



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 02:59 PM BST

PDB ID : 4IL6
Title : Structure of Sr-substituted photosystem II
Authors : Koua, F.H.M.; Umena, Y.; Kawakami, K.; Kamiya, N.; Shen, J.R.
Deposited on : 2012-12-29
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.13.1
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) : 2.13.1

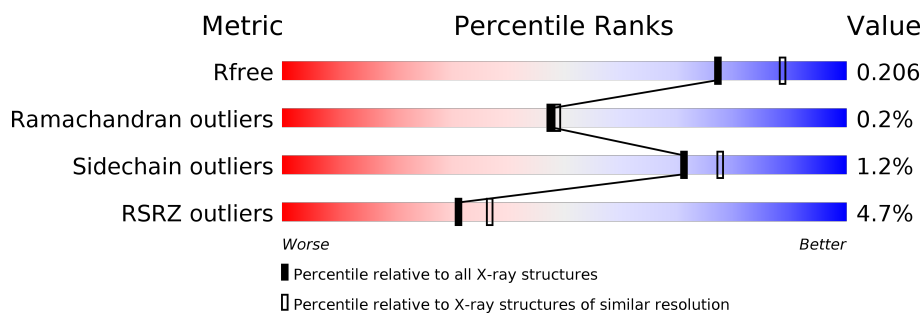
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



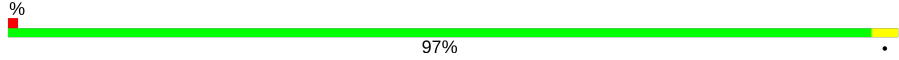
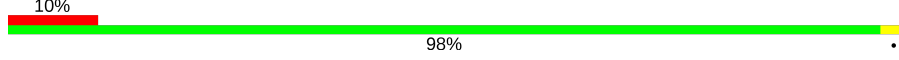
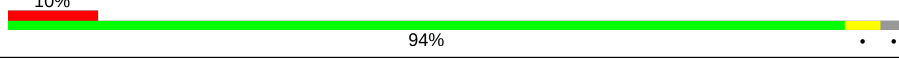
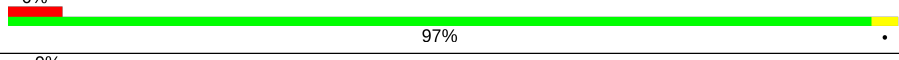

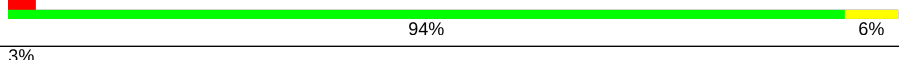
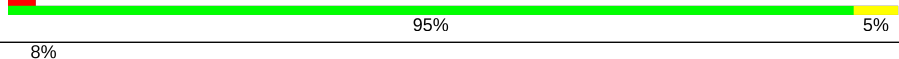
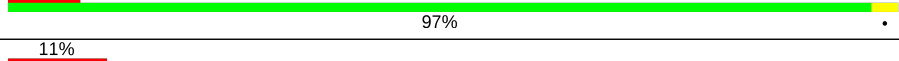
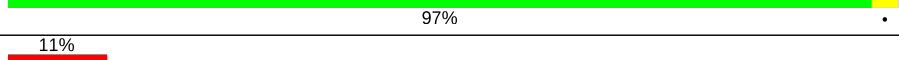
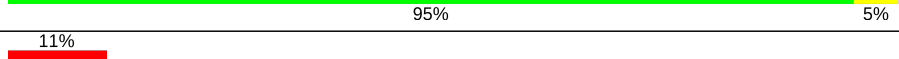
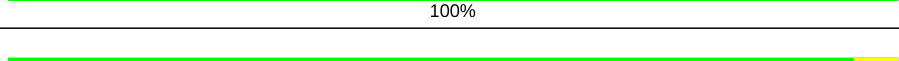
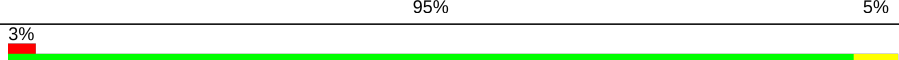
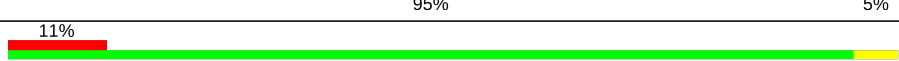
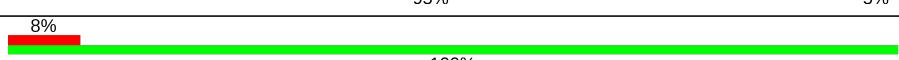
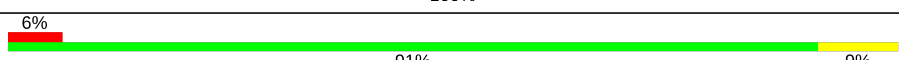
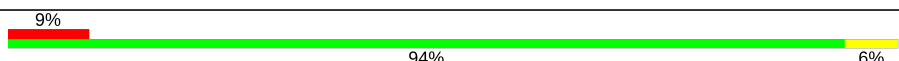
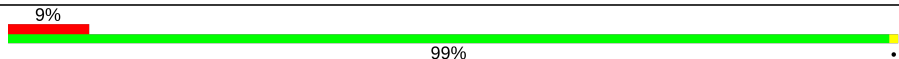
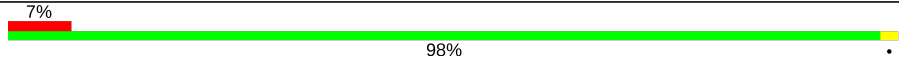
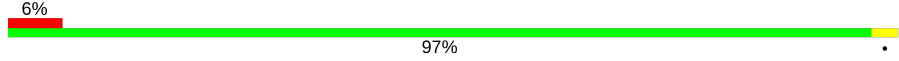
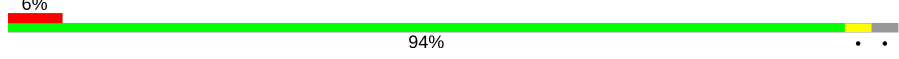
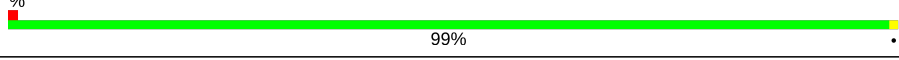
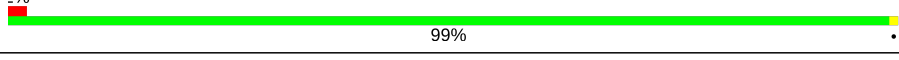
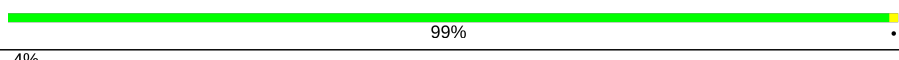
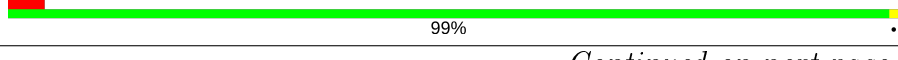

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	334	 99%
1	a	334	 99%
2	B	505	 99%
2	b	505	 98%
3	C	451	 98%
3	c	451	 97%
4	D	342	 98%

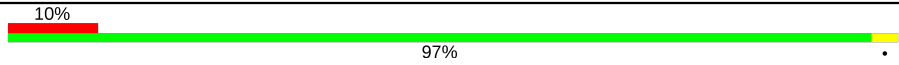
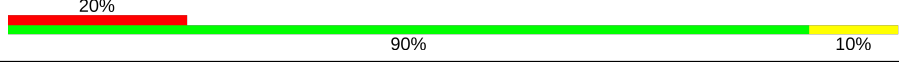
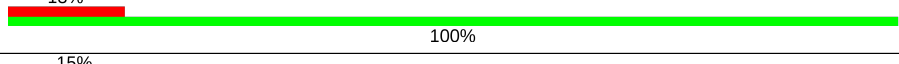
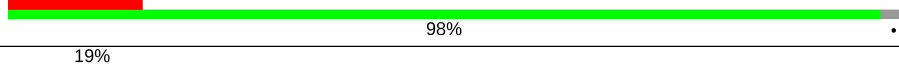
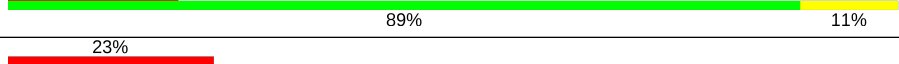

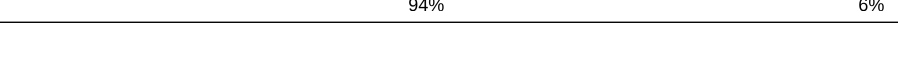
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Mol	Chain	Length	Quality of chain
4	d	342	 97%
5	E	80	 98%
5	e	80	 94%
6	F	34	 97%
6	f	34	 88%
7	H	63	 94%
7	h	63	 95%
8	I	36	 97%
8	i	36	 97%
9	J	37	 95%
9	j	37	 100%
10	K	37	 95%
10	k	37	 95%
11	L	37	 95%
11	l	37	 100%
12	M	34	 91%
12	m	34	 94%
13	O	244	 99%
13	o	244	 98%
14	T	31	 97%
14	t	31	 94%
15	U	97	 99%
15	u	97	 99%
16	V	137	 99%
16	v	137	 99%

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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	
20	R	34	

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
24	CLA	A	1005	X	-	-	-
24	CLA	A	1006	X	-	-	-
24	CLA	A	1008	X	-	-	-
24	CLA	B	601	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	D	405	X	-	-	-
24	CLA	a	407	X	-	-	-
24	CLA	a	408	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	a	412	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
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24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	c	501	X	-	-	-
24	CLA	c	502	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	d	402	X	-	-	-
24	CLA	d	403	X	-	-	-
26	BCR	D	406	-	X	-	-
26	BCR	H	101	-	X	-	-
26	BCR	J	101	-	X	-	-
26	BCR	K	101	-	X	-	-
26	BCR	d	404	-	X	-	-
26	BCR	k	101	-	X	-	-
26	BCR	y	101	-	X	-	-
32	LMT	A	1018	-	-	-	X
32	LMT	i	102	-	-	-	X
35	HTG	B	624	-	-	-	X

2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 53568 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 Q(B) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	Total 2643	C 1733	N 431	O 464	S 15	0	5	0
1	a	334	Total 2637	C 1729	N 431	O 462	S 15	0	4	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	SEE REMARK 999	UNP P51765
a	279	PRO	ARG	SEE REMARK 999	UNP P51765

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	505	Total 4040	C 2652	N 674	O 701	S 13	0	10	0
2	b	505	Total 4033	C 2646	N 676	O 698	S 13	0	9	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	451	Total 3500	C 2292	N 584	O 611	S 13	0	3	0
3	c	450	Total 3492	C 2287	N 583	O 609	S 13	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	342	Total 2726	C 1805	N 445	O 464	S 12	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	d	342	2726	1805	445	464	12	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	80	660	431	105	124		0	2	0
5	e	78	638	418	103	117		0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	34	275	187	45	42	1	0	0	0
6	f	32	257	175	43	38	1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	I	36	296	200	46	49	1	0	0	0
8	i	36	296	200	46	49	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	J	37	266	179	41	45	1	0	0	0
9	j	37	266	179	41	45	1	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	K	37	293	204	43	46	0	0	0
10	k	37	293	204	43	46	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	L	37	304	202	48	53	1	0	0	0
11	l	37	304	202	48	53	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	M	34	274	184	40	49	1	0	1	0
12	m	34	274	184	40	49	1	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	O	244	1883	1176	317	386	4	0	2	0
13	o	243	1868	1167	315	382	4	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	T	31	267	187	38	40	2	0	0	0
14	t	30	258	181	36	39	2	0	0	0

- 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
			780	495	129	156			
15	u	97	Total	C	N	O	0	1	0
			780	495	129	156			

- 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	3	0
			1081	687	179	211	4			
16	v	137	Total	C	N	O	S	0	2	0
			1076	683	177	212	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
			224	147	38	36	3			
17	y	30	Total	C	N	O	S	0	0	0
			224	147	38	36	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	40	Total	C	N	O	0	0	0
			296	197	47	52			
18	x	39	Total	C	N	O	0	0	0
			287	191	46	50			

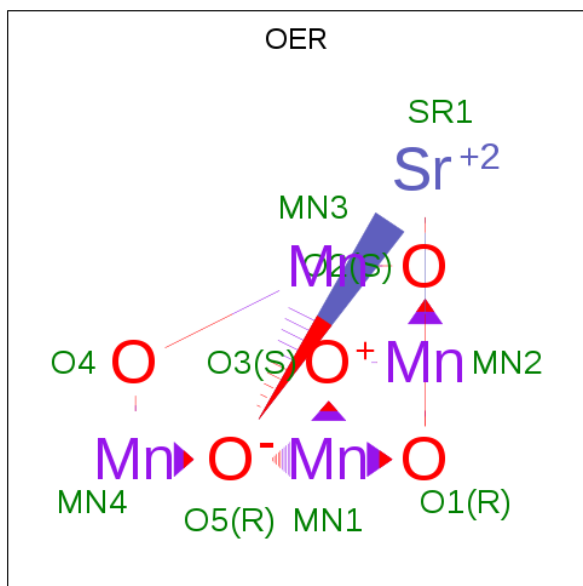
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			481	329	72	78	2			
19	z	62	Total	C	N	O	S	0	0	0
			481	329	72	78	2			

- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			273	186	47	40			

- Molecule 21 is SR-MN4-O5 CLUSTER (three-letter code: OER) (formula: $\text{Mn}_4\text{O}_5\text{Sr}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Mn	O	Sr		
21	A	1	10	4	5	1	0	0
21	a	1	10	4	5	1	0	0

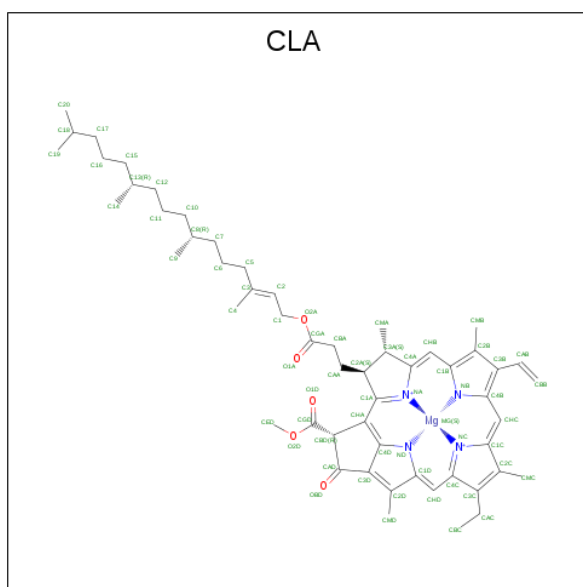
- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 23 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



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

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

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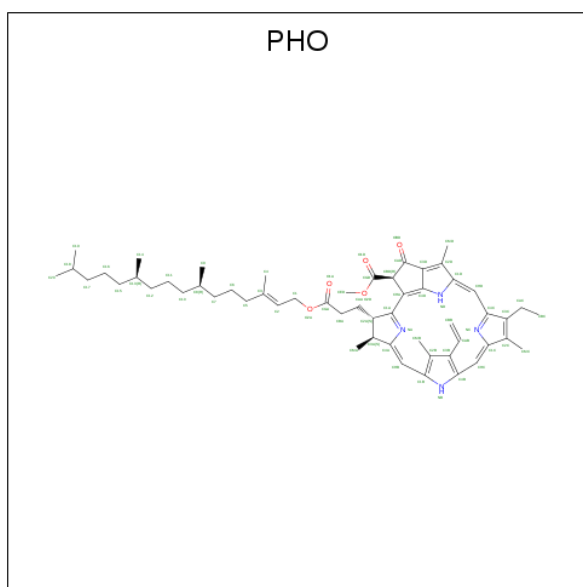
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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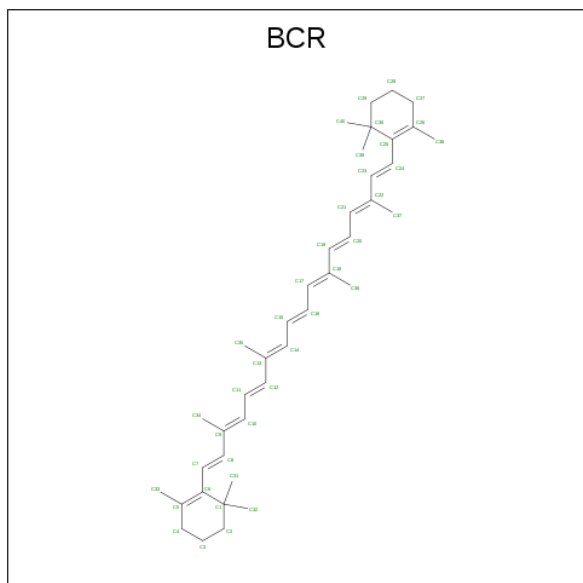
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



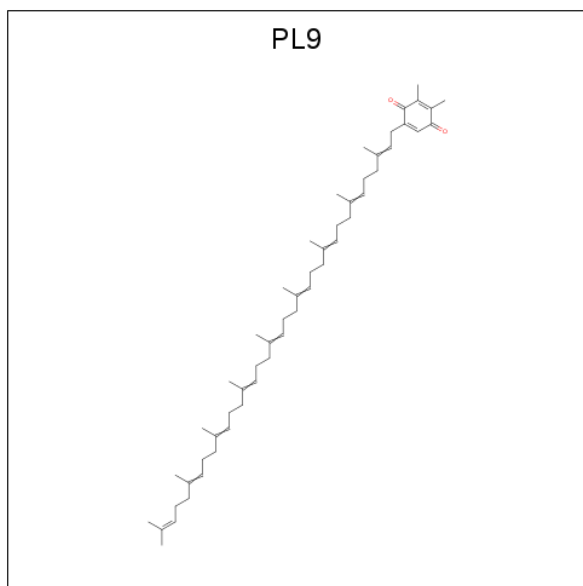
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
25	A	1	64	55	4	5	0	0
25	D	1	64	55	4	5	0	0
25	a	1	64	55	4	5	0	0
25	a	1	64	55	4	5	0	0

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



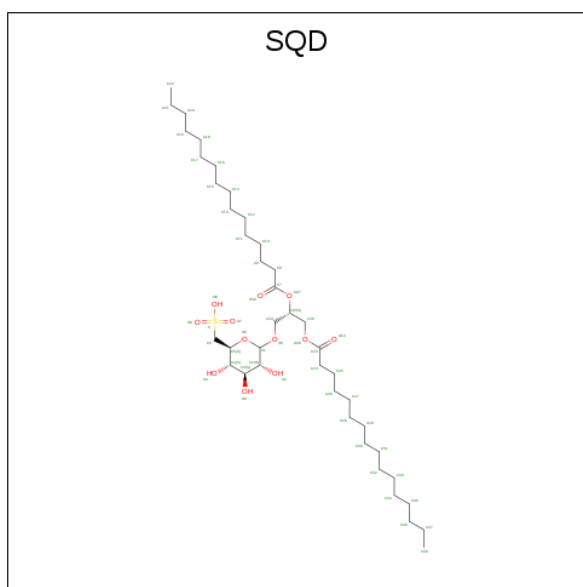
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	J	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	d	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0
26	y	1	Total C 40 40	0	0

- Molecule 27 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: $C_{53}H_{80}O_2$).



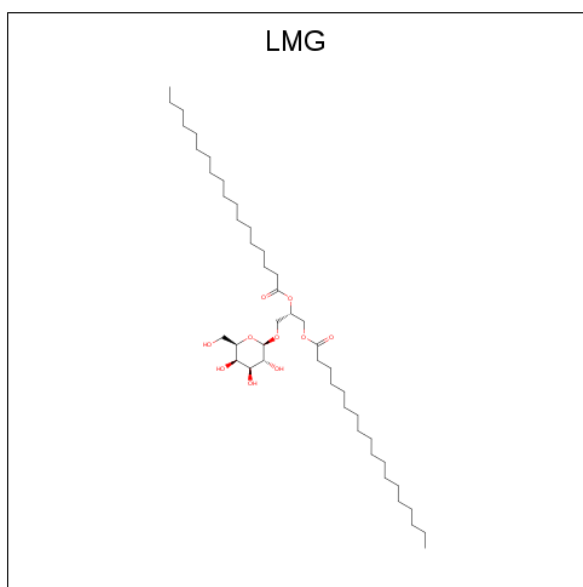
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			55	53	2		
27	D	1	Total	C	O	0	0
			55	53	2		
27	a	1	Total	C	O	0	0
			55	53	2		
27	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



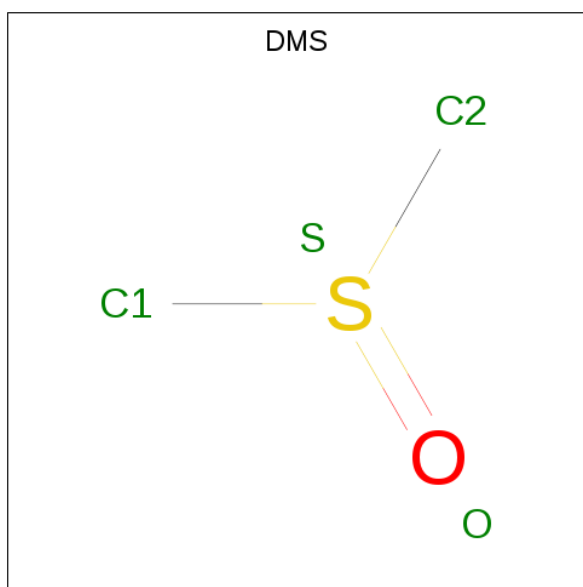
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
28	A	1	54	41	12	1	0	0
28	A	1	54	41	12	1	0	0
28	B	1	108	82	24	2	0	1
28	D	1	43	30	12	1	0	0
28	a	1	54	41	12	1	0	0
28	b	1	108	82	24	2	0	1
28	c	1	54	41	12	1	0	0
28	f	1	43	30	12	1	0	0

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
29	A	1	51	41	10	0	0
29	B	1	51	41	10	0	0
29	C	1	51	41	10	0	0
29	C	1	51	41	10	0	0
29	D	1	51	41	10	0	0
29	Z	1	51	41	10	0	0
29	a	1	51	41	10	0	0
29	c	1	51	41	10	0	0
29	c	1	51	41	10	0	0
29	c	1	51	41	10	0	0
29	d	1	51	41	10	0	0
29	m	1	51	41	10	0	0

- Molecule 30 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



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

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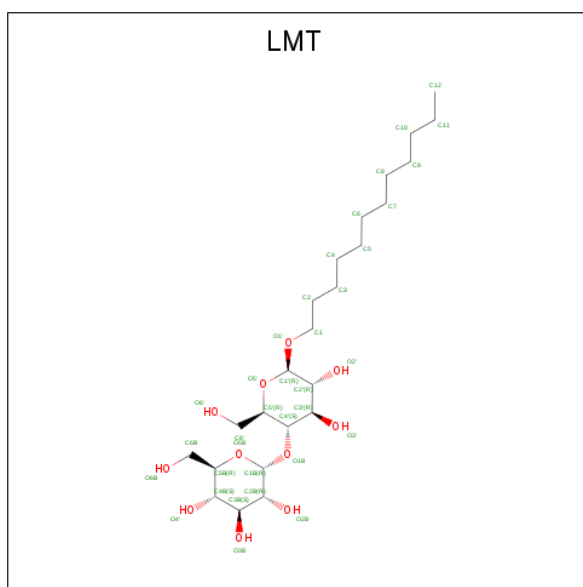
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	O	1	Total 4	C 2	O 1	S 1	0	0
30	O	1	Total 4	C 2	O 1	S 1	0	0
30	U	1	Total 4	C 2	O 1	S 1	0	0
30	V	1	Total 4	C 2	O 1	S 1	0	0
30	V	1	Total 4	C 2	O 1	S 1	0	0
30	a	1	Total 4	C 2	O 1	S 1	0	0
30	a	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	d	1	Total 4	C 2	O 1	S 1	0	0
30	d	1	Total 4	C 2	O 1	S 1	0	0
30	u	1	Total 4	C 2	O 1	S 1	0	0
30	v	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 31 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	J	1	Total C 16 16	0	0
31	i	1	Total C 16 16	0	0
31	D	2	Total C O 56 51 5	0	0
31	K	1	Total C O 34 29 5	0	0
31	y	1	Total C 16 16	0	0
31	l	1	Total C 16 16	0	0
31	B	2	Total C 32 32	0	0
31	I	2	Total C 26 26	0	0
31	c	1	Total C O 32 27 5	0	0
31	a	1	Total C O 30 25 5	0	0
31	x	1	Total C 16 16	0	0
31	A	1	Total C O 28 23 5	0	0
31	j	1	Total C 16 16	0	0
31	X	1	Total C 16 16	0	0
31	d	2	Total C O 52 47 5	0	0
31	t	1	Total C 16 16	0	0
31	Y	1	Total C 16 16	0	0
31	L	1	Total C 16 16	0	0
31	b	2	Total C 32 32	0	0

- Molecule 32 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



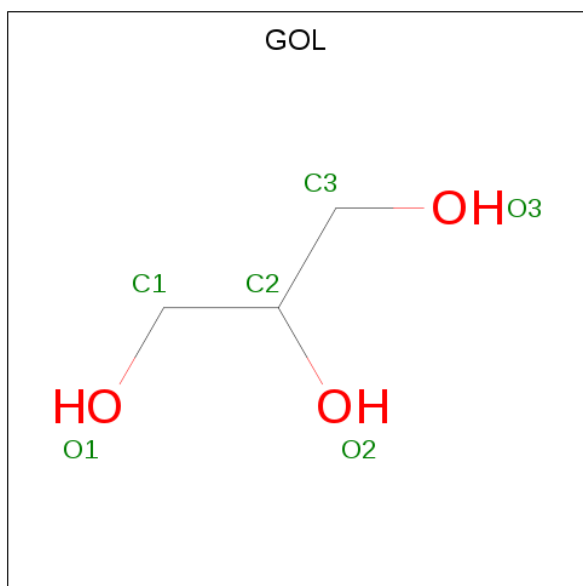
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			35	24	11		
32	A	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	C	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	a	1	Total	C	O	0	0
			35	24	11		
32	a	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			35	24	11		
32	f	1	Total	C	O	0	0
			35	24	11		
32	i	1	Total	C	O	0	0
			35	24	11		
32	m	1	Total	C	O	0	0
			35	24	11		
32	m	1	Total	C	O	0	0
			35	24	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	t	1	Total	C	O	0	0
			35	24	11		

- Molecule 33 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



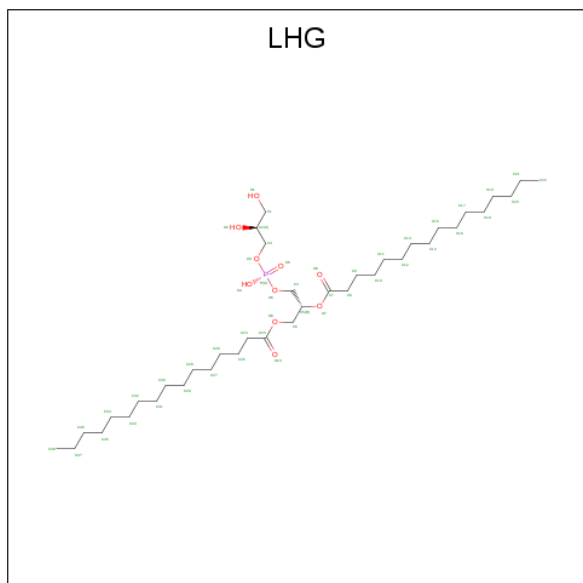
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	A	1	Total	C	O	0	0
			6	3	3		
33	B	1	Total	C	O	0	0
			6	3	3		
33	D	1	Total	C	O	0	0
			6	3	3		
33	V	1	Total	C	O	0	0
			6	3	3		
33	V	1	Total	C	O	0	0
			6	3	3		
33	V	1	Total	C	O	0	0
			6	3	3		
33	a	1	Total	C	O	0	0
			6	3	3		
33	b	1	Total	C	O	0	0
			6	3	3		
33	d	1	Total	C	O	0	0
			6	3	3		
33	d	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	v	1	Total	C	O	0	0
			6	3	3		
33	v	1	Total	C	O	0	0
			6	3	3		

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{76}O_2$).



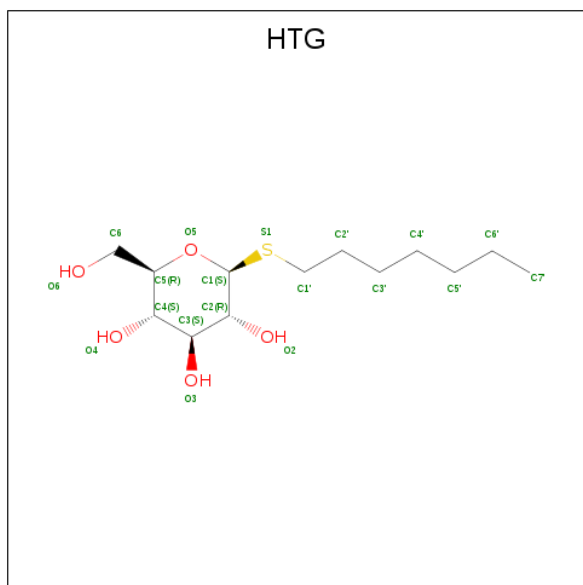
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	P	0	0
			49	38	10	1		
34	D	1	Total	C	O	P	0	0
			49	38	10	1		
34	D	1	Total	C	O	P	0	0
			49	38	10	1		
34	D	1	Total	C	O	P	0	0
			49	38	10	1		
34	E	1	Total	C	O	P	0	0
			49	38	10	1		
34	b	1	Total	C	O	P	0	0
			49	38	10	1		
34	d	1	Total	C	O	P	0	0
			49	38	10	1		
34	d	1	Total	C	O	P	0	0
			49	38	10	1		
34	d	1	Total	C	O	P	0	0
			49	38	10	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
34	e	1	49	38	10	1	0	0

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).



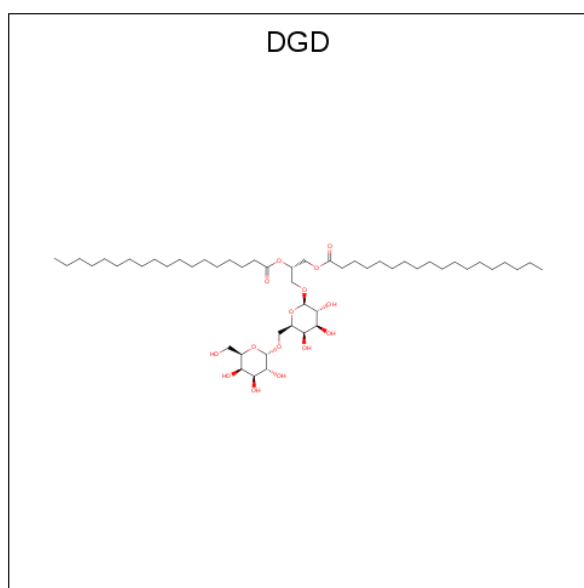
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
35	B	1	19	13	5	1	0	0
35	B	1	19	13	5	1	0	0
35	B	1	19	13	5	1	0	0
35	C	1	19	13	5	1	0	0
35	C	1	19	13	5	1	0	0
35	D	1	19	13	5	1	0	0
35	D	1	19	13	5	1	0	0
35	V	1	19	13	5	1	0	0
35	b	1	19	13	5	1	0	0
35	b	1	19	13	5	1	0	0

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

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



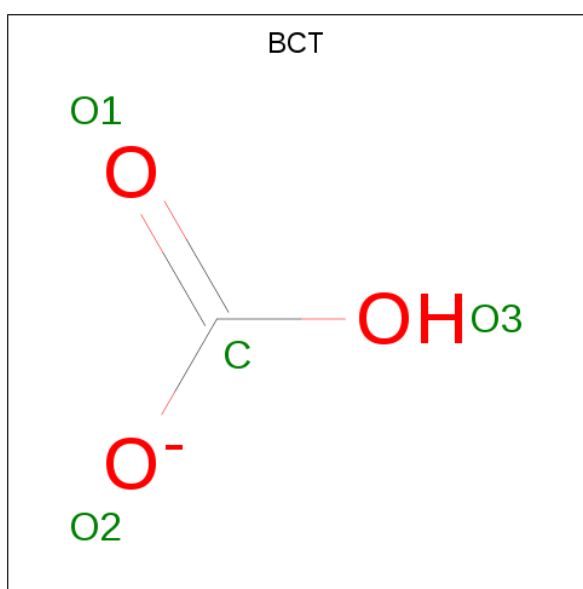
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
36	C	1	Total 62	C 47	O 15	0	0
36	C	1	Total 62	C 47	O 15	0	0
36	C	1	Total 62	C 47	O 15	0	0
36	H	1	Total 62	C 47	O 15	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 37 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	D	1	Total	C	O	0	0
			4	1	3		
37	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
40	A	134	134	134	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	B	252	Total O 253 253	0	1
40	C	168	Total O 168 168	0	0
40	D	132	Total O 132 132	0	0
40	E	22	Total O 22 22	0	0
40	F	6	Total O 6 6	0	0
40	H	31	Total O 31 31	0	0
40	I	4	Total O 4 4	0	0
40	J	7	Total O 7 7	0	0
40	K	7	Total O 7 7	0	0
40	L	11	Total O 11 11	0	0
40	M	6	Total O 6 6	0	0
40	O	119	Total O 119 119	0	0
40	T	10	Total O 10 10	0	0
40	U	63	Total O 63 63	0	0
40	V	96	Total O 96 96	0	0
40	Y	1	Total O 1 1	0	0
40	X	8	Total O 8 8	0	0
40	Z	1	Total O 1 1	0	0
40	R	1	Total O 1 1	0	0
40	a	118	Total O 118 118	0	0
40	b	209	Total O 209 209	0	0

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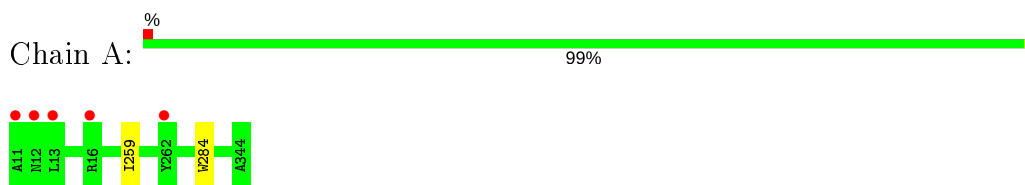
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	c	169	Total O 169 169	0	0
40	d	121	Total O 121 121	0	0
40	e	9	Total O 9 9	0	0
40	f	5	Total O 5 5	0	0
40	h	23	Total O 23 23	0	0
40	i	4	Total O 4 4	0	0
40	j	5	Total O 5 5	0	0
40	k	3	Total O 3 3	0	0
40	l	8	Total O 8 8	0	0
40	m	10	Total O 10 10	0	0
40	o	112	Total O 112 112	0	0
40	t	13	Total O 13 13	0	0
40	u	74	Total O 74 74	0	0
40	v	65	Total O 65 65	0	0
40	y	1	Total O 1 1	0	0
40	x	9	Total O 9 9	0	0

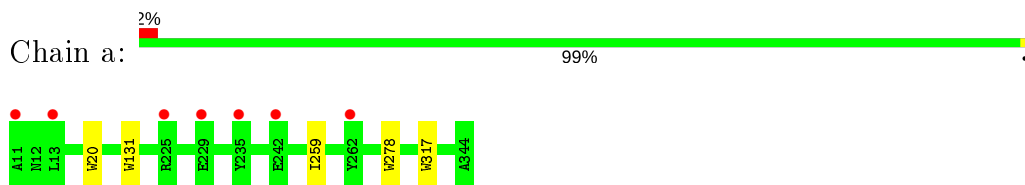
3 Residue-property plots [i](#)

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

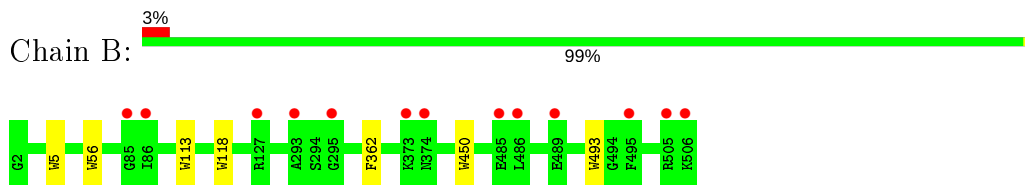
- Molecule 1: Photosystem Q(B) protein



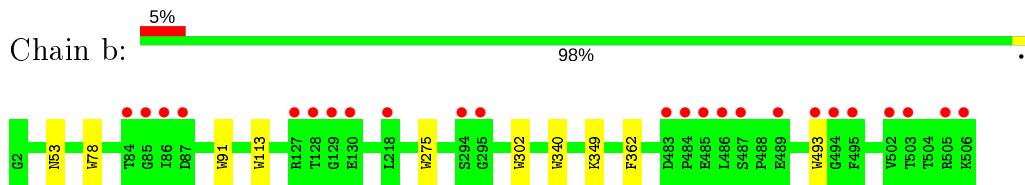
- Molecule 1: Photosystem Q(B) protein



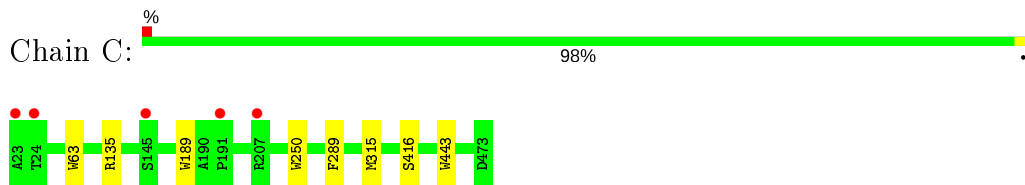
- Molecule 2: Photosystem II core light harvesting protein



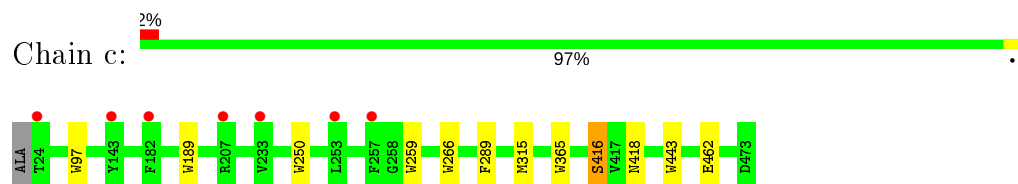
- Molecule 2: Photosystem II core light harvesting protein



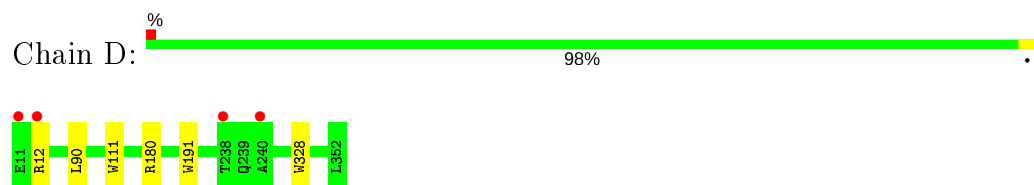
- Molecule 3: Photosystem II CP43 protein



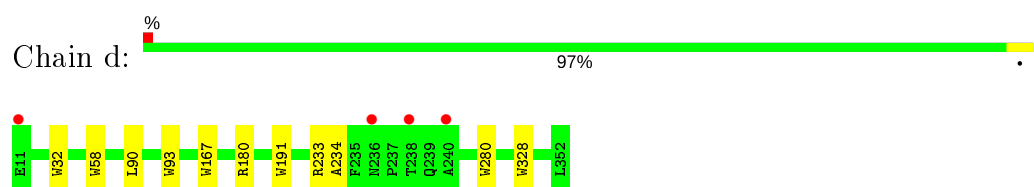
- Molecule 3: Photosystem II CP43 protein



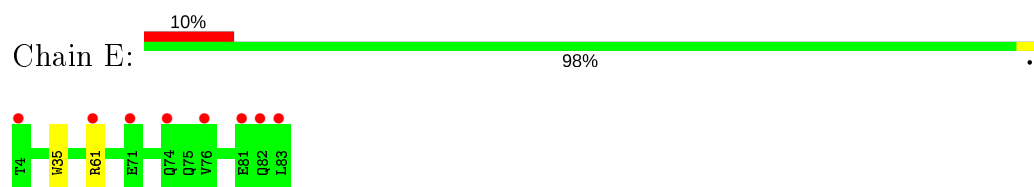
- Molecule 4: Photosystem II D2 protein



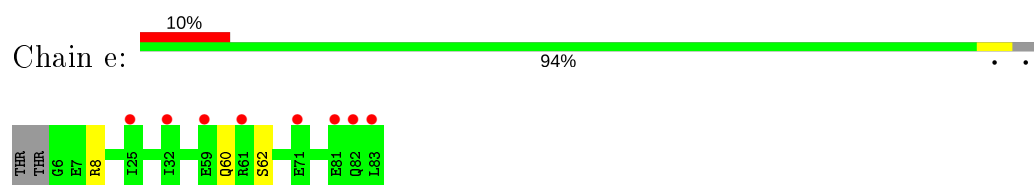
- Molecule 4: Photosystem II D2 protein



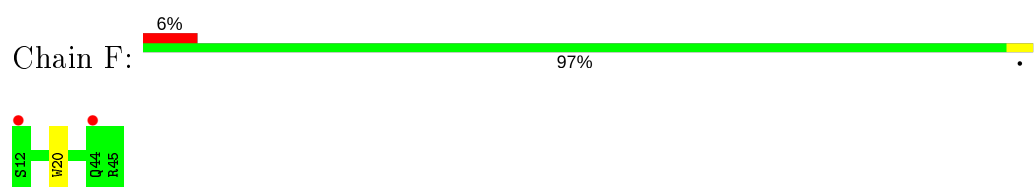
- Molecule 5: Cytochrome b559 subunit alpha



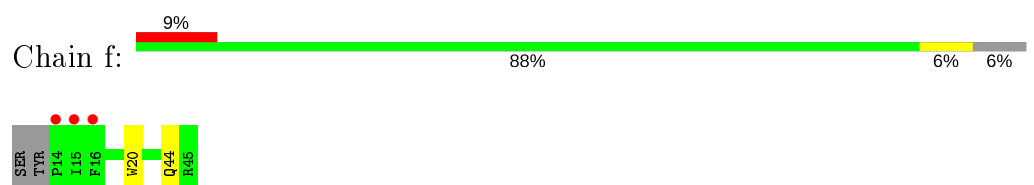
- Molecule 5: Cytochrome b559 subunit alpha



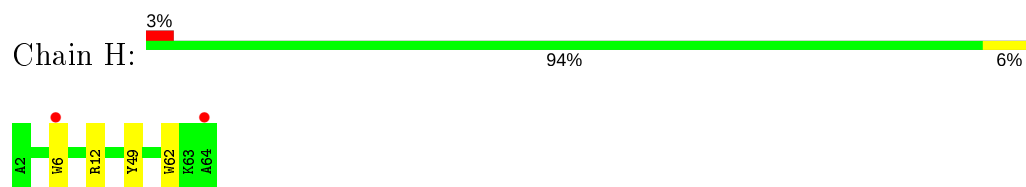
- Molecule 6: Cytochrome b559 subunit beta



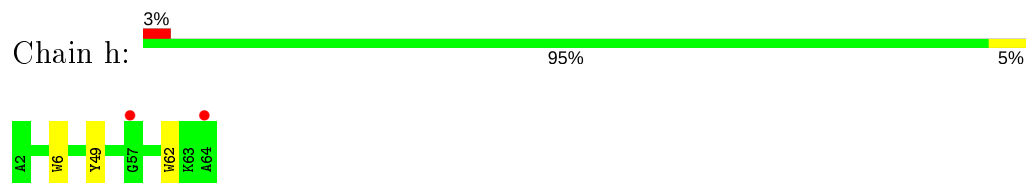
- Molecule 6: Cytochrome b559 subunit beta



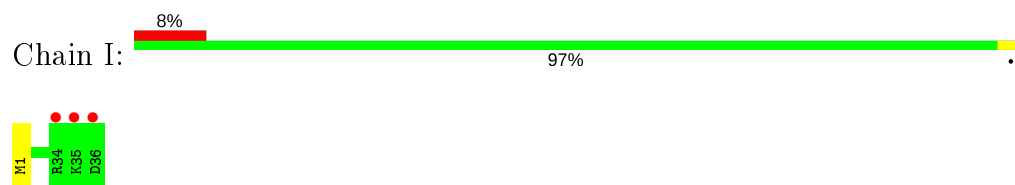
- Molecule 7: Photosystem II reaction center protein H



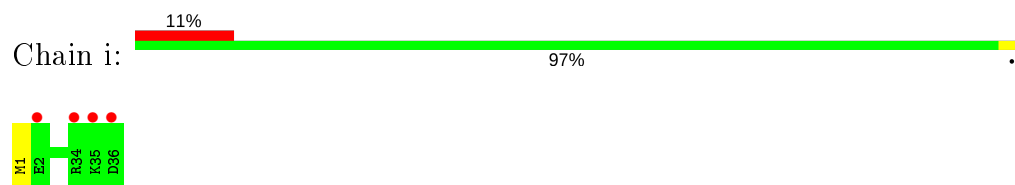
- Molecule 7: Photosystem II reaction center protein H



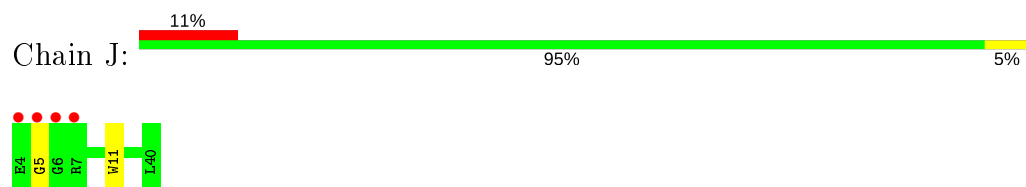
- Molecule 8: Photosystem II reaction center protein I



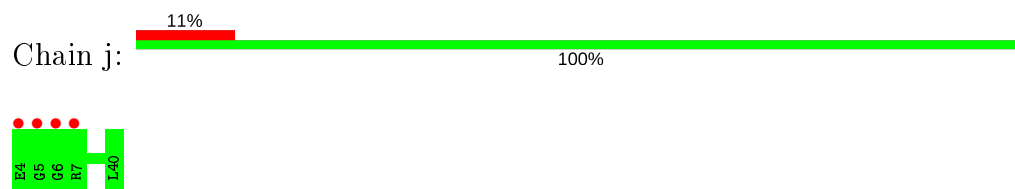
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J

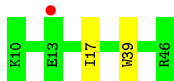


- Molecule 10: Photosystem II reaction center protein K

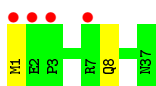




- Molecule 10: Photosystem II reaction center protein K



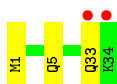
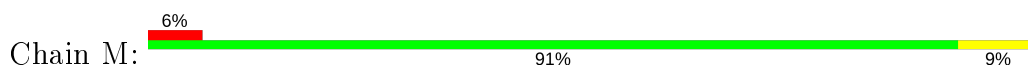
- Molecule 11: Photosystem II reaction center protein L



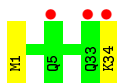
- Molecule 11: Photosystem II reaction center protein L



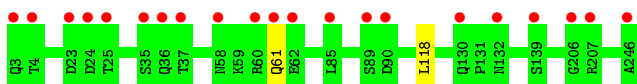
- Molecule 12: Photosystem II reaction center protein M



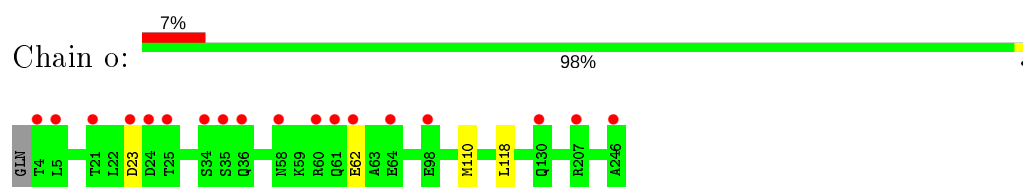
- Molecule 12: Photosystem II reaction center protein M



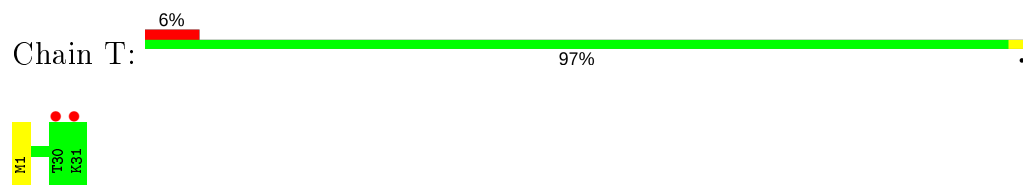
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



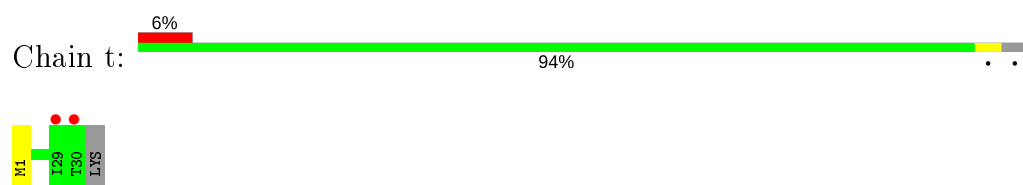
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



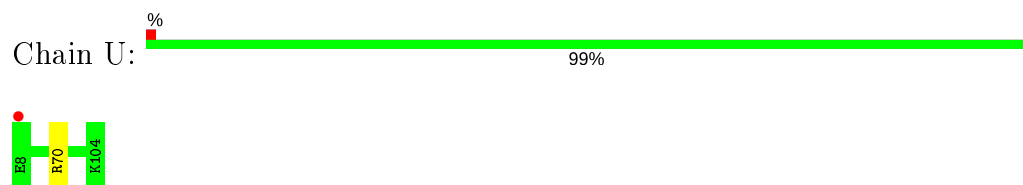
- Molecule 14: Photosystem II reaction center protein T



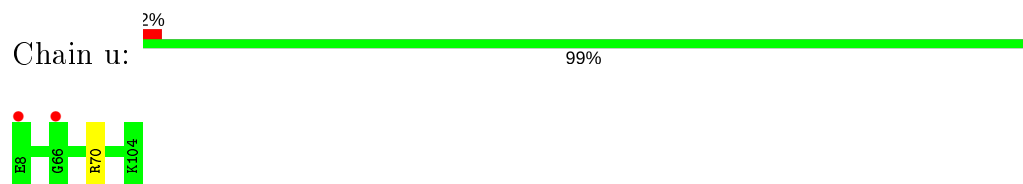
- Molecule 14: Photosystem II reaction center protein T



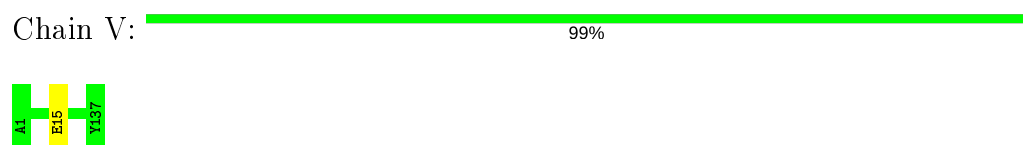
- Molecule 15: Photosystem II 12 kDa extrinsic protein



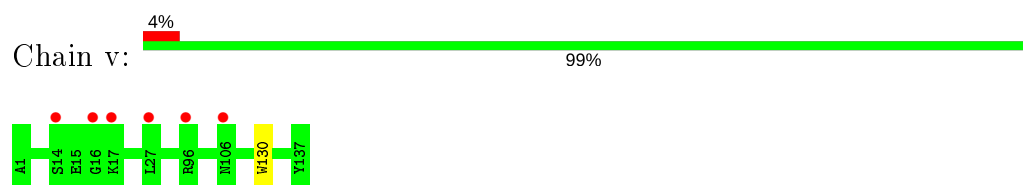
- Molecule 15: Photosystem II 12 kDa extrinsic protein



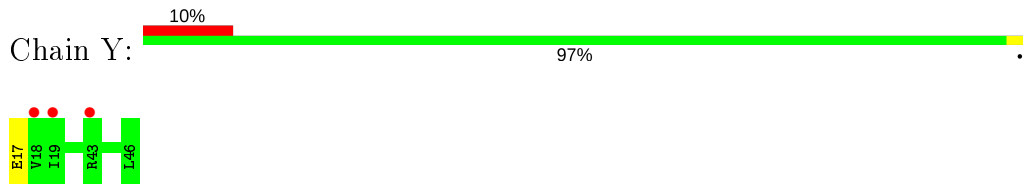
- Molecule 16: Cytochrome c-550



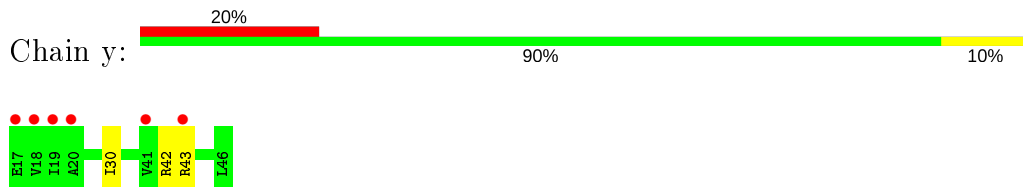
- Molecule 16: Cytochrome c-550



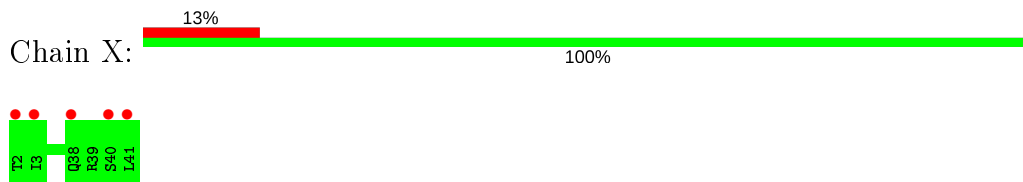
- Molecule 17: Photosystem II reaction center protein ycf12



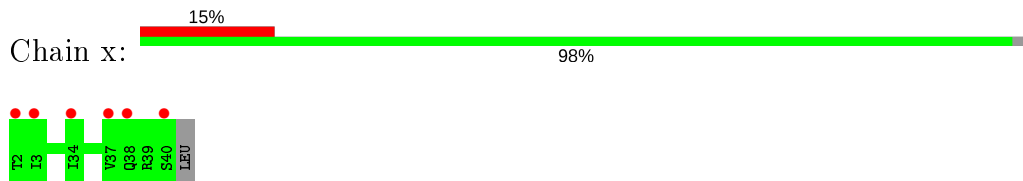
- Molecule 17: Photosystem II reaction center protein ycf12



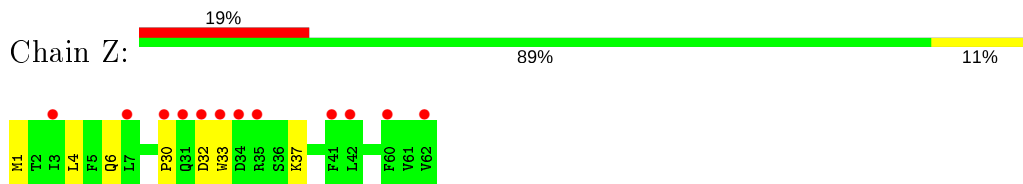
- Molecule 18: Photosystem II reaction center protein X



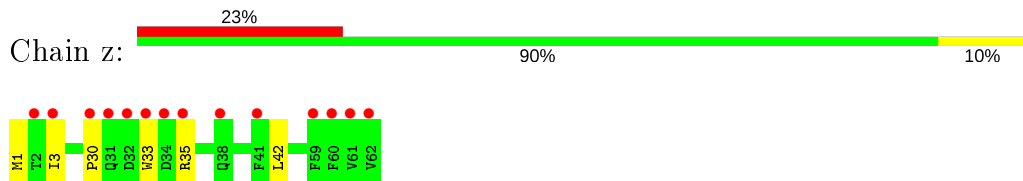
- Molecule 18: Photosystem II reaction center protein X



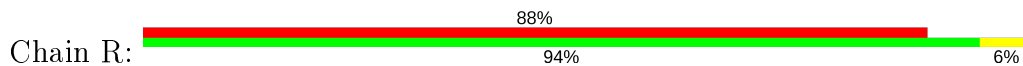
- Molecule 19: Photosystem II reaction center protein Z

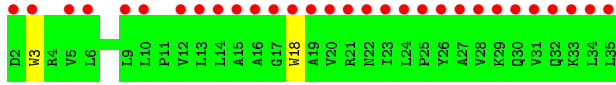


- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.86Å 228.79Å 285.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.10 19.96 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.96-2.10) 99.9 (19.96-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.09Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.176 , 0.205 0.177 , 0.206	Depositor DCC
R_{free} test set	23034 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtrriage
Anisotropy	0.137	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	53568	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, GOL, MG, PHO, DGD, CL, OER, LMT, CLA, PL9, DMS, FE2, SQD, BCT, HEM, FME, UNL, HTG, BCR, LMG

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	0.57	1/2743 (0.0%)	0.52	0/3740
1	a	0.56	4/2734 (0.1%)	0.52	0/3728
2	B	0.58	6/4210 (0.1%)	0.53	0/5731
2	b	0.58	7/4200 (0.2%)	0.52	0/5719
3	C	0.58	4/3622 (0.1%)	0.52	0/4931
3	c	0.58	7/3611 (0.2%)	0.51	0/4916
4	D	0.62	3/2821 (0.1%)	0.54	0/3844
4	d	0.60	7/2821 (0.2%)	0.53	0/3844
5	E	0.51	1/685 (0.1%)	0.51	0/936
5	e	0.49	0/657	0.49	0/897
6	F	0.57	1/284 (0.4%)	0.46	0/387
6	f	0.56	1/265 (0.4%)	0.47	0/360
7	H	0.60	2/522 (0.4%)	0.52	0/712
7	h	0.60	2/511 (0.4%)	0.53	0/697
8	I	0.34	0/293	0.42	0/396
8	i	0.35	0/293	0.44	0/396
9	J	0.54	1/272 (0.4%)	0.49	0/368
9	j	0.51	0/272	0.49	0/368
10	K	0.52	1/303 (0.3%)	0.49	0/416
10	k	0.51	1/303 (0.3%)	0.52	0/416
11	L	0.38	0/311	0.46	0/422
11	l	0.36	0/311	0.47	0/422
12	M	0.30	0/270	0.48	0/368
12	m	0.33	0/270	0.47	0/368
13	O	0.34	0/1920	0.53	0/2603
13	o	0.33	0/1902	0.52	0/2579
14	T	0.40	0/266	0.45	0/360
14	t	0.38	0/257	0.45	0/349
15	U	0.36	0/794	0.51	0/1076
15	u	0.34	0/794	0.51	0/1076
16	V	0.40	0/1111	0.49	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.40	1/1103 (0.1%)	0.48	0/1497
17	Y	0.33	0/225	0.49	0/301
17	y	0.30	0/225	0.48	0/301
18	X	0.32	0/299	0.43	0/403
18	x	0.33	0/290	0.42	0/392
19	Z	0.52	1/482 (0.2%)	0.46	0/659
19	z	0.51	1/482 (0.2%)	0.46	0/659
20	R	0.65	2/279 (0.7%)	0.52	0/383
All	All	0.53	54/43013 (0.1%)	0.51	0/58527

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	317	TRP	CD2-CE2	5.39	1.47	1.41
4	d	167	TRP	CD2-CE2	5.37	1.47	1.41
4	d	191	TRP	CD2-CE2	5.34	1.47	1.41
2	b	91	TRP	CD2-CE2	5.32	1.47	1.41
2	B	56	TRP	CD2-CE2	5.26	1.47	1.41
4	D	111	TRP	CD2-CE2	5.24	1.47	1.41
3	c	365	TRP	CD2-CE2	5.23	1.47	1.41
6	F	20	TRP	CD2-CE2	5.20	1.47	1.41
2	b	493	TRP	CD2-CE2	5.17	1.47	1.41
3	c	189	TRP	CD2-CE2	5.16	1.47	1.41
5	E	35	TRP	CD2-CE2	5.15	1.47	1.41
2	B	113	TRP	CD2-CE2	5.15	1.47	1.41
3	C	443	TRP	CD2-CE2	5.15	1.47	1.41
4	d	93	TRP	CD2-CE2	5.15	1.47	1.41
20	R	18	TRP	CD2-CE2	5.15	1.47	1.41
1	A	284	TRP	CD2-CE2	5.14	1.47	1.41
3	c	97	TRP	CD2-CE2	5.14	1.47	1.41
1	a	278	TRP	CD2-CE2	5.13	1.47	1.41
7	h	62	TRP	CD2-CE2	5.12	1.47	1.41
4	d	280	TRP	CD2-CE2	5.12	1.47	1.41
7	h	6	TRP	CD2-CE2	5.11	1.47	1.41
7	H	6	TRP	CD2-CE2	5.11	1.47	1.41
9	J	11	TRP	CD2-CE2	5.11	1.47	1.41
4	D	328	TRP	CD2-CE2	5.10	1.47	1.41
20	R	3	TRP	CD2-CE2	5.09	1.47	1.41
4	d	58	TRP	CD2-CE2	5.09	1.47	1.41
4	d	32	TRP	CD2-CE2	5.09	1.47	1.41
4	D	191	TRP	CD2-CE2	5.09	1.47	1.41
2	B	118	TRP	CD2-CE2	5.09	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	493	TRP	CD2-CE2	5.09	1.47	1.41
2	b	78	TRP	CD2-CE2	5.09	1.47	1.41
16	v	130	TRP	CD2-CE2	5.09	1.47	1.41
6	f	20	TRP	CD2-CE2	5.08	1.47	1.41
19	Z	33	TRP	CD2-CE2	5.07	1.47	1.41
19	z	33	TRP	CD2-CE2	5.07	1.47	1.41
3	c	266	TRP	CD2-CE2	5.07	1.47	1.41
3	c	259	TRP	CD2-CE2	5.06	1.47	1.41
3	c	250	TRP	CD2-CE2	5.05	1.47	1.41
7	H	62	TRP	CD2-CE2	5.05	1.47	1.41
3	c	443	TRP	CD2-CE2	5.05	1.47	1.41
3	C	250	TRP	CD2-CE2	5.04	1.47	1.41
2	b	340	TRP	CD2-CE2	5.04	1.47	1.41
10	k	39	TRP	CD2-CE2	5.04	1.47	1.41
2	b	275	TRP	CD2-CE2	5.04	1.47	1.41
2	B	450	TRP	CD2-CE2	5.04	1.47	1.41
10	K	39	TRP	CD2-CE2	5.04	1.47	1.41
3	C	63	TRP	CD2-CE2	5.03	1.47	1.41
1	a	131	TRP	CD2-CE2	5.02	1.47	1.41
2	b	113	TRP	CD2-CE2	5.02	1.47	1.41
2	B	5	TRP	CD2-CE2	5.02	1.47	1.41
1	a	20	TRP	CD2-CE2	5.01	1.47	1.41
3	C	189	TRP	CD2-CE2	5.01	1.47	1.41
2	b	302	TRP	CD2-CE2	5.00	1.47	1.41
4	d	328	TRP	CD2-CE2	5.00	1.47	1.41

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	337/334 (101%)	333 (99%)	3 (1%)	1 (0%)	41	41
1	a	336/334 (101%)	331 (98%)	4 (1%)	1 (0%)	41	41
2	B	513/505 (102%)	505 (98%)	8 (2%)	0	100	100
2	b	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
3	C	452/451 (100%)	442 (98%)	9 (2%)	1 (0%)	47	49
3	c	450/451 (100%)	441 (98%)	8 (2%)	1 (0%)	47	49
4	D	340/342 (99%)	331 (97%)	9 (3%)	0	100	100
4	d	340/342 (99%)	333 (98%)	6 (2%)	1 (0%)	41	41
5	E	80/80 (100%)	79 (99%)	1 (1%)	0	100	100
5	e	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	30/34 (88%)	30 (100%)	0	0	100	100
7	H	62/63 (98%)	59 (95%)	3 (5%)	0	100	100
7	h	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
8	I	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
8	i	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
9	J	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	4	1
9	j	35/37 (95%)	35 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	33/34 (97%)	33 (100%)	0	0	100	100
12	m	33/34 (97%)	33 (100%)	0	0	100	100
13	O	244/244 (100%)	240 (98%)	4 (2%)	0	100	100
13	o	242/244 (99%)	234 (97%)	8 (3%)	0	100	100
14	T	29/31 (94%)	29 (100%)	0	0	100	100
14	t	28/31 (90%)	28 (100%)	0	0	100	100
15	U	96/97 (99%)	93 (97%)	3 (3%)	0	100	100
15	u	96/97 (99%)	94 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	V	138/137 (101%)	134 (97%)	4 (3%)	0	100	100
16	v	137/137 (100%)	134 (98%)	3 (2%)	0	100	100
17	Y	28/30 (93%)	28 (100%)	0	0	100	100
17	y	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
18	X	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	37 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	4
19	z	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	9	4
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	5258/5296 (99%)	5151 (98%)	99 (2%)	8 (0%)	47	49

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
3	c	416	SER
9	J	5	GLY
4	d	234	ALA
19	z	30	PRO
19	Z	30	PRO
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	274/269 (102%)	274 (100%)	0	100	100
1	a	273/269 (102%)	273 (100%)	0	100	100
2	B	413/403 (102%)	412 (100%)	1 (0%)	93	96
2	b	412/403 (102%)	409 (99%)	3 (1%)	84	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	355/352 (101%)	352 (99%)	3 (1%)	81	86
3	c	354/352 (101%)	349 (99%)	5 (1%)	67	73
4	D	277/277 (100%)	274 (99%)	3 (1%)	73	79
4	d	277/277 (100%)	274 (99%)	3 (1%)	73	79
5	E	73/71 (103%)	72 (99%)	1 (1%)	67	73
5	e	69/71 (97%)	66 (96%)	3 (4%)	29	29
6	F	28/28 (100%)	28 (100%)	0	100	100
6	f	26/28 (93%)	25 (96%)	1 (4%)	33	34
7	H	54/53 (102%)	51 (94%)	3 (6%)	21	18
7	h	53/53 (100%)	52 (98%)	1 (2%)	57	63
8	I	32/32 (100%)	32 (100%)	0	100	100
8	i	32/32 (100%)	32 (100%)	0	100	100
9	J	25/25 (100%)	25 (100%)	0	100	100
9	j	25/25 (100%)	25 (100%)	0	100	100
10	K	30/30 (100%)	29 (97%)	1 (3%)	38	40
10	k	30/30 (100%)	29 (97%)	1 (3%)	38	40
11	L	35/35 (100%)	33 (94%)	2 (6%)	20	18
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	31/30 (103%)	29 (94%)	2 (6%)	17	14
12	m	31/30 (103%)	30 (97%)	1 (3%)	39	41
13	O	209/207 (101%)	207 (99%)	2 (1%)	76	82
13	o	207/207 (100%)	203 (98%)	4 (2%)	57	63
14	T	27/27 (100%)	27 (100%)	0	100	100
14	t	26/27 (96%)	26 (100%)	0	100	100
15	U	85/84 (101%)	84 (99%)	1 (1%)	71	77
15	u	85/84 (101%)	84 (99%)	1 (1%)	71	77
16	V	120/117 (103%)	119 (99%)	1 (1%)	81	86
16	v	119/117 (102%)	119 (100%)	0	100	100
17	Y	23/23 (100%)	22 (96%)	1 (4%)	29	29
17	y	23/23 (100%)	20 (87%)	3 (13%)	4	2
18	X	33/33 (100%)	33 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	x	32/33 (97%)	32 (100%)	0	100	100
19	Z	51/51 (100%)	47 (92%)	4 (8%)	12	9
19	z	51/51 (100%)	48 (94%)	3 (6%)	19	17
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4364/4323 (101%)	4310 (99%)	54 (1%)	71	77

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	362	PHE
3	C	135	ARG
3	C	289	PHE
3	C	315	MET
4	D	12	ARG
4	D	90	LEU
4	D	180	ARG
5	E	61	ARG
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	49	TYR
10	K	17	ILE
11	L	1	MET
11	L	8	GLN
12	M	5	GLN
12	M	33	GLN
13	O	61	GLN
13	O	118	LEU
15	U	70	ARG
16	V	15	GLU
17	Y	17	GLU
19	Z	4	LEU
19	Z	6	GLN
19	Z	32	ASP
19	Z	37	LYS
2	b	53	ASN
2	b	349	LYS
2	b	362	PHE
3	c	289	PHE
3	c	315	MET
3	c	416	SER
3	c	418	ASN

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Mol	Chain	Res	Type
3	c	462	GLU
4	d	90	LEU
4	d	180	ARG
4	d	233	ARG
5	e	8	ARG
5	e	60	GLN
5	e	62	SER
6	f	44	GLN
7	h	49	TYR
10	k	17	ILE
12	m	34	LYS
13	o	23	ASP
13	o	62	GLU
13	o	110	MET
13	o	118	LEU
15	u	70	ARG
17	y	30	ILE
17	y	42	ARG
17	y	43	ARG
19	z	3	ILE
19	z	35	ARG
19	z	42	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	GLN
1	A	315	ASN
2	B	14	ASN
2	B	53	ASN
2	B	331	ASN
3	C	25	ASN
4	D	83	ASN
11	L	8	GLN
12	M	33	GLN
13	O	61	GLN
13	O	82	GLN
13	O	124	ASN
13	O	147	ASN
16	V	34	GLN
16	V	118	HIS
19	Z	58	ASN

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Mol	Chain	Res	Type
1	a	315	ASN
2	b	53	ASN
2	b	331	ASN
4	d	83	ASN
4	d	332	GLN
5	e	75	GLN
13	o	124	ASN
13	o	147	ASN
16	v	34	GLN
19	z	31	GLN
19	z	58	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](#)

8 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
19	FME	Z	1	19	8,9,10	0.60	0	7,9,11	1.97	4 (57%)
8	FME	I	1	8	8,9,10	0.54	0	7,9,11	1.30	1 (14%)
12	FME	m	1	12	8,9,10	0.50	0	7,9,11	1.58	2 (28%)
14	FME	T	1	14	8,9,10	0.55	0	7,9,11	1.84	3 (42%)
8	FME	i	1	8	8,9,10	0.51	0	7,9,11	1.35	1 (14%)
19	FME	z	1	19	8,9,10	0.48	0	7,9,11	1.73	1 (14%)
12	FME	M	1	12	8,9,10	0.49	0	7,9,11	1.53	2 (28%)
14	FME	t	1	14	8,9,10	0.50	0	7,9,11	1.60	2 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	FME	Z	1	19	-	4/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
14	FME	T	1	14	-	2/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
19	FME	z	1	19	-	5/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	1	FME	CE-SD-CG	3.06	110.90	100.40
14	T	1	FME	C-CA-N	2.88	114.93	109.73
14	T	1	FME	CE-SD-CG	2.85	110.19	100.40
19	Z	1	FME	C-CA-N	2.77	114.73	109.73
19	z	1	FME	CE-SD-CG	2.74	109.81	100.40
14	t	1	FME	CE-SD-CG	2.70	109.68	100.40
12	M	1	FME	CE-SD-CG	2.58	109.27	100.40
12	m	1	FME	CE-SD-CG	2.46	108.86	100.40
8	I	1	FME	CE-SD-CG	2.19	107.93	100.40
14	T	1	FME	O-C-CA	-2.14	119.17	124.78
14	t	1	FME	O-C-CA	-2.10	119.28	124.78
12	M	1	FME	O1-CN-N	-2.08	119.80	125.27
12	m	1	FME	O1-CN-N	-2.07	119.81	125.27
8	i	1	FME	CE-SD-CG	2.07	107.52	100.40
19	Z	1	FME	O1-CN-N	-2.03	119.93	125.27
19	Z	1	FME	O-C-CA	-2.03	119.47	124.78

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	Z	1	FME	O1-CN-N-CA
19	Z	1	FME	N-CA-CB-CG
8	I	1	FME	O1-CN-N-CA

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

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 261 ligands modelled in this entry, 24 are unknown and 10 are monoatomic - leaving 227 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$
26	BCR	b	622	-	41,41,41	3.90	15 (36%)	56,56,56	8.19	36 (64%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	DGD	c	515	-	63,63,67	0.89	3 (4%)	77,77,81	0.89	2 (2%)
30	DMS	O	301	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0
34	LHG	D	410	-	48,48,48	0.87	2 (4%)	51,54,54	0.95	4 (7%)
24	CLA	C	503	-	59,73,73	2.57	14 (23%)	67,113,113	2.09	14 (20%)
30	DMS	B	634	-	3,3,3	2.68	1 (33%)	3,3,3	0.48	0
24	CLA	B	612	-	59,73,73	2.40	14 (23%)	67,113,113	1.95	15 (22%)
32	LMT	C	520	-	36,36,36	0.52	0	47,47,47	1.01	1 (2%)
34	LHG	E	101	-	48,48,48	0.96	2 (4%)	51,54,54	0.96	3 (5%)
26	BCR	D	406	-	41,41,41	3.87	14 (34%)	56,56,56	8.13	45 (80%)
28	SQD	a	401	-	53,54,54	1.04	3 (5%)	62,65,65	1.16	5 (8%)
24	CLA	c	502	-	59,73,73	2.41	15 (25%)	67,113,113	2.05	16 (23%)
24	CLA	b	618	-	59,73,73	2.44	14 (23%)	67,113,113	2.13	15 (22%)
24	CLA	b	617	-	59,73,73	2.60	15 (25%)	67,113,113	2.16	20 (29%)
33	GOL	b	632	-	5,5,5	0.22	0	5,5,5	0.28	0
24	CLA	A	1005	-	59,73,73	2.29	14 (23%)	67,113,113	1.94	13 (19%)
24	CLA	C	504	40	59,73,73	2.51	15 (25%)	67,113,113	2.10	17 (25%)
24	CLA	b	607	-	59,73,73	2.47	14 (23%)	67,113,113	2.33	13 (19%)
26	BCR	b	620	-	41,41,41	3.82	14 (34%)	56,56,56	8.09	40 (71%)
26	BCR	a	413	-	41,41,41	3.75	14 (34%)	56,56,56	8.51	40 (71%)
24	CLA	a	408	40	59,73,73	2.21	13 (22%)	67,113,113	1.95	16 (23%)
30	DMS	u	201	-	3,3,3	2.63	1 (33%)	3,3,3	0.51	0
35	HTG	C	521	-	19,19,19	1.05	2 (10%)	23,24,24	1.23	1 (4%)
26	BCR	K	101	-	41,41,41	3.85	15 (36%)	56,56,56	8.01	41 (73%)
32	LMT	a	402	-	36,36,36	0.58	1 (2%)	47,47,47	0.86	3 (6%)
30	DMS	c	528	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0
32	LMT	m	101	-	36,36,36	0.47	0	47,47,47	0.69	0
24	CLA	B	601	40	59,73,73	2.43	16 (27%)	67,113,113	2.14	17 (25%)
36	DGD	C	517	-	63,63,67	0.85	2 (3%)	77,77,81	0.87	2 (2%)
30	DMS	O	302	-	3,3,3	2.67	1 (33%)	3,3,3	0.58	0
26	BCR	B	619	-	41,41,41	3.87	15 (36%)	56,56,56	7.98	35 (62%)
24	CLA	B	611	-	59,73,73	2.52	14 (23%)	67,113,113	2.04	14 (20%)
33	GOL	v	204	-	5,5,5	0.25	0	5,5,5	0.31	0
28	SQD	c	518	-	53,54,54	1.04	3 (5%)	62,65,65	1.30	7 (11%)
35	HTG	D	413	-	19,19,19	1.05	2 (10%)	23,24,24	1.29	1 (4%)
34	LHG	d	406	-	48,48,48	0.94	2 (4%)	51,54,54	0.92	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	SQD	f	102	-	42,43,54	1.20	4 (9%)	51,54,65	1.37	7 (13%)
26	BCR	T	101	-	41,41,41	3.90	15 (36%)	56,56,56	8.04	38 (67%)
35	HTG	d	416	-	19,19,19	1.01	2 (10%)	23,24,24	1.59	1 (4%)
24	CLA	b	608	-	59,73,73	2.14	14 (23%)	67,113,113	1.94	15 (22%)
33	GOL	A	1019	-	5,5,5	0.26	0	5,5,5	0.30	0
30	DMS	c	529	-	3,3,3	2.60	1 (33%)	3,3,3	0.48	0
30	DMS	c	526	-	3,3,3	2.65	1 (33%)	3,3,3	0.46	0
36	DGD	h	102	-	63,63,67	0.91	3 (4%)	77,77,81	0.84	3 (3%)
26	BCR	y	101	-	41,41,41	3.91	15 (36%)	56,56,56	8.83	44 (78%)
24	CLA	b	604	40	59,73,73	2.79	15 (25%)	67,113,113	2.12	17 (25%)
32	LMT	a	416	-	36,36,36	0.50	0	47,47,47	0.76	1 (2%)
24	CLA	c	508	-	59,73,73	2.63	16 (27%)	67,113,113	2.05	16 (23%)
27	PL9	D	407	-	55,55,55	0.73	2 (3%)	68,69,69	1.43	13 (19%)
32	LMT	i	102	-	36,36,36	0.51	0	47,47,47	1.02	2 (4%)
26	BCR	t	101	-	41,41,41	3.89	15 (36%)	56,56,56	8.09	40 (71%)
33	GOL	d	417	-	5,5,5	0.32	0	5,5,5	0.17	0
36	DGD	c	516	-	63,63,67	0.92	3 (4%)	77,77,81	0.91	3 (3%)
38	HEM	V	201	16	27,50,50	2.14	6 (22%)	17,82,82	2.01	4 (23%)
30	DMS	A	1014	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
30	DMS	C	525	-	3,3,3	2.67	1 (33%)	3,3,3	0.54	0
24	CLA	C	512	-	59,73,73	3.02	14 (23%)	67,113,113	2.08	17 (25%)
29	LMG	A	1012	-	51,51,55	0.95	2 (3%)	59,59,63	0.92	2 (3%)
24	CLA	c	501	-	59,73,73	2.49	15 (25%)	67,113,113	2.14	16 (23%)
34	LHG	D	409	-	48,48,48	0.91	2 (4%)	51,54,54	0.96	3 (5%)
35	HTG	b	626	-	19,19,19	1.00	1 (5%)	23,24,24	1.18	2 (8%)
24	CLA	B	615	-	59,73,73	2.58	16 (27%)	67,113,113	2.20	16 (23%)
24	CLA	C	506	-	59,73,73	2.41	15 (25%)	67,113,113	2.07	14 (20%)
24	CLA	B	606	-	59,73,73	2.63	16 (27%)	67,113,113	2.20	17 (25%)
30	DMS	c	524	-	3,3,3	2.58	1 (33%)	3,3,3	0.34	0
21	OER	a	403	1,3,40	0,15,15	0.00	-	-	-	-
30	DMS	d	413	-	3,3,3	2.68	1 (33%)	3,3,3	0.60	0
29	LMG	a	415	-	51,51,55	0.96	2 (3%)	59,59,63	0.97	2 (3%)
29	LMG	d	409	39	51,51,55	0.94	2 (3%)	59,59,63	0.87	2 (3%)
35	HTG	b	601	-	19,19,19	1.01	2 (10%)	23,24,24	1.36	1 (4%)
24	CLA	c	512	-	59,73,73	2.55	15 (25%)	67,113,113	2.15	17 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	C	507	40	59,73,73	2.73	14 (23%)	67,113,113	2.29	15 (22%)
34	LHG	e	101	-	48,48,48	0.97	2 (4%)	51,54,54	0.99	2 (3%)
24	CLA	b	614	-	59,73,73	2.35	14 (23%)	67,113,113	1.94	15 (22%)
26	BCR	k	102	-	41,41,41	3.81	15 (36%)	56,56,56	8.37	37 (66%)
26	BCR	c	514	-	41,41,41	3.91	15 (36%)	56,56,56	8.73	41 (73%)
30	DMS	B	632	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
24	CLA	B	608	-	59,73,73	2.42	15 (25%)	67,113,113	2.01	15 (22%)
33	GOL	V	206	-	5,5,5	0.28	0	5,5,5	0.24	0
24	CLA	c	513	-	59,73,73	2.53	15 (25%)	67,113,113	2.00	16 (23%)
24	CLA	d	403	-	59,73,73	2.54	15 (25%)	67,113,113	1.92	16 (23%)
24	CLA	b	615	-	59,73,73	2.36	14 (23%)	67,113,113	2.10	15 (22%)
35	HTG	c	522	-	19,19,19	1.00	2 (10%)	23,24,24	1.19	1 (4%)
30	DMS	a	417	-	3,3,3	2.55	1 (33%)	3,3,3	0.38	0
35	HTG	D	419	-	19,19,19	1.01	1 (5%)	23,24,24	1.55	1 (4%)
24	CLA	A	1006	40	59,73,73	2.16	14 (23%)	67,113,113	1.94	17 (25%)
36	DGD	C	515	-	63,63,67	0.87	2 (3%)	77,77,81	0.87	3 (3%)
24	CLA	b	613	40	59,73,73	2.36	14 (23%)	67,113,113	2.00	13 (19%)
32	LMT	M	101	-	36,36,36	0.48	0	47,47,47	0.89	0
24	CLA	c	503	-	59,73,73	2.71	15 (25%)	67,113,113	2.07	15 (22%)
34	LHG	b	624	-	48,48,48	0.91	2 (4%)	51,54,54	0.95	2 (3%)
30	DMS	B	626	-	3,3,3	2.54	1 (33%)	3,3,3	0.35	0
24	CLA	a	409	40	59,73,73	2.28	13 (22%)	67,113,113	1.95	15 (22%)
24	CLA	B	602	-	59,73,73	2.35	15 (25%)	67,113,113	1.99	16 (23%)
30	DMS	V	203	-	3,3,3	2.68	1 (33%)	3,3,3	0.51	0
24	CLA	c	507	40	59,73,73	2.51	15 (25%)	67,113,113	2.33	17 (25%)
30	DMS	b	633	-	3,3,3	2.66	1 (33%)	3,3,3	0.65	0
27	PL9	A	1010	-	55,55,55	0.68	2 (3%)	68,69,69	1.63	17 (25%)
24	CLA	c	509	-	59,73,73	2.47	15 (25%)	67,113,113	2.14	17 (25%)
35	HTG	o	301	-	19,19,19	1.04	1 (5%)	23,24,24	1.30	1 (4%)
34	LHG	d	408	-	48,48,48	0.95	2 (4%)	51,54,54	0.94	2 (3%)
24	CLA	A	1008	-	59,73,73	2.40	15 (25%)	67,113,113	2.04	16 (23%)
38	HEM	f	101	5,6	27,50,50	2.14	6 (22%)	17,82,82	1.90	3 (17%)
24	CLA	C	510	-	59,73,73	2.29	15 (25%)	67,113,113	2.10	15 (22%)
35	HTG	b	630	-	19,19,19	1.08	2 (10%)	23,24,24	1.69	2 (8%)
29	LMG	Z	101	-	51,51,55	0.98	2 (3%)	59,59,63	0.99	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	SQD	A	1016	-	53,54,54	1.04	3 (5%)	62,65,65	1.16	5 (8%)
30	DMS	C	526	-	3,3,3	2.65	1 (33%)	3,3,3	0.50	0
29	LMG	c	521	-	51,51,55	1.00	3 (5%)	59,59,63	1.06	3 (5%)
36	DGD	H	102	-	63,63,67	0.88	3 (4%)	77,77,81	0.82	3 (3%)
33	GOL	a	420	-	5,5,5	0.28	0	5,5,5	0.27	0
33	GOL	d	415	-	5,5,5	0.28	0	5,5,5	0.33	0
24	CLA	C	508	-	59,73,73	2.46	16 (27%)	67,113,113	1.99	15 (22%)
24	CLA	B	614	-	59,73,73	2.46	15 (25%)	67,113,113	2.22	19 (28%)
29	LMG	B	622	-	51,51,55	0.98	2 (3%)	59,59,63	0.90	2 (3%)
35	HTG	b	602	-	19,19,19	1.02	2 (10%)	23,24,24	1.38	1 (4%)
24	CLA	B	607	40	59,73,73	2.44	15 (25%)	67,113,113	2.10	17 (25%)
29	LMG	D	412	39	51,51,55	0.90	2 (3%)	59,59,63	0.79	1 (1%)
28	SQD	D	408	-	42,43,54	1.17	3 (7%)	51,54,65	1.61	9 (17%)
24	CLA	b	605	-	59,73,73	2.46	15 (25%)	67,113,113	2.00	16 (23%)
34	LHG	D	411	-	48,48,48	0.94	2 (4%)	51,54,54	0.93	2 (3%)
26	BCR	d	404	-	41,41,41	3.92	15 (36%)	56,56,56	8.26	40 (71%)
24	CLA	b	612	-	59,73,73	2.69	15 (25%)	67,113,113	2.12	13 (19%)
24	CLA	c	505	-	59,73,73	2.39	15 (25%)	67,113,113	2.10	15 (22%)
24	CLA	B	604	-	59,73,73	2.41	13 (22%)	67,113,113	2.22	18 (26%)
38	HEM	F	101	5,6	27,50,50	2.17	5 (18%)	17,82,82	1.83	3 (17%)
33	GOL	V	204	-	5,5,5	0.29	0	5,5,5	0.22	0
24	CLA	B	605	-	59,73,73	2.31	14 (23%)	67,113,113	2.00	16 (23%)
33	GOL	B	631	-	5,5,5	0.24	0	5,5,5	0.25	0
24	CLA	c	511	3	59,73,73	2.76	14 (23%)	67,113,113	2.11	15 (22%)
35	HTG	B	624	-	19,19,19	1.03	2 (10%)	23,24,24	1.52	1 (4%)
24	CLA	C	502	-	59,73,73	2.34	14 (23%)	67,113,113	2.04	15 (22%)
26	BCR	A	1009	-	41,41,41	3.83	14 (34%)	56,56,56	8.21	41 (73%)
24	CLA	B	613	-	59,73,73	2.27	14 (23%)	67,113,113	2.07	18 (26%)
26	BCR	J	101	-	41,41,41	3.89	14 (34%)	56,56,56	8.75	39 (69%)
24	CLA	a	407	-	59,73,73	2.23	14 (23%)	67,113,113	1.83	11 (16%)
24	CLA	C	501	-	59,73,73	2.38	15 (25%)	67,113,113	2.09	16 (23%)
21	OER	A	1001	1,3,40	0,15,15	0.00	-	-	-	-
30	DMS	B	627	-	3,3,3	2.57	1 (33%)	3,3,3	0.45	0
24	CLA	D	402	-	59,73,73	2.17	14 (23%)	67,113,113	2.14	19 (28%)
24	CLA	C	505	-	59,73,73	2.58	15 (25%)	67,113,113	2.13	13 (19%)
37	BCT	d	401	22	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	616	-	59,73,73	2.54	14 (23%)	67,113,113	2.10	16 (23%)
35	HTG	B	629	-	19,19,19	1.02	2 (10%)	23,24,24	1.34	1 (4%)
32	LMT	t	103	-	36,36,36	0.45	0	47,47,47	1.03	2 (4%)
30	DMS	B	633	-	3,3,3	2.69	1 (33%)	3,3,3	0.57	0
24	CLA	B	610	40	59,73,73	2.22	15 (25%)	67,113,113	1.99	13 (19%)
27	PL9	a	414	-	55,55,55	0.70	2 (3%)	68,69,69	1.49	14 (20%)
32	LMT	A	1017	-	36,36,36	0.53	1 (2%)	47,47,47	0.86	1 (2%)
32	LMT	f	103	-	36,36,36	0.52	0	47,47,47	0.66	0
26	BCR	k	101	-	41,41,41	3.87	15 (36%)	56,56,56	8.62	40 (71%)
30	DMS	U	201	-	3,3,3	2.64	1 (33%)	3,3,3	0.48	0
36	DGD	C	516	-	63,63,67	0.91	3 (4%)	77,77,81	0.93	4 (5%)
24	CLA	c	510	-	59,73,73	2.35	15 (25%)	67,113,113	2.03	16 (23%)
29	LMG	C	518	-	51,51,55	0.98	2 (3%)	59,59,63	0.87	2 (3%)
24	CLA	C	513	-	59,73,73	2.59	16 (27%)	67,113,113	2.04	17 (25%)
30	DMS	b	628	-	3,3,3	2.51	1 (33%)	3,3,3	0.50	0
36	DGD	c	517	-	63,63,67	0.89	2 (3%)	77,77,81	0.82	3 (3%)
24	CLA	B	609	-	59,73,73	2.45	14 (23%)	67,113,113	2.02	14 (20%)
24	CLA	B	603	-	59,73,73	2.22	14 (23%)	67,113,113	2.15	16 (23%)
24	CLA	b	611	-	59,73,73	2.38	14 (23%)	67,113,113	2.03	16 (23%)
24	CLA	b	610	40	59,73,73	2.43	15 (25%)	67,113,113	2.15	16 (23%)
24	CLA	C	511	3	59,73,73	2.64	15 (25%)	67,113,113	2.22	15 (22%)
35	HTG	B	628	-	19,19,19	1.05	2 (10%)	23,24,24	1.26	1 (4%)
33	GOL	D	418	-	5,5,5	0.29	0	5,5,5	0.31	0
32	LMT	B	623	-	36,36,36	0.48	0	47,47,47	1.00	2 (4%)
30	DMS	b	635	-	3,3,3	2.67	1 (33%)	3,3,3	0.45	0
32	LMT	b	631	-	36,36,36	0.50	0	47,47,47	0.84	2 (4%)
29	LMG	C	519	-	51,51,55	0.99	2 (3%)	59,59,63	1.06	4 (6%)
28	SQD	A	1011	-	53,54,54	1.02	3 (5%)	62,65,65	1.32	9 (14%)
24	CLA	c	504	40	59,73,73	2.53	15 (25%)	67,113,113	2.06	16 (23%)
25	PHO	A	1007	-	67,69,69	2.04	14 (20%)	85,99,99	1.86	15 (17%)
28	SQD	B	620[B]	-	53,54,54	1.02	3 (5%)	62,65,65	1.17	6 (9%)
24	CLA	b	609	-	59,73,73	2.71	16 (27%)	67,113,113	2.22	17 (25%)
33	GOL	V	207	-	5,5,5	0.24	0	5,5,5	0.35	0
28	SQD	B	620[A]	-	53,54,54	1.04	3 (5%)	62,65,65	1.10	7 (11%)
35	HTG	d	410	-	19,19,19	1.05	2 (10%)	23,24,24	1.29	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	C	509	-	59,73,73	2.31	15 (25%)	67,113,113	2.14	17 (25%)
26	BCR	K	102	-	41,41,41	3.94	15 (36%)	56,56,56	8.47	39 (69%)
24	CLA	b	606	-	59,73,73	2.35	14 (23%)	67,113,113	2.07	17 (25%)
30	DMS	d	414	-	3,3,3	2.65	1 (33%)	3,3,3	0.41	0
35	HTG	V	202	-	19,19,19	0.99	2 (10%)	23,24,24	1.61	3 (13%)
29	LMG	c	519	-	51,51,55	0.98	2 (3%)	59,59,63	0.88	2 (3%)
38	HEM	v	201	16	27,50,50	2.17	6 (22%)	17,82,82	1.69	3 (17%)
28	SQD	b	623[B]	-	53,54,54	1.02	3 (5%)	62,65,65	1.12	7 (11%)
26	BCR	b	621	-	41,41,41	3.84	14 (34%)	56,56,56	8.44	42 (75%)
25	PHO	a	410	-	67,69,69	2.08	15 (22%)	85,99,99	1.84	16 (18%)
24	CLA	d	402	-	59,73,73	2.30	14 (23%)	67,113,113	1.98	15 (22%)
33	GOL	v	203	-	5,5,5	0.33	0	5,5,5	0.32	0
24	CLA	B	616	-	59,73,73	2.27	14 (23%)	67,113,113	2.09	19 (28%)
32	LMT	m	103	-	36,36,36	0.53	1 (2%)	47,47,47	0.78	1 (2%)
35	HTG	C	522	-	19,19,19	1.02	2 (10%)	23,24,24	1.91	5 (21%)
34	LHG	d	407	-	48,48,48	0.88	2 (4%)	51,54,54	0.91	3 (5%)
34	LHG	B	621	-	48,48,48	0.93	2 (4%)	51,54,54	0.92	2 (3%)
30	DMS	b	634	-	3,3,3	2.71	1 (33%)	3,3,3	0.63	0
30	DMS	C	527	-	3,3,3	2.66	1 (33%)	3,3,3	0.55	0
30	DMS	C	524	-	3,3,3	2.59	1 (33%)	3,3,3	0.45	0
37	BCT	D	401	22	0,3,3	0.00	-	0,3,3	0.00	-
30	DMS	v	202	-	3,3,3	2.62	1 (33%)	3,3,3	0.50	0
30	DMS	b	629	-	3,3,3	2.66	1 (33%)	3,3,3	0.44	0
30	DMS	D	417	-	3,3,3	2.68	1 (33%)	3,3,3	0.44	0
26	BCR	H	101	-	41,41,41	3.84	14 (34%)	56,56,56	8.40	42 (75%)
25	PHO	D	404	-	67,69,69	2.11	15 (22%)	85,99,99	1.90	19 (22%)
26	BCR	B	618	-	41,41,41	3.81	14 (34%)	56,56,56	8.43	41 (73%)
28	SQD	b	623[A]	-	53,54,54	1.02	3 (5%)	62,65,65	1.14	7 (11%)
32	LMT	b	625	-	36,36,36	0.51	0	47,47,47	1.20	6 (12%)
26	BCR	B	617	-	41,41,41	3.82	15 (36%)	56,56,56	8.16	37 (66%)
35	HTG	c	525	-	19,19,19	1.05	2 (10%)	23,24,24	1.18	1 (4%)
29	LMG	m	102	-	51,51,55	0.99	2 (3%)	59,59,63	1.10	4 (6%)
30	DMS	V	205	-	3,3,3	2.67	1 (33%)	3,3,3	0.50	0
25	PHO	a	411	-	67,69,69	2.11	15 (22%)	85,99,99	1.93	19 (22%)
24	CLA	b	619	-	59,73,73	2.43	14 (23%)	67,113,113	2.06	15 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	C	514	-	41,41,41	3.93	15 (36%)	56,56,56	8.28	38 (67%)
32	LMT	M	102	-	36,36,36	0.50	0	47,47,47	0.73	0
30	DMS	a	418	-	3,3,3	2.68	1 (33%)	3,3,3	0.59	0
26	BCR	h	101	-	41,41,41	3.87	14 (34%)	56,56,56	8.48	42 (75%)
24	CLA	D	405	-	59,73,73	2.55	15 (25%)	67,113,113	1.96	15 (22%)
29	LMG	c	520	-	51,51,55	0.99	3 (5%)	59,59,63	1.02	3 (5%)
30	DMS	D	416	-	3,3,3	2.70	1 (33%)	3,3,3	0.75	0
27	PL9	d	405	-	55,55,55	0.73	2 (3%)	68,69,69	1.38	10 (14%)
24	CLA	D	403	40	59,73,73	2.05	13 (22%)	67,113,113	2.11	15 (22%)
32	LMT	A	1018	-	36,36,36	0.53	0	47,47,47	1.00	5 (10%)
30	DMS	c	527	-	3,3,3	2.68	1 (33%)	3,3,3	0.59	0
24	CLA	a	412	-	59,73,73	2.19	14 (23%)	67,113,113	2.05	16 (23%)
30	DMS	A	1013	-	3,3,3	2.53	1 (33%)	3,3,3	0.57	0
30	DMS	C	523	-	3,3,3	2.54	1 (33%)	3,3,3	0.38	0
24	CLA	c	506	-	59,73,73	2.58	14 (23%)	67,113,113	2.09	14 (20%)

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
26	BCR	b	622	-	-	6/29/63/63	0/2/2/2
36	DGD	c	515	-	-	22/51/91/95	0/2/2/2
33	GOL	b	632	-	-	2/4/4/4	-
34	LHG	D	410	-	-	15/53/53/53	-
24	CLA	C	503	-	2/2/20/25	4/37/135/135	-
28	SQD	c	518	-	-	22/49/69/69	0/1/1/1
24	CLA	B	612	-	3/3/20/25	4/37/135/135	-
32	LMT	C	520	-	-	9/21/61/61	0/2/2/2
34	LHG	E	101	-	-	32/53/53/53	-
26	BCR	D	406	-	-	6/29/63/63	0/2/2/2
28	SQD	a	401	-	-	25/49/69/69	0/1/1/1
24	CLA	c	502	-	1/1/20/25	7/37/135/135	-
24	CLA	b	617	-	3/3/20/25	21/37/135/135	-
34	LHG	d	408	-	-	14/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	1005	-	3/3/20/25	1/37/135/135	-
24	CLA	C	504	40	3/3/20/25	10/37/135/135	-
24	CLA	b	607	-	3/3/20/25	5/37/135/135	-
26	BCR	b	620	-	-	5/29/63/63	0/2/2/2
26	BCR	a	413	-	-	5/29/63/63	0/2/2/2
24	CLA	a	408	40	1/1/20/25	3/37/135/135	-
35	HTG	C	521	-	-	5/10/30/30	0/1/1/1
26	BCR	K	101	-	-	9/29/63/63	0/2/2/2
32	LMT	a	402	-	-	7/21/61/61	0/2/2/2
32	LMT	m	101	-	-	0/21/61/61	0/2/2/2
24	CLA	B	601	40	3/3/20/25	14/37/135/135	-
36	DGD	C	517	-	-	10/51/91/95	0/2/2/2
26	BCR	B	619	-	-	2/29/63/63	0/2/2/2
38	HEM	f	101	5,6	-	1/6/54/54	-
33	GOL	v	204	-	-	3/4/4/4	-
35	HTG	D	413	-	-	5/10/30/30	0/1/1/1
34	LHG	d	406	-	-	16/53/53/53	-
28	SQD	f	102	-	-	23/38/58/69	0/1/1/1
26	BCR	T	101	-	-	6/29/63/63	0/2/2/2
35	HTG	d	416	-	-	4/10/30/30	0/1/1/1
24	CLA	b	608	-	3/3/20/25	7/37/135/135	-
33	GOL	A	1019	-	-	2/4/4/4	-
25	PHO	a	411	-	-	5/53/103/103	0/5/6/6
36	DGD	h	102	-	-	18/51/91/95	0/2/2/2
26	BCR	y	101	-	-	11/29/63/63	0/2/2/2
24	CLA	c	510	-	3/3/20/25	11/37/135/135	-
32	LMT	a	416	-	-	8/21/61/61	0/2/2/2
24	CLA	c	508	-	2/2/20/25	14/37/135/135	-
27	PL9	D	407	-	-	1/53/73/73	0/1/1/1
32	LMT	i	102	-	-	12/21/61/61	0/2/2/2
26	BCR	t	101	-	-	5/29/63/63	0/2/2/2
33	GOL	d	417	-	-	2/4/4/4	-
36	DGD	c	516	-	-	27/51/91/95	0/2/2/2
38	HEM	V	201	16	-	0/6/54/54	-
33	GOL	B	631	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	607	40	3/3/20/25	3/37/135/135	-
29	LMG	A	1012	-	-	27/46/66/70	0/1/1/1
24	CLA	c	501	-	3/3/20/25	3/37/135/135	-
24	CLA	B	611	-	3/3/20/25	7/37/135/135	-
35	HTG	b	626	-	-	5/10/30/30	0/1/1/1
24	CLA	B	615	-	3/3/20/25	7/37/135/135	-
24	CLA	C	506	-	3/3/20/25	12/37/135/135	-
24	CLA	C	513	-	2/2/20/25	10/37/135/135	-
35	HTG	c	525	-	-	5/10/30/30	0/1/1/1
29	LMG	a	415	-	-	23/46/66/70	0/1/1/1
29	LMG	d	409	39	-	17/46/66/70	0/1/1/1
24	CLA	c	512	-	3/3/20/25	16/37/135/135	-
36	DGD	c	517	-	-	19/51/91/95	0/2/2/2
26	BCR	H	101	-	-	9/29/63/63	0/2/2/2
34	LHG	e	101	-	-	28/53/53/53	-
24	CLA	b	614	-	1/1/20/25	3/37/135/135	-
26	BCR	k	102	-	-	9/29/63/63	0/2/2/2
26	BCR	c	514	-	-	7/29/63/63	0/2/2/2
24	CLA	B	608	-	1/1/20/25	1/37/135/135	-
33	GOL	V	206	-	-	3/4/4/4	-
24	CLA	c	513	-	1/1/20/25	20/37/135/135	-
24	CLA	d	403	-	2/2/20/25	15/37/135/135	-
35	HTG	c	522	-	-	5/10/30/30	0/1/1/1
35	HTG	D	419	-	-	7/10/30/30	0/1/1/1
24	CLA	A	1006	40	2/2/20/25	11/37/135/135	-
36	DGD	C	515	-	-	26/51/91/95	0/2/2/2
24	CLA	b	613	40	3/3/20/25	5/37/135/135	-
32	LMT	M	101	-	-	9/21/61/61	0/2/2/2
24	CLA	c	503	-	1/1/20/25	3/37/135/135	-
34	LHG	b	624	-	-	20/53/53/53	-
35	HTG	V	202	-	-	6/10/30/30	0/1/1/1
24	CLA	a	409	40	2/2/20/25	8/37/135/135	-
24	CLA	B	602	-	3/3/20/25	4/37/135/135	-
24	CLA	b	605	-	3/3/20/25	5/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PL9	A	1010	-	-	6/53/73/73	0/1/1/1
24	CLA	c	509	-	3/3/20/25	11/37/135/135	-
35	HTG	o	301	-	-	4/10/30/30	0/1/1/1
24	CLA	A	1008	-	1/1/20/25	8/37/135/135	-
24	CLA	C	510	-	3/3/20/25	6/37/135/135	-
35	HTG	b	630	-	-	7/10/30/30	0/1/1/1
29	LMG	Z	101	-	-	27/46/66/70	0/1/1/1
28	SQD	A	1016	-	-	23/49/69/69	0/1/1/1
29	LMG	c	521	-	-	25/46/66/70	0/1/1/1
36	DGD	H	102	-	-	16/51/91/95	0/2/2/2
33	GOL	a	420	-	-	2/4/4/4	-
33	GOL	d	415	-	-	2/4/4/4	-
24	CLA	C	508	-	3/3/20/25	13/37/135/135	-
24	CLA	B	614	-	3/3/20/25	11/37/135/135	-
29	LMG	B	622	-	-	22/46/66/70	0/1/1/1
35	HTG	b	602	-	-	2/10/30/30	0/1/1/1
29	LMG	D	412	39	-	15/46/66/70	0/1/1/1
28	SQD	D	408	-	-	22/38/58/69	0/1/1/1
24	CLA	c	507	40	3/3/20/25	9/37/135/135	-
34	LHG	D	411	-	-	16/53/53/53	-
26	BCR	d	404	-	-	10/29/63/63	0/2/2/2
24	CLA	b	612	-	-	2/37/135/135	-
24	CLA	c	505	-	2/2/20/25	9/37/135/135	-
24	CLA	B	604	-	3/3/20/25	11/37/135/135	-
38	HEM	F	101	5,6	-	0/6/54/54	-
33	GOL	V	204	-	-	2/4/4/4	-
24	CLA	B	605	-	3/3/20/25	3/37/135/135	-
24	CLA	c	511	3	2/2/20/25	2/37/135/135	-
35	HTG	B	624	-	-	7/10/30/30	0/1/1/1
24	CLA	C	502	-	1/1/20/25	10/37/135/135	-
26	BCR	A	1009	-	-	6/29/63/63	0/2/2/2
24	CLA	B	613	-	3/3/20/25	4/37/135/135	-
26	BCR	J	101	-	-	12/29/63/63	0/2/2/2
24	CLA	a	407	-	3/3/20/25	1/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	501	-	3/3/20/25	6/37/135/135	-
24	CLA	b	619	-	3/3/20/25	11/37/135/135	-
24	CLA	C	505	-	1/1/20/25	8/37/135/135	-
24	CLA	b	616	-	3/3/20/25	9/37/135/135	-
35	HTG	B	629	-	-	2/10/30/30	0/1/1/1
32	LMT	t	103	-	-	16/21/61/61	0/2/2/2
24	CLA	B	610	40	3/3/20/25	9/37/135/135	-
27	PL9	a	414	-	-	5/53/73/73	0/1/1/1
24	CLA	b	606	-	3/3/20/25	8/37/135/135	-
32	LMT	f	103	-	-	15/21/61/61	0/2/2/2
26	BCR	k	101	-	-	14/29/63/63	0/2/2/2
36	DGD	C	516	-	-	23/51/91/95	0/2/2/2
24	CLA	b	615	-	3/3/20/25	9/37/135/135	-
29	LMG	C	518	-	-	20/46/66/70	0/1/1/1
24	CLA	B	606	-	3/3/20/25	10/37/135/135	-
24	CLA	C	512	-	3/3/20/25	16/37/135/135	-
24	CLA	B	609	-	2/2/20/25	1/37/135/135	-
24	CLA	B	603	-	3/3/20/25	7/37/135/135	-
24	CLA	b	611	-	1/1/20/25	1/37/135/135	-
24	CLA	b	610	40	3/3/20/25	4/37/135/135	-
35	HTG	B	628	-	-	3/10/30/30	0/1/1/1
33	GOL	D	418	-	-	4/4/4/4	-
32	LMT	B	623	-	-	14/21/61/61	0/2/2/2
32	LMT	b	631	-	-	10/21/61/61	0/2/2/2
29	LMG	C	519	-	-	22/46/66/70	0/1/1/1
28	SQD	A	1011	-	-	20/49/69/69	0/1/1/1
33	GOL	v	203	-	-	2/4/4/4	-
24	CLA	c	504	40	2/2/20/25	12/37/135/135	-
25	PHO	A	1007	-	-	1/53/103/103	0/5/6/6
28	SQD	B	620[B]	-	-	24/49/69/69	0/1/1/1
24	CLA	b	609	-	3/3/20/25	9/37/135/135	-
33	GOL	V	207	-	-	2/4/4/4	-
28	SQD	B	620[A]	-	-	29/49/69/69	0/1/1/1
35	HTG	d	410	-	-	4/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	509	-	3/3/20/25	7/37/135/135	-
32	LMT	A	1017	-	-	10/21/61/61	0/2/2/2
26	BCR	K	102	-	-	8/29/63/63	0/2/2/2
28	SQD	b	623[A]	-	-	22/49/69/69	0/1/1/1
29	LMG	c	519	-	-	25/46/66/70	0/1/1/1
38	HEM	v	201	16	-	0/6/54/54	-
28	SQD	b	623[B]	-	-	29/49/69/69	0/1/1/1
26	BCR	b	621	-	-	5/29/63/63	0/2/2/2
24	CLA	D	405	-	2/2/20/25	14/37/135/135	-
24	CLA	d	402	-	1/1/20/25	6/37/135/135	-
24	CLA	b	618	-	3/3/20/25	5/37/135/135	-
24	CLA	B	616	-	3/3/20/25	14/37/135/135	-
32	LMT	m	103	-	-	7/21/61/61	0/2/2/2
35	HTG	C	522	-	-	6/10/30/30	0/1/1/1
34	LHG	d	407	-	-	15/53/53/53	-
34	LHG	B	621	-	-	19/53/53/53	-
32	LMT	A	1018	-	-	13/21/61/61	0/2/2/2
34	LHG	D	409	-	-	16/53/53/53	-
35	HTG	b	601	-	-	3/10/30/30	0/1/1/1
24	CLA	C	507	40	3/3/20/25	17/37/135/135	-
25	PHO	D	404	-	-	6/53/103/103	0/5/6/6
26	BCR	B	618	-	-	5/29/63/63	0/2/2/2
32	LMT	b	625	-	-	11/21/61/61	0/2/2/2
26	BCR	B	617	-	-	4/29/63/63	0/2/2/2
29	LMG	m	102	-	-	22/46/66/70	0/1/1/1
24	CLA	C	511	3	2/2/20/25	7/37/135/135	-
24	CLA	D	402	-	2/2/20/25	4/37/135/135	-
26	BCR	C	514	-	-	6/29/63/63	0/2/2/2
32	LMT	M	102	-	-	6/21/61/61	0/2/2/2
26	BCR	h	101	-	-	8/29/63/63	0/2/2/2
29	LMG	c	520	-	-	17/46/66/70	0/1/1/1
27	PL9	d	405	-	-	2/53/73/73	0/1/1/1
24	CLA	D	403	40	1/1/20/25	3/37/135/135	-
24	CLA	c	506	-	3/3/20/25	13/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PHO	a	410	-	-	4/53/103/103	0/5/6/6
24	CLA	a	412	-	1/1/20/25	14/37/135/135	-
24	CLA	b	604	40	1/1/20/25	19/37/135/135	-

All (1598) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	MG-NA	17.54	2.47	2.06
24	b	604	CLA	MG-NC	13.70	2.38	2.06
24	b	617	CLA	MG-NA	13.60	2.38	2.06
24	C	505	CLA	MG-NA	13.03	2.37	2.06
24	C	507	CLA	MG-NA	12.84	2.36	2.06
24	b	616	CLA	MG-NA	12.82	2.36	2.06
24	c	506	CLA	MG-NC	12.80	2.36	2.06
24	B	615	CLA	MG-NA	12.41	2.35	2.06
24	b	609	CLA	MG-NA	12.31	2.35	2.06
24	C	511	CLA	MG-NA	12.27	2.35	2.06
24	B	606	CLA	MG-NA	11.83	2.34	2.06
24	B	611	CLA	MG-NA	11.83	2.34	2.06
24	d	403	CLA	MG-NC	11.58	2.33	2.06
24	D	405	CLA	MG-NC	11.46	2.33	2.06
24	B	607	CLA	MG-NA	11.36	2.33	2.06
24	b	605	CLA	MG-NC	11.06	2.32	2.06
24	c	511	CLA	MG-NC	11.05	2.32	2.06
24	c	504	CLA	MG-NA	11.04	2.32	2.06
24	B	604	CLA	MG-NA	10.91	2.32	2.06
24	c	508	CLA	MG-NC	10.90	2.32	2.06
24	c	509	CLA	MG-NA	10.76	2.31	2.06
24	B	612	CLA	MG-NA	10.61	2.31	2.06
24	c	503	CLA	MG-NA	10.53	2.31	2.06
24	b	612	CLA	MG-NC	10.51	2.31	2.06
24	c	512	CLA	MG-NC	10.48	2.31	2.06
24	b	610	CLA	MG-NA	10.38	2.30	2.06
24	C	504	CLA	MG-NA	10.32	2.30	2.06
24	B	608	CLA	MG-NA	10.10	2.30	2.06
24	c	507	CLA	MG-NC	10.09	2.30	2.06
24	b	619	CLA	MG-NA	10.06	2.30	2.06
24	B	614	CLA	MG-NC	10.06	2.30	2.06
24	C	503	CLA	MG-NA	9.86	2.29	2.06
24	b	612	CLA	MG-NA	9.84	2.29	2.06
24	C	513	CLA	MG-NC	9.76	2.29	2.06
24	b	611	CLA	MG-NA	9.68	2.29	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	511	CLA	MG-NA	9.67	2.29	2.06
24	b	607	CLA	MG-NA	9.65	2.29	2.06
24	B	609	CLA	MG-NC	9.54	2.28	2.06
24	A	1008	CLA	MG-NA	9.51	2.28	2.06
24	c	501	CLA	MG-NA	9.48	2.28	2.06
24	c	503	CLA	MG-NC	9.41	2.28	2.06
24	b	618	CLA	MG-NA	9.16	2.28	2.06
24	b	614	CLA	MG-NA	9.11	2.27	2.06
24	c	513	CLA	MG-NC	9.11	2.27	2.06
24	C	510	CLA	MG-NA	9.08	2.27	2.06
26	c	514	BCR	C8-C9	-8.97	1.26	1.45
24	A	1005	CLA	MG-NC	8.96	2.27	2.06
24	C	509	CLA	MG-NC	8.93	2.27	2.06
26	t	101	BCR	C8-C9	-8.89	1.26	1.45
26	k	102	BCR	C12-C13	-8.88	1.26	1.45
26	K	101	BCR	C8-C9	-8.87	1.26	1.45
26	D	406	BCR	C19-C18	-8.87	1.26	1.45
26	b	622	BCR	C8-C9	-8.85	1.26	1.45
26	d	404	BCR	C19-C18	-8.85	1.26	1.45
26	B	618	BCR	C8-C9	-8.83	1.27	1.45
24	C	502	CLA	MG-NA	8.83	2.27	2.06
26	k	101	BCR	C8-C9	-8.83	1.27	1.45
26	B	619	BCR	C8-C9	-8.82	1.27	1.45
26	C	514	BCR	C8-C9	-8.82	1.27	1.45
26	k	102	BCR	C8-C9	-8.81	1.27	1.45
26	b	622	BCR	C12-C13	-8.80	1.27	1.45
26	K	102	BCR	C12-C13	-8.79	1.27	1.45
26	C	514	BCR	C19-C18	-8.77	1.27	1.45
26	c	514	BCR	C12-C13	-8.76	1.27	1.45
26	K	102	BCR	C19-C18	-8.76	1.27	1.45
26	t	101	BCR	C19-C18	-8.76	1.27	1.45
26	H	101	BCR	C8-C9	-8.76	1.27	1.45
26	B	617	BCR	C8-C9	-8.75	1.27	1.45
26	y	101	BCR	C12-C13	-8.74	1.27	1.45
26	y	101	BCR	C19-C18	-8.74	1.27	1.45
26	d	404	BCR	C8-C9	-8.73	1.27	1.45
24	a	409	CLA	MG-NA	8.73	2.27	2.06
26	T	101	BCR	C8-C9	-8.73	1.27	1.45
26	T	101	BCR	C19-C18	-8.73	1.27	1.45
26	K	102	BCR	C8-C9	-8.72	1.27	1.45
26	C	514	BCR	C12-C13	-8.70	1.27	1.45
26	b	622	BCR	C19-C18	-8.69	1.27	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	619	BCR	C12-C13	-8.68	1.27	1.45
26	y	101	BCR	C8-C9	-8.68	1.27	1.45
26	h	101	BCR	C19-C18	-8.67	1.27	1.45
26	t	101	BCR	C12-C13	-8.67	1.27	1.45
26	K	101	BCR	C19-C18	-8.66	1.27	1.45
26	k	102	BCR	C19-C18	-8.66	1.27	1.45
26	b	620	BCR	C8-C9	-8.65	1.27	1.45
26	J	101	BCR	C12-C13	-8.65	1.27	1.45
26	k	101	BCR	C19-C18	-8.65	1.27	1.45
26	A	1009	BCR	C8-C9	-8.64	1.27	1.45
26	B	617	BCR	C12-C13	-8.64	1.27	1.45
26	d	404	BCR	C12-C13	-8.64	1.27	1.45
26	h	101	BCR	C8-C9	-8.63	1.27	1.45
26	B	618	BCR	C12-C13	-8.63	1.27	1.45
26	k	101	BCR	C12-C13	-8.63	1.27	1.45
26	T	101	BCR	C12-C13	-8.62	1.27	1.45
26	b	620	BCR	C12-C13	-8.61	1.27	1.45
26	D	406	BCR	C8-C9	-8.61	1.27	1.45
26	h	101	BCR	C12-C13	-8.60	1.27	1.45
26	J	101	BCR	C19-C18	-8.60	1.27	1.45
26	H	101	BCR	C12-C13	-8.60	1.27	1.45
26	J	101	BCR	C8-C9	-8.59	1.27	1.45
26	D	406	BCR	C12-C13	-8.59	1.27	1.45
26	H	101	BCR	C19-C18	-8.58	1.27	1.45
26	b	621	BCR	C8-C9	-8.57	1.27	1.45
26	b	620	BCR	C19-C18	-8.57	1.27	1.45
26	A	1009	BCR	C19-C18	-8.56	1.27	1.45
26	c	514	BCR	C19-C18	-8.56	1.27	1.45
24	B	605	CLA	MG-NA	8.56	2.26	2.06
26	A	1009	BCR	C12-C13	-8.55	1.27	1.45
26	b	621	BCR	C19-C18	-8.54	1.27	1.45
26	B	618	BCR	C19-C18	-8.54	1.27	1.45
26	b	621	BCR	C12-C13	-8.52	1.27	1.45
26	B	619	BCR	C19-C18	-8.51	1.27	1.45
26	K	101	BCR	C12-C13	-8.49	1.27	1.45
26	a	413	BCR	C8-C9	-8.47	1.27	1.45
24	B	602	CLA	MG-NC	8.46	2.26	2.06
26	a	413	BCR	C12-C13	-8.42	1.27	1.45
26	B	617	BCR	C19-C18	-8.42	1.27	1.45
24	c	502	CLA	MG-NA	8.35	2.26	2.06
26	a	413	BCR	C19-C18	-8.31	1.28	1.45
24	d	402	CLA	MG-NA	8.26	2.25	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	610	CLA	MG-NC	8.21	2.25	2.06
24	B	601	CLA	MG-NC	8.21	2.25	2.06
24	C	508	CLA	MG-NA	8.18	2.25	2.06
24	c	510	CLA	MG-NA	8.02	2.25	2.06
24	C	508	CLA	MG-NC	7.94	2.25	2.06
24	C	503	CLA	MG-NC	7.94	2.25	2.06
24	b	613	CLA	MG-NA	7.86	2.24	2.06
24	C	506	CLA	MG-NC	7.83	2.24	2.06
24	C	513	CLA	MG-NA	7.80	2.24	2.06
26	C	514	BCR	C20-C21	-7.76	1.19	1.43
26	K	102	BCR	C20-C21	-7.75	1.19	1.43
24	C	501	CLA	MG-NA	7.74	2.24	2.06
24	c	513	CLA	MG-NA	7.73	2.24	2.06
24	b	615	CLA	MG-NA	7.71	2.24	2.06
26	y	101	BCR	C20-C21	-7.71	1.19	1.43
26	K	102	BCR	C16-C17	-7.69	1.19	1.43
26	J	101	BCR	C16-C17	-7.69	1.19	1.43
24	c	505	CLA	MG-NA	7.69	2.24	2.06
26	d	404	BCR	C20-C21	-7.68	1.19	1.43
26	D	406	BCR	C20-C21	-7.68	1.19	1.43
26	b	622	BCR	C20-C21	-7.65	1.19	1.43
26	c	514	BCR	C16-C17	-7.63	1.19	1.43
26	B	619	BCR	C20-C21	-7.61	1.19	1.43
26	h	101	BCR	C20-C21	-7.61	1.19	1.43
26	H	101	BCR	C20-C21	-7.60	1.19	1.43
26	B	618	BCR	C20-C21	-7.60	1.19	1.43
24	c	508	CLA	MG-NA	7.60	2.24	2.06
26	T	101	BCR	C16-C17	-7.60	1.19	1.43
26	A	1009	BCR	C20-C21	-7.60	1.19	1.43
26	k	101	BCR	C20-C21	-7.59	1.19	1.43
26	C	514	BCR	C16-C17	-7.59	1.19	1.43
26	c	514	BCR	C20-C21	-7.59	1.19	1.43
26	K	101	BCR	C20-C21	-7.59	1.19	1.43
26	b	620	BCR	C20-C21	-7.58	1.19	1.43
26	J	101	BCR	C20-C21	-7.58	1.20	1.43
26	b	621	BCR	C20-C21	-7.58	1.20	1.43
26	y	101	BCR	C16-C17	-7.58	1.20	1.43
26	T	101	BCR	C20-C21	-7.56	1.20	1.43
26	K	101	BCR	C16-C17	-7.55	1.20	1.43
26	B	617	BCR	C16-C17	-7.54	1.20	1.43
26	t	101	BCR	C20-C21	-7.53	1.20	1.43
26	h	101	BCR	C16-C17	-7.52	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	k	101	BCR	C16-C17	-7.51	1.20	1.43
26	d	404	BCR	C16-C17	-7.50	1.20	1.43
26	D	406	BCR	C16-C17	-7.50	1.20	1.43
26	H	101	BCR	C16-C17	-7.49	1.20	1.43
26	b	622	BCR	C16-C17	-7.49	1.20	1.43
26	B	619	BCR	C16-C17	-7.48	1.20	1.43
24	B	601	CLA	MG-NA	7.47	2.24	2.06
26	t	101	BCR	C16-C17	-7.47	1.20	1.43
26	b	621	BCR	C16-C17	-7.47	1.20	1.43
26	k	102	BCR	C20-C21	-7.44	1.20	1.43
26	B	617	BCR	C20-C21	-7.42	1.20	1.43
24	c	501	CLA	MG-NC	7.39	2.23	2.06
24	c	505	CLA	MG-NC	7.38	2.23	2.06
26	b	620	BCR	C16-C17	-7.37	1.20	1.43
26	a	413	BCR	C16-C17	-7.34	1.20	1.43
26	B	618	BCR	C16-C17	-7.34	1.20	1.43
26	A	1009	BCR	C16-C17	-7.34	1.20	1.43
24	b	606	CLA	MG-NC	7.34	2.23	2.06
26	a	413	BCR	C20-C21	-7.32	1.20	1.43
24	C	506	CLA	MG-NA	7.26	2.23	2.06
24	C	501	CLA	MG-NC	7.21	2.23	2.06
24	c	502	CLA	MG-NC	7.16	2.23	2.06
24	b	606	CLA	MG-NA	7.16	2.23	2.06
24	A	1006	CLA	MG-NA	7.14	2.23	2.06
24	a	408	CLA	MG-NA	7.13	2.23	2.06
24	b	613	CLA	MG-NC	7.11	2.23	2.06
24	b	607	CLA	MG-NC	7.05	2.23	2.06
24	B	616	CLA	MG-NA	7.05	2.23	2.06
24	b	609	CLA	MG-NC	6.96	2.22	2.06
24	B	613	CLA	MG-NA	6.88	2.22	2.06
24	b	615	CLA	MG-NC	6.86	2.22	2.06
24	b	618	CLA	MG-NC	6.85	2.22	2.06
24	B	603	CLA	MG-NA	6.81	2.22	2.06
24	B	613	CLA	MG-NC	6.77	2.22	2.06
24	a	407	CLA	MG-NC	6.72	2.22	2.06
24	B	616	CLA	MG-NC	6.72	2.22	2.06
26	D	406	BCR	C21-C22	-6.72	1.26	1.35
24	C	504	CLA	MG-NC	6.71	2.22	2.06
24	c	512	CLA	MG-NA	6.66	2.22	2.06
26	K	102	BCR	C21-C22	-6.65	1.27	1.35
26	d	404	BCR	C21-C22	-6.64	1.27	1.35
24	c	510	CLA	MG-NC	6.63	2.22	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	606	CLA	MG-NC	6.63	2.22	2.06
26	b	622	BCR	C21-C22	-6.61	1.27	1.35
24	B	609	CLA	MG-NA	6.60	2.22	2.06
24	a	412	CLA	MG-NA	6.60	2.21	2.06
24	b	608	CLA	MG-NC	6.57	2.21	2.06
26	k	102	BCR	C21-C22	-6.55	1.27	1.35
24	C	507	CLA	MG-NC	6.52	2.21	2.06
26	t	101	BCR	C17-C18	-6.51	1.27	1.35
26	c	514	BCR	C17-C18	-6.50	1.27	1.35
26	d	404	BCR	C17-C18	-6.50	1.27	1.35
26	T	101	BCR	C17-C18	-6.46	1.27	1.35
26	K	102	BCR	C17-C18	-6.46	1.27	1.35
26	b	621	BCR	C21-C22	-6.46	1.27	1.35
26	A	1009	BCR	C21-C22	-6.46	1.27	1.35
26	C	514	BCR	C21-C22	-6.46	1.27	1.35
26	y	101	BCR	C21-C22	-6.42	1.27	1.35
26	T	101	BCR	C16-C15	-6.40	1.19	1.36
26	y	101	BCR	C17-C18	-6.39	1.27	1.35
26	B	617	BCR	C21-C22	-6.38	1.27	1.35
26	T	101	BCR	C21-C22	-6.36	1.27	1.35
26	J	101	BCR	C17-C18	-6.36	1.27	1.35
26	h	101	BCR	C21-C22	-6.36	1.27	1.35
26	b	622	BCR	C17-C18	-6.36	1.27	1.35
26	H	101	BCR	C21-C22	-6.36	1.27	1.35
26	C	514	BCR	C17-C18	-6.35	1.27	1.35
24	c	507	CLA	MG-NA	6.35	2.21	2.06
26	J	101	BCR	C16-C15	-6.34	1.19	1.36
26	J	101	BCR	C21-C22	-6.32	1.27	1.35
26	c	514	BCR	C16-C15	-6.30	1.19	1.36
26	y	101	BCR	C16-C15	-6.29	1.19	1.36
26	C	514	BCR	C16-C15	-6.29	1.19	1.36
26	K	101	BCR	C21-C22	-6.29	1.27	1.35
26	K	102	BCR	C16-C15	-6.28	1.19	1.36
26	k	102	BCR	C17-C18	-6.28	1.27	1.35
24	B	603	CLA	MG-NC	6.27	2.21	2.06
26	h	101	BCR	C17-C18	-6.26	1.27	1.35
26	b	621	BCR	C17-C18	-6.26	1.27	1.35
26	d	404	BCR	C16-C15	-6.25	1.19	1.36
26	k	101	BCR	C17-C18	-6.25	1.27	1.35
26	B	619	BCR	C21-C22	-6.23	1.27	1.35
26	k	101	BCR	C21-C22	-6.21	1.27	1.35
24	D	402	CLA	MG-NC	6.21	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	t	101	BCR	C21-C22	-6.19	1.27	1.35
26	k	102	BCR	C16-C17	-6.19	1.24	1.43
26	B	618	BCR	C21-C22	-6.18	1.27	1.35
26	B	619	BCR	C17-C18	-6.17	1.27	1.35
26	A	1009	BCR	C17-C18	-6.17	1.27	1.35
26	b	620	BCR	C21-C22	-6.17	1.27	1.35
26	t	101	BCR	C16-C15	-6.17	1.19	1.36
26	a	413	BCR	C17-C18	-6.15	1.27	1.35
26	B	617	BCR	C17-C18	-6.15	1.27	1.35
26	A	1009	BCR	C16-C15	-6.15	1.20	1.36
26	c	514	BCR	C21-C22	-6.14	1.27	1.35
26	h	101	BCR	C16-C15	-6.13	1.20	1.36
26	B	619	BCR	C16-C15	-6.12	1.20	1.36
26	H	101	BCR	C16-C15	-6.11	1.20	1.36
26	k	101	BCR	C16-C15	-6.11	1.20	1.36
26	K	101	BCR	C16-C15	-6.11	1.20	1.36
26	H	101	BCR	C17-C18	-6.11	1.27	1.35
24	d	402	CLA	MG-NC	6.11	2.20	2.06
26	b	620	BCR	C16-C15	-6.10	1.20	1.36
26	b	620	BCR	C17-C18	-6.10	1.27	1.35
26	b	621	BCR	C16-C15	-6.09	1.20	1.36
26	b	622	BCR	C16-C15	-6.06	1.20	1.36
26	B	617	BCR	C16-C15	-6.06	1.20	1.36
26	B	618	BCR	C17-C18	-6.04	1.27	1.35
24	B	614	CLA	MG-NA	6.01	2.20	2.06
26	D	406	BCR	C16-C15	-6.00	1.20	1.36
26	a	413	BCR	C16-C15	-5.98	1.20	1.36
26	D	406	BCR	C17-C18	-5.97	1.27	1.35
26	K	101	BCR	C17-C18	-5.97	1.27	1.35
24	b	614	CLA	MG-NC	5.92	2.20	2.06
26	a	413	BCR	C21-C22	-5.91	1.28	1.35
26	C	514	BCR	C20-C19	-5.90	1.19	1.34
26	k	102	BCR	C11-C12	-5.87	1.19	1.34
26	B	618	BCR	C16-C15	-5.86	1.20	1.36
26	J	101	BCR	C11-C12	-5.85	1.19	1.34
24	C	507	CLA	C3B-C2B	5.85	1.48	1.40
26	B	619	BCR	C11-C12	-5.84	1.19	1.34
24	B	612	CLA	C3B-C2B	5.83	1.48	1.40
24	A	1008	CLA	MG-NC	5.83	2.20	2.06
24	B	615	CLA	C3B-C2B	5.82	1.48	1.40
26	C	514	BCR	C11-C12	-5.81	1.19	1.34
26	K	102	BCR	C20-C19	-5.80	1.19	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	t	101	BCR	C11-C12	-5.80	1.19	1.34
24	a	408	CLA	C3B-C2B	5.79	1.48	1.40
26	b	622	BCR	C11-C12	-5.79	1.19	1.34
26	K	102	BCR	C11-C12	-5.77	1.19	1.34
26	h	101	BCR	C20-C19	-5.76	1.19	1.34
24	B	605	CLA	MG-NC	5.76	2.19	2.06
26	c	514	BCR	C11-C12	-5.74	1.19	1.34
26	k	101	BCR	C11-C12	-5.73	1.19	1.34
26	y	101	BCR	C11-C12	-5.73	1.19	1.34
26	y	101	BCR	C20-C19	-5.73	1.19	1.34
26	d	404	BCR	C20-C19	-5.73	1.19	1.34
24	d	403	CLA	C3B-C2B	5.72	1.48	1.40
24	b	609	CLA	C3B-C2B	5.72	1.48	1.40
26	c	514	BCR	C20-C19	-5.71	1.19	1.34
24	C	502	CLA	MG-NC	5.71	2.19	2.06
26	T	101	BCR	C20-C19	-5.71	1.19	1.34
26	T	101	BCR	C11-C12	-5.71	1.19	1.34
26	b	621	BCR	C11-C12	-5.69	1.19	1.34
26	K	101	BCR	C20-C19	-5.69	1.19	1.34
24	c	507	CLA	C3B-C2B	5.68	1.48	1.40
26	h	101	BCR	C11-C12	-5.68	1.19	1.34
26	B	618	BCR	C11-C12	-5.68	1.19	1.34
24	b	619	CLA	C3B-C2B	5.67	1.48	1.40
26	b	621	BCR	C20-C19	-5.67	1.20	1.34
26	d	404	BCR	C11-C12	-5.67	1.20	1.34
26	K	101	BCR	C11-C12	-5.66	1.20	1.34
26	D	406	BCR	C20-C19	-5.66	1.20	1.34
26	b	620	BCR	C11-C12	-5.64	1.20	1.34
26	J	101	BCR	C20-C19	-5.64	1.20	1.34
26	b	622	BCR	C20-C19	-5.64	1.20	1.34
24	A	1006	CLA	C3B-C2B	5.62	1.48	1.40
24	B	602	CLA	MG-NA	5.62	2.19	2.06
24	C	513	CLA	C3B-C2B	5.61	1.48	1.40
26	B	619	BCR	C20-C19	-5.61	1.20	1.34
26	k	101	BCR	C20-C19	-5.60	1.20	1.34
24	B	608	CLA	MG-NC	5.59	2.19	2.06
26	D	406	BCR	C11-C12	-5.59	1.20	1.34
26	H	101	BCR	C20-C19	-5.58	1.20	1.34
26	A	1009	BCR	C11-C12	-5.58	1.20	1.34
24	c	511	CLA	CHC-C1C	5.58	1.49	1.35
26	H	101	BCR	C11-C12	-5.57	1.20	1.34
26	A	1009	BCR	C20-C19	-5.57	1.20	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	504	CLA	MG-NC	5.55	2.19	2.06
24	c	503	CLA	CHC-C1C	5.55	1.49	1.35
26	t	101	BCR	C20-C19	-5.55	1.20	1.34
24	D	402	CLA	MG-NA	5.53	2.19	2.06
25	A	1007	PHO	C3C-C2C	5.52	1.48	1.36
24	C	503	CLA	CHC-C1C	5.52	1.49	1.35
24	b	606	CLA	CHC-C1C	5.52	1.49	1.35
24	c	503	CLA	C3B-C2B	5.51	1.48	1.40
24	c	508	CLA	C3C-C2C	5.51	1.48	1.36
26	B	617	BCR	C11-C12	-5.51	1.20	1.34
25	D	404	PHO	CHB-C1B	5.51	1.49	1.38
26	b	620	BCR	C20-C19	-5.50	1.20	1.34
26	B	618	BCR	C20-C19	-5.50	1.20	1.34
24	C	508	CLA	CHC-C1C	5.49	1.49	1.35
24	b	604	CLA	CHC-C1C	5.48	1.49	1.35
24	C	507	CLA	CHC-C1C	5.48	1.49	1.35
24	b	618	CLA	C3B-C2B	5.48	1.48	1.40
25	a	410	PHO	C3C-C2C	5.47	1.48	1.36
24	C	511	CLA	C3B-C2B	5.47	1.48	1.40
24	C	512	CLA	C3C-C2C	5.47	1.48	1.36
24	c	505	CLA	C3B-C2B	5.47	1.48	1.40
24	c	512	CLA	CHC-C1C	5.47	1.49	1.35
24	C	503	CLA	C3B-C2B	5.47	1.48	1.40
24	c	512	CLA	C3B-C2B	5.47	1.48	1.40
24	a	407	CLA	C3B-C2B	5.46	1.48	1.40
26	a	413	BCR	C11-C12	-5.46	1.20	1.34
24	B	606	CLA	C3B-C2B	5.45	1.47	1.40
24	C	512	CLA	C3B-C2B	5.45	1.47	1.40
24	c	501	CLA	C3C-C2C	5.45	1.48	1.36
24	C	513	CLA	C3C-C2C	5.45	1.48	1.36
24	c	513	CLA	C3B-C2B	5.45	1.47	1.40
24	b	610	CLA	MG-NC	5.44	2.19	2.06
24	b	604	CLA	MG-NA	5.44	2.19	2.06
24	b	604	CLA	O2D-CGD	5.44	1.46	1.33
24	a	407	CLA	MG-NA	5.43	2.19	2.06
25	D	404	PHO	C3B-C2B	5.43	1.48	1.37
24	B	605	CLA	CHC-C1C	5.43	1.48	1.35
24	c	509	CLA	C3B-C2B	5.43	1.47	1.40
24	c	507	CLA	CHC-C1C	5.43	1.48	1.35
24	c	511	CLA	C3B-C2B	5.43	1.47	1.40
24	c	502	CLA	C3B-C2B	5.42	1.47	1.40
24	C	511	CLA	C3C-C2C	5.41	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	410	PHO	CHB-C1B	5.41	1.49	1.38
24	c	503	CLA	C3C-C2C	5.41	1.48	1.36
24	d	403	CLA	CHC-C1C	5.41	1.48	1.35
24	c	512	CLA	C3C-C2C	5.41	1.48	1.36
24	c	504	CLA	O2D-CGD	5.41	1.46	1.33
24	C	513	CLA	CHC-C1C	5.40	1.48	1.35
24	c	508	CLA	O2D-CGD	5.40	1.46	1.33
24	b	607	CLA	C3B-C2B	5.40	1.47	1.40
24	b	611	CLA	C3C-C2C	5.40	1.48	1.36
24	c	513	CLA	C3C-C2C	5.40	1.48	1.36
38	f	101	HEM	C3D-C2D	5.40	1.53	1.37
24	b	605	CLA	C3B-C2B	5.40	1.47	1.40
24	B	602	CLA	C3C-C2C	5.40	1.48	1.36
24	D	405	CLA	CHC-C1C	5.40	1.48	1.35
24	C	506	CLA	C3C-C2C	5.39	1.48	1.36
24	b	605	CLA	CHC-C1C	5.39	1.48	1.35
24	B	608	CLA	C3C-C2C	5.39	1.48	1.36
25	a	411	PHO	C3B-C2B	5.38	1.48	1.37
26	T	101	BCR	C11-C10	-5.38	1.26	1.43
24	B	610	CLA	C3C-C2C	5.38	1.48	1.36
24	c	513	CLA	CHC-C1C	5.38	1.48	1.35
24	c	506	CLA	C3B-C2B	5.38	1.47	1.40
24	C	504	CLA	C3C-C2C	5.38	1.48	1.36
24	D	405	CLA	C3C-C2C	5.38	1.48	1.36
24	B	609	CLA	CHC-C1C	5.38	1.48	1.35
26	a	413	BCR	C20-C19	-5.38	1.20	1.34
24	B	616	CLA	C3B-C2B	5.38	1.47	1.40
24	C	511	CLA	MG-NC	5.37	2.19	2.06
24	b	611	CLA	CHC-C1C	5.37	1.48	1.35
24	B	606	CLA	C3C-C2C	5.37	1.48	1.36
24	C	508	CLA	C3C-C2C	5.37	1.48	1.36
24	C	506	CLA	CHC-C1C	5.37	1.48	1.35
24	c	511	CLA	C3C-C2C	5.37	1.48	1.36
24	B	613	CLA	C3B-C2B	5.36	1.47	1.40
24	b	605	CLA	C3C-C2C	5.36	1.48	1.36
24	b	619	CLA	MG-NC	5.36	2.19	2.06
24	c	505	CLA	CHC-C1C	5.36	1.48	1.35
26	k	102	BCR	C11-C10	-5.36	1.26	1.43
25	a	411	PHO	CHB-C1B	5.36	1.49	1.38
24	B	603	CLA	C3C-C2C	5.36	1.48	1.36
24	C	511	CLA	CHC-C1C	5.35	1.48	1.35
24	B	601	CLA	C3C-C2C	5.35	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	601	CLA	CHC-C1C	5.34	1.48	1.35
24	b	604	CLA	C3C-C2C	5.34	1.48	1.36
24	b	604	CLA	C3B-C2B	5.34	1.47	1.40
24	a	407	CLA	C3C-C2C	5.34	1.48	1.36
24	b	613	CLA	C3C-C2C	5.34	1.48	1.36
26	k	102	BCR	C15-C14	-5.34	1.26	1.43
38	F	101	HEM	C3D-C2D	5.33	1.53	1.37
24	b	609	CLA	C3C-C2C	5.33	1.48	1.36
24	C	503	CLA	C3C-C2C	5.33	1.48	1.36
24	A	1005	CLA	C3B-C2B	5.33	1.47	1.40
26	B	617	BCR	C20-C19	-5.33	1.20	1.34
25	A	1007	PHO	CHB-C1B	5.33	1.49	1.38
24	b	613	CLA	CHC-C1C	5.33	1.48	1.35
25	A	1007	PHO	C3B-C2B	5.33	1.48	1.37
24	B	613	CLA	CHC-C1C	5.32	1.48	1.35
24	C	512	CLA	CHC-C1C	5.32	1.48	1.35
24	a	409	CLA	MG-NC	5.32	2.18	2.06
24	c	502	CLA	CHC-C1C	5.32	1.48	1.35
24	B	615	CLA	O2D-CGD	5.31	1.46	1.33
26	k	102	BCR	C20-C19	-5.31	1.20	1.34
24	C	509	CLA	C3C-C2C	5.31	1.48	1.36
24	c	506	CLA	C3C-C2C	5.31	1.48	1.36
26	B	619	BCR	C11-C10	-5.31	1.27	1.43
24	A	1008	CLA	C3C-C2C	5.30	1.48	1.36
24	C	508	CLA	O2D-CGD	5.30	1.46	1.33
26	h	101	BCR	C11-C10	-5.30	1.27	1.43
24	b	612	CLA	CHC-C1C	5.30	1.48	1.35
26	b	622	BCR	C11-C10	-5.30	1.27	1.43
25	D	404	PHO	C3C-C2C	5.30	1.48	1.36
24	c	504	CLA	CHC-C1C	5.29	1.48	1.35
24	b	609	CLA	CHC-C1C	5.29	1.48	1.35
24	C	507	CLA	C3C-C2C	5.29	1.48	1.36
24	b	615	CLA	C3B-C2B	5.29	1.47	1.40
24	a	412	CLA	MG-NC	5.29	2.18	2.06
26	c	514	BCR	C11-C10	-5.29	1.27	1.43
24	b	608	CLA	C3C-C2C	5.29	1.48	1.36
26	K	102	BCR	C11-C10	-5.29	1.27	1.43
24	c	511	CLA	O2D-CGD	5.29	1.46	1.33
26	C	514	BCR	C11-C10	-5.29	1.27	1.43
24	B	611	CLA	C3C-C2C	5.29	1.48	1.36
24	D	405	CLA	C3B-C2B	5.28	1.47	1.40
26	k	101	BCR	C11-C10	-5.28	1.27	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	CHC-C1C	5.28	1.48	1.35
24	B	604	CLA	C3C-C2C	5.28	1.47	1.36
24	C	501	CLA	CHC-C1C	5.27	1.48	1.35
24	B	611	CLA	O2D-CGD	5.27	1.46	1.33
24	C	509	CLA	C3B-C2B	5.27	1.47	1.40
24	B	606	CLA	CHC-C1C	5.27	1.48	1.35
24	B	614	CLA	C3C-C2C	5.27	1.47	1.36
24	C	504	CLA	C3B-C2B	5.27	1.47	1.40
38	v	201	HEM	C3D-C2D	5.27	1.53	1.37
24	c	505	CLA	C3C-C2C	5.26	1.47	1.36
24	C	506	CLA	O2D-CGD	5.26	1.46	1.33
24	c	504	CLA	C3C-C2C	5.26	1.47	1.36
24	b	606	CLA	C3C-C2C	5.26	1.47	1.36
24	c	508	CLA	C3B-C2B	5.26	1.47	1.40
24	C	513	CLA	O2D-CGD	5.26	1.46	1.33
24	a	409	CLA	CHC-C1C	5.26	1.48	1.35
24	B	601	CLA	O2D-CGD	5.26	1.46	1.33
26	c	514	BCR	C15-C14	-5.26	1.27	1.43
26	d	404	BCR	C11-C10	-5.26	1.27	1.43
24	c	510	CLA	C3C-C2C	5.26	1.47	1.36
24	C	508	CLA	C3B-C2B	5.26	1.47	1.40
24	b	615	CLA	C3C-C2C	5.25	1.47	1.36
24	B	612	CLA	CHC-C1C	5.25	1.48	1.35
25	a	411	PHO	C3C-C2C	5.25	1.47	1.36
24	b	606	CLA	O2D-CGD	5.25	1.46	1.33
26	t	101	BCR	C11-C10	-5.25	1.27	1.43
24	a	412	CLA	CHC-C1C	5.25	1.48	1.35
26	y	101	BCR	C11-C10	-5.25	1.27	1.43
24	C	511	CLA	O2D-CGD	5.24	1.46	1.33
26	J	101	BCR	C11-C10	-5.24	1.27	1.43
24	d	402	CLA	C3C-C2C	5.24	1.47	1.36
24	C	505	CLA	C3C-C2C	5.24	1.47	1.36
24	D	403	CLA	C3B-C2B	5.24	1.47	1.40
24	C	502	CLA	CHC-C1C	5.24	1.48	1.35
26	C	514	BCR	C15-C14	-5.24	1.27	1.43
24	B	611	CLA	C3B-C2B	5.24	1.47	1.40
26	K	102	BCR	C15-C14	-5.24	1.27	1.43
24	c	513	CLA	O2D-CGD	5.23	1.46	1.33
26	T	101	BCR	C15-C14	-5.23	1.27	1.43
24	d	403	CLA	C3C-C2C	5.23	1.47	1.36
24	b	618	CLA	C3C-C2C	5.23	1.47	1.36
24	C	505	CLA	CHC-C1C	5.23	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	J	101	BCR	C15-C14	-5.23	1.27	1.43
24	b	614	CLA	C3B-C2B	5.23	1.47	1.40
24	B	610	CLA	CHC-C1C	5.23	1.48	1.35
24	C	502	CLA	C3B-C2B	5.23	1.47	1.40
24	b	608	CLA	CHC-C1C	5.22	1.48	1.35
24	d	402	CLA	CHC-C1C	5.21	1.48	1.35
26	B	618	BCR	C11-C10	-5.21	1.27	1.43
24	b	610	CLA	C3C-C2C	5.21	1.47	1.36
24	b	615	CLA	CHC-C1C	5.21	1.48	1.35
26	k	102	BCR	C16-C15	-5.21	1.22	1.36
24	C	501	CLA	C3C-C2C	5.21	1.47	1.36
24	b	612	CLA	C3C-C2C	5.20	1.47	1.36
24	c	508	CLA	CHC-C1C	5.20	1.48	1.35
26	A	1009	BCR	C11-C10	-5.20	1.27	1.43
25	a	411	PHO	CHC-C1C	5.20	1.48	1.38
24	c	509	CLA	CHC-C1C	5.20	1.48	1.35
24	c	507	CLA	C3C-C2C	5.20	1.47	1.36
24	A	1005	CLA	CHC-C1C	5.20	1.48	1.35
24	b	616	CLA	CHC-C1C	5.20	1.48	1.35
24	c	509	CLA	O2D-CGD	5.20	1.45	1.33
25	a	410	PHO	C3B-C2B	5.20	1.47	1.37
24	B	602	CLA	C3B-C2B	5.19	1.47	1.40
24	B	610	CLA	C3B-C2B	5.19	1.47	1.40
24	A	1008	CLA	CHC-C1C	5.19	1.48	1.35
24	b	616	CLA	C3B-C2B	5.19	1.47	1.40
24	B	609	CLA	O2D-CGD	5.19	1.45	1.33
24	B	603	CLA	O2D-CGD	5.19	1.45	1.33
24	B	616	CLA	CHC-C1C	5.18	1.48	1.35
24	C	506	CLA	C3B-C2B	5.18	1.47	1.40
26	h	101	BCR	C15-C14	-5.18	1.27	1.43
24	b	615	CLA	OBD-CAD	5.18	1.29	1.22
24	a	412	CLA	C3C-C2C	5.18	1.47	1.36
26	y	101	BCR	C15-C14	-5.18	1.27	1.43
38	V	201	HEM	C3D-C2D	5.18	1.53	1.37
24	b	617	CLA	C3C-C2C	5.18	1.47	1.36
24	C	504	CLA	O2D-CGD	5.17	1.45	1.33
26	B	619	BCR	C15-C14	-5.17	1.27	1.43
24	b	618	CLA	CHC-C1C	5.17	1.48	1.35
26	k	101	BCR	C15-C14	-5.17	1.27	1.43
24	D	405	CLA	MG-NA	5.17	2.18	2.06
26	H	101	BCR	C11-C10	-5.17	1.27	1.43
24	B	606	CLA	O2D-CGD	5.16	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	617	BCR	C11-C10	-5.16	1.27	1.43
26	K	101	BCR	C11-C10	-5.16	1.27	1.43
26	b	620	BCR	C11-C10	-5.15	1.27	1.43
24	C	510	CLA	O2D-CGD	5.15	1.45	1.33
24	B	614	CLA	C3B-C2B	5.14	1.47	1.40
24	B	607	CLA	C3C-C2C	5.14	1.47	1.36
26	t	101	BCR	C15-C14	-5.14	1.27	1.43
24	c	506	CLA	O2D-CGD	5.14	1.45	1.33
24	b	607	CLA	O2D-CGD	5.14	1.45	1.33
25	D	404	PHO	O2D-CGD	5.14	1.45	1.33
24	b	613	CLA	O2D-CGD	5.14	1.45	1.33
24	B	602	CLA	CHC-C1C	5.14	1.48	1.35
24	b	619	CLA	CHC-C1C	5.14	1.48	1.35
24	c	510	CLA	C3B-C2B	5.14	1.47	1.40
25	a	411	PHO	C1A-NA	-5.14	1.27	1.37
24	b	617	CLA	CHC-C1C	5.14	1.48	1.35
24	B	612	CLA	C3C-C2C	5.13	1.47	1.36
24	b	611	CLA	C3B-C2B	5.13	1.47	1.40
24	C	512	CLA	O2D-CGD	5.13	1.45	1.33
24	c	501	CLA	C3B-C2B	5.13	1.47	1.40
24	B	605	CLA	O2D-CGD	5.13	1.45	1.33
24	B	604	CLA	CHC-C1C	5.13	1.48	1.35
26	D	406	BCR	C11-C10	-5.13	1.27	1.43
24	a	409	CLA	C3C-C2C	5.13	1.47	1.36
26	d	404	BCR	C15-C14	-5.12	1.27	1.43
24	b	615	CLA	O2D-CGD	5.12	1.45	1.33
24	c	510	CLA	O2D-CGD	5.12	1.45	1.33
24	c	510	CLA	CHC-C1C	5.12	1.48	1.35
24	b	608	CLA	O2D-CGD	5.12	1.45	1.33
26	B	617	BCR	C15-C14	-5.12	1.27	1.43
24	a	408	CLA	C3C-C2C	5.12	1.47	1.36
26	K	101	BCR	C15-C14	-5.11	1.27	1.43
24	A	1006	CLA	CHC-C1C	5.11	1.48	1.35
24	B	605	CLA	C3C-C2C	5.11	1.47	1.36
24	c	506	CLA	CHC-C1C	5.11	1.48	1.35
24	b	614	CLA	CHC-C1C	5.10	1.48	1.35
24	B	615	CLA	C3C-C2C	5.10	1.47	1.36
24	c	509	CLA	C3C-C2C	5.10	1.47	1.36
25	D	404	PHO	CHC-C1C	5.10	1.48	1.38
24	b	607	CLA	CHC-C1C	5.10	1.48	1.35
26	b	622	BCR	C15-C14	-5.10	1.27	1.43
24	a	407	CLA	CHC-C1C	5.09	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	504	CLA	CHC-C1C	5.09	1.48	1.35
24	c	512	CLA	O2D-CGD	5.09	1.45	1.33
24	B	609	CLA	C3C-C2C	5.09	1.47	1.36
24	b	606	CLA	C3B-C2B	5.09	1.47	1.40
24	D	402	CLA	C3B-C2B	5.09	1.47	1.40
24	A	1008	CLA	C3B-C2B	5.08	1.47	1.40
24	B	608	CLA	C3B-C2B	5.08	1.47	1.40
26	b	621	BCR	C15-C14	-5.07	1.27	1.43
24	b	616	CLA	C3C-C2C	5.07	1.47	1.36
24	B	614	CLA	CHC-C1C	5.07	1.48	1.35
24	b	608	CLA	C3B-C2B	5.07	1.47	1.40
24	b	612	CLA	O2D-CGD	5.06	1.45	1.33
25	a	411	PHO	O2D-CGD	5.06	1.45	1.33
26	b	621	BCR	C11-C10	-5.06	1.27	1.43
24	A	1005	CLA	O2D-CGD	5.06	1.45	1.33
24	b	610	CLA	O2D-CGD	5.06	1.45	1.33
25	A	1007	PHO	C1A-NA	-5.05	1.27	1.37
25	D	404	PHO	C1A-NA	-5.05	1.27	1.37
26	a	413	BCR	C15-C14	-5.05	1.27	1.43
26	D	406	BCR	C15-C14	-5.05	1.27	1.43
24	c	504	CLA	C3B-C2B	5.05	1.47	1.40
24	c	507	CLA	O2D-CGD	5.05	1.45	1.33
24	B	612	CLA	O2D-CGD	5.05	1.45	1.33
24	B	601	CLA	C3B-C2B	5.04	1.47	1.40
24	c	501	CLA	CHC-C1C	5.04	1.47	1.35
24	b	617	CLA	C3B-C2B	5.04	1.47	1.40
24	b	613	CLA	C3B-C2B	5.04	1.47	1.40
24	C	510	CLA	C3B-C2B	5.03	1.47	1.40
24	B	607	CLA	MG-NC	5.03	2.18	2.06
24	A	1006	CLA	C3C-C2C	5.03	1.47	1.36
24	B	616	CLA	C3C-C2C	5.03	1.47	1.36
24	b	614	CLA	O2D-CGD	5.03	1.45	1.33
24	A	1005	CLA	C3C-C2C	5.03	1.47	1.36
24	c	501	CLA	O2D-CGD	5.02	1.45	1.33
24	B	604	CLA	O2D-CGD	5.02	1.45	1.33
24	C	501	CLA	O2D-CGD	5.02	1.45	1.33
24	b	609	CLA	O2D-CGD	5.02	1.45	1.33
24	C	501	CLA	C3B-C2B	5.02	1.47	1.40
26	H	101	BCR	C15-C14	-5.01	1.27	1.43
24	B	603	CLA	C3B-C2B	5.01	1.47	1.40
26	d	404	BCR	C23-C22	-5.01	1.35	1.45
24	C	505	CLA	C3B-C2B	5.01	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	C3C-C2C	5.01	1.47	1.36
24	D	402	CLA	OBD-CAD	5.00	1.29	1.22
24	b	607	CLA	C3C-C2C	5.00	1.47	1.36
24	b	618	CLA	O2D-CGD	5.00	1.45	1.33
24	d	402	CLA	O2D-CGD	5.00	1.45	1.33
24	b	619	CLA	O2D-CGD	4.99	1.45	1.33
24	b	611	CLA	MG-NC	4.99	2.18	2.06
24	c	509	CLA	OBD-CAD	4.99	1.29	1.22
26	A	1009	BCR	C15-C14	-4.98	1.28	1.43
26	a	413	BCR	C11-C10	-4.98	1.28	1.43
24	C	509	CLA	O2D-CGD	4.98	1.45	1.33
24	B	616	CLA	O2D-CGD	4.98	1.45	1.33
24	c	502	CLA	OBD-CAD	4.98	1.29	1.22
24	a	412	CLA	C3B-C2B	4.98	1.47	1.40
24	b	610	CLA	C3B-C2B	4.98	1.47	1.40
24	b	617	CLA	O2D-CGD	4.97	1.45	1.33
24	c	503	CLA	O2D-CGD	4.97	1.45	1.33
26	B	618	BCR	C15-C14	-4.97	1.28	1.43
24	A	1005	CLA	OBD-CAD	4.97	1.29	1.22
24	C	503	CLA	O2D-CGD	4.97	1.45	1.33
24	B	605	CLA	C3B-C2B	4.97	1.47	1.40
24	B	614	CLA	O2D-CGD	4.97	1.45	1.33
24	b	610	CLA	CHC-C1C	4.97	1.47	1.35
24	B	613	CLA	C3C-C2C	4.97	1.47	1.36
24	a	407	CLA	O2D-CGD	4.97	1.45	1.33
24	b	614	CLA	C3C-C2C	4.97	1.47	1.36
26	D	406	BCR	C23-C22	-4.96	1.35	1.45
26	a	413	BCR	C23-C22	-4.96	1.35	1.45
24	B	603	CLA	CHC-C1C	4.96	1.47	1.35
24	a	407	CLA	OBD-CAD	4.96	1.29	1.22
24	c	502	CLA	O2D-CGD	4.96	1.45	1.33
24	C	502	CLA	O2D-CGD	4.96	1.45	1.33
24	C	510	CLA	C3C-C2C	4.96	1.47	1.36
24	B	615	CLA	CHC-C1C	4.95	1.47	1.35
24	A	1006	CLA	O2D-CGD	4.95	1.45	1.33
24	B	611	CLA	OBD-CAD	4.95	1.29	1.22
26	b	620	BCR	C15-C14	-4.95	1.28	1.43
24	C	510	CLA	CHC-C1C	4.95	1.47	1.35
24	A	1008	CLA	O2D-CGD	4.94	1.45	1.33
24	B	607	CLA	CHC-C1C	4.94	1.47	1.35
24	C	509	CLA	CHC-C1C	4.94	1.47	1.35
24	c	502	CLA	C3C-C2C	4.93	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	619	CLA	C3C-C2C	4.92	1.47	1.36
24	C	505	CLA	O2D-CGD	4.92	1.45	1.33
24	a	412	CLA	O2D-CGD	4.91	1.45	1.33
24	b	611	CLA	O2D-CGD	4.91	1.45	1.33
25	a	410	PHO	C1A-NA	-4.91	1.27	1.37
26	k	101	BCR	C23-C22	-4.90	1.35	1.45
26	k	102	BCR	C23-C22	-4.89	1.35	1.45
24	D	403	CLA	C3C-C2C	4.89	1.47	1.36
24	D	402	CLA	C3C-C2C	4.89	1.47	1.36
25	a	410	PHO	CHD-C1D	4.89	1.48	1.38
24	D	402	CLA	CHC-C1C	4.89	1.47	1.35
26	b	621	BCR	C23-C22	-4.89	1.35	1.45
24	d	402	CLA	C3B-C2B	4.89	1.47	1.40
26	y	101	BCR	C23-C22	-4.89	1.35	1.45
25	a	410	PHO	O2D-CGD	4.88	1.45	1.33
24	b	605	CLA	O2D-CGD	4.88	1.45	1.33
25	a	410	PHO	CHC-C1C	4.87	1.48	1.38
24	C	507	CLA	O2D-CGD	4.87	1.45	1.33
26	T	101	BCR	C23-C22	-4.86	1.35	1.45
26	K	102	BCR	C23-C22	-4.85	1.35	1.45
24	a	408	CLA	CHC-C1C	4.85	1.47	1.35
24	D	405	CLA	O2D-CGD	4.85	1.45	1.33
24	c	505	CLA	O2D-CGD	4.85	1.45	1.33
24	b	616	CLA	O2D-CGD	4.84	1.45	1.33
25	A	1007	PHO	CHC-C1C	4.83	1.48	1.38
24	B	608	CLA	O2D-CGD	4.83	1.45	1.33
24	C	507	CLA	OBD-CAD	4.82	1.29	1.22
26	t	101	BCR	C23-C22	-4.82	1.35	1.45
24	B	610	CLA	O2D-CGD	4.81	1.44	1.33
24	C	502	CLA	OBD-CAD	4.81	1.29	1.22
26	B	619	BCR	C23-C22	-4.81	1.35	1.45
24	C	510	CLA	OBD-CAD	4.81	1.29	1.22
26	b	620	BCR	C23-C22	-4.80	1.35	1.45
26	J	101	BCR	C23-C22	-4.80	1.35	1.45
24	d	403	CLA	O2D-CGD	4.79	1.44	1.33
24	B	614	CLA	OBD-CAD	4.79	1.29	1.22
24	B	604	CLA	C3B-C2B	4.79	1.47	1.40
24	B	613	CLA	O2D-CGD	4.79	1.44	1.33
26	H	101	BCR	C23-C22	-4.78	1.35	1.45
24	a	409	CLA	C3B-C2B	4.77	1.47	1.40
24	b	612	CLA	C3B-C2B	4.77	1.47	1.40
24	c	510	CLA	OBD-CAD	4.77	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	609	CLA	OBD-CAD	4.76	1.29	1.22
24	B	608	CLA	CHC-C1C	4.76	1.47	1.35
24	D	402	CLA	O2D-CGD	4.76	1.44	1.33
24	D	403	CLA	MG-NA	4.76	2.17	2.06
24	B	604	CLA	OBD-CAD	4.76	1.29	1.22
26	B	617	BCR	C23-C22	-4.75	1.35	1.45
26	K	101	BCR	C23-C22	-4.75	1.35	1.45
24	b	616	CLA	OBD-CAD	4.75	1.28	1.22
24	b	604	CLA	OBD-CAD	4.74	1.28	1.22
26	C	514	BCR	C23-C22	-4.74	1.35	1.45
26	h	101	BCR	C23-C22	-4.74	1.35	1.45
24	c	508	CLA	OBD-CAD	4.73	1.28	1.22
24	B	612	CLA	OBD-CAD	4.73	1.28	1.22
24	b	605	CLA	OBD-CAD	4.73	1.28	1.22
24	c	505	CLA	OBD-CAD	4.73	1.28	1.22
24	c	511	CLA	OBD-CAD	4.73	1.28	1.22
24	a	408	CLA	O2D-CGD	4.73	1.44	1.33
24	B	602	CLA	OBD-CAD	4.72	1.28	1.22
24	B	609	CLA	C3B-C2B	4.72	1.46	1.40
24	a	409	CLA	O2D-CGD	4.72	1.44	1.33
24	B	615	CLA	OBD-CAD	4.72	1.28	1.22
24	b	612	CLA	OBD-CAD	4.72	1.28	1.22
24	B	602	CLA	O2D-CGD	4.72	1.44	1.33
26	c	514	BCR	C23-C22	-4.70	1.35	1.45
24	c	507	CLA	OBD-CAD	4.70	1.28	1.22
26	b	622	BCR	C23-C22	-4.70	1.35	1.45
24	B	601	CLA	OBD-CAD	4.69	1.28	1.22
24	c	513	CLA	OBD-CAD	4.69	1.28	1.22
24	a	408	CLA	OBD-CAD	4.69	1.28	1.22
24	B	607	CLA	C3B-C2B	4.69	1.46	1.40
24	D	403	CLA	O2D-CGD	4.68	1.44	1.33
24	C	509	CLA	OBD-CAD	4.67	1.28	1.22
24	b	604	CLA	O2A-CGA	4.67	1.47	1.33
24	D	403	CLA	OBD-CAD	4.67	1.28	1.22
24	C	503	CLA	OBD-CAD	4.66	1.28	1.22
24	c	506	CLA	OBD-CAD	4.66	1.28	1.22
24	b	607	CLA	OBD-CAD	4.65	1.28	1.22
24	D	403	CLA	CHC-C1C	4.65	1.46	1.35
24	d	403	CLA	OBD-CAD	4.65	1.28	1.22
24	B	607	CLA	O2D-CGD	4.64	1.44	1.33
24	C	511	CLA	OBD-CAD	4.64	1.28	1.22
24	C	513	CLA	OBD-CAD	4.64	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	OBD-CAD	4.61	1.28	1.22
24	c	512	CLA	OBD-CAD	4.61	1.28	1.22
26	B	618	BCR	C23-C22	-4.61	1.36	1.45
24	a	408	CLA	MG-NC	4.61	2.17	2.06
24	b	618	CLA	OBD-CAD	4.61	1.28	1.22
24	A	1008	CLA	OBD-CAD	4.60	1.28	1.22
26	A	1009	BCR	C23-C22	-4.60	1.36	1.45
24	B	609	CLA	OBD-CAD	4.60	1.28	1.22
25	A	1007	PHO	O2D-CGD	4.59	1.44	1.33
24	C	506	CLA	OBD-CAD	4.59	1.28	1.22
24	b	613	CLA	OBD-CAD	4.57	1.28	1.22
25	D	404	PHO	CHD-C1D	4.56	1.47	1.38
24	a	412	CLA	OBD-CAD	4.56	1.28	1.22
24	B	613	CLA	OBD-CAD	4.55	1.28	1.22
30	b	634	DMS	O-S	4.55	1.81	1.50
24	c	504	CLA	OBD-CAD	4.55	1.28	1.22
29	m	102	LMG	O8-C28	4.54	1.46	1.33
30	D	416	DMS	O-S	4.54	1.80	1.50
38	F	101	HEM	C3C-C2C	-4.54	1.34	1.40
29	c	521	LMG	O7-C10	4.54	1.47	1.34
30	D	417	DMS	O-S	4.52	1.80	1.50
30	d	413	DMS	O-S	4.52	1.80	1.50
24	C	505	CLA	OBD-CAD	4.52	1.28	1.22
30	B	634	DMS	O-S	4.51	1.80	1.50
29	Z	101	LMG	O8-C28	4.51	1.46	1.33
24	D	405	CLA	OBD-CAD	4.51	1.28	1.22
30	B	633	DMS	O-S	4.51	1.80	1.50
30	a	418	DMS	O-S	4.51	1.80	1.50
30	A	1014	DMS	O-S	4.51	1.80	1.50
24	D	403	CLA	MG-NC	4.51	2.17	2.06
30	V	203	DMS	O-S	4.51	1.80	1.50
29	c	520	LMG	O8-C28	4.50	1.46	1.33
24	d	402	CLA	O2A-CGA	4.50	1.46	1.33
29	B	622	LMG	O8-C28	4.50	1.46	1.33
30	O	301	DMS	O-S	4.49	1.80	1.50
30	c	527	DMS	O-S	4.49	1.80	1.50
30	O	302	DMS	O-S	4.49	1.80	1.50
25	A	1007	PHO	CHD-C1D	4.49	1.47	1.38
30	V	205	DMS	O-S	4.48	1.80	1.50
30	b	629	DMS	O-S	4.48	1.80	1.50
30	b	635	DMS	O-S	4.48	1.80	1.50
24	b	610	CLA	C3D-C2D	4.48	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	619	CLA	O2A-CGA	4.47	1.46	1.33
30	C	525	DMS	O-S	4.47	1.80	1.50
30	b	633	DMS	O-S	4.47	1.80	1.50
24	B	608	CLA	O2A-CGA	4.47	1.46	1.33
24	C	501	CLA	OBD-CAD	4.47	1.28	1.22
30	c	528	DMS	O-S	4.46	1.80	1.50
38	v	201	HEM	C3B-C2B	-4.46	1.34	1.40
24	c	503	CLA	OBD-CAD	4.46	1.28	1.22
30	C	526	DMS	O-S	4.46	1.80	1.50
30	B	632	DMS	O-S	4.46	1.80	1.50
30	C	527	DMS	O-S	4.46	1.80	1.50
30	d	414	DMS	O-S	4.45	1.80	1.50
24	b	619	CLA	OBD-CAD	4.45	1.28	1.22
30	c	526	DMS	O-S	4.45	1.80	1.50
29	C	518	LMG	O8-C28	4.45	1.46	1.33
24	C	509	CLA	O2A-CGA	4.44	1.46	1.33
28	D	408	SQD	O47-C7	4.44	1.46	1.34
29	c	521	LMG	O8-C28	4.44	1.46	1.33
34	d	406	LHG	O8-C23	4.44	1.46	1.33
25	a	411	PHO	CHD-C1D	4.43	1.47	1.38
24	b	606	CLA	OBD-CAD	4.43	1.28	1.22
30	U	201	DMS	O-S	4.43	1.80	1.50
24	D	403	CLA	C3D-C2D	4.42	1.47	1.39
30	u	201	DMS	O-S	4.42	1.80	1.50
28	f	102	SQD	O48-C23	4.42	1.46	1.33
29	C	519	LMG	O8-C28	4.41	1.46	1.33
24	C	511	CLA	C3D-C2D	4.41	1.47	1.39
24	B	602	CLA	C3D-C2D	4.41	1.47	1.39
24	b	611	CLA	OBD-CAD	4.41	1.28	1.22
30	v	202	DMS	O-S	4.40	1.80	1.50
29	c	519	LMG	O7-C10	4.40	1.46	1.34
24	d	403	CLA	O2A-CGA	4.39	1.46	1.33
24	c	501	CLA	O2A-CGA	4.39	1.46	1.33
24	C	509	CLA	MG-NA	4.39	2.16	2.06
24	a	408	CLA	O2A-CGA	4.39	1.46	1.33
24	c	507	CLA	O2A-CGA	4.38	1.46	1.33
24	c	501	CLA	OBD-CAD	4.38	1.28	1.22
29	B	622	LMG	O7-C10	4.37	1.46	1.34
34	e	101	LHG	O8-C23	4.37	1.46	1.33
28	a	401	SQD	O48-C23	4.36	1.46	1.33
24	a	409	CLA	C3D-C2D	4.36	1.47	1.39
29	c	519	LMG	O8-C28	4.36	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	603	CLA	OBD-CAD	4.36	1.28	1.22
30	c	529	DMS	O-S	4.35	1.79	1.50
24	a	412	CLA	O2A-CGA	4.35	1.46	1.33
34	E	101	LHG	O8-C23	4.35	1.46	1.33
24	C	504	CLA	OBD-CAD	4.35	1.28	1.22
24	c	512	CLA	O2A-CGA	4.35	1.46	1.33
24	B	609	CLA	O2A-CGA	4.35	1.46	1.33
24	B	610	CLA	OBD-CAD	4.35	1.28	1.22
30	c	524	DMS	O-S	4.35	1.79	1.50
28	c	518	SQD	O47-C7	4.35	1.46	1.34
24	c	509	CLA	O2A-CGA	4.34	1.46	1.33
29	C	519	LMG	O7-C10	4.34	1.46	1.34
24	C	513	CLA	O2A-CGA	4.33	1.46	1.33
24	B	601	CLA	O2A-CGA	4.33	1.46	1.33
24	B	614	CLA	O2A-CGA	4.33	1.46	1.33
28	D	408	SQD	O48-C23	4.33	1.46	1.33
34	e	101	LHG	O7-C7	4.33	1.46	1.34
28	b	623[B]	SQD	O48-C23	4.33	1.46	1.33
30	B	627	DMS	O-S	4.33	1.79	1.50
29	A	1012	LMG	O8-C28	4.32	1.46	1.33
30	C	524	DMS	O-S	4.32	1.79	1.50
29	a	415	LMG	O7-C10	4.32	1.46	1.34
24	b	617	CLA	OBD-CAD	4.32	1.28	1.22
28	a	401	SQD	O47-C7	4.31	1.46	1.34
28	A	1016	SQD	O48-C23	4.31	1.45	1.33
24	A	1006	CLA	OBD-CAD	4.31	1.28	1.22
24	C	506	CLA	O2A-CGA	4.31	1.45	1.33
24	A	1006	CLA	C3D-C2D	4.31	1.47	1.39
28	A	1011	SQD	O48-C23	4.31	1.45	1.33
28	B	620[A]	SQD	O48-C23	4.31	1.45	1.33
29	C	518	LMG	O7-C10	4.31	1.46	1.34
24	c	504	CLA	C3D-C2D	4.30	1.47	1.39
24	C	504	CLA	C3D-C2D	4.30	1.47	1.39
24	b	608	CLA	MG-NA	4.30	2.16	2.06
28	A	1016	SQD	O47-C7	4.30	1.46	1.34
24	b	605	CLA	O2A-CGA	4.30	1.45	1.33
28	B	620[B]	SQD	O48-C23	4.29	1.45	1.33
24	C	512	CLA	OBD-CAD	4.29	1.28	1.22
28	c	518	SQD	O48-C23	4.29	1.45	1.33
24	B	606	CLA	OBD-CAD	4.29	1.28	1.22
24	A	1008	CLA	O2A-CGA	4.28	1.45	1.33
36	c	517	DGD	O1G-C1A	4.28	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	f	101	HEM	C3C-C2C	-4.28	1.34	1.40
28	b	623[A]	SQD	O48-C23	4.28	1.45	1.33
38	V	201	HEM	C3B-C2B	-4.27	1.34	1.40
28	f	102	SQD	O47-C7	4.27	1.46	1.34
24	c	506	CLA	O2A-CGA	4.27	1.45	1.33
29	a	415	LMG	O8-C28	4.27	1.45	1.33
30	B	626	DMS	O-S	4.27	1.79	1.50
24	B	616	CLA	OBD-CAD	4.27	1.28	1.22
24	B	608	CLA	OBD-CAD	4.27	1.28	1.22
30	a	417	DMS	O-S	4.26	1.79	1.50
30	C	523	DMS	O-S	4.26	1.79	1.50
24	B	615	CLA	C3D-C2D	4.26	1.47	1.39
29	A	1012	LMG	O7-C10	4.26	1.46	1.34
24	b	608	CLA	OBD-CAD	4.26	1.28	1.22
24	c	513	CLA	O2A-CGA	4.26	1.45	1.33
24	D	405	CLA	O2A-CGA	4.25	1.45	1.33
36	c	516	DGD	O1G-C1A	4.25	1.45	1.33
25	D	404	PHO	O2A-CGA	4.25	1.45	1.33
25	a	411	PHO	O2A-CGA	4.25	1.45	1.33
24	D	403	CLA	O2A-CGA	4.25	1.45	1.33
24	a	408	CLA	C3D-C2D	4.24	1.47	1.39
29	c	520	LMG	O7-C10	4.24	1.46	1.34
29	d	409	LMG	O7-C10	4.24	1.46	1.34
24	c	509	CLA	MG-NC	4.24	2.16	2.06
24	C	508	CLA	O2A-CGA	4.24	1.45	1.33
24	A	1005	CLA	O2A-CGA	4.24	1.45	1.33
24	B	616	CLA	O2A-CGA	4.24	1.45	1.33
24	b	618	CLA	O2A-CGA	4.23	1.45	1.33
30	A	1013	DMS	O-S	4.23	1.78	1.50
34	D	409	LHG	O8-C23	4.23	1.45	1.33
24	c	505	CLA	O2A-CGA	4.23	1.45	1.33
24	c	511	CLA	O2A-CGA	4.23	1.45	1.33
24	B	608	CLA	C3D-C2D	4.23	1.47	1.39
34	E	101	LHG	O7-C7	4.23	1.46	1.34
24	C	507	CLA	O2A-CGA	4.23	1.45	1.33
24	D	402	CLA	O2A-CGA	4.23	1.45	1.33
24	C	512	CLA	O2A-CGA	4.22	1.45	1.33
29	d	409	LMG	O8-C28	4.21	1.45	1.33
24	b	609	CLA	O2A-CGA	4.21	1.45	1.33
28	B	620[A]	SQD	O47-C7	4.21	1.46	1.34
28	b	623[A]	SQD	O47-C7	4.20	1.46	1.34
29	m	102	LMG	O7-C10	4.20	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	515	DGD	O1G-C1A	4.20	1.45	1.33
24	d	402	CLA	OBD-CAD	4.20	1.28	1.22
34	d	408	LHG	O7-C7	4.20	1.46	1.34
30	b	628	DMS	O-S	4.19	1.78	1.50
36	h	102	DGD	O1G-C1A	4.19	1.45	1.33
24	C	505	CLA	O2A-CGA	4.19	1.45	1.33
38	V	201	HEM	C3C-C2C	-4.19	1.34	1.40
24	C	503	CLA	C3D-C2D	4.18	1.46	1.39
34	D	411	LHG	O8-C23	4.18	1.45	1.33
24	b	612	CLA	O2A-CGA	4.18	1.45	1.33
29	Z	101	LMG	O7-C10	4.18	1.46	1.34
34	d	408	LHG	O8-C23	4.17	1.45	1.33
24	c	510	CLA	O2A-CGA	4.17	1.45	1.33
24	B	613	CLA	O2A-CGA	4.17	1.45	1.33
36	h	102	DGD	O2G-C1B	4.17	1.46	1.34
34	B	621	LHG	O8-C23	4.17	1.45	1.33
28	B	620[B]	SQD	O47-C7	4.17	1.46	1.34
24	a	412	CLA	C3D-C2D	4.16	1.46	1.39
24	b	612	CLA	C3D-C2D	4.16	1.46	1.39
34	b	624	LHG	O8-C23	4.16	1.45	1.33
24	c	503	CLA	O2A-CGA	4.16	1.45	1.33
24	C	501	CLA	O2A-CGA	4.15	1.45	1.33
24	b	609	CLA	C3D-C2D	4.15	1.46	1.39
28	b	623[B]	SQD	O47-C7	4.15	1.46	1.34
24	a	409	CLA	O2A-CGA	4.15	1.45	1.33
24	C	501	CLA	C3D-C2D	4.15	1.46	1.39
24	b	614	CLA	O2A-CGA	4.15	1.45	1.33
38	F	101	HEM	C3B-C2B	-4.15	1.34	1.40
24	c	508	CLA	O2A-CGA	4.15	1.45	1.33
24	B	611	CLA	O2A-CGA	4.14	1.45	1.33
24	b	617	CLA	O2A-CGA	4.14	1.45	1.33
24	C	512	CLA	C3D-C2D	4.14	1.46	1.39
24	C	510	CLA	O2A-CGA	4.14	1.45	1.33
24	b	614	CLA	C3D-C2D	4.14	1.46	1.39
24	A	1005	CLA	C3D-C2D	4.14	1.46	1.39
24	C	511	CLA	O2A-CGA	4.13	1.45	1.33
24	b	608	CLA	C3D-C2D	4.13	1.46	1.39
36	C	517	DGD	O2G-C1B	4.13	1.45	1.34
24	C	509	CLA	C3D-C2D	4.12	1.46	1.39
24	b	614	CLA	OBD-CAD	4.12	1.28	1.22
24	B	612	CLA	C3D-C2D	4.11	1.46	1.39
28	A	1011	SQD	O47-C7	4.11	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	OBD-CAD	4.11	1.28	1.22
24	b	607	CLA	O2A-CGA	4.10	1.45	1.33
24	d	403	CLA	C3D-C2D	4.10	1.46	1.39
24	b	611	CLA	O2A-CGA	4.10	1.45	1.33
38	v	201	HEM	C3C-C2C	-4.10	1.34	1.40
24	c	504	CLA	O2A-CGA	4.10	1.45	1.33
24	C	502	CLA	O2A-CGA	4.10	1.45	1.33
36	c	516	DGD	O2G-C1B	4.10	1.45	1.34
24	c	513	CLA	C3D-C2D	4.09	1.46	1.39
24	C	504	CLA	O2A-CGA	4.08	1.45	1.33
24	b	615	CLA	O2A-CGA	4.08	1.45	1.33
24	B	615	CLA	O2A-CGA	4.08	1.45	1.33
24	B	607	CLA	C3D-C2D	4.08	1.46	1.39
24	a	407	CLA	C3D-C2D	4.08	1.46	1.39
24	b	613	CLA	O2A-CGA	4.08	1.45	1.33
24	B	606	CLA	C3D-C2D	4.08	1.46	1.39
25	a	410	PHO	O2A-CGA	4.08	1.45	1.33
24	B	611	CLA	C3D-C2D	4.07	1.46	1.39
24	A	1006	CLA	O2A-CGA	4.07	1.45	1.33
24	C	506	CLA	C3D-C2D	4.06	1.46	1.39
24	c	502	CLA	C3D-C2D	4.06	1.46	1.39
24	b	605	CLA	C3D-C2D	4.06	1.46	1.39
34	D	411	LHG	O7-C7	4.06	1.45	1.34
24	C	503	CLA	O2A-CGA	4.06	1.45	1.33
24	B	609	CLA	C3D-C2D	4.06	1.46	1.39
24	b	610	CLA	O2A-CGA	4.06	1.45	1.33
24	b	604	CLA	C3D-C2D	4.06	1.46	1.39
24	c	502	CLA	O2A-CGA	4.06	1.45	1.33
24	C	513	CLA	C3D-C2D	4.05	1.46	1.39
24	c	508	CLA	C3D-C2D	4.05	1.46	1.39
24	D	405	CLA	C3D-C2D	4.05	1.46	1.39
24	B	602	CLA	O2A-CGA	4.05	1.45	1.33
36	c	517	DGD	O2G-C1B	4.05	1.45	1.34
34	B	621	LHG	O7-C7	4.05	1.45	1.34
24	c	506	CLA	C3D-C2D	4.04	1.46	1.39
36	C	517	DGD	O1G-C1A	4.04	1.45	1.33
24	B	607	CLA	OBD-CAD	4.03	1.27	1.22
24	b	607	CLA	C3D-C2D	4.03	1.46	1.39
24	c	503	CLA	C3D-C2D	4.03	1.46	1.39
24	c	509	CLA	C3D-C2D	4.03	1.46	1.39
24	b	608	CLA	O2A-CGA	4.03	1.45	1.33
24	b	606	CLA	C3D-C2D	4.02	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	516	DGD	O1G-C1A	4.02	1.45	1.33
24	b	618	CLA	C3D-C2D	4.02	1.46	1.39
24	B	605	CLA	C3D-C2D	4.01	1.46	1.39
24	C	505	CLA	C3D-C2D	4.01	1.46	1.39
36	C	515	DGD	O2G-C1B	4.01	1.45	1.34
29	D	412	LMG	O7-C10	4.01	1.45	1.34
24	b	616	CLA	C3D-C2D	4.01	1.46	1.39
36	C	516	DGD	O2G-C1B	4.00	1.45	1.34
24	C	510	CLA	C3D-C2D	4.00	1.46	1.39
24	B	601	CLA	C3D-C2D	3.99	1.46	1.39
29	D	412	LMG	O8-C28	3.99	1.45	1.33
36	H	102	DGD	O1G-C1A	3.99	1.45	1.33
36	C	515	DGD	O1G-C1A	3.99	1.45	1.33
25	A	1007	PHO	O2A-CGA	3.98	1.45	1.33
38	v	201	HEM	C3C-CAC	3.98	1.56	1.47
24	B	606	CLA	O2A-CGA	3.97	1.44	1.33
24	A	1008	CLA	C3D-C2D	3.97	1.46	1.39
24	c	511	CLA	C3D-C2D	3.97	1.46	1.39
36	c	515	DGD	O2G-C1B	3.96	1.45	1.34
24	b	611	CLA	C3D-C2D	3.96	1.46	1.39
24	b	619	CLA	C3D-C2D	3.96	1.46	1.39
24	B	604	CLA	MG-NC	3.95	2.15	2.06
24	C	508	CLA	C3D-C2D	3.95	1.46	1.39
24	C	502	CLA	C3D-C2D	3.95	1.46	1.39
24	B	604	CLA	C3D-C2D	3.95	1.46	1.39
24	b	616	CLA	O2A-CGA	3.95	1.44	1.33
24	B	607	CLA	O2A-CGA	3.95	1.44	1.33
24	B	604	CLA	O2A-CGA	3.95	1.44	1.33
34	d	407	LHG	O8-C23	3.94	1.44	1.33
24	B	612	CLA	O2A-CGA	3.94	1.44	1.33
24	B	610	CLA	O2A-CGA	3.93	1.44	1.33
24	c	507	CLA	C3D-C2D	3.93	1.46	1.39
24	B	613	CLA	C3D-C2D	3.92	1.46	1.39
24	c	501	CLA	C3D-C2D	3.92	1.46	1.39
24	b	606	CLA	O2A-CGA	3.91	1.44	1.33
24	B	610	CLA	MG-NA	3.89	2.15	2.06
24	c	512	CLA	C3D-C2D	3.87	1.46	1.39
34	D	410	LHG	O8-C23	3.87	1.44	1.33
24	B	605	CLA	O2A-CGA	3.86	1.44	1.33
24	b	615	CLA	C3D-C2D	3.85	1.46	1.39
24	a	407	CLA	O2A-CGA	3.85	1.44	1.33
38	f	101	HEM	C3B-C2B	-3.84	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	H	102	DGD	O2G-C1B	3.83	1.45	1.34
24	B	616	CLA	C3D-C2D	3.83	1.46	1.39
24	C	507	CLA	C3D-C2D	3.83	1.46	1.39
24	b	610	CLA	OBD-CAD	3.83	1.27	1.22
38	f	101	HEM	C3B-CAB	3.82	1.55	1.47
38	F	101	HEM	C3B-CAB	3.82	1.55	1.47
34	b	624	LHG	O7-C7	3.82	1.45	1.34
24	b	613	CLA	C3D-C2D	3.81	1.46	1.39
34	d	406	LHG	O7-C7	3.81	1.45	1.34
24	B	603	CLA	C3D-C2D	3.80	1.46	1.39
24	B	610	CLA	C3D-C2D	3.80	1.46	1.39
24	C	510	CLA	MG-NC	3.79	2.15	2.06
35	o	301	HTG	C1'-S1	-3.79	1.76	1.81
35	b	630	HTG	C1'-S1	-3.78	1.76	1.81
24	c	505	CLA	C3D-C2D	3.77	1.46	1.39
38	V	201	HEM	C3B-CAB	3.77	1.55	1.47
24	B	603	CLA	O2A-CGA	3.77	1.44	1.33
25	a	410	PHO	OBD-CAD	3.76	1.29	1.22
34	d	407	LHG	O7-C7	3.76	1.44	1.34
24	D	402	CLA	C3D-C2D	3.75	1.46	1.39
38	V	201	HEM	C3C-CAC	3.75	1.55	1.47
24	c	510	CLA	C3D-C2D	3.74	1.46	1.39
35	d	410	HTG	C1'-S1	-3.71	1.76	1.81
24	B	614	CLA	C3D-C2D	3.71	1.46	1.39
34	D	410	LHG	O7-C7	3.70	1.44	1.34
24	d	402	CLA	C3D-C2D	3.70	1.46	1.39
35	b	626	HTG	C1'-S1	-3.68	1.76	1.81
24	A	1006	CLA	MG-NC	3.68	2.15	2.06
24	a	409	CLA	OBD-CAD	3.68	1.27	1.22
24	d	403	CLA	MG-NA	3.68	2.15	2.06
35	D	413	HTG	C1'-S1	-3.67	1.76	1.81
24	b	617	CLA	C3D-C2D	3.66	1.46	1.39
34	D	409	LHG	O7-C7	3.66	1.44	1.34
38	F	101	HEM	C3C-CAC	3.66	1.55	1.47
35	B	628	HTG	C1'-S1	-3.64	1.76	1.81
25	a	411	PHO	OBD-CAD	3.63	1.28	1.22
35	c	525	HTG	C1'-S1	-3.63	1.76	1.81
25	D	404	PHO	OBD-CAD	3.62	1.28	1.22
38	f	101	HEM	C3C-CAC	3.61	1.55	1.47
35	C	521	HTG	C1'-S1	-3.61	1.76	1.81
35	b	601	HTG	C1'-S1	-3.59	1.76	1.81
35	B	629	HTG	C1'-S1	-3.57	1.76	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	501	CLA	C1D-C2D	3.57	1.50	1.42
24	C	501	CLA	C1D-C2D	3.57	1.50	1.42
25	A	1007	PHO	OBD-CAD	3.55	1.28	1.22
24	b	604	CLA	C1D-C2D	3.54	1.50	1.42
35	B	624	HTG	C1'-S1	-3.54	1.76	1.81
24	d	403	CLA	C1D-C2D	3.51	1.50	1.42
35	D	419	HTG	C1'-S1	-3.51	1.76	1.81
24	c	504	CLA	C1D-C2D	3.51	1.50	1.42
35	d	416	HTG	C1'-S1	-3.49	1.77	1.81
24	B	609	CLA	C1D-C2D	3.48	1.50	1.42
35	b	602	HTG	C1'-S1	-3.47	1.77	1.81
24	c	513	CLA	C1D-C2D	3.46	1.50	1.42
24	b	612	CLA	C1D-C2D	3.46	1.50	1.42
24	A	1005	CLA	MG-NA	3.46	2.14	2.06
24	b	609	CLA	C1D-C2D	3.45	1.50	1.42
24	D	405	CLA	C1D-C2D	3.44	1.50	1.42
35	c	522	HTG	C1'-S1	-3.43	1.77	1.81
24	B	602	CLA	C1D-C2D	3.42	1.50	1.42
24	D	403	CLA	C1D-C2D	3.42	1.50	1.42
38	v	201	HEM	C3B-CAB	3.42	1.54	1.47
35	V	202	HTG	C1'-S1	-3.42	1.77	1.81
24	B	606	CLA	C1D-C2D	3.41	1.50	1.42
24	a	408	CLA	C1D-C2D	3.41	1.50	1.42
24	c	503	CLA	C1D-C2D	3.41	1.50	1.42
25	D	404	PHO	CHC-C4B	3.40	1.48	1.40
24	c	508	CLA	C1D-C2D	3.40	1.50	1.42
24	c	506	CLA	C1D-C2D	3.38	1.50	1.42
24	C	506	CLA	C1D-C2D	3.38	1.50	1.42
24	a	409	CLA	C1D-C2D	3.38	1.50	1.42
24	A	1005	CLA	C1D-C2D	3.37	1.50	1.42
24	c	505	CLA	C1D-C2D	3.37	1.50	1.42
24	C	504	CLA	C1D-C2D	3.36	1.50	1.42
24	b	605	CLA	C1D-C2D	3.35	1.50	1.42
35	C	522	HTG	C1'-S1	-3.35	1.77	1.81
24	C	507	CLA	C1D-C2D	3.33	1.50	1.42
25	a	410	PHO	CHC-C4B	3.32	1.48	1.40
24	B	601	CLA	C1D-C2D	3.32	1.50	1.42
25	a	410	PHO	CHD-C4C	3.32	1.48	1.40
25	D	404	PHO	CHD-C4C	3.32	1.48	1.40
24	C	513	CLA	C1D-C2D	3.31	1.50	1.42
25	a	411	PHO	CHD-C4C	3.31	1.48	1.40
24	C	508	CLA	C1D-C2D	3.30	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	606	CLA	C1D-C2D	3.30	1.50	1.42
24	B	615	CLA	C1D-C2D	3.30	1.50	1.42
24	b	607	CLA	C1D-C2D	3.30	1.50	1.42
24	c	509	CLA	C1D-C2D	3.29	1.50	1.42
24	b	608	CLA	C1D-C2D	3.29	1.50	1.42
24	D	402	CLA	C1D-C2D	3.29	1.50	1.42
25	a	411	PHO	CHC-C4B	3.28	1.48	1.40
24	C	505	CLA	C1D-C2D	3.28	1.50	1.42
24	b	611	CLA	C1D-C2D	3.26	1.50	1.42
24	B	607	CLA	C1D-C2D	3.26	1.49	1.42
24	C	509	CLA	C1D-C2D	3.25	1.49	1.42
24	c	510	CLA	C1D-C2D	3.22	1.49	1.42
24	b	619	CLA	C1D-C2D	3.22	1.49	1.42
24	B	611	CLA	C1D-C2D	3.22	1.49	1.42
24	b	616	CLA	C1D-C2D	3.20	1.49	1.42
24	B	615	CLA	MG-NC	3.19	2.13	2.06
24	b	618	CLA	C1D-C2D	3.19	1.49	1.42
24	d	402	CLA	C1D-C2D	3.19	1.49	1.42
24	B	611	CLA	MG-NC	3.19	2.13	2.06
24	A	1006	CLA	C1D-C2D	3.18	1.49	1.42
24	c	511	CLA	C1D-C2D	3.18	1.49	1.42
24	C	503	CLA	C1D-C2D	3.18	1.49	1.42
24	a	407	CLA	C1D-C2D	3.17	1.49	1.42
24	c	507	CLA	C1D-C2D	3.16	1.49	1.42
25	A	1007	PHO	CHD-C4C	3.16	1.47	1.40
24	B	613	CLA	C1D-C2D	3.16	1.49	1.42
24	C	510	CLA	C1D-C2D	3.16	1.49	1.42
24	c	502	CLA	C1D-C2D	3.14	1.49	1.42
24	B	612	CLA	C1D-C2D	3.13	1.49	1.42
24	b	615	CLA	C1B-CHB	3.12	1.49	1.41
25	A	1007	PHO	CHC-C4B	3.12	1.47	1.40
24	C	502	CLA	C1D-C2D	3.12	1.49	1.42
24	b	610	CLA	C1B-CHB	3.12	1.49	1.41
24	A	1008	CLA	C1D-C2D	3.12	1.49	1.42
24	b	610	CLA	C1D-C2D	3.11	1.49	1.42
24	B	613	CLA	C1B-CHB	3.11	1.49	1.41
24	B	608	CLA	C1D-C2D	3.09	1.49	1.42
24	B	603	CLA	C1D-C2D	3.09	1.49	1.42
24	c	512	CLA	C1D-C2D	3.09	1.49	1.42
24	C	513	CLA	C1B-CHB	3.09	1.49	1.41
24	c	510	CLA	C1B-CHB	3.08	1.49	1.41
24	B	616	CLA	C1D-C2D	3.08	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	C1D-C2D	3.07	1.49	1.42
24	B	615	CLA	C1B-CHB	3.07	1.49	1.41
24	C	512	CLA	C1D-C2D	3.07	1.49	1.42
24	B	604	CLA	C1D-C2D	3.06	1.49	1.42
24	b	614	CLA	C1D-C2D	3.06	1.49	1.42
24	a	408	CLA	C1B-CHB	3.05	1.49	1.41
24	C	511	CLA	C1B-CHB	3.05	1.49	1.41
24	b	618	CLA	C1B-CHB	3.04	1.49	1.41
24	B	614	CLA	C1B-CHB	3.04	1.49	1.41
24	c	507	CLA	C1B-CHB	3.04	1.49	1.41
24	b	613	CLA	C1D-C2D	3.04	1.49	1.42
24	b	615	CLA	C1D-C2D	3.04	1.49	1.42
24	B	612	CLA	C1B-CHB	3.03	1.49	1.41
24	a	412	CLA	C1D-C2D	3.03	1.49	1.42
24	C	505	CLA	C1B-CHB	3.03	1.49	1.41
24	C	512	CLA	C1B-CHB	3.03	1.49	1.41
24	b	617	CLA	C1D-C2D	3.02	1.49	1.42
24	C	510	CLA	C1B-CHB	3.01	1.49	1.41
24	c	513	CLA	C1B-CHB	3.01	1.49	1.41
24	c	506	CLA	C1B-CHB	3.01	1.49	1.41
25	a	411	PHO	C3D-C4D	-3.01	1.34	1.43
24	c	505	CLA	C1B-CHB	3.01	1.49	1.41
24	c	501	CLA	C1B-CHB	3.01	1.49	1.41
24	C	507	CLA	C1B-CHB	3.00	1.49	1.41
24	B	610	CLA	C1D-C2D	2.98	1.49	1.42
24	A	1008	CLA	C1B-CHB	2.98	1.49	1.41
24	C	511	CLA	C1D-C2D	2.98	1.49	1.42
24	c	509	CLA	C1B-CHB	2.98	1.49	1.41
24	B	609	CLA	C1B-CHB	2.97	1.49	1.41
24	B	614	CLA	C1D-C2D	2.97	1.49	1.42
24	b	607	CLA	C1B-CHB	2.97	1.49	1.41
24	b	604	CLA	C1B-CHB	2.97	1.49	1.41
24	C	503	CLA	C1B-CHB	2.96	1.49	1.41
24	C	507	CLA	C4B-CHC	2.96	1.49	1.41
24	b	616	CLA	C1B-CHB	2.96	1.49	1.41
24	D	405	CLA	C1B-CHB	2.96	1.49	1.41
24	b	609	CLA	C1B-CHB	2.96	1.49	1.41
24	b	619	CLA	C1B-CHB	2.95	1.49	1.41
24	C	502	CLA	C1B-CHB	2.95	1.49	1.41
24	b	606	CLA	C1B-CHB	2.95	1.49	1.41
25	D	404	PHO	C3D-C4D	-2.95	1.34	1.43
24	C	513	CLA	C4B-CHC	2.95	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	605	CLA	C1B-CHB	2.95	1.49	1.41
24	b	613	CLA	C1B-CHB	2.94	1.49	1.41
24	b	612	CLA	C1B-CHB	2.94	1.49	1.41
24	B	610	CLA	C1B-CHB	2.93	1.49	1.41
24	B	604	CLA	C1B-CHB	2.93	1.49	1.41
24	B	611	CLA	C1B-CHB	2.93	1.49	1.41
24	c	512	CLA	C1B-CHB	2.93	1.49	1.41
24	c	504	CLA	C1B-CHB	2.93	1.49	1.41
24	c	503	CLA	C1B-CHB	2.93	1.49	1.41
24	c	511	CLA	C1B-CHB	2.92	1.49	1.41
24	B	606	CLA	C1B-CHB	2.92	1.49	1.41
24	c	508	CLA	C1B-CHB	2.92	1.49	1.41
24	c	511	CLA	C4B-CHC	2.91	1.49	1.41
24	c	512	CLA	C4B-CHC	2.91	1.49	1.41
24	C	501	CLA	C1B-CHB	2.91	1.49	1.41
24	c	503	CLA	C4B-CHC	2.91	1.49	1.41
24	C	504	CLA	C1B-CHB	2.90	1.49	1.41
24	C	506	CLA	C1B-CHB	2.90	1.49	1.41
24	d	403	CLA	C1B-CHB	2.90	1.49	1.41
24	C	512	CLA	C4B-CHC	2.89	1.49	1.41
24	c	507	CLA	C4B-CHC	2.89	1.49	1.41
24	b	604	CLA	C4B-CHC	2.89	1.49	1.41
24	B	603	CLA	C1B-CHB	2.89	1.49	1.41
24	A	1006	CLA	C1B-CHB	2.89	1.49	1.41
24	C	503	CLA	C4B-CHC	2.88	1.49	1.41
24	C	508	CLA	C1B-CHB	2.88	1.49	1.41
24	B	601	CLA	C1B-CHB	2.87	1.49	1.41
24	b	611	CLA	C1B-CHB	2.87	1.49	1.41
24	C	513	CLA	C1C-C2C	2.87	1.50	1.44
24	B	605	CLA	C1B-CHB	2.86	1.48	1.41
24	b	617	CLA	C1B-CHB	2.86	1.48	1.41
28	a	401	SQD	C6-S	-2.85	1.66	1.77
24	D	402	CLA	C1B-CHB	2.85	1.48	1.41
24	b	613	CLA	C4B-CHC	2.85	1.48	1.41
28	A	1016	SQD	C6-S	-2.84	1.66	1.77
24	B	614	CLA	C4B-CHC	2.84	1.48	1.41
24	B	608	CLA	C1B-CHB	2.83	1.48	1.41
24	a	409	CLA	C1B-CHB	2.83	1.48	1.41
28	A	1011	SQD	C6-S	-2.83	1.67	1.77
24	b	611	CLA	C4B-CHC	2.82	1.48	1.41
24	b	614	CLA	C1B-CHB	2.82	1.48	1.41
25	D	404	PHO	C3D-C2D	2.82	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	502	CLA	C1B-CHB	2.82	1.48	1.41
24	c	512	CLA	C1C-C2C	2.81	1.50	1.44
24	B	602	CLA	C1B-CHB	2.81	1.48	1.41
24	B	616	CLA	C1B-CHB	2.81	1.48	1.41
24	c	501	CLA	C4B-CHC	2.80	1.48	1.41
25	a	410	PHO	C3D-C2D	2.80	1.46	1.39
24	C	511	CLA	C4B-CHC	2.80	1.48	1.41
28	b	623[A]	SQD	C6-S	-2.80	1.67	1.77
24	c	508	CLA	C4B-CHC	2.80	1.48	1.41
24	B	605	CLA	C4B-CHC	2.80	1.48	1.41
24	b	617	CLA	C4B-CHC	2.80	1.48	1.41
25	A	1007	PHO	C3D-C4D	-2.80	1.34	1.43
24	c	513	CLA	C4B-CHC	2.79	1.48	1.41
25	a	411	PHO	C3D-C2D	2.78	1.46	1.39
24	B	610	CLA	C4B-CHC	2.78	1.48	1.41
28	f	102	SQD	C6-S	-2.77	1.67	1.77
24	D	403	CLA	C1B-CHB	2.77	1.48	1.41
28	B	620[B]	SQD	C6-S	-2.77	1.67	1.77
24	c	510	CLA	C4B-CHC	2.77	1.48	1.41
24	A	1005	CLA	C1B-CHB	2.77	1.48	1.41
24	a	412	CLA	C1B-CHB	2.76	1.48	1.41
28	B	620[A]	SQD	C6-S	-2.76	1.67	1.77
28	c	518	SQD	C6-S	-2.75	1.67	1.77
24	a	407	CLA	C1B-CHB	2.75	1.48	1.41
24	b	608	CLA	C1B-CHB	2.75	1.48	1.41
24	d	403	CLA	C4B-CHC	2.75	1.48	1.41
24	D	405	CLA	C4B-CHC	2.74	1.48	1.41
28	b	623[B]	SQD	C6-S	-2.74	1.67	1.77
24	C	501	CLA	C4B-CHC	2.74	1.48	1.41
24	b	606	CLA	C4B-CHC	2.74	1.48	1.41
24	B	607	CLA	C1B-CHB	2.73	1.48	1.41
24	c	504	CLA	C4B-CHC	2.73	1.48	1.41
24	B	601	CLA	C4B-CHC	2.73	1.48	1.41
24	c	505	CLA	C4B-CHC	2.73	1.48	1.41
24	B	602	CLA	CHD-C4C	2.72	1.48	1.41
27	D	407	PL9	C6-C5	2.72	1.49	1.35
24	d	402	CLA	C1B-CHB	2.72	1.48	1.41
27	a	414	PL9	C6-C5	2.72	1.49	1.35
24	C	512	CLA	C1C-C2C	2.72	1.49	1.44
25	a	410	PHO	C3D-C4D	-2.71	1.35	1.43
24	B	602	CLA	C4B-CHC	2.71	1.48	1.41
27	A	1010	PL9	C6-C5	2.71	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	C1C-C2C	2.71	1.49	1.44
24	B	611	CLA	C4B-CHC	2.71	1.48	1.41
24	c	513	CLA	CHD-C4C	2.70	1.48	1.41
24	B	606	CLA	C4B-CHC	2.70	1.48	1.41
24	B	609	CLA	C4B-CHC	2.70	1.48	1.41
24	b	609	CLA	C4B-CHC	2.70	1.48	1.41
24	b	605	CLA	C4B-CHC	2.70	1.48	1.41
24	b	605	CLA	CHD-C4C	2.69	1.48	1.41
26	K	101	BCR	C24-C25	-2.69	1.35	1.45
24	b	607	CLA	C4B-CHC	2.68	1.48	1.41
24	C	508	CLA	C4B-CHC	2.68	1.48	1.41
24	b	612	CLA	C4B-CHC	2.68	1.48	1.41
24	b	617	CLA	C1C-C2C	2.68	1.49	1.44
24	b	605	CLA	MG-NA	2.68	2.12	2.06
26	k	102	BCR	C24-C25	-2.68	1.35	1.45
24	C	506	CLA	C4B-CHC	2.68	1.48	1.41
24	b	614	CLA	C4B-CHC	2.67	1.48	1.41
24	c	502	CLA	C4B-CHC	2.67	1.48	1.41
24	B	616	CLA	C4B-CHC	2.67	1.48	1.41
27	d	405	PL9	C6-C5	2.67	1.49	1.35
24	c	503	CLA	CHD-C4C	2.66	1.48	1.41
26	y	101	BCR	C24-C25	-2.66	1.35	1.45
24	A	1008	CLA	C4B-CHC	2.65	1.48	1.41
24	c	506	CLA	C4B-CHC	2.65	1.48	1.41
24	C	505	CLA	CHD-C4C	2.65	1.48	1.41
25	A	1007	PHO	C3D-C2D	2.64	1.46	1.39
24	C	501	CLA	CHD-C4C	2.64	1.48	1.41
24	a	409	CLA	C4B-CHC	2.63	1.48	1.41
24	c	507	CLA	C1C-C2C	2.63	1.49	1.44
25	a	411	PHO	C3B-C4B	2.63	1.48	1.43
26	K	102	BCR	C24-C25	-2.63	1.35	1.45
24	b	618	CLA	C4B-CHC	2.63	1.48	1.41
24	b	619	CLA	C4B-CHC	2.63	1.48	1.41
24	b	616	CLA	C4B-CHC	2.62	1.48	1.41
24	B	606	CLA	C1C-C2C	2.62	1.49	1.44
24	b	615	CLA	C4B-CHC	2.62	1.48	1.41
24	C	511	CLA	C1C-C2C	2.62	1.49	1.44
24	b	604	CLA	CHD-C4C	2.62	1.48	1.41
24	C	509	CLA	C1B-CHB	2.61	1.48	1.41
24	c	503	CLA	C1C-C2C	2.61	1.49	1.44
26	J	101	BCR	C24-C25	-2.61	1.35	1.45
24	c	509	CLA	CHD-C4C	2.60	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	621	BCR	C24-C25	-2.60	1.35	1.45
24	b	612	CLA	CHD-C4C	2.60	1.48	1.41
26	c	514	BCR	C24-C25	-2.60	1.35	1.45
26	d	404	BCR	C24-C25	-2.60	1.35	1.45
24	B	607	CLA	C4B-CHC	2.60	1.48	1.41
24	C	505	CLA	C4B-CHC	2.59	1.48	1.41
24	C	503	CLA	CHD-C4C	2.59	1.48	1.41
24	B	612	CLA	C4B-CHC	2.59	1.48	1.41
24	c	506	CLA	CHD-C4C	2.58	1.48	1.41
24	B	601	CLA	CHD-C4C	2.58	1.48	1.41
24	B	605	CLA	C1C-C2C	2.57	1.49	1.44
28	D	408	SQD	C6-S	-2.57	1.67	1.77
24	c	504	CLA	CHD-C4C	2.57	1.48	1.41
24	c	509	CLA	C4B-CHC	2.57	1.48	1.41
24	B	613	CLA	C4B-CHC	2.57	1.48	1.41
26	b	622	BCR	C24-C25	-2.56	1.36	1.45
26	b	620	BCR	C24-C25	-2.56	1.36	1.45
26	t	101	BCR	C24-C25	-2.56	1.36	1.45
24	B	608	CLA	C4B-CHC	2.56	1.48	1.41
26	k	101	BCR	C24-C25	-2.56	1.36	1.45
24	C	507	CLA	C1C-C2C	2.56	1.49	1.44
24	d	403	CLA	C1C-C2C	2.56	1.49	1.44
24	D	402	CLA	C4B-CHC	2.55	1.48	1.41
24	D	402	CLA	C1C-C2C	2.55	1.49	1.44
24	C	504	CLA	CHD-C4C	2.55	1.48	1.41
24	D	405	CLA	C1C-C2C	2.55	1.49	1.44
24	D	405	CLA	CHD-C4C	2.55	1.48	1.41
24	c	505	CLA	C1C-C2C	2.54	1.49	1.44
24	C	504	CLA	C4B-CHC	2.54	1.48	1.41
24	A	1006	CLA	C4B-CHC	2.54	1.48	1.41
26	D	406	BCR	C24-C25	-2.54	1.36	1.45
24	C	502	CLA	C4B-CHC	2.54	1.48	1.41
24	B	603	CLA	C4B-CHC	2.53	1.48	1.41
24	c	505	CLA	CHD-C4C	2.53	1.48	1.41
26	C	514	BCR	C24-C25	-2.52	1.36	1.45
24	c	513	CLA	C1C-C2C	2.52	1.49	1.44
26	h	101	BCR	C24-C25	-2.52	1.36	1.45
24	b	610	CLA	C4B-CHC	2.52	1.48	1.41
24	b	606	CLA	C1C-C2C	2.52	1.49	1.44
24	c	501	CLA	CHD-C4C	2.51	1.48	1.41
24	a	409	CLA	CHD-C4C	2.51	1.48	1.41
24	B	604	CLA	C4B-CHC	2.51	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	609	CLA	CHD-C4C	2.51	1.48	1.41
24	d	402	CLA	C4B-CHC	2.51	1.48	1.41
24	b	604	CLA	C1C-C2C	2.51	1.49	1.44
24	a	407	CLA	C4B-CHC	2.50	1.47	1.41
24	C	510	CLA	C4B-CHC	2.50	1.47	1.41
24	C	503	CLA	C1C-C2C	2.50	1.49	1.44
26	B	619	BCR	C24-C25	-2.50	1.36	1.45
24	c	502	CLA	CHD-C4C	2.50	1.48	1.41
24	b	618	CLA	CHD-C4C	2.49	1.48	1.41
26	A	1009	BCR	C24-C25	-2.49	1.36	1.45
24	b	609	CLA	C1C-C2C	2.49	1.49	1.44
25	D	404	PHO	C3B-C4B	2.49	1.48	1.43
24	c	508	CLA	C1C-C2C	2.48	1.49	1.44
24	b	608	CLA	C4B-CHC	2.48	1.47	1.41
24	C	509	CLA	C4B-CHC	2.48	1.47	1.41
24	c	511	CLA	C1C-C2C	2.48	1.49	1.44
24	c	508	CLA	CHD-C4C	2.48	1.48	1.41
24	b	605	CLA	C1C-C2C	2.47	1.49	1.44
26	B	618	BCR	C24-C25	-2.47	1.36	1.45
24	D	403	CLA	CHD-C4C	2.47	1.48	1.41
26	B	617	BCR	C24-C25	-2.47	1.36	1.45
24	d	403	CLA	CHD-C4C	2.47	1.48	1.41
24	b	616	CLA	CHD-C4C	2.46	1.48	1.41
24	b	618	CLA	C1C-C2C	2.46	1.49	1.44
24	B	608	CLA	CHD-C4C	2.46	1.48	1.41
24	A	1005	CLA	CHD-C4C	2.46	1.48	1.41
24	C	513	CLA	CHD-C4C	2.46	1.48	1.41
24	C	506	CLA	CHD-C4C	2.46	1.48	1.41
24	c	512	CLA	CHD-C4C	2.45	1.48	1.41
24	C	505	CLA	MG-NC	2.45	2.12	2.06
24	B	602	CLA	C1C-C2C	2.45	1.49	1.44
35	C	521	HTG	C1-S1	-2.44	1.77	1.80
26	a	413	BCR	C24-C25	-2.44	1.36	1.45
26	H	101	BCR	C24-C25	-2.44	1.36	1.45
24	c	511	CLA	CHD-C4C	2.44	1.48	1.41
24	C	505	CLA	C4C-C3C	2.44	1.49	1.45
24	B	609	CLA	CHD-C4C	2.44	1.48	1.41
24	B	604	CLA	CHD-C4C	2.43	1.48	1.41
24	c	510	CLA	CHD-C4C	2.43	1.48	1.41
24	C	509	CLA	CHD-C4C	2.43	1.48	1.41
24	b	613	CLA	CHD-C4C	2.43	1.48	1.41
24	b	611	CLA	CHD-C4C	2.42	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	617	CLA	MG-NC	2.42	2.12	2.06
24	B	607	CLA	CHD-C4C	2.42	1.48	1.41
24	b	608	CLA	CHD-C4C	2.42	1.48	1.41
24	C	507	CLA	CHD-C4C	2.41	1.48	1.41
24	c	508	CLA	C4C-C3C	2.41	1.49	1.45
24	b	607	CLA	CHD-C4C	2.41	1.48	1.41
24	C	508	CLA	C1C-C2C	2.41	1.49	1.44
24	C	511	CLA	CHD-C4C	2.41	1.48	1.41
24	B	601	CLA	C1C-C2C	2.41	1.49	1.44
24	c	510	CLA	C1C-C2C	2.40	1.49	1.44
25	A	1007	PHO	C3B-C4B	2.40	1.48	1.43
26	T	101	BCR	C24-C25	-2.40	1.36	1.45
24	A	1008	CLA	C1C-C2C	2.40	1.49	1.44
24	B	603	CLA	CHD-C4C	2.40	1.48	1.41
24	b	605	CLA	C4C-C3C	2.39	1.49	1.45
24	b	615	CLA	CHD-C4C	2.39	1.48	1.41
24	B	612	CLA	C1C-C2C	2.39	1.49	1.44
24	B	615	CLA	CHD-C4C	2.38	1.47	1.41
24	b	606	CLA	CHD-C4C	2.38	1.47	1.41
24	b	609	CLA	C4C-C3C	2.38	1.49	1.45
24	a	408	CLA	C4B-CHC	2.37	1.47	1.41
24	c	506	CLA	C4C-C3C	2.37	1.49	1.45
24	a	408	CLA	CHD-C4C	2.37	1.47	1.41
25	a	410	PHO	C3B-C4B	2.37	1.48	1.43
35	B	628	HTG	C1-S1	-2.37	1.77	1.80
24	C	501	CLA	C1C-C2C	2.37	1.49	1.44
24	B	615	CLA	C4B-CHC	2.37	1.47	1.41
24	b	604	CLA	C4C-C3C	2.36	1.49	1.45
24	A	1005	CLA	C4B-CHC	2.36	1.47	1.41
36	H	102	DGD	O5D-C1E	2.36	1.44	1.40
24	B	610	CLA	C1C-C2C	2.36	1.49	1.44
24	d	402	CLA	CHD-C4C	2.36	1.47	1.41
35	b	630	HTG	C1-S1	-2.36	1.77	1.80
35	c	525	HTG	C1-S1	-2.35	1.77	1.80
24	b	610	CLA	CHD-C4C	2.35	1.47	1.41
35	c	522	HTG	C1-S1	-2.35	1.77	1.80
24	a	412	CLA	C4B-CHC	2.34	1.47	1.41
24	A	1006	CLA	CHD-C4C	2.34	1.47	1.41
24	C	510	CLA	CHD-C4C	2.33	1.47	1.41
24	c	504	CLA	C4C-C3C	2.33	1.49	1.45
24	c	504	CLA	C1C-C2C	2.33	1.49	1.44
24	C	505	CLA	C1C-C2C	2.33	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	606	CLA	CHD-C4C	2.33	1.47	1.41
24	C	512	CLA	CHD-C4C	2.32	1.47	1.41
24	B	605	CLA	CHD-C4C	2.32	1.47	1.41
24	B	608	CLA	C4C-C3C	2.32	1.49	1.45
24	C	510	CLA	C1C-C2C	2.32	1.49	1.44
24	a	412	CLA	C1C-C2C	2.32	1.49	1.44
24	B	615	CLA	C1C-C2C	2.32	1.49	1.44
24	c	501	CLA	C4C-C3C	2.31	1.49	1.45
24	B	606	CLA	C4C-C3C	2.31	1.49	1.45
24	B	610	CLA	CHD-C4C	2.31	1.47	1.41
24	B	611	CLA	C1C-C2C	2.31	1.49	1.44
24	c	503	CLA	C4C-C3C	2.30	1.49	1.45
24	C	508	CLA	CHD-C4C	2.30	1.47	1.41
24	b	613	CLA	C1C-C2C	2.30	1.49	1.44
27	D	407	PL9	C2-C3	2.30	1.40	1.34
27	A	1010	PL9	C2-C3	2.30	1.40	1.34
24	A	1008	CLA	CHD-C4C	2.30	1.47	1.41
24	c	513	CLA	C4C-C3C	2.30	1.49	1.45
24	D	405	CLA	C4C-C3C	2.29	1.49	1.45
24	B	616	CLA	CHD-C4C	2.29	1.47	1.41
24	C	506	CLA	C4C-C3C	2.29	1.49	1.45
24	C	501	CLA	C4C-C3C	2.29	1.49	1.45
35	D	413	HTG	C1-S1	-2.28	1.77	1.80
24	a	412	CLA	CHD-C4C	2.28	1.47	1.41
24	B	613	CLA	C1C-C2C	2.28	1.49	1.44
24	b	610	CLA	C4C-C3C	2.28	1.49	1.45
24	B	612	CLA	CHD-C4C	2.28	1.47	1.41
35	b	602	HTG	C1-S1	-2.27	1.77	1.80
24	C	506	CLA	C1C-C2C	2.27	1.49	1.44
24	c	507	CLA	CHD-C4C	2.27	1.47	1.41
24	B	607	CLA	C1C-C2C	2.27	1.49	1.44
24	b	611	CLA	C1C-C2C	2.27	1.48	1.44
24	d	402	CLA	C1C-C2C	2.26	1.48	1.44
24	c	506	CLA	C1C-C2C	2.26	1.48	1.44
35	V	202	HTG	C1-S1	-2.26	1.77	1.80
24	c	501	CLA	C1C-C2C	2.26	1.48	1.44
24	b	614	CLA	C1C-C2C	2.26	1.48	1.44
24	a	407	CLA	CHD-C4C	2.25	1.47	1.41
24	c	509	CLA	C1C-C2C	2.25	1.48	1.44
38	V	201	HEM	CAA-C2A	2.24	1.55	1.52
24	b	616	CLA	MG-NC	2.24	2.11	2.06
24	b	619	CLA	CHD-C4C	2.24	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	504	CLA	C1C-C2C	2.24	1.48	1.44
24	b	612	CLA	C1C-C2C	2.23	1.48	1.44
24	b	614	CLA	CHD-C4C	2.23	1.47	1.41
24	B	611	CLA	CHD-C4C	2.23	1.47	1.41
24	b	615	CLA	C1C-C2C	2.22	1.48	1.44
24	c	509	CLA	C4C-C3C	2.22	1.48	1.45
35	B	624	HTG	C1-S1	-2.22	1.77	1.80
24	B	615	CLA	C1C-NC	-2.21	1.34	1.37
24	B	609	CLA	C1C-C2C	2.21	1.48	1.44
24	b	607	CLA	C1C-C2C	2.21	1.48	1.44
28	f	102	SQD	O6-C1	2.21	1.44	1.40
24	b	617	CLA	CHD-C4C	2.20	1.47	1.41
38	f	101	HEM	CAA-C2A	2.20	1.55	1.52
36	h	102	DGD	O5D-C1E	2.20	1.43	1.40
24	b	610	CLA	C1C-C2C	2.19	1.48	1.44
24	B	615	CLA	C4C-C3C	2.19	1.48	1.45
38	v	201	HEM	CAA-C2A	2.19	1.55	1.52
24	B	602	CLA	C4C-C3C	2.19	1.48	1.45
27	a	414	PL9	C2-C3	2.19	1.40	1.34
24	D	402	CLA	CHD-C4C	2.19	1.47	1.41
25	a	411	PHO	C4C-C3C	2.18	1.49	1.45
35	B	629	HTG	C1-S1	-2.18	1.77	1.80
32	m	103	LMT	O1'-C1'	2.18	1.43	1.40
32	a	402	LMT	O1'-C1'	2.18	1.43	1.40
24	b	608	CLA	C1C-C2C	2.18	1.48	1.44
24	D	403	CLA	C4B-CHC	2.18	1.47	1.41
24	c	505	CLA	C4C-C3C	2.18	1.48	1.45
24	B	614	CLA	CHD-C4C	2.17	1.47	1.41
24	B	608	CLA	C1C-C2C	2.17	1.48	1.44
24	c	502	CLA	C4C-C3C	2.17	1.48	1.45
24	b	612	CLA	C4C-C3C	2.16	1.48	1.45
24	B	613	CLA	CHD-C4C	2.15	1.47	1.41
24	C	502	CLA	C1C-C2C	2.15	1.48	1.44
24	C	509	CLA	C1C-C2C	2.15	1.48	1.44
35	d	410	HTG	C1-S1	-2.14	1.77	1.80
24	c	510	CLA	C4C-C3C	2.14	1.48	1.45
24	C	504	CLA	C4C-C3C	2.13	1.48	1.45
36	c	515	DGD	O5D-C1E	2.13	1.43	1.40
24	b	619	CLA	C1C-C2C	2.12	1.48	1.44
24	C	502	CLA	CHD-C4C	2.12	1.47	1.41
24	C	513	CLA	C4C-C3C	2.12	1.48	1.45
24	B	603	CLA	C1C-C2C	2.12	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	616	CLA	C1C-C2C	2.12	1.48	1.44
35	d	416	HTG	C1-S1	-2.12	1.77	1.80
27	d	405	PL9	C2-C3	2.11	1.40	1.34
26	b	622	BCR	C8-C7	-2.11	1.26	1.33
24	C	512	CLA	C4C-C3C	2.11	1.48	1.45
24	d	403	CLA	C4C-C3C	2.11	1.48	1.45
24	B	616	CLA	C1C-C2C	2.11	1.48	1.44
36	C	516	DGD	O5D-C1E	2.11	1.43	1.40
24	B	601	CLA	C4C-C3C	2.10	1.48	1.45
24	A	1006	CLA	C1C-C2C	2.10	1.48	1.44
24	c	512	CLA	C4C-C3C	2.10	1.48	1.45
24	B	612	CLA	MG-NC	2.10	2.11	2.06
29	c	520	LMG	O1-C1	2.10	1.43	1.40
24	b	617	CLA	C1C-NC	-2.09	1.34	1.37
24	c	508	CLA	C1C-NC	-2.09	1.34	1.37
24	B	614	CLA	C1C-NC	-2.09	1.34	1.37
35	b	601	HTG	C1-S1	-2.09	1.77	1.80
24	A	1005	CLA	C1C-C2C	2.09	1.48	1.44
32	A	1017	LMT	O1'-C1'	2.09	1.43	1.40
26	K	101	BCR	C8-C7	-2.08	1.26	1.33
24	B	610	CLA	C4C-C3C	2.08	1.48	1.45
26	d	404	BCR	C8-C7	-2.08	1.26	1.33
24	A	1008	CLA	C4C-C3C	2.07	1.48	1.45
24	C	511	CLA	C4C-C3C	2.07	1.48	1.45
24	C	508	CLA	C1C-NC	-2.07	1.34	1.37
26	K	102	BCR	C8-C7	-2.07	1.26	1.33
25	a	410	PHO	CHB-C4A	-2.07	1.34	1.40
26	c	514	BCR	C8-C7	-2.07	1.26	1.33
35	C	522	HTG	C1-S1	-2.07	1.77	1.80
26	t	101	BCR	C8-C7	-2.06	1.26	1.33
24	B	601	CLA	C1C-NC	-2.06	1.34	1.37
24	c	502	CLA	C1C-C2C	2.06	1.48	1.44
26	k	101	BCR	C8-C7	-2.05	1.26	1.33
36	c	516	DGD	O5D-C1E	2.04	1.43	1.40
26	C	514	BCR	C8-C7	-2.04	1.26	1.33
24	c	507	CLA	C1C-NC	-2.04	1.34	1.37
24	C	513	CLA	C1C-NC	-2.03	1.34	1.37
29	c	521	LMG	O1-C1	2.03	1.43	1.40
26	B	617	BCR	C8-C7	-2.03	1.26	1.33
26	k	102	BCR	C8-C7	-2.03	1.26	1.33
26	y	101	BCR	C8-C7	-2.02	1.26	1.33
24	a	407	CLA	C1C-C2C	2.02	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	C4C-C3C	2.02	1.48	1.45
26	T	101	BCR	C8-C7	-2.02	1.26	1.33
26	B	619	BCR	C8-C7	-2.02	1.27	1.33
24	b	609	CLA	C1C-NC	-2.02	1.34	1.37
25	D	404	PHO	C1B-C2B	2.01	1.50	1.45
24	B	606	CLA	C1C-NC	-2.01	1.34	1.37
24	C	509	CLA	C4C-C3C	2.01	1.48	1.45
24	C	510	CLA	C1C-NC	-2.00	1.34	1.37
24	B	607	CLA	C4C-C3C	2.00	1.48	1.45

All (2311) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1009	BCR	C20-C21-C22	28.08	167.39	127.31
26	J	101	BCR	C16-C17-C18	28.03	167.31	127.31
26	y	101	BCR	C20-C21-C22	27.20	166.12	127.31
26	k	101	BCR	C15-C16-C17	27.02	178.83	123.47
26	c	514	BCR	C16-C17-C18	26.99	165.84	127.31
26	b	621	BCR	C20-C21-C22	26.96	165.78	127.31
26	h	101	BCR	C20-C21-C22	26.67	165.37	127.31
26	y	101	BCR	C16-C17-C18	26.62	165.30	127.31
26	B	618	BCR	C20-C21-C22	26.40	164.98	127.31
26	c	514	BCR	C15-C16-C17	26.38	177.52	123.47
26	c	514	BCR	C20-C21-C22	26.37	164.94	127.31
26	C	514	BCR	C15-C16-C17	26.24	177.23	123.47
26	K	102	BCR	C15-C16-C17	26.18	177.10	123.47
26	b	620	BCR	C20-C21-C22	26.17	164.67	127.31
26	d	404	BCR	C20-C21-C22	26.00	164.42	127.31
26	J	101	BCR	C20-C21-C22	25.98	164.40	127.31
26	d	404	BCR	C15-C16-C17	25.95	176.62	123.47
26	B	617	BCR	C20-C21-C22	25.64	163.91	127.31
26	y	101	BCR	C15-C16-C17	25.52	175.76	123.47
26	b	622	BCR	C15-C16-C17	25.45	175.61	123.47
26	C	514	BCR	C20-C21-C22	25.36	163.51	127.31
26	K	102	BCR	C20-C21-C22	25.23	163.32	127.31
26	h	101	BCR	C16-C17-C18	25.23	163.32	127.31
26	J	101	BCR	C15-C16-C17	25.23	175.15	123.47
26	H	101	BCR	C20-C21-C22	25.15	163.20	127.31
26	k	102	BCR	C20-C21-C22	25.10	163.13	127.31
26	k	102	BCR	C15-C16-C17	24.95	174.58	123.47
26	b	621	BCR	C16-C17-C18	24.90	162.84	127.31
26	B	619	BCR	C20-C21-C22	24.83	162.75	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	t	101	BCR	C20-C21-C22	24.67	162.52	127.31
26	a	413	BCR	C16-C17-C18	24.49	162.26	127.31
26	h	101	BCR	C15-C16-C17	24.42	173.49	123.47
26	k	101	BCR	C16-C17-C18	24.36	162.07	127.31
26	H	101	BCR	C15-C16-C17	24.31	173.27	123.47
26	b	622	BCR	C20-C21-C22	24.22	161.88	127.31
26	k	102	BCR	C16-C17-C18	24.17	161.80	127.31
26	T	101	BCR	C20-C21-C22	24.15	161.78	127.31
26	b	621	BCR	C15-C16-C17	24.15	172.95	123.47
26	T	101	BCR	C15-C16-C17	24.14	172.93	123.47
26	D	406	BCR	C20-C21-C22	24.02	161.59	127.31
26	H	101	BCR	C16-C17-C18	23.85	161.35	127.31
26	k	101	BCR	C20-C21-C22	23.66	161.08	127.31
26	D	406	BCR	C16-C17-C18	23.55	160.92	127.31
26	B	618	BCR	C16-C17-C18	23.34	160.62	127.31
26	a	413	BCR	C15-C16-C17	23.18	170.97	123.47
26	t	101	BCR	C15-C16-C17	23.14	170.87	123.47
26	b	620	BCR	C15-C16-C17	22.90	170.39	123.47
26	B	618	BCR	C15-C16-C17	22.80	170.19	123.47
26	b	622	BCR	C16-C15-C14	22.79	170.15	123.47
26	T	101	BCR	C16-C15-C14	22.77	170.11	123.47
26	K	101	BCR	C20-C21-C22	22.67	159.66	127.31
26	B	617	BCR	C16-C17-C18	22.44	159.34	127.31
26	D	406	BCR	C15-C16-C17	22.36	169.28	123.47
26	C	514	BCR	C16-C15-C14	22.33	169.22	123.47
26	B	619	BCR	C15-C16-C17	22.27	169.09	123.47
26	B	617	BCR	C15-C16-C17	21.96	168.46	123.47
26	K	102	BCR	C16-C15-C14	21.92	168.38	123.47
26	a	413	BCR	C20-C21-C22	21.87	158.52	127.31
26	K	102	BCR	C16-C17-C18	21.83	158.46	127.31
26	b	620	BCR	C16-C17-C18	21.72	158.31	127.31
26	K	101	BCR	C15-C16-C17	21.71	167.94	123.47
26	d	404	BCR	C16-C15-C14	21.22	166.94	123.47
26	t	101	BCR	C16-C17-C18	21.17	157.52	127.31
26	K	101	BCR	C16-C17-C18	21.07	157.38	127.31
26	t	101	BCR	C16-C15-C14	21.07	166.63	123.47
26	A	1009	BCR	C16-C17-C18	20.96	157.22	127.31
26	C	514	BCR	C16-C17-C18	20.81	157.00	127.31
26	c	514	BCR	C16-C15-C14	20.69	165.86	123.47
26	d	404	BCR	C16-C17-C18	20.58	156.68	127.31
26	B	619	BCR	C16-C17-C18	20.51	156.57	127.31
26	y	101	BCR	C16-C15-C14	20.48	165.43	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	J	101	BCR	C16-C15-C14	20.47	165.41	123.47
26	k	101	BCR	C16-C15-C14	20.45	165.36	123.47
26	b	622	BCR	C16-C17-C18	20.30	156.28	127.31
26	a	413	BCR	C16-C15-C14	20.21	164.87	123.47
26	T	101	BCR	C16-C17-C18	20.06	155.94	127.31
26	B	617	BCR	C16-C15-C14	19.96	164.35	123.47
26	h	101	BCR	C16-C15-C14	19.90	164.24	123.47
26	A	1009	BCR	C15-C16-C17	19.80	164.03	123.47
26	k	102	BCR	C16-C15-C14	19.57	163.56	123.47
26	B	618	BCR	C16-C15-C14	19.53	163.48	123.47
26	K	101	BCR	C16-C15-C14	19.51	163.44	123.47
26	B	619	BCR	C16-C15-C14	19.38	163.17	123.47
26	H	101	BCR	C16-C15-C14	18.80	161.99	123.47
26	A	1009	BCR	C16-C15-C14	18.73	161.83	123.47
26	b	620	BCR	C16-C15-C14	18.59	161.56	123.47
26	y	101	BCR	C21-C20-C19	17.79	178.74	123.22
26	b	621	BCR	C16-C15-C14	17.63	159.58	123.47
26	K	102	BCR	C21-C20-C19	17.56	178.01	123.22
26	k	101	BCR	C21-C20-C19	17.31	177.23	123.22
26	B	618	BCR	C21-C20-C19	16.98	176.20	123.22
26	H	101	BCR	C21-C20-C19	16.84	175.76	123.22
26	h	101	BCR	C21-C20-C19	16.70	175.34	123.22
26	K	101	BCR	C21-C20-C19	16.58	174.96	123.22
26	T	101	BCR	C21-C20-C19	16.31	174.13	123.22
26	J	101	BCR	C21-C20-C19	16.12	173.53	123.22
26	c	514	BCR	C21-C20-C19	16.00	173.15	123.22
26	D	406	BCR	C16-C15-C14	15.88	156.00	123.47
26	b	621	BCR	C21-C20-C19	15.79	172.49	123.22
26	a	413	BCR	C21-C20-C19	15.77	172.44	123.22
26	d	404	BCR	C21-C20-C19	15.73	172.31	123.22
26	B	619	BCR	C21-C20-C19	15.66	172.09	123.22
26	k	102	BCR	C21-C20-C19	15.62	171.96	123.22
26	C	514	BCR	C21-C20-C19	15.41	171.32	123.22
26	B	617	BCR	C21-C20-C19	15.00	170.02	123.22
26	A	1009	BCR	C21-C20-C19	14.98	169.96	123.22
26	k	102	BCR	C7-C8-C9	14.71	148.46	126.23
26	k	102	BCR	C10-C11-C12	14.58	168.72	123.22
26	D	406	BCR	C21-C20-C19	14.53	168.57	123.22
26	b	622	BCR	C21-C20-C19	14.52	168.54	123.22
26	t	101	BCR	C21-C20-C19	14.07	167.12	123.22
26	t	101	BCR	C11-C12-C13	13.98	165.68	126.42
26	J	101	BCR	C11-C12-C13	13.92	165.52	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	620	BCR	C21-C20-C19	13.84	166.39	123.22
26	y	101	BCR	C7-C8-C9	13.83	147.14	126.23
26	A	1009	BCR	C19-C18-C17	13.70	139.97	118.94
26	K	102	BCR	C10-C11-C12	13.69	165.95	123.22
26	a	413	BCR	C19-C18-C17	13.63	139.85	118.94
26	y	101	BCR	C20-C19-C18	13.63	164.70	126.42
26	c	514	BCR	C20-C19-C18	13.62	164.66	126.42
26	A	1009	BCR	C20-C19-C18	13.53	164.41	126.42
26	K	102	BCR	C20-C19-C18	13.53	164.41	126.42
26	a	413	BCR	C10-C11-C12	13.49	165.31	123.22
26	K	101	BCR	C11-C12-C13	13.46	164.22	126.42
26	h	101	BCR	C20-C19-C18	13.42	164.13	126.42
26	b	621	BCR	C11-C10-C9	13.20	146.15	127.31
26	B	617	BCR	C19-C18-C17	13.19	139.19	118.94
26	C	514	BCR	C10-C11-C12	13.19	164.38	123.22
26	k	102	BCR	C11-C12-C13	13.15	163.35	126.42
26	B	619	BCR	C10-C11-C12	13.12	164.16	123.22
26	a	413	BCR	C11-C10-C9	13.03	145.91	127.31
26	k	101	BCR	C10-C11-C12	13.01	163.80	123.22
26	B	619	BCR	C11-C12-C13	13.00	162.94	126.42
26	H	101	BCR	C20-C19-C18	12.99	162.91	126.42
26	K	101	BCR	C15-C14-C13	12.94	145.77	127.31
26	t	101	BCR	C10-C11-C12	12.85	163.31	123.22
26	B	618	BCR	C19-C18-C17	12.78	138.55	118.94
26	a	413	BCR	C15-C14-C13	12.78	145.54	127.31
26	a	413	BCR	C20-C19-C18	12.54	161.64	126.42
26	c	514	BCR	C10-C11-C12	12.48	162.17	123.22
26	K	101	BCR	C20-C19-C18	12.43	161.35	126.42
26	K	101	BCR	C10-C11-C12	12.43	162.00	123.22
26	D	406	BCR	C19-C18-C17	12.41	137.98	118.94
26	T	101	BCR	C20-C19-C18	12.39	161.21	126.42
24	b	607	CLA	C4A-NA-C1A	12.30	112.24	106.71
26	b	622	BCR	C20-C19-C18	12.28	160.91	126.42
26	H	101	BCR	C11-C10-C9	12.28	144.83	127.31
26	t	101	BCR	C20-C19-C18	12.23	160.77	126.42
26	B	619	BCR	C19-C18-C17	12.22	137.69	118.94
26	b	622	BCR	C11-C12-C13	12.20	160.68	126.42
26	C	514	BCR	C20-C19-C18	12.16	160.58	126.42
26	B	617	BCR	C15-C14-C13	12.09	144.57	127.31
26	d	404	BCR	C11-C12-C13	12.06	160.31	126.42
26	k	102	BCR	C20-C19-C18	12.05	160.27	126.42
26	b	621	BCR	C10-C11-C12	12.04	160.78	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	y	101	BCR	C11-C12-C13	11.99	160.11	126.42
24	C	511	CLA	C4A-NA-C1A	11.99	112.09	106.71
26	k	101	BCR	C11-C12-C13	11.99	160.09	126.42
26	K	102	BCR	C11-C12-C13	11.98	160.07	126.42
26	H	101	BCR	C19-C18-C17	11.96	137.30	118.94
26	b	621	BCR	C19-C18-C17	11.95	137.28	118.94
24	c	507	CLA	C4A-NA-C1A	11.92	112.07	106.71
26	J	101	BCR	C10-C11-C12	11.92	160.42	123.22
26	B	617	BCR	C11-C10-C9	11.80	144.15	127.31
26	d	404	BCR	C20-C19-C18	11.74	159.40	126.42
26	D	406	BCR	C15-C14-C13	11.72	144.04	127.31
26	J	101	BCR	C20-C19-C18	11.67	159.21	126.42
26	B	617	BCR	C20-C19-C18	11.61	159.04	126.42
26	B	618	BCR	C20-C19-C18	11.58	158.96	126.42
24	C	507	CLA	C4A-NA-C1A	11.56	111.91	106.71
26	J	101	BCR	C19-C18-C17	11.44	136.50	118.94
26	k	101	BCR	C20-C19-C18	11.42	158.50	126.42
26	C	514	BCR	C11-C10-C9	11.41	143.59	127.31
26	t	101	BCR	C19-C18-C17	11.39	136.42	118.94
26	a	413	BCR	C11-C12-C13	11.38	158.38	126.42
26	D	406	BCR	C7-C8-C9	11.37	143.42	126.23
26	k	101	BCR	C7-C8-C9	11.36	143.40	126.23
26	b	622	BCR	C10-C11-C12	11.24	158.28	123.22
26	A	1009	BCR	C10-C11-C12	11.21	158.21	123.22
26	B	618	BCR	C7-C8-C9	11.21	143.17	126.23
26	C	514	BCR	C11-C12-C13	11.20	157.88	126.42
26	b	621	BCR	C20-C19-C18	11.20	157.88	126.42
24	b	618	CLA	C4A-NA-C1A	11.15	111.72	106.71
24	C	503	CLA	C4A-NA-C1A	11.14	111.71	106.71
24	B	615	CLA	C4A-NA-C1A	11.07	111.69	106.71
26	D	406	BCR	C20-C19-C18	11.02	157.38	126.42
26	A	1009	BCR	C7-C8-C9	10.97	142.82	126.23
26	A	1009	BCR	C11-C12-C13	10.95	157.19	126.42
26	D	406	BCR	C11-C12-C13	10.94	157.16	126.42
26	a	413	BCR	C7-C8-C9	10.92	142.74	126.23
24	b	609	CLA	C4A-NA-C1A	10.90	111.61	106.71
26	h	101	BCR	C11-C12-C13	10.87	156.97	126.42
26	B	619	BCR	C20-C19-C18	10.87	156.95	126.42
26	k	101	BCR	C15-C14-C13	10.86	142.80	127.31
26	h	101	BCR	C19-C18-C17	10.80	135.51	118.94
26	y	101	BCR	C10-C11-C12	10.79	156.89	123.22
26	b	620	BCR	C19-C18-C17	10.78	135.49	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	514	BCR	C11-C12-C13	10.78	156.70	126.42
26	b	620	BCR	C20-C19-C18	10.75	156.60	126.42
26	T	101	BCR	C11-C12-C13	10.74	156.58	126.42
26	b	620	BCR	C10-C11-C12	10.72	156.66	123.22
24	c	503	CLA	C4A-NA-C1A	10.71	111.52	106.71
26	T	101	BCR	C10-C11-C12	10.70	156.60	123.22
26	d	404	BCR	C7-C8-C9	10.64	142.31	126.23
26	A	1009	BCR	C11-C10-C9	10.63	142.48	127.31
24	b	612	CLA	C4A-NA-C1A	10.63	111.48	106.71
26	b	622	BCR	C19-C18-C17	10.60	135.20	118.94
24	c	511	CLA	C4A-NA-C1A	10.57	111.46	106.71
26	H	101	BCR	C11-C12-C13	10.56	156.08	126.42
26	K	101	BCR	C11-C10-C9	10.54	142.36	127.31
26	b	620	BCR	C15-C14-C13	10.52	142.32	127.31
26	K	101	BCR	C19-C18-C17	10.50	135.06	118.94
26	b	620	BCR	C11-C12-C13	10.50	155.91	126.42
26	h	101	BCR	C11-C10-C9	10.48	142.26	127.31
26	k	101	BCR	C19-C18-C17	10.47	135.00	118.94
26	B	617	BCR	C10-C11-C12	10.43	155.77	123.22
26	B	618	BCR	C15-C14-C13	10.43	142.19	127.31
26	t	101	BCR	C7-C8-C9	10.42	141.98	126.23
24	C	505	CLA	C4A-NA-C1A	10.40	111.38	106.71
24	B	604	CLA	C4A-NA-C1A	10.33	111.35	106.71
26	T	101	BCR	C11-C10-C9	10.31	142.02	127.31
26	B	618	BCR	C10-C11-C12	10.24	155.16	123.22
26	d	404	BCR	C15-C14-C13	10.23	141.91	127.31
26	K	101	BCR	C7-C8-C9	10.21	141.67	126.23
26	b	622	BCR	C15-C14-C13	10.20	141.87	127.31
26	K	102	BCR	C7-C8-C9	10.18	141.62	126.23
26	b	620	BCR	C11-C10-C9	10.16	141.81	127.31
26	y	101	BCR	C19-C18-C17	10.15	134.52	118.94
26	A	1009	BCR	C15-C14-C13	10.14	141.78	127.31
26	c	514	BCR	C7-C8-C9	10.14	141.56	126.23
26	J	101	BCR	C7-C8-C9	10.14	141.56	126.23
26	D	406	BCR	C11-C10-C9	10.13	141.76	127.31
24	B	606	CLA	C4A-NA-C1A	10.12	111.26	106.71
26	b	621	BCR	C11-C12-C13	10.10	154.79	126.42
26	B	619	BCR	C15-C14-C13	10.09	141.72	127.31
26	b	621	BCR	C15-C14-C13	10.07	141.68	127.31
26	b	622	BCR	C7-C8-C9	10.05	141.43	126.23
26	H	101	BCR	C15-C14-C13	9.99	141.57	127.31
24	B	613	CLA	C4A-NA-C1A	9.96	111.18	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	617	BCR	C36-C18-C17	-9.95	108.99	122.92
24	c	512	CLA	C4A-NA-C1A	9.94	111.18	106.71
26	k	101	BCR	C11-C10-C9	9.93	141.48	127.31
26	B	619	BCR	C7-C8-C9	9.85	141.12	126.23
26	T	101	BCR	C15-C14-C13	9.81	141.31	127.31
24	b	604	CLA	C4A-NA-C1A	9.80	111.11	106.71
26	J	101	BCR	C36-C18-C17	-9.80	109.20	122.92
24	c	501	CLA	C4A-NA-C1A	9.76	111.09	106.71
24	c	506	CLA	C4A-NA-C1A	9.74	111.08	106.71
26	D	406	BCR	C10-C11-C12	9.70	153.49	123.22
24	B	601	CLA	C4A-NA-C1A	9.69	111.06	106.71
24	c	509	CLA	C4A-NA-C1A	9.67	111.06	106.71
24	b	610	CLA	C4A-NA-C1A	9.67	111.05	106.71
26	K	102	BCR	C15-C14-C13	9.60	141.01	127.31
26	B	618	BCR	C11-C12-C13	9.52	153.16	126.42
26	B	618	BCR	C12-C13-C14	9.51	133.54	118.94
24	B	611	CLA	C4A-NA-C1A	9.51	110.98	106.71
26	b	622	BCR	C11-C10-C9	9.50	140.87	127.31
26	c	514	BCR	C19-C18-C17	9.50	133.52	118.94
24	C	506	CLA	C4A-NA-C1A	9.48	110.97	106.71
24	C	512	CLA	C4A-NA-C1A	9.47	110.97	106.71
26	B	619	BCR	C11-C10-C9	9.45	140.80	127.31
26	c	514	BCR	C15-C14-C13	9.45	140.79	127.31
26	C	514	BCR	C15-C14-C13	9.44	140.78	127.31
26	b	620	BCR	C7-C8-C9	9.43	140.48	126.23
24	B	614	CLA	C4A-NA-C1A	9.40	110.93	106.71
24	C	504	CLA	C4A-NA-C1A	9.39	110.93	106.71
24	c	508	CLA	C4A-NA-C1A	9.36	110.91	106.71
24	b	616	CLA	C4A-NA-C1A	9.35	110.91	106.71
24	B	609	CLA	C4A-NA-C1A	9.35	110.91	106.71
26	K	102	BCR	C19-C18-C17	9.33	133.26	118.94
26	t	101	BCR	C15-C14-C13	9.32	140.61	127.31
26	B	618	BCR	C11-C10-C9	9.31	140.60	127.31
24	C	501	CLA	C4A-NA-C1A	9.28	110.88	106.71
26	B	617	BCR	C23-C22-C21	9.20	133.06	118.94
26	b	621	BCR	C7-C8-C9	9.20	140.13	126.23
26	h	101	BCR	C15-C14-C13	9.17	140.39	127.31
24	c	502	CLA	C4A-NA-C1A	9.15	110.82	106.71
26	H	101	BCR	C12-C13-C14	9.13	132.96	118.94
24	c	504	CLA	C4A-NA-C1A	9.10	110.80	106.71
26	b	620	BCR	C12-C13-C14	9.08	132.88	118.94
24	C	513	CLA	C4A-NA-C1A	9.06	110.78	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	413	BCR	C36-C18-C17	-9.04	110.27	122.92
26	K	102	BCR	C11-C10-C9	9.02	140.19	127.31
24	b	613	CLA	C4A-NA-C1A	9.01	110.75	106.71
26	b	621	BCR	C12-C13-C14	8.97	132.71	118.94
26	C	514	BCR	C7-C8-C9	8.97	139.79	126.23
24	b	615	CLA	C4A-NA-C1A	8.97	110.74	106.71
24	C	502	CLA	C4A-NA-C1A	8.95	110.73	106.71
24	C	509	CLA	C4A-NA-C1A	8.95	110.73	106.71
24	c	505	CLA	C4A-NA-C1A	8.93	110.72	106.71
26	T	101	BCR	C24-C23-C22	8.90	139.68	126.23
26	T	101	BCR	C19-C18-C17	8.89	132.58	118.94
26	B	617	BCR	C11-C12-C13	8.86	151.30	126.42
26	y	101	BCR	C11-C10-C9	8.85	139.94	127.31
26	B	619	BCR	C36-C18-C17	-8.81	110.58	122.92
24	b	605	CLA	C4A-NA-C1A	8.79	110.66	106.71
26	d	404	BCR	C10-C11-C12	8.78	150.61	123.22
26	J	101	BCR	C11-C10-C9	8.75	139.80	127.31
24	C	508	CLA	C4A-NA-C1A	8.74	110.64	106.71
24	C	510	CLA	C4A-NA-C1A	8.69	110.61	106.71
24	b	606	CLA	C4A-NA-C1A	8.69	110.61	106.71
26	h	101	BCR	C24-C23-C22	8.69	139.37	126.23
26	c	514	BCR	C11-C10-C9	8.68	139.69	127.31
26	d	404	BCR	C19-C18-C17	8.67	132.25	118.94
26	H	101	BCR	C7-C8-C9	8.67	139.34	126.23
26	c	514	BCR	C36-C18-C17	-8.60	110.88	122.92
24	D	402	CLA	C4A-NA-C1A	8.57	110.56	106.71
26	T	101	BCR	C7-C8-C9	8.55	139.16	126.23
24	b	619	CLA	C4A-NA-C1A	8.54	110.54	106.71
25	D	404	PHO	CMD-C2D-C1D	8.48	138.13	125.06
24	c	513	CLA	C4A-NA-C1A	8.45	110.51	106.71
24	D	405	CLA	C4A-NA-C1A	8.45	110.50	106.71
26	h	101	BCR	C10-C11-C12	8.45	149.57	123.22
25	a	411	PHO	CMD-C2D-C1D	8.41	138.02	125.06
26	D	406	BCR	C29-C30-C25	8.41	123.42	110.48
26	y	101	BCR	C15-C14-C13	8.36	139.25	127.31
24	B	605	CLA	C4A-NA-C1A	8.36	110.47	106.71
26	t	101	BCR	C36-C18-C17	-8.35	111.22	122.92
26	C	514	BCR	C37-C22-C21	-8.34	111.25	122.92
26	J	101	BCR	C15-C14-C13	8.33	139.20	127.31
26	H	101	BCR	C23-C22-C21	8.33	131.72	118.94
26	J	101	BCR	C33-C5-C4	-8.33	97.62	113.62
24	B	607	CLA	C4A-NA-C1A	8.32	110.45	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
26	k	101	BCR	C23-C22-C21	8.26	131.62	118.94
26	A	1009	BCR	C12-C13-C14	8.21	131.53	118.94
26	D	406	BCR	C36-C18-C19	-8.19	105.18	118.08
24	B	602	CLA	C4A-NA-C1A	8.16	110.37	106.71
26	k	102	BCR	C37-C22-C21	-8.15	111.51	122.92
26	d	404	BCR	C32-C1-C6	8.11	123.45	110.30
24	b	617	CLA	C4A-NA-C1A	8.09	110.34	106.71
26	a	413	BCR	C24-C23-C22	8.09	138.46	126.23
24	D	403	CLA	C4A-NA-C1A	8.07	110.33	106.71
24	A	1008	CLA	C4A-NA-C1A	8.04	110.32	106.71
24	c	510	CLA	C4A-NA-C1A	8.03	110.31	106.71
26	C	514	BCR	C19-C18-C17	8.03	131.26	118.94
24	a	409	CLA	C4A-NA-C1A	8.02	110.31	106.71
26	D	406	BCR	C12-C13-C14	8.01	131.24	118.94
26	a	413	BCR	C23-C22-C21	8.01	131.23	118.94
25	a	410	PHO	CMD-C2D-C1D	8.00	137.39	125.06
26	A	1009	BCR	C23-C22-C21	7.99	131.21	118.94
24	b	614	CLA	C4A-NA-C1A	7.89	110.25	106.71
24	d	403	CLA	C4A-NA-C1A	7.89	110.25	106.71
26	H	101	BCR	C10-C11-C12	7.89	147.83	123.22
24	B	616	CLA	C4A-NA-C1A	7.86	110.24	106.71
24	b	611	CLA	C4A-NA-C1A	7.83	110.23	106.71
26	h	101	BCR	C7-C8-C9	7.83	138.06	126.23
25	A	1007	PHO	CMD-C2D-C1D	7.81	137.09	125.06
26	K	101	BCR	C12-C13-C14	7.80	130.91	118.94
26	k	102	BCR	C19-C18-C17	7.73	130.80	118.94
26	B	617	BCR	C24-C23-C22	7.72	137.90	126.23
24	B	610	CLA	C4A-NA-C1A	7.69	110.16	106.71
24	B	603	CLA	C4A-NA-C1A	7.66	110.15	106.71
26	k	101	BCR	C36-C18-C17	-7.63	112.23	122.92
26	d	404	BCR	C12-C13-C14	7.59	130.59	118.94
26	d	404	BCR	C11-C10-C9	7.58	138.13	127.31
24	a	408	CLA	C4A-NA-C1A	7.57	110.11	106.71
26	h	101	BCR	C23-C22-C21	7.51	130.46	118.94
24	B	608	CLA	C4A-NA-C1A	7.51	110.08	106.71
24	a	412	CLA	C4A-NA-C1A	7.50	110.08	106.71
26	h	101	BCR	C12-C13-C14	7.50	130.45	118.94
24	B	612	CLA	C4A-NA-C1A	7.48	110.07	106.71
26	b	622	BCR	C23-C22-C21	7.47	130.40	118.94
26	C	514	BCR	C23-C22-C21	7.42	130.33	118.94
26	t	101	BCR	C11-C10-C9	7.40	137.88	127.31
26	h	101	BCR	C37-C22-C21	-7.40	112.56	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	y	101	BCR	C33-C5-C6	7.39	132.83	124.53
26	k	102	BCR	C11-C10-C9	7.37	137.83	127.31
26	b	620	BCR	C38-C26-C27	-7.34	99.52	113.62
26	y	101	BCR	C33-C5-C4	-7.28	99.62	113.62
26	a	413	BCR	C12-C13-C14	7.21	130.00	118.94
26	B	618	BCR	C23-C22-C21	7.16	129.93	118.94
26	B	619	BCR	C29-C30-C25	7.16	121.51	110.48
26	d	404	BCR	C30-C25-C26	-7.16	112.53	122.61
26	A	1009	BCR	C36-C18-C17	-7.11	112.96	122.92
24	D	403	CLA	C2C-C1C-NC	7.03	116.55	109.97
26	A	1009	BCR	C36-C18-C19	-6.98	107.08	118.08
24	d	402	CLA	C4A-NA-C1A	6.96	109.84	106.71
26	B	618	BCR	C36-C18-C19	-6.95	107.13	118.08
35	D	419	HTG	C1'-S1-C1	6.93	113.06	100.09
26	b	621	BCR	C23-C22-C21	6.93	129.57	118.94
26	B	619	BCR	C24-C23-C22	6.93	136.70	126.23
26	y	101	BCR	C12-C13-C14	6.92	129.56	118.94
35	d	416	HTG	C1'-S1-C1	6.91	113.02	100.09
26	b	620	BCR	C23-C22-C21	6.91	129.54	118.94
26	c	514	BCR	C38-C26-C27	-6.90	100.36	113.62
26	T	101	BCR	C8-C7-C6	6.89	146.56	127.20
24	b	608	CLA	C4A-NA-C1A	6.88	109.80	106.71
26	t	101	BCR	C23-C22-C21	6.87	129.49	118.94
26	c	514	BCR	C24-C23-C22	6.83	136.56	126.23
26	K	102	BCR	C38-C26-C25	6.79	132.15	124.53
26	d	404	BCR	C29-C30-C25	6.78	120.91	110.48
26	b	622	BCR	C37-C22-C21	-6.77	113.43	122.92
26	D	406	BCR	C8-C9-C10	6.75	129.29	118.94
26	H	101	BCR	C37-C22-C21	-6.75	113.47	122.92
26	K	101	BCR	C23-C22-C21	6.71	129.24	118.94
26	k	101	BCR	C12-C13-C14	6.68	129.20	118.94
24	A	1005	CLA	C4A-NA-C1A	6.63	109.69	106.71
26	T	101	BCR	C23-C22-C21	6.61	129.08	118.94
26	b	622	BCR	C12-C13-C14	6.59	129.05	118.94
26	T	101	BCR	C36-C18-C17	-6.56	113.74	122.92
26	K	101	BCR	C37-C22-C21	-6.54	113.77	122.92
35	b	630	HTG	C1'-S1-C1	6.50	112.24	100.09
26	t	101	BCR	C12-C13-C14	6.48	128.89	118.94
26	H	101	BCR	C8-C7-C6	6.44	145.28	127.20
26	t	101	BCR	C24-C23-C22	6.39	135.89	126.23
26	B	617	BCR	C12-C13-C14	6.37	128.72	118.94
26	A	1009	BCR	C24-C23-C22	6.37	135.86	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k	102	BCR	C38-C26-C25	6.37	131.68	124.53
35	B	624	HTG	C1'-S1-C1	6.35	111.96	100.09
26	b	621	BCR	C36-C18-C19	-6.34	108.08	118.08
24	A	1006	CLA	C4A-NA-C1A	6.34	109.56	106.71
26	J	101	BCR	C24-C23-C22	6.33	135.81	126.23
26	k	101	BCR	C38-C26-C27	-6.32	101.48	113.62
26	K	102	BCR	C38-C26-C27	-6.31	101.50	113.62
26	B	618	BCR	C24-C23-C22	6.31	135.77	126.23
26	b	620	BCR	C38-C26-C25	6.30	131.61	124.53
26	B	617	BCR	C7-C8-C9	6.30	135.76	126.23
26	B	618	BCR	C23-C24-C25	6.30	144.90	127.20
26	c	514	BCR	C23-C22-C21	6.29	128.60	118.94
26	k	102	BCR	C36-C18-C17	-6.28	114.13	122.92
26	b	620	BCR	C2-C1-C6	6.26	120.12	110.48
26	k	102	BCR	C33-C5-C4	-6.25	101.60	113.62
26	J	101	BCR	C4-C5-C6	6.25	131.81	122.73
26	D	406	BCR	C2-C1-C6	6.25	120.10	110.48
26	k	101	BCR	C33-C5-C6	6.23	131.52	124.53
26	k	102	BCR	C15-C14-C13	6.22	136.19	127.31
26	B	618	BCR	C35-C13-C12	-6.22	108.28	118.08
26	H	101	BCR	C36-C18-C19	-6.21	108.30	118.08
24	a	407	CLA	C4A-NA-C1A	6.21	109.50	106.71
26	B	619	BCR	C12-C13-C14	6.20	128.45	118.94
24	b	610	CLA	C2C-C1C-NC	6.18	115.76	109.97
26	k	101	BCR	C24-C23-C22	6.18	135.57	126.23
26	C	514	BCR	C8-C7-C6	6.16	144.50	127.20
24	a	408	CLA	C2C-C1C-NC	6.15	115.74	109.97
26	K	102	BCR	C29-C30-C25	6.15	119.95	110.48
26	B	618	BCR	C36-C18-C17	-6.15	114.31	122.92
26	c	514	BCR	C37-C22-C21	-6.15	114.31	122.92
24	A	1005	CLA	C2C-C1C-NC	6.14	115.72	109.97
26	D	406	BCR	C23-C22-C21	6.14	128.36	118.94
26	K	101	BCR	C36-C18-C17	-6.12	114.35	122.92
26	h	101	BCR	C38-C26-C27	-6.10	101.90	113.62
24	D	402	CLA	C2C-C1C-NC	6.09	115.68	109.97
26	b	622	BCR	C2-C1-C6	6.08	119.85	110.48
26	H	101	BCR	C36-C18-C17	-6.08	114.41	122.92
26	B	618	BCR	C29-C30-C25	6.06	119.81	110.48
26	k	101	BCR	C33-C5-C4	-6.06	101.98	113.62
24	B	608	CLA	C2C-C1C-NC	6.05	115.64	109.97
24	B	603	CLA	O2D-CGD-CBD	6.05	122.02	111.27
26	c	514	BCR	C29-C30-C25	6.04	119.78	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	618	BCR	C38-C26-C27	-6.03	102.03	113.62
26	c	514	BCR	C38-C26-C25	6.01	131.28	124.53
24	B	607	CLA	C2C-C1C-NC	6.01	115.60	109.97
35	b	602	HTG	C1'-S1-C1	6.00	111.32	100.09
24	C	510	CLA	C2C-C1C-NC	5.95	115.55	109.97
26	k	102	BCR	C33-C5-C6	5.94	131.20	124.53
24	B	603	CLA	C2C-C1C-NC	5.93	115.52	109.97
26	b	621	BCR	C36-C18-C17	-5.92	114.64	122.92
26	b	622	BCR	C35-C13-C12	-5.91	108.77	118.08
26	H	101	BCR	C24-C23-C22	5.91	135.16	126.23
38	V	201	HEM	CBD-CAD-C3D	-5.90	101.60	112.48
26	b	620	BCR	C35-C13-C12	-5.90	108.78	118.08
26	y	101	BCR	C37-C22-C21	-5.89	114.68	122.92
26	b	622	BCR	C36-C18-C17	-5.88	114.68	122.92
26	B	619	BCR	C30-C25-C26	-5.86	114.36	122.61
24	A	1006	CLA	C2C-C1C-NC	5.85	115.46	109.97
26	a	413	BCR	C33-C5-C6	5.85	131.10	124.53
26	K	102	BCR	C37-C22-C21	-5.85	114.73	122.92
26	C	514	BCR	C12-C13-C14	5.85	127.91	118.94
26	y	101	BCR	C38-C26-C27	-5.83	102.41	113.62
26	A	1009	BCR	C38-C26-C27	-5.80	102.47	113.62
24	a	407	CLA	C2C-C1C-NC	5.79	115.39	109.97
26	y	101	BCR	C36-C18-C17	-5.79	114.82	122.92
38	f	101	HEM	CBD-CAD-C3D	-5.78	101.82	112.48
26	J	101	BCR	C23-C22-C21	5.78	127.81	118.94
26	B	617	BCR	C8-C7-C6	5.76	143.37	127.20
26	A	1009	BCR	C37-C22-C21	-5.75	114.87	122.92
26	h	101	BCR	C36-C18-C17	-5.75	114.88	122.92
26	d	404	BCR	C23-C22-C21	5.74	127.75	118.94
24	C	509	CLA	C2C-C1C-NC	5.74	115.35	109.97
26	b	622	BCR	C24-C23-C22	5.74	134.91	126.23
24	a	412	CLA	C2C-C1C-NC	5.71	115.33	109.97
24	A	1008	CLA	C2C-C1C-NC	5.70	115.31	109.97
26	d	404	BCR	C8-C9-C10	5.69	127.67	118.94
35	d	410	HTG	C1'-S1-C1	5.69	110.73	100.09
26	d	404	BCR	C37-C22-C21	-5.69	114.96	122.92
26	b	620	BCR	C24-C23-C22	5.68	134.82	126.23
26	k	102	BCR	C24-C23-C22	5.66	134.79	126.23
26	K	102	BCR	C32-C1-C6	5.66	119.48	110.30
26	b	620	BCR	C36-C18-C19	-5.66	109.16	118.08
26	h	101	BCR	C8-C7-C6	5.66	143.09	127.20
26	B	619	BCR	C23-C22-C21	5.66	127.62	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	622	BCR	C8-C7-C6	5.65	143.06	127.20
26	y	101	BCR	C8-C7-C6	5.64	143.04	127.20
26	b	620	BCR	C8-C7-C6	5.64	143.03	127.20
26	b	621	BCR	C37-C22-C21	-5.63	115.03	122.92
26	t	101	BCR	C8-C7-C6	5.63	143.02	127.20
26	b	620	BCR	C8-C9-C10	5.63	127.58	118.94
24	C	505	CLA	C2C-C1C-NC	5.61	115.23	109.97
24	b	607	CLA	C2C-C1C-NC	5.60	115.22	109.97
26	C	514	BCR	C38-C26-C27	-5.60	102.86	113.62
26	y	101	BCR	C29-C30-C25	5.59	119.08	110.48
24	B	615	CLA	C2C-C1C-NC	5.58	115.20	109.97
24	c	506	CLA	C2C-C1C-NC	5.57	115.19	109.97
26	c	514	BCR	C8-C7-C6	5.55	142.78	127.20
24	c	505	CLA	O2D-CGD-CBD	5.54	121.12	111.27
24	B	604	CLA	C2C-C1C-NC	5.54	115.16	109.97
24	b	616	CLA	C2C-C1C-NC	5.53	115.15	109.97
26	J	101	BCR	C12-C13-C14	5.52	127.42	118.94
26	k	101	BCR	C38-C26-C25	5.52	130.72	124.53
24	d	402	CLA	C2C-C1C-NC	5.51	115.13	109.97
26	b	621	BCR	C40-C30-C25	5.50	119.22	110.30
24	b	608	CLA	C2C-C1C-NC	5.50	115.12	109.97
24	b	612	CLA	C2C-C1C-NC	5.49	115.11	109.97
24	c	501	CLA	C2C-C1C-NC	5.47	115.09	109.97
26	A	1009	BCR	C8-C7-C6	5.46	142.54	127.20
26	d	404	BCR	C36-C18-C19	-5.46	109.48	118.08
24	C	504	CLA	C2C-C1C-NC	5.46	115.08	109.97
26	a	413	BCR	C38-C26-C27	-5.44	103.17	113.62
26	y	101	BCR	C38-C26-C25	5.43	130.63	124.53
24	B	616	CLA	O2D-CGD-CBD	5.43	120.92	111.27
26	a	413	BCR	C33-C5-C4	-5.43	103.19	113.62
26	J	101	BCR	C1-C6-C5	-5.42	114.97	122.61
26	B	618	BCR	C30-C25-C26	-5.42	114.97	122.61
26	a	413	BCR	C37-C22-C23	-5.42	109.54	118.08
26	k	102	BCR	C23-C22-C21	5.42	127.25	118.94
26	b	620	BCR	C36-C18-C17	-5.41	115.35	122.92
26	H	101	BCR	C38-C26-C27	-5.40	103.24	113.62
26	h	101	BCR	C29-C30-C25	5.39	118.78	110.48
24	c	510	CLA	C2C-C1C-NC	5.39	115.02	109.97
26	t	101	BCR	C35-C13-C12	-5.39	109.59	118.08
26	b	622	BCR	C38-C26-C27	-5.39	103.27	113.62
26	J	101	BCR	C33-C5-C6	5.38	130.57	124.53
24	B	601	CLA	O2D-CGD-CBD	5.38	120.83	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	509	CLA	C2C-C1C-NC	5.38	115.01	109.97
26	h	101	BCR	C36-C18-C19	-5.37	109.61	118.08
35	B	629	HTG	C1'-S1-C1	5.37	110.14	100.09
26	k	102	BCR	C38-C26-C27	-5.36	103.31	113.62
24	b	609	CLA	C2C-C1C-NC	5.36	114.99	109.97
24	D	402	CLA	C3C-C4C-NC	5.36	116.58	110.57
24	B	610	CLA	C2C-C1C-NC	5.35	114.99	109.97
24	a	409	CLA	C2C-C1C-NC	5.35	114.98	109.97
26	T	101	BCR	C38-C26-C27	-5.35	103.35	113.62
24	b	615	CLA	C2C-C1C-NC	5.34	114.98	109.97
26	J	101	BCR	C40-C30-C25	5.34	118.96	110.30
26	B	619	BCR	C35-C13-C12	-5.33	109.67	118.08
35	D	413	HTG	C1'-S1-C1	5.32	110.05	100.09
24	B	609	CLA	C2C-C1C-NC	5.32	114.96	109.97
24	C	502	CLA	C2C-C1C-NC	5.31	114.95	109.97
35	C	521	HTG	C1'-S1-C1	5.31	110.03	100.09
24	b	611	CLA	C2C-C1C-NC	5.31	114.95	109.97
24	C	506	CLA	C2C-C1C-NC	5.30	114.94	109.97
24	C	501	CLA	C2C-C1C-NC	5.30	114.93	109.97
35	C	522	HTG	C1'-S1-C1	5.29	109.99	100.09
24	B	602	CLA	C2C-C1C-NC	5.29	114.93	109.97
26	B	617	BCR	C37-C22-C21	-5.29	115.52	122.92
26	D	406	BCR	C38-C26-C27	-5.28	103.48	113.62
26	B	618	BCR	C34-C9-C8	-5.28	109.76	118.08
24	B	606	CLA	C2C-C1C-NC	5.27	114.91	109.97
35	b	601	HTG	C1'-S1-C1	5.27	109.95	100.09
26	k	101	BCR	C8-C7-C6	5.26	141.99	127.20
24	B	614	CLA	O2D-CGD-CBD	5.26	120.61	111.27
24	b	614	CLA	C2C-C1C-NC	5.26	114.90	109.97
26	b	621	BCR	C38-C26-C27	-5.26	103.52	113.62
24	D	403	CLA	C1C-C2C-C3C	-5.26	101.43	106.96
24	c	507	CLA	O2D-CGD-CBD	5.25	120.60	111.27
26	b	621	BCR	C8-C7-C6	5.24	141.93	127.20
26	K	102	BCR	C24-C23-C22	5.23	134.14	126.23
26	K	102	BCR	C8-C7-C6	5.23	141.90	127.20
26	D	406	BCR	C40-C30-C25	5.23	118.78	110.30
24	c	504	CLA	O2D-CGD-CBD	5.23	120.56	111.27
24	B	613	CLA	C2C-C1C-NC	5.20	114.85	109.97
26	a	413	BCR	C36-C18-C19	-5.20	109.88	118.08
26	T	101	BCR	C2-C1-C6	5.20	118.49	110.48
35	B	628	HTG	C1'-S1-C1	5.19	109.79	100.09
26	d	404	BCR	C8-C7-C6	5.19	141.77	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	404	PHO	O2D-CGD-CBD	5.17	120.46	111.27
35	C	522	HTG	C1-O5-C5	5.17	122.11	112.58
26	h	101	BCR	C32-C1-C6	5.17	118.68	110.30
26	C	514	BCR	C36-C18-C19	-5.16	109.95	118.08
24	b	611	CLA	O2D-CGD-CBD	5.15	120.43	111.27
24	b	606	CLA	C2C-C1C-NC	5.15	114.80	109.97
26	a	413	BCR	C8-C7-C6	5.15	141.67	127.20
26	H	101	BCR	C8-C9-C10	5.15	126.84	118.94
35	o	301	HTG	C1'-S1-C1	5.14	109.71	100.09
24	c	507	CLA	C2C-C1C-NC	5.14	114.79	109.97
24	B	614	CLA	C2C-C1C-NC	5.14	114.78	109.97
26	a	413	BCR	C8-C9-C10	5.13	126.82	118.94
26	C	514	BCR	C40-C30-C25	5.13	118.62	110.30
24	b	619	CLA	C2C-C1C-NC	5.13	114.78	109.97
26	c	514	BCR	C12-C13-C14	5.13	126.81	118.94
38	F	101	HEM	CBD-CAD-C3D	-5.13	103.03	112.48
24	c	501	CLA	O2D-CGD-CBD	5.13	120.38	111.27
26	D	406	BCR	C33-C5-C4	-5.13	103.77	113.62
24	B	611	CLA	C2C-C1C-NC	5.11	114.76	109.97
35	c	522	HTG	C1'-S1-C1	5.11	109.65	100.09
26	J	101	BCR	C8-C7-C6	5.10	141.54	127.20
26	y	101	BCR	C23-C22-C21	5.10	126.77	118.94
26	B	617	BCR	C37-C22-C23	-5.10	110.05	118.08
26	H	101	BCR	C30-C25-C26	-5.09	115.44	122.61
26	B	618	BCR	C37-C22-C21	-5.08	115.80	122.92
24	b	604	CLA	O2D-CGD-CBD	5.08	120.30	111.27
26	c	514	BCR	C1-C6-C5	-5.08	115.46	122.61
24	C	507	CLA	C2C-C1C-NC	5.07	114.73	109.97
24	b	618	CLA	C2C-C1C-NC	5.07	114.72	109.97
24	b	617	CLA	C2C-C1C-NC	5.07	114.72	109.97
26	k	101	BCR	C37-C22-C23	-5.07	110.09	118.08
26	t	101	BCR	C38-C26-C27	-5.07	103.88	113.62
26	b	621	BCR	C35-C13-C14	-5.06	115.83	122.92
26	D	406	BCR	C30-C25-C26	-5.06	115.48	122.61
24	d	403	CLA	C2C-C1C-NC	5.06	114.71	109.97
26	b	622	BCR	C36-C18-C19	-5.05	110.12	118.08
26	D	406	BCR	C8-C7-C6	5.05	141.38	127.20
26	B	619	BCR	C2-C1-C6	5.05	118.25	110.48
26	B	618	BCR	C31-C1-C6	5.05	118.48	110.30
26	B	617	BCR	C38-C26-C27	-5.04	103.94	113.62
24	B	616	CLA	C2C-C1C-NC	5.03	114.69	109.97
26	K	102	BCR	C36-C18-C17	-5.02	115.89	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	606	CLA	O2D-CGD-CBD	5.02	120.18	111.27
24	c	504	CLA	C2C-C1C-NC	5.02	114.67	109.97
25	a	411	PHO	O2D-CGD-CBD	5.01	120.17	111.27
24	c	505	CLA	C2C-C1C-NC	5.00	114.66	109.97
26	K	102	BCR	C33-C5-C4	-5.00	104.01	113.62
26	b	621	BCR	C23-C24-C25	4.99	141.23	127.20
26	B	618	BCR	C33-C5-C6	4.99	130.13	124.53
24	B	601	CLA	C2C-C1C-NC	4.98	114.64	109.97
26	H	101	BCR	C35-C13-C12	-4.98	110.22	118.08
25	A	1007	PHO	O2D-CGD-CBD	4.98	120.12	111.27
26	c	514	BCR	C33-C5-C4	-4.98	104.05	113.62
24	c	502	CLA	C2C-C1C-NC	4.96	114.62	109.97
24	C	507	CLA	O2D-CGD-CBD	4.96	120.08	111.27
24	b	613	CLA	C2C-C1C-NC	4.95	114.61	109.97
26	b	622	BCR	C30-C25-C26	-4.95	115.64	122.61
26	b	621	BCR	C30-C25-C26	-4.94	115.65	122.61
26	k	101	BCR	C8-C9-C10	4.94	126.53	118.94
24	D	405	CLA	C2C-C1C-NC	4.94	114.60	109.97
26	k	102	BCR	C2-C1-C6	4.93	118.07	110.48
35	c	525	HTG	C1'-S1-C1	4.92	109.30	100.09
24	b	619	CLA	O2D-CGD-CBD	4.92	120.01	111.27
26	D	406	BCR	C38-C26-C25	4.91	130.04	124.53
24	b	609	CLA	O2D-CGD-CBD	4.90	119.98	111.27
24	c	508	CLA	C2C-C1C-NC	4.90	114.56	109.97
24	a	412	CLA	O2D-CGD-CBD	4.89	119.95	111.27
24	B	612	CLA	C2C-C1C-NC	4.89	114.55	109.97
26	K	102	BCR	C23-C22-C21	4.88	126.43	118.94
26	J	101	BCR	C37-C22-C21	-4.88	116.09	122.92
24	c	502	CLA	O2D-CGD-CBD	4.87	119.92	111.27
26	t	101	BCR	C33-C5-C4	-4.87	104.27	113.62
24	b	608	CLA	O2D-CGD-CBD	4.87	119.92	111.27
29	c	521	LMG	O7-C10-C11	4.85	121.96	111.50
26	B	619	BCR	C8-C7-C6	4.85	140.83	127.20
26	c	514	BCR	C30-C25-C26	-4.85	115.78	122.61
26	H	101	BCR	C32-C1-C6	4.85	118.16	110.30
24	b	617	CLA	O2D-CGD-CBD	4.85	119.88	111.27
26	h	101	BCR	C30-C25-C26	-4.84	115.80	122.61
24	C	508	CLA	C2C-C1C-NC	4.84	114.50	109.97
26	c	514	BCR	C2-C1-C6	4.84	117.93	110.48
26	B	618	BCR	C38-C26-C25	4.83	129.96	124.53
24	C	509	CLA	O2D-CGD-CBD	4.83	119.85	111.27
24	B	612	CLA	C3C-C4C-NC	4.83	115.99	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	101	BCR	C12-C13-C14	4.83	126.35	118.94
24	a	408	CLA	C1C-C2C-C3C	-4.82	101.89	106.96
26	A	1009	BCR	C30-C25-C26	-4.81	115.84	122.61
24	C	502	CLA	O2D-CGD-CBD	4.80	119.80	111.27
26	k	102	BCR	C8-C7-C6	4.80	140.68	127.20
28	D	408	SQD	O7-S-C6	4.80	112.64	106.94
35	V	202	HTG	C1'-S1-C1	4.79	109.05	100.09
25	a	410	PHO	O2D-CGD-CBD	4.79	119.77	111.27
24	B	605	CLA	C3C-C4C-NC	4.78	115.94	110.57
26	K	101	BCR	C31-C1-C6	4.78	118.05	110.30
24	B	605	CLA	O2D-CGD-CBD	4.77	119.74	111.27
24	C	504	CLA	O2D-CGD-CBD	4.76	119.73	111.27
26	h	101	BCR	C35-C13-C12	-4.76	110.58	118.08
26	K	101	BCR	C8-C9-C10	4.76	126.24	118.94
24	b	604	CLA	C2C-C1C-NC	4.76	114.43	109.97
26	D	406	BCR	C37-C22-C21	-4.76	116.26	122.92
26	K	101	BCR	C36-C18-C19	-4.75	110.60	118.08
26	k	101	BCR	C35-C13-C12	-4.75	110.60	118.08
26	K	102	BCR	C2-C1-C6	4.74	117.78	110.48
24	B	614	CLA	C3C-C4C-NC	4.74	115.89	110.57
24	B	610	CLA	C3C-C4C-NC	4.74	115.88	110.57
24	b	606	CLA	O2D-CGD-CBD	4.73	119.68	111.27
24	c	513	CLA	C2C-C1C-NC	4.73	114.40	109.97
25	D	404	PHO	C3D-C2D-C1D	-4.72	98.99	105.87
26	d	404	BCR	C33-C5-C4	-4.72	104.55	113.62
26	J	101	BCR	C29-C30-C25	4.72	117.75	110.48
26	t	101	BCR	C2-C1-C6	4.72	117.74	110.48
29	C	519	LMG	O7-C10-C11	4.71	121.66	111.50
26	T	101	BCR	C37-C22-C21	-4.71	116.32	122.92
24	B	614	CLA	C4D-C3D-CAD	4.71	111.10	108.47
24	c	513	CLA	O2D-CGD-CBD	4.71	119.64	111.27
24	b	605	CLA	C2C-C1C-NC	4.71	114.38	109.97
24	b	604	CLA	C4D-C3D-CAD	4.71	111.10	108.47
26	y	101	BCR	C36-C18-C19	-4.70	110.66	118.08
24	B	607	CLA	C1C-C2C-C3C	-4.70	102.01	106.96
24	C	511	CLA	C2C-C1C-NC	4.70	114.37	109.97
24	c	512	CLA	C2C-C1C-NC	4.69	114.37	109.97
26	A	1009	BCR	C37-C22-C23	-4.69	110.69	118.08
24	c	512	CLA	O2D-CGD-CBD	4.69	119.60	111.27
26	T	101	BCR	C29-C30-C25	4.68	117.69	110.48
24	B	605	CLA	C2C-C1C-NC	4.68	114.36	109.97
25	a	411	PHO	C3D-C2D-C1D	-4.68	99.05	105.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1009	BCR	C35-C13-C14	-4.67	116.38	122.92
24	C	503	CLA	C2C-C1C-NC	4.67	114.35	109.97
24	d	402	CLA	C3C-C4C-NC	4.66	115.80	110.57
24	C	502	CLA	C3C-C4C-NC	4.65	115.79	110.57
26	T	101	BCR	C33-C5-C4	-4.65	104.68	113.62
24	C	505	CLA	O2D-CGD-CBD	4.65	119.53	111.27
26	d	404	BCR	C24-C23-C22	4.64	133.25	126.23
26	A	1009	BCR	C27-C26-C25	4.64	129.47	122.73
24	B	616	CLA	C3C-C4C-NC	4.62	115.76	110.57
24	C	501	CLA	O2D-CGD-CBD	4.62	119.48	111.27
24	A	1006	CLA	C1C-C2C-C3C	-4.61	102.11	106.96
24	b	607	CLA	O2D-CGD-CBD	4.61	119.46	111.27
26	k	101	BCR	C23-C24-C25	4.61	140.14	127.20
24	C	510	CLA	C1C-C2C-C3C	-4.61	102.11	106.96
24	D	403	CLA	C3C-C4C-NC	4.61	115.74	110.57
24	B	616	CLA	C4D-C3D-CAD	4.60	111.03	108.47
24	b	617	CLA	C4D-C3D-CAD	4.59	111.03	108.47
24	a	412	CLA	C3C-C4C-NC	4.59	115.72	110.57
26	K	102	BCR	C36-C18-C19	-4.59	110.85	118.08
26	T	101	BCR	C30-C25-C26	-4.58	116.16	122.61
26	t	101	BCR	C40-C30-C25	4.58	117.73	110.30
24	c	503	CLA	C2C-C1C-NC	4.58	114.26	109.97
26	J	101	BCR	C23-C24-C25	4.58	140.06	127.20
26	H	101	BCR	C33-C5-C4	-4.58	104.82	113.62
24	C	506	CLA	O2D-CGD-CBD	4.58	119.40	111.27
26	b	621	BCR	C32-C1-C6	4.57	117.71	110.30
24	B	602	CLA	O2D-CGD-CBD	4.57	119.39	111.27
24	B	612	CLA	O2D-CGD-CBD	4.57	119.39	111.27
26	y	101	BCR	C30-C25-C26	-4.57	116.18	122.61
24	b	614	CLA	C3C-C4C-NC	4.56	115.69	110.57
26	J	101	BCR	C35-C13-C12	-4.56	110.89	118.08
24	C	512	CLA	C2C-C1C-NC	4.56	114.24	109.97
26	B	618	BCR	C8-C7-C6	4.55	139.99	127.20
26	K	102	BCR	C40-C30-C25	4.55	117.69	110.30
24	A	1005	CLA	C1C-C2C-C3C	-4.55	102.17	106.96
24	b	615	CLA	C3C-C4C-NC	4.54	115.67	110.57
26	k	102	BCR	C29-C30-C25	4.54	117.46	110.48
26	H	101	BCR	C29-C30-C25	4.53	117.46	110.48
26	K	102	BCR	C12-C13-C14	4.53	125.89	118.94
24	C	513	CLA	C2C-C1C-NC	4.53	114.22	109.97
26	y	101	BCR	C40-C30-C25	4.52	117.64	110.30
26	B	617	BCR	C40-C30-C25	4.52	117.64	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	512	CLA	O2D-CGD-CBD	4.52	119.30	111.27
26	K	101	BCR	C35-C13-C14	-4.52	116.59	122.92
24	b	613	CLA	C3C-C4C-NC	4.52	115.64	110.57
35	b	626	HTG	C1'-S1-C1	4.52	108.54	100.09
38	v	201	HEM	CBD-CAD-C3D	-4.51	104.16	112.48
28	c	518	SQD	O9-S-C6	4.51	112.30	106.94
24	C	510	CLA	O2D-CGD-CBD	4.51	119.28	111.27
26	b	620	BCR	C33-C5-C4	-4.51	104.96	113.62
26	J	101	BCR	C38-C26-C27	-4.50	104.97	113.62
24	A	1008	CLA	O2D-CGD-CBD	4.50	119.27	111.27
25	a	410	PHO	C3D-C2D-C1D	-4.50	99.31	105.87
26	b	620	BCR	C37-C22-C21	-4.50	116.62	122.92
24	c	505	CLA	C4D-C3D-CAD	4.50	110.98	108.47
24	C	511	CLA	C3C-C4C-NC	4.49	115.61	110.57
24	c	507	CLA	C3C-C4C-NC	4.49	115.61	110.57
24	c	511	CLA	C2C-C1C-NC	4.49	114.18	109.97
26	B	618	BCR	C8-C9-C10	4.49	125.83	118.94
24	B	601	CLA	C4D-C3D-CAD	4.49	110.97	108.47
24	B	615	CLA	C3C-C4C-NC	4.49	115.60	110.57
26	d	404	BCR	C32-C1-C2	-4.49	90.97	108.91
24	b	617	CLA	C3C-C4C-NC	4.48	115.60	110.57
24	B	611	CLA	C3C-C4C-NC	4.48	115.60	110.57
26	J	101	BCR	C30-C25-C26	-4.48	116.30	122.61
25	A	1007	PHO	C3D-C2D-C1D	-4.48	99.35	105.87
24	B	611	CLA	O2D-CGD-CBD	4.48	119.22	111.27
26	k	101	BCR	C29-C30-C25	4.48	117.37	110.48
24	a	407	CLA	C3C-C4C-NC	4.47	115.59	110.57
28	A	1011	SQD	O47-C7-C8	4.47	121.13	111.50
24	C	508	CLA	C3C-C4C-NC	4.46	115.57	110.57
26	h	101	BCR	C27-C26-C25	4.46	129.21	122.73
26	H	101	BCR	C39-C30-C25	4.45	117.52	110.30
24	b	607	CLA	C3C-C4C-NC	4.44	115.55	110.57
26	D	406	BCR	C35-C13-C12	-4.44	111.08	118.08
26	C	514	BCR	C31-C1-C6	4.44	117.50	110.30
28	B	620[A]	SQD	O47-C7-C8	4.43	121.04	111.50
24	b	619	CLA	C3C-C4C-NC	4.43	115.53	110.57
26	d	404	BCR	C33-C5-C6	4.42	129.49	124.53
24	c	510	CLA	C4D-C3D-CAD	4.41	110.93	108.47
24	c	501	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
26	y	101	BCR	C23-C24-C25	4.41	139.58	127.20
24	c	509	CLA	C4D-C3D-CAD	4.41	110.93	108.47
24	b	618	CLA	C3C-C4C-NC	4.40	115.51	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1008	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
24	b	615	CLA	O2D-CGD-CBD	4.39	119.06	111.27
24	C	513	CLA	C3C-C4C-NC	4.39	115.49	110.57
24	b	613	CLA	C4D-C3D-CAD	4.38	110.91	108.47
24	B	603	CLA	C3C-C4C-NC	4.38	115.48	110.57
24	A	1008	CLA	C3C-C4C-NC	4.38	115.48	110.57
24	b	610	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
24	a	409	CLA	O2D-CGD-CBD	4.37	119.04	111.27
26	t	101	BCR	C33-C5-C6	4.37	129.44	124.53
24	B	603	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
26	k	101	BCR	C31-C1-C6	4.37	117.38	110.30
24	D	402	CLA	C1C-C2C-C3C	-4.36	102.37	106.96
24	C	512	CLA	C3C-C4C-NC	4.36	115.46	110.57
26	H	101	BCR	C35-C13-C14	-4.36	116.82	122.92
26	J	101	BCR	C8-C9-C10	4.36	125.62	118.94
24	c	512	CLA	C4D-C3D-CAD	4.35	110.89	108.47
24	b	612	CLA	O2D-CGD-CBD	4.34	118.99	111.27
26	B	617	BCR	C8-C9-C10	4.34	125.61	118.94
24	C	510	CLA	C4D-C3D-CAD	4.34	110.89	108.47
26	D	406	BCR	C36-C18-C17	-4.34	116.84	122.92
24	A	1006	CLA	O2D-CGD-CBD	4.34	118.98	111.27
26	K	102	BCR	C33-C5-C6	4.34	129.40	124.53
24	b	610	CLA	C3C-C4C-NC	4.34	115.43	110.57
26	D	406	BCR	C23-C24-C25	4.33	139.38	127.20
24	c	512	CLA	C3C-C4C-NC	4.33	115.43	110.57
24	b	610	CLA	O2D-CGD-CBD	4.33	118.97	111.27
26	t	101	BCR	C37-C22-C23	-4.33	111.26	118.08
26	B	617	BCR	C23-C24-C25	4.33	139.35	127.20
26	D	406	BCR	C1-C6-C5	-4.32	116.53	122.61
26	C	514	BCR	C24-C23-C22	4.32	132.76	126.23
24	B	610	CLA	O2D-CGD-CBD	4.32	118.94	111.27
24	A	1005	CLA	C3C-C4C-NC	4.31	115.41	110.57
24	c	511	CLA	C4D-C3D-CAD	4.31	110.88	108.47
26	B	619	BCR	C38-C26-C27	-4.31	105.33	113.62
24	C	513	CLA	O2D-CGD-CBD	4.31	118.93	111.27
24	B	604	CLA	C3C-C4C-NC	4.31	115.40	110.57
24	b	606	CLA	C3C-C4C-NC	4.30	115.39	110.57
29	m	102	LMG	O7-C10-C11	4.29	120.76	111.50
24	C	511	CLA	O2D-CGD-CBD	4.29	118.89	111.27
24	a	407	CLA	C1C-C2C-C3C	-4.29	102.44	106.96
26	b	621	BCR	C8-C9-C10	4.29	125.52	118.94
24	C	513	CLA	C4D-C3D-CAD	4.27	110.85	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	101	BCR	C38-C26-C27	-4.27	105.41	113.62
36	C	516	DGD	O2G-C1B-C2B	4.27	120.70	111.50
24	c	510	CLA	C3C-C4C-NC	4.27	115.36	110.57
24	a	408	CLA	O2D-CGD-CBD	4.27	118.85	111.27
24	C	506	CLA	C3C-C4C-NC	4.27	115.36	110.57
24	B	609	CLA	O2D-CGD-CBD	4.26	118.84	111.27
24	b	605	CLA	O2D-CGD-CBD	4.26	118.84	111.27
24	b	608	CLA	C3C-C4C-NC	4.25	115.34	110.57
24	B	608	CLA	C3C-C4C-NC	4.25	115.33	110.57
26	d	404	BCR	C35-C13-C12	-4.24	111.39	118.08
24	b	616	CLA	C3C-C4C-NC	4.24	115.33	110.57
26	t	101	BCR	C38-C26-C25	4.24	129.29	124.53
26	A	1009	BCR	C33-C5-C4	-4.24	105.47	113.62
24	B	604	CLA	C4D-C3D-CAD	4.24	110.83	108.47
24	c	508	CLA	C3C-C4C-NC	4.24	115.32	110.57
28	c	518	SQD	O47-C7-C8	4.24	120.63	111.50
24	b	611	CLA	C3C-C4C-NC	4.24	115.32	110.57
26	K	101	BCR	C34-C9-C8	-4.23	111.41	118.08
26	b	620	BCR	C27-C26-C25	4.23	128.87	122.73
24	c	508	CLA	O2D-CGD-CBD	4.23	118.78	111.27
26	C	514	BCR	C30-C25-C26	-4.22	116.66	122.61
24	B	613	CLA	C3C-C4C-NC	4.22	115.30	110.57
26	K	101	BCR	C2-C1-C6	4.22	116.97	110.48
26	k	102	BCR	C32-C1-C6	4.21	117.12	110.30
24	b	609	CLA	C1C-C2C-C3C	-4.21	102.53	106.96
24	C	507	CLA	C1C-C2C-C3C	-4.21	102.53	106.96
24	C	509	CLA	C3C-C4C-NC	4.20	115.29	110.57
25	A	1007	PHO	C4A-NA-C1A	4.20	111.53	108.14
26	b	621	BCR	C35-C13-C12	-4.20	111.46	118.08
26	H	101	BCR	C34-C9-C10	-4.20	117.04	122.92
26	J	101	BCR	C38-C26-C25	4.19	129.24	124.53
26	h	101	BCR	C33-C5-C4	-4.19	105.57	113.62
24	b	608	CLA	C1C-C2C-C3C	-4.19	102.56	106.96
24	B	606	CLA	C3C-C4C-NC	4.18	115.26	110.57
32	C	520	LMT	O1B-C4'-C3'	4.18	118.40	107.28
28	b	623[B]	SQD	O47-C7-C8	4.18	120.51	111.50
24	C	507	CLA	C4D-C3D-CAD	4.18	110.80	108.47
24	B	609	CLA	C3C-C4C-NC	4.17	115.25	110.57
26	A	1009	BCR	C8-C9-C10	4.17	125.35	118.94
26	h	101	BCR	C23-C24-C25	4.17	138.92	127.20
24	D	403	CLA	O2D-CGD-CBD	4.17	118.68	111.27
24	C	507	CLA	C3C-C4C-NC	4.17	115.25	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	409	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
26	d	404	BCR	C38-C26-C25	4.17	129.21	124.53
26	b	621	BCR	C29-C30-C25	4.16	116.88	110.48
24	b	612	CLA	C1C-C2C-C3C	-4.16	102.59	106.96
26	T	101	BCR	C27-C26-C25	4.15	128.76	122.73
26	c	514	BCR	C23-C24-C25	4.15	138.85	127.20
26	D	406	BCR	C32-C1-C6	4.15	117.02	110.30
24	c	509	CLA	C3C-C4C-NC	4.15	115.22	110.57
26	b	622	BCR	C29-C30-C25	4.14	116.86	110.48
26	a	413	BCR	C2-C1-C6	4.14	116.86	110.48
24	c	506	CLA	C3C-C4C-NC	4.13	115.21	110.57
24	b	606	CLA	C1C-C2C-C3C	-4.13	102.61	106.96
24	a	412	CLA	C1C-C2C-C3C	-4.13	102.62	106.96
26	K	101	BCR	C30-C25-C26	-4.12	116.81	122.61
24	C	509	CLA	C1C-C2C-C3C	-4.12	102.62	106.96
28	b	623[A]	SQD	O47-C7-C8	4.12	120.38	111.50
24	c	505	CLA	C3C-C4C-NC	4.11	115.18	110.57
26	k	102	BCR	C12-C13-C14	4.10	125.24	118.94
24	c	510	CLA	O2D-CGD-CBD	4.10	118.56	111.27
24	b	616	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
24	A	1006	CLA	C3C-C4C-NC	4.10	115.17	110.57
29	Z	101	LMG	O7-C10-C11	4.10	120.33	111.50
24	B	602	CLA	C3C-C4C-NC	4.09	115.15	110.57
28	f	102	SQD	O47-C7-C8	4.09	120.31	111.50
24	c	510	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
24	C	503	CLA	C3C-C4C-NC	4.09	115.15	110.57
26	b	621	BCR	C27-C26-C25	4.08	128.66	122.73
26	K	101	BCR	C23-C24-C25	4.08	138.67	127.20
24	c	511	CLA	C3C-C4C-NC	4.08	115.15	110.57
28	B	620[B]	SQD	O47-C7-C8	4.08	120.29	111.50
26	k	101	BCR	C30-C25-C26	-4.08	116.87	122.61
24	B	606	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
24	B	608	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
24	d	403	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
24	c	511	CLA	O2D-CGD-CBD	4.05	118.47	111.27
34	e	101	LHG	O7-C7-C8	4.05	120.24	111.50
24	C	501	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
26	y	101	BCR	C24-C23-C22	4.05	132.35	126.23
24	C	504	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
24	c	509	CLA	O2D-CGD-CBD	4.05	118.46	111.27
24	d	402	CLA	C4D-C3D-CAD	4.04	110.72	108.47
26	B	619	BCR	C36-C18-C19	-4.03	111.72	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	510	CLA	C3C-C4C-NC	4.03	115.09	110.57
28	D	408	SQD	O47-C7-C8	4.03	120.19	111.50
26	D	406	BCR	C4-C5-C6	4.03	128.58	122.73
24	B	604	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
24	d	402	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
24	c	507	CLA	C1C-C2C-C3C	-4.02	102.72	106.96
24	C	505	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
24	C	504	CLA	C3C-C4C-NC	4.02	115.07	110.57
24	D	403	CLA	C3B-C4B-NB	4.01	114.40	109.21
24	B	613	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
26	k	102	BCR	C23-C24-C25	4.01	138.46	127.20
24	B	602	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
24	b	617	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
24	C	505	CLA	C3C-C4C-NC	4.00	115.05	110.57
24	b	604	CLA	C3C-C4C-NC	4.00	115.05	110.57
26	B	617	BCR	C35-C13-C12	-4.00	111.78	118.08
24	c	506	CLA	C4D-C3D-CAD	3.99	110.70	108.47
24	B	614	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
24	c	502	CLA	C3C-C4C-NC	3.99	115.05	110.57
24	b	619	CLA	C4D-C3D-CAD	3.98	110.69	108.47
25	D	404	PHO	C4C-C3C-C2C	-3.98	102.38	106.78
26	a	413	BCR	C37-C22-C21	-3.98	117.35	122.92
36	c	516	DGD	O2G-C1B-C2B	3.97	120.07	111.50
24	B	608	CLA	O2D-CGD-CBD	3.97	118.33	111.27
26	B	617	BCR	C36-C18-C19	-3.97	111.82	118.08
26	T	101	BCR	C33-C5-C6	3.97	128.99	124.53
24	b	616	CLA	O2D-CGD-CBD	3.97	118.32	111.27
24	D	405	CLA	C3C-C4C-NC	3.96	115.02	110.57
24	b	607	CLA	C1C-C2C-C3C	-3.96	102.79	106.96
26	C	514	BCR	C29-C30-C25	3.96	116.58	110.48
24	c	501	CLA	C4D-C3D-CAD	3.96	110.68	108.47
26	b	621	BCR	C2-C1-C6	3.96	116.58	110.48
26	H	101	BCR	C27-C26-C25	3.95	128.47	122.73
24	B	601	CLA	C3C-C4C-NC	3.95	115.00	110.57
24	d	402	CLA	O2D-CGD-CBD	3.94	118.28	111.27
26	d	404	BCR	C40-C30-C29	-3.94	93.14	108.91
24	a	409	CLA	C3C-C4C-NC	3.94	114.99	110.57
24	B	607	CLA	C3C-C4C-NC	3.94	114.99	110.57
24	B	603	CLA	C4-C3-C5	3.94	121.89	115.27
24	C	509	CLA	C4D-C3D-CAD	3.93	110.66	108.47
24	d	403	CLA	C3C-C4C-NC	3.93	114.98	110.57
24	C	505	CLA	C4D-C3D-CAD	3.93	110.66	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	614	CLA	O2D-CGD-CBD	3.93	118.25	111.27
26	b	620	BCR	C30-C25-C26	-3.93	117.08	122.61
24	b	611	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
24	c	506	CLA	O2D-CGD-CBD	3.92	118.24	111.27
26	B	617	BCR	C30-C25-C26	-3.92	117.09	122.61
25	a	410	PHO	C4A-NA-C1A	3.92	111.30	108.14
24	d	403	CLA	C4D-C3D-CAD	3.91	110.65	108.47
24	B	603	CLA	C4D-C3D-CAD	3.91	110.65	108.47
26	C	514	BCR	C38-C26-C25	3.91	128.92	124.53
24	c	505	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
24	a	412	CLA	C4D-C3D-CAD	3.90	110.64	108.47
24	b	605	CLA	C4D-C3D-CAD	3.90	110.64	108.47
24	b	609	CLA	C3C-C4C-NC	3.89	114.94	110.57
26	b	622	BCR	C27-C26-C25	3.89	128.38	122.73
26	C	514	BCR	C2-C1-C6	3.89	116.47	110.48
26	h	101	BCR	C38-C26-C25	3.89	128.89	124.53
26	C	514	BCR	C1-C6-C5	-3.88	117.15	122.61
26	c	514	BCR	C27-C26-C25	3.88	128.36	122.73
24	a	408	CLA	C3C-C4C-NC	3.87	114.92	110.57
24	D	405	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
26	c	514	BCR	C40-C30-C25	3.86	116.57	110.30
24	c	506	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
26	a	413	BCR	C35-C13-C14	-3.86	117.52	122.92
26	a	413	BCR	C30-C25-C26	-3.86	117.18	122.61
26	C	514	BCR	C31-C1-C2	-3.86	93.48	108.91
24	b	612	CLA	C3C-C4C-NC	3.85	114.89	110.57
24	b	618	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
24	C	503	CLA	O2D-CGD-CBD	3.85	118.11	111.27
25	A	1007	PHO	C4C-C3C-C2C	-3.85	102.52	106.78
24	C	508	CLA	C4D-C3D-CAD	3.85	110.62	108.47
24	A	1008	CLA	C4D-C3D-CAD	3.84	110.61	108.47
24	c	509	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
36	C	515	DGD	O2G-C1B-C2B	3.83	119.76	111.50
26	a	413	BCR	C29-C30-C25	3.83	116.38	110.48
34	E	101	LHG	O7-C7-C8	3.83	119.75	111.50
24	b	607	CLA	C4D-C3D-CAD	3.83	110.60	108.47
26	y	101	BCR	C1-C6-C5	-3.82	117.23	122.61
25	a	411	PHO	C4C-C3C-C2C	-3.82	102.56	106.78
26	b	620	BCR	C1-C6-C5	-3.82	117.24	122.61
28	A	1016	SQD	O47-C7-C8	3.82	119.73	111.50
24	C	501	CLA	C4D-C3D-CAD	3.81	110.59	108.47
27	D	407	PL9	C40-C39-C41	3.81	121.67	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	512	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
26	A	1009	BCR	C35-C13-C12	-3.80	112.08	118.08
28	D	408	SQD	O6-C1-C2	3.80	114.24	108.30
24	b	605	CLA	C3C-C4C-NC	3.80	114.83	110.57
26	k	102	BCR	C40-C30-C25	3.79	116.45	110.30
24	B	601	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
24	a	408	CLA	C3B-C4B-NB	3.79	114.11	109.21
26	a	413	BCR	C27-C26-C25	3.79	128.23	122.73
24	c	513	CLA	C4D-C3D-CAD	3.79	110.58	108.47
26	C	514	BCR	C27-C26-C25	3.78	128.22	122.73
26	B	617	BCR	C29-C30-C25	3.78	116.30	110.48
26	K	101	BCR	C29-C30-C25	3.78	116.29	110.48
25	a	411	PHO	O2D-CGD-O1D	-3.77	116.47	123.84
24	B	615	CLA	O2D-CGD-CBD	3.76	117.96	111.27
24	B	604	CLA	O2D-CGD-CBD	3.76	117.96	111.27
24	B	615	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
24	c	504	CLA	C3C-C4C-NC	3.76	114.79	110.57
24	b	613	CLA	O2D-CGD-CBD	3.76	117.95	111.27
24	c	503	CLA	C3C-C4C-NC	3.76	114.79	110.57
26	b	622	BCR	C39-C30-C25	3.76	116.40	110.30
24	C	506	CLA	C4D-C3D-CAD	3.76	110.56	108.47
24	A	1005	CLA	C4D-C3D-CAD	3.75	110.56	108.47
24	c	513	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
24	b	617	CLA	C4-C3-C5	3.75	121.58	115.27
26	D	406	BCR	C35-C13-C14	-3.74	117.68	122.92
26	B	619	BCR	C39-C30-C29	-3.74	93.94	108.91
24	B	609	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
35	V	202	HTG	O5-C1-C2	-3.74	105.61	110.31
26	b	620	BCR	C29-C30-C25	3.73	116.23	110.48
26	y	101	BCR	C8-C9-C10	3.73	124.67	118.94
24	C	512	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
24	b	611	CLA	C4D-C3D-CAD	3.72	110.54	108.47
26	y	101	BCR	C35-C13-C12	-3.72	112.22	118.08
34	d	408	LHG	O7-C7-C8	3.71	119.50	111.50
26	B	617	BCR	C32-C1-C6	3.71	116.31	110.30
24	c	503	CLA	C4D-C3D-CAD	3.71	110.54	108.47
36	h	102	DGD	O2G-C1B-C2B	3.71	119.49	111.50
24	B	611	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
24	c	504	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
28	a	401	SQD	O47-C7-C8	3.70	119.47	111.50
32	b	625	LMT	O1B-C1B-C2B	3.69	117.67	108.10
24	c	503	CLA	C1C-C2C-C3C	-3.69	103.08	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	513	CLA	C3C-C4C-NC	3.68	114.70	110.57
26	t	101	BCR	C1-C6-C5	-3.68	117.43	122.61
26	K	102	BCR	C30-C25-C26	-3.68	117.43	122.61
26	C	514	BCR	C35-C13-C12	-3.68	112.28	118.08
28	A	1011	SQD	O9-S-C6	3.68	111.31	106.94
24	C	502	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
26	K	102	BCR	C35-C13-C12	-3.67	112.30	118.08
24	C	503	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
25	a	410	PHO	C4C-C3C-C2C	-3.67	102.72	106.78
24	C	506	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
24	c	507	CLA	C4D-C3D-CAD	3.66	110.51	108.47
24	C	509	CLA	C3B-C4B-NB	3.66	113.94	109.21
24	B	607	CLA	O2D-CGD-CBD	3.66	117.76	111.27
24	B	614	CLA	O2D-CGD-O1D	-3.65	116.69	123.84
24	C	501	CLA	C3C-C4C-NC	3.65	114.67	110.57
25	a	410	PHO	C2C-C1C-NC	3.65	115.30	109.79
24	b	613	CLA	C1C-C2C-C3C	-3.64	103.12	106.96
24	D	402	CLA	C3B-C4B-NB	3.64	113.91	109.21
26	B	618	BCR	C27-C26-C25	3.63	128.01	122.73
26	K	101	BCR	C8-C7-C6	3.63	137.39	127.20
25	A	1007	PHO	C2D-C1D-ND	3.63	115.26	109.79
26	t	101	BCR	C36-C18-C19	-3.63	112.36	118.08
24	c	502	CLA	C4D-C3D-CAD	3.63	110.49	108.47
24	C	508	CLA	O2D-CGD-CBD	3.62	117.71	111.27
26	a	413	BCR	C38-C26-C25	3.62	128.60	124.53
26	A	1009	BCR	C2-C1-C6	3.62	116.05	110.48
24	b	606	CLA	C4D-C3D-CAD	3.62	110.49	108.47
32	i	102	LMT	C1'-O5'-C5'	3.62	120.79	113.69
26	k	102	BCR	C30-C25-C26	-3.62	117.52	122.61
26	J	101	BCR	C34-C9-C10	-3.61	117.86	122.92
24	b	615	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
24	c	508	CLA	C4D-C3D-CAD	3.61	110.48	108.47
26	a	413	BCR	C34-C9-C8	-3.60	112.40	118.08
29	c	519	LMG	O7-C10-C11	3.60	119.26	111.50
24	c	503	CLA	O2D-CGD-CBD	3.60	117.66	111.27
26	C	514	BCR	C8-C9-C10	3.60	124.46	118.94
26	K	101	BCR	C24-C23-C22	3.60	131.67	126.23
36	c	515	DGD	O2G-C1B-C2B	3.60	119.25	111.50
24	B	605	CLA	C4-C3-C5	3.60	121.32	115.27
24	C	513	CLA	C1C-C2C-C3C	-3.60	103.18	106.96
25	A	1007	PHO	C2C-C1C-NC	3.60	115.22	109.79
24	B	610	CLA	C1C-C2C-C3C	-3.59	103.18	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	514	BCR	C33-C5-C4	-3.58	106.74	113.62
24	b	604	CLA	C1C-C2C-C3C	-3.58	103.20	106.96
24	b	619	CLA	C3B-C4B-NB	3.58	113.83	109.21
26	b	620	BCR	C33-C5-C6	3.57	128.54	124.53
24	b	615	CLA	C4D-C3D-CAD	3.57	110.46	108.47
26	b	620	BCR	C39-C30-C25	3.56	116.08	110.30
24	b	609	CLA	C4D-C3D-CAD	3.56	110.46	108.47
24	C	508	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
24	A	1005	CLA	CMB-C2B-C3B	3.56	131.33	124.68
26	b	620	BCR	C23-C24-C25	3.55	137.18	127.20
26	a	413	BCR	C35-C13-C12	-3.55	112.48	118.08
26	h	101	BCR	C39-C30-C25	3.55	116.06	110.30
26	K	101	BCR	C33-C5-C4	-3.55	106.79	113.62
24	B	610	CLA	C4D-C3D-CAD	3.55	110.45	108.47
26	b	622	BCR	C23-C24-C25	3.55	137.17	127.20
24	c	511	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
28	A	1011	SQD	O6-C1-C2	3.55	113.84	108.30
24	c	501	CLA	C3C-C4C-NC	3.54	114.54	110.57
26	K	101	BCR	C35-C13-C12	-3.54	112.50	118.08
24	B	603	CLA	C3B-C4B-NB	3.53	113.78	109.21
26	d	404	BCR	C40-C30-C39	3.53	119.36	108.53
26	B	618	BCR	C33-C5-C4	-3.53	106.84	113.62
24	b	616	CLA	C3B-C4B-NB	3.53	113.77	109.21
24	c	502	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
25	D	404	PHO	C1-C2-C3	-3.52	119.95	126.04
38	F	101	HEM	CBA-CAA-C2A	-3.52	105.99	112.49
24	B	616	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
24	b	605	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
24	c	508	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
25	a	411	PHO	C2B-C1B-NB	3.51	115.09	109.79
24	c	502	CLA	CAC-C3C-C4C	3.51	129.36	124.81
29	d	409	LMG	O7-C10-C11	3.51	119.06	111.50
36	c	517	DGD	O2G-C1B-C2B	3.50	119.05	111.50
26	D	406	BCR	C34-C9-C10	-3.50	118.02	122.92
26	d	404	BCR	C35-C13-C14	-3.50	118.02	122.92
29	a	415	LMG	O7-C10-C11	3.50	119.04	111.50
26	k	101	BCR	C2-C1-C6	3.50	115.86	110.48
35	b	630	HTG	C1-O5-C5	3.50	119.03	112.58
28	c	518	SQD	O6-C1-C2	3.49	113.76	108.30
24	b	610	CLA	C3B-C4B-NB	3.49	113.73	109.21
24	B	608	CLA	C3B-C4B-NB	3.49	113.73	109.21
26	k	101	BCR	C27-C26-C25	3.49	127.80	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	613	CLA	O2D-CGD-CBD	3.48	117.46	111.27
24	C	510	CLA	C3B-C4B-NB	3.48	113.71	109.21
24	b	606	CLA	C4-C3-C5	3.48	121.12	115.27
26	h	101	BCR	C39-C30-C29	-3.48	95.00	108.91
24	C	504	CLA	C3B-C4B-NB	3.48	113.70	109.21
29	A	1012	LMG	O7-C10-C11	3.47	118.99	111.50
24	B	607	CLA	C3B-C4B-NB	3.47	113.70	109.21
26	D	406	BCR	C40-C30-C29	-3.46	95.05	108.91
26	K	102	BCR	C40-C30-C29	-3.46	95.07	108.91
24	A	1006	CLA	C3B-C4B-NB	3.46	113.68	109.21
26	C	514	BCR	C23-C24-C25	3.46	136.91	127.20
24	C	511	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
24	D	405	CLA	C4D-C3D-CAD	3.45	110.39	108.47
24	b	614	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
26	y	101	BCR	C32-C1-C6	3.45	115.89	110.30
24	a	412	CLA	C3B-C4B-NB	3.45	113.67	109.21
27	A	1010	PL9	C7-C3-C4	3.45	119.68	116.88
29	c	520	LMG	O7-C10-C11	3.44	118.92	111.50
26	B	617	BCR	C27-C26-C25	3.44	127.73	122.73
24	B	612	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
26	t	101	BCR	C23-C24-C25	3.43	136.84	127.20
26	K	101	BCR	C27-C26-C25	3.43	127.71	122.73
26	k	102	BCR	C39-C30-C25	3.43	115.86	110.30
24	a	412	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
24	C	512	CLA	C4D-C3D-CAD	3.43	110.38	108.47
26	H	101	BCR	C23-C24-C25	3.42	136.82	127.20
26	D	406	BCR	C34-C9-C8	-3.42	112.69	118.08
24	B	613	CLA	C3B-C4B-NB	3.42	113.63	109.21
26	c	514	BCR	C4-C5-C6	3.42	127.69	122.73
24	C	503	CLA	C4D-C3D-CAD	3.41	110.37	108.47
24	b	619	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
24	b	618	CLA	O2D-CGD-CBD	3.41	117.33	111.27
26	b	622	BCR	C38-C26-C25	3.41	128.35	124.53
28	a	401	SQD	O9-S-C6	3.40	110.98	106.94
25	D	404	PHO	C2D-C1D-ND	3.40	114.92	109.79
29	C	518	LMG	O7-C10-C11	3.39	118.81	111.50
26	T	101	BCR	C23-C24-C25	3.39	136.72	127.20
26	B	617	BCR	C38-C26-C25	3.39	128.33	124.53
26	B	618	BCR	C35-C13-C14	-3.39	118.18	122.92
24	A	1005	CLA	C3B-C4B-NB	3.39	113.59	109.21
26	B	619	BCR	C37-C22-C21	-3.39	118.18	122.92
24	D	402	CLA	CMC-C2C-C1C	3.39	130.19	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	607	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
26	A	1009	BCR	C1-C6-C5	-3.38	117.85	122.61
26	c	514	BCR	C31-C1-C2	-3.38	95.38	108.91
24	b	616	CLA	C4D-C3D-CAD	3.37	110.35	108.47
26	k	101	BCR	C39-C30-C25	3.37	115.77	110.30
24	B	607	CLA	C4-C3-C5	3.37	120.95	115.27
34	D	411	LHG	O7-C7-C8	3.37	118.77	111.50
26	a	413	BCR	C31-C1-C6	3.37	115.77	110.30
26	k	101	BCR	C36-C18-C19	-3.37	112.76	118.08
26	y	101	BCR	C35-C13-C14	-3.36	118.22	122.92
26	A	1009	BCR	C29-C30-C25	3.36	115.65	110.48
26	H	101	BCR	C38-C26-C25	3.35	128.29	124.53
24	b	608	CLA	C4-C3-C5	3.35	120.90	115.27
28	A	1016	SQD	O9-S-C6	3.34	110.91	106.94
24	c	508	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
25	a	410	PHO	C2D-C1D-ND	3.34	114.82	109.79
24	b	615	CLA	C3B-C4B-NB	3.33	113.52	109.21
24	a	407	CLA	C3B-C4B-NB	3.33	113.52	109.21
26	k	101	BCR	C37-C22-C21	-3.33	118.25	122.92
24	D	402	CLA	O2D-CGD-CBD	3.33	117.19	111.27
24	B	612	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
24	C	502	CLA	C4D-C3D-CAD	3.33	110.33	108.47
29	m	102	LMG	O8-C28-C29	3.33	122.35	111.91
24	D	403	CLA	CMB-C2B-C3B	3.33	130.90	124.68
35	C	522	HTG	O5-C1-C2	3.32	114.49	110.31
26	c	514	BCR	C33-C5-C6	3.32	128.26	124.53
25	a	411	PHO	C2D-C1D-ND	3.32	114.80	109.79
26	D	406	BCR	C39-C30-C25	-3.32	104.91	110.30
29	B	622	LMG	O7-C10-C11	3.32	118.66	111.50
26	y	101	BCR	C4-C5-C6	3.32	127.55	122.73
24	B	615	CLA	C3B-C4B-NB	3.32	113.50	109.21
24	a	407	CLA	CMB-C2B-C3B	3.32	130.88	124.68
26	d	404	BCR	C36-C18-C17	-3.32	118.28	122.92
25	a	411	PHO	C4A-NA-C1A	3.31	110.82	108.14
24	C	508	CLA	C3B-C4B-NB	3.31	113.49	109.21
24	b	614	CLA	C3B-C4B-NB	3.31	113.48	109.21
25	A	1007	PHO	C3C-C4C-NC	3.30	115.40	110.28
24	B	604	CLA	C3B-C4B-NB	3.30	113.48	109.21
24	B	605	CLA	C4C-C3C-C2C	-3.30	102.09	106.90
24	C	508	CLA	C4C-C3C-C2C	-3.30	102.09	106.90
24	D	405	CLA	O2D-CGD-CBD	3.30	117.13	111.27
25	A	1007	PHO	C2B-C1B-NB	3.28	114.74	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	411	PHO	C2C-C1C-NC	3.28	114.74	109.79
24	c	504	CLA	C4D-C3D-CAD	3.28	110.30	108.47
24	C	511	CLA	C4D-C3D-CAD	3.28	110.30	108.47
24	A	1006	CLA	CMB-C2B-C3B	3.28	130.81	124.68
26	b	621	BCR	C33-C5-C4	-3.28	107.32	113.62
27	A	1010	PL9	C25-C24-C26	3.27	120.78	115.27
26	b	620	BCR	C35-C13-C14	-3.27	118.34	122.92
26	c	514	BCR	C35-C13-C12	-3.27	112.92	118.08
24	B	605	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
24	b	619	CLA	CAC-C3C-C4C	3.27	129.05	124.81
24	B	608	CLA	CAC-C3C-C4C	3.27	129.05	124.81
24	B	606	CLA	C4D-C3D-CAD	3.26	110.29	108.47
25	a	410	PHO	C3C-C4C-NC	3.26	115.33	110.28
24	B	610	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
24	b	612	CLA	C4D-C3D-CAD	3.25	110.28	108.47
24	b	618	CLA	C4D-C3D-CAD	3.25	110.28	108.47
25	a	411	PHO	C3C-C4C-NC	3.25	115.32	110.28
24	B	615	CLA	C4D-C3D-CAD	3.25	110.28	108.47
24	c	506	CLA	C3B-C4B-NB	3.25	113.42	109.21
24	C	511	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
32	t	103	LMT	C2'-C3'-C4'	3.25	117.10	109.68
24	d	403	CLA	C3B-C4B-NB	3.25	113.41	109.21
28	D	408	SQD	O9-S-C6	3.24	110.80	106.94
24	c	509	CLA	C3B-C4B-NB	3.24	113.40	109.21
26	b	622	BCR	C1-C6-C5	-3.24	118.05	122.61
27	d	405	PL9	C7-C8-C9	-3.24	121.40	126.79
24	B	611	CLA	C4D-C3D-CAD	3.24	110.28	108.47
24	c	504	CLA	CAC-C3C-C4C	3.24	129.01	124.81
26	c	514	BCR	C28-C27-C26	3.24	119.86	114.08
24	A	1008	CLA	C3B-C4B-NB	3.24	113.39	109.21
24	C	502	CLA	C3B-C4B-NB	3.23	113.39	109.21
24	A	1005	CLA	O2D-CGD-CBD	3.23	117.01	111.27
27	a	414	PL9	C7-C3-C4	3.23	119.50	116.88
25	D	404	PHO	C4A-NA-C1A	3.23	110.75	108.14
24	B	615	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
27	A	1010	PL9	C37-C38-C39	-3.22	119.90	127.66
24	C	513	CLA	C4C-C3C-C2C	-3.22	102.21	106.90
24	B	616	CLA	C4C-C3C-C2C	-3.21	102.21	106.90
24	C	506	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
26	K	101	BCR	C31-C1-C2	-3.21	96.06	108.91
24	C	501	CLA	C3B-C4B-NB	3.21	113.35	109.21
24	b	619	CLA	C4C-C3C-C2C	-3.20	102.23	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	619	BCR	C38-C26-C25	3.20	128.12	124.53
26	d	404	BCR	C2-C1-C6	3.20	115.41	110.48
24	C	501	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
24	B	602	CLA	C4D-C3D-CAD	3.20	110.25	108.47
24	B	616	CLA	C3B-C4B-NB	3.20	113.35	109.21
26	b	620	BCR	C40-C30-C25	3.20	115.49	110.30
25	a	410	PHO	C1C-C2C-C3C	-3.20	102.84	106.51
24	B	612	CLA	C4D-C3D-CAD	3.20	110.25	108.47
24	c	501	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
24	b	607	CLA	CAC-C3C-C4C	3.20	128.96	124.81
26	h	101	BCR	C8-C9-C10	3.19	123.84	118.94
24	B	608	CLA	CMB-C2B-C3B	3.19	130.65	124.68
24	c	504	CLA	C3B-C4B-NB	3.18	113.33	109.21
24	d	402	CLA	C3B-C4B-NB	3.18	113.32	109.21
26	B	617	BCR	C33-C5-C4	-3.18	107.50	113.62
25	D	404	PHO	C2B-C1B-NB	3.18	114.59	109.79
24	C	505	CLA	CAC-C3C-C4C	3.18	128.93	124.81
26	H	101	BCR	C39-C30-C29	-3.18	96.21	108.91
24	C	505	CLA	C3B-C4B-NB	3.17	113.31	109.21
25	a	410	PHO	C2B-C1B-NB	3.17	114.57	109.79
24	c	508	CLA	C3B-C4B-NB	3.17	113.30	109.21
26	B	618	BCR	C40-C30-C25	3.17	115.44	110.30
24	b	614	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
24	b	613	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
26	B	617	BCR	C2-C1-C6	3.16	115.34	110.48
28	f	102	SQD	C3-C4-C5	3.15	115.86	110.24
24	B	614	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
24	b	615	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
24	C	502	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
26	A	1009	BCR	C38-C26-C25	3.15	128.06	124.53
24	b	615	CLA	C4-C3-C5	3.14	120.55	115.27
24	D	402	CLA	C4-C3-C5	3.13	120.54	115.27
24	c	510	CLA	C3B-C4B-NB	3.13	113.26	109.21
24	B	612	CLA	C3B-C4B-NB	3.13	113.25	109.21
24	A	1006	CLA	CMC-C2C-C1C	3.12	129.80	125.04
25	D	404	PHO	C2C-C1C-NC	3.12	114.50	109.79
24	C	512	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
36	C	517	DGD	O2G-C1B-C2B	3.12	118.22	111.50
24	d	403	CLA	O2D-CGD-O1D	-3.12	117.75	123.84
24	B	609	CLA	CAC-C3C-C4C	3.12	128.85	124.81
26	H	101	BCR	C4-C5-C6	3.11	127.25	122.73
35	V	202	HTG	C1-C2-C3	-3.11	104.44	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	603	CLA	CMB-C2B-C3B	3.11	130.50	124.68
34	b	624	LHG	O7-C7-C8	3.11	118.21	111.50
25	A	1007	PHO	C1C-C2C-C3C	-3.11	102.94	106.51
26	T	101	BCR	C1-C6-C5	-3.11	118.24	122.61
24	b	604	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
24	b	614	CLA	CAC-C3C-C4C	3.11	128.84	124.81
24	b	605	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
24	B	611	CLA	C4C-C3C-C2C	-3.10	102.37	106.90
24	B	603	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
26	B	617	BCR	C33-C5-C6	3.10	128.01	124.53
32	b	631	LMT	C1B-O5B-C5B	3.10	119.78	113.69
26	y	101	BCR	C39-C30-C29	-3.10	96.51	108.91
24	A	1005	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
26	k	101	BCR	C39-C30-C29	-3.10	96.52	108.91
24	a	409	CLA	C3B-C4B-NB	3.09	113.21	109.21
24	B	604	CLA	CAC-C3C-C4C	3.09	128.82	124.81
28	D	408	SQD	C1-O5-C5	-3.09	107.62	113.69
24	b	608	CLA	C3B-C4B-NB	3.09	113.20	109.21
26	c	514	BCR	C31-C1-C6	3.09	115.31	110.30
24	b	607	CLA	C3B-C4B-NB	3.08	113.20	109.21
24	B	609	CLA	C4D-C3D-CAD	3.08	110.19	108.47
26	k	102	BCR	C4-C5-C6	3.08	127.20	122.73
25	D	404	PHO	C3C-C4C-NC	3.08	115.05	110.28
24	B	606	CLA	C3B-C4B-NB	3.07	113.18	109.21
24	b	617	CLA	C3B-C4B-NB	3.07	113.18	109.21
34	B	621	LHG	O7-C7-C8	3.07	118.11	111.50
26	h	101	BCR	C1-C6-C5	-3.07	118.29	122.61
24	c	506	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
24	C	509	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
26	c	514	BCR	C39-C30-C29	-3.06	96.65	108.91
24	B	604	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
24	D	402	CLA	C4D-C3D-CAD	3.06	110.18	108.47
24	c	512	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
25	A	1007	PHO	C4D-ND-C1D	-3.06	101.26	106.76
24	c	511	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
34	d	406	LHG	O8-C23-C24	3.06	121.51	111.91
26	b	622	BCR	C32-C1-C6	3.06	115.26	110.30
25	a	411	PHO	C4-C3-C5	3.06	120.42	115.27
32	i	102	LMT	O5'-C5'-C4'	3.05	116.19	109.75
26	b	621	BCR	C34-C9-C8	-3.05	113.27	118.08
26	B	618	BCR	C39-C30-C29	-3.05	96.70	108.91
24	c	501	CLA	C3B-C4B-NB	3.05	113.15	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	620	BCR	C34-C9-C10	-3.05	118.66	122.92
26	h	101	BCR	C34-C9-C10	-3.05	118.66	122.92
24	d	402	CLA	C4-C3-C5	3.04	120.39	115.27
24	b	609	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
25	D	404	PHO	O2D-CGD-O1D	-3.04	117.89	123.84
24	b	615	CLA	CAC-C3C-C4C	3.04	128.76	124.81
26	b	621	BCR	C31-C1-C6	3.04	115.23	110.30
24	B	601	CLA	O2A-CGA-CBA	3.04	121.46	111.91
35	C	522	HTG	O5-C5-C4	3.04	115.21	109.69
26	t	101	BCR	C8-C9-C10	3.04	123.60	118.94
24	B	604	CLA	CED-O2D-CGD	3.03	122.80	115.94
24	B	606	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
26	K	102	BCR	C39-C30-C29	-3.03	96.79	108.91
24	a	407	CLA	C4D-C3D-CAD	3.03	110.16	108.47
26	H	101	BCR	C33-C5-C6	3.03	127.93	124.53
24	B	609	CLA	C3B-C4B-NB	3.03	113.12	109.21
34	D	409	LHG	O7-C7-C8	3.02	118.02	111.50
26	d	404	BCR	C23-C24-C25	3.02	135.69	127.20
24	b	617	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
24	C	509	CLA	CMB-C2B-C3B	3.02	130.33	124.68
26	H	101	BCR	C28-C27-C26	3.02	119.47	114.08
24	c	502	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
24	C	513	CLA	CMB-C2B-C3B	3.01	130.31	124.68
24	b	611	CLA	CMB-C2B-C3B	3.01	130.30	124.68
27	A	1010	PL9	C10-C9-C11	3.00	120.32	115.27
26	B	618	BCR	C31-C1-C2	-3.00	96.92	108.91
26	T	101	BCR	C38-C26-C25	2.99	127.89	124.53
26	T	101	BCR	C8-C9-C10	2.99	123.53	118.94
24	B	608	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
24	D	402	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
24	c	513	CLA	CMB-C2B-C3B	2.99	130.27	124.68
24	C	504	CLA	C4D-C3D-CAD	2.99	110.14	108.47
24	b	609	CLA	C3B-C4B-NB	2.99	113.07	109.21
24	b	612	CLA	CAC-C3C-C4C	2.98	128.68	124.81
24	B	606	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
34	D	409	LHG	O8-C23-C24	2.98	121.27	111.91
24	d	403	CLA	CMB-C2B-C3B	2.98	130.25	124.68
26	B	617	BCR	C39-C30-C25	2.98	115.13	110.30
26	y	101	BCR	C2-C1-C6	2.98	115.06	110.48
24	C	512	CLA	C4-C3-C5	2.98	120.28	115.27
26	d	404	BCR	C34-C9-C10	-2.98	118.75	122.92
24	c	502	CLA	C3B-C4B-NB	2.97	113.06	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	402	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
29	B	622	LMG	O8-C28-C29	2.97	121.22	111.91
24	B	610	CLA	C3B-C4B-NB	2.97	113.04	109.21
24	B	608	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
24	c	508	CLA	C4-C3-C5	2.97	120.26	115.27
26	B	618	BCR	C39-C30-C25	2.96	115.11	110.30
26	b	622	BCR	C39-C30-C29	-2.96	97.05	108.91
24	B	601	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
24	b	618	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
26	k	102	BCR	C39-C30-C29	-2.96	97.06	108.91
24	C	502	CLA	CAC-C3C-C4C	2.96	128.65	124.81
24	c	507	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
24	b	618	CLA	C3B-C4B-NB	2.96	113.03	109.21
24	C	506	CLA	C3B-C4B-NB	2.96	113.03	109.21
24	c	509	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
26	C	514	BCR	C36-C18-C17	-2.95	118.79	122.92
24	c	512	CLA	C4-C3-C5	2.95	120.23	115.27
24	c	510	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
24	b	606	CLA	C3B-C4B-NB	2.94	113.02	109.21
24	b	611	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
24	c	509	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
24	c	509	CLA	CAC-C3C-C4C	2.94	128.62	124.81
27	a	414	PL9	C25-C24-C26	2.94	120.22	115.27
27	d	405	PL9	C40-C39-C41	2.94	120.21	115.27
24	b	607	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
26	k	101	BCR	C34-C9-C8	-2.93	113.45	118.08
24	C	503	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
24	B	607	CLA	CMC-C2C-C1C	2.93	129.50	125.04
24	A	1008	CLA	C4-C3-C5	2.93	120.20	115.27
26	b	621	BCR	C38-C26-C25	2.93	127.82	124.53
24	B	604	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
28	b	623[A]	SQD	O7-S-C6	2.93	110.42	106.94
26	K	102	BCR	C8-C9-C10	2.93	123.43	118.94
26	t	101	BCR	C39-C30-C25	2.93	115.05	110.30
24	C	509	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
24	b	605	CLA	CMB-C2B-C3B	2.92	130.15	124.68
34	D	410	LHG	O7-C7-C8	2.92	117.80	111.50
26	B	617	BCR	C34-C9-C10	-2.92	118.83	122.92
24	b	619	CLA	CMB-C2B-C3B	2.92	130.14	124.68
24	a	407	CLA	C4C-C3C-C2C	-2.92	102.65	106.90
24	B	612	CLA	CMB-C2B-C3B	2.92	130.13	124.68
24	C	511	CLA	C3B-C4B-NB	2.91	112.98	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	615	CLA	CED-O2D-CGD	2.91	122.53	115.94
26	y	101	BCR	C27-C26-C25	2.91	126.96	122.73
27	D	407	PL9	C25-C24-C26	2.91	120.17	115.27
24	B	611	CLA	C3B-C4B-NB	2.91	112.98	109.21
24	C	504	CLA	C4-C3-C5	2.91	120.17	115.27
24	b	605	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
24	C	501	CLA	CAC-C3C-C4C	2.91	128.59	124.81
24	c	507	CLA	C3B-C4B-NB	2.91	112.97	109.21
24	C	504	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
36	H	102	DGD	O2G-C1B-C2B	2.91	117.77	111.50
24	D	405	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
24	c	510	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
34	d	406	LHG	O7-C7-C8	2.90	117.74	111.50
24	D	405	CLA	C3B-C4B-NB	2.90	112.95	109.21
27	A	1010	PL9	C32-C33-C34	-2.90	120.69	127.66
27	A	1010	PL9	C35-C34-C36	2.90	120.14	115.27
24	b	610	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
24	c	505	CLA	CAC-C3C-C4C	2.89	128.56	124.81
24	C	507	CLA	CMB-C2B-C3B	2.89	130.09	124.68
24	B	613	CLA	CMC-C2C-C1C	2.89	129.44	125.04
24	B	609	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
26	b	622	BCR	C8-C9-C10	2.89	123.37	118.94
24	c	503	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
24	a	407	CLA	O2D-CGD-CBD	2.89	116.39	111.27
24	B	606	CLA	C1-O2A-CGA	2.88	124.01	116.44
36	c	515	DGD	O1G-C1A-C2A	2.88	120.96	111.91
24	D	405	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
28	b	623[A]	SQD	O48-C23-C24	2.88	120.95	111.91
24	b	610	CLA	CED-O2D-CGD	2.88	122.46	115.94
24	c	504	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
24	c	505	CLA	C3B-C4B-NB	2.88	112.93	109.21
26	a	413	BCR	C23-C24-C25	2.88	135.29	127.20
24	D	403	CLA	CMC-C2C-C1C	2.87	129.42	125.04
24	A	1006	CLA	C4-C3-C5	2.87	120.10	115.27
26	h	101	BCR	C33-C5-C6	2.87	127.75	124.53
24	a	412	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
24	C	510	CLA	CBC-CAC-C3C	-2.87	104.52	112.43
24	B	607	CLA	CBC-CAC-C3C	-2.87	104.52	112.43
24	c	505	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
24	D	402	CLA	C1-C2-C3	-2.86	121.09	126.04
26	d	404	BCR	C34-C9-C8	-2.86	113.57	118.08
26	t	101	BCR	C37-C22-C21	-2.86	118.92	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	504	CLA	CAC-C3C-C4C	2.85	128.51	124.81
24	c	508	CLA	CMB-C2B-C3B	2.85	130.01	124.68
24	b	612	CLA	C3B-C4B-NB	2.85	112.89	109.21
24	c	507	CLA	CMB-C2B-C3B	2.85	130.01	124.68
26	A	1009	BCR	C4-C5-C6	2.85	126.87	122.73
24	c	509	CLA	CMB-C2B-C3B	2.85	130.01	124.68
24	b	606	CLA	CMC-C2C-C1C	2.85	129.38	125.04
24	B	606	CLA	CMB-C2B-C3B	2.85	130.00	124.68
26	d	404	BCR	C39-C30-C29	-2.85	97.52	108.91
24	B	610	CLA	C4-C3-C5	2.84	120.05	115.27
24	C	505	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
24	B	616	CLA	O2A-CGA-CBA	2.84	120.82	111.91
24	B	606	CLA	C4-C3-C5	2.84	120.05	115.27
24	b	606	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
24	B	601	CLA	C3B-C4B-NB	2.84	112.88	109.21
24	B	602	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
24	b	604	CLA	O2A-CGA-CBA	2.84	120.81	111.91
24	c	511	CLA	C4-C3-C5	2.83	120.04	115.27
24	b	605	CLA	C3B-C4B-NB	2.83	112.87	109.21
24	B	614	CLA	C4-C3-C5	2.83	120.04	115.27
24	B	602	CLA	CMB-C2B-C3B	2.83	129.97	124.68
24	c	513	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
28	B	620[B]	SQD	O8-S-C6	2.83	110.25	105.74
24	A	1006	CLA	C4D-C3D-CAD	2.83	110.05	108.47
26	b	620	BCR	C31-C1-C2	-2.83	97.59	108.91
28	D	408	SQD	C44-O6-C1	-2.83	108.21	113.74
36	c	517	DGD	O1G-C1A-C2A	2.83	120.78	111.91
34	E	101	LHG	O8-C23-C24	2.83	120.78	111.91
24	B	615	CLA	CMB-C2B-C3B	2.83	129.97	124.68
27	A	1010	PL9	C53-C6-C1	2.83	120.77	114.99
24	D	403	CLA	CBC-CAC-C3C	-2.83	104.64	112.43
24	B	614	CLA	O1D-CGD-CBD	-2.82	118.70	124.48
24	b	609	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
24	a	412	CLA	CAC-C3C-C4C	2.82	128.47	124.81
38	v	201	HEM	C1D-C2D-C3D	-2.82	105.03	107.00
26	t	101	BCR	C27-C26-C25	2.82	126.83	122.73
24	b	616	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
24	B	612	CLA	C4-C3-C5	2.82	120.02	115.27
26	h	101	BCR	C35-C13-C14	-2.82	118.97	122.92
26	b	620	BCR	C37-C22-C23	-2.82	113.64	118.08
24	B	613	CLA	C4D-C3D-CAD	2.82	110.04	108.47
24	C	506	CLA	CMB-C2B-C3B	2.82	129.95	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	614	CLA	C3B-C4B-NB	2.82	112.85	109.21
32	A	1018	LMT	C1B-O5B-C5B	2.82	119.22	113.69
27	a	414	PL9	C53-C6-C1	2.82	120.75	114.99
28	b	623[B]	SQD	O48-C23-C24	2.82	120.74	111.91
26	K	101	BCR	C39-C30-C25	2.82	114.86	110.30
24	B	602	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
26	b	621	BCR	C33-C5-C6	2.81	127.69	124.53
38	V	201	HEM	C1D-C2D-C3D	-2.81	105.04	107.00
24	d	402	CLA	CMB-C2B-C3B	2.81	129.93	124.68
26	t	101	BCR	C1-C6-C7	2.81	123.71	115.78
24	c	502	CLA	CMB-C2B-C3B	2.80	129.92	124.68
24	c	512	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
24	B	604	CLA	O1D-CGD-CBD	-2.80	118.75	124.48
24	b	607	CLA	O2A-CGA-CBA	2.80	120.69	111.91
28	f	102	SQD	O6-C1-C2	2.80	112.67	108.30
24	C	508	CLA	CMB-C2B-C3B	2.80	129.91	124.68
26	K	101	BCR	C33-C5-C6	2.80	127.67	124.53
24	c	503	CLA	CMB-C2B-C3B	2.80	129.91	124.68
24	C	507	CLA	C3B-C4B-NB	2.79	112.82	109.21
24	B	616	CLA	CAC-C3C-C4C	2.79	128.43	124.81
24	B	613	CLA	CMB-C2B-C3B	2.79	129.90	124.68
24	c	510	CLA	CMB-C2B-C3B	2.79	129.90	124.68
26	A	1009	BCR	C33-C5-C6	2.79	127.66	124.53
26	T	101	BCR	C36-C18-C19	-2.79	113.68	118.08
28	f	102	SQD	O7-S-C6	2.79	110.25	106.94
32	B	623	LMT	C2'-C3'-C4'	2.79	116.05	109.68
24	A	1008	CLA	C4C-C3C-C2C	-2.79	102.84	106.90
24	b	617	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
24	C	513	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
24	b	615	CLA	CED-O2D-CGD	2.78	122.24	115.94
24	B	603	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
24	d	402	CLA	O2A-CGA-CBA	2.78	120.64	111.91
25	a	411	PHO	C1C-C2C-C3C	-2.78	103.31	106.51
24	c	506	CLA	CAC-C3C-C4C	2.78	128.42	124.81
24	B	602	CLA	C3B-C4B-NB	2.78	112.80	109.21
24	c	501	CLA	C4-C3-C5	2.78	119.94	115.27
24	C	512	CLA	CMB-C2B-C3B	2.78	129.88	124.68
24	b	615	CLA	CMC-C2C-C1C	2.78	129.27	125.04
26	D	406	BCR	C33-C5-C6	2.78	127.64	124.53
24	b	613	CLA	C3B-C4B-NB	2.78	112.80	109.21
24	B	616	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
24	C	510	CLA	C4-C3-C5	2.77	119.93	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	614	CLA	CMB-C2B-C3B	2.77	129.86	124.68
32	b	625	LMT	C3B-C4B-C5B	2.77	115.17	110.24
24	B	612	CLA	CAC-C3C-C4C	2.76	128.40	124.81
24	B	615	CLA	CAC-C3C-C4C	2.76	128.40	124.81
25	D	404	PHO	CAC-C3C-C4C	2.76	128.24	125.22
24	C	503	CLA	C4-C3-C5	2.76	119.92	115.27
24	b	617	CLA	CMC-C2C-C1C	2.76	129.24	125.04
29	c	521	LMG	O8-C28-C29	2.76	120.56	111.91
24	a	412	CLA	CMC-C2C-C1C	2.75	129.23	125.04
24	b	619	CLA	CBC-CAC-C3C	-2.75	104.84	112.43
24	C	513	CLA	C3B-C4B-NB	2.75	112.77	109.21
24	c	505	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
24	C	506	CLA	CAC-C3C-C4C	2.75	128.38	124.81
24	c	504	CLA	C4-C3-C5	2.75	119.89	115.27
24	b	606	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
24	b	617	CLA	CMB-C2B-C3B	2.75	129.81	124.68
26	H	101	BCR	C1-C6-C5	-2.74	118.75	122.61
26	D	406	BCR	C32-C1-C2	-2.74	97.94	108.91
26	B	619	BCR	C23-C24-C25	2.74	134.90	127.20
26	d	404	BCR	C30-C25-C24	2.74	123.53	115.78
26	H	101	BCR	C2-C1-C6	2.74	114.70	110.48
24	c	504	CLA	CMB-C2B-C3B	2.74	129.80	124.68
26	b	620	BCR	C34-C9-C8	-2.74	113.76	118.08
24	d	403	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
26	k	101	BCR	C31-C1-C2	-2.74	97.96	108.91
25	a	410	PHO	C4D-ND-C1D	-2.74	101.84	106.76
26	T	101	BCR	C35-C13-C12	-2.74	113.77	118.08
24	C	512	CLA	CMC-C2C-C1C	2.73	129.20	125.04
24	a	412	CLA	CMB-C2B-C3B	2.73	129.79	124.68
24	c	501	CLA	CAC-C3C-C4C	2.73	128.36	124.81
24	C	501	CLA	C4-C3-C5	2.73	119.87	115.27
24	D	405	CLA	CMB-C2B-C3B	2.73	129.79	124.68
24	C	503	CLA	CMB-C2B-C3B	2.73	129.78	124.68
24	D	403	CLA	CHD-C4C-C3C	-2.73	120.83	124.84
24	B	605	CLA	CMC-C2C-C1C	2.73	129.19	125.04
26	b	621	BCR	C1-C6-C5	-2.72	118.78	122.61
24	c	508	CLA	CAC-C3C-C4C	2.72	128.34	124.81
24	B	614	CLA	CMB-C2B-C3B	2.72	129.77	124.68
25	a	411	PHO	C4D-ND-C1D	-2.72	101.87	106.76
24	b	616	CLA	CMC-C2C-C1C	2.72	129.18	125.04
26	h	101	BCR	C4-C5-C6	2.72	126.68	122.73
24	b	611	CLA	C3B-C4B-NB	2.72	112.72	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	509	CLA	CAC-C3C-C4C	2.72	128.34	124.81
24	b	614	CLA	C4D-C3D-CAD	2.72	109.98	108.47
24	a	412	CLA	C4-C3-C5	2.72	119.84	115.27
29	C	518	LMG	O8-C28-C29	2.72	120.43	111.91
24	c	505	CLA	CMB-C2B-C3B	2.72	129.76	124.68
26	k	102	BCR	C8-C9-C10	2.72	123.11	118.94
24	B	601	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
24	D	405	CLA	C4-C3-C5	2.71	119.84	115.27
26	B	619	BCR	C31-C1-C2	-2.71	98.05	108.91
24	C	507	CLA	C4-C3-C5	2.71	119.83	115.27
26	A	1009	BCR	C32-C1-C6	2.71	114.69	110.30
28	A	1016	SQD	O6-C1-C2	2.71	112.53	108.30
24	c	511	CLA	C3B-C4B-NB	2.71	112.71	109.21
26	y	101	BCR	C28-C27-C26	2.71	118.91	114.08
24	B	604	CLA	C4-C3-C5	2.71	119.83	115.27
24	a	408	CLA	CMC-C2C-C1C	2.71	129.16	125.04
29	D	412	LMG	O7-C10-C11	2.71	117.33	111.50
25	A	1007	PHO	CMB-C2B-C1B	2.71	129.23	125.06
28	A	1016	SQD	O48-C23-C24	2.70	120.39	111.91
29	A	1012	LMG	O8-C28-C29	2.70	120.39	111.91
24	b	606	CLA	CMB-C2B-C3B	2.70	129.73	124.68
24	a	409	CLA	CMC-C2C-C1C	2.70	129.15	125.04
34	D	411	LHG	O8-C23-C24	2.70	120.38	111.91
24	c	513	CLA	CAC-C3C-C4C	2.70	128.31	124.81
24	C	504	CLA	CMB-C2B-C3B	2.70	129.72	124.68
27	a	414	PL9	C40-C39-C41	2.70	119.81	115.27
26	D	406	BCR	C39-C30-C29	-2.69	98.13	108.91
24	B	610	CLA	O2A-CGA-CBA	2.69	120.36	111.91
25	D	404	PHO	C4D-ND-C1D	-2.69	101.92	106.76
24	b	608	CLA	C4D-C3D-CAD	2.69	109.97	108.47
24	B	605	CLA	CAC-C3C-C4C	2.69	128.30	124.81
26	K	101	BCR	C28-C27-C26	2.69	118.88	114.08
26	y	101	BCR	C34-C9-C8	-2.69	113.84	118.08
24	b	612	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
24	C	510	CLA	CMC-C2C-C1C	2.69	129.13	125.04
24	b	605	CLA	C1-O2A-CGA	2.69	123.49	116.44
26	J	101	BCR	C40-C30-C29	-2.68	98.17	108.91
24	b	613	CLA	CMB-C2B-C3B	2.68	129.69	124.68
24	C	507	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
26	b	622	BCR	C32-C1-C2	-2.68	98.20	108.91
25	a	411	PHO	CAC-C3C-C4C	2.68	128.14	125.22
24	C	501	CLA	C4C-C3C-C2C	-2.68	103.00	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	402	CLA	CMC-C2C-C1C	2.67	129.11	125.04
24	B	613	CLA	C4C-C3C-C2C	-2.67	103.00	106.90
24	C	511	CLA	C4-C3-C5	2.67	119.76	115.27
26	d	404	BCR	C38-C26-C27	-2.67	108.49	113.62
29	a	415	LMG	O8-C28-C29	2.67	120.28	111.91
24	a	409	CLA	C4-C3-C5	2.66	119.75	115.27
27	a	414	PL9	C10-C9-C11	2.66	119.75	115.27
24	c	503	CLA	C4-C3-C5	2.66	119.74	115.27
27	A	1010	PL9	C30-C29-C31	2.66	119.74	115.27
26	K	102	BCR	C4-C5-C6	2.66	126.59	122.73
24	c	512	CLA	CMC-C2C-C1C	2.65	129.08	125.04
24	c	505	CLA	CMC-C2C-C1C	2.65	129.08	125.04
28	a	401	SQD	O48-C23-C24	2.65	120.23	111.91
24	b	610	CLA	C4-C3-C5	2.65	119.73	115.27
27	a	414	PL9	C35-C34-C36	2.65	119.73	115.27
24	c	513	CLA	O2A-CGA-CBA	2.65	120.22	111.91
24	B	604	CLA	O2A-CGA-CBA	2.65	120.22	111.91
24	C	506	CLA	C4-C3-C5	2.64	119.72	115.27
24	c	507	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
26	c	514	BCR	C8-C9-C10	2.64	123.00	118.94
27	a	414	PL9	C37-C38-C39	-2.64	121.30	127.66
24	B	616	CLA	C4-C3-C5	2.64	119.72	115.27
28	f	102	SQD	O48-C23-C24	2.64	120.20	111.91
24	B	615	CLA	C1-O2A-CGA	2.64	123.37	116.44
34	d	407	LHG	O7-C7-C8	2.64	117.19	111.50
27	d	405	PL9	C53-C6-C1	2.64	120.38	114.99
24	A	1005	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
24	b	609	CLA	CMB-C2B-C3B	2.63	129.61	124.68
24	b	604	CLA	C1-O2A-CGA	2.63	123.35	116.44
29	Z	101	LMG	O8-C28-C29	2.63	120.17	111.91
28	B	620[B]	SQD	O48-C23-C24	2.63	120.16	111.91
29	c	520	LMG	O1-C1-C2	2.63	112.41	108.30
24	b	608	CLA	C4C-C3C-C2C	-2.63	103.07	106.90
26	B	619	BCR	C27-C26-C25	2.63	126.55	122.73
24	b	604	CLA	C3B-C4B-NB	2.63	112.61	109.21
24	b	611	CLA	CAC-C3C-C4C	2.63	128.22	124.81
24	c	501	CLA	C4C-C3C-C2C	-2.63	103.07	106.90
24	b	615	CLA	O2A-CGA-CBA	2.63	120.15	111.91
24	b	604	CLA	CAC-C3C-C4C	2.62	128.22	124.81
24	C	501	CLA	C1-O2A-CGA	2.62	123.33	116.44
24	c	507	CLA	O1D-CGD-CBD	-2.62	119.12	124.48
27	d	405	PL9	C25-C24-C26	2.62	119.68	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	615	CLA	CMB-C2B-C3B	2.62	129.58	124.68
24	C	512	CLA	O2A-CGA-CBA	2.62	120.13	111.91
24	c	510	CLA	O2A-CGA-CBA	2.62	120.13	111.91
28	B	620[A]	SQD	O48-C23-C24	2.62	120.13	111.91
24	B	611	CLA	CAC-C3C-C4C	2.62	128.21	124.81
24	c	506	CLA	CMB-C2B-C3B	2.62	129.57	124.68
24	B	616	CLA	CMB-C2B-C3B	2.62	129.57	124.68
24	A	1006	CLA	CBC-CAC-C3C	-2.61	105.22	112.43
24	a	408	CLA	C4-C3-C5	2.61	119.67	115.27
24	C	510	CLA	O2A-CGA-CBA	2.61	120.11	111.91
24	b	618	CLA	CMC-C2C-C1C	2.61	129.02	125.04
24	a	408	CLA	CMB-C2B-C3B	2.61	129.57	124.68
24	c	506	CLA	C4-C3-C5	2.61	119.67	115.27
29	C	519	LMG	O8-C28-C29	2.61	120.10	111.91
24	c	512	CLA	CMB-C2B-C3B	2.61	129.56	124.68
25	D	404	PHO	C4-C3-C5	2.61	119.66	115.27
27	d	405	PL9	C35-C34-C36	2.60	119.65	115.27
24	b	617	CLA	CED-O2D-CGD	2.60	121.83	115.94
26	a	413	BCR	C3-C4-C5	2.60	118.73	114.08
24	A	1008	CLA	CED-O2D-CGD	2.60	121.82	115.94
26	h	101	BCR	C2-C1-C6	2.60	114.49	110.48
29	c	520	LMG	O8-C28-C29	2.60	120.06	111.91
26	k	101	BCR	C4-C5-C6	2.60	126.50	122.73
26	b	620	BCR	C4-C5-C6	2.60	126.50	122.73
24	b	604	CLA	CED-O2D-CGD	2.60	121.81	115.94
34	e	101	LHG	O8-C23-C24	2.59	120.05	111.91
28	b	623[B]	SQD	O8-S-C6	2.59	109.87	105.74
24	d	403	CLA	C1-O2A-CGA	2.59	123.25	116.44
26	k	102	BCR	C1-C6-C5	-2.59	118.96	122.61
36	C	517	DGD	O1G-C1A-C2A	2.59	120.04	111.91
24	b	609	CLA	CAC-C3C-C4C	2.58	128.16	124.81
24	c	511	CLA	CMB-C2B-C3B	2.58	129.51	124.68
26	b	621	BCR	C37-C22-C23	-2.58	114.01	118.08
24	B	602	CLA	O2A-CGA-CBA	2.58	120.00	111.91
26	D	406	BCR	C27-C26-C25	2.58	126.48	122.73
24	C	507	CLA	O2A-CGA-CBA	2.58	119.99	111.91
32	A	1018	LMT	C2'-C3'-C4'	2.57	115.56	109.68
24	B	601	CLA	C4-C3-C5	2.57	119.60	115.27
26	K	101	BCR	C39-C30-C29	-2.57	98.61	108.91
26	b	620	BCR	C39-C30-C29	-2.57	98.62	108.91
24	B	607	CLA	C4D-C3D-CAD	2.57	109.90	108.47
26	a	413	BCR	C1-C6-C5	-2.57	119.00	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
24	c	512	CLA	O2A-CGA-CBA	2.57	119.96	111.91
24	b	605	CLA	O2A-CGA-CBA	2.56	119.95	111.91
36	h	102	DGD	O1G-C1A-C2A	2.56	119.95	111.91
26	B	617	BCR	C39-C30-C29	-2.56	98.66	108.91
24	b	610	CLA	CAC-C3C-C4C	2.56	128.13	124.81
25	D	404	PHO	CED-O2D-CGD	2.56	121.72	115.94
24	b	608	CLA	CMC-C2C-C1C	2.56	128.93	125.04
24	C	502	CLA	C4-C3-C5	2.55	119.57	115.27
34	d	407	LHG	O8-C23-C24	2.55	119.92	111.91
26	K	102	BCR	C32-C1-C2	-2.55	98.70	108.91
26	b	621	BCR	C28-C29-C30	2.55	123.73	114.60
24	a	407	CLA	CAC-C3C-C4C	2.55	128.12	124.81
25	D	404	PHO	CMB-C2B-C1B	2.55	128.99	125.06
29	c	519	LMG	O8-C28-C29	2.55	119.91	111.91
27	D	407	PL9	C20-C19-C21	2.55	119.56	115.27
24	A	1008	CLA	CMC-C2C-C1C	2.55	128.92	125.04
24	a	409	CLA	C4C-C3C-C2C	-2.55	103.18	106.90
24	C	512	CLA	C3B-C4B-NB	2.55	112.50	109.21
24	c	513	CLA	C3B-C4B-NB	2.54	112.50	109.21
24	b	616	CLA	O2A-CGA-CBA	2.54	119.89	111.91
24	c	503	CLA	C3B-C4B-NB	2.54	112.50	109.21
24	B	614	CLA	C1-O2A-CGA	2.54	123.11	116.44
24	C	513	CLA	CMC-C2C-C1C	2.54	128.91	125.04
24	B	602	CLA	CMC-C2C-C1C	2.54	128.91	125.04
24	B	611	CLA	C1-C2-C3	-2.54	121.66	126.04
24	B	605	CLA	C4D-C3D-CAD	2.54	109.88	108.47
26	A	1009	BCR	C40-C30-C29	-2.54	98.76	108.91
27	A	1010	PL9	C40-C39-C41	2.53	119.53	115.27
24	b	612	CLA	C1-O2A-CGA	2.53	123.09	116.44
25	a	410	PHO	CMB-C2B-C1B	2.53	128.97	125.06
27	a	414	PL9	C30-C29-C31	2.53	119.53	115.27
26	J	101	BCR	C2-C1-C6	2.53	114.38	110.48
26	D	406	BCR	C37-C22-C23	-2.53	114.09	118.08
24	B	607	CLA	CMB-C2B-C3B	2.53	129.41	124.68
26	T	101	BCR	C3-C4-C5	2.53	118.59	114.08
26	c	514	BCR	C34-C9-C8	-2.53	114.09	118.08
24	c	504	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
26	C	514	BCR	C4-C5-C6	2.53	126.40	122.73
24	B	610	CLA	CMB-C2B-C3B	2.52	129.40	124.68
24	c	506	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
24	B	608	CLA	C4D-C3D-CAD	2.52	109.88	108.47
26	B	619	BCR	C1-C6-C5	-2.52	119.06	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	605	CLA	CED-O2D-CGD	2.52	121.64	115.94
24	c	507	CLA	CMC-C2C-C1C	2.52	128.88	125.04
24	b	607	CLA	CMC-C2C-C1C	2.52	128.87	125.04
29	C	519	LMG	O7-C10-O9	-2.52	117.62	123.70
24	b	614	CLA	C1-C2-C3	-2.52	121.69	126.04
26	K	102	BCR	C1-C6-C5	-2.51	119.07	122.61
24	B	603	CLA	O2A-CGA-O1A	-2.51	117.25	123.59
24	b	616	CLA	CMB-C2B-C3B	2.51	129.38	124.68
24	c	509	CLA	C4-C3-C5	2.51	119.50	115.27
24	C	505	CLA	CMC-C2C-C1C	2.51	128.86	125.04
26	A	1009	BCR	C23-C24-C25	2.51	134.25	127.20
24	c	503	CLA	CAC-C3C-C4C	2.51	128.06	124.81
24	B	602	CLA	C1-O2A-CGA	2.51	123.03	116.44
24	B	612	CLA	CMC-C2C-C1C	2.51	128.86	125.04
24	c	508	CLA	C1-C2-C3	-2.51	121.71	126.04
24	C	501	CLA	CMB-C2B-C3B	2.51	129.37	124.68
28	B	620[A]	SQD	O9-S-C6	2.50	109.92	106.94
24	b	608	CLA	CMB-C2B-C3B	2.50	129.36	124.68
32	b	625	LMT	C4B-C3B-C2B	2.50	115.19	110.82
24	C	502	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
24	B	616	CLA	CBC-CAC-C3C	-2.50	105.55	112.43
26	t	101	BCR	C31-C1-C2	-2.50	98.92	108.91
25	D	404	PHO	C1C-C2C-C3C	-2.50	103.64	106.51
24	c	510	CLA	C4-C3-C5	2.49	119.47	115.27
26	t	101	BCR	C34-C9-C8	-2.49	114.15	118.08
26	K	102	BCR	C27-C26-C25	2.49	126.35	122.73
24	B	607	CLA	C4C-C3C-C2C	-2.49	103.27	106.90
24	b	616	CLA	CAC-C3C-C4C	2.49	128.04	124.81
24	C	503	CLA	C3B-C4B-NB	2.49	112.43	109.21
26	h	101	BCR	C28-C27-C26	2.49	118.52	114.08
24	b	611	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
24	a	409	CLA	CAC-C3C-C4C	2.49	128.03	124.81
27	d	405	PL9	C20-C19-C21	2.48	119.45	115.27
34	D	410	LHG	O8-C23-C24	2.48	119.70	111.91
24	b	618	CLA	C4-C3-C5	2.48	119.45	115.27
24	C	504	CLA	CED-O2D-CGD	2.48	121.55	115.94
32	A	1018	LMT	C1'-C2'-C3'	2.48	115.17	110.00
24	C	509	CLA	C4-C3-C5	2.48	119.45	115.27
24	A	1008	CLA	CMB-C2B-C3B	2.48	129.32	124.68
24	c	509	CLA	CED-O2D-CGD	2.48	121.55	115.94
27	A	1010	PL9	C45-C44-C46	2.48	119.44	115.27
26	T	101	BCR	C4-C5-C6	2.48	126.33	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	507	CLA	O2A-CGA-CBA	2.48	119.69	111.91
24	c	505	CLA	C1-O2A-CGA	2.48	122.95	116.44
24	a	408	CLA	CHD-C4C-C3C	-2.48	121.20	124.84
27	A	1010	PL9	C20-C19-C21	2.48	119.44	115.27
34	d	408	LHG	O8-C23-C24	2.48	119.68	111.91
24	B	612	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
24	b	614	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
24	b	618	CLA	CMB-C2B-C3B	2.47	129.31	124.68
24	c	512	CLA	O1D-CGD-CBD	-2.47	119.42	124.48
24	b	618	CLA	CAC-C3C-C4C	2.47	128.02	124.81
24	D	405	CLA	CAC-C3C-C4C	2.47	128.02	124.81
24	c	502	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
24	b	617	CLA	CAC-C3C-C4C	2.47	128.01	124.81
26	B	619	BCR	C34-C9-C8	-2.47	114.19	118.08
24	C	507	CLA	CMC-C2C-C1C	2.47	128.80	125.04
26	t	101	BCR	C3-C4-C5	2.47	118.48	114.08
24	B	608	CLA	C4-C3-C5	2.47	119.42	115.27
24	c	511	CLA	C1-O2A-CGA	2.47	122.91	116.44
27	D	407	PL9	C10-C9-C11	2.47	119.42	115.27
27	D	407	PL9	C37-C38-C39	-2.46	121.72	127.66
26	K	102	BCR	C29-C28-C27	2.46	116.89	111.38
26	k	102	BCR	C35-C13-C12	-2.46	114.19	118.08
24	c	513	CLA	CMC-C2C-C1C	2.46	128.79	125.04
24	C	512	CLA	CAC-C3C-C4C	2.46	128.01	124.81
26	K	102	BCR	C23-C24-C25	2.46	134.12	127.20
24	C	502	CLA	CMB-C2B-C3B	2.46	129.28	124.68
26	B	619	BCR	C37-C22-C23	-2.46	114.20	118.08
24	C	507	CLA	CED-O2D-CGD	2.46	121.50	115.94
24	c	502	CLA	C1-C2-C3	-2.46	121.79	126.04
24	b	609	CLA	CMC-C2C-C1C	2.46	128.78	125.04
26	b	621	BCR	C31-C1-C2	-2.46	99.07	108.91
26	t	101	BCR	C4-C5-C6	2.46	126.30	122.73
24	b	607	CLA	CMB-C2B-C3B	2.46	129.27	124.68
26	a	413	BCR	C40-C30-C25	2.45	114.28	110.30
25	a	411	PHO	CHD-C1D-ND	-2.45	119.47	124.58
24	C	510	CLA	C4C-C3C-C2C	-2.45	103.32	106.90
27	D	407	PL9	C53-C6-C1	2.45	120.00	114.99
36	H	102	DGD	O1G-C1A-O1A	-2.45	117.40	123.59
27	d	405	PL9	C22-C23-C24	-2.45	121.77	127.66
26	B	617	BCR	C35-C13-C14	-2.45	119.50	122.92
24	A	1005	CLA	CMC-C2C-C1C	2.45	128.76	125.04
26	b	621	BCR	C24-C23-C22	2.45	129.93	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	507	CLA	C4-C3-C5	2.44	119.38	115.27
24	B	603	CLA	O2A-CGA-CBA	2.44	119.58	111.91
24	D	402	CLA	CMB-C2B-C3B	2.44	129.25	124.68
24	c	504	CLA	CED-O2D-CGD	2.44	121.46	115.94
24	B	606	CLA	CAC-C3C-C4C	2.44	127.98	124.81
24	c	510	CLA	C1-C2-C3	-2.44	121.82	126.04
24	b	606	CLA	O2A-CGA-CBA	2.44	119.57	111.91
24	c	513	CLA	C4-C3-C5	2.44	119.38	115.27
24	b	607	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
26	y	101	BCR	C3-C4-C5	2.44	118.43	114.08
24	b	616	CLA	C1-C2-C3	-2.43	121.83	126.04
24	C	511	CLA	CAC-C3C-C4C	2.43	127.97	124.81
25	a	411	PHO	CMB-C2B-C1B	2.43	128.81	125.06
24	C	507	CLA	O1D-CGD-CBD	-2.43	119.50	124.48
24	B	613	CLA	O2A-CGA-CBA	2.43	119.55	111.91
24	b	616	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
36	C	515	DGD	O1G-C1A-C2A	2.43	119.54	111.91
24	b	610	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
24	d	403	CLA	CMC-C2C-C1C	2.43	128.74	125.04
28	f	102	SQD	C4-C3-C2	2.43	115.06	110.82
25	D	404	PHO	CHD-C1D-ND	-2.43	119.53	124.58
24	c	509	CLA	C1-O2A-CGA	2.42	122.80	116.44
24	b	605	CLA	CAC-C3C-C4C	2.42	127.95	124.81
32	t	103	LMT	C1'-C2'-C3'	2.42	115.04	110.00
26	D	406	BCR	C28-C27-C26	2.42	118.40	114.08
24	C	505	CLA	C1-O2A-CGA	2.42	122.80	116.44
24	B	605	CLA	C3B-C4B-NB	2.42	112.34	109.21
26	B	618	BCR	C37-C22-C23	-2.42	114.27	118.08
24	c	513	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
24	C	506	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
24	C	508	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
24	b	617	CLA	CBC-CAC-C3C	-2.42	105.77	112.43
24	B	602	CLA	CAC-C3C-C4C	2.42	127.94	124.81
24	B	607	CLA	CED-O2D-CGD	2.41	121.40	115.94
24	c	510	CLA	CMC-C2C-C1C	2.41	128.71	125.04
24	b	611	CLA	C6-C5-C3	-2.41	107.13	113.45
26	k	102	BCR	C2-C3-C4	2.41	116.77	111.38
24	c	506	CLA	O2A-CGA-CBA	2.41	119.48	111.91
24	b	605	CLA	C4-C3-C5	2.41	119.33	115.27
24	b	609	CLA	C4-C3-C5	2.41	119.33	115.27
24	C	507	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
24	B	607	CLA	C1-O2A-CGA	2.41	122.76	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	611	CLA	C4-C3-C5	2.41	119.32	115.27
27	a	414	PL9	C32-C33-C34	-2.41	121.87	127.66
24	b	613	CLA	C4-C3-C5	2.40	119.32	115.27
28	b	623[B]	SQD	O9-S-C6	2.40	109.80	106.94
24	B	601	CLA	CMB-C2B-C3B	2.40	129.17	124.68
24	a	408	CLA	C4D-C3D-CAD	2.40	109.81	108.47
24	D	402	CLA	CHD-C4C-C3C	-2.40	121.31	124.84
24	a	409	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
24	C	503	CLA	CMC-C2C-C1C	2.40	128.69	125.04
24	B	603	CLA	C5-C3-C2	-2.40	116.26	121.12
26	J	101	BCR	C36-C18-C19	-2.40	114.30	118.08
24	c	502	CLA	CMC-C2C-C1C	2.40	128.69	125.04
28	D	408	SQD	O48-C23-C24	2.40	119.43	111.91
27	D	407	PL9	C22-C23-C24	-2.40	121.89	127.66
24	B	614	CLA	CMC-C2C-C1C	2.40	128.69	125.04
24	B	609	CLA	CMC-C2C-C1C	2.39	128.69	125.04
26	T	101	BCR	C30-C25-C24	2.39	122.55	115.78
24	C	513	CLA	O2A-CGA-CBA	2.39	119.42	111.91
26	c	514	BCR	C28-C29-C30	2.39	123.15	114.60
27	d	405	PL9	C10-C9-C11	2.39	119.29	115.27
26	H	101	BCR	C32-C1-C2	-2.39	99.35	108.91
24	b	608	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
25	a	410	PHO	CED-O2D-CGD	2.39	121.34	115.94
36	H	102	DGD	O1G-C1A-C2A	2.39	119.40	111.91
24	c	506	CLA	CED-O2D-CGD	2.39	121.34	115.94
24	B	608	CLA	CMC-C2C-C1C	2.39	128.67	125.04
26	K	101	BCR	C30-C25-C24	2.39	122.53	115.78
24	c	502	CLA	C4-C3-C5	2.38	119.28	115.27
24	B	602	CLA	C4-C3-C5	2.38	119.28	115.27
38	V	201	HEM	CMA-C3A-C4A	-2.38	124.80	128.46
24	c	511	CLA	CMC-C2C-C1C	2.38	128.66	125.04
27	A	1010	PL9	C7-C3-C2	-2.38	120.17	123.30
28	c	518	SQD	O5-C1-C2	-2.38	105.32	110.35
24	B	613	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
24	c	504	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
27	A	1010	PL9	C15-C14-C16	2.37	119.27	115.27
36	c	516	DGD	O1G-C1A-C2A	2.37	119.36	111.91
24	c	511	CLA	CAC-C3C-C4C	2.37	127.89	124.81
24	b	604	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
24	A	1005	CLA	O2A-CGA-CBA	2.37	119.35	111.91
24	C	513	CLA	CAC-C3C-C4C	2.37	127.89	124.81
24	b	611	CLA	O2A-CGA-CBA	2.37	119.35	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	1010	PL9	C42-C43-C44	-2.37	121.95	127.66
26	h	101	BCR	C32-C1-C31	-2.37	101.26	108.53
38	f	101	HEM	C1D-C2D-C3D	-2.37	105.35	107.00
24	C	512	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
24	b	604	CLA	CMB-C2B-C3B	2.37	129.11	124.68
26	k	101	BCR	C40-C30-C25	2.37	114.14	110.30
24	B	603	CLA	O1D-CGD-CBD	-2.37	119.64	124.48
24	C	508	CLA	CED-O2D-CGD	2.37	121.29	115.94
24	b	611	CLA	CMC-C2C-C1C	2.36	128.64	125.04
24	B	610	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
24	C	513	CLA	CED-O2D-CGD	2.36	121.28	115.94
26	t	101	BCR	C40-C30-C29	-2.36	99.47	108.91
28	B	620[B]	SQD	O6-C1-C2	2.36	111.99	108.30
24	c	501	CLA	CMB-C2B-C3B	2.36	129.09	124.68
24	B	615	CLA	C4-C3-C5	2.36	119.24	115.27
24	b	617	CLA	O2A-CGA-CBA	2.36	119.31	111.91
24	C	511	CLA	C1-O2A-CGA	2.36	122.62	116.44
24	b	617	CLA	O2A-CGA-O1A	-2.36	117.65	123.59
24	C	509	CLA	C1-O2A-CGA	2.35	122.62	116.44
24	c	512	CLA	C3B-C4B-NB	2.35	112.25	109.21
24	d	402	CLA	CED-O2D-CGD	2.35	121.26	115.94
26	k	102	BCR	C30-C25-C24	2.35	122.42	115.78
24	c	509	CLA	CMC-C2C-C1C	2.35	128.61	125.04
24	B	604	CLA	CMB-C2B-C3B	2.35	129.07	124.68
26	B	618	BCR	C2-C1-C6	2.35	114.09	110.48
24	b	616	CLA	CED-O2D-CGD	2.35	121.24	115.94
24	D	402	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
24	b	614	CLA	CMC-C2C-C1C	2.34	128.61	125.04
24	B	611	CLA	CMB-C2B-C3B	2.34	129.06	124.68
24	a	409	CLA	C1-O2A-CGA	2.34	122.58	116.44
38	F	101	HEM	C1D-C2D-C3D	-2.34	105.37	107.00
26	B	619	BCR	C31-C1-C6	2.34	114.09	110.30
28	B	620[B]	SQD	O7-S-C6	2.34	109.72	106.94
24	c	513	CLA	CED-O2D-CGD	2.34	121.22	115.94
24	C	501	CLA	CED-O2D-CGD	2.34	121.22	115.94
24	c	501	CLA	CMC-C2C-C1C	2.34	128.60	125.04
25	a	410	PHO	O2D-CGD-O1D	-2.34	119.27	123.84
26	B	618	BCR	C3-C4-C5	2.33	118.24	114.08
24	c	503	CLA	O1D-CGD-CBD	-2.33	119.71	124.48
32	A	1017	LMT	C3'-C4'-C5'	-2.33	105.58	110.93
26	c	514	BCR	C7-C6-C5	2.33	127.11	121.46
24	D	402	CLA	O2A-CGA-CBA	2.33	119.22	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	610	CLA	CBC-CAC-C3C	-2.33	106.00	112.43
24	B	609	CLA	C1-O2A-CGA	2.33	122.55	116.44
24	b	614	CLA	CBC-CAC-C3C	-2.33	106.02	112.43
26	H	101	BCR	C37-C22-C23	-2.33	114.41	118.08
24	a	409	CLA	CMB-C2B-C3B	2.33	129.03	124.68
24	b	613	CLA	O2A-CGA-CBA	2.32	119.20	111.91
26	T	101	BCR	C37-C22-C23	-2.32	114.42	118.08
26	d	404	BCR	C3-C2-C1	2.32	122.90	114.60
24	C	503	CLA	CAC-C3C-C4C	2.32	127.82	124.81
27	a	414	PL9	C20-C19-C21	2.32	119.18	115.27
24	C	504	CLA	C1-O2A-CGA	2.32	122.53	116.44
28	a	401	SQD	O6-C1-C2	2.32	111.92	108.30
24	c	512	CLA	C1-C2-C3	-2.32	122.03	126.04
26	k	101	BCR	C1-C6-C5	-2.32	119.35	122.61
24	b	608	CLA	CED-O2D-CGD	2.32	121.18	115.94
32	a	402	LMT	C1B-O5B-C5B	2.32	118.24	113.69
32	b	625	LMT	O1'-C1'-C2'	2.32	111.92	108.30
24	b	604	CLA	C4-C3-C5	2.32	119.17	115.27
24	d	402	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
25	a	411	PHO	C1-C2-C3	-2.32	122.04	126.04
24	b	610	CLA	C1-O2A-CGA	2.31	122.52	116.44
24	c	503	CLA	CMC-C2C-C1C	2.31	128.56	125.04
26	A	1009	BCR	C3-C4-C5	2.31	118.21	114.08
24	A	1008	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
24	a	409	CLA	C4D-C3D-CAD	2.31	109.76	108.47
28	B	620[A]	SQD	O7-S-C6	2.31	109.69	106.94
26	B	619	BCR	C30-C25-C24	2.31	122.31	115.78
24	b	609	CLA	C1-O2A-CGA	2.31	122.50	116.44
24	b	614	CLA	CED-O2D-CGD	2.31	121.16	115.94
24	C	504	CLA	CHD-C4C-NC	-2.31	120.57	124.20
24	c	510	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
24	C	502	CLA	CMC-C2C-C1C	2.31	128.55	125.04
24	B	607	CLA	CHC-C1C-NC	-2.30	120.71	124.20
24	C	511	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
24	b	616	CLA	C4-C3-C5	2.30	119.14	115.27
24	D	405	CLA	CMC-C2C-C1C	2.30	128.53	125.04
36	C	516	DGD	O1G-C1A-O1A	-2.29	117.80	123.59
27	D	407	PL9	C7-C3-C4	2.29	118.74	116.88
24	B	615	CLA	CMC-C2C-C1C	2.29	128.52	125.04
24	C	509	CLA	CED-O2D-CGD	2.29	121.11	115.94
28	f	102	SQD	O8-S-C6	2.29	109.38	105.74
36	C	516	DGD	O1G-C1A-C2A	2.29	119.08	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	611	CLA	CED-O2D-CGD	2.29	121.11	115.94
24	D	403	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
27	a	414	PL9	C51-C49-C50	2.28	119.65	114.60
27	a	414	PL9	C45-C44-C46	2.28	119.11	115.27
26	k	102	BCR	C31-C1-C2	-2.28	99.78	108.91
24	A	1008	CLA	O2A-CGA-CBA	2.28	119.07	111.91
24	b	612	CLA	CMC-C2C-C1C	2.28	128.51	125.04
24	B	615	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
26	B	618	BCR	C32-C1-C6	2.28	114.00	110.30
27	D	407	PL9	C35-C34-C36	2.28	119.11	115.27
36	C	516	DGD	O2G-C1B-O1B	-2.28	118.19	123.70
24	b	613	CLA	O1D-CGD-CBD	-2.28	119.82	124.48
34	D	410	LHG	C5-O7-C7	-2.28	112.19	117.79
34	d	407	LHG	O8-C23-O10	-2.28	117.85	123.59
24	c	507	CLA	CBC-CAC-C3C	-2.27	106.16	112.43
24	C	508	CLA	C4-C3-C5	2.27	119.10	115.27
24	b	619	CLA	O2A-CGA-CBA	2.27	119.04	111.91
24	B	605	CLA	CMB-C2B-C3B	2.27	128.93	124.68
24	c	509	CLA	O2A-CGA-CBA	2.27	119.04	111.91
26	A	1009	BCR	C32-C1-C2	-2.27	99.82	108.91
28	b	623[A]	SQD	O8-S-C6	2.27	109.36	105.74
24	a	408	CLA	O2A-CGA-CBA	2.27	119.03	111.91
26	y	101	BCR	C31-C1-C6	2.27	113.98	110.30
24	b	617	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
24	b	606	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
24	B	601	CLA	CAC-C3C-C4C	2.26	127.74	124.81
26	H	101	BCR	C30-C25-C24	2.26	122.16	115.78
24	B	613	CLA	C4-C3-C5	2.26	119.06	115.27
24	D	403	CLA	C4C-C3C-C2C	-2.25	103.61	106.90
24	B	604	CLA	CMC-C2C-C1C	2.25	128.47	125.04
28	B	620[B]	SQD	C45-O47-C7	-2.25	112.25	117.79
24	C	509	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
26	c	514	BCR	C39-C30-C25	2.25	113.95	110.30
24	B	611	CLA	CBC-CAC-C3C	-2.25	106.23	112.43
24	B	601	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
24	C	509	CLA	O2A-CGA-CBA	2.25	118.96	111.91
24	b	606	CLA	C1-O2A-CGA	2.25	122.34	116.44
28	A	1011	SQD	C45-O47-C7	-2.24	112.27	117.79
36	c	517	DGD	O1G-C1A-O1A	-2.24	117.93	123.59
24	b	619	CLA	O1D-CGD-CBD	-2.24	119.89	124.48
24	B	604	CLA	CHD-C4C-NC	-2.24	120.68	124.20
24	b	610	CLA	CMB-C2B-C3B	2.24	128.87	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	606	CLA	CMC-C2C-C1C	2.24	128.45	125.04
24	d	403	CLA	O2D-CGD-CBD	2.24	115.24	111.27
34	b	624	LHG	O8-C23-C24	2.24	118.93	111.91
24	D	402	CLA	C1-O2A-CGA	2.24	122.31	116.44
24	B	616	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
26	y	101	BCR	C30-C25-C24	2.23	122.10	115.78
24	C	508	CLA	CAC-C3C-C4C	2.23	127.71	124.81
24	B	607	CLA	CAC-C3C-C4C	2.23	127.70	124.81
24	b	608	CLA	C1-O2A-CGA	2.23	122.30	116.44
24	D	403	CLA	CHC-C1C-C2C	-2.23	120.55	126.72
24	D	402	CLA	CED-O2D-CGD	2.23	120.98	115.94
24	c	512	CLA	C1-O2A-CGA	2.23	122.29	116.44
24	C	503	CLA	O2A-CGA-CBA	2.22	118.89	111.91
24	B	613	CLA	CED-O2D-CGD	2.22	120.97	115.94
24	B	601	CLA	CMC-C2C-C1C	2.22	128.42	125.04
26	A	1009	BCR	C34-C9-C8	-2.22	114.58	118.08
26	C	514	BCR	C35-C13-C14	-2.22	119.81	122.92
24	B	613	CLA	CAC-C3C-C4C	2.22	127.69	124.81
26	d	404	BCR	C4-C5-C6	2.22	125.96	122.73
34	d	406	LHG	O8-C23-O10	-2.22	117.98	123.59
24	B	609	CLA	C1-C2-C3	-2.22	122.20	126.04
24	C	501	CLA	CMC-C2C-C1C	2.22	128.42	125.04
28	A	1011	SQD	O5-C1-C2	-2.22	105.66	110.35
24	b	605	CLA	C1-C2-C3	-2.22	122.21	126.04
24	B	601	CLA	CED-O2D-CGD	2.22	120.95	115.94
24	C	504	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
24	A	1006	CLA	C4C-C3C-C2C	-2.21	103.67	106.90
24	B	612	CLA	CED-O2D-CGD	2.21	120.94	115.94
26	h	101	BCR	C40-C30-C25	2.21	113.88	110.30
27	A	1010	PL9	C51-C49-C50	2.21	119.48	114.60
24	C	511	CLA	CMB-C2B-C3B	2.21	128.81	124.68
28	A	1016	SQD	O8-S-C6	2.21	109.26	105.74
26	C	514	BCR	C34-C9-C8	-2.21	114.60	118.08
28	D	408	SQD	O5-C1-C2	-2.20	105.68	110.35
26	y	101	BCR	C1-C6-C7	2.20	122.01	115.78
26	b	621	BCR	C30-C25-C24	2.20	122.01	115.78
26	t	101	BCR	C30-C25-C26	-2.20	119.51	122.61
25	a	411	PHO	CED-O2D-CGD	2.20	120.92	115.94
24	c	512	CLA	CAC-C3C-C4C	2.20	127.67	124.81
28	A	1011	SQD	O8-S-C6	2.20	109.25	105.74
32	A	1018	LMT	O1B-C4'-C3'	2.20	113.13	107.28
24	B	612	CLA	O2A-CGA-CBA	2.20	118.81	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	509	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
24	b	604	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
38	f	101	HEM	CMA-C3A-C4A	-2.20	125.09	128.46
26	D	406	BCR	C40-C30-C39	2.20	115.27	108.53
24	B	610	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
24	D	405	CLA	C1-O2A-CGA	2.20	122.20	116.44
24	b	619	CLA	CED-O2D-CGD	2.20	120.90	115.94
24	C	506	CLA	CED-O2D-CGD	2.19	120.90	115.94
26	c	514	BCR	C40-C30-C29	-2.19	100.14	108.91
24	b	617	CLA	CHC-C1C-NC	-2.19	120.88	124.20
32	a	402	LMT	C3'-C4'-C5'	-2.19	105.91	110.93
24	C	506	CLA	O2A-CGA-CBA	2.19	118.78	111.91
26	B	619	BCR	C28-C27-C26	2.19	117.99	114.08
26	a	413	BCR	C31-C1-C2	-2.19	100.15	108.91
24	c	504	CLA	CHD-C4C-NC	-2.19	120.76	124.20
28	A	1011	SQD	O48-C23-C24	2.19	118.77	111.91
26	D	406	BCR	C3-C4-C5	2.19	117.98	114.08
24	b	610	CLA	CMC-C2C-C1C	2.18	128.37	125.04
24	b	612	CLA	CED-O2D-CGD	2.18	120.87	115.94
24	C	510	CLA	CMB-C2B-C3B	2.18	128.76	124.68
26	D	406	BCR	C31-C1-C2	-2.18	100.18	108.91
24	b	605	CLA	CED-O2D-CGD	2.18	120.87	115.94
24	c	510	CLA	CAC-C3C-C4C	2.18	127.64	124.81
26	b	621	BCR	C32-C1-C31	-2.18	101.84	108.53
24	B	614	CLA	O2A-CGA-CBA	2.18	118.74	111.91
24	A	1008	CLA	CAC-C3C-C4C	2.18	127.64	124.81
24	c	505	CLA	CED-O2D-CGD	2.18	120.86	115.94
24	b	618	CLA	CED-O2D-CGD	2.18	120.86	115.94
24	B	614	CLA	CED-O2D-CGD	2.17	120.85	115.94
26	h	101	BCR	C30-C25-C24	2.17	121.92	115.78
24	c	508	CLA	CED-O2D-CGD	2.17	120.85	115.94
24	B	613	CLA	C1-O2A-CGA	2.17	122.14	116.44
24	c	508	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
24	B	616	CLA	CMC-C2C-C1C	2.17	128.34	125.04
24	c	511	CLA	O2A-CGA-CBA	2.17	118.71	111.91
26	T	101	BCR	C35-C13-C14	-2.17	119.89	122.92
24	d	403	CLA	CAC-C3C-C4C	2.17	127.62	124.81
24	C	513	CLA	C1-O2A-CGA	2.17	122.13	116.44
26	J	101	BCR	C1-C6-C7	2.17	121.91	115.78
34	D	409	LHG	O8-C23-O10	-2.17	118.12	123.59
24	A	1006	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
26	h	101	BCR	C28-C29-C30	2.17	122.35	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	405	CLA	O2A-CGA-CBA	2.16	118.70	111.91
24	C	513	CLA	C4-C3-C5	2.16	118.91	115.27
28	c	518	SQD	O48-C23-C24	2.16	118.69	111.91
24	c	501	CLA	O2A-CGA-CBA	2.16	118.69	111.91
24	a	408	CLA	C4C-C3C-C2C	-2.16	103.75	106.90
24	B	608	CLA	CHD-C4C-NC	-2.16	120.80	124.20
24	B	602	CLA	C1-C2-C3	-2.16	122.31	126.04
24	B	611	CLA	CMC-C2C-C1C	2.16	128.33	125.04
24	b	609	CLA	C1D-CHD-C4C	2.16	125.41	122.56
24	B	605	CLA	O2A-CGA-O1A	-2.15	118.15	123.59
24	c	508	CLA	O2A-CGA-CBA	2.15	118.66	111.91
24	C	512	CLA	C1-C2-C3	-2.15	122.32	126.04
24	b	604	CLA	CHD-C4C-NC	-2.15	120.82	124.20
27	d	405	PL9	C51-C49-C50	2.15	119.35	114.60
26	J	101	BCR	C32-C1-C6	2.15	113.79	110.30
32	B	623	LMT	C1B-O5B-C5B	2.15	117.91	113.69
24	C	505	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
26	b	622	BCR	C28-C27-C26	2.15	117.91	114.08
24	a	408	CLA	CED-O2D-CGD	2.15	120.79	115.94
24	b	618	CLA	C1-O2A-CGA	2.15	122.07	116.44
24	A	1006	CLA	CHD-C4C-C3C	-2.14	121.69	124.84
24	b	610	CLA	C1-C2-C3	-2.14	122.34	126.04
26	t	101	BCR	C31-C1-C6	2.14	113.77	110.30
26	y	101	BCR	C40-C30-C29	-2.14	100.34	108.91
24	B	613	CLA	CBC-CAC-C3C	-2.14	106.53	112.43
26	b	622	BCR	C30-C25-C24	2.14	121.83	115.78
25	A	1007	PHO	CED-O2D-CGD	2.14	120.77	115.94
24	c	505	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
24	a	408	CLA	CBC-CAC-C3C	-2.14	106.54	112.43
26	K	101	BCR	C1-C6-C7	2.14	121.82	115.78
24	c	502	CLA	CHD-C4C-NC	-2.14	120.84	124.20
26	A	1009	BCR	C1-C6-C7	2.14	121.82	115.78
26	J	101	BCR	C39-C30-C29	-2.14	100.36	108.91
27	A	1010	PL9	C27-C28-C29	-2.14	122.52	127.66
24	D	402	CLA	CAC-C3C-C4C	2.13	127.58	124.81
24	C	504	CLA	CMC-C2C-C1C	2.13	128.29	125.04
24	C	512	CLA	CED-O2D-CGD	2.13	120.77	115.94
32	b	631	LMT	O5B-C5B-C6B	2.13	111.74	106.44
24	c	513	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
24	A	1008	CLA	C1-O2A-CGA	2.13	122.04	116.44
25	A	1007	PHO	O1D-CGD-CBD	-2.13	120.12	124.48
29	d	409	LMG	O8-C28-C29	2.13	118.59	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	512	CLA	C1-O2A-CGA	2.13	122.03	116.44
36	c	516	DGD	O1G-C1A-O1A	-2.13	118.22	123.59
28	b	623[A]	SQD	C45-O47-C7	-2.13	112.55	117.79
24	B	605	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
24	b	619	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
26	b	621	BCR	C40-C30-C29	-2.13	100.40	108.91
32	A	1018	LMT	O5B-C5B-C4B	2.12	113.55	109.69
29	m	102	LMG	O8-C28-O10	-2.12	118.23	123.59
24	b	606	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
26	y	101	BCR	C39-C30-C25	2.12	113.74	110.30
24	d	402	CLA	CAC-C3C-C4C	2.12	127.56	124.81
34	B	621	LHG	O8-C23-C24	2.12	118.57	111.91
27	A	1010	PL9	C7-C8-C9	-2.12	123.26	126.79
24	a	412	CLA	CED-O2D-CGD	2.12	120.73	115.94
24	b	606	CLA	CAC-C3C-C4C	2.12	127.56	124.81
26	C	514	BCR	C30-C25-C24	2.12	121.77	115.78
32	a	416	LMT	C1B-O5B-C5B	2.12	117.85	113.69
27	D	407	PL9	C42-C43-C44	-2.12	122.56	127.66
24	b	617	CLA	C1-O2A-CGA	2.12	122.00	116.44
24	c	501	CLA	CHD-C4C-NC	-2.12	120.87	124.20
24	B	606	CLA	CHC-C1C-NC	-2.12	120.99	124.20
24	B	613	CLA	CHD-C4C-C3C	-2.11	121.73	124.84
26	J	101	BCR	C27-C26-C25	2.11	125.80	122.73
24	c	504	CLA	CMC-C2C-C1C	2.11	128.25	125.04
24	a	412	CLA	O2A-CGA-CBA	2.11	118.53	111.91
24	A	1006	CLA	C1-O2A-CGA	2.11	121.98	116.44
24	A	1005	CLA	C4-C3-C5	2.11	118.82	115.27
26	T	101	BCR	C1-C6-C7	2.11	121.74	115.78
24	C	510	CLA	CAC-C3C-C4C	2.11	127.54	124.81
24	B	609	CLA	CED-O2D-CGD	2.10	120.70	115.94
28	A	1011	SQD	C1-O5-C5	-2.10	109.56	113.69
24	c	501	CLA	C1-O2A-CGA	2.10	121.96	116.44
24	C	502	CLA	O2A-CGA-CBA	2.10	118.50	111.91
24	a	407	CLA	C4-C3-C5	2.10	118.81	115.27
26	K	101	BCR	C40-C30-C25	2.10	113.70	110.30
24	C	508	CLA	C1-C2-C3	-2.10	122.41	126.04
25	A	1007	PHO	O2D-CGD-O1D	-2.10	119.74	123.84
24	C	510	CLA	CED-O2D-CGD	2.10	120.68	115.94
24	C	508	CLA	O2A-CGA-CBA	2.09	118.48	111.91
26	K	101	BCR	C2-C3-C4	2.09	116.05	111.38
26	T	101	BCR	C31-C1-C2	-2.09	100.53	108.91
26	K	101	BCR	C38-C26-C25	2.09	126.88	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	613	CLA	CED-O2D-CGD	2.09	120.67	115.94
24	C	501	CLA	CBC-CAC-C3C	-2.09	106.67	112.43
24	c	503	CLA	CHD-C4C-NC	-2.09	120.91	124.20
26	a	413	BCR	C1-C6-C7	2.09	121.69	115.78
24	B	605	CLA	CHD-C4C-C3C	-2.09	121.77	124.84
24	B	608	CLA	O2A-CGA-CBA	2.09	118.45	111.91
24	c	502	CLA	O2A-CGA-CBA	2.09	118.45	111.91
24	b	608	CLA	CAC-C3C-C4C	2.08	127.52	124.81
24	C	503	CLA	CED-O2D-CGD	2.08	120.65	115.94
24	a	408	CLA	O2D-CGD-O1D	-2.08	119.76	123.84
24	A	1006	CLA	CED-O2D-CGD	2.08	120.65	115.94
26	C	514	BCR	C33-C5-C6	2.08	126.86	124.53
27	D	407	PL9	C51-C49-C50	2.08	119.19	114.60
28	b	623[B]	SQD	C45-O47-C7	-2.08	112.67	117.79
29	C	519	LMG	O6-C5-C6	2.08	111.59	106.44
27	a	414	PL9	C15-C14-C16	2.07	118.76	115.27
24	c	511	CLA	CED-O2D-CGD	2.07	120.63	115.94
26	k	101	BCR	C34-C9-C10	-2.07	120.02	122.92
24	B	615	CLA	O2A-CGA-CBA	2.07	118.41	111.91
32	m	103	LMT	O1'-C1'-C2'	2.07	111.53	108.30
24	d	403	CLA	CED-O2D-CGD	2.07	120.61	115.94
24	D	403	CLA	C4-C3-C5	2.06	118.74	115.27
24	B	601	CLA	C4-C3-C2	-2.06	118.38	123.68
27	D	407	PL9	C12-C13-C14	-2.06	122.69	127.66
24	C	511	CLA	CMC-C2C-C1C	2.06	128.18	125.04
35	C	522	HTG	O5-C5-C6	2.06	111.56	106.44
24	A	1006	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
24	d	403	CLA	C4-C3-C5	2.06	118.73	115.27
24	b	612	CLA	O2A-CGA-CBA	2.06	118.37	111.91
24	c	507	CLA	CHA-C1A-NA	-2.06	121.68	126.40
24	C	509	CLA	CHD-C4C-NC	-2.06	120.96	124.20
25	D	404	PHO	CMD-C2D-C3D	-2.06	122.88	127.61
25	a	410	PHO	O1D-CGD-CBD	-2.06	120.28	124.48
38	v	201	HEM	CMA-C3A-C4A	-2.06	125.31	128.46
24	B	614	CLA	C1-C2-C3	-2.05	122.49	126.04
24	c	507	CLA	C1-O2A-CGA	2.05	121.83	116.44
24	C	511	CLA	CED-O2D-CGD	2.05	120.57	115.94
26	a	413	BCR	C4-C5-C6	2.05	125.71	122.73
24	C	505	CLA	CMB-C2B-C3B	2.05	128.51	124.68
27	D	407	PL9	C7-C8-C9	-2.05	123.38	126.79
34	D	410	LHG	O8-C23-O10	-2.04	118.43	123.59
24	B	606	CLA	O2A-CGA-CBA	2.04	118.32	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	102	BCR	C39-C30-C25	2.04	113.61	110.30
28	b	623[B]	SQD	O48-C23-O10	-2.04	118.44	123.59
28	A	1011	SQD	O47-C7-O49	-2.04	118.77	123.70
24	B	616	CLA	C1-C2-C3	-2.04	122.52	126.04
26	H	101	BCR	C28-C29-C30	2.04	121.89	114.60
28	b	623[A]	SQD	O9-S-C6	2.04	109.36	106.94
27	a	414	PL9	C7-C3-C2	-2.04	120.62	123.30
25	a	411	PHO	CMD-C2D-C3D	-2.04	122.93	127.61
24	B	606	CLA	C1D-CHD-C4C	2.04	125.24	122.56
28	B	620[A]	SQD	O8-S-C6	2.03	108.98	105.74
24	B	616	CLA	O1D-CGD-CBD	-2.03	120.32	124.48
32	b	625	LMT	C1-O1'-C1'	-2.03	110.47	113.84
24	a	412	CLA	CBC-CAC-C3C	-2.03	106.83	112.43
28	D	408	SQD	C1-C2-C3	-2.03	105.77	110.00
26	A	1009	BCR	C34-C9-C10	-2.03	120.08	122.92
24	B	609	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
24	B	614	CLA	CBC-CAC-C3C	-2.03	106.83	112.43
24	d	403	CLA	CBC-CAC-C3C	-2.03	106.84	112.43
36	h	102	DGD	O1G-C1A-O1A	-2.03	118.47	123.59
24	B	604	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
32	a	402	LMT	O5'-C5'-C6'	2.03	111.48	106.44
27	d	405	PL9	C7-C3-C4	2.03	118.52	116.88
24	D	402	CLA	CBC-CAC-C3C	-2.03	106.84	112.43
24	C	513	CLA	CHC-C1C-NC	-2.03	121.13	124.20
29	m	102	LMG	O7-C10-O9	-2.03	118.81	123.70
28	c	518	SQD	O8-S-C6	2.02	108.97	105.74
24	c	503	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
28	B	620[A]	SQD	O47-C7-O49	-2.02	118.81	123.70
38	V	201	HEM	CBA-CAA-C2A	-2.02	108.75	112.49
28	c	518	SQD	O9-S-O7	-2.02	106.95	113.95
24	B	614	CLA	CAC-C3C-C4C	2.02	127.43	124.81
26	b	622	BCR	C31-C1-C2	-2.02	100.82	108.91
24	b	618	CLA	O2A-CGA-CBA	2.02	118.25	111.91
24	a	409	CLA	CBC-CAC-C3C	-2.02	106.86	112.43
24	b	609	CLA	O2A-CGA-CBA	2.02	118.24	111.91
24	c	508	CLA	CHD-C4C-NC	-2.02	121.03	124.20
24	C	502	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
29	c	521	LMG	O7-C10-O9	-2.02	118.83	123.70
24	B	616	CLA	C1-O2A-CGA	2.02	121.73	116.44
28	b	623[A]	SQD	O48-C23-O10	-2.01	118.51	123.59
24	C	504	CLA	C7-C6-C5	-2.01	107.89	113.36
35	b	626	HTG	O5-C5-C6	2.01	111.43	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	615	CLA	C1-C2-C3	-2.01	122.57	126.04
32	b	625	LMT	O5B-C5B-C6B	2.01	111.43	106.44
25	a	410	PHO	C1-O2A-CGA	2.01	121.71	116.44
24	b	611	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
26	J	101	BCR	C28-C27-C26	2.01	117.66	114.08
24	B	603	CLA	CMC-C2C-C1C	2.00	128.09	125.04
28	B	620[A]	SQD	C45-O47-C7	-2.00	112.86	117.79
24	b	609	CLA	CED-O2D-CGD	2.00	120.47	115.94
24	D	403	CLA	O2A-CGA-CBA	2.00	118.19	111.91
26	B	618	BCR	C40-C30-C29	-2.00	100.90	108.91
34	E	101	LHG	O8-C23-O10	-2.00	118.54	123.59
36	C	515	DGD	O1G-C1A-O1A	-2.00	118.54	123.59
28	b	623[B]	SQD	O47-C7-O49	-2.00	118.87	123.70
28	a	401	SQD	O8-S-C6	2.00	108.93	105.74

All (166) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	C	503	CLA	NC
24	C	503	CLA	NA
24	B	612	CLA	NA
24	B	612	CLA	NC
24	B	612	CLA	ND
24	c	502	CLA	NA
24	b	617	CLA	NC
24	b	617	CLA	ND
24	b	617	CLA	NA
24	A	1005	CLA	NC
24	A	1005	CLA	ND
24	A	1005	CLA	NA
24	C	504	CLA	NC
24	C	504	CLA	ND
24	C	504	CLA	NA
24	b	607	CLA	NC
24	b	607	CLA	ND
24	b	607	CLA	NA
24	C	510	CLA	NC
24	C	510	CLA	ND
24	C	510	CLA	NA
24	a	408	CLA	NA
24	B	601	CLA	NC
24	B	601	CLA	ND

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Mol	Chain	Res	Type	Atom
24	B	601	CLA	NA
24	B	611	CLA	NC
24	B	611	CLA	ND
24	B	611	CLA	NA
24	b	608	CLA	NC
24	b	608	CLA	ND
24	b	608	CLA	NA
24	c	508	CLA	NC
24	c	508	CLA	NA
24	B	607	CLA	NC
24	B	607	CLA	ND
24	B	607	CLA	NA
24	c	501	CLA	NC
24	c	501	CLA	ND
24	c	501	CLA	NA
24	B	615	CLA	NC
24	B	615	CLA	ND
24	B	615	CLA	NA
24	C	506	CLA	NC
24	C	506	CLA	ND
24	C	506	CLA	NA
24	B	606	CLA	NC
24	B	606	CLA	ND
24	B	606	CLA	NA
24	c	512	CLA	NC
24	c	512	CLA	NA
24	c	512	CLA	ND
24	b	614	CLA	NC
24	B	608	CLA	NC
24	c	513	CLA	NC
24	d	403	CLA	NC
24	d	403	CLA	NA
24	A	1006	CLA	NC
24	A	1006	CLA	NA
24	b	613	CLA	NC
24	b	613	CLA	ND
24	b	613	CLA	NA
24	c	503	CLA	NC
24	a	409	CLA	NC
24	a	409	CLA	NA
24	B	602	CLA	NC
24	B	602	CLA	ND

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Mol	Chain	Res	Type	Atom
24	B	602	CLA	NA
24	c	507	CLA	NC
24	c	507	CLA	ND
24	c	507	CLA	NA
24	c	509	CLA	NC
24	c	509	CLA	ND
24	c	509	CLA	NA
24	A	1008	CLA	NC
24	B	605	CLA	NC
24	B	605	CLA	ND
24	B	605	CLA	NA
24	C	512	CLA	NC
24	C	512	CLA	NA
24	C	512	CLA	ND
24	C	508	CLA	NC
24	C	508	CLA	ND
24	C	508	CLA	NA
24	B	614	CLA	NC
24	B	614	CLA	ND
24	B	614	CLA	NA
24	b	605	CLA	NC
24	b	605	CLA	ND
24	b	605	CLA	NA
24	c	505	CLA	ND
24	c	505	CLA	NA
24	b	615	CLA	NA
24	b	615	CLA	NC
24	b	615	CLA	ND
24	c	511	CLA	NC
24	c	511	CLA	NA
24	C	502	CLA	NA
24	B	613	CLA	NC
24	B	613	CLA	ND
24	B	613	CLA	NA
24	a	407	CLA	NC
24	a	407	CLA	ND
24	a	407	CLA	NA
24	C	501	CLA	NC
24	C	501	CLA	ND
24	C	501	CLA	NA
24	D	402	CLA	ND
24	D	402	CLA	NA

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Mol	Chain	Res	Type	Atom
24	C	505	CLA	ND
24	b	616	CLA	NC
24	b	616	CLA	ND
24	b	616	CLA	NA
24	B	604	CLA	NC
24	B	604	CLA	ND
24	B	604	CLA	NA
24	B	610	CLA	NC
24	B	610	CLA	ND
24	B	610	CLA	NA
24	c	504	CLA	NC
24	c	504	CLA	NA
24	c	510	CLA	NC
24	c	510	CLA	ND
24	c	510	CLA	NA
24	C	513	CLA	NC
24	C	513	CLA	NA
24	B	609	CLA	NC
24	B	609	CLA	ND
24	B	603	CLA	NC
24	B	603	CLA	ND
24	B	603	CLA	NA
24	b	611	CLA	NC
24	b	610	CLA	NC
24	b	610	CLA	ND
24	b	610	CLA	NA
24	b	606	CLA	NC
24	b	606	CLA	ND
24	b	606	CLA	NA
24	b	609	CLA	NC
24	b	609	CLA	ND
24	b	609	CLA	NA
24	C	509	CLA	NC
24	C	509	CLA	ND
24	C	509	CLA	NA
24	D	405	CLA	NC
24	D	405	CLA	NA
24	d	402	CLA	ND
24	b	618	CLA	NC
24	b	618	CLA	ND
24	b	618	CLA	NA
24	B	616	CLA	NC

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Mol	Chain	Res	Type	Atom
24	B	616	CLA	ND
24	B	616	CLA	NA
24	C	507	CLA	NA
24	C	507	CLA	NC
24	C	507	CLA	ND
24	C	511	CLA	NC
24	C	511	CLA	NA
24	b	619	CLA	NC
24	b	619	CLA	ND
24	b	619	CLA	NA
24	D	403	CLA	NA
24	b	604	CLA	NA
24	a	412	CLA	NC
24	c	506	CLA	NC
24	c	506	CLA	ND
24	c	506	CLA	NA

All (1872) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	b	622	BCR	C14-C15-C16-C17
26	b	622	BCR	C15-C16-C17-C18
34	D	410	LHG	C4-O6-P-O4
26	D	406	BCR	C37-C22-C23-C24
26	D	406	BCR	C22-C23-C24-C25
28	a	401	SQD	O6-C44-C45-O47
24	c	502	CLA	CHA-CBD-CGD-O1D
24	b	617	CLA	CHA-CBD-CGD-O1D
24	b	617	CLA	CAD-CBD-CGD-O1D
24	b	617	CLA	CAD-CBD-CGD-O2D
26	a	413	BCR	C14-C15-C16-C17
26	a	413	BCR	C18-C19-C20-C21
26	a	413	BCR	C19-C20-C21-C22
24	a	408	CLA	CHA-CBD-CGD-O1D
35	C	521	HTG	C2'-C1'-S1-C1
26	K	101	BCR	C10-C11-C12-C13
26	K	101	BCR	C18-C19-C20-C21
32	a	402	LMT	C2'-C1'-O1'-C1
32	a	402	LMT	O5'-C1'-O1'-C1
24	B	601	CLA	CHA-CBD-CGD-O1D
24	B	601	CLA	CHA-CBD-CGD-O2D
24	B	601	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
32	f	103	LMT	C2-C1-O1'-C1'
26	B	619	BCR	C10-C11-C12-C13
26	T	101	BCR	C14-C15-C16-C17
26	T	101	BCR	C18-C19-C20-C21
28	f	102	SQD	C8-C7-O47-C45
35	d	416	HTG	O5-C1-S1-C1'
32	A	1017	LMT	C2'-C1'-O1'-C1
32	A	1017	LMT	O5'-C1'-O1'-C1
26	y	101	BCR	C10-C11-C12-C13
26	y	101	BCR	C18-C19-C20-C21
26	y	101	BCR	C19-C20-C21-C22
26	y	101	BCR	C20-C21-C22-C37
24	c	508	CLA	CHA-CBD-CGD-O1D
24	c	508	CLA	CHA-CBD-CGD-O2D
32	i	102	LMT	C2'-C1'-O1'-C1
26	t	101	BCR	C14-C15-C16-C17
26	t	101	BCR	C18-C19-C20-C21
33	d	415	GOL	C1-C2-C3-O3
24	B	606	CLA	CHA-CBD-CGD-O1D
26	H	101	BCR	C10-C11-C12-C13
26	H	101	BCR	C14-C15-C16-C17
26	H	101	BCR	C18-C19-C20-C21
26	H	101	BCR	C19-C20-C21-C22
34	e	101	LHG	C4-O6-P-O4
34	e	101	LHG	C8-C7-O7-C5
26	k	102	BCR	C10-C11-C12-C13
26	k	102	BCR	C14-C15-C16-C17
26	k	102	BCR	C18-C19-C20-C21
26	c	514	BCR	C14-C15-C16-C17
26	c	514	BCR	C18-C19-C20-C21
34	E	101	LHG	C4-O6-P-O4
33	V	206	GOL	C1-C2-C3-O3
32	b	625	LMT	C2B-C1B-O1B-C4'
35	c	522	HTG	C2-C1-S1-C1'
35	c	522	HTG	O5-C1-S1-C1'
35	c	522	HTG	C2'-C1'-S1-C1
35	D	419	HTG	C2-C1-S1-C1'
35	D	419	HTG	O5-C1-S1-C1'
34	b	624	LHG	C4-O6-P-O4
34	b	624	LHG	C4-O6-P-O5
27	A	1010	PL9	C24-C26-C27-C28
38	f	101	HEM	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
35	b	630	HTG	C2-C1-S1-C1'
35	b	630	HTG	O5-C1-S1-C1'
28	A	1016	SQD	O6-C44-C45-O47
29	c	521	LMG	O6-C1-O1-C7
29	c	521	LMG	C11-C10-O7-C8
24	C	508	CLA	CHA-CBD-CGD-O1D
24	B	614	CLA	CHA-CBD-CGD-O1D
24	B	614	CLA	CAD-CBD-CGD-O1D
24	B	614	CLA	CAD-CBD-CGD-O2D
24	b	605	CLA	CHA-CBD-CGD-O1D
26	d	404	BCR	C14-C15-C16-C17
26	d	404	BCR	C18-C19-C20-C21
26	d	404	BCR	C37-C22-C23-C24
25	a	411	PHO	CHA-CBD-CGD-O2D
24	C	502	CLA	CHA-CBD-CGD-O2D
26	A	1009	BCR	C14-C15-C16-C17
26	A	1009	BCR	C18-C19-C20-C21
26	A	1009	BCR	C19-C20-C21-C22
26	J	101	BCR	C10-C11-C12-C13
26	J	101	BCR	C11-C12-C13-C14
26	J	101	BCR	C11-C12-C13-C35
26	J	101	BCR	C14-C15-C16-C17
26	J	101	BCR	C18-C19-C20-C21
32	t	103	LMT	C2'-C1'-O1'-C1
32	t	103	LMT	O5'-C1'-O1'-C1
26	k	101	BCR	C10-C11-C12-C13
26	k	101	BCR	C18-C19-C20-C21
26	k	101	BCR	C19-C20-C21-C22
26	k	101	BCR	C21-C22-C23-C24
26	k	101	BCR	C37-C22-C23-C24
33	D	418	GOL	O1-C1-C2-C3
32	B	623	LMT	C2'-C1'-O1'-C1
32	B	623	LMT	C2-C1-O1'-C1'
29	C	519	LMG	O9-C10-O7-C8
28	B	620[B]	SQD	O49-C7-O47-C45
28	B	620[B]	SQD	C8-C7-O47-C45
28	B	620[B]	SQD	O5-C5-C6-S
24	b	609	CLA	CHA-CBD-CGD-O1D
24	b	609	CLA	CHA-CBD-CGD-O2D
28	B	620[A]	SQD	O5-C1-O6-C44
28	B	620[A]	SQD	O49-C7-O47-C45
28	B	620[A]	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
28	B	620[A]	SQD	O5-C5-C6-S
26	K	102	BCR	C14-C15-C16-C17
26	K	102	BCR	C18-C19-C20-C21
26	K	102	BCR	C37-C22-C23-C24
28	b	623[A]	SQD	C46-C45-O47-C7
28	b	623[A]	SQD	C8-C7-O47-C45
28	b	623[A]	SQD	O5-C5-C6-S
35	V	202	HTG	C2-C1-S1-C1'
35	V	202	HTG	O5-C1-S1-C1'
28	b	623[B]	SQD	O49-C7-O47-C45
28	b	623[B]	SQD	C5-C6-S-O7
28	b	623[B]	SQD	C5-C6-S-O8
28	b	623[B]	SQD	C5-C6-S-O9
35	C	522	HTG	C2'-C1'-S1-C1
34	d	407	LHG	C4-O6-P-O4
34	B	621	LHG	C4-O6-P-O4
34	B	621	LHG	C4-O6-P-O5
24	C	507	CLA	CHA-CBD-CGD-O1D
35	c	525	HTG	C2'-C1'-S1-C1
26	C	514	BCR	C14-C15-C16-C17
26	h	101	BCR	C18-C19-C20-C21
29	c	520	LMG	C2-C1-O1-C7
29	c	520	LMG	O6-C1-O1-C7
29	c	520	LMG	C8-C7-O1-C1
24	b	604	CLA	CHA-CBD-CGD-O1D
24	b	604	CLA	CHA-CBD-CGD-O2D
32	A	1018	LMT	C3'-C4'-O1B-C1B
24	c	513	CLA	CBD-CGD-O2D-CED
24	C	513	CLA	CBD-CGD-O2D-CED
32	b	631	LMT	O5B-C1B-O1B-C4'
24	b	615	CLA	C13-C15-C16-C17
29	m	102	LMG	O10-C28-O8-C9
28	B	620[B]	SQD	O10-C23-O48-C46
24	C	513	CLA	O1D-CGD-O2D-CED
32	C	520	LMT	C3'-C4'-O1B-C1B
24	c	512	CLA	CBD-CGD-O2D-CED
24	c	512	CLA	O1D-CGD-O2D-CED
28	f	102	SQD	O49-C7-O47-C45
34	e	101	LHG	O9-C7-O7-C5
29	c	521	LMG	O9-C10-O7-C8
28	b	623[A]	SQD	O49-C7-O47-C45
24	b	617	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
29	m	102	LMG	C29-C28-O8-C9
28	D	408	SQD	C24-C23-O48-C46
32	A	1018	LMT	O5'-C5'-C6'-O6'
29	C	519	LMG	C11-C10-O7-C8
28	b	623[B]	SQD	C8-C7-O47-C45
35	D	419	HTG	O5-C5-C6-O6
24	c	508	CLA	CBD-CGD-O2D-CED
24	C	511	CLA	CBD-CGD-O2D-CED
34	E	101	LHG	O10-C23-O8-C6
24	B	614	CLA	C3-C5-C6-C7
29	a	415	LMG	C29-C28-O8-C9
34	e	101	LHG	C24-C23-O8-C6
28	B	620[B]	SQD	C24-C23-O48-C46
24	C	502	CLA	CBD-CGD-O2D-CED
35	B	624	HTG	S1-C1'-C2'-C3'
35	C	521	HTG	S1-C1'-C2'-C3'
35	D	419	HTG	S1-C1'-C2'-C3'
29	a	415	LMG	O10-C28-O8-C9
28	D	408	SQD	O10-C23-O48-C46
29	c	519	LMG	O10-C28-O8-C9
24	B	616	CLA	O1A-CGA-O2A-C1
26	K	101	BCR	C19-C20-C21-C22
26	T	101	BCR	C19-C20-C21-C22
26	b	620	BCR	C19-C20-C21-C22
26	J	101	BCR	C15-C16-C17-C18
26	J	101	BCR	C19-C20-C21-C22
26	K	102	BCR	C19-C20-C21-C22
26	C	514	BCR	C19-C20-C21-C22
26	h	101	BCR	C15-C16-C17-C18
32	A	1018	LMT	C4'-C5'-C6'-O6'
25	a	411	PHO	O1D-CGD-O2D-CED
34	D	410	LHG	O2-C2-C3-O3
34	d	407	LHG	O2-C2-C3-O3
34	E	101	LHG	C24-C23-O8-C6
24	B	616	CLA	CBA-CGA-O2A-C1
32	a	402	LMT	O5B-C5B-C6B-O6B
35	B	629	HTG	O5-C5-C6-O6
32	i	102	LMT	C4'-C5'-C6'-O6'
35	d	410	HTG	C4-C5-C6-O6
32	C	520	LMT	O5B-C5B-C6B-O6B
32	A	1017	LMT	O5'-C5'-C6'-O6'
35	d	410	HTG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
29	C	519	LMG	O6-C5-C6-O5
32	a	402	LMT	C4B-C5B-C6B-O6B
28	B	620[B]	SQD	C30-C31-C32-C33
26	y	101	BCR	C14-C15-C16-C17
32	f	103	LMT	C4B-C5B-C6B-O6B
29	c	521	LMG	C29-C28-O8-C9
29	c	519	LMG	C29-C28-O8-C9
35	c	522	HTG	S1-C1'-C2'-C3'
35	B	624	HTG	O5-C5-C6-O6
29	c	521	LMG	O6-C5-C6-O5
34	e	101	LHG	O10-C23-O8-C6
32	b	631	LMT	O5B-C5B-C6B-O6B
24	b	617	CLA	C4-C3-C5-C6
35	D	419	HTG	C4-C5-C6-O6
24	b	617	CLA	C2-C3-C5-C6
24	C	502	CLA	O1D-CGD-O2D-CED
32	m	103	LMT	O5B-C5B-C6B-O6B
29	c	521	LMG	O10-C28-O8-C9
32	f	103	LMT	C4'-C5'-C6'-O6'
32	i	102	LMT	O5'-C1'-O1'-C1
32	B	623	LMT	O5'-C1'-O1'-C1
28	b	623[B]	SQD	O5-C1-O6-C44
27	a	414	PL9	C24-C26-C27-C28
29	A	1012	LMG	C29-C28-O8-C9
28	D	408	SQD	C8-C7-O47-C45
35	b	630	HTG	O5-C5-C6-O6
24	C	513	CLA	C3-C5-C6-C7
24	B	601	CLA	CBA-CGA-O2A-C1
24	c	513	CLA	CBA-CGA-O2A-C1
28	B	620[A]	SQD	C24-C23-O48-C46
25	a	411	PHO	CBD-CGD-O2D-CED
32	b	631	LMT	C4B-C5B-C6B-O6B
26	B	617	BCR	C19-C20-C21-C22
29	A	1012	LMG	O10-C28-O8-C9
34	d	408	LHG	C30-C31-C32-C33
35	B	624	HTG	C4-C5-C6-O6
35	B	629	HTG	C4-C5-C6-O6
32	m	103	LMT	C4B-C5B-C6B-O6B
24	B	601	CLA	C5-C6-C7-C8
24	C	506	CLA	C15-C16-C17-C18
24	D	405	CLA	C10-C11-C12-C13
28	f	102	SQD	C2-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
28	b	623[B]	SQD	C2-C1-O6-C44
24	B	601	CLA	O1A-CGA-O2A-C1
32	f	103	LMT	O5B-C5B-C6B-O6B
24	c	513	CLA	C14-C13-C15-C16
24	c	509	CLA	C6-C7-C8-C9
24	B	610	CLA	C14-C13-C15-C16
24	c	504	CLA	C11-C12-C13-C14
24	C	507	CLA	C14-C13-C15-C16
24	c	510	CLA	O1D-CGD-O2D-CED
24	c	508	CLA	C13-C15-C16-C17
24	B	606	CLA	C2A-CAA-CBA-CGA
24	b	609	CLA	C2A-CAA-CBA-CGA
26	y	101	BCR	C11-C12-C13-C35
26	k	101	BCR	C7-C8-C9-C34
24	c	513	CLA	O1A-CGA-O2A-C1
24	B	614	CLA	C5-C6-C7-C8
32	A	1017	LMT	O5B-C5B-C6B-O6B
24	b	604	CLA	CBA-CGA-O2A-C1
24	b	617	CLA	C8-C10-C11-C12
24	b	614	CLA	C13-C15-C16-C17
24	c	509	CLA	C13-C15-C16-C17
24	b	609	CLA	C15-C16-C17-C18
29	C	518	LMG	C10-C11-C12-C13
29	C	518	LMG	C28-C29-C30-C31
28	b	623[B]	SQD	C7-C8-C9-C10
35	C	521	HTG	C1'-C2'-C3'-C4'
26	B	618	BCR	C14-C15-C16-C17
24	C	506	CLA	C13-C15-C16-C17
24	B	606	CLA	C10-C11-C12-C13
24	B	606	CLA	C15-C16-C17-C18
24	C	509	CLA	C15-C16-C17-C18
24	B	616	CLA	C5-C6-C7-C8
24	b	619	CLA	C10-C11-C12-C13
24	b	604	CLA	C15-C16-C17-C18
33	D	418	GOL	O1-C1-C2-O2
33	D	418	GOL	O2-C2-C3-O3
28	f	102	SQD	C23-C24-C25-C26
36	C	516	DGD	C1B-C2B-C3B-C4B
36	C	515	DGD	C1B-C2B-C3B-C4B
28	A	1016	SQD	C23-C24-C25-C26
29	m	102	LMG	C28-C29-C30-C31
28	B	620[A]	SQD	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
29	c	519	LMG	C28-C29-C30-C31
32	f	103	LMT	O5'-C5'-C6'-O6'
36	H	102	DGD	C6B-C7B-C8B-C9B
24	c	513	CLA	O1D-CGD-O2D-CED
24	c	508	CLA	C10-C11-C12-C13
24	B	606	CLA	C13-C15-C16-C17
24	C	508	CLA	C10-C11-C12-C13
24	c	506	CLA	C5-C6-C7-C8
32	C	520	LMT	O1'-C1-C2-C3
35	b	601	HTG	S1-C1'-C2'-C3'
28	D	408	SQD	O49-C7-O47-C45
24	b	604	CLA	C2-C1-O2A-CGA
24	C	509	CLA	C10-C11-C12-C13
24	b	619	CLA	C5-C6-C7-C8
36	c	517	DGD	C1A-C2A-C3A-C4A
34	e	101	LHG	C23-C24-C25-C26
35	C	522	HTG	O5-C5-C6-O6
34	D	411	LHG	C31-C32-C33-C34
24	B	616	CLA	C15-C16-C17-C18
24	c	502	CLA	C11-C12-C13-C15
24	C	506	CLA	C12-C13-C15-C16
24	c	513	CLA	C12-C13-C15-C16
24	C	512	CLA	C12-C13-C15-C16
24	b	606	CLA	C6-C7-C8-C10
24	a	412	CLA	C11-C12-C13-C15
24	a	412	CLA	C12-C13-C15-C16
28	B	620[A]	SQD	O10-C23-O48-C46
26	c	514	BCR	C15-C16-C17-C18
26	d	404	BCR	C13-C14-C15-C16
24	d	403	CLA	O1D-CGD-O2D-CED
24	C	506	CLA	C5-C6-C7-C8
24	c	513	CLA	C15-C16-C17-C18
24	A	1008	CLA	C10-C11-C12-C13
24	b	619	CLA	C13-C15-C16-C17
29	c	521	LMG	C4-C5-C6-O5
32	i	102	LMT	O5'-C5'-C6'-O6'
24	C	511	CLA	O1D-CGD-O2D-CED
32	b	625	LMT	O1'-C1-C2-C3
26	b	622	BCR	C10-C11-C12-C13
26	b	622	BCR	C18-C19-C20-C21
26	D	406	BCR	C18-C19-C20-C21
26	B	619	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
26	b	620	BCR	C10-C11-C12-C13
26	b	620	BCR	C18-C19-C20-C21
26	d	404	BCR	C10-C11-C12-C13
26	B	618	BCR	C18-C19-C20-C21
35	b	626	HTG	C4-C5-C6-O6
24	B	610	CLA	C8-C10-C11-C12
24	c	504	CLA	C10-C11-C12-C13
24	b	609	CLA	C10-C11-C12-C13
24	b	604	CLA	C10-C11-C12-C13
24	a	412	CLA	C8-C10-C11-C12
24	c	506	CLA	C15-C16-C17-C18
32	f	103	LMT	O1'-C1-C2-C3
24	B	615	CLA	C5-C6-C7-C8
24	B	604	CLA	C13-C15-C16-C17
24	D	405	CLA	C8-C10-C11-C12
24	b	619	CLA	C15-C16-C17-C18
24	c	508	CLA	O1D-CGD-O2D-CED
29	Z	101	LMG	C11-C10-O7-C8
32	A	1018	LMT	O1'-C1-C2-C3
24	c	508	CLA	C15-C16-C17-C18
24	B	613	CLA	C13-C15-C16-C17
24	b	616	CLA	C10-C11-C12-C13
34	e	101	LHG	C4-O6-P-O3
34	E	101	LHG	C4-O6-P-O3
34	b	624	LHG	C4-O6-P-O3
34	B	621	LHG	C4-O6-P-O3
35	b	626	HTG	O5-C5-C6-O6
24	B	607	CLA	C3-C5-C6-C7
24	C	512	CLA	CBA-CGA-O2A-C1
28	b	623[B]	SQD	C13-C14-C15-C16
24	b	617	CLA	C5-C6-C7-C8
24	A	1008	CLA	C8-C10-C11-C12
24	c	506	CLA	O1D-CGD-O2D-CED
32	b	631	LMT	O1'-C1-C2-C3
35	o	301	HTG	S1-C1'-C2'-C3'
29	d	409	LMG	O6-C5-C6-O5
34	d	407	LHG	C1-C2-C3-O3
29	Z	101	LMG	O9-C10-O7-C8
32	M	101	LMT	C2B-C1B-O1B-C4'
24	B	601	CLA	C3-C5-C6-C7
24	a	412	CLA	CBA-CGA-O2A-C1
26	k	102	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
26	k	102	BCR	C19-C20-C21-C22
26	K	102	BCR	C15-C16-C17-C18
26	C	514	BCR	C15-C16-C17-C18
34	e	101	LHG	C7-C8-C9-C10
28	D	408	SQD	C23-C24-C25-C26
36	c	515	DGD	C3A-C4A-C5A-C6A
36	c	516	DGD	C5B-C6B-C7B-C8B
29	A	1012	LMG	C15-C16-C17-C18
36	C	515	DGD	CBA-CCA-CDA-CEA
29	Z	101	LMG	C15-C16-C17-C18
29	m	102	LMG	C31-C32-C33-C34
26	b	622	BCR	C20-C21-C22-C37
26	a	413	BCR	C16-C17-C18-C36
26	k	102	BCR	C16-C17-C18-C36
26	k	102	BCR	C20-C21-C22-C37
32	b	625	LMT	O5B-C5B-C6B-O6B
26	A	1009	BCR	C16-C17-C18-C36
26	k	101	BCR	C20-C21-C22-C37
26	B	618	BCR	C20-C21-C22-C37
26	B	617	BCR	C20-C21-C22-C37
26	C	514	BCR	C20-C21-C22-C37
35	D	419	HTG	C1'-C2'-C3'-C4'
36	c	515	DGD	CBA-CCA-CDA-CEA
34	D	410	LHG	C14-C15-C16-C17
28	a	401	SQD	C17-C18-C19-C20
32	f	103	LMT	C2-C3-C4-C5
32	i	102	LMT	C7-C8-C9-C10
32	i	102	LMT	C11-C10-C9-C8
36	c	516	DGD	C7B-C8B-C9B-CAB
29	a	415	LMG	C16-C17-C18-C19
29	a	415	LMG	C30-C31-C32-C33
29	d	409	LMG	C15-C16-C17-C18
29	d	409	LMG	C36-C37-C38-C39
34	e	101	LHG	C11-C10-C9-C8
34	e	101	LHG	C13-C14-C15-C16
34	E	101	LHG	C9-C10-C11-C12
34	E	101	LHG	C32-C33-C34-C35
32	b	625	LMT	C3-C4-C5-C6
34	b	624	LHG	C13-C14-C15-C16
29	Z	101	LMG	C21-C22-C23-C24
29	Z	101	LMG	C34-C35-C36-C37
29	B	622	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
28	D	408	SQD	C32-C33-C34-C35
34	D	411	LHG	C26-C27-C28-C29
32	t	103	LMT	C5-C6-C7-C8
32	t	103	LMT	C6-C7-C8-C9
35	B	628	HTG	C2'-C3'-C4'-C5'
29	C	519	LMG	C33-C34-C35-C36
28	A	1011	SQD	C32-C33-C34-C35
28	B	620[B]	SQD	C12-C13-C14-C15
28	B	620[B]	SQD	C31-C32-C33-C34
28	b	623[B]	SQD	C14-C15-C16-C17
32	A	1018	LMT	C11-C10-C9-C8
24	C	506	CLA	O1D-CGD-O2D-CED
24	B	606	CLA	C16-C17-C18-C20
24	A	1006	CLA	C16-C17-C18-C19
24	B	604	CLA	C16-C17-C18-C20
28	b	623[A]	SQD	C24-C23-O48-C46
36	c	515	DGD	C5A-C6A-C7A-C8A
28	c	518	SQD	C30-C31-C32-C33
36	C	516	DGD	C9A-CAA-CBA-CCA
36	C	516	DGD	C3B-C4B-C5B-C6B
36	c	516	DGD	C9B-CAB-CBB-CCB
29	d	409	LMG	C20-C21-C22-C23
36	c	517	DGD	C7B-C8B-C9B-CAB
34	e	101	LHG	C10-C11-C12-C13
34	E	101	LHG	C18-C19-C20-C21
32	b	625	LMT	C7-C8-C9-C10
29	Z	101	LMG	C18-C19-C20-C21
29	B	622	LMG	C34-C35-C36-C37
32	B	623	LMT	C6-C7-C8-C9
29	C	519	LMG	C11-C12-C13-C14
28	b	623[A]	SQD	C34-C35-C36-C37
35	C	522	HTG	C2'-C3'-C4'-C5'
34	B	621	LHG	C14-C15-C16-C17
28	B	620[B]	SQD	C46-C45-O47-C7
28	B	620[A]	SQD	C46-C45-O47-C7
24	b	611	CLA	C13-C15-C16-C17
29	C	519	LMG	C10-C11-C12-C13
32	M	101	LMT	O5B-C1B-O1B-C4'
28	a	401	SQD	C10-C11-C12-C13
28	a	401	SQD	C26-C27-C28-C29
28	c	518	SQD	C9-C10-C11-C12
28	c	518	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
29	A	1012	LMG	C19-C20-C21-C22
36	C	517	DGD	CCB-CDB-CEB-CFB
34	e	101	LHG	C34-C35-C36-C37
29	Z	101	LMG	C20-C21-C22-C23
29	c	521	LMG	C11-C12-C13-C14
29	C	518	LMG	C19-C20-C21-C22
29	c	519	LMG	C14-C15-C16-C17
28	c	518	SQD	C12-C13-C14-C15
34	d	406	LHG	C11-C12-C13-C14
29	A	1012	LMG	C12-C13-C14-C15
29	a	415	LMG	C29-C30-C31-C32
29	a	415	LMG	C32-C33-C34-C35
29	a	415	LMG	C39-C40-C41-C42
35	o	301	HTG	C3'-C4'-C5'-C6'
29	C	518	LMG	C33-C34-C35-C36
28	A	1011	SQD	C14-C15-C16-C17
24	c	513	CLA	C13-C15-C16-C17
34	e	101	LHG	O2-C2-C3-O3
28	a	401	SQD	C30-C31-C32-C33
32	f	103	LMT	C6-C7-C8-C9
36	c	516	DGD	C4A-C5A-C6A-C7A
36	c	516	DGD	C6A-C7A-C8A-C9A
29	d	409	LMG	C35-C36-C37-C38
34	e	101	LHG	C17-C18-C19-C20
36	C	515	DGD	C5B-C6B-C7B-C8B
34	b	624	LHG	C12-C13-C14-C15
32	b	631	LMT	C5-C6-C7-C8
32	m	103	LMT	C5-C6-C7-C8
26	a	413	BCR	C16-C17-C18-C19
26	K	101	BCR	C20-C21-C22-C23
26	y	101	BCR	C20-C21-C22-C23
32	a	416	LMT	C2'-C1'-O1'-C1
26	k	102	BCR	C16-C17-C18-C19
29	m	102	LMG	C2-C1-O1-C7
26	A	1009	BCR	C16-C17-C18-C19
26	A	1009	BCR	C20-C21-C22-C23
26	k	101	BCR	C20-C21-C22-C23
32	b	631	LMT	C2'-C1'-O1'-C1
26	K	102	BCR	C20-C21-C22-C23
32	A	1018	LMT	C2'-C1'-O1'-C1
26	B	618	BCR	C20-C21-C22-C23
26	C	514	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
36	c	515	DGD	C9A-CAA-CBA-CCA
28	a	401	SQD	C25-C26-C27-C28
28	f	102	SQD	C30-C31-C32-C33
36	c	516	DGD	CAA-CBA-CCA-CDA
34	e	101	LHG	C27-C28-C29-C30
34	E	101	LHG	C25-C26-C27-C28
36	C	515	DGD	CAB-CBB-CCB-CDB
34	d	408	LHG	C31-C32-C33-C34
29	C	519	LMG	C30-C31-C32-C33
28	B	620[B]	SQD	C29-C30-C31-C32
35	V	202	HTG	C3'-C4'-C5'-C6'
29	c	519	LMG	C21-C22-C23-C24
29	c	519	LMG	C33-C34-C35-C36
34	B	621	LHG	C33-C34-C35-C36
24	b	604	CLA	O1A-CGA-O2A-C1
24	b	607	CLA	C16-C17-C18-C19
24	a	409	CLA	C16-C17-C18-C19
24	C	508	CLA	C16-C17-C18-C20
24	b	605	CLA	C16-C17-C18-C19
24	b	616	CLA	C16-C17-C18-C19
24	b	619	CLA	C16-C17-C18-C19
24	c	505	CLA	C4-C3-C5-C6
28	a	401	SQD	C15-C16-C17-C18
34	d	406	LHG	C30-C31-C32-C33
28	f	102	SQD	C24-C25-C26-C27
36	C	516	DGD	C8A-C9A-CAA-CBA
36	c	516	DGD	CBA-CCA-CDA-CEA
36	C	517	DGD	C8B-C9B-CAB-CBB
29	a	415	LMG	C17-C18-C19-C20
29	a	415	LMG	C36-C37-C38-C39
29	d	409	LMG	C29-C30-C31-C32
36	c	517	DGD	C2A-C3A-C4A-C5A
34	e	101	LHG	C15-C16-C17-C18
34	e	101	LHG	C25-C26-C27-C28
29	c	521	LMG	C39-C40-C41-C42
29	B	622	LMG	C21-C22-C23-C24
29	B	622	LMG	C35-C36-C37-C38
29	C	519	LMG	C39-C40-C41-C42
24	c	508	CLA	C11-C10-C8-C9
24	B	614	CLA	C11-C12-C13-C14
24	c	505	CLA	C11-C12-C13-C14
24	B	603	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	A	1011	SQD	C7-C8-C9-C10
36	H	102	DGD	C7A-C8A-C9A-CAA
36	c	517	DGD	C6B-C7B-C8B-C9B
34	e	101	LHG	C24-C25-C26-C27
32	b	625	LMT	C5-C6-C7-C8
35	c	522	HTG	C2'-C3'-C4'-C5'
29	m	102	LMG	C30-C31-C32-C33
34	D	409	LHG	C32-C33-C34-C35
29	C	519	LMG	C37-C38-C39-C40
28	b	623[A]	SQD	C32-C33-C34-C35
24	b	606	CLA	C5-C6-C7-C8
26	k	101	BCR	C11-C12-C13-C35
29	d	409	LMG	C39-C40-C41-C42
36	c	517	DGD	C7A-C8A-C9A-CAA
34	e	101	LHG	C31-C32-C33-C34
29	Z	101	LMG	C37-C38-C39-C40
28	A	1016	SQD	C14-C15-C16-C17
32	t	103	LMT	C7-C8-C9-C10
29	C	519	LMG	C35-C36-C37-C38
28	B	620[A]	SQD	C34-C35-C36-C37
35	B	624	HTG	C1'-C2'-C3'-C4'
33	v	204	GOL	O1-C1-C2-C3
34	d	406	LHG	O1-C1-C2-C3
33	d	417	GOL	O1-C1-C2-C3
34	E	101	LHG	O1-C1-C2-C3
34	d	408	LHG	O1-C1-C2-C3
35	b	630	HTG	C1'-C2'-C3'-C4'
33	a	420	GOL	C1-C2-C3-O3
33	V	204	GOL	C1-C2-C3-O3
34	D	409	LHG	O1-C1-C2-C3
33	D	418	GOL	C1-C2-C3-O3
33	V	207	GOL	O1-C1-C2-C3
26	d	404	BCR	C21-C22-C23-C24
24	B	604	CLA	C3-C5-C6-C7
29	c	519	LMG	O9-C10-O7-C8
24	c	507	CLA	C5-C6-C7-C8
29	c	519	LMG	C11-C10-O7-C8
36	c	515	DGD	C4B-C5B-C6B-C7B
36	h	102	DGD	C6A-C7A-C8A-C9A
34	E	101	LHG	C14-C15-C16-C17
34	E	101	LHG	C30-C31-C32-C33
29	C	518	LMG	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
28	A	1011	SQD	C12-C13-C14-C15
28	A	1011	SQD	C18-C19-C20-C21
28	b	623[B]	SQD	C29-C30-C31-C32
32	A	1017	LMT	C4'-C5'-C6'-O6'
29	C	519	LMG	C28-C29-C30-C31
28	b	623[A]	SQD	C7-C8-C9-C10
36	c	515	DGD	C2B-C3B-C4B-C5B
28	c	518	SQD	C33-C34-C35-C36
36	C	516	DGD	CCA-CDA-CEA-CFA
32	a	416	LMT	C7-C8-C9-C10
36	c	516	DGD	C8A-C9A-CAA-CBA
36	c	516	DGD	C2B-C3B-C4B-C5B
29	a	415	LMG	C15-C16-C17-C18
34	e	101	LHG	C18-C19-C20-C21
35	D	419	HTG	C3'-C4'-C5'-C6'
36	C	515	DGD	C5A-C6A-C7A-C8A
34	b	624	LHG	C11-C10-C9-C8
29	Z	101	LMG	C17-C18-C19-C20
29	Z	101	LMG	C33-C34-C35-C36
28	A	1016	SQD	C27-C28-C29-C30
28	A	1016	SQD	C29-C30-C31-C32
28	A	1016	SQD	C34-C35-C36-C37
29	B	622	LMG	C30-C31-C32-C33
29	D	412	LMG	C35-C36-C37-C38
28	D	408	SQD	C28-C29-C30-C31
34	D	409	LHG	C11-C10-C9-C8
34	D	409	LHG	C25-C26-C27-C28
29	C	518	LMG	C31-C32-C33-C34
29	C	518	LMG	C34-C35-C36-C37
32	B	623	LMT	C11-C10-C9-C8
28	A	1011	SQD	C25-C26-C27-C28
29	c	519	LMG	C11-C12-C13-C14
29	c	519	LMG	C19-C20-C21-C22
29	c	519	LMG	C36-C37-C38-C39
28	b	623[B]	SQD	C15-C16-C17-C18
32	m	103	LMT	C7-C8-C9-C10
34	d	407	LHG	C34-C35-C36-C37
34	B	621	LHG	C13-C14-C15-C16
34	B	621	LHG	C30-C31-C32-C33
29	D	412	LMG	O6-C5-C6-O5
24	b	607	CLA	C16-C17-C18-C20
24	d	403	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
24	B	604	CLA	C16-C17-C18-C19
24	C	507	CLA	C16-C17-C18-C19
24	C	507	CLA	C16-C17-C18-C20
29	m	102	LMG	O6-C1-O1-C7
32	b	631	LMT	O5'-C1'-O1'-C1
34	D	410	LHG	C11-C10-C9-C8
28	c	518	SQD	C16-C17-C18-C19
36	h	102	DGD	C9A-CAA-CBA-CCA
29	A	1012	LMG	C29-C30-C31-C32
34	e	101	LHG	C14-C15-C16-C17
36	C	515	DGD	C8B-C9B-CAB-CBB
29	C	518	LMG	C36-C37-C38-C39
28	A	1011	SQD	C15-C16-C17-C18
35	V	202	HTG	C2'-C3'-C4'-C5'
32	C	520	LMT	C6-C7-C8-C9
36	C	517	DGD	C2A-C3A-C4A-C5A
34	E	101	LHG	C15-C16-C17-C18
29	B	622	LMG	C36-C37-C38-C39
29	B	622	LMG	C38-C39-C40-C41
29	D	412	LMG	C36-C37-C38-C39
28	D	408	SQD	C25-C26-C27-C28
28	A	1011	SQD	C28-C29-C30-C31
28	B	620[B]	SQD	C32-C33-C34-C35
28	B	620[A]	SQD	C12-C13-C14-C15
29	c	519	LMG	C39-C40-C41-C42
34	d	407	LHG	C30-C31-C32-C33
28	c	518	SQD	C23-C24-C25-C26
34	B	621	LHG	C7-C8-C9-C10
24	b	607	CLA	C13-C15-C16-C17
24	a	409	CLA	C13-C15-C16-C17
24	c	509	CLA	C10-C11-C12-C13
24	C	512	CLA	O1A-CGA-O2A-C1
36	C	517	DGD	CAB-CBB-CCB-CDB
29	B	622	LMG	C31-C32-C33-C34
28	B	620[B]	SQD	C24-C25-C26-C27
28	b	623[B]	SQD	C24-C25-C26-C27
28	c	518	SQD	C29-C30-C31-C32
34	d	406	LHG	C25-C26-C27-C28
34	E	101	LHG	C11-C12-C13-C14
29	D	412	LMG	C12-C13-C14-C15
28	B	620[B]	SQD	C11-C12-C13-C14
24	B	604	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	c	514	BCR	C19-C20-C21-C22
32	b	625	LMT	C2-C1-O1'-C1'
36	H	102	DGD	C9B-CAB-CBB-CCB
29	A	1012	LMG	C18-C19-C20-C21
29	A	1012	LMG	C21-C22-C23-C24
29	a	415	LMG	C20-C21-C22-C23
29	d	409	LMG	C13-C14-C15-C16
34	E	101	LHG	C29-C30-C31-C32
36	C	515	DGD	C7B-C8B-C9B-CAB
32	M	101	LMT	C3-C4-C5-C6
34	b	624	LHG	C27-C28-C29-C30
29	D	412	LMG	C18-C19-C20-C21
28	D	408	SQD	C24-C25-C26-C27
34	D	411	LHG	C32-C33-C34-C35
28	b	623[B]	SQD	C9-C10-C11-C12
28	b	623[B]	SQD	C28-C29-C30-C31
24	d	403	CLA	C16-C17-C18-C19
24	C	508	CLA	C16-C17-C18-C19
34	D	410	LHG	C16-C17-C18-C19
36	c	517	DGD	C8A-C9A-CAA-CBA
36	c	517	DGD	C9B-CAB-CBB-CCB
29	c	521	LMG	C19-C20-C21-C22
29	B	622	LMG	C14-C15-C16-C17
28	B	620[A]	SQD	C15-C16-C17-C18
29	c	520	LMG	C31-C32-C33-C34
32	M	101	LMT	O5B-C5B-C6B-O6B
25	D	404	PHO	CBD-CGD-O2D-CED
28	a	401	SQD	C16-C17-C18-C19
36	C	516	DGD	C7A-C8A-C9A-CAA
29	A	1012	LMG	C38-C39-C40-C41
35	b	626	HTG	C3'-C4'-C5'-C6'
29	c	521	LMG	C16-C17-C18-C19
26	k	101	BCR	C14-C15-C16-C17
24	B	616	CLA	C3-C5-C6-C7
32	f	103	LMT	C5-C6-C7-C8
29	Z	101	LMG	C29-C30-C31-C32
24	a	412	CLA	O1A-CGA-O2A-C1
29	A	1012	LMG	C11-C10-O7-C8
28	a	401	SQD	C11-C12-C13-C14
36	C	516	DGD	C3A-C4A-C5A-C6A
29	A	1012	LMG	C32-C33-C34-C35
34	D	411	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
36	C	515	DGD	O6E-C5E-C6E-O5E
32	b	631	LMT	C1-C2-C3-C4
34	d	406	LHG	O1-C1-C2-O2
33	d	415	GOL	O2-C2-C3-O3
33	V	206	GOL	O2-C2-C3-O3
32	A	1017	LMT	C4-C5-C6-C7
36	H	102	DGD	CBA-CCA-CDA-CEA
32	a	416	LMT	C5-C6-C7-C8
29	c	521	LMG	C13-C14-C15-C16
29	c	521	LMG	C18-C19-C20-C21
29	m	102	LMG	C19-C20-C21-C22
29	m	102	LMG	C35-C36-C37-C38
34	D	411	LHG	C29-C30-C31-C32
32	t	103	LMT	C11-C10-C9-C8
29	c	519	LMG	C30-C31-C32-C33
24	B	606	CLA	C16-C17-C18-C19
24	b	616	CLA	C16-C17-C18-C20
29	Z	101	LMG	C16-C17-C18-C19
32	i	102	LMT	C1-C2-C3-C4
28	b	623[A]	SQD	C31-C32-C33-C34
32	C	520	LMT	C1-C2-C3-C4
32	C	520	LMT	C4B-C5B-C6B-O6B
29	d	409	LMG	C14-C15-C16-C17
28	B	620[B]	SQD	C34-C35-C36-C37
35	b	626	HTG	S1-C1'-C2'-C3'
29	c	520	LMG	C28-C29-C30-C31
24	B	613	CLA	C15-C16-C17-C18
34	D	410	LHG	C1-C2-C3-O3
36	h	102	DGD	CAA-CBA-CCA-CDA
29	a	415	LMG	C19-C20-C21-C22
36	c	517	DGD	CBB-CCB-CDB-CEB
34	E	101	LHG	C26-C27-C28-C29
28	A	1011	SQD	C13-C14-C15-C16
29	A	1012	LMG	O9-C10-O7-C8
36	c	515	DGD	O6D-C5D-C6D-O5D
24	C	509	CLA	C2-C1-O2A-CGA
28	c	518	SQD	C14-C15-C16-C17
28	f	102	SQD	C33-C34-C35-C36
36	c	516	DGD	C9A-CAA-CBA-CCA
36	C	515	DGD	C7A-C8A-C9A-CAA
29	c	521	LMG	C36-C37-C38-C39
32	t	103	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
29	C	519	LMG	C31-C32-C33-C34
24	B	611	CLA	C15-C16-C17-C18
28	b	623[A]	SQD	O10-C23-O48-C46
32	B	623	LMT	C1-C2-C3-C4
28	f	102	SQD	C29-C30-C31-C32
29	A	1012	LMG	C34-C35-C36-C37
29	A	1012	LMG	C36-C37-C38-C39
34	e	101	LHG	C26-C27-C28-C29
28	B	620[A]	SQD	C28-C29-C30-C31
34	d	407	LHG	C14-C15-C16-C17
32	A	1018	LMT	C6-C7-C8-C9
24	b	619	CLA	C16-C17-C18-C20
26	K	101	BCR	C1-C6-C7-C8
26	K	101	BCR	C5-C6-C7-C8
26	b	620	BCR	C1-C6-C7-C8
26	b	620	BCR	C5-C6-C7-C8
26	d	404	BCR	C23-C24-C25-C26
26	B	617	BCR	C1-C6-C7-C8
26	B	617	BCR	C5-C6-C7-C8
32	C	520	LMT	C11-C10-C9-C8
34	d	406	LHG	C29-C30-C31-C32
36	c	517	DGD	CBA-CCA-CDA-CEA
34	E	101	LHG	C34-C35-C36-C37
28	b	623[A]	SQD	C30-C31-C32-C33
29	C	518	LMG	C29-C28-O8-C9
24	C	504	CLA	C13-C15-C16-C17
24	C	508	CLA	C13-C15-C16-C17
24	D	405	CLA	C13-C15-C16-C17
36	H	102	DGD	CCA-CDA-CEA-CFA
32	i	102	LMT	C2-C3-C4-C5
29	A	1012	LMG	C37-C38-C39-C40
36	C	517	DGD	C9B-CAB-CBB-CCB
34	e	101	LHG	C29-C30-C31-C32
29	Z	101	LMG	C38-C39-C40-C41
32	t	103	LMT	C3-C4-C5-C6
32	C	520	LMT	C3-C4-C5-C6
36	C	516	DGD	C5B-C6B-C7B-C8B
29	B	622	LMG	C39-C40-C41-C42
24	B	608	CLA	C13-C15-C16-C17
29	Z	101	LMG	C12-C13-C14-C15
28	A	1016	SQD	C15-C16-C17-C18
24	c	510	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	B	611	CLA	C12-C13-C15-C16
24	c	508	CLA	C11-C10-C8-C7
24	B	615	CLA	C12-C13-C15-C16
24	c	513	CLA	C11-C10-C8-C7
24	A	1006	CLA	C6-C7-C8-C10
24	A	1008	CLA	C11-C12-C13-C15
24	B	614	CLA	C11-C12-C13-C15
24	c	505	CLA	C2-C3-C5-C6
24	c	505	CLA	C11-C12-C13-C15
24	C	505	CLA	C11-C12-C13-C15
24	B	604	CLA	C6-C7-C8-C10
24	c	504	CLA	C11-C12-C13-C15
24	c	510	CLA	C2-C3-C5-C6
24	B	603	CLA	C6-C7-C8-C10
24	D	405	CLA	C11-C10-C8-C7
24	B	616	CLA	C11-C12-C13-C15
24	c	513	CLA	C8-C10-C11-C12
24	C	512	CLA	C8-C10-C11-C12
24	C	507	CLA	C5-C6-C7-C8
26	D	406	BCR	C13-C14-C15-C16
26	K	101	BCR	C9-C10-C11-C12
24	c	502	CLA	C16-C17-C18-C19
24	c	513	CLA	C16-C17-C18-C19
24	A	1006	CLA	C16-C17-C18-C20
24	b	618	CLA	C16-C17-C18-C19
25	D	404	PHO	O1D-CGD-O2D-CED
36	C	515	DGD	C3B-C4B-C5B-C6B
24	c	506	CLA	C10-C11-C12-C13
29	D	412	LMG	C20-C21-C22-C23
34	D	411	LHG	C9-C10-C11-C12
34	D	411	LHG	C33-C34-C35-C36
35	C	522	HTG	C1'-C2'-C3'-C4'
36	c	515	DGD	C2A-C3A-C4A-C5A
28	c	518	SQD	C11-C12-C13-C14
36	h	102	DGD	C9B-CAB-CBB-CCB
34	E	101	LHG	C11-C10-C9-C8
28	A	1011	SQD	C33-C34-C35-C36
36	c	516	DGD	C1A-C2A-C3A-C4A
28	c	518	SQD	C34-C35-C36-C37
32	a	416	LMT	C11-C10-C9-C8
29	D	412	LMG	C30-C31-C32-C33
28	D	408	SQD	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
34	D	409	LHG	C29-C30-C31-C32
35	d	410	HTG	C3'-C4'-C5'-C6'
29	c	520	LMG	C37-C38-C39-C40
32	t	103	LMT	C1-C2-C3-C4
34	D	409	LHG	C15-C16-C17-C18
24	b	609	CLA	CBD-CGD-O2D-CED
24	C	502	CLA	C16-C17-C18-C19
24	c	506	CLA	C16-C17-C18-C19
32	f	103	LMT	O5'-C1'-O1'-C1
32	a	416	LMT	O5'-C1'-O1'-C1
24	c	512	CLA	C15-C16-C17-C18
24	b	616	CLA	C8-C10-C11-C12
36	c	515	DGD	CAB-CBB-CCB-CDB
28	f	102	SQD	C32-C33-C34-C35
36	C	516	DGD	C5A-C6A-C7A-C8A
29	m	102	LMG	C29-C30-C31-C32
34	D	411	LHG	C34-C35-C36-C37
28	B	620[A]	SQD	C27-C28-C29-C30
29	c	519	LMG	C18-C19-C20-C21
29	m	102	LMG	C10-C11-C12-C13
34	E	101	LHG	C8-C7-O7-C5
28	A	1011	SQD	C8-C7-O47-C45
36	C	516	DGD	CAA-CBA-CCA-CDA
29	A	1012	LMG	C20-C21-C22-C23
35	d	410	HTG	C2'-C3'-C4'-C5'
32	t	103	LMT	C4'-C5'-C6'-O6'
29	C	519	LMG	C4-C5-C6-O5
32	a	402	LMT	C1-C2-C3-C4
24	C	503	CLA	C8-C10-C11-C12
36	H	102	DGD	CCB-CDB-CEB-CFB
34	b	624	LHG	C14-C15-C16-C17
28	B	620[A]	SQD	C16-C17-C18-C19
28	A	1011	SQD	O49-C7-O47-C45
24	c	513	CLA	C3-C5-C6-C7
24	a	412	CLA	C3-C5-C6-C7
24	a	412	CLA	O1D-CGD-O2D-CED
32	f	103	LMT	C2'-C1'-O1'-C1
34	e	101	LHG	O7-C5-C6-O8
32	A	1018	LMT	O5B-C5B-C6B-O6B
28	a	401	SQD	C32-C33-C34-C35
36	H	102	DGD	C5B-C6B-C7B-C8B
29	Z	101	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
24	a	409	CLA	C16-C17-C18-C20
28	a	401	SQD	C31-C32-C33-C34
28	D	408	SQD	C27-C28-C29-C30
28	b	623[B]	SQD	C17-C18-C19-C20
29	c	520	LMG	C38-C39-C40-C41
24	c	503	CLA	C8-C10-C11-C12
24	C	505	CLA	C13-C15-C16-C17
24	B	603	CLA	C5-C6-C7-C8
27	A	1010	PL9	C4-C3-C7-C8
28	A	1016	SQD	C24-C25-C26-C27
24	c	502	CLA	C11-C12-C13-C14
24	B	615	CLA	C14-C13-C15-C16
24	b	614	CLA	C14-C13-C15-C16
24	A	1006	CLA	C6-C7-C8-C9
24	C	512	CLA	C14-C13-C15-C16
24	b	615	CLA	C14-C13-C15-C16
24	C	505	CLA	C11-C12-C13-C14
24	B	604	CLA	C6-C7-C8-C9
24	B	604	CLA	C11-C12-C13-C14
24	b	606	CLA	C6-C7-C8-C9
24	D	405	CLA	C11-C10-C8-C9
24	B	616	CLA	C11-C12-C13-C14
24	b	619	CLA	C11-C12-C13-C14
24	b	619	CLA	C14-C13-C15-C16
24	b	604	CLA	C11-C10-C8-C9
24	a	412	CLA	C11-C12-C13-C14
24	a	412	CLA	C14-C13-C15-C16
29	m	102	LMG	C16-C17-C18-C19
34	E	101	LHG	C13-C14-C15-C16
29	m	102	LMG	C33-C34-C35-C36
36	c	515	DGD	O6E-C5E-C6E-O5E
29	C	518	LMG	C15-C16-C17-C18
32	b	631	LMT	C7-C8-C9-C10
29	c	520	LMG	C33-C34-C35-C36
29	C	518	LMG	O10-C28-O8-C9
24	C	503	CLA	C1A-C2A-CAA-CBA
24	c	508	CLA	C1A-C2A-CAA-CBA
24	C	506	CLA	C1A-C2A-CAA-CBA
24	c	506	CLA	C1A-C2A-CAA-CBA
24	b	605	CLA	C16-C17-C18-C20
24	b	618	CLA	C16-C17-C18-C20
36	c	515	DGD	C8A-C9A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	f	102	SQD	C34-C35-C36-C37
28	b	623[A]	SQD	C10-C11-C12-C13
26	b	621	BCR	C19-C20-C21-C22
34	D	410	LHG	C34-C35-C36-C37
28	a	401	SQD	C28-C29-C30-C31
29	d	409	LMG	C38-C39-C40-C41
32	M	101	LMT	C7-C8-C9-C10
34	d	408	LHG	C17-C18-C19-C20
29	a	415	LMG	C10-C11-C12-C13
34	b	624	LHG	C7-C8-C9-C10
24	b	615	CLA	C8-C10-C11-C12
24	a	412	CLA	C13-C15-C16-C17
29	m	102	LMG	C34-C35-C36-C37
29	c	520	LMG	C30-C31-C32-C33
28	f	102	SQD	C26-C27-C28-C29
29	D	412	LMG	C17-C18-C19-C20
32	b	625	LMT	C1-C2-C3-C4
29	c	520	LMG	C4-C5-C6-O5
34	d	408	LHG	C9-C10-C11-C12
36	C	515	DGD	O6D-C5D-C6D-O5D
34	D	410	LHG	C10-C11-C12-C13
29	B	622	LMG	C12-C13-C14-C15
28	A	1011	SQD	C9-C10-C11-C12
32	f	103	LMT	C1-C2-C3-C4
36	c	516	DGD	C8B-C9B-CAB-CBB
29	C	519	LMG	C34-C35-C36-C37
32	C	520	LMT	C5-C6-C7-C8
24	c	505	CLA	C15-C16-C17-C18
24	c	507	CLA	C16-C17-C18-C19
28	c	518	SQD	C19-C20-C21-C22
29	A	1012	LMG	C7-C8-C9-O8
34	E	101	LHG	C4-C5-C6-O8
29	C	519	LMG	C7-C8-C9-O8
28	b	623[A]	SQD	C44-C45-C46-O48
29	c	519	LMG	C7-C8-C9-O8
29	c	520	LMG	C7-C8-C9-O8
24	c	509	CLA	C15-C16-C17-C18
36	h	102	DGD	CCB-CDB-CEB-CFB
36	H	102	DGD	CDB-CEB-CFB-CGB
29	c	519	LMG	C17-C18-C19-C20
36	C	516	DGD	C2G-C3G-O3G-C1D
36	C	516	DGD	C5D-C6D-O5D-C1E

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Mol	Chain	Res	Type	Atoms
36	c	516	DGD	C2G-C3G-O3G-C1D
36	c	516	DGD	C5D-C6D-O5D-C1E
29	C	519	LMG	C8-C7-O1-C1
26	h	101	BCR	C14-C15-C16-C17
36	c	517	DGD	CDB-CEB-CFB-CGB
29	D	412	LMG	C21-C22-C23-C24
28	D	408	SQD	C35-C36-C37-C38
29	c	519	LMG	C31-C32-C33-C34
32	t	103	LMT	O5'-C5'-C6'-O6'
36	h	102	DGD	C7A-C8A-C9A-CAA
32	a	416	LMT	C9-C10-C11-C12
36	H	102	DGD	O2G-C1B-C2B-C3B
29	A	1012	LMG	C10-C11-C12-C13
34	d	408	LHG	C29-C30-C31-C32
28	B	620[A]	SQD	C35-C36-C37-C38
36	h	102	DGD	CDB-CEB-CFB-CGB
33	a	420	GOL	O2-C2-C3-O3
33	V	207	GOL	O1-C1-C2-O2
29	d	409	LMG	C19-C20-C21-C22
29	C	518	LMG	C40-C41-C42-C43
28	b	623[A]	SQD	C35-C36-C37-C38
28	b	623[B]	SQD	C33-C34-C35-C36
29	a	415	LMG	C13-C14-C15-C16
29	B	622	LMG	C15-C16-C17-C18
29	B	622	LMG	C40-C41-C42-C43
28	A	1011	SQD	C10-C11-C12-C13
24	B	615	CLA	C10-C11-C12-C13
29	C	519	LMG	C40-C41-C42-C43
34	d	406	LHG	C7-C8-C9-C10
36	c	516	DGD	C1B-C2B-C3B-C4B
34	E	101	LHG	C23-C24-C25-C26
24	b	604	CLA	C16-C17-C18-C20
36	c	517	DGD	CDA-CEA-CFA-CGA
24	c	509	CLA	C8-C10-C11-C12
34	D	411	LHG	C35-C36-C37-C38
28	B	620[A]	SQD	C18-C19-C20-C21
24	c	509	CLA	C2-C1-O2A-CGA
36	C	515	DGD	C4A-C5A-C6A-C7A
34	D	411	LHG	C28-C29-C30-C31
24	C	512	CLA	O1D-CGD-O2D-CED
36	c	515	DGD	CCB-CDB-CEB-CFB
36	C	516	DGD	C8B-C9B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	A	1016	SQD	C18-C19-C20-C21
34	B	621	LHG	C12-C13-C14-C15
32	m	103	LMT	C1-C2-C3-C4
24	d	403	CLA	C10-C11-C12-C13
34	E	101	LHG	C35-C36-C37-C38
34	b	624	LHG	C28-C29-C30-C31
34	b	624	LHG	C32-C33-C34-C35
29	c	521	LMG	C34-C35-C36-C37
24	c	513	CLA	C16-C17-C18-C20
24	b	606	CLA	C16-C17-C18-C20
24	c	506	CLA	C16-C17-C18-C20
28	A	1016	SQD	C16-C17-C18-C19
34	D	409	LHG	C9-C10-C11-C12
28	b	623[B]	SQD	C35-C36-C37-C38
29	C	518	LMG	C22-C23-C24-C25
32	B	623	LMT	O5B-C1B-O1B-C4'
24	c	503	CLA	O1D-CGD-O2D-CED
24	c	509	CLA	O1D-CGD-O2D-CED
36	C	516	DGD	C7B-C8B-C9B-CAB
36	C	517	DGD	CBB-CCB-CDB-CEB
28	A	1011	SQD	C35-C36-C37-C38
36	C	516	DGD	C2E-C1E-O5D-C6D
32	M	101	LMT	C2'-C1'-O1'-C1
26	J	101	BCR	C20-C21-C22-C23
32	m	103	LMT	C2'-C1'-O1'-C1
29	a	415	LMG	O7-C8-C9-O8
29	Z	101	LMG	O7-C8-C9-O8
29	C	519	LMG	O7-C8-C9-O8
28	b	623[B]	SQD	O6-C44-C45-O47
29	c	520	LMG	O7-C8-C9-O8
34	E	101	LHG	O9-C7-O7-C5
29	c	521	LMG	C40-C41-C42-C43
29	A	1012	LMG	C30-C31-C32-C33
24	b	617	CLA	C6-C7-C8-C10
24	c	512	CLA	C11-C10-C8-C7
24	b	614	CLA	C12-C13-C15-C16
24	d	403	CLA	C12-C13-C15-C16
24	a	409	CLA	C6-C7-C8-C10
24	C	508	CLA	C11-C12-C13-C15
24	b	615	CLA	C12-C13-C15-C16
24	b	616	CLA	C11-C10-C8-C7
24	B	604	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	c	504	CLA	C12-C13-C15-C16
24	d	402	CLA	C11-C12-C13-C15
24	C	507	CLA	C11-C12-C13-C15
24	b	619	CLA	C11-C12-C13-C15
24	b	619	CLA	C12-C13-C15-C16
34	D	409	LHG	C10-C11-C12-C13
28	b	623[A]	SQD	C17-C18-C19-C20
24	b	617	CLA	C14-C13-C15-C16
24	B	611	CLA	C14-C13-C15-C16
24	C	506	CLA	C14-C13-C15-C16
24	c	513	CLA	C11-C10-C8-C9
24	a	409	CLA	C6-C7-C8-C9
24	a	409	CLA	C11-C10-C8-C9
24	A	1008	CLA	C11-C12-C13-C14
24	C	512	CLA	C11-C10-C8-C9
24	C	508	CLA	C11-C10-C8-C9
24	B	614	CLA	C14-C13-C15-C16
24	b	616	CLA	C11-C10-C8-C9
24	D	405	CLA	C6-C7-C8-C9
24	D	405	CLA	C14-C13-C15-C16
24	B	616	CLA	C14-C13-C15-C16
24	C	511	CLA	C6-C7-C8-C9
34	d	406	LHG	C34-C35-C36-C37
36	H	102	DGD	C7B-C8B-C9B-CAB
28	B	620[B]	SQD	C19-C20-C21-C22
34	B	621	LHG	C17-C18-C19-C20
28	a	401	SQD	C24-C23-O48-C46
35	V	202	HTG	C4'-C5'-C6'-C7'
36	c	515	DGD	C4D-C5D-C6D-O5D
24	c	502	CLA	C16-C17-C18-C20
24	C	502	CLA	C16-C17-C18-C20
35	o	301	HTG	C4'-C5'-C6'-C7'
32	B	623	LMT	C3'-C4'-O1B-C1B
28	A	1011	SQD	C19-C20-C21-C22
26	y	101	BCR	C11-C12-C13-C14
26	k	101	BCR	C7-C8-C9-C10
28	f	102	SQD	C11-C10-C9-C8
29	B	622	LMG	C20-C21-C22-C23
24	c	511	CLA	CBA-CGA-O2A-C1
28	c	518	SQD	C17-C18-C19-C20
25	D	404	PHO	C2C-C3C-CAC-CBC
24	C	513	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
32	i	102	LMT	C4B-C5B-C6B-O6B
29	B	622	LMG	C37-C38-C39-C40
34	d	407	LHG	C12-C13-C14-C15
24	b	604	CLA	C8-C10-C11-C12
28	f	102	SQD	C27-C28-C29-C30
29	a	415	LMG	C38-C39-C40-C41
34	D	409	LHG	C24-C25-C26-C27
28	B	620[A]	SQD	C17-C18-C19-C20
29	c	521	LMG	C28-C29-C30-C31
34	D	409	LHG	C7-C8-C9-C10
36	c	516	DGD	C6B-C7B-C8B-C9B
35	d	416	HTG	C1'-C2'-C3'-C4'
28	A	1016	SQD	C19-C20-C21-C22
28	D	408	SQD	C31-C32-C33-C34
24	B	603	CLA	C16-C17-C18-C20
35	B	624	HTG	C2'-C3'-C4'-C5'
29	a	415	LMG	C22-C23-C24-C25
32	t	103	LMT	C2B-C1B-O1B-C4'
24	b	608	CLA	CBA-CGA-O2A-C1
36	c	517	DGD	C2A-C1A-O1G-C1G
29	c	520	LMG	C29-C28-O8-C9
34	D	409	LHG	C23-C24-C25-C26
29	A	1012	LMG	C16-C17-C18-C19
29	d	409	LMG	C34-C35-C36-C37
32	m	103	LMT	C4-C5-C6-C7
24	C	501	CLA	O1D-CGD-O2D-CED
35	B	628	HTG	C4'-C5'-C6'-C7'
34	B	621	LHG	C10-C11-C12-C13
26	t	101	BCR	C19-C20-C21-C22
26	k	101	BCR	C15-C16-C17-C18
26	h	101	BCR	C9-C10-C11-C12
32	b	631	LMT	C2-C1-O1'-C1'
32	M	102	LMT	C2-C1-O1'-C1'
34	E	101	LHG	C19-C20-C21-C22
29	Z	101	LMG	C13-C14-C15-C16
29	m	102	LMG	C12-C13-C14-C15
28	A	1011	SQD	C11-C10-C9-C8
28	B	620[A]	SQD	C24-C25-C26-C27
32	a	416	LMT	C4B-C5B-C6B-O6B
34	d	408	LHG	C28-C29-C30-C31
24	c	507	CLA	C16-C17-C18-C20
24	D	405	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	C	503	CLA	CBA-CGA-O2A-C1
24	b	618	CLA	C10-C11-C12-C13
34	e	101	LHG	C4-C5-C6-O8
29	Z	101	LMG	C7-C8-C9-O8
28	A	1016	SQD	O6-C44-C45-C46
29	C	519	LMG	O1-C7-C8-C9
29	c	519	LMG	O1-C7-C8-C9
36	c	515	DGD	C5B-C6B-C7B-C8B
36	h	102	DGD	CCA-CDA-CEA-CFA
36	C	515	DGD	CCA-CDA-CEA-CFA
32	t	103	LMT	O5B-C1B-O1B-C4'
24	b	609	CLA	O1D-CGD-O2D-CED
32	t	103	LMT	C4-C5-C6-C7
25	a	410	PHO	C8-C10-C11-C12
34	d	406	LHG	C24-C25-C26-C27
24	B	613	CLA	C3-C5-C6-C7
24	b	604	CLA	C3-C5-C6-C7
29	c	521	LMG	C31-C32-C33-C34
28	D	408	SQD	C30-C31-C32-C33
25	a	410	PHO	C4-C3-C5-C6
24	C	510	CLA	C4-C3-C5-C6
36	c	515	DGD	CDA-CEA-CFA-CGA
29	m	102	LMG	C37-C38-C39-C40
29	B	622	LMG	C22-C23-C24-C25
32	B	623	LMT	C9-C10-C11-C12
34	D	410	LHG	C4-O6-P-O3
34	d	407	LHG	C4-O6-P-O3
28	D	408	SQD	C7-C8-C9-C10
36	c	515	DGD	CBB-CCB-CDB-CEB
34	D	410	LHG	C12-C13-C14-C15
35	b	630	HTG	C4-C5-C6-O6
33	v	203	GOL	O2-C2-C3-O3
36	C	515	DGD	C9A-CAA-CBA-CCA
32	a	402	LMT	C4-C5-C6-C7
28	B	620[A]	SQD	C26-C27-C28-C29
24	B	604	CLA	O1D-CGD-O2D-CED
36	C	516	DGD	C1A-C2A-C3A-C4A
29	B	622	LMG	C10-C11-C12-C13
29	a	415	LMG	C14-C15-C16-C17
28	B	620[B]	SQD	C10-C11-C12-C13
32	M	102	LMT	C3-C4-C5-C6
32	f	103	LMT	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
34	d	406	LHG	C17-C18-C19-C20
32	B	623	LMT	C5'-C4'-O1B-C1B
28	B	620[B]	SQD	C14-C15-C16-C17
34	E	101	LHG	C31-C32-C33-C34
29	c	521	LMG	O1-C7-C8-O7
29	c	519	LMG	O1-C7-C8-O7
29	c	519	LMG	O7-C8-C9-O8
26	y	101	BCR	C15-C16-C17-C18
26	H	101	BCR	C15-C16-C17-C18
26	h	101	BCR	C19-C20-C21-C22
24	b	604	CLA	C16-C17-C18-C19
34	D	411	LHG	C17-C18-C19-C20
28	f	102	SQD	O5-C1-O6-C44
32	A	1018	LMT	O5'-C1'-O1'-C1
24	b	606	CLA	C13-C15-C16-C17
34	d	406	LHG	C1-C2-C3-O3
27	A	1010	PL9	C19-C21-C22-C23
27	a	414	PL9	C14-C16-C17-C18
27	a	414	PL9	C19-C21-C22-C23
27	d	405	PL9	C39-C41-C42-C43
36	h	102	DGD	C5B-C6B-C7B-C8B
36	h	102	DGD	CBB-CCB-CDB-CEB
29	C	518	LMG	C13-C14-C15-C16
24	D	402	CLA	C2-C1-O2A-CGA
24	b	617	CLA	C6-C7-C8-C9
24	c	508	CLA	C11-C12-C13-C14
24	C	506	CLA	C6-C7-C8-C9
24	C	506	CLA	C11-C12-C13-C14
24	A	1006	CLA	C11-C10-C8-C9
24	c	507	CLA	C11-C10-C8-C9
24	C	508	CLA	C14-C13-C15-C16
24	c	510	CLA	C6-C7-C8-C9
24	d	402	CLA	C11-C12-C13-C14
35	C	521	HTG	C2'-C3'-C4'-C5'
29	d	409	LMG	C17-C18-C19-C20
34	D	409	LHG	C33-C34-C35-C36
28	A	1011	SQD	C34-C35-C36-C37
24	b	608	CLA	C13-C15-C16-C17
28	a	401	SQD	O10-C23-O48-C46
34	d	406	LHG	C18-C19-C20-C21
34	D	409	LHG	C34-C35-C36-C37
24	b	617	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
24	B	601	CLA	C16-C17-C18-C20
26	K	101	BCR	C23-C24-C25-C30
26	y	101	BCR	C5-C6-C7-C8
26	d	404	BCR	C23-C24-C25-C30
26	b	621	BCR	C23-C24-C25-C30
26	h	101	BCR	C23-C24-C25-C26
24	C	509	CLA	C13-C15-C16-C17
26	K	102	BCR	C7-C8-C9-C34
36	C	515	DGD	C8A-C9A-CAA-CBA
28	b	623[A]	SQD	C26-C27-C28-C29
26	D	406	BCR	C21-C22-C23-C24
36	C	515	DGD	C4D-C5D-C6D-O5D
26	D	406	BCR	C14-C15-C16-C17
34	B	621	LHG	C28-C29-C30-C31
24	c	510	CLA	C8-C10-C11-C12
36	C	516	DGD	CDA-CEA-CFA-CGA
24	b	606	CLA	C16-C17-C18-C19
24	C	504	CLA	C3-C5-C6-C7
29	Z	101	LMG	C4-C5-C6-O5
34	b	624	LHG	C17-C18-C19-C20
24	c	511	CLA	O1A-CGA-O2A-C1
29	A	1012	LMG	C13-C14-C15-C16
29	d	409	LMG	C30-C31-C32-C33
24	C	506	CLA	C10-C11-C12-C13
34	b	624	LHG	O6-C4-C5-C6
29	C	518	LMG	C35-C36-C37-C38
25	a	410	PHO	C2-C3-C5-C6
24	b	617	CLA	C12-C13-C15-C16
24	C	504	CLA	C6-C7-C8-C10
24	c	508	CLA	C11-C12-C13-C15
24	C	506	CLA	C6-C7-C8-C10
24	C	506	CLA	C11-C12-C13-C15
24	B	606	CLA	C11-C10-C8-C7
24	d	403	CLA	C11-C12-C13-C15
24	A	1006	CLA	C11-C10-C8-C7
24	a	409	CLA	C11-C10-C8-C7
24	c	507	CLA	C11-C10-C8-C7
24	C	512	CLA	C11-C10-C8-C7
24	C	508	CLA	C11-C10-C8-C7
24	C	508	CLA	C12-C13-C15-C16
24	B	614	CLA	C12-C13-C15-C16
24	c	504	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
24	C	513	CLA	C6-C7-C8-C10
24	b	609	CLA	C11-C10-C8-C7
24	D	405	CLA	C6-C7-C8-C10
24	D	405	CLA	C12-C13-C15-C16
24	B	616	CLA	C12-C13-C15-C16
24	C	507	CLA	C12-C13-C15-C16
24	b	604	CLA	C6-C7-C8-C10
24	c	506	CLA	C11-C12-C13-C15
35	c	525	HTG	S1-C1'-C2'-C3'
28	a	401	SQD	C9-C10-C11-C12
28	b	623[B]	SQD	C26-C27-C28-C29
26	H	101	BCR	C9-C10-C11-C12
26	k	102	BCR	C9-C10-C11-C12
26	k	101	BCR	C9-C10-C11-C12
26	B	618	BCR	C15-C16-C17-C18
24	c	508	CLA	C16-C17-C18-C20
34	d	406	LHG	C23-C24-C25-C26
29	D	412	LMG	C40-C41-C42-C43
35	B	624	HTG	O5-C1-S1-C1'
35	B	624	HTG	C2'-C1'-S1-C1
26	J	101	BCR	C20-C21-C22-C37
35	C	522	HTG	O5-C1-S1-C1'
29	d	409	LMG	C10-C11-C12-C13
29	Z	101	LMG	C40-C41-C42-C43
29	B	622	LMG	C28-C29-C30-C31
35	C	521	HTG	C3'-C4'-C5'-C6'
36	c	516	DGD	C3B-C4B-C5B-C6B
34	b	624	LHG	C30-C31-C32-C33
32	A	1017	LMT	C11-C10-C9-C8
28	b	623[B]	SQD	C30-C31-C32-C33
24	A	1005	CLA	CAD-CBD-CGD-O2D
24	b	607	CLA	CAD-CBD-CGD-O2D
29	c	521	LMG	C7-C8-O7-C10
24	B	610	CLA	CAD-CBD-CGD-O2D
25	A	1007	PHO	CAD-CBD-CGD-O2D
28	b	623[B]	SQD	C46-C45-O47-C7
24	b	604	CLA	CAD-CBD-CGD-O2D
36	c	517	DGD	CAA-CBA-CCA-CDA
28	B	620[A]	SQD	C11-C10-C9-C8
24	C	504	CLA	C15-C16-C17-C18
24	C	510	CLA	C8-C10-C11-C12
35	b	626	HTG	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
36	c	516	DGD	CBB-CCB-CDB-CEB
36	C	516	DGD	O6E-C1E-O5D-C6D
32	M	101	LMT	O5'-C1'-O1'-C1
28	b	623[A]	SQD	C19-C20-C21-C22
32	M	102	LMT	C7-C8-C9-C10
28	a	401	SQD	O6-C44-C45-C46
34	d	408	LHG	C2-C3-O3-P
29	c	521	LMG	O1-C7-C8-C9
28	D	408	SQD	C44-C45-C46-O48
34	D	411	LHG	C2-C3-O3-P
24	C	503	CLA	O1A-CGA-O2A-C1
34	d	408	LHG	C34-C35-C36-C37
28	A	1016	SQD	C26-C27-C28-C29
34	d	407	LHG	C26-C27-C28-C29
28	A	1011	SQD	C30-C31-C32-C33
28	B	620[A]	SQD	C32-C33-C34-C35
34	D	411	LHG	C24-C23-O8-C6
24	B	601	CLA	C15-C16-C17-C18
24	c	506	CLA	C13-C15-C16-C17
36	H	102	DGD	C2B-C3B-C4B-C5B
32	B	623	LMT	C3-C4-C5-C6
28	B	620[B]	SQD	C15-C16-C17-C18
34	B	621	LHG	C11-C10-C9-C8
34	B	621	LHG	C11-C12-C13-C14
24	c	502	CLA	CHA-CBD-CGD-O2D
24	B	607	CLA	CHA-CBD-CGD-O2D
24	B	606	CLA	CHA-CBD-CGD-O2D
24	B	602	CLA	CHA-CBD-CGD-O2D
24	c	507	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O2D
24	C	502	CLA	CHA-CBD-CGD-O1D
24	D	403	CLA	CHA-CBD-CGD-O2D
24	c	506	CLA	CHA-CBD-CGD-O1D
24	b	608	CLA	O1A-CGA-O2A-C1
26	T	101	BCR	C20-C21-C22-C23
26	t	101	BCR	C20-C21-C22-C23
36	c	516	DGD	C2E-C1E-O5D-C6D
34	E	101	LHG	O7-C5-C6-O8
34	d	407	LHG	C28-C29-C30-C31
32	a	416	LMT	C4'-C5'-C6'-O6'
36	c	517	DGD	O1A-C1A-O1G-C1G
29	c	520	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
34	B	621	LHG	C25-C26-C27-C28
35	D	413	HTG	C1'-C2'-C3'-C4'
33	A	1019	GOL	O2-C2-C3-O3
33	d	417	GOL	O1-C1-C2-O2
29	d	409	LMG	C21-C22-C23-C24
34	E	101	LHG	C28-C29-C30-C31
29	c	519	LMG	C10-C11-C12-C13
24	C	510	CLA	C2-C3-C5-C6
24	B	605	CLA	O1D-CGD-O2D-CED
27	a	414	PL9	C4-C3-C7-C8
28	a	401	SQD	O49-C7-O47-C45
32	A	1018	LMT	C1-C2-C3-C4
24	c	505	CLA	C14-C13-C15-C16
24	c	504	CLA	C11-C10-C8-C9
24	C	513	CLA	C6-C7-C8-C9
24	c	506	CLA	C11-C12-C13-C14
34	D	410	LHG	C32-C33-C34-C35
29	Z	101	LMG	C22-C23-C24-C25
35	D	413	HTG	O5-C5-C6-O6
24	C	511	CLA	CBA-CGA-O2A-C1
26	b	621	BCR	C37-C22-C23-C24
26	h	101	BCR	C37-C22-C23-C24
33	b	632	GOL	O1-C1-C2-C3
33	V	206	GOL	O1-C1-C2-C3
24	b	617	CLA	CBD-CGD-O2D-CED
29	D	412	LMG	C22-C23-C24-C25
26	k	101	BCR	C11-C12-C13-C14
36	c	516	DGD	C4B-C5B-C6B-C7B
29	C	519	LMG	C32-C33-C34-C35
35	b	601	HTG	O5-C5-C6-O6
24	c	512	CLA	C1A-C2A-CAA-CBA
24	c	503	CLA	C1A-C2A-CAA-CBA
24	B	612	CLA	C8-C10-C11-C12
36	c	516	DGD	C3A-C4A-C5A-C6A
29	C	518	LMG	C18-C19-C20-C21
28	b	623[B]	SQD	C25-C26-C27-C28
29	c	520	LMG	C40-C41-C42-C43
36	H	102	DGD	CDA-CEA-CFA-CGA
36	c	516	DGD	CAB-CBB-CCB-CDB
34	D	410	LHG	C4-O6-P-O5
34	d	407	LHG	C4-O6-P-O5
24	B	611	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
24	C	505	CLA	C16-C17-C18-C20
24	D	405	CLA	C16-C17-C18-C20
32	M	102	LMT	C9-C10-C11-C12
35	b	630	HTG	S1-C1'-C2'-C3'
24	b	605	CLA	C3-C5-C6-C7
24	b	616	CLA	C3-C5-C6-C7
24	b	617	CLA	C10-C11-C12-C13
36	h	102	DGD	C6B-C7B-C8B-C9B
36	C	515	DGD	CBB-CCB-CDB-CEB
24	D	402	CLA	C16-C17-C18-C20
35	D	413	HTG	C3'-C4'-C5'-C6'
36	C	515	DGD	C6B-C7B-C8B-C9B
24	c	502	CLA	CAD-CBD-CGD-O1D
24	C	504	CLA	CAD-CBD-CGD-O1D
28	f	102	SQD	C5-C6-S-O7
24	b	608	CLA	CAD-CBD-CGD-O1D
24	B	605	CLA	CAD-CBD-CGD-O1D
24	b	612	CLA	CAD-CBD-CGD-O1D
24	C	502	CLA	CAD-CBD-CGD-O1D
24	b	604	CLA	CAD-CBD-CGD-O1D
24	C	501	CLA	C13-C15-C16-C17
28	f	102	SQD	C31-C32-C33-C34
34	b	624	LHG	C31-C32-C33-C34
35	d	416	HTG	S1-C1'-C2'-C3'
34	D	410	LHG	C26-C27-C28-C29
28	a	401	SQD	C18-C19-C20-C21
29	c	520	LMG	O6-C5-C6-O5
36	c	516	DGD	C2A-C3A-C4A-C5A
29	a	415	LMG	C12-C13-C14-C15
28	a	401	SQD	C23-C24-C25-C26
24	b	617	CLA	C11-C10-C8-C7
24	B	615	CLA	C11-C10-C8-C7
24	c	513	CLA	C6-C7-C8-C10
24	c	513	CLA	C11-C12-C13-C15
24	A	1006	CLA	C12-C13-C15-C16
24	c	507	CLA	C11-C12-C13-C15
24	C	512	CLA	C11-C12-C13-C15
24	c	505	CLA	C12-C13-C15-C16
24	C	505	CLA	C12-C13-C15-C16
35	C	522	HTG	C2-C1-S1-C1'
24	C	507	CLA	C6-C7-C8-C10
24	b	604	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	a	412	CLA	C11-C10-C8-C7
24	c	506	CLA	C11-C10-C8-C7
29	m	102	LMG	C13-C14-C15-C16
25	a	411	PHO	C2C-C3C-CAC-CBC
34	D	411	LHG	O10-C23-O8-C6
36	C	517	DGD	C7A-C8A-C9A-CAA
35	o	301	HTG	C4-C5-C6-O6
28	b	623[B]	SQD	O6-C44-C45-C46
29	A	1012	LMG	O7-C8-C9-O8
28	D	408	SQD	O47-C45-C46-O48
28	B	620[A]	SQD	O6-C44-C45-O47
28	b	623[B]	SQD	C11-C10-C9-C8
36	h	102	DGD	CBA-CCA-CDA-CEA
29	C	518	LMG	C32-C33-C34-C35
24	B	601	CLA	C16-C17-C18-C19
24	B	603	CLA	C16-C17-C18-C19
24	B	614	CLA	C13-C15-C16-C17
24	b	618	CLA	C13-C15-C16-C17
24	C	511	CLA	O1A-CGA-O2A-C1
27	A	1010	PL9	C15-C14-C16-C17
24	C	504	CLA	C6-C7-C8-C9
24	C	504	CLA	C11-C12-C13-C14
24	B	606	CLA	C11-C10-C8-C9
24	d	403	CLA	C14-C13-C15-C16
24	b	609	CLA	C11-C10-C8-C9
29	c	519	LMG	C32-C33-C34-C35
29	c	519	LMG	C34-C35-C36-C37
27	D	407	PL9	C39-C41-C42-C43
33	b	632	GOL	O1-C1-C2-O2
33	v	204	GOL	O1-C1-C2-O2
34	E	101	LHG	O1-C1-C2-O2
24	D	403	CLA	C2C-C3C-CAC-CBC
24	b	617	CLA	C16-C17-C18-C19
24	b	615	CLA	C16-C17-C18-C20
28	b	623[A]	SQD	C14-C15-C16-C17
35	B	628	HTG	C1'-C2'-C3'-C4'
36	h	102	DGD	O2G-C1B-C2B-C3B
35	D	413	HTG	C2'-C3'-C4'-C5'
32	A	1017	LMT	C3-C4-C5-C6
29	Z	101	LMG	C36-C37-C38-C39
32	i	102	LMT	O5B-C5B-C6B-O6B
34	E	101	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
28	A	1016	SQD	C35-C36-C37-C38
28	D	408	SQD	C11-C10-C9-C8
36	c	515	DGD	CAA-CBA-CCA-CDA
24	B	601	CLA	C2-C1-O2A-CGA
24	d	402	CLA	C2-C1-O2A-CGA
24	B	616	CLA	C2-C1-O2A-CGA
24	c	508	CLA	C16-C17-C18-C19
36	h	102	DGD	CDA-CEA-CFA-CGA
29	B	622	LMG	O8-C28-C29-C30
34	d	408	LHG	C11-C10-C9-C8
29	B	622	LMG	C13-C14-C15-C16
28	D	408	SQD	C33-C34-C35-C36
24	c	512	CLA	O1A-CGA-O2A-C1
34	b	624	LHG	O6-C4-C5-O7
36	C	517	DGD	CBA-CCA-CDA-CEA
34	e	101	LHG	C33-C34-C35-C36
24	b	618	CLA	C5-C6-C7-C8
32	t	103	LMT	C9-C10-C11-C12
35	b	601	HTG	C1'-C2'-C3'-C4'
24	C	510	CLA	C16-C17-C18-C19
24	d	402	CLA	C16-C17-C18-C20
28	a	401	SQD	C8-C7-O47-C45
36	c	516	DGD	O6E-C1E-O5D-C6D
35	D	413	HTG	C4'-C5'-C6'-C7'
32	M	102	LMT	O1'-C1-C2-C3
29	A	1012	LMG	O1-C7-C8-O7
28	b	623[A]	SQD	O47-C45-C46-O48
32	f	103	LMT	C11-C10-C9-C8
36	c	515	DGD	CDB-CEB-CFB-CGB
24	a	412	CLA	C10-C11-C12-C13
24	b	616	CLA	C15-C16-C17-C18
29	a	415	LMG	C40-C41-C42-C43
29	m	102	LMG	C21-C22-C23-C24
29	a	415	LMG	C7-C8-C9-O8
29	c	519	LMG	C12-C13-C14-C15
24	b	613	CLA	C15-C16-C17-C18
24	A	1008	CLA	C13-C15-C16-C17
24	C	504	CLA	C11-C12-C13-C15
24	d	403	CLA	C6-C7-C8-C10
24	C	511	CLA	C6-C7-C8-C10
32	B	623	LMT	C2B-C1B-O1B-C4'
28	A	1016	SQD	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
34	d	408	LHG	C12-C13-C14-C15
29	C	519	LMG	C36-C37-C38-C39
32	A	1018	LMT	C5-C6-C7-C8
24	b	617	CLA	C11-C10-C8-C9
24	b	617	CLA	C11-C12-C13-C14
24	c	512	CLA	C11-C10-C8-C9
24	C	512	CLA	C11-C12-C13-C14
24	C	508	CLA	C11-C12-C13-C14
24	C	505	CLA	C14-C13-C15-C16
24	C	507	CLA	C11-C12-C13-C14
24	b	604	CLA	C6-C7-C8-C9
24	a	412	CLA	C11-C10-C8-C9
24	B	610	CLA	C10-C11-C12-C13
26	d	404	BCR	C19-C20-C21-C22
24	c	510	CLA	C16-C17-C18-C19
34	D	409	LHG	C11-C12-C13-C14
35	b	602	HTG	C4-C5-C6-O6
24	c	512	CLA	CBA-CGA-O2A-C1
24	D	405	CLA	O1A-CGA-O2A-C1
36	c	517	DGD	C9A-CAA-CBA-CCA
24	D	402	CLA	C16-C17-C18-C19
24	C	505	CLA	C16-C17-C18-C19
34	E	101	LHG	C16-C17-C18-C19
33	v	204	GOL	C1-C2-C3-O3
34	E	101	LHG	C2-C3-O3-P
28	A	1011	SQD	C16-C17-C18-C19
24	B	611	CLA	C16-C17-C18-C19
24	C	512	CLA	C16-C17-C18-C20
24	D	405	CLA	CBA-CGA-O2A-C1
24	c	510	CLA	O1A-CGA-O2A-C1
36	H	102	DGD	O1B-C1B-C2B-C3B
29	Z	101	LMG	C32-C33-C34-C35
36	c	515	DGD	O6E-C1E-O5D-C6D
28	a	401	SQD	O5-C1-O6-C44
32	b	625	LMT	O5'-C1'-O1'-C1
28	A	1016	SQD	O5-C1-O6-C44
32	M	101	LMT	C1-C2-C3-C4
34	D	409	LHG	C26-C27-C28-C29
34	B	621	LHG	C34-C35-C36-C37
24	C	501	CLA	C15-C16-C17-C18
36	c	517	DGD	C6A-C7A-C8A-C9A
28	A	1016	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
29	C	518	LMG	C12-C13-C14-C15
26	b	621	BCR	C18-C19-C20-C21
24	C	513	CLA	C16-C17-C18-C19
34	D	409	LHG	C30-C31-C32-C33
24	C	507	CLA	C4-C3-C5-C6
28	A	1016	SQD	O49-C7-O47-C45
28	a	401	SQD	C34-C35-C36-C37
24	C	507	CLA	C8-C10-C11-C12
36	c	515	DGD	C2E-C1E-O5D-C6D
28	a	401	SQD	C2-C1-O6-C44
34	D	411	LHG	C27-C28-C29-C30
28	b	623[B]	SQD	O47-C45-C46-O48
34	d	406	LHG	C26-C27-C28-C29
36	H	102	DGD	CBB-CCB-CDB-CEB
25	D	404	PHO	C4C-C3C-CAC-CBC
24	c	512	CLA	C3A-C2A-CAA-CBA
36	C	515	DGD	C6A-C7A-C8A-C9A
24	b	608	CLA	C4-C3-C5-C6
34	d	406	LHG	C31-C32-C33-C34
36	C	515	DGD	C2A-C3A-C4A-C5A
24	B	615	CLA	C11-C10-C8-C9
24	b	613	CLA	C11-C12-C13-C14
24	c	504	CLA	C14-C13-C15-C16
24	b	615	CLA	C16-C17-C18-C19
24	b	610	CLA	CBA-CGA-O2A-C1
35	c	525	HTG	C4'-C5'-C6'-C7'
36	h	102	DGD	O1G-C1G-C2G-C3G
24	B	602	CLA	C3-C5-C6-C7
29	m	102	LMG	C14-C15-C16-C17
24	d	402	CLA	C16-C17-C18-C19
36	C	515	DGD	O6E-C1E-O5D-C6D
34	b	624	LHG	C33-C34-C35-C36
26	K	102	BCR	C7-C8-C9-C10
28	f	102	SQD	C25-C26-C27-C28
24	c	513	CLA	C1A-C2A-CAA-CBA
24	C	513	CLA	C1A-C2A-CAA-CBA
24	c	510	CLA	CBA-CGA-O2A-C1
32	t	103	LMT	C4B-C5B-C6B-O6B
24	B	601	CLA	C6-C7-C8-C10
24	c	509	CLA	C6-C7-C8-C10
24	D	402	CLA	C11-C12-C13-C15
24	B	610	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	c	510	CLA	C6-C7-C8-C10
24	b	606	CLA	C11-C10-C8-C7
24	B	616	CLA	C11-C10-C8-C7
32	b	625	LMT	C2-C3-C4-C5
24	d	403	CLA	C15-C16-C17-C18
28	A	1016	SQD	C28-C29-C30-C31
29	D	412	LMG	C38-C39-C40-C41
35	c	525	HTG	C4-C5-C6-O6
29	Z	101	LMG	C30-C31-C32-C33
34	D	410	LHG	O6-C4-C5-C6
34	e	101	LHG	O6-C4-C5-C6
34	d	407	LHG	O6-C4-C5-C6
24	C	502	CLA	C15-C16-C17-C18
24	B	613	CLA	C10-C11-C12-C13
28	B	620[B]	SQD	C23-C24-C25-C26
28	c	518	SQD	O49-C7-O47-C45
29	C	519	LMG	O1-C7-C8-O7
29	Z	101	LMG	C31-C32-C33-C34
35	b	602	HTG	C1'-C2'-C3'-C4'
26	t	101	BCR	C9-C10-C11-C12
26	J	101	BCR	C13-C14-C15-C16
34	B	621	LHG	C18-C19-C20-C21
32	A	1017	LMT	C4B-C5B-C6B-O6B
36	c	516	DGD	C7A-C8A-C9A-CAA
24	B	616	CLA	C10-C11-C12-C13
24	b	610	CLA	O1A-CGA-O2A-C1
27	A	1010	PL9	C9-C11-C12-C13
28	c	518	SQD	C15-C16-C17-C18
36	C	516	DGD	CCB-CDB-CEB-CFB
35	b	630	HTG	C2'-C3'-C4'-C5'
24	B	610	CLA	C2A-CAA-CBA-CGA
26	y	101	BCR	C1-C6-C7-C8
26	H	101	BCR	C23-C24-C25-C26
26	H	101	BCR	C23-C24-C25-C30
26	c	514	BCR	C23-C24-C25-C30
26	J	101	BCR	C1-C6-C7-C8
26	h	101	BCR	C23-C24-C25-C30
24	B	601	CLA	CAA-CBA-CGA-O2A
24	b	604	CLA	CAA-CBA-CGA-O2A
29	A	1012	LMG	O1-C7-C8-C9
34	d	407	LHG	C32-C33-C34-C35
34	d	407	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
26	d	404	BCR	C15-C16-C17-C18
28	b	623[A]	SQD	C15-C16-C17-C18
24	C	510	CLA	C16-C17-C18-C20
24	c	510	CLA	C16-C17-C18-C20
24	C	508	CLA	C15-C16-C17-C18
36	c	517	DGD	C4A-C5A-C6A-C7A
27	A	1010	PL9	C13-C14-C16-C17
36	H	102	DGD	C9A-CAA-CBA-CCA
29	D	412	LMG	C8-C7-O1-C1
28	b	623[A]	SQD	C45-C44-O6-C1
24	C	511	CLA	C8-C10-C11-C12
24	B	615	CLA	C8-C10-C11-C12
28	b	623[B]	SQD	C32-C33-C34-C35
32	i	102	LMT	C9-C10-C11-C12
29	c	521	LMG	C12-C13-C14-C15
29	d	409	LMG	C4-C5-C6-O5
24	B	602	CLA	C8-C10-C11-C12
34	b	624	LHG	C11-C12-C13-C14
24	b	617	CLA	C11-C12-C13-C15
24	A	1008	CLA	C11-C10-C8-C7
33	V	204	GOL	O2-C2-C3-O3
28	c	518	SQD	C10-C11-C12-C13
32	b	625	LMT	C2'-C1'-O1'-C1
28	A	1016	SQD	C2-C1-O6-C44
34	e	101	LHG	C1-C2-C3-O3
28	B	620[B]	SQD	O47-C45-C46-O48
36	C	515	DGD	O2G-C1B-C2B-C3B
29	c	519	LMG	C35-C36-C37-C38
24	C	512	CLA	C16-C17-C18-C19
26	c	514	BCR	C20-C21-C22-C37
28	B	620[A]	SQD	O48-C23-C24-C25
28	B	620[A]	SQD	C31-C32-C33-C34
24	A	1008	CLA	C15-C16-C17-C18
35	c	525	HTG	C2'-C3'-C4'-C5'
24	C	512	CLA	CAA-CBA-CGA-O2A
24	c	512	CLA	C14-C13-C15-C16
24	c	513	CLA	C6-C7-C8-C9
24	d	403	CLA	C11-C12-C13-C14
24	c	507	CLA	C11-C12-C13-C14
24	c	504	CLA	C6-C7-C8-C9
24	b	606	CLA	C11-C10-C8-C9
24	C	507	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	b	604	CLA	C11-C12-C13-C14
24	c	506	CLA	C11-C10-C8-C9
36	C	516	DGD	C6A-C7A-C8A-C9A
32	B	623	LMT	O5'-C5'-C6'-O6'
36	C	516	DGD	CAB-CBB-CCB-CDB
24	B	612	CLA	O1A-CGA-O2A-C1
36	c	517	DGD	O6D-C5D-C6D-O5D
29	C	518	LMG	C39-C40-C41-C42
24	B	601	CLA	CAD-CBD-CGD-O2D
24	c	512	CLA	CAD-CBD-CGD-O2D
24	d	403	CLA	CAD-CBD-CGD-O2D
24	b	613	CLA	CAD-CBD-CGD-O2D
24	c	509	CLA	CAD-CBD-CGD-O2D
24	C	512	CLA	CAD-CBD-CGD-O2D
24	b	612	CLA	CAD-CBD-CGD-O2D
24	b	615	CLA	CAD-CBD-CGD-O2D
24	a	407	CLA	CAD-CBD-CGD-O2D
24	C	501	CLA	CAD-CBD-CGD-O2D
24	C	505	CLA	CAD-CBD-CGD-O2D
24	B	604	CLA	CAD-CBD-CGD-O2D
24	c	510	CLA	CAD-CBD-CGD-O2D
24	B	603	CLA	CAD-CBD-CGD-O2D
24	C	509	CLA	CAD-CBD-CGD-O2D
24	D	405	CLA	CAD-CBD-CGD-O2D
24	B	616	CLA	CAD-CBD-CGD-O2D
24	b	619	CLA	CAD-CBD-CGD-O2D
28	f	102	SQD	C7-C8-C9-C10
34	B	621	LHG	C9-C10-C11-C12
34	d	408	LHG	C32-C33-C34-C35
32	A	1018	LMT	C5'-C4'-O1B-C1B
28	B	620[B]	SQD	C18-C19-C20-C21
28	B	620[A]	SQD	C11-C12-C13-C14
28	b	623[A]	SQD	C33-C34-C35-C36
36	C	517	DGD	O1G-C1A-C2A-C3A
29	a	415	LMG	O7-C10-C11-C12
28	c	518	SQD	C25-C26-C27-C28
32	a	402	LMT	C5-C6-C7-C8
32	f	103	LMT	C3-C4-C5-C6
29	Z	101	LMG	O8-C28-C29-C30
34	b	624	LHG	C16-C17-C18-C19
28	B	620[A]	SQD	O6-C44-C45-C46
28	b	623[B]	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
28	B	620[A]	SQD	C19-C20-C21-C22
29	c	521	LMG	O8-C28-C29-C30
25	a	410	PHO	O2A-C1-C2-C3
24	b	607	CLA	O2A-C1-C2-C3
24	d	403	CLA	O2A-C1-C2-C3
24	d	402	CLA	O2A-C1-C2-C3
24	B	612	CLA	CBA-CGA-O2A-C1
24	C	507	CLA	C2A-CAA-CBA-CGA
24	B	605	CLA	C13-C15-C16-C17
24	C	513	CLA	C16-C17-C18-C20
24	b	617	CLA	CHA-CBD-CGD-O2D
24	C	504	CLA	CHA-CBD-CGD-O1D
24	C	504	CLA	CHA-CBD-CGD-O2D
24	a	408	CLA	CHA-CBD-CGD-O2D
24	b	608	CLA	CHA-CBD-CGD-O1D
26	H	101	BCR	C13-C14-C15-C16
24	A	1006	CLA	CHA-CBD-CGD-O2D
24	a	409	CLA	CHA-CBD-CGD-O2D
24	B	602	CLA	CHA-CBD-CGD-O1D
24	c	507	CLA	CHA-CBD-CGD-O2D
24	c	509	CLA	CHA-CBD-CGD-O1D
24	B	614	CLA	CHA-CBD-CGD-O2D
24	b	605	CLA	CHA-CBD-CGD-O2D
25	a	411	PHO	CHA-CBD-CGD-O1D
24	c	504	CLA	CHA-CBD-CGD-O2D
25	D	404	PHO	CHA-CBD-CGD-O1D
25	D	404	PHO	CHA-CBD-CGD-O2D
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D
28	b	623[B]	SQD	C27-C28-C29-C30
32	M	102	LMT	O5'-C5'-C6'-O6'
24	B	610	CLA	C15-C16-C17-C18
36	c	516	DGD	O2G-C1B-C2B-C3B
34	D	410	LHG	C30-C31-C32-C33
29	c	520	LMG	C12-C13-C14-C15
29	m	102	LMG	O1-C7-C8-O7
28	B	620[B]	SQD	O6-C44-C45-O47
28	B	620[A]	SQD	C7-C8-C9-C10
32	i	102	LMT	C5-C6-C7-C8
24	c	504	CLA	C15-C16-C17-C18
24	C	507	CLA	C15-C16-C17-C18
28	a	401	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
34	b	624	LHG	C29-C30-C31-C32
29	D	412	LMG	C34-C35-C36-C37
32	M	101	LMT	C4-C5-C6-C7
28	f	102	SQD	O47-C7-C8-C9
24	c	512	CLA	CAA-CBA-CGA-O2A
36	h	102	DGD	CAB-CBB-CCB-CDB
24	C	512	CLA	C2C-C3C-CAC-CBC
32	B	623	LMT	C2-C3-C4-C5
24	B	611	CLA	C2-C3-C5-C6
24	c	512	CLA	C12-C13-C15-C16
24	d	403	CLA	C11-C10-C8-C7
24	A	1006	CLA	C11-C12-C13-C15
24	C	502	CLA	C11-C12-C13-C15
24	c	504	CLA	C6-C7-C8-C10
24	b	613	CLA	C16-C17-C18-C19
29	C	518	LMG	C29-C30-C31-C32
24	c	512	CLA	C11-C12-C13-C14
24	c	513	CLA	C11-C12-C13-C14
24	d	403	CLA	C6-C7-C8-C9
24	A	1006	CLA	C14-C13-C15-C16
24	C	502	CLA	C11-C12-C13-C14
24	B	616	CLA	C11-C10-C8-C9
36	C	515	DGD	O1B-C1B-C2B-C3B
24	a	412	CLA	C5-C6-C7-C8
29	Z	101	LMG	O10-C28-C29-C30
28	c	518	SQD	C5-C6-S-O8
28	f	102	SQD	C5-C6-S-O8
32	A	1017	LMT	C9-C10-C11-C12
28	c	518	SQD	C8-C7-O47-C45
28	A	1016	SQD	C8-C7-O47-C45
36	C	515	DGD	O1G-C1A-C2A-C3A
36	h	102	DGD	C7B-C8B-C9B-CAB
26	b	622	BCR	C37-C22-C23-C24
24	C	512	CLA	CAA-CBA-CGA-O1A
24	b	613	CLA	C16-C17-C18-C20
33	A	1019	GOL	C1-C2-C3-O3
33	v	203	GOL	C1-C2-C3-O3
28	B	620[A]	SQD	O10-C23-C24-C25
34	d	406	LHG	C9-C10-C11-C12
28	A	1016	SQD	C24-C23-O48-C46
29	A	1012	LMG	C40-C41-C42-C43
36	C	517	DGD	O1A-C1A-C2A-C3A

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Mol	Chain	Res	Type	Atoms
29	c	521	LMG	O10-C28-C29-C30
24	b	615	CLA	O1A-CGA-O2A-C1
28	f	102	SQD	C24-C23-O48-C46
29	m	102	LMG	O1-C7-C8-C9
28	B	620[B]	SQD	O6-C44-C45-C46
28	B	620[B]	SQD	C44-C45-C46-O48
28	A	1016	SQD	O10-C23-O48-C46
24	c	501	CLA	C13-C15-C16-C17
29	B	622	LMG	O9-C10-O7-C8
29	a	415	LMG	O9-C10-C11-C12
24	b	608	CLA	C2-C3-C5-C6
24	C	507	CLA	C2-C3-C5-C6
36	C	515	DGD	C2E-C1E-O5D-C6D
36	h	102	DGD	O1G-C1G-C2G-O2G
34	E	101	LHG	O7-C7-C8-C9
26	c	514	BCR	C16-C17-C18-C36
26	b	621	BCR	C20-C21-C22-C37
34	B	621	LHG	O6-C4-C5-C6
26	K	101	BCR	C23-C24-C25-C26
26	T	101	BCR	C1-C6-C7-C8
26	T	101	BCR	C5-C6-C7-C8
26	J	101	BCR	C5-C6-C7-C8
26	C	514	BCR	C23-C24-C25-C30
24	C	507	CLA	C10-C11-C12-C13
24	b	610	CLA	C16-C17-C18-C20
28	f	102	SQD	O10-C23-O48-C46
29	A	1012	LMG	C33-C34-C35-C36
36	c	517	DGD	O1G-C1A-C2A-C3A
28	f	102	SQD	O49-C7-C8-C9
24	C	513	CLA	C4-C3-C5-C6
36	H	102	DGD	C3B-C4B-C5B-C6B
27	a	414	PL9	C36-C37-C38-C39
24	a	408	CLA	C15-C16-C17-C18
28	a	401	SQD	C5-C6-S-O9
28	c	518	SQD	C5-C6-S-O7
28	c	518	SQD	C5-C6-S-O9
24	B	607	CLA	CAD-CBD-CGD-O1D
24	A	1006	CLA	CAD-CBD-CGD-O1D
24	c	504	CLA	CAD-CBD-CGD-O1D
24	B	609	CLA	CAD-CBD-CGD-O1D
24	b	610	CLA	CAD-CBD-CGD-O1D
24	c	512	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
34	d	407	LHG	C11-C10-C9-C8
24	c	513	CLA	C5-C6-C7-C8
24	d	403	CLA	C11-C10-C8-C9
24	A	1008	CLA	C11-C10-C8-C9
24	b	616	CLA	C11-C12-C13-C14
24	B	610	CLA	C11-C12-C13-C14
24	B	603	CLA	C11-C12-C13-C14
28	c	518	SQD	O47-C7-C8-C9
24	c	505	CLA	CAA-CBA-CGA-O2A
29	B	622	LMG	C33-C34-C35-C36
24	C	501	CLA	C2A-CAA-CBA-CGA
29	A	1012	LMG	C22-C23-C24-C25
28	D	408	SQD	C29-C30-C31-C32
29	m	102	LMG	O7-C10-C11-C12
28	D	408	SQD	O47-C7-C8-C9
36	c	515	DGD	O1B-C1B-C2B-C3B
36	C	515	DGD	O1A-C1A-C2A-C3A
24	b	615	CLA	C10-C11-C12-C13
35	d	416	HTG	C2-C1-S1-C1'
24	c	512	CLA	C11-C12-C13-C15
24	c	509	CLA	C11-C10-C8-C7
24	B	610	CLA	C12-C13-C15-C16
24	C	509	CLA	C11-C10-C8-C7
36	c	516	DGD	O1B-C1B-C2B-C3B
36	c	515	DGD	O2G-C1B-C2B-C3B
36	C	516	DGD	O2G-C1B-C2B-C3B
24	c	501	CLA	CAA-CBA-CGA-O2A
34	d	408	LHG	O8-C23-C24-C25
34	D	411	LHG	O8-C23-C24-C25
24	C	501	CLA	CAA-CBA-CGA-O2A
36	C	516	DGD	O1B-C1B-C2B-C3B
34	d	408	LHG	O10-C23-C24-C25
28	D	408	SQD	O49-C7-C8-C9
24	c	505	CLA	CAA-CBA-CGA-O1A
32	A	1018	LMT	C2-C1-O1'-C1'
24	C	510	CLA	CAA-CBA-CGA-O2A
29	D	412	LMG	O7-C10-C11-C12
24	B	612	CLA	C10-C11-C12-C13
24	c	501	CLA	CAA-CBA-CGA-O1A
35	V	202	HTG	C4-C5-C6-O6
27	d	405	PL9	C11-C12-C13-C14
29	c	521	LMG	C35-C36-C37-C38

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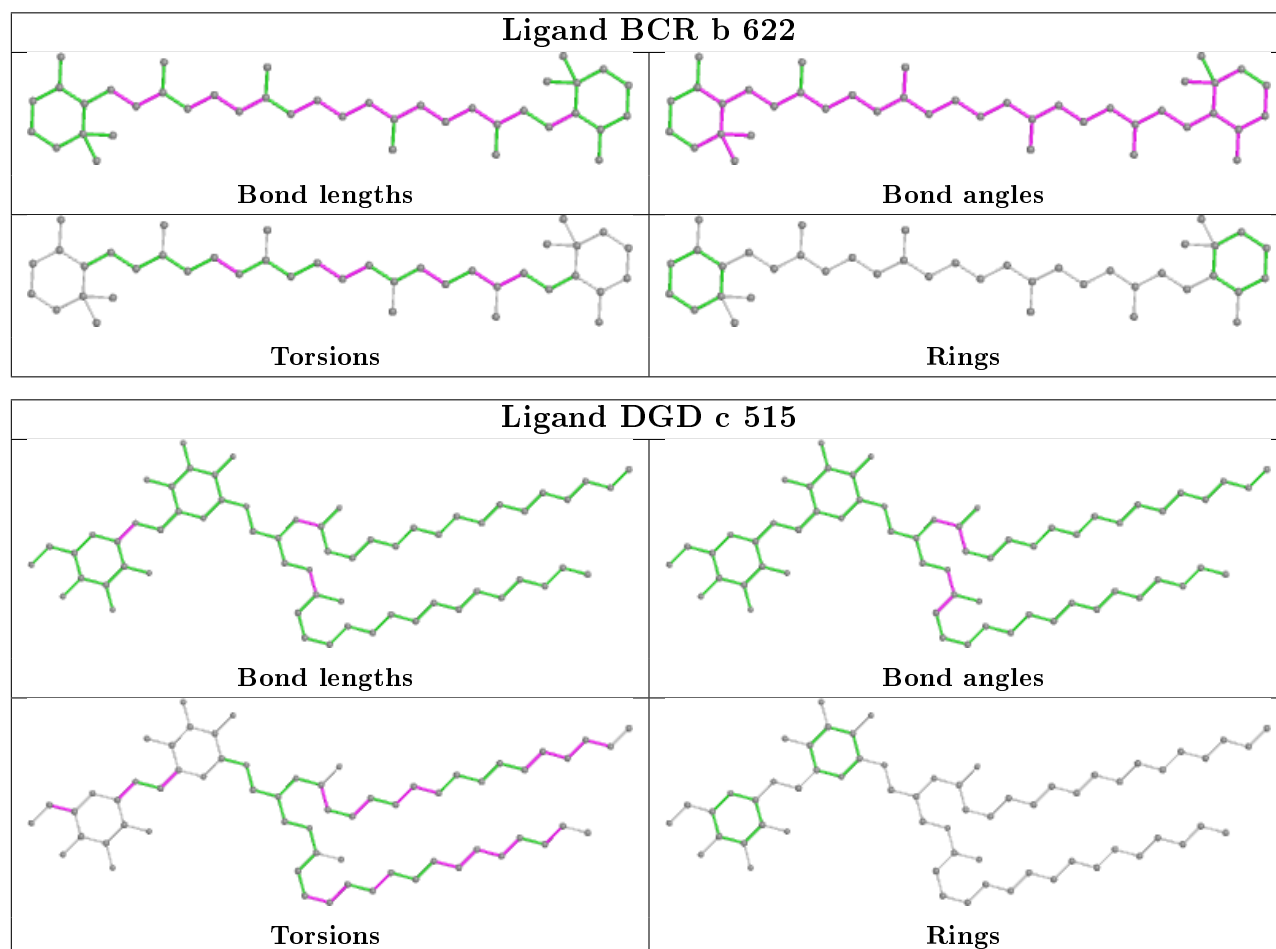
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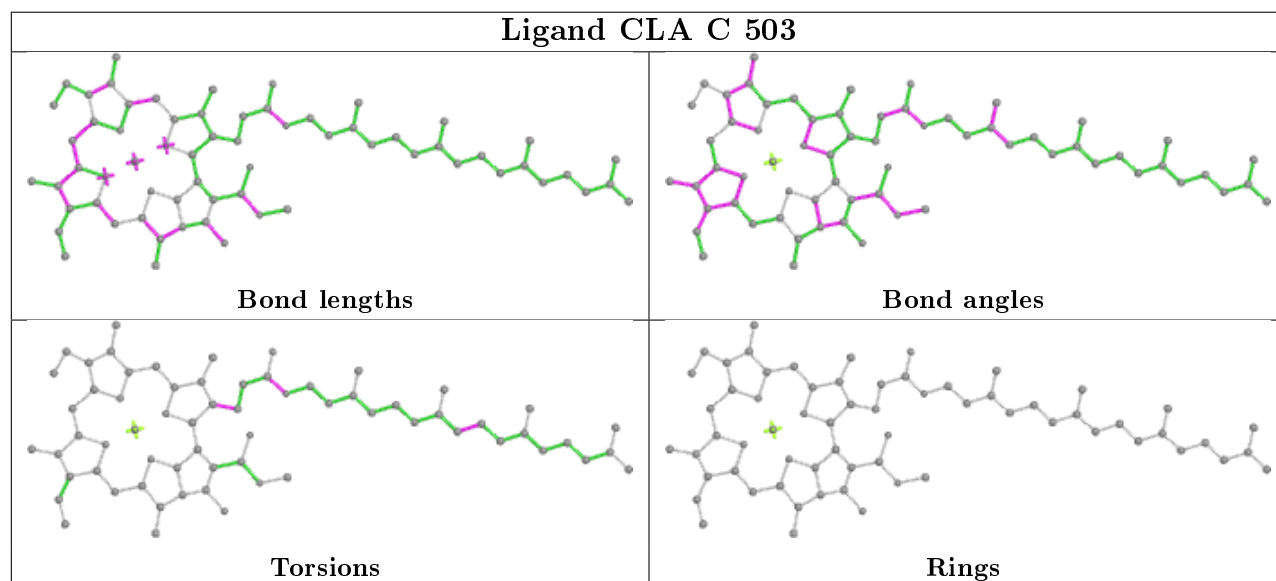
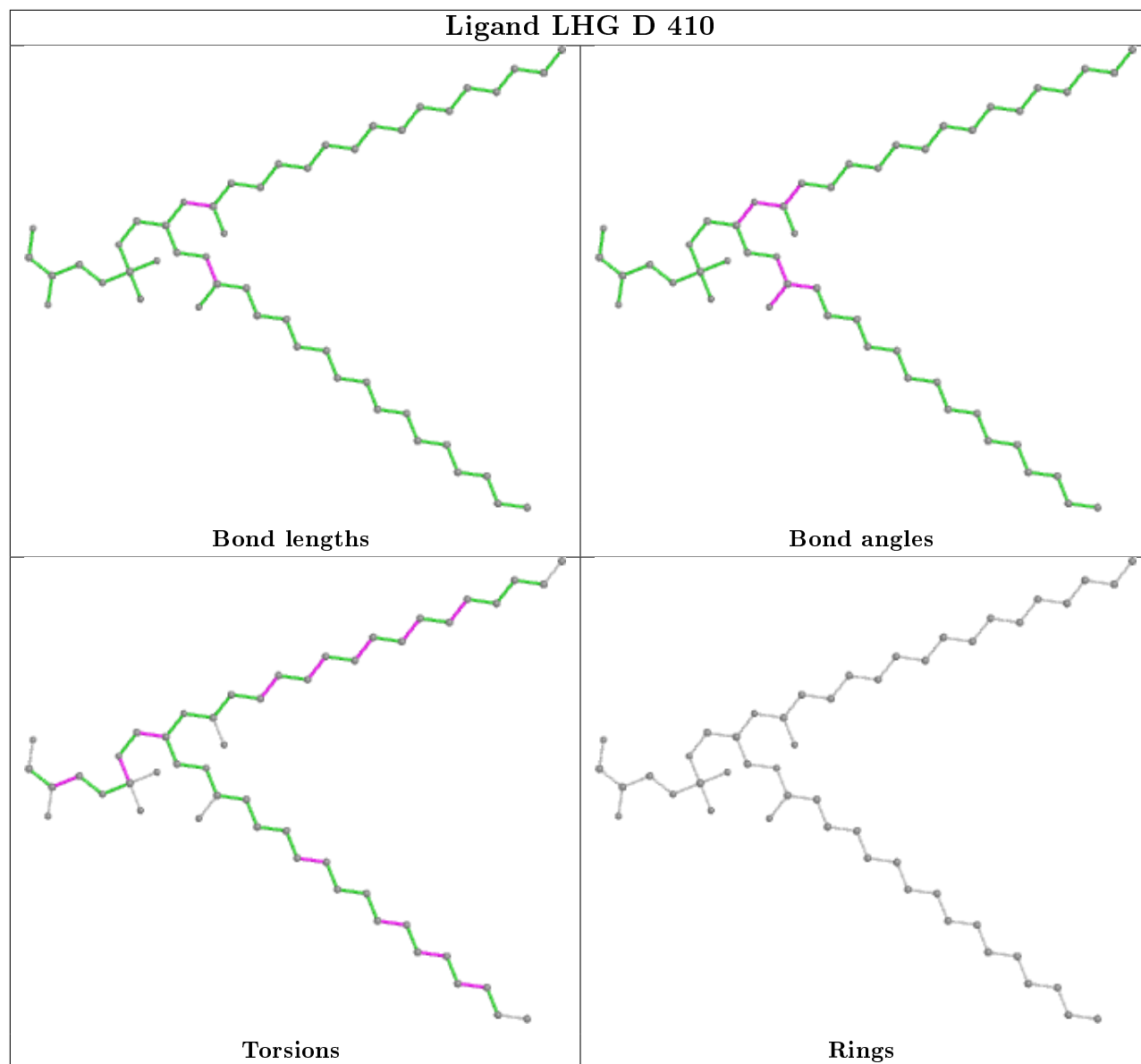
Mol	Chain	Res	Type	Atoms
24	D	403	CLA	C15-C16-C17-C18
24	B	611	CLA	C4-C3-C5-C6

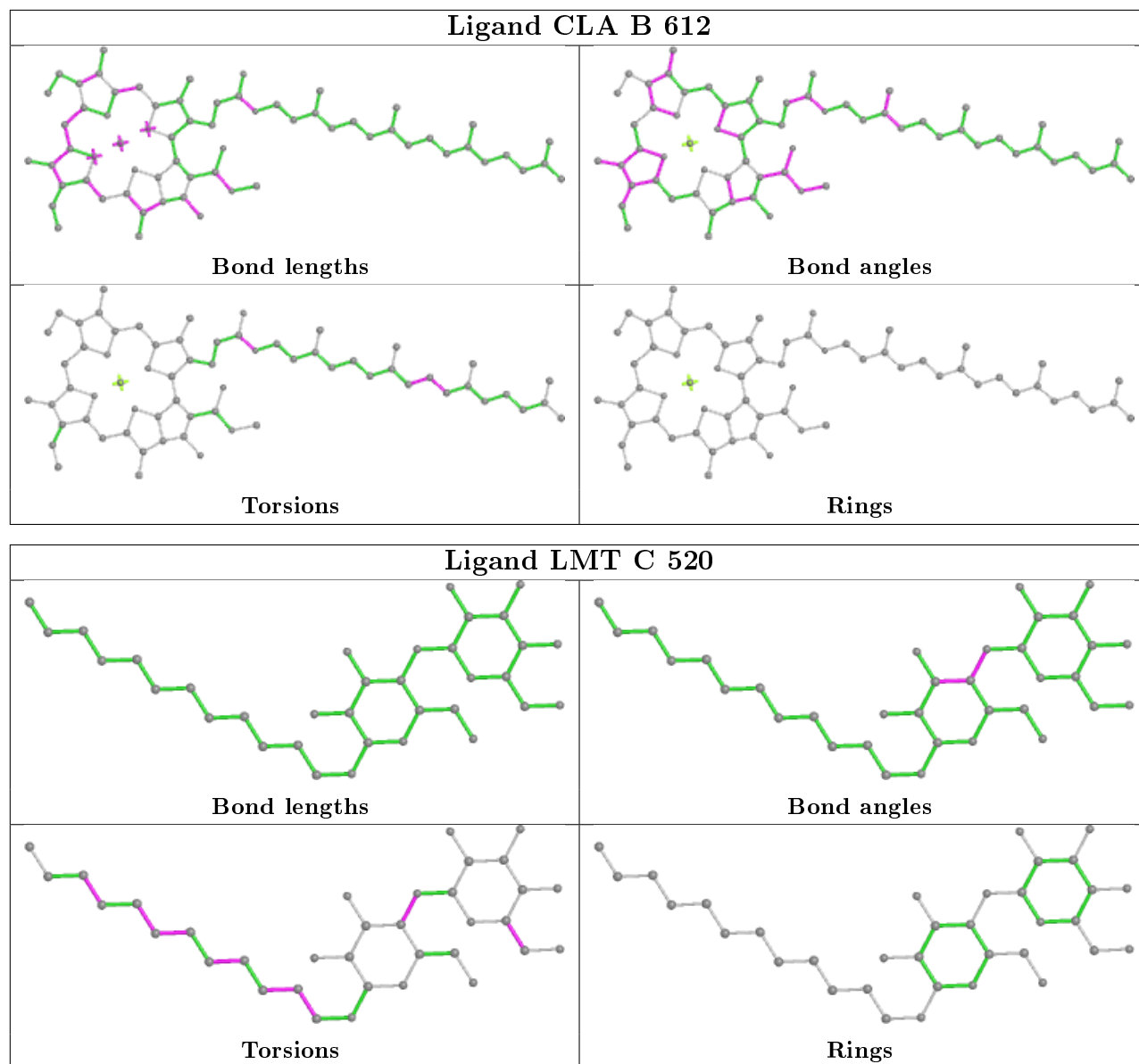
There are no ring outliers.

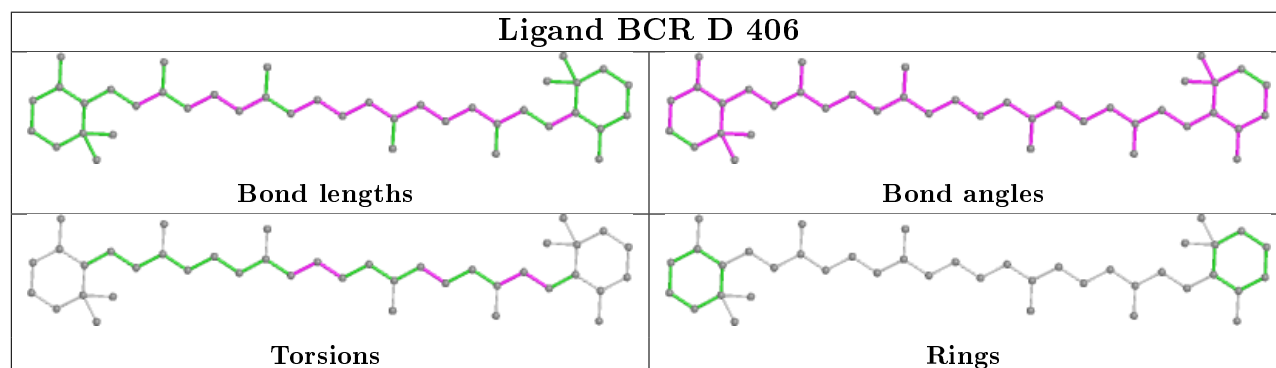
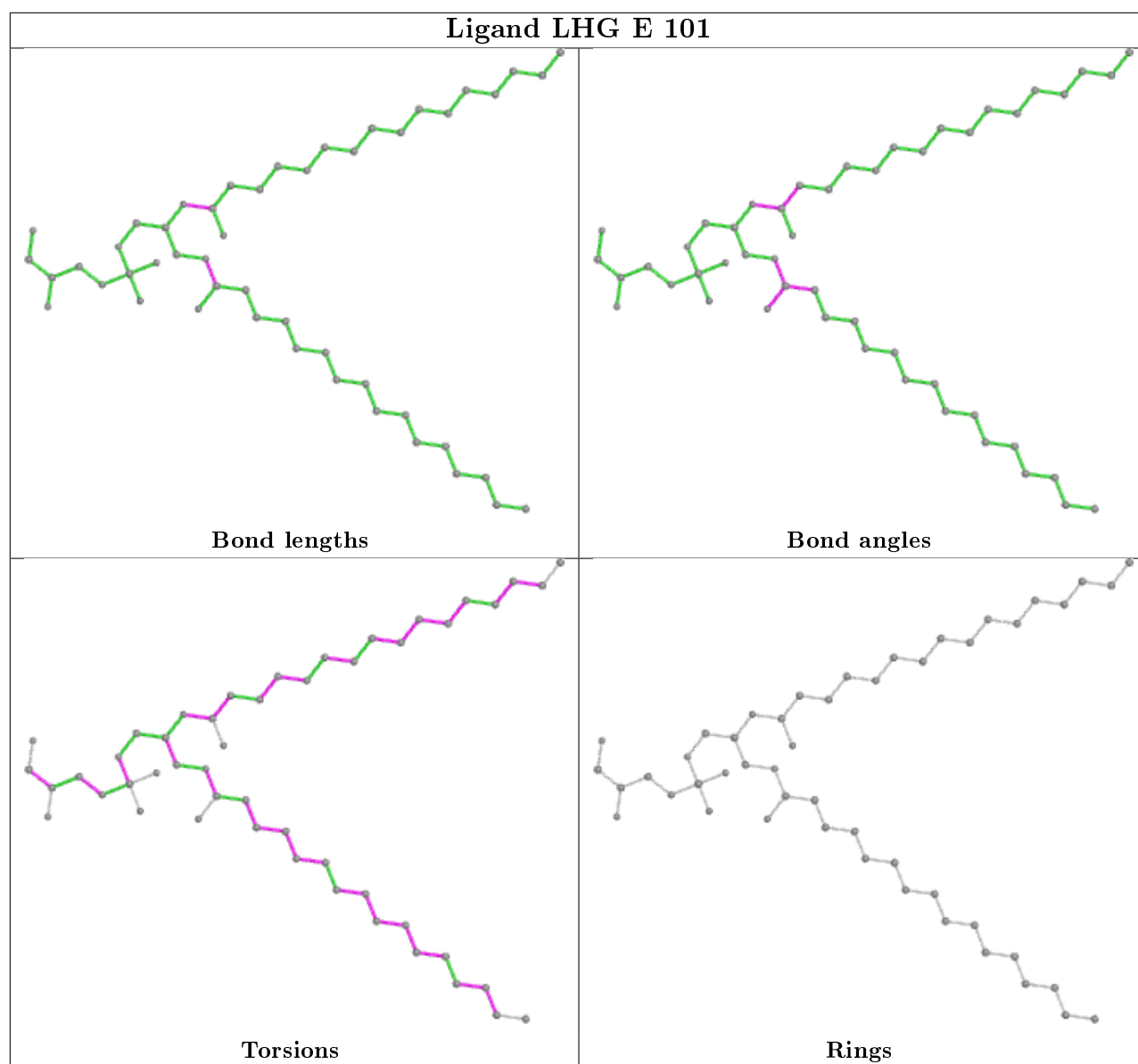
No monomer is involved in short contacts.

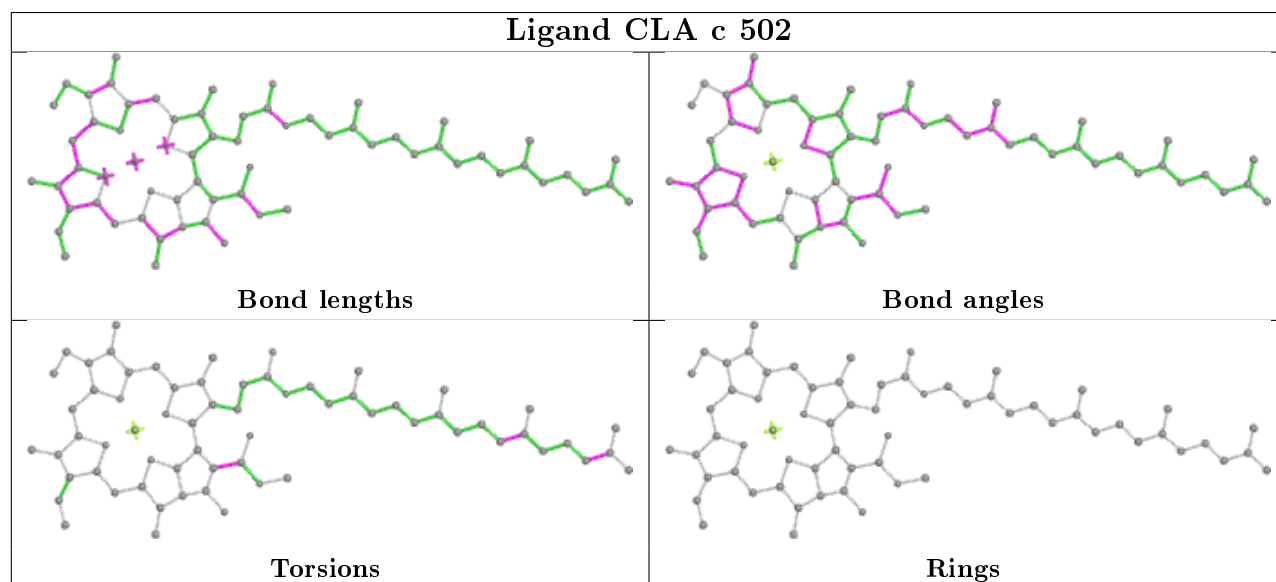
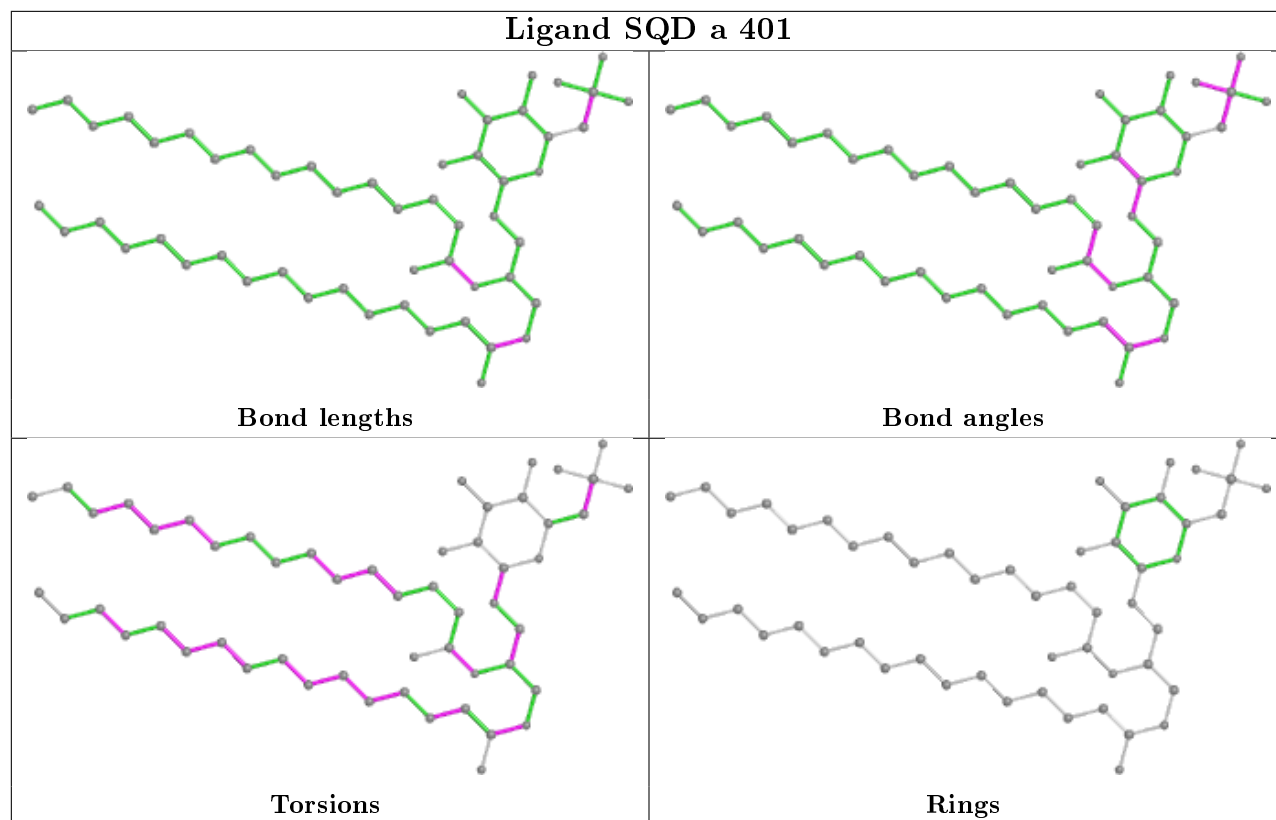
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

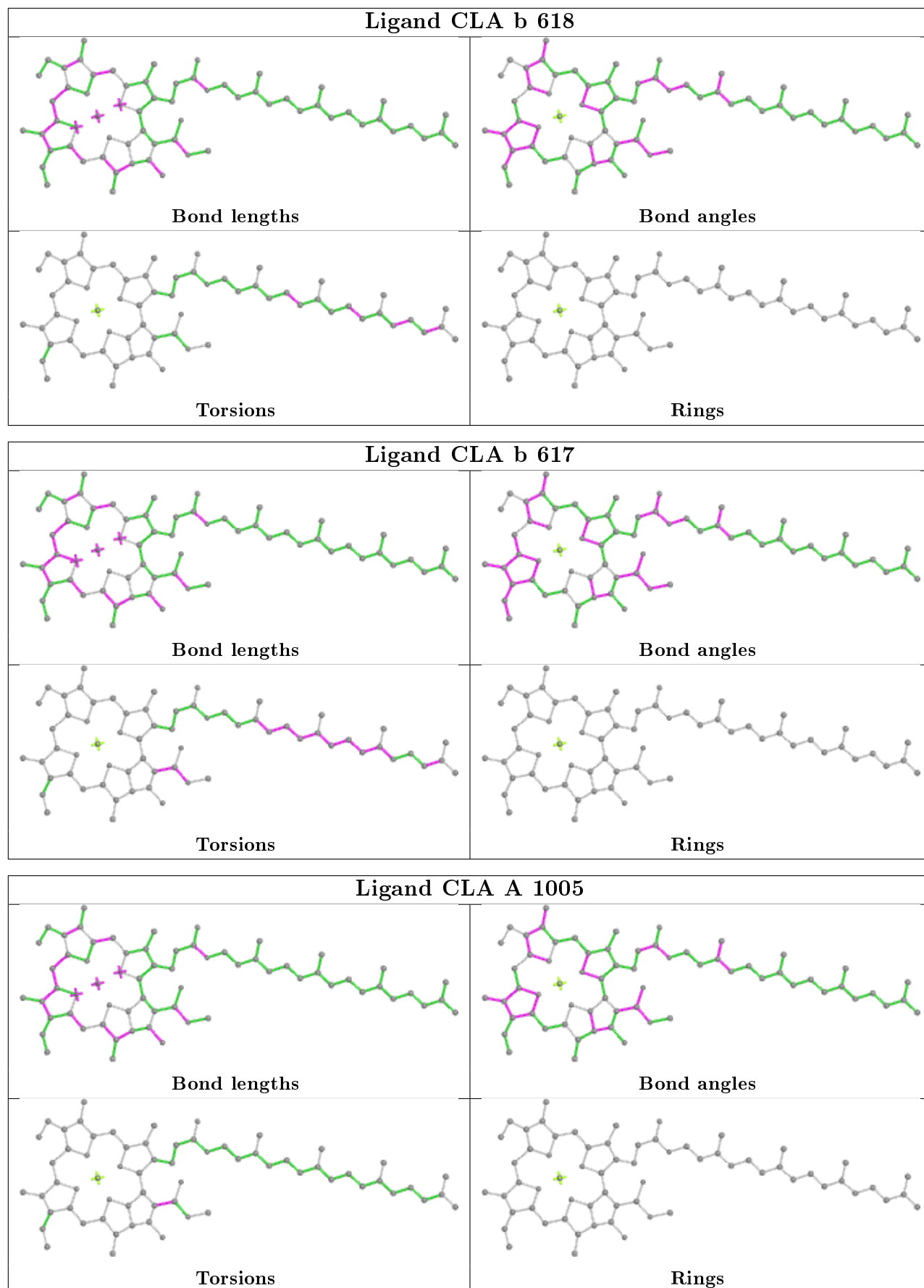


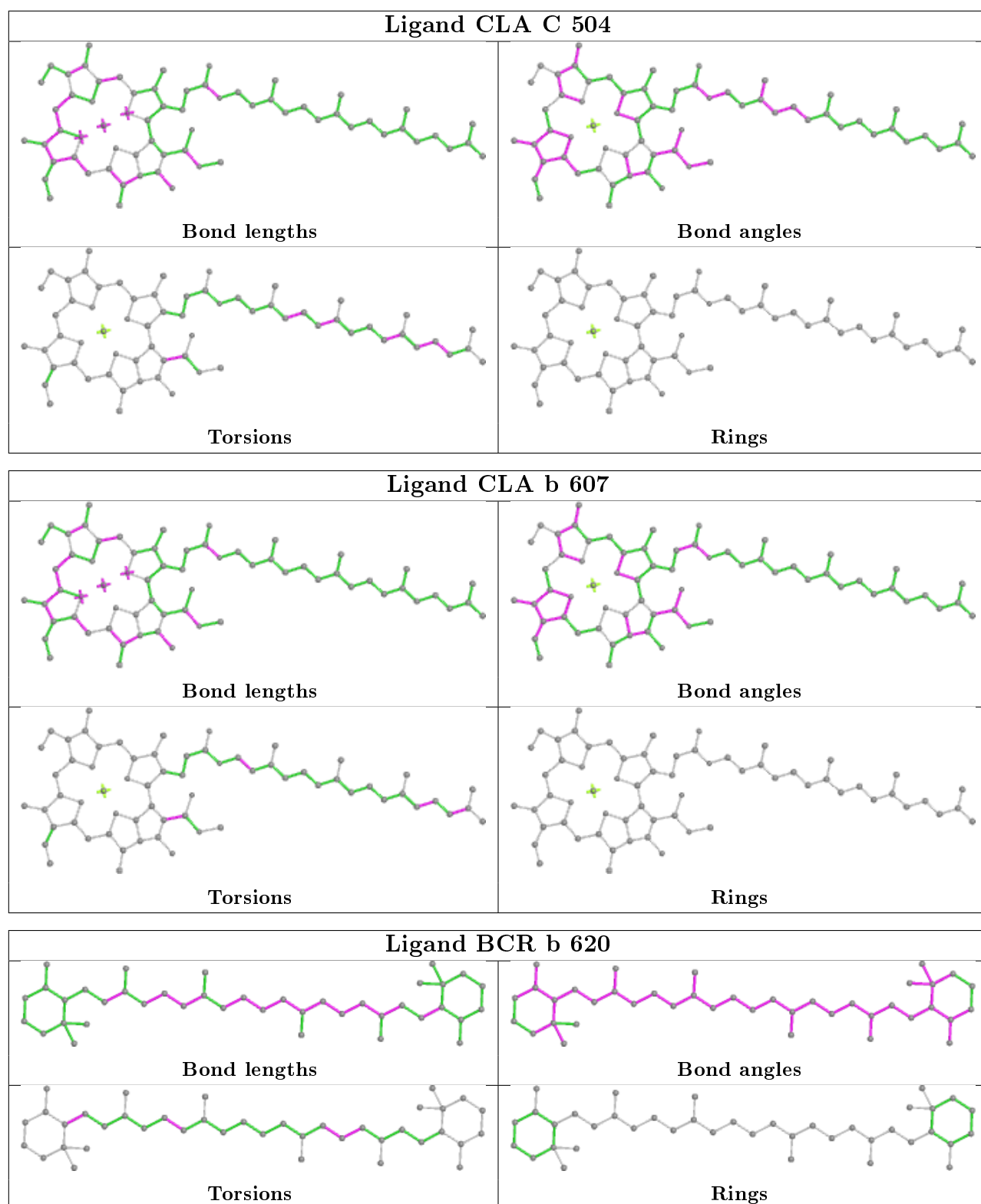


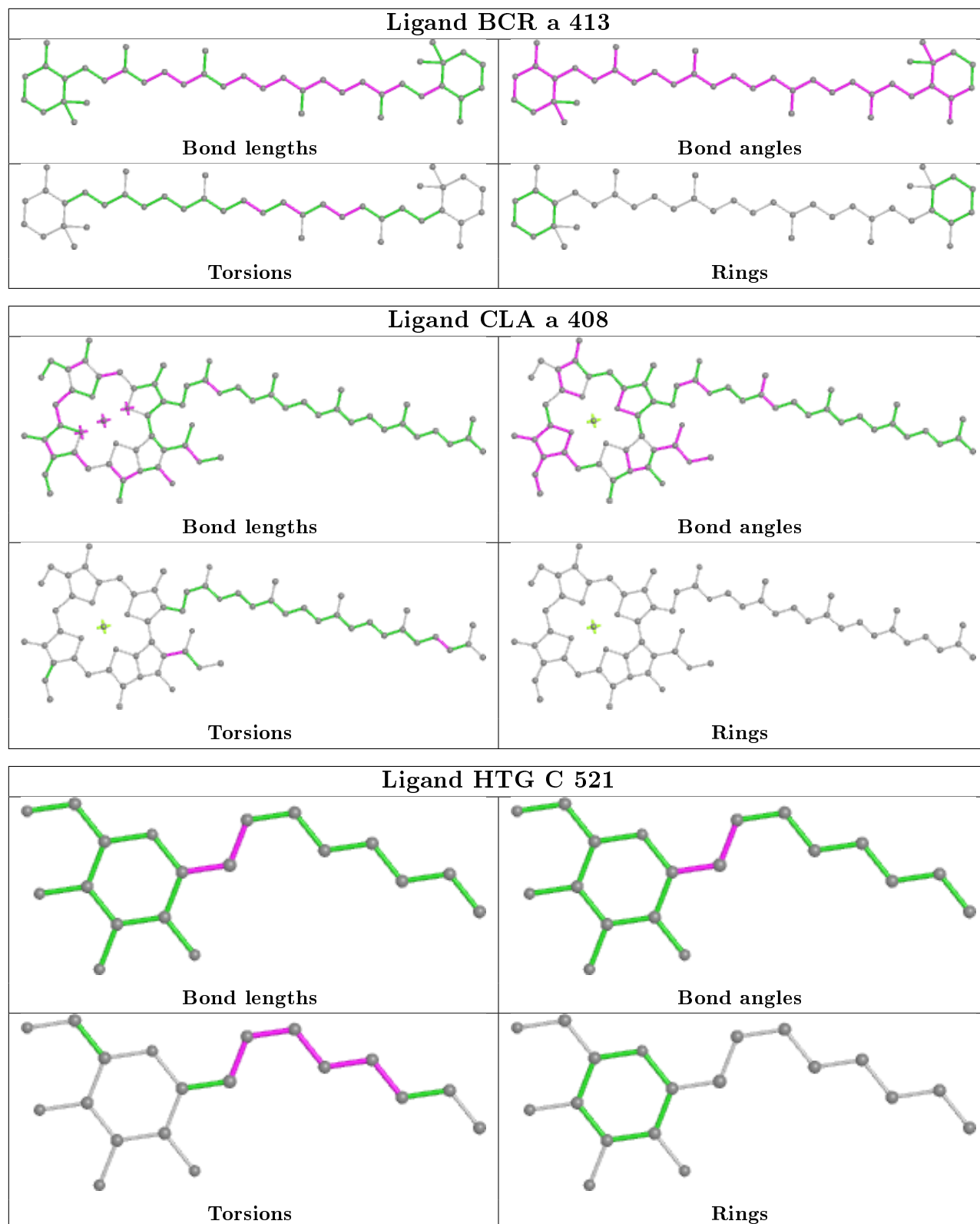


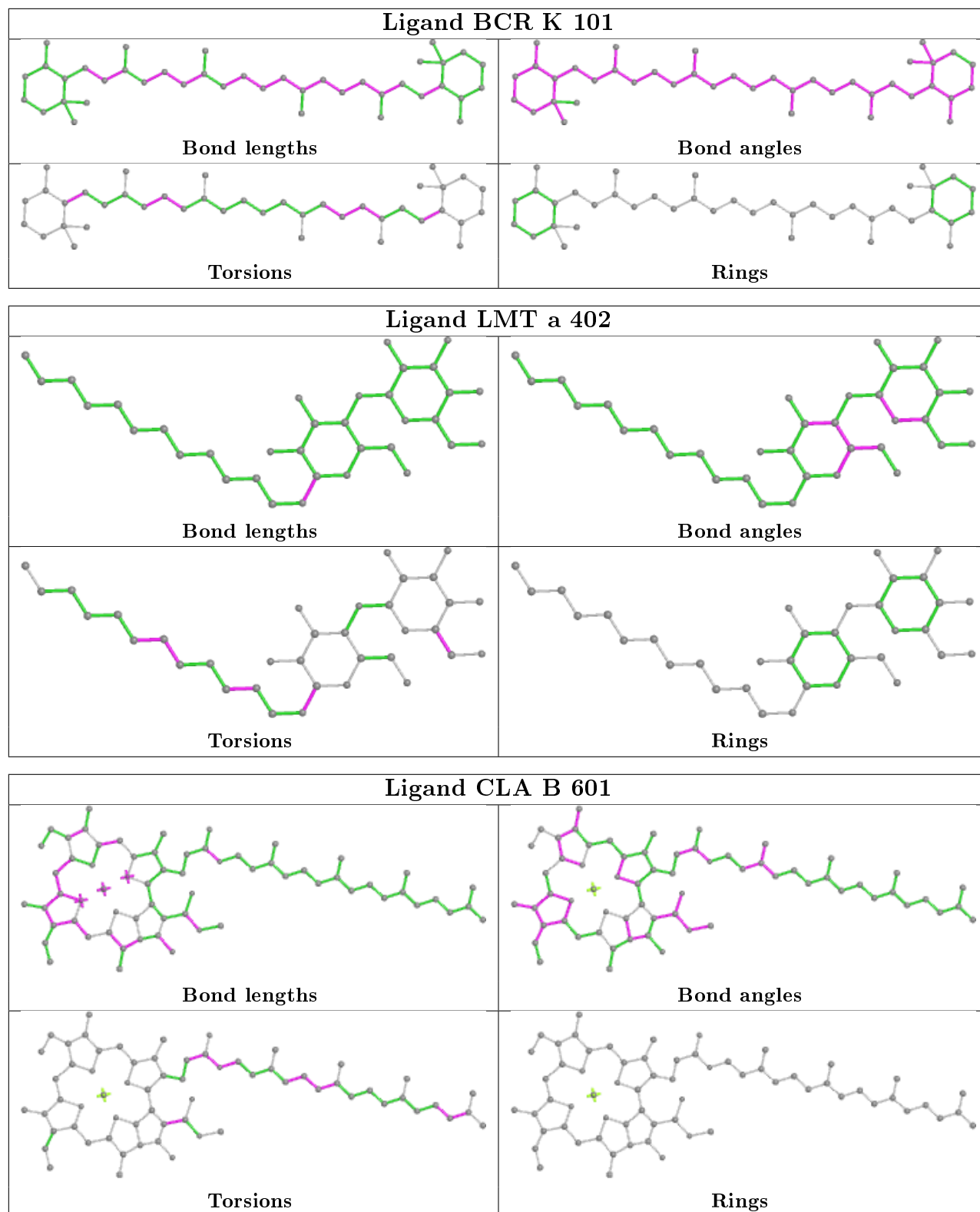


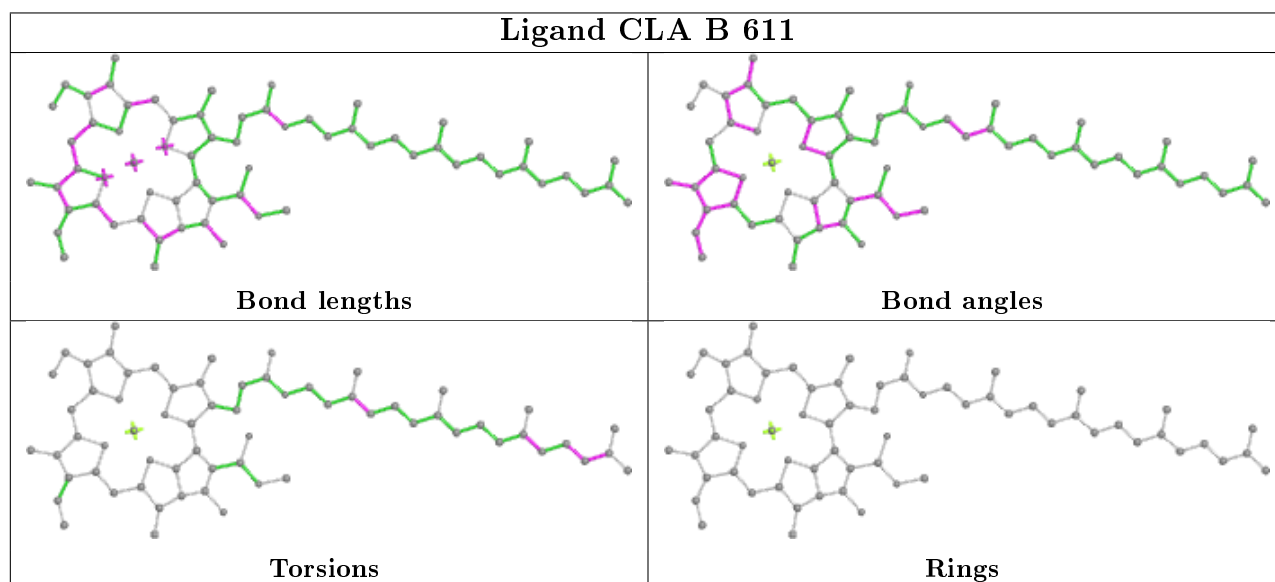
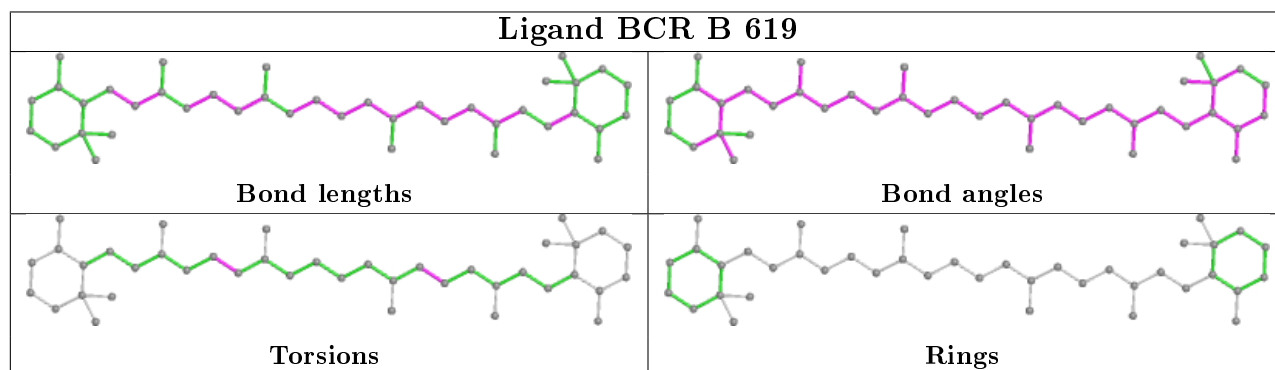
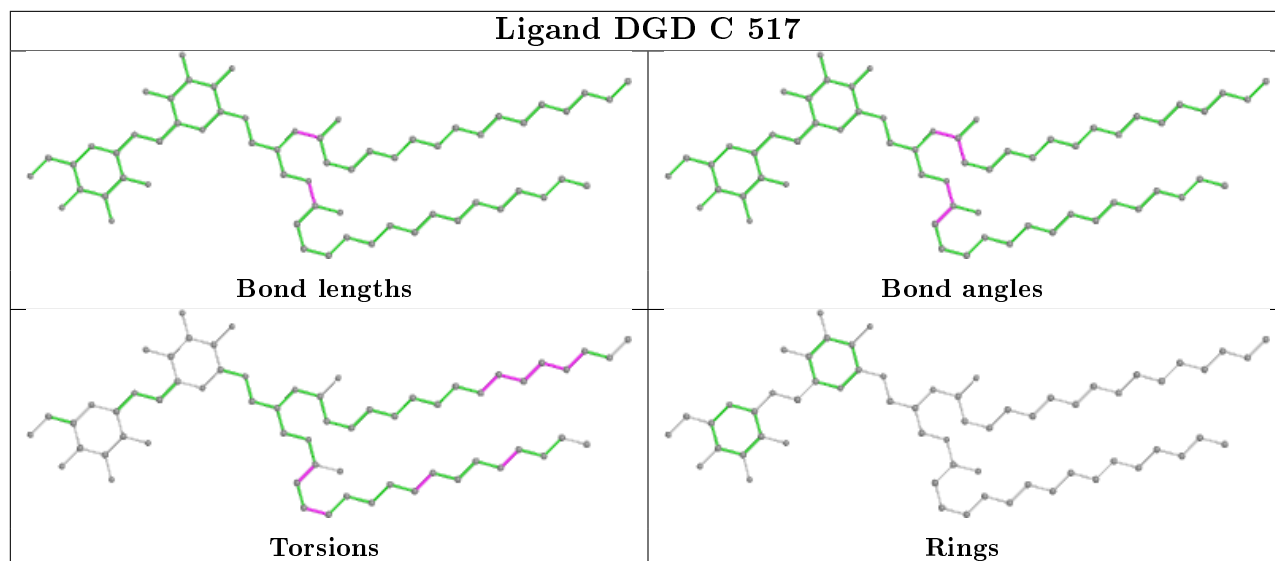


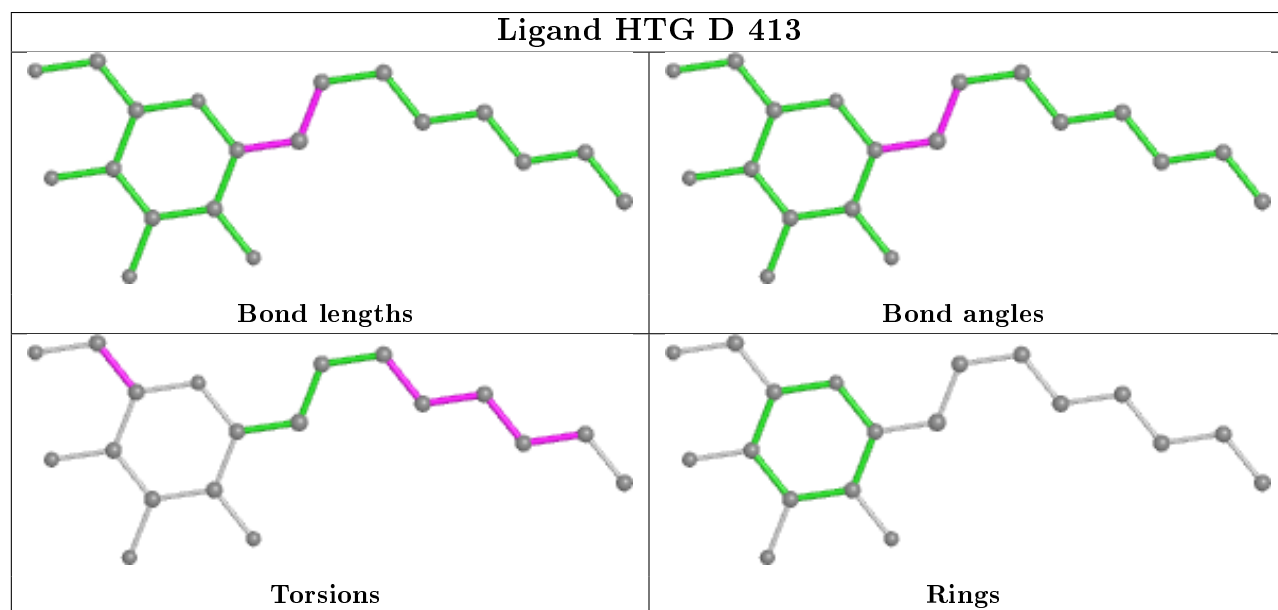
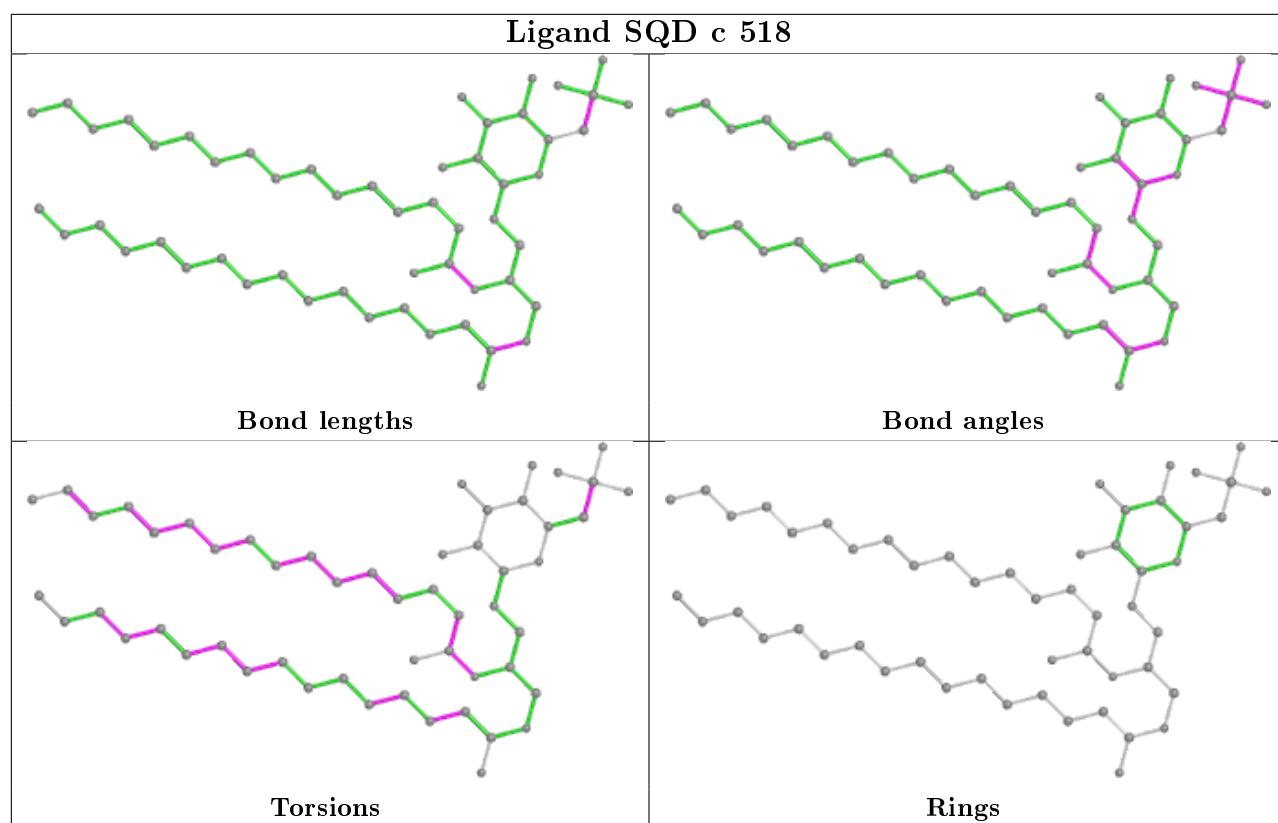


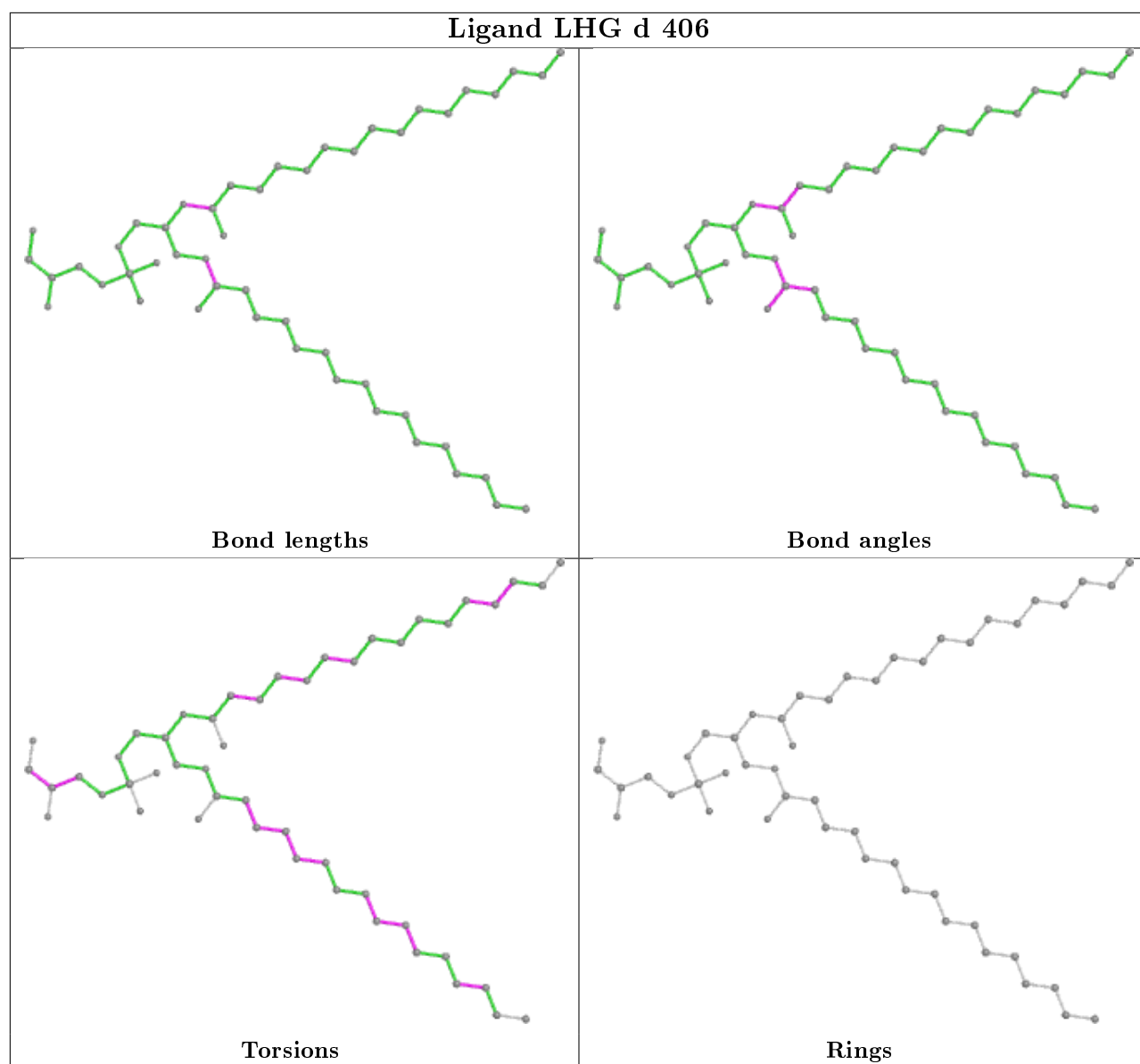


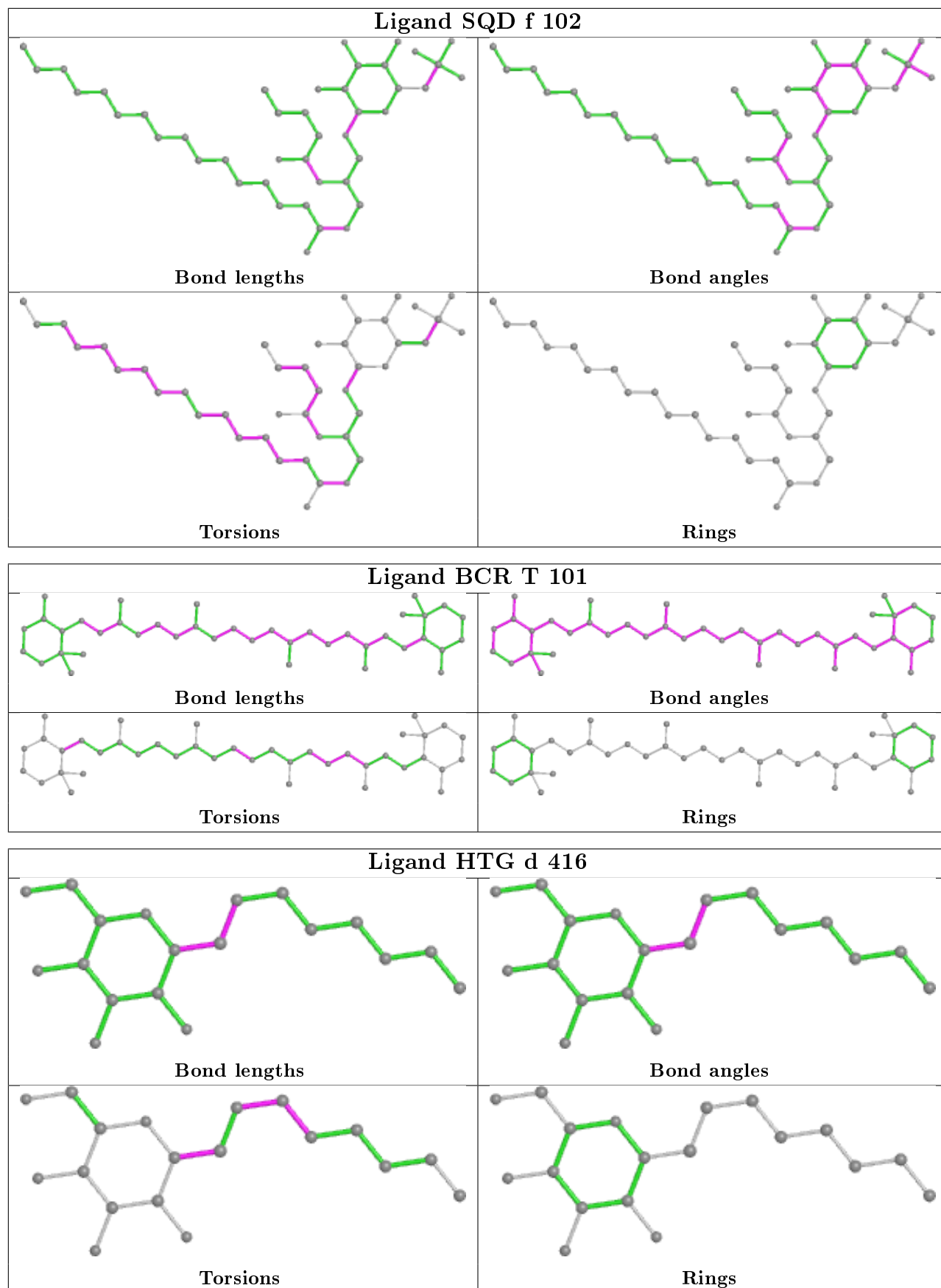


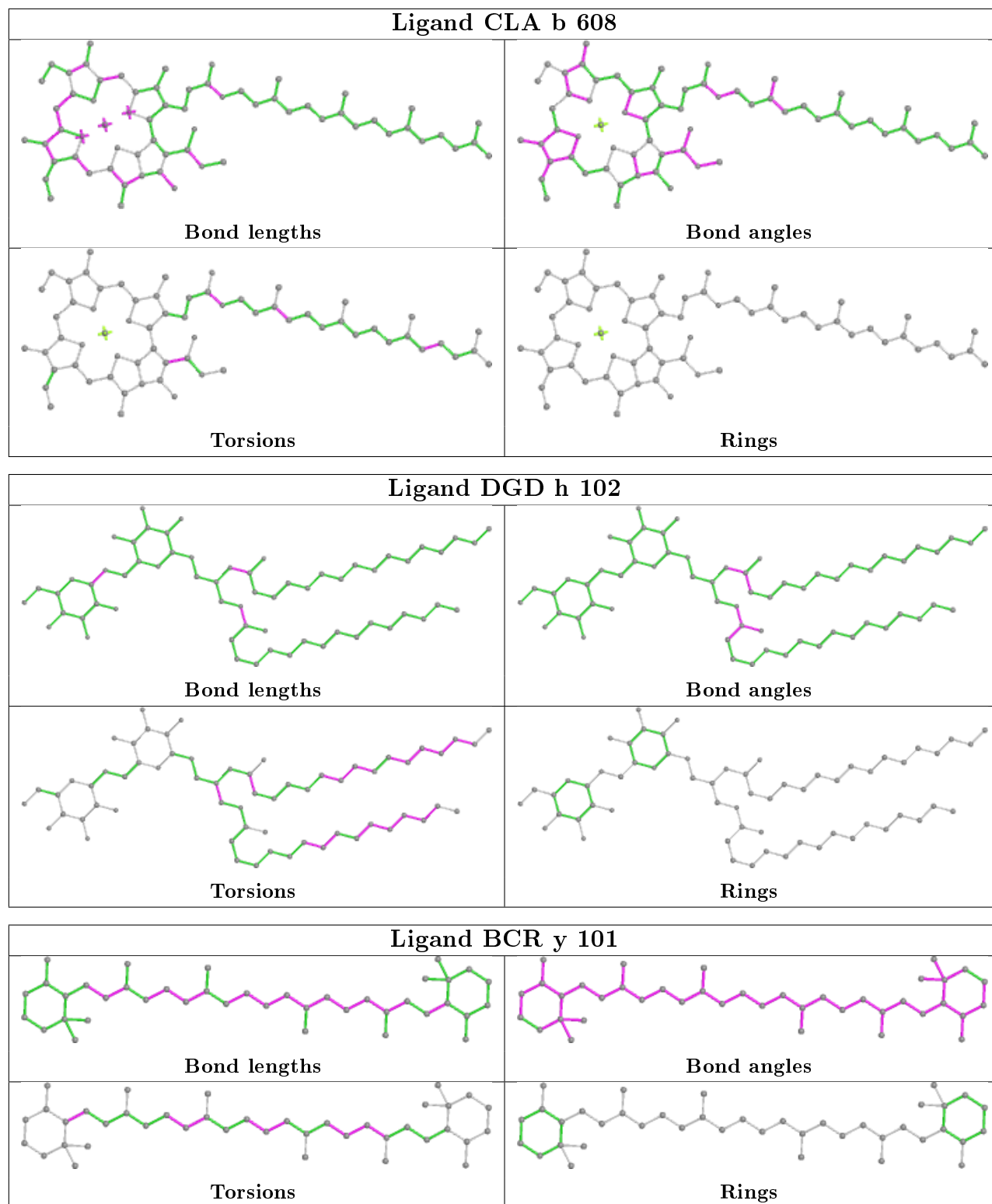


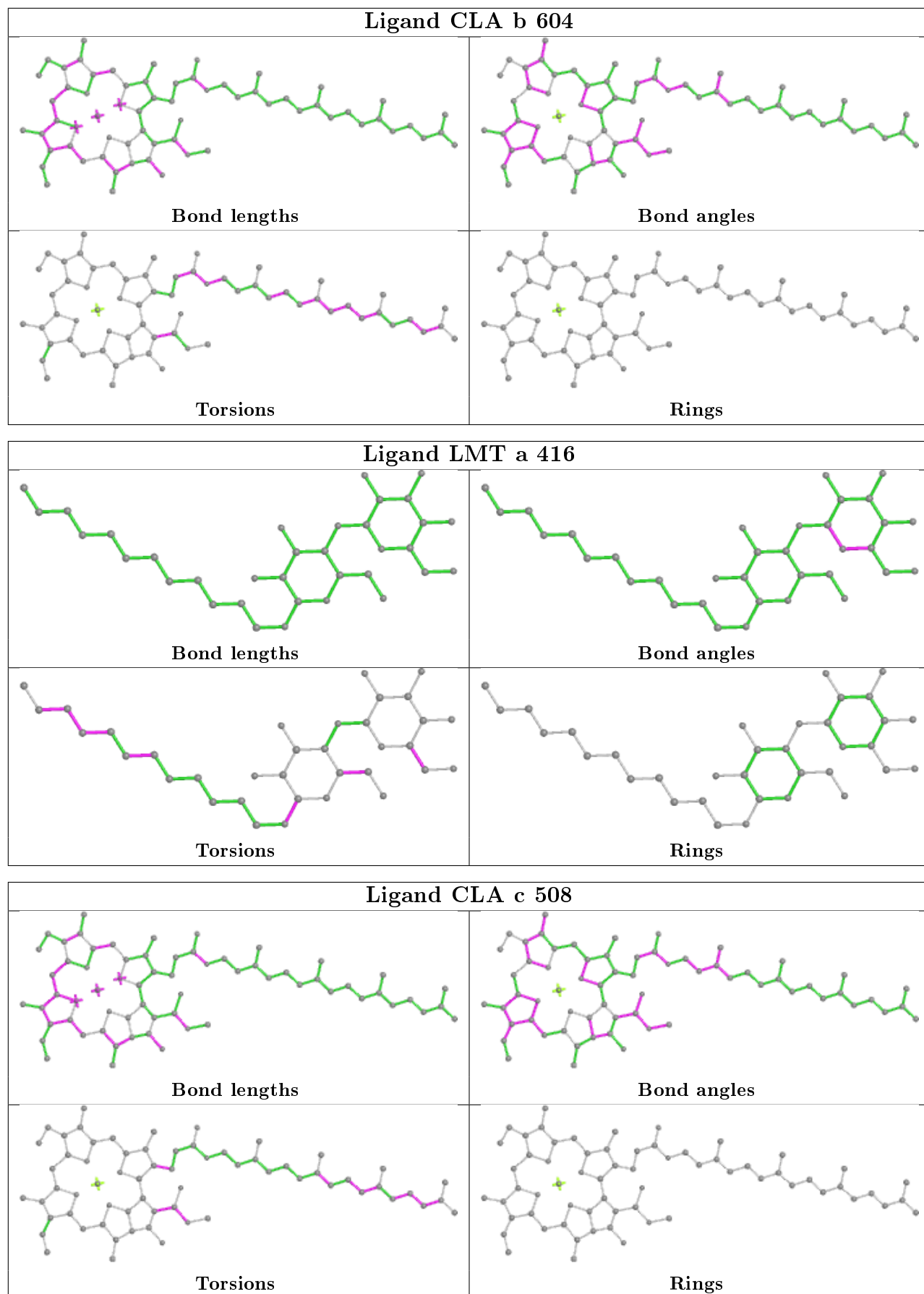


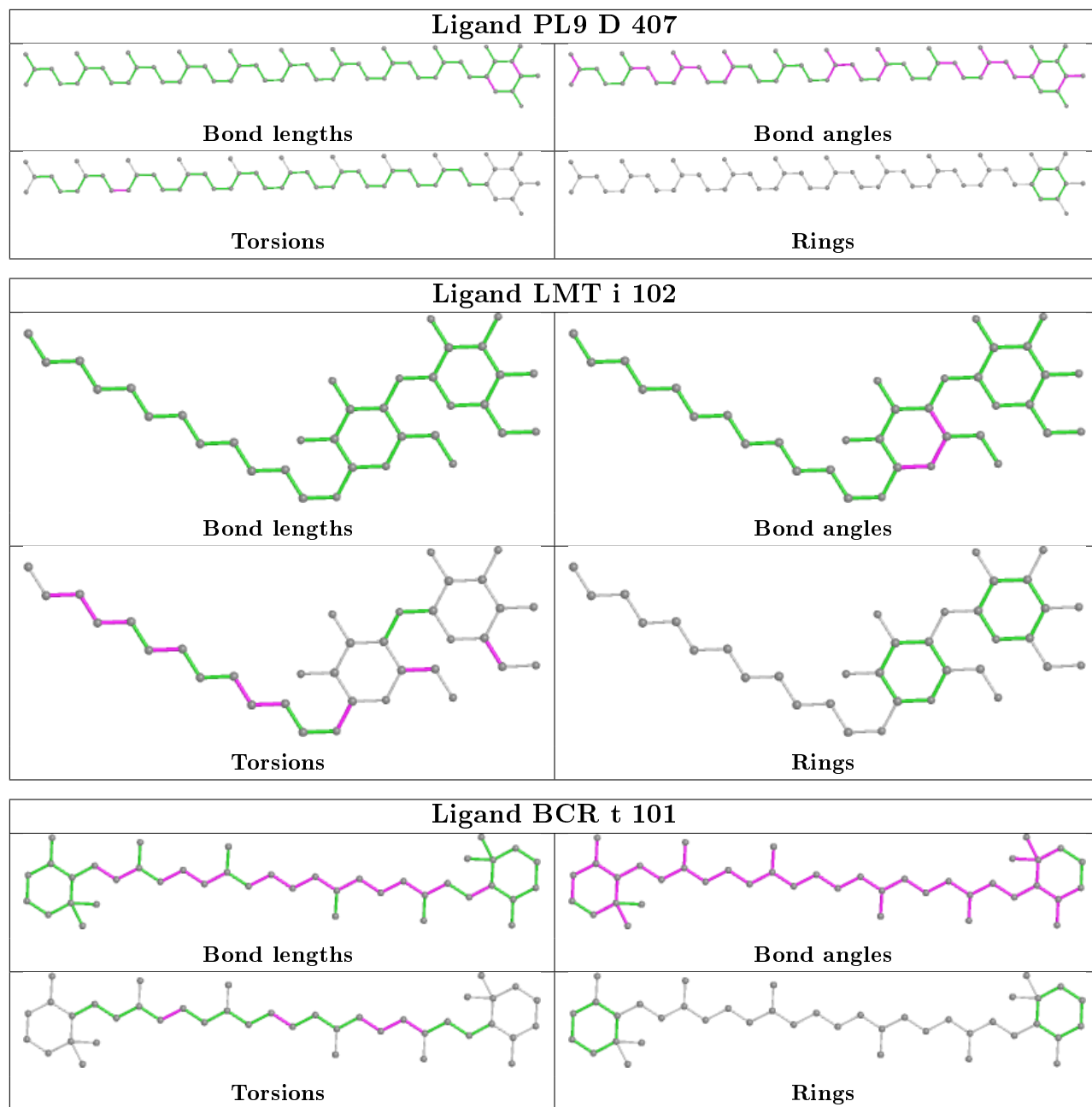


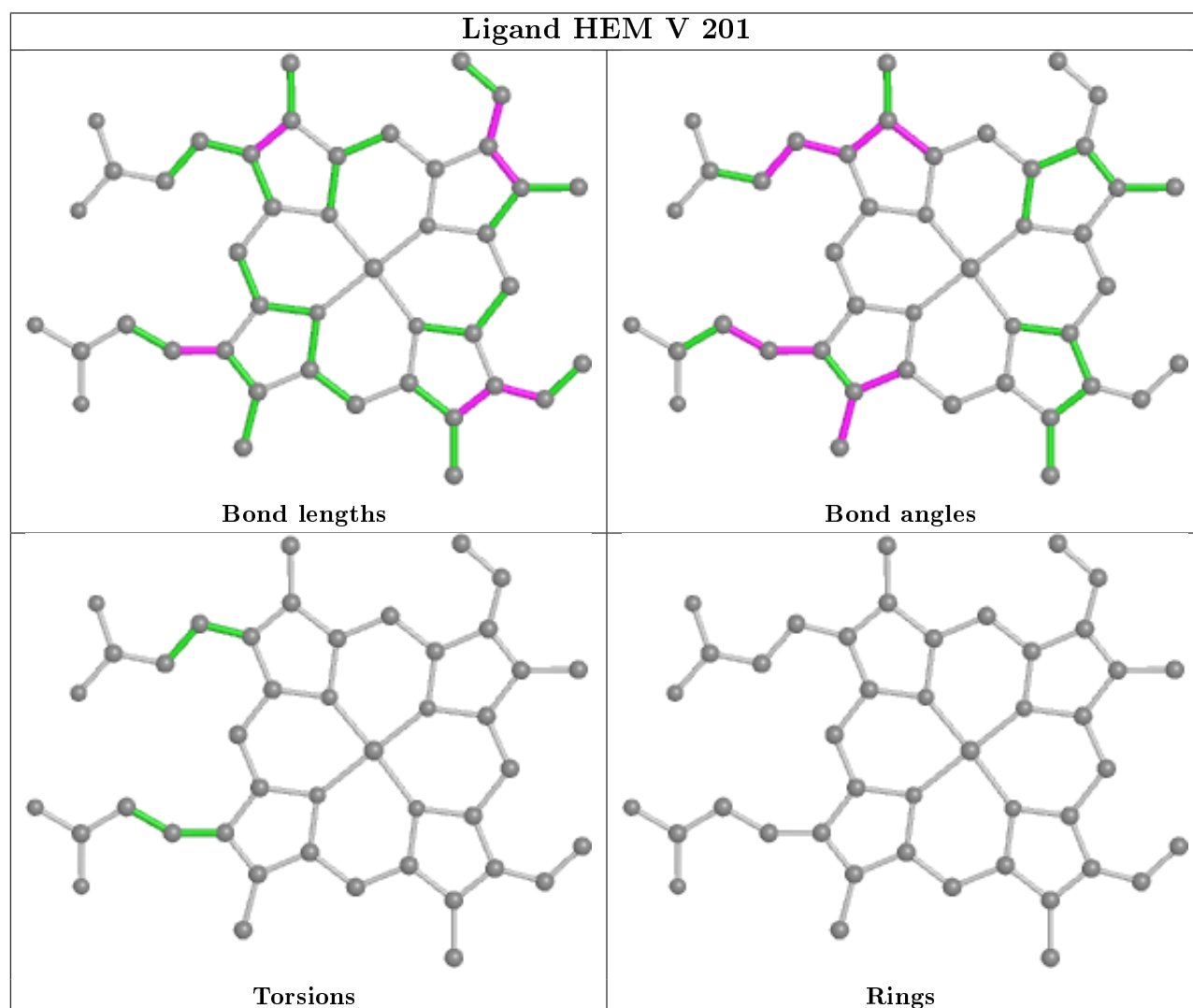
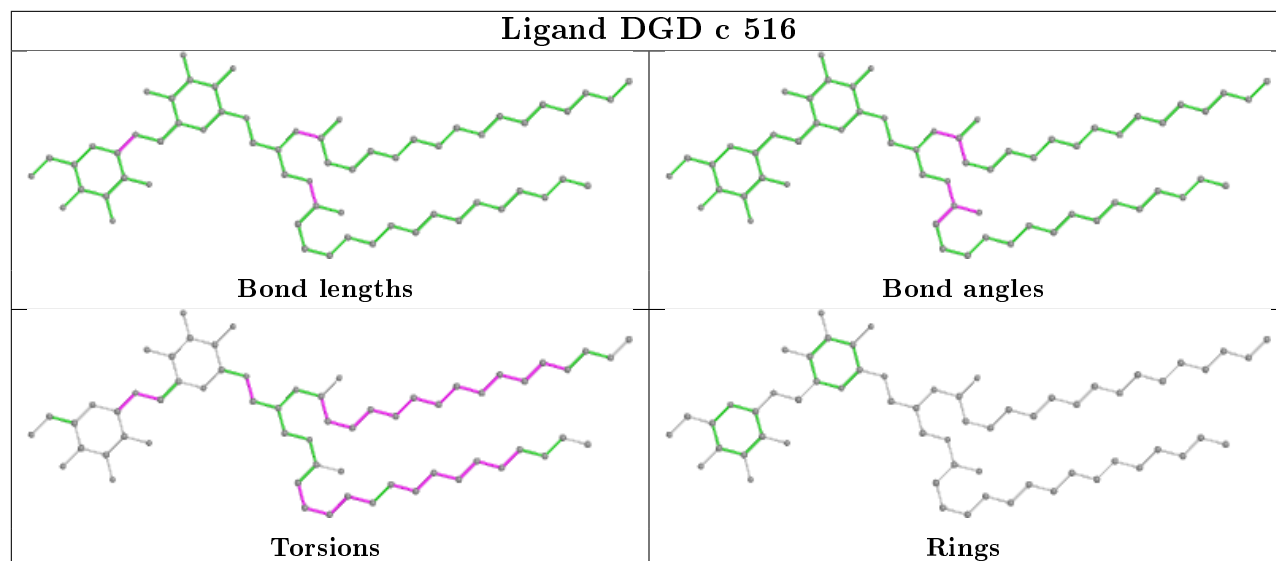


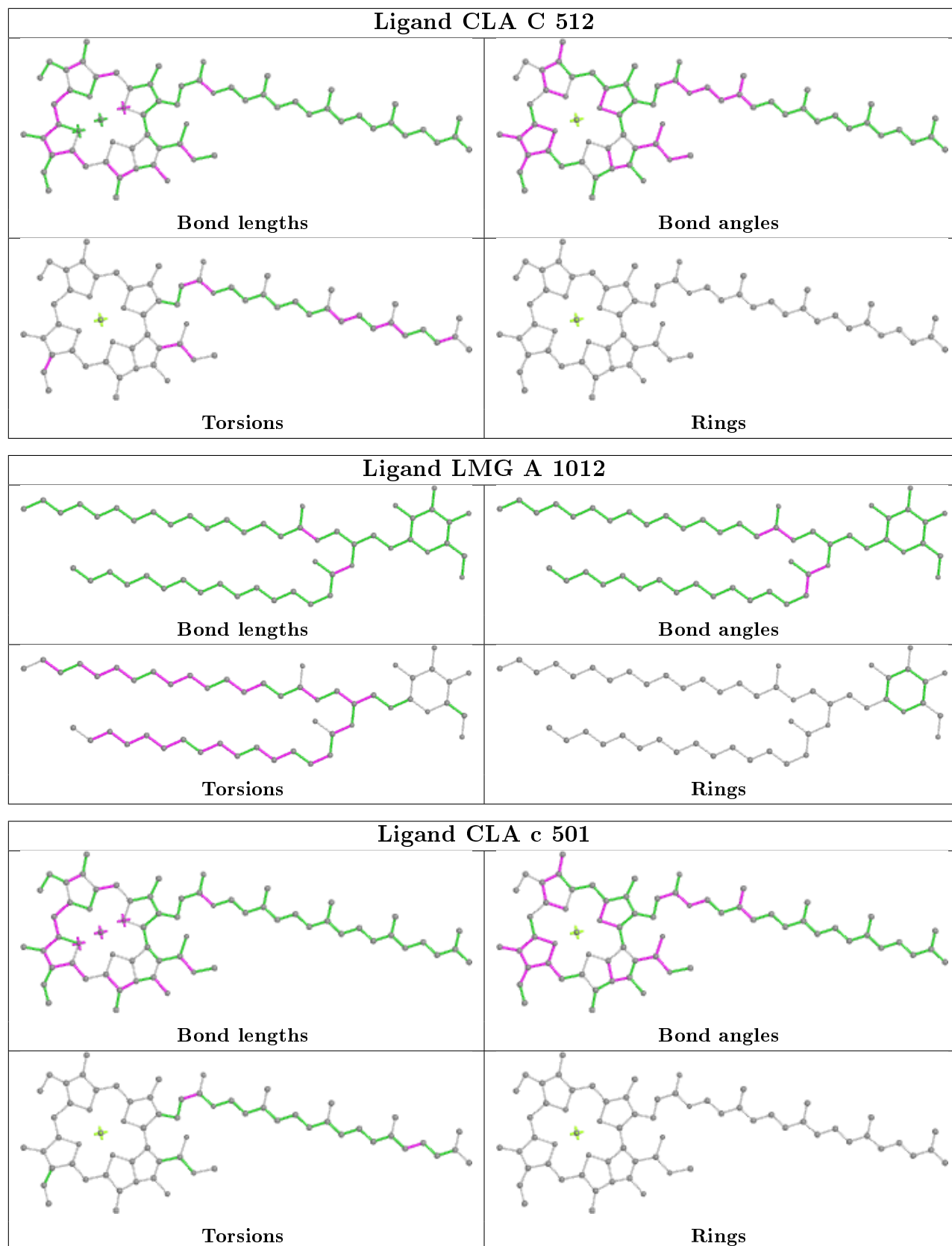


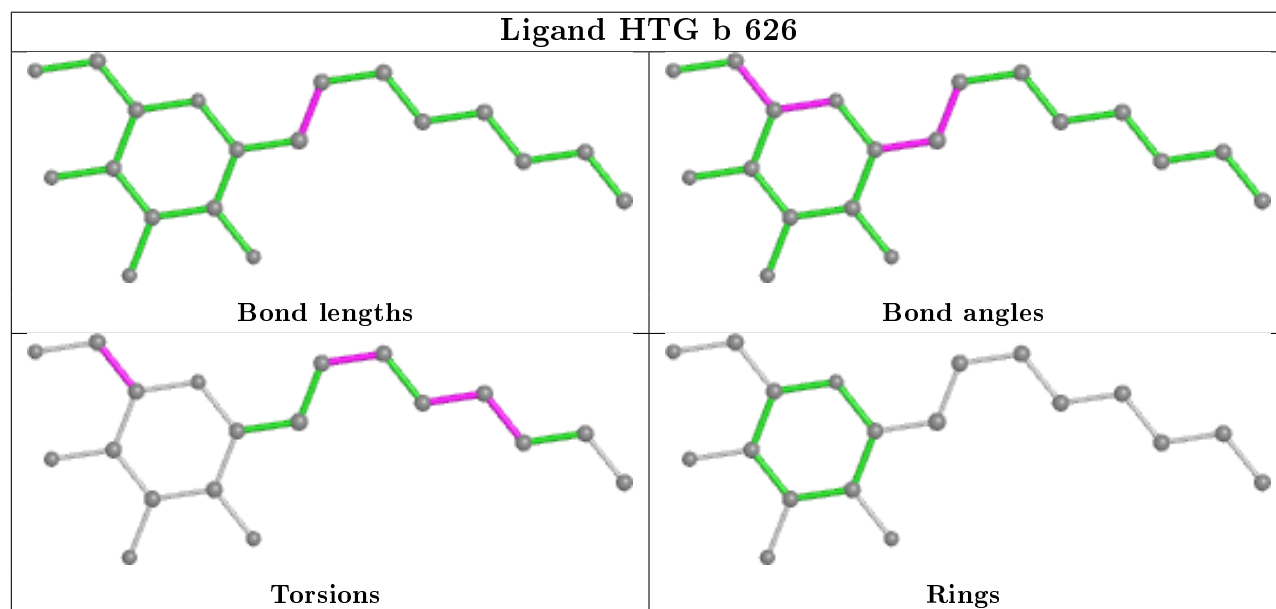
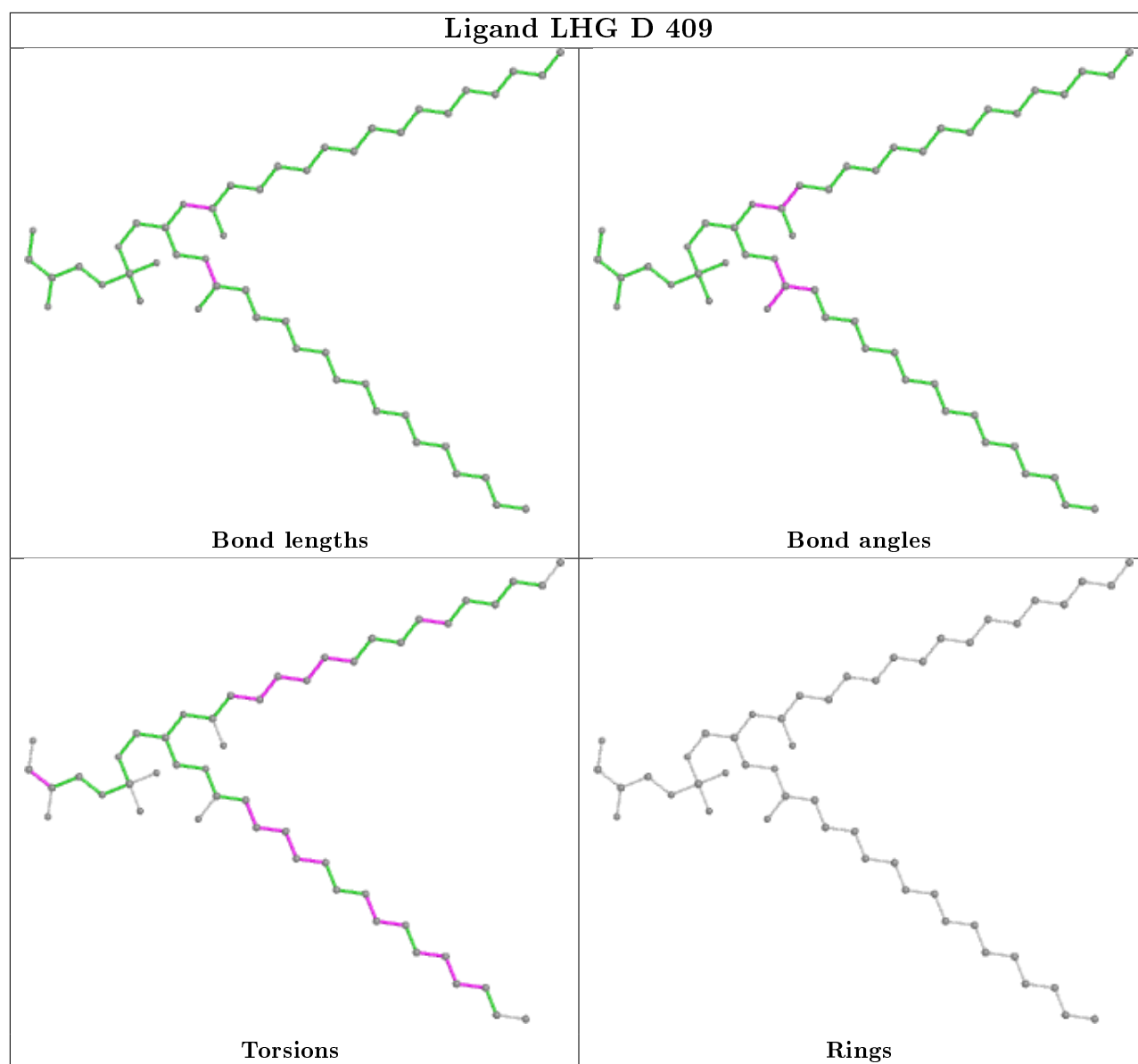


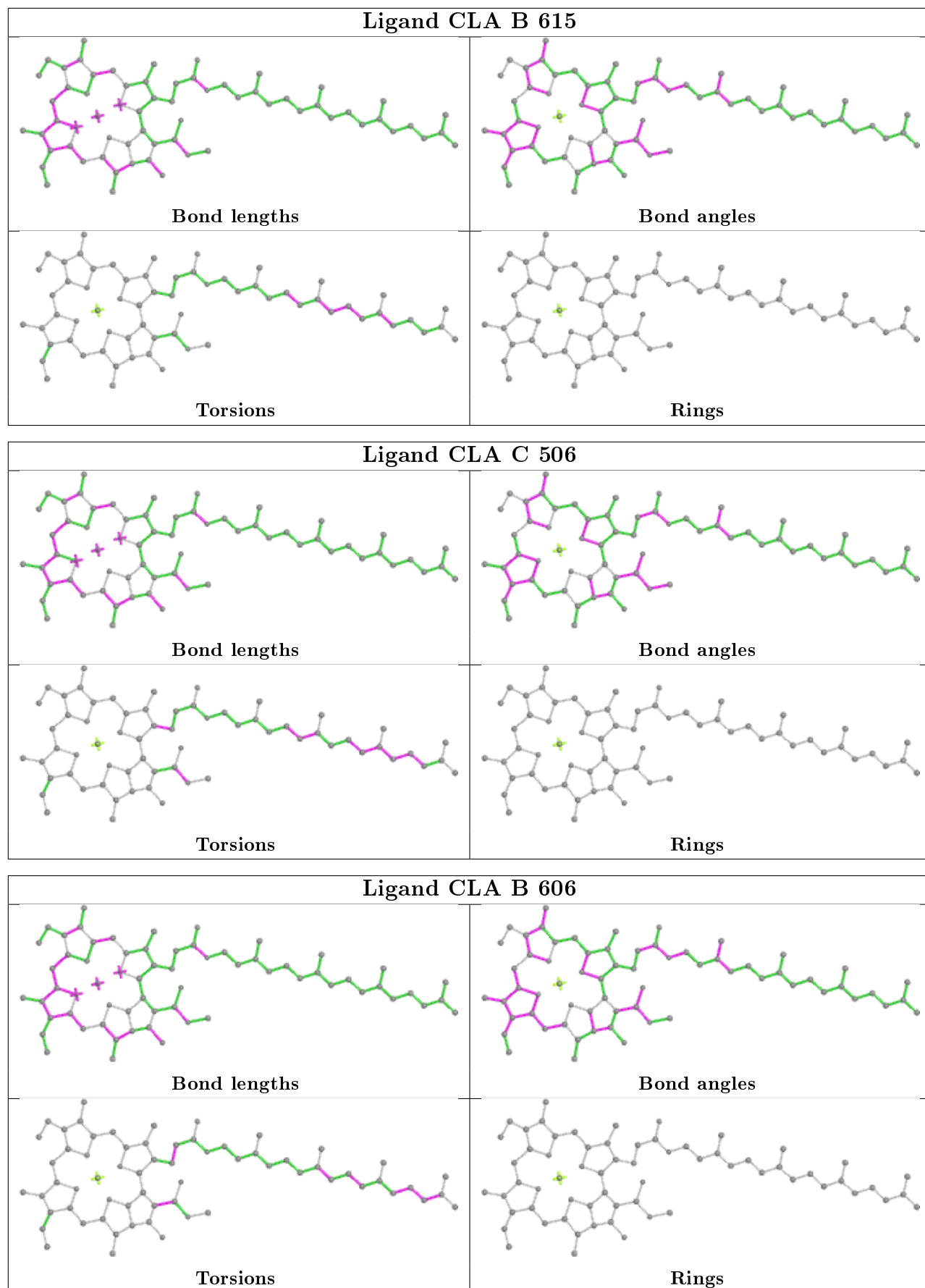


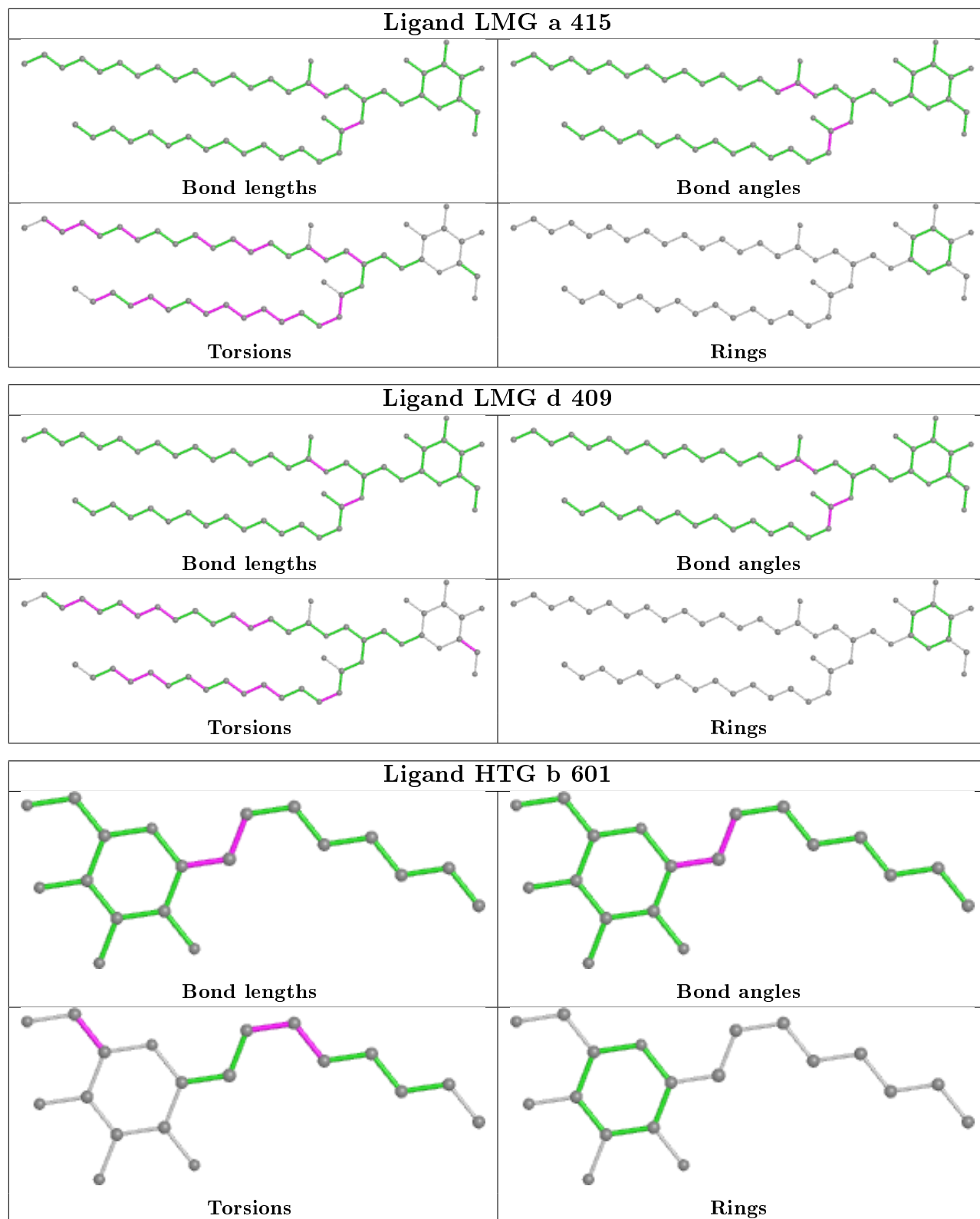


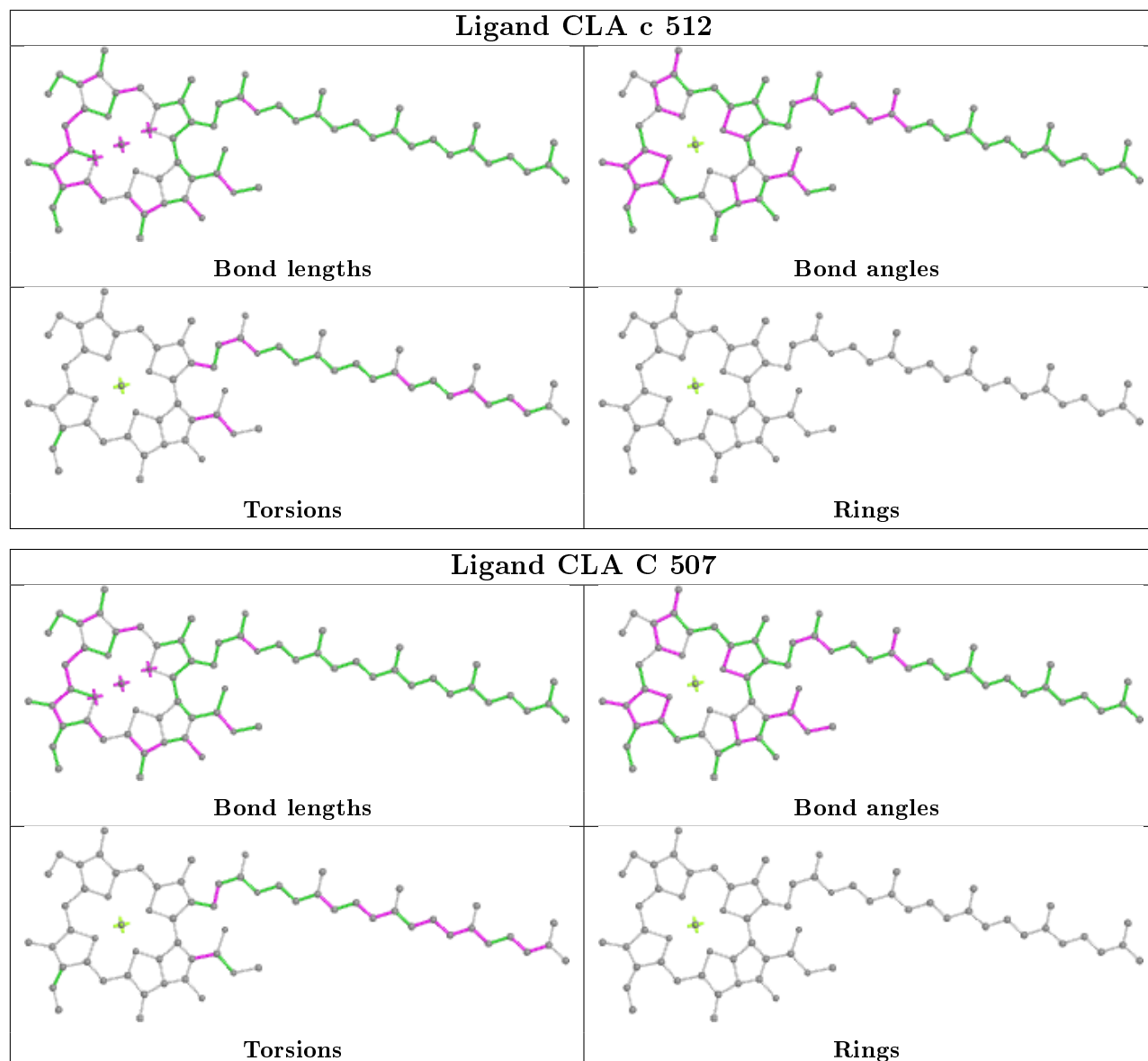


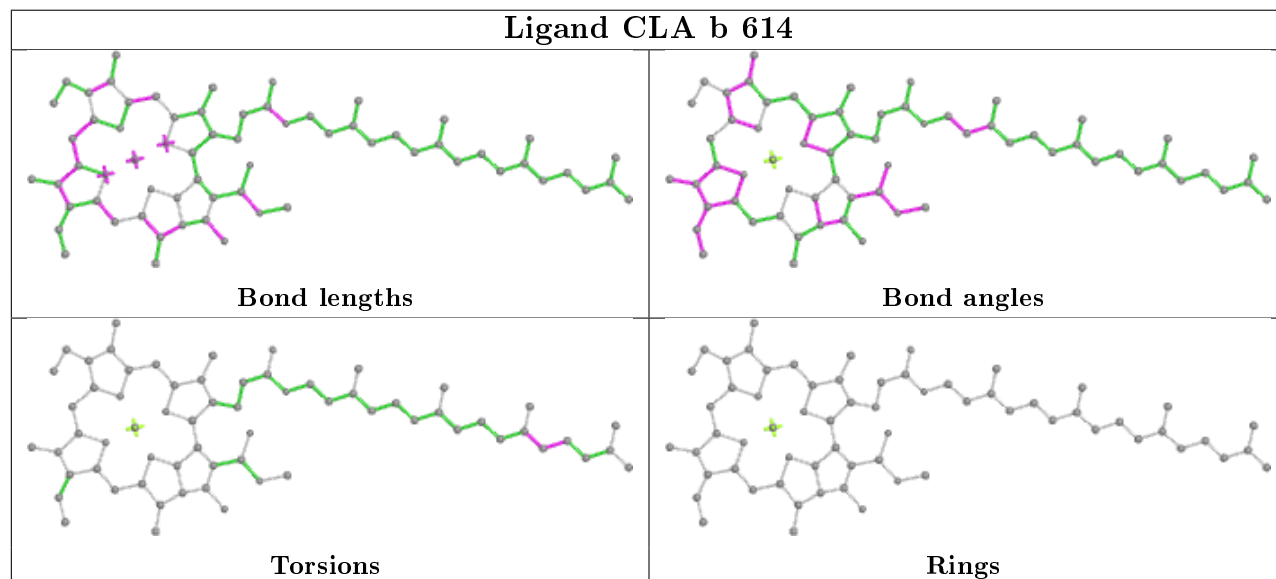
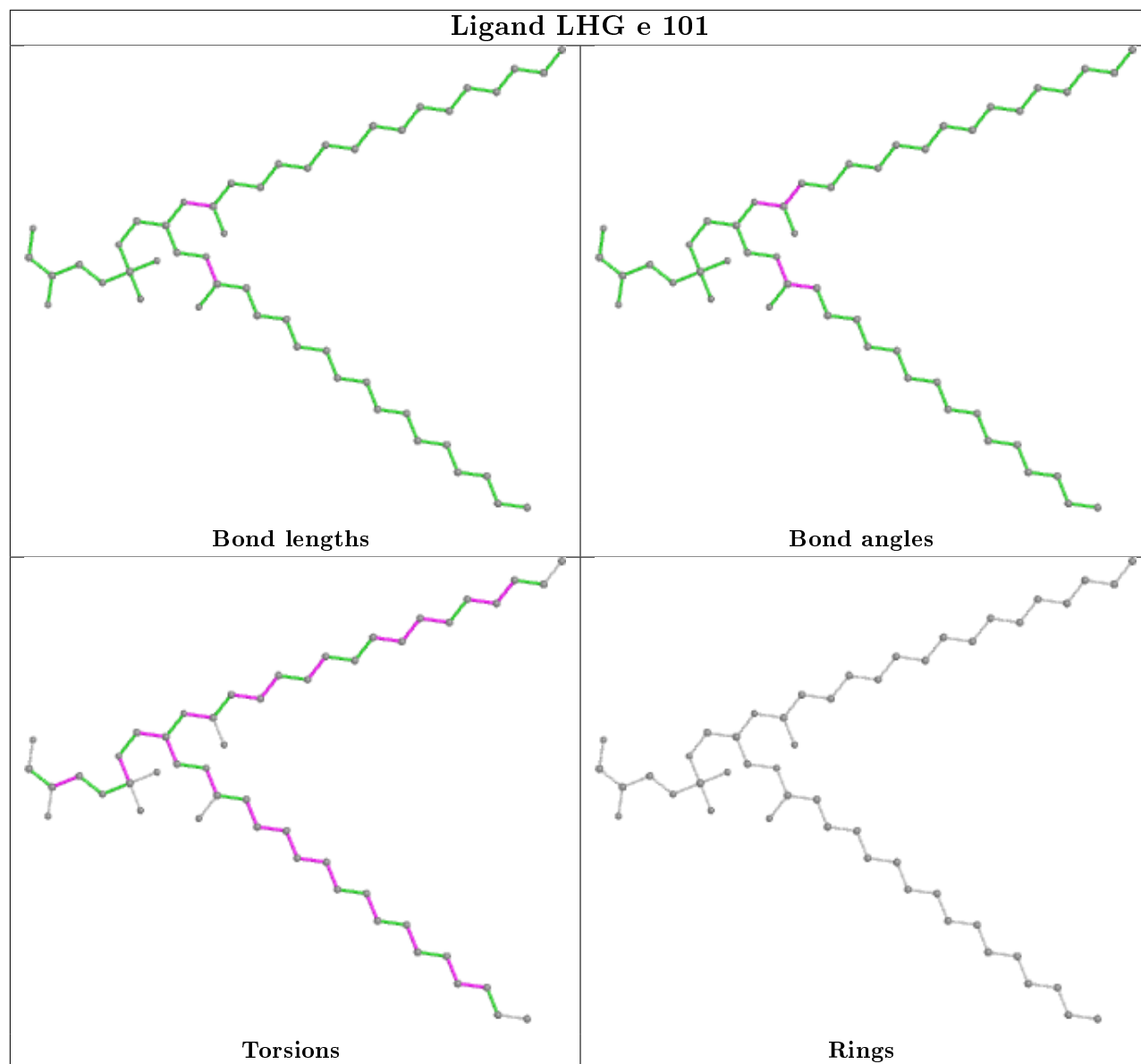


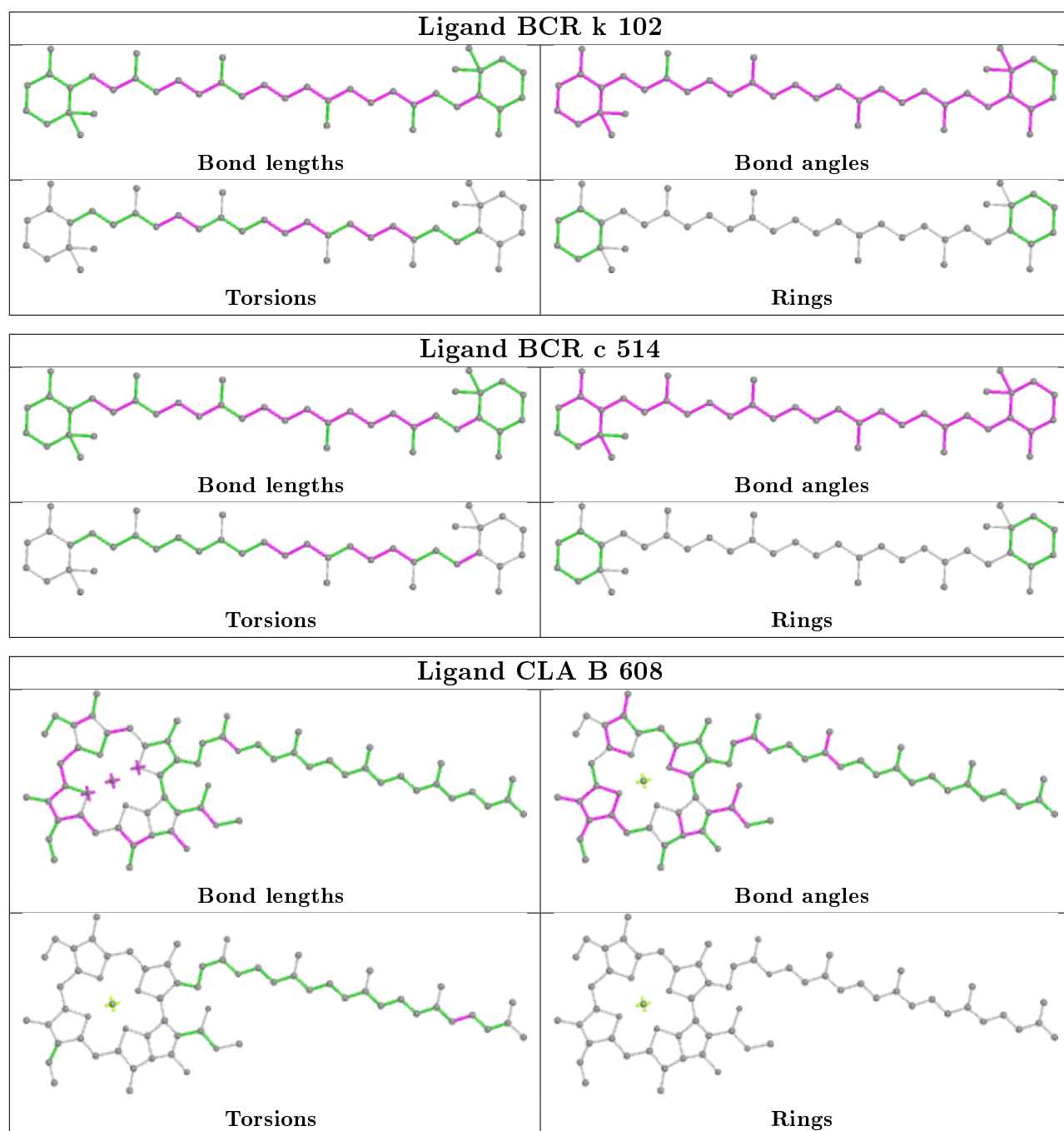


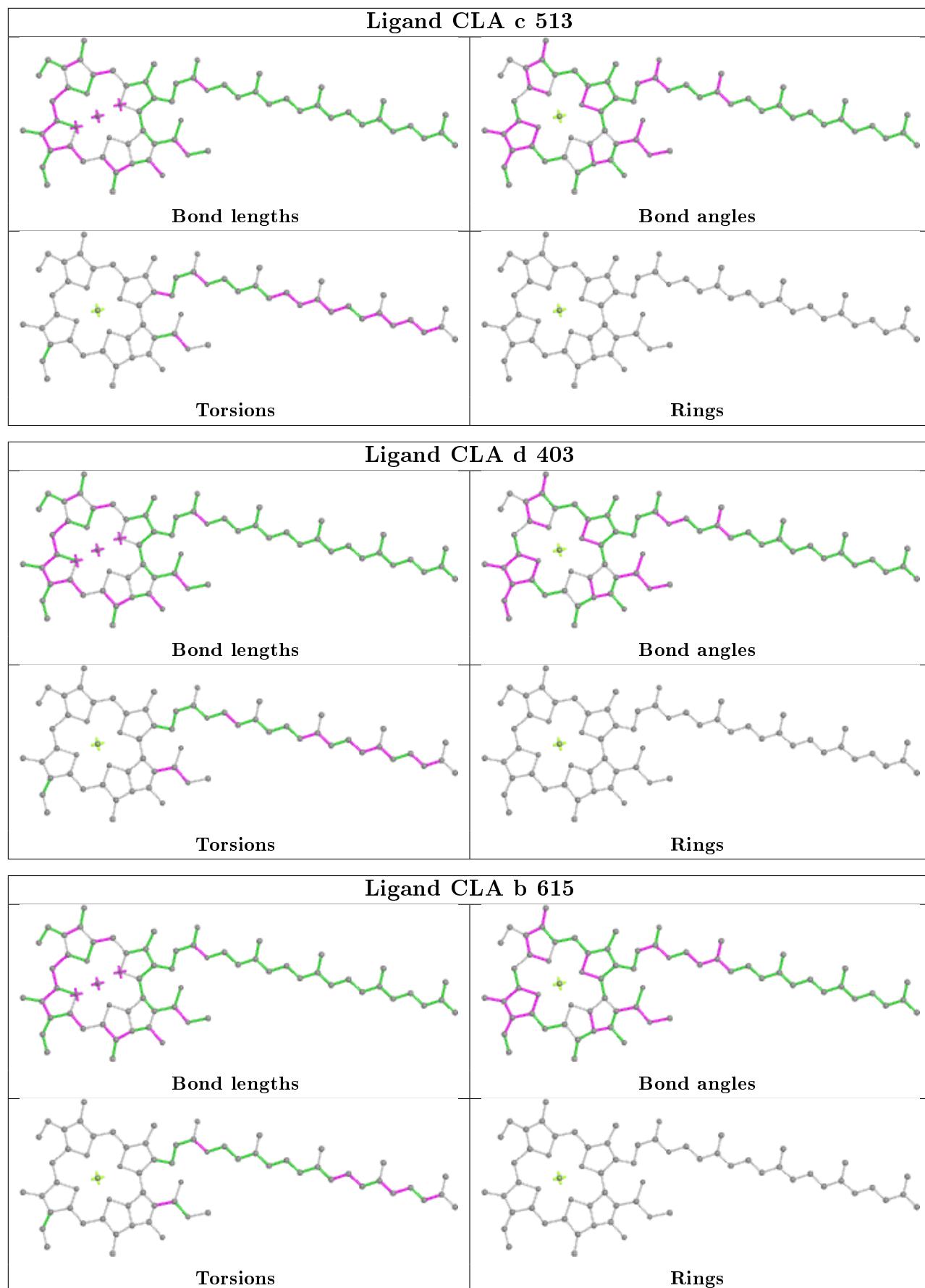


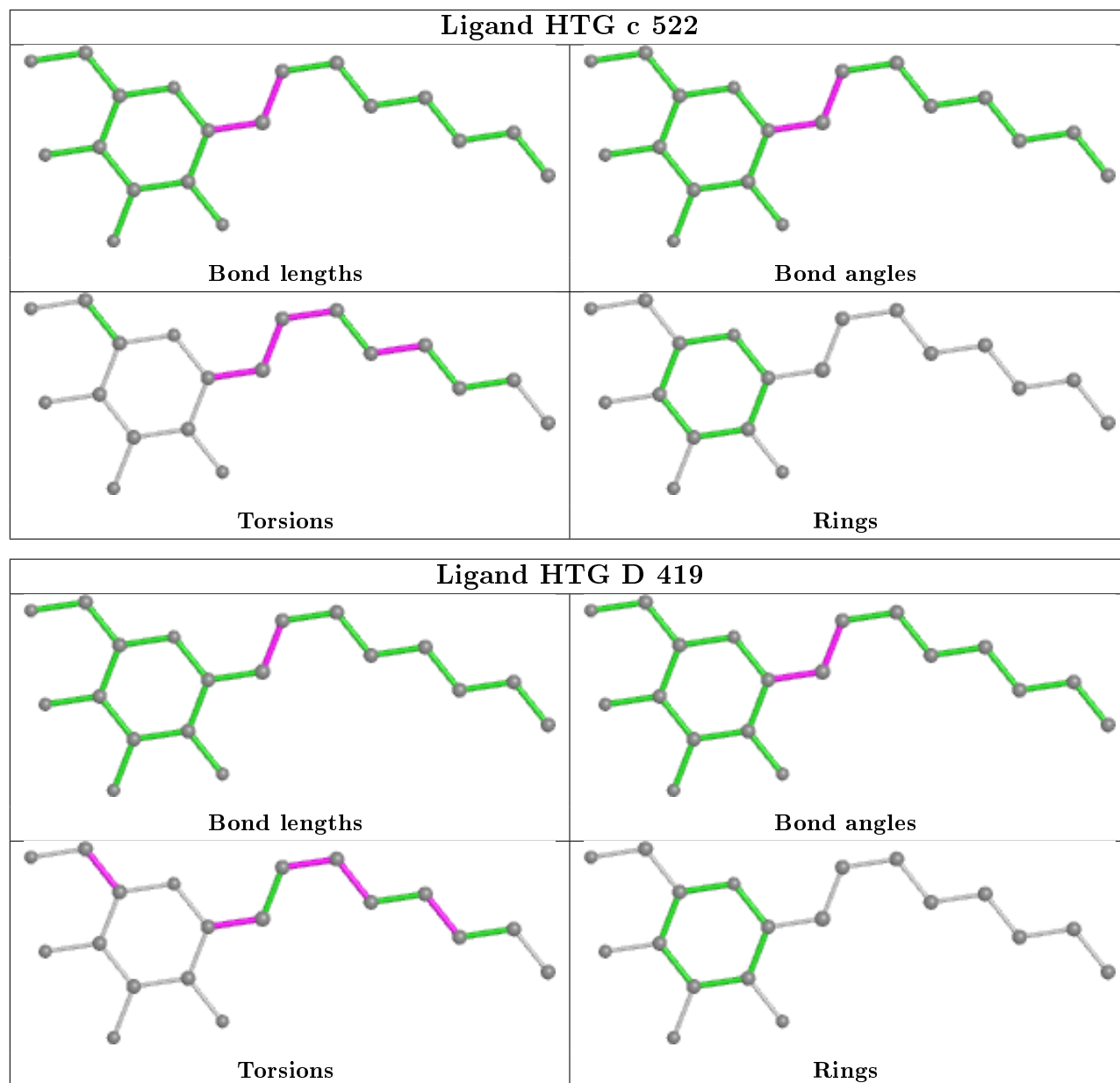


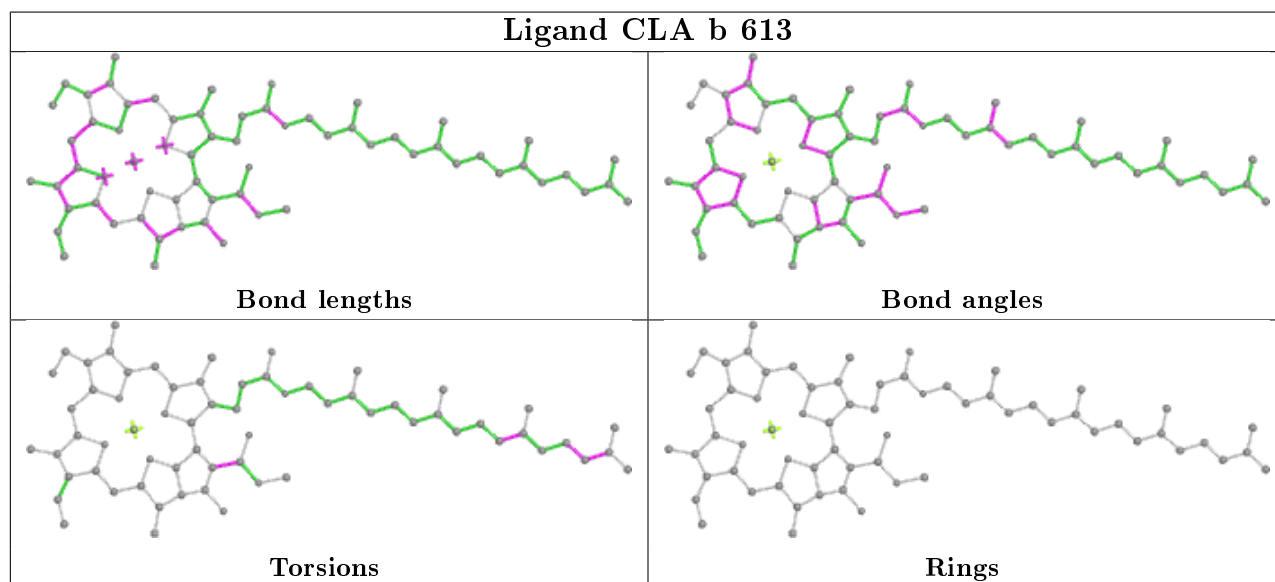
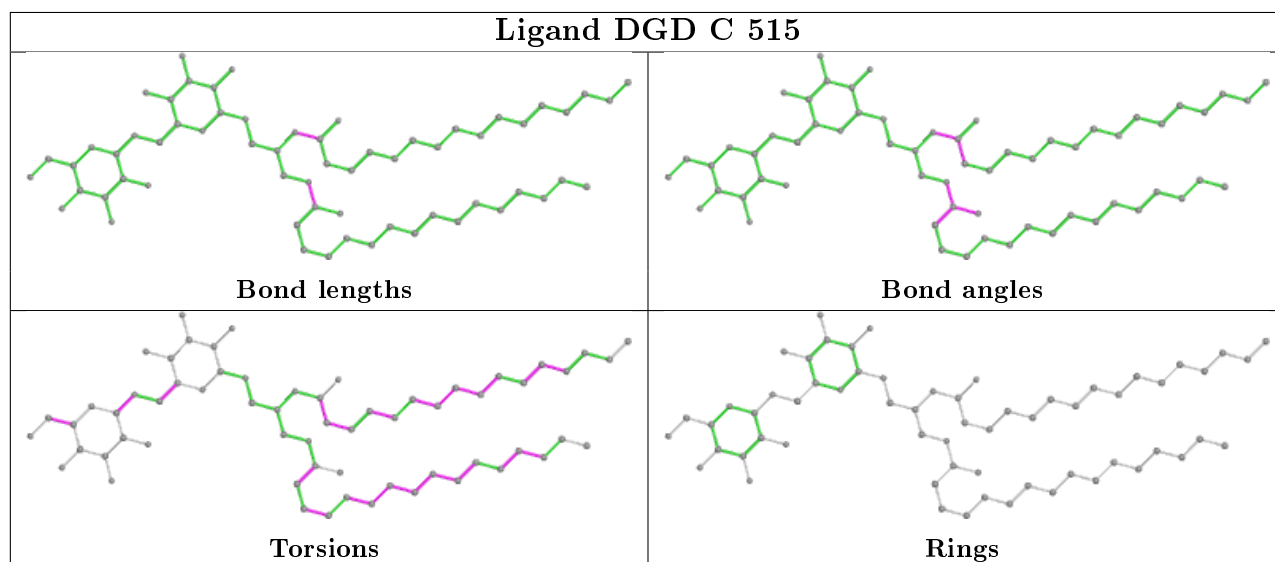
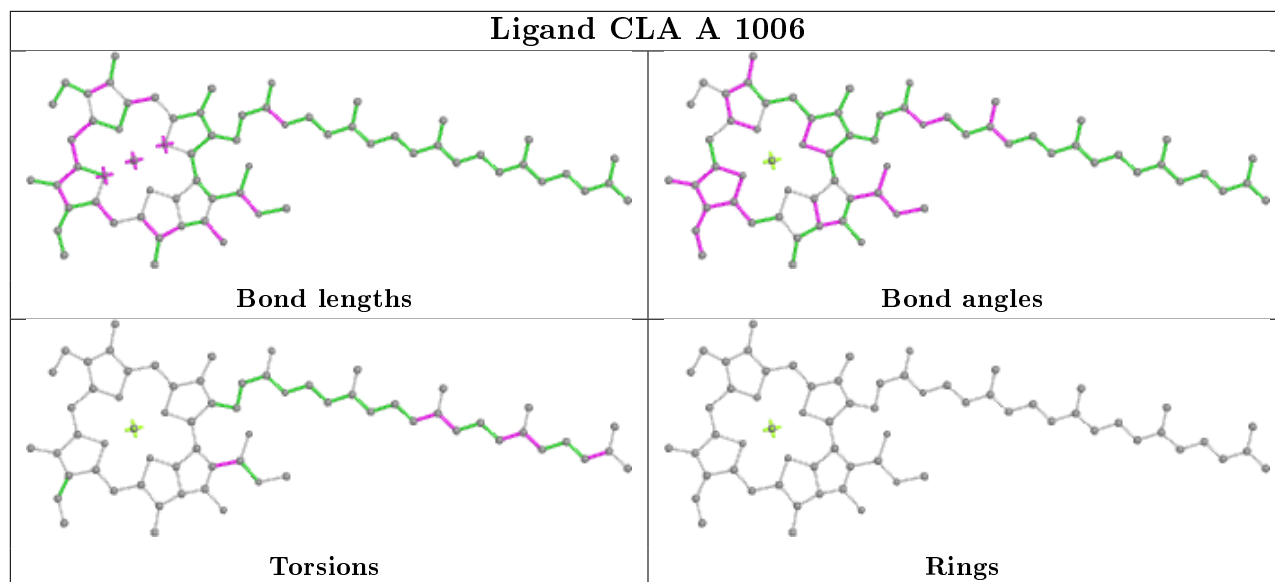


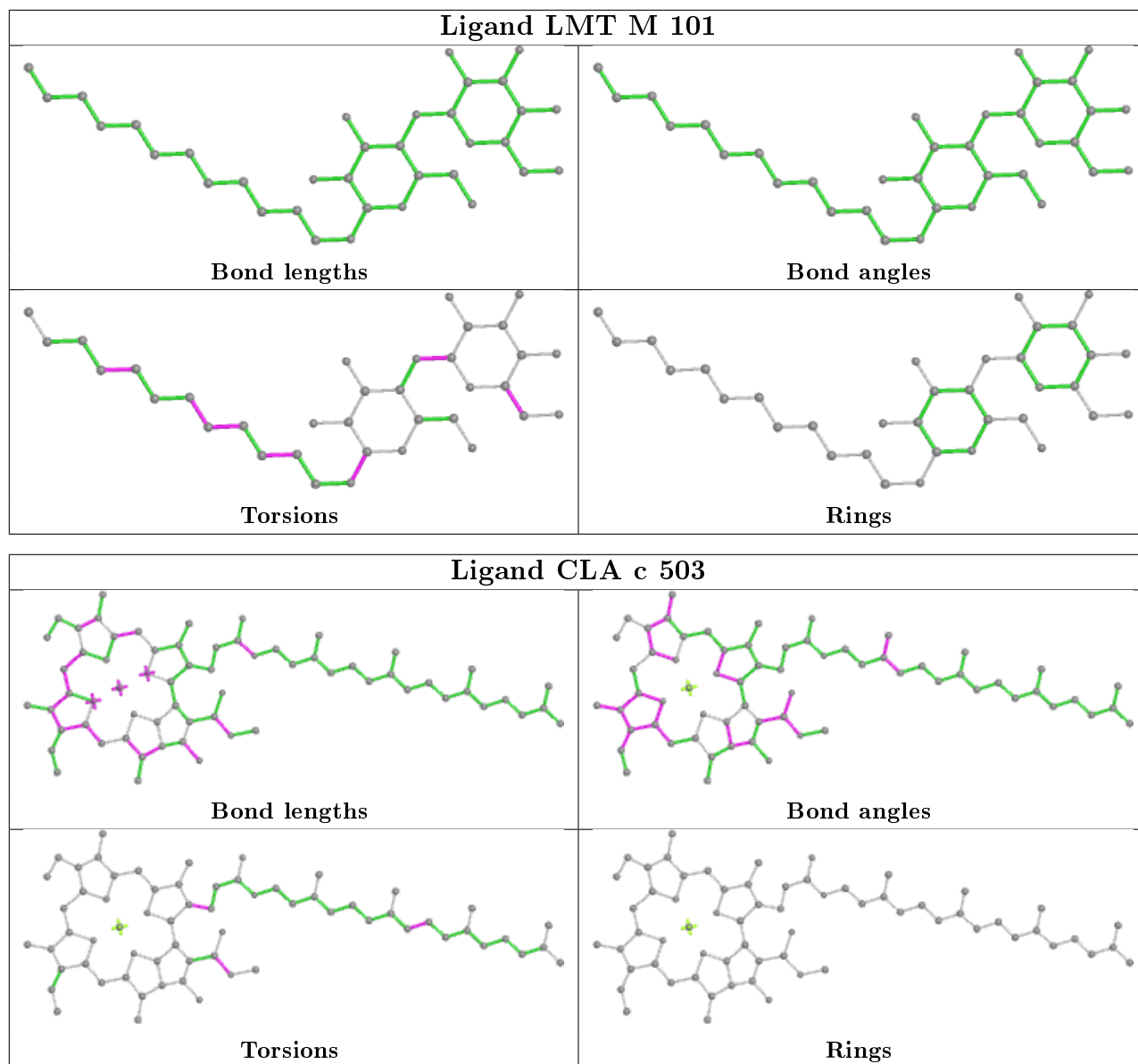


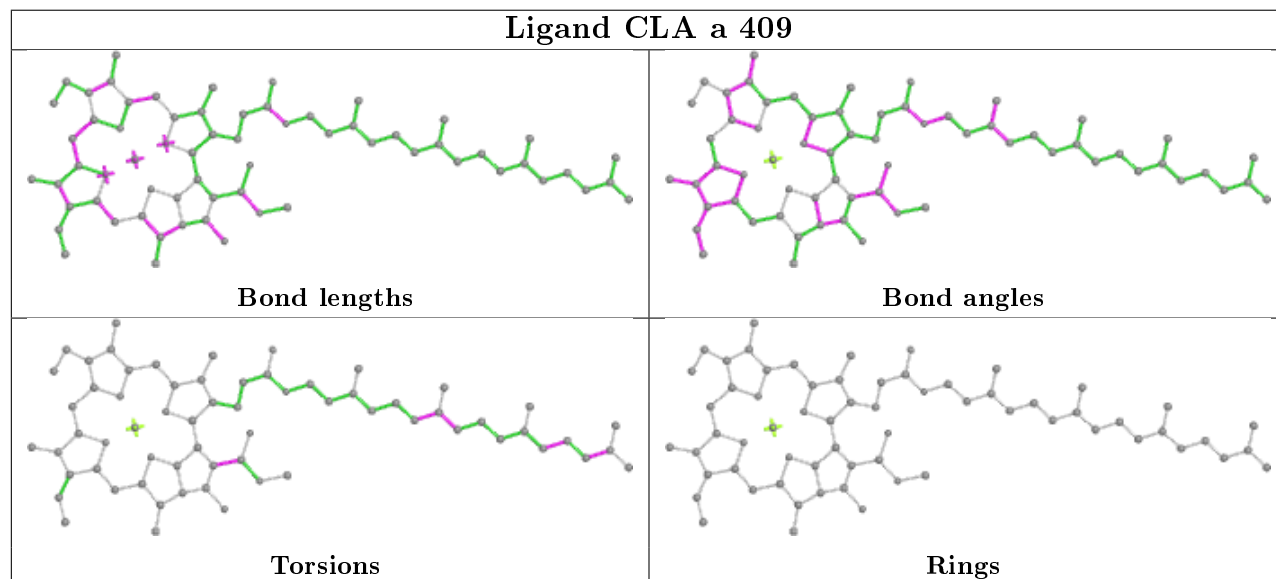
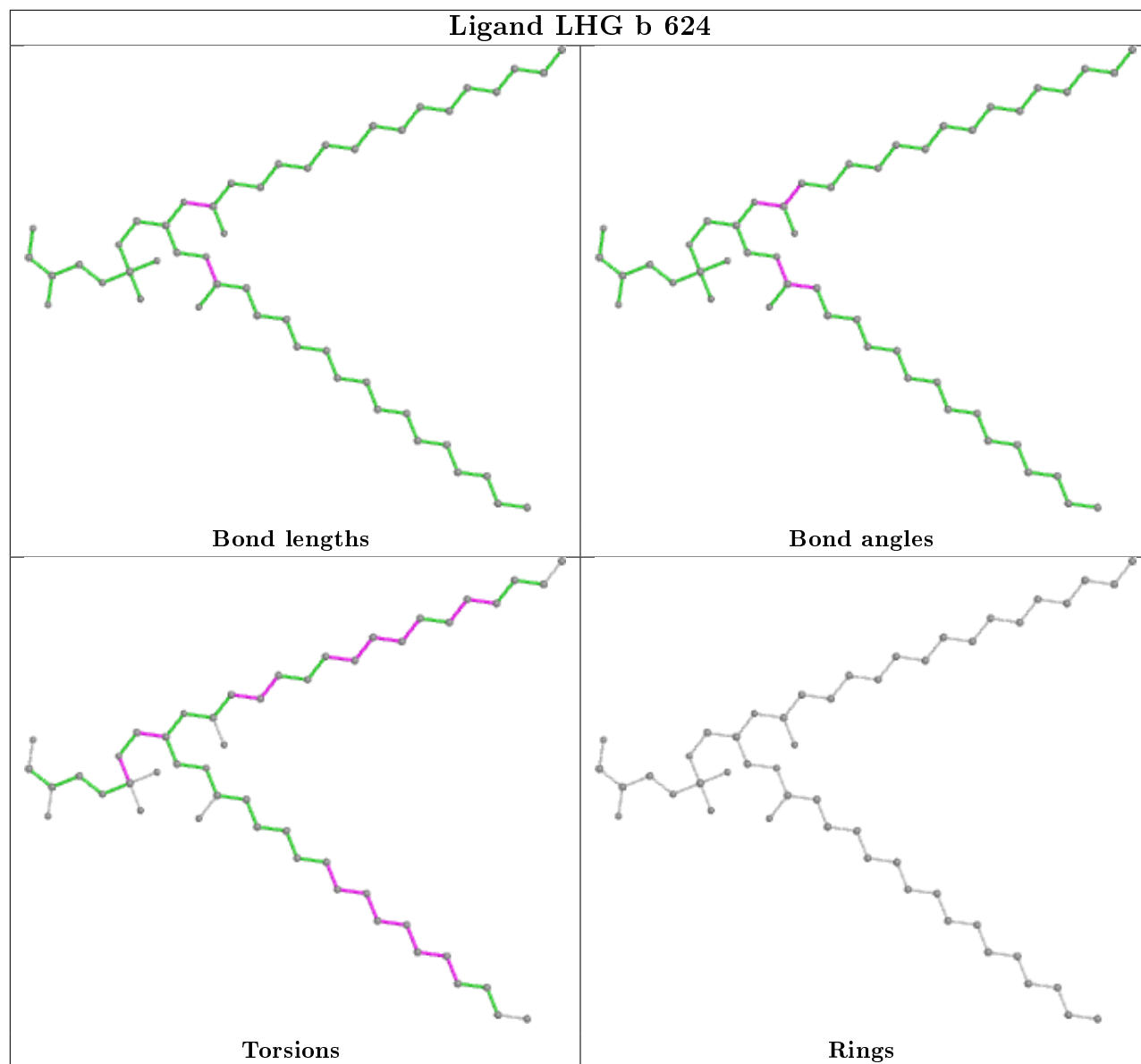


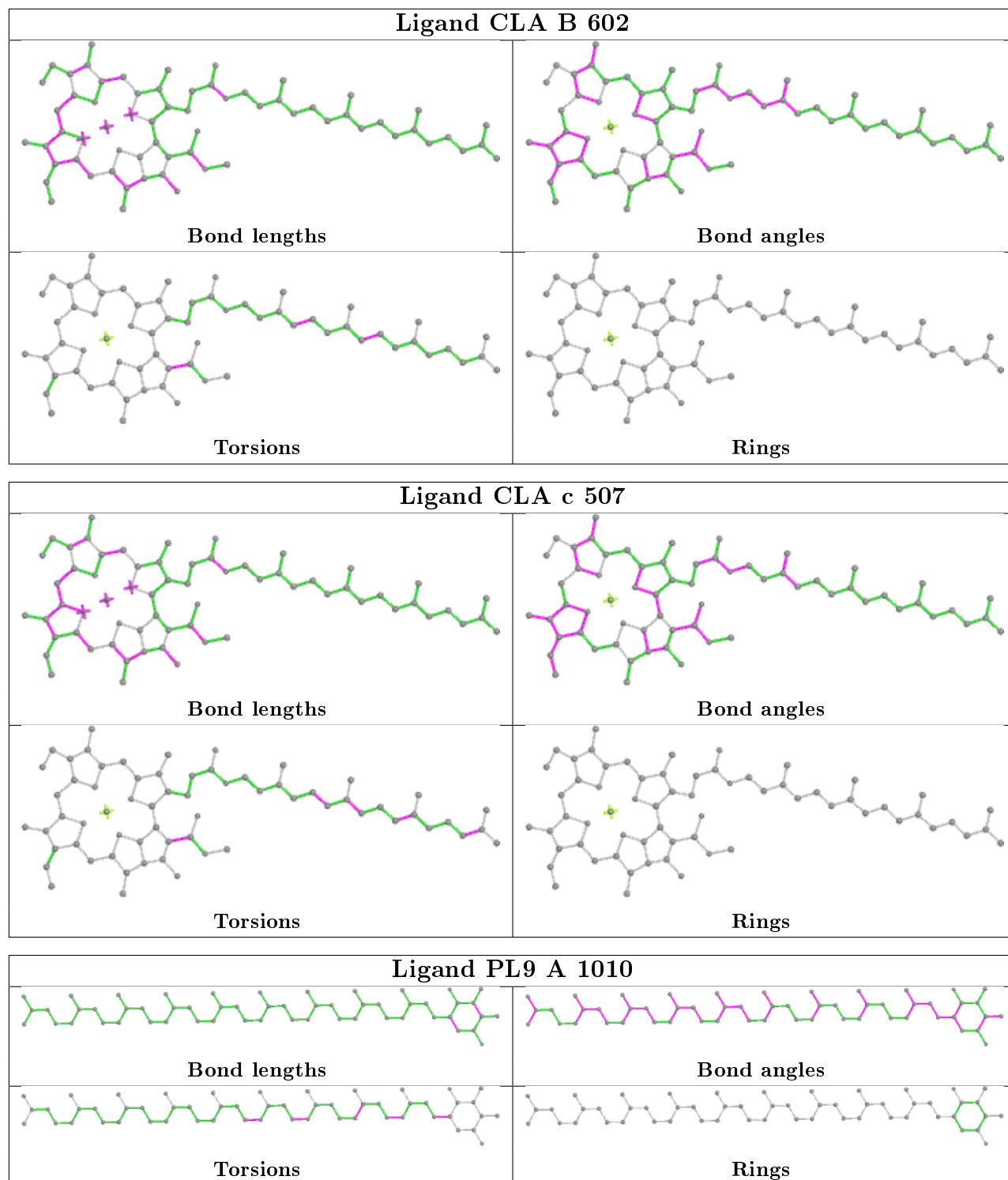


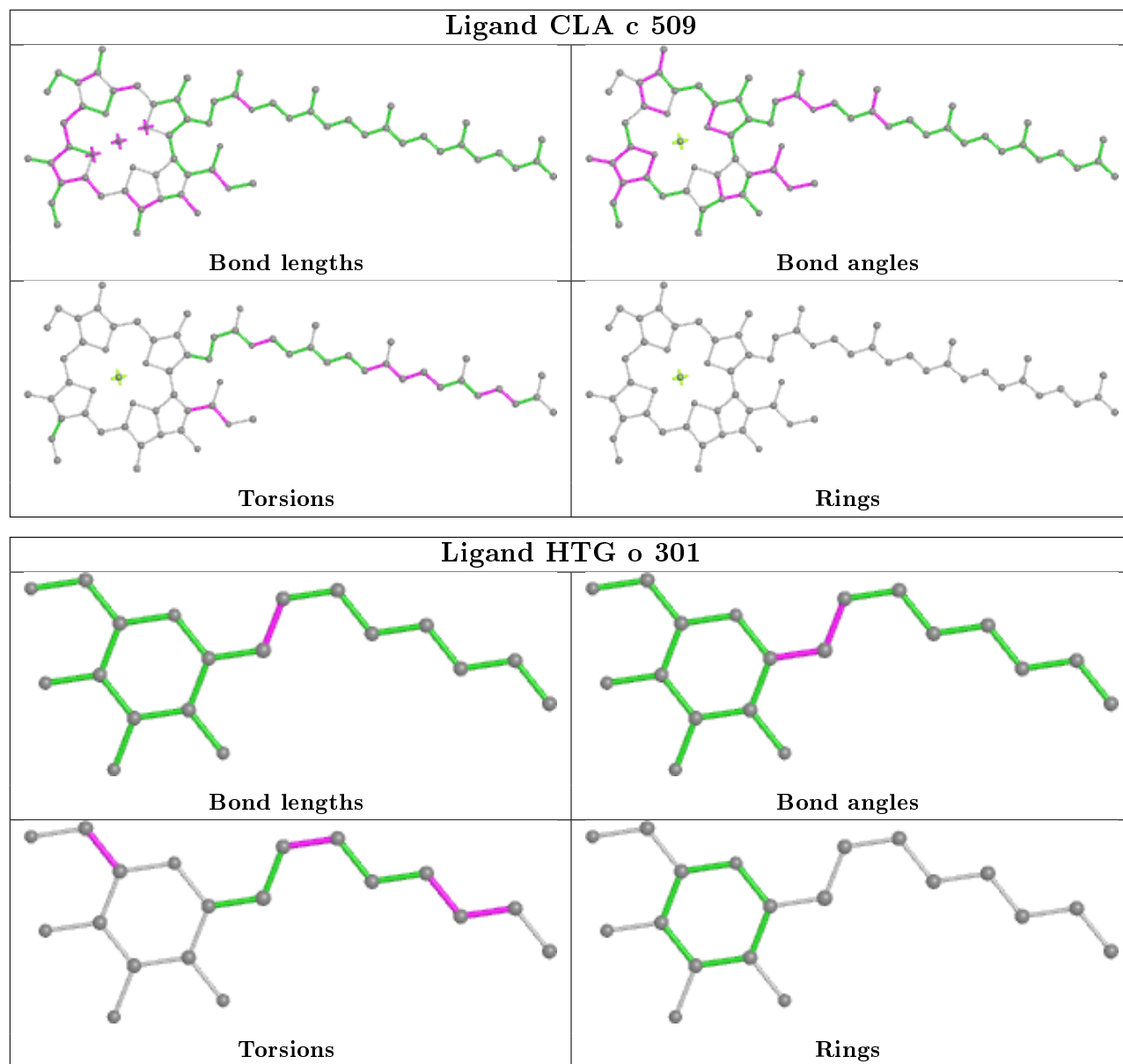


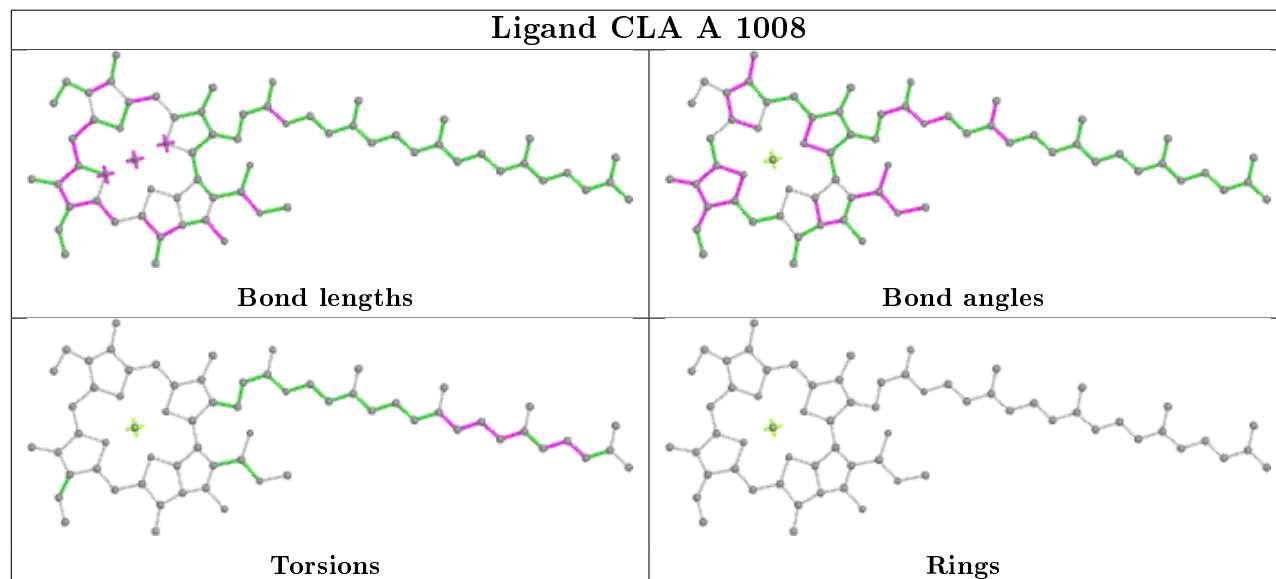
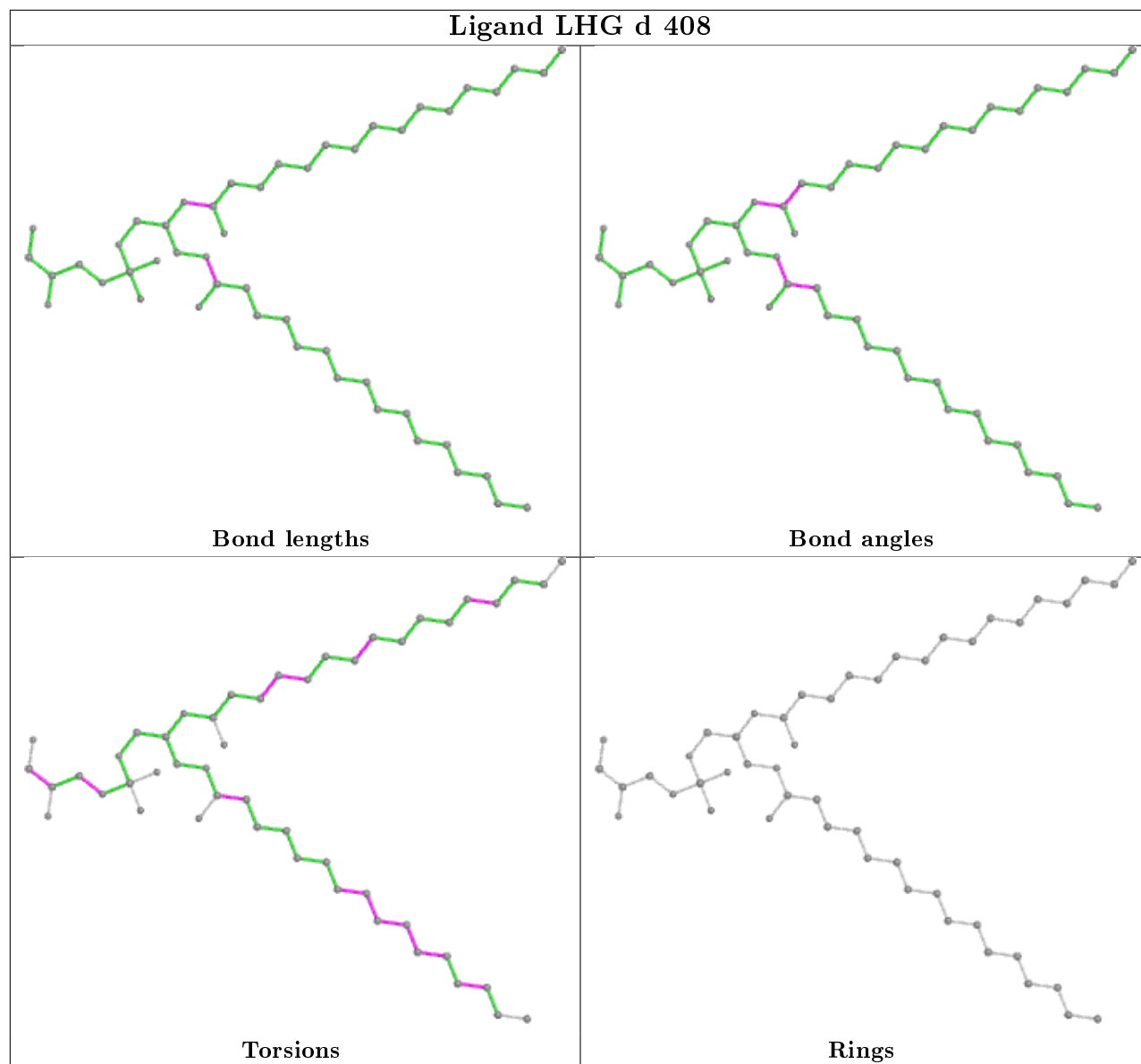


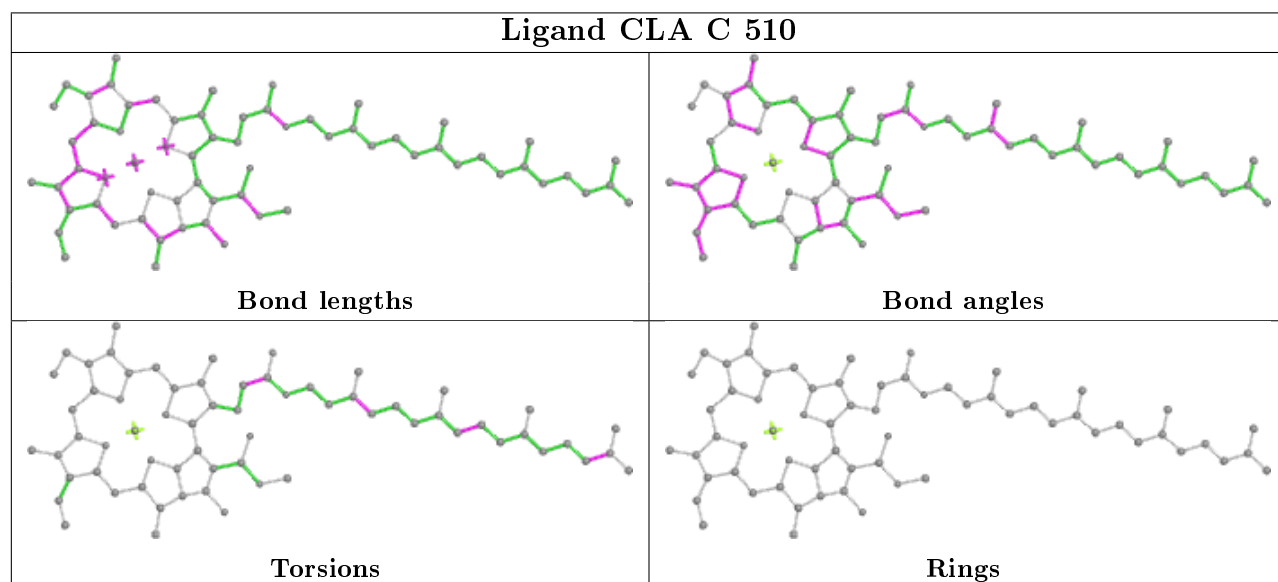
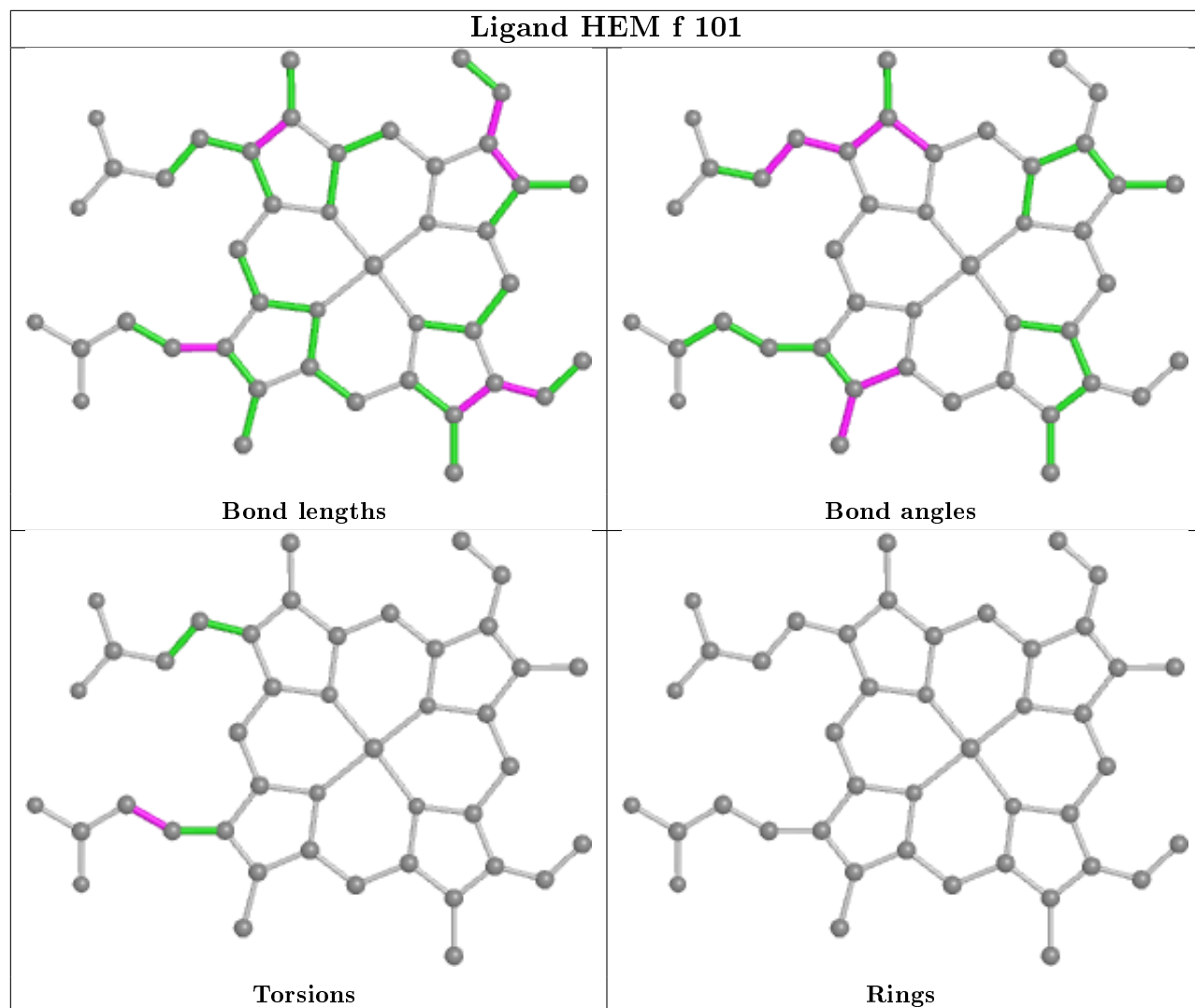


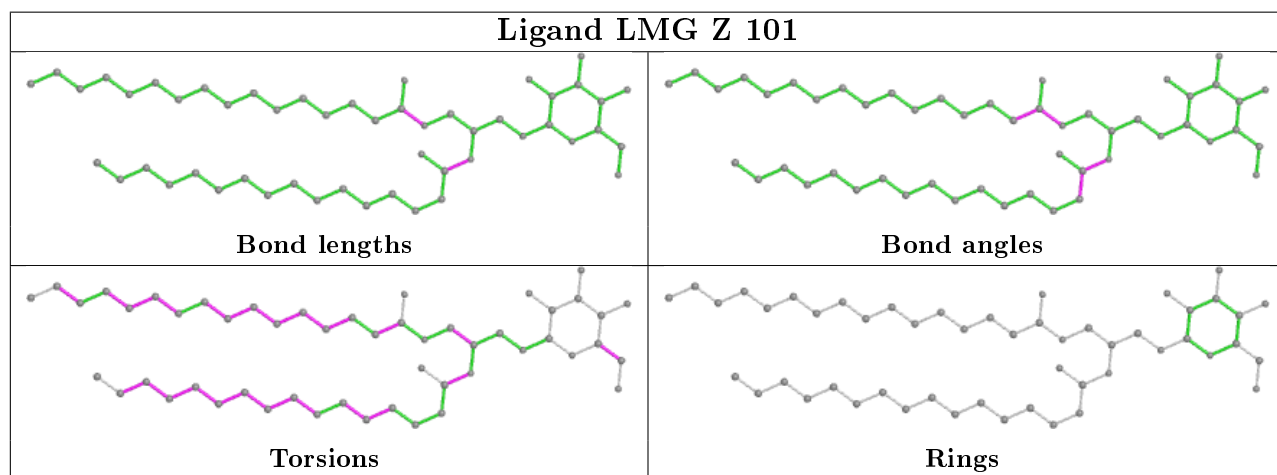
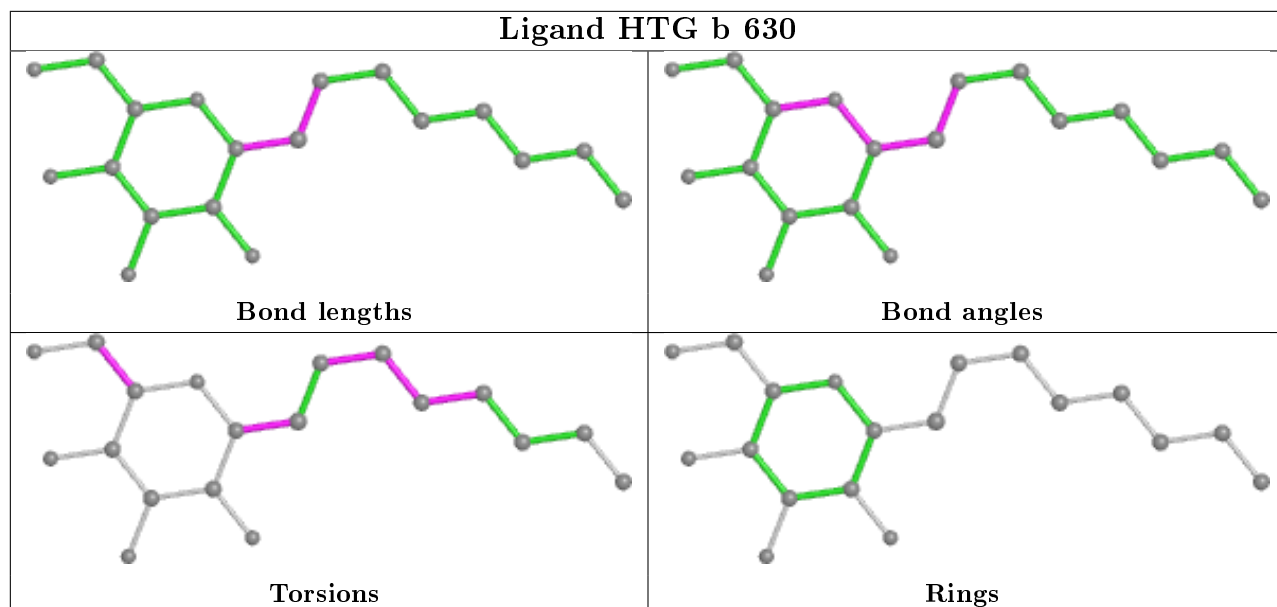


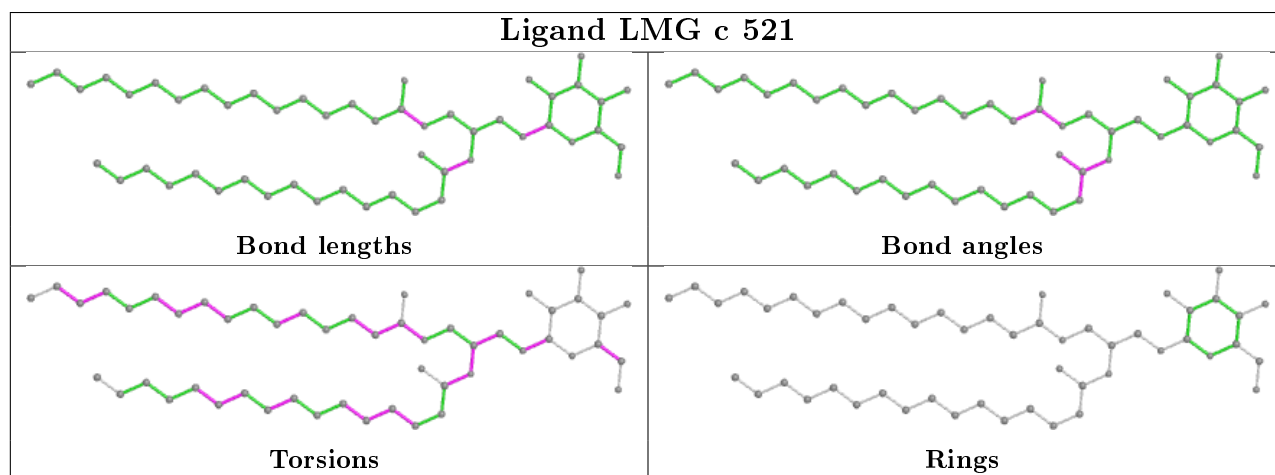
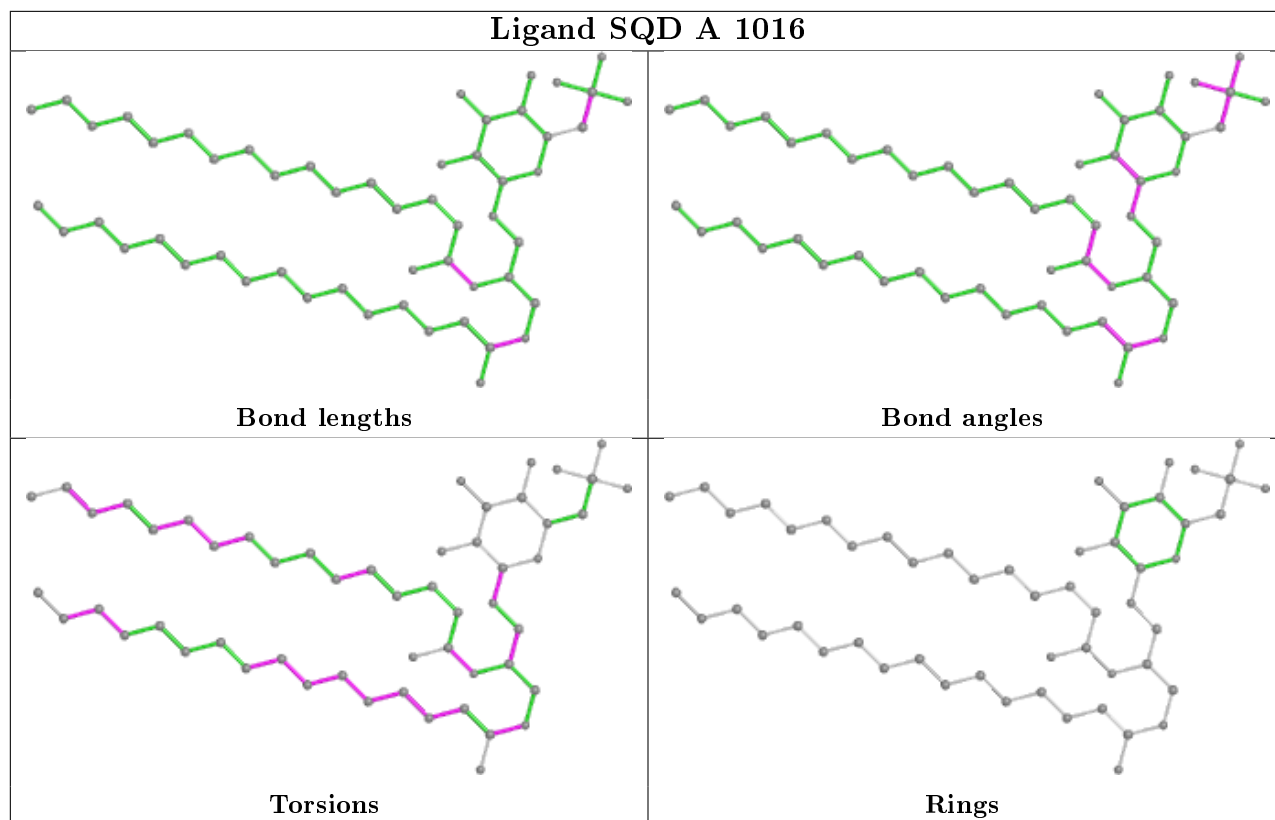


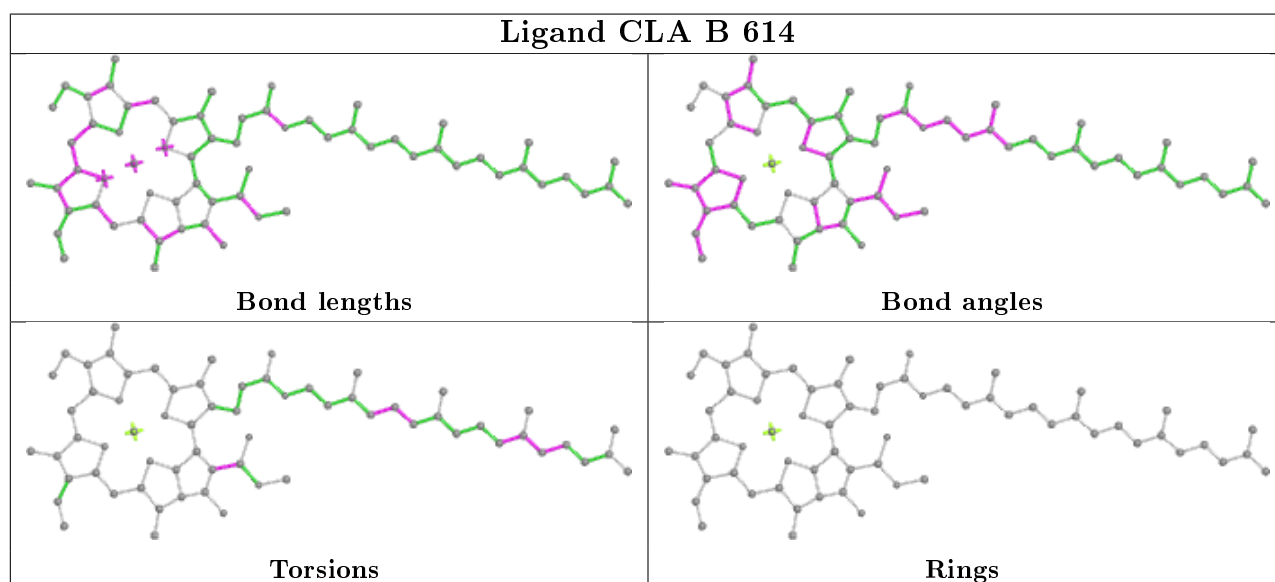
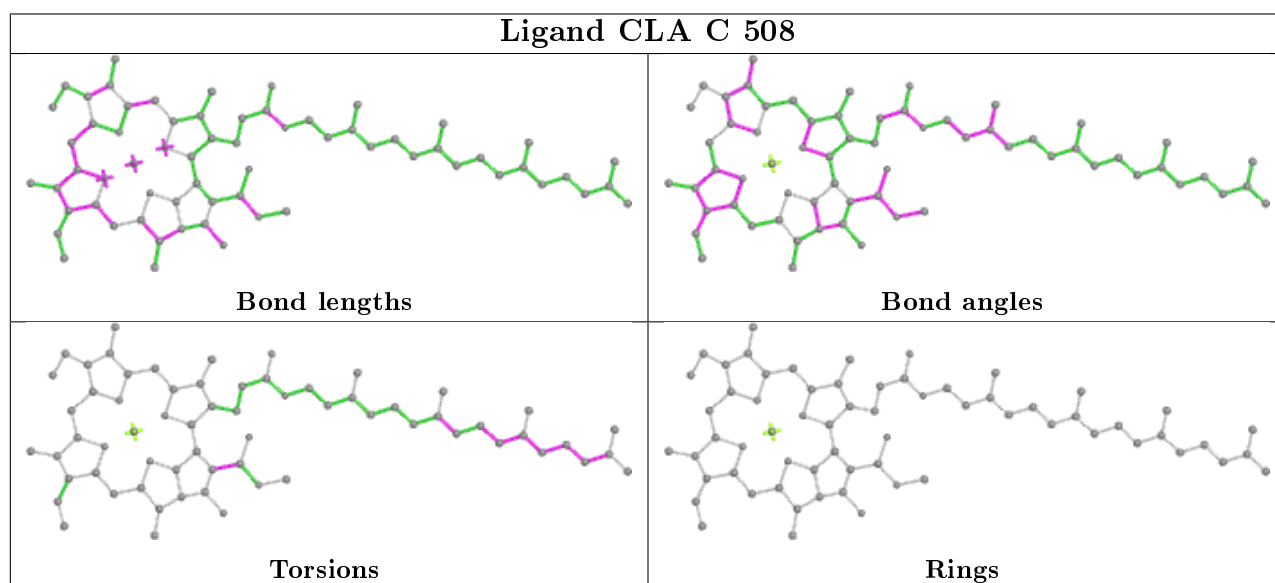
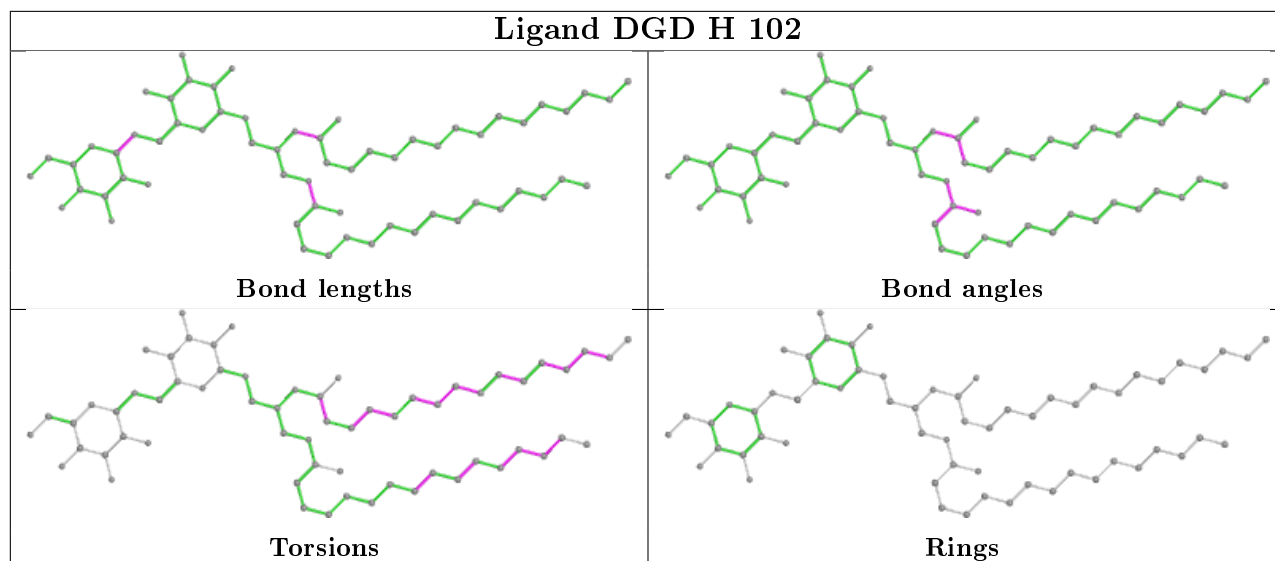


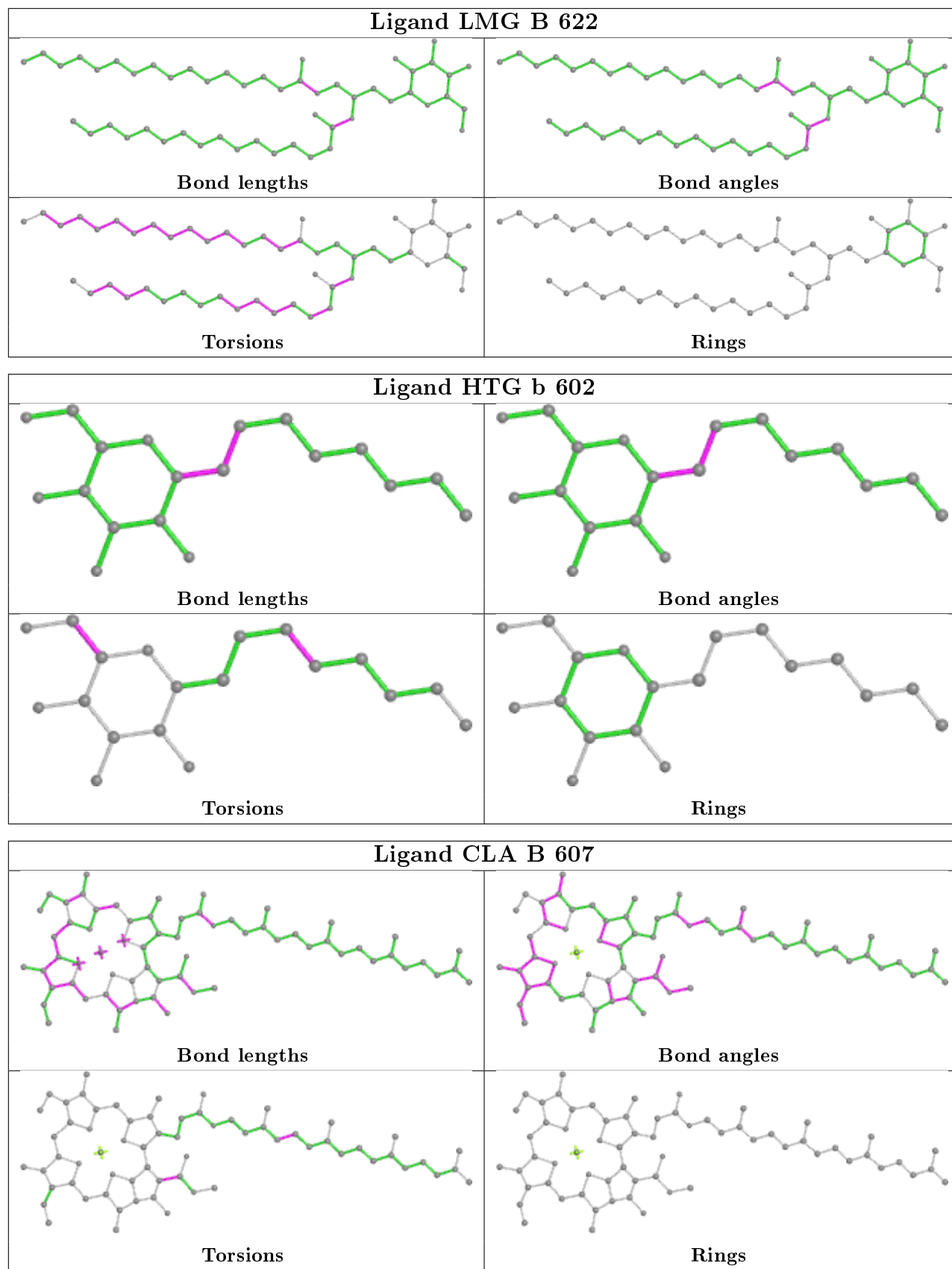


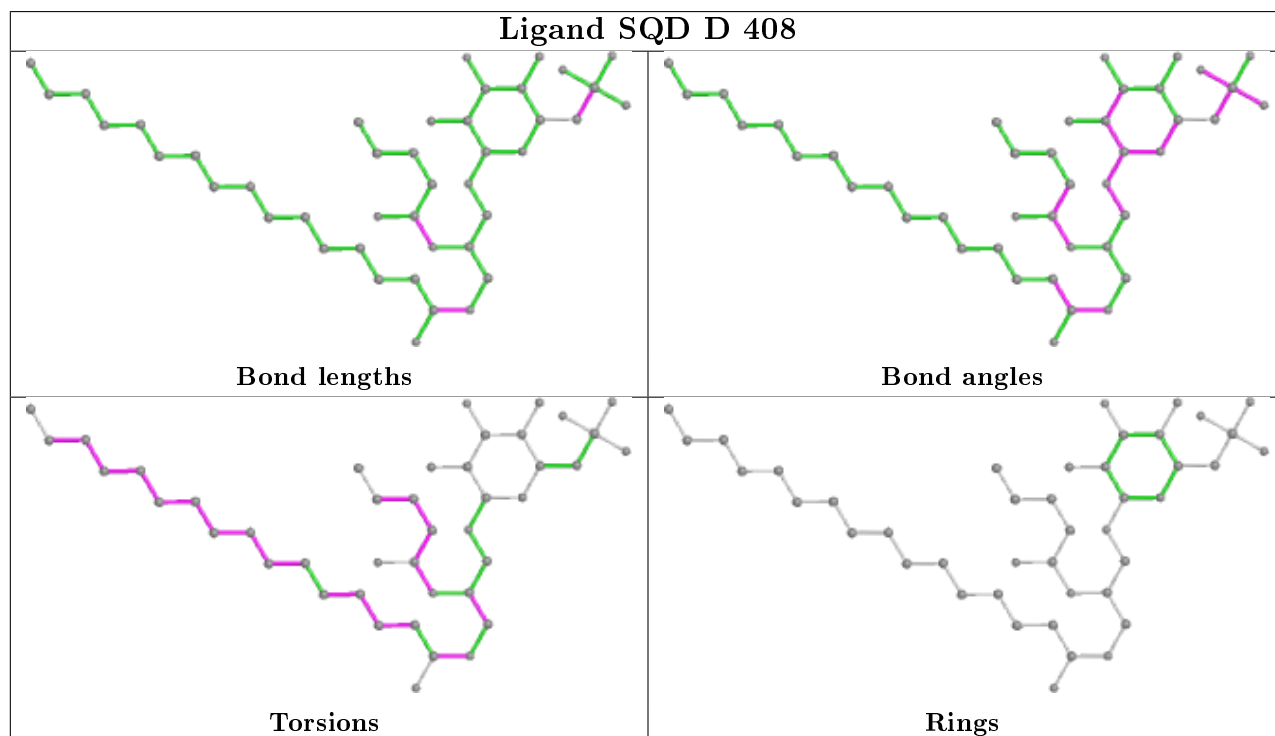
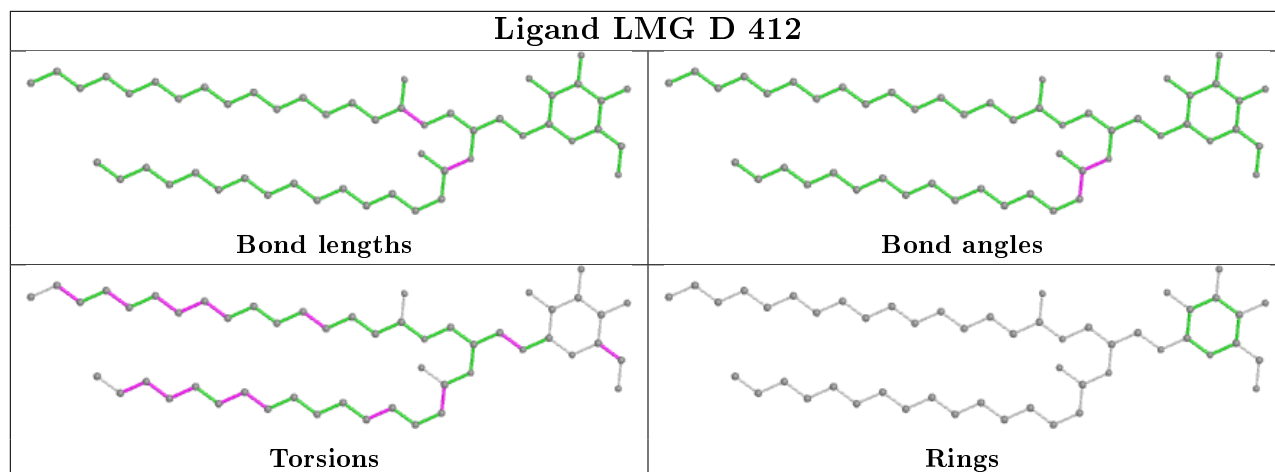


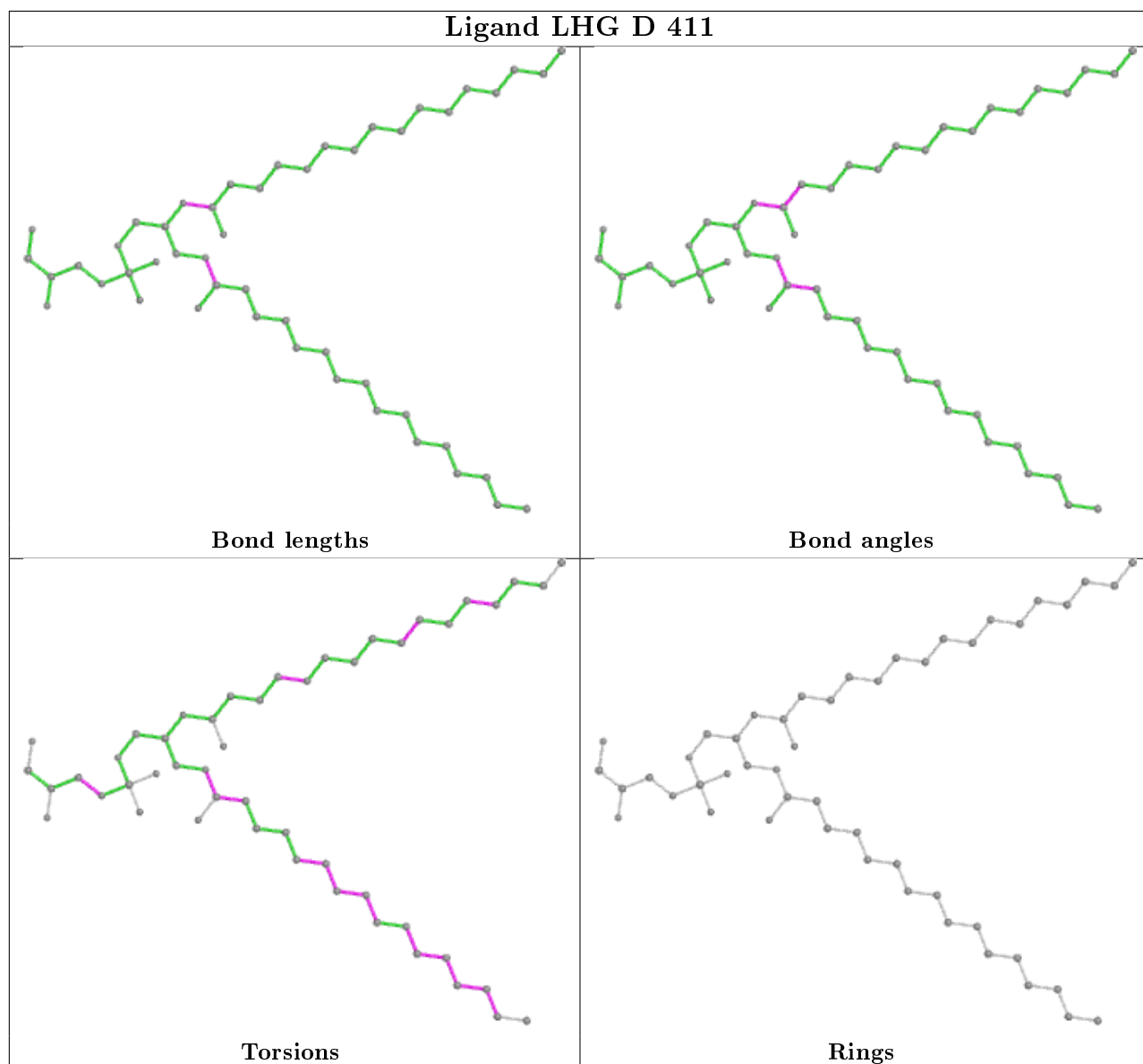
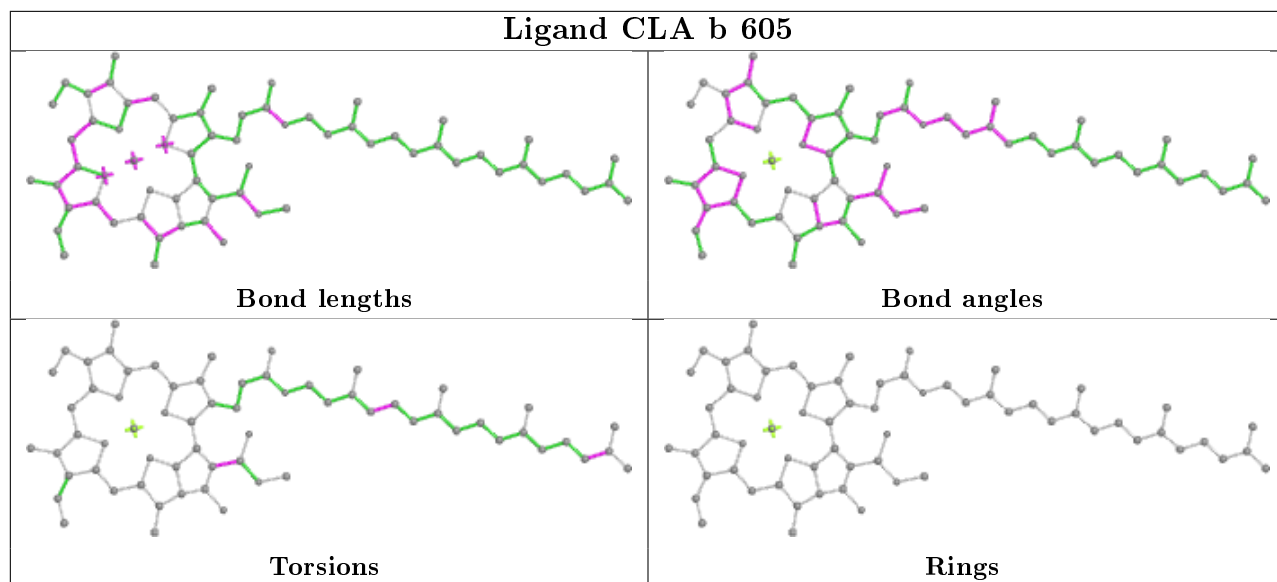


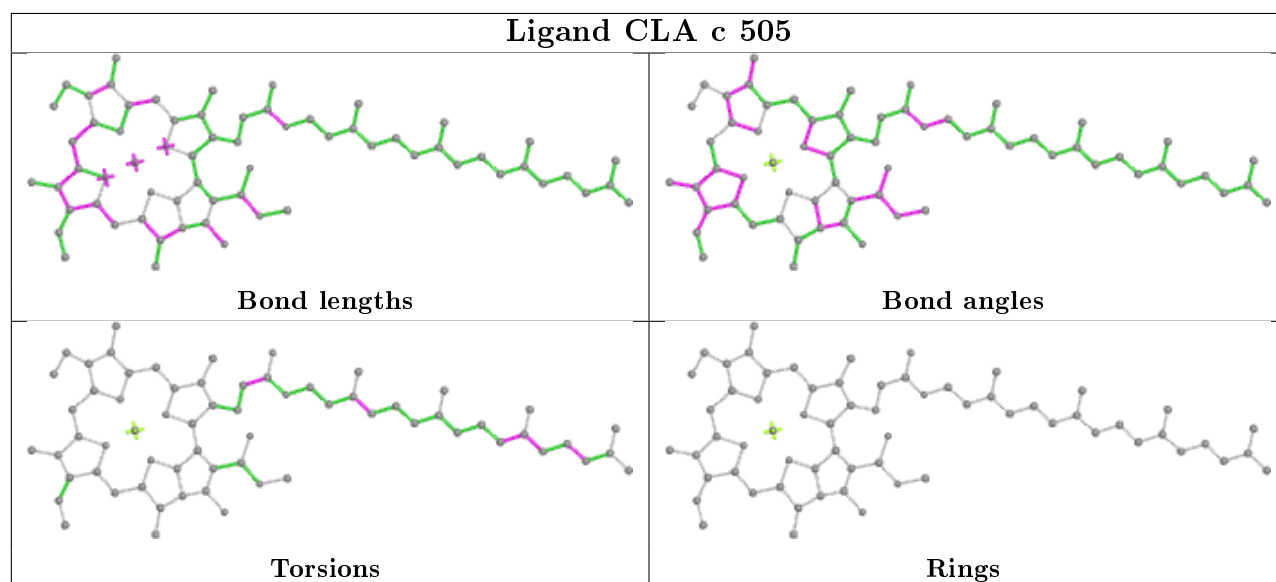
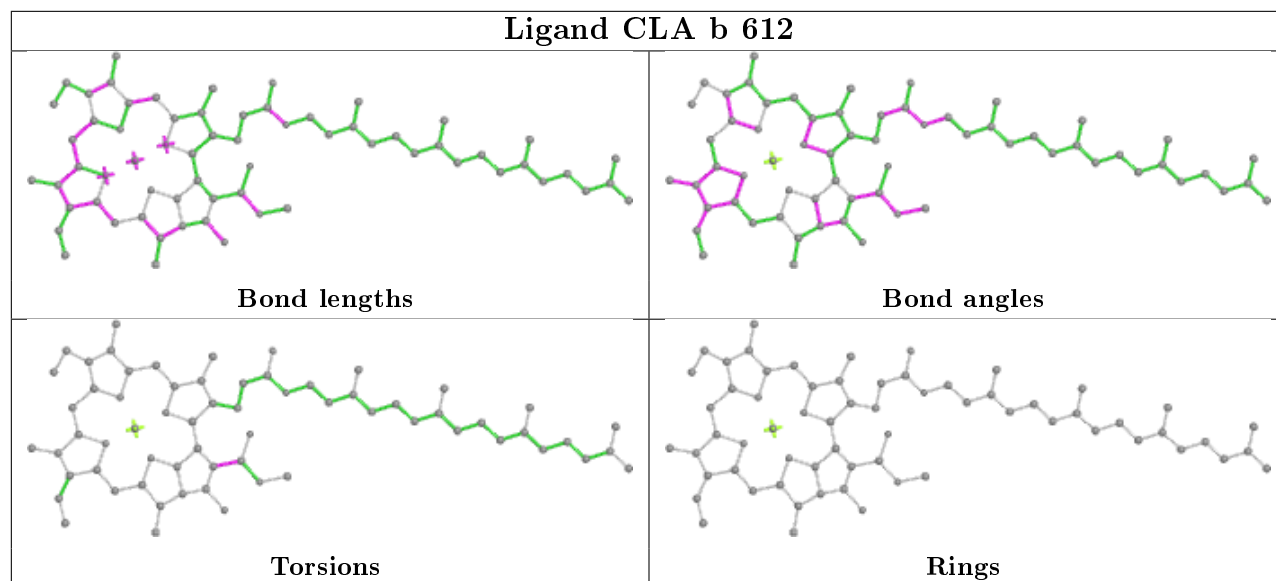
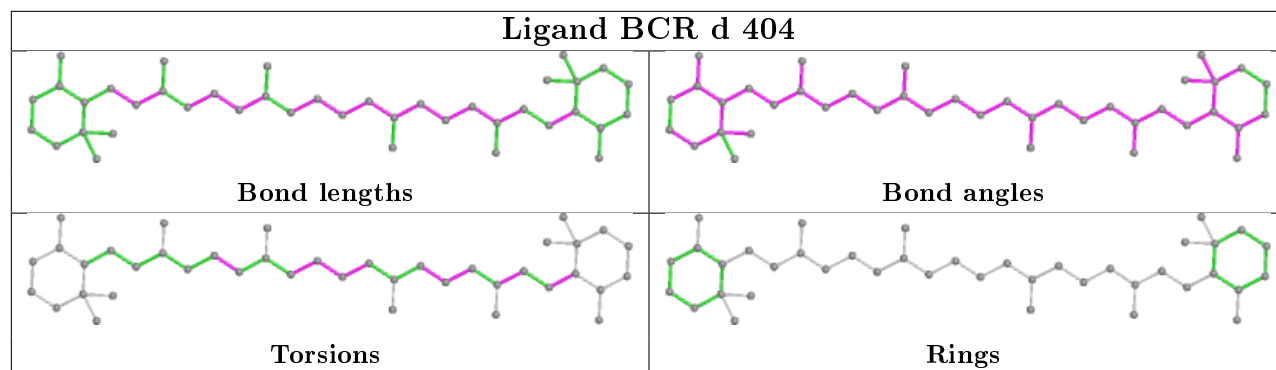


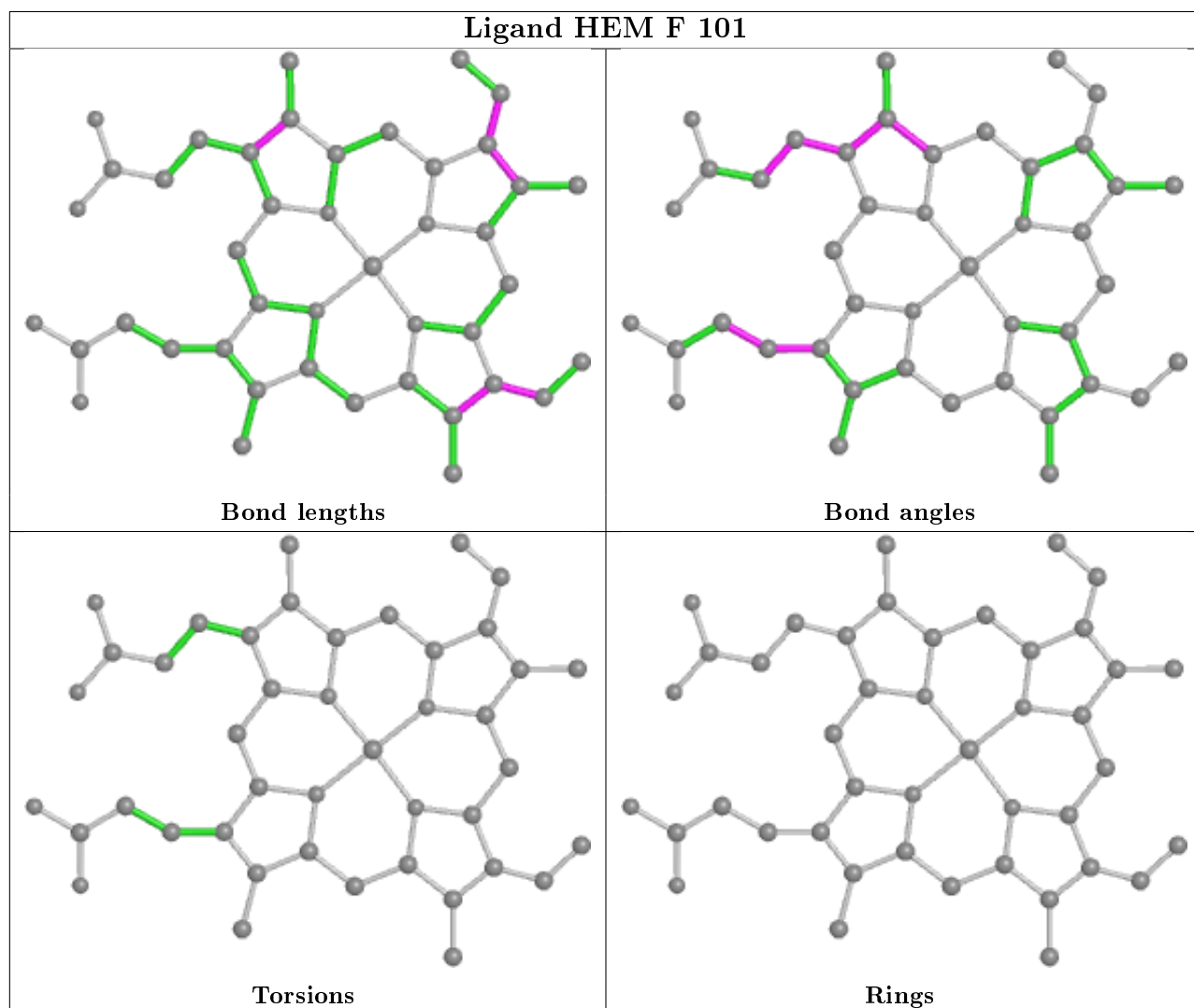
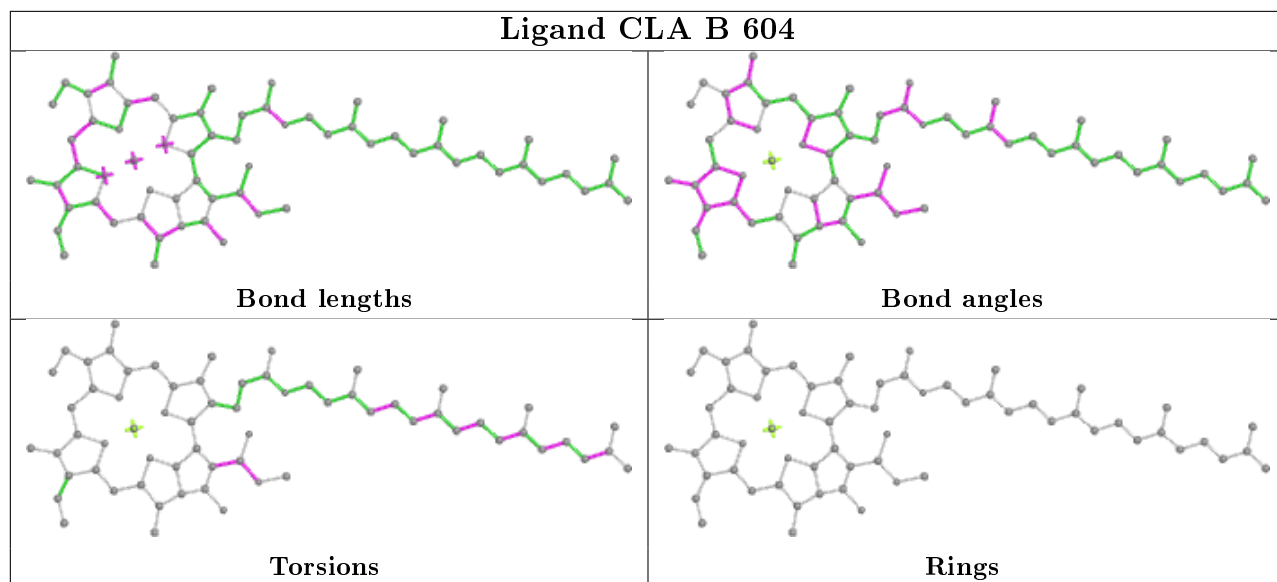


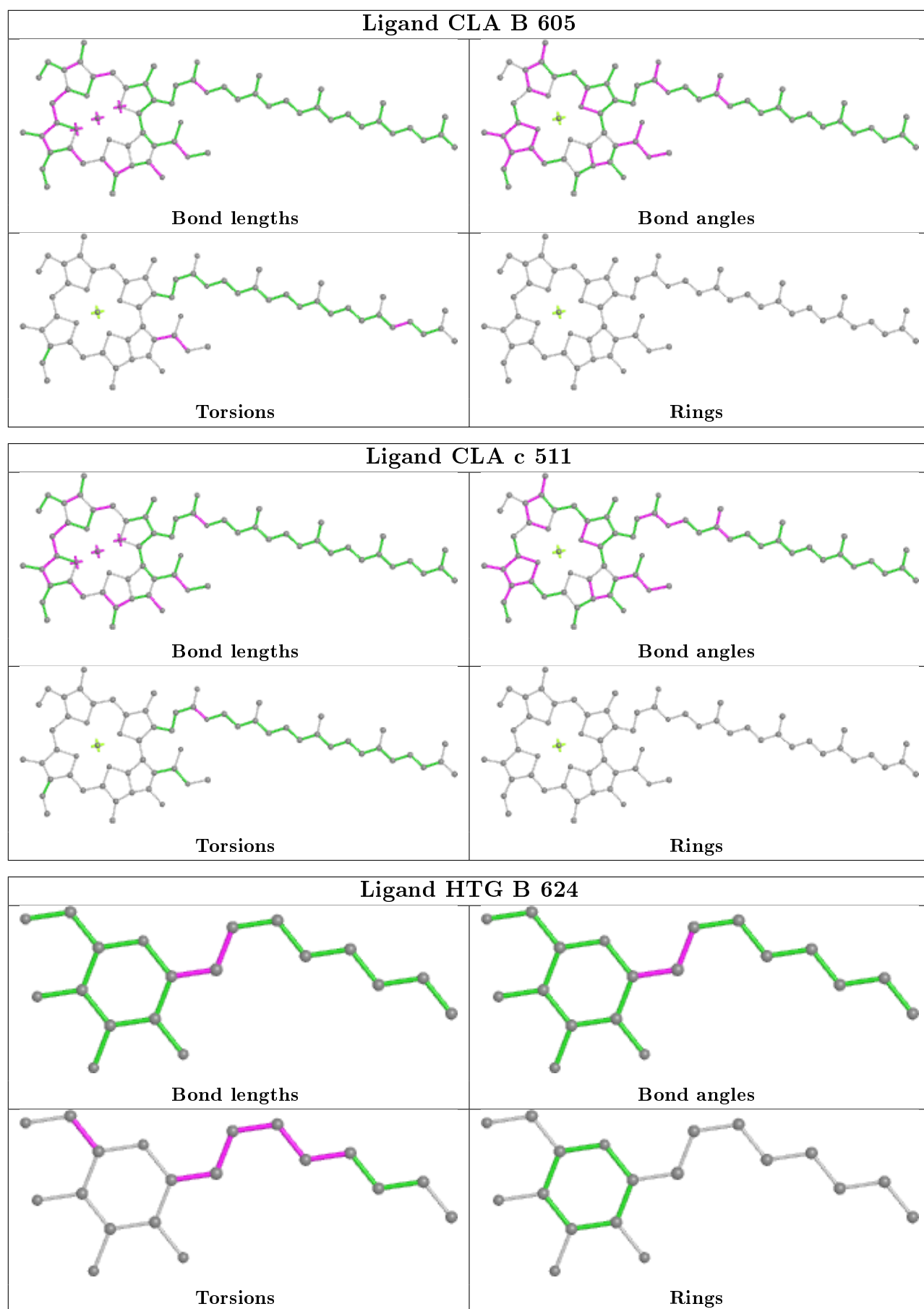


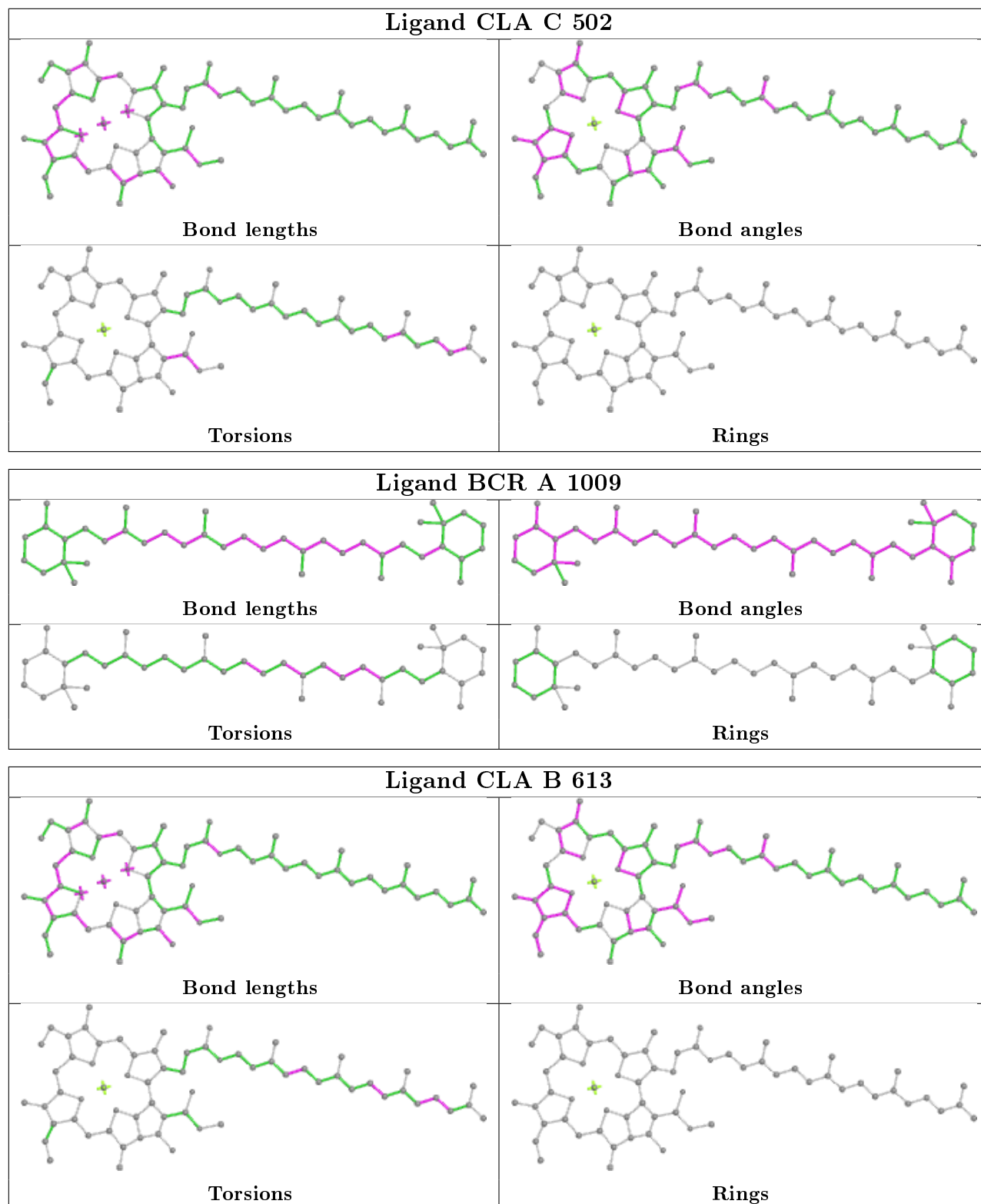


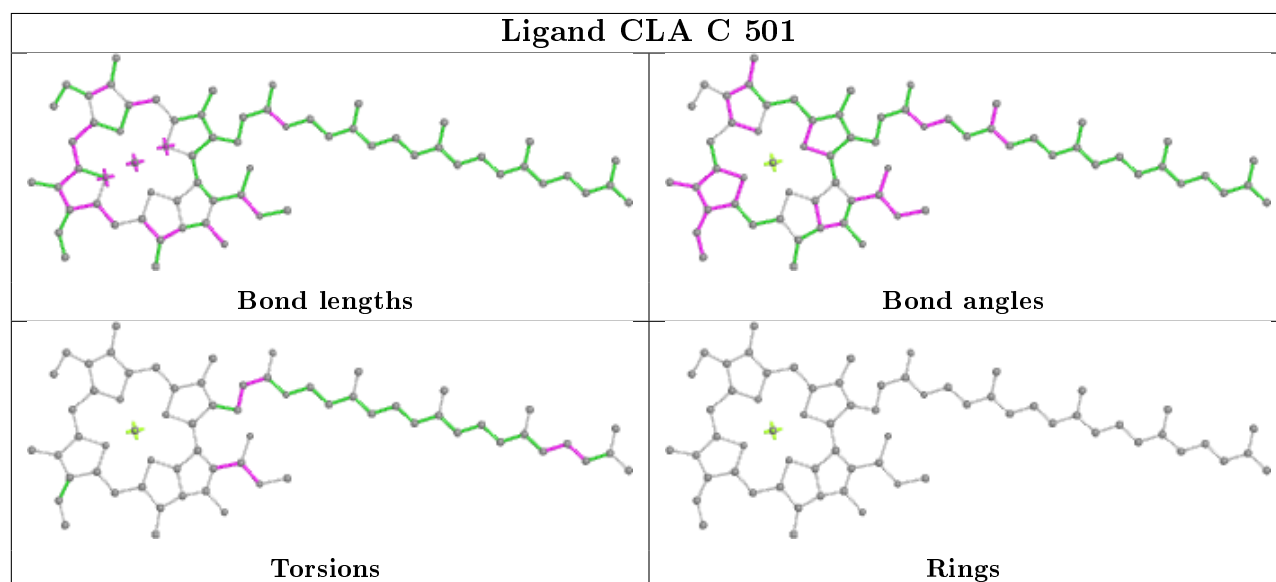
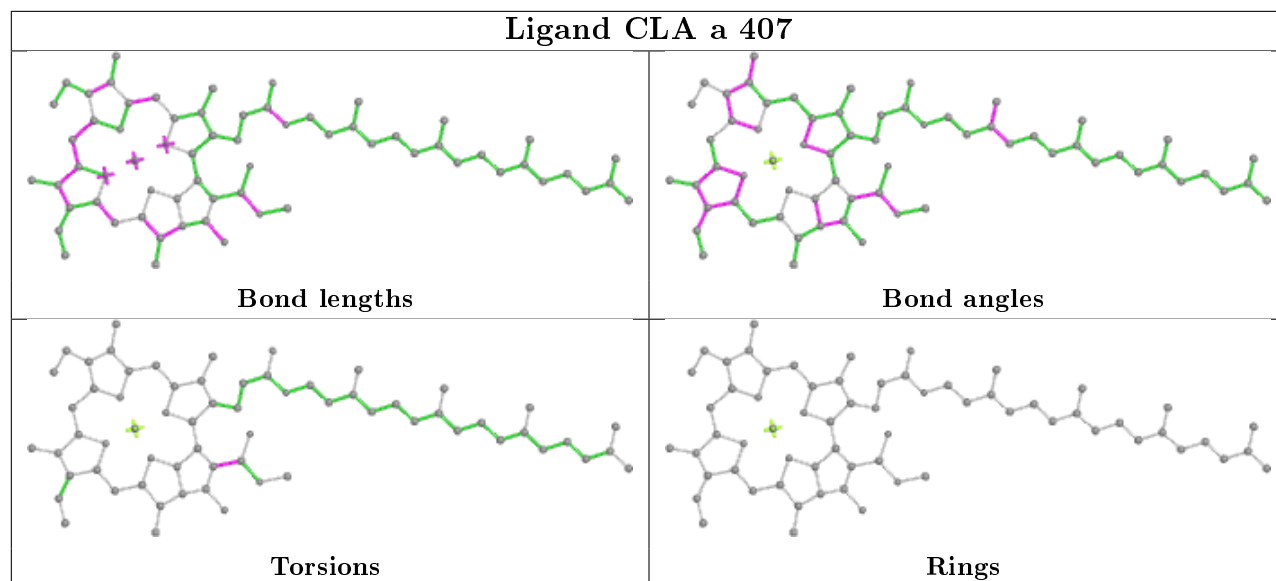
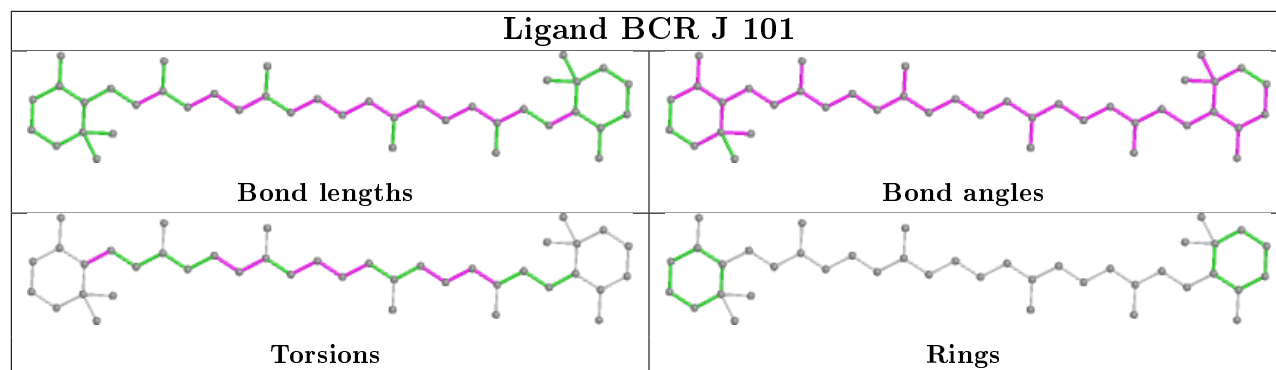


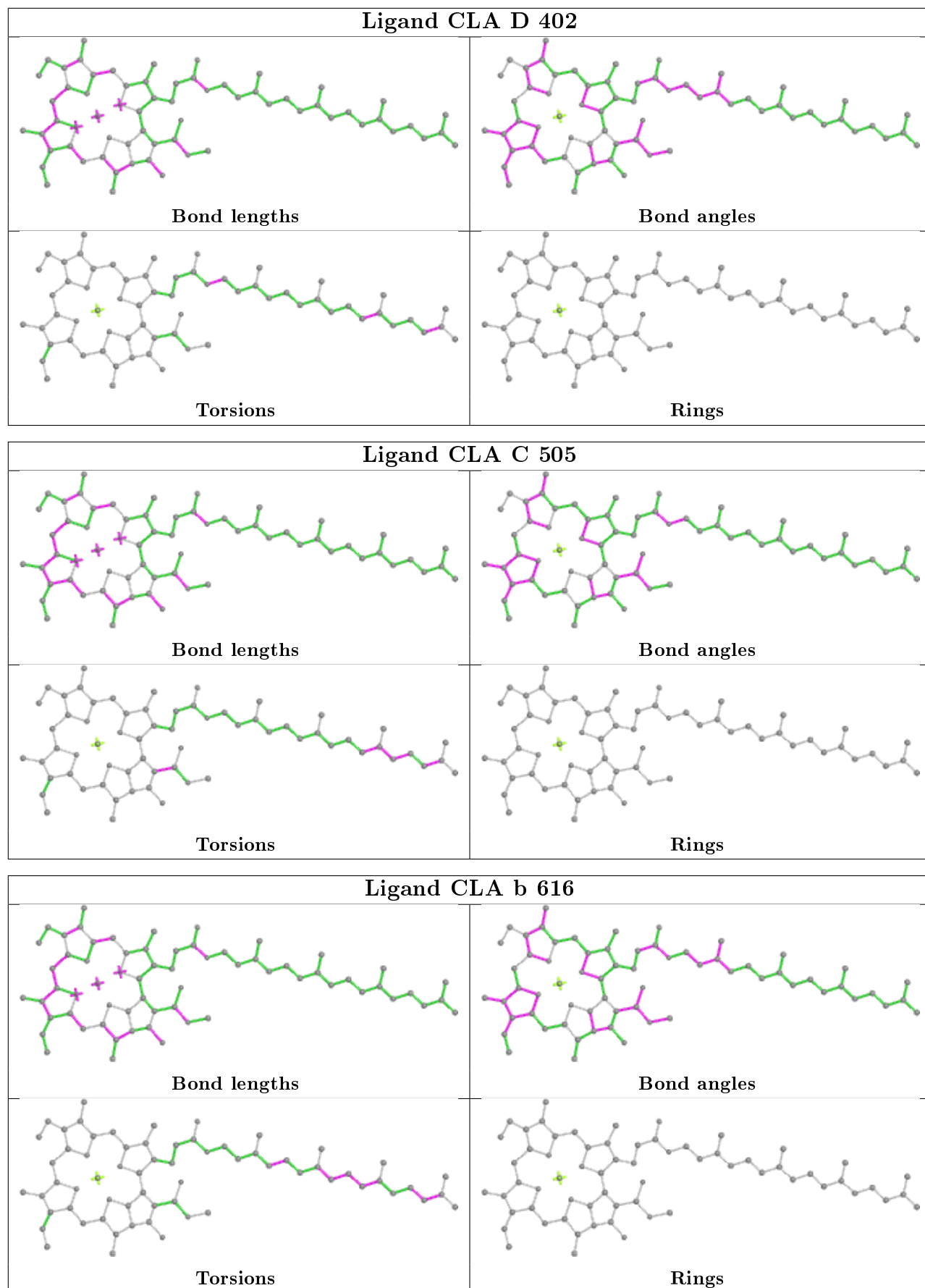


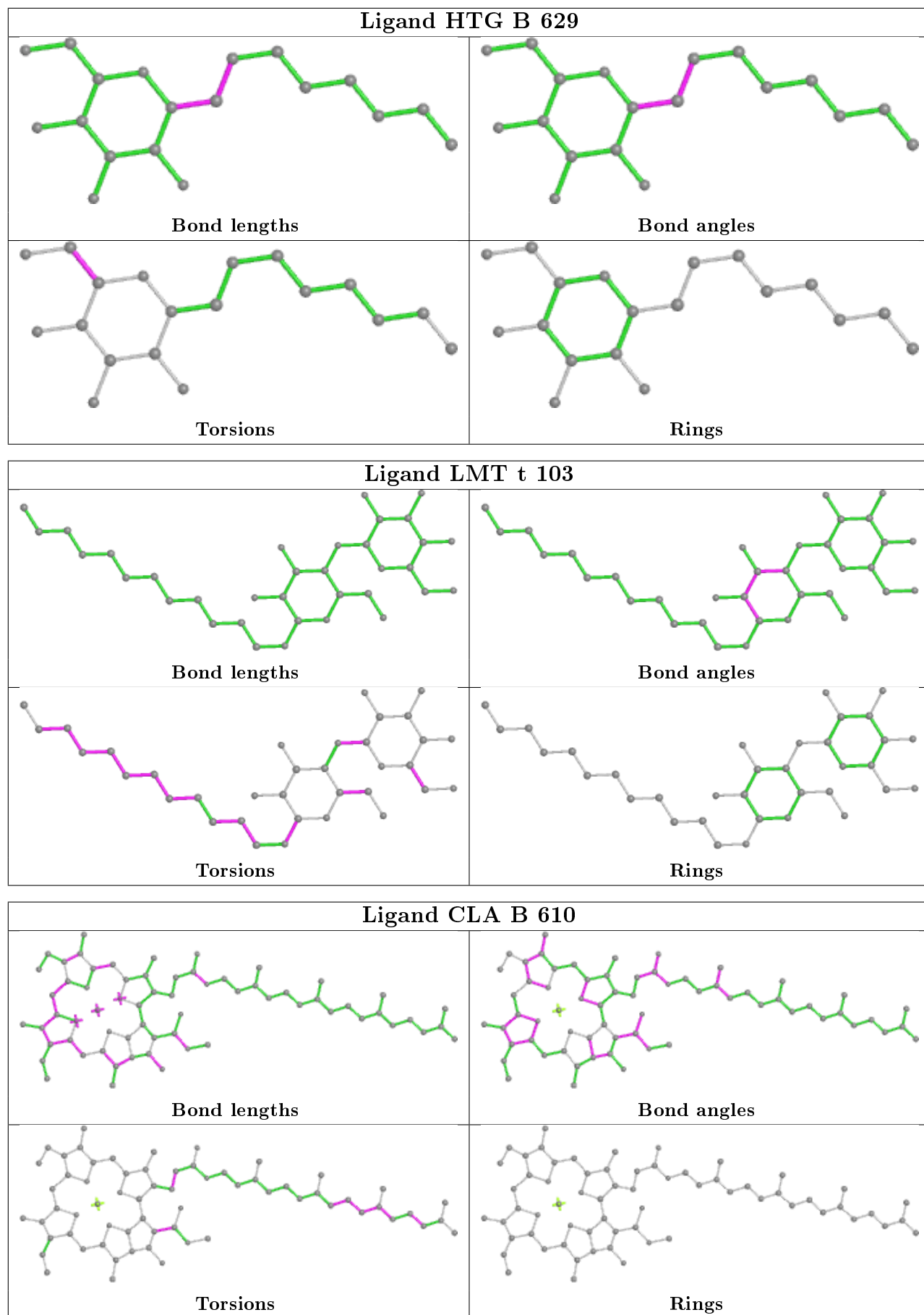


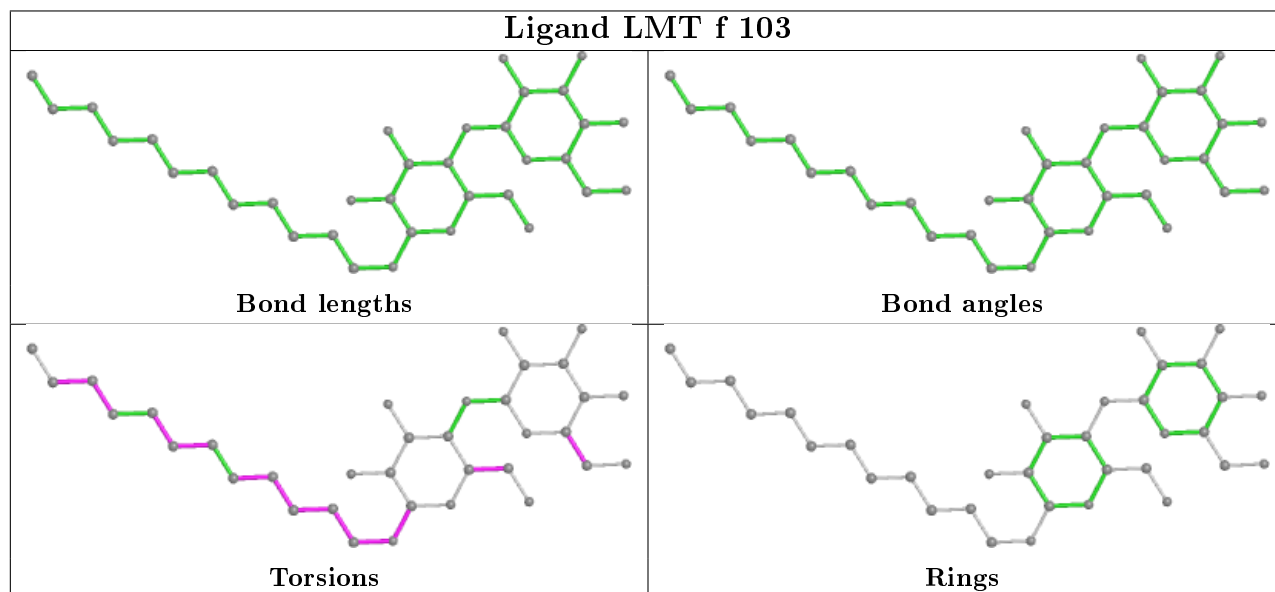
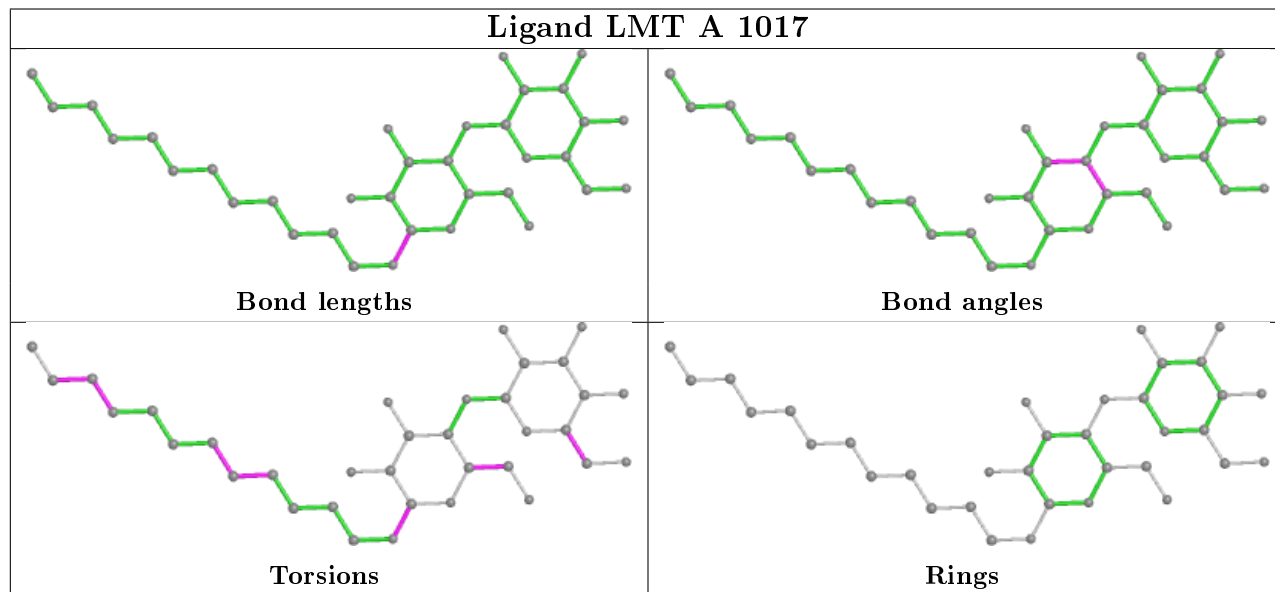
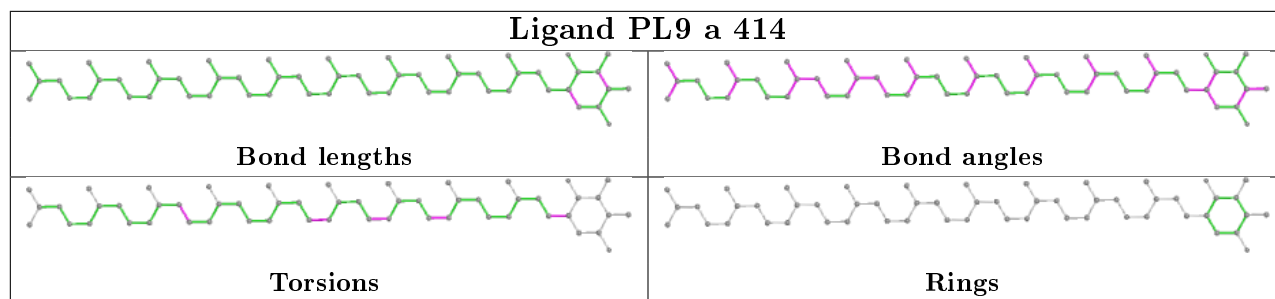


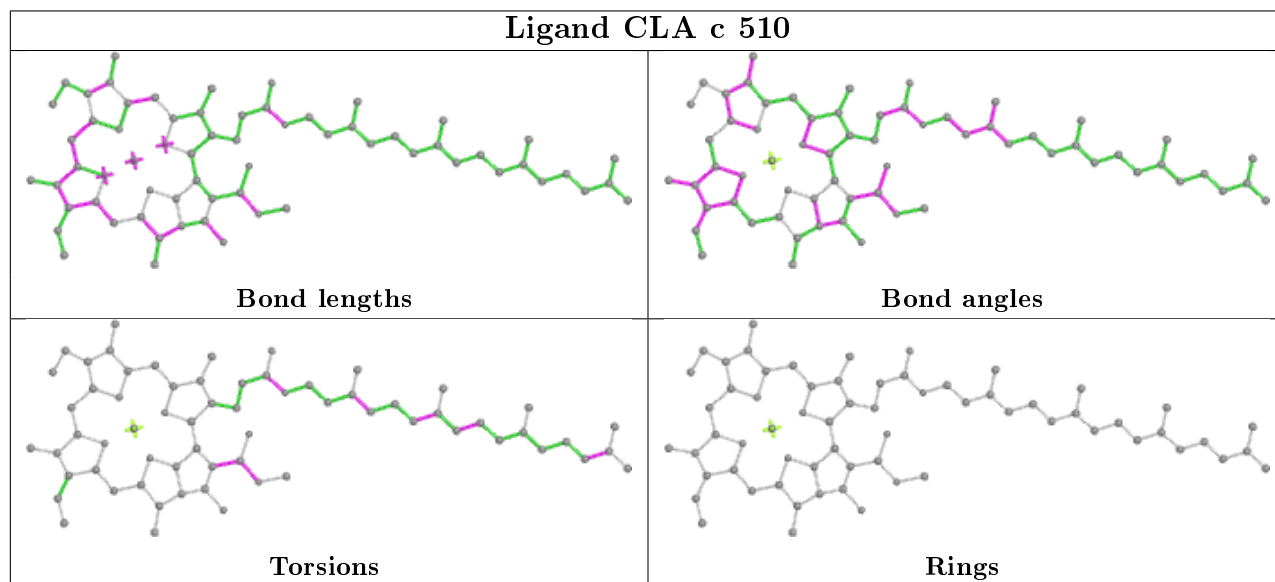
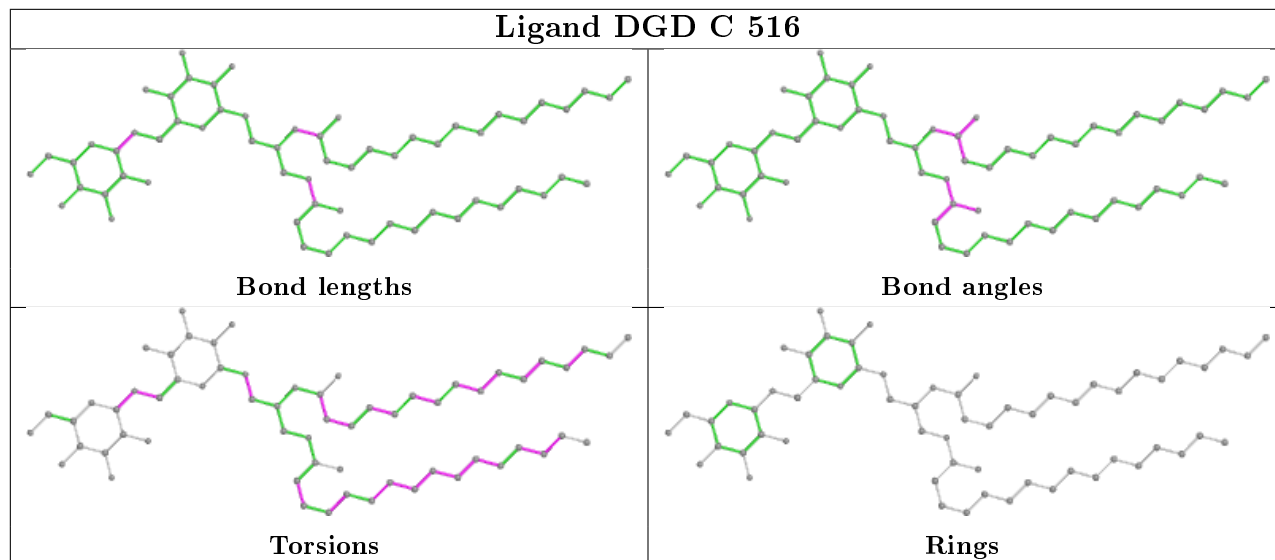
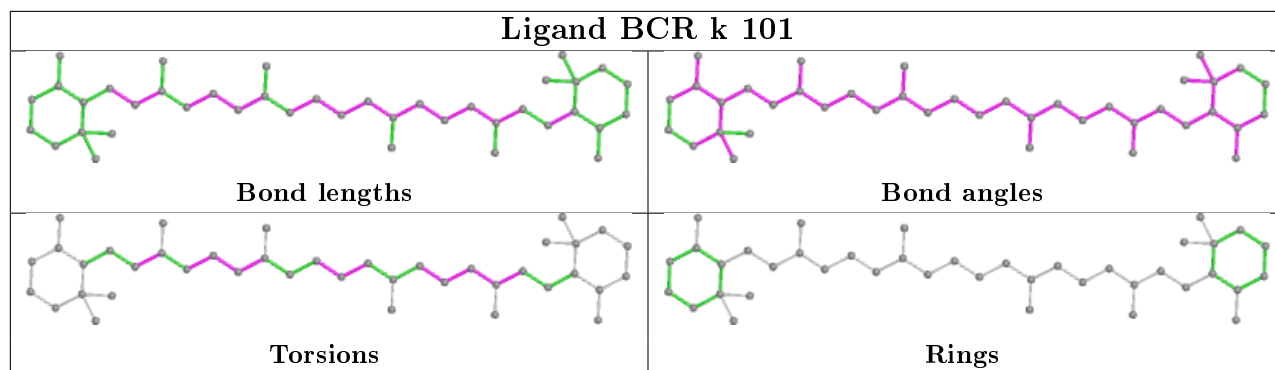


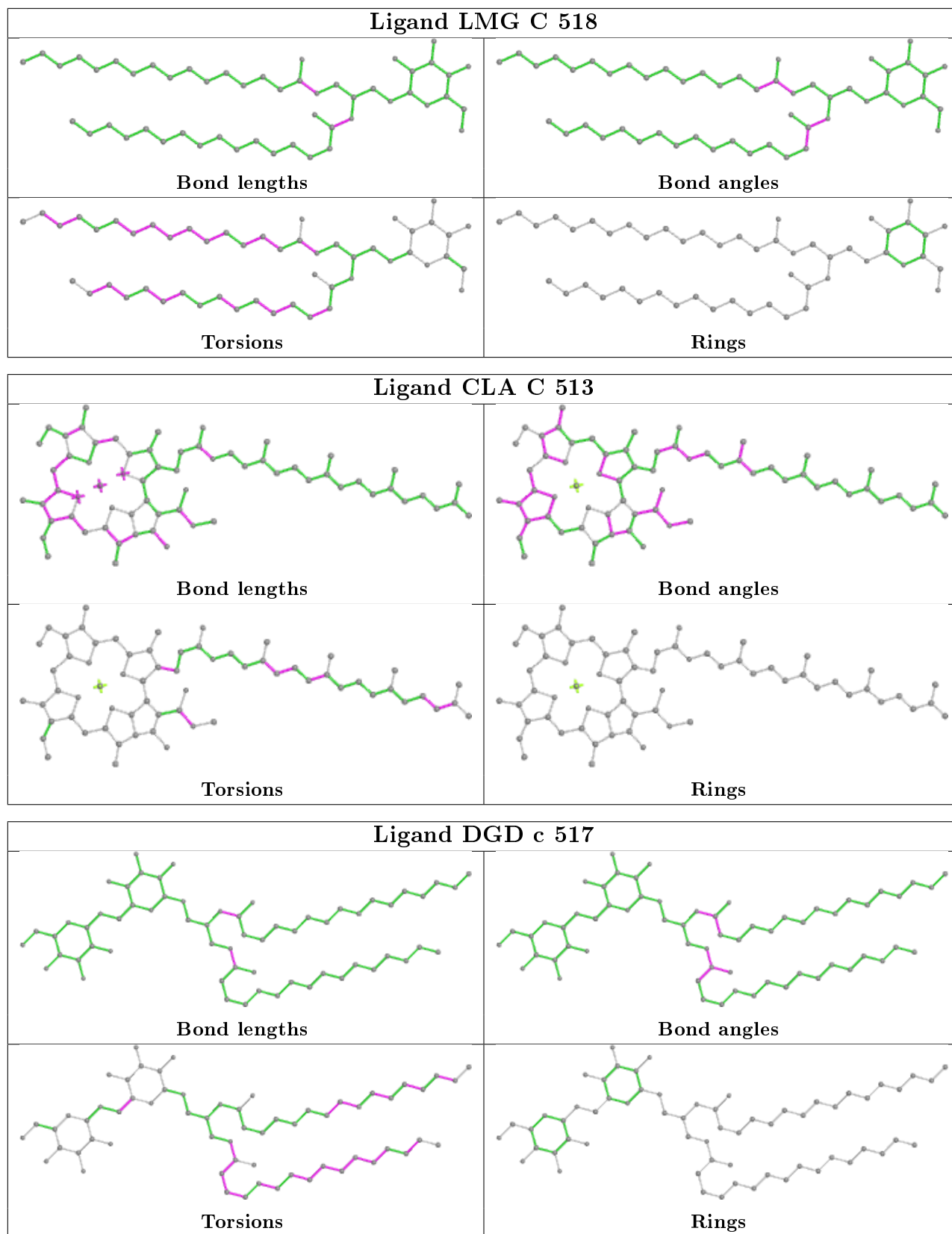


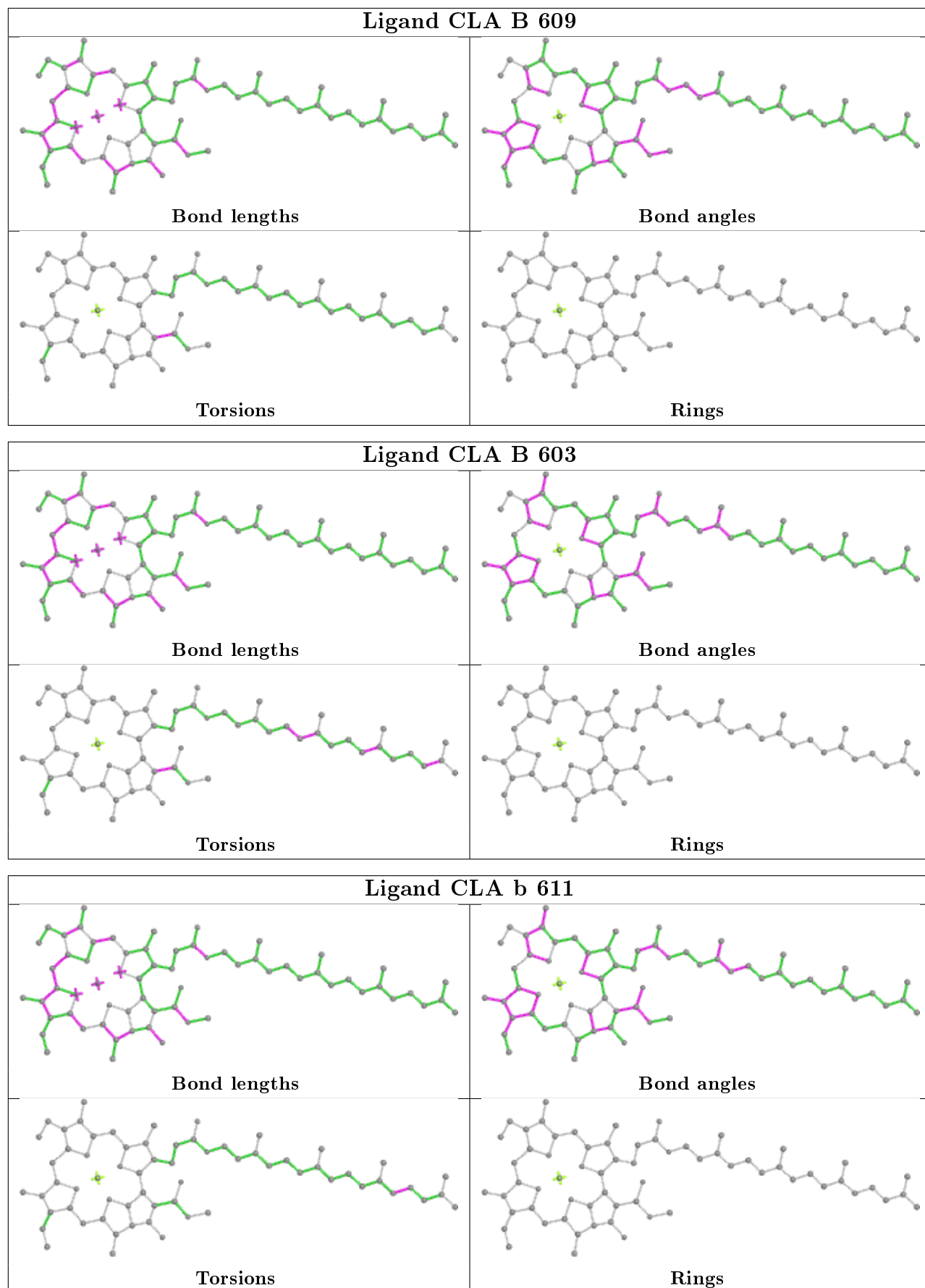


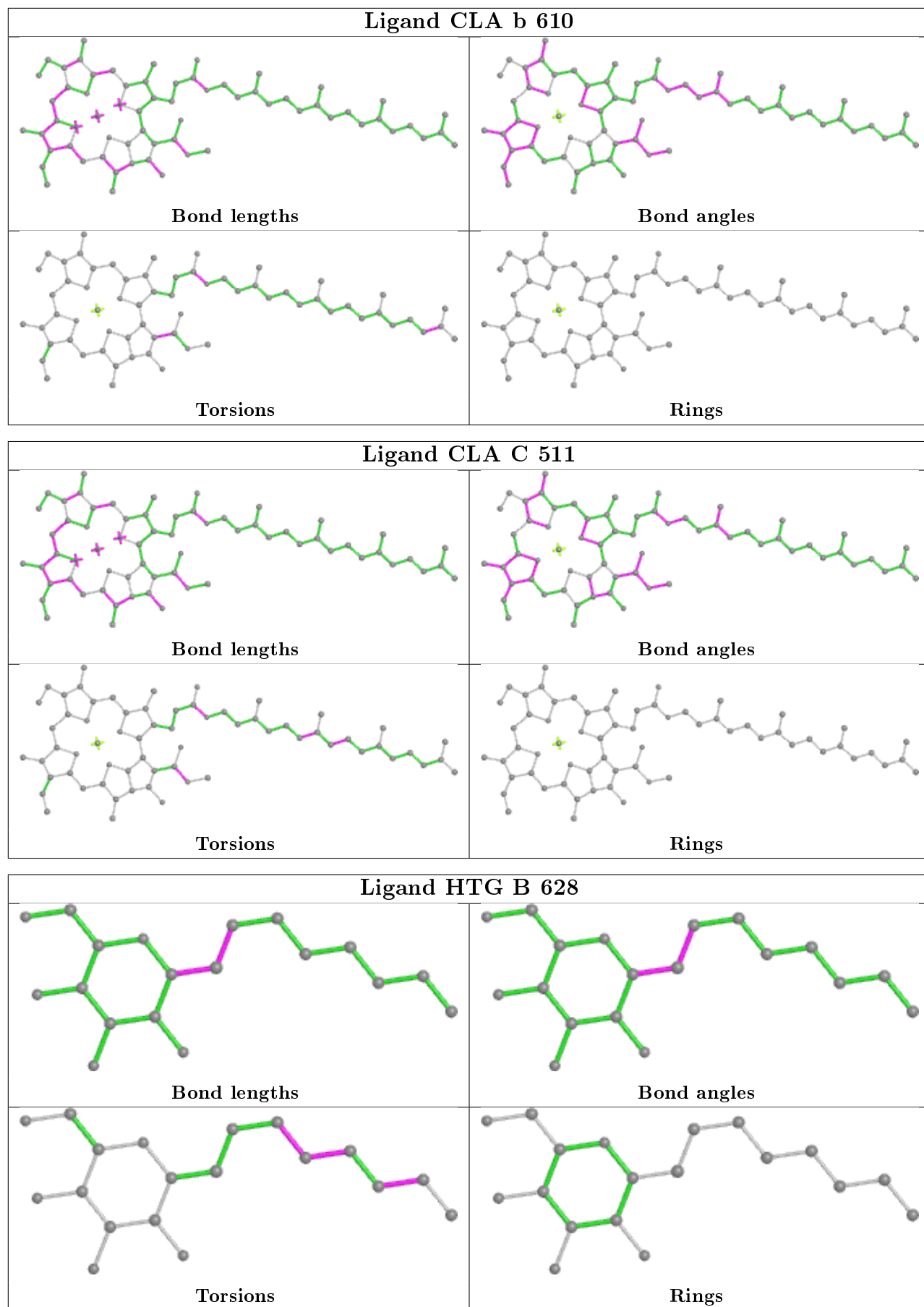


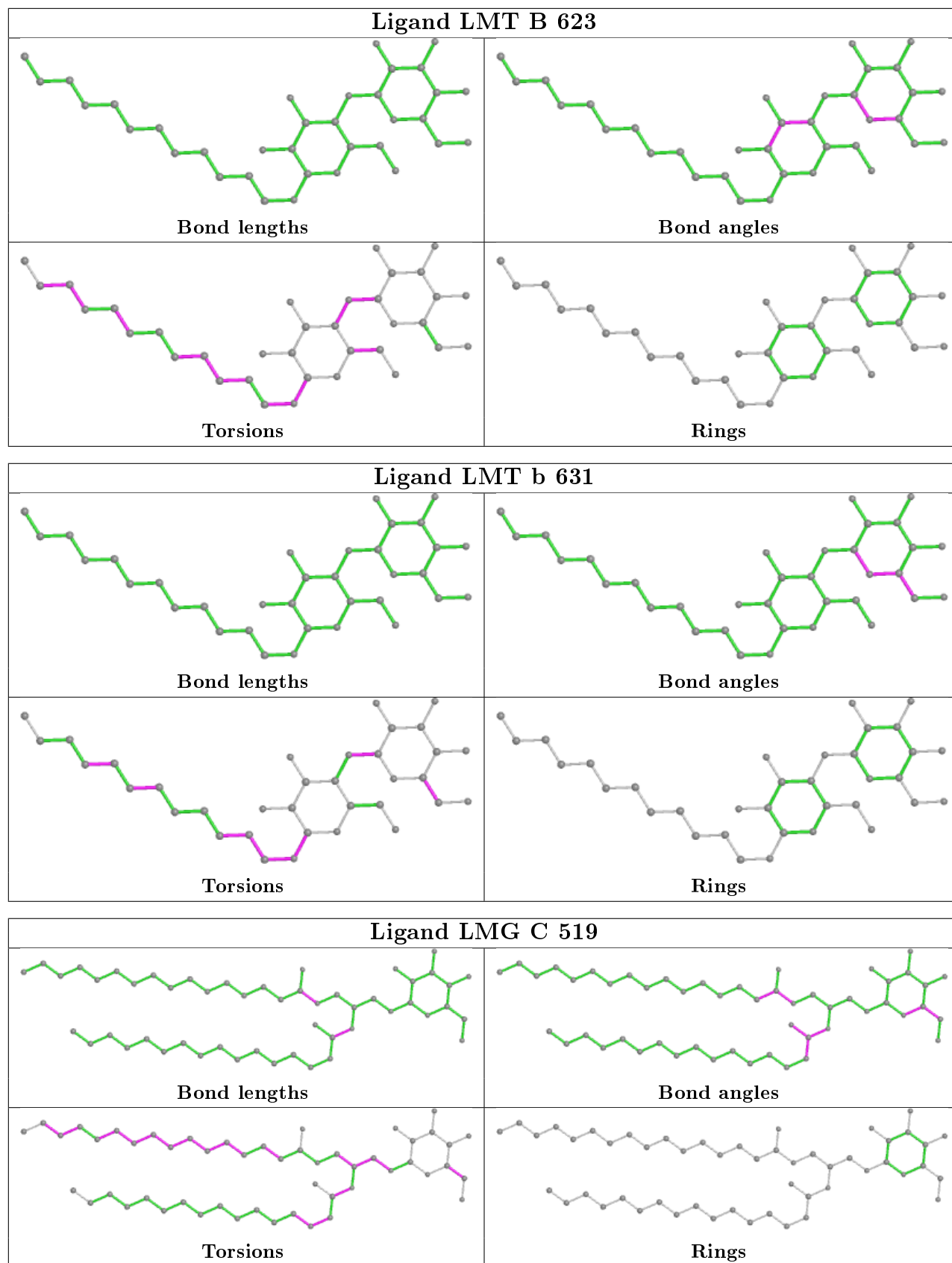


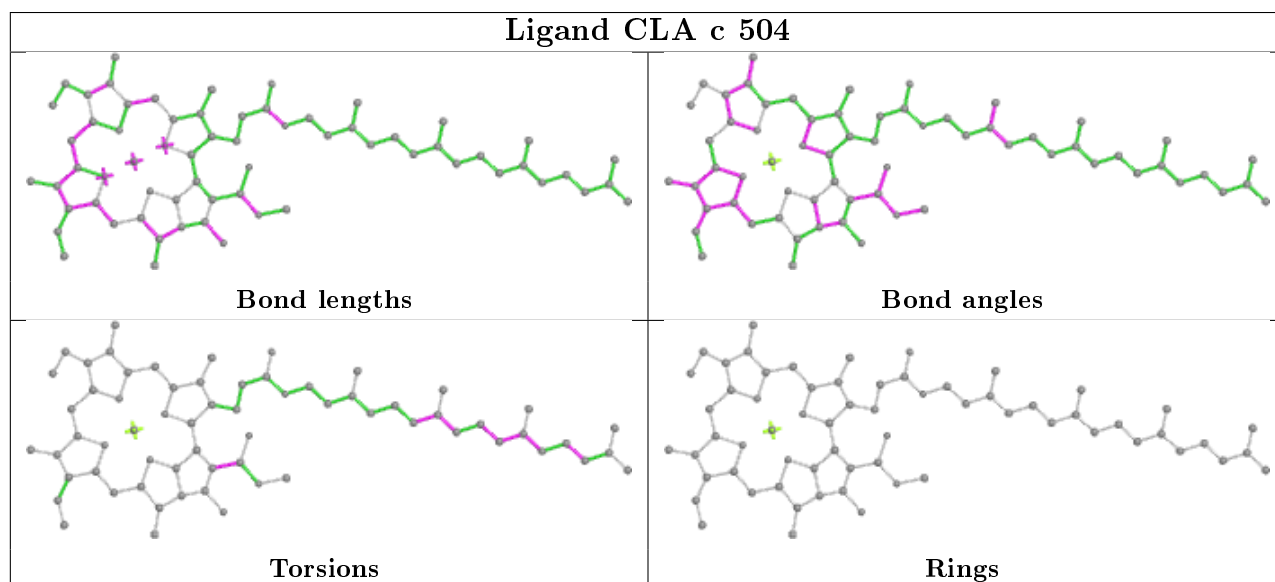
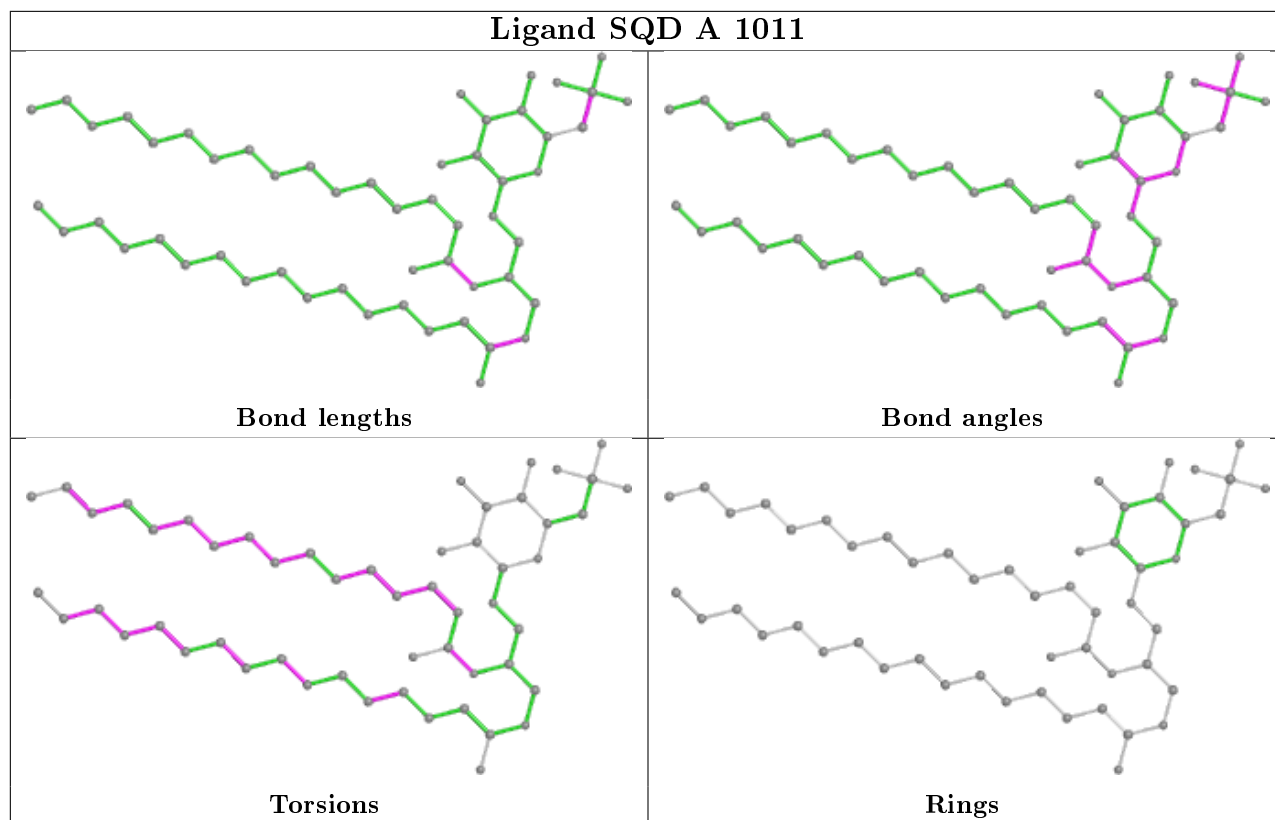


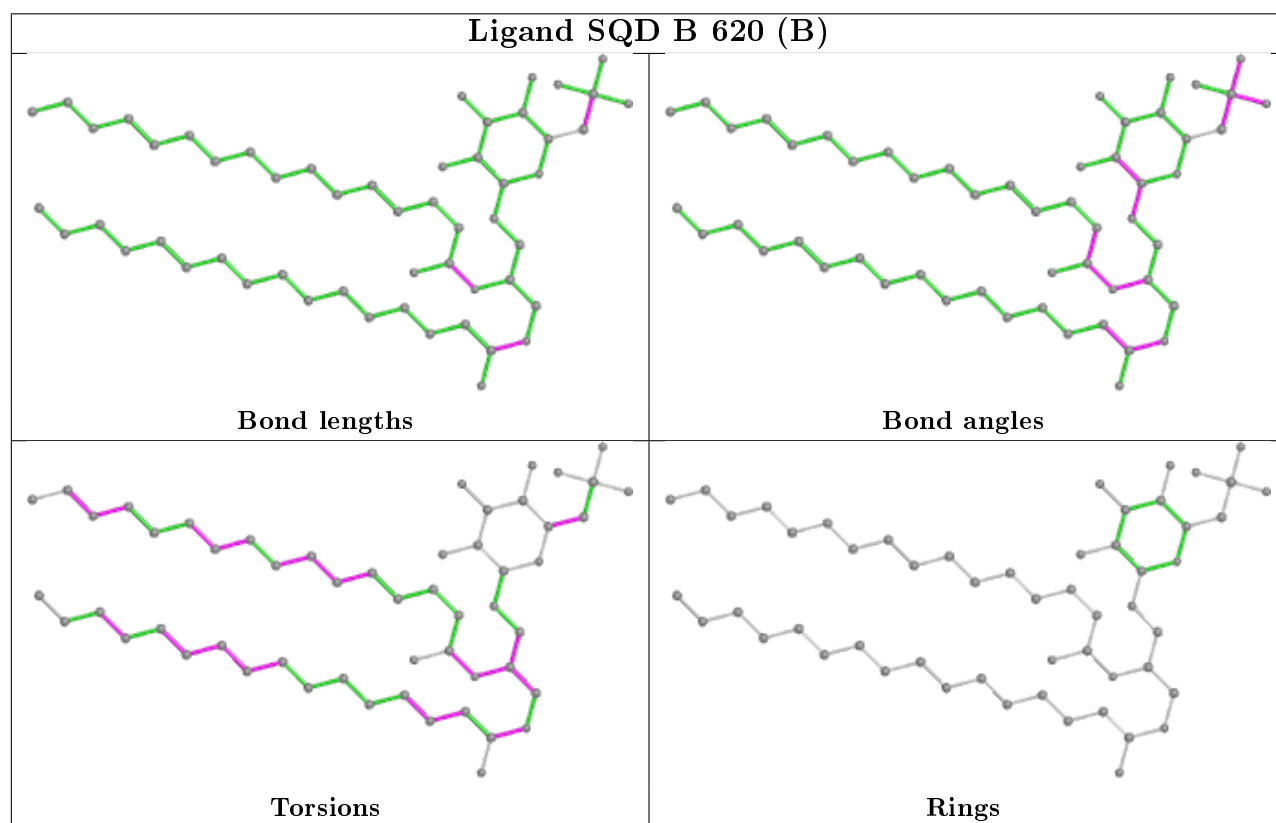
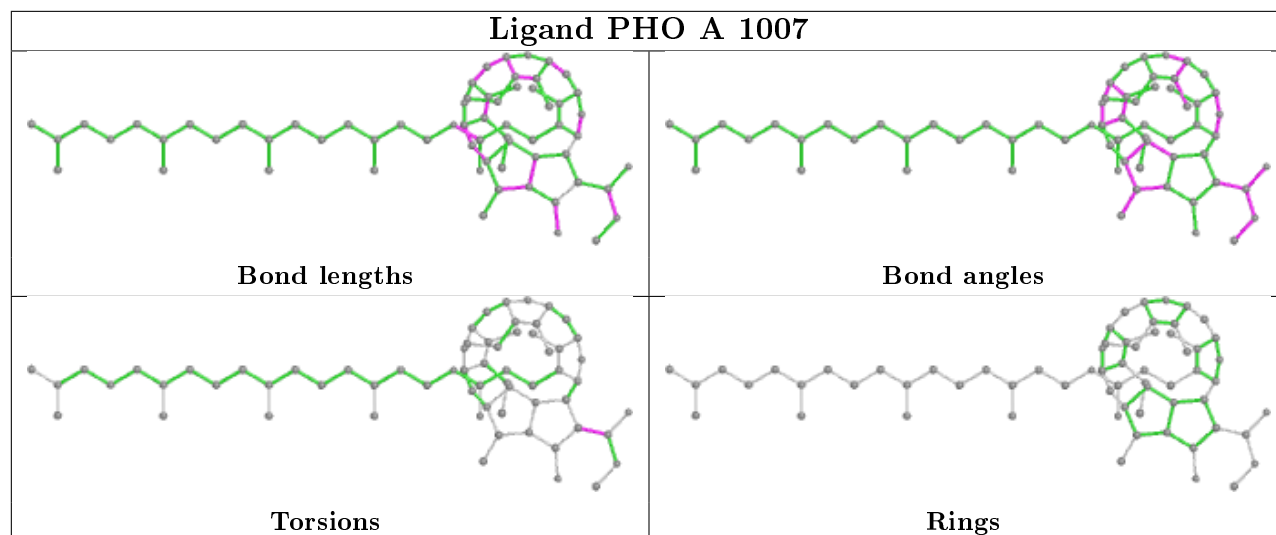


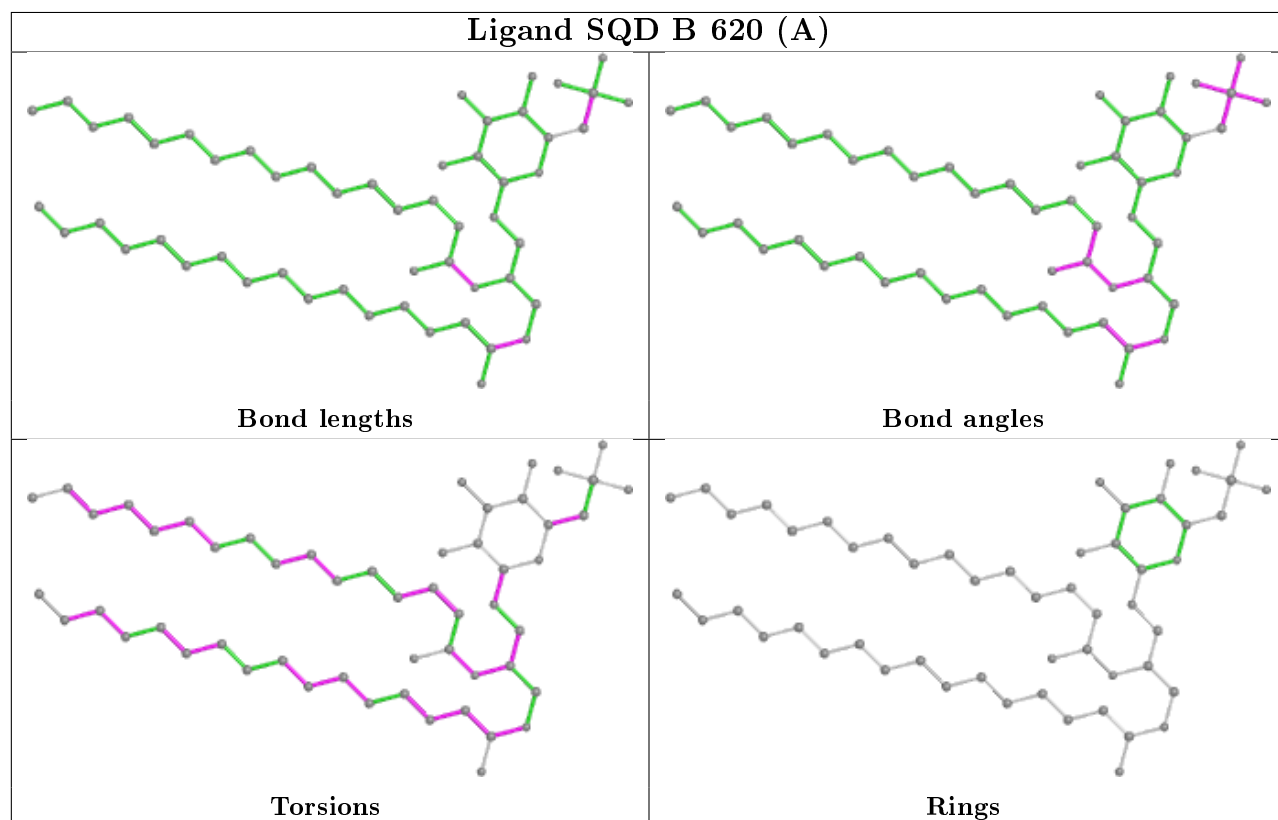
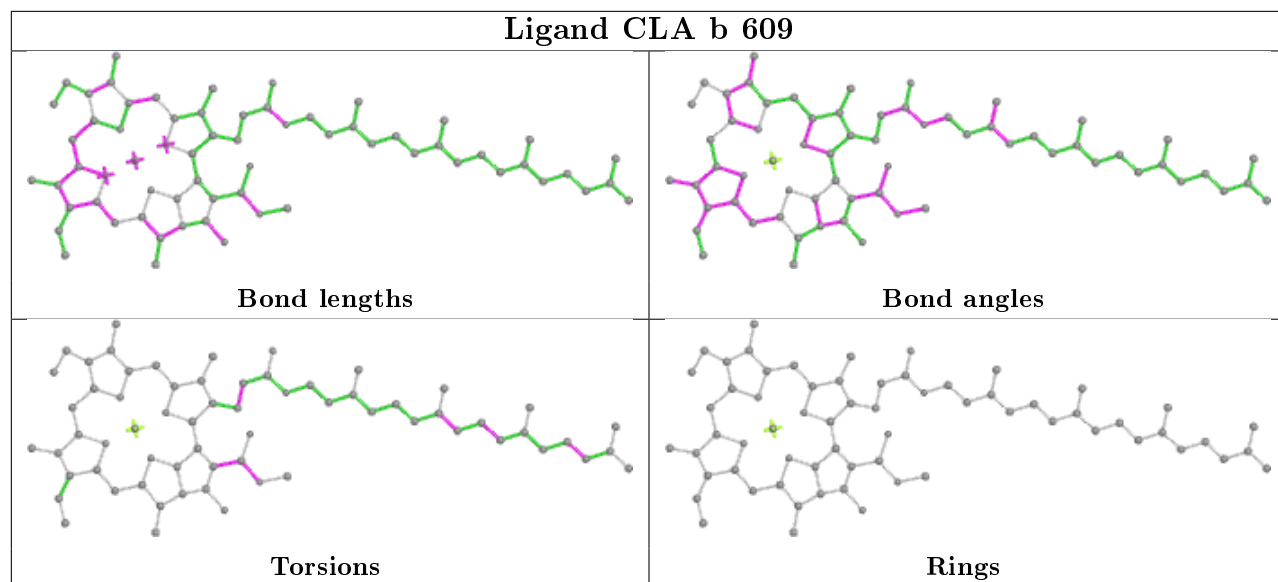


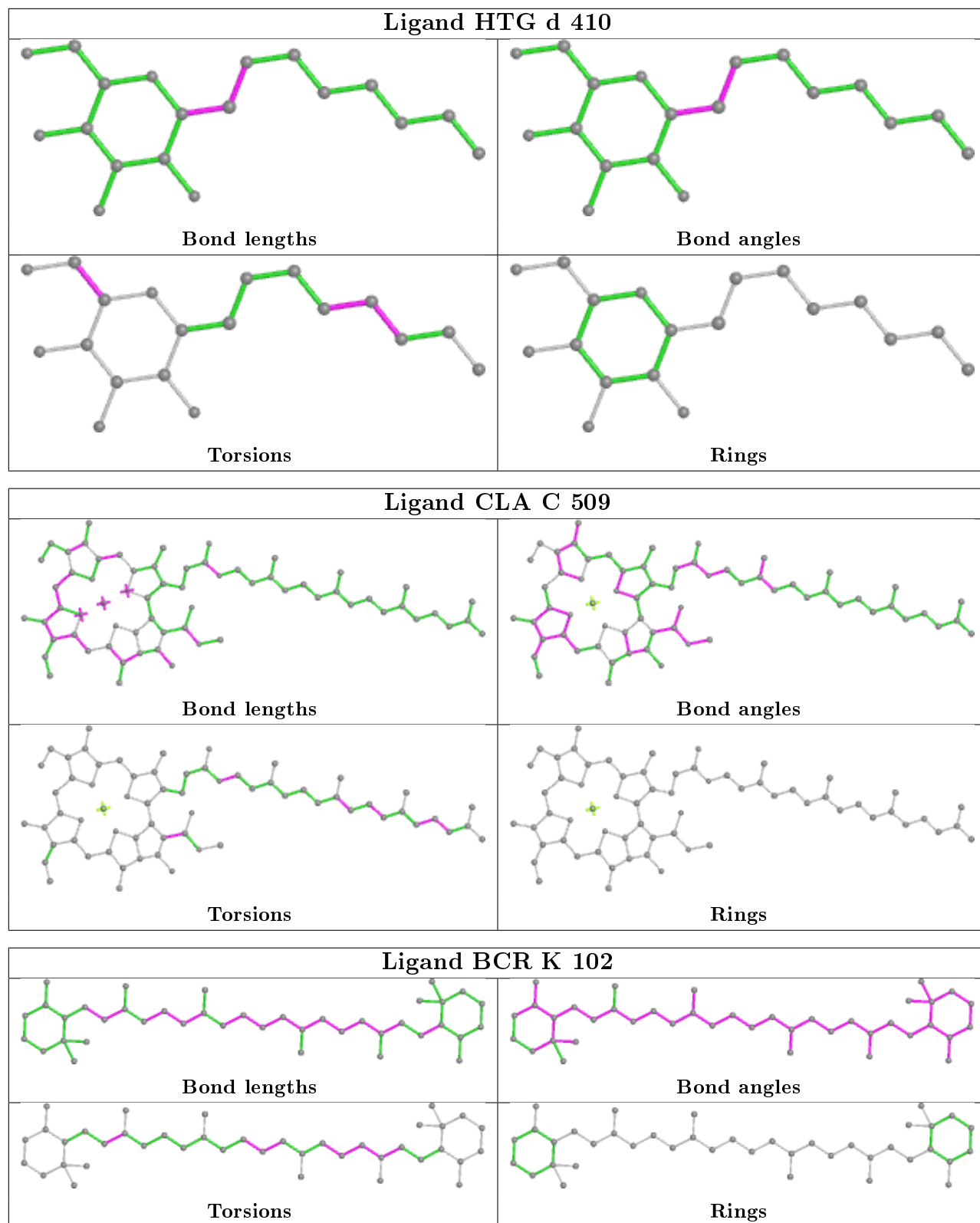


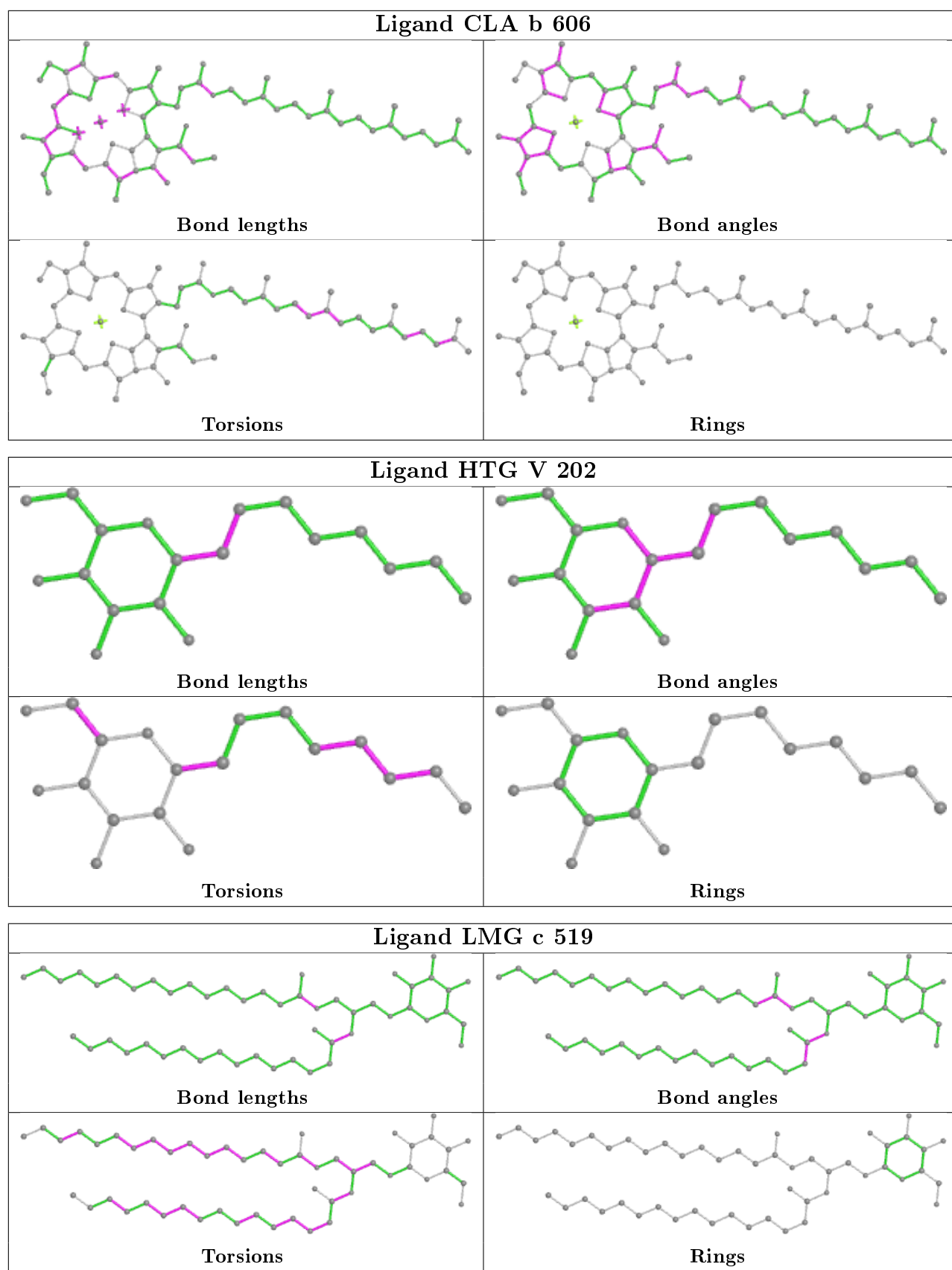


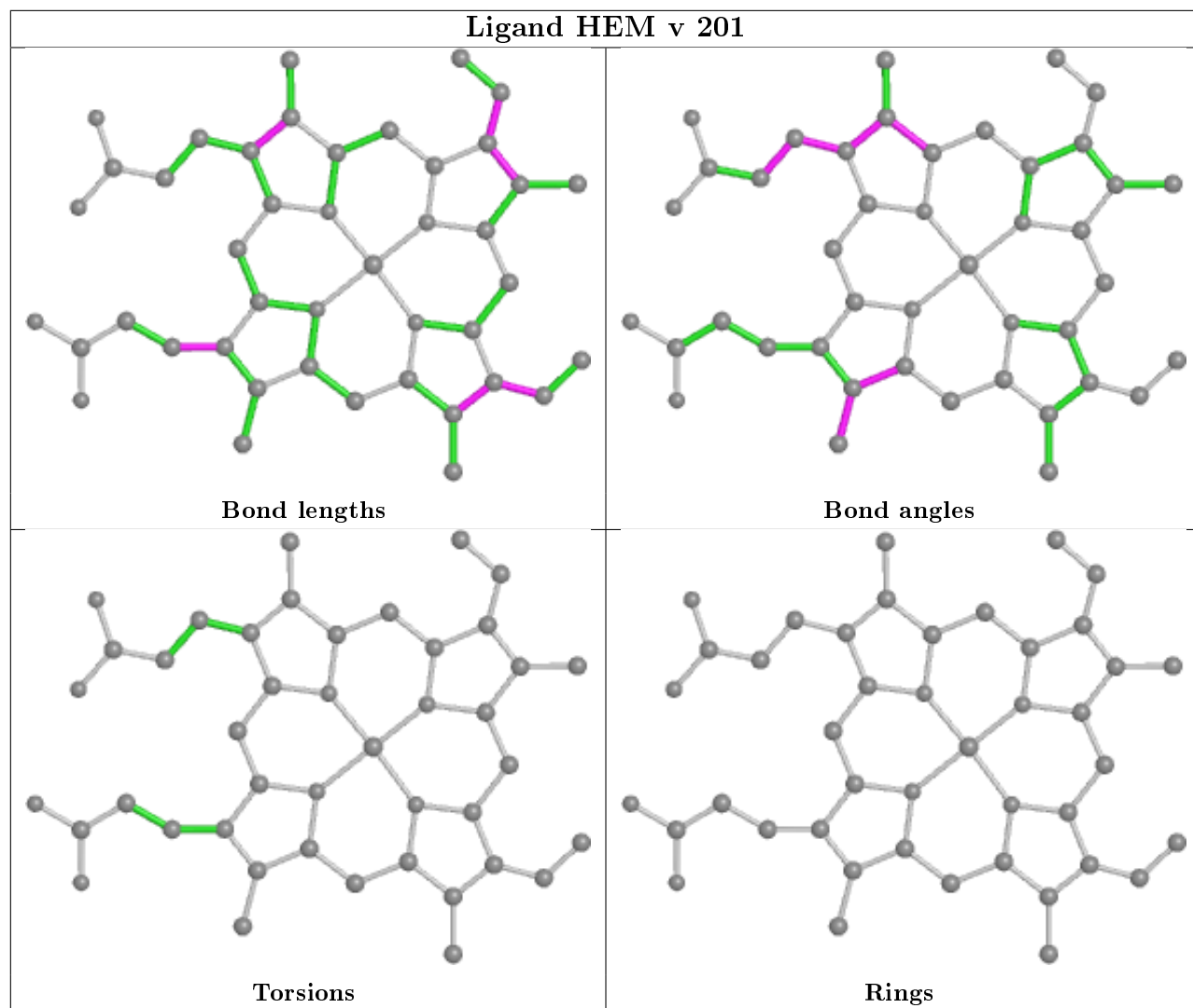


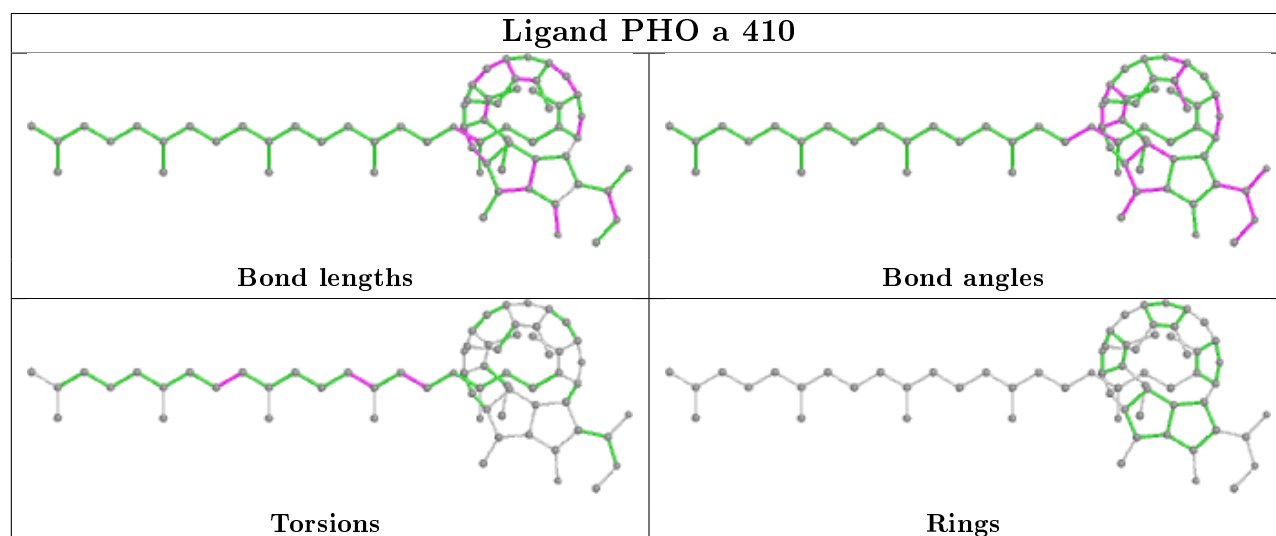
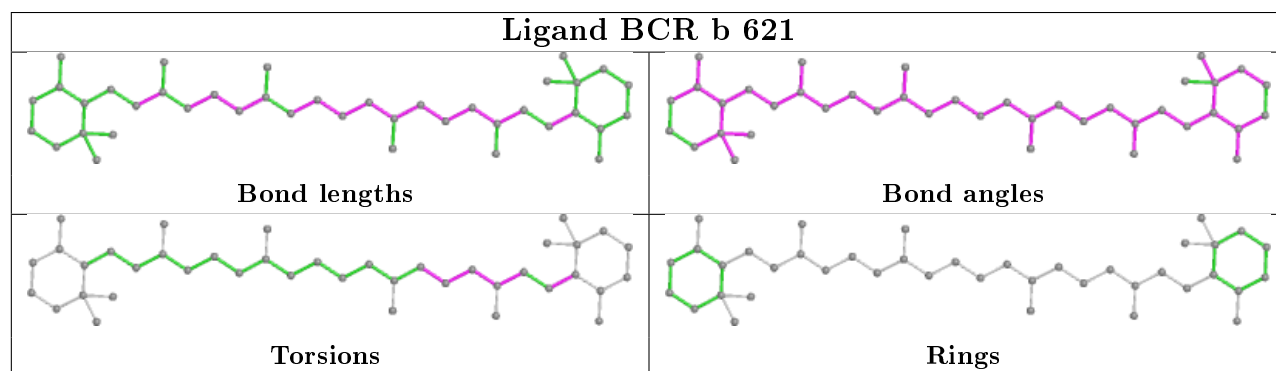
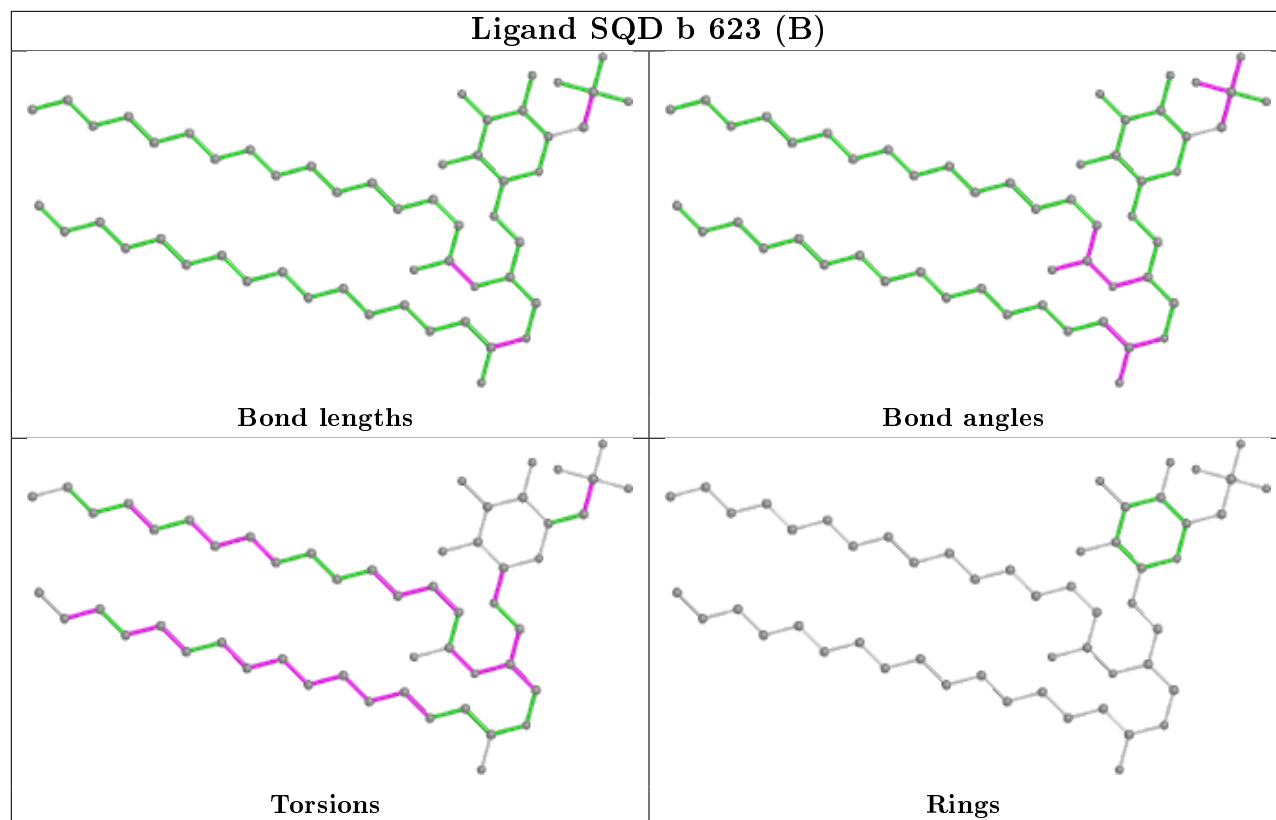


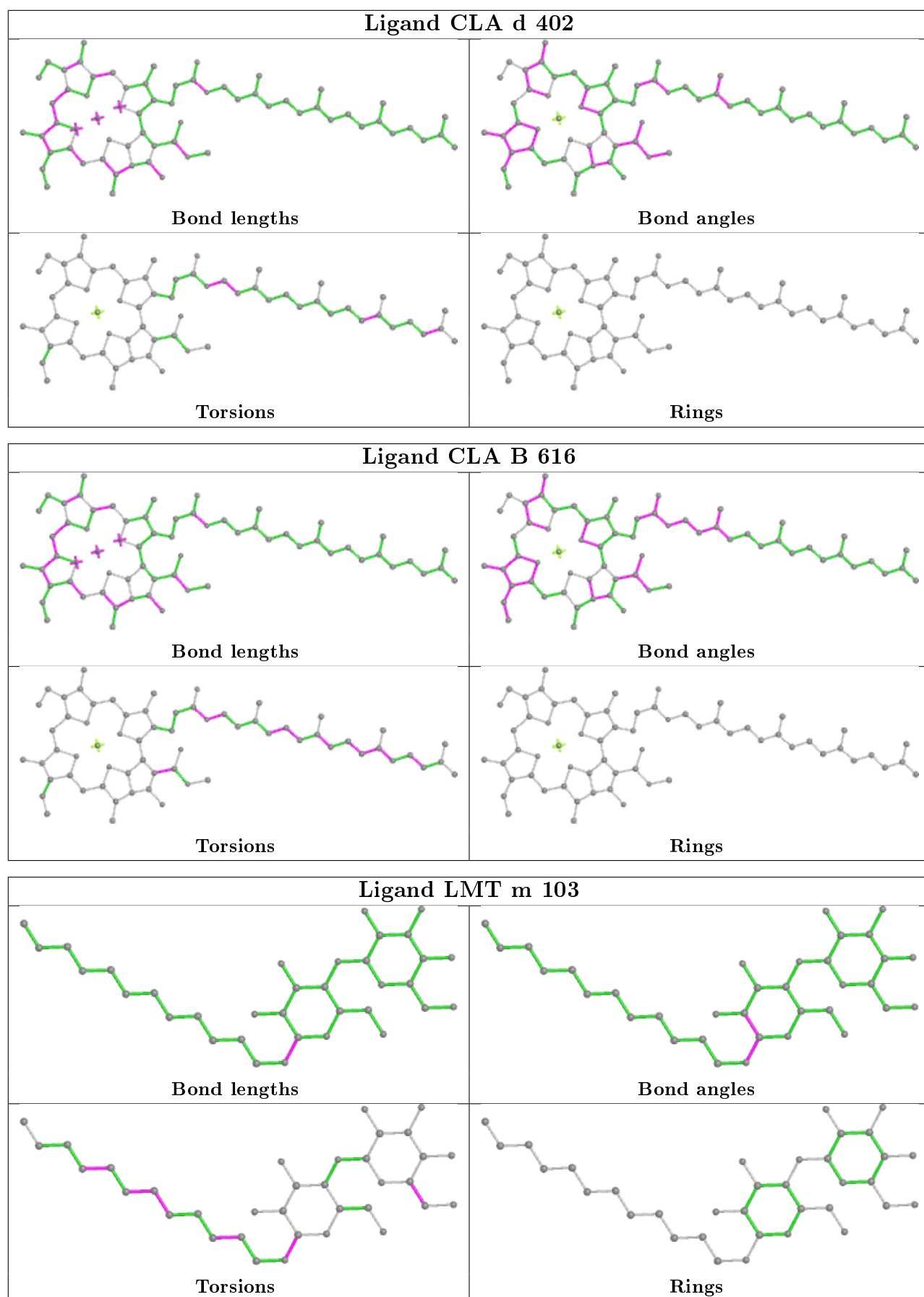


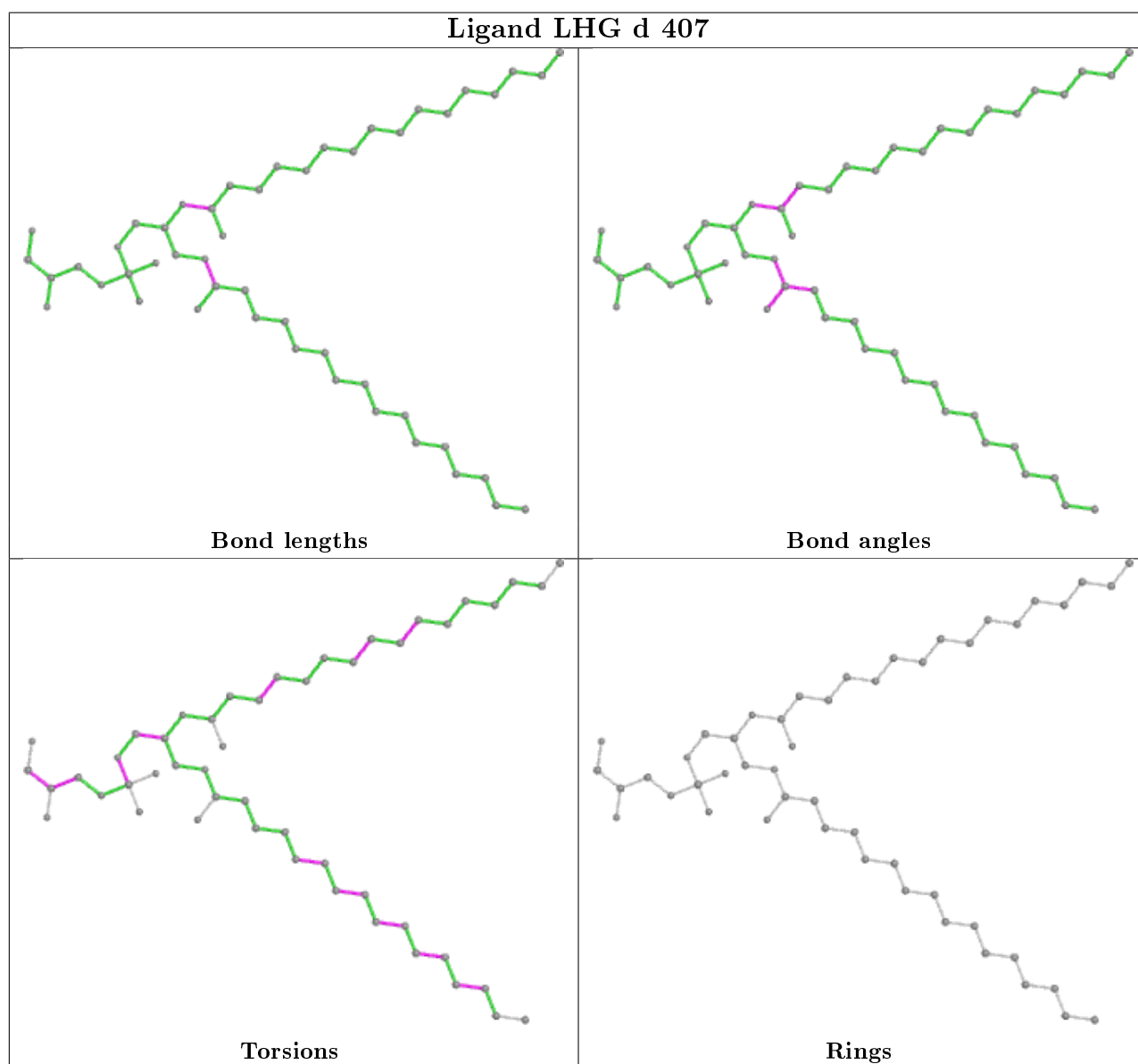
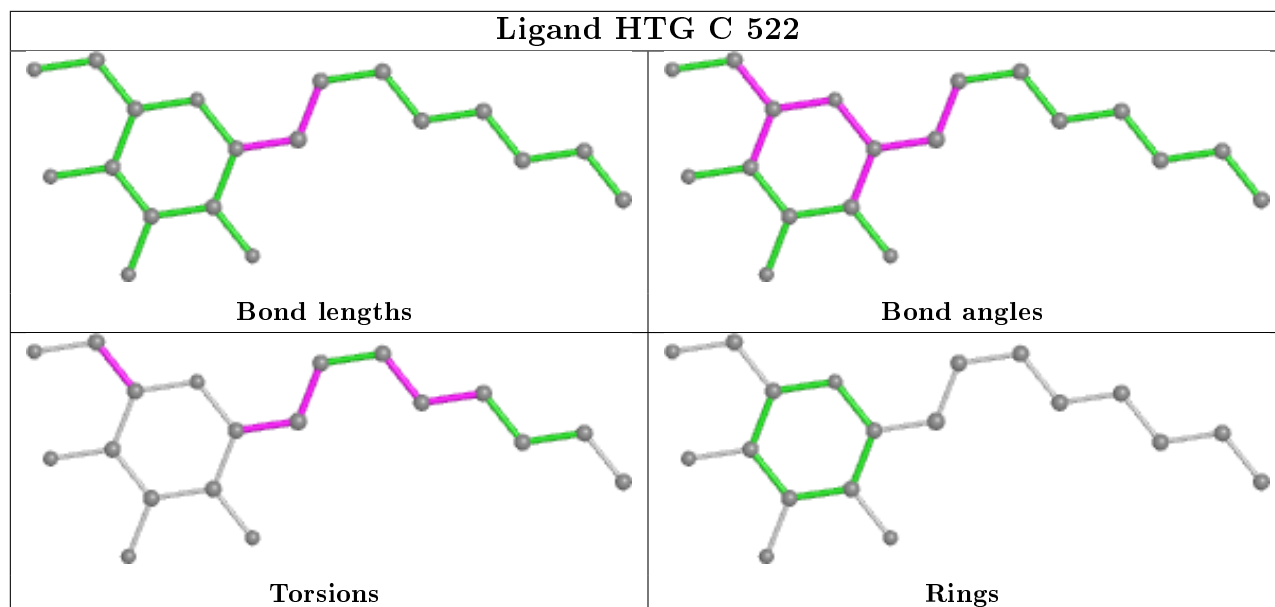


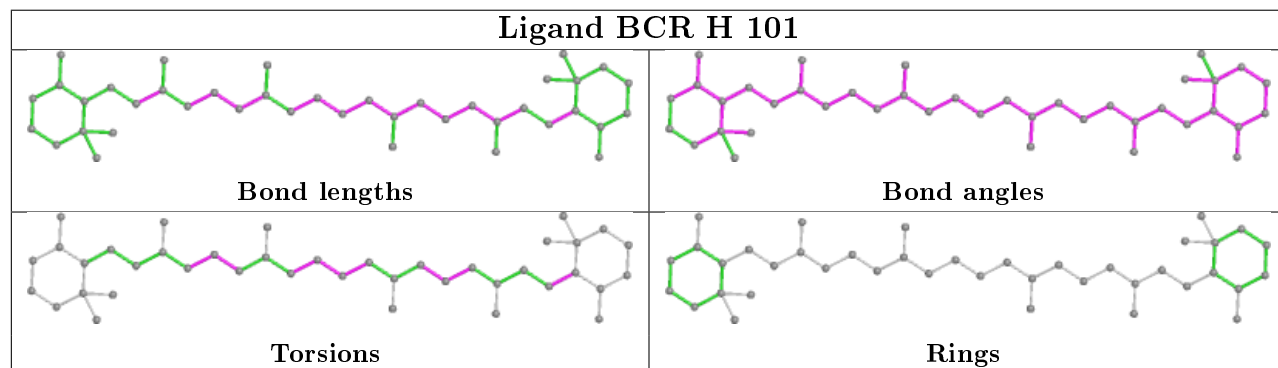
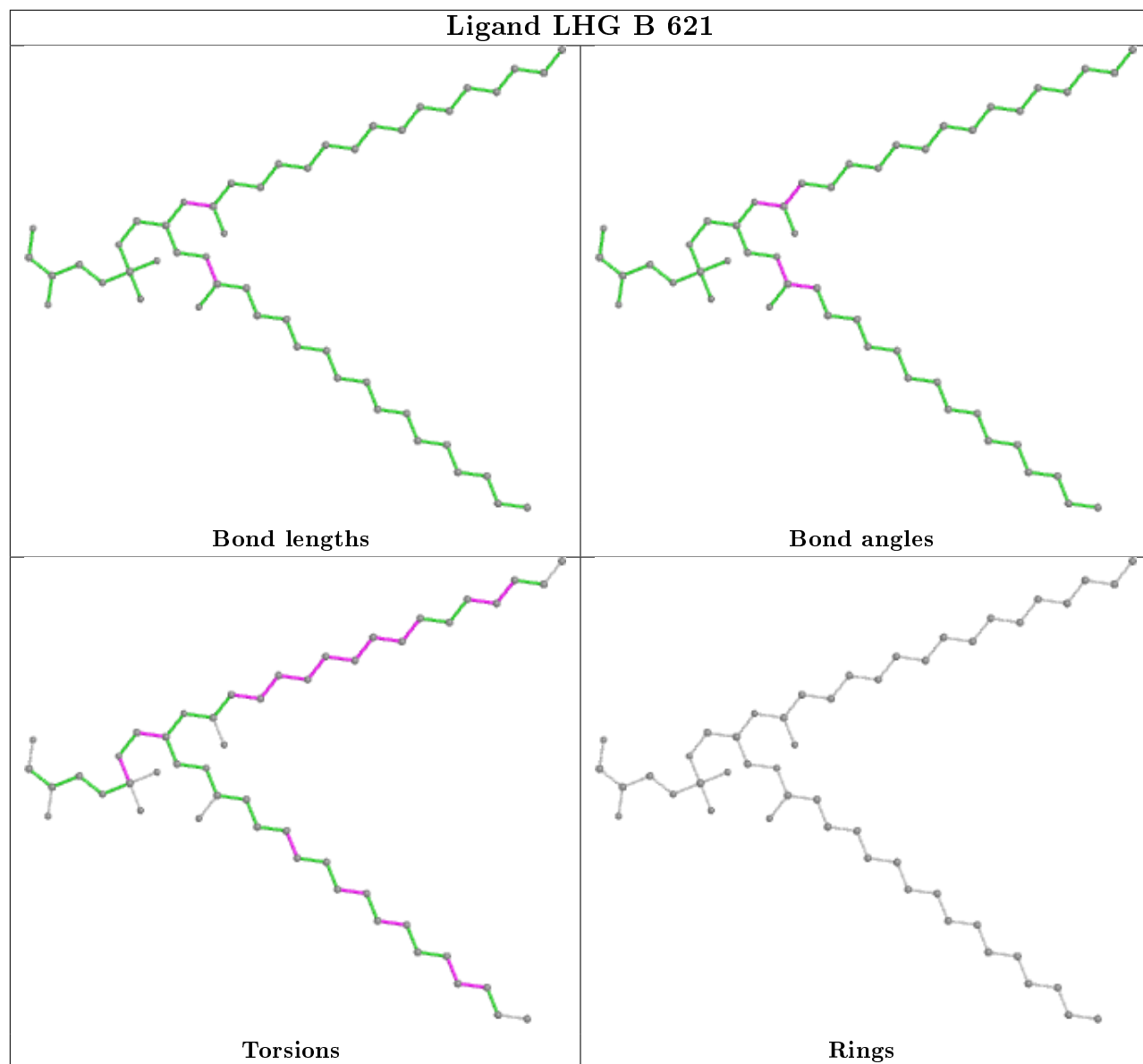


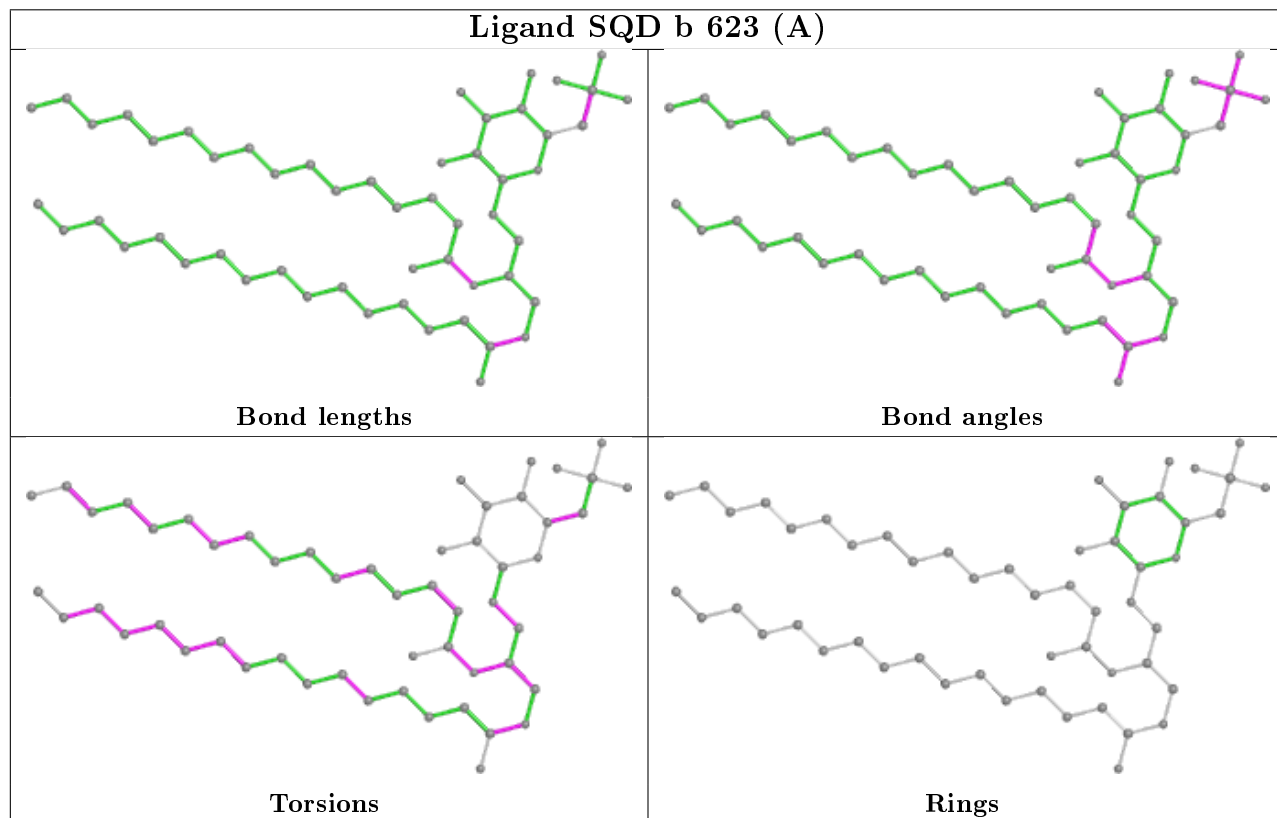
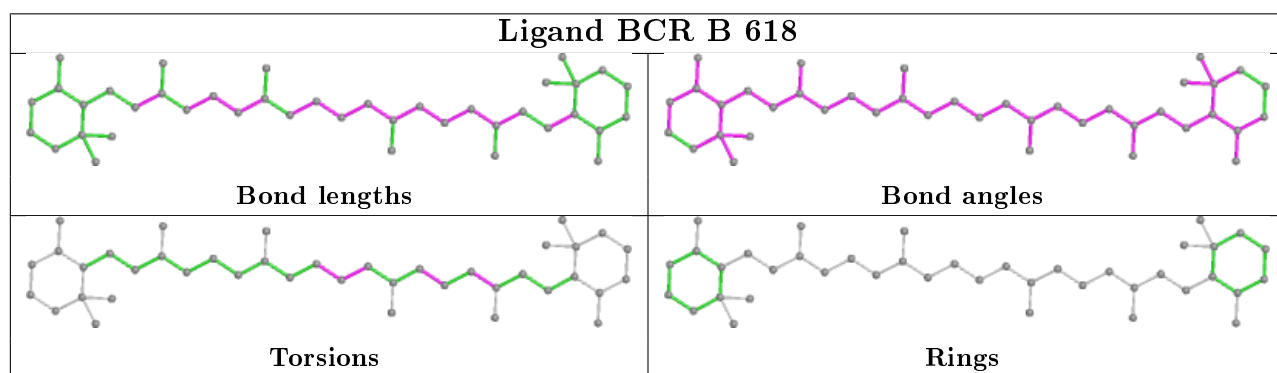
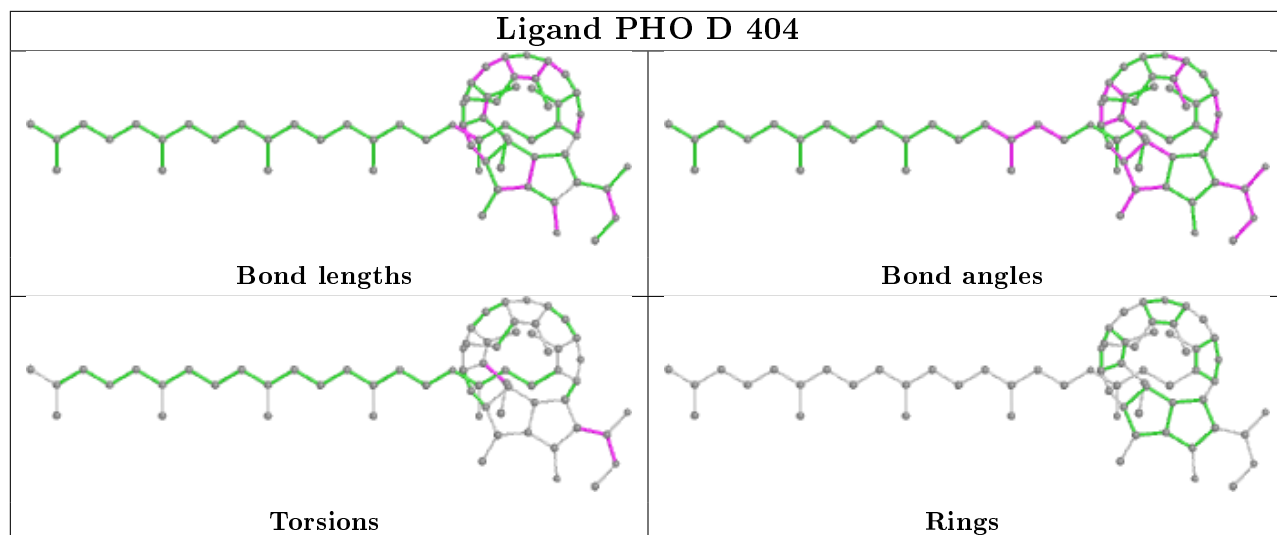


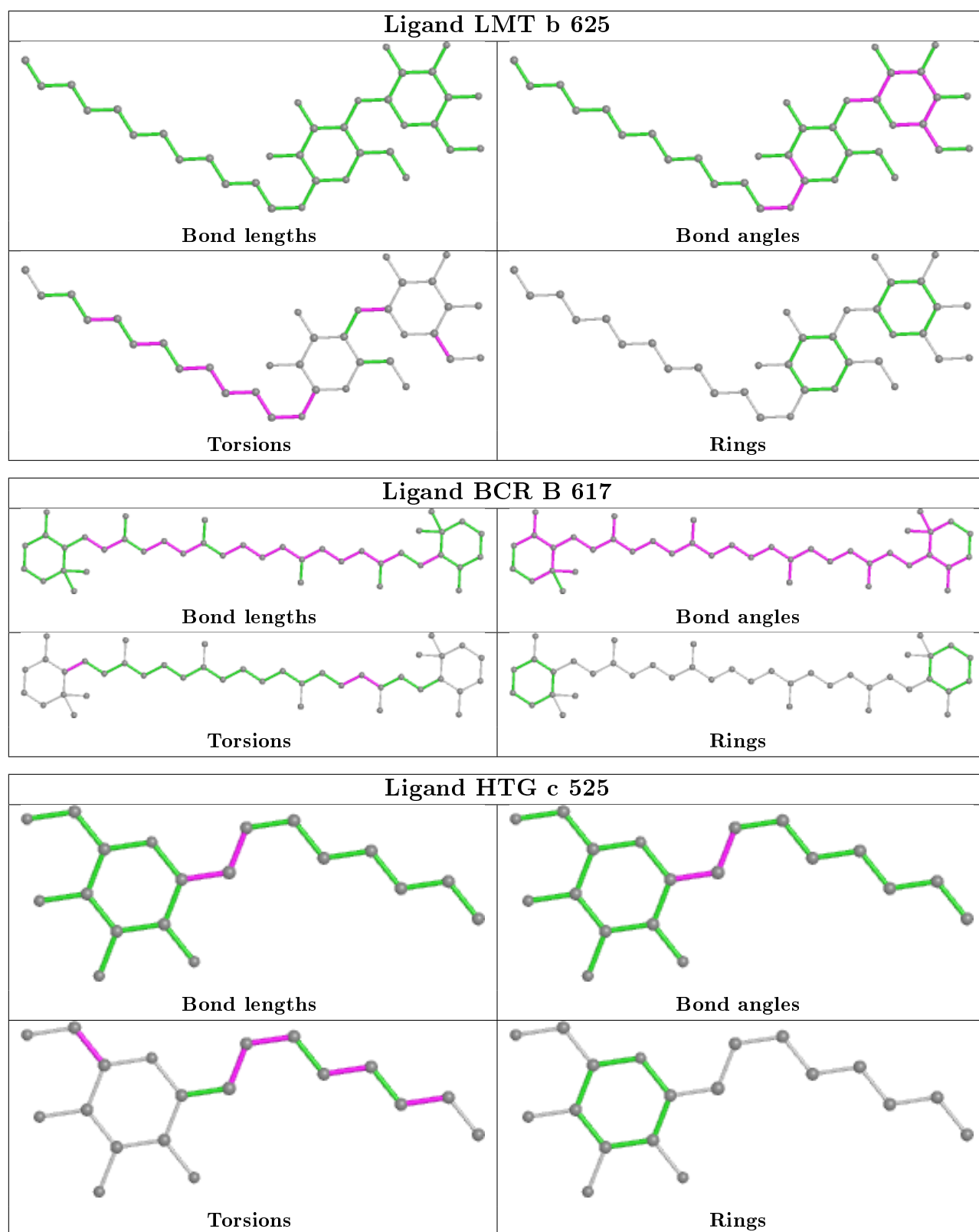


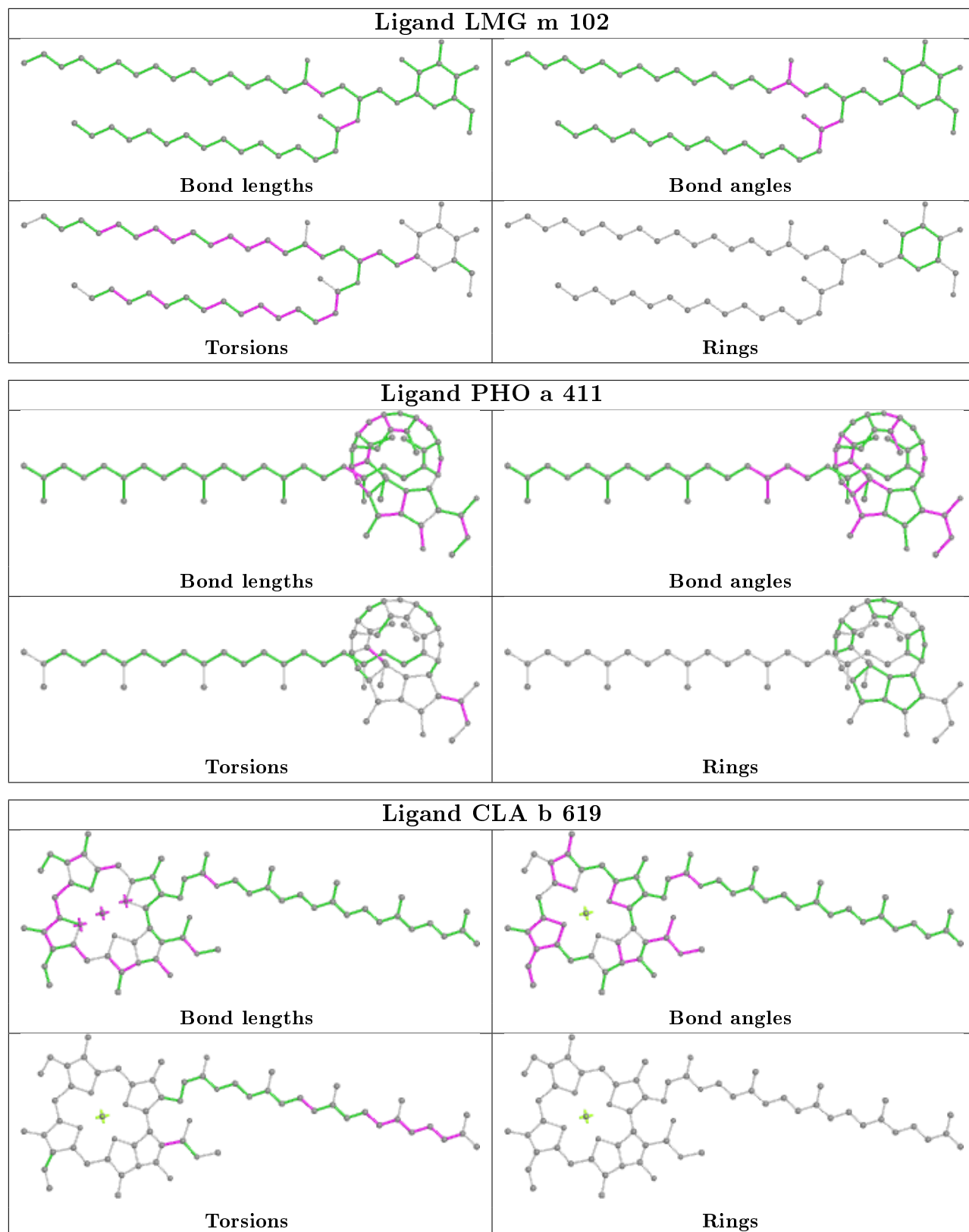


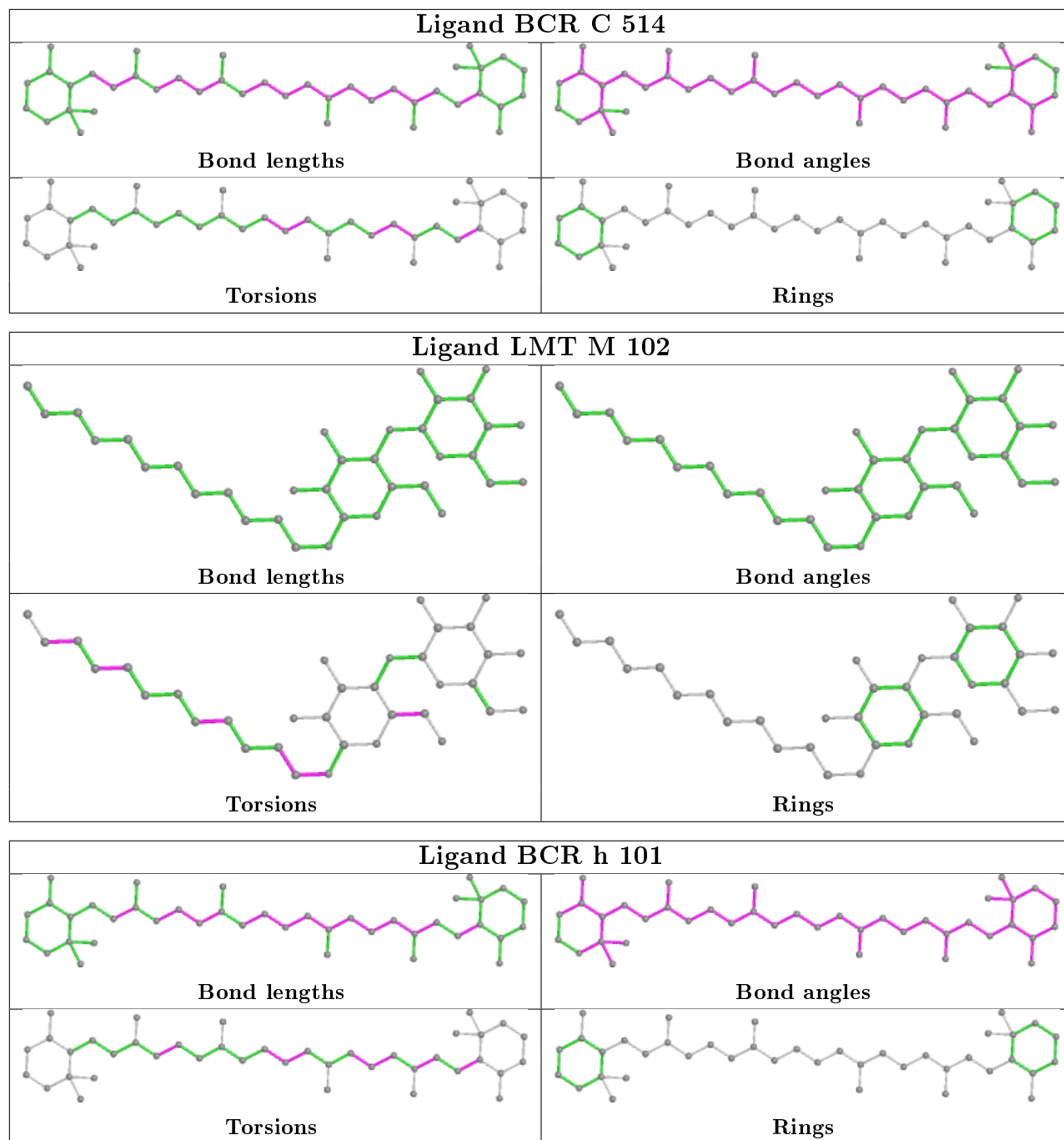


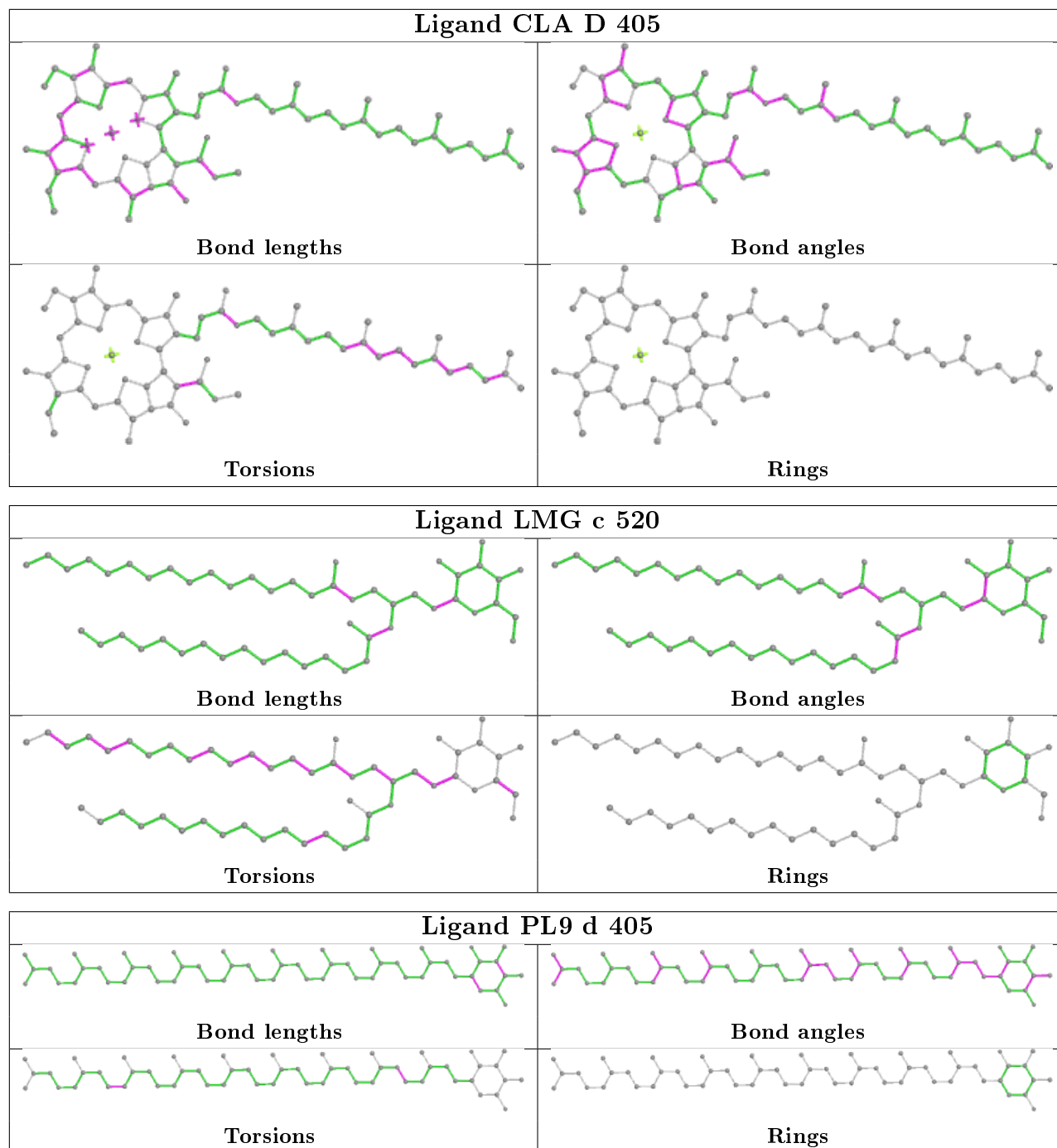


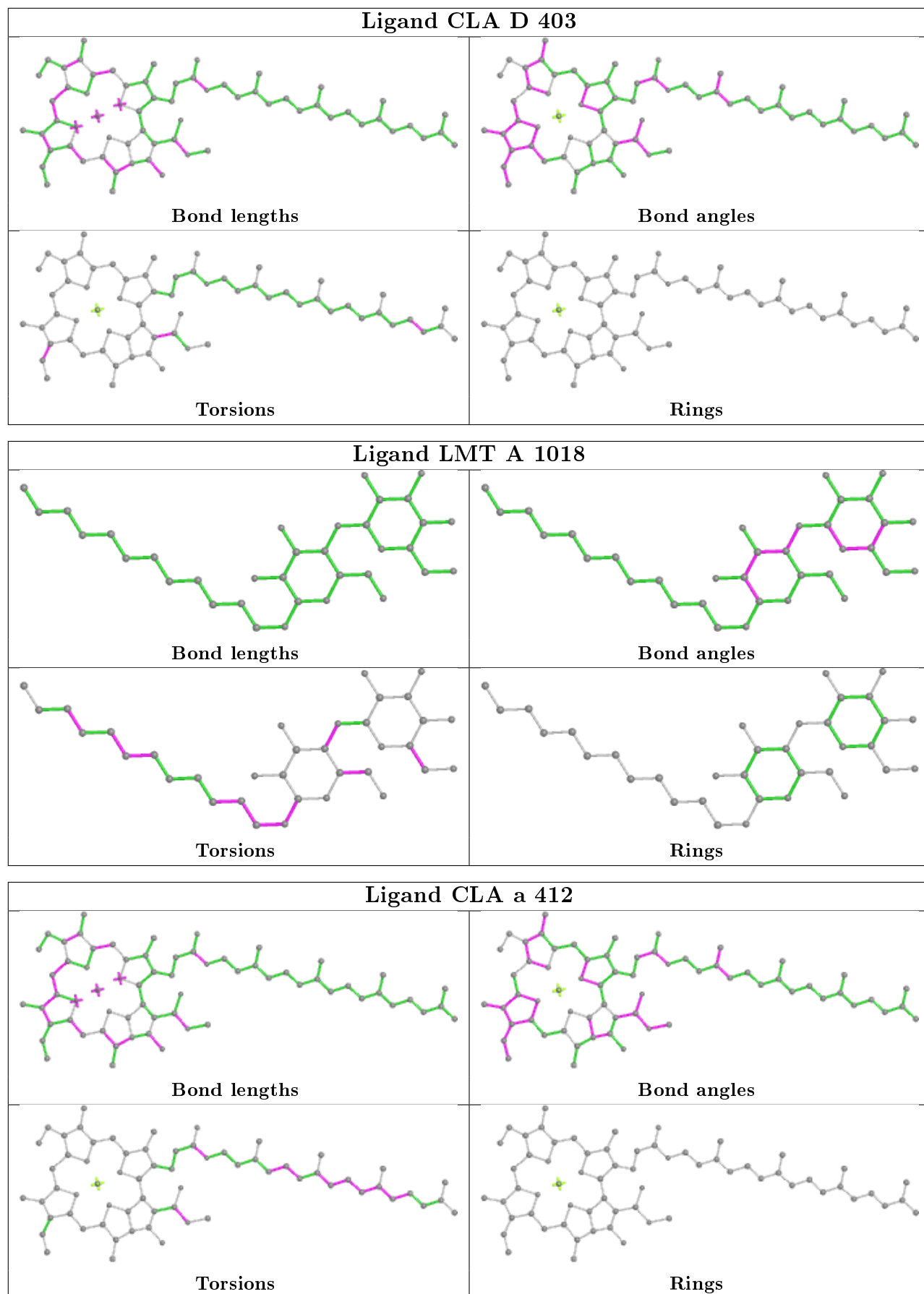


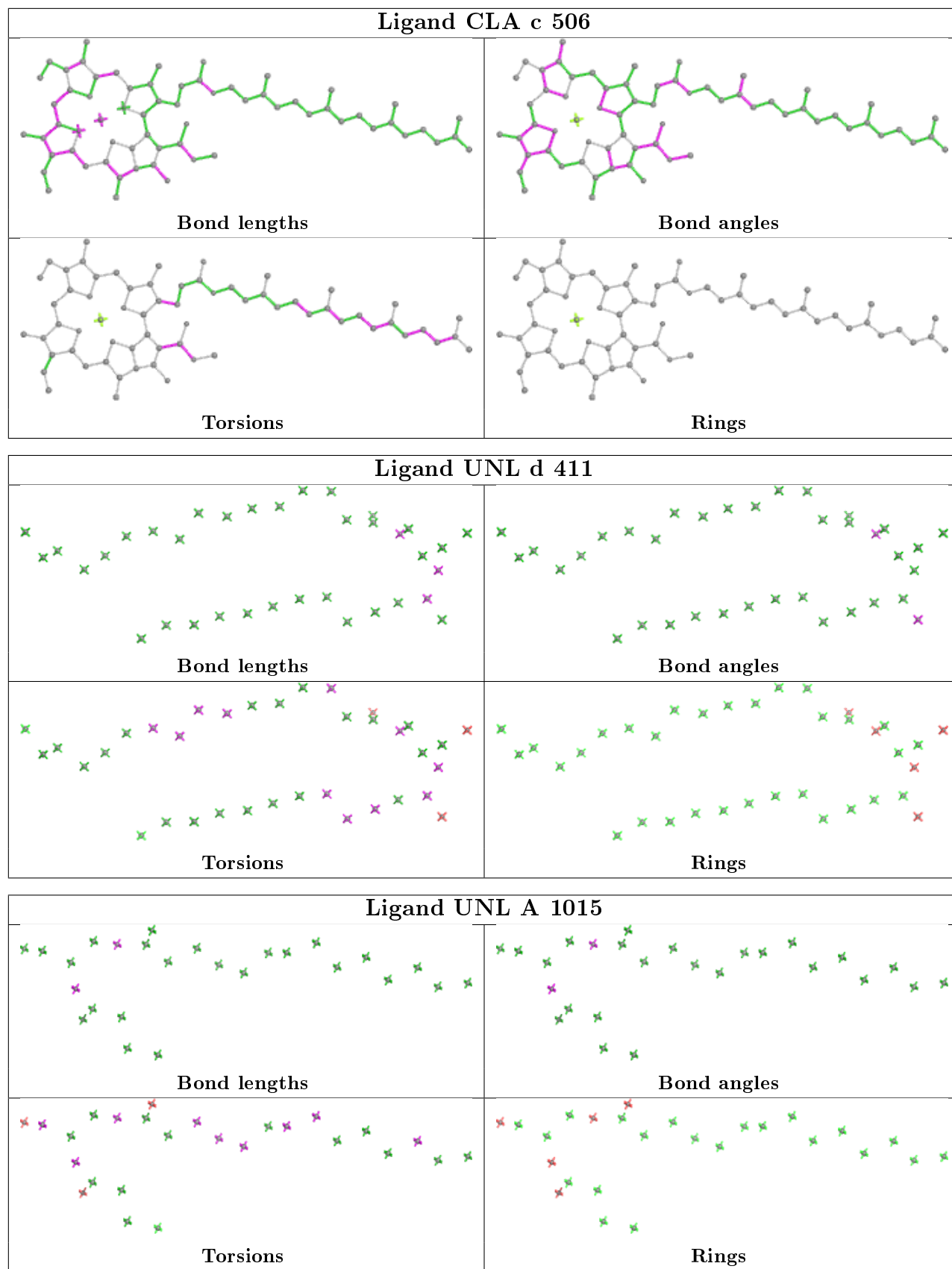


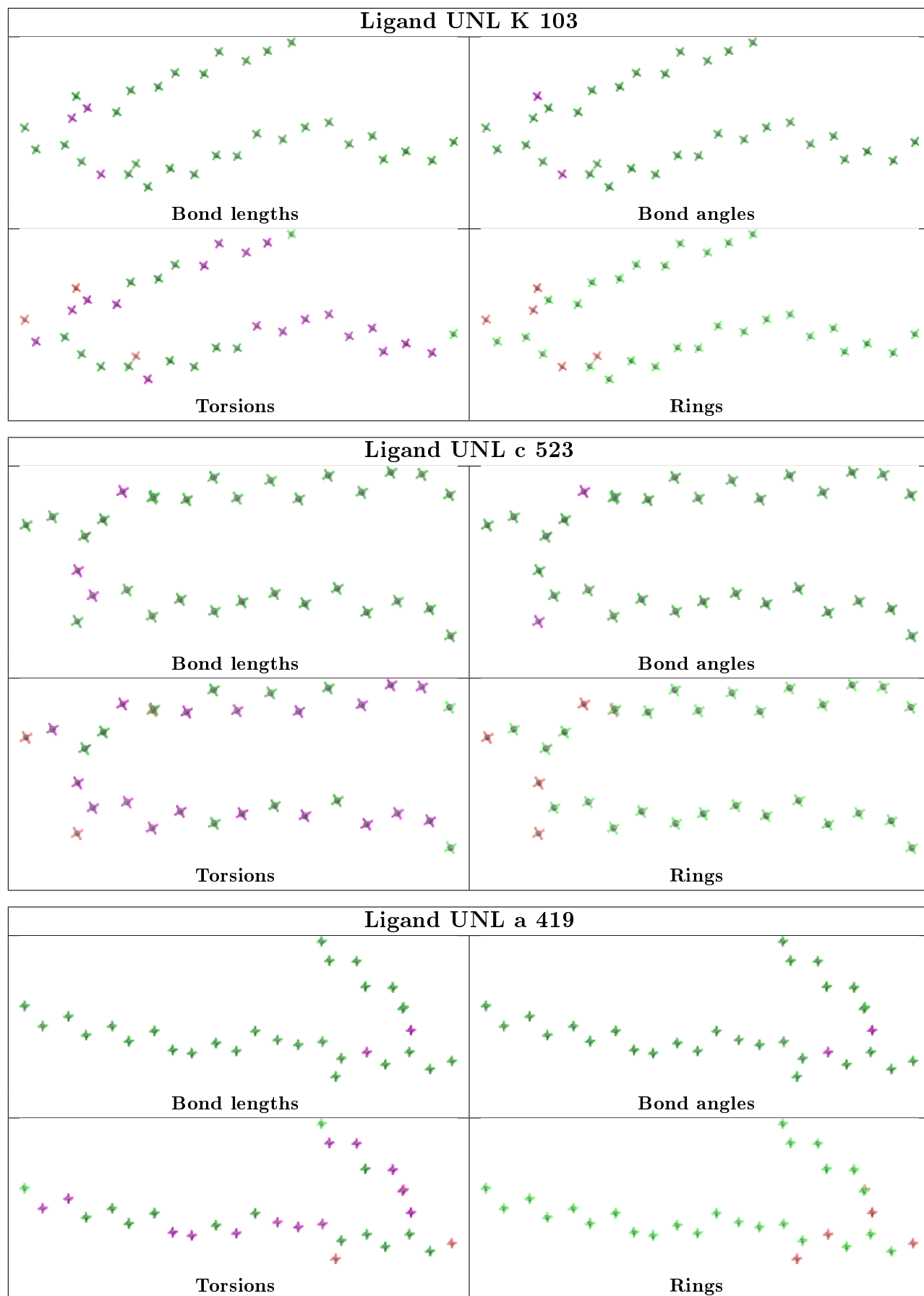


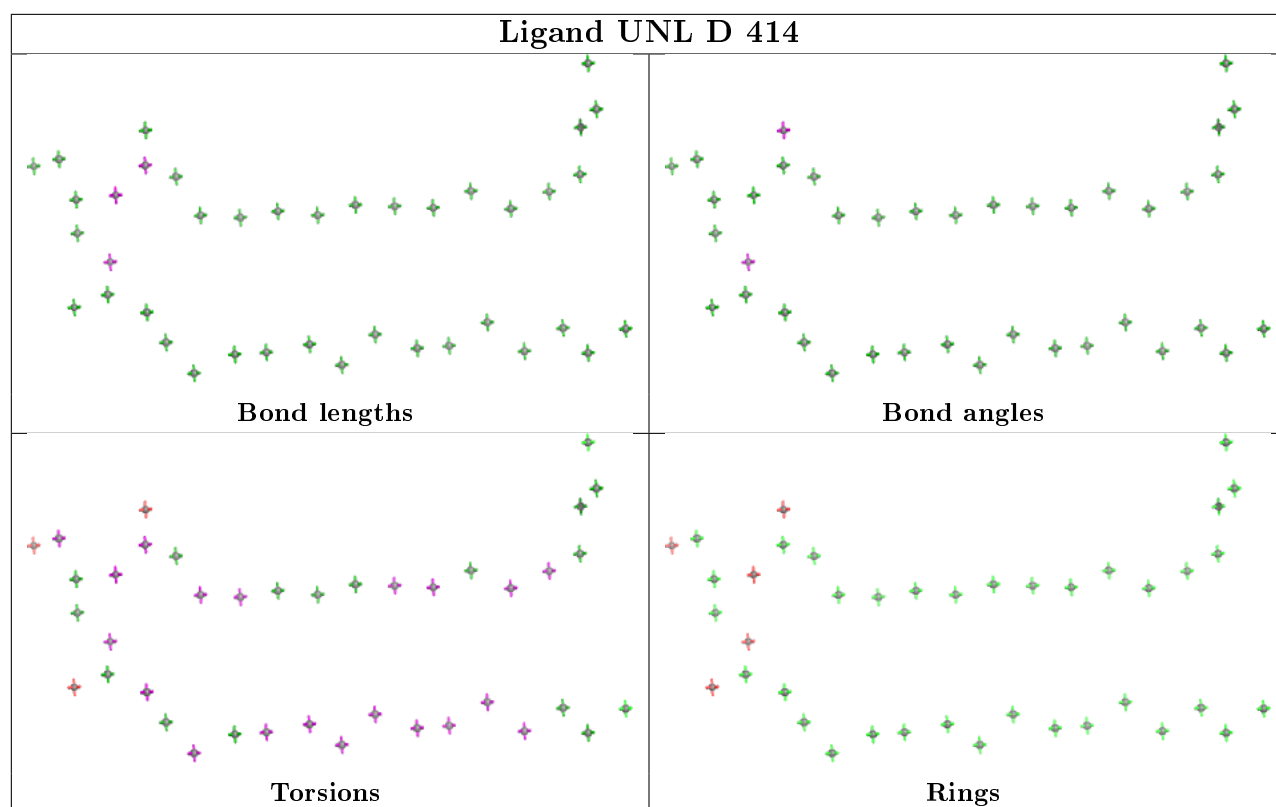












5.7 Other polymers [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/334 (100%)	-0.72	5 (1%) 73 77	19, 25, 44, 64	0
1	a	334/334 (100%)	-0.59	7 (2%) 63 68	21, 28, 51, 72	0
2	B	505/505 (100%)	-0.52	13 (2%) 56 61	20, 29, 50, 69	0
2	b	505/505 (100%)	-0.34	24 (4%) 30 36	21, 31, 59, 88	0
3	C	451/451 (100%)	-0.54	5 (1%) 80 84	22, 33, 47, 72	0
3	c	450/451 (99%)	-0.38	7 (1%) 72 75	26, 38, 51, 68	0
4	D	342/342 (100%)	-0.70	4 (1%) 79 82	18, 26, 39, 88	0
4	d	342/342 (100%)	-0.66	4 (1%) 79 82	21, 29, 46, 80	0
5	E	80/80 (100%)	0.22	8 (10%) 7 9	29, 43, 65, 74	0
5	e	78/80 (97%)	0.51	8 (10%) 6 8	35, 47, 68, 75	0
6	F	34/34 (100%)	-0.36	2 (5%) 22 27	29, 34, 55, 67	0
6	f	32/34 (94%)	-0.04	3 (9%) 8 11	33, 40, 69, 78	0
7	H	63/63 (100%)	-0.21	2 (3%) 47 54	27, 36, 45, 54	0
7	h	63/63 (100%)	-0.14	2 (3%) 47 54	30, 39, 49, 56	0
8	I	35/36 (97%)	-0.04	3 (8%) 10 13	32, 37, 71, 87	0
8	i	35/36 (97%)	0.01	4 (11%) 5 6	32, 37, 71, 92	0
9	J	37/37 (100%)	-0.12	4 (10%) 5 7	28, 37, 84, 92	0
9	j	37/37 (100%)	0.15	4 (10%) 5 7	33, 44, 68, 75	0
10	K	37/37 (100%)	-0.54	0 100 100	33, 38, 50, 52	0
10	k	37/37 (100%)	-0.05	1 (2%) 54 60	38, 44, 61, 71	0
11	L	37/37 (100%)	-0.34	4 (10%) 5 7	21, 24, 57, 73	0
11	l	37/37 (100%)	-0.25	3 (8%) 12 15	22, 25, 63, 88	0
12	M	33/34 (97%)	-0.29	2 (6%) 21 26	24, 27, 51, 76	0
12	m	33/34 (97%)	-0.35	3 (9%) 9 12	25, 29, 52, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/244 (100%)	0.07	21 (8%) 10 13	20, 37, 68, 88	0
13	o	243/244 (99%)	0.02	18 (7%) 14 18	24, 38, 68, 78	0
14	T	30/31 (96%)	-0.26	2 (6%) 17 22	22, 27, 56, 84	0
14	t	29/31 (93%)	-0.33	2 (6%) 16 21	23, 27, 53, 66	0
15	U	97/97 (100%)	-0.33	1 (1%) 82 85	25, 31, 48, 66	0
15	u	97/97 (100%)	-0.37	2 (2%) 63 68	28, 32, 42, 71	0
16	V	137/137 (100%)	-0.57	0 100 100	24, 30, 43, 62	0
16	v	137/137 (100%)	-0.12	6 (4%) 34 40	30, 40, 57, 66	0
17	Y	30/30 (100%)	0.45	3 (10%) 7 9	40, 47, 58, 63	0
17	y	30/30 (100%)	0.63	6 (20%) 1 1	45, 56, 69, 75	0
18	X	40/40 (100%)	0.20	5 (12%) 3 5	33, 40, 65, 80	0
18	x	39/40 (97%)	0.37	6 (15%) 2 2	38, 47, 76, 83	0
19	Z	61/62 (98%)	0.52	12 (19%) 1 1	37, 45, 77, 86	0
19	z	61/62 (98%)	1.01	14 (22%) 0 0	49, 59, 90, 96	0
20	R	34/34 (100%)	3.95	30 (88%) 0 0	71, 86, 100, 101	0
All	All	5280/5296 (99%)	-0.32	250 (4%) 31 37	18, 33, 61, 101	0

All (250) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	494	GLY	8.7
19	z	62	VAL	8.1
18	x	2	THR	7.5
3	C	23	ALA	7.4
20	R	18	TRP	7.2
11	l	1	MET	6.8
18	X	41	LEU	6.7
20	R	6	LEU	6.7
20	R	28	VAL	6.6
14	T	30	THR	6.5
2	b	85	GLY	6.3
12	M	33	GLN	6.1
1	a	11	ALA	6.0
7	H	64	ALA	6.0
13	O	60	ARG	6.0
19	Z	31	GLN	6.0
8	I	36	ASP	6.0

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Mol	Chain	Res	Type	RSRZ
2	b	503	THR	6.0
2	b	486	LEU	6.0
19	z	31	GLN	5.9
20	R	16	ALA	5.9
18	X	2	THR	5.9
20	R	13	LEU	5.8
20	R	20	VAL	5.8
13	o	4	THR	5.8
12	M	34	LYS	5.6
9	J	4	GLU	5.6
20	R	25	PRO	5.5
7	h	64	ALA	5.5
4	D	11	GLU	5.5
18	x	40	SER	5.5
1	A	11	ALA	5.5
6	f	14	PRO	5.5
20	R	35	LEU	5.5
5	e	61	ARG	5.4
2	b	495	PHE	5.3
20	R	32	GLN	5.3
19	z	3	ILE	5.2
13	o	35	SER	5.1
14	T	31	LYS	5.1
13	O	61	GLN	5.1
9	J	5	GLY	5.1
8	i	36	ASP	5.0
13	O	3	GLN	5.0
2	b	84	THR	5.0
13	o	246	ALA	5.0
20	R	3	TRP	5.0
2	b	506	LYS	4.9
2	b	127	ARG	4.8
15	u	8	GLU	4.8
19	z	32	ASP	4.8
20	R	26	TYR	4.8
17	y	18	VAL	4.8
11	L	1	MET	4.7
19	z	61	VAL	4.6
12	m	33	GLN	4.6
13	O	4	THR	4.6
20	R	14	LEU	4.6
19	z	60	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
13	o	62	GLU	4.5
16	v	16	GLY	4.5
2	b	86	ILE	4.5
20	R	24	LEU	4.5
18	x	38	GLN	4.4
20	R	10	LEU	4.4
20	R	31	VAL	4.4
17	y	19	ILE	4.4
11	l	2	GLU	4.4
2	B	86	ILE	4.4
17	Y	19	ILE	4.4
19	Z	32	ASP	4.3
14	t	29	ILE	4.3
2	b	484	PRO	4.3
13	o	36	GLN	4.3
6	F	12	SER	4.3
8	I	34	ARG	4.2
20	R	29	LYS	4.2
20	R	17	GLY	4.2
2	B	85	GLY	4.2
9	j	6	GLY	4.2
9	j	4	GLU	4.1
19	Z	30	PRO	4.1
5	E	61	ARG	4.0
13	O	246	ALA	4.0
14	t	30	THR	4.0
4	d	11	GLU	4.0
8	i	35	LYS	4.0
2	B	485	GLU	3.9
19	Z	62	VAL	3.9
13	O	35	SER	3.9
13	O	62	GLU	3.9
11	l	3	PRO	3.9
1	A	13	LEU	3.9
5	E	83	LEU	3.9
2	b	485	GLU	3.8
2	b	502	VAL	3.8
3	C	24	THR	3.8
3	c	207	ARG	3.8
20	R	21	ARG	3.8
20	R	33	LYS	3.7
17	y	41	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
19	z	35	ARG	3.7
20	R	27	ALA	3.7
9	j	5	GLY	3.7
2	b	87	ASP	3.7
19	Z	7	LEU	3.6
2	b	295	GLY	3.6
12	m	34	LYS	3.6
11	L	2	GLU	3.6
19	Z	34	ASP	3.6
5	e	59	GLU	3.6
13	o	207	ARG	3.5
15	U	8	GLU	3.5
19	Z	33	TRP	3.5
20	R	23	ILE	3.5
19	z	34	ASP	3.5
13	o	58	ASN	3.5
5	E	81	GLU	3.4
20	R	12	VAL	3.4
13	O	36	GLN	3.4
5	e	25	ILE	3.4
20	R	34	LEU	3.4
5	E	82	GLN	3.4
18	X	40	SER	3.3
9	J	7	ARG	3.3
3	C	145	SER	3.3
9	J	6	GLY	3.3
4	D	240	ALA	3.3
20	R	15	ALA	3.3
13	o	23	ASP	3.2
13	O	89	SER	3.2
20	R	2	ASP	3.2
9	j	7	ARG	3.2
1	A	262	TYR	3.2
6	f	15	ILE	3.2
13	o	5	LEU	3.2
4	D	12	ARG	3.2
13	O	132	ASN	3.1
19	Z	60	PHE	3.1
3	C	207	ARG	3.1
13	o	25	THR	3.1
13	o	61	GLN	3.1
1	a	235	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	506	LYS	3.1
2	b	129	GLY	3.1
19	Z	3	ILE	3.1
5	e	71	GLU	3.0
13	o	60	ARG	3.0
20	R	9	LEU	3.0
1	a	262	TYR	3.0
6	f	16	PHE	3.0
3	c	143	TYR	3.0
2	B	127[A]	ARG	3.0
13	O	130	GLN	3.0
13	o	130	GLN	3.0
3	c	24	THR	2.9
17	y	43	ARG	2.9
2	b	128	THR	2.9
13	O	58	ASN	2.9
16	v	106	ASN	2.9
4	d	240	ALA	2.8
5	e	81	GLU	2.8
19	z	38	GLN	2.8
2	B	486	LEU	2.8
13	O	85	LEU	2.8
8	I	35	LYS	2.8
2	B	295	GLY	2.8
13	O	207	ARG	2.8
3	c	257	PHE	2.8
4	d	236	ASN	2.8
19	Z	41	PHE	2.7
8	i	34	ARG	2.7
19	Z	35	ARG	2.7
19	z	2	THR	2.7
1	A	16	ARG	2.7
17	Y	18	VAL	2.7
2	b	493	TRP	2.7
2	b	218	LEU	2.7
17	Y	43	ARG	2.7
5	E	4	THR	2.7
5	e	82	GLN	2.6
20	R	30	GLN	2.6
17	y	20	ALA	2.6
13	o	34	SER	2.6
11	L	7	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
19	z	30	PRO	2.6
4	D	238	THR	2.6
5	E	74	GLN	2.6
5	e	83	LEU	2.6
20	R	5	VAL	2.5
2	B	293	ALA	2.5
2	b	487	SER	2.5
3	C	191	PRO	2.5
13	o	24	ASP	2.5
18	x	34	ILE	2.5
16	v	17	LYS	2.5
18	X	38	GLN	2.5
3	c	253	LEU	2.5
19	Z	42	LEU	2.5
19	z	33	TRP	2.5
13	O	25	THR	2.5
2	b	489	GLU	2.5
2	B	373	LYS	2.4
2	B	505	ARG	2.4
5	E	71	GLU	2.4
10	k	13	GLU	2.4
18	X	3	ILE	2.4
3	c	182	PHE	2.4
11	L	3	PRO	2.4
1	a	242	GLU	2.4
7	h	57	GLY	2.4
1	a	229	GLU	2.3
4	d	238	THR	2.3
16	v	96	ARG	2.3
13	O	139	SER	2.3
13	O	90	ASP	2.3
12	m	5	GLN	2.3
15	u	66	GLY	2.3
16	v	14	SER	2.3
2	B	495	PHE	2.3
18	x	37	VAL	2.3
7	H	6	TRP	2.3
1	A	12	ASN	2.3
13	O	24	ASP	2.2
1	a	225	ARG	2.2
2	B	489[A]	GLU	2.2
19	z	41	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
13	o	64	GLU	2.2
16	v	27	LEU	2.2
3	c	233	VAL	2.2
13	O	206	GLY	2.2
13	o	21	THR	2.2
1	a	13	LEU	2.1
2	b	130[A]	GLU	2.1
5	E	76	VAL	2.1
2	b	505[A]	ARG	2.1
2	b	294	SER	2.1
17	y	17	GLU	2.1
20	R	22	ASN	2.1
8	i	2	GLU	2.1
13	o	98	GLU	2.1
13	O	37	THR	2.1
20	R	19	ALA	2.1
19	z	59	PHE	2.1
6	F	44	GLN	2.0
2	B	374	ASN	2.0
2	b	483	ASP	2.0
13	O	23	ASP	2.0
5	e	32	ILE	2.0
18	x	3	ILE	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
19	FME	z	1	10/11	0.71	0.34	87,91,94,95	0
19	FME	Z	1	10/11	0.75	0.23	69,71,74,78	0
14	FME	t	1	10/11	0.89	0.14	28,30,46,49	0
12	FME	M	1	10/11	0.91	0.12	33,36,43,49	0
12	FME	m	1	10/11	0.92	0.12	35,38,49,54	0
14	FME	T	1	10/11	0.95	0.09	27,29,44,46	0
8	FME	i	1	10/11	0.96	0.08	36,38,40,40	0
8	FME	I	1	10/11	0.97	0.07	34,39,40,40	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	LMT	i	102	35/35	0.22	0.41	52,88,111,111	0
32	LMT	A	1018	35/35	0.24	0.44	51,93,113,116	0
31	UNL	b	603	16/-	0.45	0.36	64,67,71,71	0
33	GOL	D	418	6/6	0.46	0.31	70,72,73,74	0
29	LMG	Z	101	51/55	0.48	0.35	47,77,104,110	0
32	LMT	a	402	35/35	0.50	0.32	52,65,69,70	0
32	LMT	m	103	35/35	0.52	0.29	55,90,100,101	0
32	LMT	t	103	35/35	0.53	0.30	46,75,96,99	0
35	HTG	B	624	19/19	0.53	0.41	58,86,92,92	0
32	LMT	b	625	35/35	0.53	0.29	52,82,103,104	0
35	HTG	B	629	19/19	0.53	0.28	52,86,90,90	0
35	HTG	D	413	19/19	0.54	0.31	69,80,85,86	0
35	HTG	c	525	19/19	0.55	0.36	76,90,95,96	0
29	LMG	c	521	51/55	0.56	0.30	53,81,93,97	0
32	LMT	M	101	35/35	0.56	0.29	52,85,95,97	0
35	HTG	d	410	19/19	0.57	0.32	74,84,91,91	0
32	LMT	f	103	35/35	0.58	0.35	71,92,104,104	0
31	UNL	K	103	34/-	0.58	0.23	57,76,82,83	0
31	UNL	Y	101	16/-	0.58	0.28	66,68,70,70	0
35	HTG	b	602	19/19	0.58	0.26	60,89,94,94	0
32	LMT	b	631	35/35	0.59	0.28	40,74,94,96	0
35	HTG	b	630	19/19	0.59	0.35	66,83,88,90	0
33	GOL	d	417	6/6	0.60	0.26	58,61,62,62	0
31	UNL	A	1015	28/-	0.61	0.27	62,73,78,78	0
30	DMS	b	635	4/4	0.61	0.29	66,70,72,74	0
34	LHG	e	101	49/49	0.61	0.31	66,97,101,102	0
35	HTG	D	419	19/19	0.62	0.27	59,79,83,84	0
31	UNL	a	419	30/-	0.62	0.29	62,74,87,89	0
32	LMT	A	1017	35/35	0.62	0.31	54,72,75,80	0
31	UNL	c	523	32/-	0.64	0.30	63,75,84,87	0
31	UNL	D	414	40/-	0.64	0.24	48,58,72,73	0
31	UNL	d	411	36/-	0.65	0.21	46,56,78,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	LHG	E	101	49/49	0.67	0.26	51,77,83,85	0
35	HTG	d	416	19/19	0.68	0.33	70,92,94,96	0
31	UNL	j	101	16/-	0.68	0.16	58,60,62,63	0
33	GOL	d	415	6/6	0.69	0.20	63,66,66,67	0
32	LMT	B	623	35/35	0.69	0.24	48,65,71,72	0
31	UNL	i	101	16/-	0.69	0.22	55,57,62,62	0
29	LMG	c	520	51/55	0.69	0.26	42,74,84,89	0
33	GOL	V	204	6/6	0.70	0.34	57,58,59,60	0
30	DMS	b	634	4/4	0.70	0.24	61,63,65,68	0
33	GOL	b	632	6/6	0.70	0.26	51,56,61,63	0
31	UNL	y	102	16/-	0.72	0.20	63,65,67,67	0
32	LMT	m	101	35/35	0.73	0.20	38,51,56,57	0
32	LMT	M	102	35/35	0.73	0.20	39,58,64,66	0
29	LMG	C	519	51/55	0.73	0.28	38,74,84,85	0
30	DMS	O	301	4/4	0.73	0.30	72,73,75,76	0
31	UNL	t	102	16/-	0.74	0.18	68,72,74,74	0
28	SQD	b	623[B]	54/54	0.75	0.25	49,57,77,80	54
33	GOL	v	204	6/6	0.75	0.24	74,75,76,76	0
28	SQD	b	623[A]	54/54	0.75	0.25	41,53,70,71	54
33	GOL	V	207	6/6	0.76	0.19	60,63,64,64	0
32	LMT	C	520	35/35	0.77	0.27	68,75,79,79	0
35	HTG	B	628	19/19	0.77	0.20	45,68,72,74	0
31	UNL	J	102	16/-	0.78	0.16	50,52,58,59	0
31	UNL	x	101	16/-	0.78	0.17	41,45,59,60	0
28	SQD	B	620[A]	54/54	0.79	0.24	42,56,75,76	54
30	DMS	B	633	4/4	0.79	0.24	67,69,70,75	0
28	SQD	B	620[B]	54/54	0.79	0.24	40,54,66,66	54
28	SQD	f	102	43/54	0.79	0.28	61,80,89,91	0
29	LMG	c	519	51/55	0.80	0.18	45,62,77,80	0
27	PL9	a	414	55/55	0.80	0.21	53,63,77,78	0
32	LMT	a	416	35/35	0.80	0.32	73,75,79,79	0
35	HTG	C	522	19/19	0.80	0.26	65,75,80,80	0
31	UNL	l	101	16/-	0.80	0.21	49,58,68,69	0
33	GOL	v	203	6/6	0.80	0.20	48,52,53,53	0
31	UNL	b	627	16/-	0.80	0.12	47,48,50,50	0
31	UNL	B	630	16/-	0.81	0.24	53,56,60,60	0
35	HTG	o	301	19/19	0.81	0.18	47,49,53,53	0
31	UNL	I	101	13/-	0.81	0.27	54,56,56,57	0
29	LMG	a	415	51/55	0.81	0.17	50,60,70,71	0
35	HTG	V	202	19/19	0.81	0.30	56,63,77,77	0
35	HTG	c	522	19/19	0.81	0.28	82,85,89,90	0
35	HTG	b	626	19/19	0.82	0.17	43,48,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	SQD	A	1016	54/54	0.82	0.17	46,60,72,73	0
27	PL9	A	1010	55/55	0.83	0.19	43,55,72,72	0
30	DMS	c	528	4/4	0.83	0.21	83,85,86,88	0
29	LMG	A	1012	51/55	0.83	0.17	49,56,67,71	0
31	UNL	L	101	16/-	0.83	0.21	53,56,63,63	0
29	LMG	C	518	51/55	0.83	0.18	36,62,70,70	0
30	DMS	a	418	4/4	0.84	0.20	62,63,66,69	0
28	SQD	a	401	54/54	0.84	0.16	42,60,74,76	0
24	CLA	B	601	65/65	0.84	0.16	34,42,66,69	0
35	HTG	C	521	19/19	0.84	0.22	69,71,74,75	0
33	GOL	V	206	6/6	0.84	0.30	53,56,57,58	0
24	CLA	b	604	65/65	0.84	0.17	40,48,69,70	0
31	UNL	B	625	16/-	0.85	0.13	44,46,52,54	0
31	UNL	X	101	16/-	0.85	0.14	39,43,51,51	0
26	BCR	K	102	40/40	0.85	0.12	39,49,52,52	0
31	UNL	I	102	13/-	0.85	0.14	55,57,60,60	0
24	CLA	c	513	65/65	0.86	0.16	45,54,69,70	0
24	CLA	C	513	65/65	0.86	0.15	41,48,66,68	0
29	LMG	B	622	51/55	0.86	0.14	38,47,58,64	0
29	LMG	m	102	51/55	0.87	0.13	35,49,57,59	0
33	GOL	A	1019	6/6	0.87	0.20	60,61,62,62	0
26	BCR	k	102	40/40	0.87	0.14	48,54,64,66	0
30	DMS	C	525	4/4	0.87	0.24	71,73,73,74	0
29	LMG	d	409	51/55	0.87	0.16	33,42,72,76	0
30	DMS	b	633	4/4	0.87	0.15	55,55,56,62	0
24	CLA	b	619	65/65	0.88	0.15	31,35,80,81	0
30	DMS	C	527	4/4	0.88	0.26	75,75,77,80	0
24	CLA	C	512	65/65	0.88	0.13	39,42,71,72	0
30	DMS	d	413	4/4	0.88	0.21	57,62,62,63	0
30	DMS	c	527	4/4	0.88	0.25	65,65,66,66	0
24	CLA	c	506	65/65	0.88	0.15	38,40,78,81	0
30	DMS	V	205	4/4	0.89	0.17	61,62,64,65	0
33	GOL	B	631	6/6	0.89	0.24	56,57,60,62	0
35	HTG	b	601	19/19	0.89	0.14	44,60,67,67	0
31	UNL	d	412	16/-	0.89	0.18	48,53,62,63	0
26	BCR	d	404	40/40	0.89	0.11	31,36,59,59	0
31	UNL	D	415	16/-	0.89	0.13	39,42,48,49	0
24	CLA	B	616	65/65	0.89	0.16	27,31,79,80	0
24	CLA	d	403	65/65	0.89	0.14	31,34,76,77	0
36	DGD	c	516	62/66	0.90	0.12	36,42,75,79	0
29	LMG	D	412	51/55	0.90	0.15	27,38,77,78	0
26	BCR	D	406	40/40	0.90	0.11	28,32,50,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	SQD	c	518	54/54	0.90	0.14	41,59,74,76	0
26	BCR	h	101	40/40	0.90	0.12	32,39,47,48	0
30	DMS	D	417	4/4	0.91	0.19	57,58,62,64	0
33	GOL	a	420	6/6	0.91	0.15	53,56,57,59	0
30	DMS	U	201	4/4	0.91	0.19	56,56,58,58	0
30	DMS	A	1014	4/4	0.91	0.20	54,54,55,61	0
24	CLA	c	512	65/65	0.91	0.12	42,46,65,67	0
26	BCR	K	101	40/40	0.91	0.13	32,35,37,38	0
30	DMS	B	634	4/4	0.91	0.27	54,57,59,59	0
30	DMS	C	526	4/4	0.91	0.18	71,71,72,72	0
28	SQD	D	408	43/54	0.91	0.18	41,67,74,76	0
28	SQD	A	1011	54/54	0.91	0.15	43,57,69,69	0
26	BCR	c	514	40/40	0.91	0.11	34,41,43,44	0
36	DGD	h	102	62/66	0.91	0.11	32,38,46,48	0
24	CLA	b	609	65/65	0.91	0.12	29,32,65,68	0
30	DMS	D	416	4/4	0.91	0.26	55,55,56,59	0
26	BCR	B	618	40/40	0.92	0.09	27,32,41,41	0
24	CLA	C	506	65/65	0.92	0.11	36,43,73,76	0
26	BCR	J	101	40/40	0.92	0.10	35,37,41,41	0
36	DGD	c	517	62/66	0.92	0.12	29,38,64,73	0
24	CLA	B	606	65/65	0.92	0.12	27,30,51,53	0
24	CLA	D	405	65/65	0.92	0.12	28,30,70,71	0
36	DGD	C	516	62/66	0.92	0.10	28,36,70,72	0
26	BCR	a	413	40/40	0.93	0.09	24,30,34,34	0
26	BCR	y	101	40/40	0.93	0.09	40,44,46,47	0
26	BCR	H	101	40/40	0.93	0.09	27,36,42,42	0
26	BCR	t	101	40/40	0.93	0.09	26,39,46,47	0
26	BCR	A	1009	40/40	0.93	0.10	25,29,32,32	0
34	LHG	d	408	49/49	0.93	0.15	32,41,72,74	0
24	CLA	A	1008	65/65	0.93	0.13	25,27,79,81	0
39	MG	K	104	1/1	0.93	0.07	48,48,48,48	0
36	DGD	H	102	62/66	0.93	0.11	27,34,38,39	0
36	DGD	c	515	62/66	0.93	0.12	28,38,69,71	0
24	CLA	c	508	65/65	0.93	0.10	32,35,65,72	0
26	BCR	k	101	40/40	0.93	0.12	36,45,47,48	0
30	DMS	u	201	4/4	0.93	0.24	56,57,57,59	0
24	CLA	a	412	65/65	0.93	0.15	26,28,90,92	0
24	CLA	b	612	65/65	0.93	0.13	30,34,37,38	0
24	CLA	C	507	65/65	0.94	0.11	34,37,51,53	0
34	LHG	d	406	49/49	0.94	0.13	38,41,46,46	0
24	CLA	C	508	65/65	0.94	0.10	28,31,65,70	0
36	DGD	C	517	62/66	0.94	0.10	24,33,62,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	CLA	a	409	65/65	0.94	0.12	24,26,85,90	0
26	BCR	C	514	40/40	0.94	0.11	31,38,41,41	0
24	CLA	C	505	65/65	0.94	0.10	32,35,44,48	0
24	CLA	c	507	65/65	0.94	0.12	33,34,50,51	0
26	BCR	b	621	40/40	0.94	0.08	28,31,41,42	0
30	DMS	O	302	4/4	0.94	0.27	58,59,62,62	0
26	BCR	B	619	40/40	0.94	0.08	31,34,42,43	0
39	MG	j	102	1/1	0.94	0.06	37,37,37,37	0
24	CLA	c	504	65/65	0.94	0.10	32,35,57,59	0
24	CLA	C	504	65/65	0.94	0.10	27,30,55,57	0
26	BCR	b	622	40/40	0.94	0.09	33,36,40,41	0
36	DGD	C	515	62/66	0.94	0.11	27,36,63,64	0
34	LHG	D	409	49/49	0.94	0.11	35,38,43,45	0
24	CLA	b	605	65/65	0.95	0.10	29,32,37,37	0
30	DMS	v	202	4/4	0.95	0.14	55,56,58,58	0
34	LHG	D	411	49/49	0.95	0.14	29,38,73,76	0
24	CLA	B	615	65/65	0.95	0.10	27,28,44,46	0
30	DMS	c	529	4/4	0.95	0.21	51,51,53,54	0
24	CLA	c	505	65/65	0.95	0.10	34,36,48,48	0
26	BCR	B	617	40/40	0.95	0.08	28,30,33,33	0
25	PHO	a	411	64/64	0.95	0.11	24,30,35,36	0
24	CLA	C	511	65/65	0.95	0.10	29,35,40,42	0
24	CLA	c	503	65/65	0.95	0.09	33,39,42,44	0
27	PL9	D	407	55/55	0.95	0.09	21,25,32,33	0
38	HEM	f	101	43/43	0.95	0.12	42,44,57,63	0
24	CLA	b	615	65/65	0.95	0.08	25,28,32,35	0
24	CLA	B	609	65/65	0.95	0.11	28,31,33,35	0
26	BCR	T	101	40/40	0.95	0.08	27,37,42,43	0
24	CLA	c	511	65/65	0.95	0.10	36,39,43,46	0
24	CLA	B	614	65/65	0.95	0.10	24,27,67,68	0
27	PL9	d	405	55/55	0.95	0.09	21,27,32,33	0
24	CLA	c	501	65/65	0.95	0.10	35,36,43,44	0
24	CLA	A	1006	65/65	0.95	0.10	22,23,66,69	0
34	LHG	d	407	49/49	0.95	0.11	26,31,40,45	0
30	DMS	c	526	4/4	0.95	0.19	73,74,74,75	0
24	CLA	b	613	65/65	0.95	0.10	28,31,38,40	0
24	CLA	b	611	65/65	0.96	0.08	26,28,38,39	0
24	CLA	b	610	65/65	0.96	0.08	23,25,34,35	0
30	DMS	V	203	4/4	0.96	0.15	50,51,51,52	0
24	CLA	c	502	65/65	0.96	0.09	28,31,50,51	0
24	CLA	C	501	65/65	0.96	0.08	31,35,41,42	0
30	DMS	C	524	4/4	0.96	0.17	40,41,41,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
38	HEM	F	101	43/43	0.96	0.11	39,41,44,46	0
30	DMS	b	629	4/4	0.96	0.11	48,49,52,53	0
24	CLA	C	503	65/65	0.96	0.08	28,33,36,38	0
37	BCT	d	401	4/4	0.96	0.09	40,40,41,42	0
26	BCR	b	620	40/40	0.96	0.09	28,34,35,35	0
24	CLA	b	607	65/65	0.96	0.09	24,26,50,51	0
24	CLA	B	604	65/65	0.96	0.10	22,24,53,55	0
24	CLA	c	509	65/65	0.96	0.11	33,35,50,51	0
24	CLA	B	610	65/65	0.96	0.09	24,26,34,36	0
24	CLA	b	608	65/65	0.96	0.10	24,26,35,35	0
34	LHG	D	410	49/49	0.96	0.11	26,30,38,41	0
24	CLA	C	509	65/65	0.96	0.10	28,31,52,53	0
24	CLA	b	617	65/65	0.96	0.10	24,28,67,68	0
24	CLA	B	607	65/65	0.96	0.09	20,22,36,37	0
30	DMS	d	414	4/4	0.96	0.11	58,59,59,60	0
34	LHG	b	624	49/49	0.96	0.09	27,32,48,53	0
24	CLA	c	510	65/65	0.96	0.09	33,35,41,43	0
24	CLA	b	614	65/65	0.96	0.09	24,26,40,41	0
24	CLA	B	605	65/65	0.96	0.10	23,26,31,32	0
24	CLA	B	602	65/65	0.96	0.09	25,27,34,35	0
24	CLA	b	618	65/65	0.96	0.08	30,32,44,46	0
25	PHO	D	404	64/64	0.96	0.09	22,25,29,30	0
24	CLA	C	502	65/65	0.96	0.09	26,28,42,44	0
25	PHO	a	410	64/64	0.97	0.08	22,24,29,31	0
24	CLA	B	611	65/65	0.97	0.09	22,24,36,37	0
24	CLA	a	408	65/65	0.97	0.08	20,23,31,34	0
39	MG	k	103	1/1	0.97	0.05	45,45,45,45	0
24	CLA	B	613	65/65	0.97	0.08	23,25,49,53	0
38	HEM	v	201	43/43	0.97	0.10	31,32,36,37	0
24	CLA	A	1005	65/65	0.97	0.10	17,20,29,33	0
24	CLA	a	407	65/65	0.97	0.10	21,23,30,35	0
30	DMS	a	417	4/4	0.97	0.09	31,32,33,33	0
24	CLA	d	402	65/65	0.97	0.10	21,23,39,43	0
30	DMS	B	627	4/4	0.97	0.10	41,41,42,44	0
24	CLA	D	402	65/65	0.97	0.09	17,20,35,37	0
24	CLA	b	606	65/65	0.97	0.09	26,29,35,39	0
25	PHO	A	1007	64/64	0.97	0.08	21,24,26,28	0
30	DMS	B	632	4/4	0.97	0.18	57,58,60,61	0
34	LHG	B	621	49/49	0.97	0.09	26,32,45,49	0
24	CLA	B	608	65/65	0.97	0.08	25,27,31,31	0
24	CLA	D	403	65/65	0.97	0.07	18,20,29,33	0
24	CLA	C	510	65/65	0.97	0.09	27,31,38,39	0

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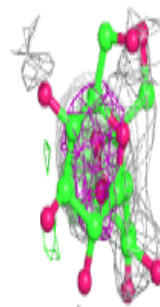
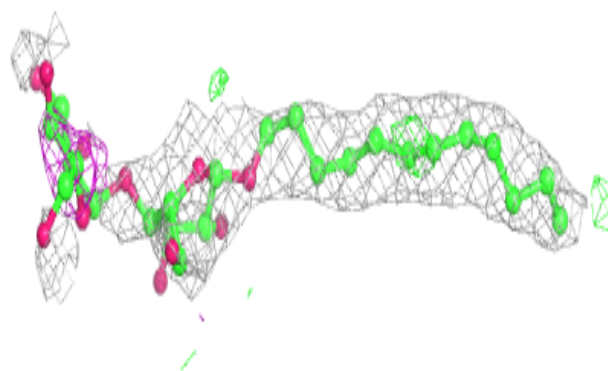
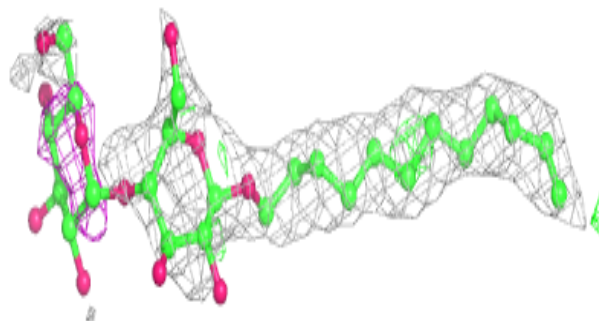
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	CLA	b	616	65/65	0.97	0.09	25,25,50,52	0
24	CLA	B	612	65/65	0.97	0.09	24,26,30,31	0
37	BCT	D	401	4/4	0.97	0.16	37,38,38,41	0
24	CLA	B	603	65/65	0.97	0.08	25,26,32,34	0
38	HEM	V	201	43/43	0.98	0.12	25,26,28,29	0
39	MG	J	103	1/1	0.98	0.04	32,32,32,32	0
30	DMS	c	524	4/4	0.98	0.18	43,43,43,43	0
30	DMS	b	628	4/4	0.98	0.07	30,31,31,32	0
30	DMS	A	1013	4/4	0.98	0.09	29,29,30,31	0
30	DMS	B	626	4/4	0.98	0.07	25,26,26,27	0
23	CL	A	1003	1/1	0.99	0.03	25,25,25,25	0
30	DMS	C	523	4/4	0.99	0.10	36,37,38,38	0
23	CL	a	405	1/1	0.99	0.03	26,26,26,26	0
21	OER	A	1001	10/10	1.00	0.06	24,25,28,28	1
21	OER	a	403	10/10	1.00	0.05	27,28,29,31	1
23	CL	A	1004	1/1	1.00	0.02	22,22,22,22	0
22	FE2	a	404	1/1	1.00	0.05	29,29,29,29	0
22	FE2	A	1002	1/1	1.00	0.03	29,29,29,29	0
23	CL	a	406	1/1	1.00	0.05	27,27,27,27	0

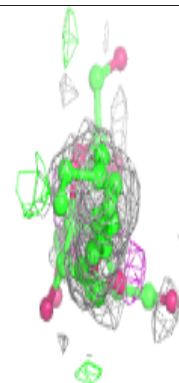
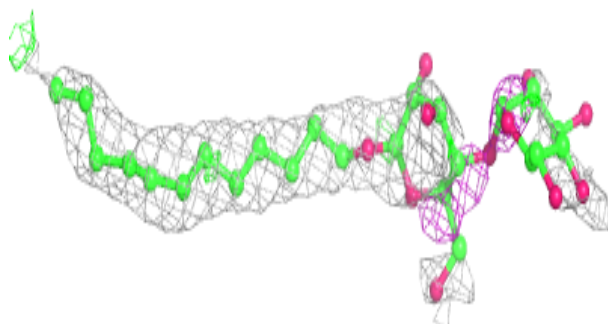
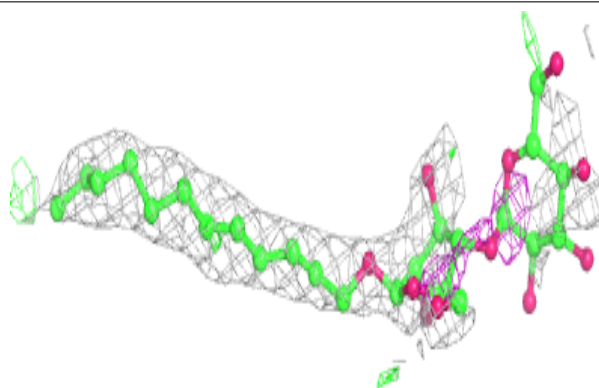
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT 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)

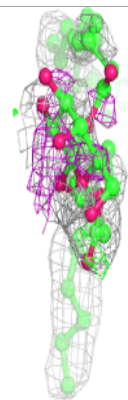
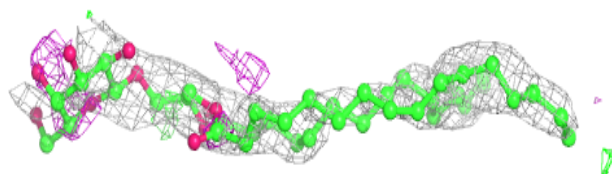
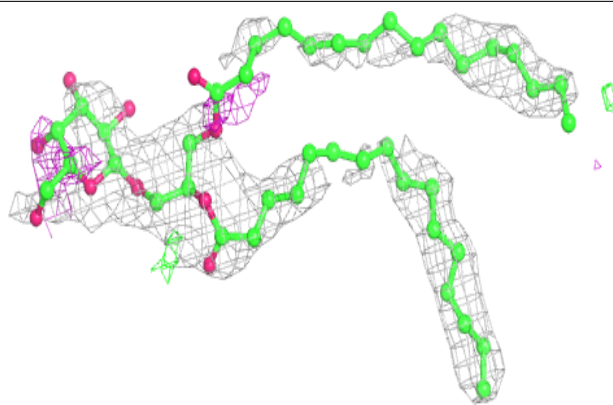
**Electron density around LMT A 1018:**

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

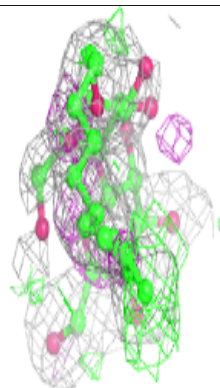
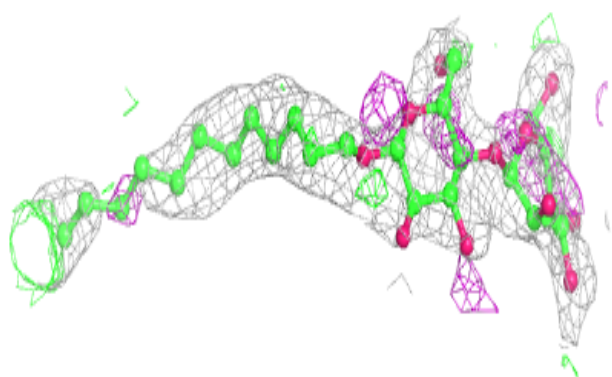
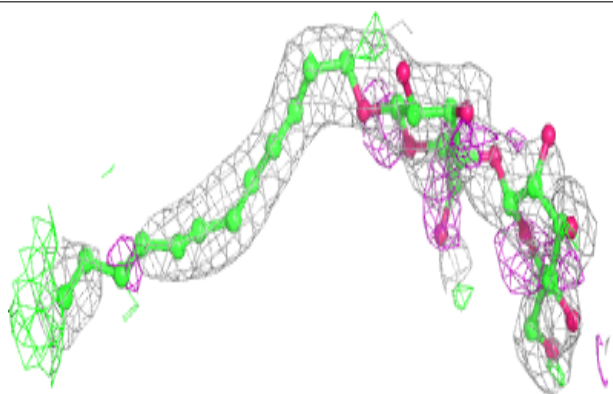


Electron density around LMG Z 101:

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

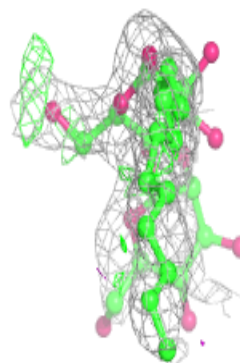
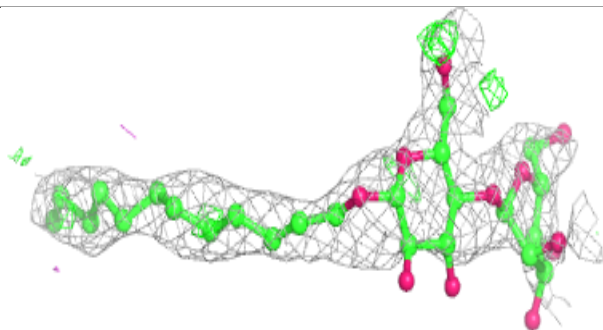
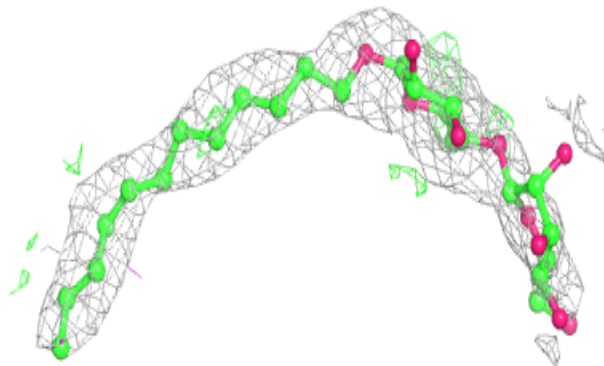
**Electron density around LMT a 402:**

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

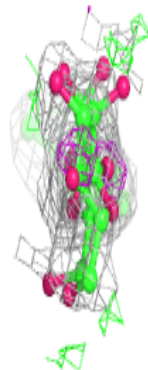
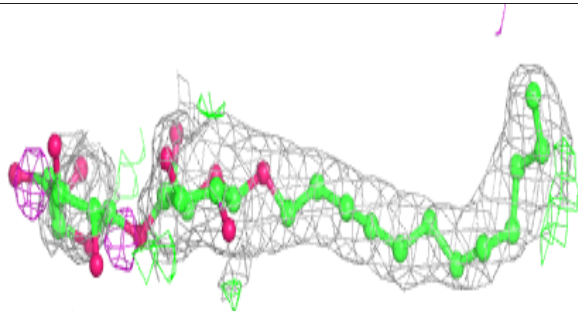
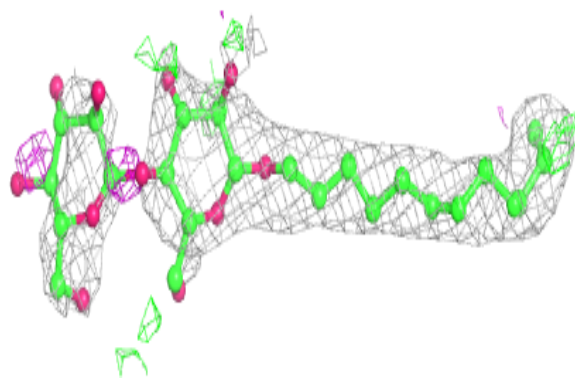


Electron density around LMT m 103:

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

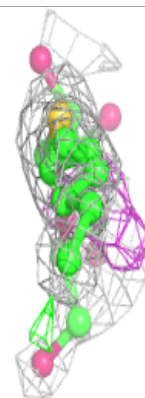
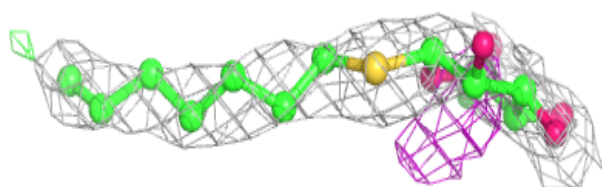
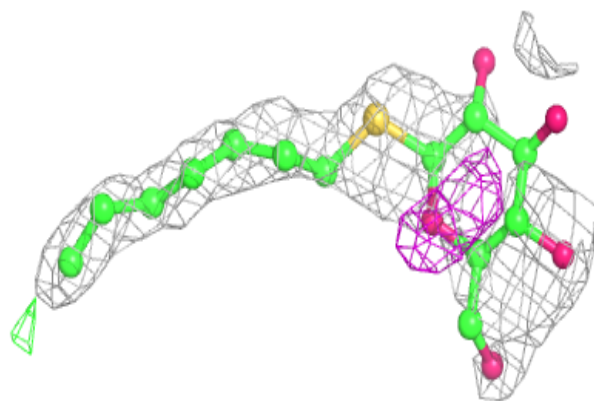
**Electron density around LMT t 103:**

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

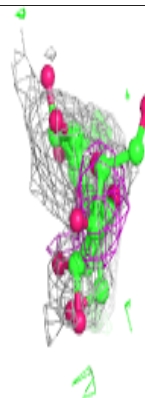
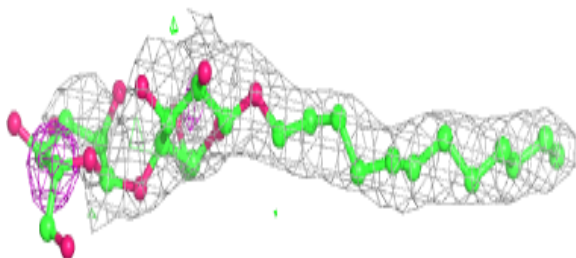
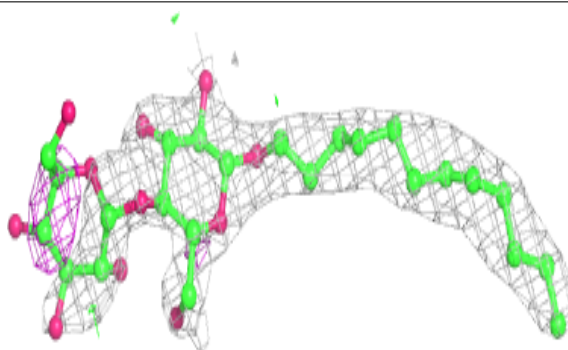


Electron density around HTG B 624:

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

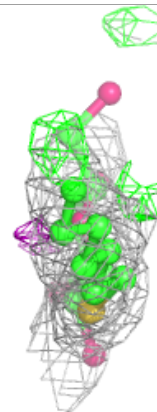
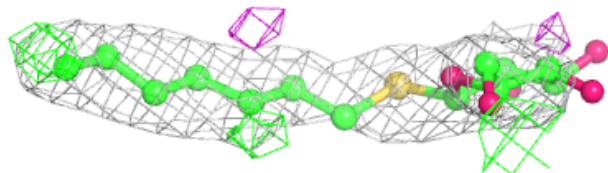
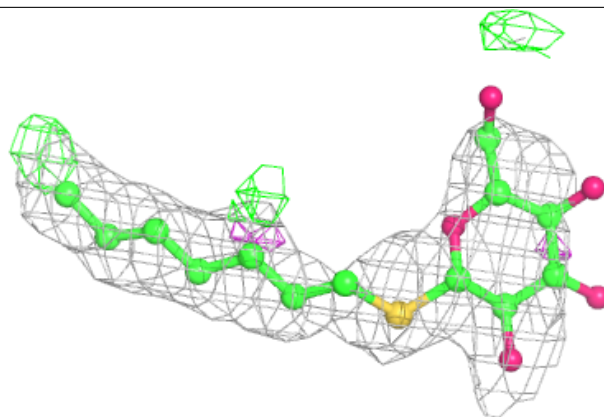
**Electron density around LMT b 625:**

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

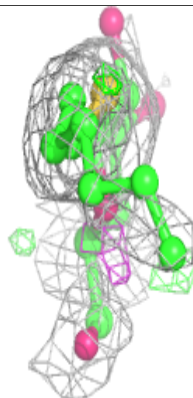
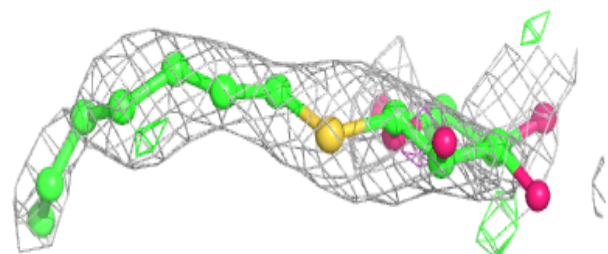
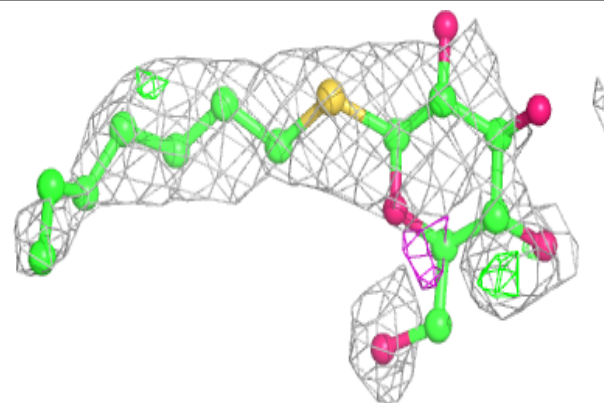


Electron density around HTG B 629:

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

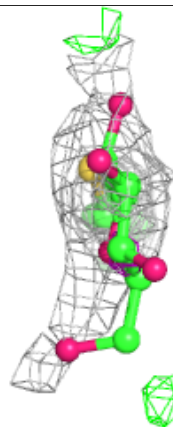
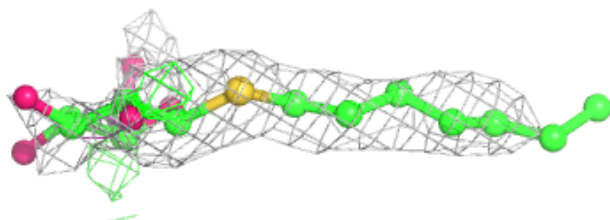
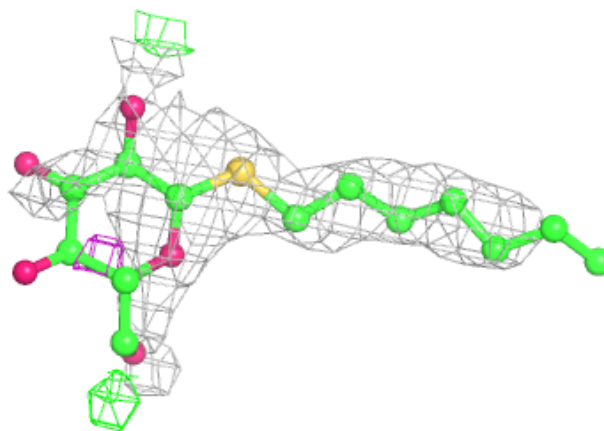
**Electron density around HTG D 413:**

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

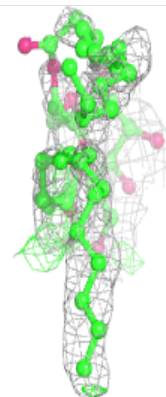
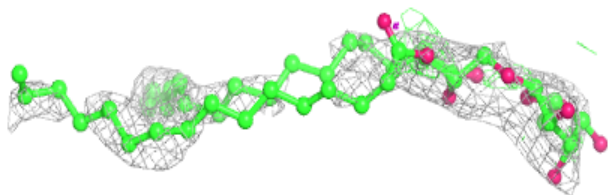
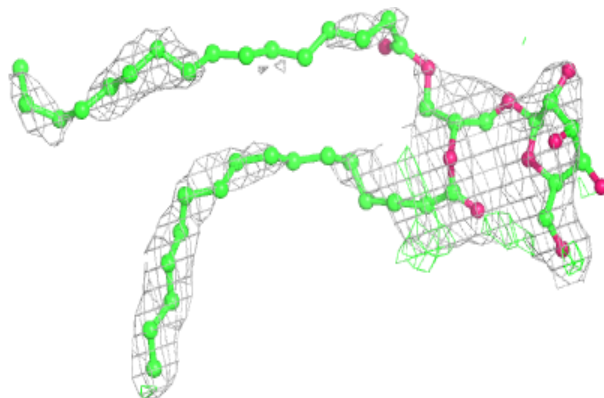


Electron density around HTG c 525:

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

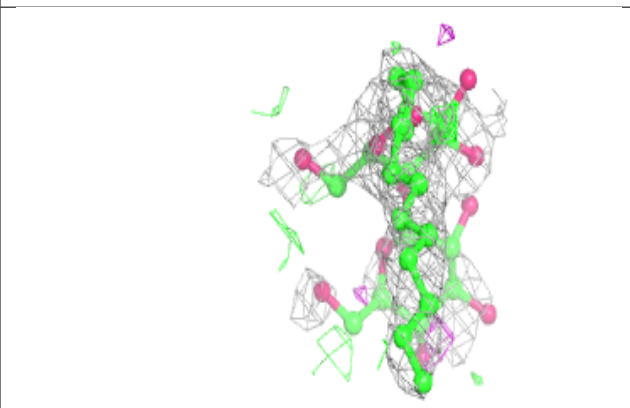
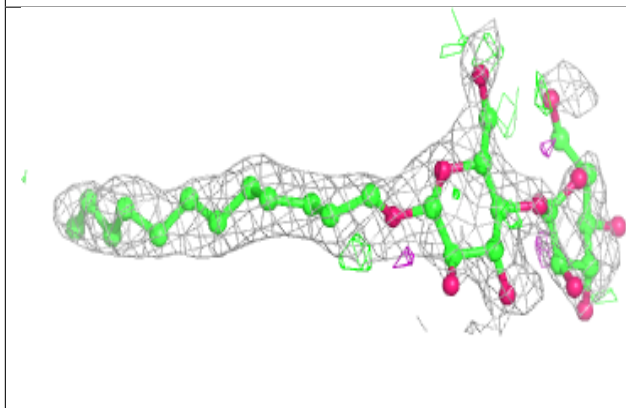
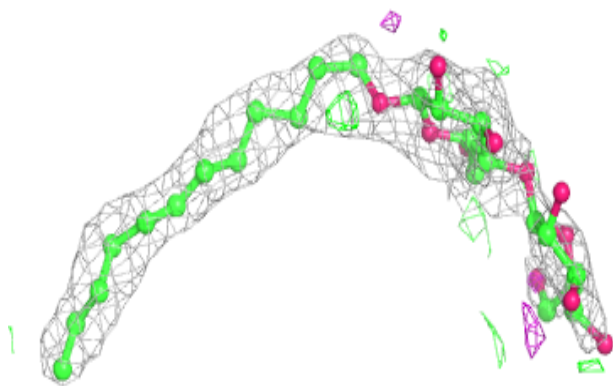
**Electron density around LMG c 521:**

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

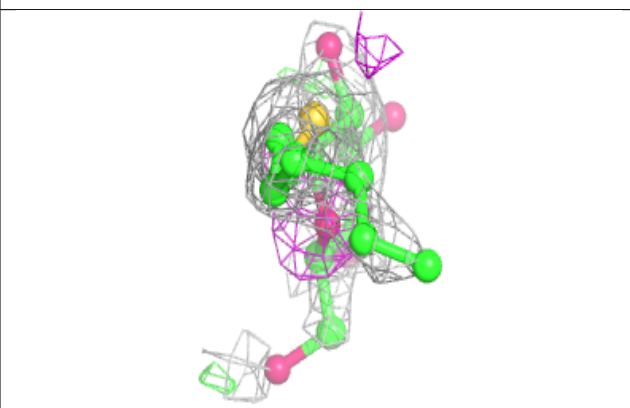
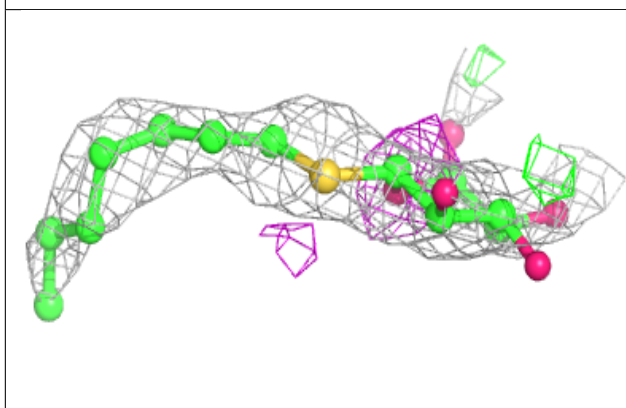
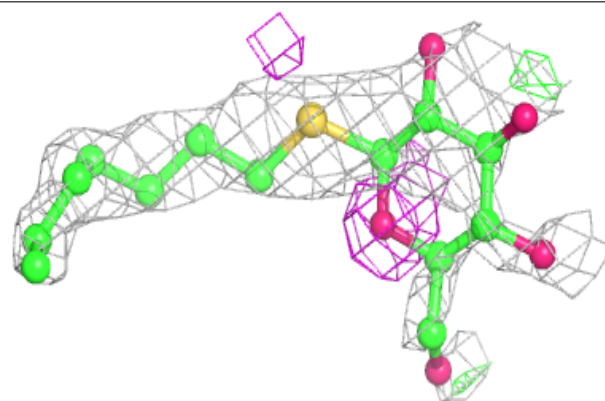


Electron density around LMT M 101:

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

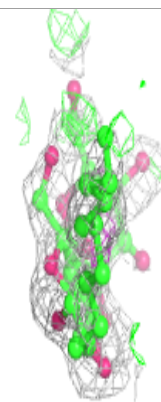
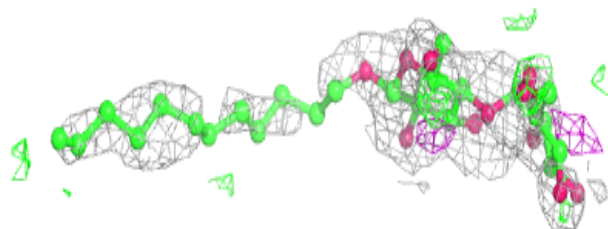
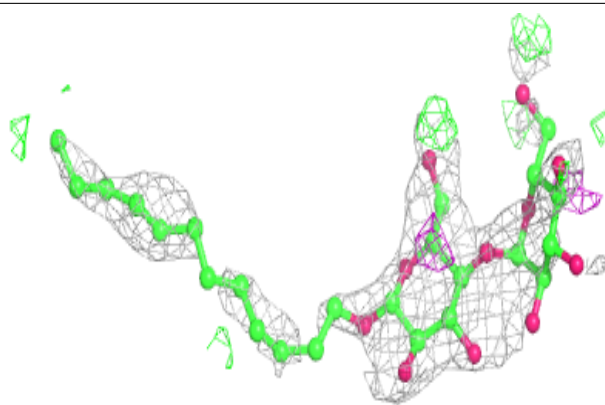
**Electron density around HTG d 410:**

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

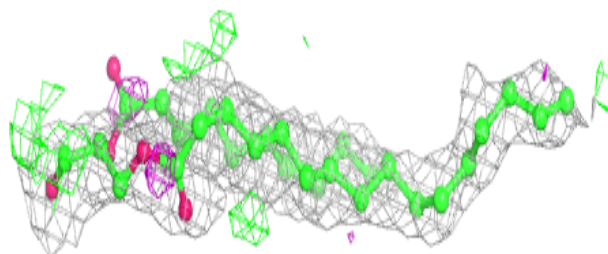
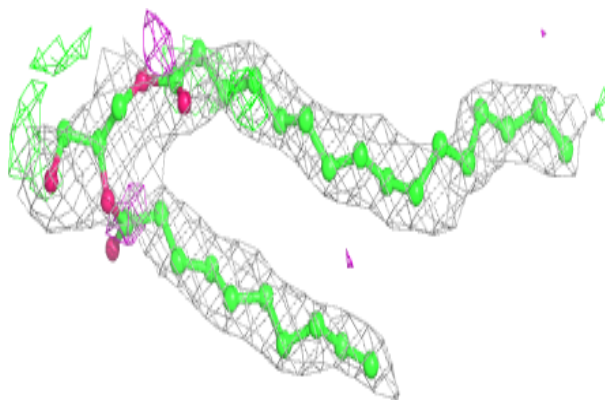


Electron density around LMT f 103:

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

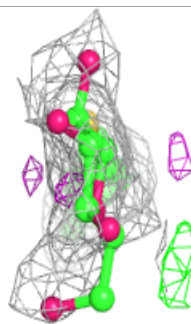
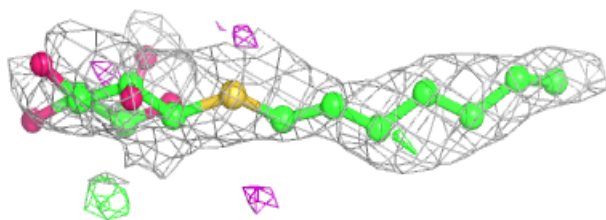
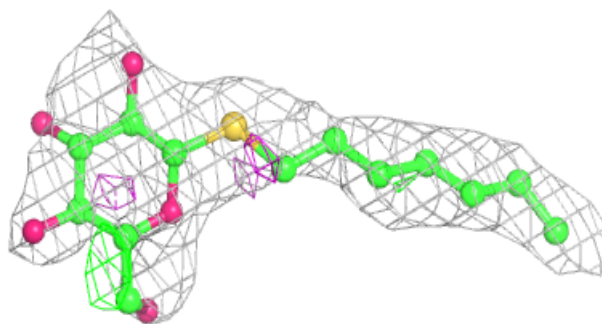
**Electron density around UNL K 103:**

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

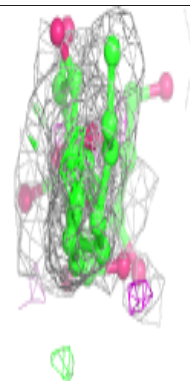
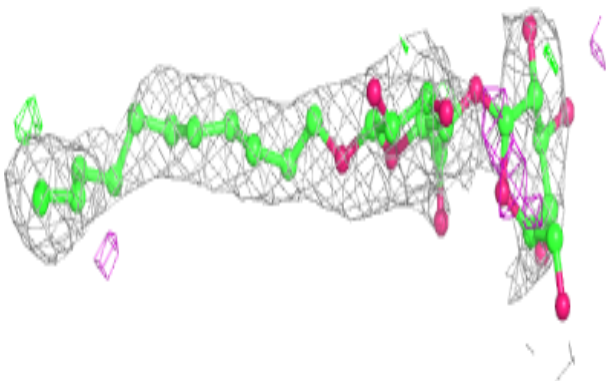
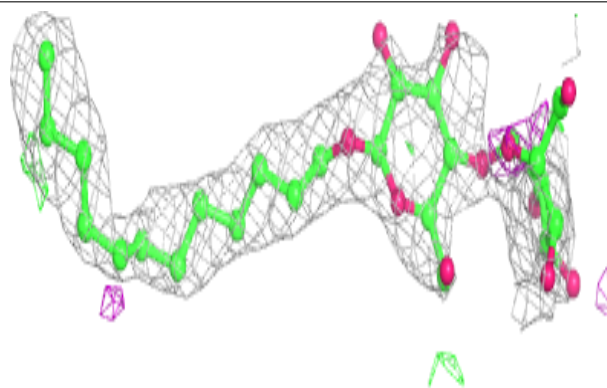


Electron density around HTG b 602:

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

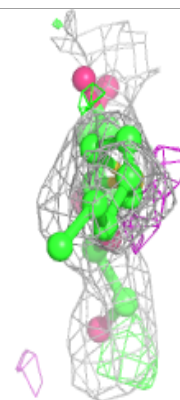
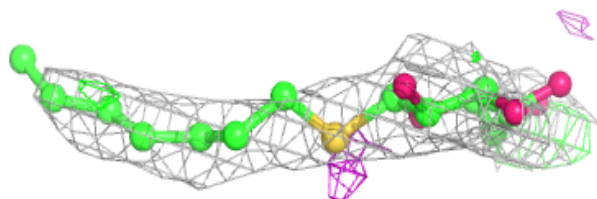
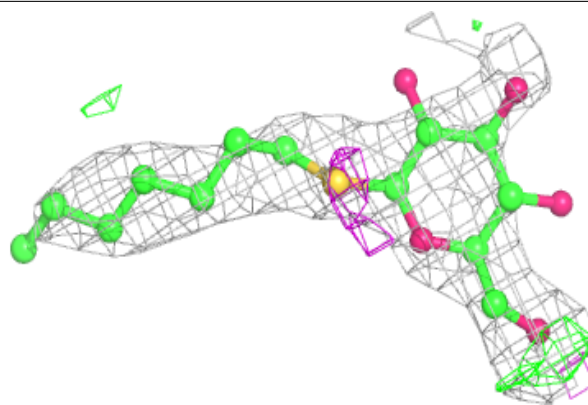
**Electron density around LMT b 631:**

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

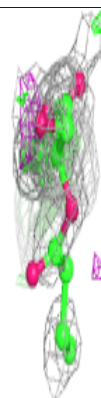
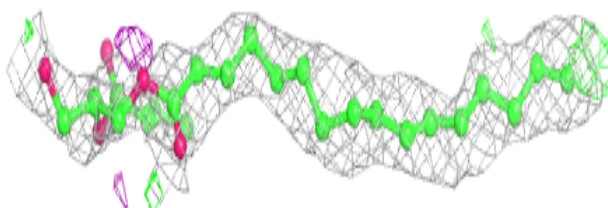
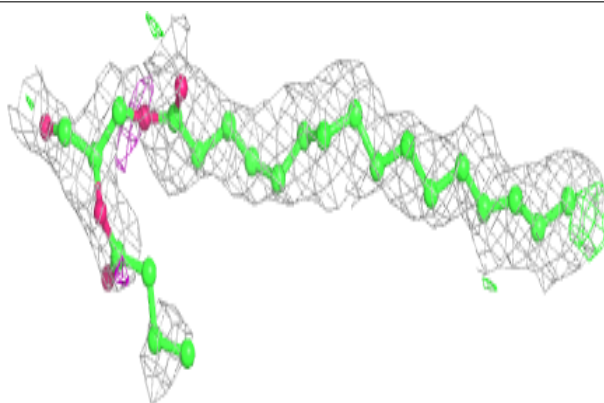


Electron density around HTG b 630:

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

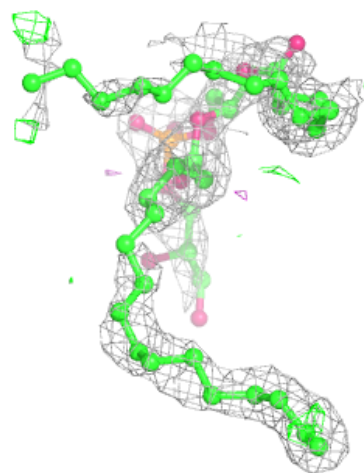
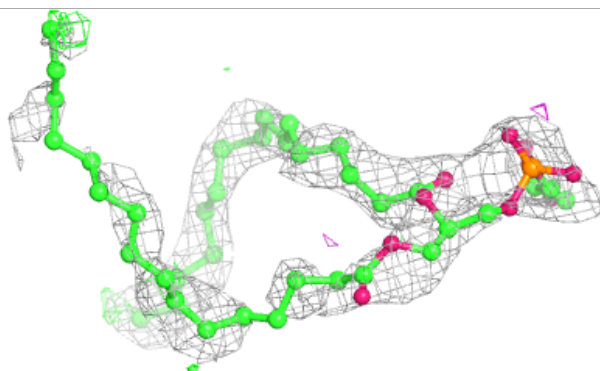
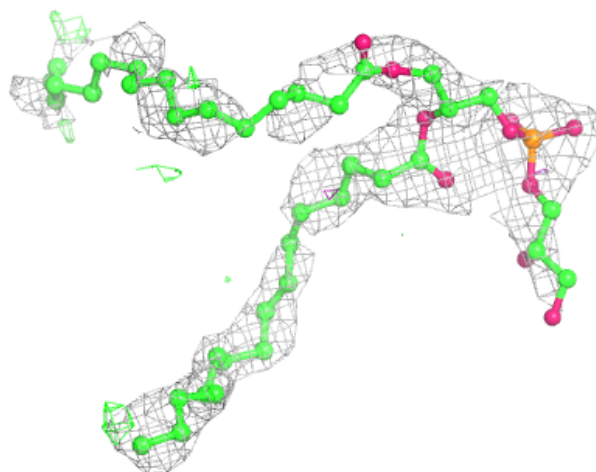
**Electron density around UNL A 1015:**

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



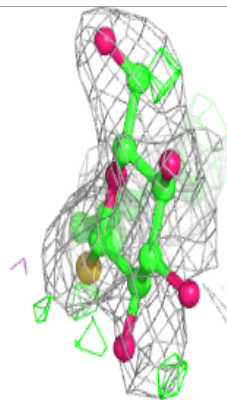
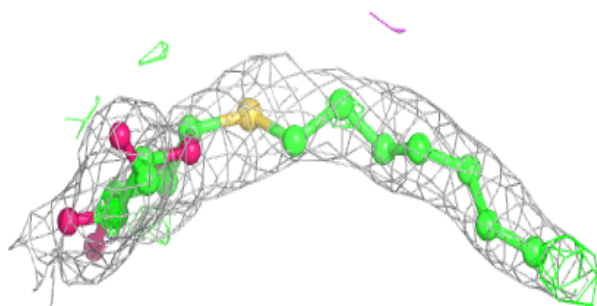
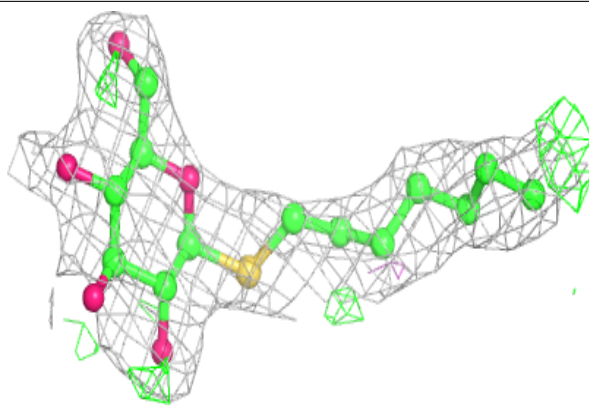
Electron density around LHG e 101:

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

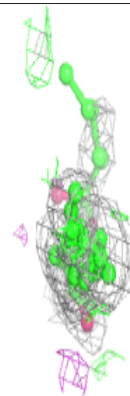
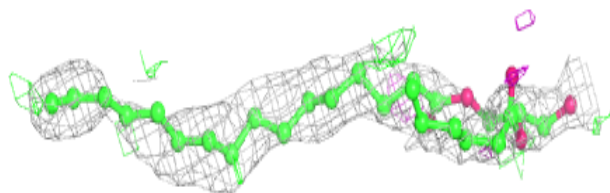
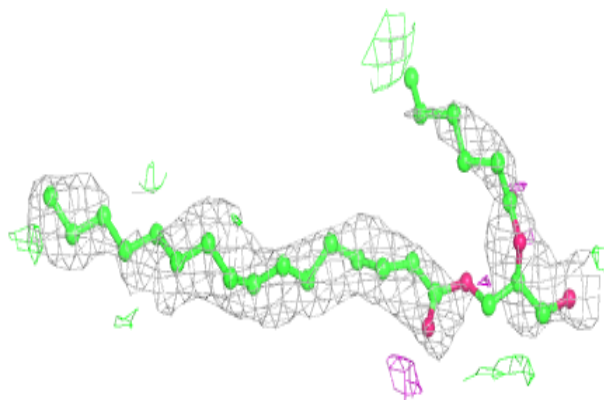


Electron density around HTG D 419:

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

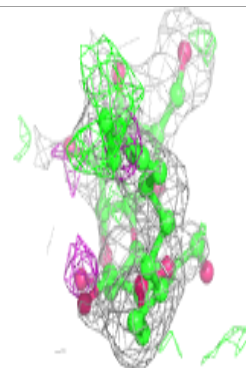
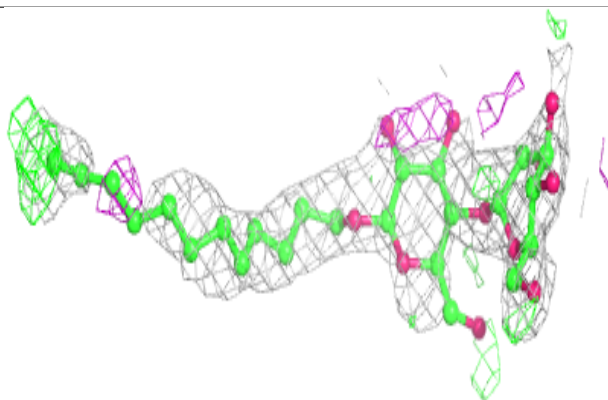
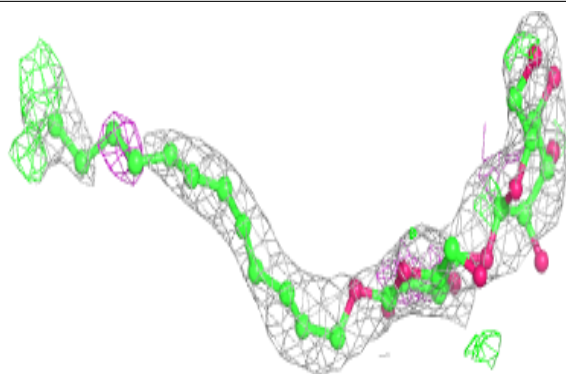
**Electron density around UNL a 419:**

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

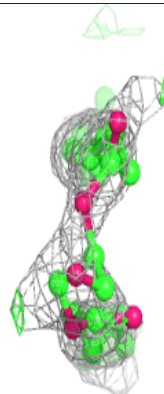
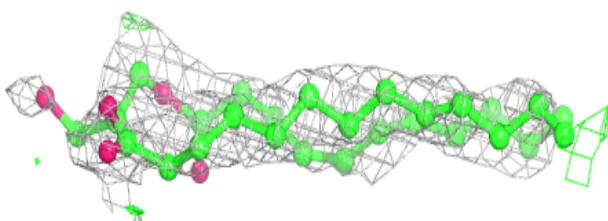
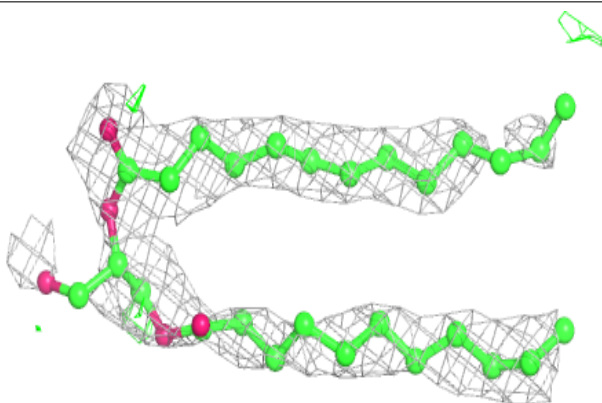


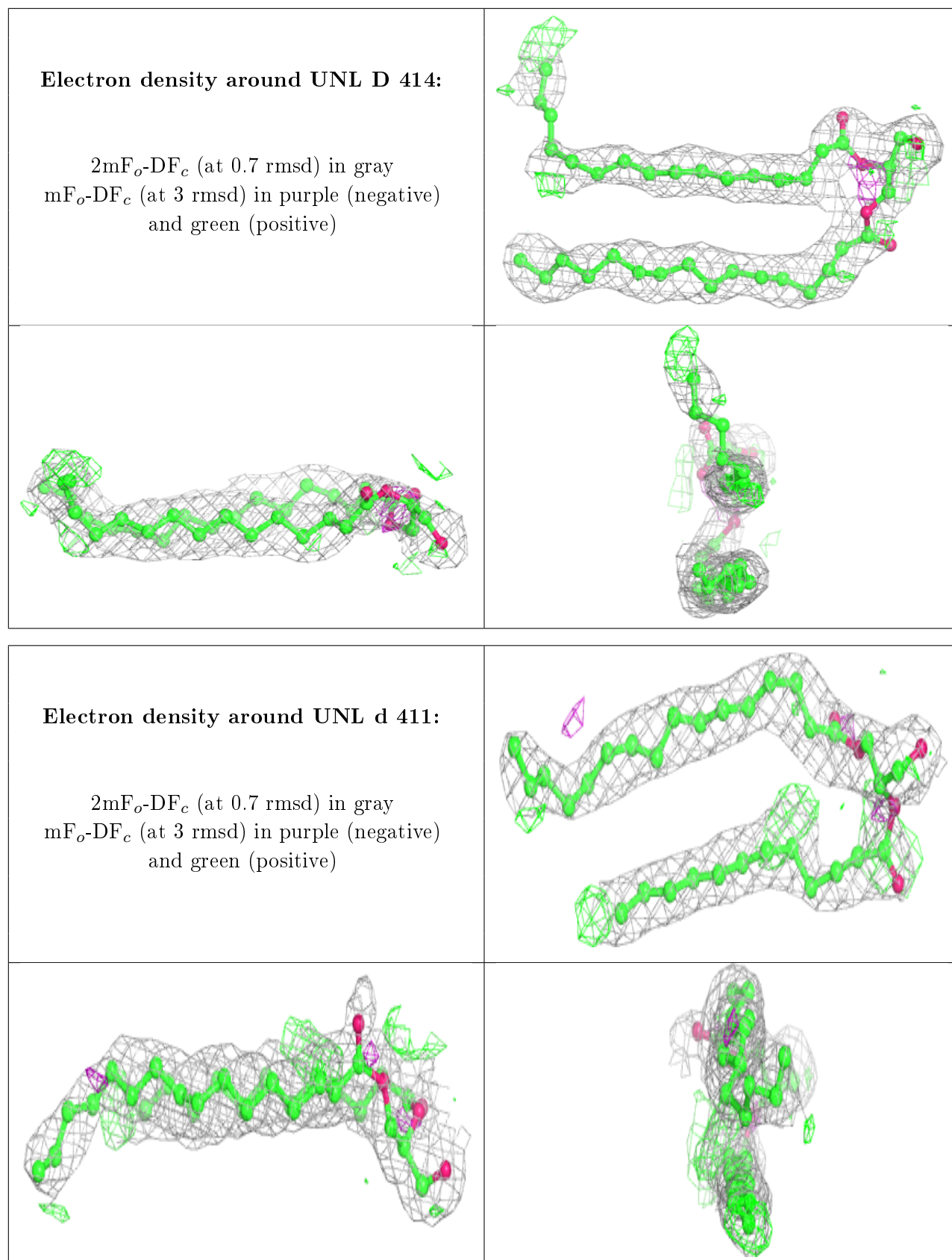
Electron density around LMT A 1017:

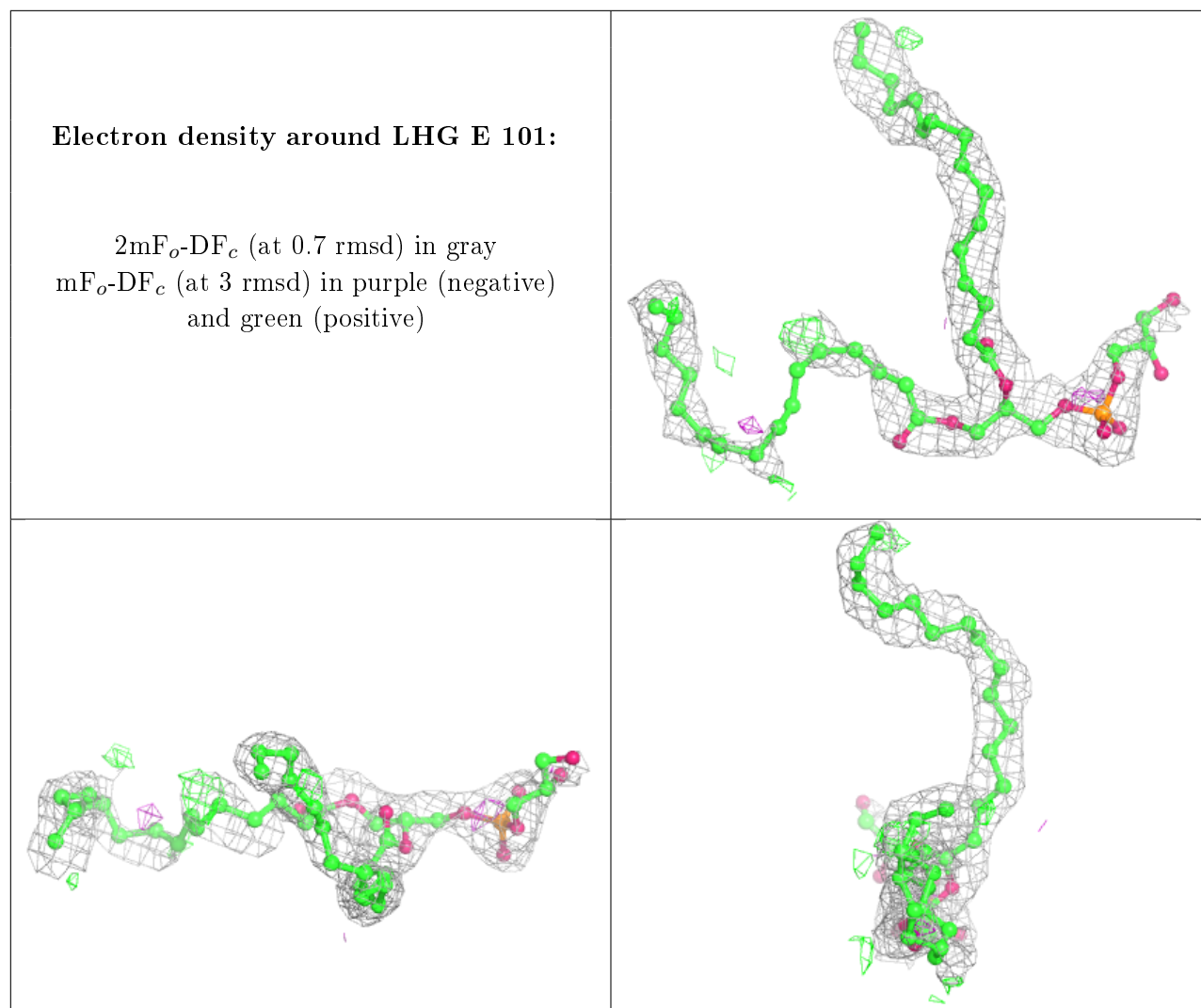
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around UNL 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)

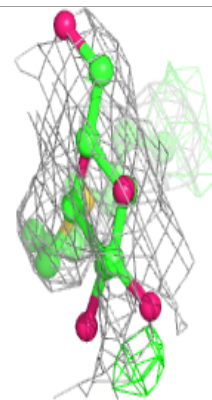
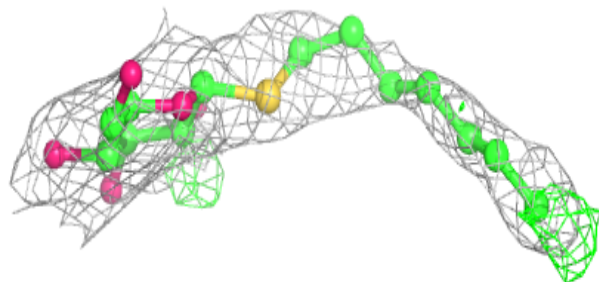
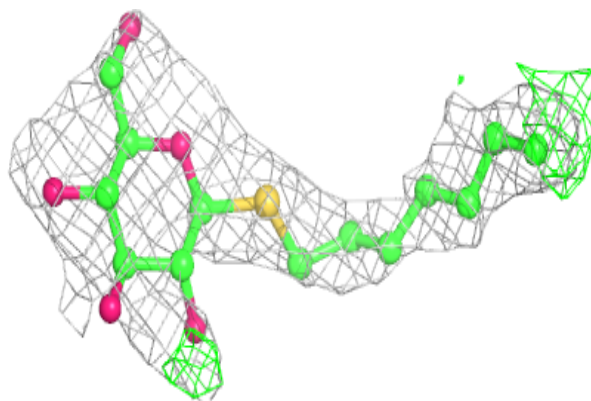




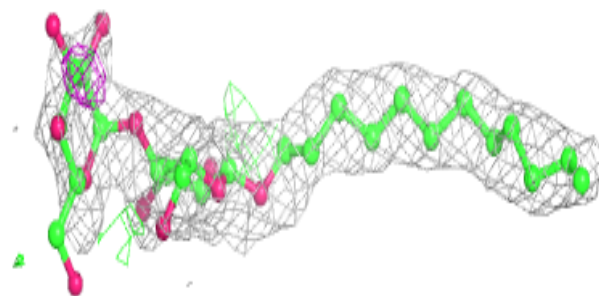
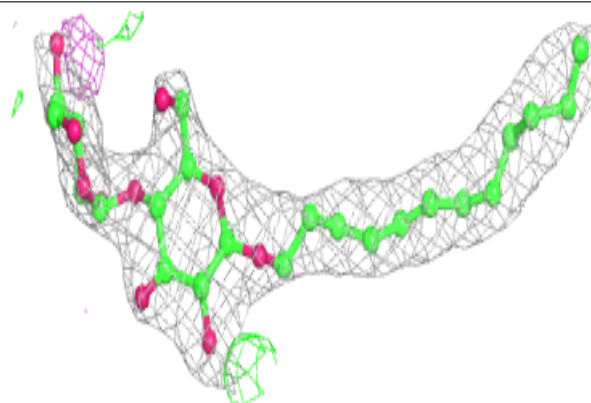


Electron density around HTG d 416:

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

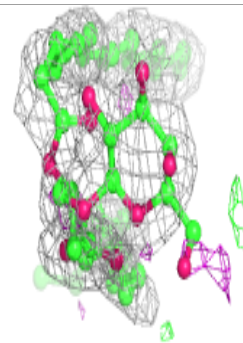
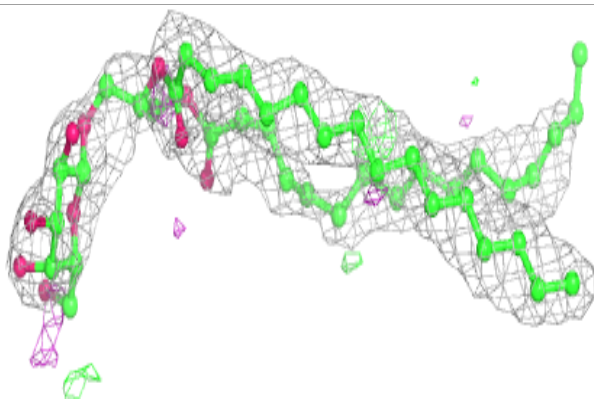
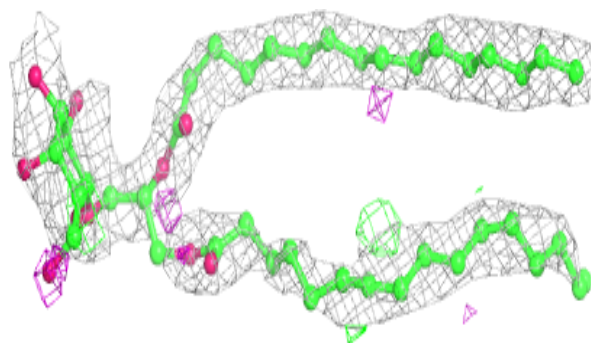
**Electron density around LMT B 623:**

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

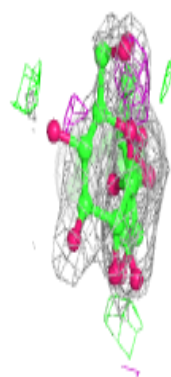
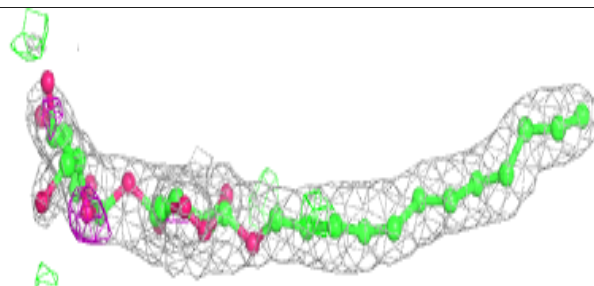
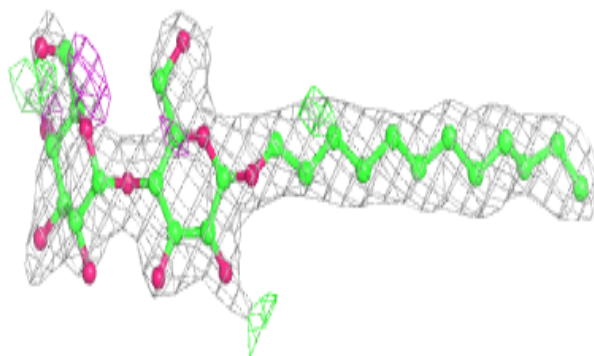


Electron density around LMG c 520:

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

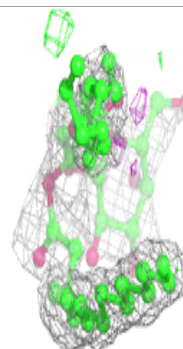
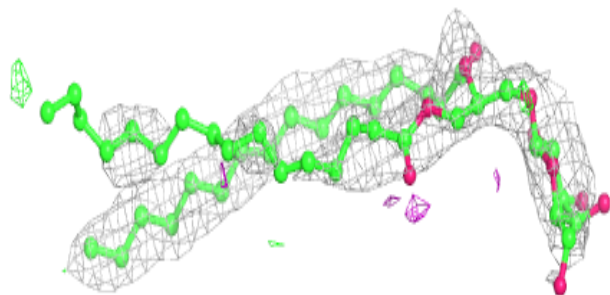
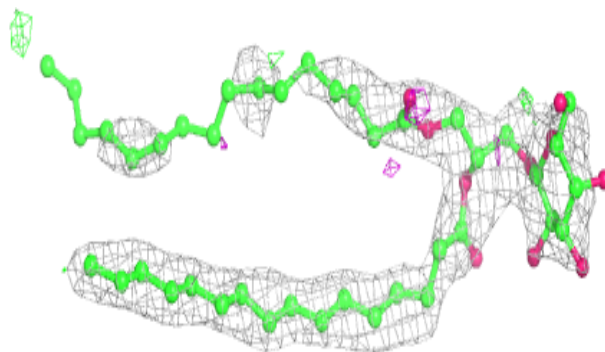
**Electron density around LMT M 102:**

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

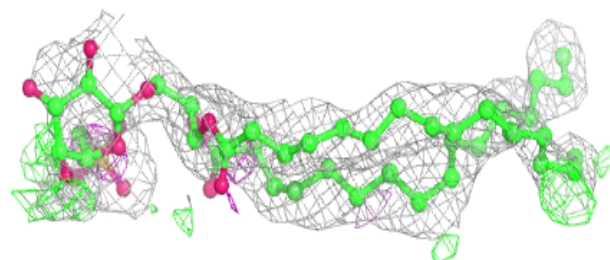
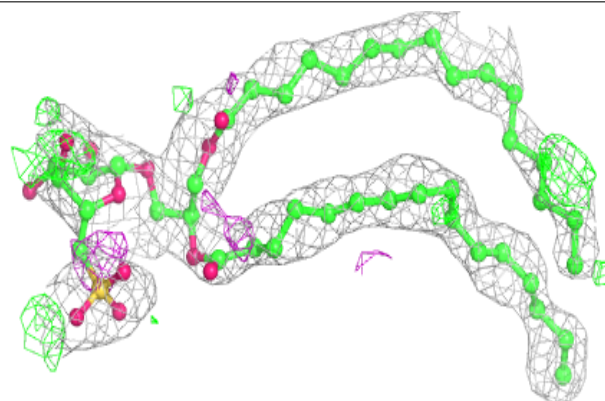


Electron density around LMG C 519:

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

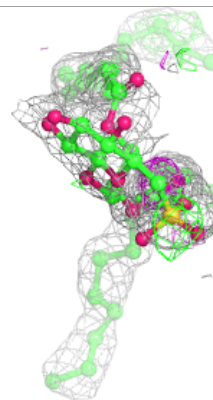
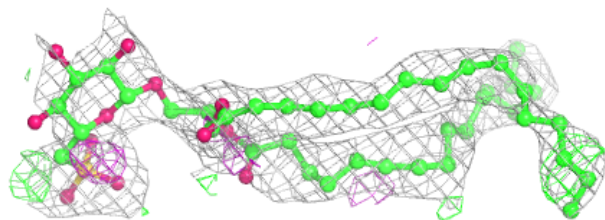
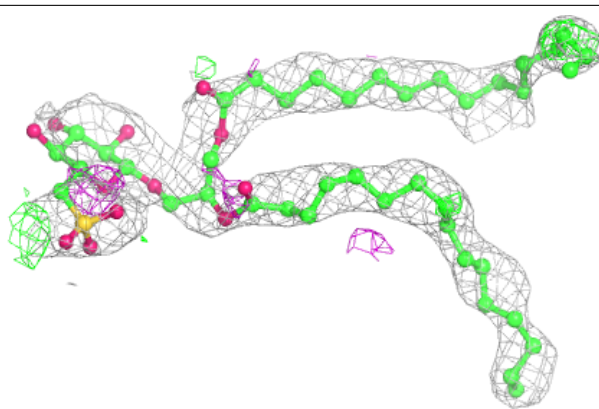
**Electron density around SQD b 623 (B):**

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

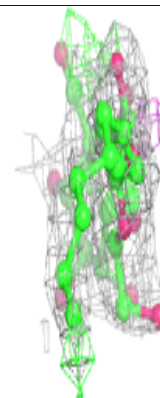
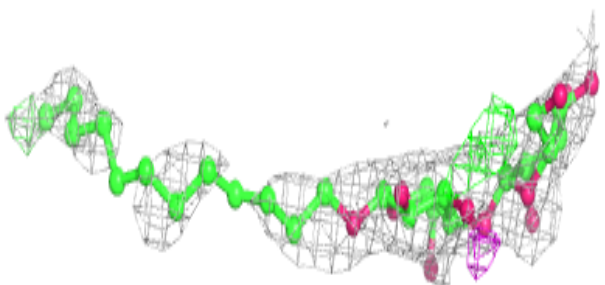
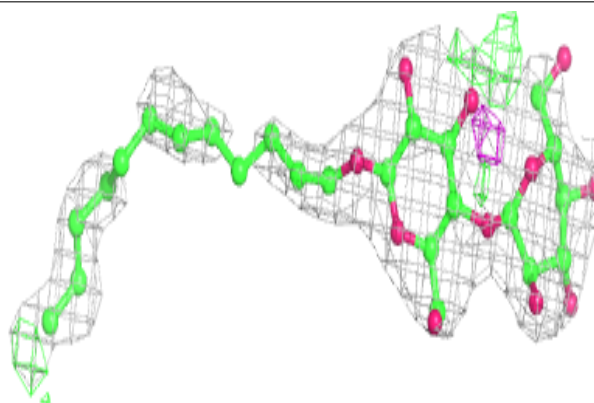


Electron density around SQD b 623 (A):

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

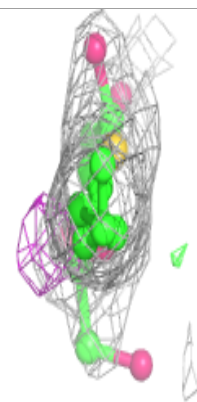
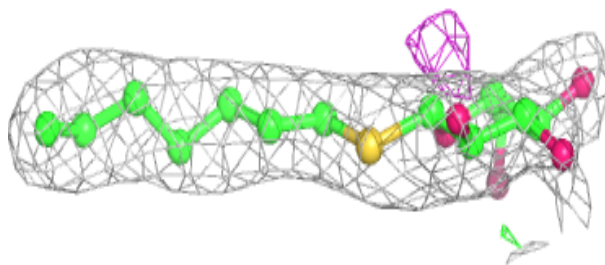
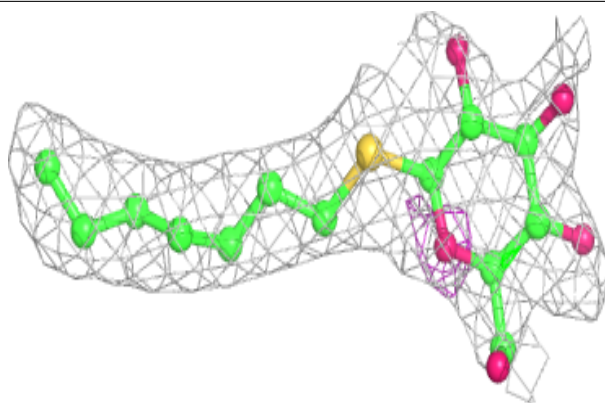
**Electron density around LMT C 520:**

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

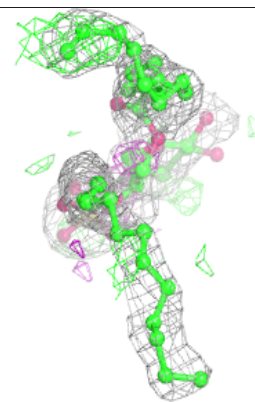
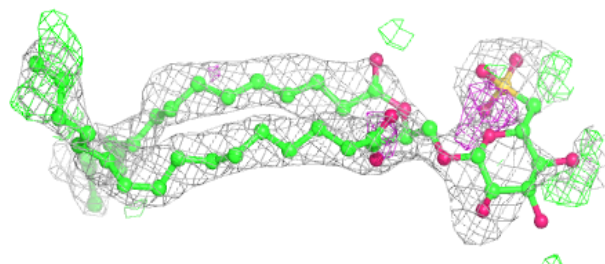
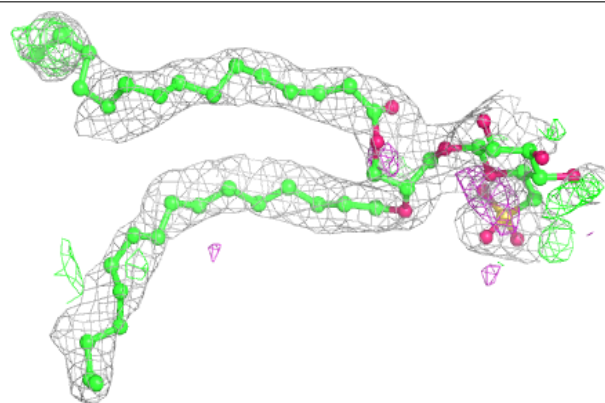


Electron density around HTG B 628:

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

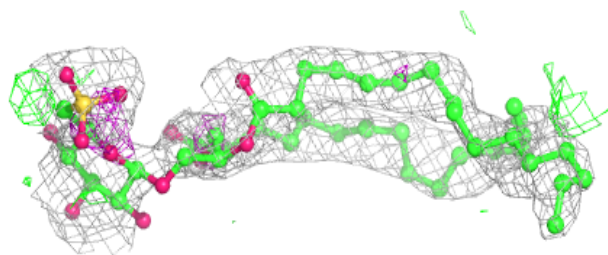
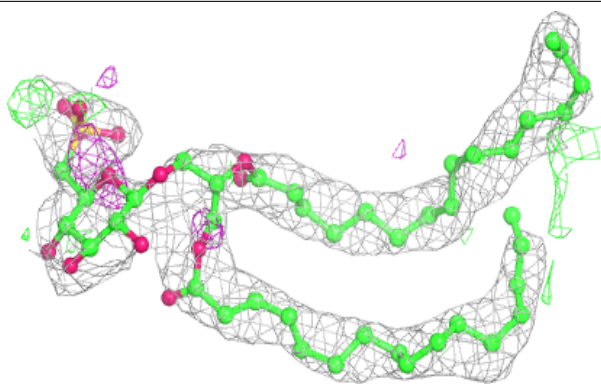
**Electron density around SQD B 620 (A):**

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

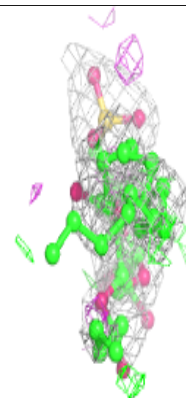
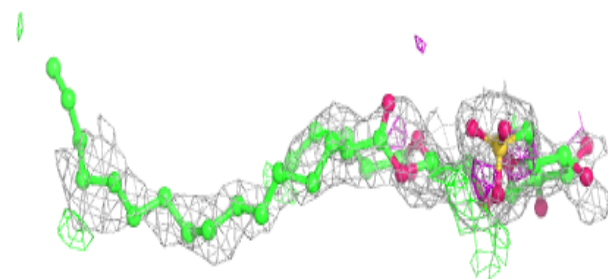
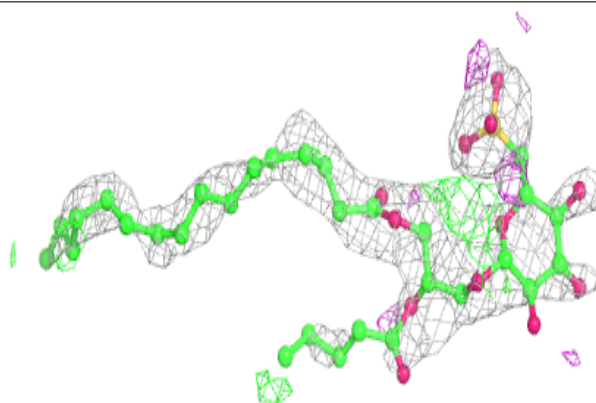


Electron density around SQD B 620 (B):

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

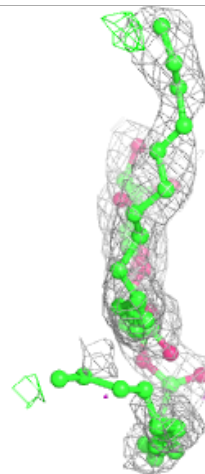
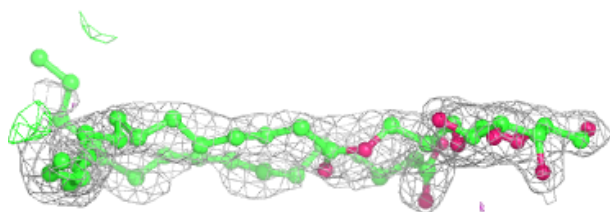
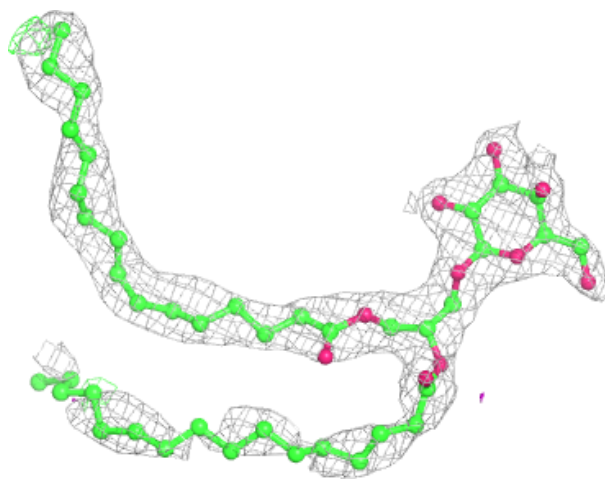
**Electron density around SQD f 102:**

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



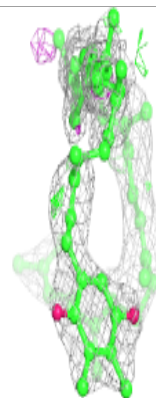
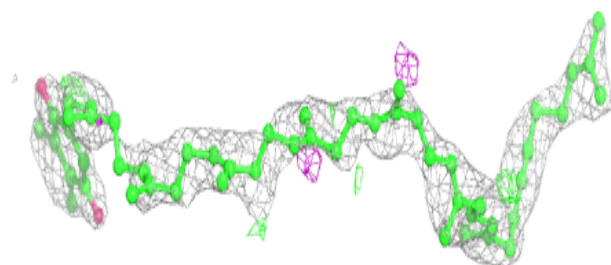
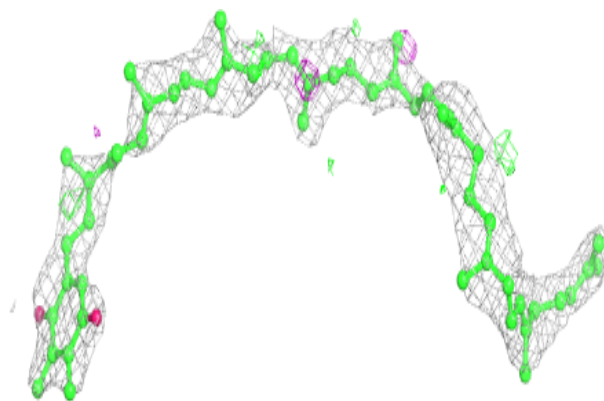
Electron density around LMG c 519:

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

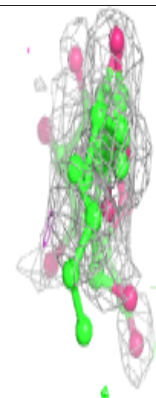
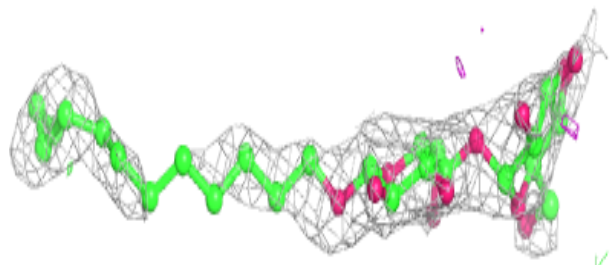
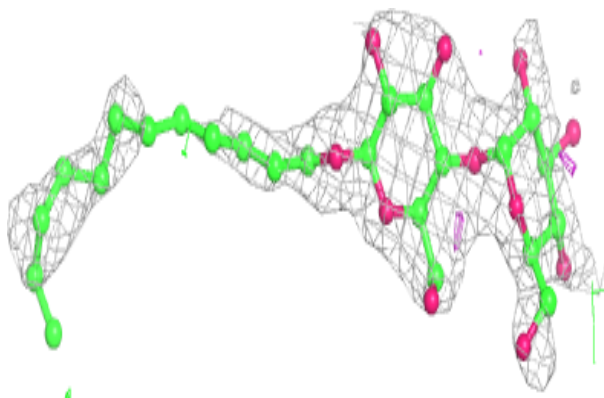


Electron density around PL9 a 414:

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

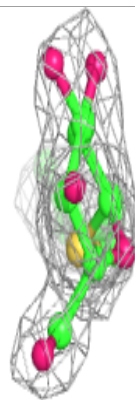
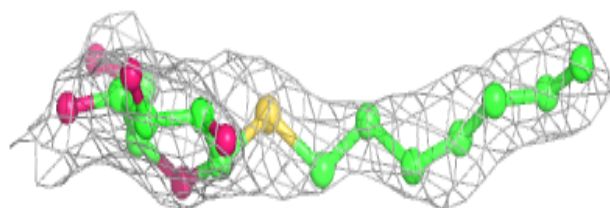
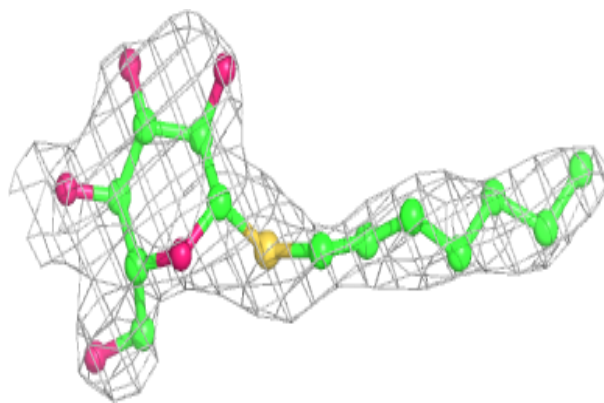
**Electron density around LMT a 416:**

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

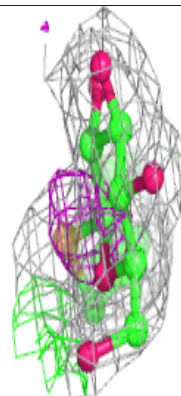
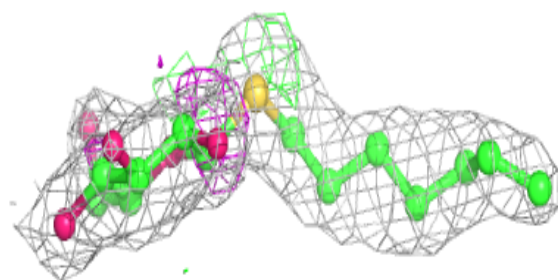
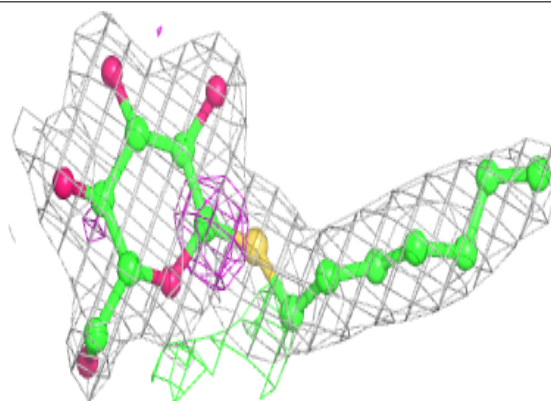


Electron density around HTG C 522:

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

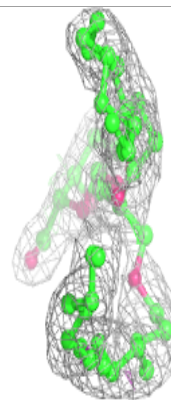
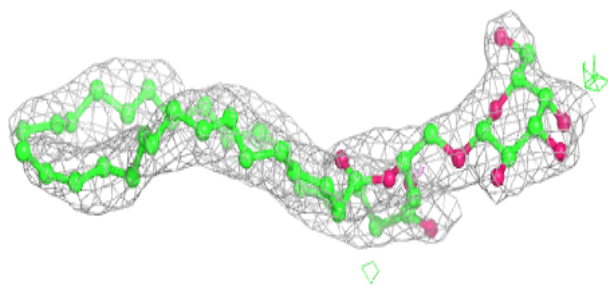
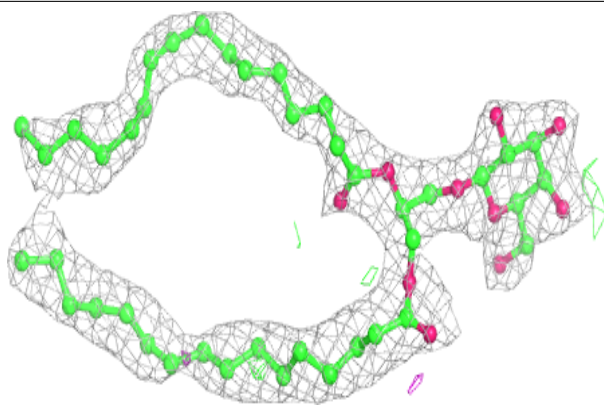
**Electron density around HTG o 301:**

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

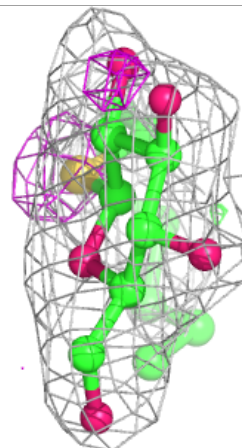
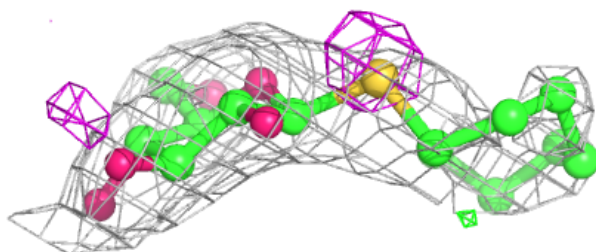
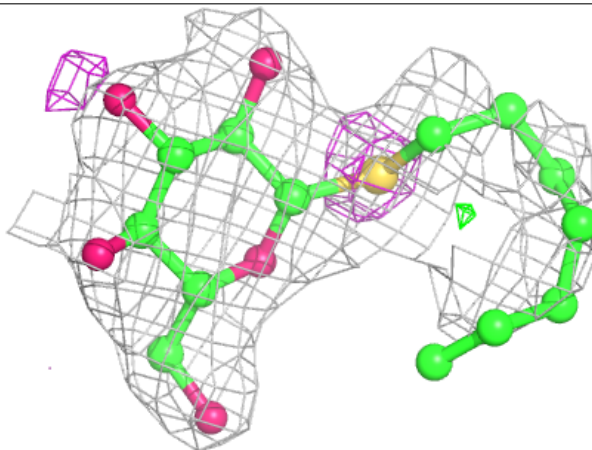


Electron density around LMG a 415:

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

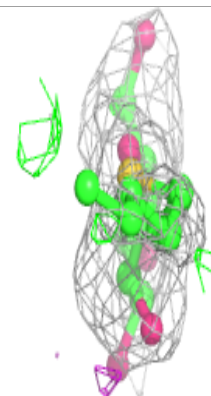
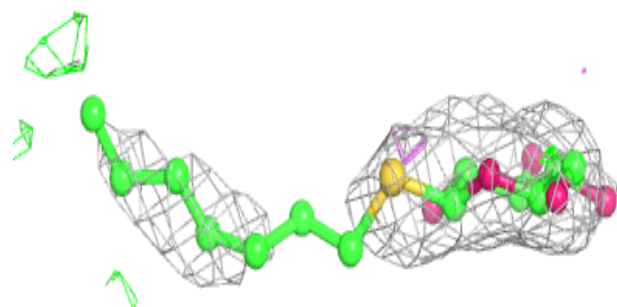
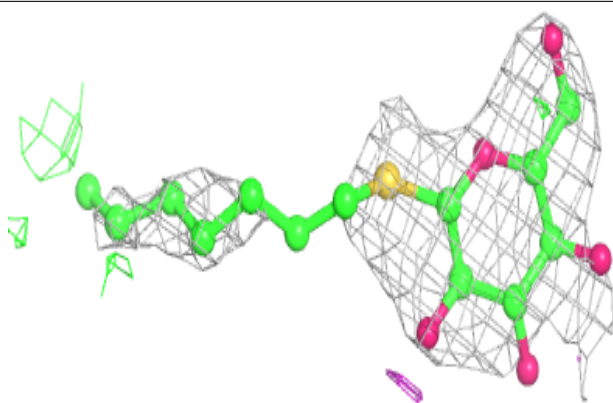
**Electron density around HTG V 202:**

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

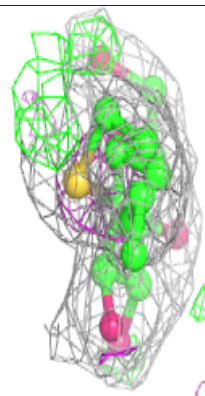
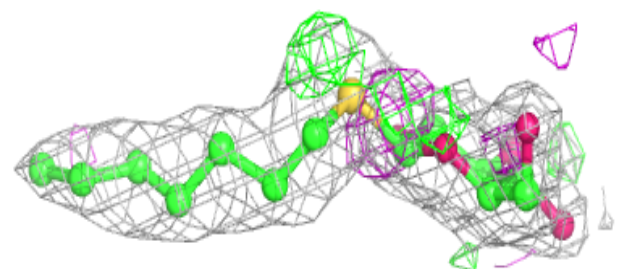
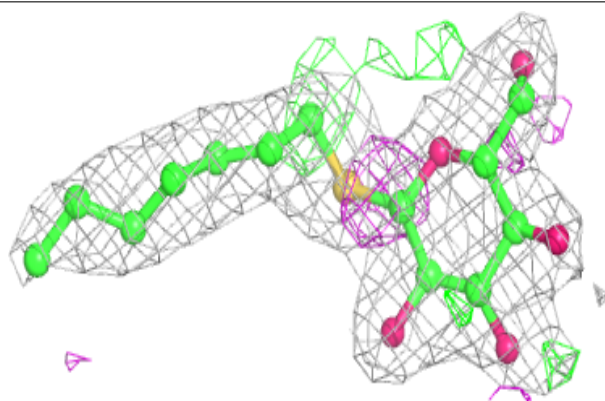


Electron density around HTG c 522:

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

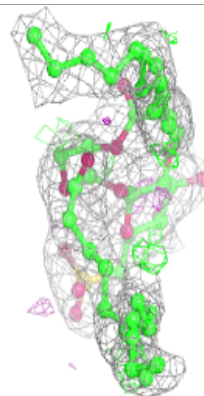
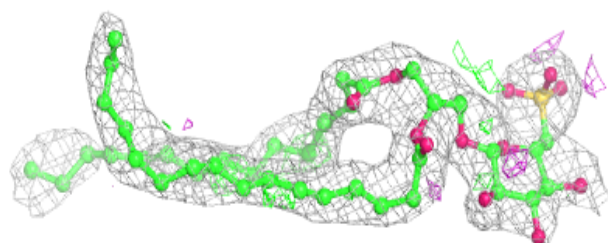
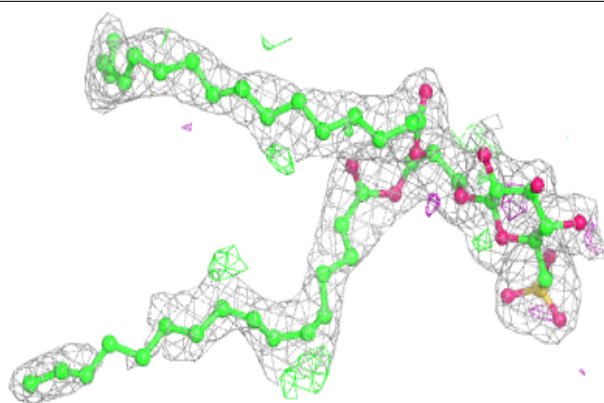
**Electron density around HTG b 626:**

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

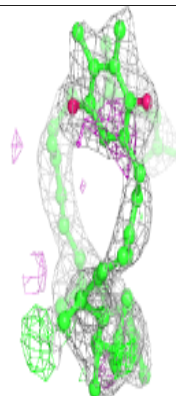
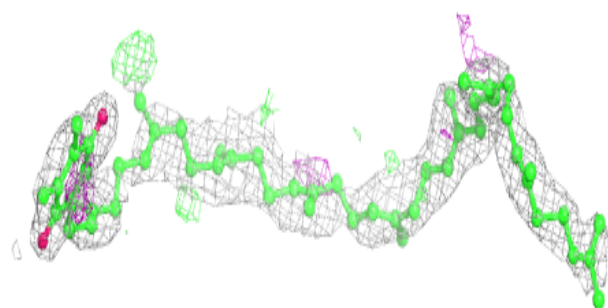
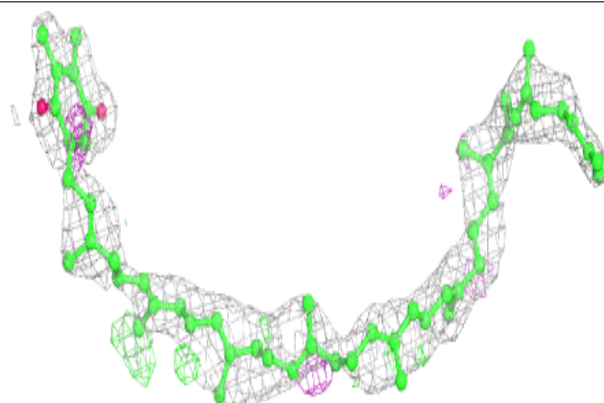


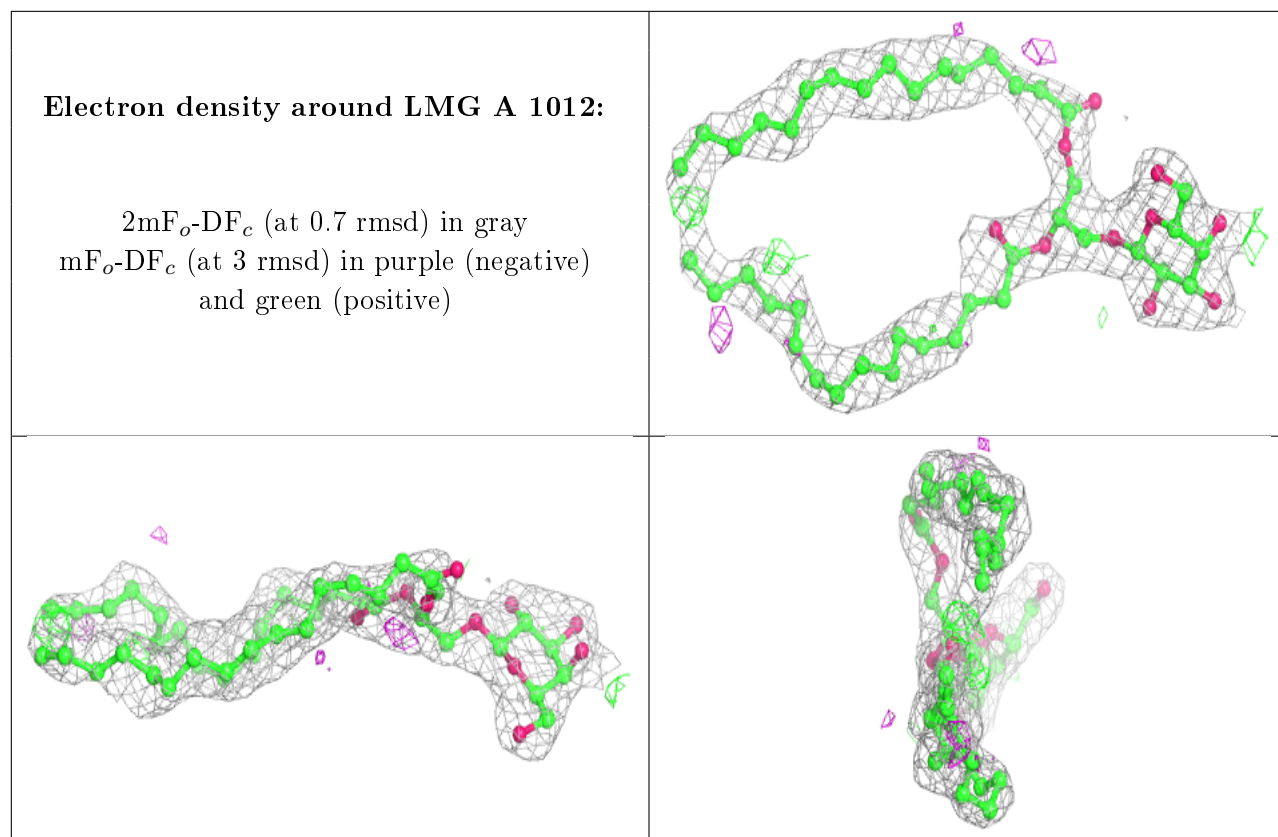
Electron density around SQD A 1016:

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

**Electron density around PL9 A 1010:**

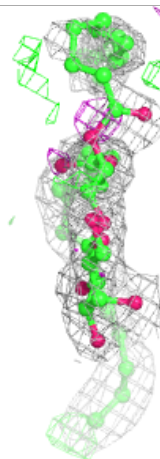
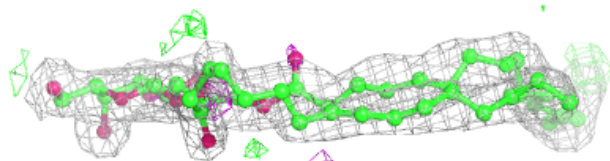
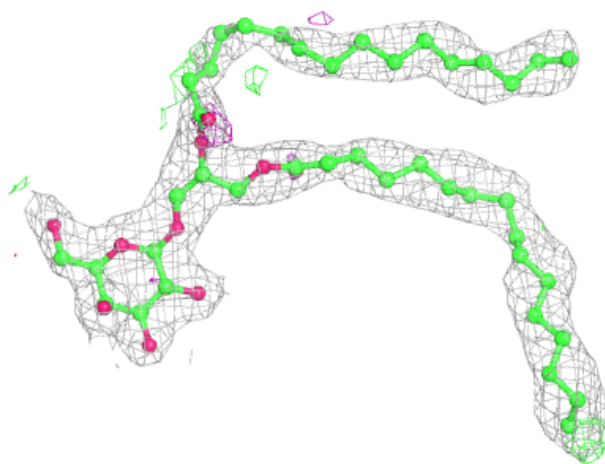
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





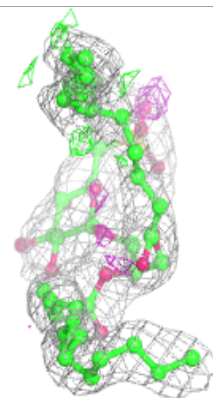
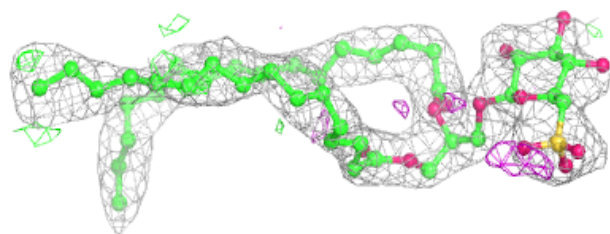
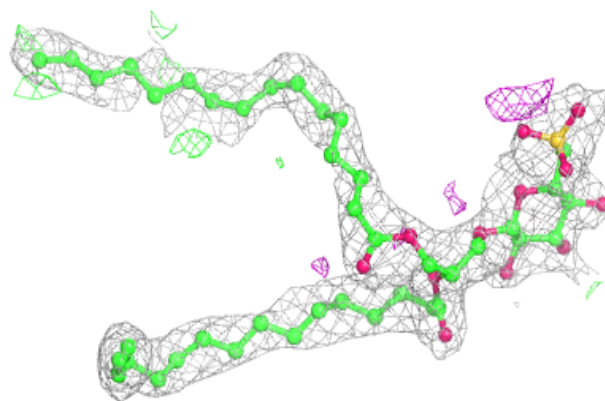
Electron density around LMG C 518:

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



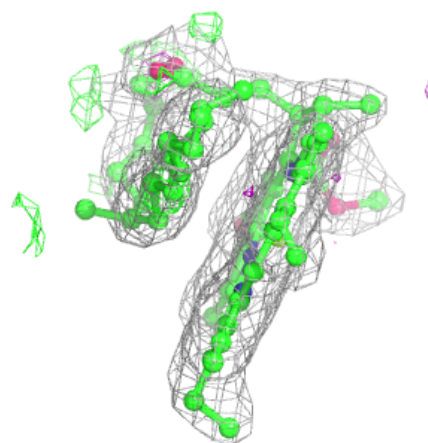
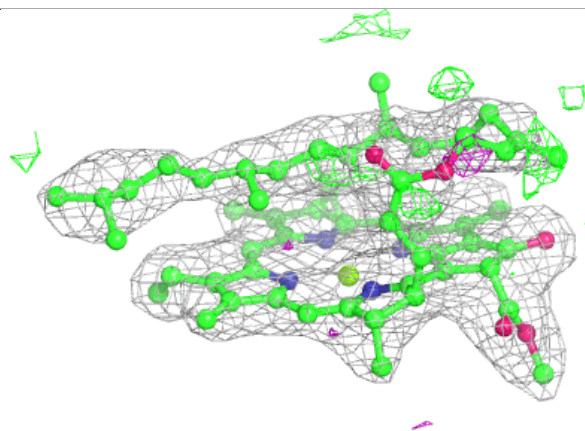
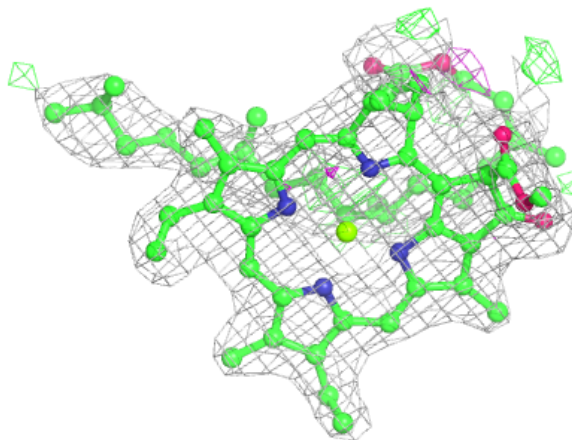
Electron density around SQD a 401:

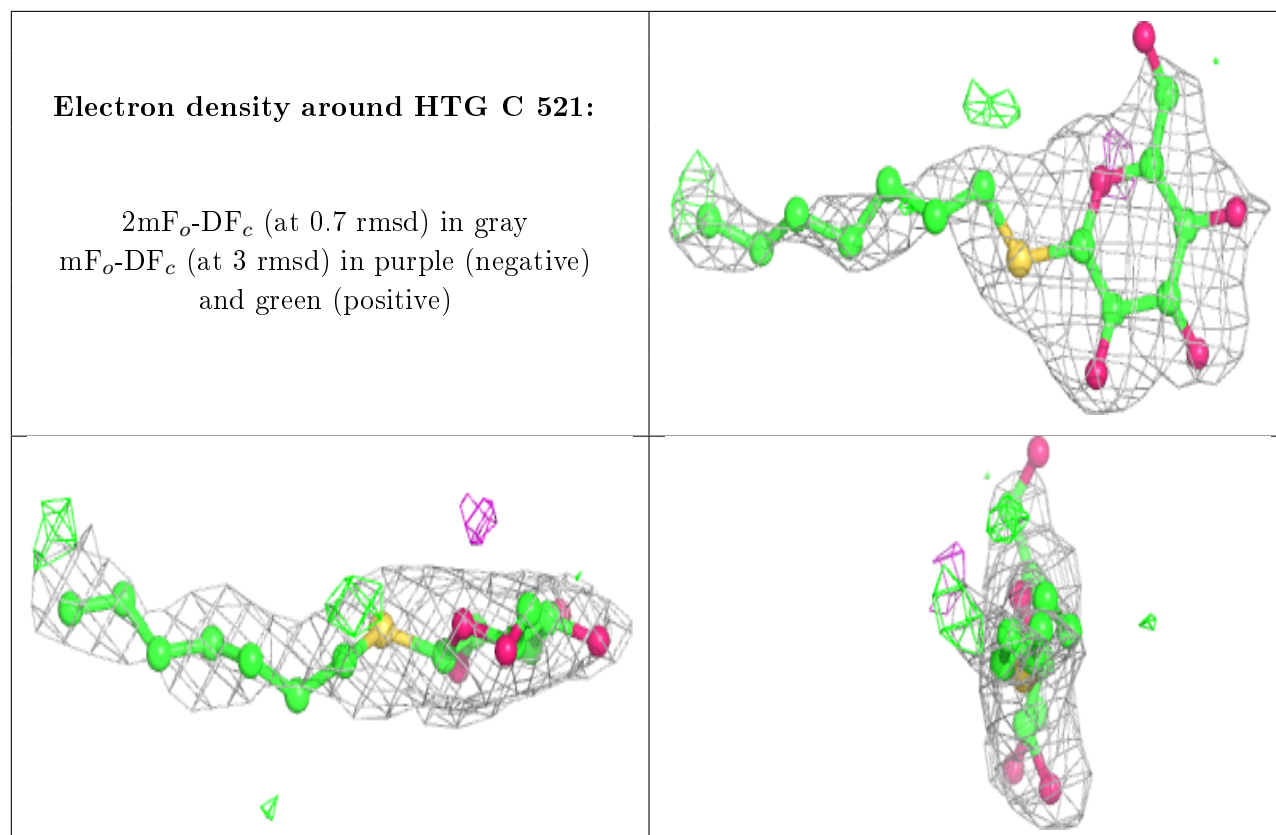
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 601:

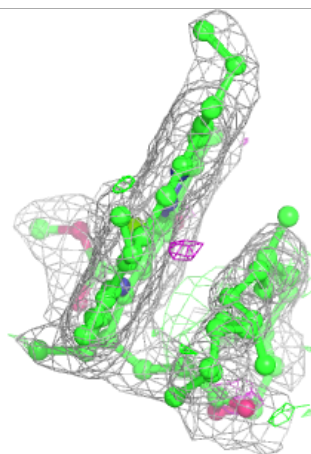
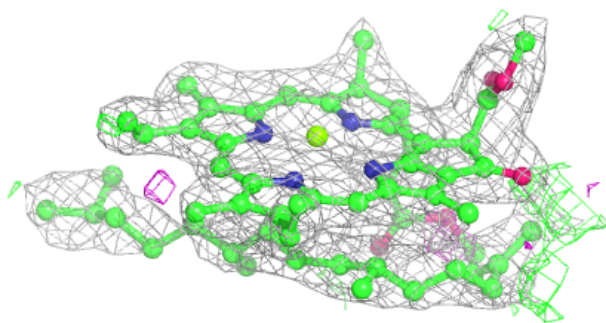
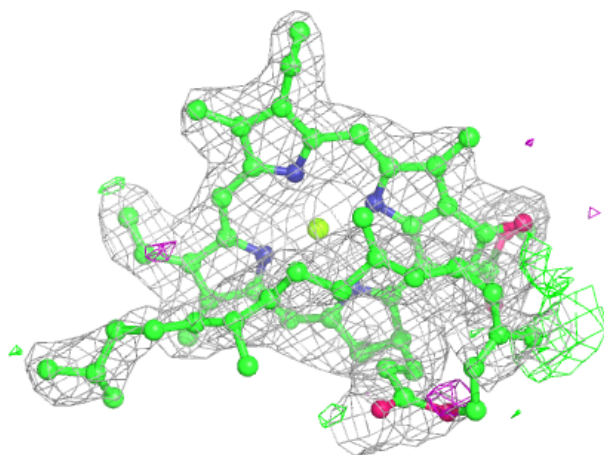
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





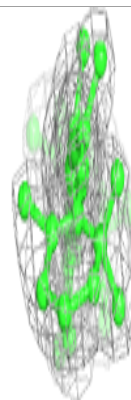
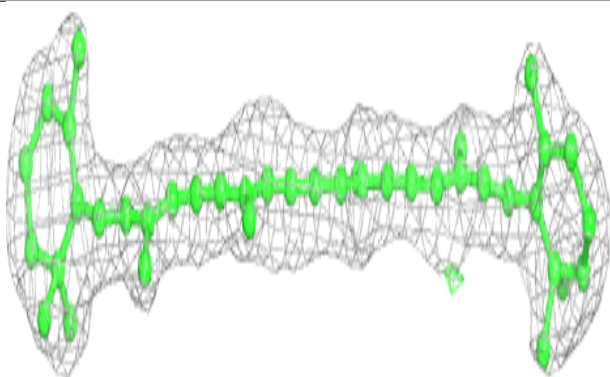
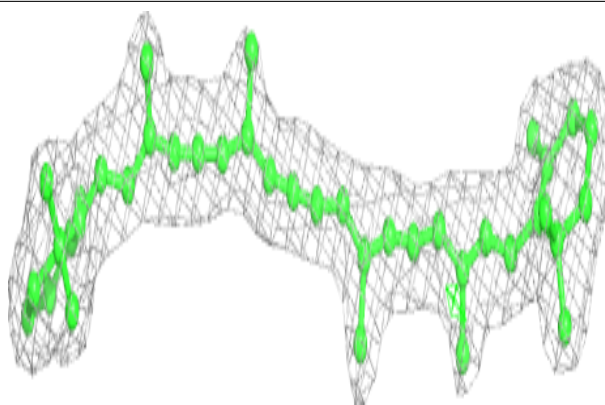
Electron density around CLA b 604:

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

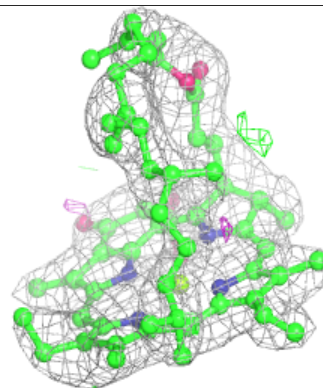
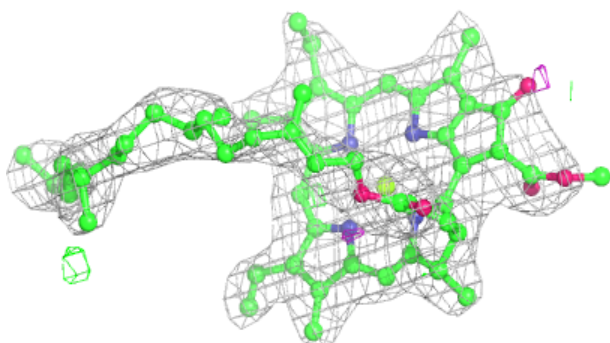
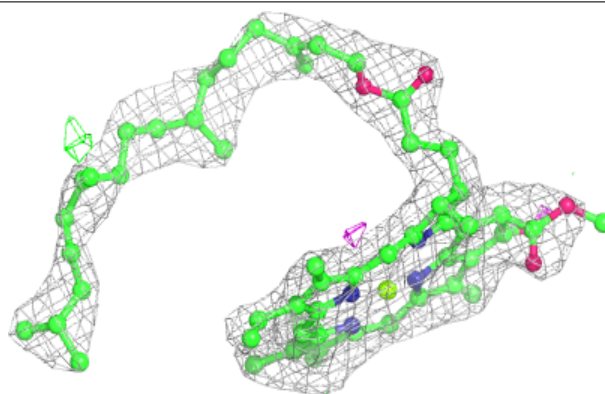


Electron density around BCR K 102:

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

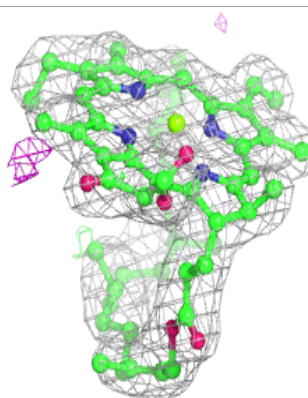
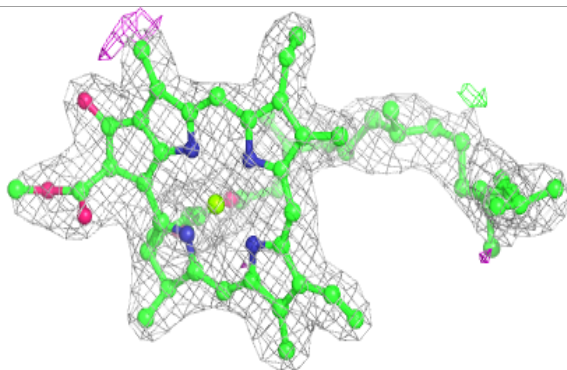
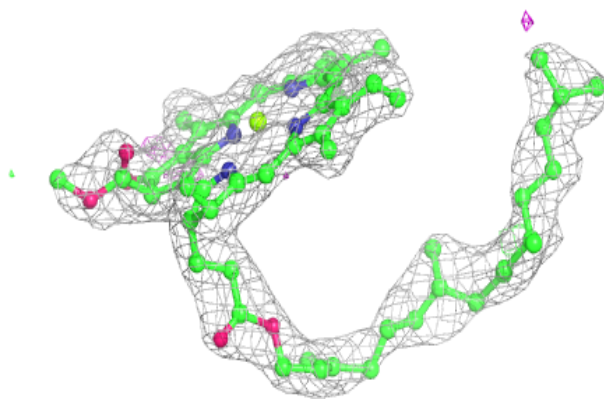
**Electron density around CLA c 513:**

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

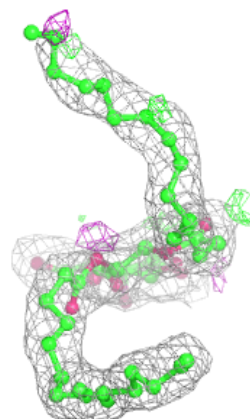
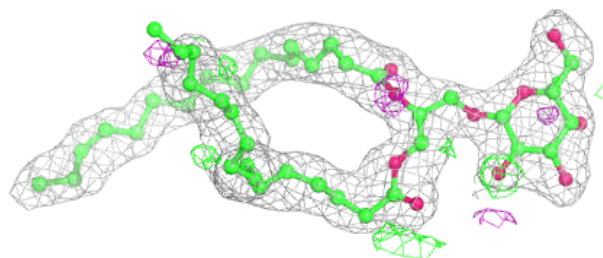
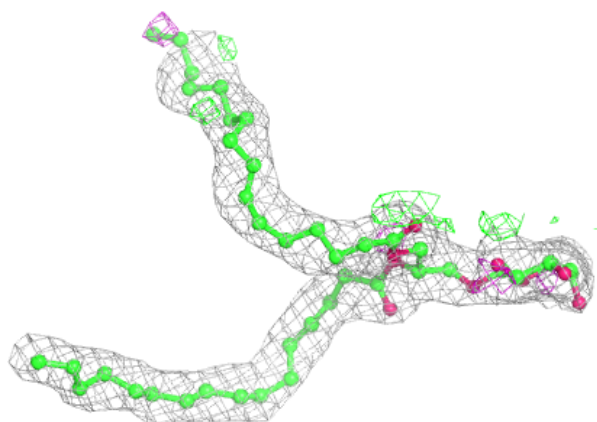


Electron density around CLA C 513:

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

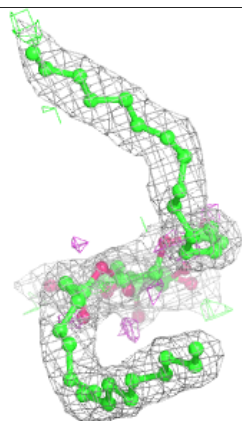
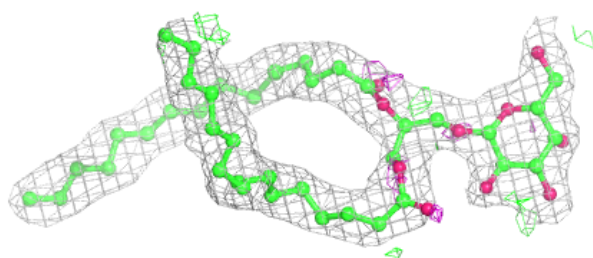
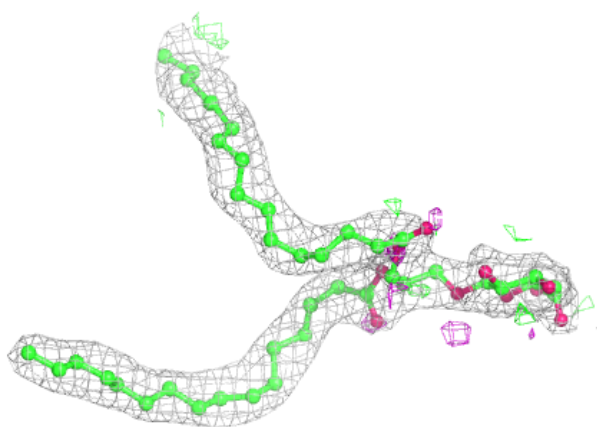
**Electron density around LMG B 622:**

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

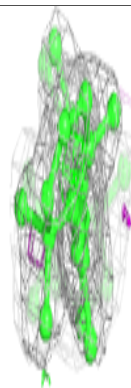
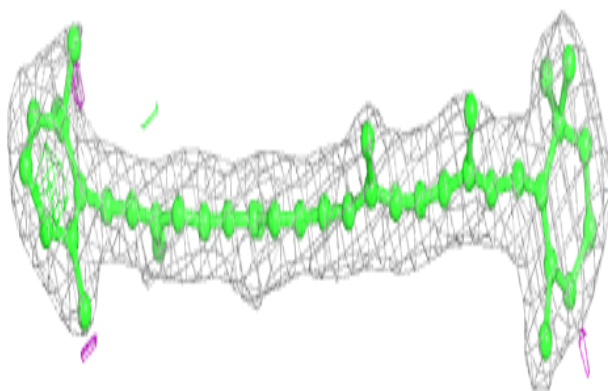
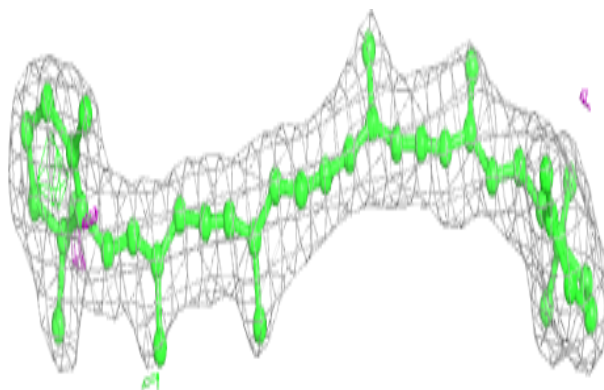


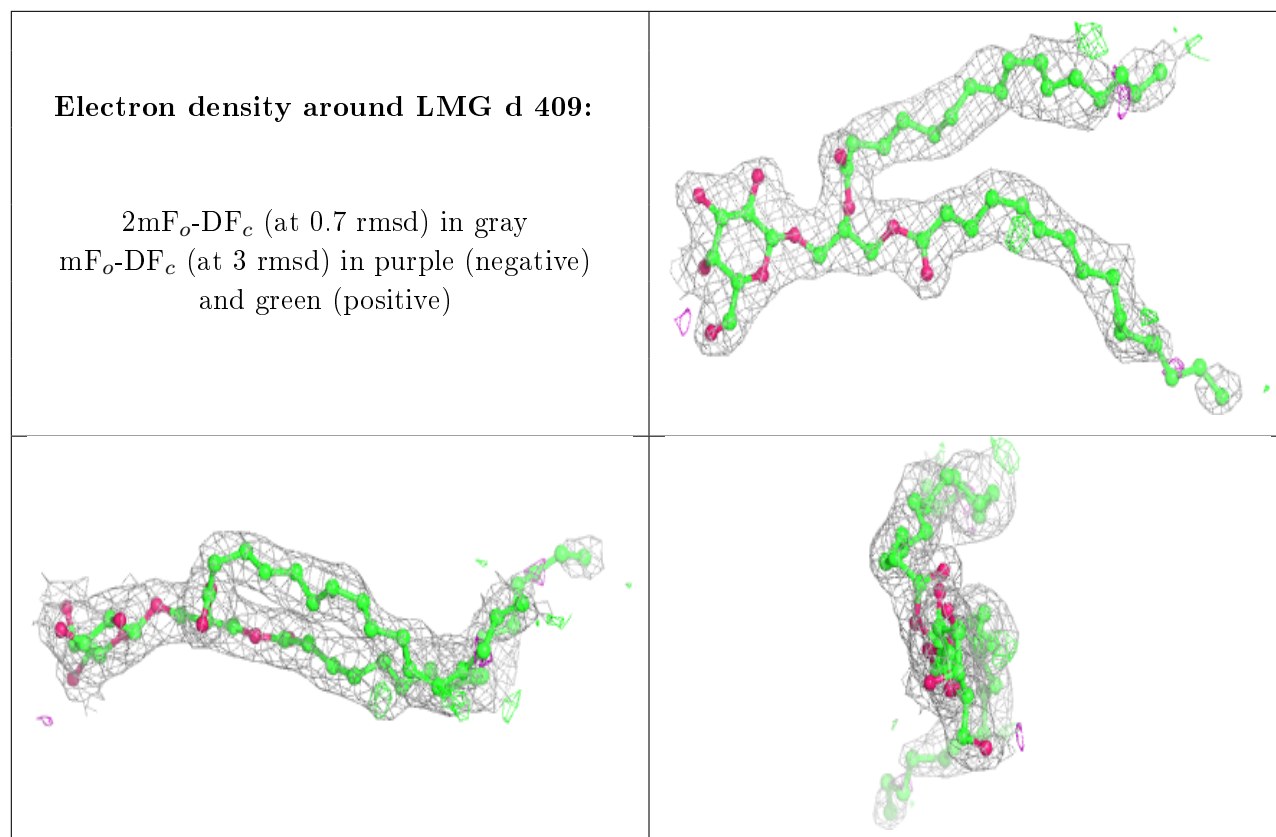
Electron density around LMG m 102:

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

**Electron density around BCR k 102:**

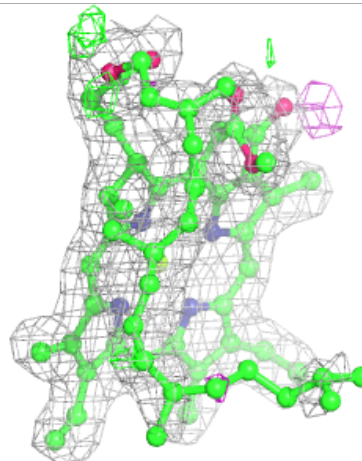
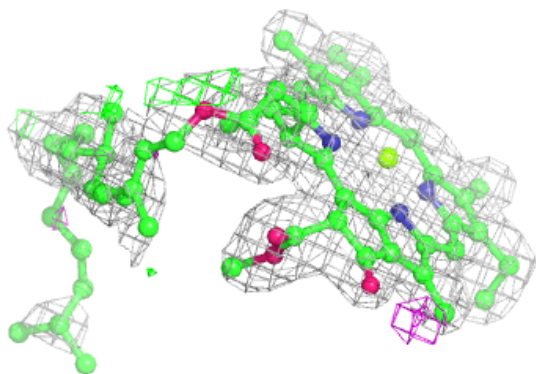
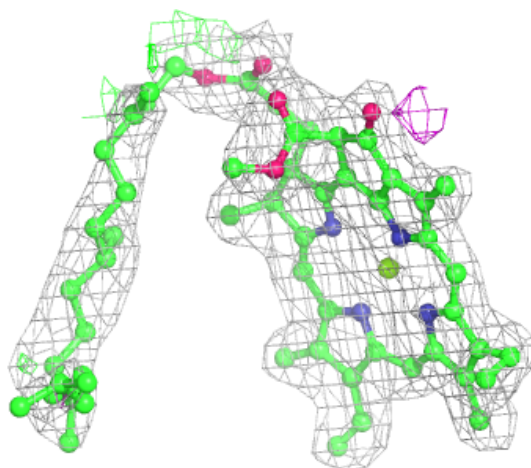
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





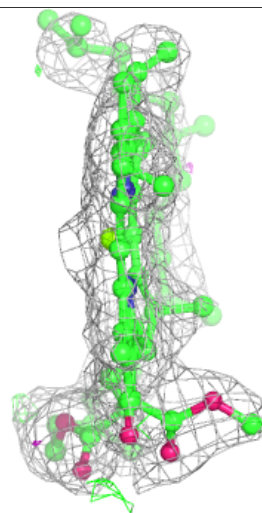
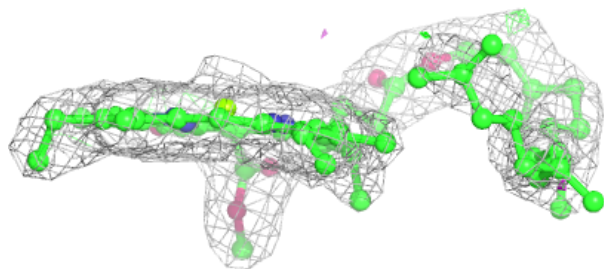
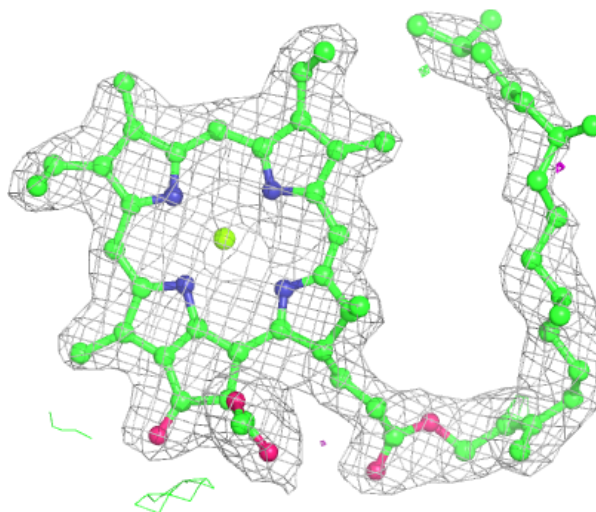
Electron density around CLA b 619:

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



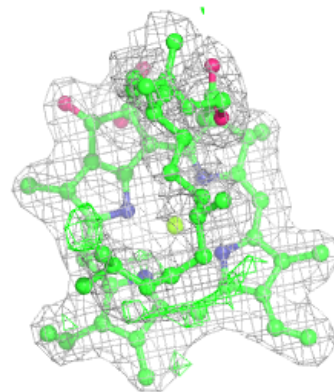
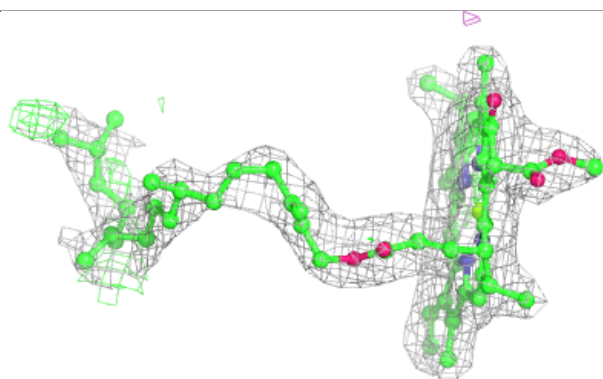
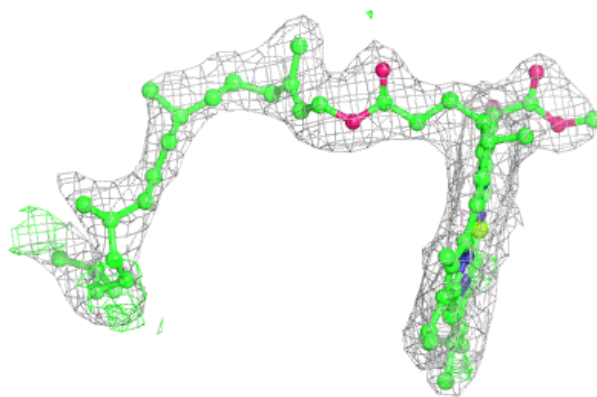
Electron density around CLA C 512:

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

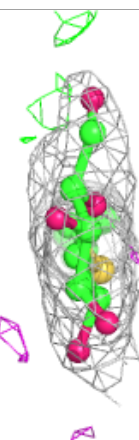
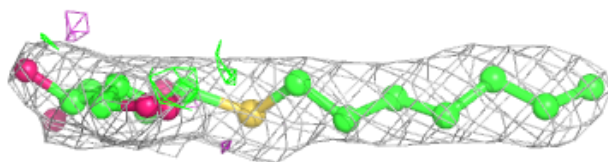
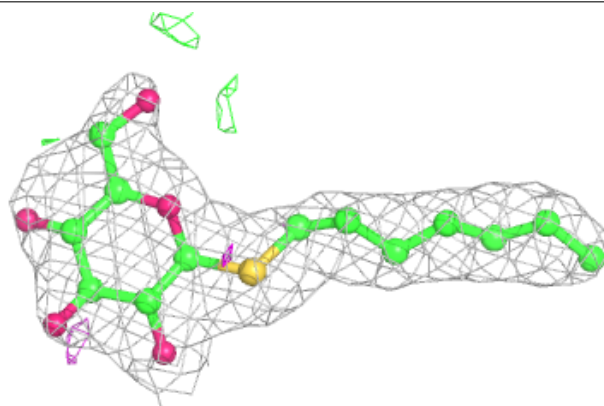


Electron density around CLA c 506:

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

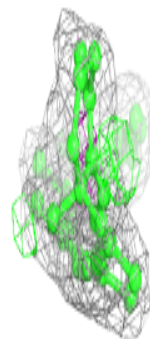
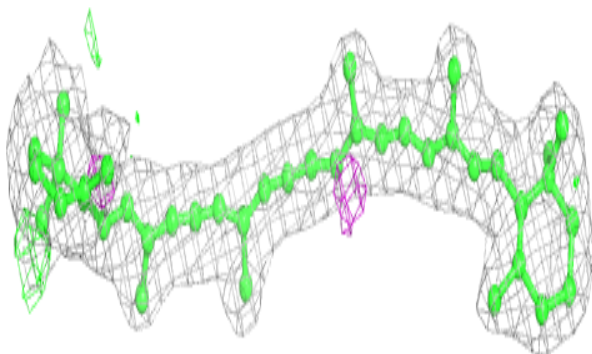
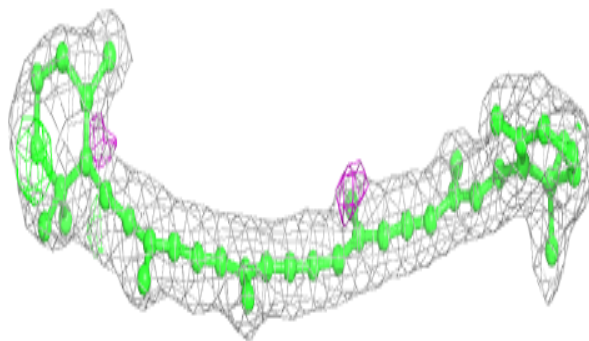
**Electron density around HTG b 601:**

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



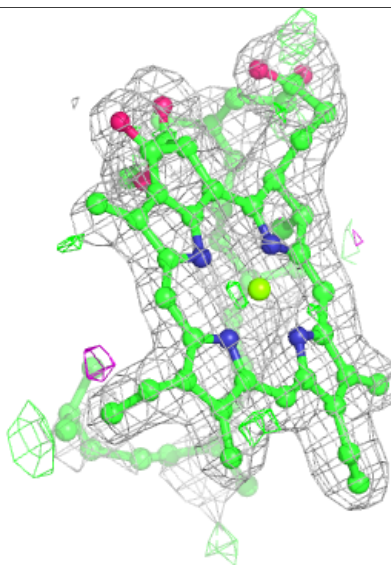
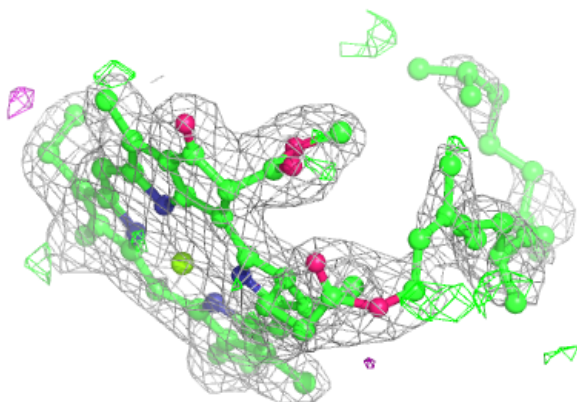
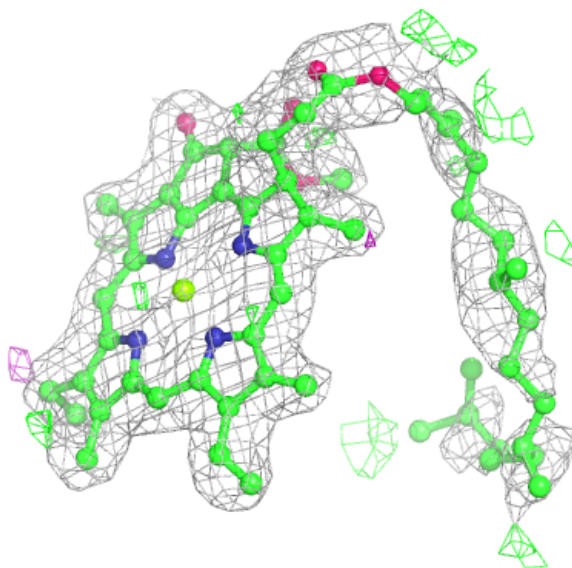
Electron density around BCR d 404:

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



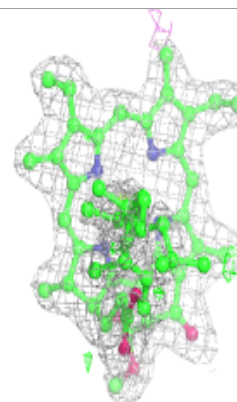
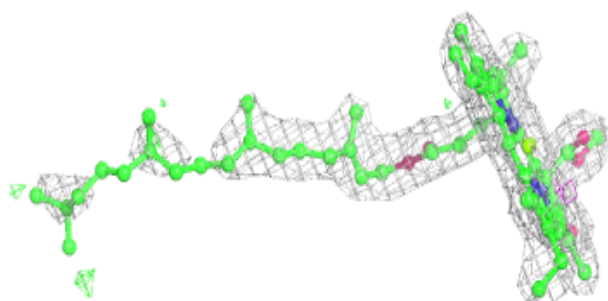
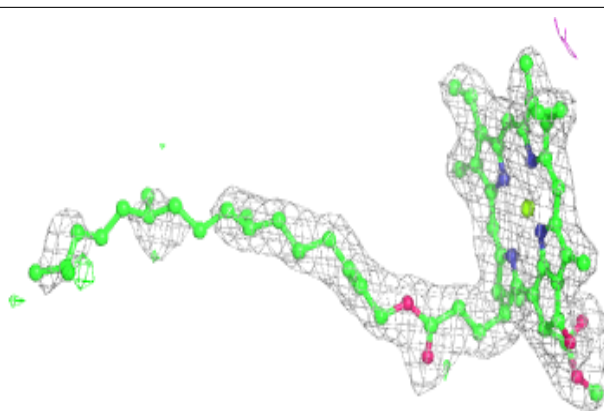
Electron density around CLA B 616:

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

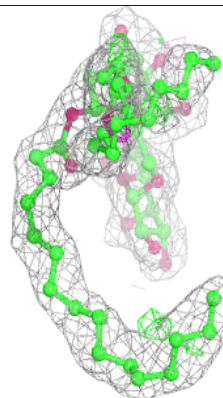
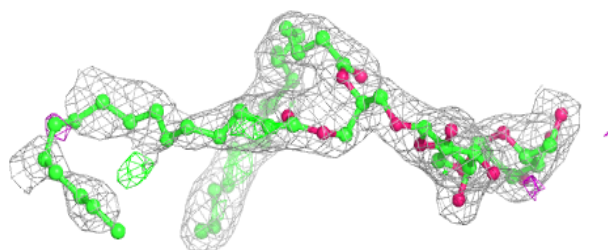
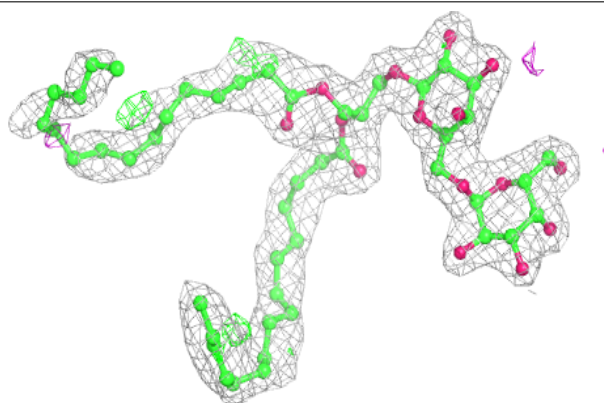


Electron density around CLA d 403:

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

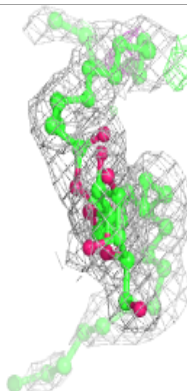
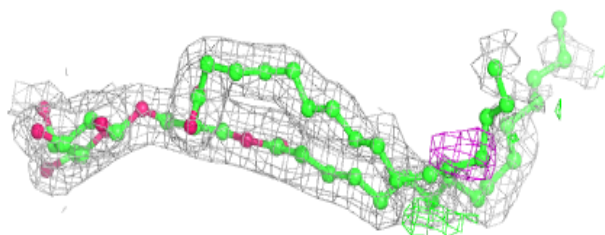
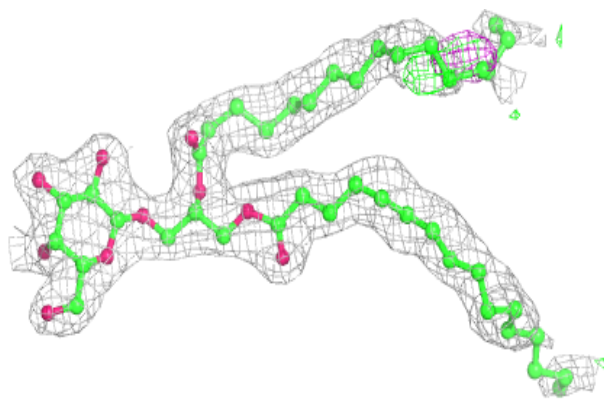
**Electron density around DGD c 516:**

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

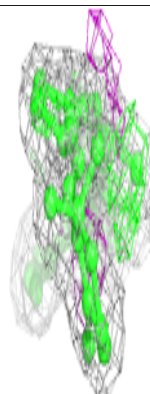
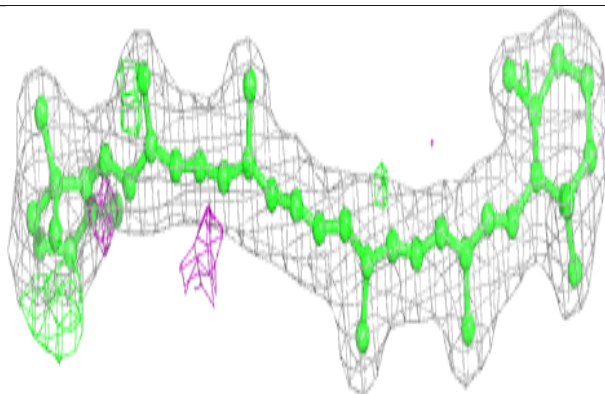
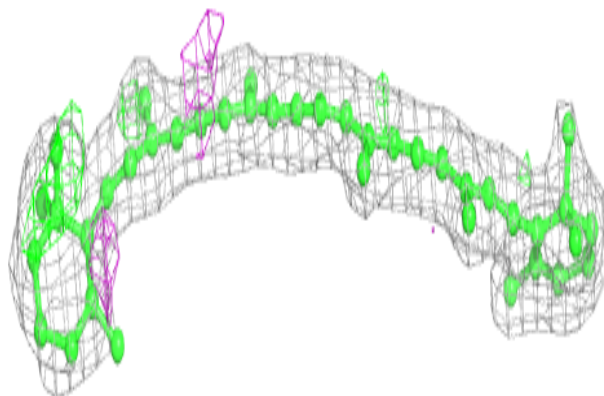


Electron density around LMG D 412:

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

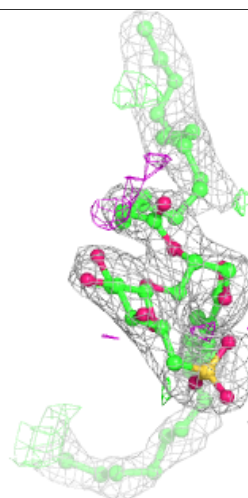
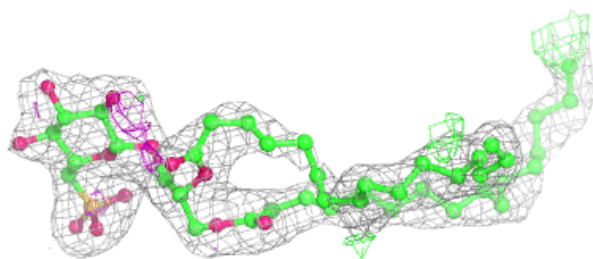
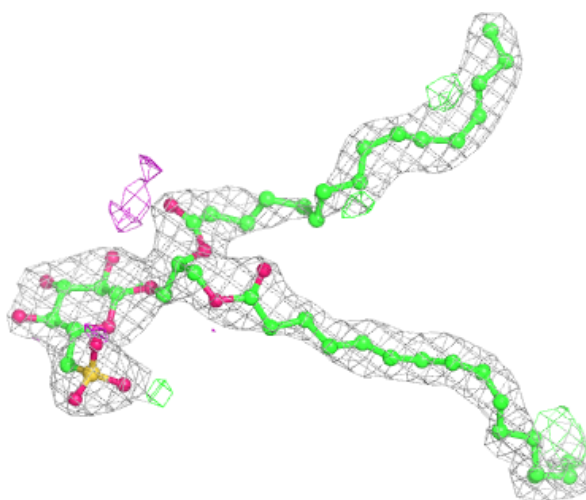
**Electron density around BCR D 406:**

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



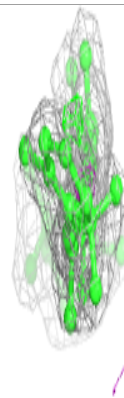
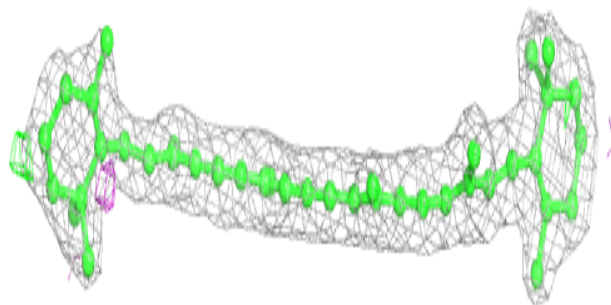
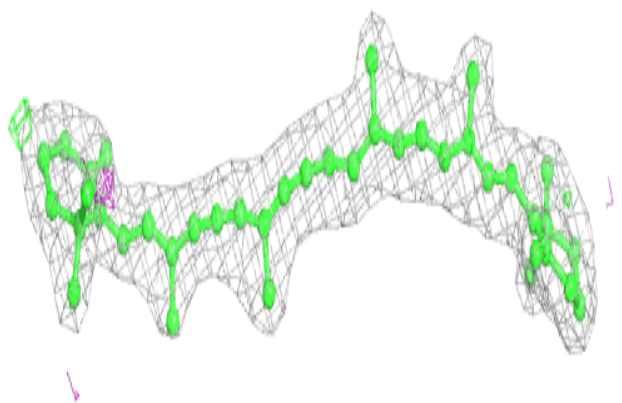
Electron density around SQD c 518:

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



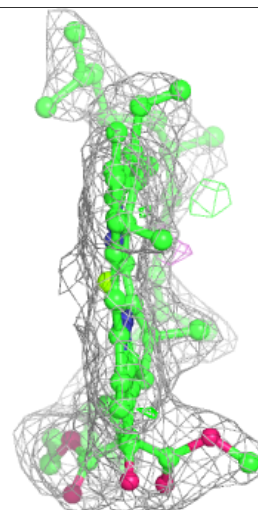
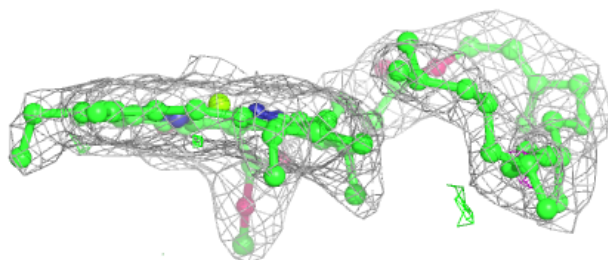
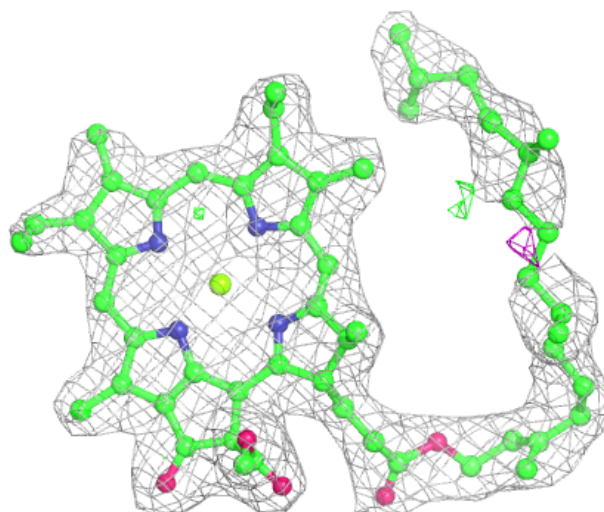
Electron density around BCR h 101:

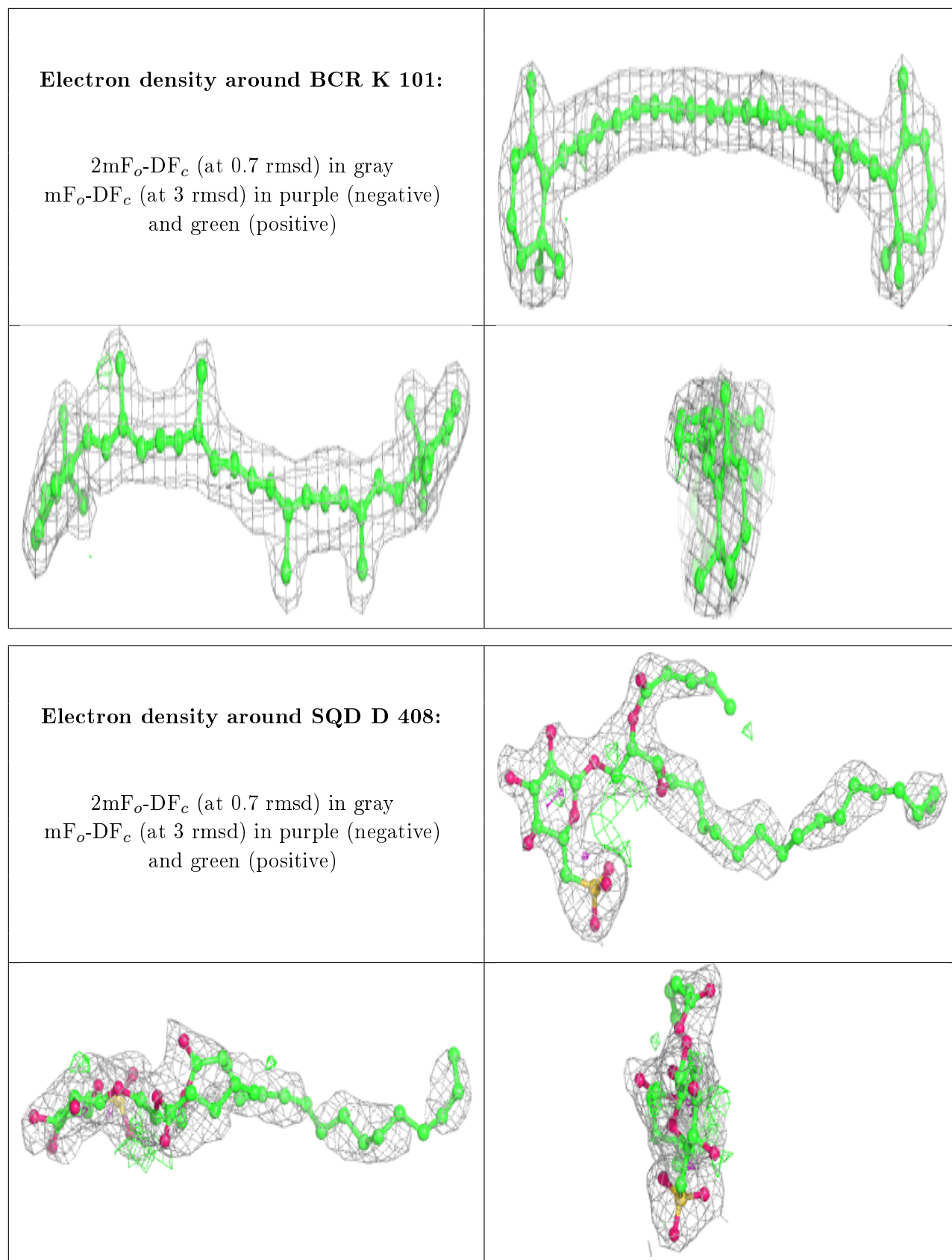
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA c 512:

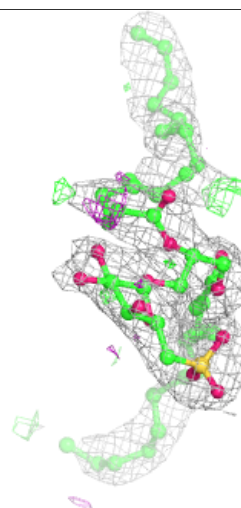
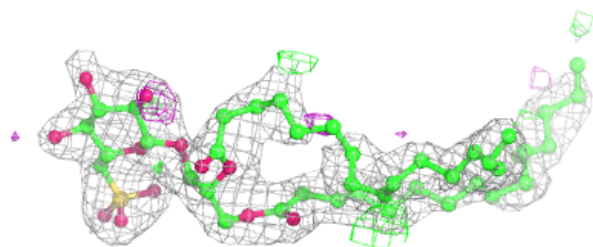
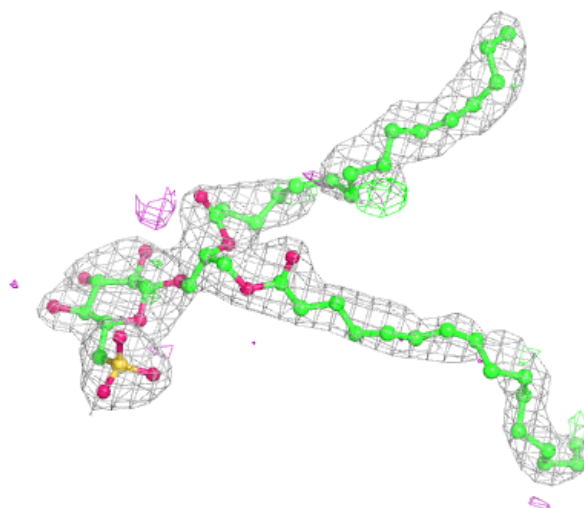
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





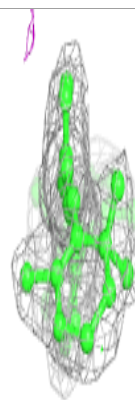
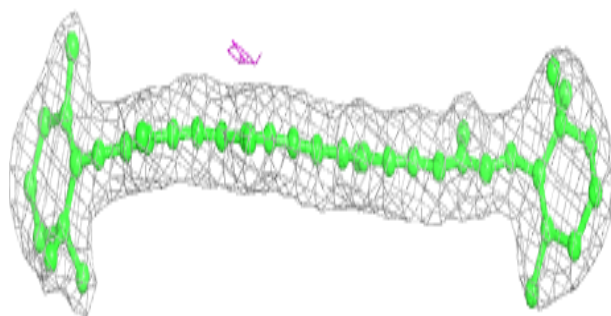
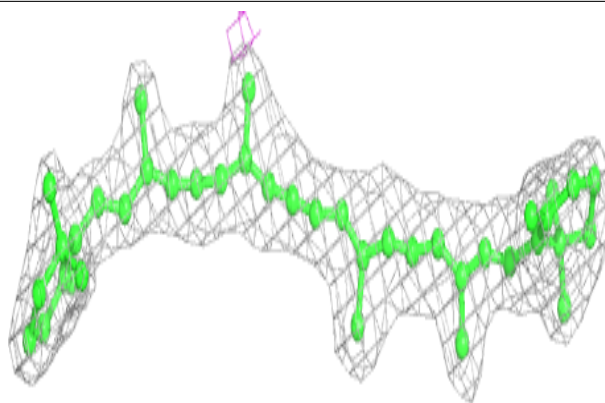
Electron density around SQD A 1011:

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

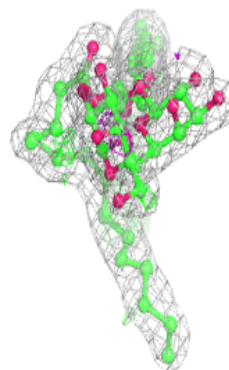
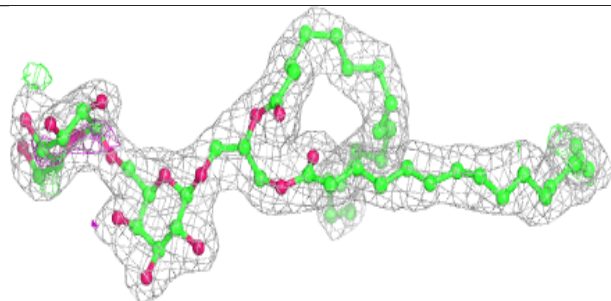
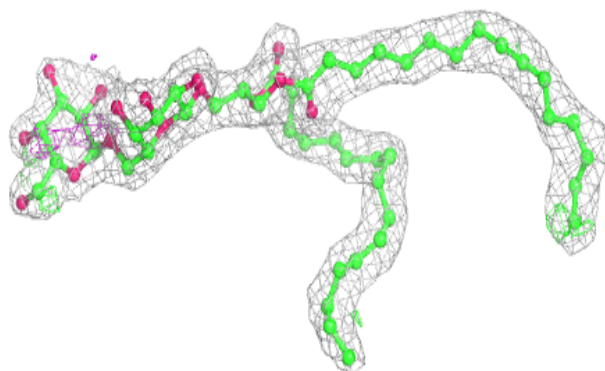


Electron density around BCR c 514:

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

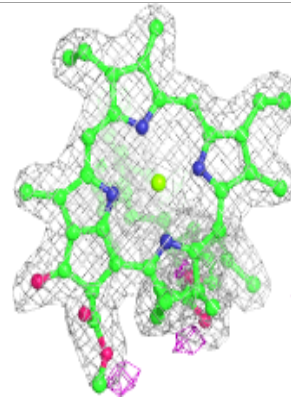
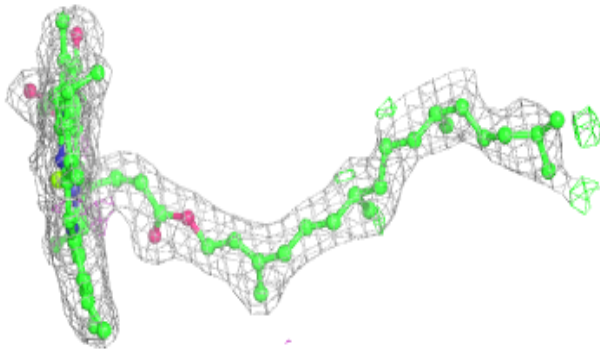
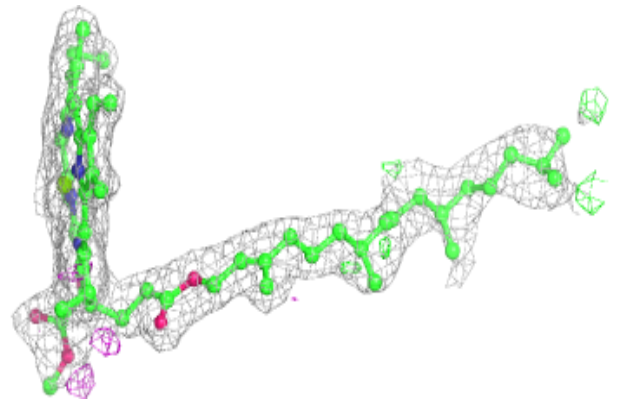
**Electron density around DGD h 102:**

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

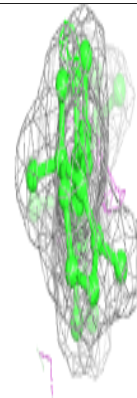
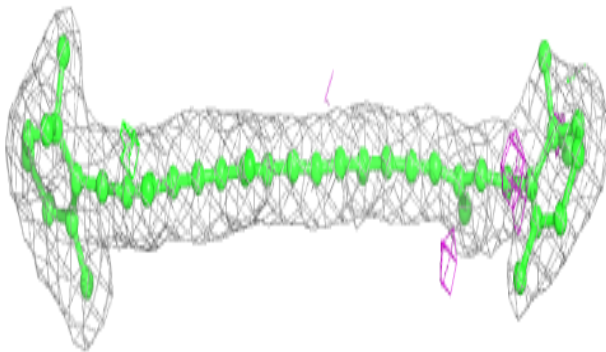
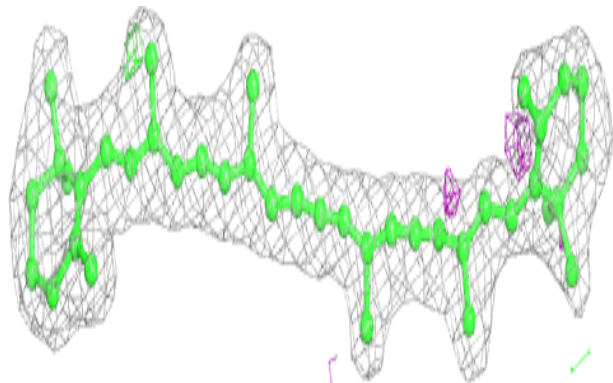


Electron density around CLA b 609:

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

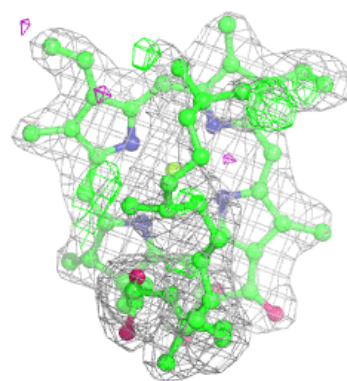
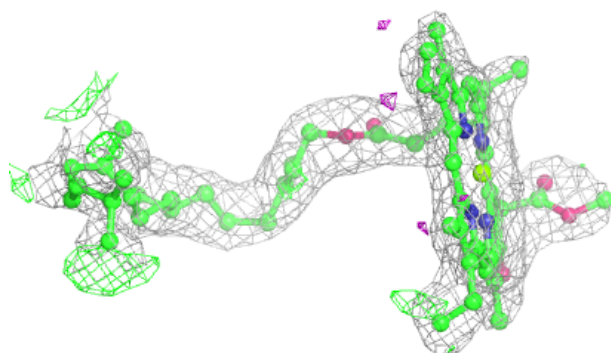
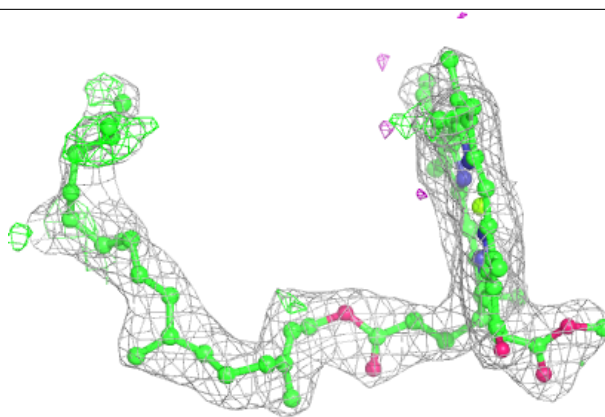
**Electron density around BCR B 618:**

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

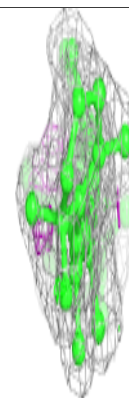
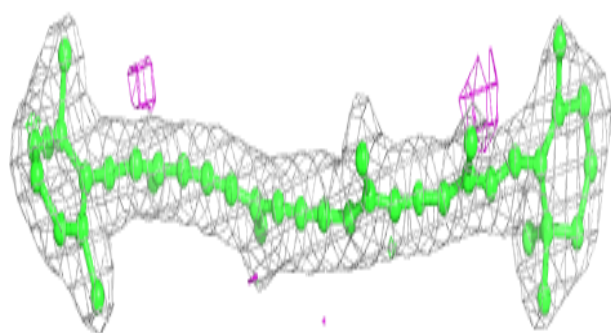
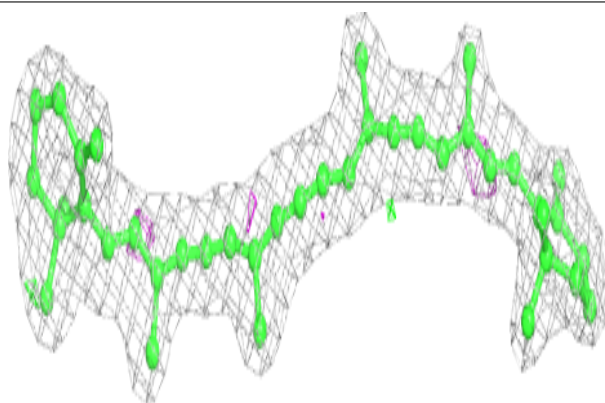


Electron density around CLA C 506:

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

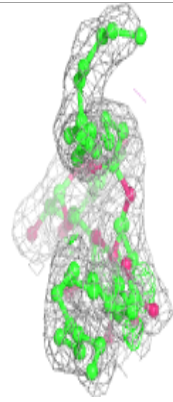
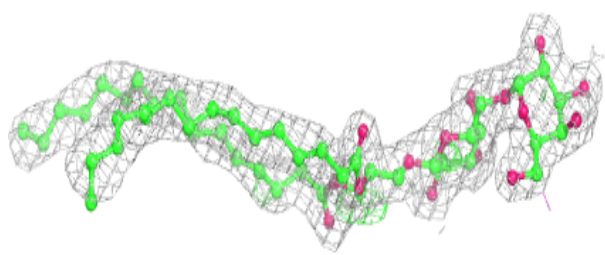
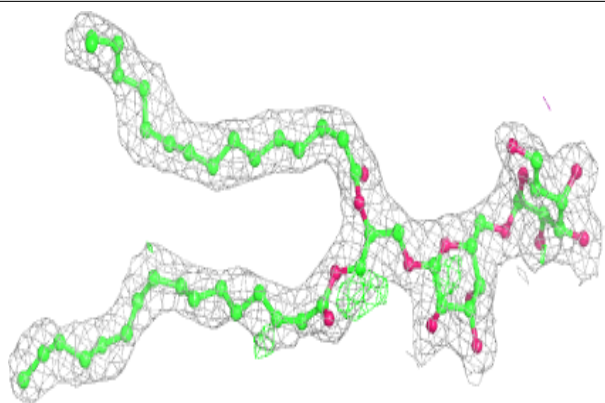
**Electron density around BCR J 101:**

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

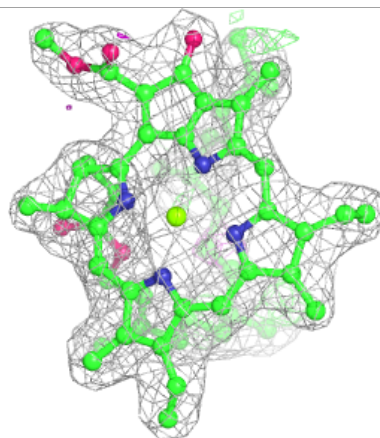
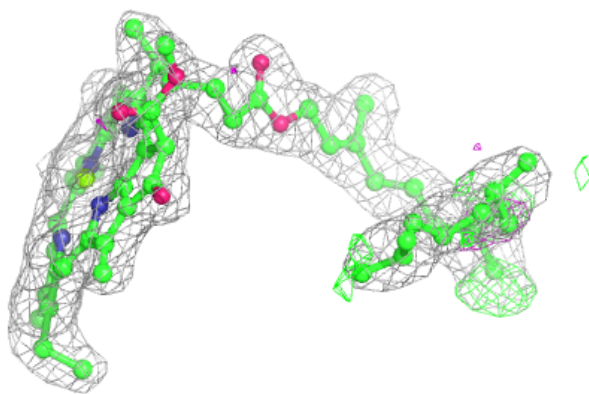
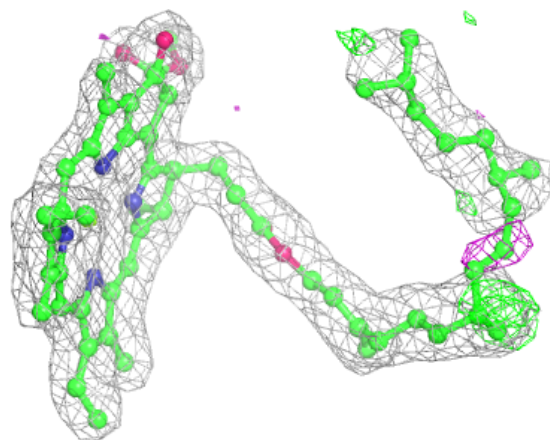


Electron density around DGD c 517:

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

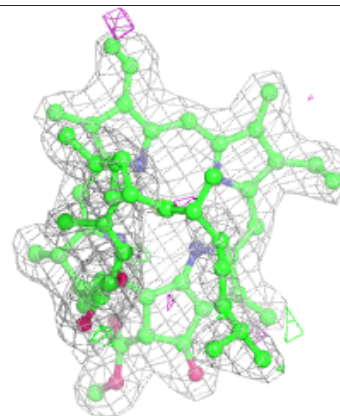
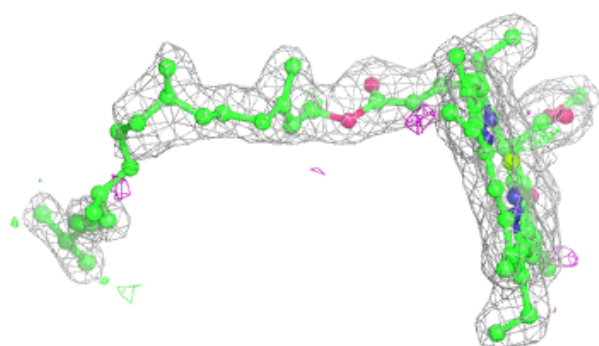
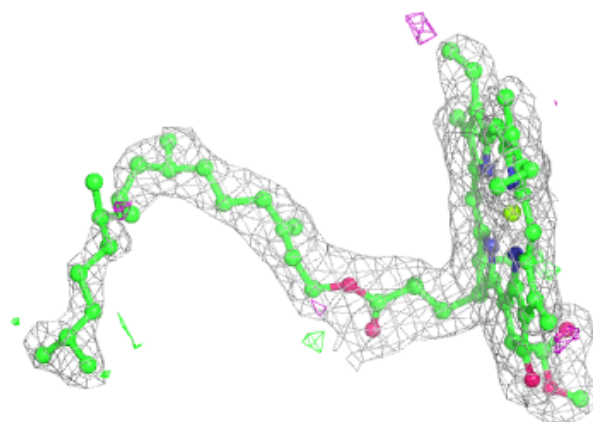
**Electron density around CLA B 606:**

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

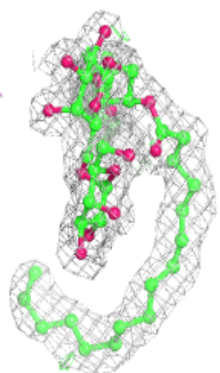
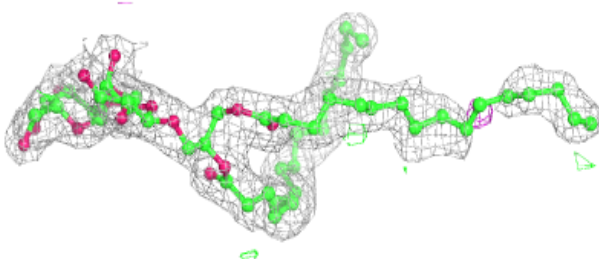
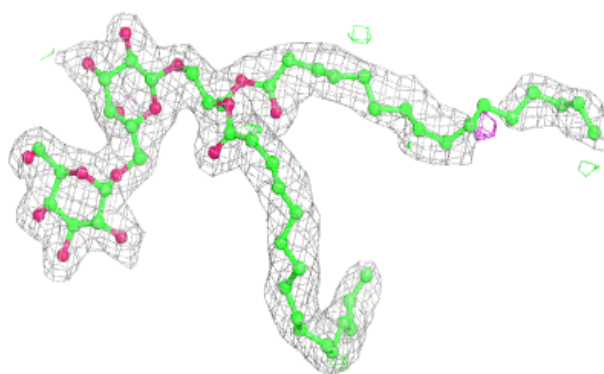


Electron density around CLA D 405:

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

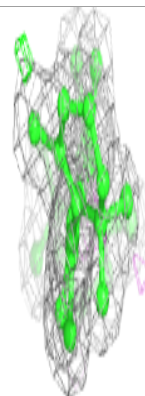
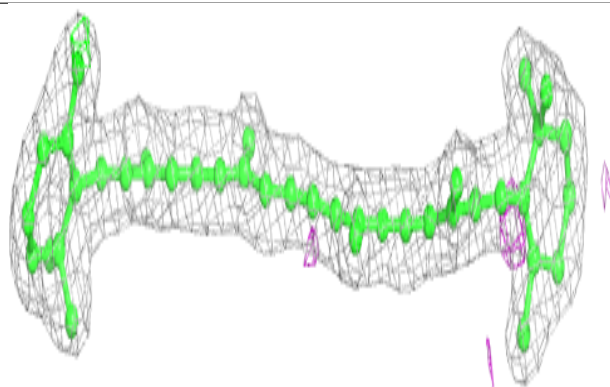
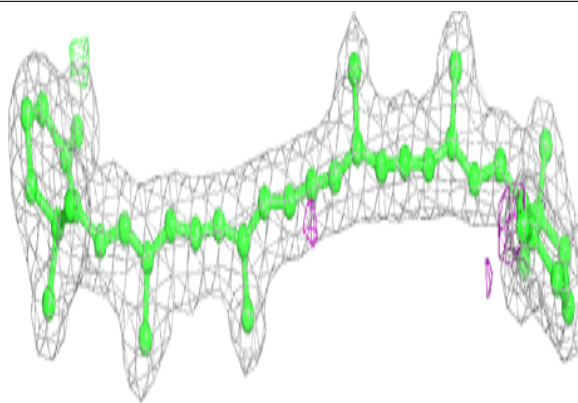
**Electron density around DGD C 516:**

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

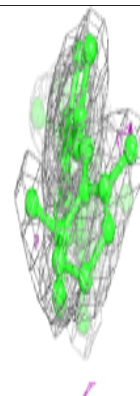
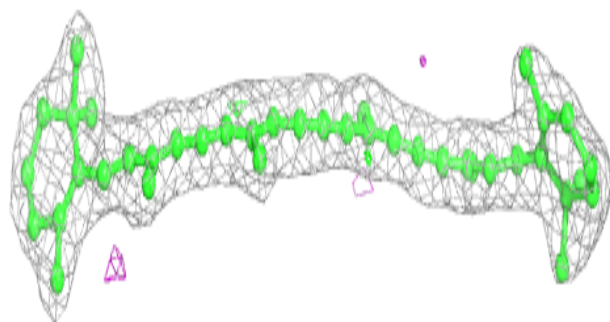
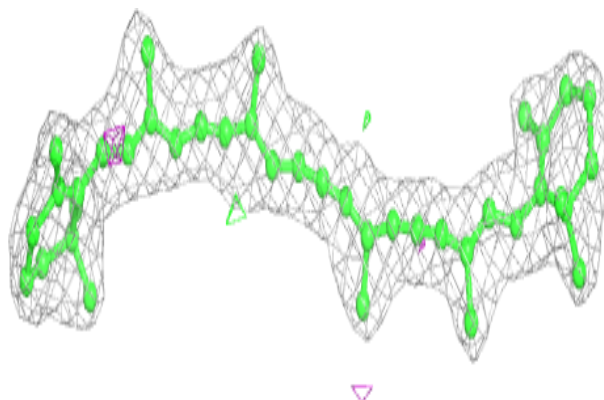


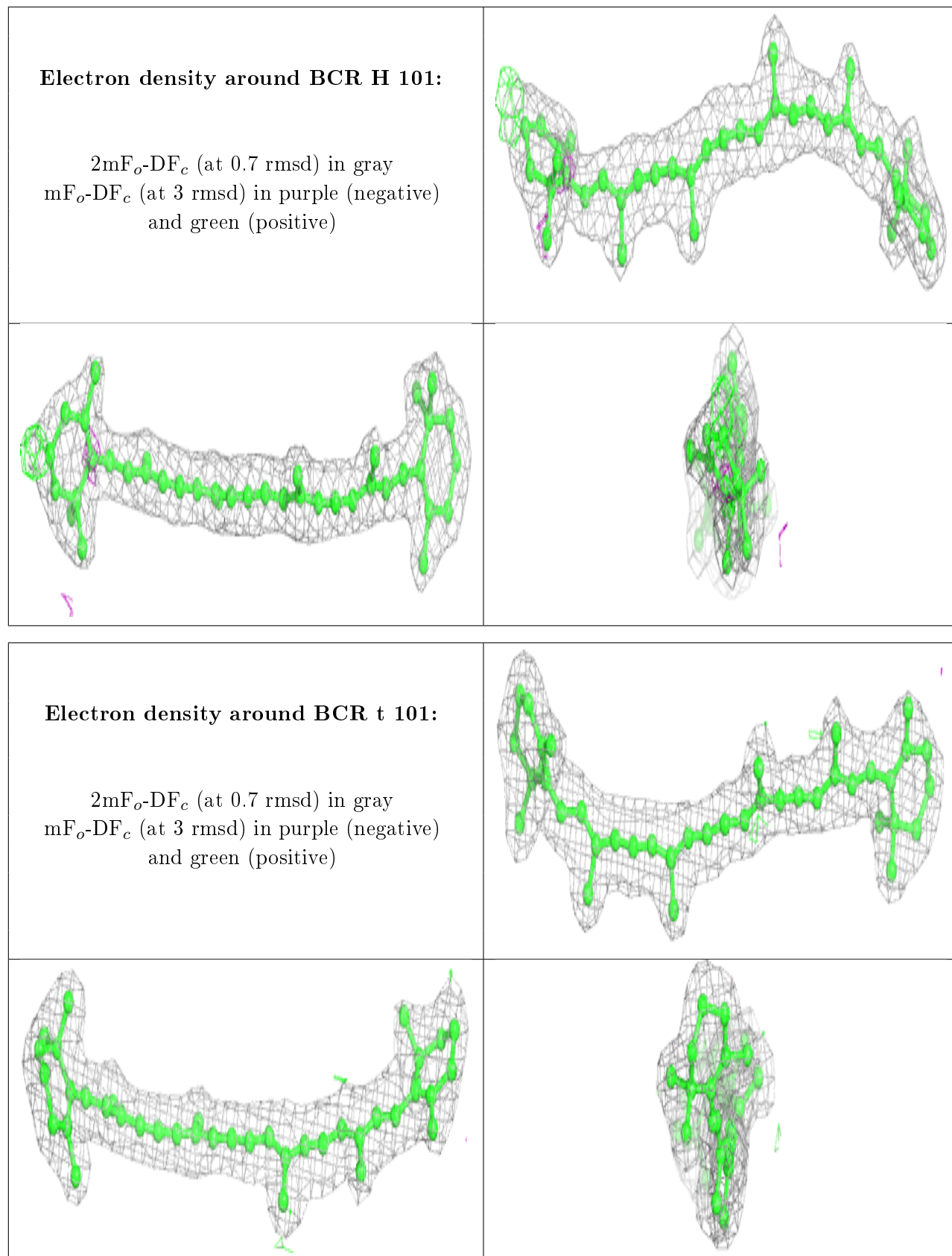
Electron density around BCR a 413:

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

**Electron density around BCR y 101:**

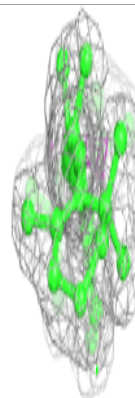
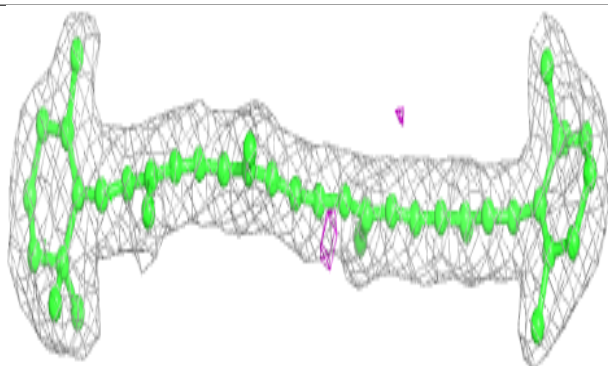
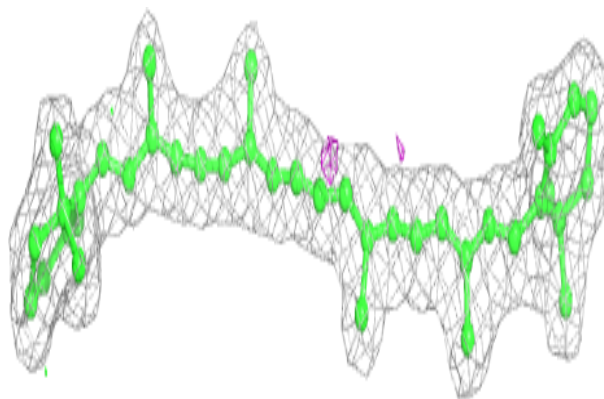
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



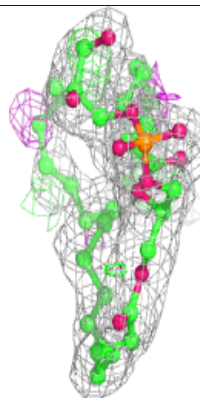
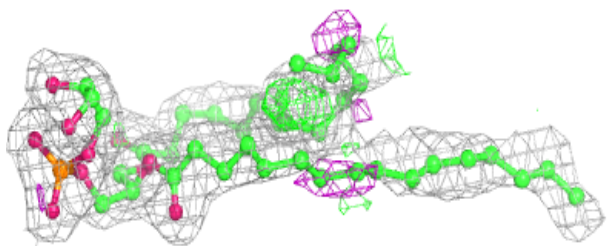
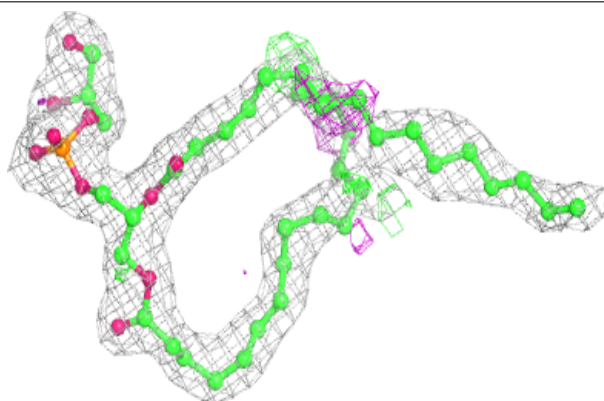


Electron density around BCR A 1009:

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

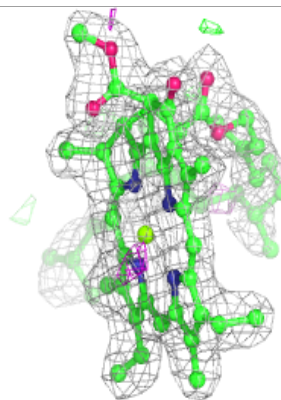
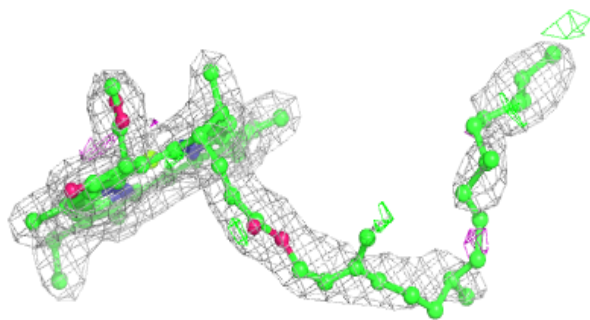
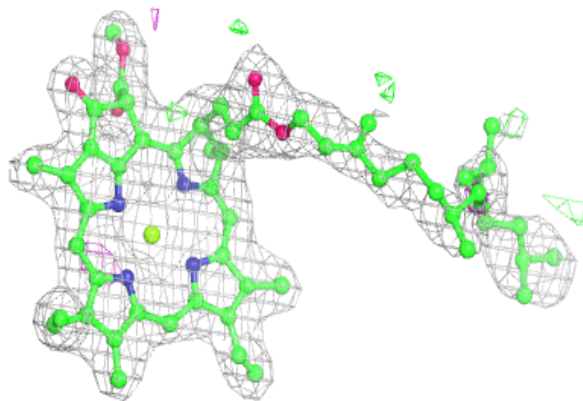
**Electron density around LHG d 408:**

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

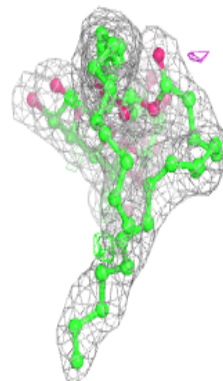
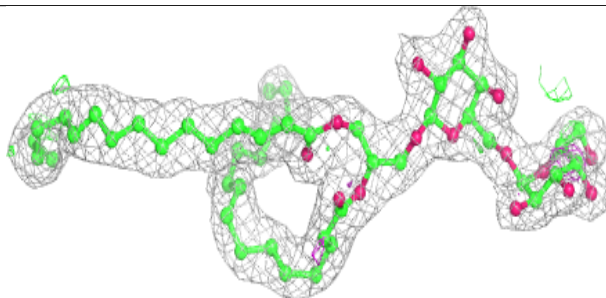
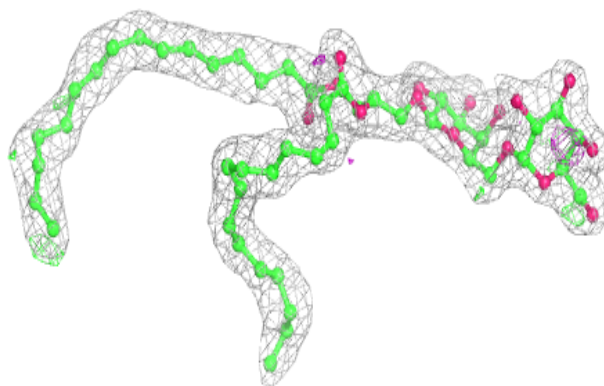


Electron density around CLA A 1008:

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

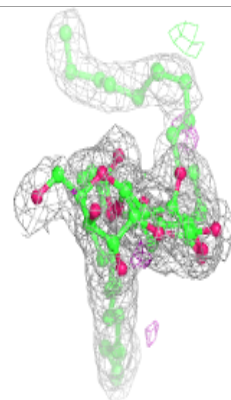
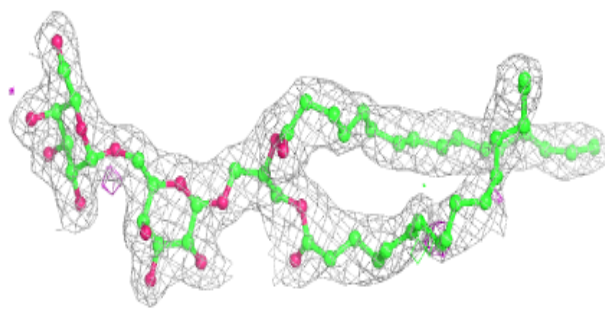
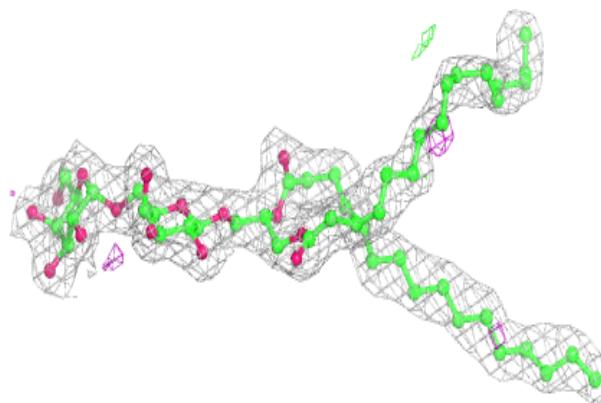
**Electron density around DGD H 102:**

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

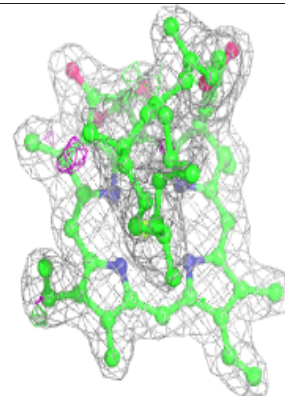
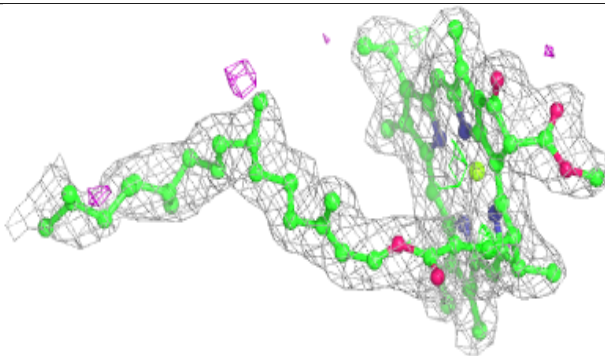
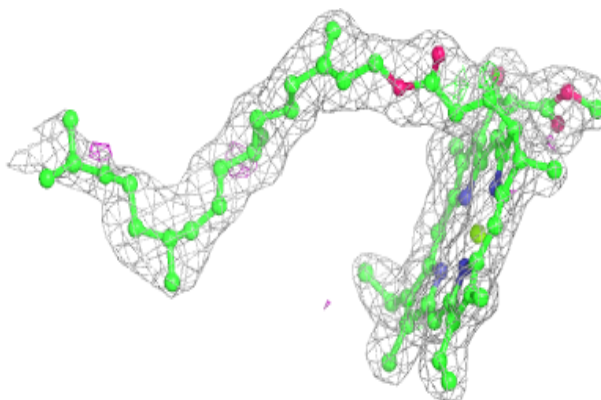


Electron density around DGD c 515:

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

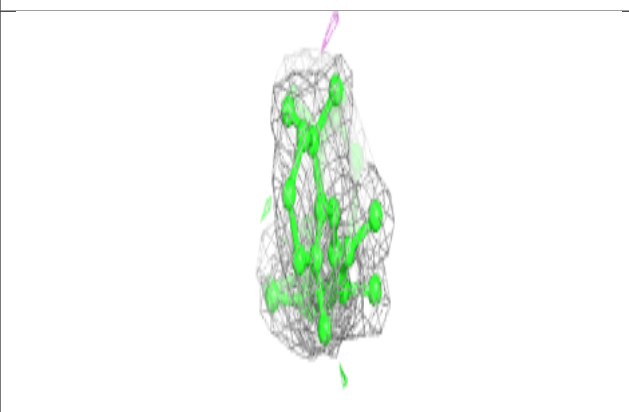
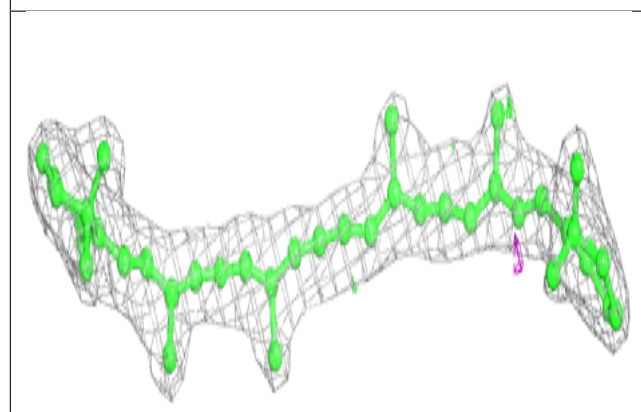
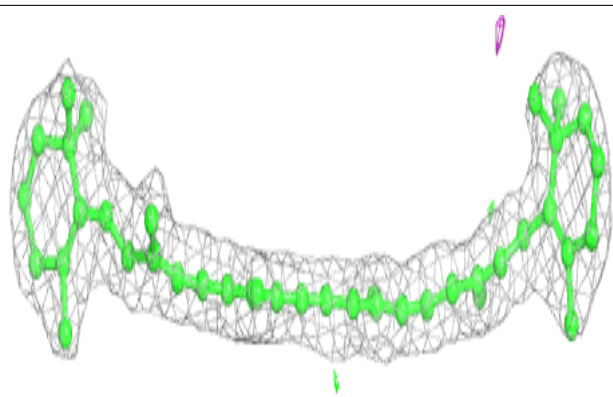
**Electron density around CLA c 508:**

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

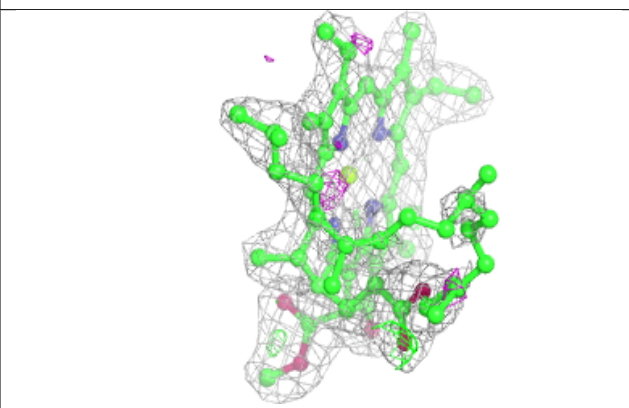
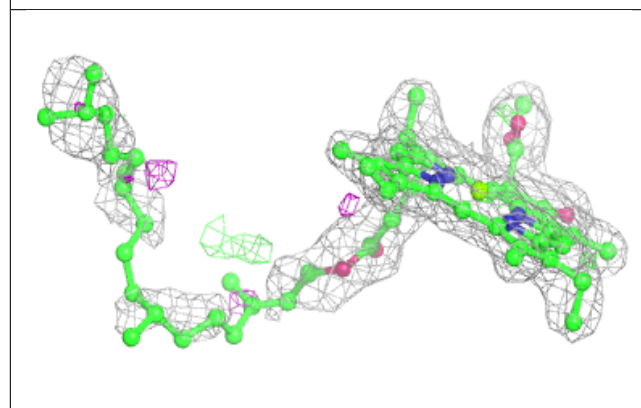
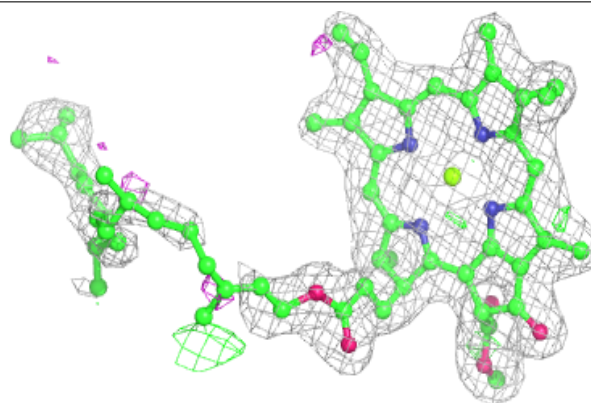


Electron density around BCR k 101:

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

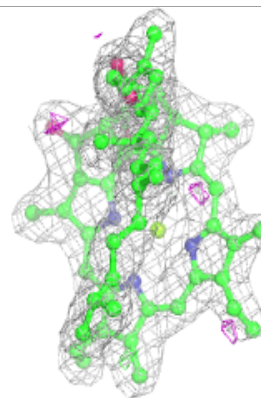
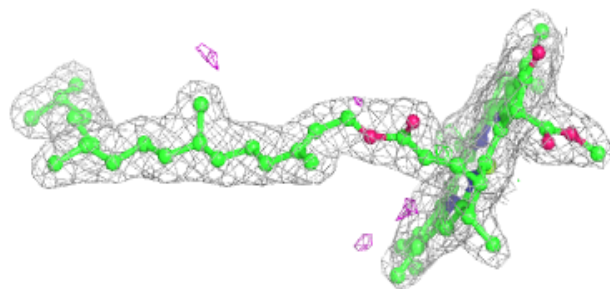
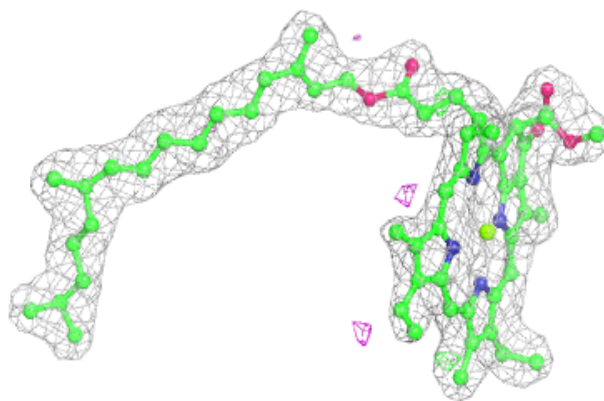
**Electron density around CLA a 412:**

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



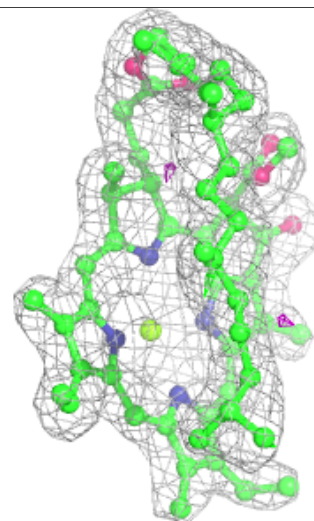
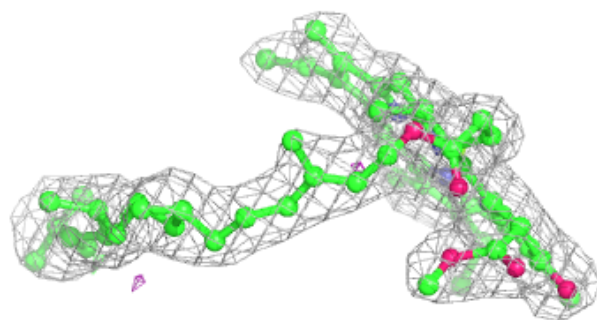
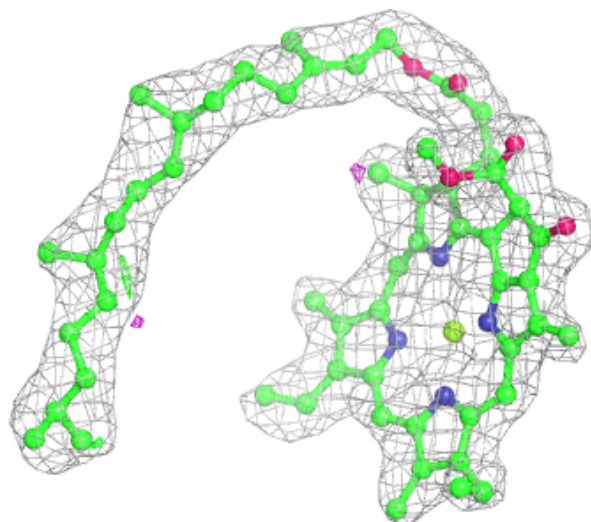
Electron density around CLA b 612:

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



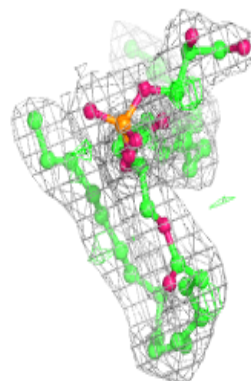
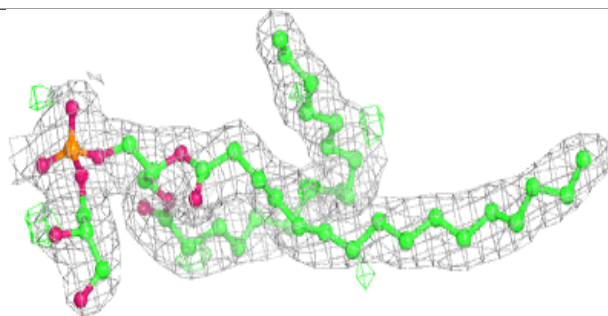
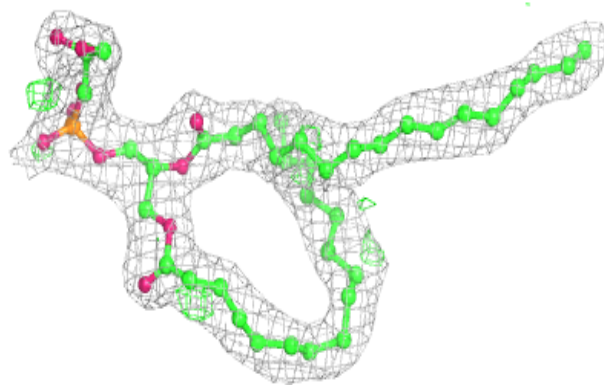
Electron density around CLA C 507:

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

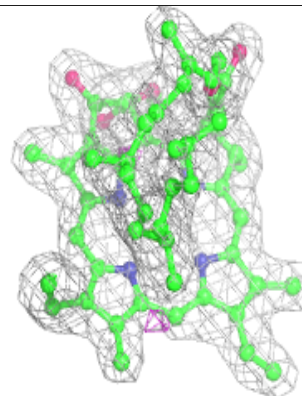
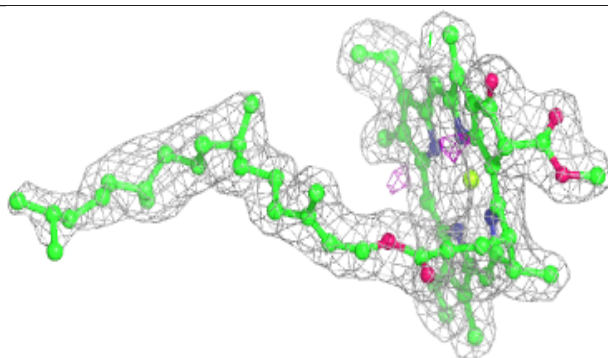
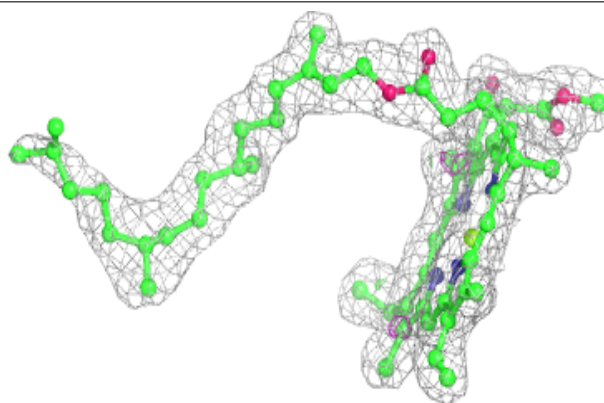


Electron density around LHG d 406:

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

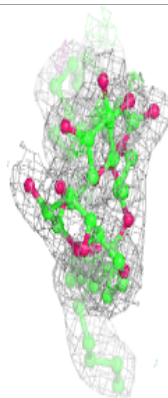
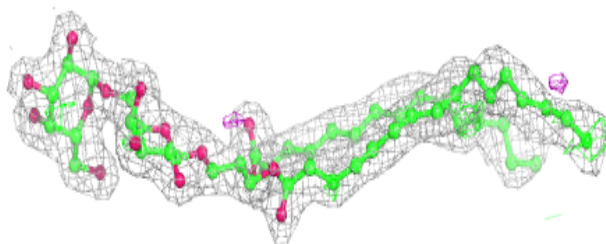
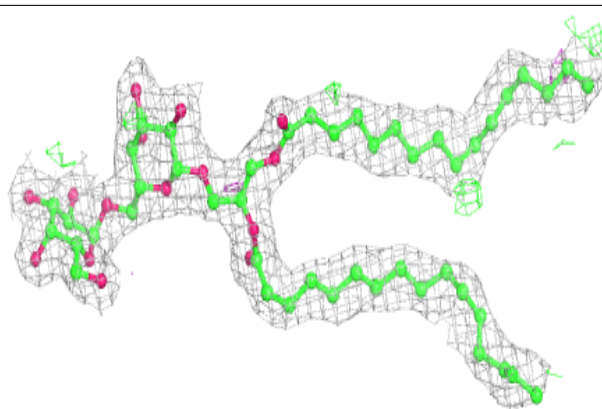
**Electron density around CLA C 508:**

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

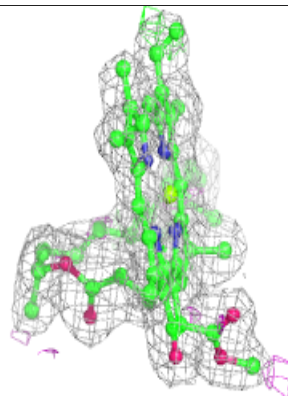
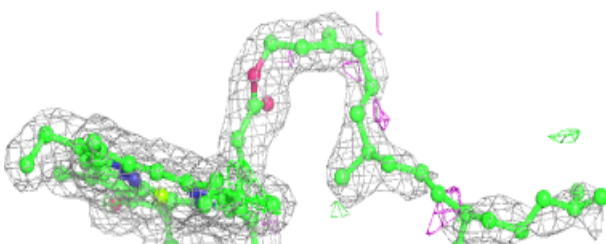
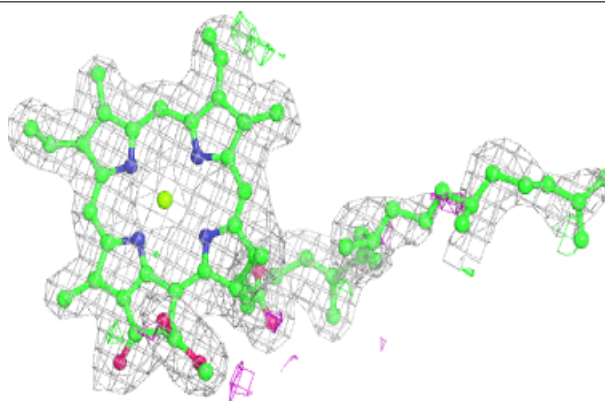


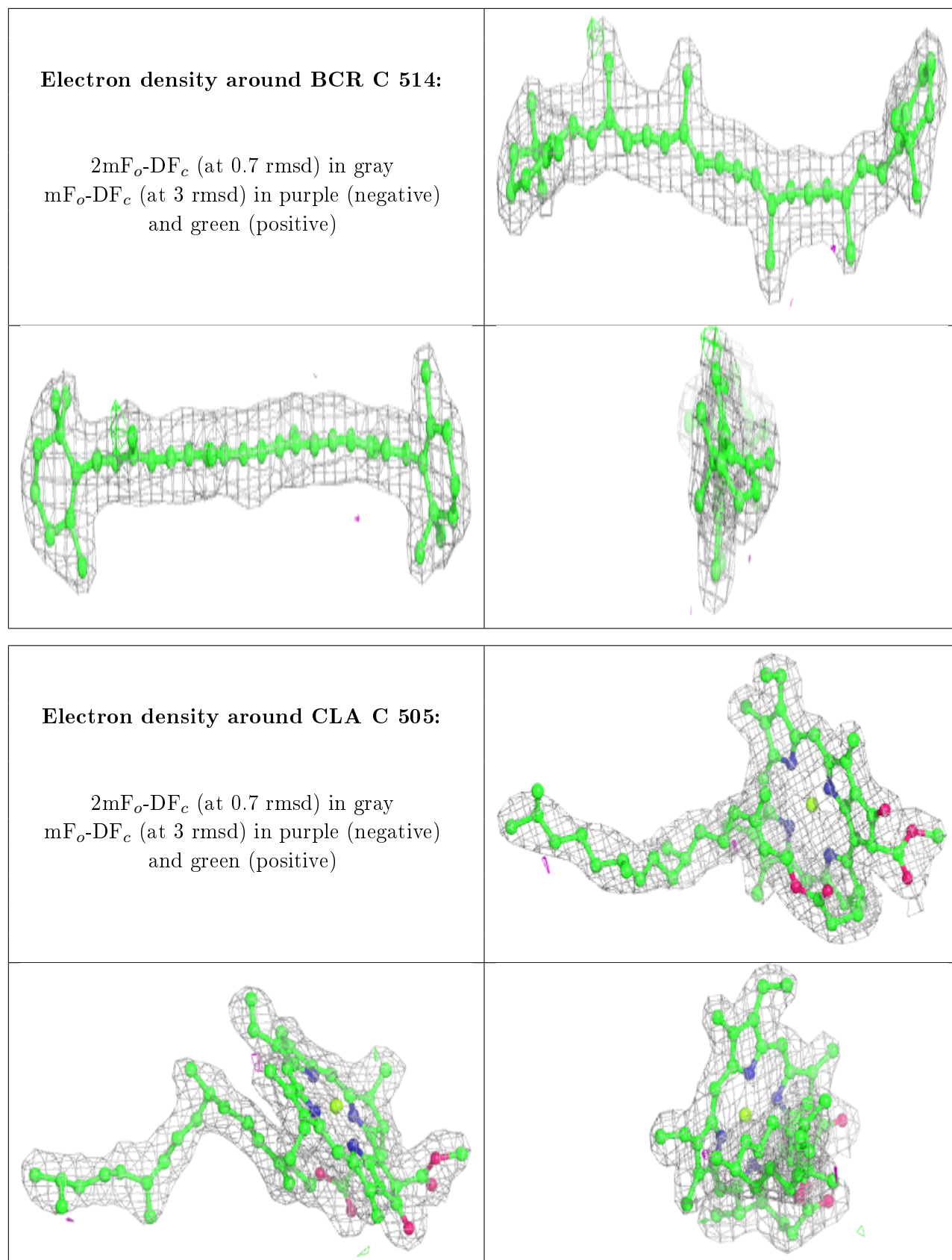
Electron density around DGD C 517:

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

**Electron density around CLA a 409:**

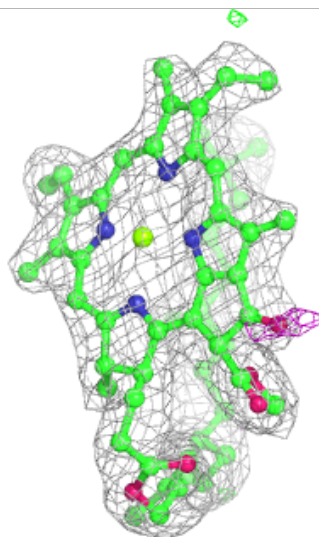
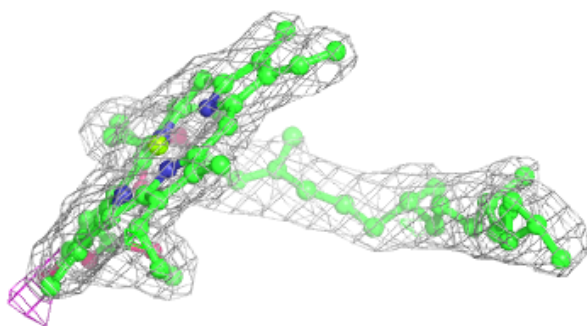
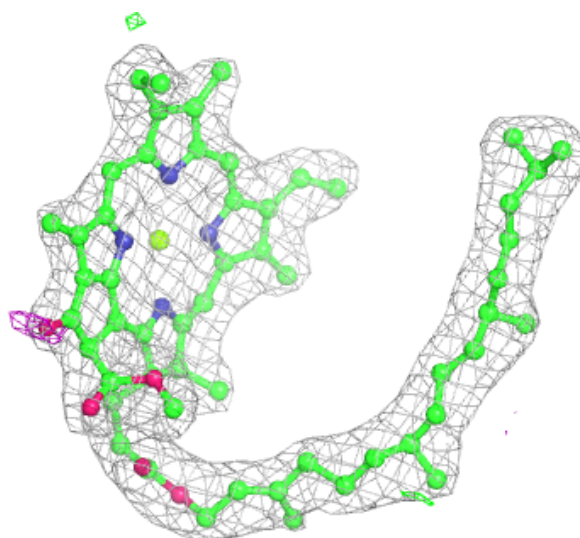
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





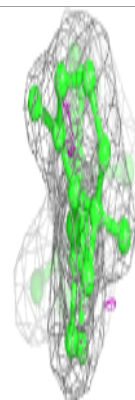
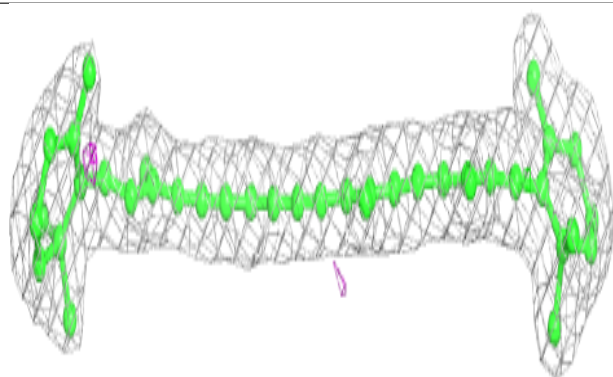
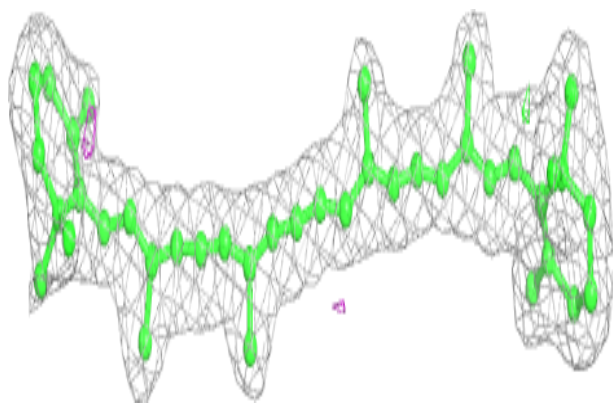
Electron density around CLA c 507:

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

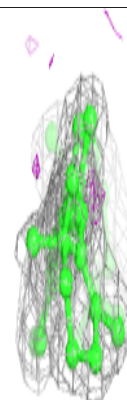
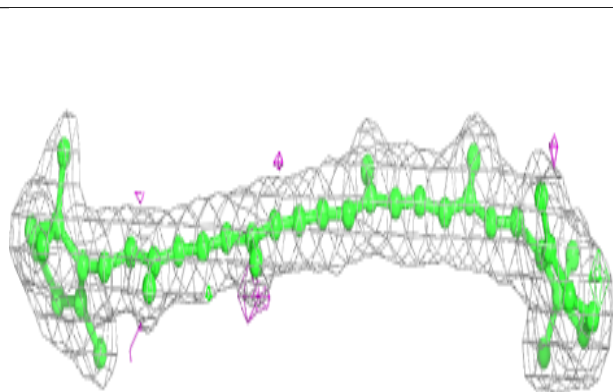
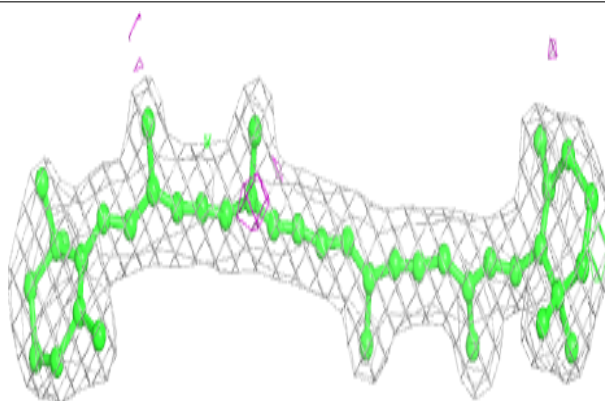


Electron density around BCR b 621:

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

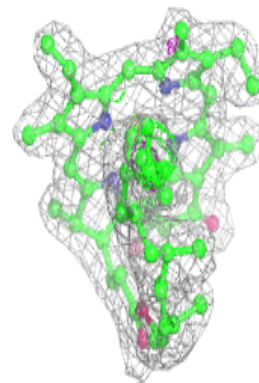
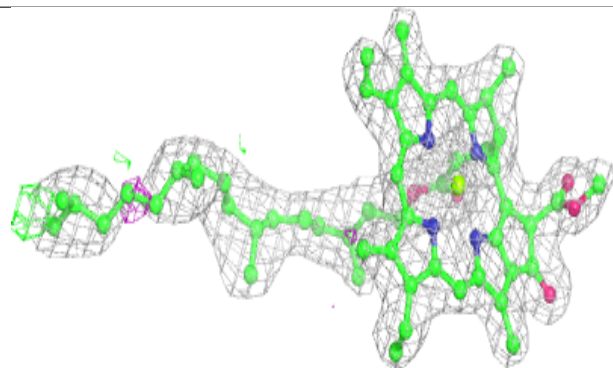
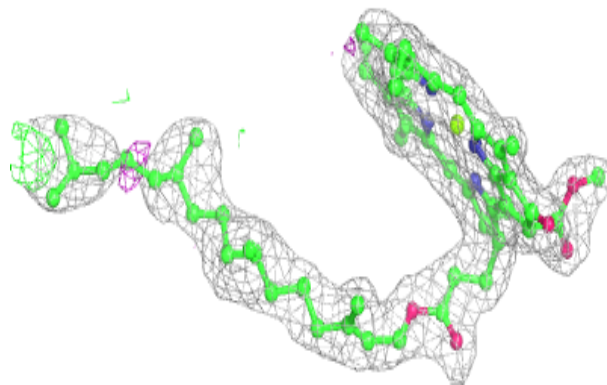
**Electron density around BCR B 619:**

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

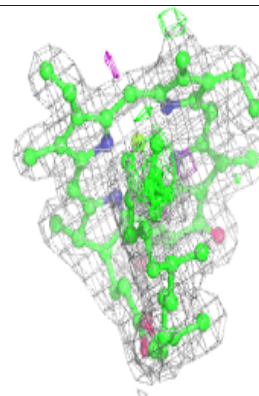
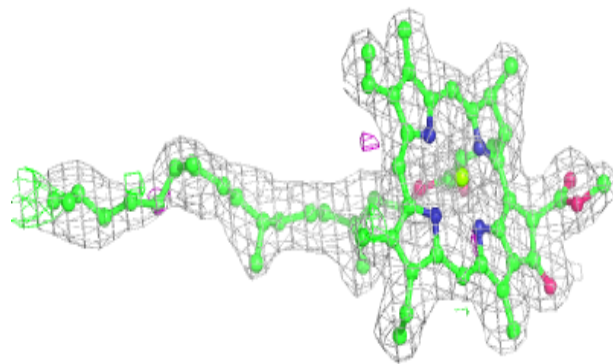
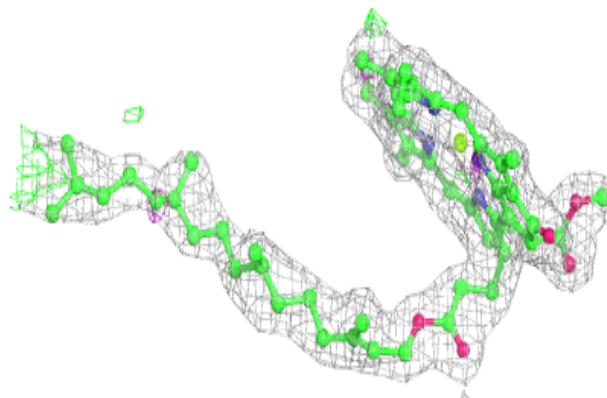


Electron density around CLA c 504:

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

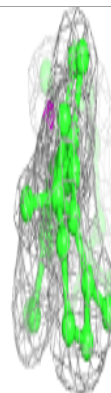
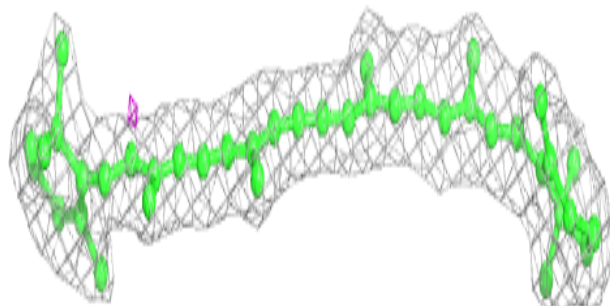
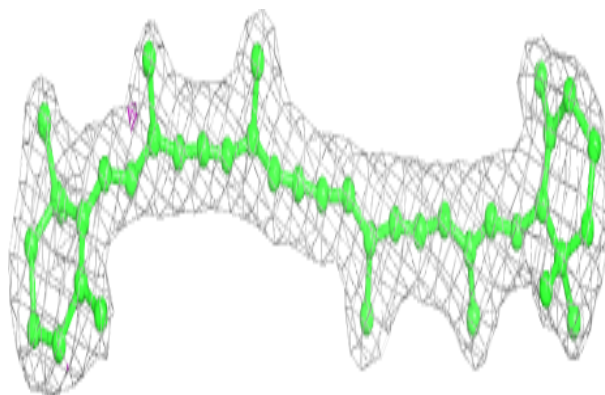
**Electron density around CLA C 504:**

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

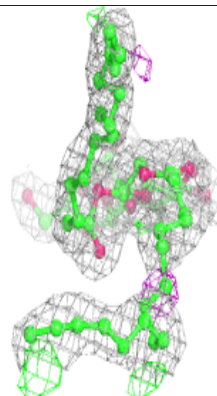
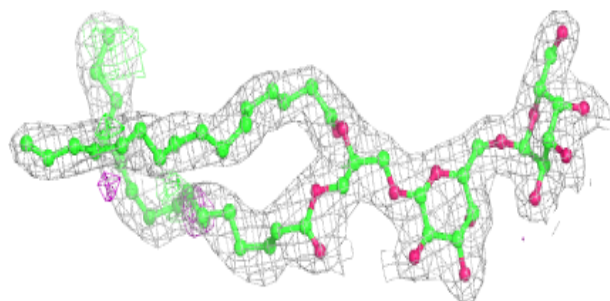
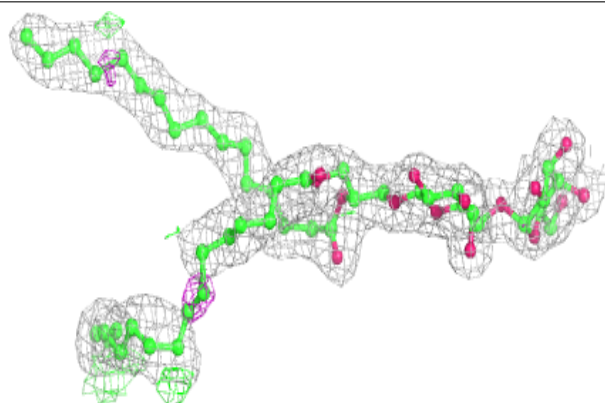


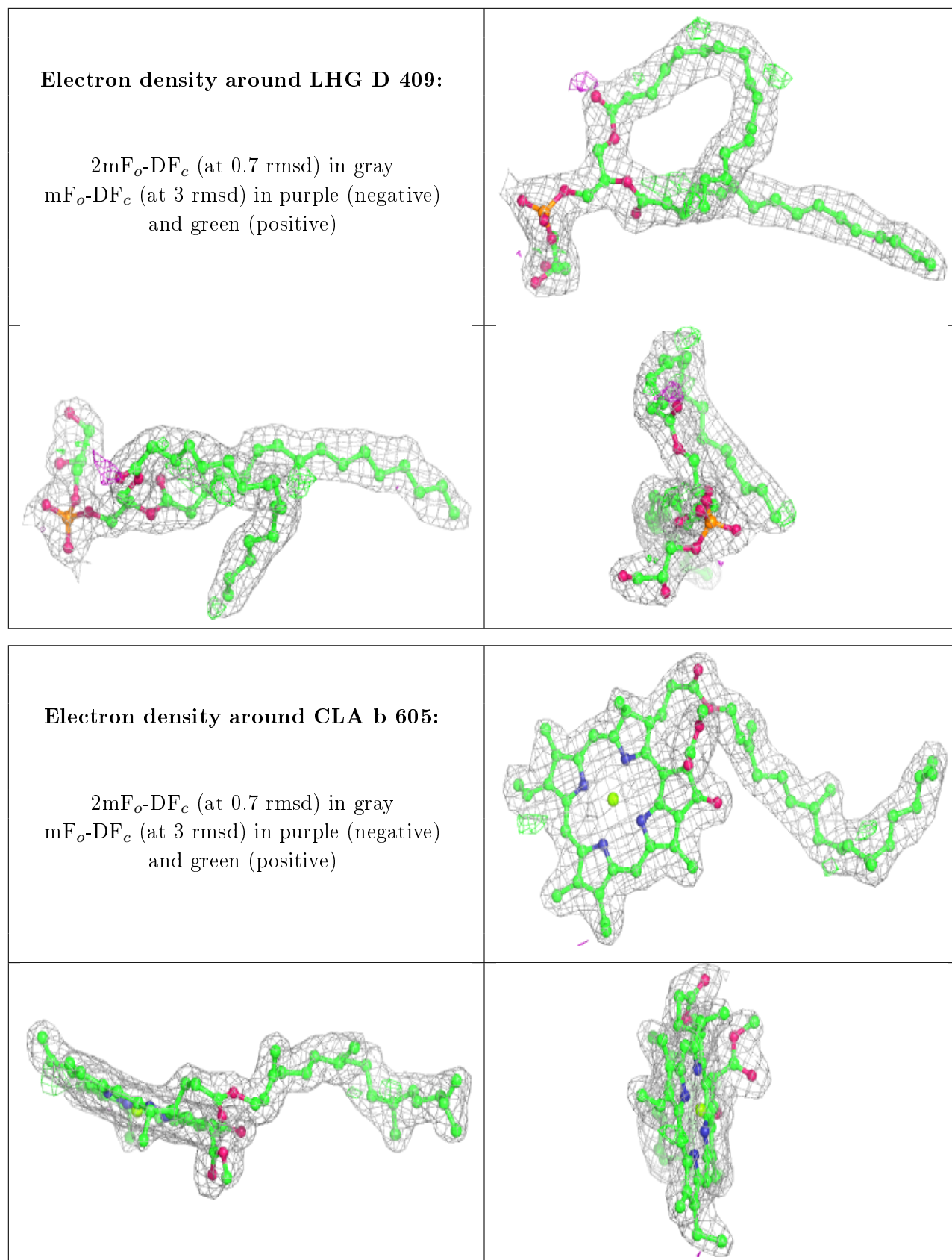
Electron density around BCR b 622:

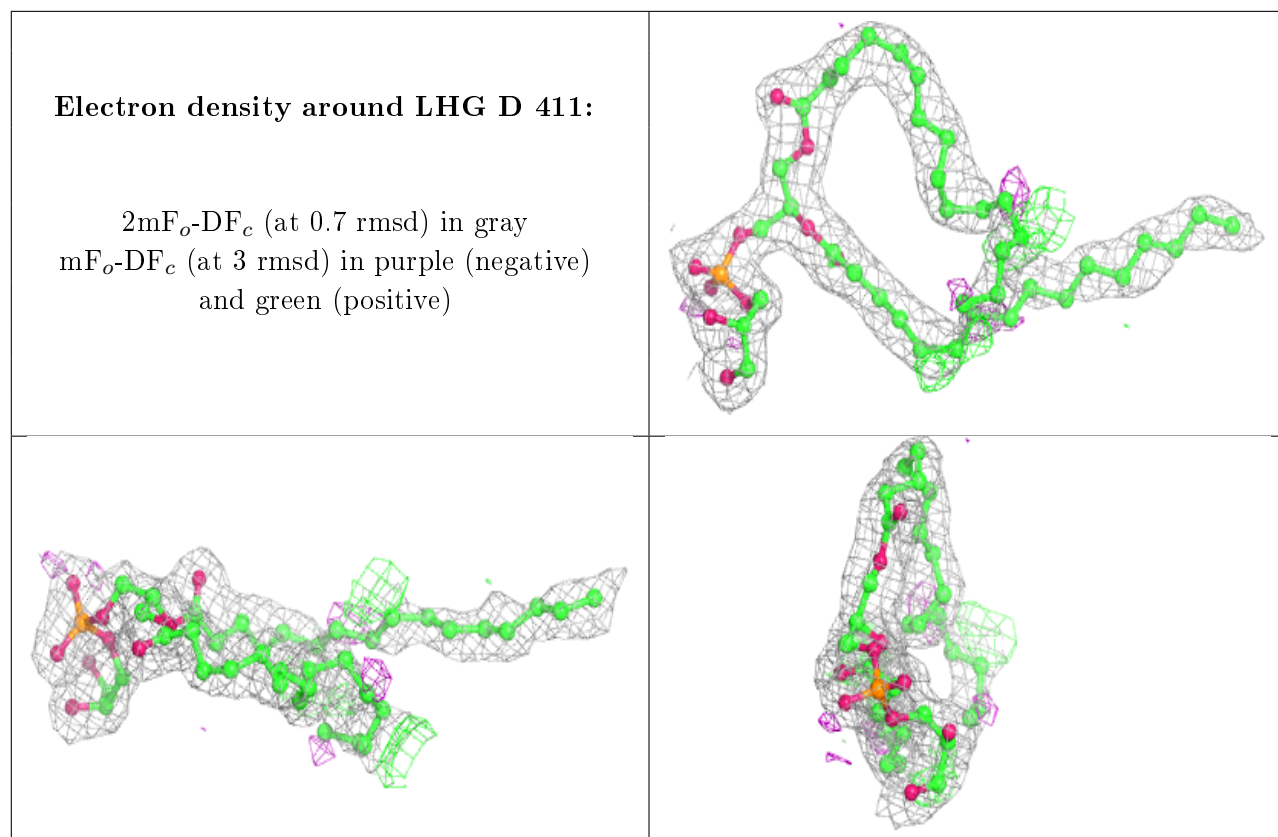
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around DGD 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)

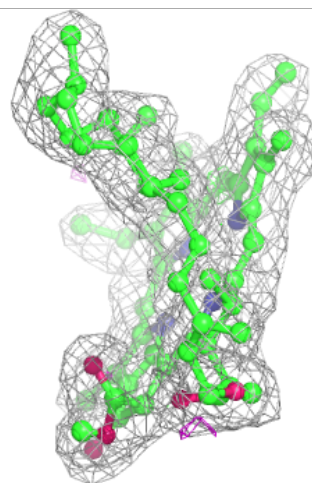
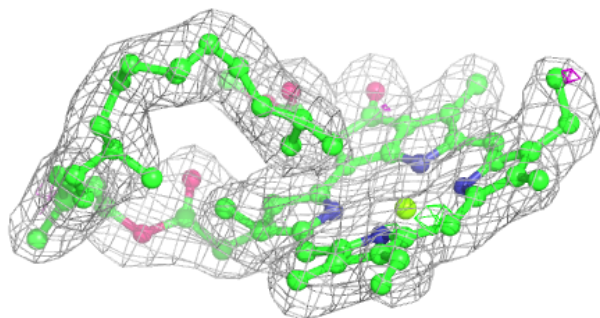
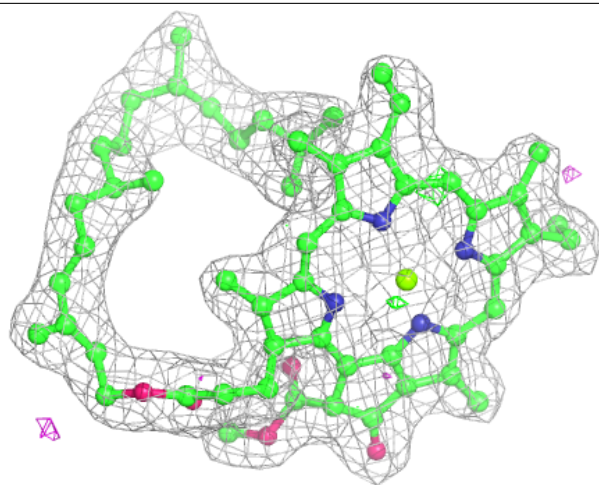






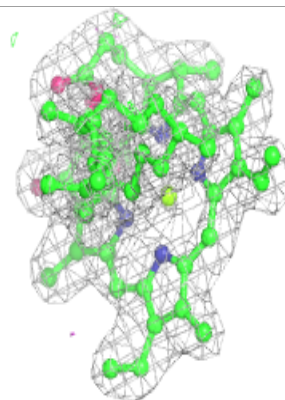
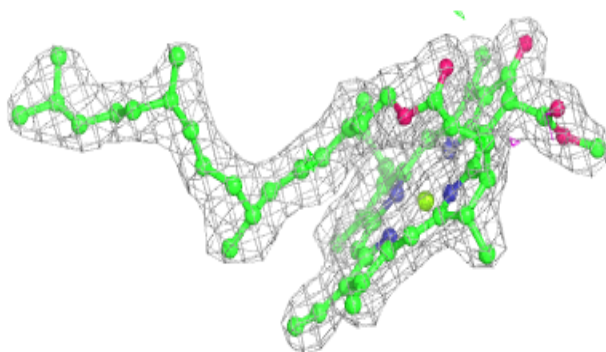
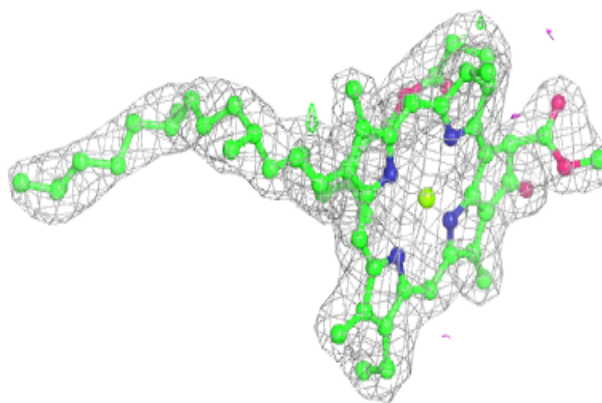
Electron density around CLA B 615:

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

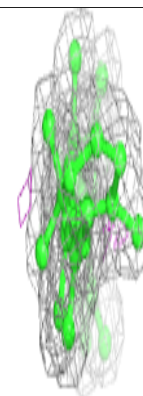
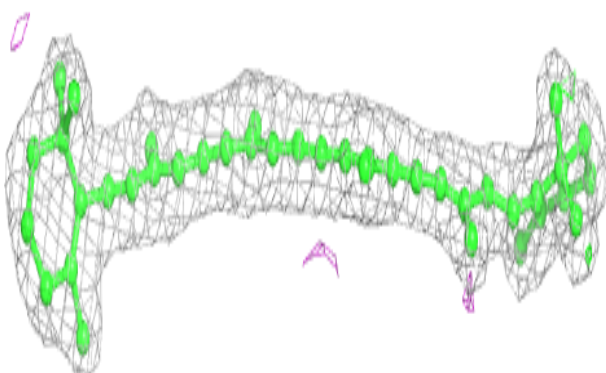
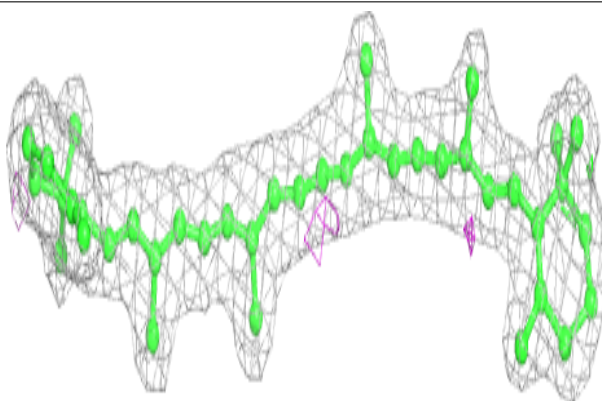


Electron density around CLA c 505:

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

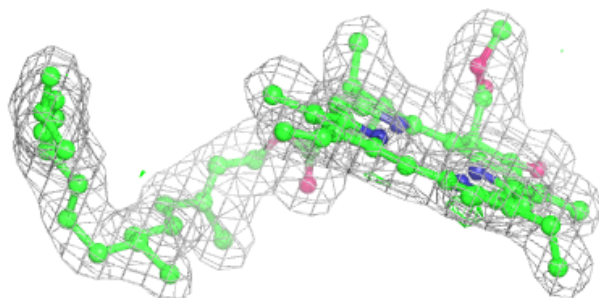
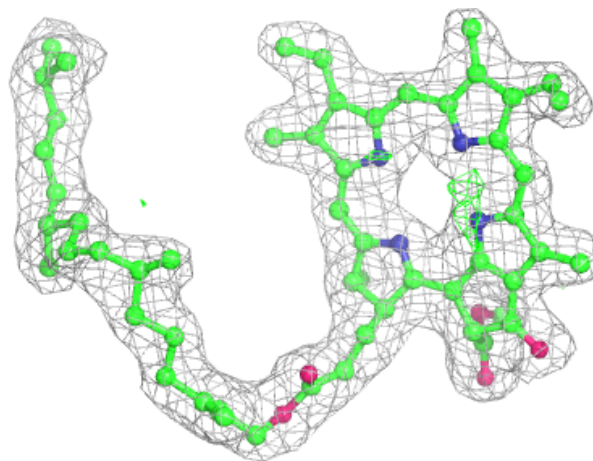
**Electron density around BCR B 617:**

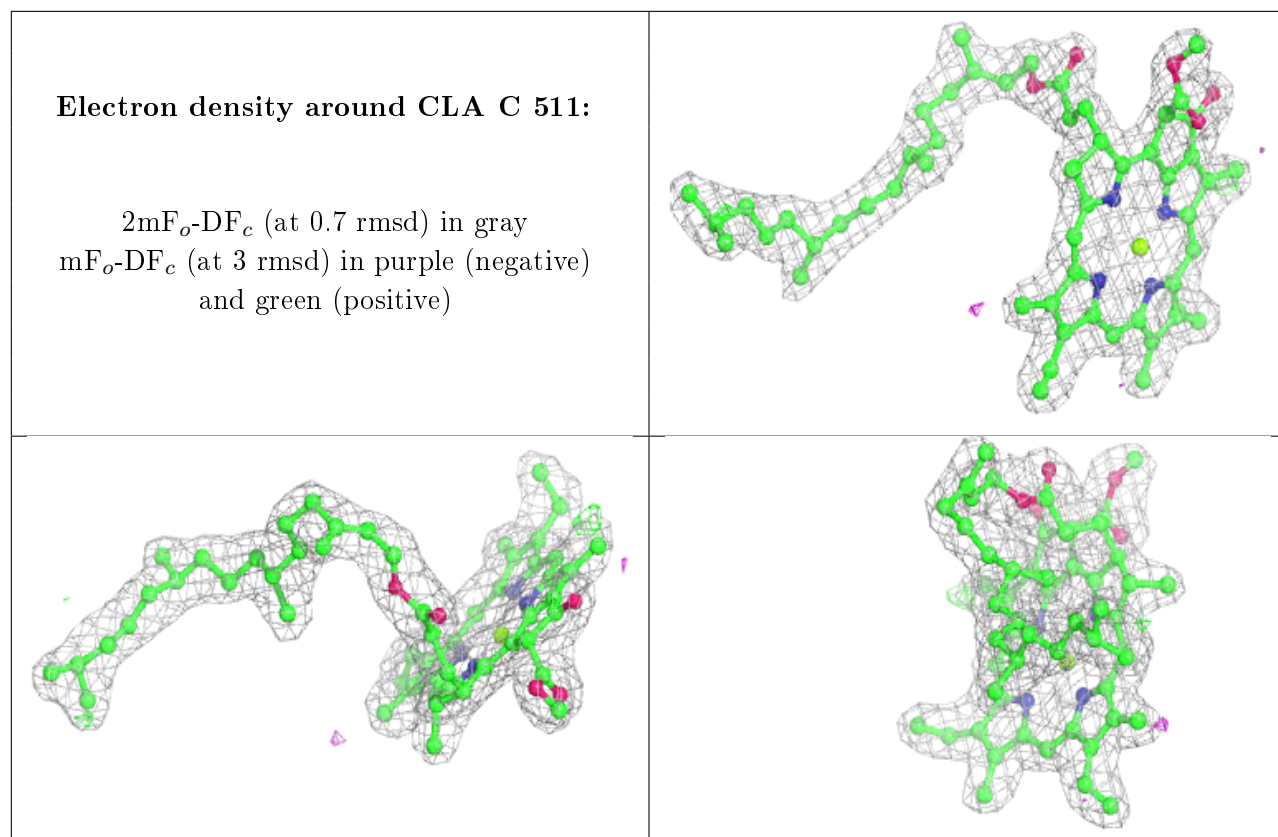
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PHO a 411:

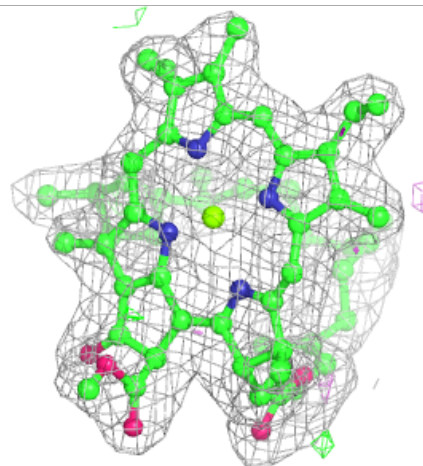
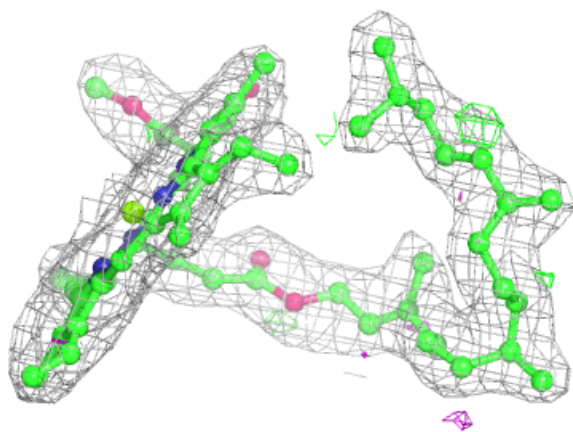
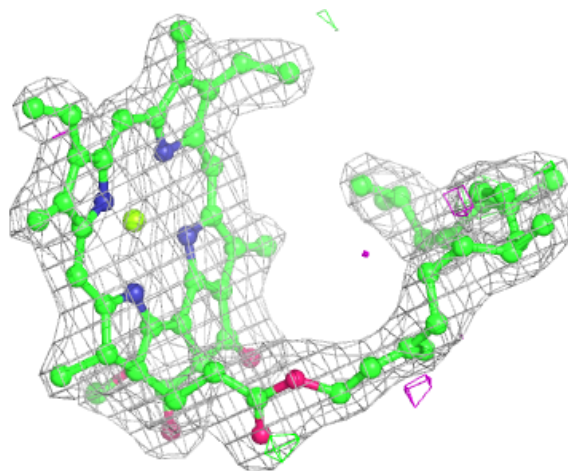
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





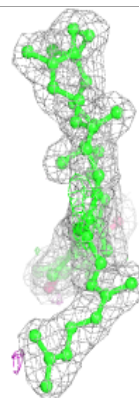
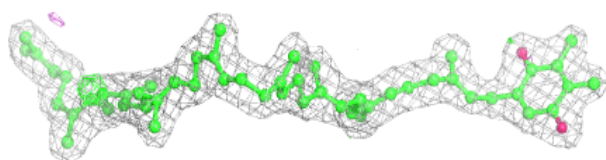
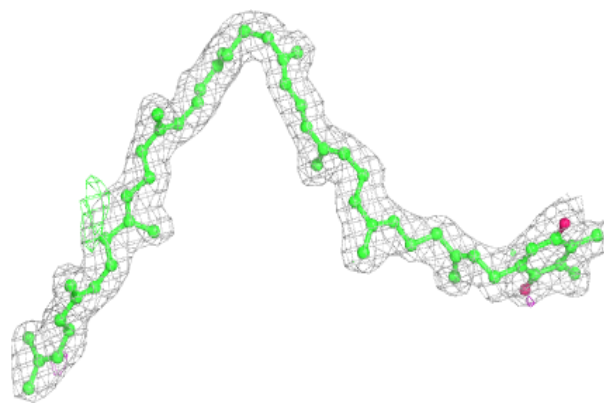
Electron density around CLA c 503:

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



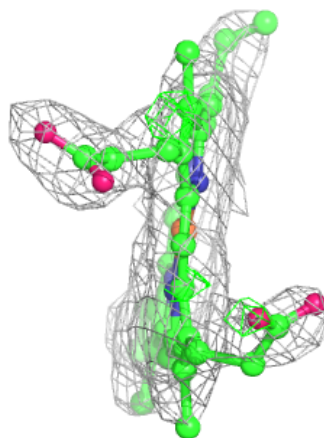
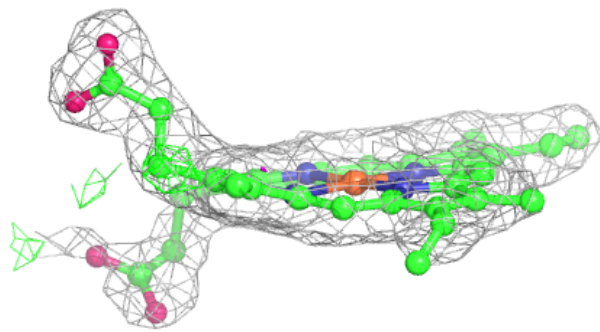
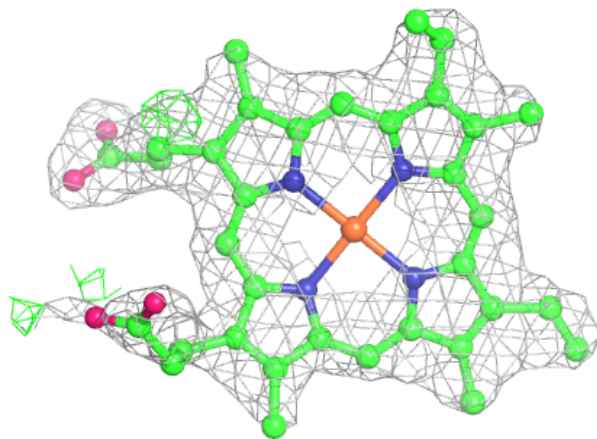
Electron density around PL9 D 407:

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



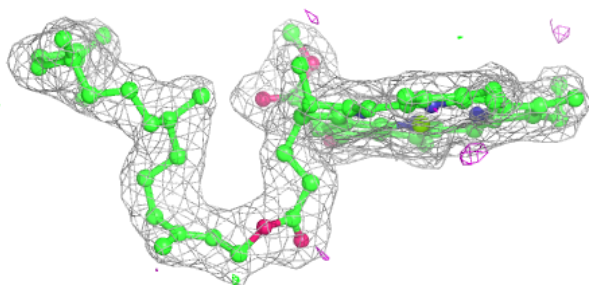
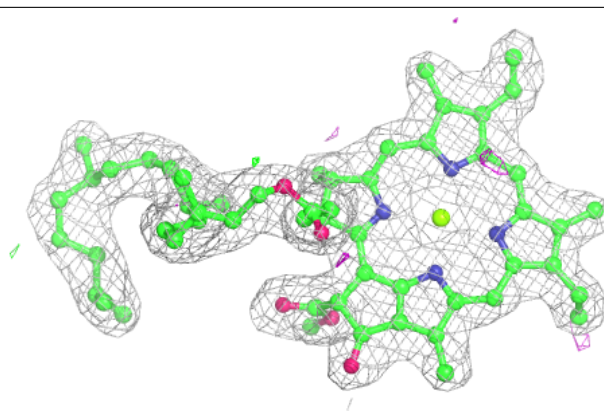
Electron density around HEM f 101:

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

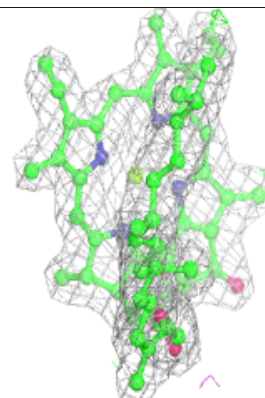
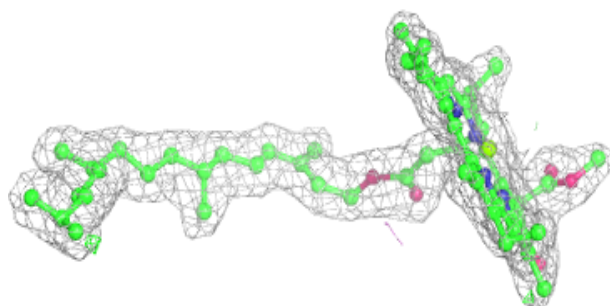
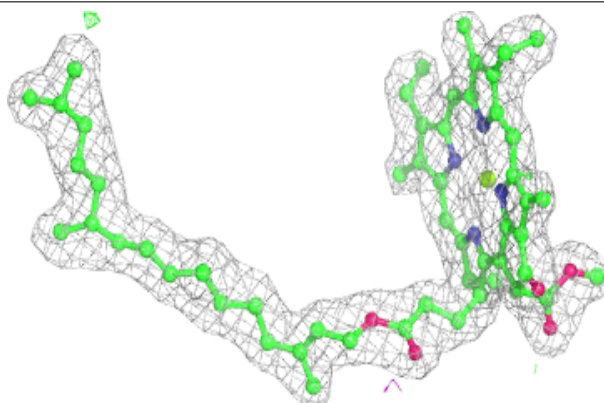


Electron density around CLA b 615:

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

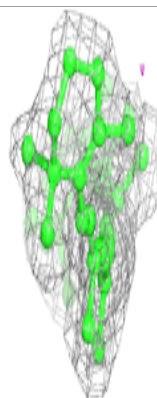
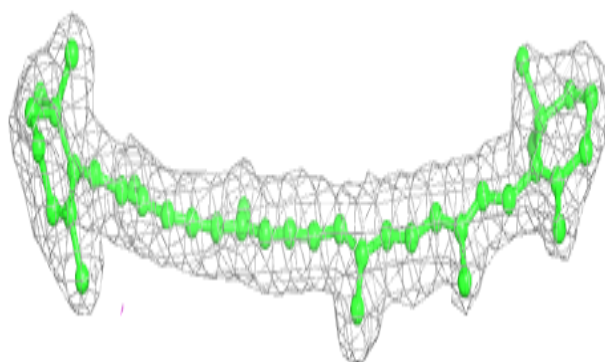
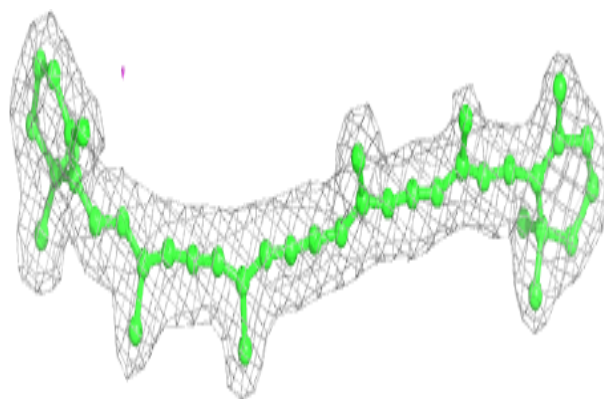
**Electron density around CLA B 609:**

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

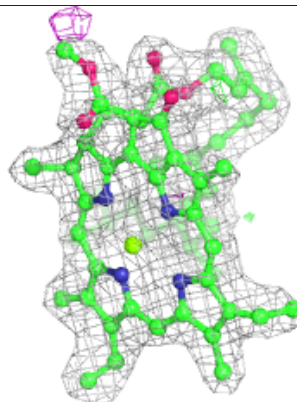
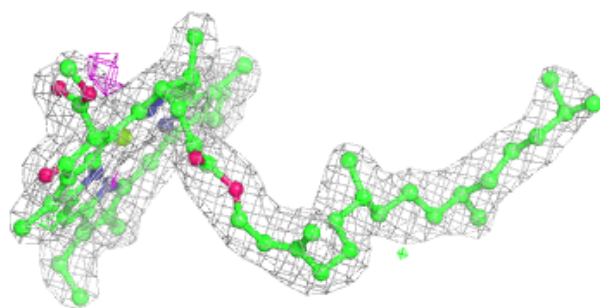
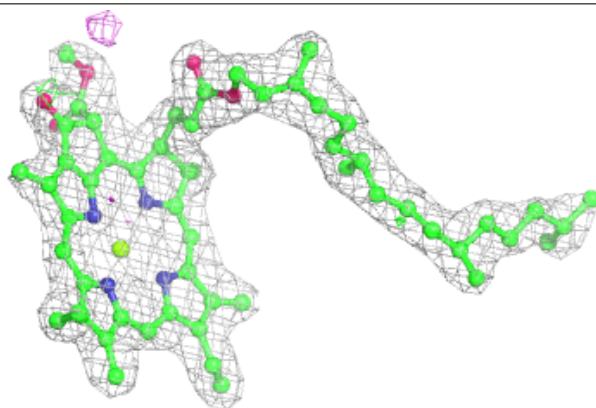


Electron density around BCR T 101:

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

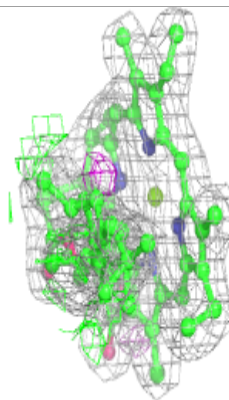
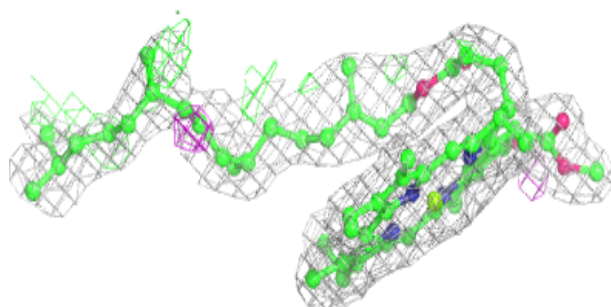
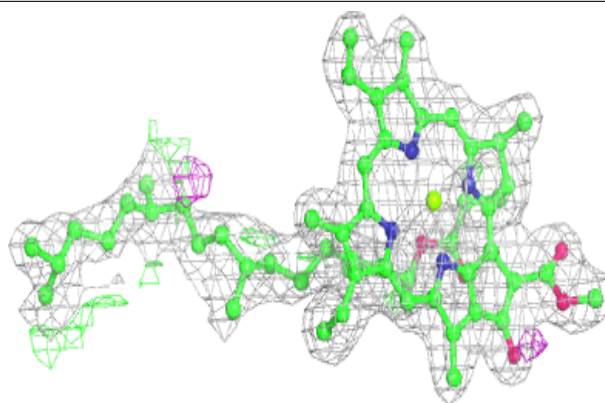
**Electron density around CLA c 511:**

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

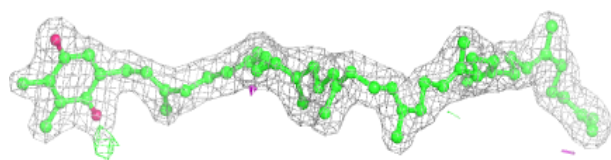
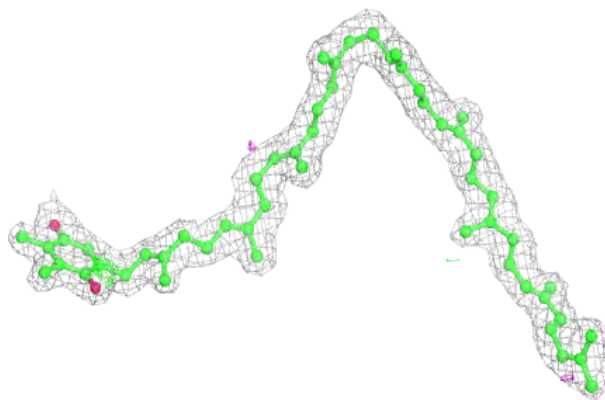


Electron density around CLA B 614:

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

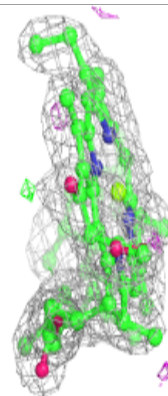
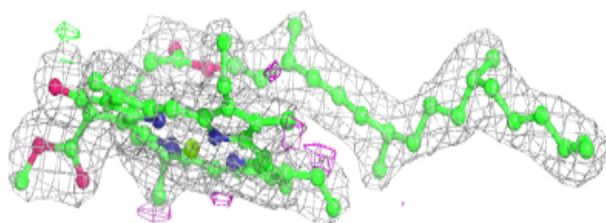
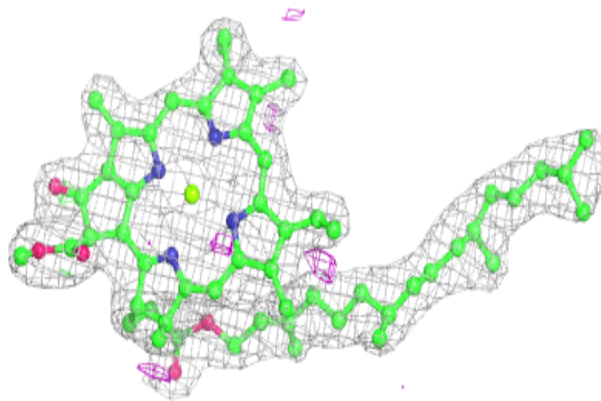
**Electron density around PL9 d 405:**

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

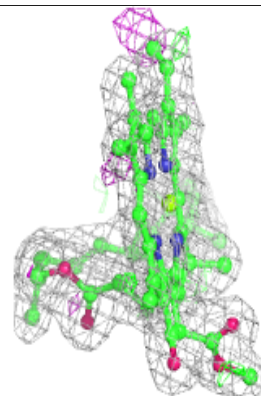
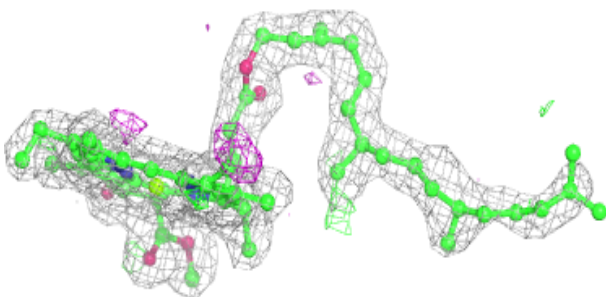
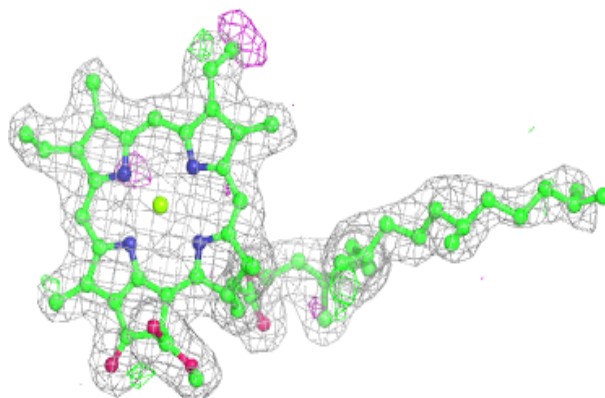


Electron density around CLA c 501:

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

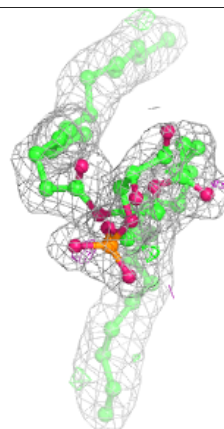
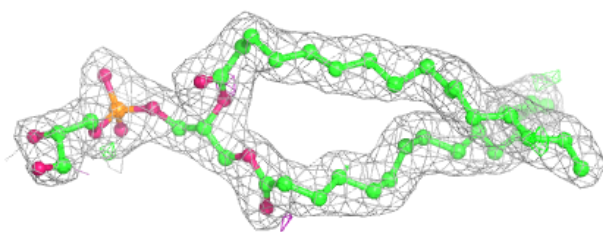
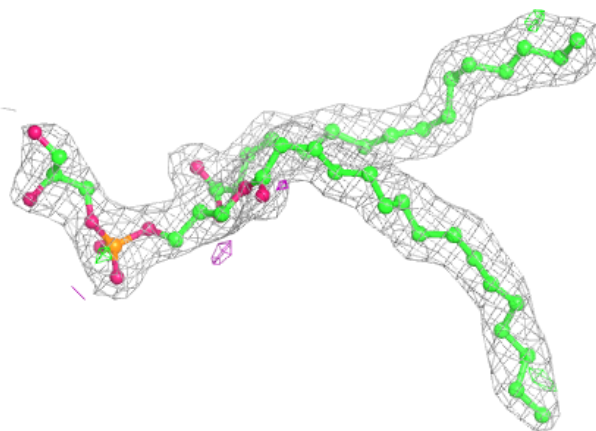
**Electron density around CLA A 1006:**

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



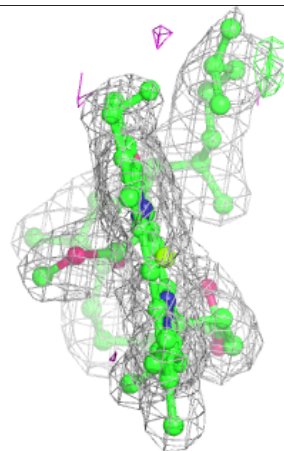
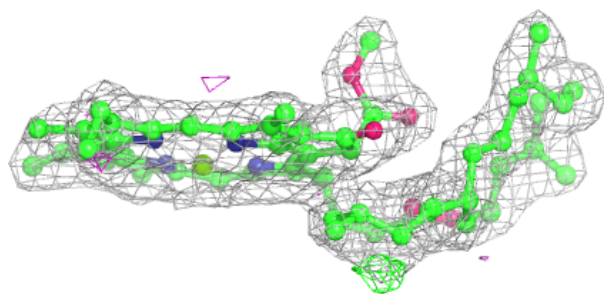
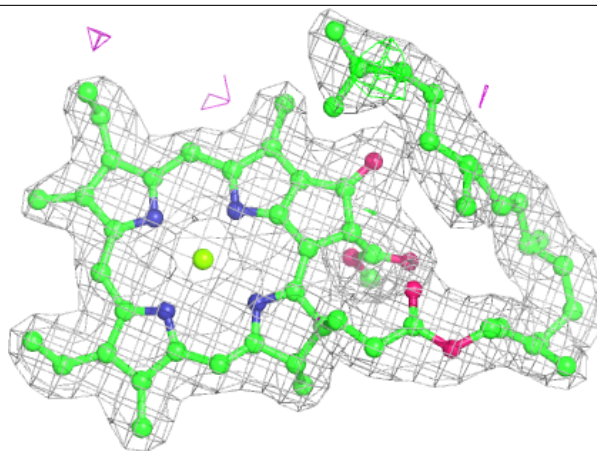
Electron density around LHG d 407:

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

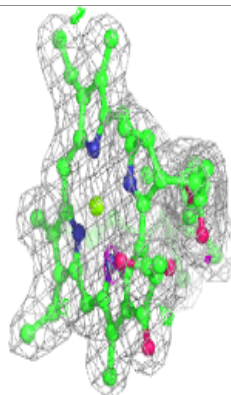
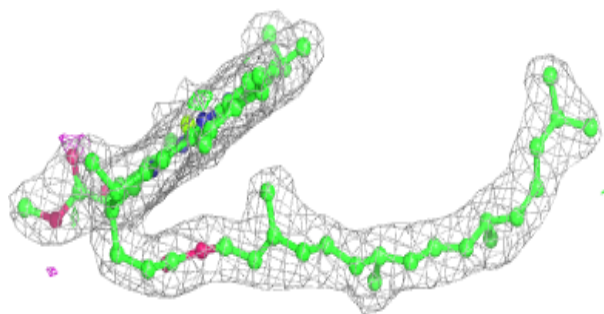
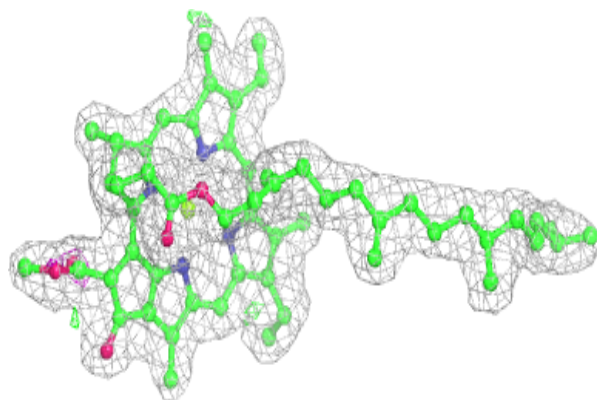


Electron density around CLA b 613:

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

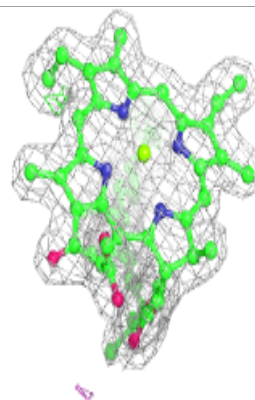
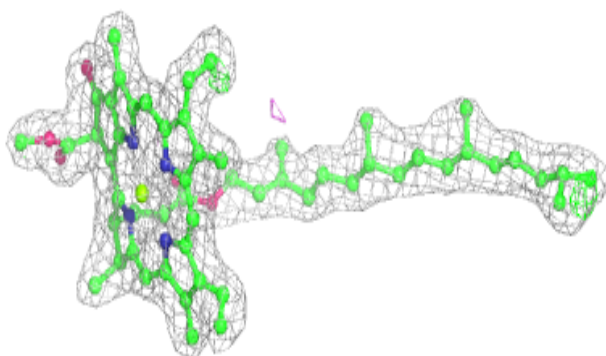
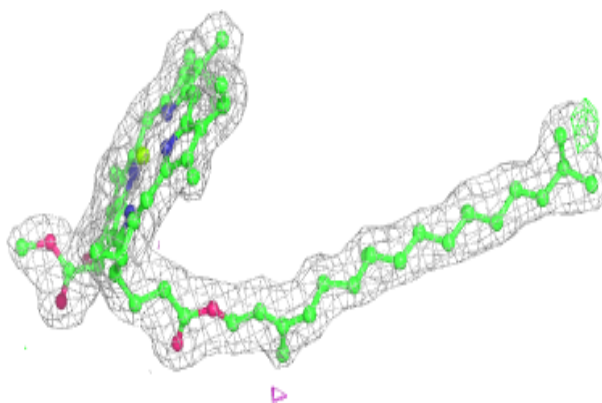
**Electron density around CLA b 611:**

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

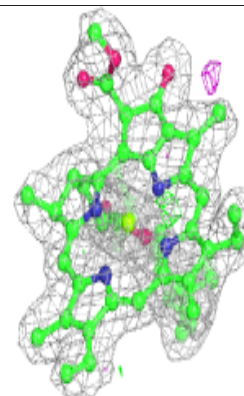
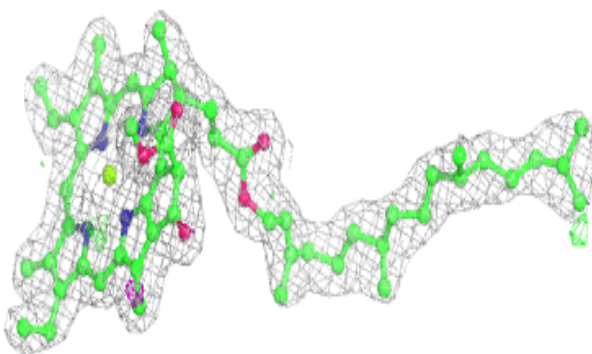
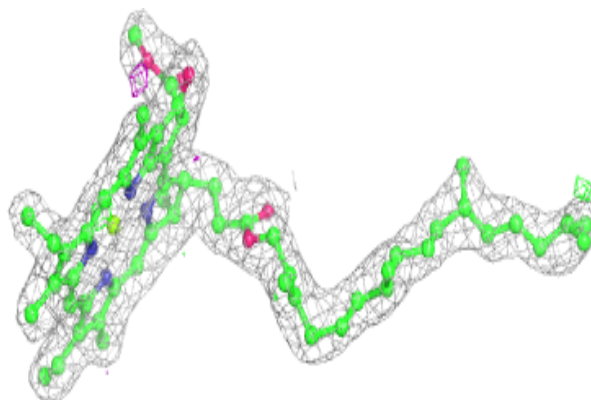


Electron density around CLA b 610:

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

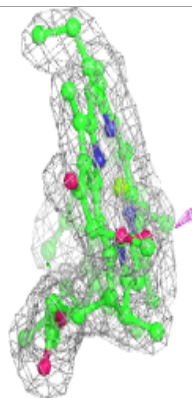
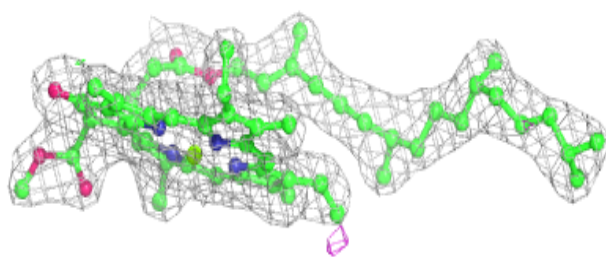
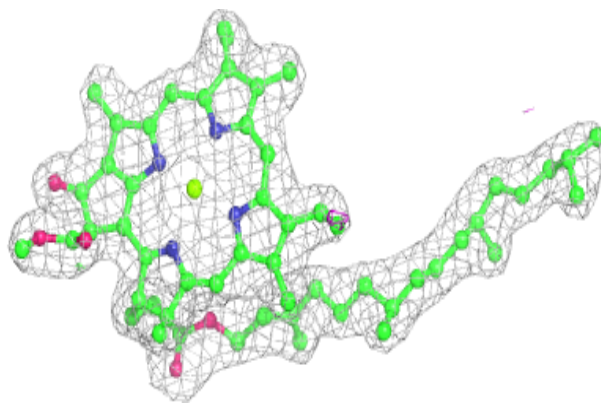
**Electron density around CLA c 502:**

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

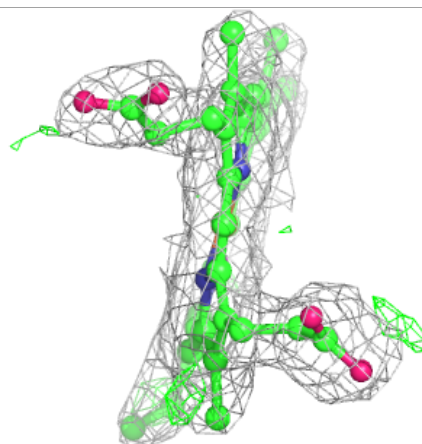
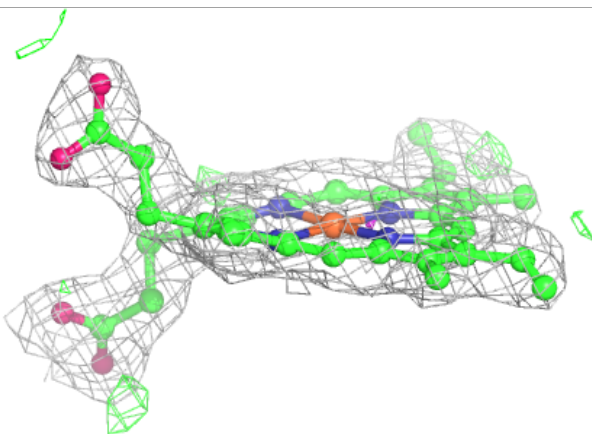
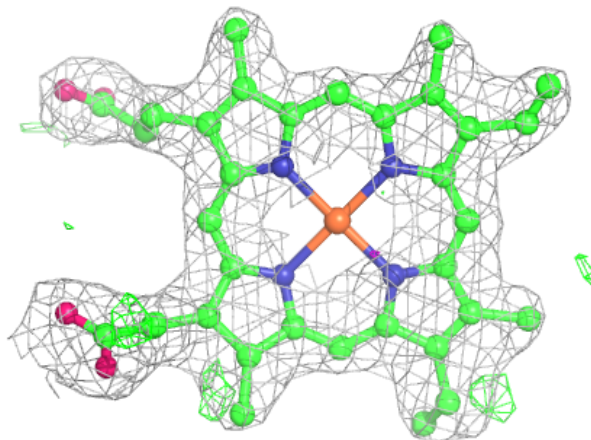


Electron density around CLA C 501:

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

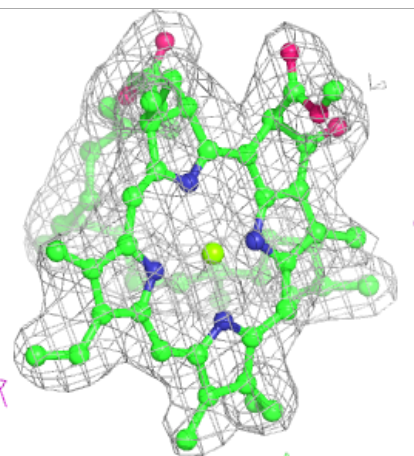
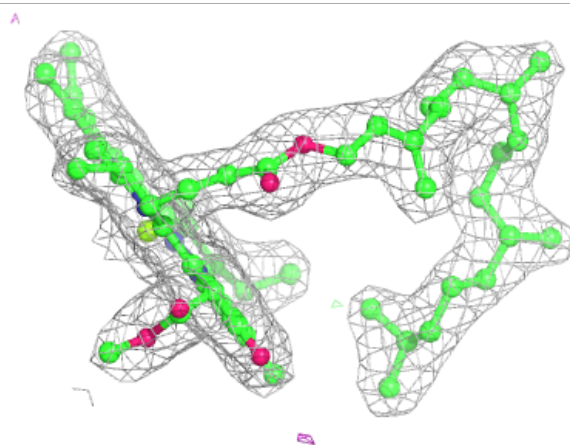
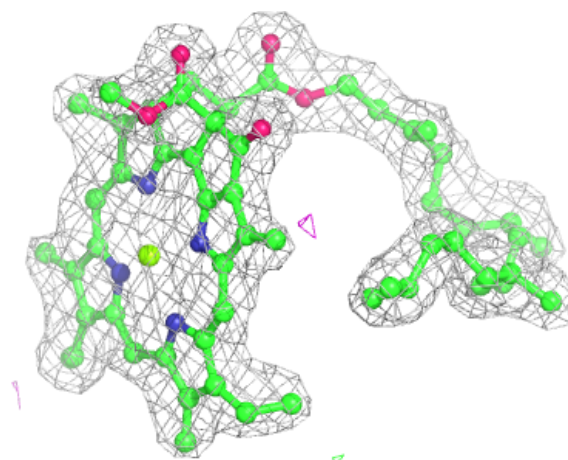
**Electron density around HEM F 101:**

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



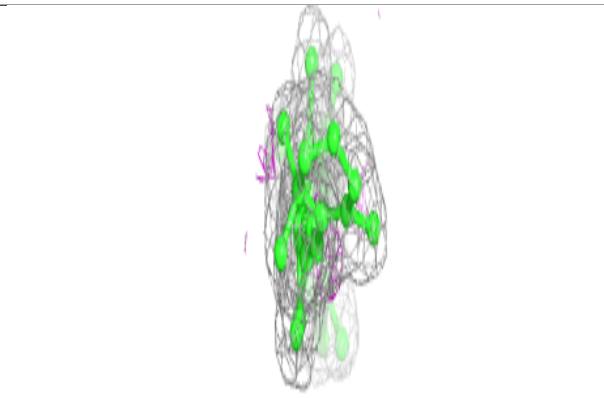
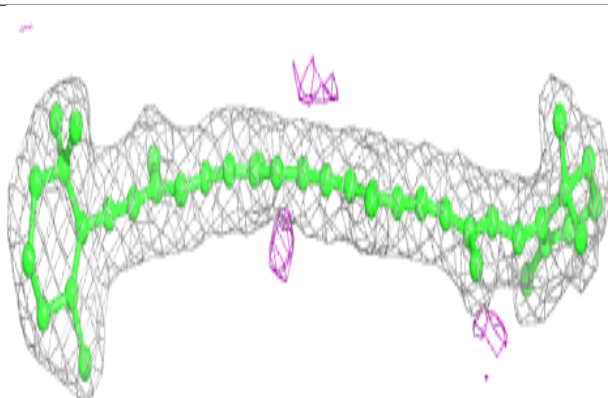
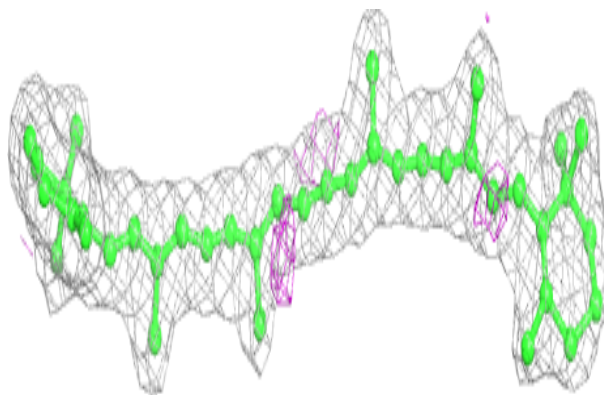
Electron density around CLA C 503:

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

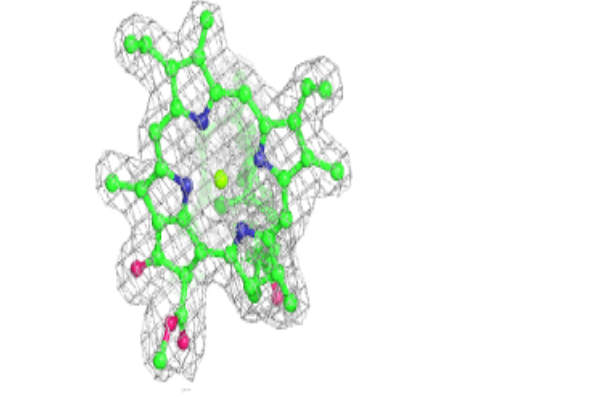
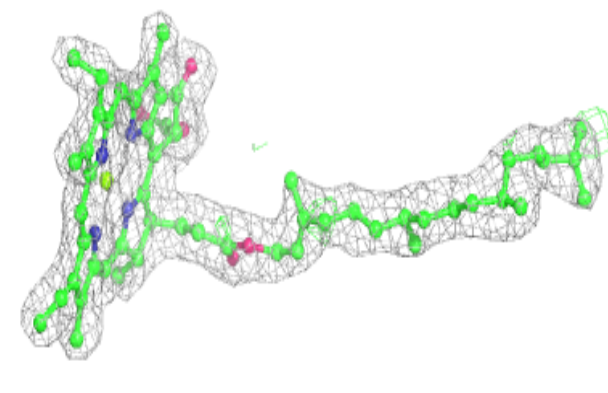
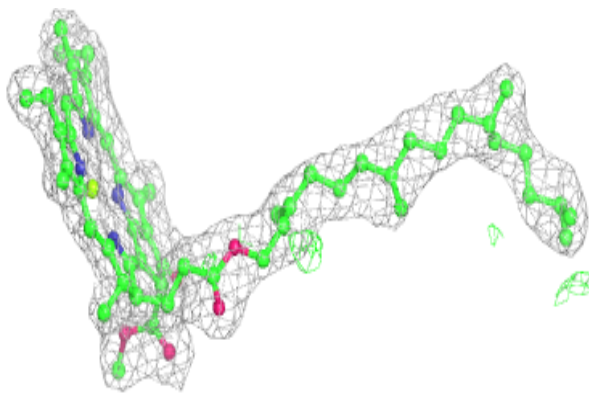


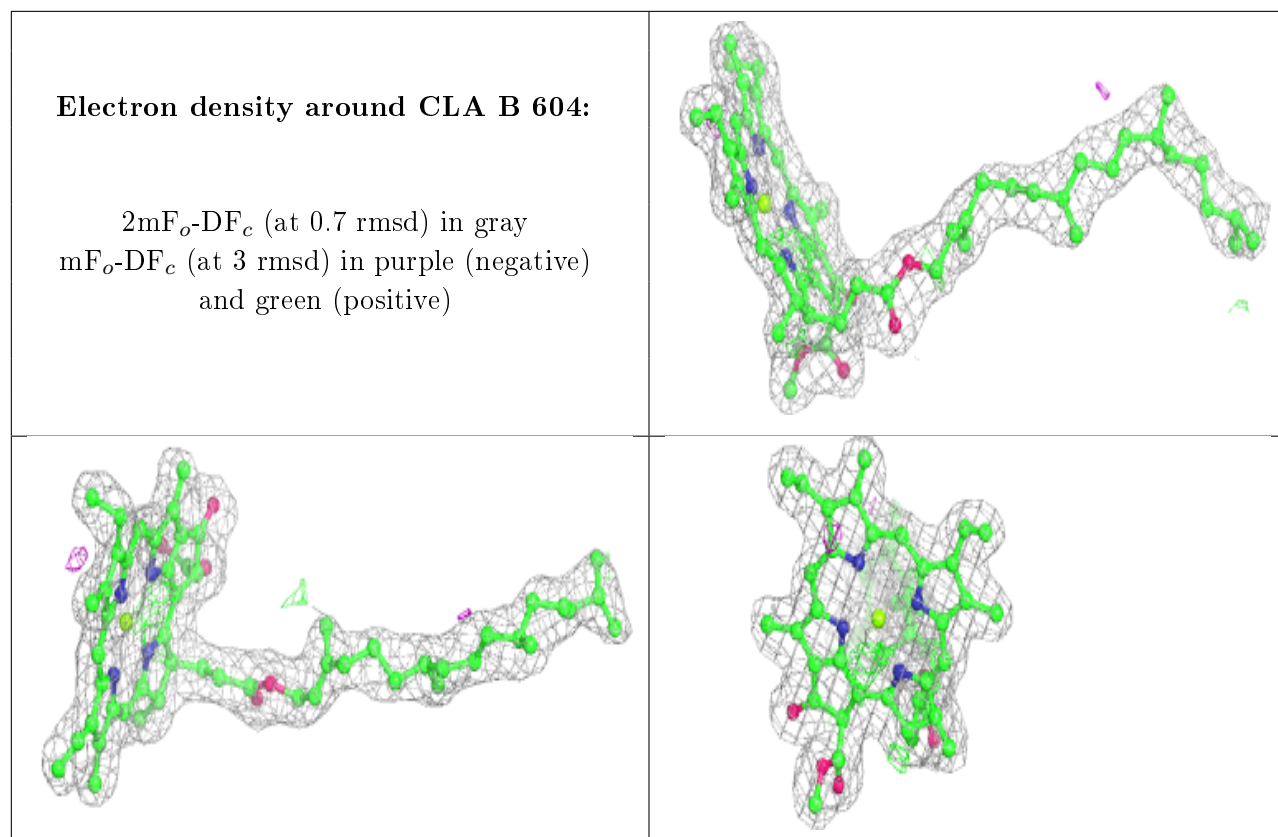
Electron density around BCR b 620:

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

**Electron density around CLA b 607:**

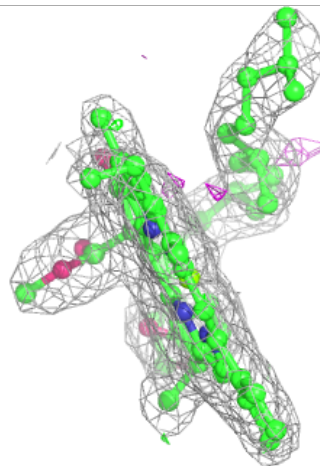
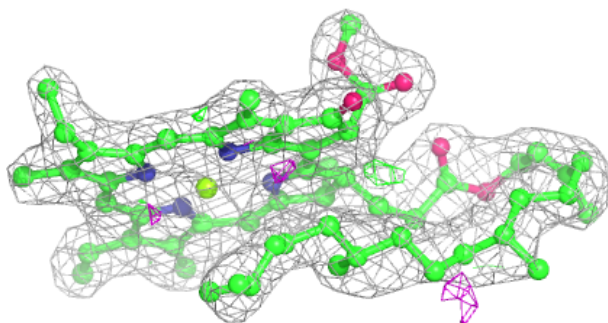
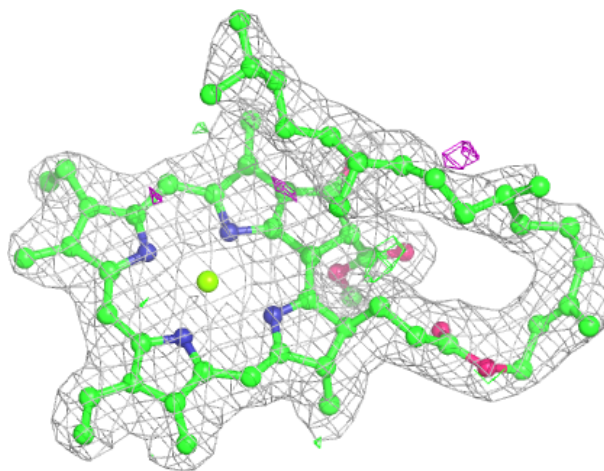
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





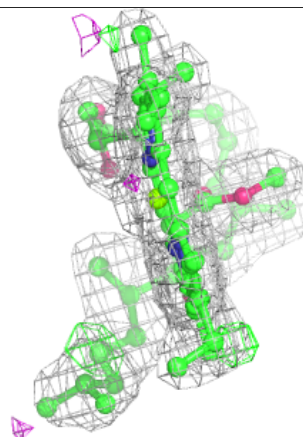
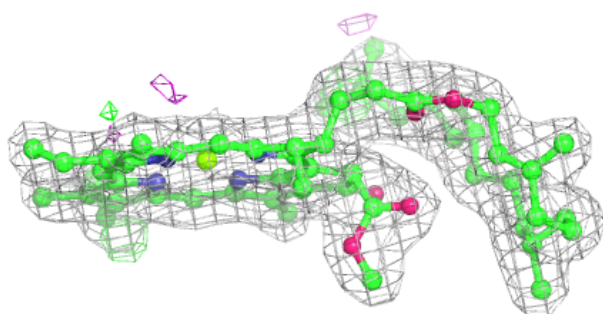
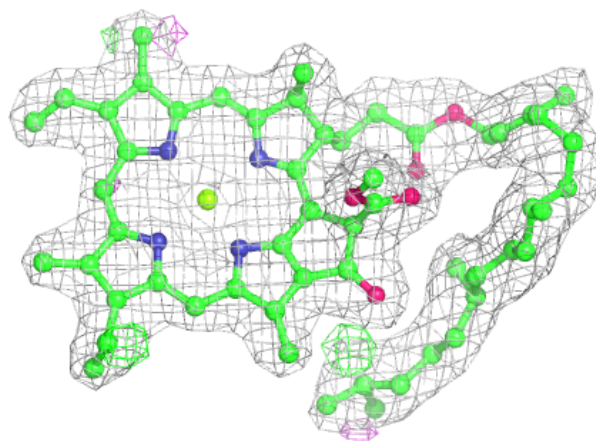
Electron density around CLA c 509:

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

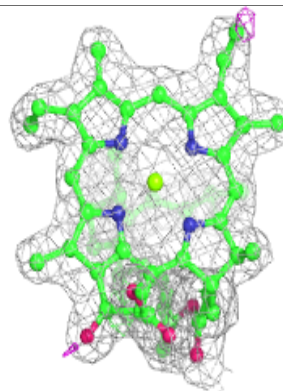
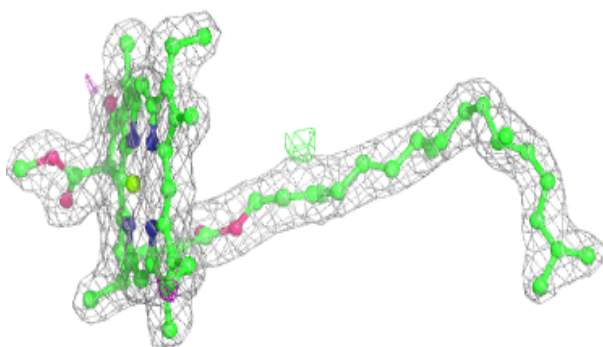
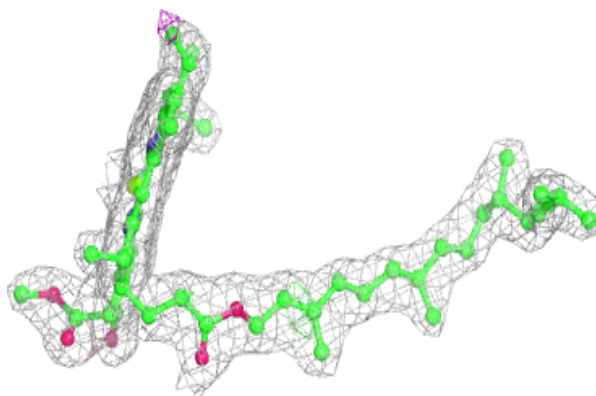


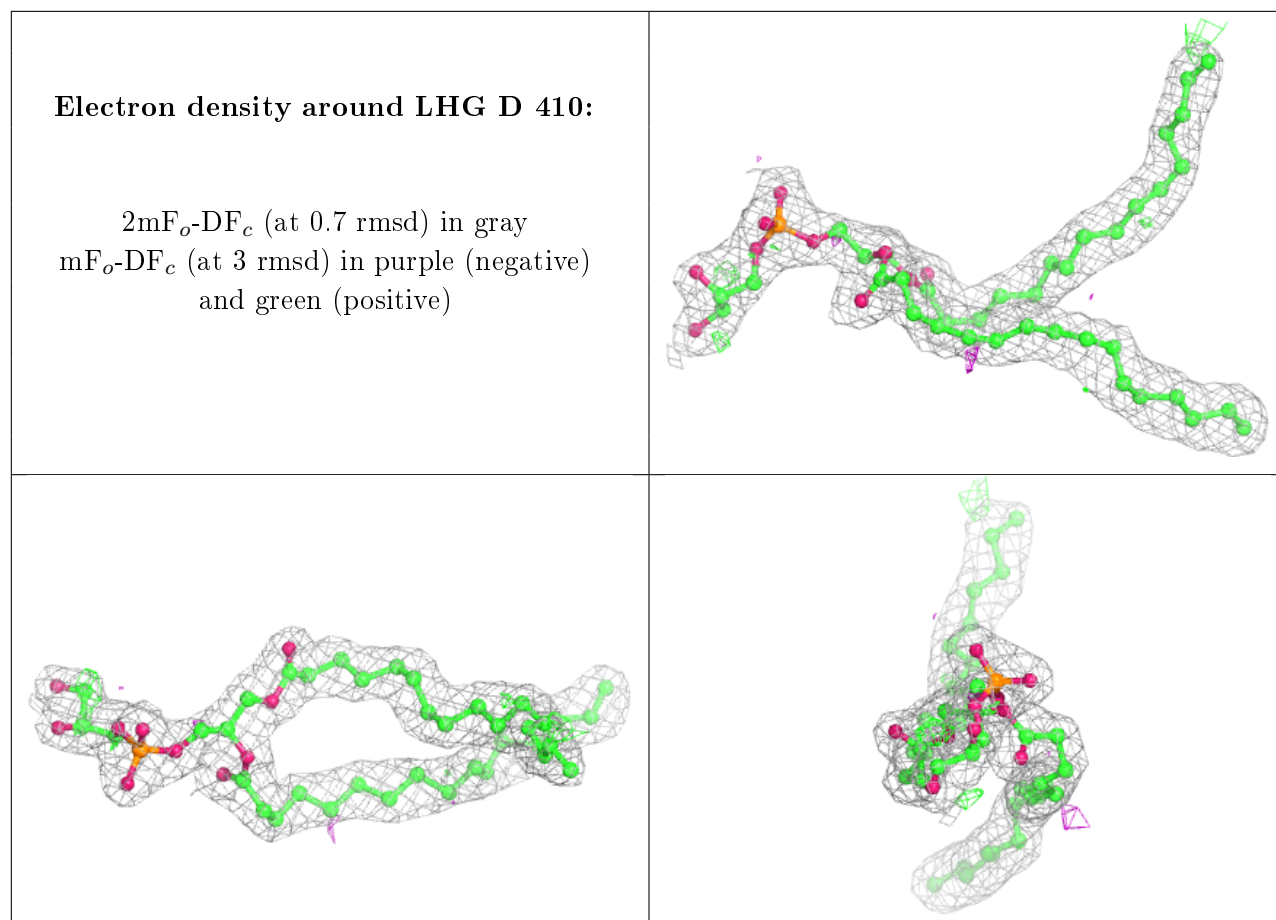
Electron density around CLA B 610:

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

**Electron density around CLA b 608:**

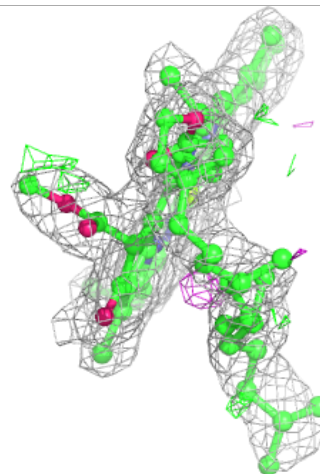
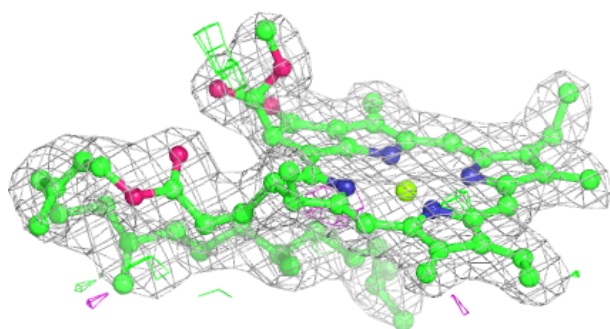
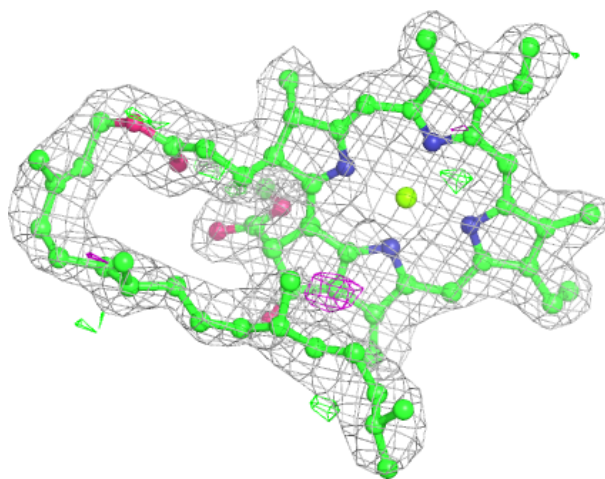
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





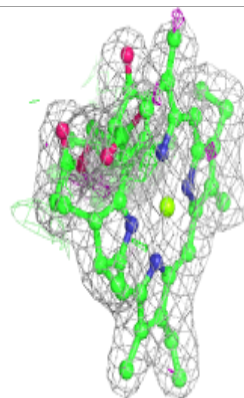
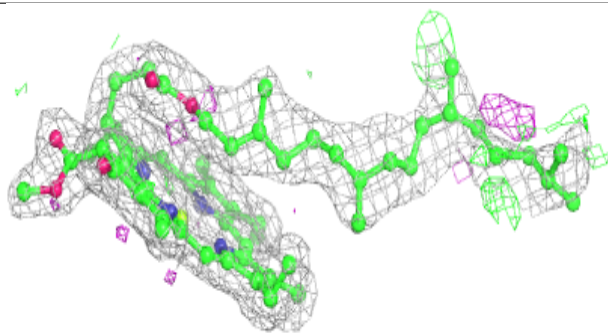
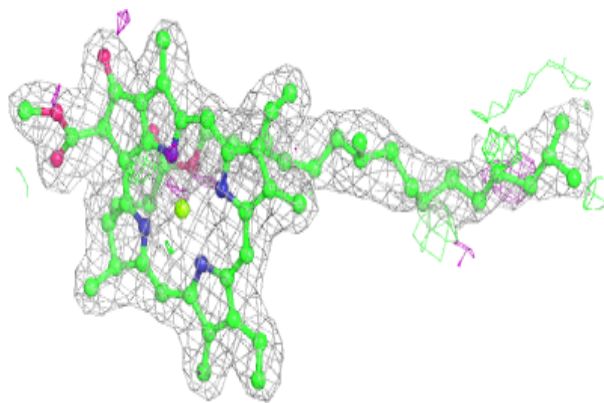
Electron density around CLA C 509:

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

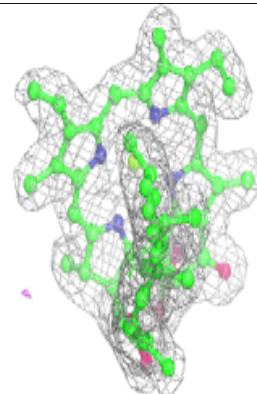
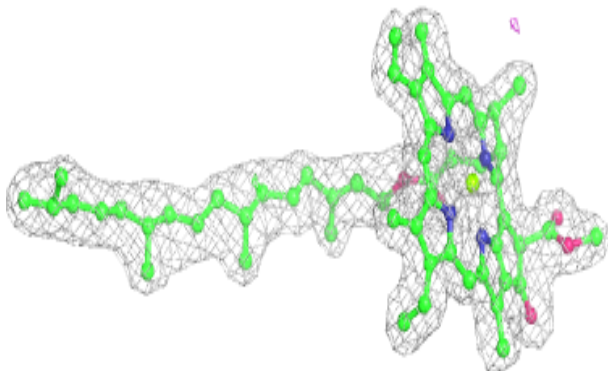
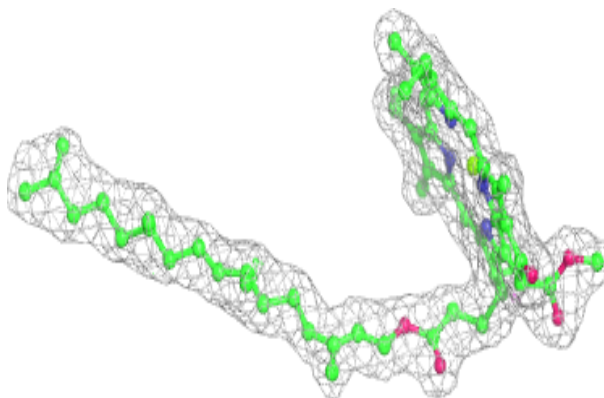


Electron density around CLA b 617:

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

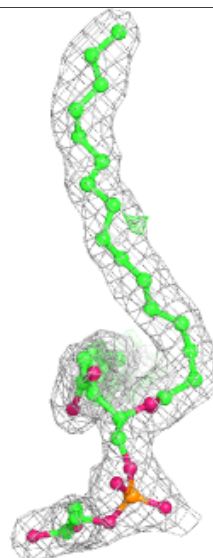
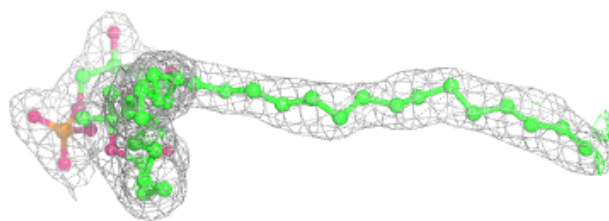
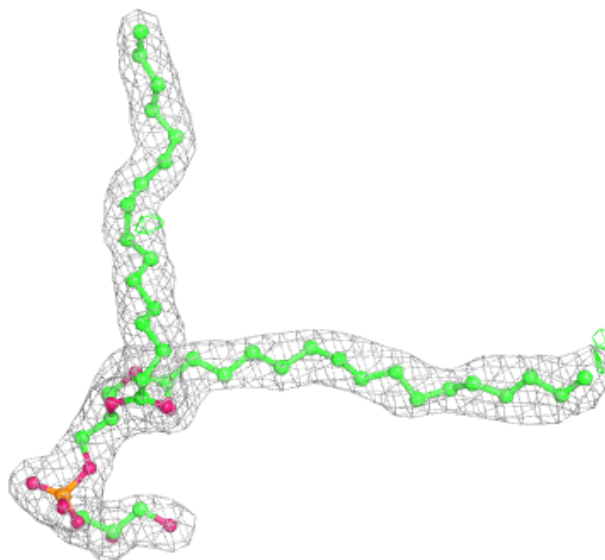
**Electron density around CLA B 607:**

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



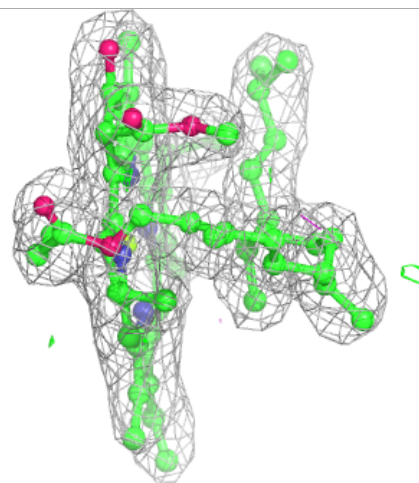
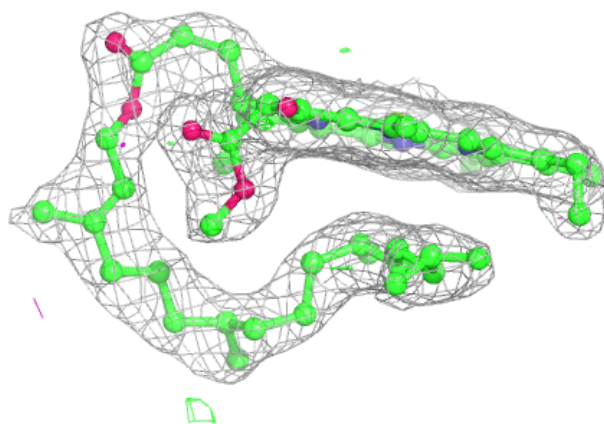
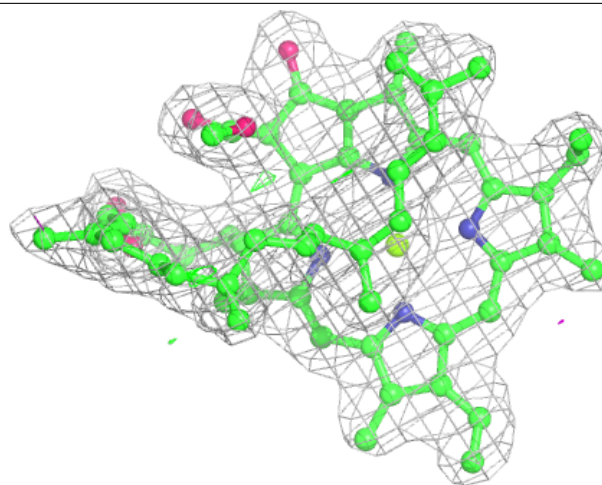
Electron density around LHG b 624:

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



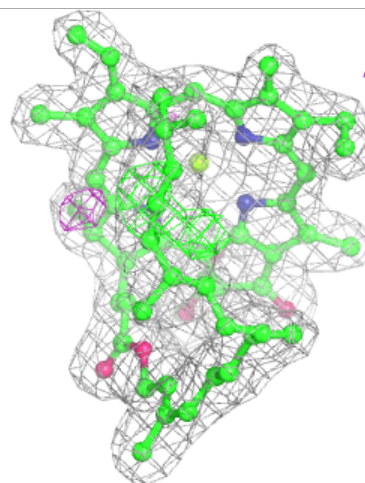
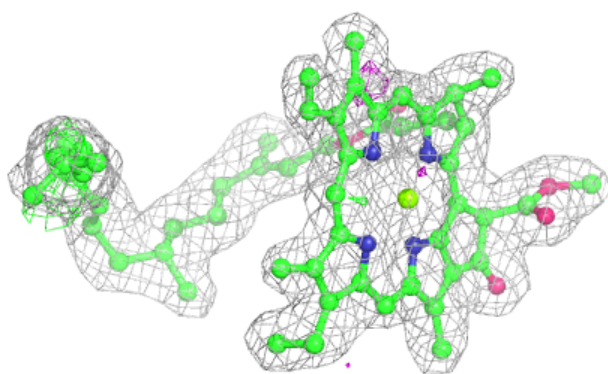
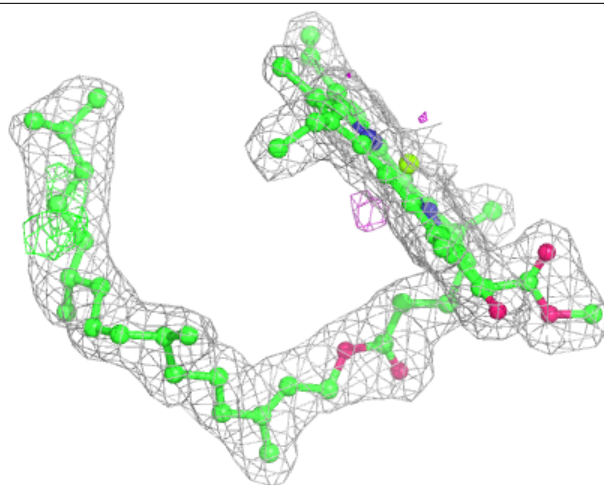
Electron density around CLA c 510:

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



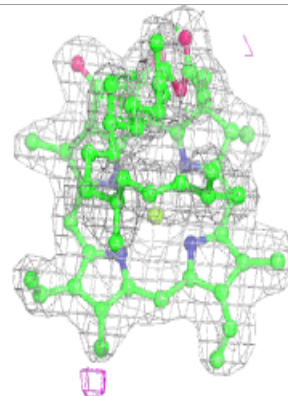
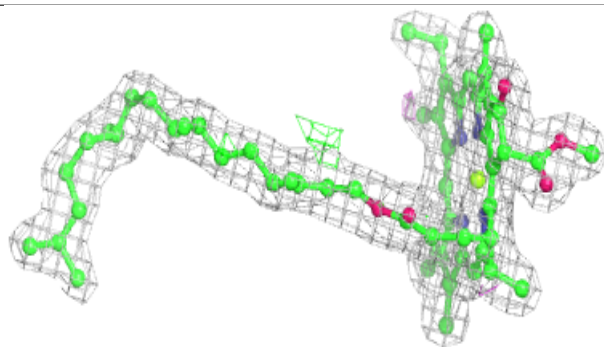
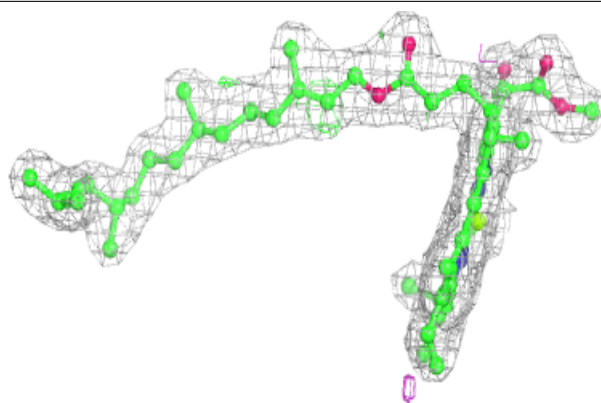
Electron density around CLA b 614:

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

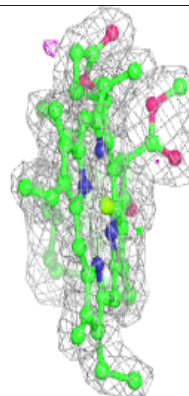
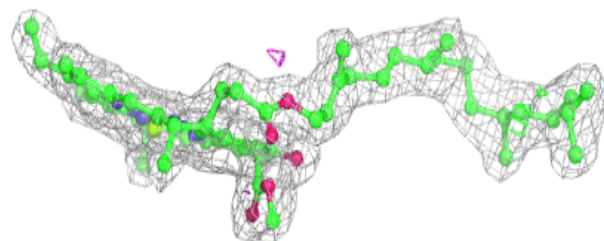
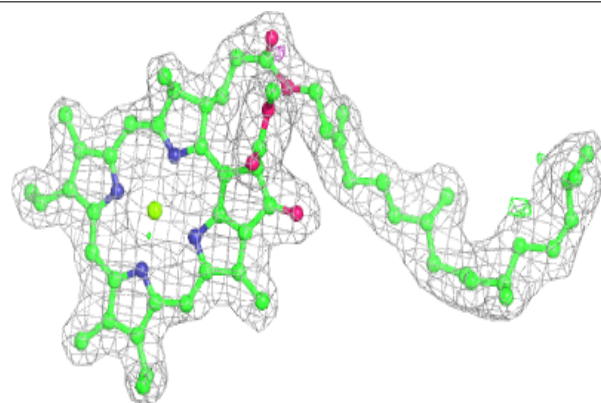


Electron density around CLA B 605:

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

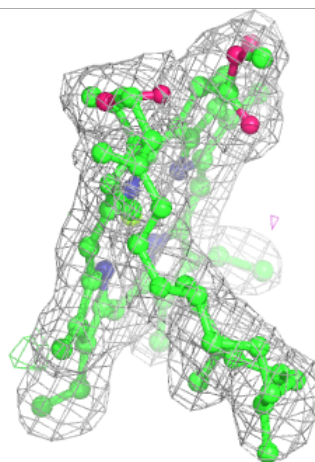
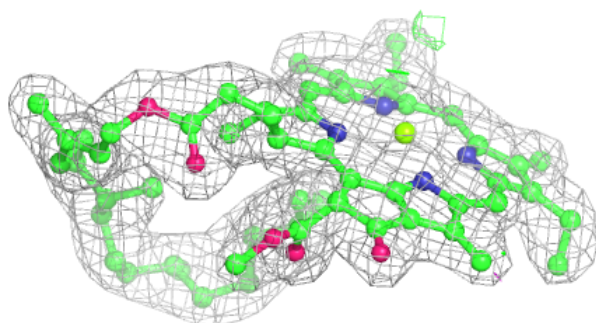
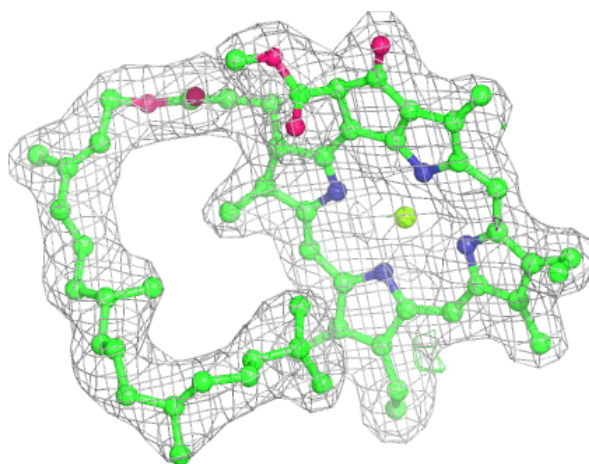
**Electron density around CLA B 602:**

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



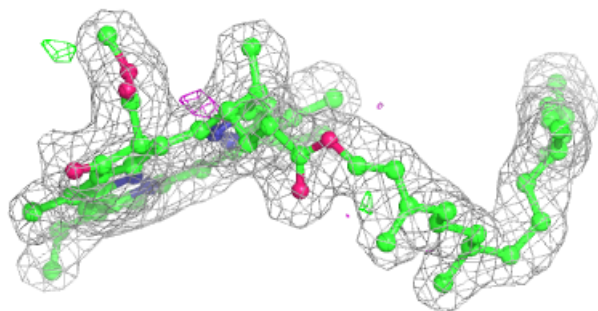
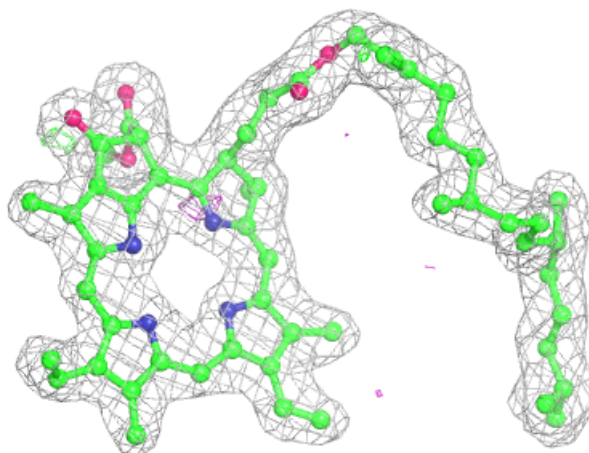
Electron density around CLA b 618:

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



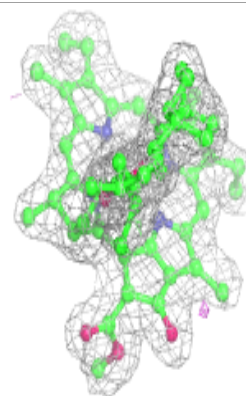
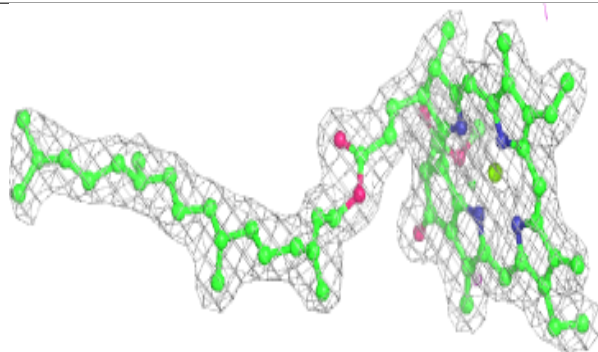
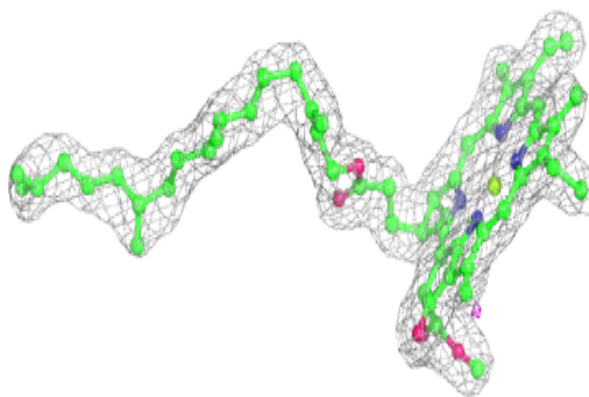
Electron density around PHO D 404:

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

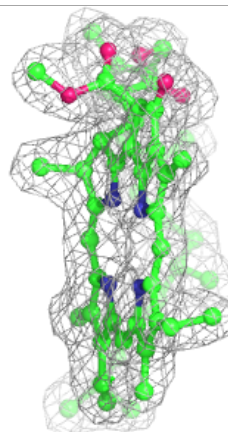
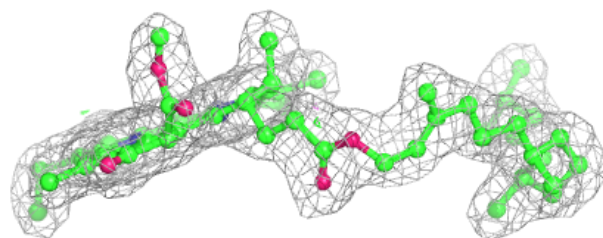
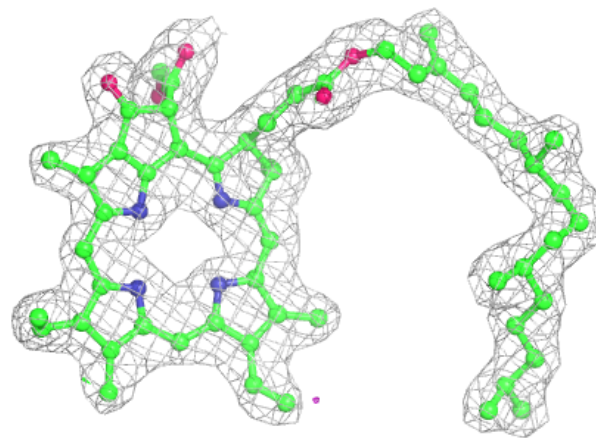


Electron density around CLA C 502:

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

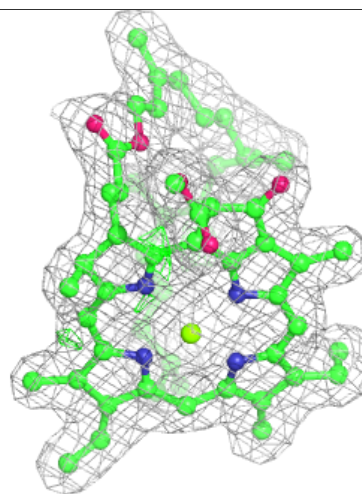
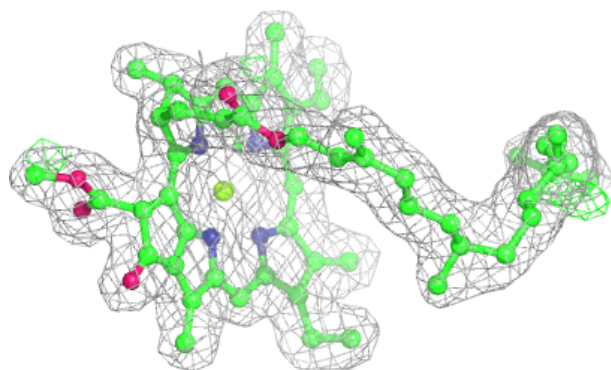
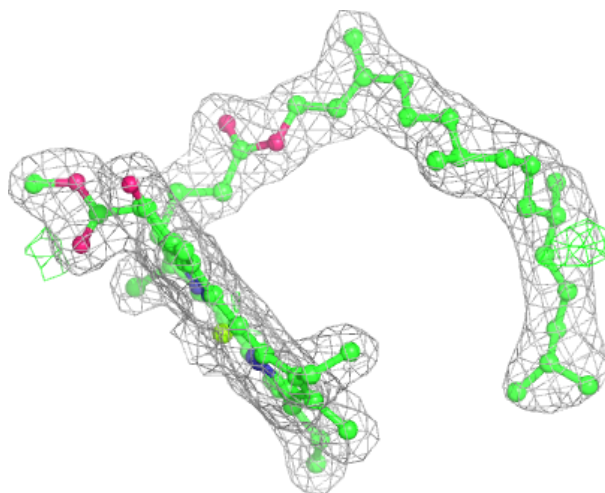
**Electron density around PHO a 410:**

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



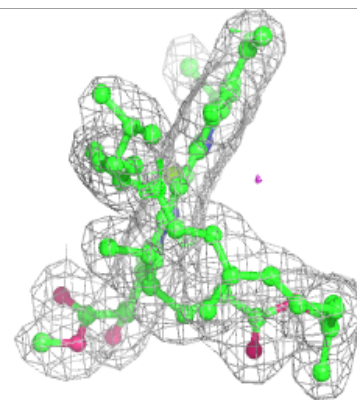
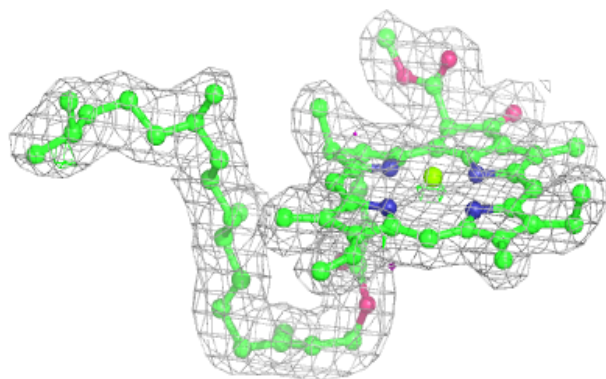
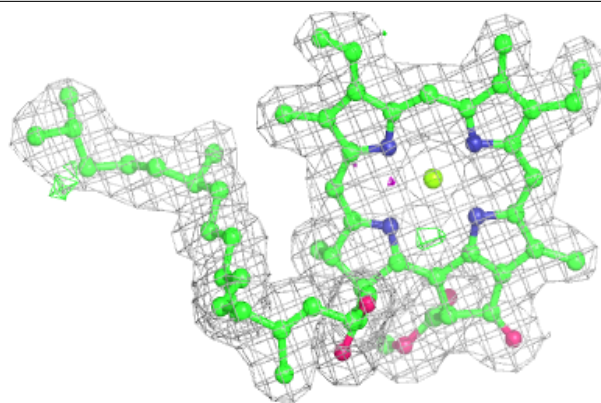
Electron density around CLA B 611:

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



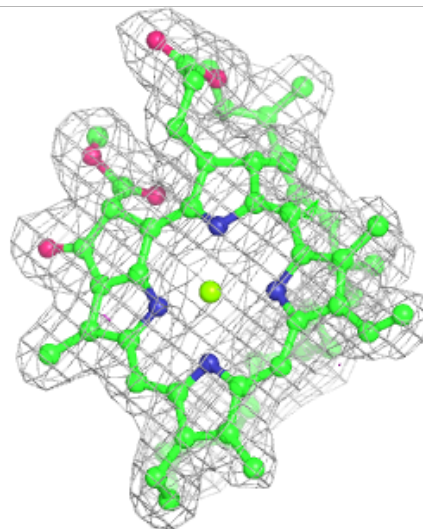
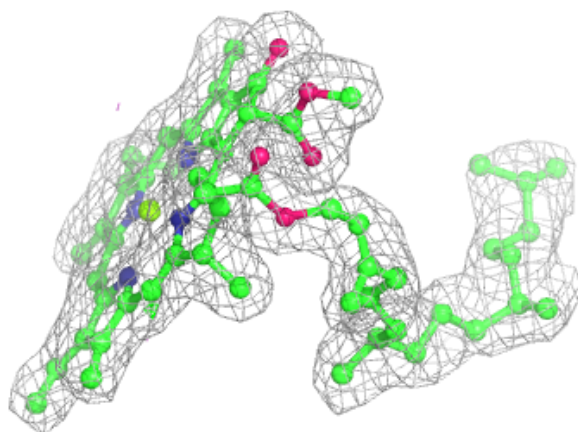
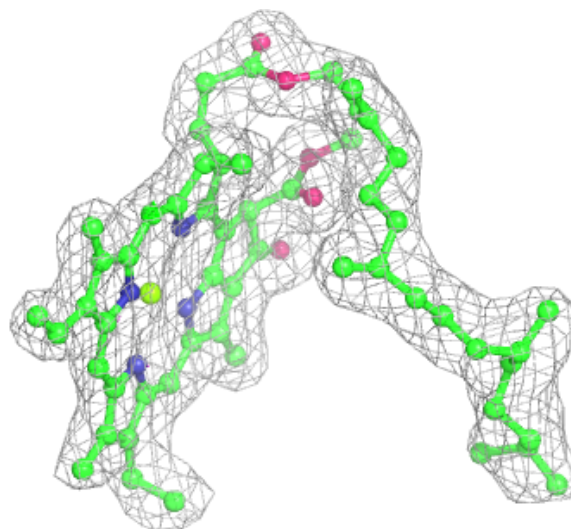
Electron density around CLA a 408:

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



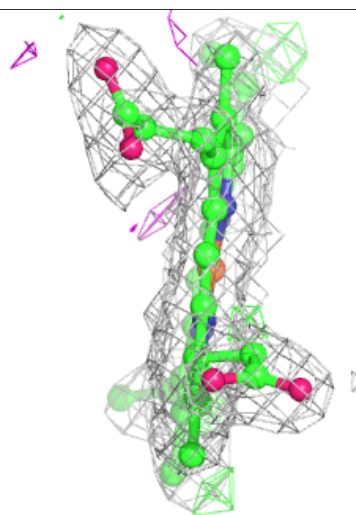
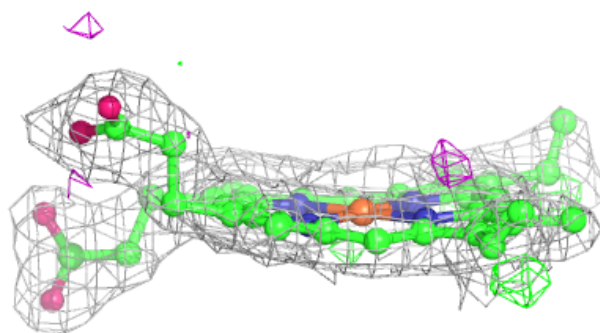
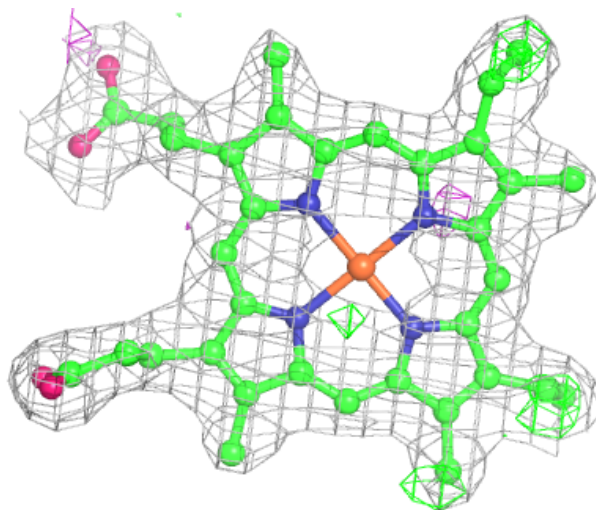
Electron density around CLA B 613:

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



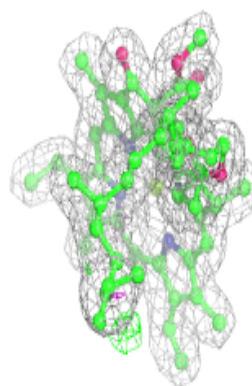
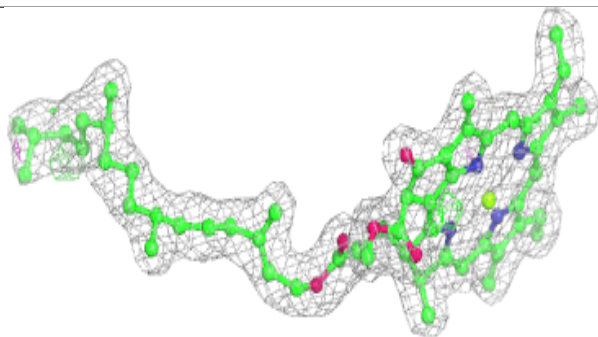
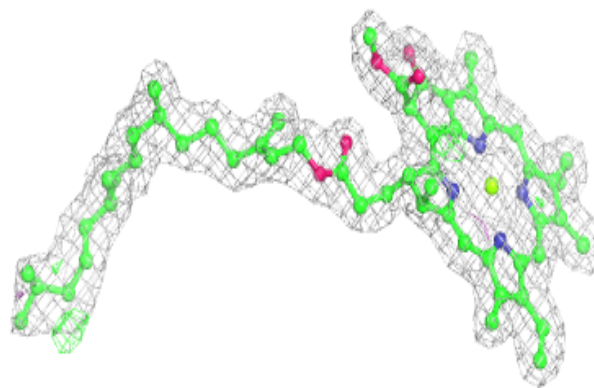
Electron density around HEM v 201:

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

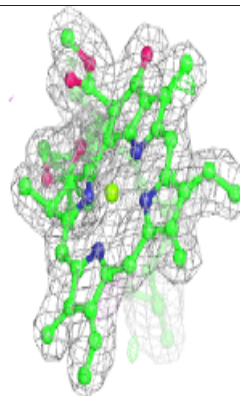
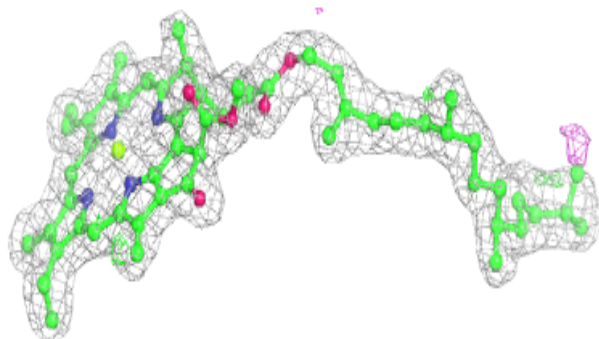
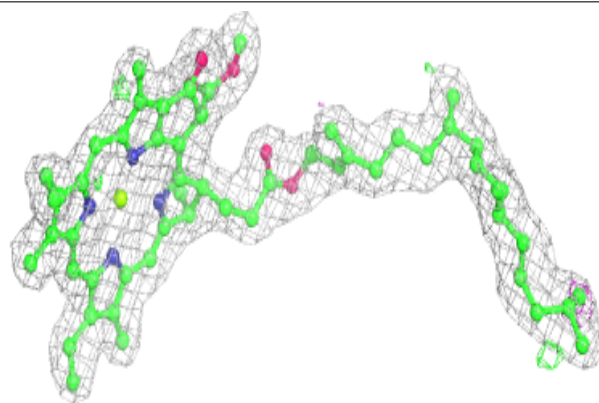


Electron density around CLA A 1005:

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

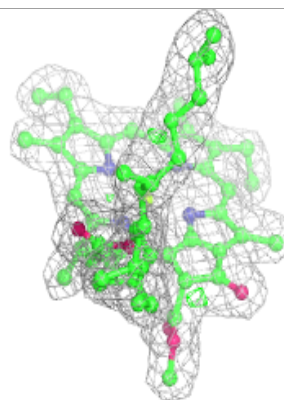
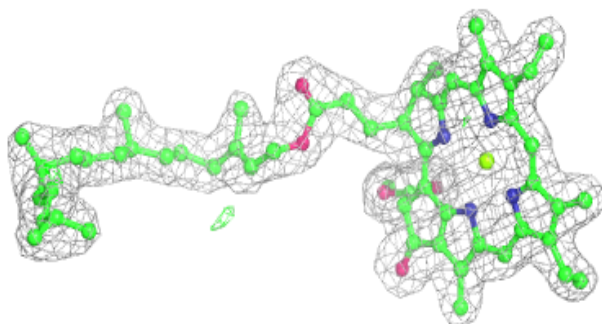
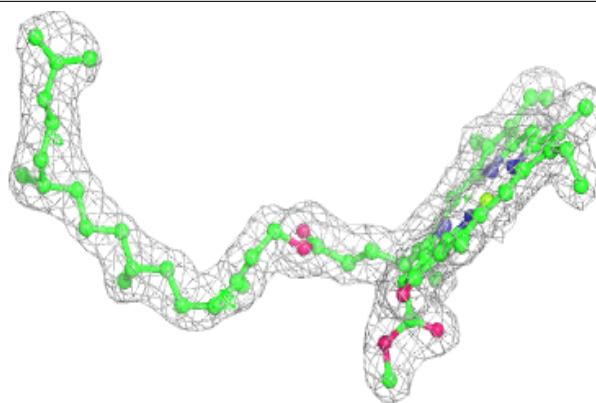
**Electron density around CLA a 407:**

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

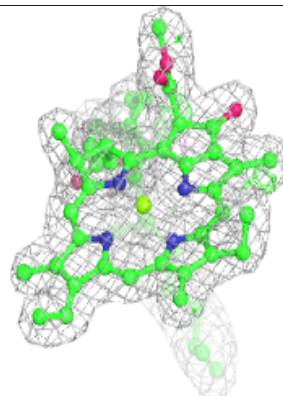
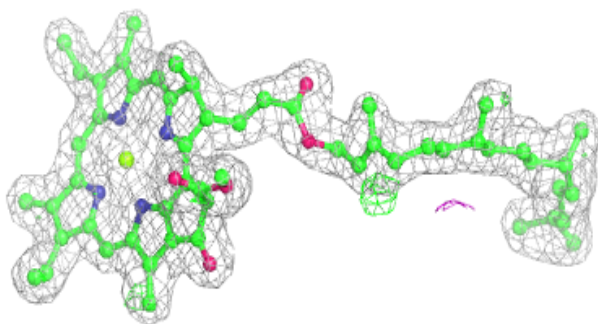
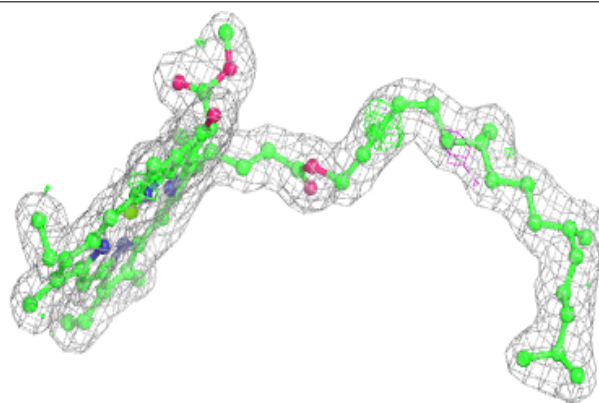


Electron density around CLA d 402:

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

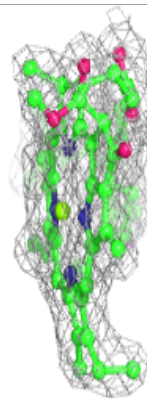
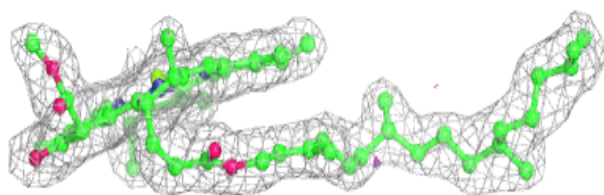
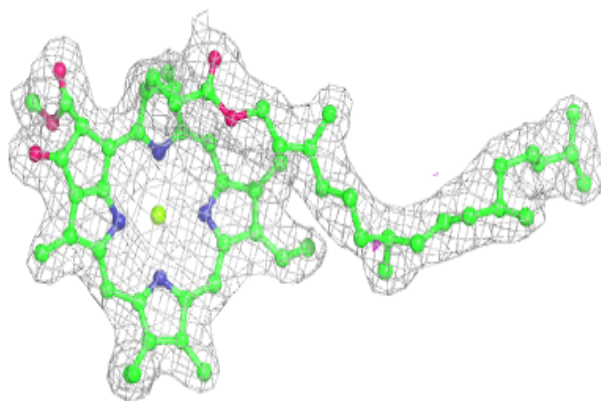
**Electron density around CLA D 402:**

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

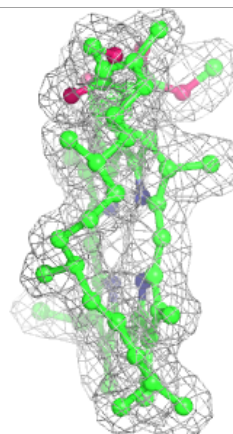
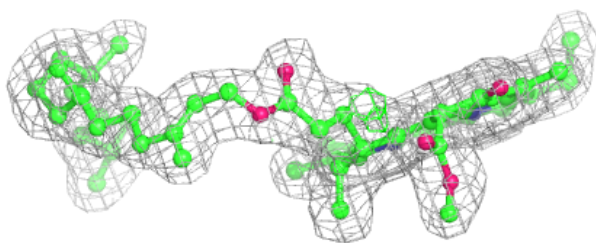
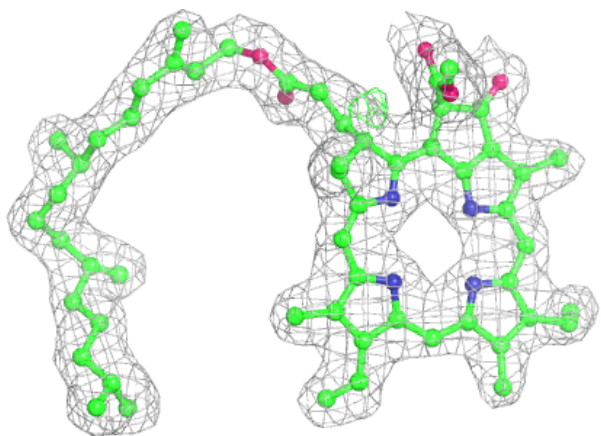


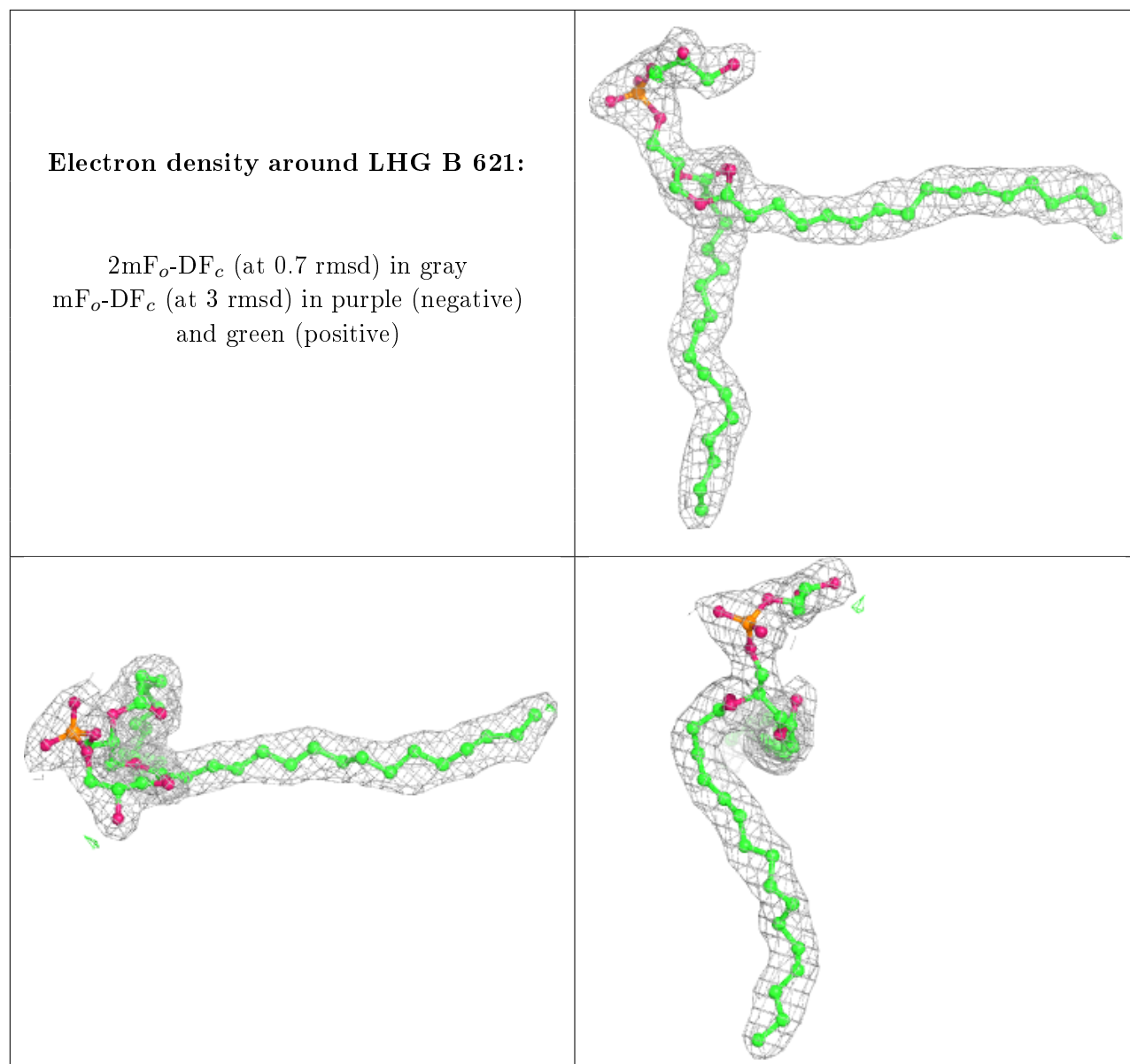
Electron density around CLA b 606:

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

**Electron density around PHO A 1007:**

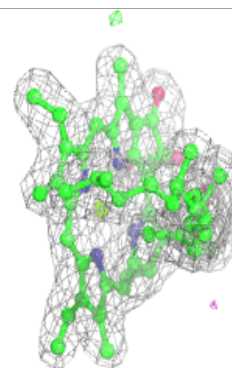
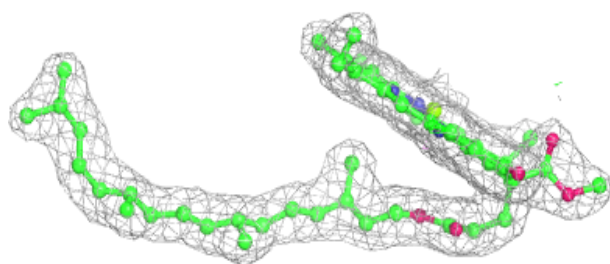
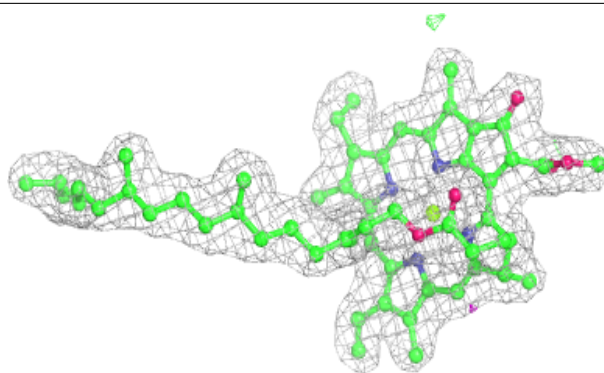
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



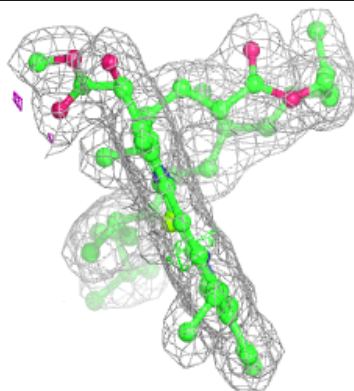
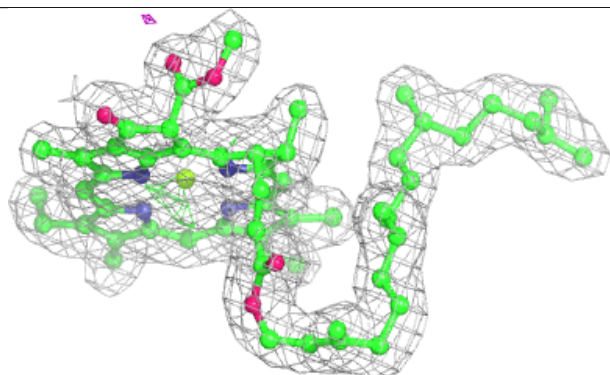
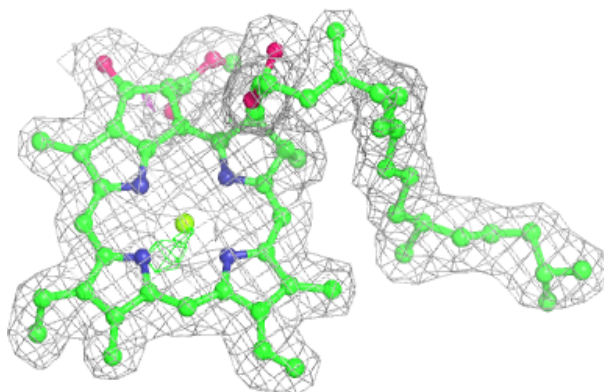


Electron density around CLA B 608:

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

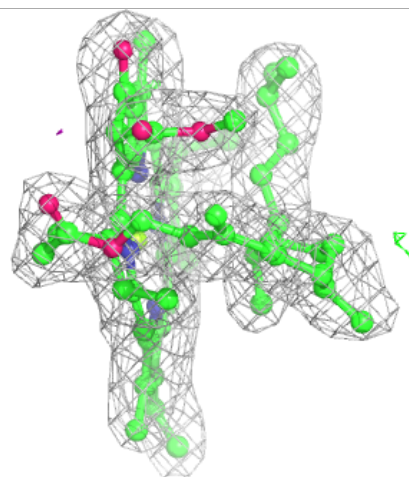
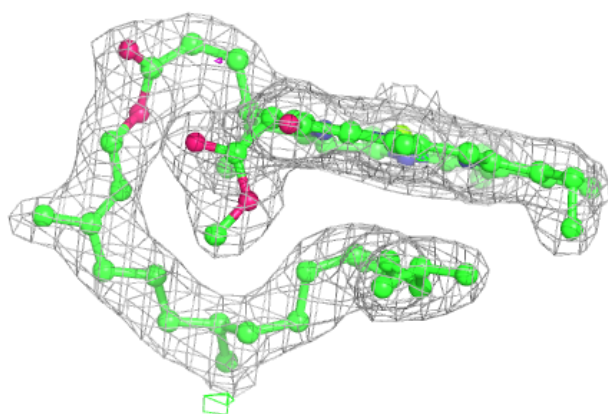
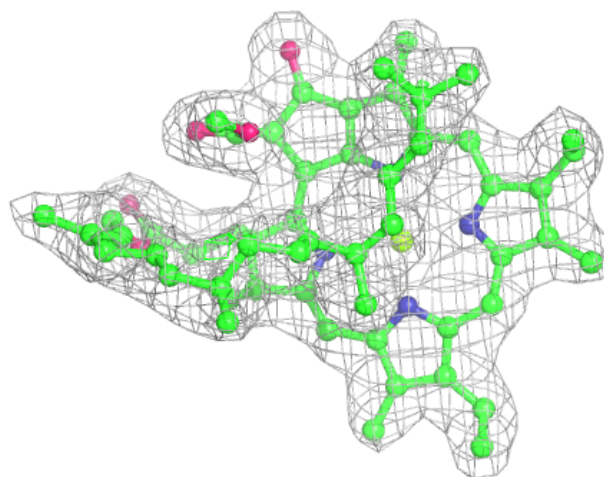
**Electron density around CLA D 403:**

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



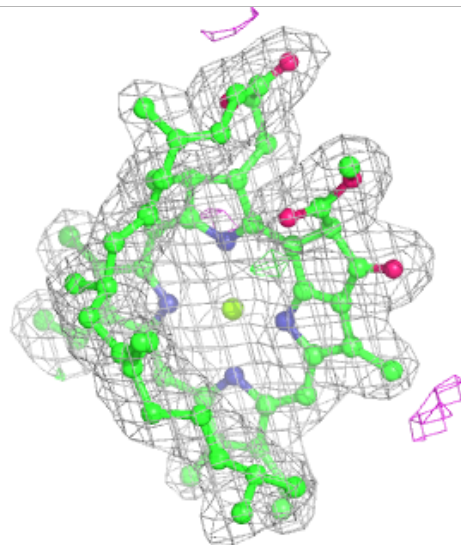
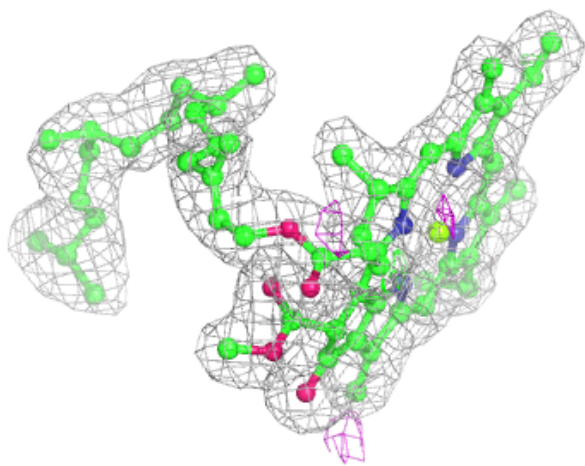
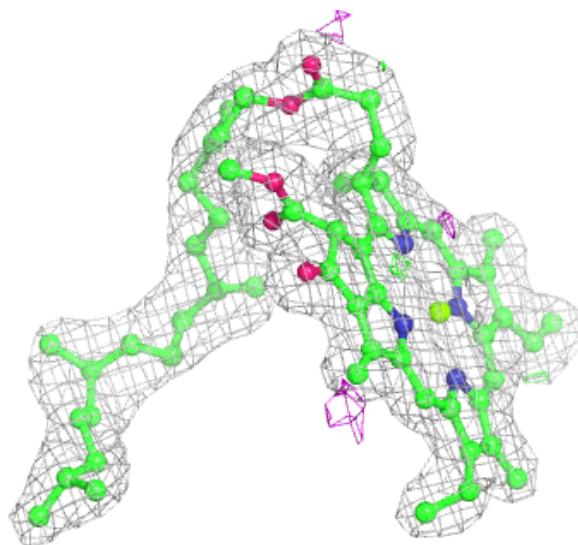
Electron density around CLA C 510:

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



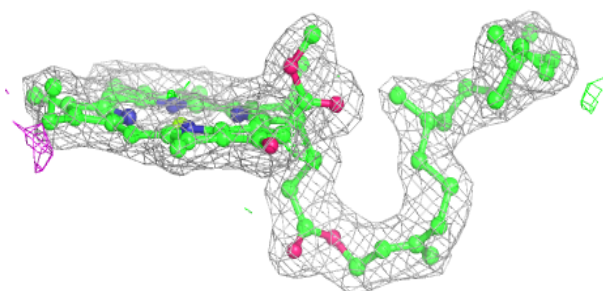
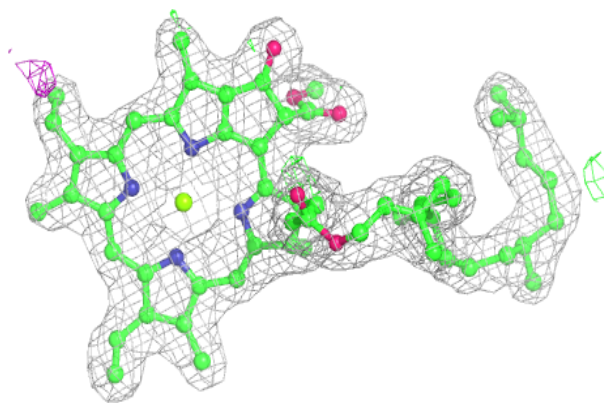
Electron density around CLA b 616:

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

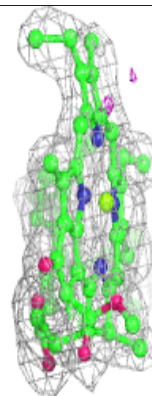
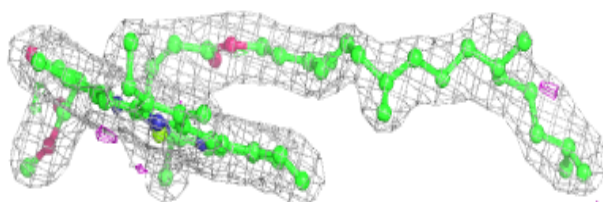
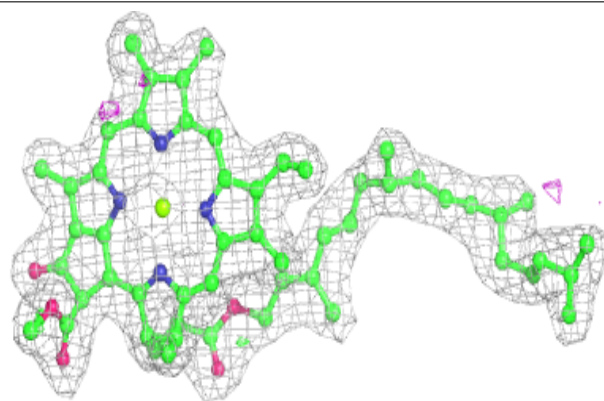


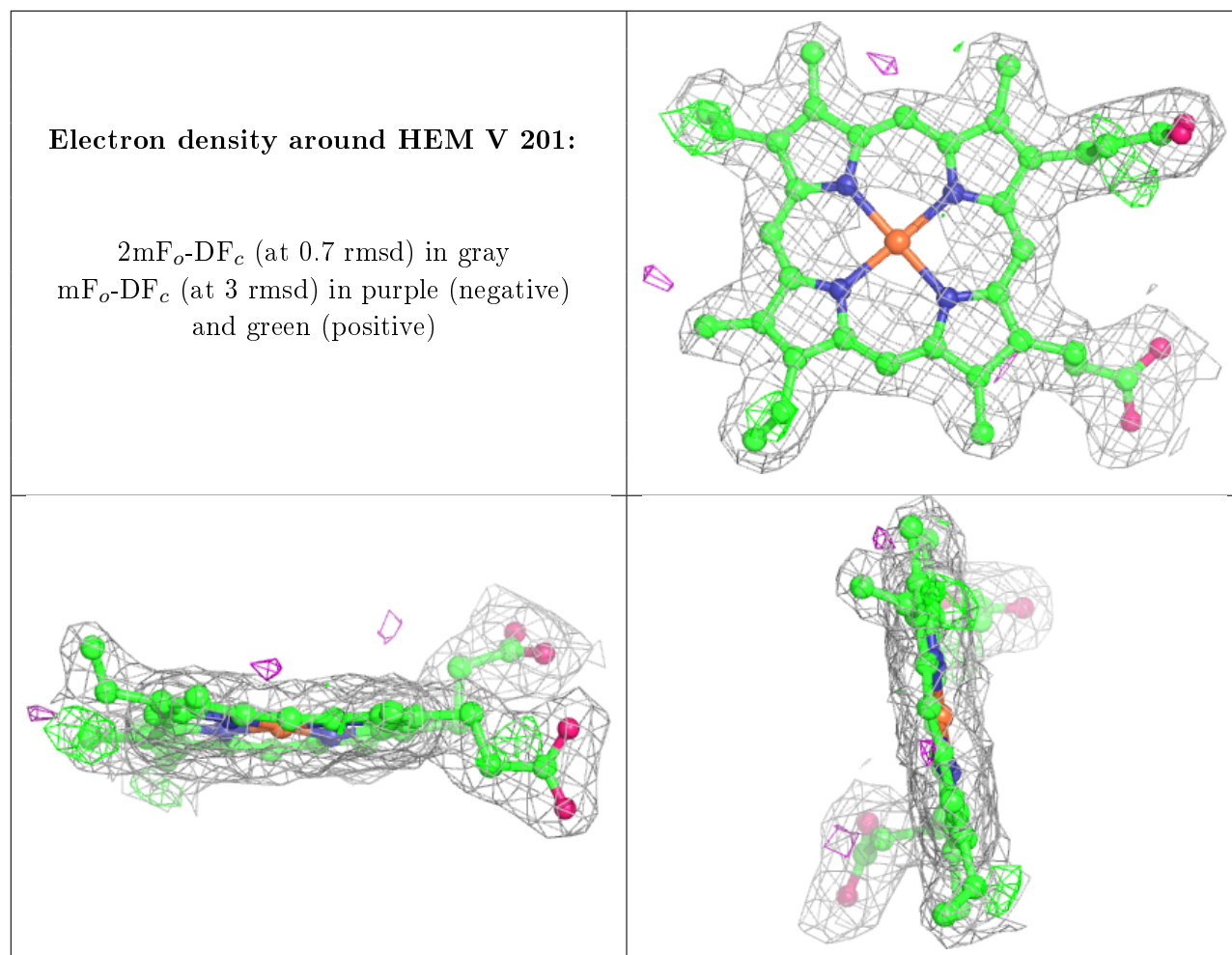
Electron density around CLA B 612:

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

**Electron density around CLA 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.