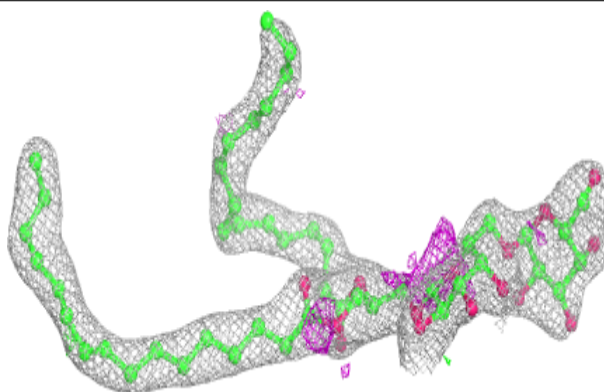


**Electron density around LMG c 521:**

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

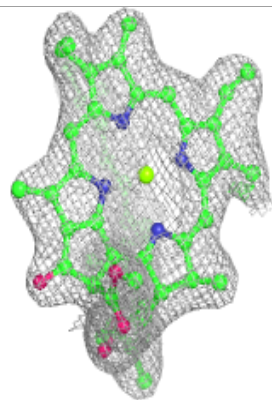
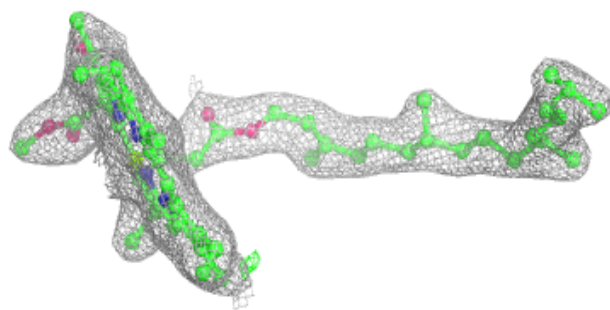
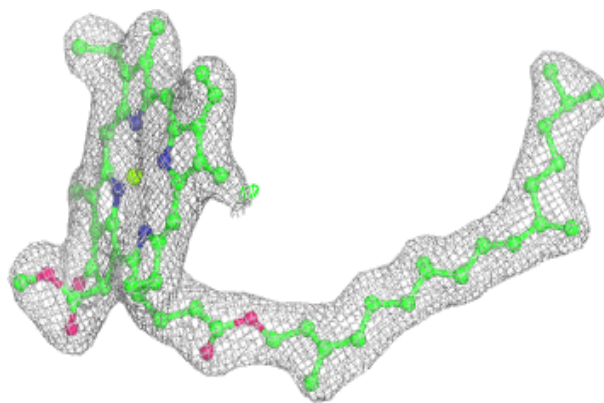
**Electron density around DGD H 103:**

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

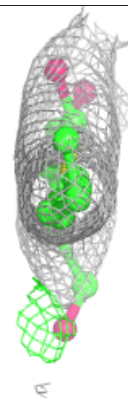
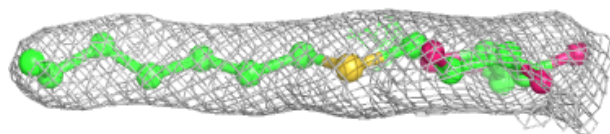
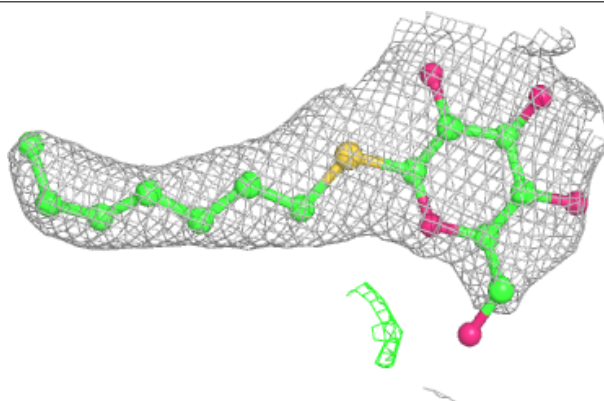


**Electron density around CLA B 610:**

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

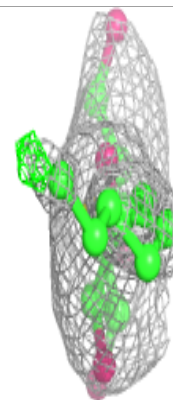
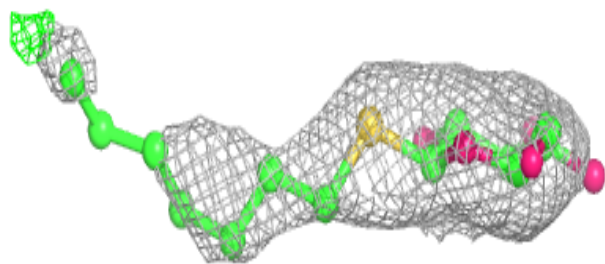
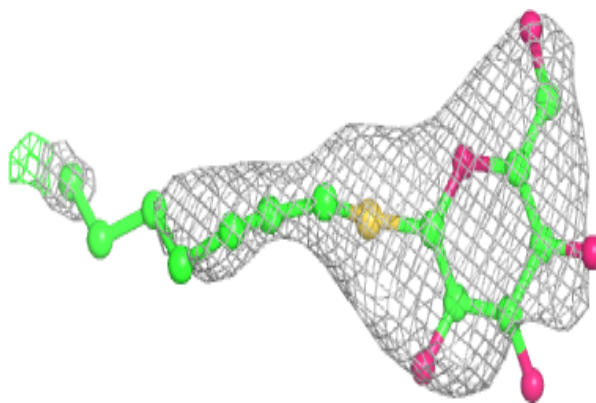
**Electron density around HTG b 603:**

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



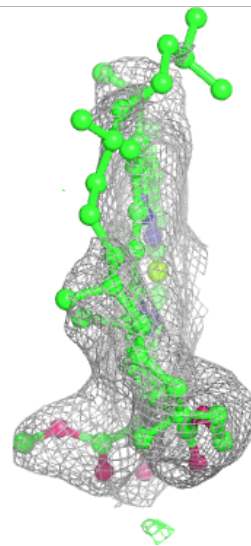
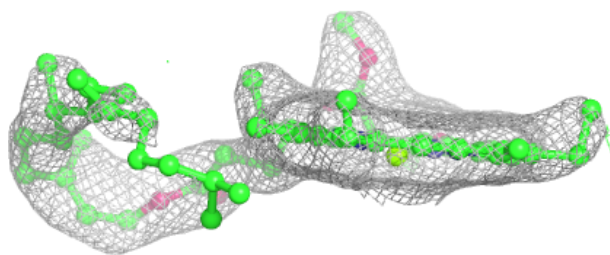
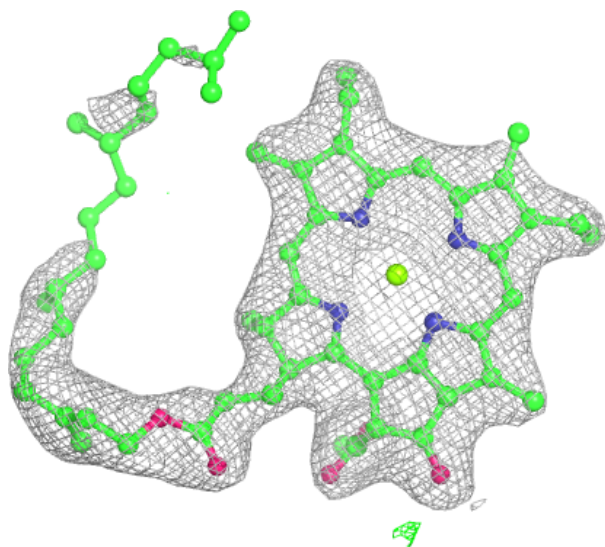
**Electron density around HTG c 523:**

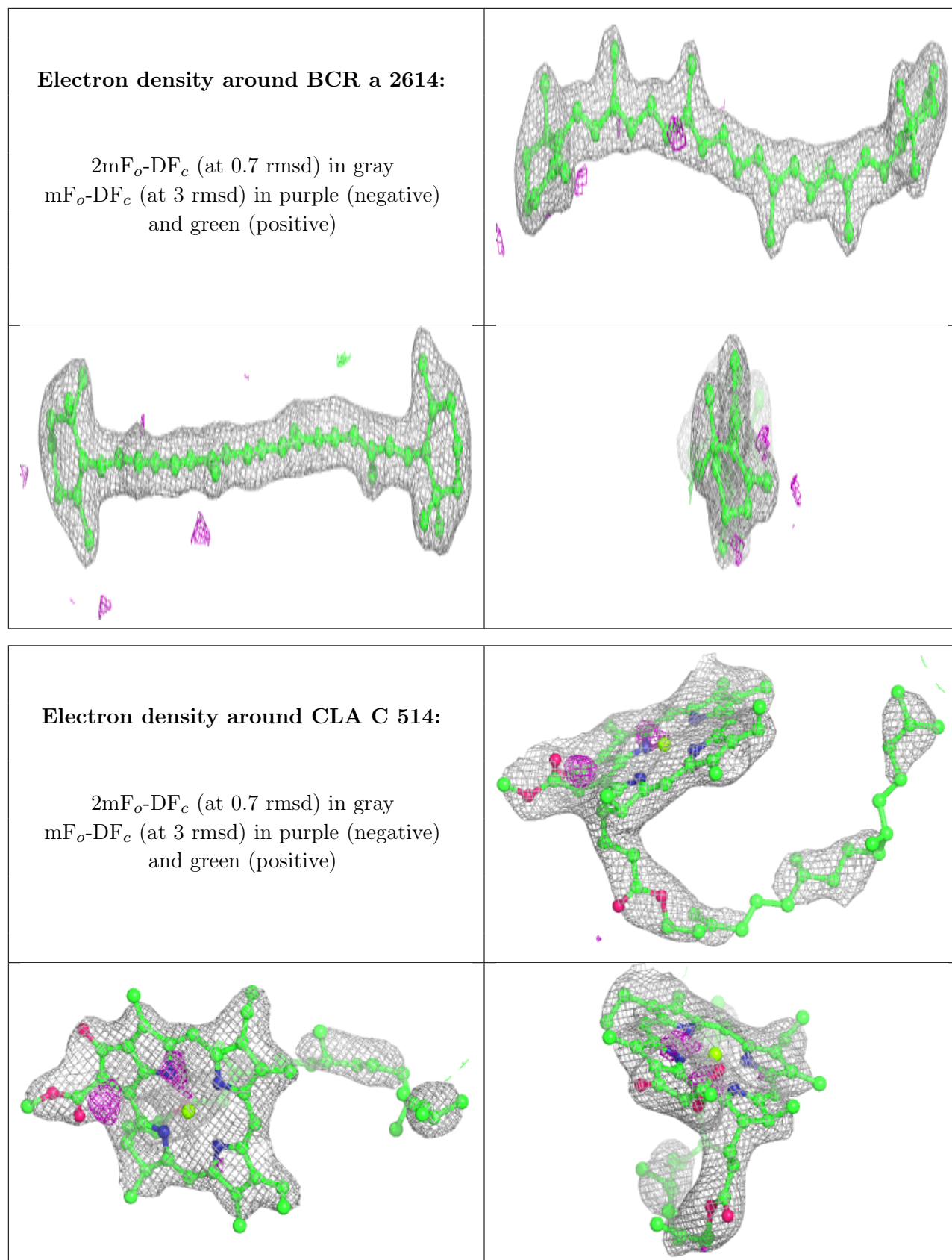
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA c 515:**

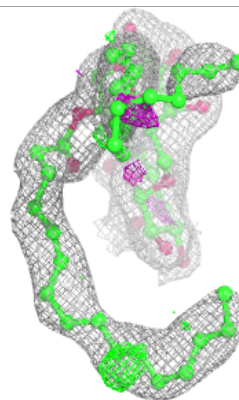
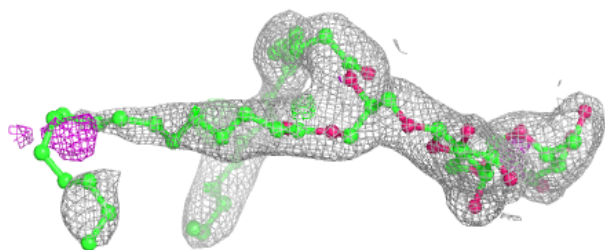
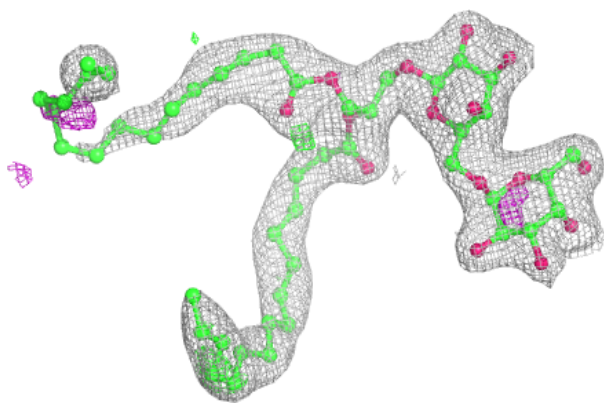
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



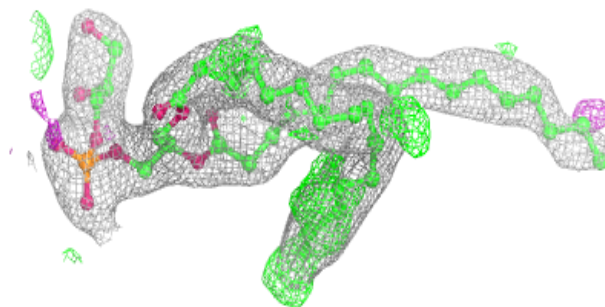
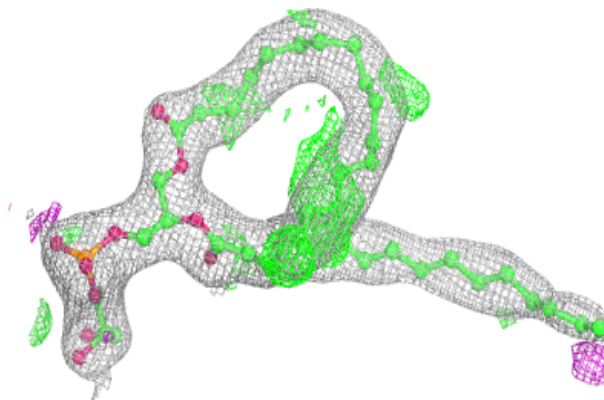


**Electron density around DGD C 518:**

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

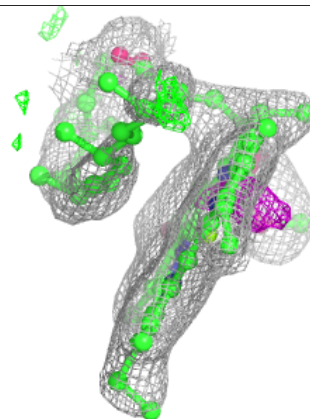
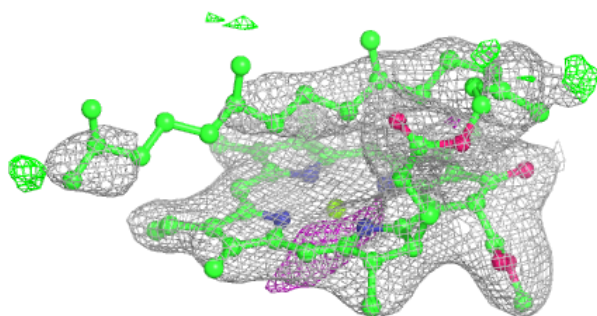
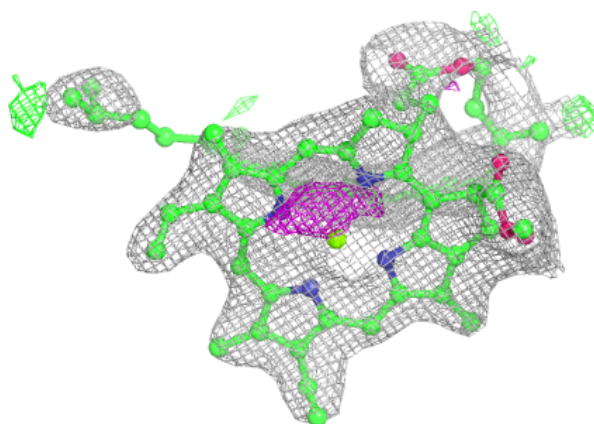
**Electron density around LHG D 2309:**

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



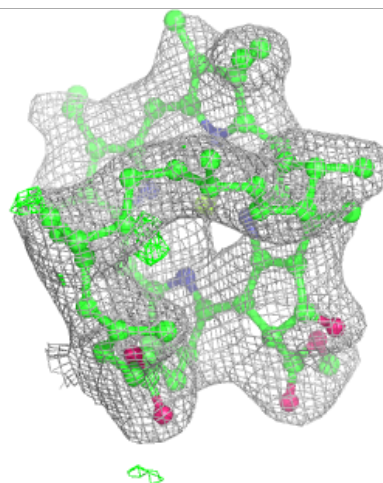
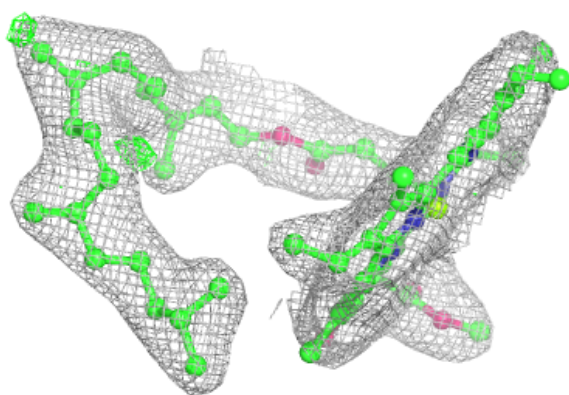
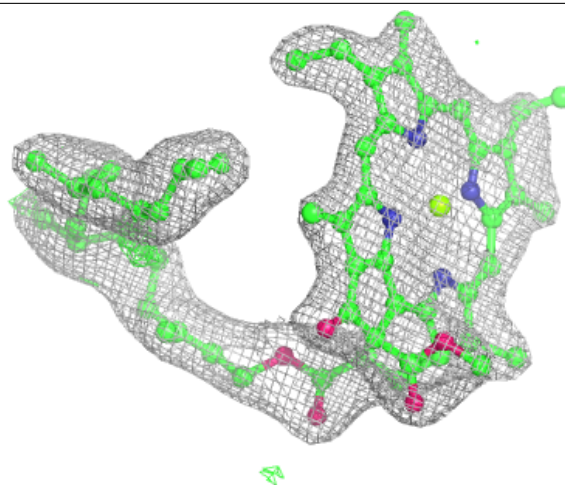
**Electron density around CLA B 602:**

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



**Electron density around CLA c 506:**

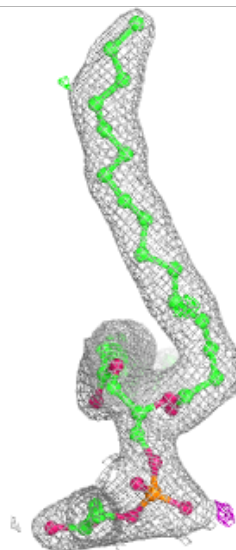
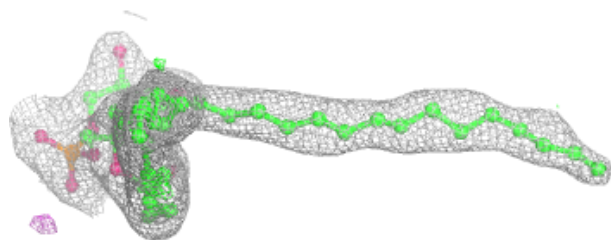
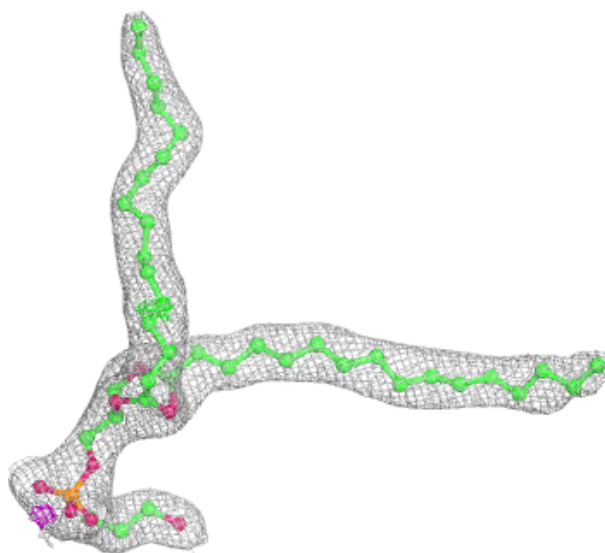
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





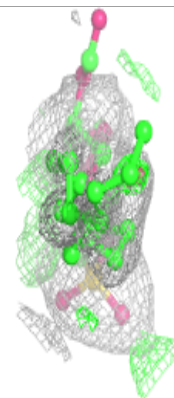
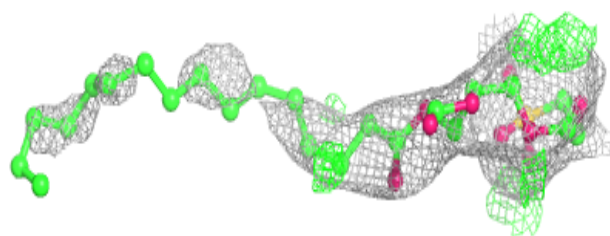
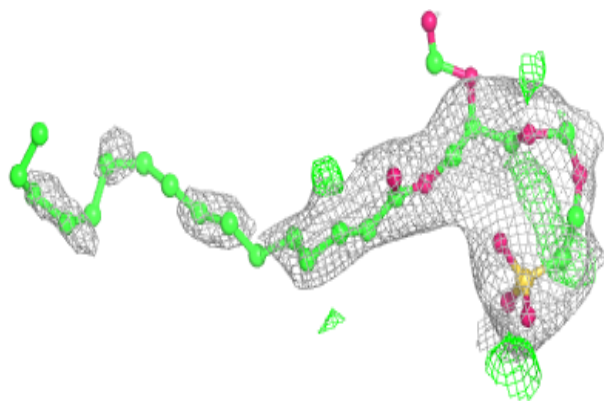
**Electron density around LHG 1 103:**

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

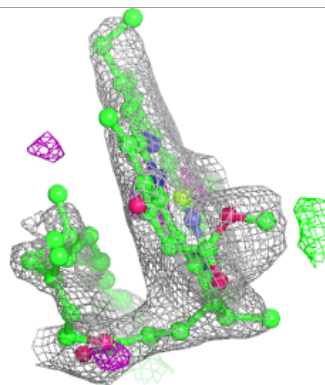
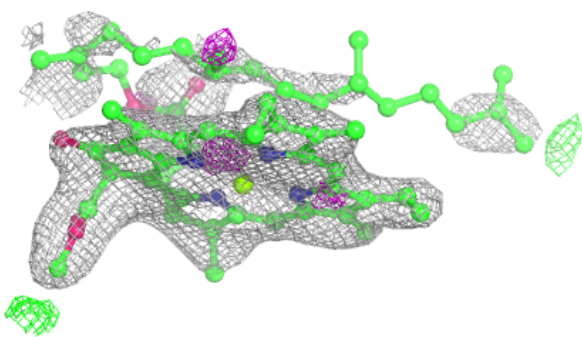
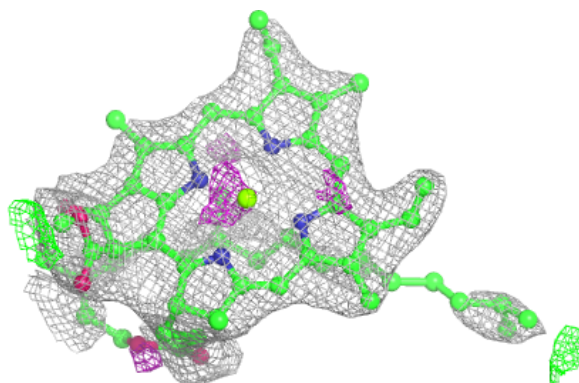


**Electron density around SQD d 417:**

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

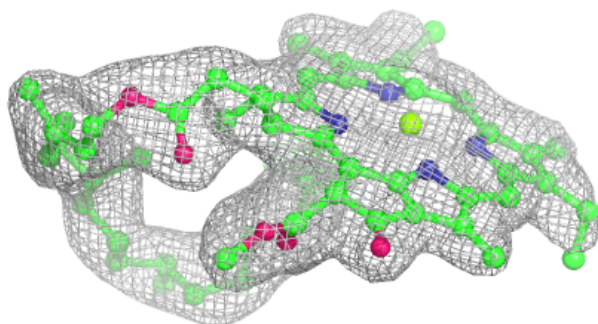
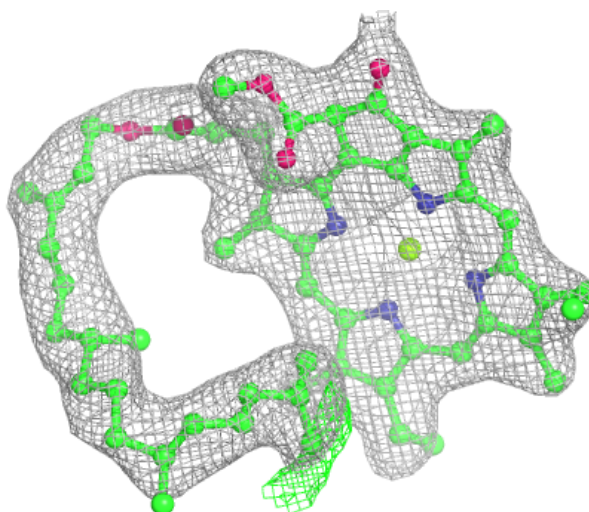
**Electron density around CLA b 606:**

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



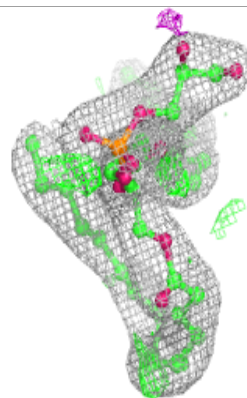
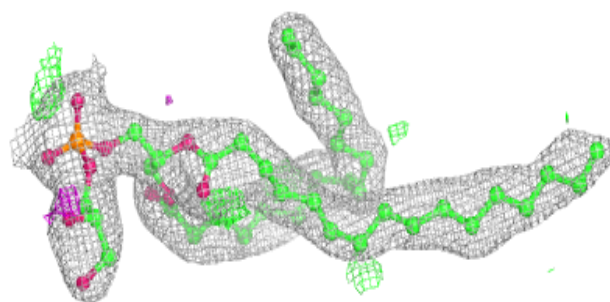
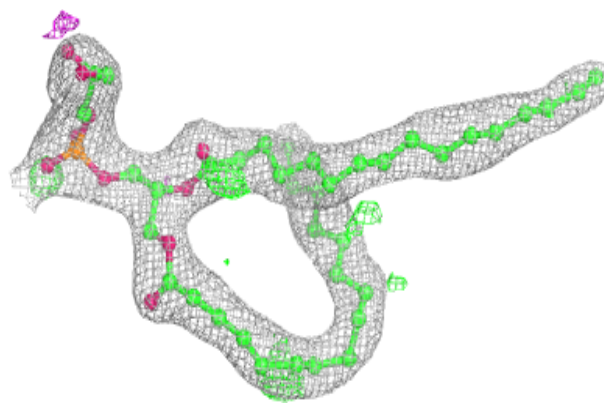
**Electron density around CLA b 620:**

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



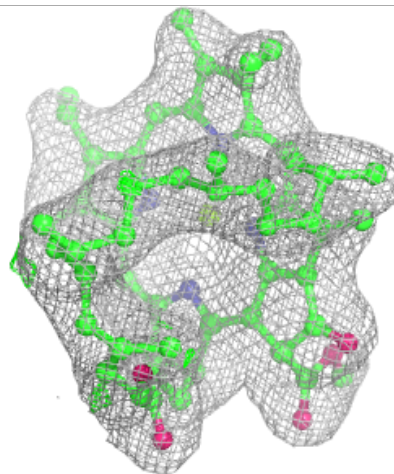
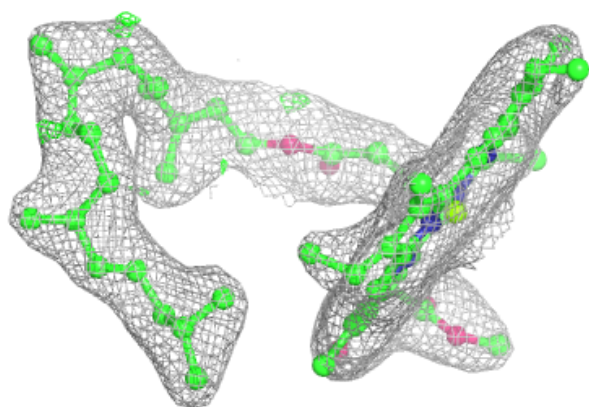
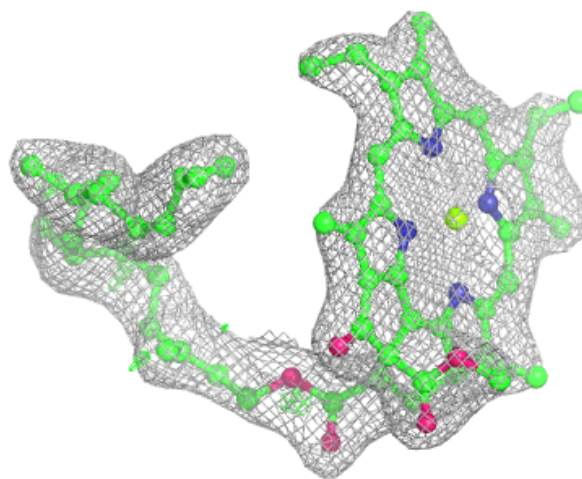
**Electron density around LHG d 412:**

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



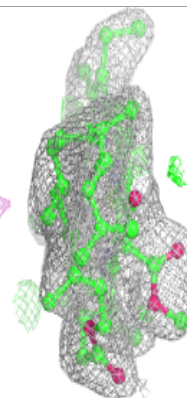
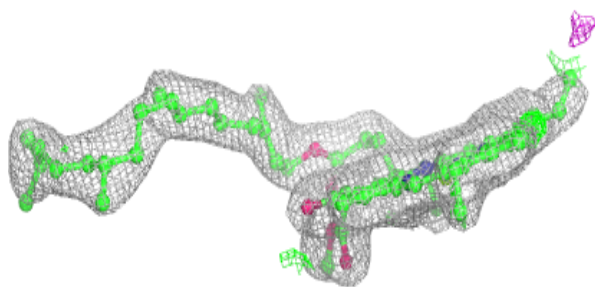
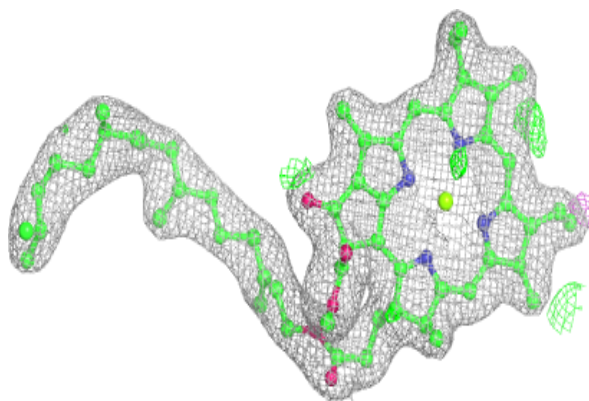
**Electron density around CLA C 504:**

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

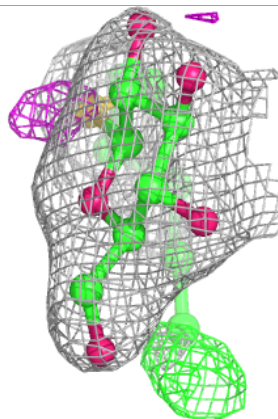
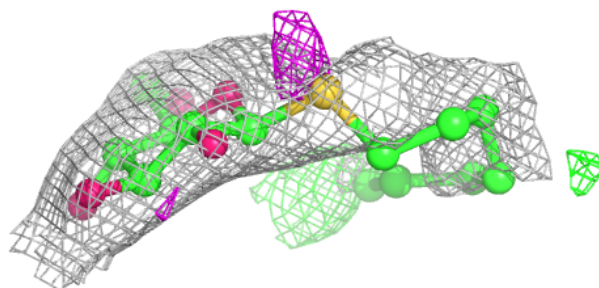
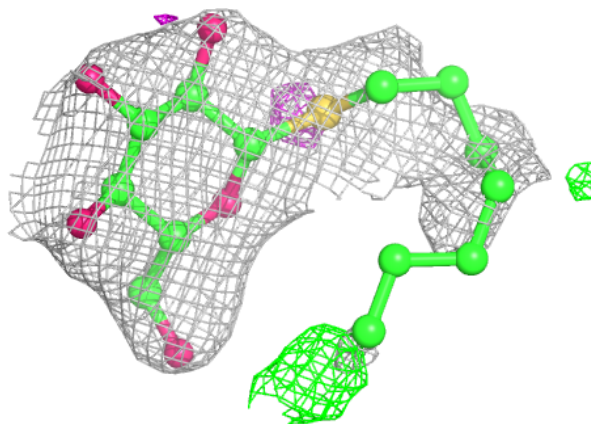


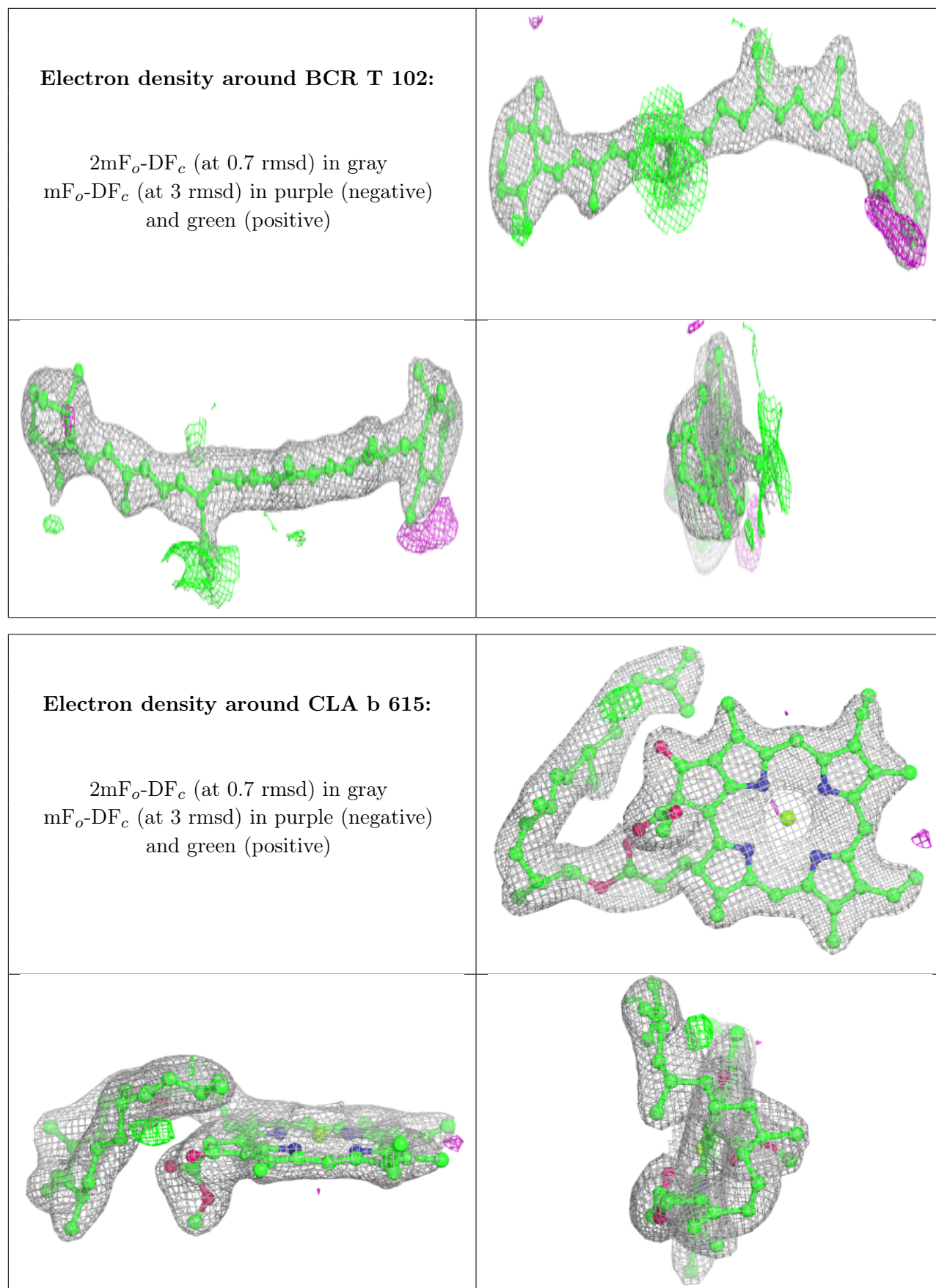
**Electron density around CLA B 603:**

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

**Electron density around HTG V 204:**

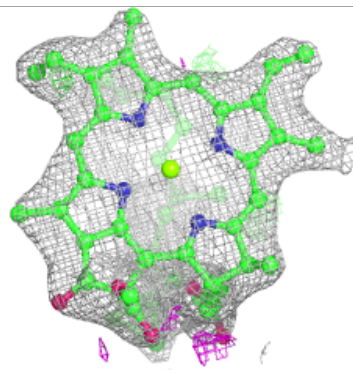
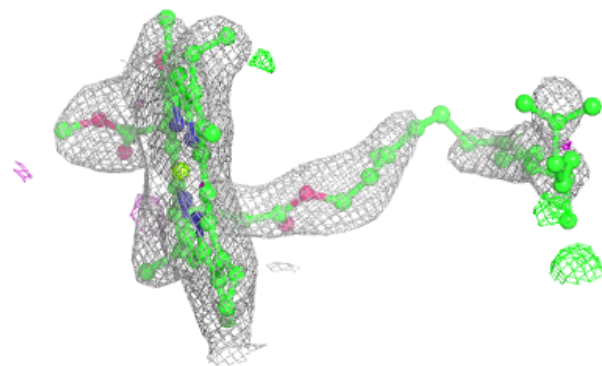
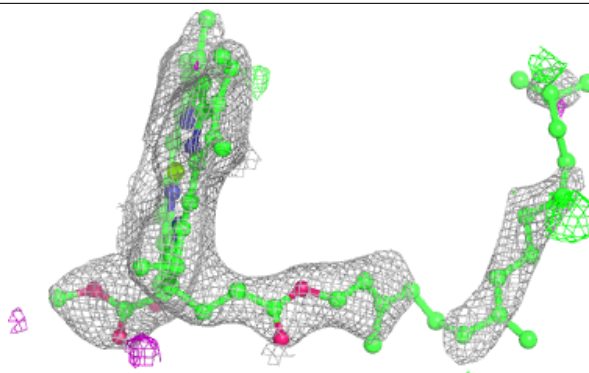
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA C 507:**

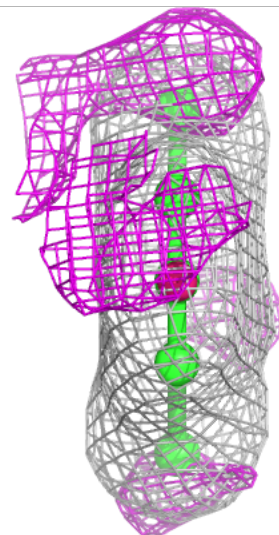
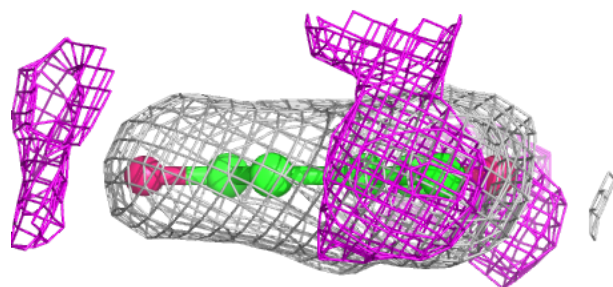
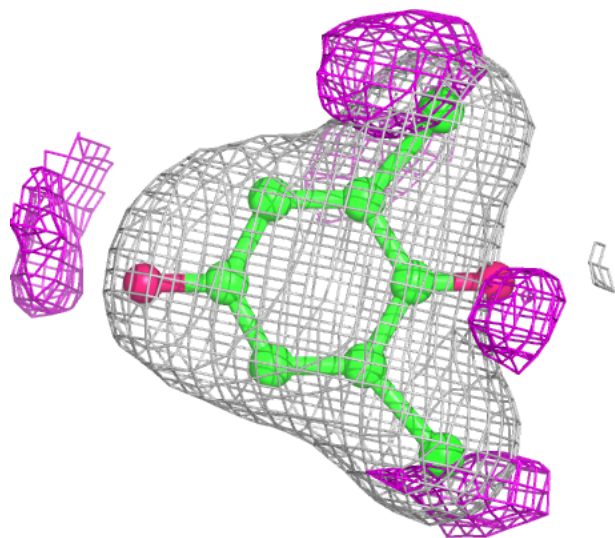
$2mF_o-DF_c$  (at 0.7 rnsd) in gray  
 $mF_o-DF_c$  (at 3 rnsd) in purple (negative)  
and green (positive)





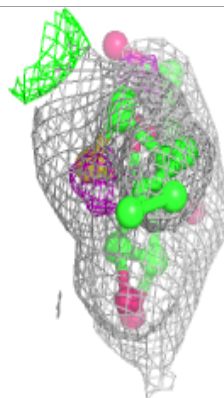
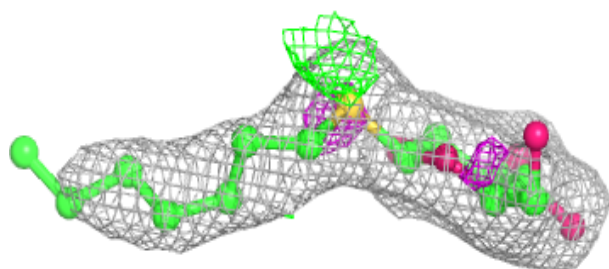
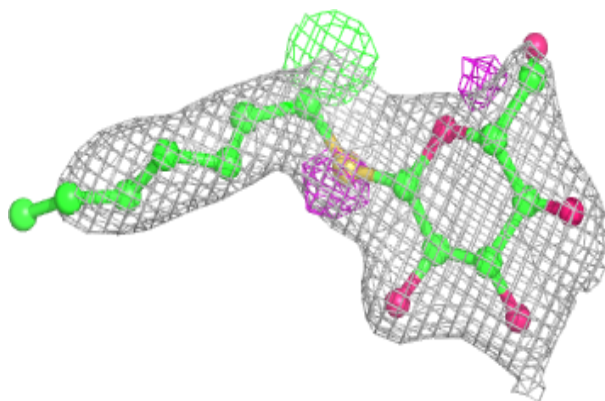
**Electron density around JOX a 2617:**

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



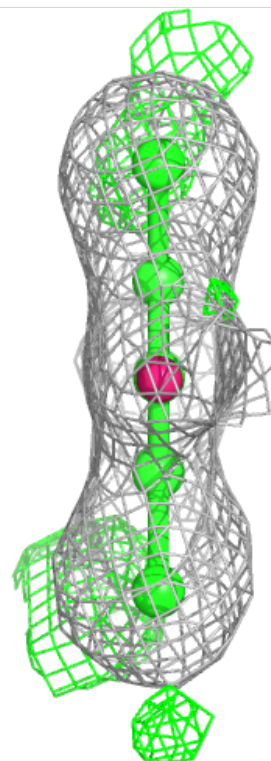
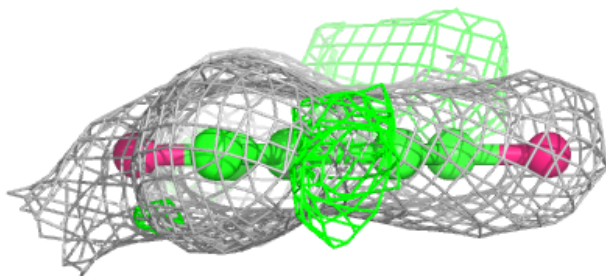
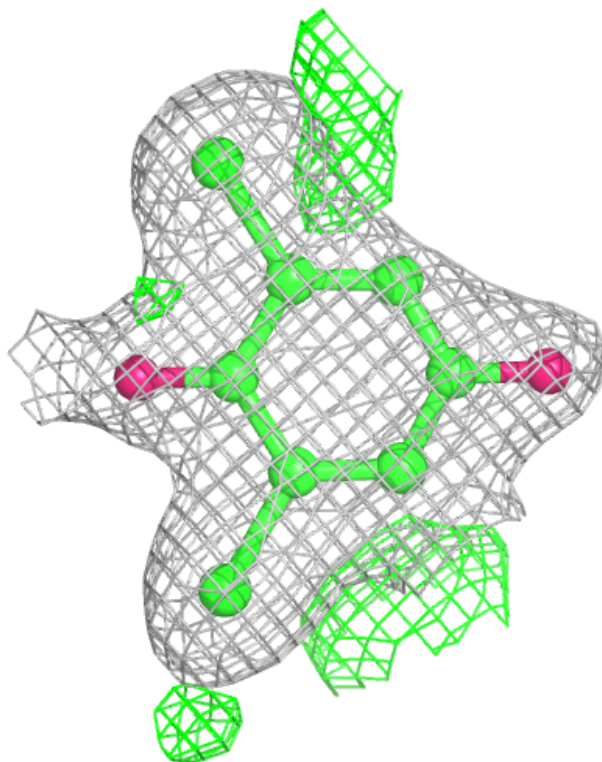
**Electron density around HTG o 301:**

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



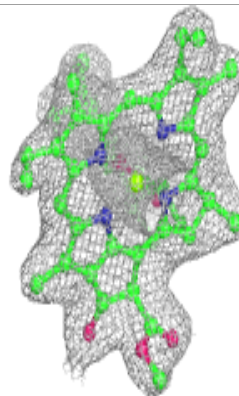
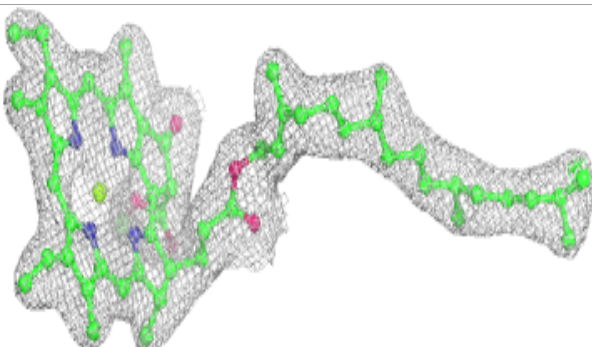
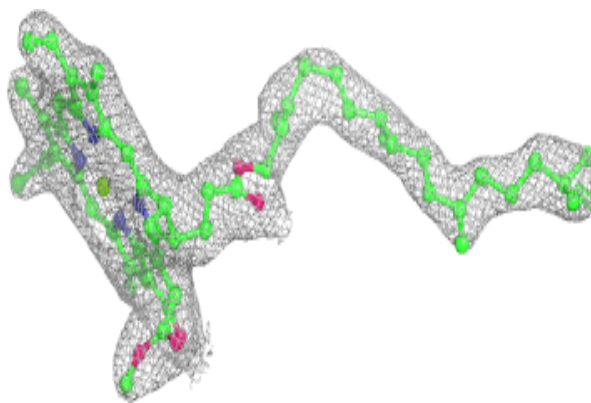
**Electron density around JOX a 2619:**

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

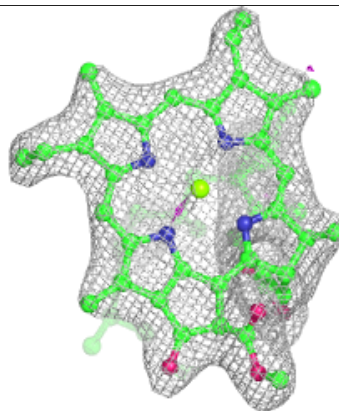
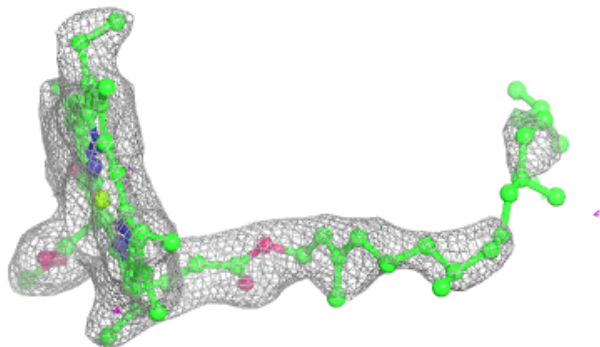
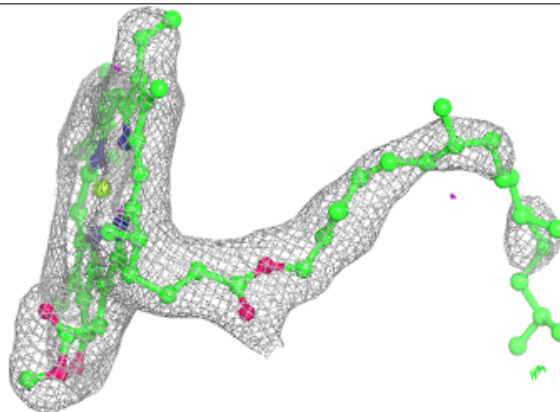


**Electron density around CLA c 505:**

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

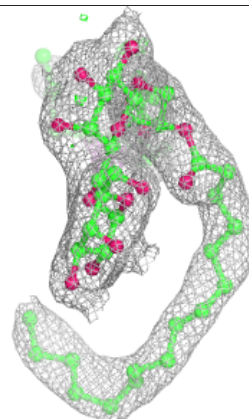
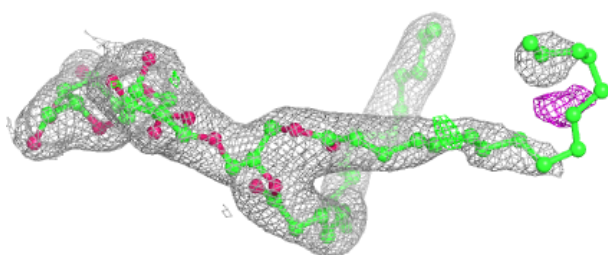
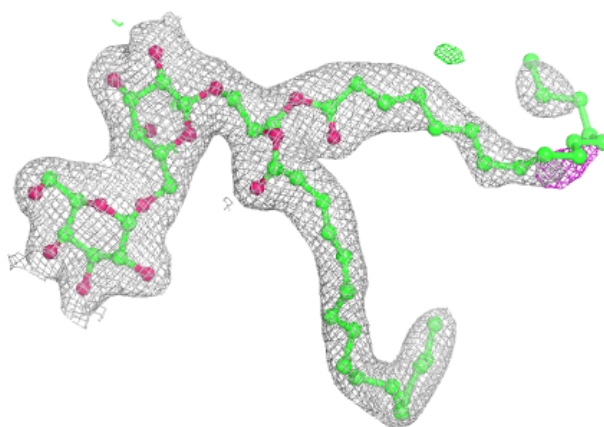
**Electron density around CLA D 2304:**

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

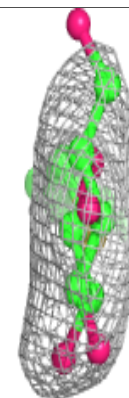
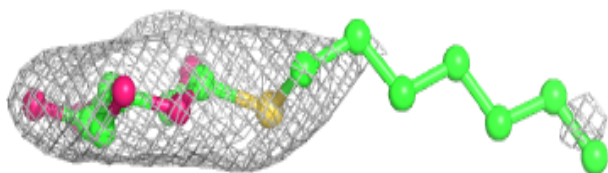
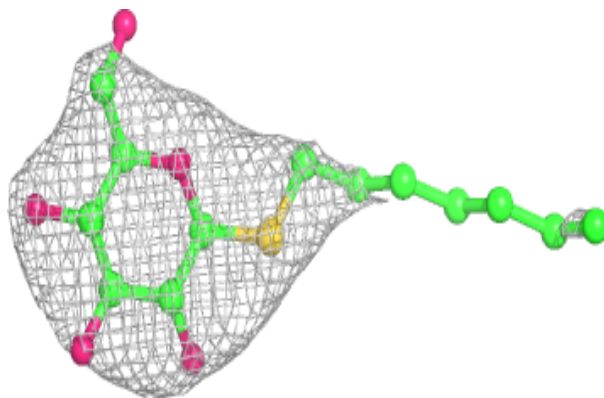


**Electron density around DGD c 519:**

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

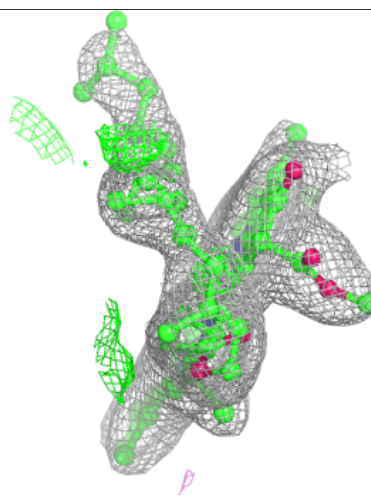
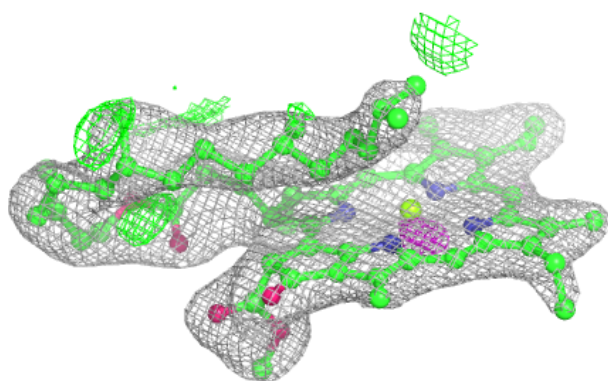
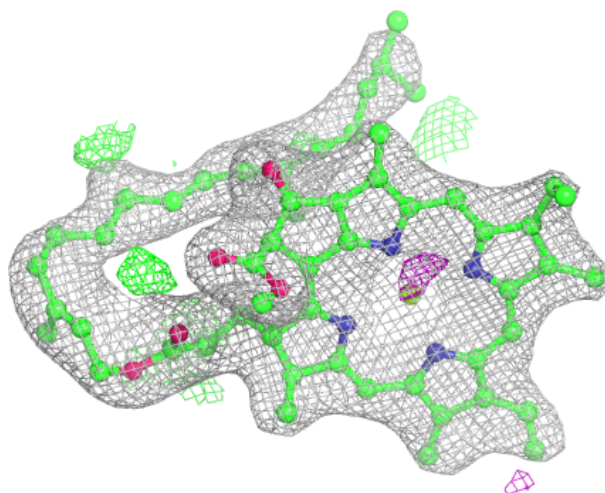
**Electron density around HTG C 521:**

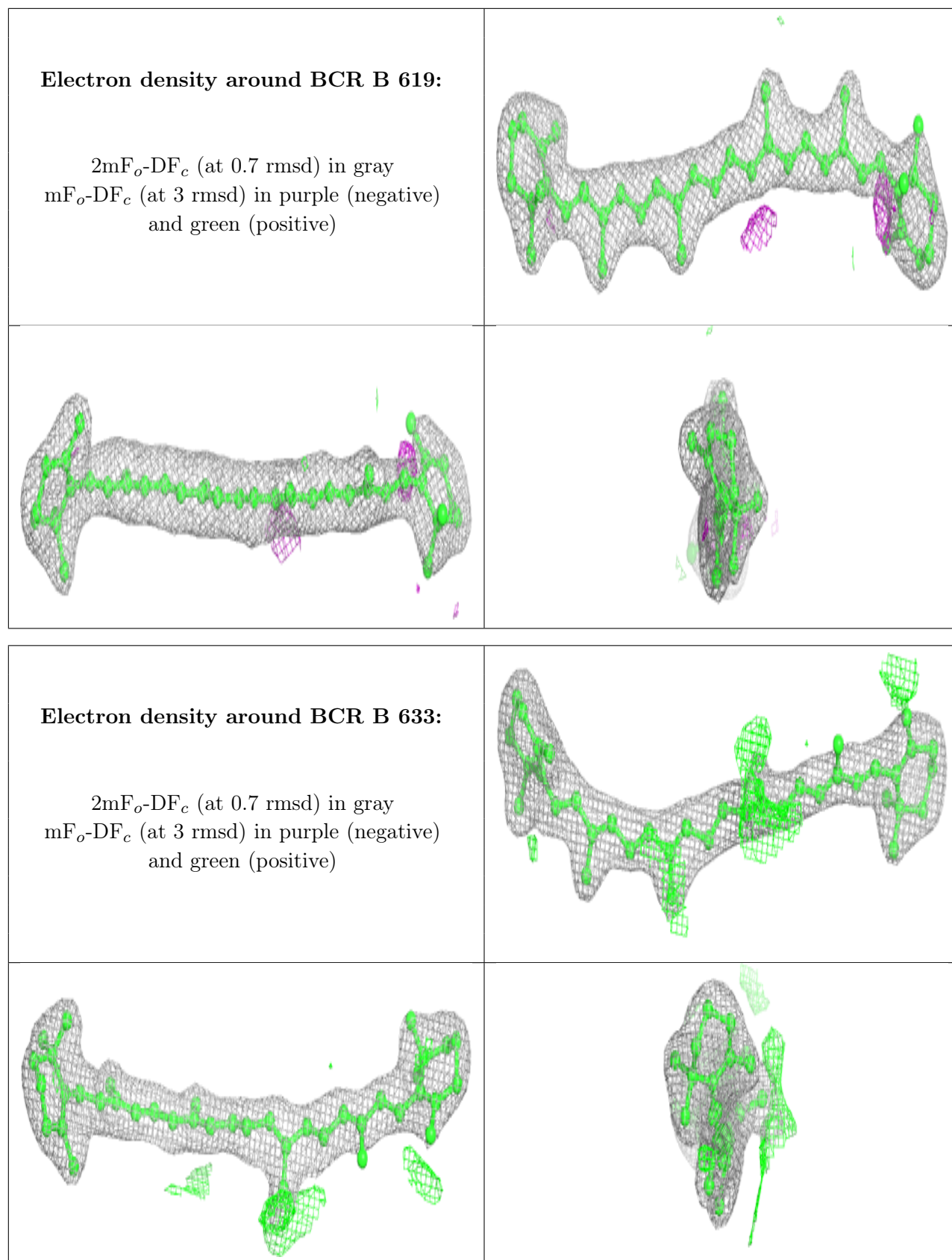
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

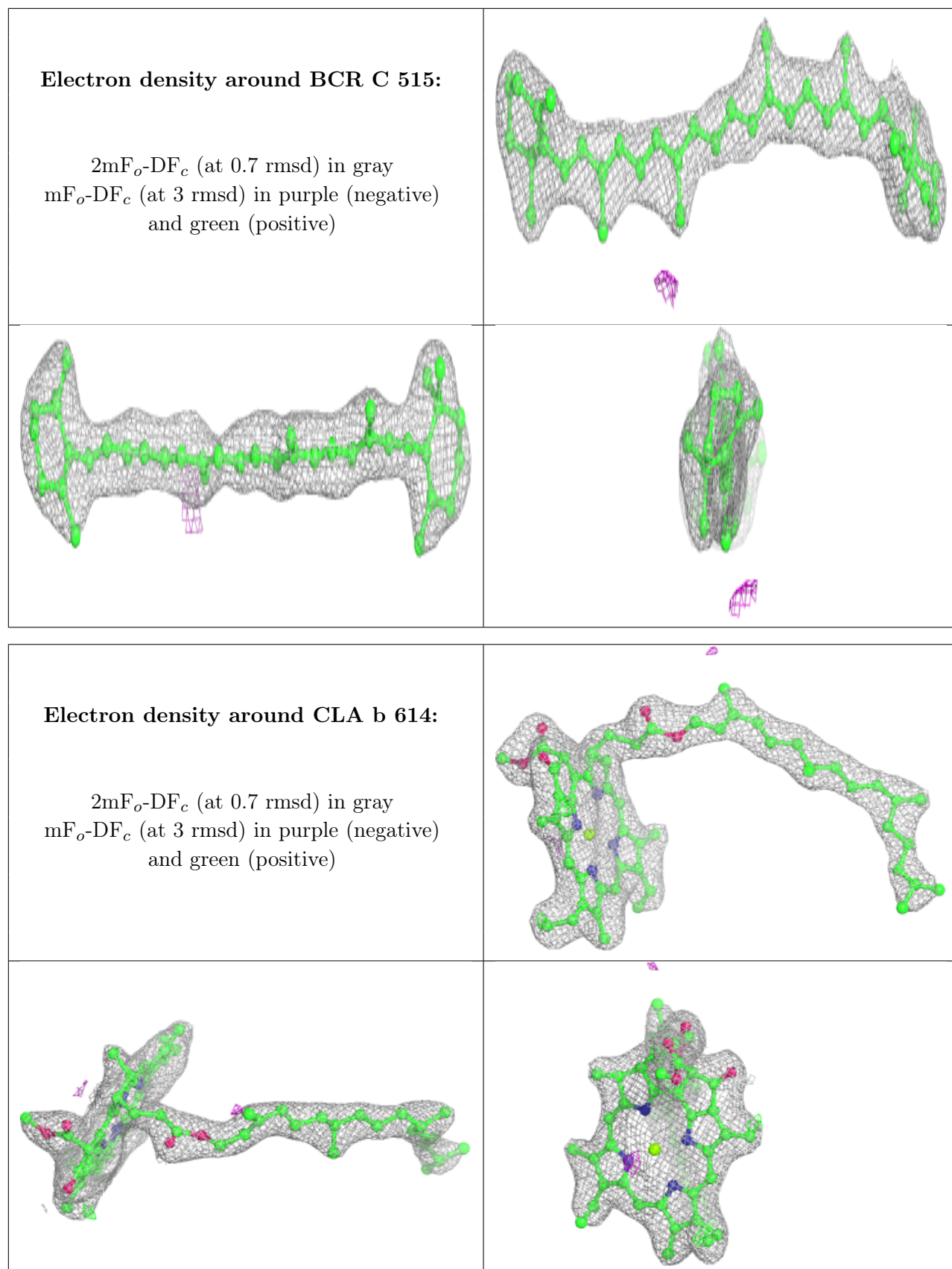


**Electron density around CLA C 510:**

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



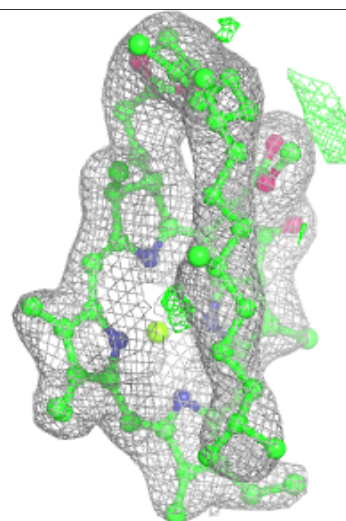
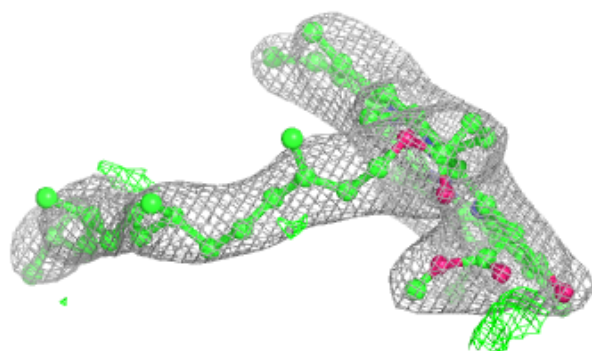
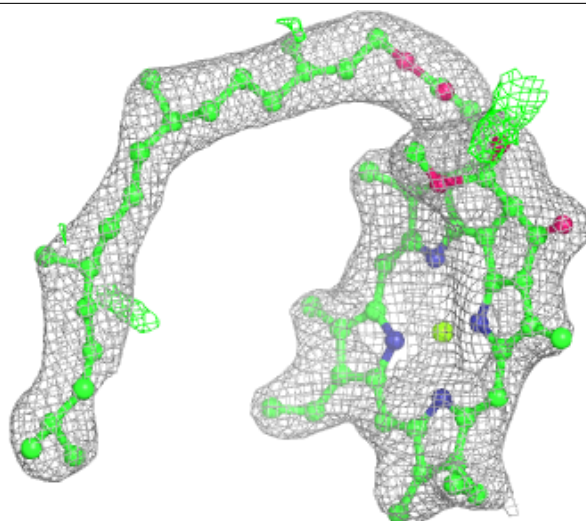






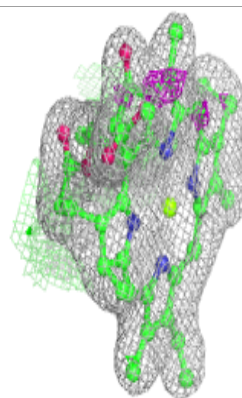
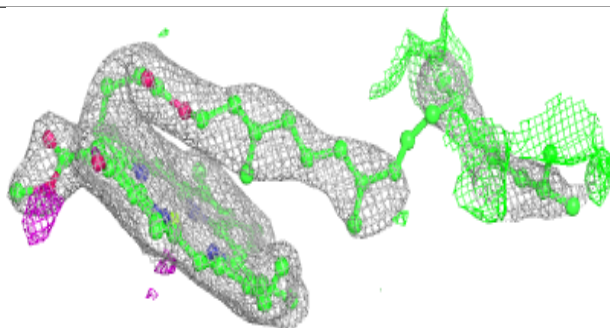
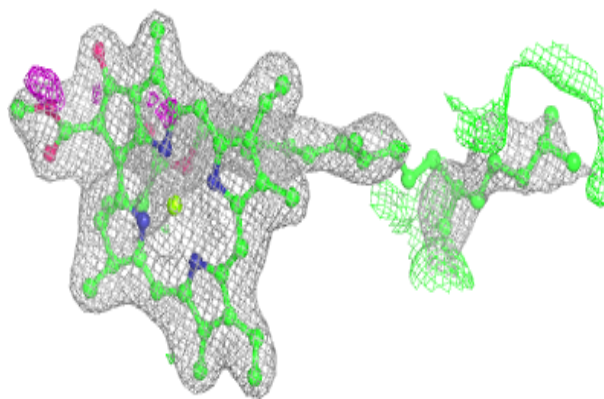
**Electron density around CLA C 508:**

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

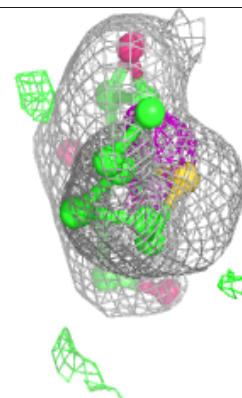
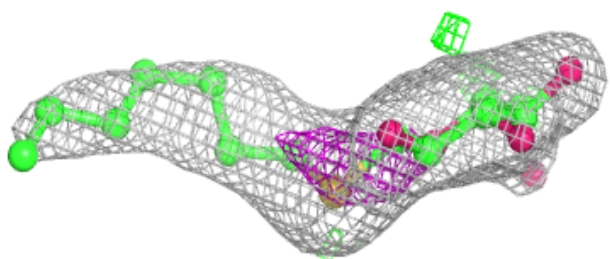
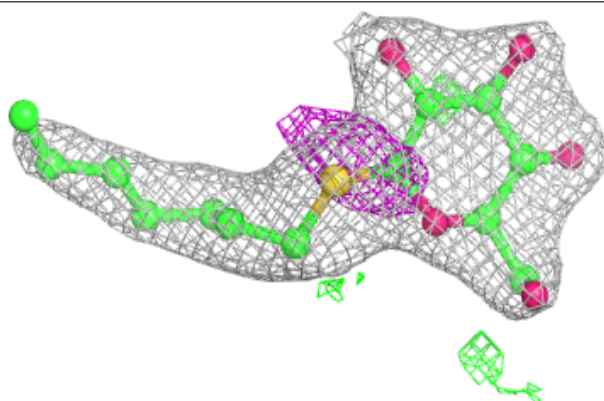


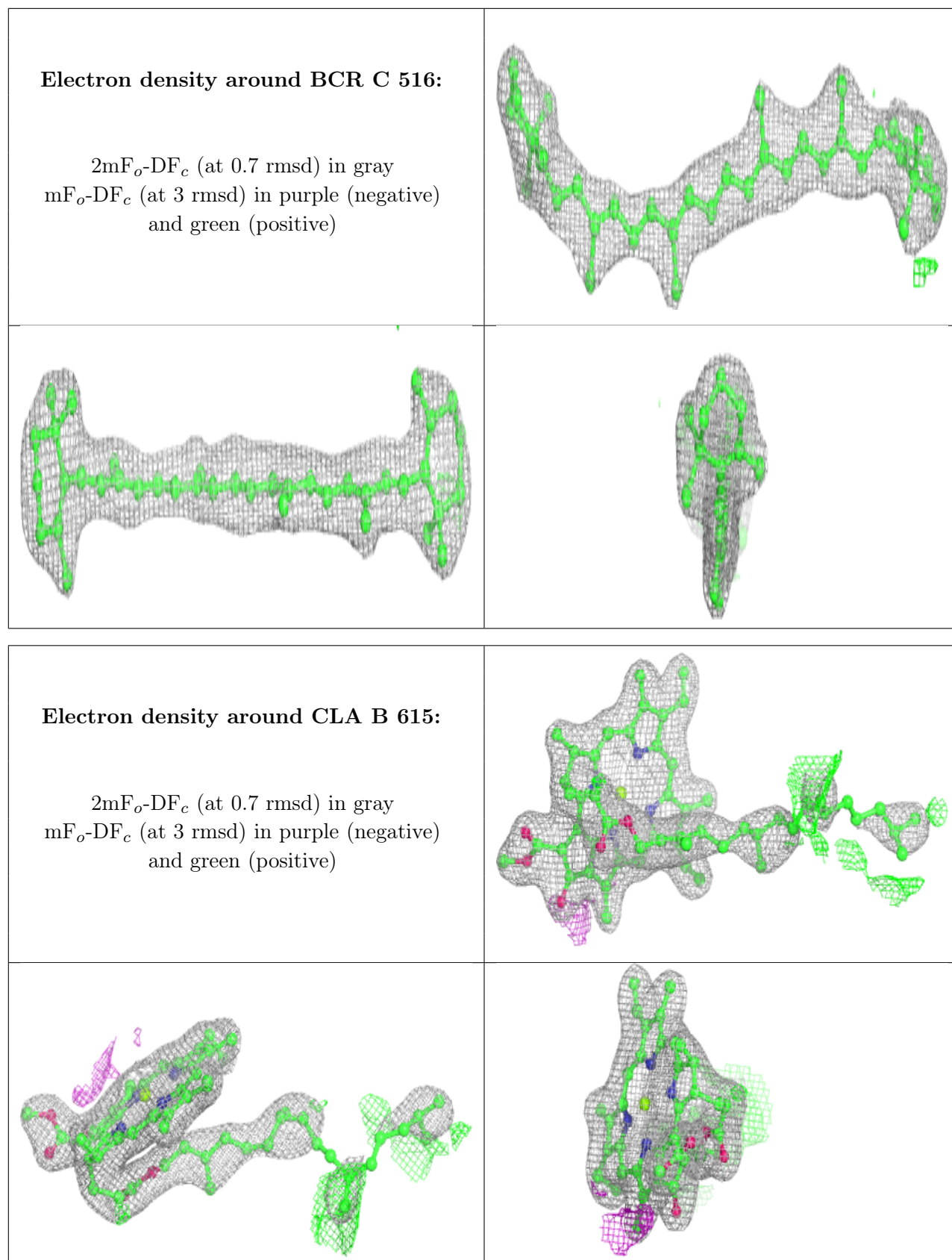
**Electron density around CLA b 619:**

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

**Electron density around HTG b 602:**

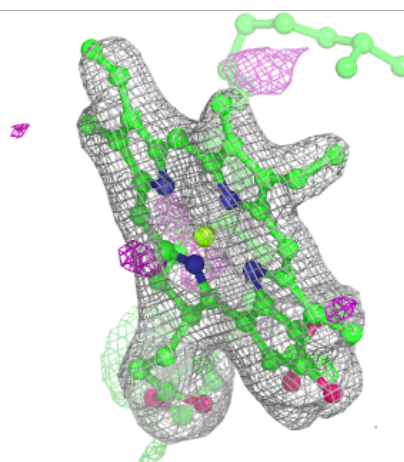
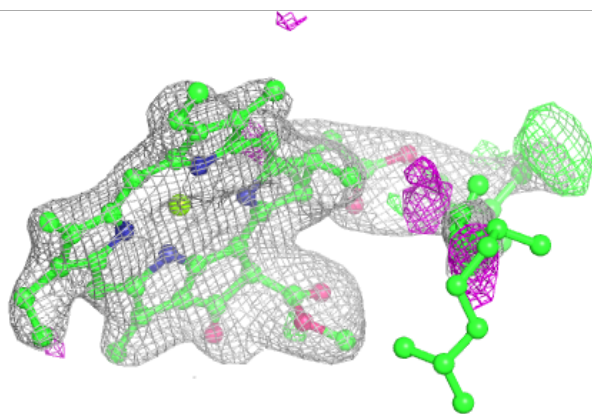
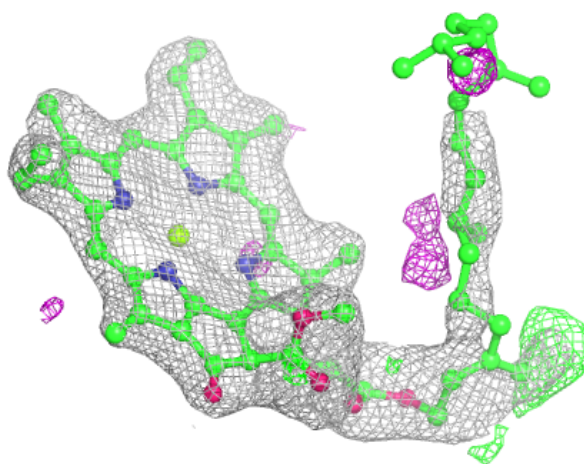
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





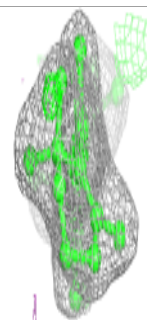
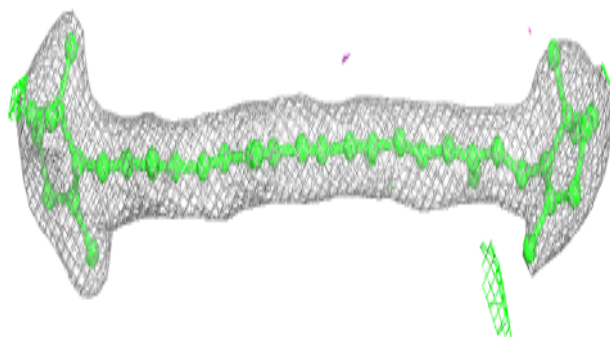
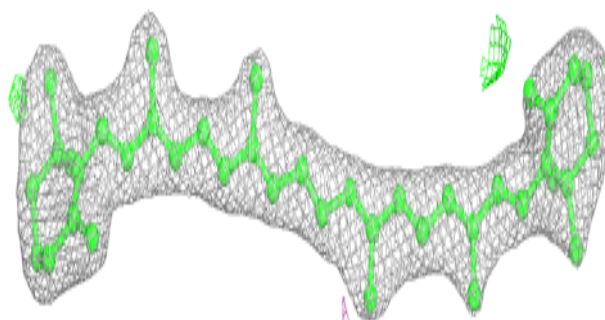
**Electron density around CLA B 617:**

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

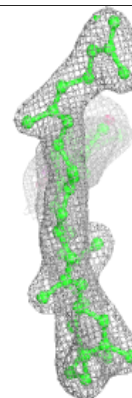
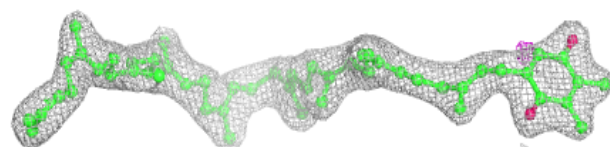
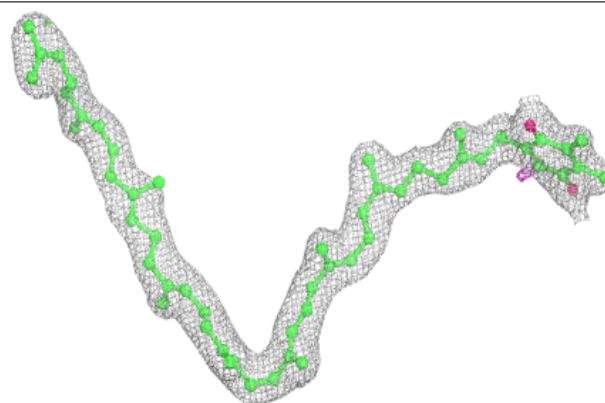


**Electron density around BCR b 623:**

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

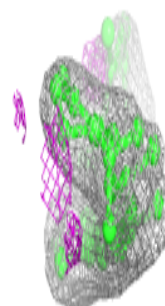
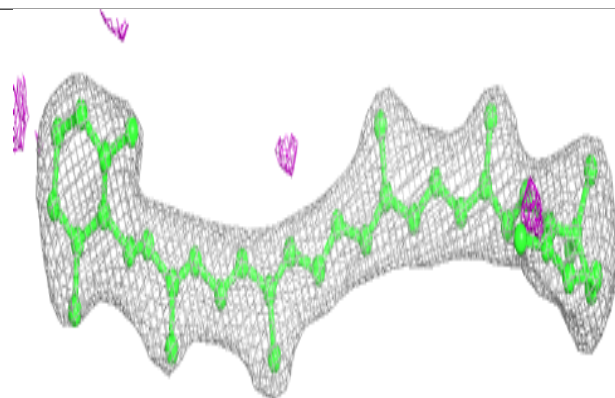
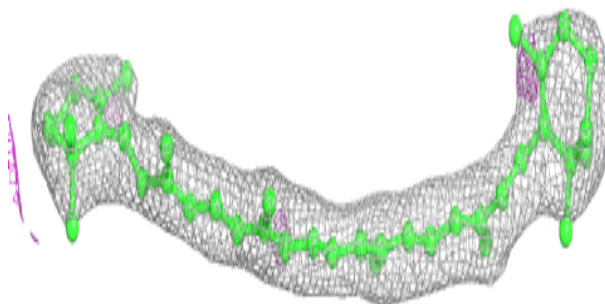
**Electron density around PL9 d 411:**

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



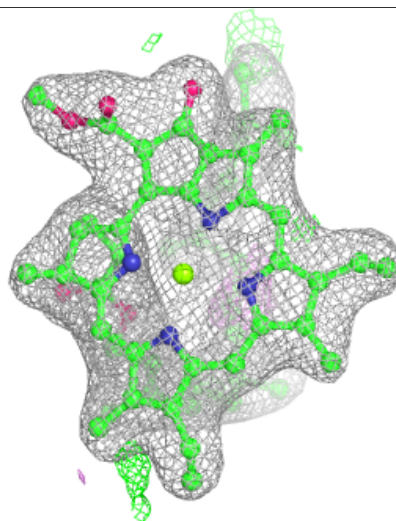
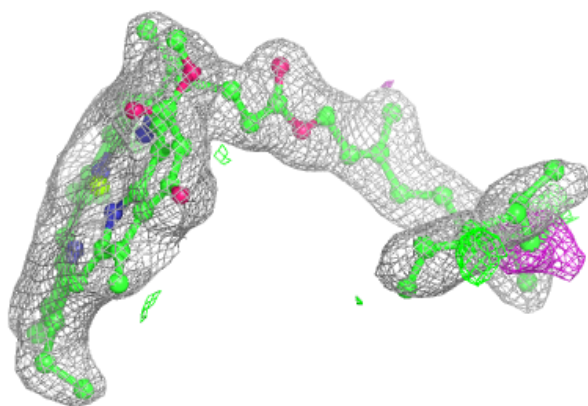
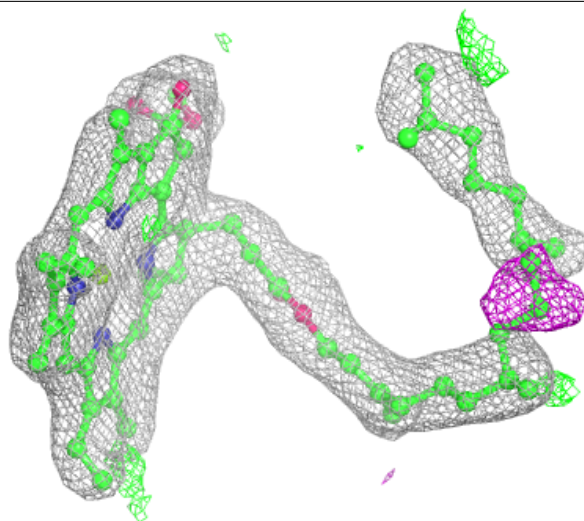
**Electron density around BCR d 410:**

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



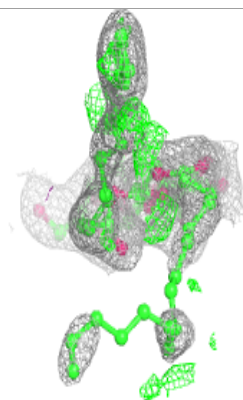
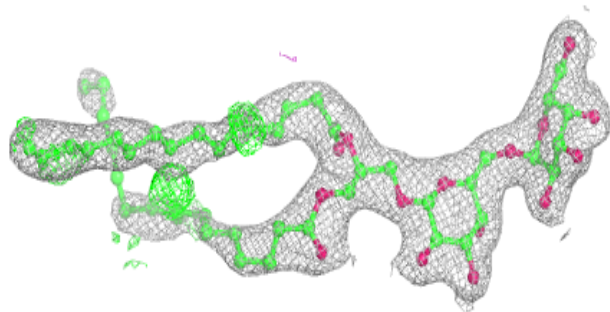
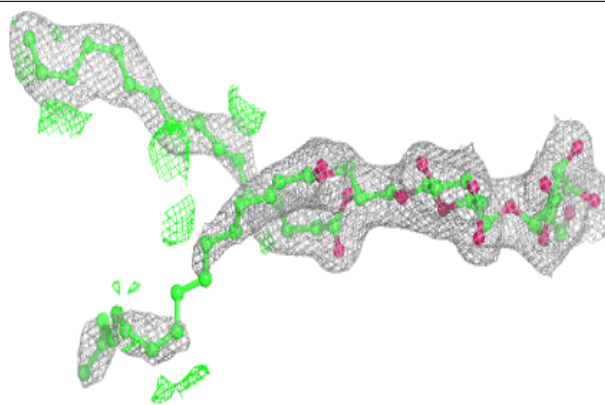
**Electron density around CLA B 607:**

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

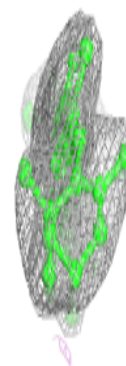
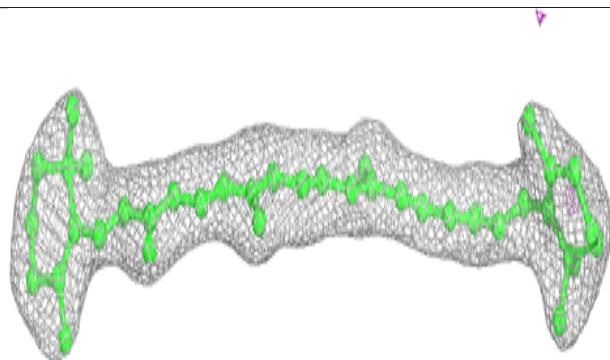
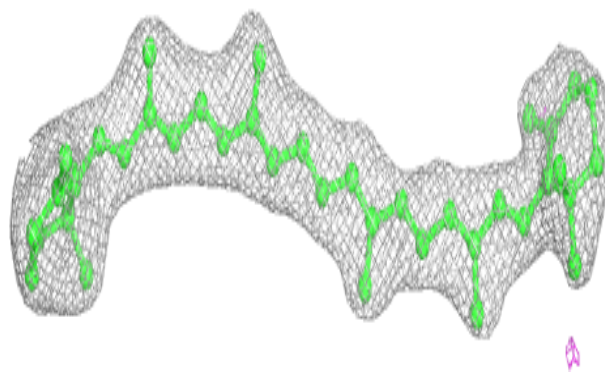


**Electron density around DGD c 518:**

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

**Electron density around BCR y 101:**

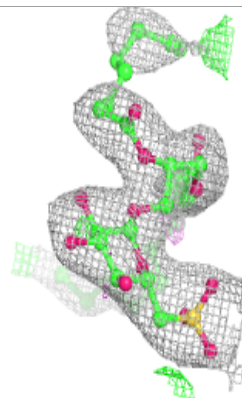
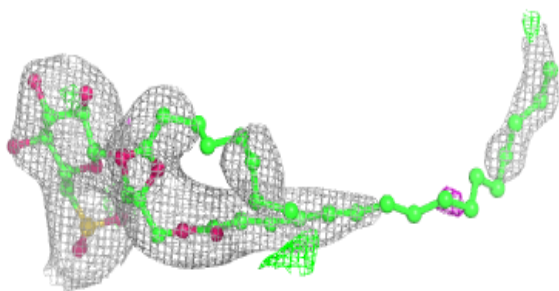
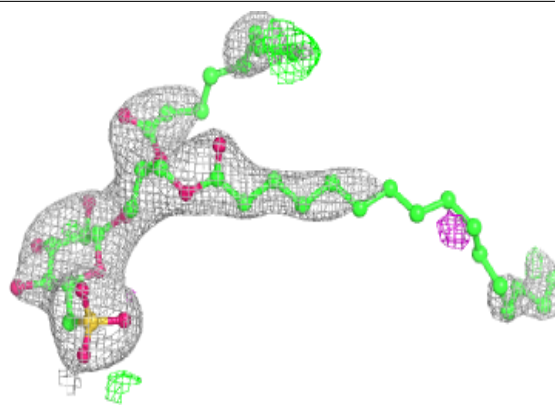
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



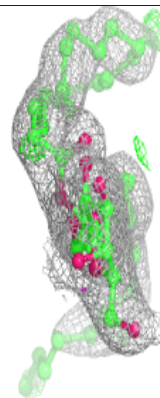
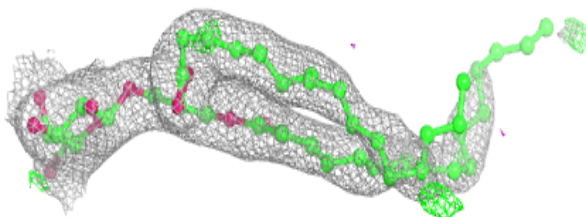
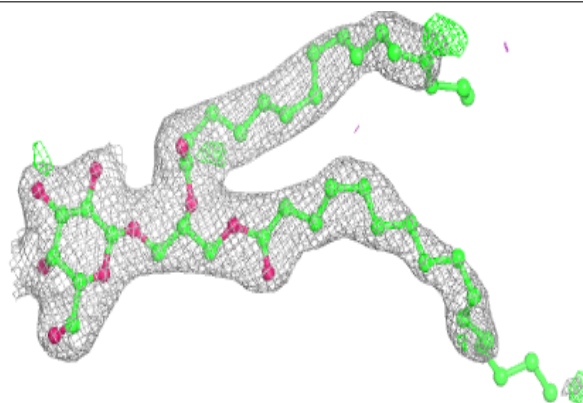


**Electron density around SQD A 412:**

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

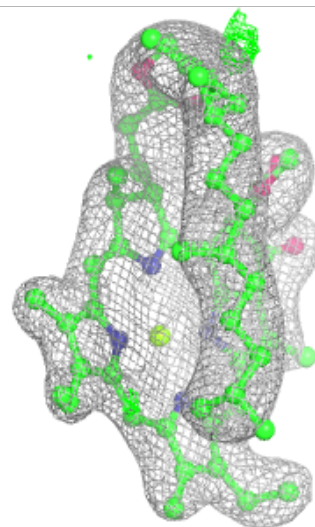
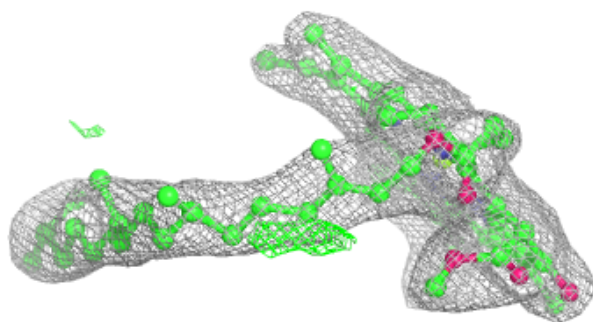
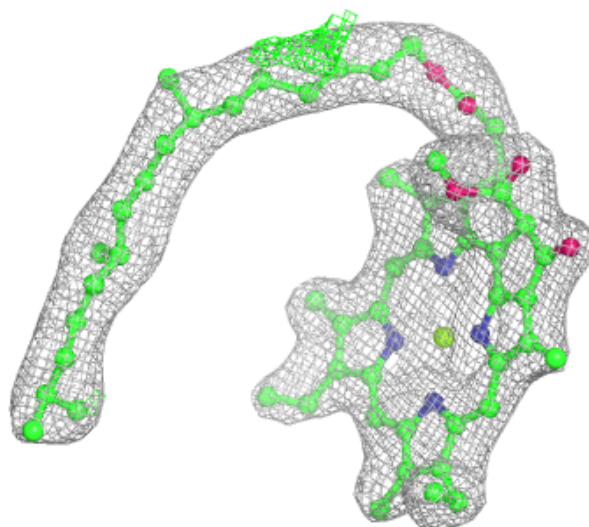
**Electron density around LMG d 414:**

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



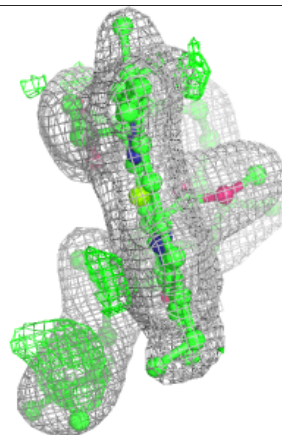
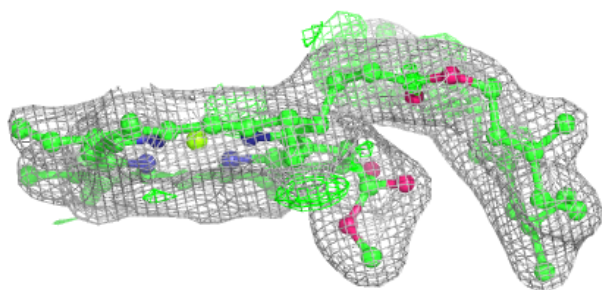
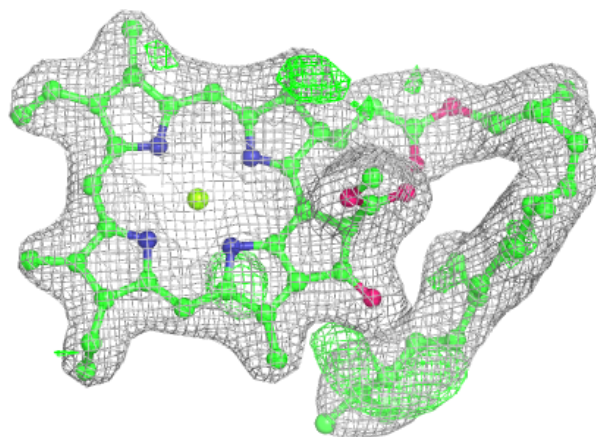
**Electron density around CLA c 510:**

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



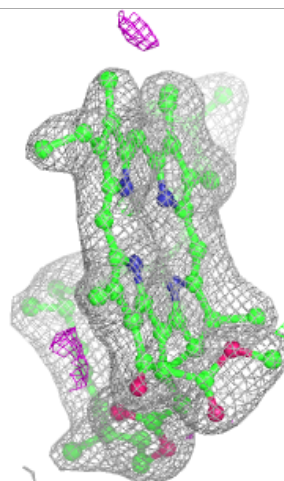
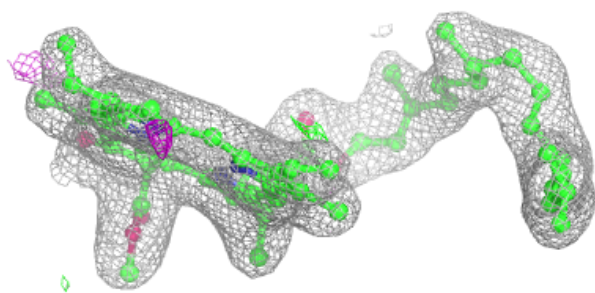
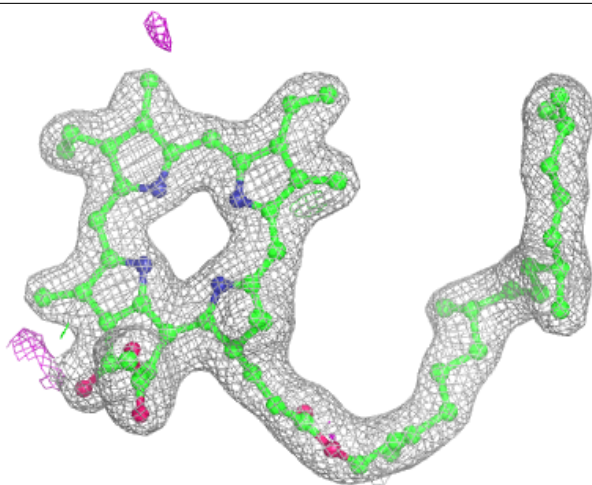
**Electron density around CLA B 611:**

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



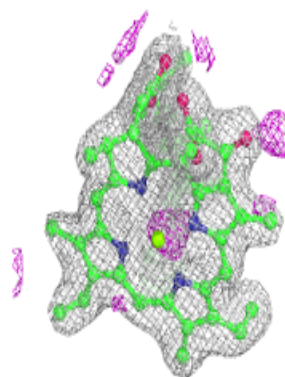
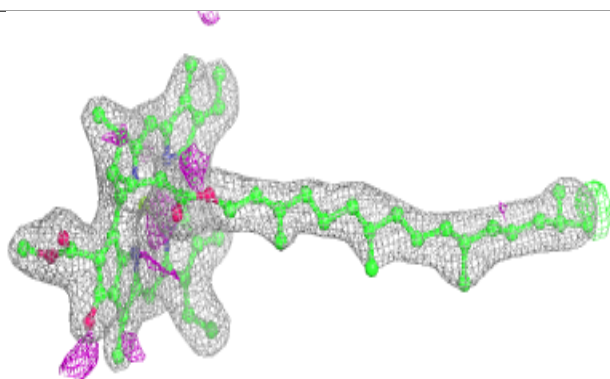
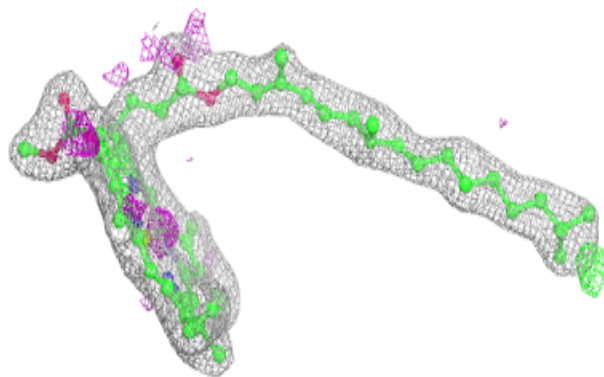
**Electron density around PHO A 409:**

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

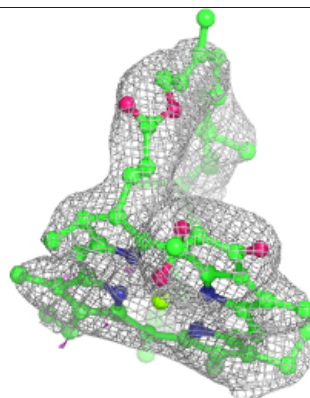
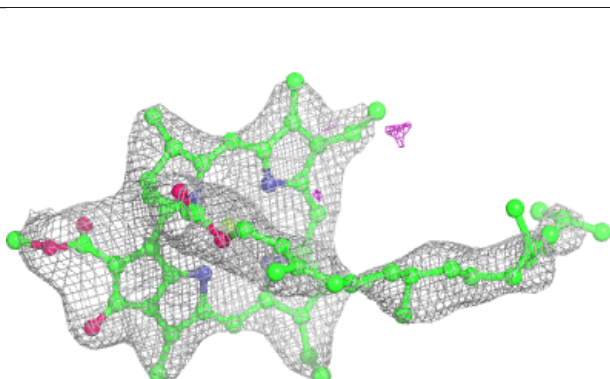
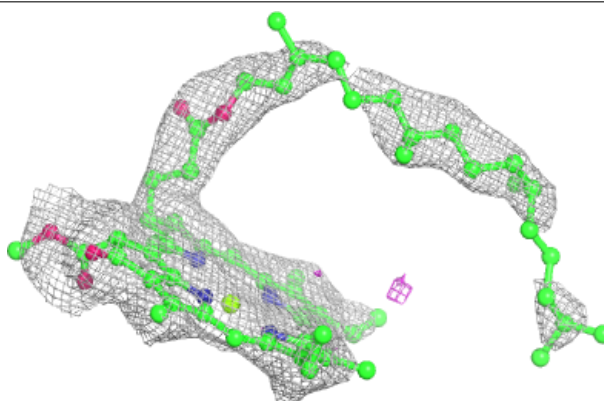


**Electron density around CLA b 612:**

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

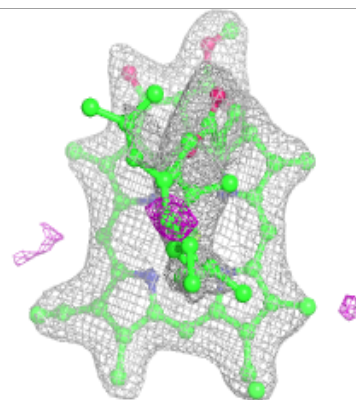
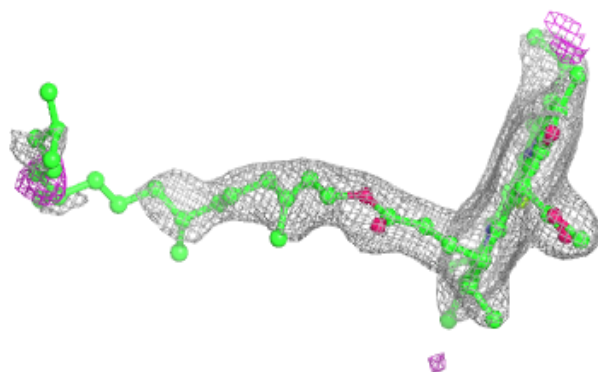
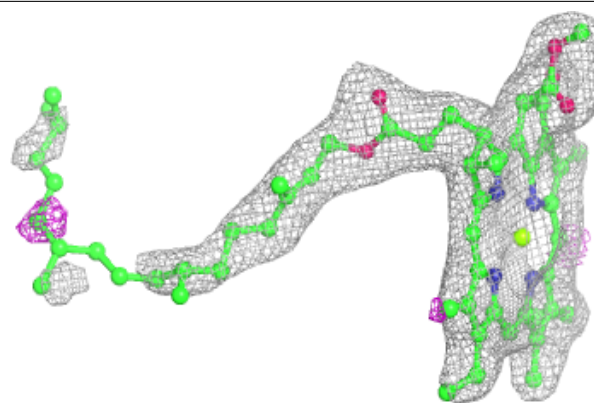
**Electron density around CLA c 516:**

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



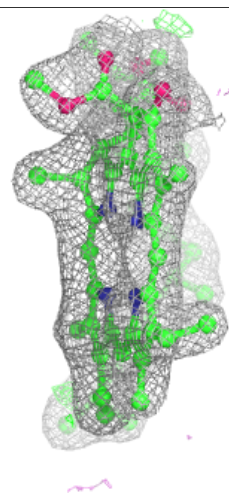
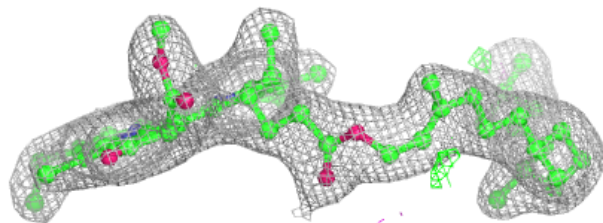
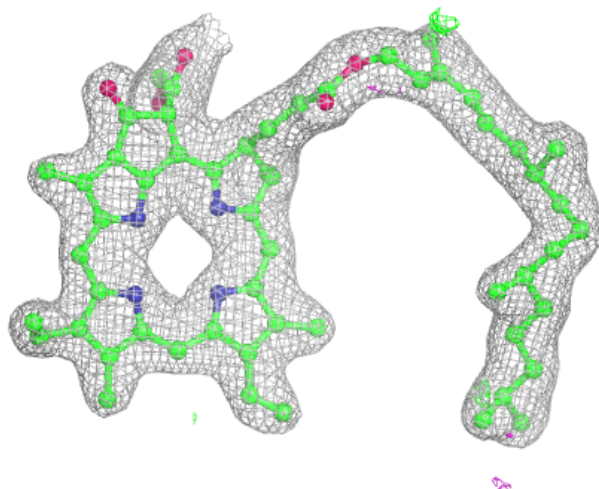
**Electron density around CLA d 409:**

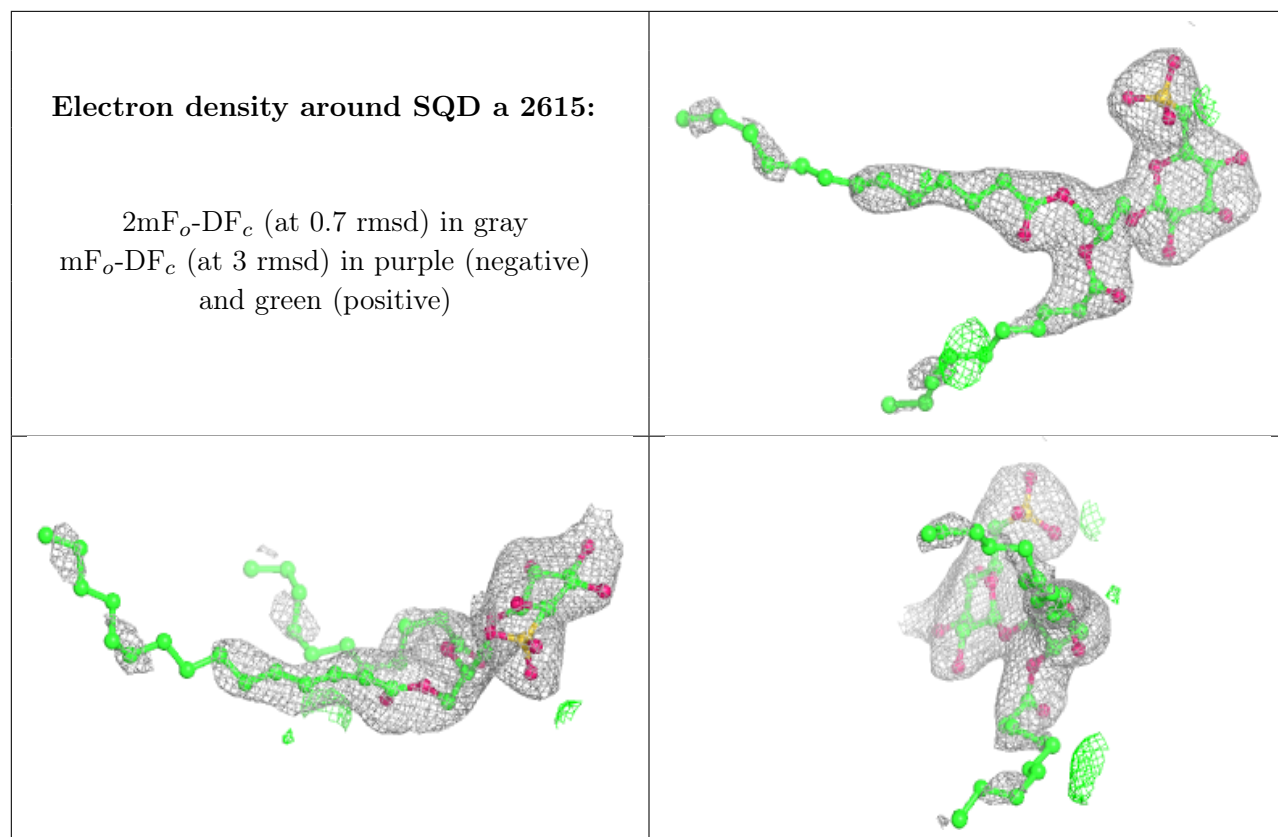
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PHO A 408:**

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

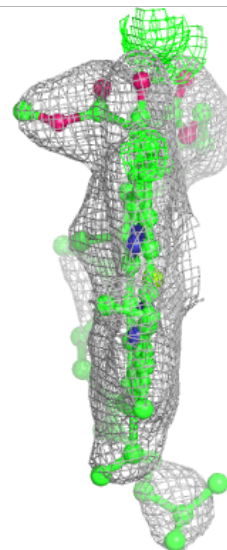
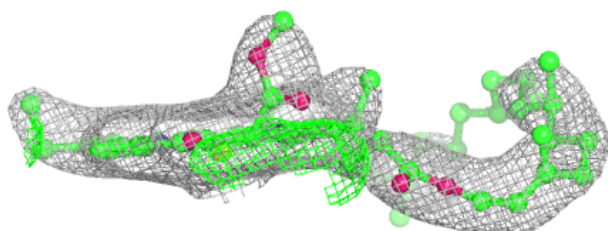
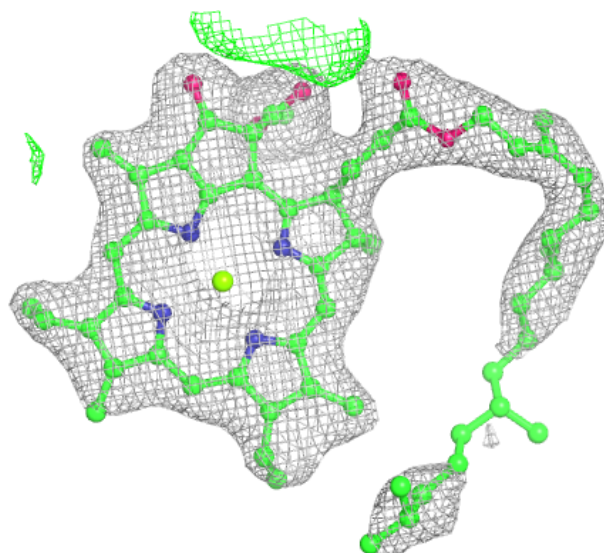


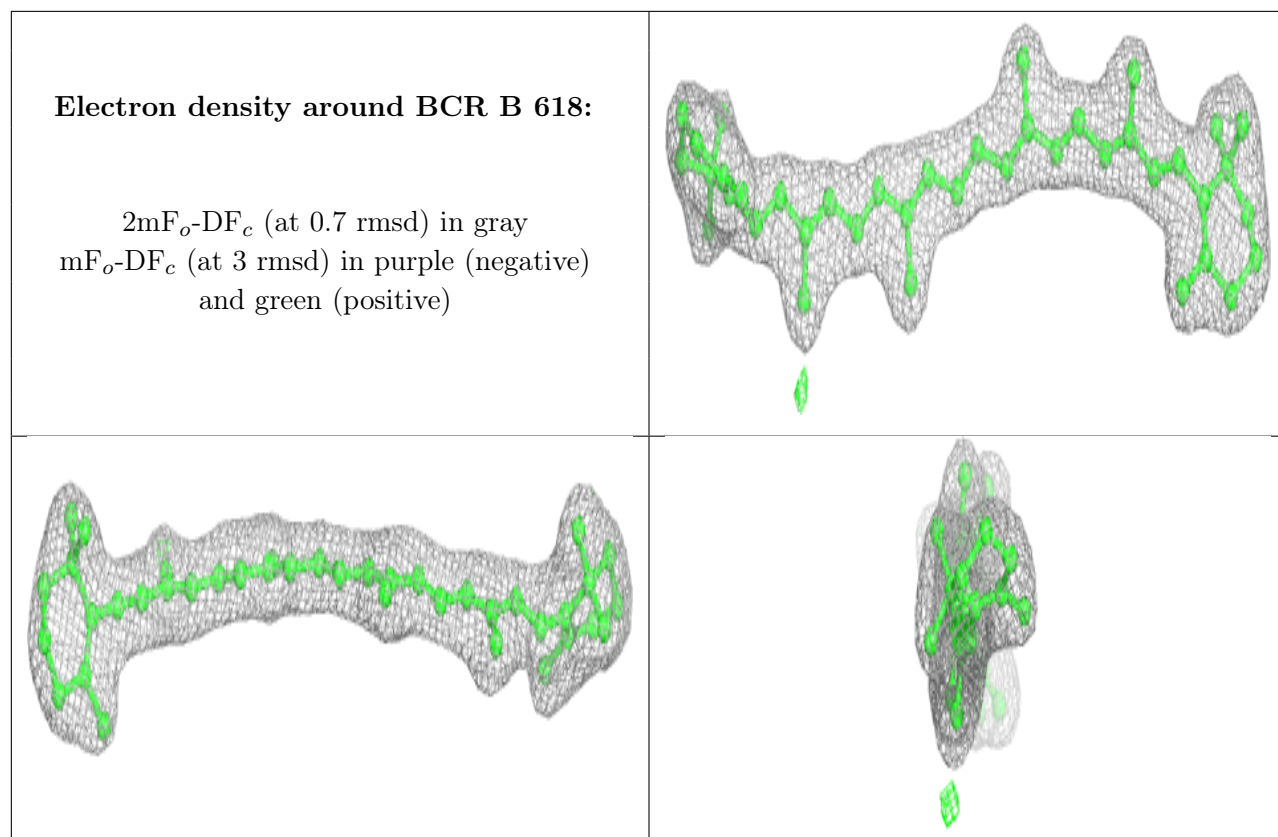




**Electron density around CLA C 513:**

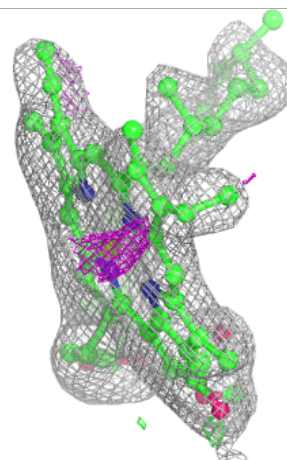
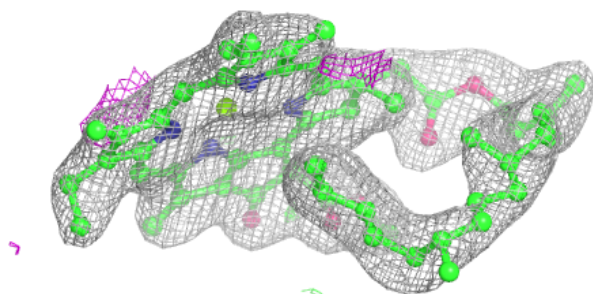
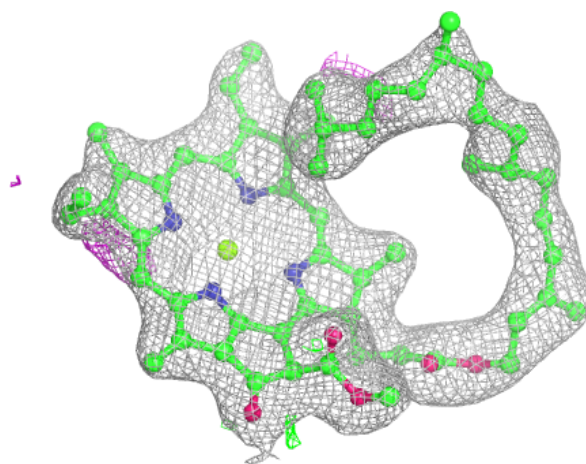
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

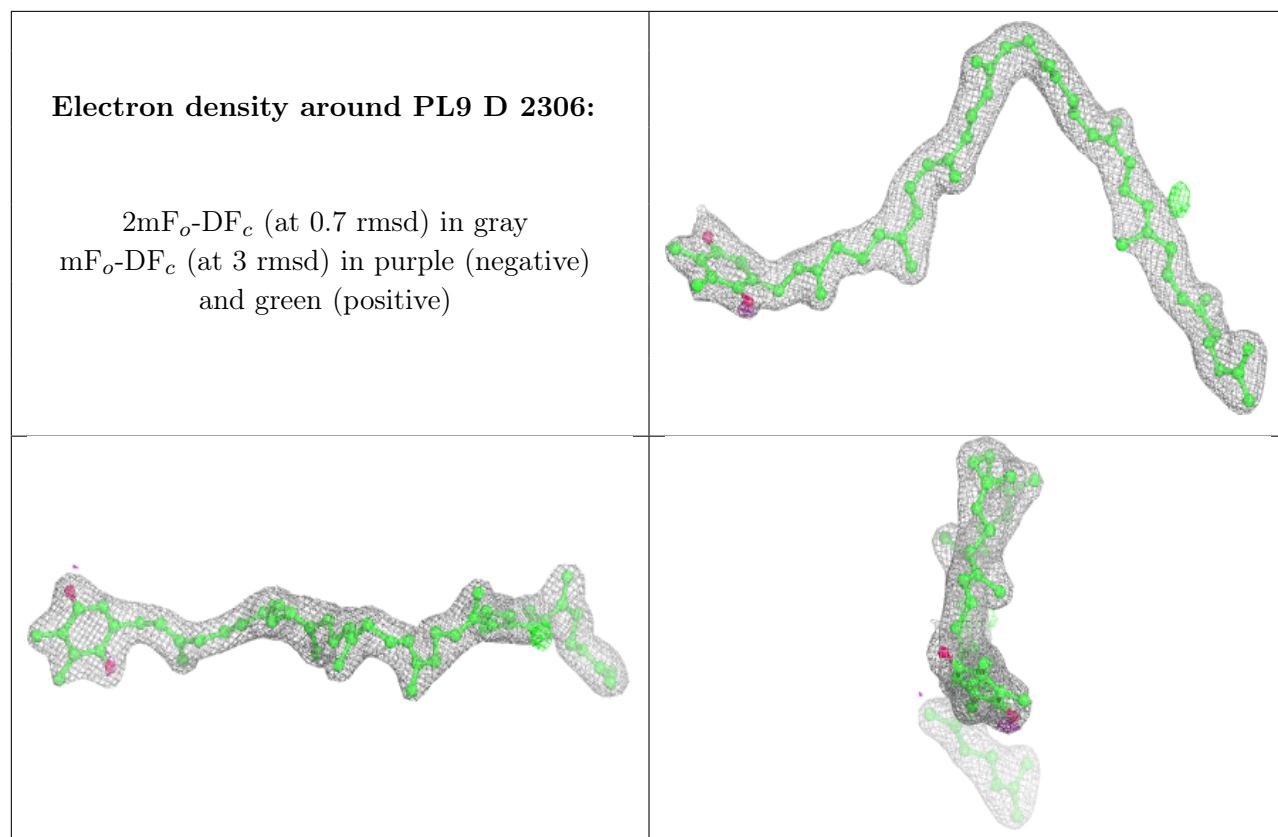




**Electron density around CLA B 616:**

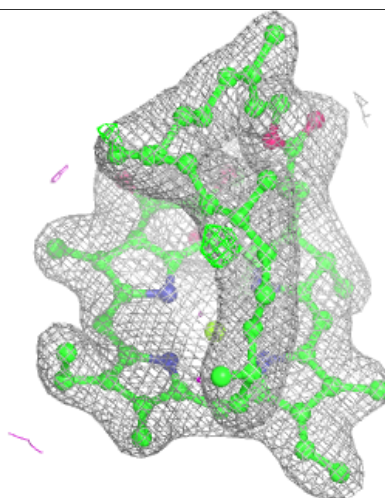
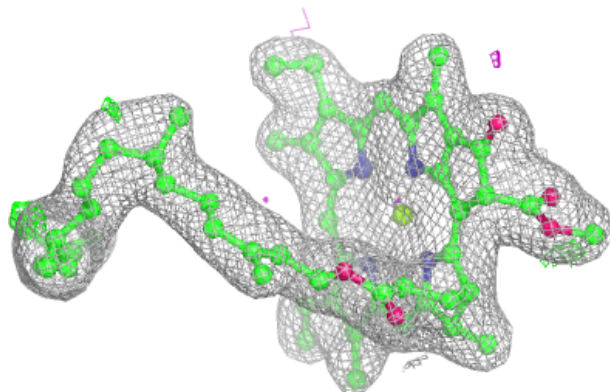
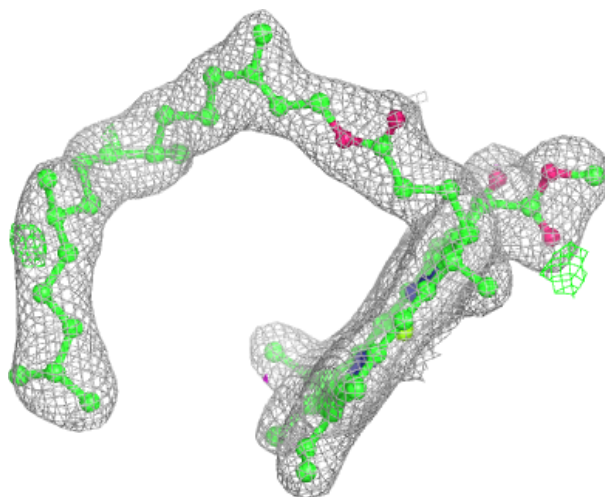
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





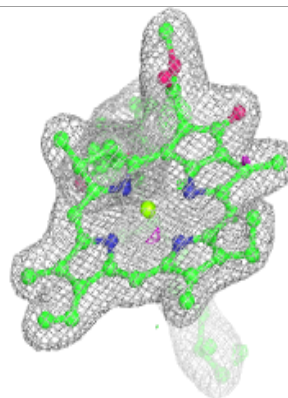
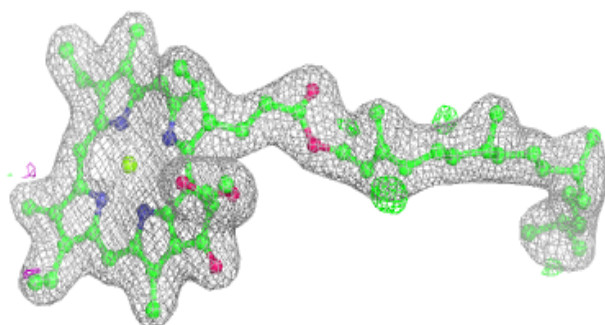
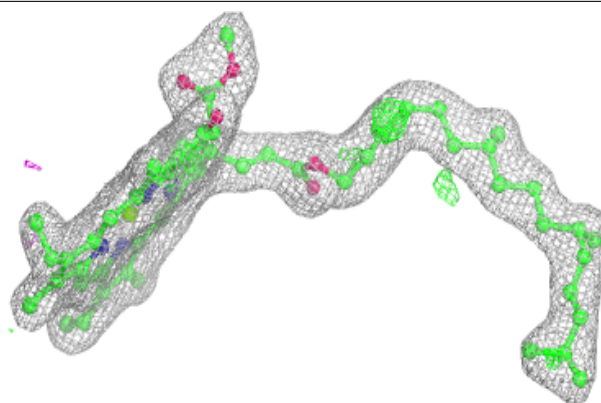
**Electron density around CLA b 616:**

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

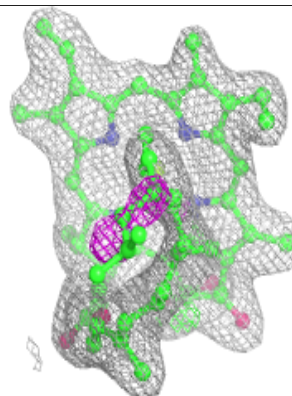
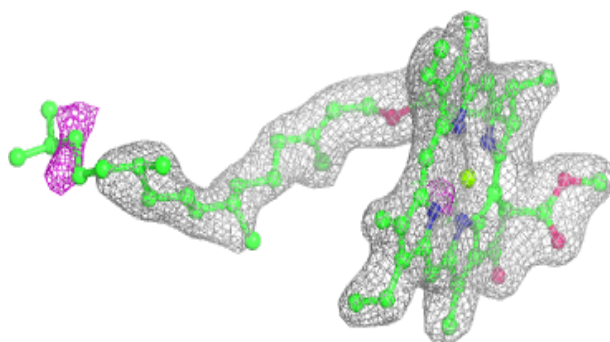
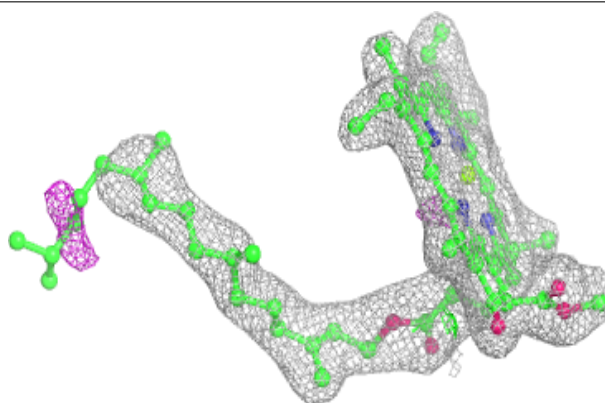


**Electron density around CLA D 2303:**

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

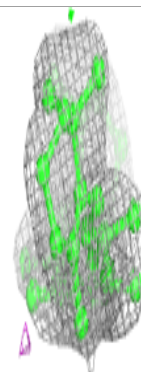
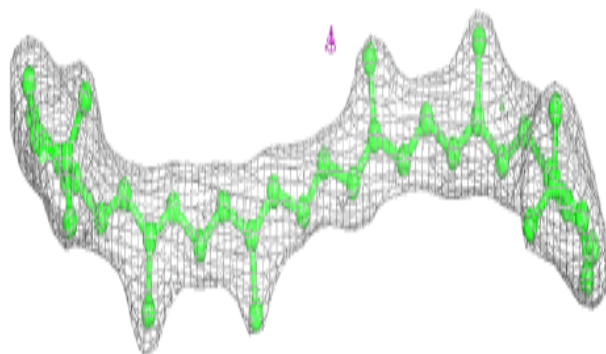
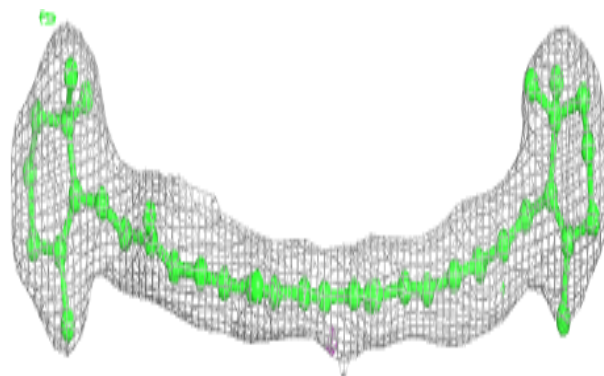
**Electron density around CLA C 509:**

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

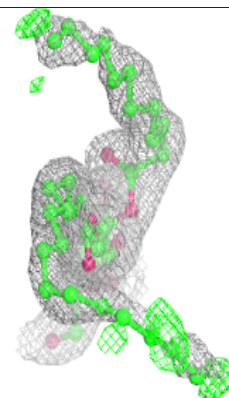
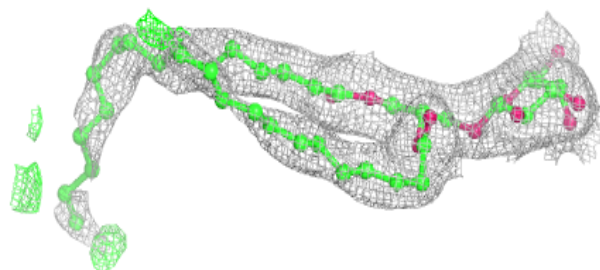
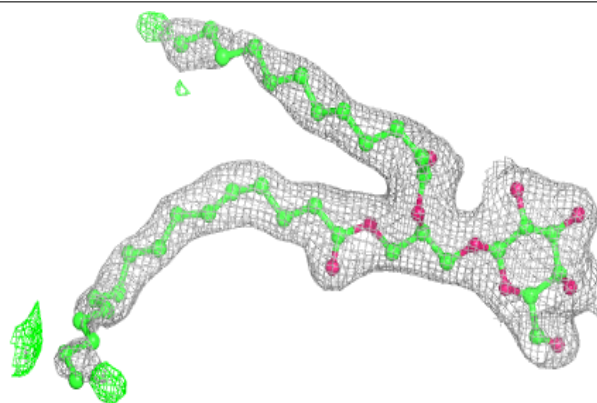


**Electron density around BCR K 101:**

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

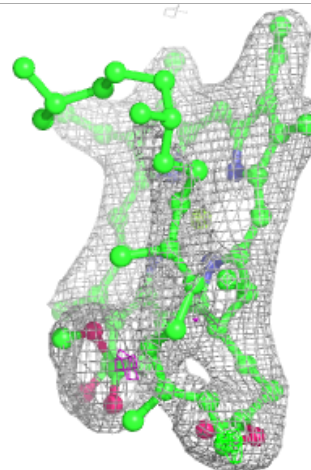
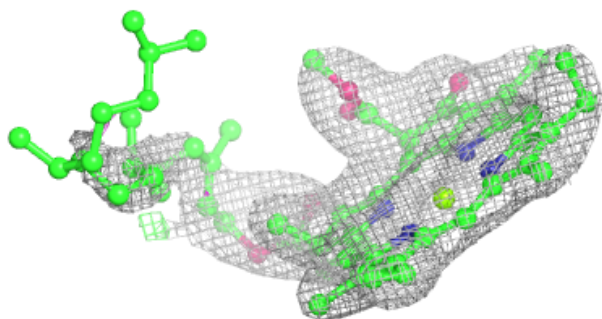
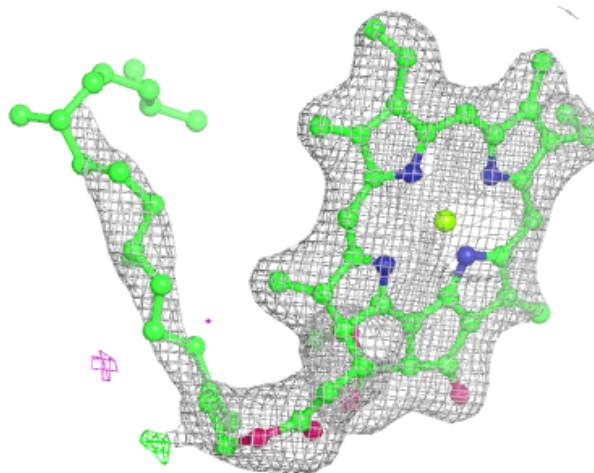
**Electron density around LMG D 2312:**

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

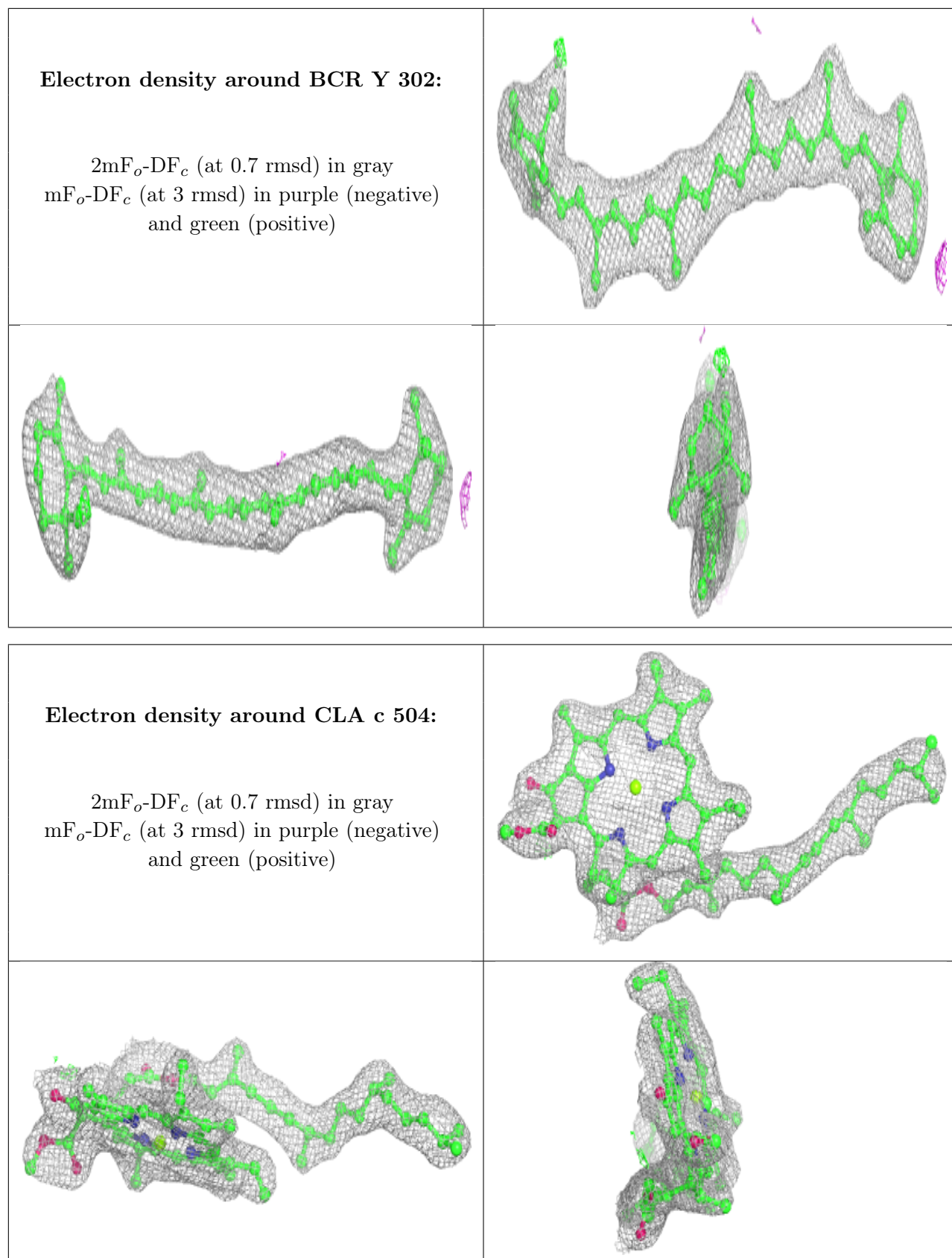


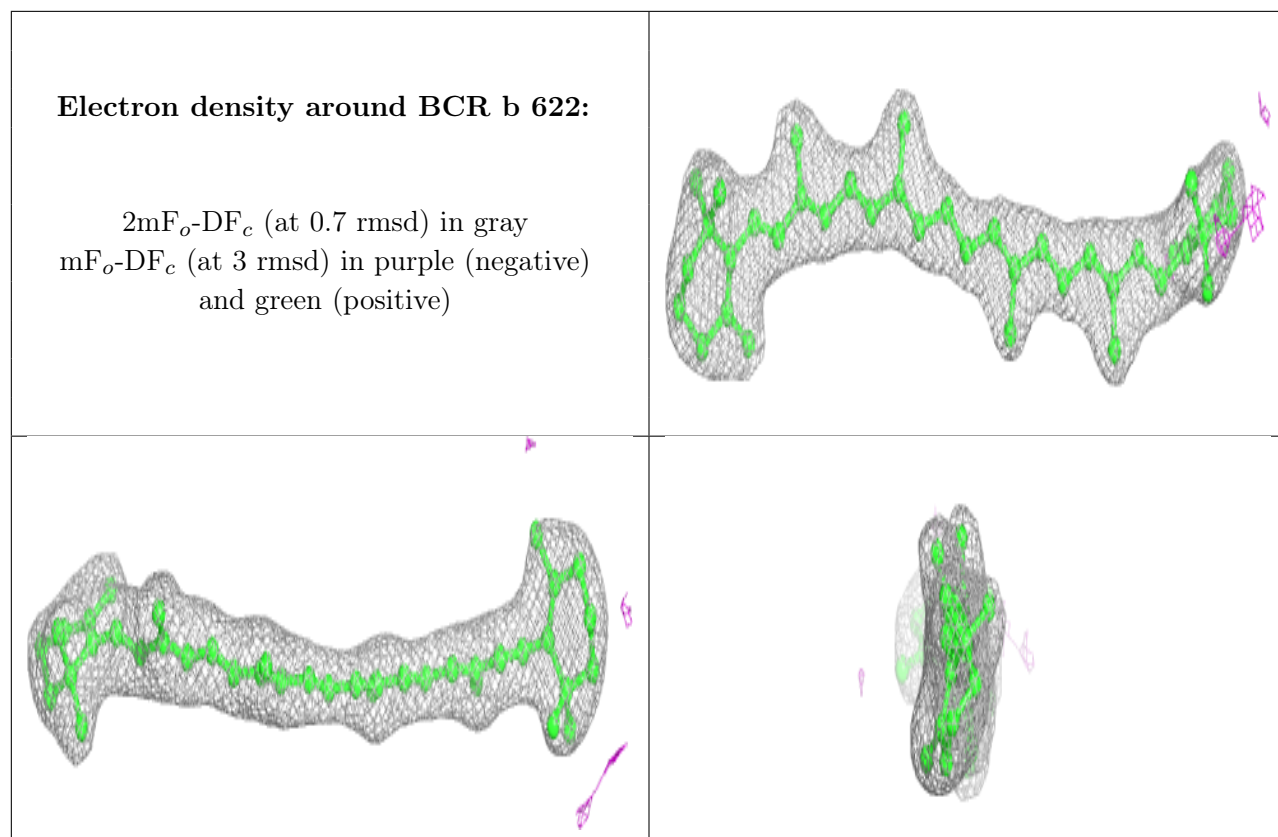
**Electron density around CLA b 621:**

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



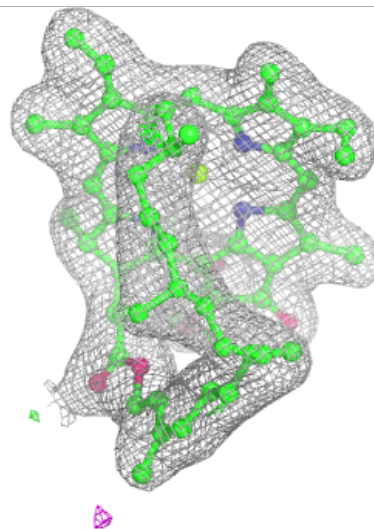
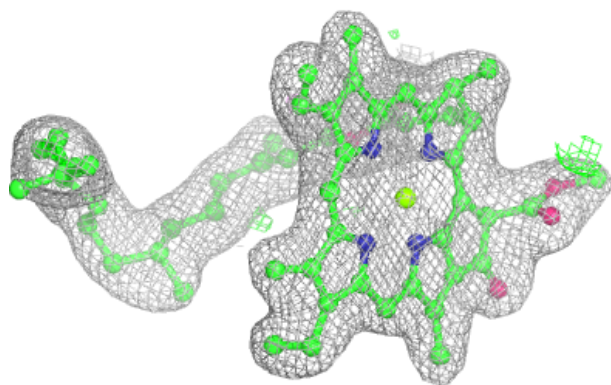
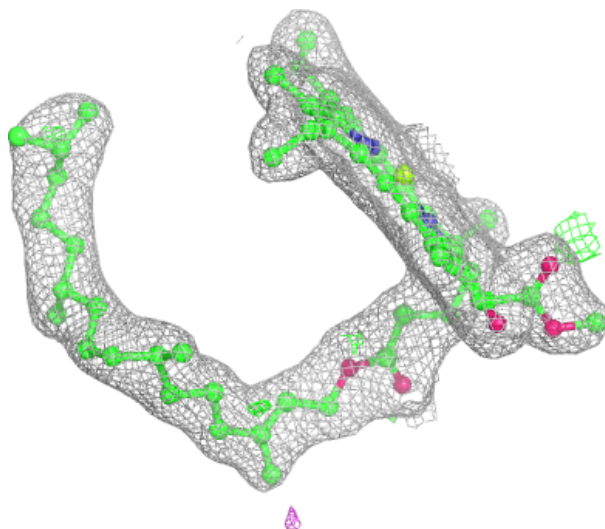






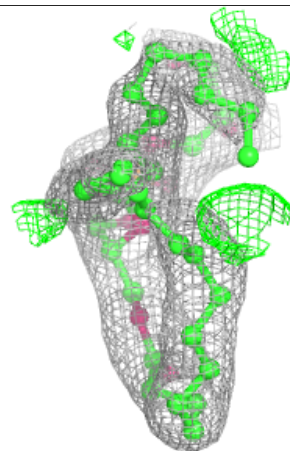
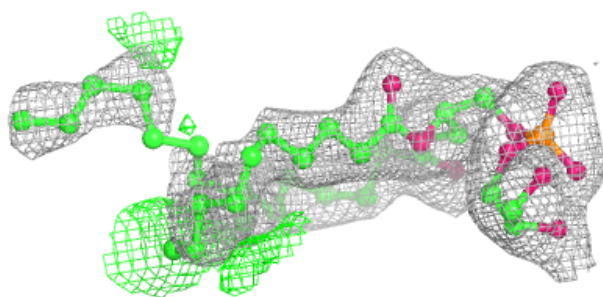
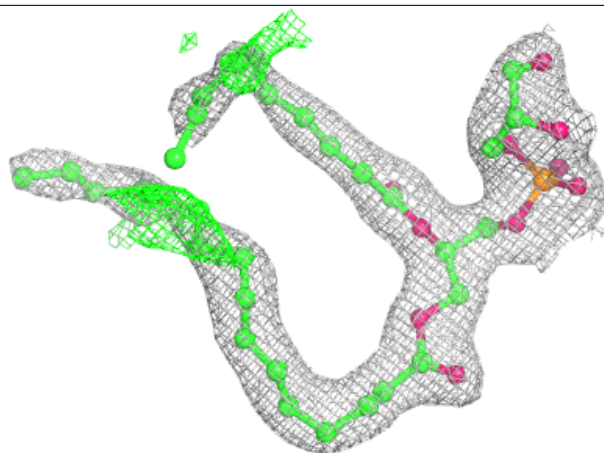
**Electron density around CLA B 612:**

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

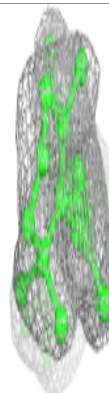
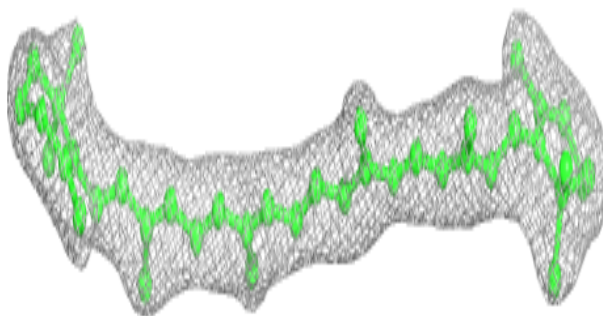
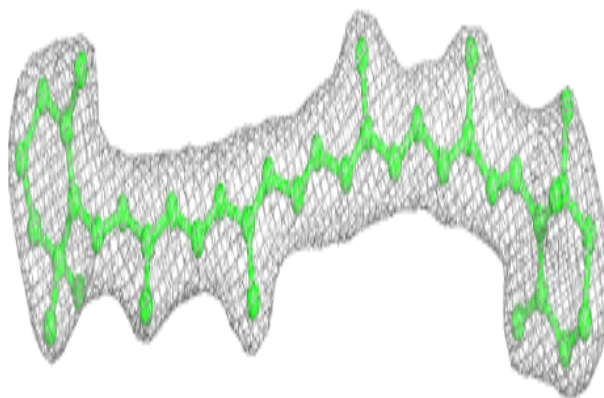


**Electron density around LHG d 403:**

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

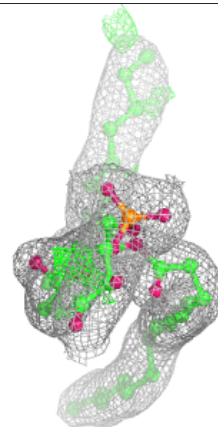
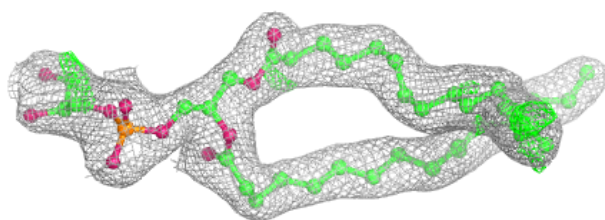
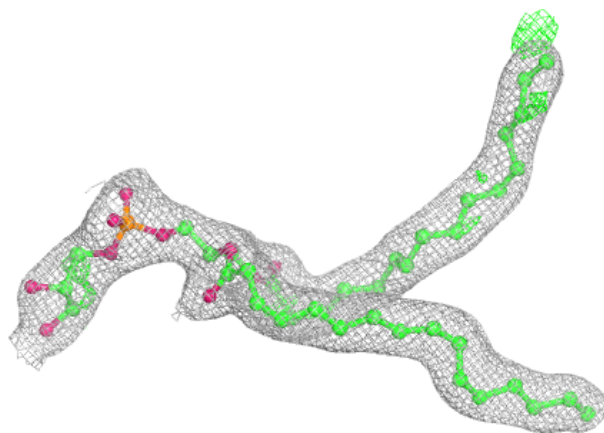
**Electron density around BCR b 624:**

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

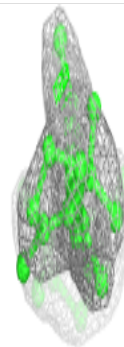
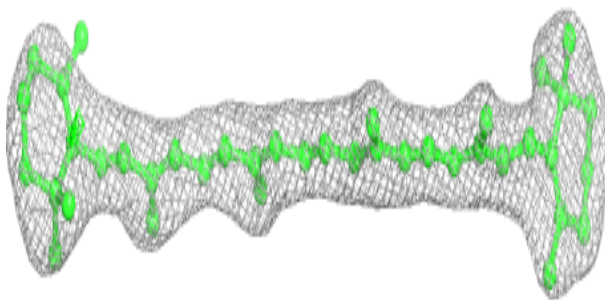
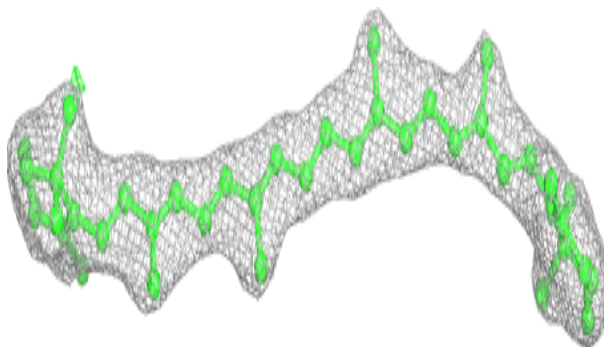


**Electron density around LHG d 413:**

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

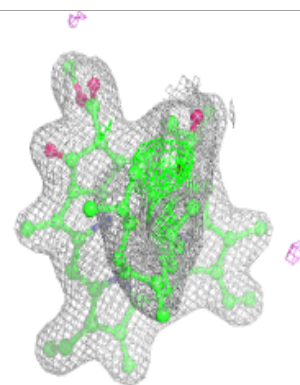
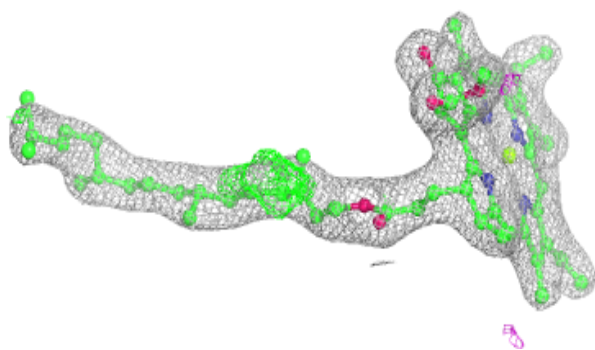
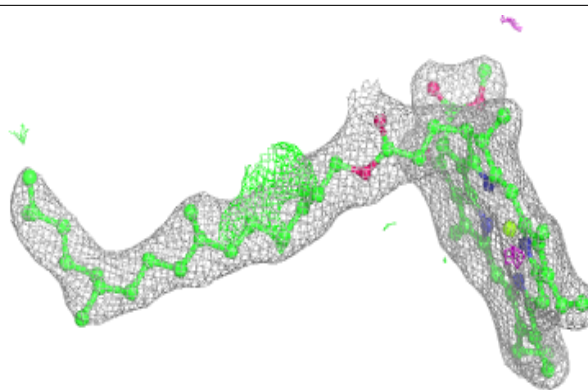
**Electron density around BCR c 517:**

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

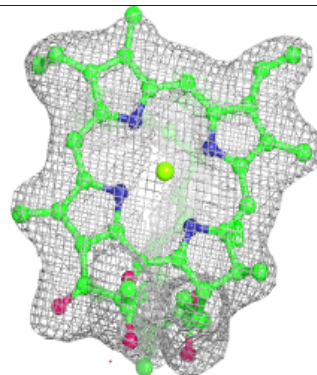
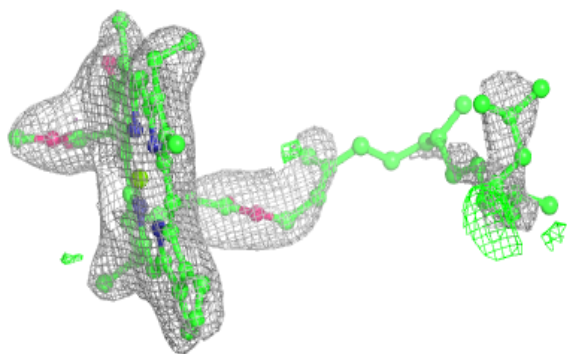
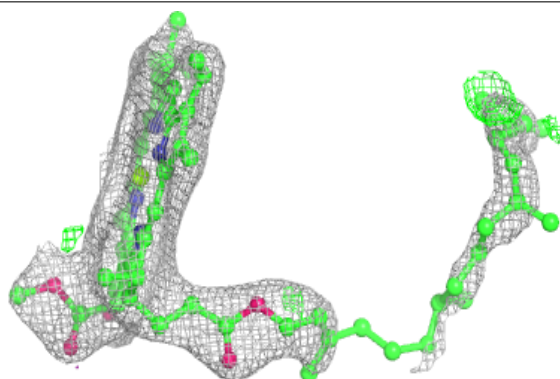


**Electron density around CLA b 609:**

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

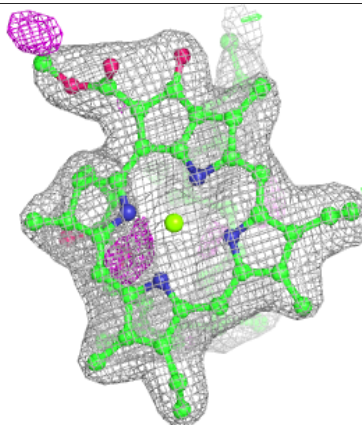
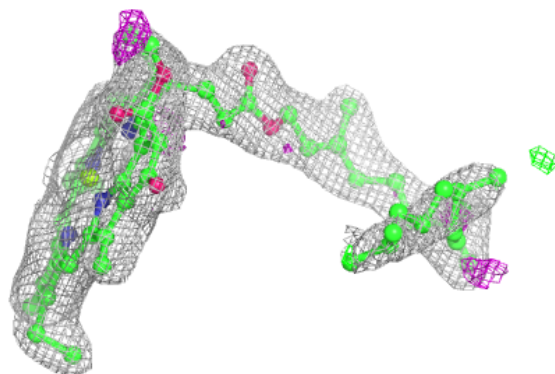
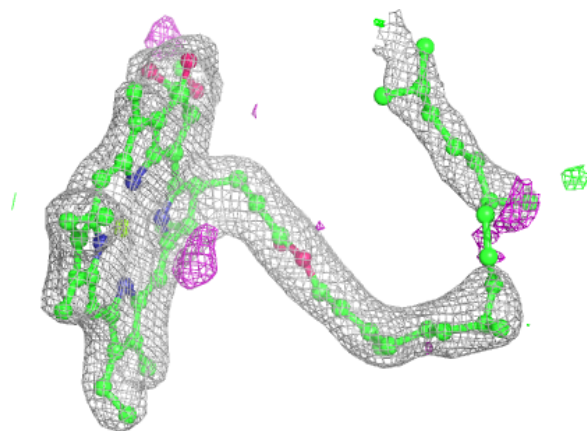
**Electron density around CLA c 509:**

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

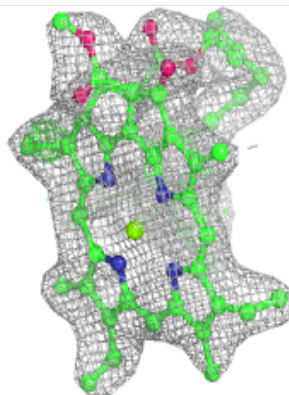
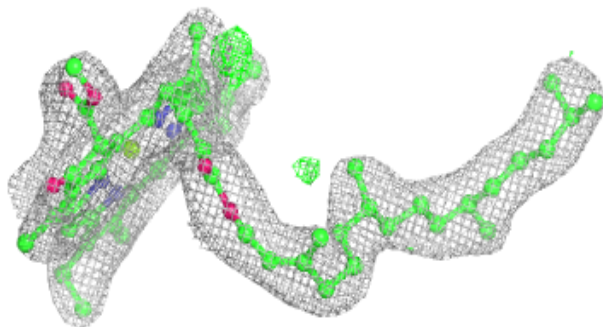
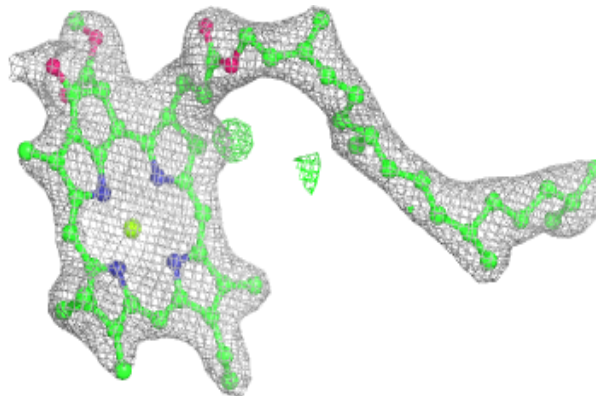


**Electron density around CLA b 611:**

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

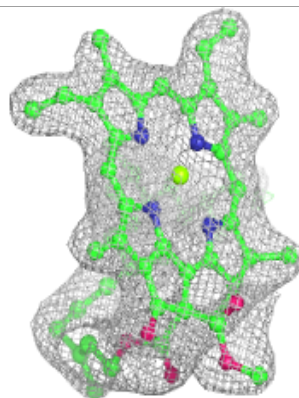
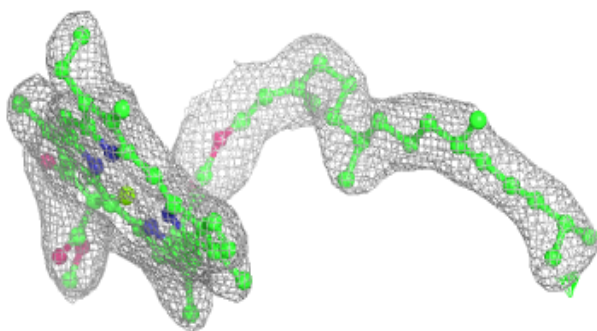
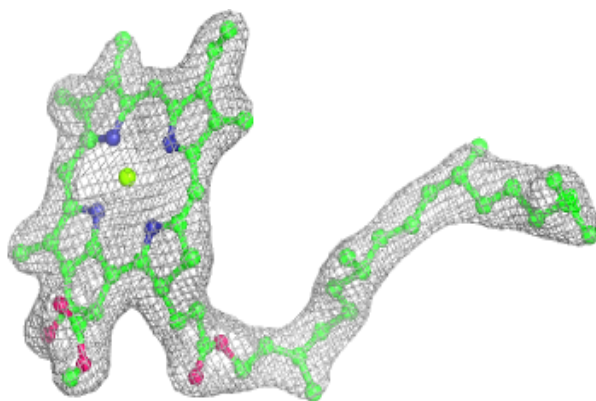
**Electron density around CLA c 514:**

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

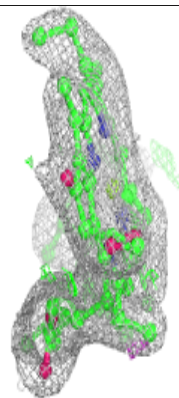
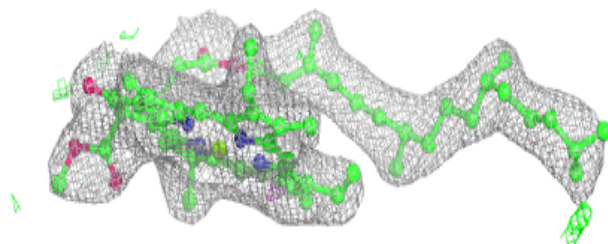
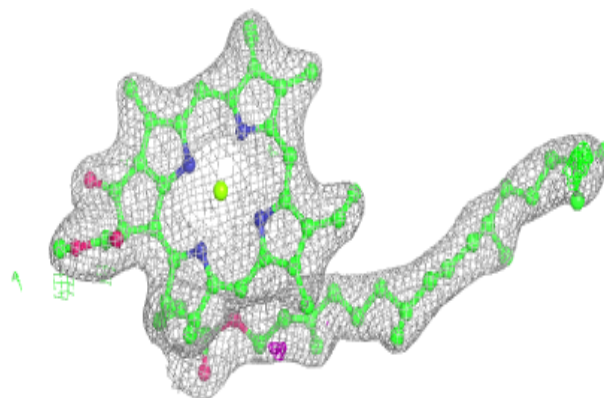


**Electron density around CLA C 512:**

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

**Electron density around CLA C 502:**

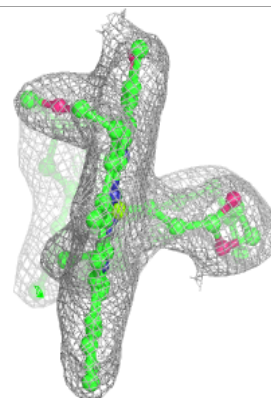
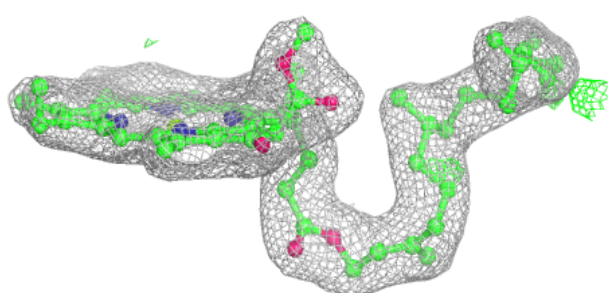
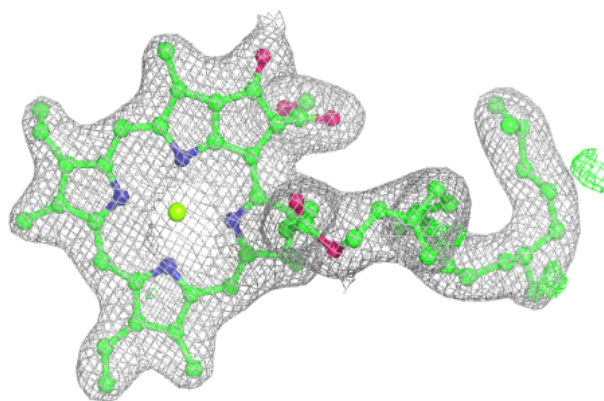
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



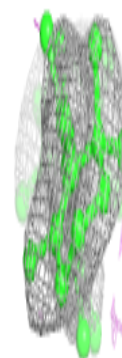
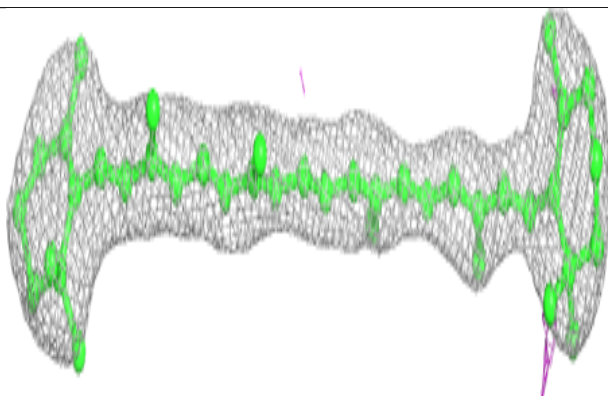
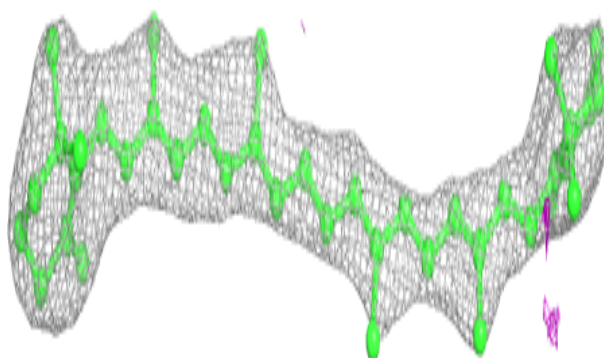


**Electron density around CLA b 617:**

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

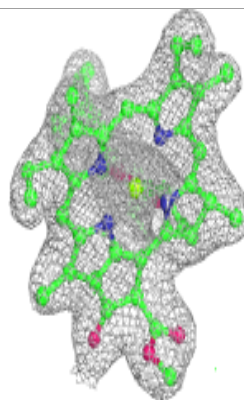
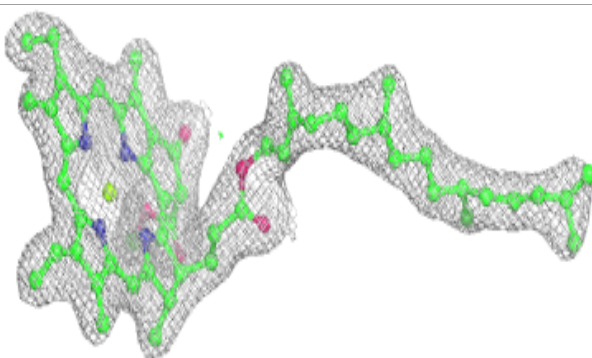
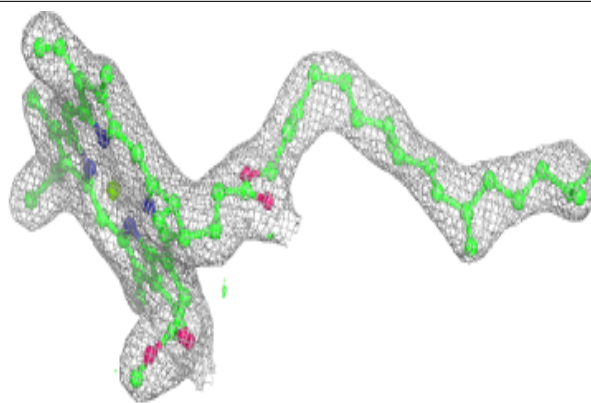
**Electron density around BCR z 101:**

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

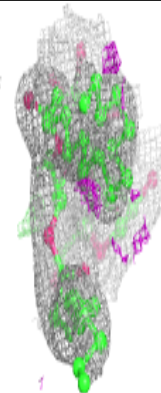
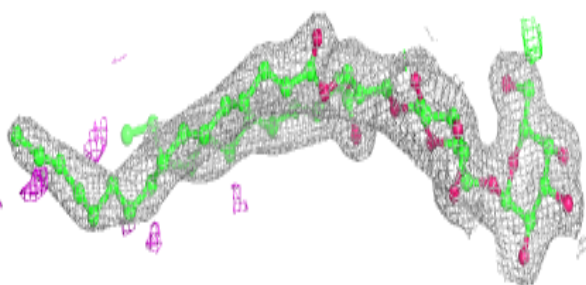
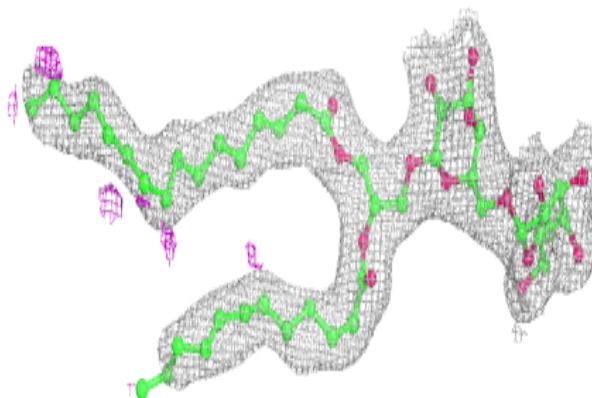


**Electron density around CLA C 503:**

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

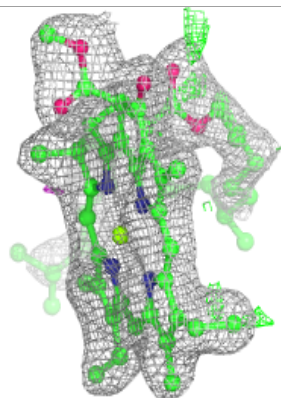
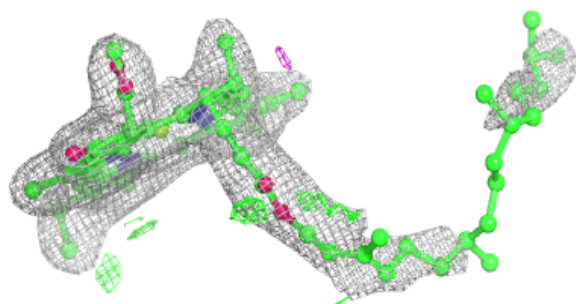
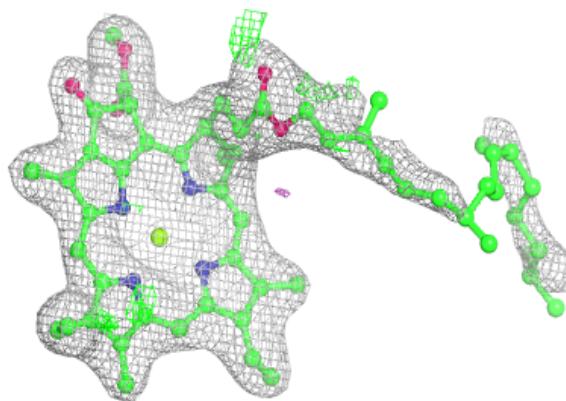
**Electron density around DGD C 519:**

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

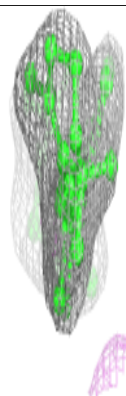
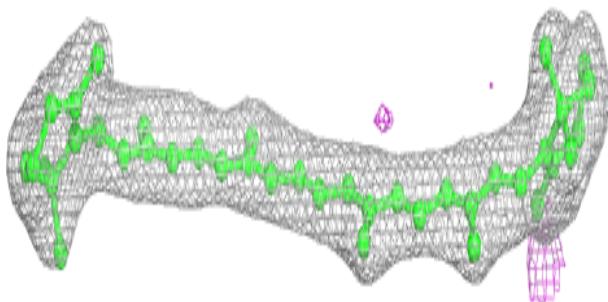
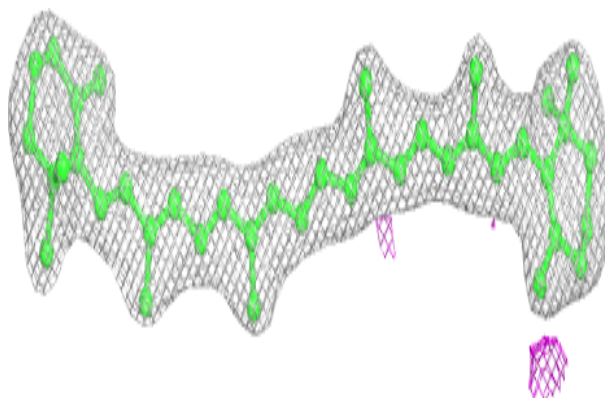


**Electron density around CLA A 410:**

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

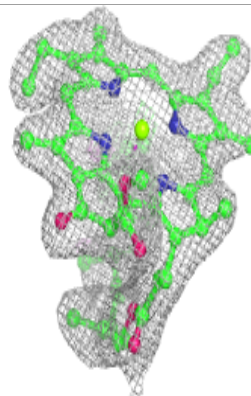
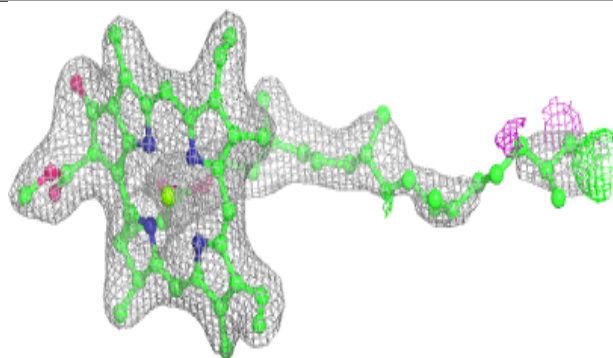
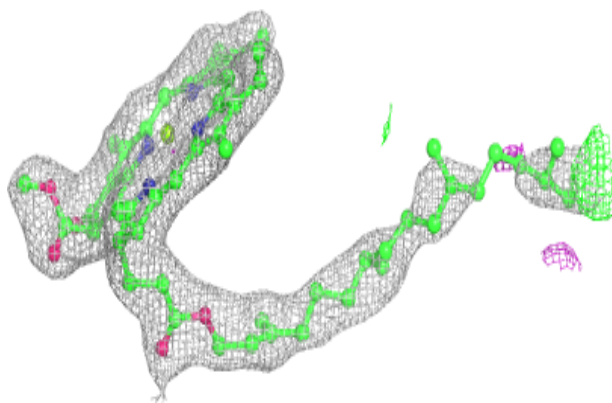
**Electron density around BCR B 620:**

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

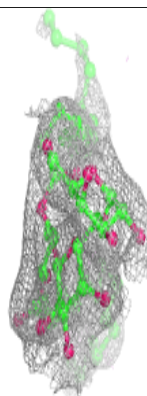
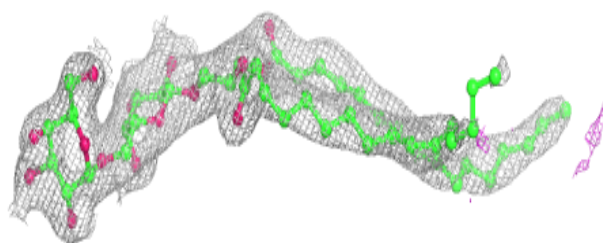
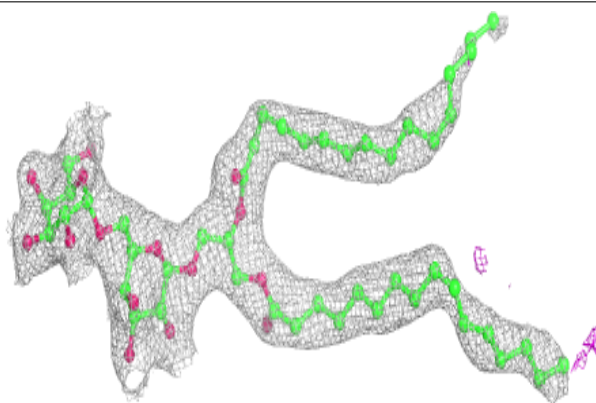


**Electron density around CLA C 505:**

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

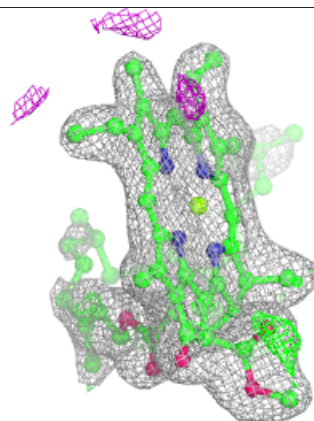
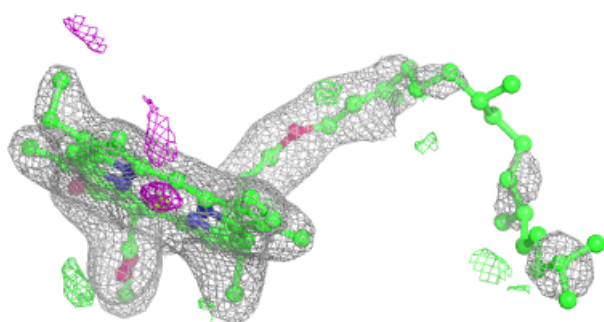
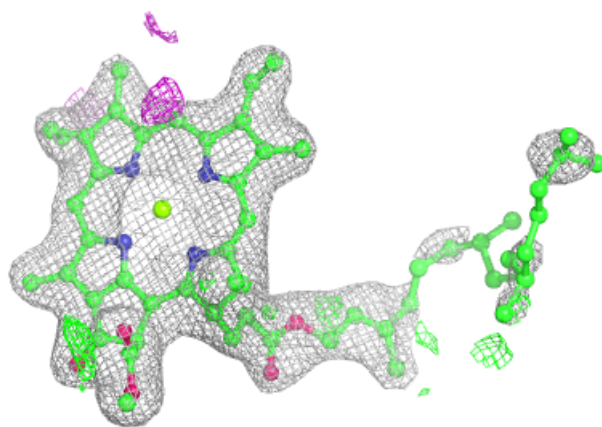
**Electron density around DGD c 520:**

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

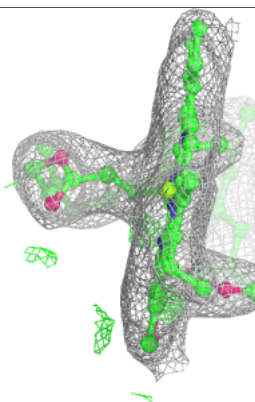
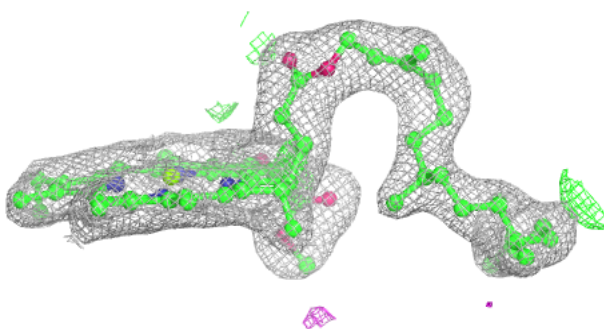
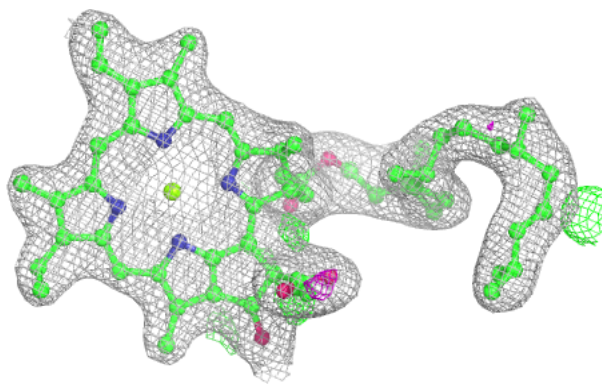


**Electron density around CLA a 2613:**

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

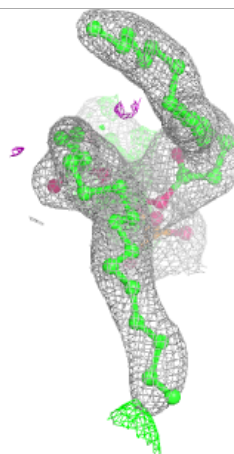
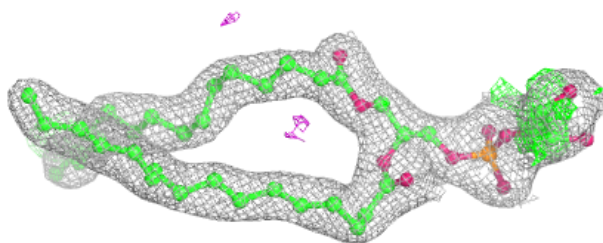
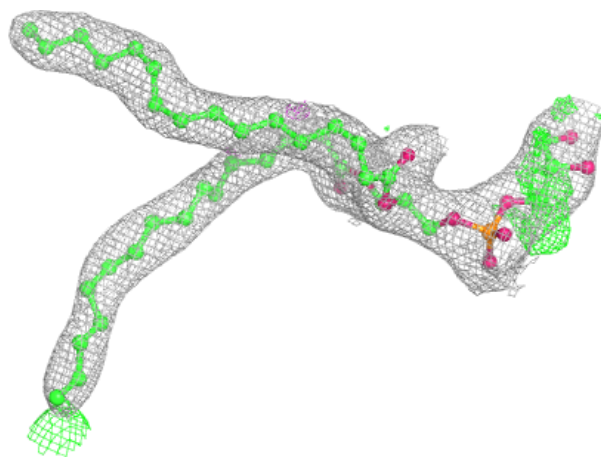
**Electron density around CLA B 613:**

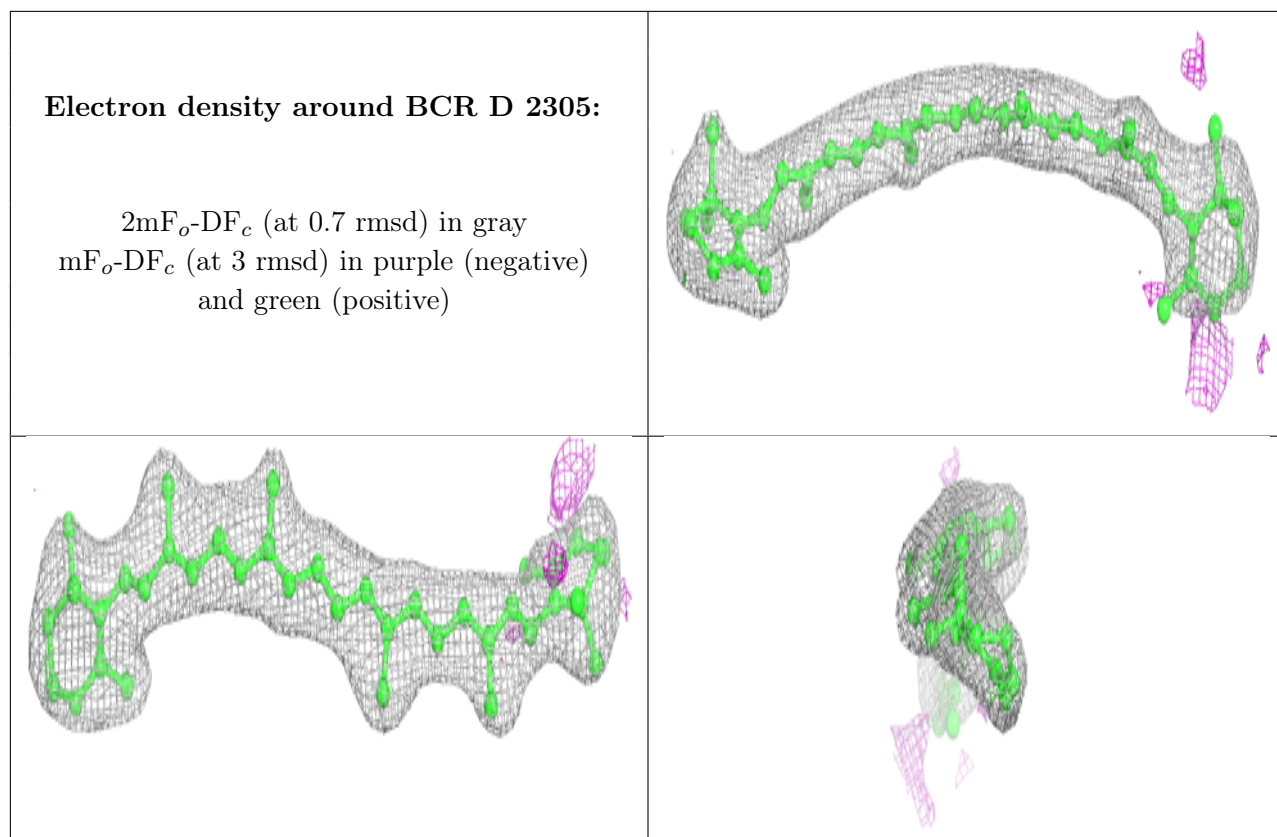
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around LHG D 2310:**

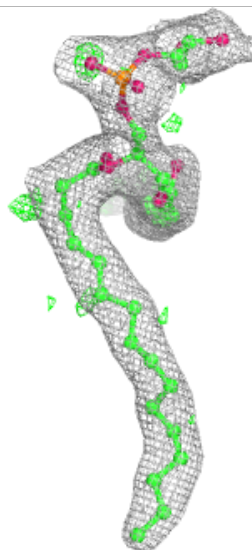
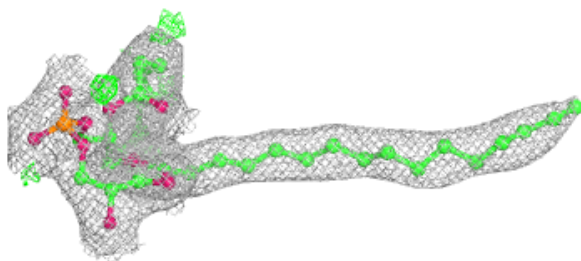
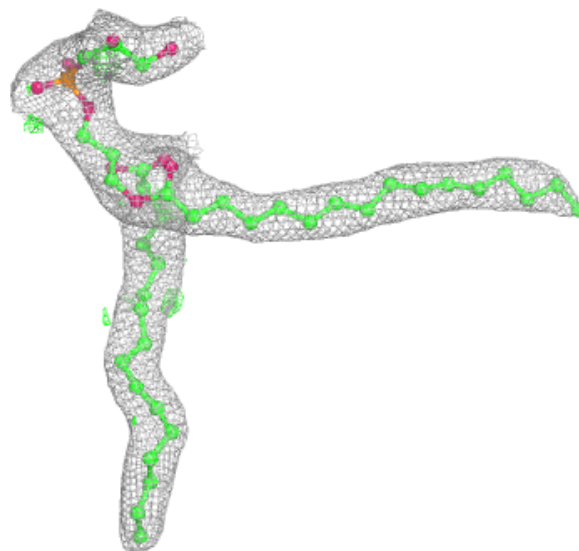
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around LHG L 101:**

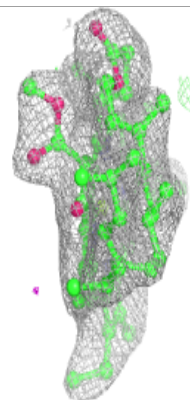
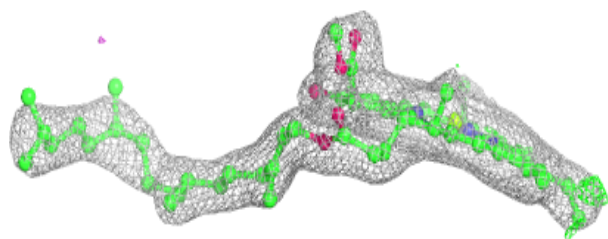
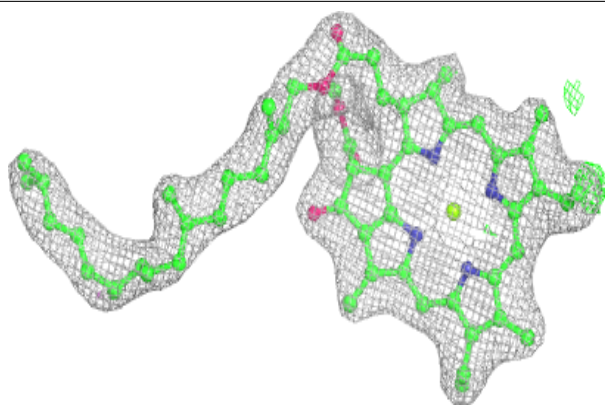
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



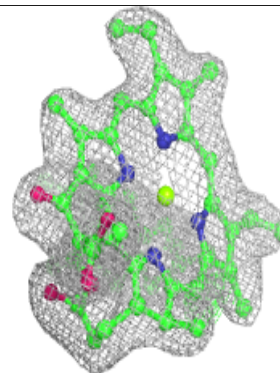
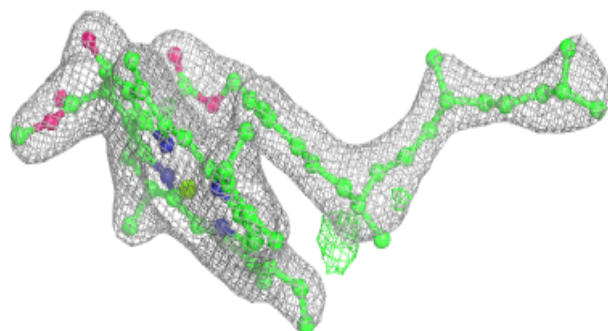
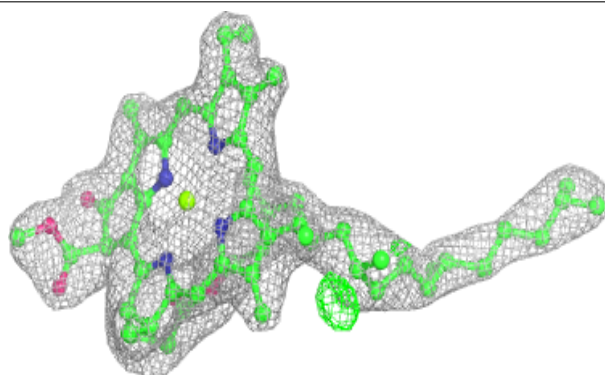


**Electron density around CLA b 607:**

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

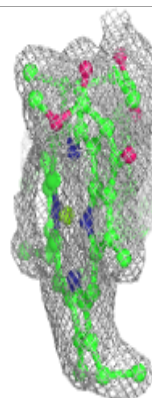
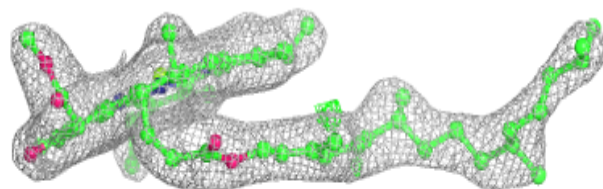
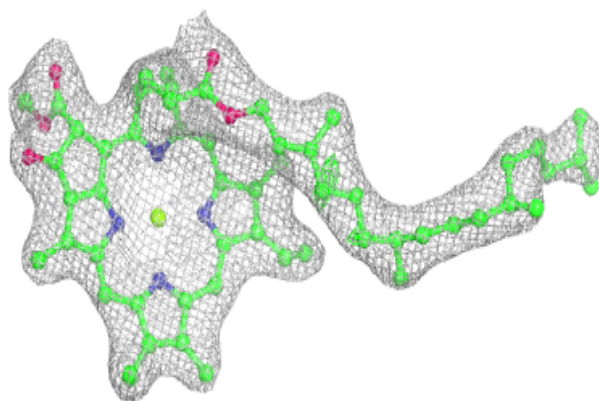
**Electron density around CLA c 508:**

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

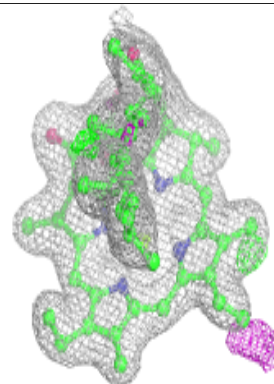
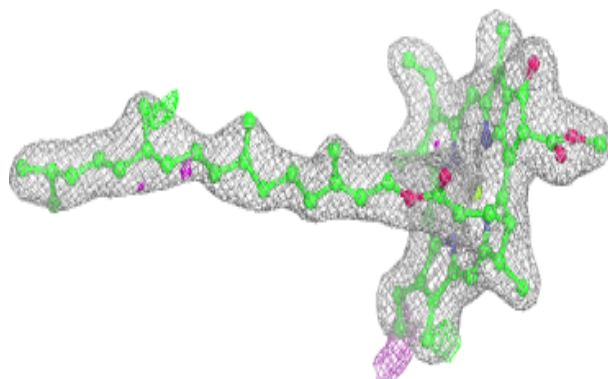
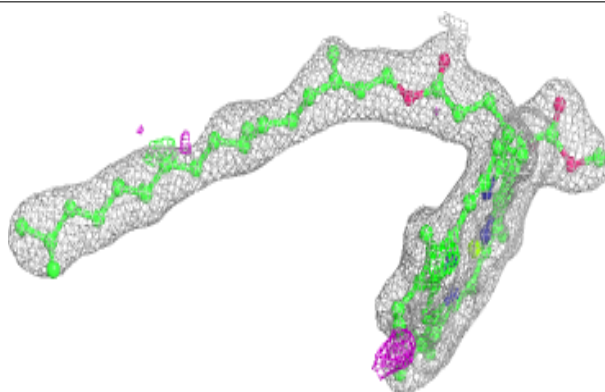


**Electron density around CLA b 608:**

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

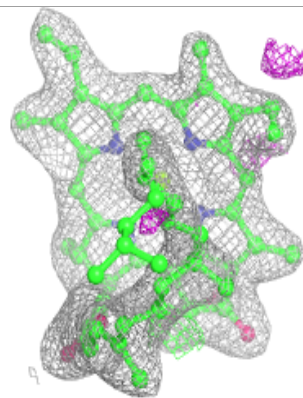
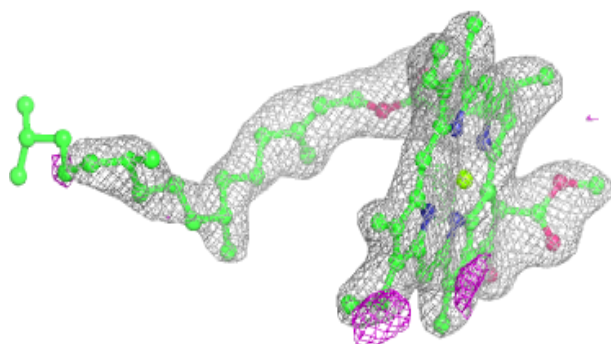
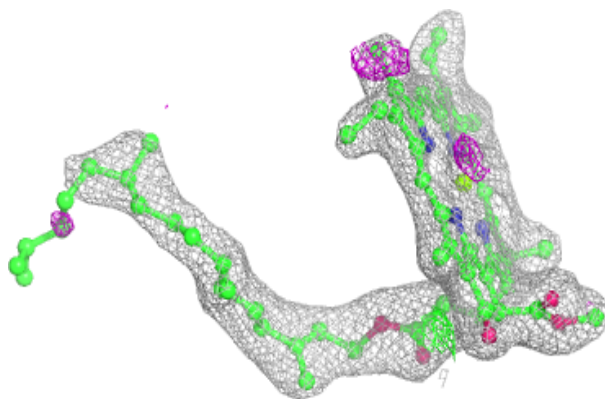
**Electron density around CLA B 608:**

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

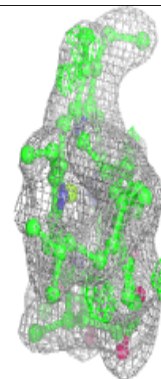
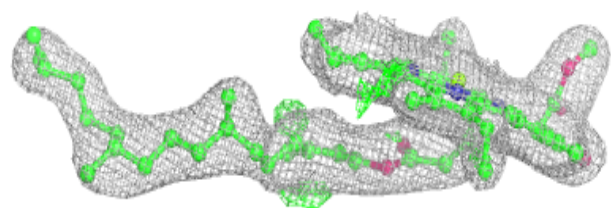
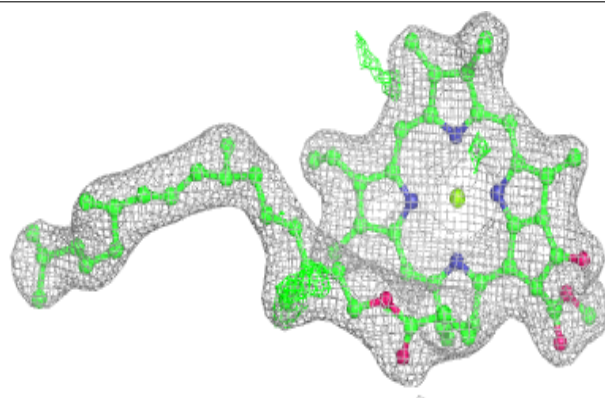


**Electron density around CLA c 511:**

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

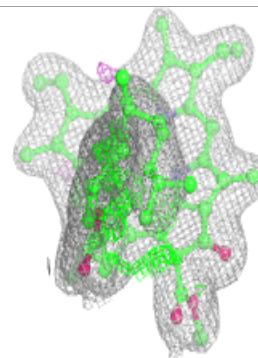
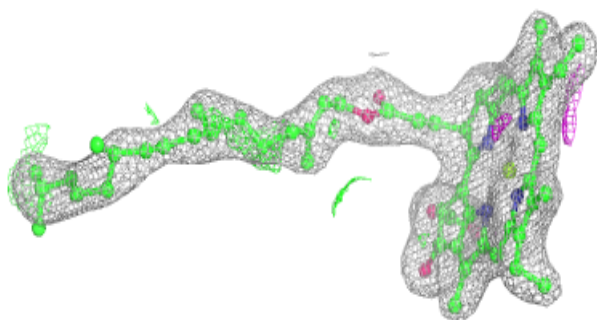
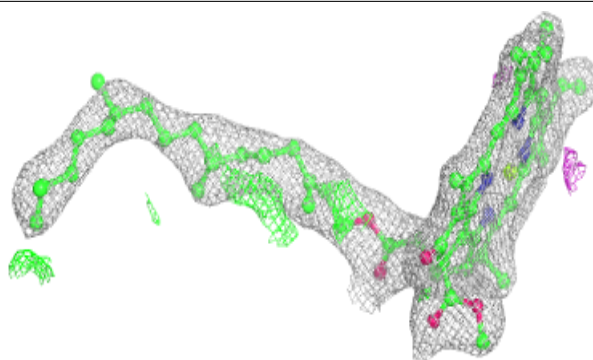
**Electron density around CLA B 604:**

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

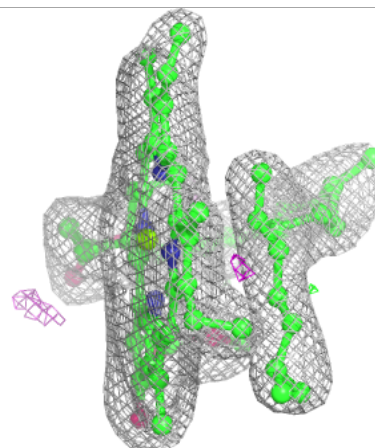
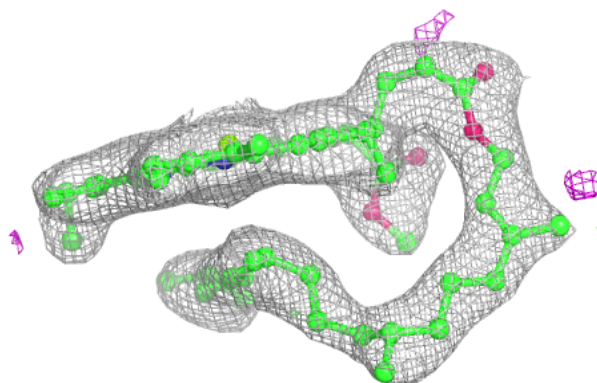
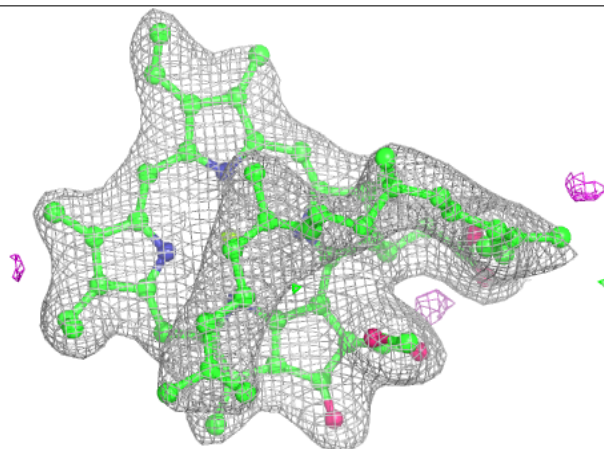


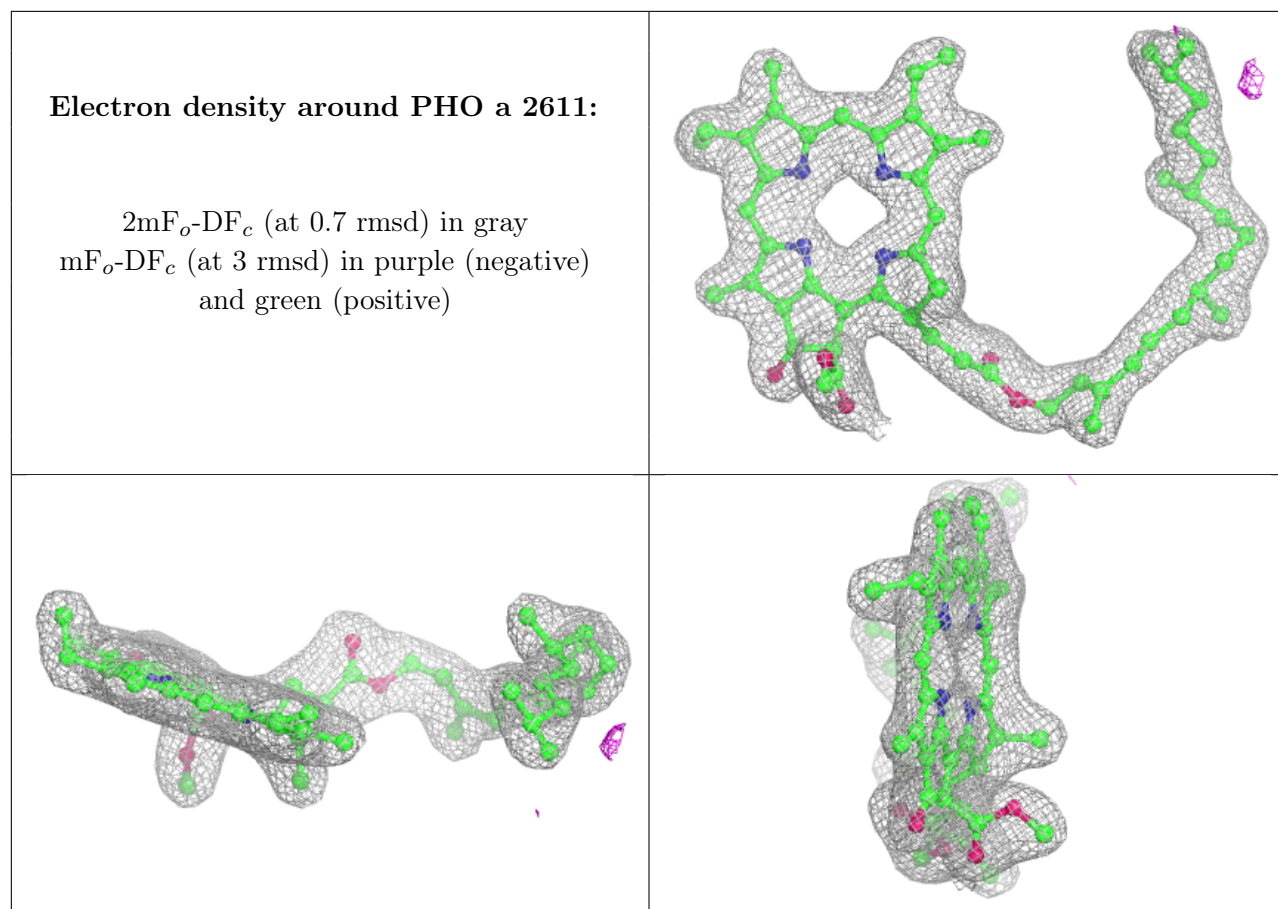
**Electron density around CLA B 605:**

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

**Electron density around CLA C 511:**

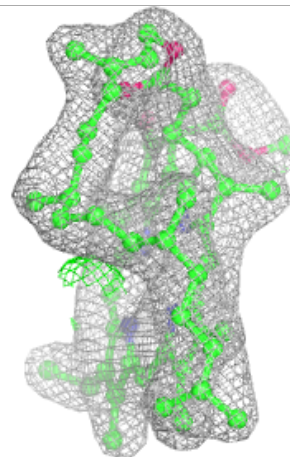
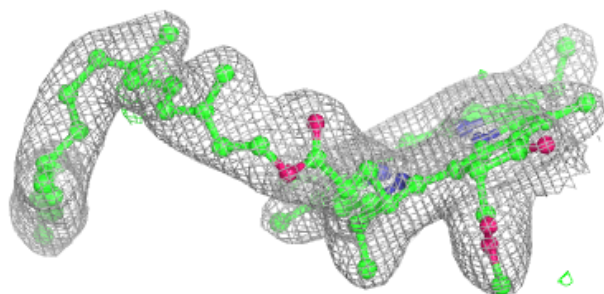
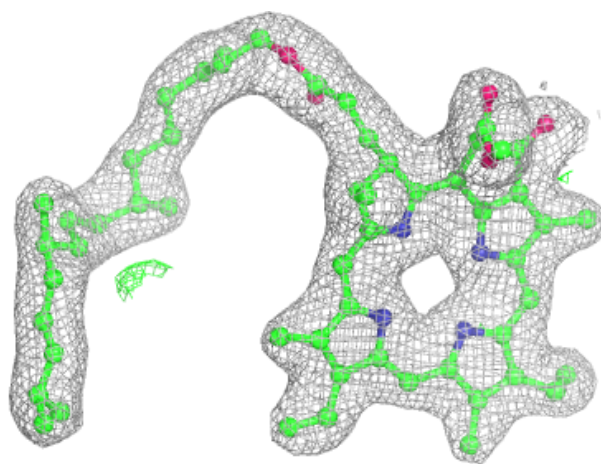
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

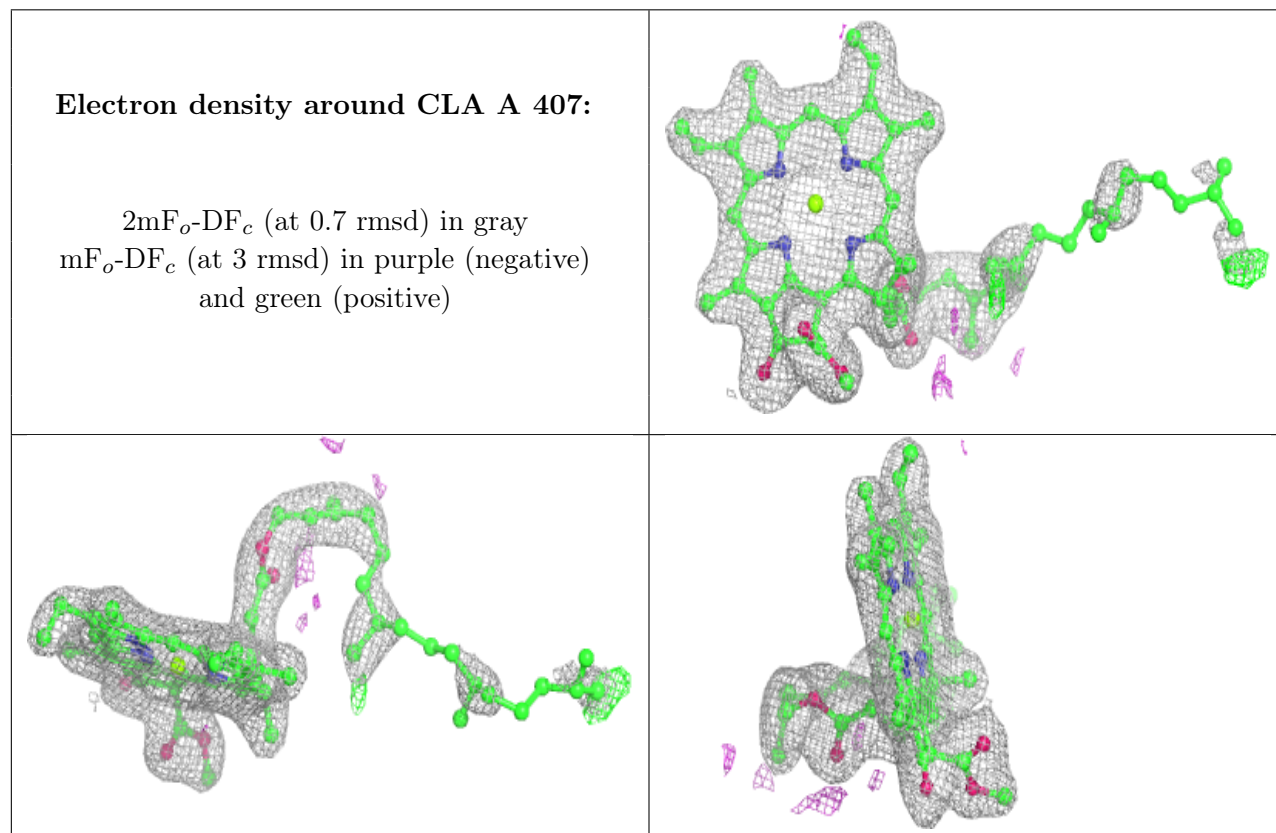
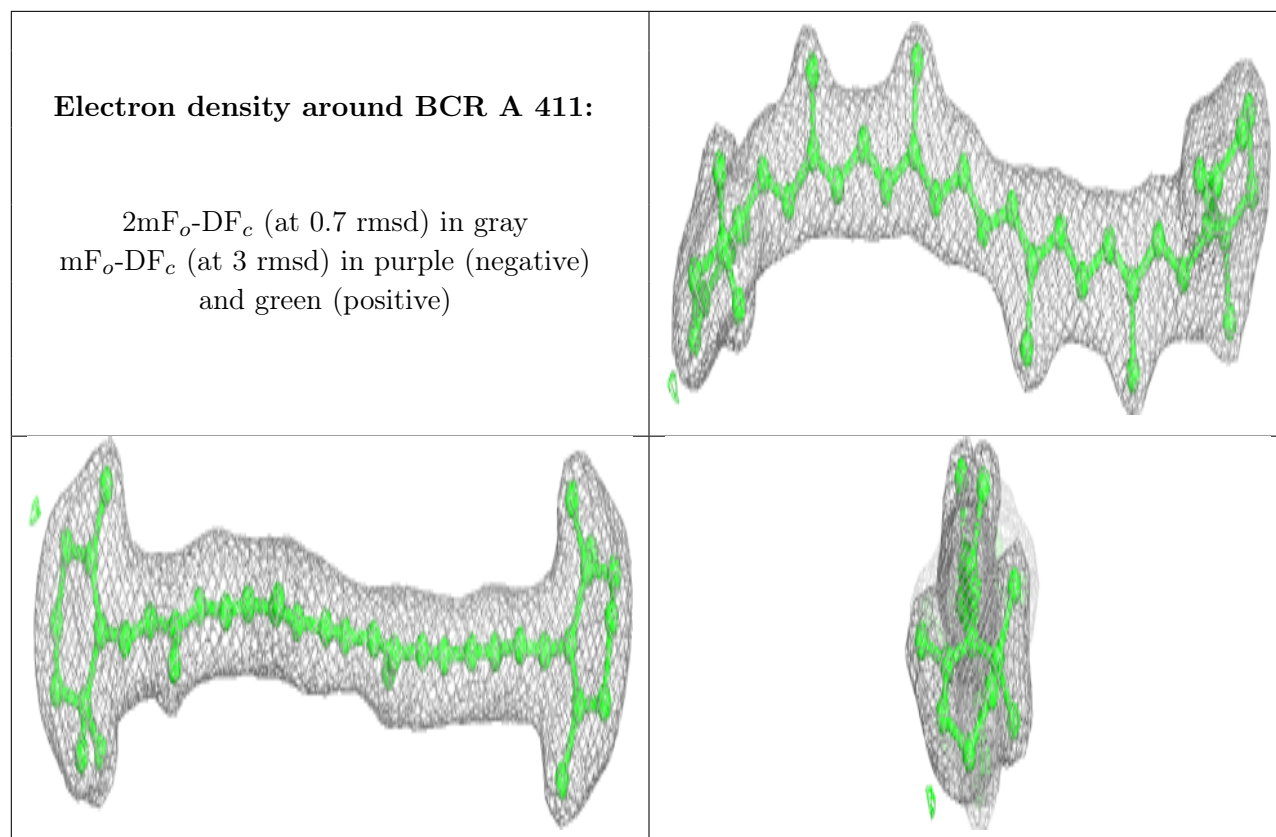


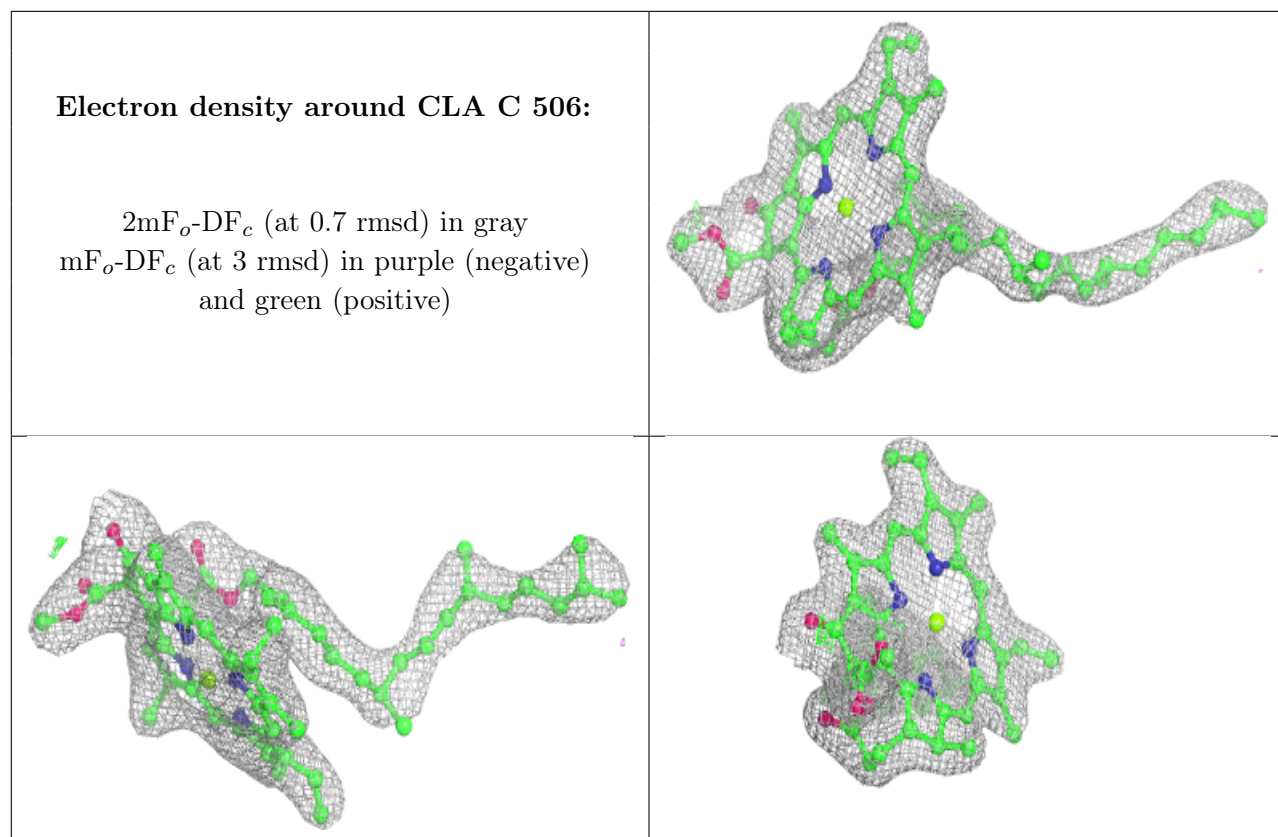


**Electron density around PHO a 2612:**

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



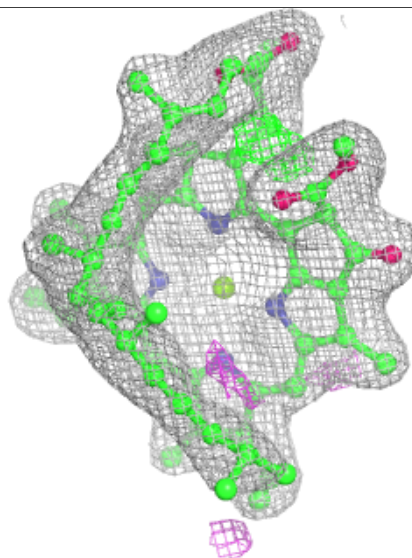
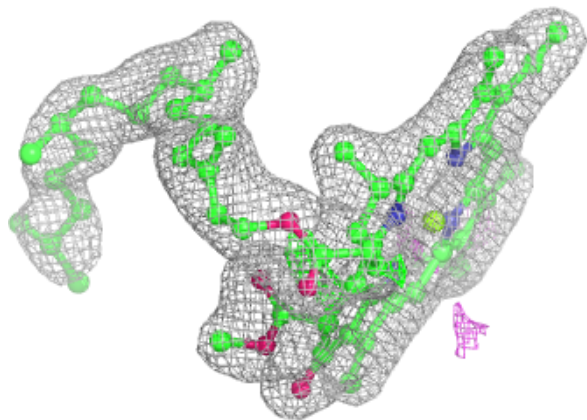
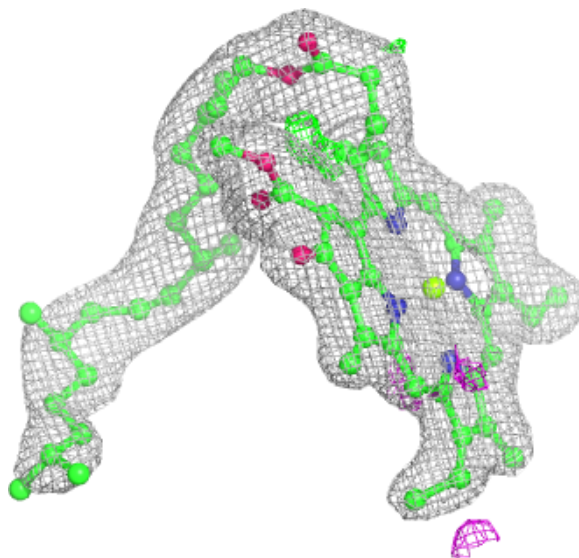






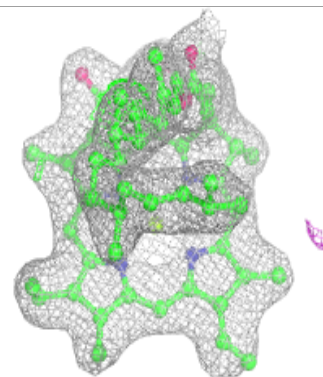
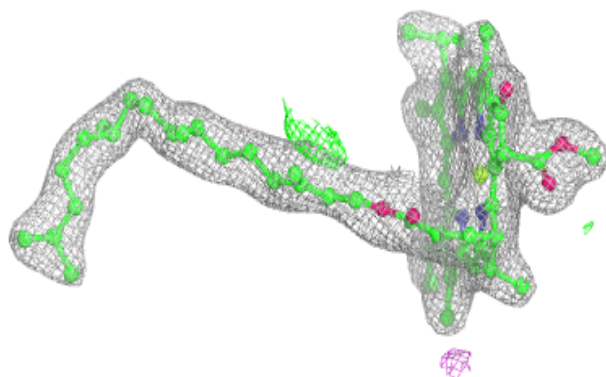
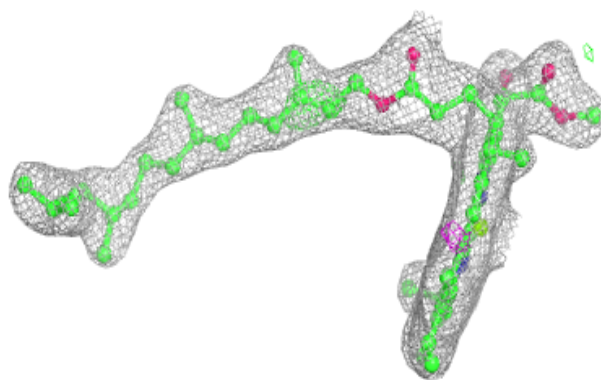
**Electron density around CLA b 618:**

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

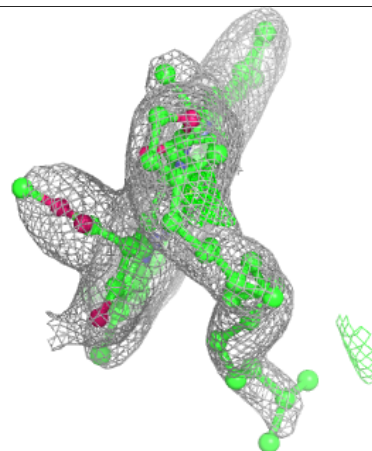
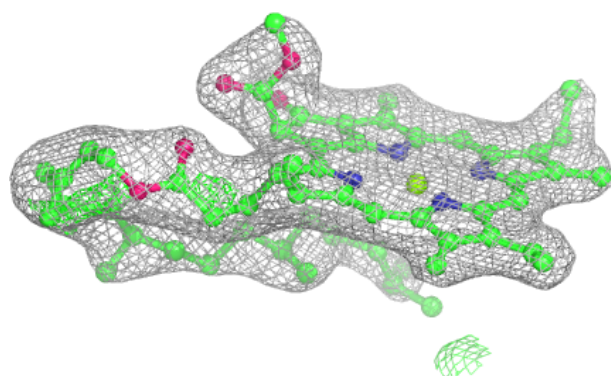
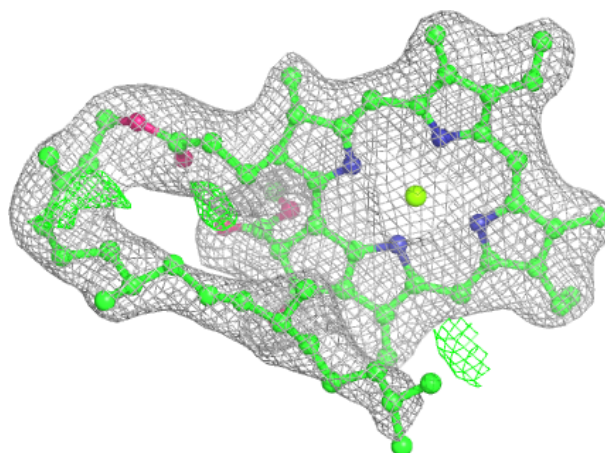


**Electron density around CLA b 610:**

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

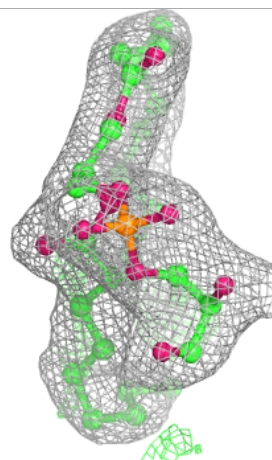
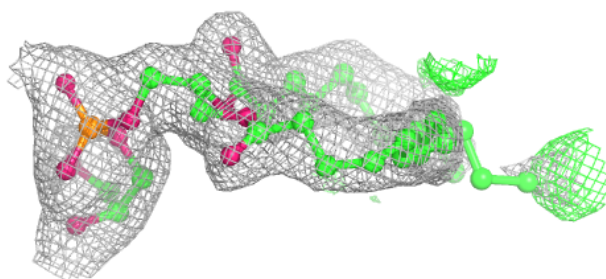
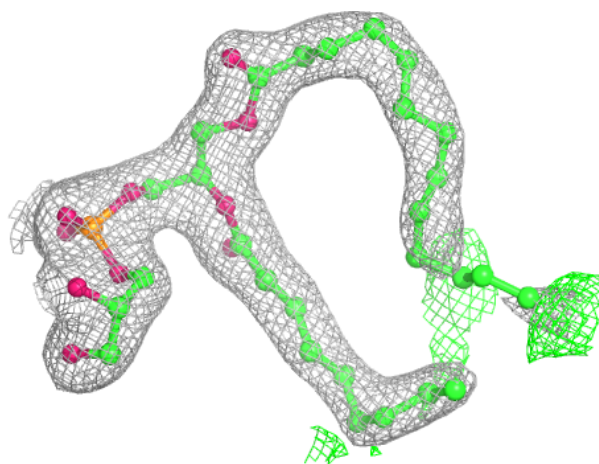
**Electron density around CLA c 512:**

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



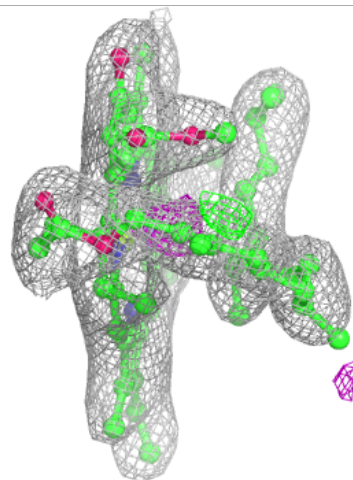
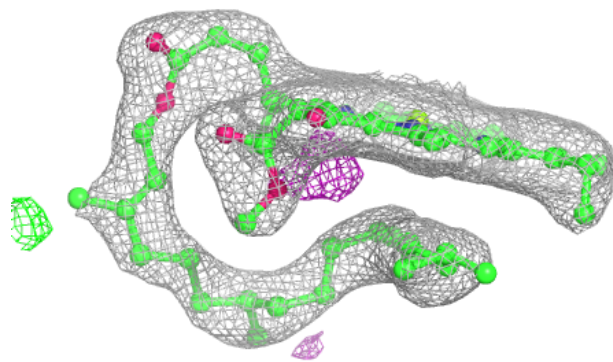
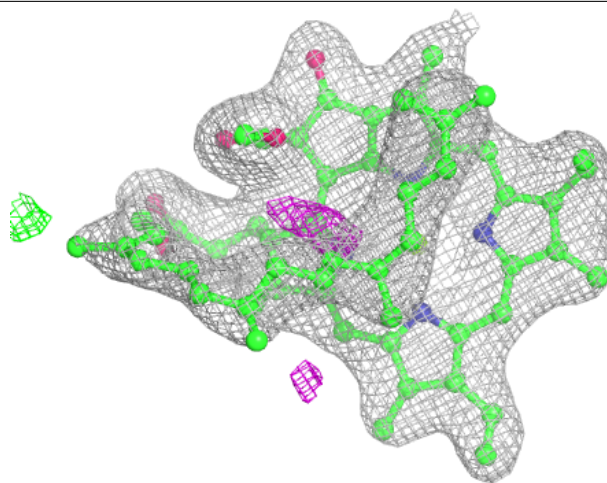
**Electron density around LHG D 2311:**

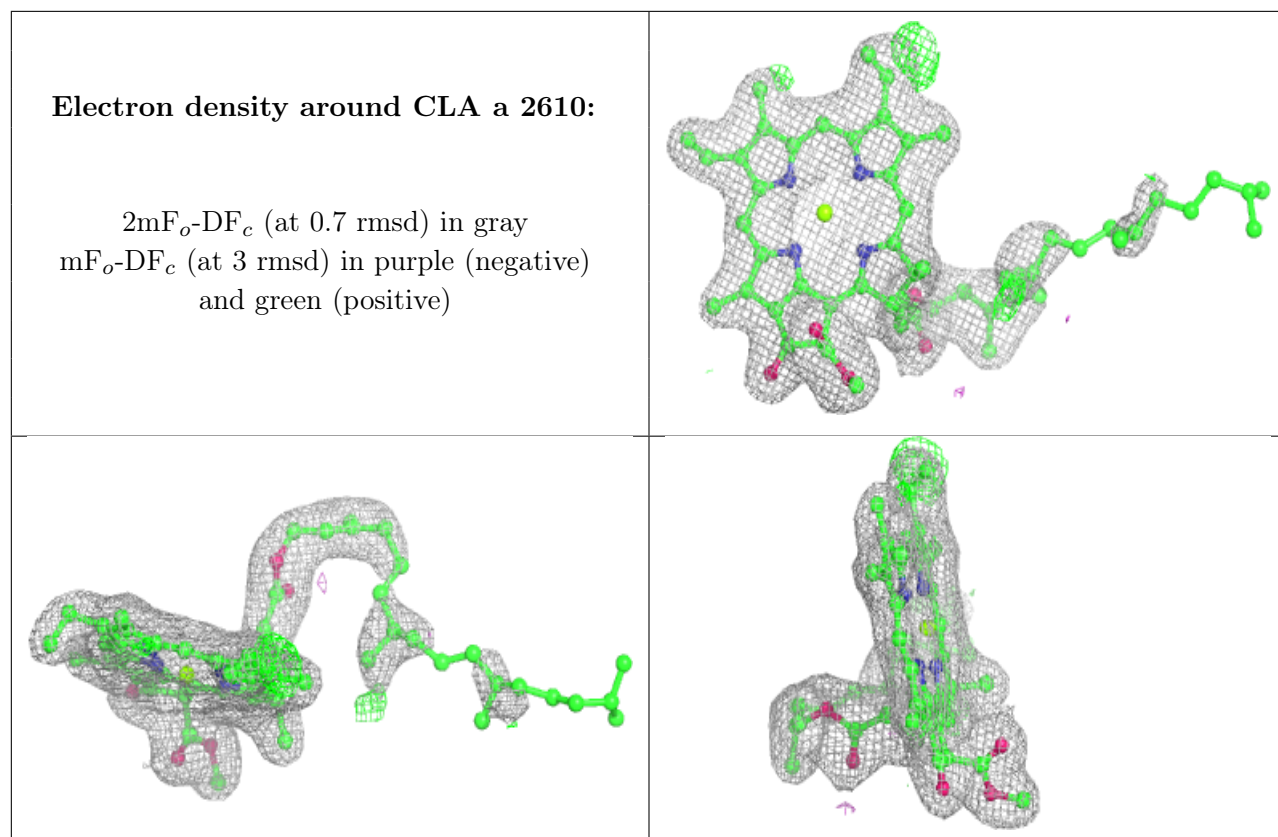
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA c 513:**

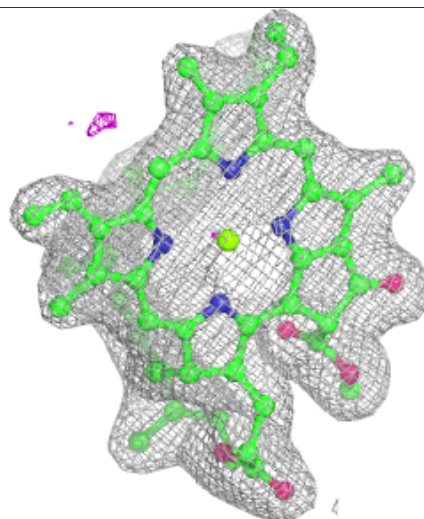
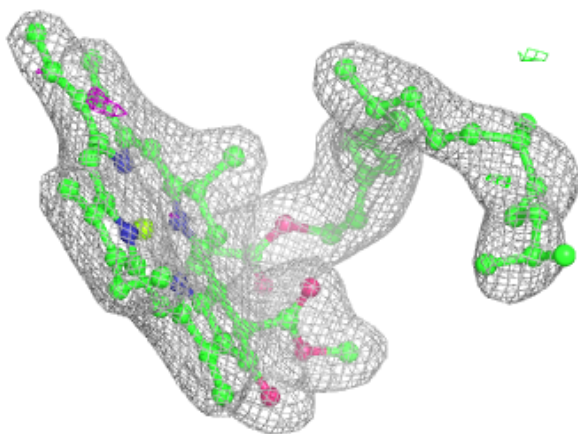
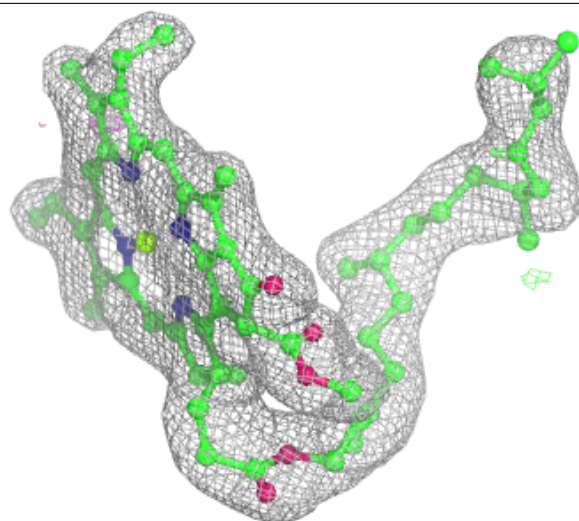
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





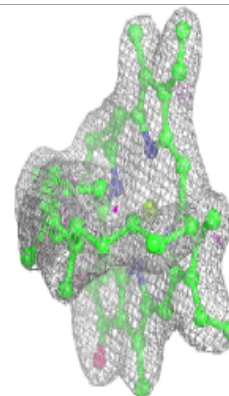
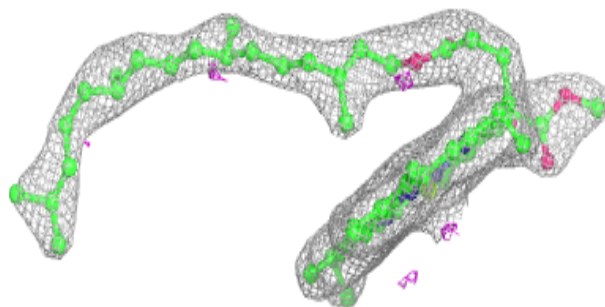
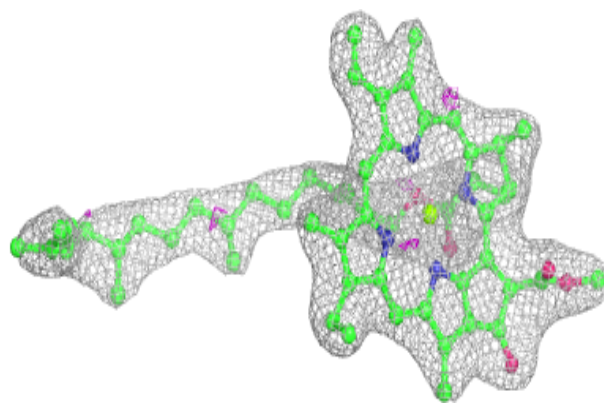
**Electron density around CLA B 614:**

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

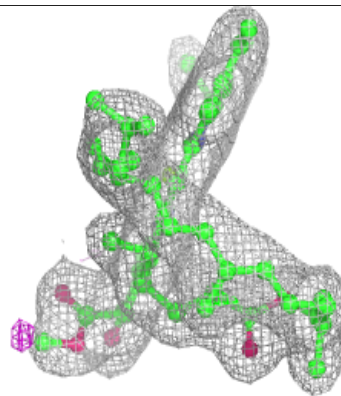
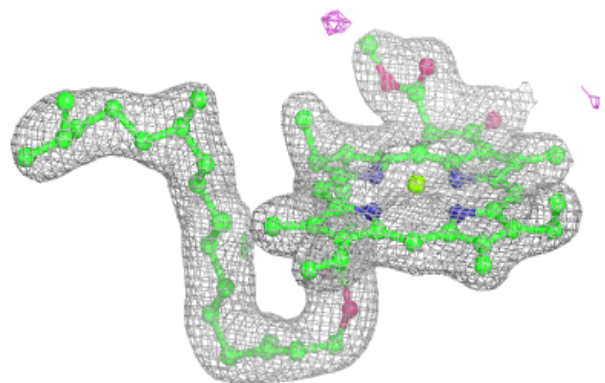
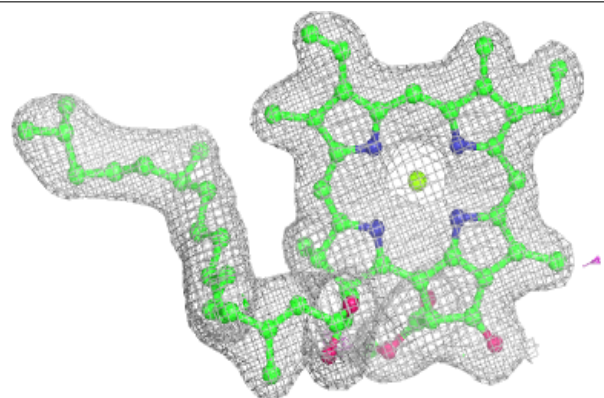


**Electron density around CLA b 613:**

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

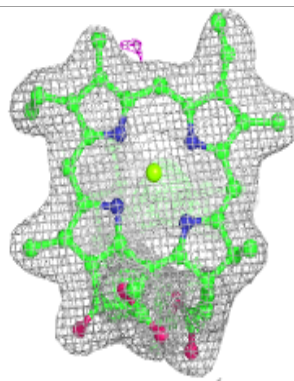
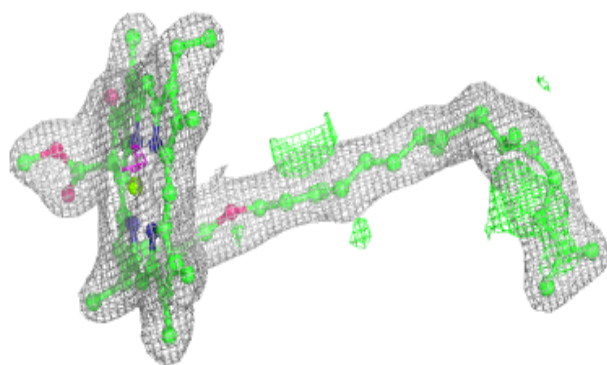
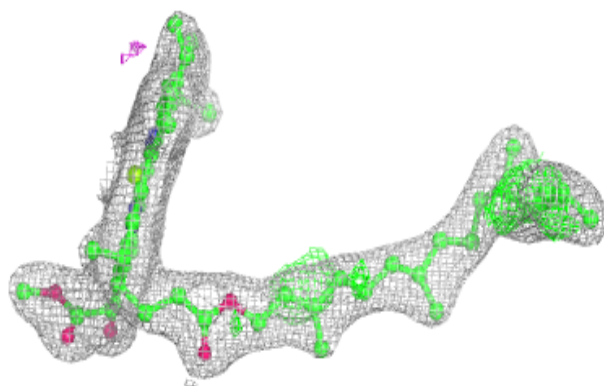
**Electron density around CLA d 402:**

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

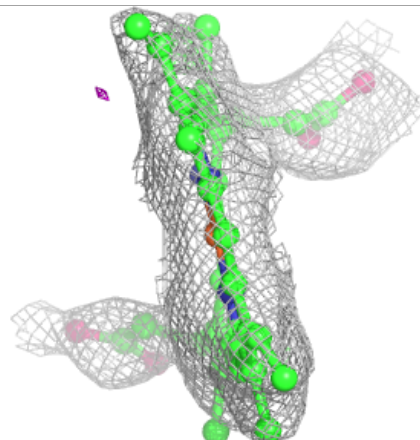
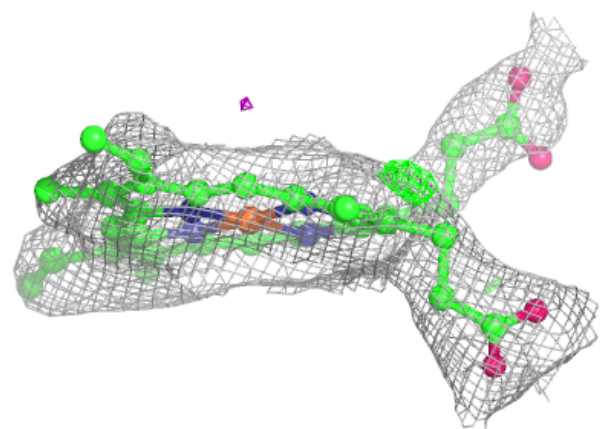
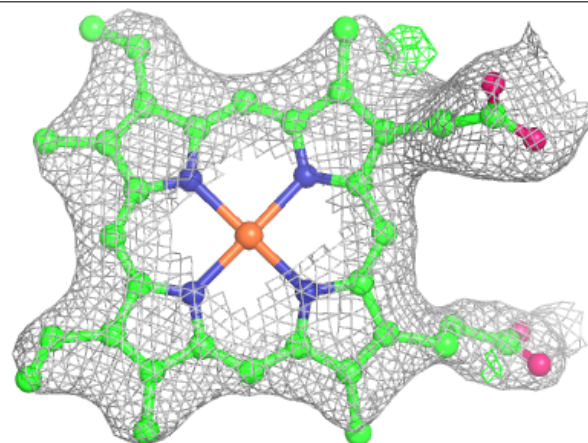


**Electron density around CLA B 606:**

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

**Electron density around HEM F 101:**

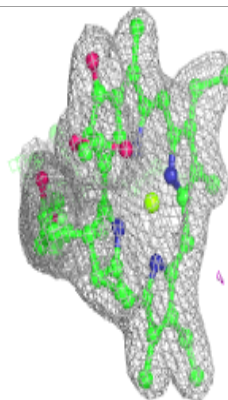
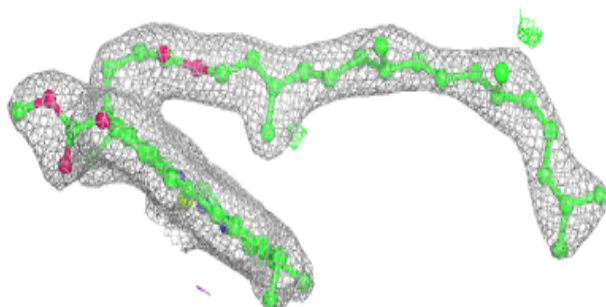
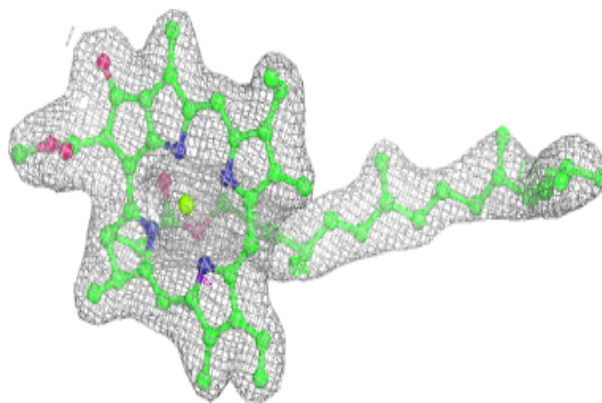
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



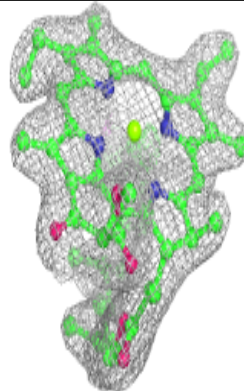
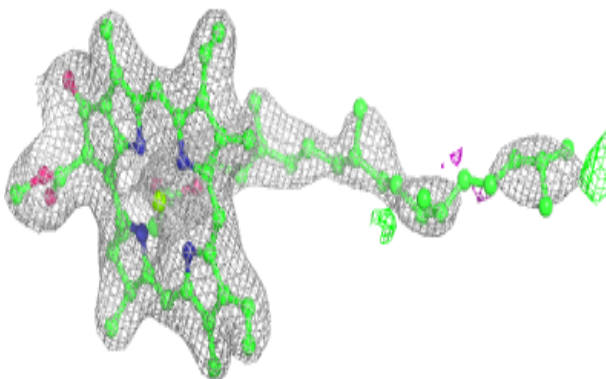
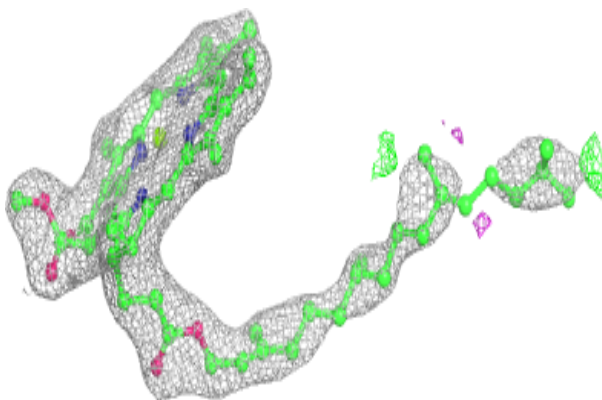


**Electron density around CLA B 609:**

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

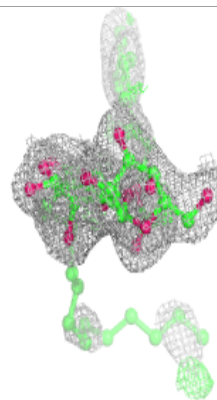
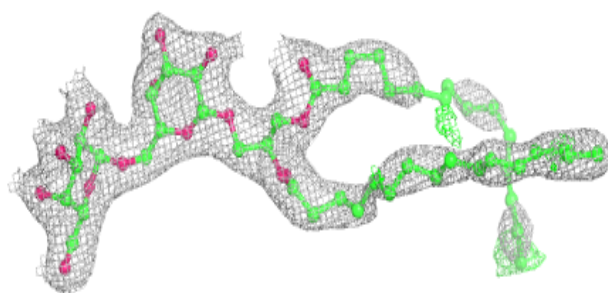
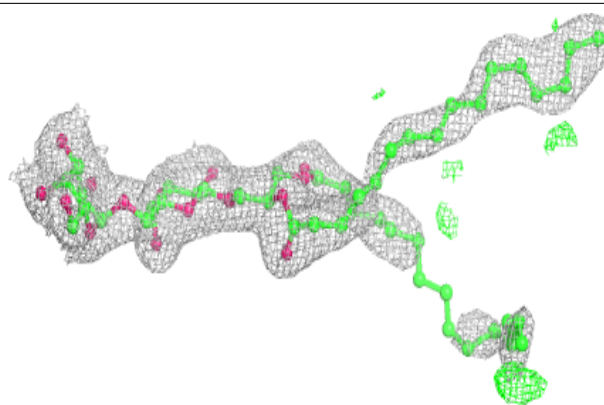
**Electron density around CLA c 507:**

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

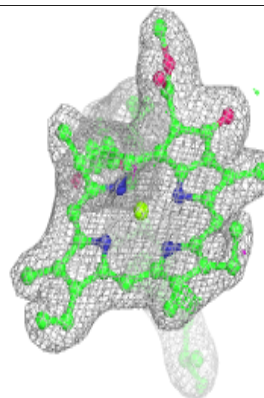
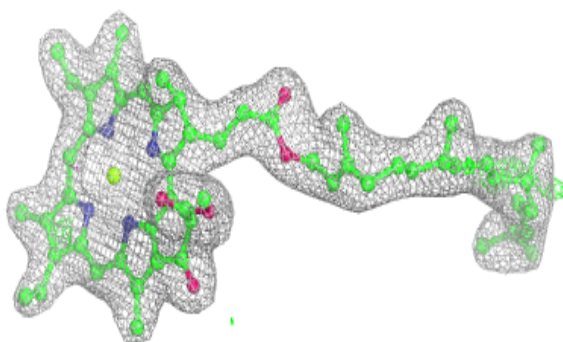
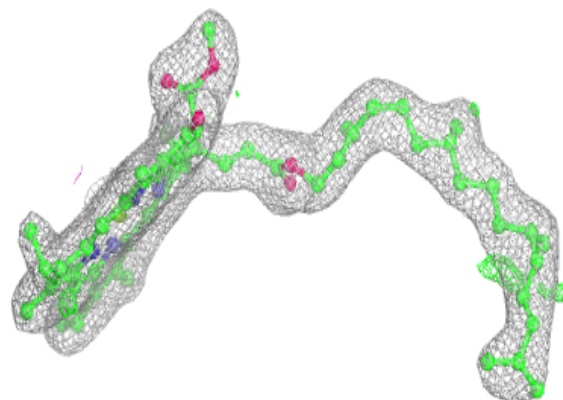


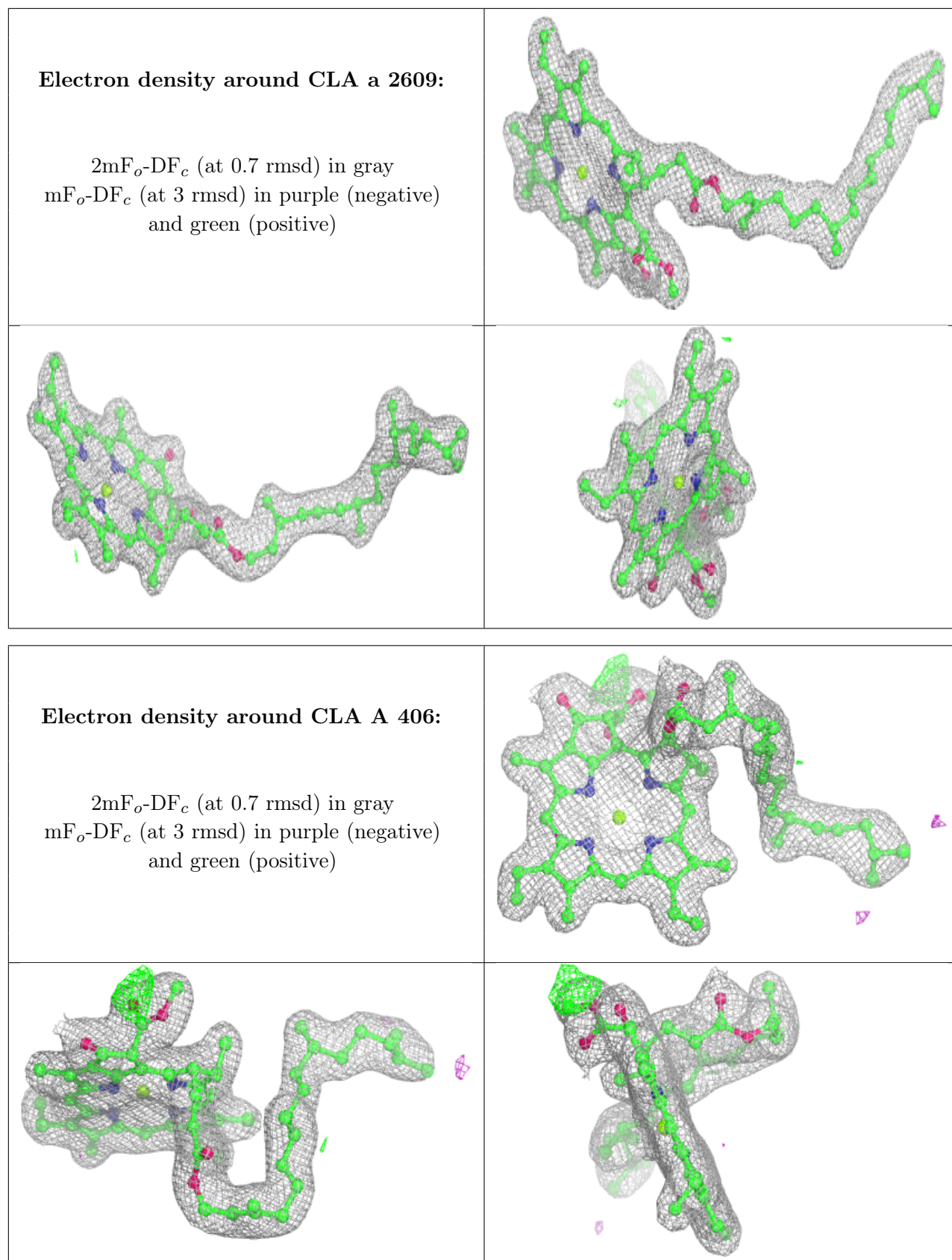
**Electron density around DGD C 517:**

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

**Electron density around CLA d 408:**

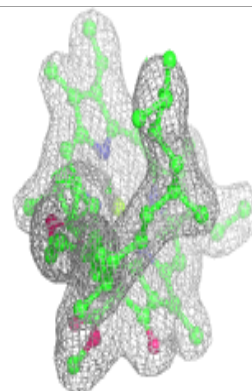
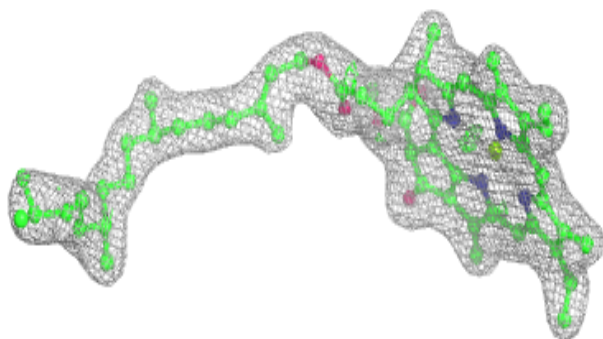
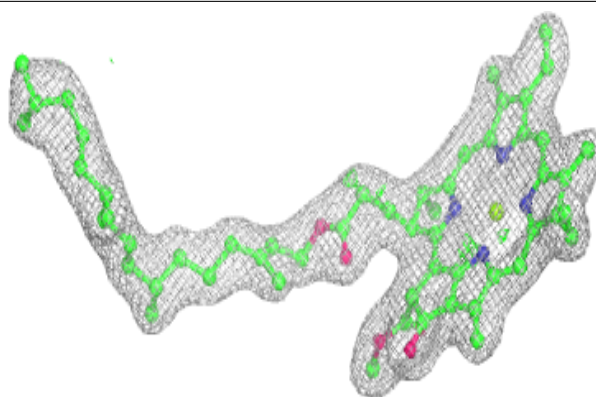
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



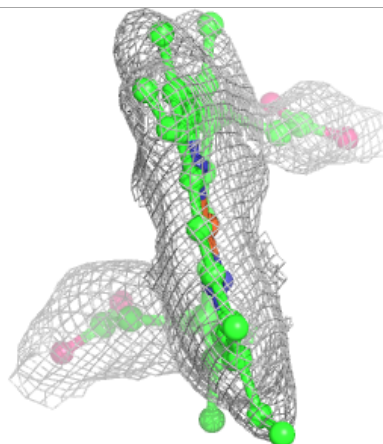
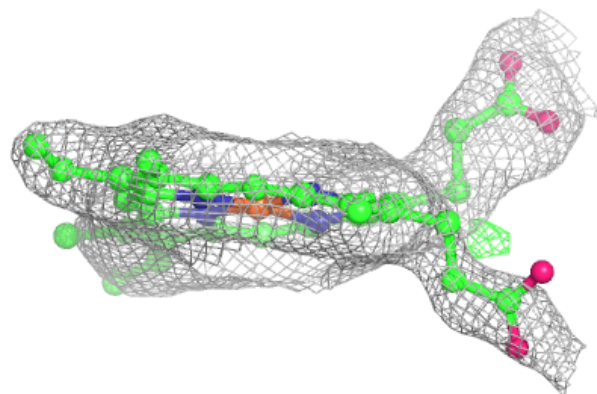
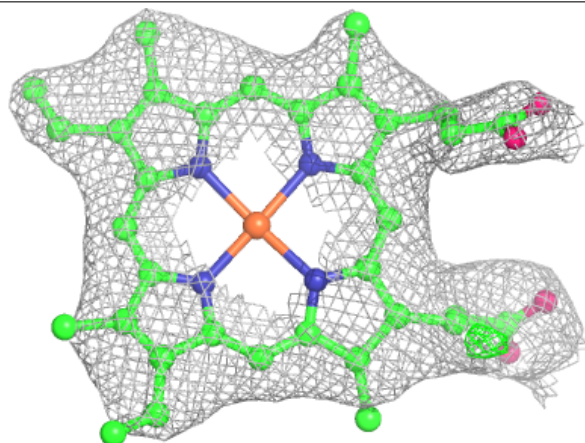


**Electron density around CLA A 405:**

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

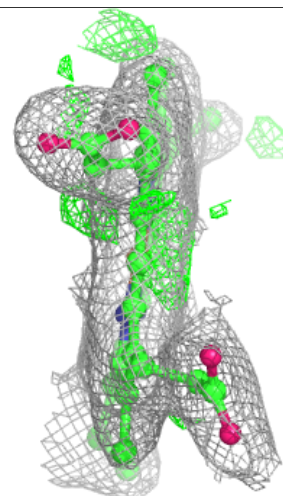
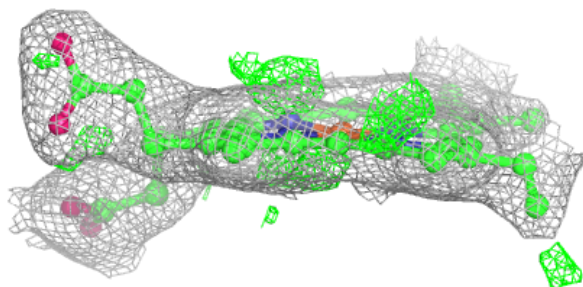
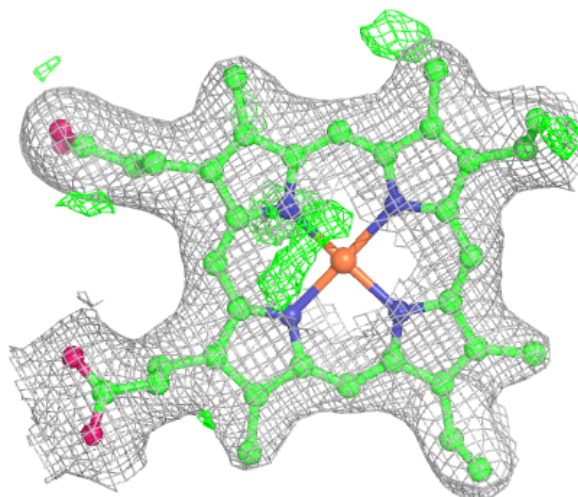
**Electron density around HEM e 103:**

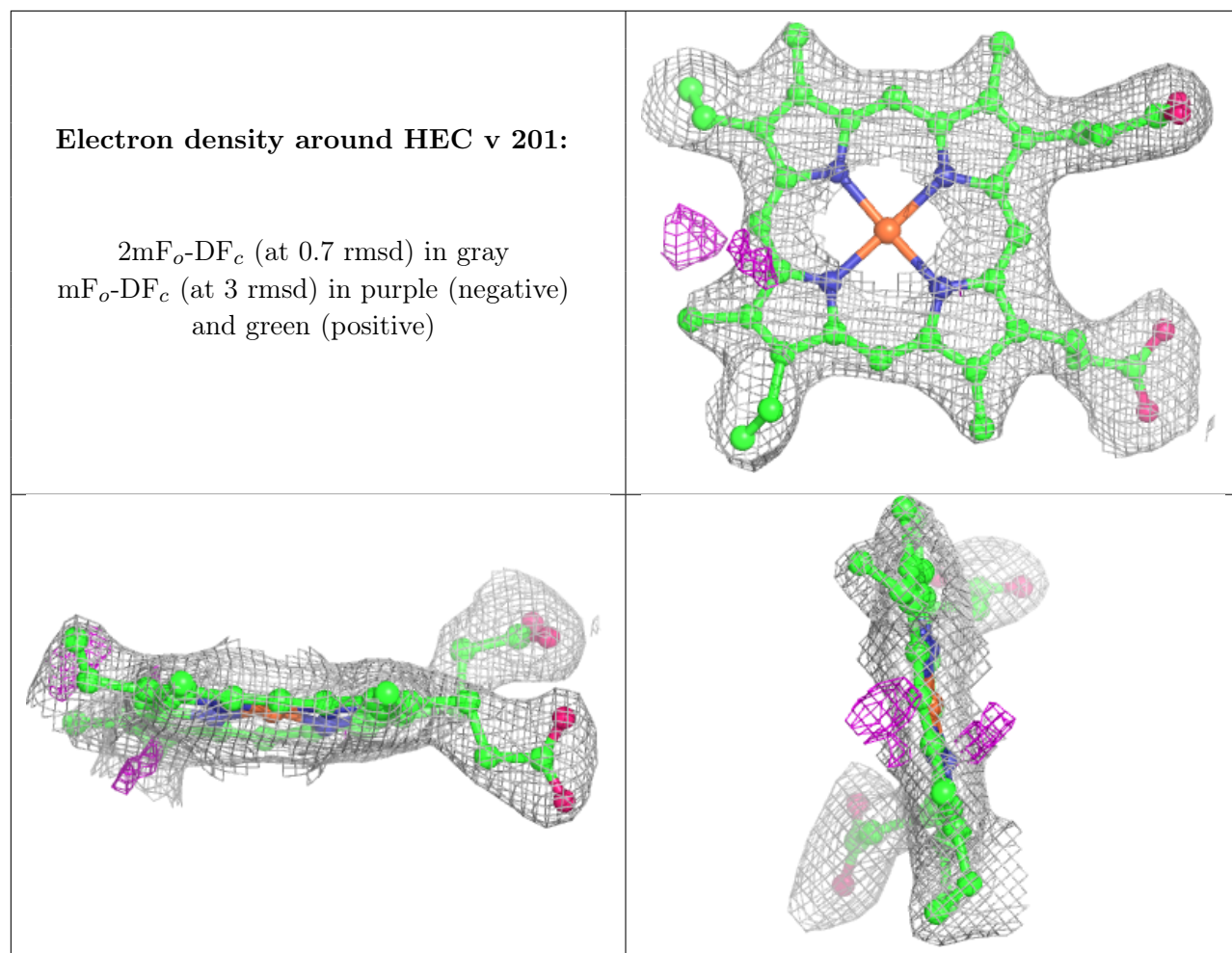
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC V 201:**

$2mF_o-DF_c$  (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.