



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2025 – 03:20 AM EDT

PDB ID : 8EZ5 / pdb_00008ez5
Title : RT XFEL structure of the two-flash state of Photosystem II (2F, S3-rich) at 2.09 Angstrom resolution
Authors : Bhowmick, A.; Hussein, R.; Bogacz, I.; Simon, P.S.; Ibrahim, M.; Chatterjee, R.; Doyle, M.D.; Cheah, M.H.; Fransson, T.; Chernev, P.; Kim, I.-S.; Makita, H.; Dasgupta, M.; Kaminsky, C.J.; Zhang, M.; Gatcke, J.; Haupt, S.; Nangca, I.I.; Keable, S.M.; Aydin, O.; Tono, K.; Owada, S.; Gee, L.B.; Fuller, F.D.; Batyuk, A.; Alonso-Mori, R.; Holton, J.M.; Paley, D.W.; Moriarty, N.W.; Mamedov, F.; Adams, P.D.; Brewster, A.S.; Dobbek, H.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yano, J.; Yachandra, V.K.
Deposited on : 2022-10-31
Resolution : 2.09 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0

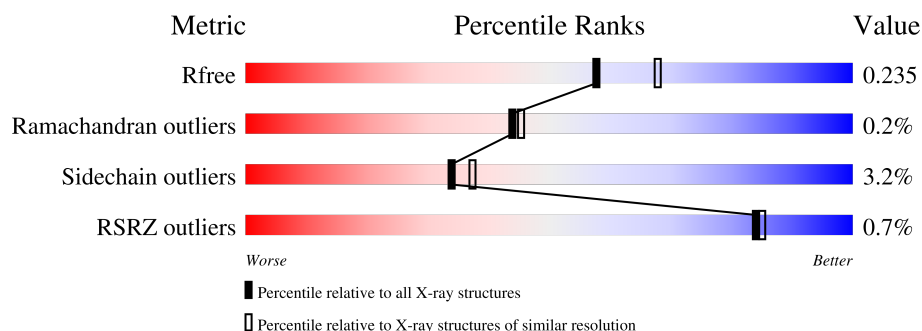
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	6234 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	

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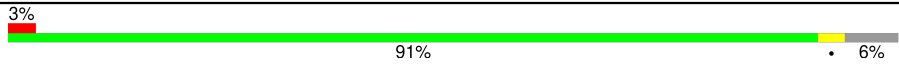



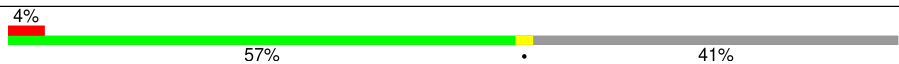

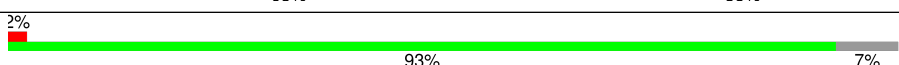
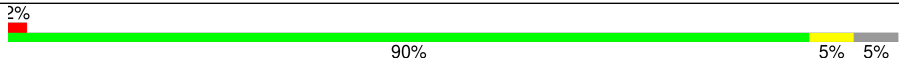
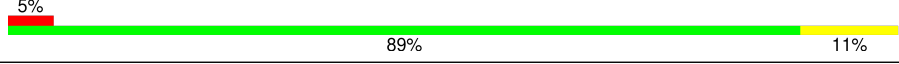
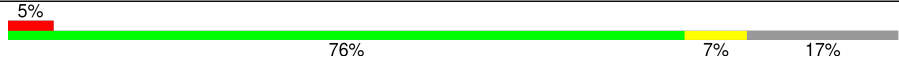
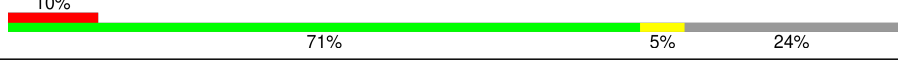
buster-report : 1.1.7 (2018)
 Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
 CCP4 : 9.0.006 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.42

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Mol	Chain	Length	Quality of chain
2	B	510	98% ..
2	b	510	97% ..
3	C	461	95% . .
3	c	461	95% . .
4	D	352	96% . .
4	d	352	95% . .
5	E	84	4% 95% . .
5	e	84	% 92% 6% .
6	F	45	2% 76% 24%
6	f	45	71% . 24%
7	H	66	3% 92% 6% .
7	h	66	2% 89% 6% 5%
8	I	38	87% 8% 5%
8	i	38	89% 5% 5%
9	J	40	90% 10%
9	j	40	2% 88% . 10%
10	K	46	78% . 20%
10	k	46	74% 7% 20%
11	L	37	97% .
11	l	37	89% 8% .
12	M	36	83% 8% 8%
12	m	36	78% 11% 11%
13	O	272	% 86% . 10%
13	o	272	86% . 10%
14	T	32	3% 91% . 6%

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Mol	Chain	Length	Quality of chain
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

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
25	CLA	A	606	X	-	-	-
25	CLA	A	609	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	D	404	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	609	X	-	-	-
25	CLA	a	612	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	d	404	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 53041 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	64	0
			3113	2030	513	551	19			
1	a	334	Total	C	N	O	S	0	64	0
			3110	2027	513	551	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	4	0
			4005	2631	666	695	13			
2	b	505	Total	C	N	O	S	0	0	0
			3978	2610	665	690	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	442	Total	C	N	O	S	0	11	0
			3509	2302	586	607	14			
3	c	451	Total	C	N	O	S	0	12	0
			3583	2343	602	624	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	2	0
			2731	1809	446	464	12			
4	d	341	Total	C	N	O	S	0	3	0
			2737	1813	446	466	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	1	0
			666	436	107	123			
5	e	82	Total	C	N	O	0	0	0
			664	434	108	122			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			510	341	82	85	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			257	174	40	42	1			
9	j	36	Total	C	N	O	S	0	0	0
			257	174	40	42	1			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	l	36	Total	C	N	O		0	0	0
			296	197	47	52				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	0	0
			256	171	37	47	1			
12	m	32	Total	C	N	O	S	0	0	0
			251	168	36	46	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	1	0
			1870	1168	313	385	4			
13	o	244	Total	C	N	O	S	0	0	0
			1874	1170	317	383	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0	0
			196	128	35	30	3			
17	y	30	Total	C	N	O	S	0	0	0
			218	144	35	36	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O		0	0	0
			281	188	45	48				
18	x	39	Total	C	N	O		0	0	0
			286	191	46	49				

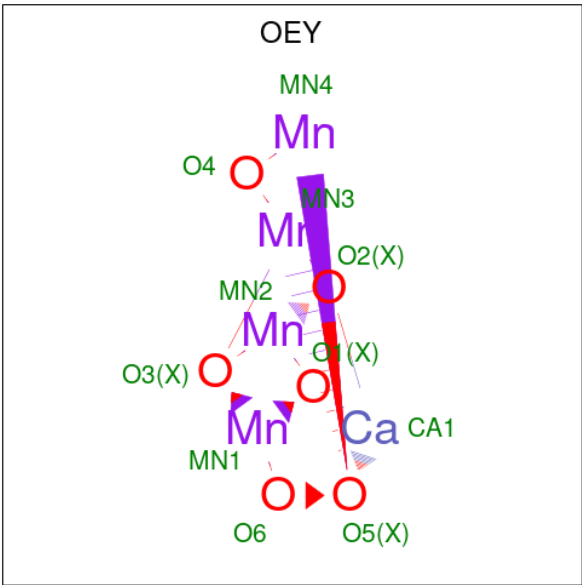
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			477	326	72	77	2			

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

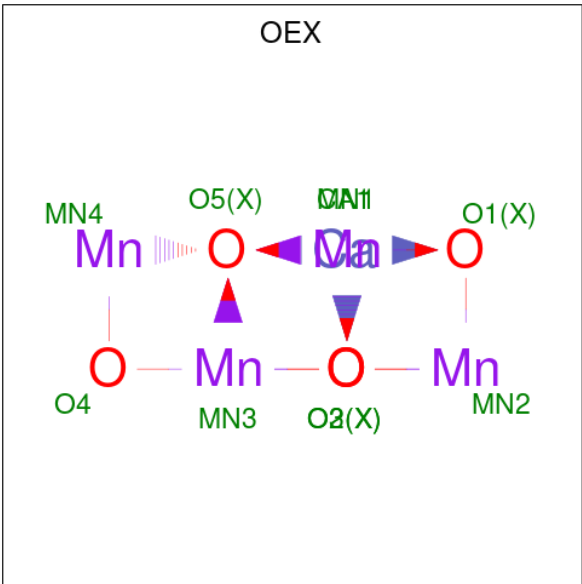
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O		0	0	0
			271	184	47	40				
20	r	31	Total	C	N	O		0	0	0
			246	166	43	37				

- Molecule 21 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
21	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

- Molecule 22 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

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

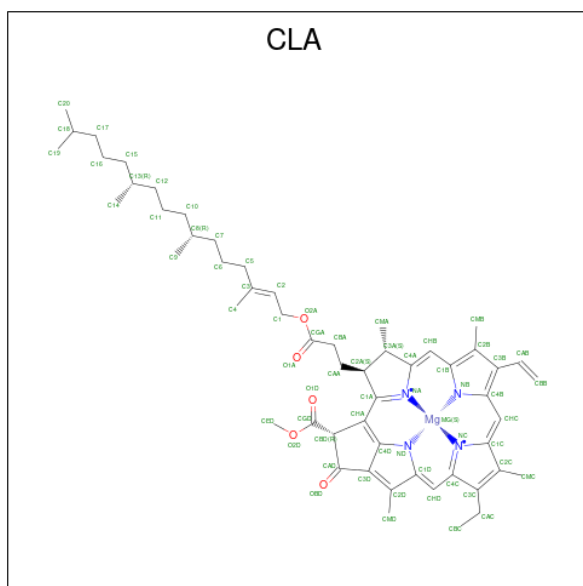
- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 24 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		

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

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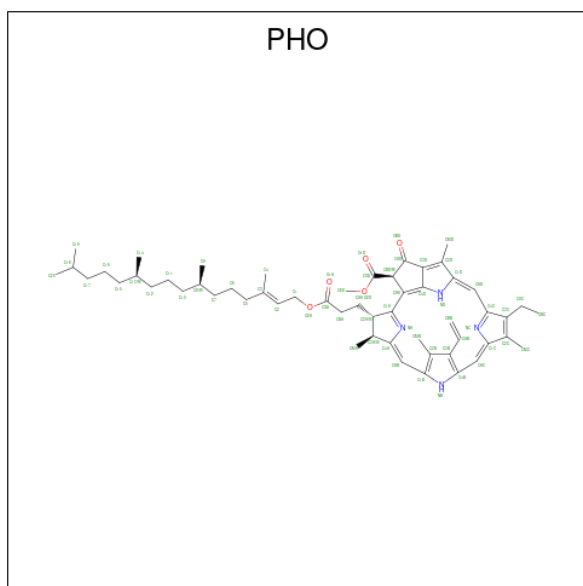
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 64	C 54	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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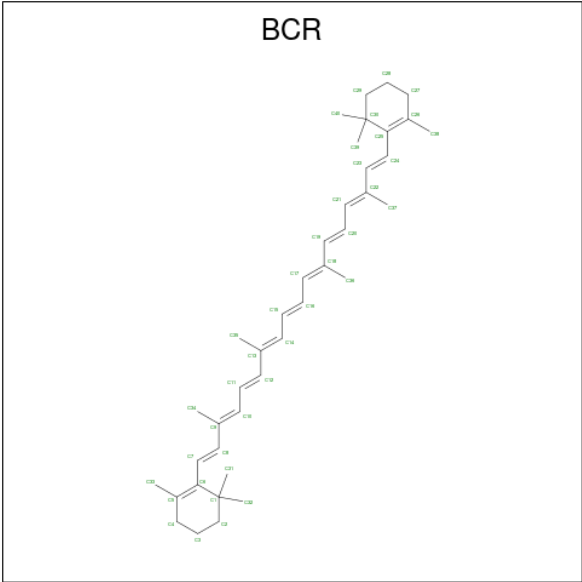
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 26 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



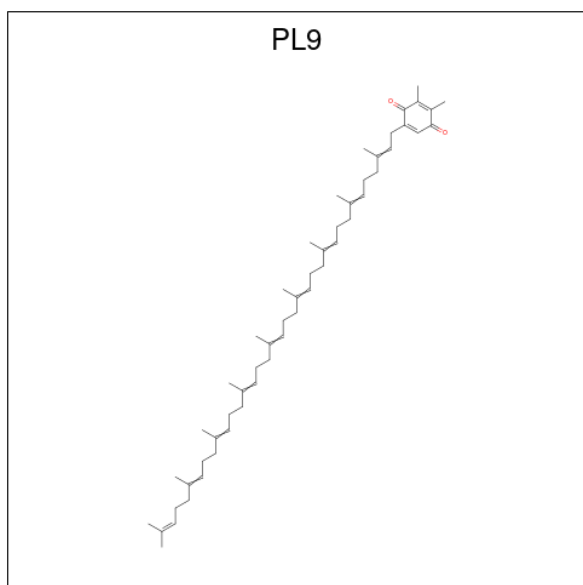
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	Y	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	d	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0
27	t	1	Total C 40 40	0	0
27	x	1	Total C 40 40	0	0

- Molecule 28 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 (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



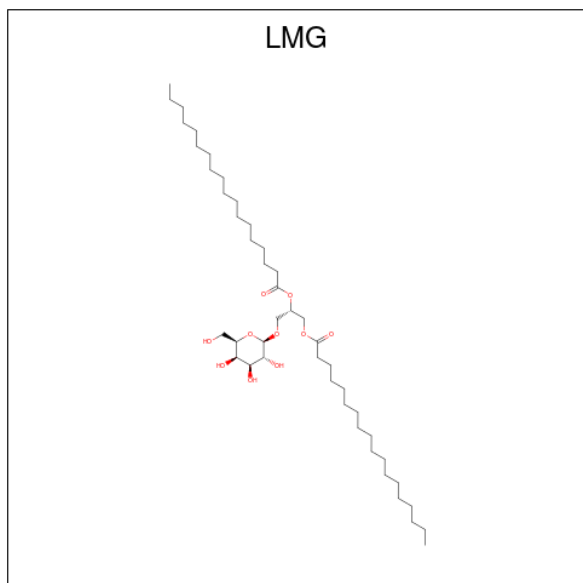
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 55 53 2	0	0
28	D	1	Total C O 55 53 2	0	0

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

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



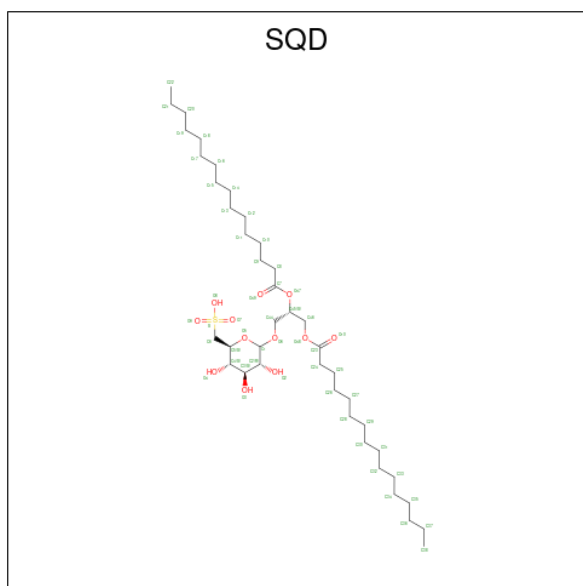
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			48	38	10		
29	B	1	Total	C	O	0	0
			28	24	4		
29	C	1	Total	C	O	0	0
			48	38	10		
29	D	1	Total	C	O	0	0
			51	41	10		
29	D	1	Total	C	O	0	0
			33	27	6		
29	M	1	Total	C	O	0	0
			51	41	10		
29	b	1	Total	C	O	0	0
			55	45	10		
29	c	1	Total	C	O	0	0
			37	27	10		
29	c	1	Total	C	O	0	0
			48	38	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	c	1	Total	C	O	0	0
			49	39	10		
29	d	1	Total	C	O	0	0
			23	21	2		
29	d	1	Total	C	O	0	0
			44	34	10		
29	m	1	Total	C	O	0	0
			51	41	10		

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



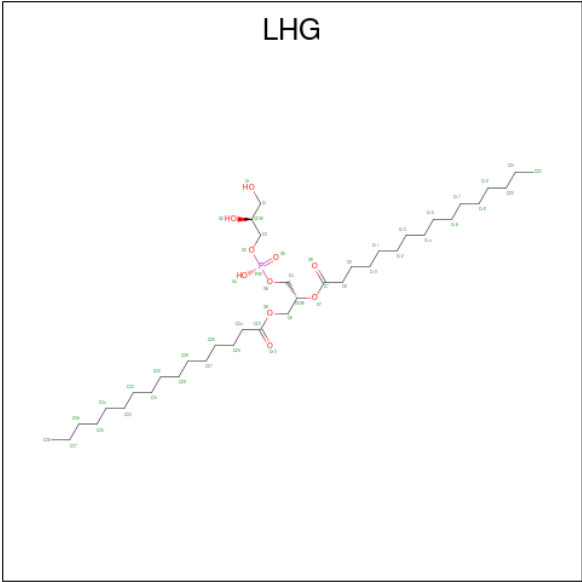
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			52	39	12	1		
30	A	1	Total	C	O		0	0
			39	35	4			
30	B	1	Total	C	O	S	0	0
			54	41	12	1		
30	F	1	Total	C	O	S	0	0
			36	25	10	1		
30	L	1	Total	C	O	S	0	0
			49	36	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O		0	0
			36	31	5			

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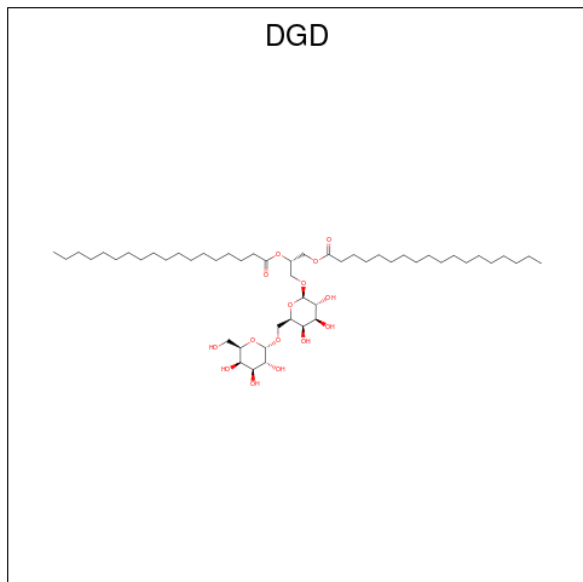
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	f	1	Total	C	O	S	0	0
			41	28	12	1		

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



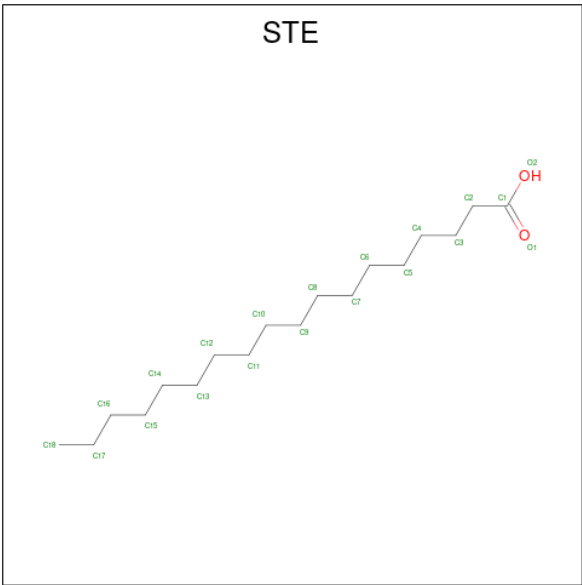
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			47	36	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			39	28	10	1		
31	e	1	Total	C	O	P	0	0
			42	31	10	1		
31	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			66	51	15		
32	C	1	Total	C	O	0	0
			62	47	15		
32	C	1	Total	C	O	0	0
			62	47	15		
32	C	1	Total	C	O	0	0
			62	47	15		
32	H	1	Total	C	O	0	0
			62	47	15		
32	a	1	Total	C	O	0	0
			44	39	5		
32	c	1	Total	C	O	0	0
			62	47	15		
32	c	1	Total	C	O	0	0
			62	47	15		
32	c	1	Total	C	O	0	0
			62	47	15		
32	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 33 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



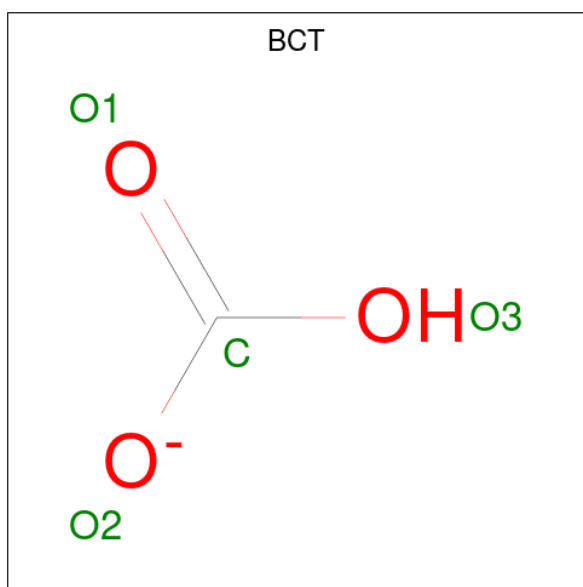
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			17	15	2		
33	B	1	Total	C	O	0	0
			12	10	2		
33	B	1	Total	C	O	0	0
			18	16	2		
33	B	1	Total	C	O	0	0
			12	10	2		
33	B	1	Total	C		0	0
			16	16			
33	C	1	Total	C	O	0	0
			12	10	2		
33	C	1	Total	C	O	0	0
			12	10	2		
33	C	1	Total	C		0	0
			16	16			
33	D	1	Total	C	O	0	0
			20	18	2		
33	E	1	Total	C	O	0	0
			12	10	2		
33	H	1	Total	C		0	0
			18	18			
33	I	1	Total	C		0	0
			15	15			
33	J	1	Total	C	O	0	0
			12	10	2		
33	M	1	Total	C	O	0	0
			15	13	2		

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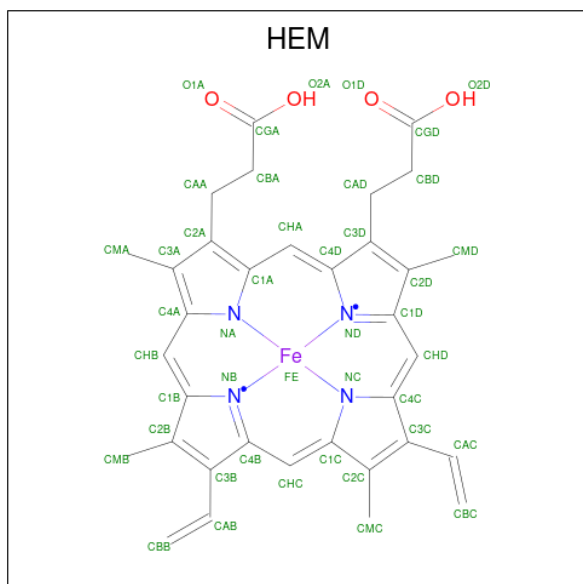
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	M	1	Total C 10 10	0	0
33	T	1	Total C 16 16	0	0
33	T	1	Total C 15 15	0	0
33	a	1	Total C 10 10	0	0
33	a	1	Total C O 12 10 2	0	0
33	b	1	Total C O 20 18 2	0	0
33	b	1	Total C O 20 18 2	0	0
33	b	1	Total C 10 10	0	0
33	c	1	Total C O 20 18 2	0	0
33	c	1	Total C O 12 10 2	0	0
33	d	1	Total C O 16 14 2	0	0
33	d	1	Total C O 17 15 2	0	0
33	j	1	Total C O 12 10 2	0	0
33	l	1	Total C 18 18	0	0
33	m	1	Total C O 12 10 2	0	0
33	t	1	Total C O 14 12 2	0	0
33	x	1	Total C O 20 18 2	0	0

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	D	1	Total	C	O	0	0
			4	1	3		
34	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



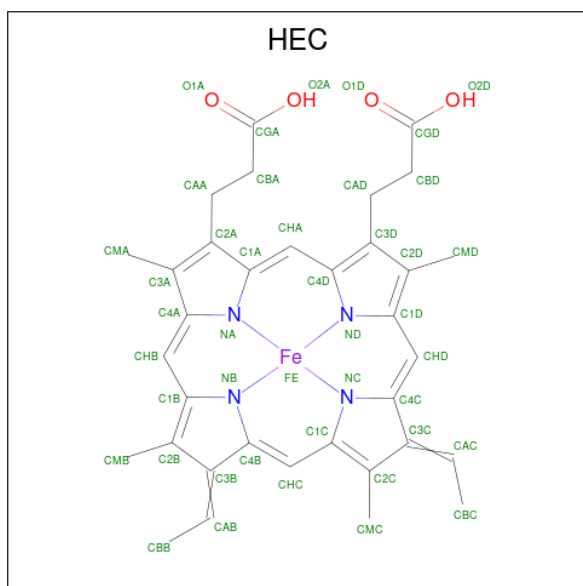
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
35	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
35	f	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 36 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	119	Total	O	0	4
			123	123		
37	B	197	Total	O	0	0
			197	197		
37	C	142	Total	O	0	0
			142	142		
37	D	106	Total	O	0	0
			106	106		
37	E	29	Total	O	0	0
			29	29		
37	F	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	H	27	Total 27	O 27	0	0
37	I	13	Total 13	O 13	0	0
37	J	12	Total 12	O 12	0	0
37	K	2	Total 2	O 2	0	0
37	L	9	Total 9	O 9	0	0
37	M	5	Total 5	O 5	0	0
37	O	73	Total 73	O 73	0	0
37	T	9	Total 9	O 9	0	0
37	U	29	Total 29	O 29	0	0
37	V	51	Total 51	O 51	0	0
37	Y	1	Total 1	O 1	0	0
37	X	8	Total 8	O 8	0	0
37	Z	3	Total 3	O 3	0	0
37	R	6	Total 6	O 6	0	0
37	a	100	Total 104	O 104	0	4
37	b	163	Total 163	O 163	0	0
37	c	160	Total 160	O 160	0	0
37	d	95	Total 95	O 95	0	0
37	e	13	Total 13	O 13	0	0
37	f	3	Total 3	O 3	0	0
37	h	20	Total 20	O 20	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	i	17	Total 17	O 17	0	0
37	j	5	Total 5	O 5	0	0
37	k	1	Total 1	O 1	0	0
37	l	12	Total 12	O 12	0	0
37	m	8	Total 8	O 8	0	0
37	o	72	Total 72	O 72	0	0
37	t	6	Total 6	O 6	0	0
37	u	50	Total 50	O 50	0	0
37	v	42	Total 42	O 42	0	0
37	x	5	Total 5	O 5	0	0
37	z	3	Total 3	O 3	0	0
37	r	7	Total 7	O 7	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 II protein D1 1

Chain A:  96%



- Molecule 1: Photosystem II protein D1 1

Chain a:  94%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  98%



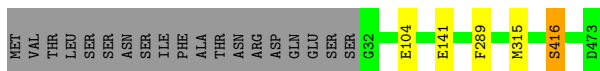
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  97%



- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  95%



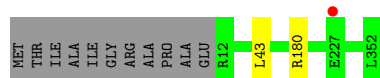
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  95% . .



- Molecule 4: Photosystem II D2 protein

Chain D:  96% . .



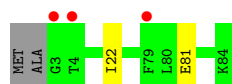
- Molecule 4: Photosystem II D2 protein

Chain d:  95% . .




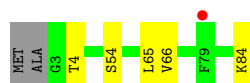
- Molecule 5: Cytochrome b559 subunit alpha

Chain E:  4% 95% . .




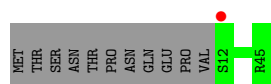
- Molecule 5: Cytochrome b559 subunit alpha

Chain e:  % 92% 6% .



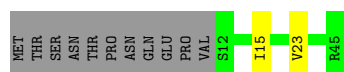
- Molecule 6: Cytochrome b559 subunit beta

Chain F:  2% 76% 24%

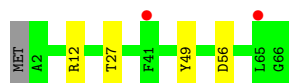
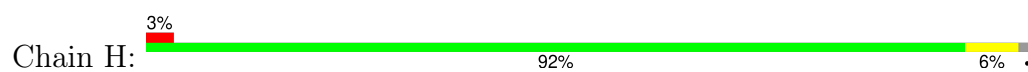


- Molecule 6: Cytochrome b559 subunit beta

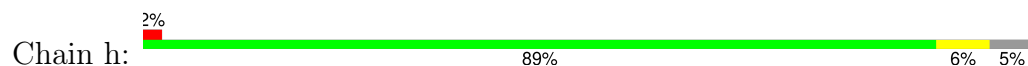
Chain f:  71% 24%



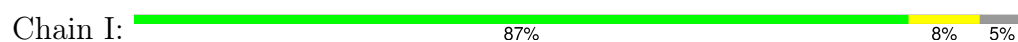
- Molecule 7: Photosystem II reaction center protein H



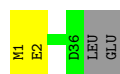
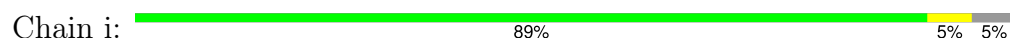
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



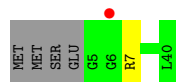
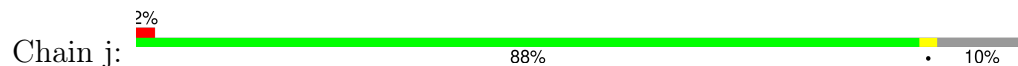
- Molecule 8: Photosystem II reaction center protein I



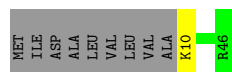
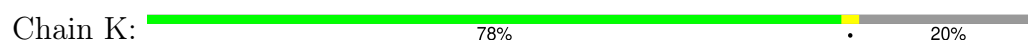
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J

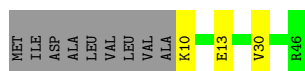


- Molecule 10: Photosystem II reaction center protein K



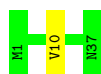
- Molecule 10: Photosystem II reaction center protein K

Chain k:  74% 7% 20%




- Molecule 11: Photosystem II reaction center protein L

Chain L:  97%




- Molecule 11: Photosystem II reaction center protein L

Chain l:  89% 8%




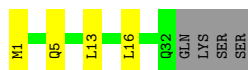
- Molecule 12: Photosystem II reaction center protein M

Chain M:  83% 8% 8%




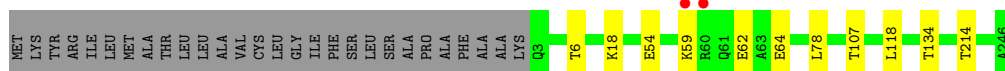
- Molecule 12: Photosystem II reaction center protein M

Chain m:  78% 11% 11%




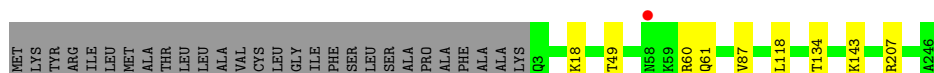
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  86% 10%

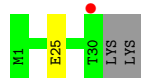
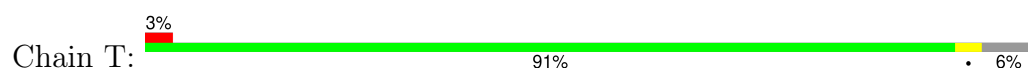


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

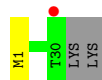
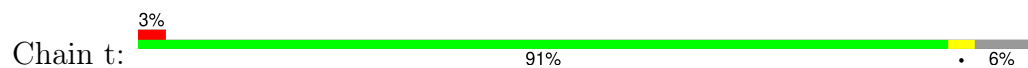
Chain o:  86% 10%



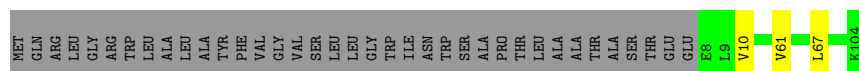
- Molecule 14: Photosystem II reaction center protein T



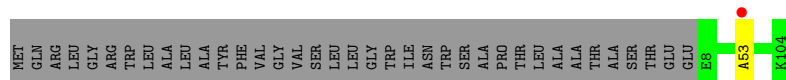
- Molecule 14: Photosystem II reaction center protein T



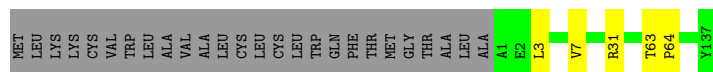
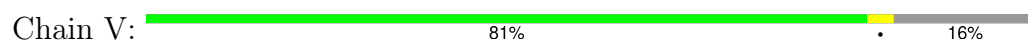
- Molecule 15: Photosystem II 12 kDa extrinsic protein



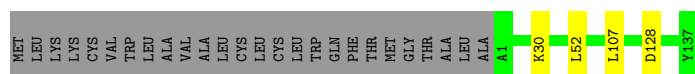
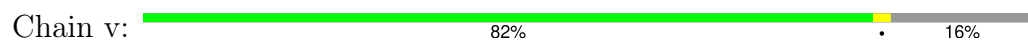
- Molecule 15: Photosystem II 12 kDa extrinsic protein



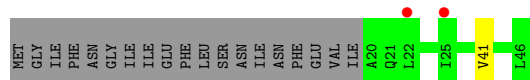
- Molecule 16: Cytochrome c-550



- Molecule 16: Cytochrome c-550

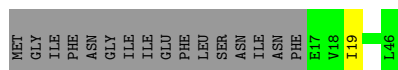


- Molecule 17: Photosystem II reaction center protein Ycf12



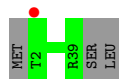
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  63% 35%

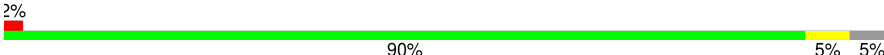


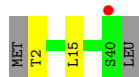
- Molecule 18: Photosystem II reaction center X protein

Chain X:  93% 7% 2%




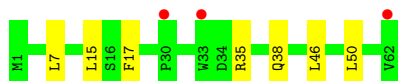
- Molecule 18: Photosystem II reaction center X protein

Chain x:  90% 5% 5% 2%

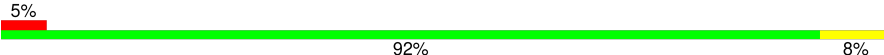


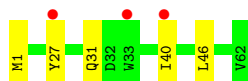
- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  89% 11% 5%




- Molecule 19: Photosystem II reaction center protein Z

Chain z:  92% 8% 5%



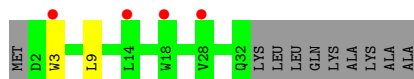
- Molecule 20: Photosystem II protein Y

Chain R:  76% 7% 17% 5%



- Molecule 20: Photosystem II protein Y

Chain r:  71% 5% 24% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.96Å 221.65Å 307.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.65 – 2.09 33.65 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.3 (33.65-2.09) 85.3 (33.65-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.51 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.186 , 0.234 0.186 , 0.235	Depositor DCC
R_{free} test set	4165 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	53041	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: DGD, OEY, CLA, HEC, CL, OEX, SQD, PL9, BCR, STE, BCT, PHO, FE2, HEM, LMG, FME, LHG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.43	0/3212	0.58	0/4376
1	a	0.42	0/3209	0.58	0/4372
2	B	0.40	0/4155	0.58	0/5661
2	b	0.39	0/4118	0.58	1/5611 (0.0%)
3	C	0.40	0/3625	0.55	0/4935
3	c	0.38	0/3705	0.54	0/5042
4	D	0.43	0/2825	0.57	0/3847
4	d	0.40	0/2834	0.58	0/3859
5	E	0.36	0/688	0.51	0/940
5	e	0.33	0/683	0.52	0/932
6	F	0.34	0/284	0.45	0/387
6	f	0.33	0/284	0.55	0/387
7	H	0.42	0/523	0.57	0/713
7	h	0.40	0/511	0.58	0/697
8	I	0.36	0/293	0.55	0/396
8	i	0.42	0/293	0.56	0/396
9	J	0.38	0/263	0.54	0/356
9	j	0.33	0/263	0.53	0/356
10	K	0.38	0/303	0.52	0/416
10	k	0.36	0/303	0.57	0/416
11	L	0.36	0/311	0.59	0/422
11	l	0.40	0/303	0.62	0/412
12	M	0.39	0/249	0.51	0/341
12	m	0.44	0/244	0.53	0/334
13	O	0.38	0/1904	0.63	0/2585
13	o	0.39	0/1905	0.62	0/2583
14	T	0.46	0/257	0.57	0/349
14	t	0.46	0/255	0.57	0/346
15	U	0.36	0/785	0.58	0/1064
15	u	0.37	0/785	0.59	0/1064
16	V	0.37	0/1085	0.59	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.35	0/1085	0.55	0/1473
17	Y	0.31	0/197	0.54	0/264
17	y	0.29	0/219	0.47	0/294
18	X	0.37	0/284	0.51	0/384
18	x	0.31	0/289	0.44	0/391
19	Z	0.32	0/490	0.49	0/669
19	z	0.30	0/488	0.42	0/666
20	R	0.36	0/277	0.58	0/380
20	r	0.31	0/252	0.51	0/347
All	All	0.39	0/44038	0.57	1/59936 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
16	V	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	98	LEU	CA-CB-CG	6.16	129.46	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide

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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	395/344 (115%)	387 (98%)	8 (2%)	0	100	100
1	a	395/344 (115%)	386 (98%)	8 (2%)	1 (0%)	37	37
2	B	507/510 (99%)	499 (98%)	8 (2%)	0	100	100
2	b	503/510 (99%)	491 (98%)	12 (2%)	0	100	100
3	C	451/461 (98%)	438 (97%)	12 (3%)	1 (0%)	44	45
3	c	461/461 (100%)	449 (97%)	11 (2%)	1 (0%)	44	45
4	D	340/352 (97%)	332 (98%)	8 (2%)	0	100	100
4	d	341/352 (97%)	331 (97%)	10 (3%)	0	100	100
5	E	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
5	e	80/84 (95%)	78 (98%)	2 (2%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	59 (94%)	3 (5%)	1 (2%)	8	4
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	229 (94%)	11 (4%)	3 (1%)	11	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	231 (96%)	10 (4%)	1 (0%)	30	29
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
15	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	12	8
16	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	19	16
16	v	135/163 (83%)	132 (98%)	3 (2%)	0	100	100
17	Y	25/46 (54%)	24 (96%)	1 (4%)	0	100	100
17	y	28/46 (61%)	26 (93%)	2 (7%)	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	R	32/41 (78%)	32 (100%)	0	0	100	100
20	r	29/41 (71%)	29 (100%)	0	0	100	100
All	All	5386/5700 (94%)	5235 (97%)	141 (3%)	10 (0%)	44	45

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO
3	c	416	SER
13	O	59	LYS
13	o	61	GLN
15	u	53	ALA
13	O	62	GLU
13	O	134	THR
1	a	259	ILE
7	H	12	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	322/280 (115%)	317 (98%)	5 (2%)	58	65
1	a	321/280 (115%)	311 (97%)	10 (3%)	35	39
2	B	407/407 (100%)	400 (98%)	7 (2%)	56	63
2	b	402/407 (99%)	390 (97%)	12 (3%)	36	40
3	C	353/362 (98%)	348 (99%)	5 (1%)	62	70
3	c	362/362 (100%)	350 (97%)	12 (3%)	33	36
4	D	277/283 (98%)	275 (99%)	2 (1%)	81	87
4	d	278/283 (98%)	272 (98%)	6 (2%)	47	53
5	E	72/73 (99%)	69 (96%)	3 (4%)	25	26
5	e	71/73 (97%)	66 (93%)	5 (7%)	12	10
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	26 (93%)	2 (7%)	12	10
7	H	54/55 (98%)	51 (94%)	3 (6%)	17	16
7	h	53/55 (96%)	49 (92%)	4 (8%)	11	9
8	I	32/34 (94%)	29 (91%)	3 (9%)	7	5
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	39
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	23 (96%)	1 (4%)	25	26
10	K	30/37 (81%)	29 (97%)	1 (3%)	33	36
10	k	30/37 (81%)	27 (90%)	3 (10%)	6	4
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	41
11	l	34/35 (97%)	31 (91%)	3 (9%)	8	5
12	M	28/32 (88%)	26 (93%)	2 (7%)	12	10
12	m	28/32 (88%)	25 (89%)	3 (11%)	5	3
13	O	206/228 (90%)	198 (96%)	8 (4%)	27	29
13	o	207/228 (91%)	199 (96%)	8 (4%)	27	29
14	T	26/28 (93%)	25 (96%)	1 (4%)	28	30
14	t	25/28 (89%)	25 (100%)	0	100	100
15	U	84/112 (75%)	81 (96%)	3 (4%)	30	32
15	u	84/112 (75%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	V	117/138 (85%)	114 (97%)	3 (3%)	41	46
16	v	117/138 (85%)	113 (97%)	4 (3%)	32	35
17	Y	19/37 (51%)	18 (95%)	1 (5%)	19	18
17	y	22/37 (60%)	21 (96%)	1 (4%)	23	24
18	X	31/34 (91%)	31 (100%)	0	100	100
18	x	31/34 (91%)	29 (94%)	2 (6%)	14	12
19	Z	52/52 (100%)	45 (86%)	7 (14%)	3	1
19	z	51/52 (98%)	46 (90%)	5 (10%)	6	4
20	R	28/33 (85%)	25 (89%)	3 (11%)	5	3
20	r	25/33 (76%)	23 (92%)	2 (8%)	10	7
All	All	4450/4654 (96%)	4308 (97%)	142 (3%)	34	37

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	16	ARG
1	A	134	SER
1	A	205	VAL
1	A	229	GLU
2	B	127	ARG
2	B	240	SER
2	B	362	PHE
2	B	371	THR
2	B	472	ARG
2	B	476	ARG
2	B	487	SER
3	C	104	GLU
3	C	141	GLU
3	C	289	PHE
3	C	315	MET
3	C	416	SER
4	D	43	LEU
4	D	180	ARG
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	81	GLU
7	H	27	THR

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Mol	Chain	Res	Type
7	H	49	TYR
7	H	56	ASP
8	I	4	LEU
8	I	6	ILE
8	I	36	ASP
10	K	10	LYS
11	L	10	VAL
12	M	9	ILE
12	M	25	LEU
13	O	6	THR
13	O	18	LYS
13	O	54	GLU
13	O	64	GLU
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	214	THR
14	T	25	GLU
15	U	10	VAL
15	U	61	VAL
15	U	67	LEU
16	V	3	LEU
16	V	7	VAL
16	V	31	ARG
17	Y	41	VAL
19	Z	7	LEU
19	Z	15	LEU
19	Z	17	PHE
19	Z	35	ARG
19	Z	38	GLN
19	Z	46	LEU
19	Z	50	LEU
20	R	13	LEU
20	R	21	ARG
20	R	35	LEU
1	a	16	ARG
1	a	28	LEU
1	a	42	LEU
1	a	159[A]	LEU
1	a	159[B]	LEU
1	a	200	LEU
1	a	223	LEU

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Mol	Chain	Res	Type
1	a	229	GLU
1	a	245	THR
1	a	288	LEU
2	b	83	GLU
2	b	98	LEU
2	b	128	THR
2	b	149	LEU
2	b	236	THR
2	b	266	GLU
2	b	357	ARG
2	b	362	PHE
2	b	444	ARG
2	b	492	GLU
2	b	505	ARG
2	b	506	ARG
3	c	24	THR
3	c	72	LEU
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	165	LEU
3	c	240	ILE
3	c	279	LEU
3	c	289	PHE
3	c	315	MET
3	c	413[A]	GLU
3	c	413[B]	GLU
4	d	90	LEU
4	d	180	ARG
4	d	182	LEU
4	d	259	ILE
4	d	291	LEU
4	d	321	LEU
5	e	4	THR
5	e	54	SER
5	e	65	LEU
5	e	66	VAL
5	e	84	LYS
6	f	15	ILE
6	f	23	VAL
7	h	7	LEU
7	h	27	THR

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Mol	Chain	Res	Type
7	h	38	PHE
7	h	49	TYR
8	i	2	GLU
9	j	7	ARG
10	k	10	LYS
10	k	13	GLU
10	k	30	VAL
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	5	GLN
12	m	13	LEU
12	m	16	LEU
13	o	18	LYS
13	o	49	THR
13	o	60	ARG
13	o	87	VAL
13	o	118	LEU
13	o	134	THR
13	o	143	LYS
13	o	207	ARG
16	v	30	LYS
16	v	52	LEU
16	v	107	LEU
16	v	128	ASP
17	y	19	ILE
18	x	2	THR
18	x	15	LEU
19	z	1	MET
19	z	27	TYR
19	z	31	GLN
19	z	40	ILE
19	z	46	LEU
20	r	3	TRP
20	r	9	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	61	HIS
7	H	59	ASN
13	O	36	GLN

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Mol	Chain	Res	Type
13	O	88	ASN
13	O	231	HIS
16	V	86	GLN
19	Z	38	GLN
1	a	19	ASN
1	a	234	ASN
2	b	490	GLN
5	e	60	GLN
12	m	5	GLN
13	o	61	GLN
18	x	33	GLN
19	z	31	GLN
20	r	30	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	$\# Z > 2$
14	FME	T	1	14	8,9,10	1.07	0	8,9,11	1.13	0
8	FME	I	1	8	8,9,10	1.00	0	8,9,11	1.02	0
8	FME	i	1	8	8,9,10	1.03	1 (12%)	8,9,11	0.76	0
12	FME	M	1	12	8,9,10	1.02	1 (12%)	8,9,11	1.02	0
12	FME	m	1	12	8,9,10	1.09	1 (12%)	8,9,11	0.86	0
14	FME	t	1	14	8,9,10	1.21	1 (12%)	8,9,11	0.78	0

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
14	FME	T	1	14	-	2/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
8	FME	i	1	8	-	4/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
14	FME	t	1	14	-	2/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-2.46	1.43	1.46
12	m	1	FME	CA-N	-2.34	1.43	1.46
12	M	1	FME	CA-N	-2.18	1.43	1.46
8	i	1	FME	CA-N	-2.03	1.43	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	O-C-CA-CB
8	i	1	FME	N-CA-CB-CG
8	i	1	FME	C-CA-CB-CG
14	t	1	FME	O-C-CA-CB
14	t	1	FME	CB-CG-SD-CE
14	T	1	FME	CB-CG-SD-CE
8	i	1	FME	CB-CG-SD-CE
12	M	1	FME	CB-CA-N-CN
8	i	1	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 188 ligands modelled in this entry, 6 are monoatomic - leaving 182 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$
33	STE	a	616	-	9,9,19	0.46	0	8,8,19	0.61	0
33	STE	C	519	-	11,11,19	0.61	0	11,11,19	1.48	3 (27%)
25	CLA	a	607	-	63,73,73	1.72	8 (12%)	74,113,113	1.38	9 (12%)
30	SQD	a	613	-	52,54,54	1.52	7 (13%)	62,65,65	1.95	12 (19%)
25	CLA	B	609	-	63,73,73	1.35	5 (7%)	74,113,113	1.32	7 (9%)
29	LMG	c	520	-	37,37,55	0.85	0	45,45,63	1.37	7 (15%)
30	SQD	B	622	-	52,54,54	1.60	8 (15%)	62,65,65	1.51	8 (12%)
25	CLA	c	510	-	63,73,73	1.53	8 (12%)	74,113,113	1.52	10 (13%)
30	SQD	L	101	-	47,49,54	1.62	8 (17%)	57,60,65	1.96	12 (21%)
25	CLA	B	612	-	63,73,73	1.26	5 (7%)	74,113,113	1.52	12 (16%)
25	CLA	b	606	-	63,73,73	1.55	6 (9%)	74,113,113	1.66	8 (10%)
25	CLA	C	510	-	63,73,73	1.36	8 (12%)	74,113,113	1.39	9 (12%)
25	CLA	A	607	37	63,73,73	1.35	6 (9%)	74,113,113	1.31	9 (12%)
31	LHG	e	101	-	41,41,48	0.77	1 (2%)	44,47,54	1.29	5 (11%)
33	STE	D	413	-	19,19,19	0.59	0	19,19,19	1.15	0
25	CLA	b	612	-	63,73,73	1.35	7 (11%)	74,113,113	1.46	10 (13%)
27	BCR	K	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.40	7 (12%)
32	DGD	A	617	-	67,67,67	1.10	7 (10%)	81,81,81	1.41	15 (18%)
33	STE	M	102	-	14,14,19	0.68	0	14,14,19	1.21	1 (7%)
25	CLA	c	508	-	62,72,73	1.47	8 (12%)	72,111,113	1.43	9 (12%)
27	BCR	C	514	-	41,41,41	1.10	2 (4%)	56,56,56	1.21	5 (8%)
25	CLA	B	610	37	63,73,73	1.38	5 (7%)	74,113,113	1.53	12 (16%)
25	CLA	B	615	-	63,73,73	1.55	5 (7%)	74,113,113	1.39	7 (9%)
25	CLA	b	615	-	63,73,73	1.48	8 (12%)	74,113,113	1.37	8 (10%)
33	STE	M	103	-	9,9,19	0.40	0	8,8,19	0.72	0
21	OEY	a	601[B]	37,3,1	0,16,16	-	-	-	-	-
22	OEX	A	602[A]	37,3,1	0,15,15	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	D	405	-	63,73,73	1.39	7 (11%)	74,113,113	1.52	8 (10%)
29	LMG	b	621	-	55,55,55	0.84	2 (3%)	63,63,63	1.33	8 (12%)
25	CLA	B	607	37	63,73,73	1.48	7 (11%)	74,113,113	1.42	6 (8%)
27	BCR	c	516	-	41,41,41	1.03	2 (4%)	56,56,56	1.16	6 (10%)
25	CLA	A	609	-	52,62,73	1.46	7 (13%)	60,99,113	1.57	8 (13%)
36	HEC	V	201	16	32,50,50	1.91	3 (9%)	30,82,82	2.62	7 (23%)
33	STE	x	102	-	19,19,19	0.66	0	19,19,19	0.90	1 (5%)
25	CLA	A	606	-	63,73,73	1.47	6 (9%)	74,113,113	1.38	11 (14%)
25	CLA	b	611	-	63,73,73	1.50	7 (11%)	74,113,113	1.55	9 (12%)
27	BCR	D	406	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	5 (8%)
33	STE	C	521	-	15,15,19	0.46	0	14,14,19	0.60	0
32	DGD	c	519	-	63,63,67	0.96	3 (4%)	77,77,81	1.41	8 (10%)
33	STE	m	102	-	11,11,19	0.69	0	11,11,19	1.41	1 (9%)
29	LMG	c	522	-	48,48,55	0.88	3 (6%)	56,56,63	1.33	9 (16%)
31	LHG	l	101	-	48,48,48	0.66	1 (2%)	51,54,54	1.20	6 (11%)
32	DGD	C	515	-	63,63,67	1.04	4 (6%)	77,77,81	1.39	12 (15%)
33	STE	H	103	-	17,17,19	0.40	0	16,16,19	0.73	0
25	CLA	b	601	37	63,73,73	1.52	7 (11%)	74,113,113	1.50	6 (8%)
35	HEM	f	101	5,6	42,50,50	1.47	6 (14%)	46,82,82	1.52	10 (21%)
27	BCR	B	619	-	41,41,41	1.00	2 (4%)	56,56,56	1.32	6 (10%)
25	CLA	C	509	-	63,73,73	1.42	6 (9%)	74,113,113	1.50	8 (10%)
32	DGD	c	518	-	63,63,67	1.02	4 (6%)	77,77,81	1.40	10 (12%)
21	OEY	A	601[B]	37,3,1	0,16,16	-	-	-	-	-
25	CLA	b	602	-	63,73,73	1.24	4 (6%)	74,113,113	1.48	10 (13%)
27	BCR	b	619	-	41,41,41	1.05	2 (4%)	56,56,56	1.27	4 (7%)
32	DGD	C	516	-	63,63,67	1.11	6 (9%)	77,77,81	1.41	13 (16%)
29	LMG	D	408	-	51,51,55	0.89	3 (5%)	59,59,63	1.34	6 (10%)
33	STE	c	521	-	19,19,19	0.68	0	19,19,19	0.92	0
25	CLA	c	503	-	63,73,73	1.53	7 (11%)	74,113,113	1.55	7 (9%)
29	LMG	C	518	-	48,48,55	0.82	1 (2%)	56,56,63	1.37	10 (17%)
25	CLA	B	601	37	63,73,73	1.58	9 (14%)	74,113,113	1.41	7 (9%)
27	BCR	a	610	-	41,41,41	0.98	2 (4%)	56,56,56	1.28	8 (14%)
29	LMG	d	410	-	21,21,55	0.49	0	20,20,63	1.19	2 (10%)
31	LHG	D	409	-	48,48,48	0.79	3 (6%)	51,54,54	1.32	7 (13%)
22	OEX	a	602[A]	37,3,1	0,15,15	-	-	-	-	-
29	LMG	M	101	-	51,51,55	0.86	1 (1%)	59,59,63	1.39	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	STE	a	617	-	11,11,19	0.80	0	11,11,19	1.08	1 (9%)
28	PL9	a	611	-	55,55,55	0.79	1 (1%)	68,69,69	1.51	13 (19%)
34	BCT	a	606	23	3,3,3	3.71	1 (33%)	2,3,3	2.09	1 (50%)
25	CLA	c	506	-	63,73,73	1.38	8 (12%)	74,113,113	1.46	7 (9%)
33	STE	B	623	-	11,11,19	0.75	0	11,11,19	1.07	0
25	CLA	a	608	37	63,73,73	1.37	6 (9%)	74,113,113	1.44	9 (12%)
25	CLA	B	605	-	63,73,73	1.41	8 (12%)	74,113,113	1.31	8 (10%)
28	PL9	D	407	-	55,55,55	0.94	2 (3%)	68,69,69	1.51	13 (19%)
25	CLA	b	603	-	63,73,73	1.34	6 (9%)	74,113,113	1.53	11 (14%)
27	BCR	x	101	-	41,41,41	0.98	2 (4%)	56,56,56	1.20	5 (8%)
25	CLA	C	504	37	57,67,73	1.39	5 (8%)	66,105,113	1.37	7 (10%)
29	LMG	m	101	-	51,51,55	0.87	3 (5%)	59,59,63	1.47	9 (15%)
27	BCR	k	101	-	41,41,41	1.07	4 (9%)	56,56,56	1.07	3 (5%)
33	STE	J	101	-	11,11,19	0.70	0	11,11,19	1.23	0
25	CLA	B	606	-	63,73,73	1.58	7 (11%)	74,113,113	1.44	9 (12%)
25	CLA	B	603	-	63,73,73	1.44	8 (12%)	74,113,113	1.36	11 (14%)
33	STE	I	101	-	14,14,19	0.44	0	13,13,19	0.63	0
25	CLA	d	404	-	63,73,73	1.28	5 (7%)	74,113,113	1.35	6 (8%)
25	CLA	b	614	-	63,73,73	1.40	7 (11%)	74,113,113	1.28	9 (12%)
33	STE	t	102	-	13,13,19	0.67	0	13,13,19	1.16	1 (7%)
25	CLA	C	502	-	63,73,73	1.37	8 (12%)	74,113,113	1.35	8 (10%)
25	CLA	b	607	37	63,73,73	1.35	7 (11%)	74,113,113	1.40	8 (10%)
31	LHG	d	407	-	48,48,48	0.81	2 (4%)	51,54,54	1.36	6 (11%)
31	LHG	D	412	-	48,48,48	0.92	2 (4%)	51,54,54	1.37	6 (11%)
32	DGD	a	615	-	43,43,67	0.77	2 (4%)	45,45,81	1.47	8 (17%)
33	STE	c	523	-	11,11,19	0.69	0	11,11,19	1.35	1 (9%)
29	LMG	D	411	-	31,31,55	0.73	1 (3%)	33,33,63	1.17	2 (6%)
25	CLA	B	614	-	63,73,73	1.54	6 (9%)	74,113,113	1.27	6 (8%)
25	CLA	c	513	-	63,73,73	1.41	6 (9%)	74,113,113	1.41	8 (10%)
25	CLA	b	616	-	58,68,73	1.43	6 (10%)	68,107,113	1.59	9 (13%)
25	CLA	b	610	37	63,73,73	1.40	8 (12%)	74,113,113	1.46	12 (16%)
27	BCR	b	617	-	41,41,41	0.99	3 (7%)	56,56,56	1.31	7 (12%)
29	LMG	A	612	-	48,48,55	0.78	2 (4%)	56,56,63	1.33	6 (10%)
31	LHG	A	614	-	48,48,48	0.70	1 (2%)	51,54,54	1.23	7 (13%)
27	BCR	B	618	-	41,41,41	1.07	2 (4%)	56,56,56	1.26	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	C	508	-	63,73,73	1.49	6 (9%)	74,113,113	1.47	8 (10%)
25	CLA	C	512	-	63,73,73	1.52	8 (12%)	74,113,113	1.42	11 (14%)
25	CLA	c	502	-	63,73,73	1.31	7 (11%)	74,113,113	1.45	10 (13%)
25	CLA	b	604	-	63,73,73	1.27	5 (7%)	74,113,113	1.72	10 (13%)
27	BCR	A	610	-	41,41,41	0.96	2 (4%)	56,56,56	1.39	10 (17%)
25	CLA	c	507	37	63,73,73	1.49	6 (9%)	74,113,113	1.33	8 (10%)
25	CLA	c	504	37	58,68,73	1.36	7 (12%)	68,107,113	1.49	6 (8%)
29	LMG	d	411	-	44,44,55	0.94	2 (4%)	52,52,63	1.34	6 (11%)
31	LHG	D	410	-	46,46,48	0.79	1 (2%)	49,52,54	1.23	5 (10%)
32	DGD	c	517	-	63,63,67	0.97	3 (4%)	77,77,81	1.36	7 (9%)
25	CLA	C	507	37	63,73,73	1.43	7 (11%)	74,113,113	1.59	10 (13%)
32	DGD	H	102	-	63,63,67	1.07	5 (7%)	77,77,81	1.40	8 (10%)
25	CLA	c	505	-	63,73,73	1.30	5 (7%)	74,113,113	1.31	7 (9%)
27	BCR	d	405	-	41,41,41	1.11	3 (7%)	56,56,56	1.23	7 (12%)
35	HEM	E	101	5,6	42,50,50	1.54	5 (11%)	46,82,82	1.27	3 (6%)
33	STE	B	624	-	17,17,19	0.63	0	17,17,19	1.03	0
25	CLA	B	613	-	63,73,73	1.32	7 (11%)	74,113,113	1.55	9 (12%)
25	CLA	c	512	-	63,73,73	1.42	8 (12%)	74,113,113	1.43	8 (10%)
25	CLA	b	613	-	63,73,73	1.60	7 (11%)	74,113,113	1.49	13 (17%)
25	CLA	C	503	-	63,73,73	1.65	7 (11%)	74,113,113	1.56	10 (13%)
26	PHO	A	608	-	50,69,69	0.98	3 (6%)	48,99,99	1.30	5 (10%)
26	PHO	D	402	-	50,69,69	0.98	4 (8%)	48,99,99	1.45	6 (12%)
33	STE	d	413	-	16,16,19	0.63	0	16,16,19	1.13	1 (6%)
26	PHO	d	402	-	50,69,69	0.96	3 (6%)	48,99,99	1.51	7 (14%)
33	STE	b	622	-	19,19,19	0.69	0	19,19,19	0.95	1 (5%)
27	BCR	Y	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.19	4 (7%)
33	STE	B	626	-	15,15,19	0.38	0	14,14,19	0.81	0
33	STE	j	101	-	11,11,19	0.70	0	11,11,19	1.40	2 (18%)
25	CLA	B	608	-	63,73,73	1.45	8 (12%)	74,113,113	1.60	6 (8%)
33	STE	b	623	-	9,9,19	0.40	0	8,8,19	0.67	0
25	CLA	b	605	-	63,73,73	1.34	5 (7%)	74,113,113	1.41	12 (16%)
31	LHG	d	408	-	48,48,48	0.61	1 (2%)	51,54,54	1.28	6 (11%)
31	LHG	d	409	-	38,38,48	0.77	1 (2%)	41,44,54	1.14	2 (4%)
27	BCR	c	514	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	7 (12%)
25	CLA	D	404	-	63,73,73	1.58	6 (9%)	74,113,113	1.40	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	C	506	-	63,73,73	1.41	7 (11%)	74,113,113	1.43	9 (12%)
30	SQD	A	613	-	50,52,54	1.59	6 (12%)	60,63,65	1.88	12 (20%)
27	BCR	c	515	-	41,41,41	1.10	2 (4%)	56,56,56	1.33	6 (10%)
25	CLA	a	609	-	63,73,73	1.39	8 (12%)	74,113,113	1.27	9 (12%)
28	PL9	d	406	-	55,55,55	1.06	4 (7%)	68,69,69	1.59	16 (23%)
33	STE	d	412	-	15,15,19	0.73	0	15,15,19	0.98	0
34	BCT	D	401	23	3,3,3	3.55	1 (33%)	2,3,3	2.02	1 (50%)
32	DGD	h	101	-	63,63,67	0.99	3 (4%)	77,77,81	1.47	10 (12%)
27	BCR	B	617	-	41,41,41	1.04	3 (7%)	56,56,56	1.23	5 (8%)
32	DGD	C	517	-	63,63,67	0.93	3 (4%)	77,77,81	1.34	7 (9%)
27	BCR	K	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.16	4 (7%)
33	STE	T	102	-	15,15,19	0.40	0	14,14,19	0.73	0
25	CLA	B	604	-	63,73,73	1.62	7 (11%)	74,113,113	1.73	11 (14%)
25	CLA	a	612	37	63,73,73	1.56	5 (7%)	74,113,113	1.45	8 (10%)
33	STE	T	103	-	14,14,19	0.31	0	13,13,19	0.96	0
31	LHG	A	615	-	48,48,48	0.75	3 (6%)	51,54,54	1.21	2 (3%)
30	SQD	a	614	-	35,35,54	1.74	7 (20%)	37,37,65	1.36	4 (10%)
25	CLA	c	511	3	63,73,73	1.69	5 (7%)	74,113,113	1.62	7 (9%)
26	PHO	d	401	-	50,69,69	0.93	2 (4%)	48,99,99	1.26	7 (14%)
27	BCR	b	618	-	41,41,41	1.14	2 (4%)	56,56,56	1.17	5 (8%)
25	CLA	c	509	-	63,73,73	1.49	6 (9%)	74,113,113	1.71	10 (13%)
25	CLA	D	403	37	63,73,73	1.42	5 (7%)	74,113,113	1.17	8 (10%)
27	BCR	H	101	-	41,41,41	0.99	2 (4%)	56,56,56	1.24	6 (10%)
36	HEC	v	201	16	32,50,50	2.05	3 (9%)	30,82,82	2.28	6 (20%)
30	SQD	A	616	-	38,38,54	1.77	5 (13%)	40,40,65	1.28	2 (5%)
25	CLA	B	602	-	63,73,73	1.28	5 (7%)	74,113,113	1.56	9 (12%)
25	CLA	c	501	-	63,73,73	1.34	5 (7%)	74,113,113	1.47	9 (12%)
33	STE	B	620	-	16,16,19	0.65	0	16,16,19	1.15	0
25	CLA	C	501	-	63,73,73	1.34	5 (7%)	74,113,113	1.48	7 (9%)
25	CLA	b	609	-	63,73,73	1.34	7 (11%)	74,113,113	1.35	9 (12%)
25	CLA	B	611	-	63,73,73	1.36	5 (7%)	74,113,113	1.47	9 (12%)
27	BCR	t	101	-	41,41,41	0.97	2 (4%)	56,56,56	1.34	6 (10%)
29	LMG	B	621	-	26,26,55	0.59	0	26,26,63	1.35	2 (7%)
30	SQD	f	102	-	39,41,54	1.70	8 (20%)	49,52,65	1.67	11 (22%)
29	LMG	c	524	-	49,49,55	0.84	2 (4%)	57,57,63	1.27	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	PL9	A	611	-	55,55,55	0.92	2 (3%)	68,69,69	1.41	11 (16%)
33	STE	b	620	-	19,19,19	0.63	0	19,19,19	0.98	0
25	CLA	C	513	-	63,73,73	1.42	6 (9%)	74,113,113	1.48	7 (9%)
25	CLA	B	616	-	58,68,73	1.52	7 (12%)	68,107,113	1.60	7 (10%)
25	CLA	d	403	-	63,73,73	1.40	6 (9%)	74,113,113	1.30	6 (8%)
25	CLA	C	511	3	63,73,73	1.48	5 (7%)	74,113,113	1.44	7 (9%)
27	BCR	T	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.19	4 (7%)
25	CLA	C	505	-	63,73,73	1.56	4 (6%)	74,113,113	1.33	7 (9%)
25	CLA	b	608	-	63,73,73	1.45	7 (11%)	74,113,113	1.52	12 (16%)
30	SQD	F	101	-	34,36,54	1.60	6 (17%)	42,45,65	1.93	12 (28%)
33	STE	E	102	-	11,11,19	0.79	0	11,11,19	1.00	0
33	STE	B	625	-	11,11,19	0.73	0	11,11,19	1.20	1 (9%)
33	STE	l	102	-	17,17,19	0.34	0	16,16,19	0.96	0
33	STE	C	520	-	11,11,19	0.71	0	11,11,19	1.41	2 (18%)

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
33	STE	a	616	-	-	3/7/7/17	-
33	STE	C	519	-	-	5/9/9/17	-
25	CLA	a	607	-	1/1/15/20	4/37/115/115	-
30	SQD	a	613	-	-	25/49/69/69	0/1/1/1
25	CLA	B	609	-	-	2/37/115/115	-
29	LMG	c	520	-	-	10/31/51/70	0/1/1/1
30	SQD	B	622	-	-	25/49/69/69	0/1/1/1
25	CLA	c	510	-	1/1/15/20	14/37/115/115	-
30	SQD	L	101	-	-	17/44/64/69	0/1/1/1
25	CLA	B	612	-	1/1/15/20	8/37/115/115	-
25	CLA	b	606	-	1/1/15/20	11/37/115/115	-
25	CLA	C	510	-	1/1/15/20	11/37/115/115	-
25	CLA	A	607	37	-	11/37/115/115	-
31	LHG	e	101	-	-	22/46/46/53	-
33	STE	D	413	-	-	9/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	612	-	1/1/15/20	4/37/115/115	-
27	BCR	K	101	-	-	7/29/63/63	0/2/2/2
32	DGD	A	617	-	-	28/55/95/95	0/2/2/2
33	STE	M	102	-	-	5/12/12/17	-
25	CLA	c	508	-	-	3/36/114/115	-
27	BCR	C	514	-	-	6/29/63/63	0/2/2/2
25	CLA	B	610	37	1/1/15/20	7/37/115/115	-
25	CLA	B	615	-	1/1/15/20	8/37/115/115	-
25	CLA	b	615	-	1/1/15/20	11/37/115/115	-
33	STE	M	103	-	-	3/7/7/17	-
25	CLA	D	405	-	-	6/37/115/115	-
29	LMG	b	621	-	-	26/50/70/70	0/1/1/1
25	CLA	B	607	37	1/1/15/20	12/37/115/115	-
27	BCR	c	516	-	-	3/29/63/63	0/2/2/2
25	CLA	A	609	-	1/1/12/20	3/24/102/115	-
36	HEC	V	201	16	-	2/10/54/54	-
33	STE	x	102	-	-	10/17/17/17	-
25	CLA	A	606	-	1/1/15/20	6/37/115/115	-
25	CLA	b	611	-	1/1/15/20	5/37/115/115	-
27	BCR	D	406	-	-	6/29/63/63	0/2/2/2
33	STE	C	521	-	-	7/13/13/17	-
32	DGD	c	519	-	-	21/51/91/95	0/2/2/2
33	STE	m	102	-	-	4/9/9/17	-
29	LMG	c	522	-	-	23/43/63/70	0/1/1/1
31	LHG	l	101	-	-	20/53/53/53	-
32	DGD	C	515	-	-	22/51/91/95	0/2/2/2
33	STE	H	103	-	-	6/15/15/17	-
25	CLA	b	601	37	1/1/15/20	14/37/115/115	-
35	HEM	f	101	5,6	-	5/12/54/54	-
27	BCR	B	619	-	-	5/29/63/63	0/2/2/2
25	CLA	C	509	-	1/1/15/20	11/37/115/115	-
32	DGD	c	518	-	-	22/51/91/95	0/2/2/2
25	CLA	b	602	-	-	13/37/115/115	-
27	BCR	b	619	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	DGD	C	516	-	-	21/51/91/95	0/2/2/2
29	LMG	D	408	-	-	17/46/66/70	0/1/1/1
33	STE	c	521	-	-	8/17/17/17	-
25	CLA	c	503	-	-	7/37/115/115	-
29	LMG	C	518	-	-	20/43/63/70	0/1/1/1
25	CLA	B	601	37	1/1/15/20	13/37/115/115	-
27	BCR	a	610	-	-	2/29/63/63	0/2/2/2
29	LMG	d	410	-	-	11/17/17/70	-
31	LHG	D	409	-	-	22/53/53/53	-
29	LMG	M	101	-	-	21/46/66/70	0/1/1/1
33	STE	a	617	-	-	4/9/9/17	-
28	PL9	a	611	-	-	15/53/73/73	0/1/1/1
25	CLA	c	506	-	1/1/15/20	12/37/115/115	-
33	STE	B	623	-	-	7/9/9/17	-
25	CLA	a	608	37	-	12/37/115/115	-
25	CLA	B	605	-	1/1/15/20	11/37/115/115	-
28	PL9	D	407	-	-	7/53/73/73	0/1/1/1
25	CLA	b	603	-	1/1/15/20	4/37/115/115	-
27	BCR	x	101	-	-	9/29/63/63	0/2/2/2
25	CLA	C	504	37	1/1/13/20	7/30/108/115	-
29	LMG	m	101	-	-	12/46/66/70	0/1/1/1
27	BCR	k	101	-	-	10/29/63/63	0/2/2/2
33	STE	J	101	-	-	2/9/9/17	-
25	CLA	B	606	-	1/1/15/20	12/37/115/115	-
25	CLA	B	603	-	1/1/15/20	11/37/115/115	-
33	STE	I	101	-	-	6/12/12/17	-
25	CLA	d	404	-	1/1/15/20	6/37/115/115	-
25	CLA	b	614	-	1/1/15/20	12/37/115/115	-
33	STE	t	102	-	-	5/11/11/17	-
25	CLA	C	502	-	1/1/15/20	7/37/115/115	-
25	CLA	b	607	37	1/1/15/20	16/37/115/115	-
31	LHG	d	407	-	-	22/53/53/53	-
31	LHG	D	412	-	-	15/53/53/53	-
32	DGD	a	615	-	-	28/45/45/95	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	STE	c	523	-	-	4/9/9/17	-
29	LMG	D	411	-	-	20/33/33/70	-
25	CLA	B	614	-	1/1/15/20	10/37/115/115	-
25	CLA	c	513	-	1/1/15/20	10/37/115/115	-
25	CLA	b	616	-	1/1/14/20	7/31/109/115	-
25	CLA	b	610	37	1/1/15/20	5/37/115/115	-
27	BCR	b	617	-	-	6/29/63/63	0/2/2/2
29	LMG	A	612	-	-	23/43/63/70	0/1/1/1
31	LHG	A	614	-	-	29/53/53/53	-
27	BCR	B	618	-	-	5/29/63/63	0/2/2/2
25	CLA	C	508	-	-	8/37/115/115	-
25	CLA	C	512	-	1/1/15/20	13/37/115/115	-
25	CLA	c	502	-	1/1/15/20	10/37/115/115	-
25	CLA	b	604	-	1/1/15/20	8/37/115/115	-
27	BCR	A	610	-	-	2/29/63/63	0/2/2/2
25	CLA	c	507	37	1/1/15/20	8/37/115/115	-
25	CLA	c	504	37	1/1/14/20	7/31/109/115	-
29	LMG	d	411	-	-	11/39/59/70	0/1/1/1
31	LHG	D	410	-	-	16/51/51/53	-
32	DGD	c	517	-	-	30/51/91/95	0/2/2/2
25	CLA	C	507	37	1/1/15/20	6/37/115/115	-
32	DGD	H	102	-	-	18/51/91/95	0/2/2/2
25	CLA	c	505	-	1/1/15/20	10/37/115/115	-
27	BCR	d	405	-	-	7/29/63/63	0/2/2/2
35	HEM	E	101	5,6	-	2/12/54/54	-
33	STE	B	624	-	-	9/15/15/17	-
25	CLA	B	613	-	1/1/15/20	14/37/115/115	-
25	CLA	c	512	-	1/1/15/20	20/37/115/115	-
25	CLA	b	613	-	1/1/15/20	8/37/115/115	-
25	CLA	C	503	-	1/1/15/20	6/37/115/115	-
26	PHO	A	608	-	-	5/37/103/103	0/5/6/6
26	PHO	D	402	-	-	3/37/103/103	0/5/6/6
33	STE	d	413	-	-	9/14/14/17	-
26	PHO	d	402	-	-	7/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	STE	b	622	-	-	8/17/17/17	-
27	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
33	STE	B	626	-	-	7/13/13/17	-
33	STE	j	101	-	-	4/9/9/17	-
25	CLA	B	608	-	1/1/15/20	4/37/115/115	-
33	STE	b	623	-	-	5/7/7/17	-
25	CLA	b	605	-	1/1/15/20	7/37/115/115	-
31	LHG	d	408	-	-	20/53/53/53	-
31	LHG	d	409	-	-	11/43/43/53	-
27	BCR	c	514	-	-	10/29/63/63	0/2/2/2
25	CLA	D	404	-	1/1/15/20	6/37/115/115	-
25	CLA	C	506	-	1/1/15/20	10/37/115/115	-
30	SQD	A	613	-	-	16/47/67/69	0/1/1/1
27	BCR	c	515	-	-	4/29/63/63	0/2/2/2
25	CLA	a	609	-	1/1/15/20	7/37/115/115	-
28	PL9	d	406	-	-	12/53/73/73	0/1/1/1
33	STE	d	412	-	-	6/13/13/17	-
32	DGD	h	101	-	-	16/51/91/95	0/2/2/2
27	BCR	B	617	-	-	0/29/63/63	0/2/2/2
32	DGD	C	517	-	-	14/51/91/95	0/2/2/2
27	BCR	K	102	-	-	10/29/63/63	0/2/2/2
33	STE	T	102	-	-	7/13/13/17	-
25	CLA	B	604	-	1/1/15/20	11/37/115/115	-
25	CLA	a	612	37	1/1/15/20	2/37/115/115	-
33	STE	T	103	-	-	8/12/12/17	-
31	LHG	A	615	-	-	17/53/53/53	-
30	SQD	a	614	-	-	17/37/37/69	-
25	CLA	c	511	3	1/1/15/20	11/37/115/115	-
26	PHO	d	401	-	-	6/37/103/103	0/5/6/6
27	BCR	b	618	-	-	4/29/63/63	0/2/2/2
25	CLA	c	509	-	1/1/15/20	10/37/115/115	-
25	CLA	D	403	37	1/1/15/20	11/37/115/115	-
27	BCR	H	101	-	-	6/29/63/63	0/2/2/2
36	HEC	v	201	16	-	2/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SQD	A	616	-	-	18/39/39/69	-
25	CLA	B	602	-	1/1/15/20	9/37/115/115	-
25	CLA	c	501	-	1/1/15/20	5/37/115/115	-
33	STE	B	620	-	-	8/14/14/17	-
25	CLA	C	501	-	1/1/15/20	5/37/115/115	-
25	CLA	b	609	-	1/1/15/20	8/37/115/115	-
25	CLA	B	611	-	1/1/15/20	7/37/115/115	-
27	BCR	t	101	-	-	7/29/63/63	0/2/2/2
29	LMG	B	621	-	-	14/22/22/70	-
30	SQD	f	102	-	-	12/36/56/69	0/1/1/1
29	LMG	c	524	-	-	19/44/64/70	0/1/1/1
28	PL9	A	611	-	-	26/53/73/73	0/1/1/1
33	STE	b	620	-	-	9/17/17/17	-
25	CLA	C	513	-	1/1/15/20	16/37/115/115	-
25	CLA	B	616	-	1/1/14/20	13/31/109/115	-
25	CLA	d	403	-	1/1/15/20	6/37/115/115	-
25	CLA	C	511	3	1/1/15/20	6/37/115/115	-
27	BCR	T	101	-	-	8/29/63/63	0/2/2/2
25	CLA	C	505	-	1/1/15/20	17/37/115/115	-
25	CLA	b	608	-	1/1/15/20	8/37/115/115	-
30	SQD	F	101	-	-	12/28/48/69	0/1/1/1
33	STE	E	102	-	-	4/9/9/17	-
33	STE	B	625	-	-	8/9/9/17	-
33	STE	l	102	-	-	9/15/15/17	-
33	STE	C	520	-	-	5/9/9/17	-

All (671) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	511	CLA	CHB-C4A	8.00	1.40	1.33
25	a	612	CLA	CHB-C4A	7.82	1.40	1.33
25	c	503	CLA	CHB-C4A	7.81	1.40	1.33
25	D	404	CLA	CHB-C4A	7.64	1.40	1.33
25	B	606	CLA	CHB-C4A	7.51	1.40	1.33
25	B	604	CLA	CHB-C4A	7.44	1.40	1.33
25	C	505	CLA	CHB-C4A	7.40	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	509	CLA	CHB-C4A	7.38	1.39	1.33
25	a	607	CLA	CHB-C4A	7.38	1.39	1.33
25	A	606	CLA	CHB-C4A	7.21	1.39	1.33
25	b	608	CLA	CHB-C4A	6.94	1.39	1.33
25	c	510	CLA	CHB-C4A	6.93	1.39	1.33
25	B	605	CLA	CHB-C4A	6.93	1.39	1.33
25	B	615	CLA	CHB-C4A	6.90	1.39	1.33
25	b	616	CLA	CHB-C4A	6.88	1.39	1.33
25	D	403	CLA	CHB-C4A	6.81	1.39	1.33
25	b	613	CLA	MG-NA	6.80	2.22	2.06
25	b	601	CLA	CHB-C4A	6.79	1.39	1.33
25	c	508	CLA	CHB-C4A	6.76	1.39	1.33
25	B	607	CLA	CHB-C4A	6.76	1.39	1.33
25	B	614	CLA	CHB-C4A	6.69	1.39	1.33
25	b	611	CLA	CHB-C4A	6.64	1.39	1.33
25	B	616	CLA	CHB-C4A	6.63	1.39	1.33
25	C	513	CLA	CHB-C4A	6.63	1.39	1.33
25	C	507	CLA	CHB-C4A	6.60	1.39	1.33
25	b	605	CLA	CHB-C4A	6.56	1.39	1.33
25	C	508	CLA	CHB-C4A	6.56	1.39	1.33
25	B	610	CLA	CHB-C4A	6.55	1.39	1.33
25	B	611	CLA	CHB-C4A	6.54	1.39	1.33
25	C	512	CLA	CHB-C4A	6.53	1.39	1.33
25	c	507	CLA	CHB-C4A	6.47	1.39	1.33
25	b	606	CLA	CHB-C4A	6.46	1.39	1.33
25	C	511	CLA	CHB-C4A	6.44	1.39	1.33
25	c	511	CLA	MG-NA	6.31	2.21	2.06
25	b	615	CLA	CHB-C4A	6.30	1.38	1.33
25	B	601	CLA	CHB-C4A	6.29	1.38	1.33
25	b	610	CLA	CHB-C4A	6.28	1.38	1.33
34	a	606	BCT	O1-C	6.24	1.47	1.25
25	B	603	CLA	CHB-C4A	6.14	1.38	1.33
25	b	606	CLA	MG-NA	6.14	2.20	2.06
36	v	201	HEC	C2B-C3B	-6.11	1.33	1.40
25	c	505	CLA	CHB-C4A	6.10	1.38	1.33
25	B	609	CLA	CHB-C4A	6.07	1.38	1.33
25	C	503	CLA	CHB-C4A	6.06	1.38	1.33
25	b	614	CLA	CHB-C4A	6.05	1.38	1.33
25	C	503	CLA	MG-NA	6.01	2.20	2.06
25	C	505	CLA	MG-NA	6.00	2.20	2.06
25	C	510	CLA	CHB-C4A	5.99	1.38	1.33
34	D	401	BCT	O1-C	5.97	1.46	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	513	CLA	CHB-C4A	5.94	1.38	1.33
25	B	608	CLA	CHB-C4A	5.92	1.38	1.33
25	C	506	CLA	CHB-C4A	5.85	1.38	1.33
25	C	509	CLA	CHB-C4A	5.84	1.38	1.33
25	B	601	CLA	MG-NA	5.74	2.19	2.06
25	a	609	CLA	CHB-C4A	5.73	1.38	1.33
25	c	501	CLA	CHB-C4A	5.72	1.38	1.33
36	V	201	HEC	C2B-C3B	-5.71	1.34	1.40
25	c	512	CLA	CHB-C4A	5.65	1.38	1.33
25	B	604	CLA	MG-NC	5.62	2.19	2.06
25	c	506	CLA	CHB-C4A	5.58	1.38	1.33
25	B	612	CLA	CHB-C4A	5.54	1.38	1.33
25	d	403	CLA	CHB-C4A	5.53	1.38	1.33
25	A	609	CLA	CHB-C4A	5.47	1.38	1.33
25	B	615	CLA	MG-NA	5.46	2.19	2.06
25	c	502	CLA	CHB-C4A	5.42	1.38	1.33
25	b	607	CLA	CHB-C4A	5.39	1.38	1.33
25	b	603	CLA	CHB-C4A	5.36	1.38	1.33
25	D	405	CLA	CHB-C4A	5.34	1.38	1.33
36	v	201	HEC	C3D-C2D	5.30	1.53	1.37
25	C	504	CLA	CHB-C4A	5.28	1.38	1.33
25	D	404	CLA	MG-NA	5.28	2.18	2.06
25	a	608	CLA	CHB-C4A	5.28	1.38	1.33
25	b	613	CLA	CHB-C4A	5.27	1.37	1.33
30	A	616	SQD	O47-C45	-5.26	1.38	1.47
25	b	604	CLA	CHB-C4A	5.24	1.37	1.33
25	A	607	CLA	CHB-C4A	5.24	1.37	1.33
25	B	613	CLA	CHB-C4A	5.23	1.37	1.33
25	b	611	CLA	MG-NA	5.21	2.18	2.06
25	b	602	CLA	CHB-C4A	5.18	1.37	1.33
35	E	101	HEM	C3C-C2C	-5.17	1.33	1.40
25	C	502	CLA	CHB-C4A	5.17	1.37	1.33
25	c	504	CLA	CHB-C4A	5.11	1.37	1.33
25	C	508	CLA	MG-NA	5.05	2.18	2.06
30	F	101	SQD	O48-C23	5.00	1.47	1.33
25	C	501	CLA	CHB-C4A	4.96	1.37	1.33
25	C	511	CLA	MG-NA	4.96	2.18	2.06
25	b	612	CLA	CHB-C4A	4.92	1.37	1.33
30	B	622	SQD	O48-C23	4.83	1.47	1.33
30	L	101	SQD	O48-C23	4.79	1.47	1.33
36	V	201	HEC	C3D-C2D	4.78	1.51	1.37
30	a	614	SQD	O48-C23	4.77	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	613	SQD	O48-C23	4.76	1.47	1.33
25	b	609	CLA	CHB-C4A	4.76	1.37	1.33
30	A	616	SQD	O48-C23	4.75	1.47	1.33
25	a	612	CLA	MG-NA	4.72	2.17	2.06
25	d	404	CLA	CHB-C4A	4.71	1.37	1.33
30	f	102	SQD	O48-C23	4.71	1.47	1.33
25	B	614	CLA	MG-NA	4.70	2.17	2.06
36	v	201	HEC	C3C-C2C	-4.69	1.35	1.40
25	c	507	CLA	MG-NA	4.69	2.17	2.06
25	b	615	CLA	MG-NA	4.66	2.17	2.06
25	C	503	CLA	MG-ND	4.61	2.14	2.05
30	a	613	SQD	O48-C23	4.56	1.46	1.33
25	a	607	CLA	MG-NC	4.55	2.17	2.06
25	b	601	CLA	MG-NA	4.48	2.16	2.06
36	V	201	HEC	C3C-C2C	-4.48	1.35	1.40
25	B	602	CLA	CHB-C4A	4.48	1.37	1.33
25	B	606	CLA	MG-NA	4.46	2.16	2.06
25	a	609	CLA	MG-ND	-4.42	1.97	2.05
25	a	607	CLA	C1D-ND	4.28	1.43	1.37
25	b	612	CLA	MG-ND	-4.24	1.97	2.05
25	a	607	CLA	MG-ND	-4.13	1.97	2.05
25	C	512	CLA	MG-ND	-4.06	1.97	2.05
25	d	403	CLA	C1D-ND	4.03	1.43	1.37
27	b	618	BCR	C30-C25	-4.03	1.48	1.53
25	B	609	CLA	C1D-ND	3.97	1.43	1.37
25	B	607	CLA	C1D-ND	3.95	1.43	1.37
25	A	606	CLA	MG-NA	3.95	2.15	2.06
25	B	611	CLA	CHC-C1C	3.91	1.44	1.34
27	T	101	BCR	C1-C6	-3.91	1.48	1.53
25	B	610	CLA	CHC-C1C	3.89	1.44	1.34
25	a	608	CLA	C1D-ND	3.89	1.43	1.37
30	B	622	SQD	O47-C7	3.89	1.45	1.34
25	D	405	CLA	C1D-ND	3.87	1.42	1.37
27	B	618	BCR	C30-C25	-3.86	1.48	1.53
28	d	406	PL9	C3-C4	-3.86	1.43	1.49
25	C	512	CLA	MG-NA	3.86	2.15	2.06
25	b	608	CLA	CHC-C1C	3.85	1.44	1.34
25	B	616	CLA	MG-NA	3.83	2.15	2.06
25	b	613	CLA	C1D-ND	3.82	1.42	1.37
27	C	514	BCR	C1-C6	-3.80	1.48	1.53
25	c	510	CLA	C1D-ND	3.80	1.42	1.37
25	a	607	CLA	MG-NA	3.79	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	513	CLA	C1D-ND	3.79	1.42	1.37
25	C	506	CLA	C1D-ND	3.79	1.42	1.37
25	B	608	CLA	MG-NA	3.78	2.15	2.06
25	c	504	CLA	CHC-C1C	3.78	1.43	1.34
27	c	515	BCR	C1-C6	-3.78	1.48	1.53
25	b	607	CLA	MG-NA	3.77	2.15	2.06
30	L	101	SQD	O47-C7	3.76	1.44	1.34
25	c	511	CLA	CHC-C1C	3.76	1.43	1.34
25	C	509	CLA	CHC-C1C	3.76	1.43	1.34
25	B	601	CLA	C1D-ND	3.74	1.42	1.37
31	D	412	LHG	O7-C5	-3.74	1.37	1.46
25	a	608	CLA	CHC-C1C	3.74	1.43	1.34
25	b	601	CLA	CHC-C1C	3.73	1.43	1.34
25	c	505	CLA	CHC-C1C	3.73	1.43	1.34
30	a	614	SQD	O47-C7	3.72	1.44	1.34
25	C	504	CLA	CHC-C1C	3.72	1.43	1.34
25	B	613	CLA	MG-ND	-3.71	1.98	2.05
25	B	606	CLA	CHC-C1C	3.71	1.43	1.34
25	b	601	CLA	C1D-ND	3.71	1.42	1.37
25	B	614	CLA	C1D-ND	3.70	1.42	1.37
25	B	603	CLA	CHC-C1C	3.69	1.43	1.34
35	f	101	HEM	C3C-C2C	-3.66	1.35	1.40
30	A	613	SQD	O47-C45	-3.66	1.38	1.46
25	b	612	CLA	C1D-ND	3.66	1.42	1.37
25	c	501	CLA	C1D-ND	3.66	1.42	1.37
25	C	509	CLA	MG-NA	3.65	2.14	2.06
25	B	615	CLA	CHC-C1C	3.65	1.43	1.34
25	C	505	CLA	CHC-C1C	3.64	1.43	1.34
25	A	607	CLA	C1D-ND	3.64	1.42	1.37
25	B	602	CLA	CHC-C1C	3.64	1.43	1.34
27	c	514	BCR	C1-C6	-3.63	1.49	1.53
25	B	608	CLA	MG-NC	3.63	2.14	2.06
25	b	603	CLA	C1D-ND	3.63	1.42	1.37
25	c	513	CLA	C1D-ND	3.63	1.42	1.37
25	A	609	CLA	C1D-ND	3.62	1.42	1.37
25	b	605	CLA	CHC-C1C	3.62	1.43	1.34
25	C	510	CLA	CHC-C1C	3.62	1.43	1.34
25	c	508	CLA	MG-NC	3.62	2.14	2.06
25	B	604	CLA	CHC-C1C	3.61	1.43	1.34
25	B	612	CLA	CHC-C1C	3.60	1.43	1.34
25	c	508	CLA	CHC-C1C	3.60	1.43	1.34
25	d	404	CLA	CHC-C1C	3.60	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	403	CLA	CHC-C1C	3.60	1.43	1.34
25	c	507	CLA	C1D-ND	3.60	1.42	1.37
25	D	404	CLA	C1D-ND	3.60	1.42	1.37
25	a	612	CLA	C1D-ND	3.60	1.42	1.37
25	b	614	CLA	CHC-C1C	3.60	1.43	1.34
25	C	503	CLA	CHC-C1C	3.59	1.43	1.34
25	c	513	CLA	CHC-C1C	3.59	1.43	1.34
25	C	512	CLA	CHC-C1C	3.59	1.43	1.34
25	C	502	CLA	CHC-C1C	3.58	1.43	1.34
25	a	607	CLA	CHC-C1C	3.57	1.43	1.34
25	c	503	CLA	CHC-C1C	3.57	1.43	1.34
25	c	506	CLA	C1D-ND	3.57	1.42	1.37
25	C	513	CLA	CHC-C1C	3.57	1.43	1.34
25	C	503	CLA	C1D-ND	3.56	1.42	1.37
25	c	506	CLA	CHC-C1C	3.56	1.43	1.34
25	b	614	CLA	C1D-ND	3.56	1.42	1.37
25	c	512	CLA	C1D-ND	3.56	1.42	1.37
30	f	102	SQD	O47-C7	3.55	1.44	1.34
25	b	604	CLA	CHC-C1C	3.55	1.43	1.34
30	a	613	SQD	O47-C45	-3.54	1.38	1.46
30	A	616	SQD	O47-C7	3.54	1.44	1.34
25	c	512	CLA	MG-NA	3.53	2.14	2.06
25	B	614	CLA	CHC-C1C	3.51	1.43	1.34
29	D	408	LMG	C4-C5	3.51	1.60	1.53
25	C	508	CLA	CHC-C1C	3.51	1.43	1.34
25	B	605	CLA	CHC-C1C	3.51	1.43	1.34
25	C	509	CLA	C1D-ND	3.50	1.42	1.37
25	B	616	CLA	C1D-ND	3.50	1.42	1.37
25	c	512	CLA	CHC-C1C	3.50	1.43	1.34
25	B	608	CLA	C1D-ND	3.48	1.42	1.37
27	Y	101	BCR	C1-C6	-3.48	1.49	1.53
25	b	616	CLA	C1D-ND	3.47	1.42	1.37
25	C	501	CLA	C1D-ND	3.47	1.42	1.37
32	c	517	DGD	O2G-C2G	-3.47	1.38	1.46
25	C	507	CLA	CHC-C1C	3.47	1.43	1.34
25	A	607	CLA	CHC-C1C	3.46	1.43	1.34
25	B	606	CLA	C1D-ND	3.46	1.42	1.37
25	c	502	CLA	C1D-ND	3.46	1.42	1.37
25	B	614	CLA	MG-ND	-3.44	1.99	2.05
25	B	607	CLA	MG-NA	3.44	2.14	2.06
25	d	403	CLA	CHC-C1C	3.43	1.43	1.34
25	b	606	CLA	C1D-ND	3.42	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	606	CLA	CHC-C1C	3.42	1.43	1.34
25	d	404	CLA	C1D-ND	3.42	1.42	1.37
25	B	607	CLA	CHC-C1C	3.42	1.43	1.34
25	c	501	CLA	CHC-C1C	3.42	1.43	1.34
25	C	506	CLA	CHC-C1C	3.42	1.43	1.34
25	D	403	CLA	C1D-ND	3.42	1.42	1.37
25	B	601	CLA	CHC-C1C	3.41	1.43	1.34
28	D	407	PL9	C6-C1	-3.40	1.42	1.48
25	b	607	CLA	CHC-C1C	3.40	1.42	1.34
25	B	602	CLA	C1D-ND	3.40	1.42	1.37
25	A	606	CLA	CHC-C1C	3.40	1.42	1.34
30	f	102	SQD	O47-C45	-3.39	1.38	1.46
30	F	101	SQD	C24-C23	3.39	1.60	1.50
25	B	613	CLA	CHC-C1C	3.39	1.42	1.34
25	C	504	CLA	MG-NA	3.39	2.14	2.06
25	b	602	CLA	CHC-C1C	3.39	1.42	1.34
25	b	602	CLA	C1D-ND	3.39	1.42	1.37
25	c	510	CLA	CHC-C1C	3.38	1.42	1.34
25	b	615	CLA	CHC-C1C	3.38	1.42	1.34
25	C	504	CLA	C1D-ND	3.37	1.42	1.37
27	d	405	BCR	C1-C6	-3.37	1.49	1.53
25	c	511	CLA	C1D-ND	3.37	1.42	1.37
25	B	611	CLA	C1D-ND	3.37	1.42	1.37
30	a	614	SQD	C24-C23	3.36	1.60	1.50
27	d	405	BCR	C30-C25	-3.36	1.49	1.53
25	c	503	CLA	C1D-ND	3.36	1.42	1.37
25	b	610	CLA	C1D-ND	3.35	1.42	1.37
25	b	608	CLA	C1D-ND	3.35	1.42	1.37
25	c	509	CLA	CHC-C1C	3.35	1.42	1.34
25	C	506	CLA	MG-ND	-3.34	1.99	2.05
27	D	406	BCR	C1-C6	-3.34	1.49	1.53
25	c	509	CLA	C1D-ND	3.33	1.42	1.37
25	B	615	CLA	C1D-ND	3.33	1.42	1.37
35	f	101	HEM	C3C-CAC	3.33	1.55	1.47
27	D	406	BCR	C30-C25	-3.33	1.49	1.53
25	C	508	CLA	C1D-ND	3.32	1.42	1.37
25	C	511	CLA	CHC-C1C	3.32	1.42	1.34
25	b	604	CLA	C1D-ND	3.31	1.42	1.37
25	B	604	CLA	C1D-ND	3.31	1.42	1.37
25	B	603	CLA	MG-NA	3.31	2.14	2.06
25	c	502	CLA	CHC-C1C	3.30	1.42	1.34
25	C	501	CLA	CHC-C1C	3.29	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	509	CLA	MG-ND	3.28	2.12	2.05
32	C	516	DGD	C4D-C3D	3.27	1.60	1.52
25	b	611	CLA	CHC-C1C	3.27	1.42	1.34
27	b	618	BCR	C1-C6	-3.27	1.49	1.53
27	c	514	BCR	C30-C25	-3.27	1.49	1.53
30	B	622	SQD	O5-C1	3.26	1.50	1.41
30	F	101	SQD	O5-C1	3.26	1.50	1.41
25	C	501	CLA	MG-NA	3.25	2.14	2.06
30	B	622	SQD	O47-C45	-3.25	1.38	1.46
27	k	101	BCR	C1-C6	-3.25	1.49	1.53
25	b	609	CLA	MG-ND	-3.24	1.99	2.05
25	B	603	CLA	MG-ND	3.23	2.12	2.05
27	B	617	BCR	C1-C6	-3.23	1.49	1.53
25	C	512	CLA	C1D-ND	3.22	1.42	1.37
27	K	101	BCR	C30-C25	-3.22	1.49	1.53
30	f	102	SQD	C24-C23	3.22	1.60	1.50
25	d	403	CLA	MG-NA	3.21	2.13	2.06
25	b	613	CLA	MG-ND	-3.21	1.99	2.05
25	B	616	CLA	CHC-C1C	3.21	1.42	1.34
25	D	404	CLA	CHC-C1C	3.20	1.42	1.34
25	b	616	CLA	CHC-C1C	3.20	1.42	1.34
30	A	613	SQD	C24-C23	3.19	1.60	1.50
25	c	508	CLA	C1D-ND	3.19	1.42	1.37
25	A	607	CLA	MG-NA	3.18	2.13	2.06
25	b	609	CLA	C1D-ND	3.18	1.42	1.37
25	C	502	CLA	MG-ND	-3.18	1.99	2.05
32	A	617	DGD	O5D-C6D	-3.17	1.38	1.43
25	b	607	CLA	C1D-ND	3.17	1.42	1.37
25	b	609	CLA	CHC-C1C	3.15	1.42	1.34
25	C	511	CLA	C1D-ND	3.14	1.42	1.37
25	A	606	CLA	C1D-ND	3.14	1.42	1.37
30	a	614	SQD	O47-C45	-3.14	1.39	1.46
25	a	609	CLA	CHC-C1C	3.13	1.42	1.34
25	b	611	CLA	C1D-ND	3.13	1.42	1.37
25	b	610	CLA	MG-NA	3.13	2.13	2.06
25	C	510	CLA	C1D-ND	3.12	1.42	1.37
25	C	507	CLA	C1D-ND	3.12	1.42	1.37
25	c	507	CLA	CHC-C1C	3.11	1.42	1.34
25	b	603	CLA	CHC-C1C	3.11	1.42	1.34
27	B	619	BCR	C1-C6	-3.11	1.49	1.53
25	c	509	CLA	MG-NC	3.11	2.13	2.06
25	C	502	CLA	C1D-ND	3.10	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	608	CLA	MG-NA	3.09	2.13	2.06
31	d	407	LHG	O7-C5	-3.08	1.39	1.46
25	B	610	CLA	CMB-C2B	-3.08	1.45	1.51
25	B	609	CLA	CHC-C1C	3.08	1.42	1.34
31	D	410	LHG	P-O6	3.08	1.71	1.59
25	D	405	CLA	CHC-C1C	3.08	1.42	1.34
27	H	101	BCR	C30-C25	-3.08	1.49	1.53
25	c	503	CLA	MG-NA	3.07	2.13	2.06
27	K	102	BCR	C30-C25	-3.07	1.49	1.53
35	E	101	HEM	C3C-C4C	3.06	1.45	1.41
30	L	101	SQD	O47-C45	-3.06	1.39	1.46
27	b	619	BCR	C1-C6	-3.06	1.49	1.53
30	A	616	SQD	C24-C23	3.05	1.59	1.50
25	C	505	CLA	C1D-ND	3.05	1.41	1.37
27	b	619	BCR	C30-C25	-3.04	1.49	1.53
30	A	613	SQD	O47-C7	3.04	1.42	1.34
25	B	612	CLA	C1D-ND	3.04	1.41	1.37
25	B	608	CLA	CHC-C1C	3.04	1.42	1.34
25	c	513	CLA	MG-NC	3.04	2.13	2.06
32	C	515	DGD	O2G-C2G	-3.03	1.39	1.46
30	f	102	SQD	O5-C1	3.03	1.49	1.41
30	B	622	SQD	C24-C23	3.03	1.59	1.50
30	a	613	SQD	O47-C7	3.03	1.42	1.34
25	D	405	CLA	MG-NA	3.02	2.13	2.06
30	a	613	SQD	C24-C23	3.02	1.59	1.50
25	A	609	CLA	CHC-C1C	3.01	1.42	1.34
27	c	516	BCR	C1-C6	-3.01	1.49	1.53
25	b	612	CLA	CHC-C1C	2.99	1.41	1.34
25	b	609	CLA	CMB-C2B	-2.99	1.45	1.51
35	E	101	HEM	CAB-C3B	2.99	1.55	1.47
25	b	615	CLA	C1D-ND	2.98	1.41	1.37
30	L	101	SQD	O5-C1	2.98	1.49	1.41
25	b	603	CLA	MG-NA	2.98	2.13	2.06
25	a	612	CLA	CHC-C1C	2.97	1.41	1.34
32	c	519	DGD	C6D-C5D	2.97	1.60	1.51
27	x	101	BCR	C30-C25	-2.97	1.50	1.53
27	K	101	BCR	C1-C6	-2.96	1.50	1.53
25	C	507	CLA	MG-ND	-2.94	1.99	2.05
26	d	402	PHO	CAC-C3C	-2.93	1.47	1.52
27	k	101	BCR	C30-C25	-2.93	1.50	1.53
25	b	605	CLA	C1D-ND	2.93	1.41	1.37
35	E	101	HEM	C3C-CAC	2.92	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	617	BCR	C1-C6	-2.92	1.50	1.53
27	A	610	BCR	C1-C6	-2.92	1.50	1.53
25	c	506	CLA	MG-NC	2.92	2.13	2.06
25	b	613	CLA	CHC-C1C	2.92	1.41	1.34
32	H	102	DGD	O5D-C1E	2.92	1.45	1.40
25	c	504	CLA	MG-ND	-2.91	2.00	2.05
25	B	613	CLA	C1D-ND	2.90	1.41	1.37
25	B	610	CLA	C1D-ND	2.89	1.41	1.37
27	c	516	BCR	C30-C25	-2.89	1.50	1.53
25	a	609	CLA	C1D-ND	2.87	1.41	1.37
27	c	515	BCR	C30-C25	-2.86	1.50	1.53
32	a	615	DGD	O1G-C1A	2.86	1.41	1.33
30	L	101	SQD	C24-C23	2.86	1.59	1.50
25	b	613	CLA	CMB-C2B	-2.85	1.45	1.51
25	c	505	CLA	C1D-ND	2.82	1.41	1.37
25	c	510	CLA	MG-NC	2.82	2.13	2.06
25	C	510	CLA	MG-NA	2.82	2.13	2.06
25	C	507	CLA	MG-NA	2.81	2.13	2.06
25	b	615	CLA	CMB-C2B	-2.81	1.46	1.51
25	d	403	CLA	CMB-C2B	-2.80	1.46	1.51
25	b	610	CLA	CHC-C1C	2.79	1.41	1.34
25	c	510	CLA	CMB-C2B	-2.79	1.46	1.51
27	Y	101	BCR	C30-C25	-2.78	1.50	1.53
25	a	607	CLA	CMB-C2B	-2.78	1.46	1.51
27	K	102	BCR	C1-C6	-2.77	1.50	1.53
30	A	613	SQD	O5-C1	2.77	1.49	1.41
25	B	605	CLA	MG-NA	2.76	2.12	2.06
25	B	613	CLA	MG-NA	2.76	2.12	2.06
28	D	407	PL9	C52-C5	-2.75	1.45	1.50
25	C	513	CLA	MG-NA	2.75	2.12	2.06
32	h	101	DGD	O2G-C2G	-2.74	1.40	1.46
29	m	101	LMG	C4-C3	2.73	1.59	1.52
25	c	504	CLA	C1D-ND	2.72	1.41	1.37
25	B	601	CLA	CMB-C2B	-2.72	1.46	1.51
25	B	602	CLA	CMB-C2B	-2.72	1.46	1.51
25	a	608	CLA	MG-ND	-2.72	2.00	2.05
25	C	511	CLA	CMB-C2B	-2.71	1.46	1.51
27	a	610	BCR	C1-C6	-2.70	1.50	1.53
25	B	605	CLA	C1D-ND	2.70	1.41	1.37
25	C	506	CLA	MG-NA	2.69	2.12	2.06
27	T	101	BCR	C30-C25	-2.69	1.50	1.53
32	A	617	DGD	C1E-C2E	2.67	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	402	PHO	CAC-C3C	-2.67	1.47	1.52
35	f	101	HEM	CAB-C3B	2.67	1.54	1.47
25	C	502	CLA	MG-NA	2.66	2.12	2.06
31	d	409	LHG	P-O6	2.66	1.69	1.59
27	B	617	BCR	C30-C25	-2.65	1.50	1.53
25	B	612	CLA	MG-NA	2.65	2.12	2.06
25	B	610	CLA	C3B-C2B	-2.64	1.36	1.40
29	c	524	LMG	C4-C5	2.63	1.58	1.53
28	A	611	PL9	C7-C3	-2.63	1.47	1.51
30	A	616	SQD	C46-C45	2.62	1.56	1.50
31	D	412	LHG	C24-C23	2.61	1.58	1.50
32	h	101	DGD	C1E-C2E	2.61	1.60	1.52
25	a	608	CLA	CMB-C2B	-2.61	1.46	1.51
29	d	411	LMG	C4-C5	2.60	1.58	1.53
25	B	606	CLA	C3B-C2B	-2.60	1.36	1.40
25	B	606	CLA	CMB-C2B	-2.60	1.46	1.51
31	A	614	LHG	P-O6	2.60	1.69	1.59
28	a	611	PL9	C53-C6	-2.60	1.45	1.50
25	a	612	CLA	CMB-C2B	-2.60	1.46	1.51
29	b	621	LMG	C3-C2	2.59	1.59	1.52
25	c	501	CLA	CMB-C2B	-2.59	1.46	1.51
25	D	405	CLA	MG-NC	2.59	2.12	2.06
25	b	614	CLA	MG-ND	-2.57	2.00	2.05
27	b	617	BCR	C30-C25	-2.57	1.50	1.53
27	C	514	BCR	C30-C25	-2.57	1.50	1.53
25	c	510	CLA	MG-NA	2.57	2.12	2.06
25	c	513	CLA	MG-ND	-2.56	2.00	2.05
25	A	609	CLA	MG-ND	-2.55	2.00	2.05
25	D	405	CLA	CMB-C2B	-2.55	1.46	1.51
25	b	603	CLA	CMB-C2B	-2.55	1.46	1.51
25	B	603	CLA	CMC-C2C	-2.55	1.45	1.50
32	A	617	DGD	C3E-C2E	2.55	1.58	1.52
31	D	409	LHG	P-O6	2.55	1.69	1.59
32	A	617	DGD	C4D-C5D	2.55	1.58	1.53
25	C	507	CLA	CMB-C2B	-2.54	1.46	1.51
32	c	519	DGD	O2G-C2G	-2.54	1.40	1.46
25	B	608	CLA	CMB-C2B	-2.54	1.46	1.51
25	B	614	CLA	CMB-C2B	-2.53	1.46	1.51
25	c	512	CLA	CMB-C2B	-2.53	1.46	1.51
25	c	502	CLA	CMB-C2B	-2.53	1.46	1.51
25	c	510	CLA	MG-ND	-2.52	2.00	2.05
29	m	101	LMG	O7-C8	-2.52	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	H	102	DGD	O1G-C1G	-2.52	1.39	1.45
30	a	613	SQD	O5-C1	2.51	1.48	1.41
25	d	404	CLA	CMB-C2B	-2.51	1.46	1.51
25	c	513	CLA	CMB-C2B	-2.51	1.46	1.51
25	C	509	CLA	CMB-C2B	-2.50	1.46	1.51
31	e	101	LHG	P-O6	2.50	1.69	1.59
25	c	507	CLA	CMB-C2B	-2.50	1.46	1.51
27	t	101	BCR	C1-C6	-2.49	1.50	1.53
25	c	507	CLA	C3B-C2B	-2.48	1.37	1.40
25	b	616	CLA	CMB-C2B	-2.48	1.46	1.51
29	D	411	LMG	C7-C8	2.48	1.57	1.51
32	A	617	DGD	C6E-C5E	2.47	1.60	1.51
25	C	512	CLA	CMB-C2B	-2.47	1.46	1.51
32	C	516	DGD	C1E-C2E	2.46	1.59	1.52
25	b	604	CLA	CMB-C2B	-2.45	1.46	1.51
25	b	612	CLA	CMB-C2B	-2.45	1.46	1.51
25	C	501	CLA	CMB-C2B	-2.45	1.46	1.51
25	c	510	CLA	CMD-C2D	-2.44	1.45	1.50
28	d	406	PL9	C6-C1	-2.44	1.44	1.48
25	b	608	CLA	CMB-C2B	-2.43	1.46	1.51
25	a	609	CLA	CMB-C2B	-2.43	1.46	1.51
25	c	509	CLA	CMB-C2B	-2.43	1.46	1.51
25	b	607	CLA	CMB-C2B	-2.43	1.46	1.51
30	a	613	SQD	O7-S	2.43	1.52	1.45
35	f	101	HEM	C3C-C4C	2.43	1.44	1.41
25	b	615	CLA	CMD-C2D	-2.43	1.45	1.50
32	C	515	DGD	C4D-C3D	2.42	1.58	1.52
25	b	614	CLA	MG-NA	2.41	2.12	2.06
25	C	502	CLA	CMB-C2B	-2.41	1.46	1.51
30	B	622	SQD	O9-S	2.41	1.51	1.45
25	b	601	CLA	CMB-C2B	-2.41	1.46	1.51
25	B	603	CLA	CMB-C2B	-2.41	1.46	1.51
25	B	603	CLA	C1D-ND	2.40	1.41	1.37
30	A	613	SQD	O9-S	2.40	1.51	1.45
27	B	618	BCR	C1-C6	-2.40	1.50	1.53
25	c	504	CLA	CMB-C2B	-2.39	1.46	1.51
25	b	615	CLA	MG-ND	-2.39	2.01	2.05
25	c	503	CLA	CMB-C2B	-2.39	1.46	1.51
25	D	405	CLA	CMC-C2C	-2.38	1.45	1.50
25	D	403	CLA	C1D-C2D	2.38	1.50	1.45
30	F	101	SQD	O7-S	2.38	1.51	1.45
25	B	603	CLA	CMD-C2D	-2.38	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	518	DGD	C4D-C3D	2.38	1.58	1.52
29	M	101	LMG	C4-C5	2.37	1.58	1.53
25	D	404	CLA	CMB-C2B	-2.37	1.46	1.51
32	H	102	DGD	C4D-C5D	2.37	1.58	1.53
30	F	101	SQD	O9-S	2.37	1.51	1.45
25	b	607	CLA	CMD-C2D	-2.35	1.45	1.50
25	c	506	CLA	MG-ND	-2.35	2.01	2.05
32	C	516	DGD	C1G-C2G	2.35	1.58	1.50
25	b	614	CLA	CMC-C2C	-2.35	1.45	1.50
25	a	609	CLA	CMC-C2C	-2.35	1.46	1.50
30	L	101	SQD	O9-S	2.34	1.51	1.45
25	b	610	CLA	CMB-C2B	-2.34	1.46	1.51
28	d	406	PL9	C46-C44	-2.34	1.46	1.51
30	F	101	SQD	O5-C5	2.33	1.50	1.44
25	D	404	CLA	CMD-C2D	-2.33	1.46	1.50
25	c	508	CLA	CMB-C2B	-2.33	1.47	1.51
25	B	604	CLA	CMB-C2B	-2.33	1.47	1.51
26	d	402	PHO	CMC-C2C	-2.33	1.46	1.51
30	f	102	SQD	O9-S	2.33	1.51	1.45
25	b	605	CLA	CMB-C2B	-2.32	1.47	1.51
32	C	515	DGD	C4E-C3E	2.32	1.58	1.52
32	c	518	DGD	C3D-C2D	2.32	1.58	1.52
25	B	616	CLA	CMC-C2C	-2.32	1.46	1.50
25	C	503	CLA	CMB-C2B	-2.32	1.47	1.51
25	b	611	CLA	CMB-C2B	-2.32	1.47	1.51
25	B	615	CLA	CMB-C2B	-2.32	1.47	1.51
25	B	601	CLA	CMC-C2C	-2.31	1.46	1.50
25	B	609	CLA	CMD-C2D	-2.31	1.46	1.50
25	B	616	CLA	MG-NC	2.30	2.11	2.06
25	c	512	CLA	C3B-C2B	-2.30	1.37	1.40
25	b	607	CLA	C3B-C2B	-2.30	1.37	1.40
25	C	513	CLA	CMB-C2B	-2.30	1.47	1.51
32	C	517	DGD	C6D-C5D	2.29	1.58	1.51
25	C	502	CLA	C3B-C2B	-2.29	1.37	1.40
25	b	612	CLA	MG-NC	2.29	2.11	2.06
25	b	610	CLA	C3B-C2B	-2.29	1.37	1.40
26	d	401	PHO	O2D-CGD	2.29	1.38	1.33
25	B	611	CLA	CMB-C2B	-2.29	1.47	1.51
25	b	611	CLA	CMD-C2D	-2.29	1.46	1.50
25	b	603	CLA	CMD-C2D	-2.28	1.46	1.50
25	b	604	CLA	MG-NC	2.28	2.11	2.06
25	B	608	CLA	CMD-C2D	-2.28	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	615	LHG	O8-C23	2.27	1.40	1.33
25	B	601	CLA	C3B-C2B	-2.27	1.37	1.40
25	B	605	CLA	C3B-C2B	-2.27	1.37	1.40
26	A	608	PHO	CAC-C3C	-2.27	1.48	1.52
30	B	622	SQD	O7-S	2.26	1.51	1.45
25	B	608	CLA	C1D-C2D	2.26	1.49	1.45
25	B	604	CLA	MG-NA	2.26	2.11	2.06
29	c	522	LMG	C3-C2	2.25	1.58	1.52
27	x	101	BCR	C1-C6	-2.25	1.50	1.53
25	c	504	CLA	CMD-C2D	-2.24	1.46	1.50
32	c	519	DGD	O1G-C1G	-2.24	1.40	1.45
25	b	613	CLA	CMD-C2D	-2.24	1.46	1.50
25	b	609	CLA	MG-NA	2.24	2.11	2.06
25	b	614	CLA	CMB-C2B	-2.24	1.47	1.51
25	c	503	CLA	CMC-C2C	-2.24	1.46	1.50
28	d	406	PL9	C41-C39	-2.24	1.46	1.51
30	f	102	SQD	O7-S	2.24	1.51	1.45
29	c	522	LMG	C4-C3	2.23	1.58	1.52
31	A	615	LHG	O7-C5	-2.23	1.41	1.46
32	c	518	DGD	O6D-C5D	-2.23	1.38	1.44
32	c	517	DGD	C4D-C3D	2.22	1.58	1.52
25	B	613	CLA	CMD-C2D	-2.22	1.46	1.50
25	C	508	CLA	CMB-C2B	-2.22	1.47	1.51
25	b	616	CLA	CMC-C2C	-2.22	1.46	1.50
25	C	513	CLA	CMC-C2C	-2.22	1.46	1.50
25	C	504	CLA	CMB-C2B	-2.22	1.47	1.51
25	c	506	CLA	CMB-C2B	-2.22	1.47	1.51
32	H	102	DGD	C1E-C2E	2.22	1.59	1.52
27	a	610	BCR	C30-C25	-2.22	1.50	1.53
29	d	411	LMG	O1-C7	-2.21	1.39	1.43
29	A	612	LMG	C4-C5	2.21	1.57	1.53
26	A	608	PHO	CMC-C2C	-2.21	1.46	1.51
32	c	518	DGD	O2G-C2G	-2.21	1.41	1.46
29	C	518	LMG	O7-C8	-2.20	1.41	1.46
25	d	403	CLA	CMD-C2D	-2.20	1.46	1.50
26	D	402	PHO	CMC-C2C	-2.20	1.46	1.51
27	H	101	BCR	C1-C6	-2.20	1.51	1.53
25	c	502	CLA	CMD-C2D	-2.20	1.46	1.50
25	c	506	CLA	CMC-C2C	-2.20	1.46	1.50
30	B	622	SQD	C8-C7	2.20	1.57	1.50
25	c	508	CLA	MG-ND	2.19	2.10	2.05
25	A	607	CLA	CMB-C2B	-2.19	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	516	DGD	O2G-C2G	-2.19	1.41	1.46
25	c	511	CLA	CMB-C2B	-2.18	1.47	1.51
35	f	101	HEM	C3B-C2B	-2.18	1.32	1.37
25	B	616	CLA	CMB-C2B	-2.18	1.47	1.51
29	b	621	LMG	C1-C2	2.18	1.58	1.52
32	h	101	DGD	C4D-C3D	2.18	1.58	1.52
30	f	102	SQD	O5-C5	2.18	1.49	1.44
25	C	509	CLA	O2D-CGD	2.18	1.38	1.33
25	C	510	CLA	MG-NC	2.18	2.11	2.06
25	B	611	CLA	CMD-C2D	-2.17	1.46	1.50
25	c	512	CLA	C1D-C2D	2.16	1.49	1.45
25	b	608	CLA	C3C-C2C	2.16	1.41	1.36
29	m	101	LMG	O1-C7	-2.16	1.40	1.43
25	B	607	CLA	CMB-C2B	-2.16	1.47	1.51
25	A	606	CLA	MG-ND	-2.15	2.01	2.05
25	a	609	CLA	CMD-C2D	-2.15	1.46	1.50
30	L	101	SQD	O7-S	2.15	1.51	1.45
27	B	619	BCR	C30-C25	-2.14	1.51	1.53
25	C	512	CLA	CMD-C2D	-2.14	1.46	1.50
32	c	517	DGD	C4D-C5D	2.14	1.57	1.53
29	D	408	LMG	O2-C2	-2.14	1.37	1.43
25	c	504	CLA	CMC-C2C	-2.14	1.46	1.50
25	B	605	CLA	CMB-C2B	-2.14	1.47	1.51
25	A	607	CLA	C3B-C2B	-2.14	1.37	1.40
25	d	404	CLA	MG-NA	2.14	2.11	2.06
25	C	503	CLA	MG-NC	2.14	2.11	2.06
31	d	408	LHG	O7-C5	-2.14	1.41	1.46
32	C	517	DGD	O1G-C1G	-2.13	1.40	1.45
25	B	607	CLA	CMC-C2C	-2.13	1.46	1.50
25	b	615	CLA	C3B-C2B	-2.13	1.37	1.40
26	D	402	PHO	CMB-C2B	-2.13	1.46	1.51
25	c	508	CLA	CMD-C2D	-2.13	1.46	1.50
25	A	609	CLA	CMB-C2B	-2.13	1.47	1.51
25	b	612	CLA	CMC-C2C	-2.12	1.46	1.50
30	a	614	SQD	C44-C45	2.12	1.56	1.51
32	A	617	DGD	C4E-C5E	2.12	1.57	1.53
25	D	403	CLA	MG-NC	2.12	2.11	2.06
29	c	524	LMG	C1-C2	2.12	1.58	1.52
32	C	517	DGD	O2G-C2G	-2.12	1.41	1.46
27	t	101	BCR	C30-C25	-2.11	1.51	1.53
29	c	522	LMG	C1-C2	2.11	1.58	1.52
27	B	617	BCR	C33-C5	-2.11	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	510	CLA	CMB-C2B	-2.11	1.47	1.51
27	k	101	BCR	C33-C5	-2.11	1.47	1.50
25	C	506	CLA	CMC-C2C	-2.11	1.46	1.50
35	E	101	HEM	CMD-C2D	2.11	1.55	1.50
35	f	101	HEM	FE-NB	2.10	2.09	1.98
25	B	604	CLA	CMD-C2D	-2.10	1.46	1.50
32	C	516	DGD	O5D-C6D	-2.10	1.40	1.43
25	C	506	CLA	CMB-C2B	-2.10	1.47	1.51
31	d	407	LHG	C24-C23	2.10	1.56	1.50
25	B	612	CLA	CMC-C2C	-2.10	1.46	1.50
32	H	102	DGD	O2G-C2G	-2.09	1.41	1.46
25	C	508	CLA	C1D-C2D	2.09	1.49	1.45
31	A	615	LHG	P-O6	2.09	1.67	1.59
32	A	617	DGD	O2G-C2G	-2.09	1.41	1.46
25	C	512	CLA	C1D-C2D	2.09	1.49	1.45
25	A	609	CLA	MG-NA	-2.09	2.01	2.06
25	c	508	CLA	CMC-C2C	-2.08	1.46	1.50
25	b	609	CLA	CMD-C2D	-2.08	1.46	1.50
31	l	101	LHG	P-O6	2.08	1.67	1.59
30	a	613	SQD	O9-S	2.08	1.51	1.45
25	B	605	CLA	CMC-C2C	-2.08	1.46	1.50
25	b	606	CLA	CMB-C2B	-2.08	1.47	1.51
25	A	609	CLA	CMD-C2D	-2.08	1.46	1.50
25	b	616	CLA	CMD-C2D	-2.08	1.46	1.50
25	c	506	CLA	CMD-C2D	-2.08	1.46	1.50
26	d	402	PHO	CMD-C2D	-2.08	1.46	1.51
25	c	505	CLA	CMB-C2B	-2.08	1.47	1.51
25	a	609	CLA	C4B-CHC	-2.07	1.35	1.41
32	C	516	DGD	C4D-C5D	2.07	1.57	1.53
25	c	501	CLA	MG-NC	2.07	2.11	2.06
25	B	607	CLA	C3D-C4D	2.06	1.48	1.44
25	a	608	CLA	CMC-C2C	-2.06	1.46	1.50
26	D	402	PHO	CMD-C2D	-2.06	1.46	1.51
32	a	615	DGD	C1G-C2G	2.06	1.57	1.50
25	b	610	CLA	CMD-C2D	-2.05	1.46	1.50
26	d	401	PHO	CAC-C3C	-2.05	1.48	1.52
26	A	608	PHO	CMD-C2D	-2.05	1.46	1.51
27	d	405	BCR	C38-C26	-2.05	1.47	1.50
25	b	601	CLA	C3D-C4D	2.05	1.48	1.44
25	B	606	CLA	CMD-C2D	-2.05	1.46	1.50
29	A	612	LMG	C4-C3	2.05	1.57	1.52
29	D	408	LMG	C7-C8	2.05	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	611	PL9	C25-C24	-2.04	1.45	1.50
25	A	606	CLA	CMD-C2D	-2.04	1.46	1.50
25	c	502	CLA	CMC-C2C	-2.04	1.46	1.50
27	k	101	BCR	C38-C26	-2.04	1.47	1.50
31	D	409	LHG	O8-C6	-2.04	1.40	1.45
32	C	515	DGD	C3E-C2E	2.04	1.57	1.52
25	B	613	CLA	CMB-C2B	-2.04	1.47	1.51
30	a	614	SQD	C25-C24	2.03	1.59	1.52
25	b	606	CLA	MG-ND	2.03	2.09	2.05
25	C	510	CLA	CMC-C2C	-2.03	1.46	1.50
30	a	614	SQD	C46-C45	2.03	1.57	1.50
25	b	601	CLA	CMC-C2C	-2.03	1.46	1.50
25	c	503	CLA	CMD-C2D	-2.03	1.46	1.50
25	B	601	CLA	MG-ND	-2.03	2.01	2.05
31	D	409	LHG	O7-C5	-2.03	1.41	1.46
25	a	607	CLA	C3D-C4D	2.02	1.48	1.44
25	C	510	CLA	CMD-C2D	-2.02	1.46	1.50
25	c	502	CLA	C4B-CHC	-2.02	1.35	1.41
25	c	505	CLA	CMC-C2C	-2.02	1.46	1.50
25	B	605	CLA	CMD-C2D	-2.02	1.46	1.50
25	b	605	CLA	CMD-C2D	-2.02	1.46	1.50
25	b	610	CLA	C3D-C4D	2.02	1.48	1.44
25	B	609	CLA	O2D-CGD	2.02	1.38	1.33
25	B	601	CLA	CMD-C2D	-2.02	1.46	1.50
27	b	617	BCR	C33-C5	-2.01	1.47	1.50
25	C	502	CLA	CMC-C2C	-2.01	1.46	1.50
25	c	512	CLA	CMD-C2D	-2.01	1.46	1.50
30	L	101	SQD	O6-C44	2.01	1.47	1.43
27	A	610	BCR	C33-C5	-2.01	1.47	1.50
25	C	507	CLA	MG-NC	2.01	2.11	2.06
25	b	602	CLA	CMB-C2B	-2.00	1.47	1.51
25	B	602	CLA	C1D-C2D	2.00	1.49	1.45
25	b	611	CLA	CMC-C2C	-2.00	1.46	1.50
25	b	608	CLA	C1D-C2D	2.00	1.49	1.45

All (1157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	511	CLA	C4A-NA-C1A	10.11	111.29	106.68
25	c	509	CLA	C4A-NA-C1A	9.52	111.02	106.68
25	c	503	CLA	C4A-NA-C1A	8.89	110.74	106.68
25	B	604	CLA	C4A-NA-C1A	8.88	110.73	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	601	CLA	C4A-NA-C1A	8.20	110.42	106.68
25	b	606	CLA	C4A-NA-C1A	8.11	110.38	106.68
36	V	201	HEC	CBB-CAB-C3B	-8.02	108.73	127.49
25	C	513	CLA	C4A-NA-C1A	7.99	110.33	106.68
25	b	604	CLA	C4A-NA-C1A	7.83	110.25	106.68
25	C	507	CLA	C4A-NA-C1A	7.68	110.18	106.68
25	B	601	CLA	C4A-NA-C1A	7.57	110.13	106.68
25	C	503	CLA	C4A-NA-C1A	7.34	110.03	106.68
25	B	616	CLA	C4A-NA-C1A	7.32	110.02	106.68
25	B	607	CLA	C4A-NA-C1A	7.30	110.01	106.68
25	C	511	CLA	C4A-NA-C1A	7.17	109.95	106.68
25	B	615	CLA	C4A-NA-C1A	7.13	109.93	106.68
25	C	501	CLA	C4A-NA-C1A	7.13	109.93	106.68
36	v	201	HEC	CBB-CAB-C3B	-7.05	110.99	127.49
30	L	101	SQD	O6-C1-C2	7.04	118.97	108.27
25	C	508	CLA	C4A-NA-C1A	6.92	109.83	106.68
25	b	611	CLA	C4A-NA-C1A	6.89	109.82	106.68
30	a	613	SQD	O6-C1-C2	6.73	118.50	108.27
25	D	405	CLA	C4A-NA-C1A	6.66	109.72	106.68
25	c	501	CLA	C4A-NA-C1A	6.66	109.72	106.68
36	v	201	HEC	CBC-CAC-C3C	-6.60	112.04	127.49
25	c	506	CLA	C4A-NA-C1A	6.56	109.67	106.68
25	c	510	CLA	C4A-NA-C1A	6.47	109.63	106.68
25	C	505	CLA	C4A-NA-C1A	6.46	109.62	106.68
30	a	613	SQD	C1-O5-C5	-6.32	101.38	113.72
25	B	608	CLA	C4A-NA-C1A	6.15	109.49	106.68
25	C	506	CLA	C4A-NA-C1A	6.14	109.48	106.68
30	A	613	SQD	O6-C1-C2	6.13	117.59	108.27
25	c	508	CLA	C4A-NA-C1A	6.10	109.46	106.68
25	B	606	CLA	C4A-NA-C1A	5.98	109.41	106.68
25	c	512	CLA	C4A-NA-C1A	5.98	109.41	106.68
25	c	507	CLA	C4A-NA-C1A	5.91	109.38	106.68
25	C	509	CLA	C4A-NA-C1A	5.89	109.37	106.68
36	V	201	HEC	CBC-CAC-C3C	-5.80	113.92	127.49
25	b	615	CLA	C4A-NA-C1A	5.75	109.30	106.68
25	D	404	CLA	C4A-NA-C1A	5.72	109.29	106.68
25	b	607	CLA	C4A-NA-C1A	5.71	109.29	106.68
25	c	504	CLA	C4A-NA-C1A	5.64	109.25	106.68
25	c	505	CLA	C4A-NA-C1A	5.62	109.24	106.68
25	a	612	CLA	C4A-NA-C1A	5.61	109.24	106.68
25	B	609	CLA	C4A-NA-C1A	5.60	109.23	106.68
25	b	616	CLA	CMB-C2B-C1B	-5.58	120.28	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	608	CLA	C4A-NA-C1A	5.50	109.19	106.68
28	a	611	PL9	C7-C3-C4	5.48	121.43	116.91
25	C	512	CLA	C4A-NA-C1A	5.48	109.18	106.68
36	V	201	HEC	CBD-CAD-C3D	-5.46	103.35	112.54
25	b	616	CLA	C4A-NA-C1A	5.43	109.16	106.68
25	D	405	CLA	CMB-C2B-C1B	-5.42	120.52	128.46
25	c	504	CLA	CMB-C2B-C1B	-5.38	120.57	128.46
28	D	407	PL9	C7-C3-C4	5.38	121.34	116.91
25	c	502	CLA	C4A-NA-C1A	5.33	109.11	106.68
25	b	604	CLA	C1-C2-C3	-5.33	117.46	126.20
25	d	404	CLA	CMB-C2B-C1B	-5.32	120.67	128.46
30	A	613	SQD	C1-O5-C5	-5.30	103.36	113.72
25	B	613	CLA	C1-C2-C3	-5.26	117.57	126.20
25	B	608	CLA	CMB-C2B-C1B	-5.25	120.77	128.46
25	c	513	CLA	C4A-NA-C1A	5.24	109.07	106.68
25	B	605	CLA	C4A-NA-C1A	5.21	109.06	106.68
25	B	602	CLA	CMB-C2B-C1B	-5.18	120.86	128.46
25	C	510	CLA	C4A-NA-C1A	5.18	109.04	106.68
25	B	602	CLA	C4A-NA-C1A	5.12	109.02	106.68
25	A	609	CLA	CMB-C2B-C1B	-5.07	121.02	128.46
25	a	607	CLA	C4A-NA-C1A	5.05	108.98	106.68
25	b	613	CLA	C4A-NA-C1A	5.00	108.96	106.68
25	b	603	CLA	C4A-NA-C1A	4.99	108.95	106.68
25	C	509	CLA	CMB-C2B-C1B	-4.93	121.24	128.46
25	b	609	CLA	CMB-C2B-C1B	-4.90	121.28	128.46
25	c	513	CLA	CMB-C2B-C1B	-4.88	121.31	128.46
25	c	510	CLA	CMB-C2B-C1B	-4.75	121.49	128.46
26	D	402	PHO	C1-C2-C3	-4.74	118.43	126.20
25	B	612	CLA	C4A-NA-C1A	4.70	108.83	106.68
25	a	608	CLA	C4A-NA-C1A	4.70	108.82	106.68
25	B	608	CLA	O2D-CGD-O1D	-4.69	114.71	123.85
25	B	612	CLA	CMB-C2B-C1B	-4.69	121.58	128.46
25	B	613	CLA	CMB-C2B-C1B	-4.68	121.60	128.46
25	d	403	CLA	CMB-C2B-C1B	-4.66	121.63	128.46
25	b	613	CLA	CMB-C2B-C1B	-4.66	121.63	128.46
28	A	611	PL9	C7-C3-C4	4.64	120.73	116.91
30	F	101	SQD	C1-O5-C5	-4.64	104.66	113.72
26	d	402	PHO	C1-C2-C3	-4.64	118.60	126.20
25	b	608	CLA	CMB-C2B-C1B	-4.59	121.73	128.46
31	A	615	LHG	O4-P-O5	4.58	133.76	112.44
30	a	614	SQD	O47-C7-C8	4.58	121.38	111.48
25	B	610	CLA	C4A-NA-C1A	4.57	108.77	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	622	SQD	O47-C7-C8	4.57	121.37	111.48
25	C	510	CLA	CMB-C2B-C1B	-4.56	121.78	128.46
25	B	614	CLA	C4A-NA-C1A	4.52	108.74	106.68
30	A	613	SQD	C1-C2-C3	-4.50	100.54	110.01
25	b	606	CLA	CMB-C2B-C1B	-4.50	121.87	128.46
25	c	506	CLA	CMB-C2B-C1B	-4.50	121.87	128.46
25	B	611	CLA	C4A-NA-C1A	4.47	108.72	106.68
25	b	603	CLA	CMB-C2B-C1B	-4.44	121.94	128.46
25	B	610	CLA	O2D-CGD-O1D	-4.44	115.20	123.85
30	F	101	SQD	O9-S-C6	4.44	113.39	106.76
25	C	504	CLA	CMB-C2B-C1B	-4.44	121.96	128.46
31	e	101	LHG	O4-P-O5	4.43	133.03	112.44
31	D	412	LHG	O4-P-O5	4.40	132.92	112.44
28	a	611	PL9	C7-C3-C2	-4.40	118.20	123.39
25	d	403	CLA	C4A-NA-C1A	4.39	108.68	106.68
27	K	101	BCR	C11-C10-C9	-4.38	121.14	127.28
31	A	614	LHG	O4-P-O5	4.37	132.76	112.44
25	B	604	CLA	CMB-C2B-C1B	-4.35	122.08	128.46
28	d	406	PL9	C7-C3-C4	4.35	120.50	116.91
25	b	606	CLA	O2D-CGD-O1D	-4.35	115.38	123.85
31	d	408	LHG	O4-P-O5	4.33	132.61	112.44
31	D	409	LHG	O4-P-O5	4.33	132.59	112.44
25	C	508	CLA	CMB-C2B-C1B	-4.32	122.13	128.46
30	L	101	SQD	O47-C7-C8	4.32	120.82	111.48
25	b	602	CLA	CMB-C2B-C1B	-4.31	122.14	128.46
25	b	605	CLA	C4A-NA-C1A	4.30	108.64	106.68
26	d	402	PHO	O1D-CGD-CBD	4.29	131.23	124.72
31	d	407	LHG	O4-P-O5	4.28	132.37	112.44
25	b	616	CLA	CMB-C2B-C3B	4.28	133.24	124.68
25	C	502	CLA	C4A-NA-C1A	4.27	108.63	106.68
32	a	615	DGD	O3G-C3G-C2G	-4.27	100.80	111.77
25	b	603	CLA	O2D-CGD-O1D	-4.27	115.54	123.85
30	A	613	SQD	O47-C7-C8	4.26	120.70	111.48
25	b	612	CLA	C4A-NA-C1A	4.25	108.62	106.68
30	B	622	SQD	O9-S-O7	-4.25	100.00	113.82
25	c	501	CLA	O2D-CGD-O1D	-4.25	115.58	123.85
25	a	607	CLA	CMB-C2B-C1B	-4.24	122.25	128.46
25	b	605	CLA	CMB-C2B-C1B	-4.23	122.25	128.46
25	b	607	CLA	CMB-C2B-C1B	-4.23	122.27	128.46
30	L	101	SQD	O7-S-C6	4.22	113.06	106.76
36	V	201	HEC	CMC-C2C-C1C	-4.22	122.28	128.46
25	b	614	CLA	CMB-C2B-C1B	-4.21	122.28	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	512	CLA	C1-C2-C3	-4.21	119.30	126.20
31	D	410	LHG	O4-P-O5	4.20	131.98	112.44
25	B	611	CLA	O2D-CGD-O1D	-4.19	115.68	123.85
31	d	409	LHG	O4-P-O5	4.19	131.93	112.44
25	d	404	CLA	CMB-C2B-C3B	4.18	133.04	124.68
30	B	622	SQD	O7-S-C6	4.18	113.00	106.76
25	C	504	CLA	C4A-NA-C1A	4.17	108.58	106.68
25	C	506	CLA	CMB-C2B-C1B	-4.16	122.36	128.46
25	b	612	CLA	CMB-C2B-C1B	-4.14	122.39	128.46
25	c	502	CLA	CMB-C2B-C1B	-4.13	122.40	128.46
25	B	603	CLA	C4A-NA-C1A	4.13	108.56	106.68
25	D	405	CLA	CMB-C2B-C3B	4.13	132.94	124.68
25	a	608	CLA	CMB-C2B-C1B	-4.11	122.44	128.46
32	c	518	DGD	O3G-C3G-C2G	-4.11	100.83	110.82
32	H	102	DGD	O3G-C3G-C2G	-4.10	100.85	110.82
25	B	613	CLA	C4A-NA-C1A	4.09	108.55	106.68
25	b	611	CLA	O2D-CGD-O1D	-4.08	115.90	123.85
25	c	508	CLA	CMB-C2B-C1B	-4.08	122.48	128.46
25	B	608	CLA	O2D-CGD-CBD	4.07	118.35	111.23
25	A	609	CLA	CMB-C2B-C3B	4.07	132.81	124.68
25	B	602	CLA	CMB-C2B-C3B	4.07	132.81	124.68
25	B	602	CLA	O2D-CGD-CBD	4.05	118.30	111.23
31	l	101	LHG	O4-P-O5	4.04	131.23	112.44
25	A	606	CLA	C4A-NA-C1A	4.04	108.52	106.68
25	B	612	CLA	CMB-C2B-C3B	4.03	132.73	124.68
25	B	607	CLA	CMB-C2B-C1B	-4.02	122.56	128.46
25	B	611	CLA	CMB-C2B-C1B	-4.02	122.57	128.46
25	b	612	CLA	O2D-CGD-O1D	-3.99	116.08	123.85
25	A	609	CLA	O2D-CGD-O1D	-3.99	116.08	123.85
25	B	616	CLA	CMB-C2B-C1B	-3.98	122.63	128.46
25	c	504	CLA	CMB-C2B-C3B	3.96	132.60	124.68
25	a	612	CLA	CMB-C2B-C1B	-3.96	122.66	128.46
25	A	607	CLA	C4A-NA-C1A	3.95	108.48	106.68
25	C	511	CLA	CMB-C2B-C1B	-3.95	122.67	128.46
25	a	609	CLA	CMB-C2B-C1B	-3.95	122.67	128.46
30	a	613	SQD	O9-S-O7	-3.95	100.98	113.82
30	f	102	SQD	O9-S-O7	-3.95	100.99	113.82
30	a	613	SQD	O47-C7-C8	3.93	119.98	111.48
30	f	102	SQD	O7-S-C6	3.92	112.61	106.76
25	C	509	CLA	CMB-C2B-C3B	3.91	132.49	124.68
26	d	402	PHO	O2D-CGD-O1D	-3.89	116.28	123.85
32	C	515	DGD	O3G-C3G-C2G	-3.89	101.36	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	509	CLA	O2A-CGA-O1A	-3.87	113.94	123.63
25	C	503	CLA	CMB-C2B-C1B	-3.87	122.79	128.46
32	h	101	DGD	O3G-C3G-C2G	-3.86	101.42	110.82
25	b	609	CLA	C4A-NA-C1A	3.86	108.44	106.68
25	C	513	CLA	CMB-C2B-C1B	-3.86	122.81	128.46
30	A	613	SQD	O9-S-O7	-3.85	101.29	113.82
30	F	101	SQD	C44-O6-C1	3.85	120.25	113.68
25	C	507	CLA	O2D-CGD-O1D	-3.83	116.38	123.85
25	C	501	CLA	CMB-C2B-C1B	-3.83	122.84	128.46
25	B	603	CLA	CMB-C2B-C1B	-3.82	122.86	128.46
25	B	606	CLA	CMB-C2B-C1B	-3.82	122.86	128.46
25	b	604	CLA	CMB-C2B-C1B	-3.82	122.86	128.46
25	C	507	CLA	CMB-C2B-C1B	-3.81	122.87	128.46
25	b	602	CLA	C4A-NA-C1A	3.81	108.42	106.68
25	B	610	CLA	CHB-C4A-NA	3.81	129.90	124.40
25	c	501	CLA	CMB-C2B-C1B	-3.80	122.89	128.46
32	c	519	DGD	O3G-C3G-C2G	-3.80	101.58	110.82
25	b	615	CLA	CMB-C2B-C1B	-3.80	122.89	128.46
27	b	617	BCR	C2-C1-C6	3.79	115.94	110.44
30	A	616	SQD	O47-C7-C8	3.79	119.67	111.48
25	b	616	CLA	O2D-CGD-O1D	-3.79	116.48	123.85
25	A	609	CLA	C4A-NA-C1A	3.78	108.40	106.68
25	b	611	CLA	CMB-C2B-C1B	-3.75	122.96	128.46
32	C	516	DGD	O3G-C3G-C2G	-3.75	101.69	110.82
25	b	610	CLA	C4A-NA-C1A	3.74	108.39	106.68
30	L	101	SQD	O48-C23-C24	3.73	123.20	111.83
26	A	608	PHO	O2D-CGD-CBD	3.72	115.04	110.95
25	c	510	CLA	O2D-CGD-O1D	-3.72	116.61	123.85
25	b	602	CLA	C1-C2-C3	-3.71	120.12	126.20
25	A	606	CLA	CMB-C2B-C1B	-3.71	123.02	128.46
25	c	509	CLA	CMB-C2B-C1B	-3.71	123.03	128.46
25	C	510	CLA	CMB-C2B-C3B	3.70	132.07	124.68
25	B	613	CLA	CMB-C2B-C3B	3.68	132.04	124.68
25	B	608	CLA	CMB-C2B-C3B	3.68	132.03	124.68
25	C	505	CLA	CMB-C2B-C1B	-3.65	123.10	128.46
25	b	602	CLA	CMB-C2B-C3B	3.63	131.93	124.68
30	L	101	SQD	O9-S-O7	-3.62	102.05	113.82
25	B	602	CLA	O2D-CGD-O1D	-3.61	116.82	123.85
30	a	613	SQD	O7-S-C6	3.59	112.12	106.76
25	b	610	CLA	C1-C2-C3	-3.59	120.31	126.20
25	b	603	CLA	C1B-CHB-C4A	-3.58	123.20	130.04
30	a	614	SQD	O48-C23-C24	3.58	122.75	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	614	CLA	C4A-NA-C1A	3.58	108.31	106.68
25	b	611	CLA	O2D-CGD-CBD	3.57	117.48	111.23
25	c	513	CLA	CMB-C2B-C3B	3.57	131.81	124.68
32	A	617	DGD	O3G-C3G-C2G	-3.56	102.17	110.82
30	B	622	SQD	O48-C23-C24	3.55	122.67	111.83
30	F	101	SQD	O9-S-O7	-3.55	102.27	113.82
25	d	404	CLA	C4A-NA-C1A	3.55	108.30	106.68
27	B	617	BCR	C2-C1-C6	3.54	115.59	110.44
25	b	602	CLA	CHB-C4A-NA	3.54	129.51	124.40
25	B	604	CLA	O2D-CGD-O1D	-3.54	116.95	123.85
30	F	101	SQD	O5-C1-O6	3.54	118.41	110.04
25	b	606	CLA	O2D-CGD-CBD	3.54	117.42	111.23
30	a	613	SQD	C44-O6-C1	-3.53	106.22	113.80
25	c	510	CLA	CMB-C2B-C3B	3.52	131.72	124.68
25	D	404	CLA	CMB-C2B-C1B	-3.52	123.31	128.46
25	B	611	CLA	O2D-CGD-CBD	3.51	117.37	111.23
25	B	612	CLA	O2D-CGD-O1D	-3.50	117.04	123.85
25	D	404	CLA	O2D-CGD-CBD	3.50	117.34	111.23
28	A	611	PL9	C7-C3-C2	-3.49	119.27	123.39
25	d	403	CLA	CMB-C2B-C3B	3.47	131.63	124.68
25	B	609	CLA	CMB-C2B-C1B	-3.47	123.37	128.46
30	f	102	SQD	O6-C1-C2	3.46	113.53	108.27
25	B	614	CLA	CMB-C2B-C1B	-3.46	123.39	128.46
25	b	604	CLA	O2D-CGD-O1D	-3.46	117.12	123.85
25	b	612	CLA	C1-C2-C3	-3.45	120.55	126.20
25	D	403	CLA	CMB-C2B-C1B	-3.44	123.41	128.46
25	b	603	CLA	CMB-C2B-C3B	3.42	131.53	124.68
25	B	616	CLA	O2D-CGD-O1D	-3.42	117.18	123.85
25	c	511	CLA	CMB-C2B-C1B	-3.42	123.45	128.46
30	f	102	SQD	O5-C5-C4	3.41	115.85	109.70
32	A	617	DGD	C4E-C3E-C2E	-3.40	104.85	110.83
27	A	610	BCR	C11-C10-C9	-3.40	122.52	127.28
36	V	201	HEC	CMC-C2C-C3C	3.39	129.80	125.82
32	C	517	DGD	O3G-C3G-C2G	-3.38	102.59	110.82
27	B	619	BCR	C2-C1-C6	3.38	115.35	110.44
36	V	201	HEC	C1D-C2D-C3D	-3.38	104.64	107.00
30	L	101	SQD	C1-C2-C3	-3.38	102.90	110.01
25	A	607	CLA	CMB-C2B-C1B	-3.38	123.51	128.46
26	A	608	PHO	CMB-C2B-C3B	3.37	131.42	124.68
25	b	601	CLA	CMB-C2B-C1B	-3.37	123.52	128.46
30	L	101	SQD	O5-C5-C4	3.37	115.77	109.70
30	A	616	SQD	O48-C23-C24	3.37	122.10	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	512	CLA	CMB-C2B-C1B	-3.37	123.52	128.46
32	c	517	DGD	O3G-C3G-C2G	-3.36	102.63	110.82
25	c	513	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
25	b	608	CLA	CMB-C2B-C3B	3.35	131.39	124.68
25	B	610	CLA	C1-C2-C3	-3.35	120.72	126.20
25	b	613	CLA	CMB-C2B-C3B	3.34	131.37	124.68
25	b	612	CLA	C1B-CHB-C4A	-3.34	123.67	130.04
31	D	412	LHG	O8-C23-C24	3.34	122.02	111.83
28	d	406	PL9	C40-C39-C41	3.34	121.02	115.23
25	b	606	CLA	CMB-C2B-C3B	3.34	131.35	124.68
27	K	101	BCR	C15-C16-C17	-3.33	116.71	123.52
25	C	502	CLA	CMB-C2B-C1B	-3.32	123.59	128.46
25	B	610	CLA	O2A-CGA-O1A	-3.31	115.34	123.63
25	c	506	CLA	CMB-C2B-C3B	3.31	131.31	124.68
25	B	601	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
25	b	602	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
32	H	102	DGD	C3E-C4E-C5E	-3.31	104.23	110.23
25	B	607	CLA	CMB-C2B-C3B	3.31	131.29	124.68
25	B	613	CLA	CAC-C3C-C4C	3.30	129.09	124.79
30	a	613	SQD	C1-C2-C3	-3.30	103.07	110.01
25	c	507	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
25	b	610	CLA	CAC-C3C-C4C	3.30	129.08	124.79
31	d	407	LHG	O8-C23-O10	-3.30	115.39	123.63
25	b	609	CLA	CMB-C2B-C3B	3.29	131.27	124.68
25	C	508	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
25	D	404	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
31	d	408	LHG	O8-C23-C24	3.28	121.85	111.83
25	b	610	CLA	CMB-C2B-C1B	-3.28	123.65	128.46
25	b	613	CLA	C1-C2-C3	-3.27	120.84	126.20
30	A	613	SQD	O8-S-C6	3.27	112.28	105.97
25	b	601	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
31	d	407	LHG	O8-C23-C24	3.25	121.76	111.83
25	B	610	CLA	O2D-CGD-CBD	3.25	116.91	111.23
25	A	609	CLA	C1B-CHB-C4A	-3.25	123.85	130.04
25	C	506	CLA	CMB-C2B-C3B	3.24	131.16	124.68
25	B	615	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
25	a	607	CLA	CMB-C2B-C3B	3.23	131.14	124.68
35	f	101	HEM	CBA-CAA-C2A	-3.23	107.11	112.54
25	a	608	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
30	A	613	SQD	O5-C1-C2	-3.22	103.75	110.37
25	D	403	CLA	CMB-C2B-C3B	3.21	131.10	124.68
30	F	101	SQD	O48-C23-C24	3.20	121.60	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	609	CLA	C4A-NA-C1A	3.19	108.14	106.68
25	b	605	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
25	B	603	CLA	CMB-C2B-C3B	3.19	131.06	124.68
25	a	609	CLA	CMB-C2B-C3B	3.19	131.06	124.68
25	c	502	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
25	b	607	CLA	CMB-C2B-C3B	3.18	131.04	124.68
29	c	522	LMG	O1-C1-C2	-3.17	103.46	108.27
25	B	604	CLA	CMB-C2B-C3B	3.17	131.02	124.68
25	B	605	CLA	O2D-CGD-O1D	-3.17	117.69	123.85
25	c	505	CLA	CMB-C2B-C1B	-3.16	123.82	128.46
25	c	512	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
25	b	612	CLA	CMB-C2B-C3B	3.15	130.99	124.68
25	c	502	CLA	C1-C2-C3	-3.15	121.03	126.20
25	b	604	CLA	CHB-C4A-NA	3.15	128.95	124.40
28	D	407	PL9	C7-C3-C2	-3.15	119.67	123.39
25	c	502	CLA	CMB-C2B-C3B	3.15	130.98	124.68
25	c	508	CLA	CMB-C2B-C3B	3.15	130.97	124.68
36	v	201	HEC	CBD-CAD-C3D	-3.14	107.25	112.54
27	T	101	BCR	C7-C8-C9	-3.14	121.59	126.23
25	C	510	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
25	C	506	CLA	C1-C2-C3	-3.14	121.06	126.20
25	b	610	CLA	C1B-CHB-C4A	-3.13	124.06	130.04
25	B	614	CLA	C1B-CHB-C4A	-3.13	124.06	130.04
25	c	511	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
25	a	608	CLA	C1B-CHB-C4A	-3.13	124.07	130.04
25	d	404	CLA	C1B-CHB-C4A	-3.12	124.08	130.04
25	c	502	CLA	C1B-CHB-C4A	-3.12	124.09	130.04
25	A	607	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
25	C	513	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
26	D	402	PHO	O2D-CGD-O1D	-3.11	117.79	123.85
26	D	402	PHO	CMB-C2B-C3B	3.11	130.90	124.68
25	c	505	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
28	d	406	PL9	C37-C38-C39	-3.10	120.52	127.62
25	B	613	CLA	O2A-CGA-O1A	-3.10	115.88	123.63
29	d	411	LMG	O2-C2-C1	-3.10	102.69	110.08
25	D	405	CLA	O2D-CGD-O1D	-3.09	117.82	123.85
29	m	101	LMG	O1-C7-C8	-3.09	103.29	110.82
32	c	519	DGD	O6D-C1D-O3G	-3.09	102.74	110.04
25	a	612	CLA	O2D-CGD-CBD	3.09	116.63	111.23
30	a	613	SQD	O48-C23-C24	3.09	121.24	111.83
26	A	608	PHO	O2D-CGD-O1D	-3.08	117.86	123.85
35	f	101	HEM	C3B-C2B-C1B	3.07	108.72	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	504	CLA	O2A-CGA-O1A	-3.07	115.95	123.63
26	D	402	PHO	O1D-CGD-CBD	3.07	129.37	124.72
27	a	610	BCR	C2-C1-C6	3.06	114.89	110.44
25	b	613	CLA	O2D-CGD-CBD	3.06	116.58	111.23
25	b	602	CLA	C1B-CHB-C4A	-3.06	124.21	130.04
30	L	101	SQD	O9-S-C6	3.06	111.32	106.76
27	d	405	BCR	C27-C26-C25	3.05	126.83	122.70
25	A	606	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
32	C	515	DGD	O6D-C1D-O3G	-3.05	102.84	110.04
25	C	507	CLA	CHB-C4A-NA	3.05	128.80	124.40
25	b	603	CLA	O2D-CGD-CBD	3.04	116.55	111.23
25	a	612	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
32	C	516	DGD	O6D-C1D-O3G	-3.04	102.85	110.04
25	B	611	CLA	CMB-C2B-C3B	3.04	130.77	124.68
25	b	610	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
25	b	607	CLA	C1B-CHB-C4A	-3.04	124.24	130.04
32	C	516	DGD	O5D-C6D-C5D	-3.04	102.57	109.42
25	C	507	CLA	CMB-C2B-C3B	3.04	130.76	124.68
25	C	512	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
29	D	408	LMG	O6-C1-O1	-3.03	102.87	110.04
25	c	503	CLA	CHB-C4A-NA	3.03	128.78	124.40
29	M	101	LMG	C38-C37-C36	-3.03	99.04	114.37
27	C	514	BCR	C2-C1-C6	3.03	114.84	110.44
35	E	101	HEM	CBD-CAD-C3D	-3.03	104.16	112.53
25	C	508	CLA	CMB-C2B-C3B	3.03	130.74	124.68
25	b	601	CLA	CHB-C4A-NA	3.03	128.77	124.40
25	C	502	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
25	b	609	CLA	C1B-CHB-C4A	-3.02	124.27	130.04
27	B	618	BCR	C24-C23-C22	-3.02	121.77	126.23
25	A	606	CLA	CMB-C2B-C3B	3.01	130.70	124.68
28	d	406	PL9	C7-C3-C2	-3.01	119.84	123.39
25	c	509	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
25	b	605	CLA	CMB-C2B-C3B	3.01	130.70	124.68
25	B	602	CLA	CHB-C4A-NA	3.01	128.74	124.40
25	a	608	CLA	CMB-C2B-C3B	3.01	130.69	124.68
25	A	607	CLA	C1-C2-C3	-3.01	121.27	126.20
25	D	403	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
25	B	614	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
32	c	518	DGD	O6D-C1D-O3G	-2.99	102.97	110.04
25	A	606	CLA	CHB-C4A-NA	2.99	128.72	124.40
32	C	517	DGD	O6D-C1D-O3G	-2.99	102.98	110.04
27	K	101	BCR	C15-C14-C13	-2.99	123.09	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	507	CLA	CMB-C2B-C1B	-2.98	124.09	128.46
25	b	613	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
27	T	101	BCR	C27-C26-C25	2.98	126.73	122.70
25	C	512	CLA	CHB-C4A-NA	2.97	128.69	124.40
25	C	503	CLA	CMB-C2B-C3B	2.97	130.62	124.68
25	a	612	CLA	CMB-C2B-C3B	2.97	130.61	124.68
25	B	610	CLA	C1B-CHB-C4A	-2.97	124.38	130.04
25	D	405	CLA	C1B-CHB-C4A	-2.96	124.39	130.04
25	C	509	CLA	CHB-C4A-NA	2.95	128.66	124.40
28	d	406	PL9	C42-C43-C44	-2.95	120.86	127.62
33	m	102	STE	O2-C1-C2	2.95	123.33	114.00
25	b	608	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
25	b	610	CLA	CAA-CBA-CGA	-2.95	104.83	113.21
25	C	513	CLA	CMB-C2B-C3B	2.94	130.57	124.68
27	Y	101	BCR	C27-C26-C25	2.94	126.68	122.70
25	B	616	CLA	CMB-C2B-C3B	2.94	130.56	124.68
25	B	611	CLA	C1-C2-C3	-2.94	121.39	126.20
25	B	604	CLA	CHB-C4A-NA	2.93	128.63	124.40
25	C	513	CLA	CHB-C4A-NA	2.93	128.63	124.40
29	C	518	LMG	O1-C7-C8	-2.93	103.68	110.82
25	b	605	CLA	O2A-CGA-O1A	-2.93	116.31	123.63
32	H	102	DGD	O2D-C2D-C1D	-2.93	103.10	110.08
30	B	622	SQD	O6-C1-C2	2.93	112.72	108.27
33	j	101	STE	O2-C1-C2	2.92	123.24	114.00
25	b	616	CLA	C1B-CHB-C4A	-2.92	124.48	130.04
25	b	606	CLA	C1B-CHB-C4A	-2.91	124.48	130.04
29	d	411	LMG	O6-C1-O1	-2.91	103.17	110.04
27	B	618	BCR	C15-C14-C13	-2.91	123.20	127.28
25	a	608	CLA	CHB-C4A-NA	2.90	128.59	124.40
27	D	406	BCR	C7-C8-C9	-2.90	121.94	126.23
25	c	504	CLA	O2A-CGA-O1A	-2.90	116.37	123.63
25	b	602	CLA	O2D-CGD-CBD	2.90	116.29	111.23
25	a	607	CLA	C1B-CHB-C4A	-2.89	124.52	130.04
25	c	508	CLA	C1-C2-C3	-2.89	121.46	126.20
33	C	520	STE	C3-C2-C1	-2.89	106.97	114.51
25	a	607	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
27	A	610	BCR	C27-C26-C25	2.88	126.60	122.70
25	c	509	CLA	CMB-C2B-C3B	2.87	130.42	124.68
25	C	511	CLA	CHB-C4A-NA	2.87	128.54	124.40
27	t	101	BCR	C15-C14-C13	-2.86	123.26	127.28
27	c	515	BCR	C7-C8-C9	-2.86	122.00	126.23
27	d	405	BCR	C38-C26-C25	-2.86	121.37	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	608	CLA	O2D-CGD-CBD	2.85	116.22	111.23
25	b	612	CLA	CHB-C4A-NA	2.85	128.52	124.40
25	b	614	CLA	CMB-C2B-C3B	2.85	130.38	124.68
25	d	403	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
28	d	406	PL9	C22-C23-C24	-2.85	121.10	127.62
27	D	406	BCR	C27-C26-C25	2.85	126.55	122.70
25	B	607	CLA	C1B-CHB-C4A	-2.85	124.61	130.04
25	B	612	CLA	O2A-CGA-O1A	-2.84	116.52	123.63
32	c	519	DGD	CDB-CCB-CBB	-2.84	100.00	114.37
27	D	406	BCR	C2-C1-C6	2.84	114.57	110.44
32	c	517	DGD	O3G-C1D-C2D	-2.84	103.96	108.27
25	B	612	CLA	C11-C12-C13	-2.84	106.53	115.97
29	b	621	LMG	C1-O6-C5	-2.84	108.18	113.72
25	C	503	CLA	C7-C6-C5	-2.83	105.71	113.26
25	B	603	CLA	CHD-C4C-NC	2.83	128.62	124.23
30	f	102	SQD	C1-O5-C5	-2.83	108.19	113.72
25	c	509	CLA	CHB-C4A-NA	2.83	128.49	124.40
25	C	504	CLA	CMB-C2B-C3B	2.83	130.34	124.68
30	A	613	SQD	O48-C23-C24	2.83	120.46	111.83
28	d	406	PL9	O1-C4-C3	-2.83	117.75	120.73
27	C	514	BCR	C15-C16-C17	-2.83	117.74	123.52
25	B	616	CLA	C1B-CHB-C4A	-2.83	124.65	130.04
25	A	609	CLA	O2D-CGD-CBD	2.82	116.17	111.23
25	b	607	CLA	CHB-C4A-NA	2.82	128.47	124.40
28	D	407	PL9	C22-C23-C24	-2.82	121.17	127.62
25	c	503	CLA	CMB-C2B-C1B	-2.82	124.33	128.46
27	k	101	BCR	C33-C5-C6	-2.82	121.41	124.48
26	d	401	PHO	CMB-C2B-C3B	2.82	130.31	124.68
25	B	612	CLA	C1-C2-C3	-2.82	121.58	126.20
25	A	606	CLA	C7-C6-C5	-2.82	105.76	113.26
28	A	611	PL9	C22-C23-C24	-2.81	121.18	127.62
32	H	102	DGD	CDB-CCB-CBB	-2.81	100.14	114.37
27	H	101	BCR	C27-C26-C25	2.81	126.50	122.70
27	B	617	BCR	C29-C30-C25	2.81	114.52	110.44
25	a	609	CLA	CHB-C4A-NA	2.81	128.45	124.40
29	m	101	LMG	O3-C3-C2	-2.81	103.76	110.38
25	C	508	CLA	CHD-C1D-ND	-2.80	120.86	124.80
26	d	402	PHO	CMC-C2C-C3C	2.80	130.23	124.94
28	D	407	PL9	C12-C13-C14	-2.80	121.21	127.62
29	M	101	LMG	C1-C2-C3	-2.80	104.11	110.01
34	a	606	BCT	O2-C-O1	-2.80	112.51	119.68
32	A	617	DGD	CDB-CCB-CBB	-2.80	100.23	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	621	LMG	C3-C4-C5	-2.79	105.17	110.23
36	V	201	HEC	CMB-C2B-C1B	-2.79	124.36	128.46
25	B	616	CLA	CAA-CBA-CGA	-2.79	105.28	113.21
25	c	506	CLA	CHB-C4A-NA	2.79	128.43	124.40
30	L	101	SQD	C3-C4-C5	2.79	115.30	110.23
27	c	515	BCR	C27-C26-C25	2.79	126.48	122.70
25	c	508	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
27	k	101	BCR	C27-C26-C25	2.79	126.47	122.70
25	B	609	CLA	CMB-C2B-C3B	2.78	130.25	124.68
25	C	509	CLA	CED-O2D-CGD	2.78	122.22	115.92
25	a	607	CLA	O1D-CGD-CBD	2.78	130.00	124.52
25	c	501	CLA	O2D-CGD-CBD	2.78	116.09	111.23
32	a	615	DGD	CDB-CCB-CBB	-2.78	100.33	114.37
27	c	514	BCR	C15-C14-C13	-2.78	123.39	127.28
36	v	201	HEC	CMB-C2B-C1B	-2.77	124.39	128.46
30	f	102	SQD	O5-C1-C2	-2.77	104.68	110.37
25	a	608	CLA	O2D-CGD-CBD	2.77	116.07	111.23
27	B	618	BCR	C3-C4-C5	-2.77	109.12	114.06
25	C	511	CLA	CMB-C2B-C3B	2.77	130.21	124.68
30	f	102	SQD	C1-C2-C3	-2.77	104.19	110.01
27	c	516	BCR	C27-C26-C25	2.76	126.44	122.70
27	x	101	BCR	C2-C1-C6	2.76	114.45	110.44
25	b	614	CLA	C1B-CHB-C4A	-2.76	124.78	130.04
29	b	621	LMG	O7-C10-O9	-2.75	117.26	123.70
25	C	503	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
25	b	616	CLA	CHB-C4A-NA	2.75	128.37	124.40
25	D	404	CLA	C1B-CHB-C4A	-2.75	124.80	130.04
25	B	602	CLA	O2A-CGA-O1A	-2.75	116.75	123.63
25	A	607	CLA	C1B-CHB-C4A	-2.75	124.80	130.04
25	B	609	CLA	C1B-CHB-C4A	-2.75	124.80	130.04
25	B	612	CLA	CHB-C4A-NA	2.75	128.36	124.40
25	b	604	CLA	CMB-C2B-C3B	2.75	130.17	124.68
27	b	618	BCR	C8-C7-C6	-2.75	119.67	127.00
27	B	619	BCR	C29-C30-C25	2.74	114.42	110.44
25	C	501	CLA	O2A-CGA-O1A	-2.74	116.77	123.63
25	B	606	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
25	b	610	CLA	CMB-C2B-C3B	2.74	130.16	124.68
25	a	607	CLA	O2A-CGA-O1A	-2.74	116.78	123.63
25	A	606	CLA	C1B-CHB-C4A	-2.73	124.83	130.04
25	A	607	CLA	CMB-C2B-C3B	2.73	130.15	124.68
25	B	606	CLA	CMB-C2B-C3B	2.73	130.14	124.68
25	b	603	CLA	CHD-C1D-ND	-2.73	120.96	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	515	BCR	C35-C13-C14	-2.73	118.39	122.82
27	Y	101	BCR	C33-C5-C6	-2.73	121.51	124.48
27	a	610	BCR	C24-C23-C22	-2.73	122.20	126.23
32	c	517	DGD	CDB-CCB-CBB	-2.73	100.59	114.37
27	K	102	BCR	C27-C26-C25	2.72	126.38	122.70
25	b	608	CLA	CHB-C4A-NA	2.72	128.33	124.40
29	m	101	LMG	O7-C10-O9	-2.72	117.35	123.70
25	b	612	CLA	O1D-CGD-CBD	2.72	129.88	124.52
27	x	101	BCR	C27-C26-C25	2.71	126.37	122.70
25	c	513	CLA	O2A-CGA-O1A	-2.71	116.85	123.63
25	b	615	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
27	b	617	BCR	C27-C26-C25	2.71	126.36	122.70
31	D	409	LHG	C18-C17-C16	-2.71	100.69	114.37
25	B	602	CLA	C1B-CHB-C4A	-2.70	124.88	130.04
26	d	401	PHO	OBD-CAD-CBD	-2.70	121.86	125.82
25	B	605	CLA	CHD-C1D-ND	-2.70	121.00	124.80
26	d	402	PHO	CMB-C2B-C3B	2.70	130.08	124.68
27	c	514	BCR	C24-C23-C22	-2.70	122.24	126.23
25	A	609	CLA	CHB-C4A-NA	2.70	128.30	124.40
32	C	517	DGD	CDB-CCB-CBB	-2.70	100.72	114.37
31	A	614	LHG	O8-C23-C24	2.70	120.06	111.83
36	v	201	HEC	CMC-C2C-C1C	-2.70	124.50	128.46
25	C	507	CLA	O2D-CGD-CBD	2.70	115.94	111.23
26	A	608	PHO	C1-C2-C3	-2.69	121.78	126.20
25	C	505	CLA	CMB-C2B-C3B	2.69	130.06	124.68
28	d	406	PL9	C36-C34-C33	-2.68	115.14	121.17
25	C	501	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
29	c	522	LMG	C6-C5-C4	-2.68	106.44	113.02
29	m	101	LMG	O6-C1-O1	-2.68	103.71	110.04
28	a	611	PL9	C7-C8-C9	-2.68	122.22	126.83
27	D	406	BCR	C3-C4-C5	-2.67	109.29	114.06
28	D	407	PL9	C20-C19-C21	2.67	119.87	115.23
30	A	613	SQD	O7-S-C6	2.67	110.74	106.76
33	c	523	STE	C3-C2-C1	-2.67	107.54	114.51
29	b	621	LMG	O8-C28-O10	-2.67	116.95	123.63
25	c	508	CLA	CHB-C4A-NA	2.67	128.25	124.40
32	C	515	DGD	CDB-CCB-CBB	-2.67	100.88	114.37
32	C	516	DGD	CDB-CCB-CBB	-2.67	100.88	114.37
27	a	610	BCR	C27-C26-C25	2.67	126.31	122.70
27	b	618	BCR	C15-C14-C13	-2.67	123.54	127.28
25	D	403	CLA	C4A-NA-C1A	2.67	107.89	106.68
25	C	511	CLA	O2D-CGD-O1D	-2.66	118.66	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	618	BCR	C27-C26-C25	2.66	126.30	122.70
25	b	613	CLA	O2A-CGA-O1A	-2.66	116.96	123.63
25	b	606	CLA	CHB-C4A-NA	2.66	128.24	124.40
27	b	619	BCR	C11-C10-C9	-2.66	123.55	127.28
30	a	613	SQD	O8-S-C6	2.65	111.10	105.97
28	D	407	PL9	C7-C8-C9	-2.65	122.26	126.83
25	c	505	CLA	O2D-CGD-CBD	2.65	115.86	111.23
25	B	606	CLA	O2A-CGA-O1A	-2.65	117.01	123.63
25	B	605	CLA	O2A-CGA-O1A	-2.64	117.02	123.63
29	c	520	LMG	O6-C1-O1	-2.64	103.80	110.04
28	d	406	PL9	C7-C8-C9	-2.64	122.28	126.83
25	c	501	CLA	CMB-C2B-C3B	2.64	129.95	124.68
25	c	512	CLA	CHB-C4A-NA	2.64	128.21	124.40
31	d	408	LHG	O8-C23-O10	-2.64	117.03	123.63
35	f	101	HEM	CBD-CAD-C3D	-2.64	105.24	112.53
28	A	611	PL9	C36-C34-C33	-2.64	115.25	121.17
25	B	609	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
32	h	101	DGD	CDB-CCB-CBB	-2.63	101.06	114.37
25	c	502	CLA	O2A-CGA-O1A	-2.63	117.04	123.63
27	c	515	BCR	C2-C1-C6	2.63	114.26	110.44
32	A	617	DGD	C3G-C2G-C1G	-2.63	105.65	111.78
30	a	613	SQD	C3-C4-C5	2.63	115.00	110.23
27	B	618	BCR	C2-C1-C6	2.62	114.25	110.44
25	B	609	CLA	O2A-CGA-O1A	-2.62	117.08	123.63
25	B	611	CLA	CHB-C4A-NA	2.61	128.17	124.40
25	c	506	CLA	C1B-CHB-C4A	-2.61	125.06	130.04
25	B	610	CLA	CMB-C2B-C1B	-2.61	124.63	128.46
25	C	502	CLA	CMB-C2B-C3B	2.61	129.90	124.68
32	h	101	DGD	O3E-C3E-C2E	-2.61	104.22	110.38
32	C	516	DGD	C1D-O6D-C5D	-2.61	108.63	113.72
25	b	615	CLA	CHB-C4A-NA	2.60	128.16	124.40
25	A	606	CLA	C6-C5-C3	2.60	119.80	113.47
26	d	401	PHO	O2A-CGA-O1A	-2.60	117.12	123.63
32	A	617	DGD	O6D-C1D-O3G	-2.60	103.90	110.04
25	a	609	CLA	O2D-CGD-CBD	2.60	115.77	111.23
25	C	510	CLA	C1B-CHB-C4A	-2.60	125.09	130.04
30	f	102	SQD	O48-C23-C24	2.60	119.75	111.83
25	a	609	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
28	A	611	PL9	C20-C19-C21	2.59	119.73	115.23
27	c	514	BCR	C33-C5-C6	-2.59	121.66	124.48
29	M	101	LMG	C1-O6-C5	-2.59	108.66	113.72
32	A	617	DGD	O5D-C6D-C5D	-2.59	103.59	109.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	c	517	DGD	O6D-C1D-O3G	-2.58	103.94	110.04
32	C	516	DGD	O2D-C2D-C1D	-2.58	103.92	110.08
28	D	407	PL9	C37-C38-C39	-2.58	121.71	127.62
25	C	501	CLA	CMB-C2B-C3B	2.58	129.84	124.68
31	e	101	LHG	O8-C23-C24	2.58	119.70	111.83
27	b	617	BCR	C33-C5-C6	-2.58	121.67	124.48
28	a	611	PL9	C22-C23-C24	-2.58	121.72	127.62
25	C	506	CLA	O2A-CGA-O1A	-2.58	117.18	123.63
30	F	101	SQD	C46-C45-C44	-2.58	105.34	113.67
25	B	615	CLA	O2D-CGD-CBD	2.58	115.73	111.23
25	b	616	CLA	O2D-CGD-CBD	2.58	115.73	111.23
25	b	601	CLA	CMB-C2B-C3B	2.57	129.82	124.68
27	C	514	BCR	C15-C14-C13	-2.57	123.67	127.28
25	b	605	CLA	O1D-CGD-CBD	2.57	129.59	124.52
25	c	512	CLA	CMB-C2B-C1B	-2.57	124.69	128.46
30	f	102	SQD	O9-S-C6	2.57	110.59	106.76
25	B	615	CLA	CHB-C4A-NA	2.57	128.10	124.40
25	b	614	CLA	O2A-CGA-O1A	-2.57	117.21	123.63
25	c	506	CLA	C1-O2A-CGA	2.56	122.86	116.65
25	B	612	CLA	C1B-CHB-C4A	-2.56	125.16	130.04
30	f	102	SQD	O47-C7-C8	2.56	120.33	110.93
25	c	510	CLA	C1-C2-C3	-2.55	122.01	126.20
32	h	101	DGD	C1D-C2D-C3D	-2.55	104.64	110.01
31	D	412	LHG	C18-C17-C16	-2.55	101.47	114.37
32	c	518	DGD	O2D-C2D-C1D	-2.55	104.00	110.08
30	L	101	SQD	O5-C1-C2	-2.55	105.13	110.37
25	C	508	CLA	O2D-CGD-CBD	2.55	115.68	111.23
27	K	101	BCR	C24-C23-C22	-2.54	122.47	126.23
25	b	616	CLA	CHD-C1D-ND	-2.54	121.22	124.80
31	d	408	LHG	C20-C19-C18	-2.54	101.53	114.37
30	F	101	SQD	O5-C5-C4	2.54	114.27	109.70
31	D	409	LHG	O8-C23-C24	2.54	119.58	111.83
29	c	524	LMG	C1-O6-C5	-2.54	108.76	113.72
25	b	613	CLA	C16-C15-C13	-2.54	107.53	115.97
25	b	611	CLA	CMB-C2B-C3B	2.54	129.75	124.68
29	C	518	LMG	O2-C2-C1	-2.53	104.05	110.08
25	c	502	CLA	CHD-C1D-ND	-2.53	121.24	124.80
26	d	401	PHO	C1-C2-C3	-2.53	122.05	126.20
27	H	101	BCR	C16-C15-C14	-2.53	118.35	123.52
25	C	509	CLA	C1B-CHB-C4A	-2.53	125.22	130.04
25	b	606	CLA	O2A-CGA-O1A	-2.52	117.31	123.63
29	M	101	LMG	C40-C39-C38	-2.52	101.61	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	l	101	LHG	C20-C19-C18	-2.52	101.61	114.37
31	D	410	LHG	O8-C6-C5	-2.52	101.12	108.40
27	b	617	BCR	C3-C4-C5	-2.52	109.56	114.06
32	a	615	DGD	C5B-C4B-C3B	-2.52	101.62	114.37
25	b	605	CLA	CHD-C1D-ND	-2.52	121.25	124.80
30	F	101	SQD	O5-C1-C2	-2.52	105.19	110.37
27	c	514	BCR	C15-C16-C17	-2.52	118.36	123.52
25	b	608	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
31	d	409	LHG	O8-C23-C24	2.52	119.51	111.83
27	H	101	BCR	C24-C23-C22	-2.52	122.51	126.23
27	c	515	BCR	C15-C16-C17	-2.52	118.37	123.52
29	c	524	LMG	O6-C1-O1	-2.51	104.10	110.04
25	d	404	CLA	O2A-CGA-O1A	-2.51	117.34	123.63
25	C	512	CLA	CMB-C2B-C3B	2.51	129.71	124.68
25	c	513	CLA	CHB-C4A-NA	2.51	128.03	124.40
29	m	101	LMG	O1-C1-C2	-2.51	104.46	108.27
25	B	612	CLA	C16-C15-C13	-2.51	107.62	115.97
25	a	612	CLA	C1B-CHB-C4A	-2.51	125.26	130.04
31	D	409	LHG	C11-C10-C9	-2.51	101.70	114.37
27	K	102	BCR	C2-C1-C6	2.51	114.08	110.44
32	C	515	DGD	O5D-C6D-C5D	-2.51	103.77	109.42
27	c	514	BCR	C27-C26-C25	2.51	126.09	122.70
25	c	507	CLA	O2A-CGA-O1A	-2.50	117.36	123.63
28	d	406	PL9	C27-C28-C29	-2.50	121.89	127.62
25	c	505	CLA	CMB-C2B-C3B	2.50	129.68	124.68
32	a	615	DGD	C1G-C2G-C3G	-2.50	106.03	111.80
25	D	405	CLA	CHB-C4A-NA	2.50	128.00	124.40
25	B	604	CLA	C2D-C1D-ND	-2.50	107.66	110.13
25	C	512	CLA	CAA-CBA-CGA	-2.49	106.13	113.21
32	C	515	DGD	C7B-C6B-C5B	-2.49	101.77	114.37
25	c	504	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
25	B	603	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
25	b	611	CLA	CHB-C4A-NA	2.49	127.99	124.40
31	D	409	LHG	C27-C26-C25	-2.49	101.79	114.37
25	b	609	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
32	C	517	DGD	C3G-C2G-C1G	-2.49	105.98	111.78
25	b	610	CLA	CHB-C4A-NA	2.49	127.99	124.40
27	B	619	BCR	C34-C9-C10	-2.48	118.79	122.82
29	c	520	LMG	O8-C28-O10	-2.48	117.42	123.63
25	B	605	CLA	C1B-CHB-C4A	-2.48	125.31	130.04
30	F	101	SQD	O8-S-C6	2.48	110.76	105.97
36	v	201	HEC	CBA-CAA-C2A	-2.48	108.47	112.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	614	CLA	CMB-C2B-C3B	2.48	129.63	124.68
30	f	102	SQD	C3-C4-C5	2.48	114.72	110.23
33	b	622	STE	C3-C2-C1	-2.48	108.04	114.51
29	C	518	LMG	O6-C1-O1	-2.47	104.20	110.04
25	b	613	CLA	CHA-C1A-NA	-2.47	120.79	126.39
32	c	517	DGD	C3G-C2G-C1G	-2.47	106.03	111.78
32	c	518	DGD	CDB-CCB-CBB	-2.47	101.91	114.37
31	l	101	LHG	C11-C10-C9	-2.46	101.91	114.37
26	D	402	PHO	CMC-C2C-C3C	2.46	129.59	124.94
25	B	602	CLA	C16-C15-C13	-2.46	107.78	115.97
25	D	403	CLA	CHB-C4A-NA	2.46	127.95	124.40
25	b	615	CLA	CMB-C2B-C3B	2.46	129.59	124.68
25	C	506	CLA	C1B-CHB-C4A	-2.45	125.36	130.04
28	a	611	PL9	C40-C39-C41	2.45	119.49	115.23
25	B	605	CLA	O1D-CGD-CBD	2.45	129.36	124.52
25	c	511	CLA	O2D-CGD-CBD	2.45	115.52	111.23
25	B	603	CLA	O2D-CGD-CBD	2.45	115.51	111.23
25	B	613	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
25	a	612	CLA	CHB-C4A-NA	2.45	127.93	124.40
27	x	101	BCR	C15-C16-C17	-2.45	118.52	123.52
25	A	607	CLA	O2A-CGA-O1A	-2.44	117.51	123.63
27	K	101	BCR	C7-C8-C9	-2.44	122.62	126.23
31	D	409	LHG	C20-C19-C18	-2.44	102.02	114.37
25	b	615	CLA	C1B-CHB-C4A	-2.44	125.38	130.04
25	a	607	CLA	CHB-C4A-NA	2.44	127.92	124.40
25	b	614	CLA	CHD-C1D-ND	-2.44	121.37	124.80
25	b	608	CLA	C1-C2-C3	-2.44	122.20	126.20
29	c	520	LMG	C40-C39-C38	-2.44	102.04	114.37
27	a	610	BCR	C29-C30-C25	2.44	113.98	110.44
25	C	512	CLA	C1B-CHB-C4A	-2.44	125.39	130.04
25	b	609	CLA	CHB-C4A-NA	2.44	127.92	124.40
25	C	506	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
25	c	505	CLA	CHB-C4A-NA	2.43	127.91	124.40
31	e	101	LHG	C11-C10-C9	-2.43	102.08	114.37
26	D	402	PHO	C1B-NB-C4B	2.43	112.08	107.09
32	A	617	DGD	O2D-C2D-C1D	-2.43	104.29	110.08
29	C	518	LMG	O1-C1-C2	-2.43	104.58	108.27
29	A	612	LMG	C40-C39-C38	-2.43	102.09	114.37
27	a	610	BCR	C11-C10-C9	-2.43	123.87	127.28
26	d	402	PHO	O2A-CGA-O1A	-2.43	117.56	123.63
27	B	617	BCR	C3-C4-C5	-2.43	109.73	114.06
30	a	613	SQD	O9-S-C6	2.42	110.37	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	M	102	STE	C3-C2-C1	-2.42	108.20	114.51
31	D	412	LHG	C11-C10-C9	-2.42	102.15	114.37
32	h	101	DGD	O6D-C1D-O3G	-2.41	104.34	110.04
26	A	608	PHO	CMC-C2C-C3C	2.41	129.49	124.94
25	c	513	CLA	C1-C2-C3	-2.41	122.25	126.20
27	B	619	BCR	C11-C10-C9	-2.41	123.90	127.28
25	C	509	CLA	CHD-C1D-ND	-2.41	121.41	124.80
27	t	101	BCR	C7-C8-C9	-2.41	122.67	126.23
29	m	101	LMG	O8-C28-O10	-2.41	117.61	123.63
25	b	609	CLA	O2A-CGA-O1A	-2.40	117.61	123.63
35	f	101	HEM	CHC-C4B-C3B	2.40	128.25	124.57
25	c	501	CLA	CHB-C4A-NA	2.40	127.87	124.40
30	A	613	SQD	O9-S-C6	2.40	110.34	106.76
31	d	408	LHG	C18-C17-C16	-2.40	102.23	114.37
25	B	614	CLA	CHB-C4A-NA	2.40	127.87	124.40
27	A	610	BCR	C15-C14-C13	-2.40	123.91	127.28
25	b	610	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
25	B	604	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
25	c	509	CLA	C1B-CHB-C4A	-2.40	125.47	130.04
28	a	611	PL9	O2-C1-C2	-2.40	116.38	121.83
29	D	408	LMG	C38-C37-C36	-2.40	102.26	114.37
25	C	512	CLA	C1-C2-C3	-2.40	122.27	126.20
25	D	404	CLA	CMB-C2B-C3B	2.40	129.47	124.68
29	d	411	LMG	C40-C39-C38	-2.39	102.27	114.37
30	L	101	SQD	C25-C24-C23	-2.39	104.93	113.69
25	D	404	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
25	b	614	CLA	C1-C2-C3	-2.39	122.28	126.20
27	d	405	BCR	C33-C5-C6	-2.39	121.88	124.48
25	A	607	CLA	O2D-CGD-CBD	2.39	115.41	111.23
29	m	101	LMG	C38-C37-C36	-2.39	102.30	114.37
32	C	516	DGD	C1D-C2D-C3D	-2.39	104.99	110.01
31	l	101	LHG	O8-C23-C24	2.38	119.11	111.83
25	C	501	CLA	C1B-CHB-C4A	-2.38	125.49	130.04
25	C	512	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
27	b	617	BCR	C15-C14-C13	-2.38	123.94	127.28
27	b	619	BCR	C15-C16-C17	-2.38	118.65	123.52
33	d	413	STE	O2-C1-C2	2.38	121.51	114.00
27	A	610	BCR	C15-C16-C17	-2.38	118.66	123.52
30	a	614	SQD	O48-C23-O10	-2.37	117.69	123.63
27	c	516	BCR	C33-C5-C6	-2.37	121.89	124.48
31	d	407	LHG	C11-C10-C9	-2.37	102.38	114.37
25	c	510	CLA	O2A-CGA-O1A	-2.37	117.70	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	405	BCR	C16-C15-C14	-2.37	118.67	123.52
25	b	608	CLA	C1B-CHB-C4A	-2.37	125.53	130.04
25	b	604	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
27	c	516	BCR	C2-C1-C6	2.36	113.87	110.44
27	c	516	BCR	C24-C23-C22	-2.36	122.75	126.23
25	c	503	CLA	C11-C12-C13	-2.36	108.14	115.97
29	c	520	LMG	C38-C37-C36	-2.35	102.46	114.37
27	A	610	BCR	C33-C5-C6	-2.35	121.92	124.48
25	D	403	CLA	C1B-CHB-C4A	-2.35	125.55	130.04
25	b	605	CLA	CHB-C4A-NA	2.35	127.79	124.40
27	K	101	BCR	C27-C26-C25	2.35	125.88	122.70
25	B	606	CLA	O2D-CGD-CBD	2.35	115.33	111.23
25	b	607	CLA	C6-C7-C8	-2.35	108.16	115.97
25	B	601	CLA	CMB-C2B-C1B	-2.35	125.02	128.46
31	D	412	LHG	C20-C19-C18	-2.35	102.51	114.37
25	b	603	CLA	CHB-C4A-NA	2.35	127.78	124.40
29	A	612	LMG	O1-C7-C8	-2.35	105.11	110.82
25	B	601	CLA	C1B-CHB-C4A	-2.35	125.57	130.04
27	K	102	BCR	C3-C4-C5	-2.34	109.88	114.06
32	A	617	DGD	CBB-CAB-C9B	-2.34	102.52	114.37
25	C	507	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
29	d	410	LMG	O7-C10-O9	-2.34	117.31	123.33
29	c	522	LMG	O6-C1-O1	-2.34	104.51	110.04
35	E	101	HEM	C4C-CHD-C1D	2.34	125.65	122.56
25	b	607	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
25	c	513	CLA	C1B-CHB-C4A	-2.34	125.58	130.04
28	d	406	PL9	C50-C49-C48	-2.34	115.64	122.66
32	h	101	DGD	C7B-C6B-C5B	-2.34	102.56	114.37
25	C	512	CLA	O2D-CGD-CBD	2.34	115.31	111.23
27	C	514	BCR	C27-C26-C25	2.34	125.86	122.70
32	a	615	DGD	CFB-CEB-CDB	-2.33	102.57	114.37
25	B	610	CLA	CMA-C3A-C4A	-2.33	105.51	111.77
33	C	519	STE	C3-C2-C1	-2.33	108.43	114.51
31	A	614	LHG	C11-C10-C9	-2.33	102.59	114.37
32	C	515	DGD	CAB-C9B-C8B	-2.33	102.60	114.37
25	D	403	CLA	O2D-CGD-CBD	2.33	115.30	111.23
28	d	406	PL9	C20-C19-C21	2.33	119.27	115.23
28	A	611	PL9	C7-C8-C9	-2.33	122.82	126.83
27	b	618	BCR	C24-C23-C22	-2.33	122.79	126.23
25	b	612	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
25	c	509	CLA	C1-O2A-CGA	-2.33	111.02	116.65
32	A	617	DGD	C3E-C4E-C5E	-2.32	106.02	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	511	CLA	CHB-C4A-NA	2.32	127.75	124.40
29	m	101	LMG	C40-C39-C38	-2.32	102.62	114.37
29	b	621	LMG	O2-C2-C1	-2.32	104.54	110.08
27	B	619	BCR	C15-C16-C17	-2.32	118.77	123.52
25	C	502	CLA	C1B-CHB-C4A	-2.32	125.62	130.04
27	d	405	BCR	C30-C25-C26	-2.32	119.47	122.64
25	C	504	CLA	O2D-CGD-O1D	-2.32	119.34	123.85
28	a	611	PL9	O2-C1-C6	2.31	124.16	120.48
28	d	406	PL9	O2-C1-C6	2.31	124.16	120.48
28	A	611	PL9	C12-C13-C14	-2.31	122.34	127.62
28	D	407	PL9	C32-C33-C34	-2.31	122.34	127.62
33	C	519	STE	C4-C3-C2	-2.31	104.66	113.13
25	C	507	CLA	C1B-CHB-C4A	-2.30	125.65	130.04
25	B	611	CLA	CHD-C4C-NC	2.30	127.80	124.23
32	C	517	DGD	O3E-C3E-C2E	-2.30	104.95	110.38
25	c	512	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
25	C	501	CLA	O2D-CGD-CBD	2.30	115.25	111.23
25	a	609	CLA	O2A-CGA-O1A	-2.30	117.89	123.63
27	t	101	BCR	C33-C5-C6	-2.29	121.98	124.48
25	B	604	CLA	C1D-ND-C4D	2.29	107.92	106.31
27	T	101	BCR	C33-C5-C6	-2.29	121.98	124.48
31	D	412	LHG	O8-C23-O10	-2.29	117.89	123.63
27	B	618	BCR	C27-C26-C25	2.29	125.80	122.70
31	D	410	LHG	C27-C26-C25	-2.29	102.78	114.37
25	c	507	CLA	C1B-CHB-C4A	-2.29	125.67	130.04
27	b	619	BCR	C29-C30-C25	2.29	113.76	110.44
25	b	613	CLA	CHB-C4A-NA	2.29	127.70	124.40
25	C	507	CLA	C2A-C1A-CHA	2.28	127.83	123.87
31	D	409	LHG	O8-C23-O10	-2.28	117.92	123.63
25	C	503	CLA	CHD-C1D-ND	-2.28	121.59	124.80
25	c	504	CLA	CHB-C4A-NA	2.28	127.69	124.40
25	b	605	CLA	CHD-C4C-NC	2.28	127.77	124.23
27	c	516	BCR	C11-C10-C9	-2.28	124.08	127.28
32	C	515	DGD	C6D-O5D-C1E	2.28	118.69	113.80
25	A	607	CLA	CHB-C4A-NA	2.28	127.69	124.40
25	a	612	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
29	D	408	LMG	O1-C1-C2	-2.28	104.81	108.27
25	b	603	CLA	CHD-C1D-C2D	2.28	130.22	125.49
35	E	101	HEM	CBA-CAA-C2A	-2.28	108.71	112.54
29	c	522	LMG	C40-C39-C38	-2.27	102.88	114.37
32	a	615	DGD	CAB-C9B-C8B	-2.27	102.88	114.37
27	t	101	BCR	C27-C26-C25	2.27	125.78	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	610	BCR	C2-C1-C6	2.27	113.74	110.44
27	c	514	BCR	C11-C10-C9	-2.27	124.09	127.28
25	c	510	CLA	CHB-C4A-NA	2.27	127.67	124.40
25	B	615	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
25	b	604	CLA	C11-C12-C13	-2.27	108.43	115.97
25	b	614	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
30	B	622	SQD	C25-C24-C23	-2.27	105.39	113.69
25	a	608	CLA	O2A-CGA-O1A	-2.26	117.96	123.63
31	D	410	LHG	C11-C10-C9	-2.26	102.95	114.37
25	C	505	CLA	C1B-CHB-C4A	-2.26	125.73	130.04
25	b	605	CLA	C1-C2-C3	-2.26	122.50	126.20
25	D	404	CLA	CHB-C4A-NA	2.26	127.66	124.40
25	b	608	CLA	C6-C7-C8	-2.26	108.46	115.97
25	c	511	CLA	CMB-C2B-C3B	2.26	129.19	124.68
32	a	615	DGD	C7B-C6B-C5B	-2.26	102.96	114.37
30	B	622	SQD	O8-S-C6	2.26	110.33	105.97
30	B	622	SQD	O9-S-C6	2.25	110.12	106.76
27	B	619	BCR	C1-C6-C5	-2.25	119.56	122.64
25	c	507	CLA	CMB-C2B-C3B	2.25	129.18	124.68
25	c	507	CLA	CHB-C4A-NA	2.25	127.65	124.40
34	D	401	BCT	O2-C-O1	-2.25	113.92	119.68
35	f	101	HEM	CAB-C3B-C2B	-2.25	121.12	128.43
32	H	102	DGD	C3G-C2G-C1G	-2.25	106.54	111.78
27	c	514	BCR	C2-C1-C6	2.25	113.70	110.44
29	D	408	LMG	C3-C4-C5	-2.25	106.16	110.23
29	c	522	LMG	O7-C10-O9	-2.25	118.45	123.70
27	t	101	BCR	C35-C13-C12	2.25	121.52	118.09
25	B	604	CLA	C11-C10-C8	-2.25	108.50	115.97
29	D	408	LMG	O1-C7-C8	-2.24	105.36	110.82
25	b	603	CLA	O2A-CGA-O1A	-2.24	118.01	123.63
25	c	512	CLA	CHD-C1D-ND	-2.24	121.64	124.80
25	C	510	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
26	d	401	PHO	CMA-C3A-C4A	-2.24	109.78	114.61
25	b	610	CLA	O1D-CGD-CBD	2.24	128.94	124.52
25	c	507	CLA	CHA-C1A-NA	-2.24	121.31	126.39
25	C	506	CLA	CHB-C4A-NA	2.24	127.63	124.40
32	H	102	DGD	C1D-C2D-C3D	-2.24	105.31	110.01
25	c	509	CLA	O2D-CGD-CBD	2.23	115.13	111.23
29	b	621	LMG	O6-C5-C6	2.23	111.97	106.44
25	b	601	CLA	O2D-CGD-CBD	2.23	115.13	111.23
29	c	524	LMG	C9-C8-C7	-2.23	106.58	111.78
25	B	611	CLA	CHD-C1D-ND	-2.23	121.66	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	506	CLA	O1D-CGD-CBD	2.23	128.92	124.52
27	x	101	BCR	C3-C4-C5	-2.23	110.08	114.06
25	b	604	CLA	C11-C10-C8	-2.23	108.55	115.97
28	D	407	PL9	C27-C28-C29	-2.23	122.52	127.62
25	b	604	CLA	C6-C7-C8	-2.23	108.56	115.97
32	H	102	DGD	O6D-C1D-O3G	-2.23	104.78	110.04
25	c	502	CLA	CHB-C4A-NA	2.23	127.61	124.40
32	h	101	DGD	C5B-C4B-C3B	-2.22	103.13	114.37
31	e	101	LHG	C20-C19-C18	-2.22	103.13	114.37
32	A	617	DGD	C5B-C4B-C3B	-2.22	103.15	114.37
25	c	511	CLA	C2A-C1A-CHA	2.22	127.72	123.87
28	A	611	PL9	O1-C4-C3	-2.22	118.39	120.73
31	A	615	LHG	C20-C19-C18	-2.22	103.16	114.37
25	B	612	CLA	CHD-C1D-ND	-2.22	121.68	124.80
32	c	519	DGD	C1D-C2D-C3D	-2.22	105.35	110.01
25	c	508	CLA	CHD-C1D-ND	-2.22	121.68	124.80
29	A	612	LMG	O6-C1-O1	-2.22	104.81	110.04
32	c	517	DGD	CBB-CAB-C9B	-2.22	103.17	114.37
32	C	516	DGD	CAB-C9B-C8B	-2.21	103.17	114.37
25	B	613	CLA	CHB-C4A-NA	2.21	127.60	124.40
25	B	615	CLA	CMB-C2B-C1B	-2.21	125.21	128.46
25	C	513	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
27	d	405	BCR	C24-C23-C22	-2.21	122.96	126.23
32	c	519	DGD	CBB-CAB-C9B	-2.21	103.18	114.37
32	H	102	DGD	CAB-C9B-C8B	-2.21	103.19	114.37
32	A	617	DGD	O3G-C1D-C2D	-2.21	104.92	108.27
32	C	515	DGD	C5B-C4B-C3B	-2.21	103.19	114.37
28	A	611	PL9	C40-C39-C38	-2.21	117.95	123.63
33	x	102	STE	C3-C2-C1	-2.21	108.74	114.51
25	B	605	CLA	CHB-C4A-NA	2.21	127.59	124.40
25	B	603	CLA	C1B-CHB-C4A	-2.21	125.83	130.04
25	A	606	CLA	O1D-CGD-CBD	2.21	128.87	124.52
25	c	508	CLA	C1B-CHB-C4A	-2.21	125.83	130.04
32	A	617	DGD	C8B-C7B-C6B	-2.21	103.22	114.37
32	h	101	DGD	C1D-O6D-C5D	-2.20	109.42	113.72
27	b	619	BCR	C27-C26-C25	2.20	125.68	122.70
27	B	617	BCR	C15-C14-C13	-2.20	124.19	127.28
25	c	501	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
28	a	611	PL9	C36-C34-C33	-2.20	116.22	121.17
32	h	101	DGD	CBB-CAB-C9B	-2.20	103.24	114.37
25	c	508	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
29	c	524	LMG	O7-C10-O9	-2.20	118.56	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	602	CLA	CHD-C1D-ND	-2.20	121.70	124.80
25	D	403	CLA	CHD-C1D-ND	-2.20	121.71	124.80
32	c	519	DGD	CAB-C9B-C8B	-2.20	103.26	114.37
25	B	606	CLA	CHB-C4A-NA	2.20	127.57	124.40
31	d	407	LHG	C5-O7-C7	-2.20	112.54	117.80
25	B	605	CLA	CHD-C1D-C2D	2.19	130.05	125.49
35	f	101	HEM	C3B-C4B-NB	-2.19	107.89	109.47
29	c	522	LMG	C38-C37-C36	-2.19	103.28	114.37
25	d	404	CLA	C1-C2-C3	-2.19	122.61	126.20
25	C	510	CLA	CHB-C4A-NA	2.19	127.56	124.40
25	A	609	CLA	CHD-C1D-ND	-2.19	121.72	124.80
29	C	518	LMG	C38-C37-C36	-2.19	103.30	114.37
29	D	408	LMG	O2-C2-C1	-2.19	104.86	110.08
32	C	517	DGD	O3G-C1D-C2D	-2.19	104.95	108.27
29	C	518	LMG	O7-C10-O9	-2.19	118.59	123.70
27	H	101	BCR	C2-C1-C6	2.19	113.61	110.44
27	x	101	BCR	C15-C14-C13	-2.18	124.22	127.28
25	b	608	CLA	CHD-C4C-NC	2.18	127.61	124.23
25	B	603	CLA	CHD-C1D-ND	-2.18	121.73	124.80
32	c	517	DGD	C5B-C4B-C3B	-2.18	103.35	114.37
31	A	614	LHG	C20-C19-C18	-2.18	103.37	114.37
25	c	501	CLA	C1-C2-C3	-2.18	122.63	126.20
29	b	621	LMG	C40-C39-C38	-2.17	103.38	114.37
32	a	615	DGD	CBB-CAB-C9B	-2.17	103.38	114.37
27	b	617	BCR	C29-C30-C25	2.17	113.59	110.44
29	A	612	LMG	C38-C37-C36	-2.17	103.40	114.37
29	B	621	LMG	O7-C10-O9	-2.17	117.75	123.33
25	b	615	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
28	d	406	PL9	O2-C1-C2	-2.17	116.89	121.83
27	B	618	BCR	C35-C13-C14	-2.17	119.30	122.82
27	H	101	BCR	C35-C13-C14	-2.17	119.30	122.82
25	B	604	CLA	C16-C15-C13	-2.16	108.77	115.97
29	M	101	LMG	O3-C3-C2	-2.16	105.28	110.38
28	a	611	PL9	C32-C33-C34	-2.16	122.67	127.62
29	c	520	LMG	C6-C5-C4	-2.16	107.71	113.02
25	b	607	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
29	m	101	LMG	O2-C2-C1	-2.16	104.93	110.08
25	a	608	CLA	CAC-C3C-C4C	2.16	127.60	124.79
29	A	612	LMG	C1-C2-C3	-2.16	105.47	110.01
29	d	411	LMG	O1-C1-C2	-2.16	105.00	108.27
29	d	411	LMG	C38-C37-C36	-2.16	103.46	114.37
29	C	518	LMG	C40-C39-C38	-2.16	103.47	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	510	CLA	C1B-CHB-C4A	-2.16	125.93	130.04
28	D	407	PL9	C42-C43-C44	-2.16	122.69	127.62
27	b	617	BCR	C11-C10-C9	-2.15	124.26	127.28
32	c	519	DGD	C8B-C7B-C6B	-2.15	103.48	114.37
25	b	605	CLA	CHD-C1D-C2D	2.15	129.96	125.49
27	t	101	BCR	C1-C6-C5	-2.15	119.69	122.64
25	B	616	CLA	O2D-CGD-CBD	2.15	114.99	111.23
31	d	407	LHG	C20-C19-C18	-2.15	103.50	114.37
32	C	516	DGD	C3E-C4E-C5E	-2.15	106.34	110.23
25	C	502	CLA	C1-C2-C3	-2.15	122.68	126.20
29	C	518	LMG	C6-C5-C4	-2.15	107.75	113.02
32	C	515	DGD	O1G-C1A-C2A	-2.14	105.30	111.83
25	c	510	CLA	O1D-CGD-CBD	2.14	128.75	124.52
25	b	614	CLA	CHB-C4A-NA	2.14	127.49	124.40
29	M	101	LMG	O2-C2-C1	-2.14	104.97	110.08
30	F	101	SQD	C3-C4-C5	2.14	114.12	110.23
32	c	519	DGD	C6B-C5B-C4B	-2.14	103.54	114.37
25	c	505	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
27	C	514	BCR	C33-C5-C6	-2.14	122.15	124.48
25	C	504	CLA	CHA-C1A-NA	-2.14	121.55	126.39
29	A	612	LMG	O7-C10-O9	-2.14	118.71	123.70
25	b	612	CLA	C11-C10-C8	-2.14	108.86	115.97
28	A	611	PL9	O2-C1-C6	2.14	123.88	120.48
25	C	510	CLA	O2D-CGD-CBD	2.14	114.96	111.23
27	D	406	BCR	C30-C25-C26	-2.13	119.72	122.64
25	C	505	CLA	O2D-CGD-O1D	-2.13	119.69	123.85
25	B	613	CLA	C1B-CHB-C4A	-2.13	125.97	130.04
29	c	522	LMG	O2-C2-C1	-2.13	104.99	110.08
25	B	603	CLA	CHB-C4A-NA	2.13	127.48	124.40
32	C	516	DGD	C6D-C5D-C4D	2.13	116.53	112.07
28	a	611	PL9	O1-C4-C3	-2.13	118.49	120.73
32	c	518	DGD	C5B-C4B-C3B	-2.13	103.62	114.37
25	B	604	CLA	O2D-CGD-CBD	2.13	114.94	111.23
25	b	608	CLA	C11-C10-C8	-2.12	108.91	115.97
25	B	607	CLA	CHB-C4A-NA	2.12	127.46	124.40
32	A	617	DGD	CFB-CEB-CDB	-2.12	103.64	114.37
25	C	508	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
25	C	505	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
26	d	401	PHO	O1D-CGD-CBD	2.12	127.94	124.72
27	B	618	BCR	C38-C26-C25	-2.12	122.17	124.48
25	d	403	CLA	C1B-CHB-C4A	-2.12	126.00	130.04
25	C	504	CLA	CHD-C1D-ND	-2.12	121.82	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	613	SQD	O47-C7-O49	-2.12	118.76	123.70
25	C	502	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
25	a	609	CLA	C1B-CHB-C4A	-2.11	126.01	130.04
33	a	617	STE	C3-C2-C1	-2.11	108.99	114.51
25	B	609	CLA	CAC-C3C-C4C	2.11	127.54	124.79
27	Y	101	BCR	C16-C15-C14	-2.11	119.20	123.52
33	B	625	STE	O2-C1-C2	2.11	120.67	114.00
30	L	101	SQD	C9-C8-C7	-2.11	105.96	113.69
25	b	602	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
25	B	612	CLA	O1D-CGD-CBD	2.11	128.68	124.52
25	B	606	CLA	CHD-C4C-NC	2.11	127.50	124.23
28	d	406	PL9	C32-C33-C34	-2.11	122.80	127.62
28	D	407	PL9	C36-C34-C33	-2.11	116.44	121.17
31	A	614	LHG	O8-C23-O10	-2.11	118.36	123.63
28	a	611	PL9	C27-C28-C29	-2.11	122.80	127.62
25	B	601	CLA	C4-C3-C5	2.11	118.88	115.23
30	a	614	SQD	C9-C8-C7	-2.10	105.98	113.69
25	a	607	CLA	C4-C3-C5	2.10	118.88	115.23
29	b	621	LMG	C8-O7-C10	2.10	122.83	117.80
25	B	601	CLA	CHB-C4A-NA	2.10	127.44	124.40
31	A	614	LHG	C18-C17-C16	-2.10	103.74	114.37
28	D	407	PL9	C8-C7-C3	2.10	117.46	112.03
25	b	613	CLA	CHA-C4D-ND	2.10	136.88	132.55
25	b	610	CLA	CHD-C1D-ND	-2.10	121.85	124.80
25	B	610	CLA	CHD-C1D-ND	-2.10	121.85	124.80
25	C	503	CLA	C4D-CHA-C1A	2.10	123.74	121.24
25	C	505	CLA	C1-C2-C3	-2.09	122.77	126.20
29	c	520	LMG	O1-C7-C8	-2.09	105.72	110.82
32	h	101	DGD	CAB-C9B-C8B	-2.09	103.78	114.37
25	B	603	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
32	C	516	DGD	O6E-C1E-O5D	-2.09	105.10	110.04
25	c	510	CLA	C2D-C1D-ND	-2.09	108.06	110.13
25	c	509	CLA	CHD-C1D-ND	-2.09	121.86	124.80
27	B	618	BCR	C33-C5-C6	-2.09	122.20	124.48
27	A	610	BCR	C16-C15-C14	-2.09	119.24	123.52
25	b	609	CLA	CHA-C1A-NA	-2.09	121.66	126.39
25	c	501	CLA	CHD-C1D-ND	-2.09	121.86	124.80
25	b	603	CLA	C11-C12-C13	-2.09	109.03	115.97
25	C	512	CLA	CHD-C1D-ND	-2.09	121.87	124.80
25	B	601	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
32	A	617	DGD	CAB-C9B-C8B	-2.09	103.82	114.37
27	A	610	BCR	C8-C7-C6	-2.09	121.43	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	l	101	LHG	C18-C17-C16	-2.08	103.83	114.37
31	D	410	LHG	O8-C23-C24	2.08	118.19	111.83
25	A	606	CLA	C11-C12-C13	-2.08	109.04	115.97
25	D	405	CLA	O2D-CGD-CBD	2.08	114.87	111.23
29	C	518	LMG	O3-C3-C2	-2.08	105.47	110.38
25	C	509	CLA	C1-C2-C3	-2.08	122.79	126.20
25	A	606	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
25	C	510	CLA	C16-C15-C13	-2.08	109.05	115.97
25	C	503	CLA	O1D-CGD-CBD	2.08	128.62	124.52
30	A	613	SQD	O5-C5-C4	2.08	113.45	109.70
29	D	411	LMG	O7-C10-O9	-2.08	118.85	123.70
29	c	522	LMG	C42-C41-C40	-2.08	103.86	114.37
25	b	613	CLA	C2A-C1A-CHA	2.08	127.47	123.87
26	d	402	PHO	C1B-NB-C4B	2.08	111.35	107.09
25	B	606	CLA	CGD-CBD-CAD	-2.08	104.13	110.85
25	c	503	CLA	CMB-C2B-C3B	2.07	128.83	124.68
25	C	511	CLA	CHD-C1D-ND	-2.07	121.89	124.80
25	b	611	CLA	CHC-C1C-NC	2.07	127.43	124.31
28	d	406	PL9	C8-C7-C3	2.07	117.39	112.03
29	D	411	LMG	C38-C37-C36	-2.07	103.91	114.37
28	A	611	PL9	O2-C1-C2	-2.07	117.12	121.83
27	A	610	BCR	C7-C8-C9	-2.07	123.17	126.23
25	b	616	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
25	B	615	CLA	CHD-C1D-ND	-2.07	121.89	124.80
25	b	611	CLA	CHD-C1D-ND	-2.07	121.89	124.80
25	b	605	CLA	C7-C6-C5	-2.07	107.75	113.26
31	e	101	LHG	C18-C17-C16	-2.07	103.92	114.37
33	t	102	STE	O2-C1-C2	2.07	120.53	114.00
25	a	609	CLA	CHA-C1A-NA	-2.07	121.71	126.39
25	C	503	CLA	C1B-CHB-C4A	-2.07	126.10	130.04
33	C	520	STE	O2-C1-C2	2.06	120.52	114.00
27	a	610	BCR	C40-C30-C25	2.06	113.48	110.24
35	f	101	HEM	CMA-C3A-C4A	-2.06	125.43	128.46
27	d	405	BCR	C11-C10-C9	-2.06	124.39	127.28
28	a	611	PL9	C42-C43-C44	-2.06	122.91	127.62
35	f	101	HEM	CMC-C2C-C3C	2.06	128.80	124.68
35	f	101	HEM	CHB-C1B-NB	2.06	126.92	124.37
25	B	603	CLA	CHD-C1D-C2D	2.06	129.77	125.49
25	b	611	CLA	CHD-C1D-C2D	2.06	129.77	125.49
25	C	511	CLA	C1B-CHB-C4A	-2.06	126.12	130.04
27	B	617	BCR	C33-C5-C6	-2.05	122.24	124.48
27	T	101	BCR	C15-C14-C13	-2.05	124.40	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C	517	DGD	CBB-CAB-C9B	-2.05	103.99	114.37
32	c	518	DGD	CBB-CAB-C9B	-2.05	103.99	114.37
29	c	520	LMG	O2-C2-C1	-2.05	105.19	110.08
29	d	411	LMG	C3-C4-C5	-2.05	106.52	110.23
29	c	522	LMG	O3-C3-C2	-2.05	105.55	110.38
32	c	518	DGD	O6E-C1E-O5D	-2.05	105.21	110.04
25	C	513	CLA	O1D-CGD-CBD	2.05	128.56	124.52
31	A	614	LHG	C27-C26-C25	-2.05	104.03	114.37
25	c	503	CLA	CHD-C1D-ND	-2.05	121.92	124.80
25	C	503	CLA	C1-C2-C3	2.04	129.55	126.20
27	A	610	BCR	C38-C26-C25	-2.04	122.25	124.48
33	j	101	STE	C3-C2-C1	-2.04	109.17	114.51
27	a	610	BCR	C21-C20-C19	-2.04	117.28	123.20
27	a	610	BCR	C39-C30-C25	-2.04	107.04	110.24
32	C	515	DGD	O3E-C3E-C2E	-2.04	105.56	110.38
32	C	515	DGD	CBB-CAB-C9B	-2.04	104.05	114.37
30	F	101	SQD	C1-C2-C3	-2.04	105.72	110.01
25	c	503	CLA	C7-C6-C5	-2.04	107.83	113.26
29	B	621	LMG	C38-C37-C36	-2.04	104.07	114.37
30	a	613	SQD	O47-C7-O49	-2.03	118.95	123.70
27	Y	101	BCR	C10-C11-C12	-2.03	117.31	123.20
33	C	519	STE	C6-C5-C4	-2.03	104.09	114.37
25	c	502	CLA	CED-O2D-CGD	2.03	120.53	115.92
32	c	518	DGD	C7B-C6B-C5B	-2.03	104.11	114.37
29	d	410	LMG	C38-C37-C36	-2.03	104.12	114.37
27	c	516	BCR	C38-C26-C25	-2.03	122.27	124.48
28	D	407	PL9	C40-C39-C41	2.03	118.75	115.23
31	l	101	LHG	C27-C26-C25	-2.03	104.13	114.37
27	c	515	BCR	C33-C5-C6	-2.03	122.27	124.48
25	D	404	CLA	C11-C12-C13	-2.02	109.23	115.97
25	D	405	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
25	C	507	CLA	CHA-C1A-NA	-2.02	121.81	126.39
25	C	508	CLA	CHD-C1D-C2D	2.02	129.70	125.49
25	B	610	CLA	CMB-C2B-C3B	2.02	128.73	124.68
25	c	512	CLA	CMB-C2B-C3B	2.02	128.73	124.68
25	B	607	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
32	c	518	DGD	C1D-C2D-C3D	-2.02	105.76	110.01
25	b	613	CLA	C1B-CHB-C4A	-2.02	126.19	130.04
31	d	408	LHG	C27-C26-C25	-2.02	104.17	114.37
25	d	403	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
32	C	516	DGD	C3D-C4D-C5D	-2.02	106.57	110.23
32	c	518	DGD	O2E-C2E-C1E	-2.02	105.27	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	618	BCR	C35-C13-C14	-2.02	119.55	122.82
25	b	615	CLA	CHC-C1C-NC	2.02	127.35	124.31
27	k	101	BCR	C38-C26-C25	-2.02	122.28	124.48
32	C	516	DGD	C6D-O5D-C1E	2.01	118.11	113.80
27	K	102	BCR	C11-C10-C9	-2.01	124.46	127.28
25	C	502	CLA	C16-C15-C13	-2.01	109.28	115.97
25	b	609	CLA	C1-C2-C3	-2.01	122.90	126.20
28	a	611	PL9	C20-C19-C21	2.01	118.72	115.23
32	A	617	DGD	C1D-C2D-C3D	-2.01	105.78	110.01
25	c	506	CLA	O2D-CGD-O1D	-2.01	119.94	123.85
27	K	101	BCR	C33-C5-C6	-2.01	122.29	124.48
25	D	404	CLA	C1-C2-C3	-2.01	122.91	126.20
25	B	608	CLA	C11-C12-C13	-2.01	109.30	115.97
26	d	401	PHO	CED-O2D-CGD	2.00	120.46	115.92
35	f	101	HEM	C1B-NB-C4B	2.00	107.58	105.21
27	H	101	BCR	C1-C6-C5	-2.00	119.90	122.64
32	C	515	DGD	C3G-C2G-C1G	-2.00	107.11	111.78
29	C	518	LMG	O8-C28-O10	-2.00	118.62	123.63
25	B	610	CLA	C4-C3-C5	2.00	118.70	115.23

All (62) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	606	CLA	ND
25	A	609	CLA	ND
25	B	601	CLA	ND
25	B	602	CLA	ND
25	B	603	CLA	ND
25	B	604	CLA	ND
25	B	605	CLA	ND
25	B	606	CLA	ND
25	B	607	CLA	ND
25	B	608	CLA	ND
25	B	610	CLA	ND
25	B	611	CLA	ND
25	B	612	CLA	ND
25	B	613	CLA	ND
25	B	614	CLA	ND
25	B	615	CLA	ND
25	B	616	CLA	ND
25	C	501	CLA	ND
25	C	502	CLA	ND

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Mol	Chain	Res	Type	Atom
25	C	503	CLA	ND
25	C	504	CLA	ND
25	C	505	CLA	ND
25	C	506	CLA	ND
25	C	507	CLA	ND
25	C	509	CLA	ND
25	C	510	CLA	ND
25	C	511	CLA	ND
25	C	512	CLA	ND
25	C	513	CLA	ND
25	D	403	CLA	ND
25	D	404	CLA	ND
25	a	607	CLA	ND
25	a	609	CLA	ND
25	a	612	CLA	ND
25	b	601	CLA	ND
25	b	603	CLA	ND
25	b	604	CLA	ND
25	b	605	CLA	ND
25	b	606	CLA	ND
25	b	607	CLA	ND
25	b	608	CLA	ND
25	b	609	CLA	ND
25	b	610	CLA	ND
25	b	611	CLA	ND
25	b	612	CLA	ND
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	615	CLA	ND
25	b	616	CLA	ND
25	c	501	CLA	ND
25	c	502	CLA	ND
25	c	504	CLA	ND
25	c	505	CLA	ND
25	c	506	CLA	ND
25	c	507	CLA	ND
25	c	509	CLA	ND
25	c	510	CLA	ND
25	c	511	CLA	ND
25	c	512	CLA	ND
25	c	513	CLA	ND
25	d	403	CLA	ND

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Mol	Chain	Res	Type	Atom
25	d	404	CLA	ND

All (1818) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	B	601	CLA	CAD-CBD-CGD-O1D
25	B	601	CLA	CAD-CBD-CGD-O2D
25	B	606	CLA	C11-C10-C8-C9
25	B	607	CLA	C4-C3-C5-C6
25	B	614	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	C	507	CLA	CHA-CBD-CGD-O2D
25	C	513	CLA	C12-C13-C15-C16
25	b	607	CLA	C4-C3-C5-C6
25	b	607	CLA	C11-C10-C8-C9
25	b	614	CLA	CAD-CBD-CGD-O1D
25	b	614	CLA	CAD-CBD-CGD-O2D
25	b	616	CLA	CHA-CBD-CGD-O1D
25	b	616	CLA	CHA-CBD-CGD-O2D
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O2D
25	c	509	CLA	C6-C7-C8-C9
25	c	511	CLA	C14-C13-C15-C16
27	B	618	BCR	C20-C21-C22-C37
27	C	514	BCR	C20-C21-C22-C37
27	D	406	BCR	C22-C23-C24-C25
27	D	406	BCR	C23-C24-C25-C26
27	D	406	BCR	C23-C24-C25-C30
27	H	101	BCR	C11-C12-C13-C35
27	T	101	BCR	C1-C6-C7-C8
27	T	101	BCR	C5-C6-C7-C8
27	T	101	BCR	C7-C8-C9-C10
27	Y	101	BCR	C20-C21-C22-C37
27	Y	101	BCR	C37-C22-C23-C24
27	b	617	BCR	C20-C21-C22-C37
27	d	405	BCR	C7-C8-C9-C34
27	d	405	BCR	C21-C22-C23-C24
27	k	101	BCR	C7-C8-C9-C34
27	k	101	BCR	C17-C18-C19-C20
27	k	101	BCR	C20-C21-C22-C37
28	A	611	PL9	C12-C13-C14-C15
28	A	611	PL9	C12-C13-C14-C16

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Mol	Chain	Res	Type	Atoms
28	A	611	PL9	C22-C23-C24-C25
28	A	611	PL9	C32-C33-C34-C36
28	A	611	PL9	C37-C38-C39-C40
28	A	611	PL9	C40-C39-C41-C42
28	D	407	PL9	C32-C33-C34-C36
28	a	611	PL9	C22-C23-C24-C25
28	a	611	PL9	C22-C23-C24-C26
28	a	611	PL9	C24-C26-C27-C28
28	a	611	PL9	C35-C34-C36-C37
28	a	611	PL9	C42-C43-C44-C46
28	a	611	PL9	C44-C46-C47-C48
28	d	406	PL9	C42-C43-C44-C46
28	d	406	PL9	C47-C48-C49-C51
29	A	612	LMG	O6-C1-O1-C7
29	A	612	LMG	O1-C7-C8-O7
29	A	612	LMG	O9-C10-O7-C8
29	A	612	LMG	C11-C10-O7-C8
29	c	524	LMG	O6-C1-O1-C7
30	A	616	SQD	C44-C45-C46-O48
30	A	616	SQD	C46-C45-O47-C7
30	B	622	SQD	C2-C1-O6-C44
30	B	622	SQD	O5-C1-O6-C44
30	B	622	SQD	O49-C7-O47-C45
30	B	622	SQD	C8-C7-O47-C45
30	B	622	SQD	O5-C5-C6-S
30	F	101	SQD	C45-C44-O6-C1
30	L	101	SQD	C8-C7-O47-C45
30	L	101	SQD	O10-C23-O48-C46
30	L	101	SQD	C24-C23-O48-C46
30	a	614	SQD	C8-C7-O47-C45
30	f	102	SQD	O5-C1-O6-C44
31	A	614	LHG	C3-O3-P-O5
31	A	614	LHG	O10-C23-O8-C6
31	A	615	LHG	C3-O3-P-O4
31	A	615	LHG	C4-O6-P-O4
31	D	409	LHG	C1-C2-C3-O3
31	D	409	LHG	O2-C2-C3-O3
31	D	409	LHG	C3-O3-P-O5
31	D	409	LHG	C3-O3-P-O6
31	D	409	LHG	C4-O6-P-O3
31	D	409	LHG	C4-O6-P-O4
31	D	412	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
31	D	412	LHG	C1-C2-C3-O3
31	D	412	LHG	C3-O3-P-O4
31	D	412	LHG	C3-O3-P-O5
31	D	412	LHG	C3-O3-P-O6
31	d	407	LHG	O1-C1-C2-O2
31	d	407	LHG	O1-C1-C2-C3
31	d	407	LHG	C3-O3-P-O6
31	d	408	LHG	O1-C1-C2-C3
31	d	408	LHG	C3-O3-P-O4
31	d	408	LHG	C3-O3-P-O6
31	d	408	LHG	C4-O6-P-O4
31	e	101	LHG	O1-C1-C2-O2
31	e	101	LHG	O1-C1-C2-C3
31	e	101	LHG	C3-O3-P-O4
31	e	101	LHG	C3-O3-P-O6
31	e	101	LHG	O6-C4-C5-O7
31	e	101	LHG	O10-C23-O8-C6
31	l	101	LHG	C3-O3-P-O4
31	l	101	LHG	C4-O6-P-O3
31	l	101	LHG	C4-O6-P-O4
31	l	101	LHG	C4-O6-P-O5
32	A	617	DGD	O1B-C1B-O2G-C2G
25	b	601	CLA	CBD-CGD-O2D-CED
25	c	509	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	CBD-CGD-O2D-CED
26	d	402	PHO	CBD-CGD-O2D-CED
25	B	601	CLA	O1A-CGA-O2A-C1
30	F	101	SQD	O10-C23-O48-C46
30	f	102	SQD	O10-C23-O48-C46
28	D	407	PL9	C47-C48-C49-C50
28	d	406	PL9	C47-C48-C49-C50
25	B	601	CLA	CBA-CGA-O2A-C1
30	F	101	SQD	C24-C23-O48-C46
30	f	102	SQD	C24-C23-O48-C46
31	A	614	LHG	C24-C23-O8-C6
31	e	101	LHG	C24-C23-O8-C6
25	c	510	CLA	CBD-CGD-O2D-CED
29	D	411	LMG	O9-C10-O7-C8
29	b	621	LMG	O9-C10-O7-C8
29	c	522	LMG	O9-C10-O7-C8
30	L	101	SQD	O49-C7-O47-C45
30	a	614	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
32	a	615	DGD	O1B-C1B-O2G-C2G
25	B	605	CLA	C3-C5-C6-C7
25	B	616	CLA	C3-C5-C6-C7
25	c	511	CLA	CBD-CGD-O2D-CED
25	c	512	CLA	CBD-CGD-O2D-CED
32	A	617	DGD	C2B-C1B-O2G-C2G
32	a	615	DGD	C2B-C1B-O2G-C2G
25	b	601	CLA	O1D-CGD-O2D-CED
25	A	609	CLA	C4-C3-C5-C6
25	B	614	CLA	C4-C3-C5-C6
25	C	504	CLA	C4-C3-C5-C6
25	b	614	CLA	C4-C3-C5-C6
28	d	406	PL9	C40-C39-C41-C42
25	A	609	CLA	C2-C3-C5-C6
25	B	605	CLA	C2-C3-C5-C6
25	B	607	CLA	C2-C3-C5-C6
25	b	607	CLA	C2-C3-C5-C6
25	b	614	CLA	C2-C3-C5-C6
28	D	407	PL9	C47-C48-C49-C51
29	M	101	LMG	O10-C28-O8-C9
25	b	614	CLA	C3-C5-C6-C7
25	c	510	CLA	C3-C5-C6-C7
30	B	622	SQD	C24-C23-O48-C46
28	A	611	PL9	C27-C28-C29-C30
28	A	611	PL9	C22-C23-C24-C26
28	A	611	PL9	C37-C38-C39-C41
29	c	524	LMG	O10-C28-O8-C9
30	B	622	SQD	O10-C23-O48-C46
29	c	522	LMG	O6-C5-C6-O5
25	B	608	CLA	C3-C5-C6-C7
25	b	602	CLA	C3-C5-C6-C7
25	b	606	CLA	C3-C5-C6-C7
26	d	402	PHO	O1D-CGD-O2D-CED
30	a	614	SQD	C24-C23-O48-C46
32	c	519	DGD	O1A-C1A-O1G-C1G
29	C	518	LMG	C11-C10-O7-C8
29	b	621	LMG	C11-C10-O7-C8
25	c	509	CLA	O1D-CGD-O2D-CED
29	b	621	LMG	O10-C28-O8-C9
25	c	513	CLA	O1D-CGD-O2D-CED
25	B	603	CLA	CBD-CGD-O2D-CED
25	B	605	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	C	513	CLA	C4-C3-C5-C6
25	c	507	CLA	C4-C3-C5-C6
25	B	614	CLA	C2-C3-C5-C6
25	C	504	CLA	C2-C3-C5-C6
25	C	513	CLA	C2-C3-C5-C6
25	b	605	CLA	C2-C3-C5-C6
25	c	507	CLA	C2-C3-C5-C6
28	A	611	PL9	C18-C19-C21-C22
28	A	611	PL9	C38-C39-C41-C42
28	A	611	PL9	C43-C44-C46-C47
28	d	406	PL9	C38-C39-C41-C42
28	A	611	PL9	C34-C36-C37-C38
28	D	407	PL9	C44-C46-C47-C48
29	c	524	LMG	C4-C5-C6-O5
29	c	522	LMG	C4-C5-C6-O5
30	F	101	SQD	O5-C1-O6-C44
29	M	101	LMG	C29-C28-O8-C9
30	a	614	SQD	O10-C23-O48-C46
31	D	412	LHG	C28-C29-C30-C31
25	C	501	CLA	CBD-CGD-O2D-CED
29	D	411	LMG	C11-C10-O7-C8
25	C	509	CLA	C3-C5-C6-C7
25	a	609	CLA	CBA-CGA-O2A-C1
29	C	518	LMG	C29-C28-O8-C9
29	c	524	LMG	C29-C28-O8-C9
32	a	615	DGD	C2A-C1A-O1G-C1G
25	B	610	CLA	CBD-CGD-O2D-CED
30	L	101	SQD	C12-C13-C14-C15
31	d	409	LHG	C24-C25-C26-C27
25	c	510	CLA	O1D-CGD-O2D-CED
25	c	512	CLA	O1D-CGD-O2D-CED
25	b	605	CLA	C4-C3-C5-C6
28	A	611	PL9	C20-C19-C21-C22
28	A	611	PL9	C45-C44-C46-C47
28	a	611	PL9	C33-C34-C36-C37
25	B	604	CLA	C3-C5-C6-C7
25	C	513	CLA	C3-C5-C6-C7
25	A	607	CLA	C14-C13-C15-C16
25	B	605	CLA	C11-C12-C13-C14
25	B	607	CLA	C14-C13-C15-C16
25	B	613	CLA	C11-C12-C13-C14
25	B	614	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	C	503	CLA	C11-C10-C8-C9
25	C	509	CLA	C11-C10-C8-C9
25	C	512	CLA	C6-C7-C8-C9
25	C	512	CLA	C11-C10-C8-C9
25	C	513	CLA	C6-C7-C8-C9
25	a	608	CLA	C11-C12-C13-C14
25	b	601	CLA	C14-C13-C15-C16
25	b	606	CLA	C14-C13-C15-C16
25	b	616	CLA	C11-C10-C8-C9
25	c	502	CLA	C6-C7-C8-C9
25	c	509	CLA	C11-C12-C13-C14
25	c	511	CLA	C11-C10-C8-C9
25	c	512	CLA	C6-C7-C8-C9
26	A	608	PHO	C14-C13-C15-C16
32	A	617	DGD	C4E-C5E-C6E-O5E
30	A	616	SQD	C44-C45-O47-C7
30	f	102	SQD	C2-C1-O6-C44
31	D	412	LHG	O2-C2-C3-O3
29	c	524	LMG	O6-C5-C6-O5
33	b	622	STE	C4-C5-C6-C7
32	a	615	DGD	O1A-C1A-O1G-C1G
25	D	404	CLA	CBD-CGD-O2D-CED
27	B	619	BCR	C7-C8-C9-C34
27	B	619	BCR	C37-C22-C23-C24
27	D	406	BCR	C37-C22-C23-C24
27	K	101	BCR	C7-C8-C9-C34
27	K	101	BCR	C37-C22-C23-C24
27	K	102	BCR	C11-C12-C13-C35
27	T	101	BCR	C7-C8-C9-C34
27	b	618	BCR	C7-C8-C9-C34
27	b	619	BCR	C37-C22-C23-C24
27	d	405	BCR	C37-C22-C23-C24
27	t	101	BCR	C7-C8-C9-C34
32	A	617	DGD	O6E-C5E-C6E-O5E
29	c	522	LMG	O7-C8-C9-O8
30	a	613	SQD	O6-C44-C45-O47
25	c	506	CLA	CBA-CGA-O2A-C1
28	d	406	PL9	C42-C43-C44-C45
25	B	611	CLA	C8-C10-C11-C12
25	C	510	CLA	C13-C15-C16-C17
25	b	615	CLA	C5-C6-C7-C8
32	C	515	DGD	O6E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
30	A	616	SQD	C7-C8-C9-C10
25	a	609	CLA	O1A-CGA-O2A-C1
25	D	405	CLA	C10-C11-C12-C13
25	B	611	CLA	C12-C13-C15-C16
25	C	508	CLA	C12-C13-C15-C16
25	b	606	CLA	C11-C10-C8-C7
25	b	615	CLA	C11-C12-C13-C15
30	a	613	SQD	C11-C12-C13-C14
33	T	102	STE	C3-C4-C5-C6
25	c	503	CLA	C5-C6-C7-C8
32	H	102	DGD	C1A-C2A-C3A-C4A
33	B	624	STE	C1-C2-C3-C4
28	A	611	PL9	C19-C21-C22-C23
28	d	406	PL9	C44-C46-C47-C48
25	C	503	CLA	C5-C6-C7-C8
25	C	513	CLA	C13-C15-C16-C17
29	A	612	LMG	C4-C5-C6-O5
29	D	411	LMG	C10-C11-C12-C13
30	A	613	SQD	C7-C8-C9-C10
32	c	518	DGD	C1B-C2B-C3B-C4B
25	c	506	CLA	O1A-CGA-O2A-C1
25	B	607	CLA	C8-C10-C11-C12
25	B	607	CLA	C10-C11-C12-C13
25	C	506	CLA	C8-C10-C11-C12
25	C	506	CLA	C13-C15-C16-C17
25	C	509	CLA	C8-C10-C11-C12
25	b	602	CLA	C13-C15-C16-C17
25	c	509	CLA	C10-C11-C12-C13
25	c	510	CLA	C10-C11-C12-C13
27	c	514	BCR	C18-C19-C20-C21
25	D	403	CLA	C15-C16-C17-C18
25	a	609	CLA	C5-C6-C7-C8
25	c	506	CLA	C8-C10-C11-C12
25	c	506	CLA	C13-C15-C16-C17
29	d	411	LMG	C28-C29-C30-C31
30	B	622	SQD	C23-C24-C25-C26
30	L	101	SQD	C23-C24-C25-C26
31	A	614	LHG	C7-C8-C9-C10
31	d	407	LHG	C7-C8-C9-C10
31	d	407	LHG	C23-C24-C25-C26
31	d	409	LHG	C23-C24-C25-C26
31	e	101	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
32	C	515	DGD	C1A-C2A-C3A-C4A
33	E	102	STE	C1-C2-C3-C4
29	C	518	LMG	O6-C1-O1-C7
32	C	516	DGD	O6E-C1E-O5D-C6D
32	c	519	DGD	C8A-C9A-CAA-CBA
25	B	603	CLA	C15-C16-C17-C18
25	B	607	CLA	C5-C6-C7-C8
25	C	509	CLA	C5-C6-C7-C8
25	b	611	CLA	C8-C10-C11-C12
25	b	614	CLA	C13-C15-C16-C17
25	c	503	CLA	C8-C10-C11-C12
31	d	407	LHG	O2-C2-C3-O3
31	e	101	LHG	O2-C2-C3-O3
29	b	621	LMG	C10-C11-C12-C13
32	a	615	DGD	C1A-C2A-C3A-C4A
32	c	518	DGD	C1A-C2A-C3A-C4A
25	B	606	CLA	C13-C15-C16-C17
25	c	511	CLA	O1D-CGD-O2D-CED
25	B	613	CLA	C5-C6-C7-C8
25	c	510	CLA	C15-C16-C17-C18
29	m	101	LMG	C29-C28-O8-C9
32	c	519	DGD	C2A-C1A-O1G-C1G
25	B	613	CLA	C8-C10-C11-C12
25	b	601	CLA	C10-C11-C12-C13
30	L	101	SQD	C11-C10-C9-C8
31	A	614	LHG	C1-C2-C3-O3
31	d	407	LHG	C1-C2-C3-O3
31	e	101	LHG	C1-C2-C3-O3
25	B	606	CLA	C2A-CAA-CBA-CGA
29	b	621	LMG	C29-C28-O8-C9
25	B	603	CLA	C8-C10-C11-C12
25	C	513	CLA	C5-C6-C7-C8
25	a	607	CLA	C15-C16-C17-C18
25	b	615	CLA	C15-C16-C17-C18
25	c	511	CLA	C15-C16-C17-C18
25	c	512	CLA	C13-C15-C16-C17
33	B	620	STE	C1-C2-C3-C4
25	B	607	CLA	C13-C15-C16-C17
25	D	403	CLA	C13-C15-C16-C17
25	b	601	CLA	C13-C15-C16-C17
25	c	511	CLA	C13-C15-C16-C17
29	b	621	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
25	C	509	CLA	C10-C11-C12-C13
25	b	603	CLA	C13-C15-C16-C17
25	b	614	CLA	C8-C10-C11-C12
25	d	404	CLA	C8-C10-C11-C12
29	M	101	LMG	C28-C29-C30-C31
28	d	406	PL9	C33-C34-C36-C37
25	b	607	CLA	C8-C10-C11-C12
29	c	522	LMG	C11-C10-O7-C8
29	A	612	LMG	C2-C1-O1-C7
29	C	518	LMG	C2-C1-O1-C7
29	c	524	LMG	C2-C1-O1-C7
32	C	516	DGD	C2E-C1E-O5D-C6D
32	c	518	DGD	C2E-C1E-O5D-C6D
25	B	606	CLA	C10-C11-C12-C13
25	C	505	CLA	C10-C11-C12-C13
28	A	611	PL9	C24-C26-C27-C28
25	c	512	CLA	CBA-CGA-O2A-C1
25	b	614	CLA	C16-C17-C18-C19
25	c	511	CLA	C16-C17-C18-C20
28	a	611	PL9	C32-C33-C34-C36
27	H	101	BCR	C20-C21-C22-C37
27	K	101	BCR	C16-C17-C18-C36
27	K	102	BCR	C16-C17-C18-C36
27	T	101	BCR	C20-C21-C22-C37
27	Y	101	BCR	C16-C17-C18-C36
27	b	617	BCR	C11-C10-C9-C34
27	b	618	BCR	C20-C21-C22-C37
27	b	619	BCR	C35-C13-C14-C15
27	b	619	BCR	C20-C21-C22-C37
27	c	514	BCR	C16-C17-C18-C36
27	k	101	BCR	C16-C17-C18-C36
27	t	101	BCR	C20-C21-C22-C37
29	c	522	LMG	C10-C11-C12-C13
32	a	615	DGD	C1B-C2B-C3B-C4B
25	C	512	CLA	C13-C15-C16-C17
25	b	607	CLA	C10-C11-C12-C13
27	c	515	BCR	C7-C8-C9-C34
27	x	101	BCR	C7-C8-C9-C34
27	Y	101	BCR	C21-C22-C23-C24
27	b	617	BCR	C21-C22-C23-C24
27	k	101	BCR	C7-C8-C9-C10
25	b	606	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	c	512	CLA	C2A-CAA-CBA-CGA
25	C	512	CLA	C8-C10-C11-C12
25	c	510	CLA	C8-C10-C11-C12
31	D	409	LHG	O1-C1-C2-C3
31	D	410	LHG	O1-C1-C2-C3
31	d	409	LHG	O1-C1-C2-C3
30	L	101	SQD	C46-C45-O47-C7
25	b	604	CLA	C16-C17-C18-C19
25	b	615	CLA	C16-C17-C18-C20
27	C	514	BCR	C20-C21-C22-C23
27	K	101	BCR	C20-C21-C22-C23
27	b	618	BCR	C11-C10-C9-C8
27	c	514	BCR	C12-C13-C14-C15
27	c	514	BCR	C16-C17-C18-C19
27	k	101	BCR	C20-C21-C22-C23
27	x	101	BCR	C11-C10-C9-C8
27	x	101	BCR	C16-C17-C18-C19
29	M	101	LMG	O6-C1-O1-C7
25	C	510	CLA	C15-C16-C17-C18
25	c	506	CLA	C2-C1-O2A-CGA
25	B	602	CLA	C16-C17-C18-C19
25	D	403	CLA	C16-C17-C18-C20
25	a	608	CLA	C16-C17-C18-C20
25	b	607	CLA	C16-C17-C18-C19
32	c	517	DGD	O6E-C5E-C6E-O5E
29	C	518	LMG	C17-C18-C19-C20
32	c	517	DGD	C4B-C5B-C6B-C7B
33	B	626	STE	C3-C4-C5-C6
33	H	103	STE	C11-C12-C13-C14
27	D	406	BCR	C14-C15-C16-C17
27	K	101	BCR	C14-C15-C16-C17
29	A	612	LMG	C33-C34-C35-C36
29	D	408	LMG	C14-C15-C16-C17
29	c	522	LMG	C39-C40-C41-C42
31	e	101	LHG	C27-C28-C29-C30
32	C	515	DGD	C7B-C8B-C9B-CAB
32	a	615	DGD	C8B-C9B-CAB-CBB
33	B	625	STE	C5-C6-C7-C8
33	I	101	STE	C10-C11-C12-C13
33	M	102	STE	C9-C10-C11-C12
33	l	102	STE	C3-C4-C5-C6
25	C	505	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	M	101	LMG	C37-C38-C39-C40
29	m	101	LMG	C39-C40-C41-C42
30	F	101	SQD	C25-C26-C27-C28
31	D	409	LHG	C10-C11-C12-C13
31	D	410	LHG	C25-C26-C27-C28
31	d	408	LHG	C29-C30-C31-C32
32	c	517	DGD	CBB-CCB-CDB-CEB
32	h	101	DGD	C6B-C7B-C8B-C9B
33	d	413	STE	C10-C11-C12-C13
33	x	102	STE	C2-C3-C4-C5
29	B	621	LMG	C33-C34-C35-C36
29	d	410	LMG	C35-C36-C37-C38
30	A	613	SQD	C16-C17-C18-C19
30	a	613	SQD	C17-C18-C19-C20
30	a	614	SQD	C10-C11-C12-C13
30	a	614	SQD	C18-C19-C20-C21
31	d	407	LHG	C18-C19-C20-C21
31	l	101	LHG	C32-C33-C34-C35
32	c	518	DGD	C2A-C3A-C4A-C5A
33	H	103	STE	C5-C6-C7-C8
33	a	616	STE	C2-C3-C4-C5
33	b	622	STE	C12-C13-C14-C15
33	b	622	STE	C14-C15-C16-C17
33	m	102	STE	C5-C6-C7-C8
33	x	102	STE	C12-C13-C14-C15
31	D	412	LHG	O1-C1-C2-O2
31	d	408	LHG	O1-C1-C2-O2
29	B	621	LMG	C32-C33-C34-C35
29	D	411	LMG	C34-C35-C36-C37
31	D	410	LHG	C29-C30-C31-C32
31	d	409	LHG	C26-C27-C28-C29
32	C	515	DGD	C1B-C2B-C3B-C4B
29	C	518	LMG	C13-C14-C15-C16
33	x	102	STE	C7-C8-C9-C10
25	B	602	CLA	C16-C17-C18-C20
25	b	604	CLA	C16-C17-C18-C20
28	A	611	PL9	C27-C28-C29-C31
32	c	517	DGD	C7A-C8A-C9A-CAA
33	d	413	STE	C11-C12-C13-C14
25	B	616	CLA	C5-C6-C7-C8
25	b	613	CLA	C13-C15-C16-C17
31	A	614	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
29	c	522	LMG	C16-C17-C18-C19
31	D	410	LHG	C34-C35-C36-C37
33	a	617	STE	C4-C5-C6-C7
25	D	404	CLA	C12-C13-C15-C16
29	D	408	LMG	C36-C37-C38-C39
29	b	621	LMG	C11-C12-C13-C14
30	A	616	SQD	C28-C29-C30-C31
30	a	614	SQD	C14-C15-C16-C17
31	D	410	LHG	C27-C28-C29-C30
32	c	518	DGD	CCA-CDA-CEA-CFA
33	C	520	STE	C3-C4-C5-C6
31	A	614	LHG	C23-C24-C25-C26
25	d	404	CLA	C5-C6-C7-C8
29	C	518	LMG	C31-C32-C33-C34
29	M	101	LMG	C14-C15-C16-C17
29	c	520	LMG	C31-C32-C33-C34
30	A	613	SQD	C11-C10-C9-C8
30	A	616	SQD	C18-C19-C20-C21
30	f	102	SQD	C29-C30-C31-C32
31	d	407	LHG	C16-C17-C18-C19
32	c	517	DGD	C9B-CAB-CBB-CCB
32	c	519	DGD	CCA-CDA-CEA-CFA
33	B	620	STE	C9-C10-C11-C12
25	c	512	CLA	O1A-CGA-O2A-C1
25	c	512	CLA	C3A-C2A-CAA-CBA
29	D	411	LMG	C14-C15-C16-C17
30	A	613	SQD	C10-C11-C12-C13
31	A	614	LHG	C17-C18-C19-C20
33	E	102	STE	C3-C4-C5-C6
33	b	620	STE	C14-C15-C16-C17
25	B	603	CLA	O1D-CGD-O2D-CED
25	B	612	CLA	C16-C17-C18-C20
25	b	607	CLA	C16-C17-C18-C20
25	b	614	CLA	C16-C17-C18-C20
25	c	503	CLA	C16-C17-C18-C20
31	d	408	LHG	C32-C33-C34-C35
32	H	102	DGD	CAB-CBB-CCB-CDB
32	c	518	DGD	C8A-C9A-CAA-CBA
33	J	101	STE	C3-C4-C5-C6
33	c	521	STE	C9-C10-C11-C12
31	l	101	LHG	C24-C25-C26-C27
29	D	408	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
29	b	621	LMG	C16-C17-C18-C19
31	A	615	LHG	C12-C13-C14-C15
31	A	615	LHG	C32-C33-C34-C35
31	l	101	LHG	C11-C12-C13-C14
32	C	516	DGD	C5A-C6A-C7A-C8A
33	T	103	STE	C11-C10-C9-C8
33	t	102	STE	C11-C10-C9-C8
29	D	408	LMG	C10-C11-C12-C13
30	F	101	SQD	C23-C24-C25-C26
32	c	519	DGD	C1A-C2A-C3A-C4A
33	d	412	STE	C1-C2-C3-C4
33	d	413	STE	C1-C2-C3-C4
29	A	612	LMG	C35-C36-C37-C38
29	d	410	LMG	C33-C34-C35-C36
30	a	613	SQD	C26-C27-C28-C29
31	A	615	LHG	C17-C18-C19-C20
31	D	410	LHG	C15-C16-C17-C18
31	d	407	LHG	C32-C33-C34-C35
31	d	408	LHG	C34-C35-C36-C37
31	e	101	LHG	C17-C18-C19-C20
31	l	101	LHG	C16-C17-C18-C19
32	H	102	DGD	C8B-C9B-CAB-CBB
32	a	615	DGD	C5A-C6A-C7A-C8A
32	c	517	DGD	C5B-C6B-C7B-C8B
32	h	101	DGD	C5B-C6B-C7B-C8B
33	x	102	STE	C3-C4-C5-C6
29	A	612	LMG	O6-C5-C6-O5
29	A	612	LMG	C38-C39-C40-C41
29	c	524	LMG	C12-C13-C14-C15
29	c	524	LMG	C15-C16-C17-C18
31	A	614	LHG	C25-C26-C27-C28
33	d	413	STE	C2-C3-C4-C5
32	c	517	DGD	O6D-C5D-C6D-O5D
29	B	621	LMG	C31-C32-C33-C34
32	A	617	DGD	C2B-C3B-C4B-C5B
32	a	615	DGD	C6A-C7A-C8A-C9A
33	D	413	STE	C4-C5-C6-C7
30	a	614	SQD	C11-C10-C9-C8
33	B	625	STE	C4-C5-C6-C7
25	B	601	CLA	C16-C17-C18-C20
25	C	513	CLA	C16-C17-C18-C19
25	b	615	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	c	506	CLA	C16-C17-C18-C20
27	Y	101	BCR	C1-C6-C7-C8
27	Y	101	BCR	C5-C6-C7-C8
27	k	101	BCR	C1-C6-C7-C8
27	k	101	BCR	C5-C6-C7-C8
27	t	101	BCR	C1-C6-C7-C8
27	t	101	BCR	C5-C6-C7-C8
29	b	621	LMG	C12-C13-C14-C15
32	C	516	DGD	C8B-C9B-CAB-CBB
32	h	101	DGD	C3B-C4B-C5B-C6B
33	d	413	STE	C5-C6-C7-C8
25	C	505	CLA	CBD-CGD-O2D-CED
31	e	101	LHG	C8-C7-O7-C5
32	C	515	DGD	C9B-CAB-CBB-CCB
33	C	519	STE	C6-C7-C8-C9
29	M	101	LMG	C33-C34-C35-C36
29	m	101	LMG	C17-C18-C19-C20
30	B	622	SQD	C11-C12-C13-C14
31	A	615	LHG	C18-C19-C20-C21
31	d	408	LHG	C12-C13-C14-C15
32	c	517	DGD	C4A-C5A-C6A-C7A
32	c	517	DGD	CCB-CDB-CEB-CFB
33	l	102	STE	C7-C8-C9-C10
33	x	102	STE	C1-C2-C3-C4
29	M	101	LMG	C38-C39-C40-C41
29	b	621	LMG	C37-C38-C39-C40
29	c	522	LMG	C32-C33-C34-C35
30	B	622	SQD	C18-C19-C20-C21
31	A	614	LHG	C33-C34-C35-C36
31	d	407	LHG	C11-C10-C9-C8
32	C	517	DGD	C8A-C9A-CAA-CBA
32	H	102	DGD	C6A-C7A-C8A-C9A
28	A	611	PL9	C4-C3-C7-C8
29	B	621	LMG	C34-C35-C36-C37
29	c	522	LMG	C15-C16-C17-C18
29	d	410	LMG	C36-C37-C38-C39
31	e	101	LHG	O9-C7-O7-C5
31	D	410	LHG	C11-C12-C13-C14
32	A	617	DGD	C2A-C3A-C4A-C5A
32	H	102	DGD	C6B-C7B-C8B-C9B
32	c	517	DGD	C6B-C7B-C8B-C9B
27	K	101	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
27	d	405	BCR	C10-C11-C12-C13
25	c	507	CLA	C8-C10-C11-C12
25	a	608	CLA	C16-C17-C18-C19
25	c	503	CLA	C16-C17-C18-C19
32	C	517	DGD	C8B-C9B-CAB-CBB
33	D	413	STE	C6-C7-C8-C9
33	x	102	STE	C5-C6-C7-C8
25	B	611	CLA	C11-C12-C13-C14
25	b	601	CLA	C6-C7-C8-C9
25	b	614	CLA	C6-C7-C8-C9
29	b	621	LMG	C40-C41-C42-C43
31	e	101	LHG	C11-C12-C13-C14
31	A	614	LHG	C15-C16-C17-C18
31	A	615	LHG	C27-C28-C29-C30
31	d	407	LHG	C15-C16-C17-C18
32	A	617	DGD	CCA-CDA-CEA-CFA
32	C	517	DGD	C4B-C5B-C6B-C7B
33	B	624	STE	C12-C13-C14-C15
33	b	620	STE	C2-C3-C4-C5
32	c	518	DGD	O6D-C1D-O3G-C3G
32	c	518	DGD	O6E-C1E-O5D-C6D
29	M	101	LMG	C15-C16-C17-C18
31	D	410	LHG	C9-C10-C11-C12
32	C	515	DGD	C4B-C5B-C6B-C7B
33	C	521	STE	C3-C4-C5-C6
33	D	413	STE	C7-C8-C9-C10
25	B	614	CLA	C13-C15-C16-C17
25	B	616	CLA	C8-C10-C11-C12
25	c	509	CLA	C13-C15-C16-C17
29	M	101	LMG	C13-C14-C15-C16
29	c	520	LMG	C38-C39-C40-C41
31	A	614	LHG	C29-C30-C31-C32
32	c	519	DGD	C9A-CAA-CBA-CCA
33	T	103	STE	C2-C3-C4-C5
31	l	101	LHG	C33-C34-C35-C36
33	D	413	STE	C14-C15-C16-C17
29	D	408	LMG	C15-C16-C17-C18
29	D	408	LMG	C17-C18-C19-C20
31	A	614	LHG	C13-C14-C15-C16
31	D	410	LHG	C33-C34-C35-C36
32	c	519	DGD	CBA-CCA-CDA-CEA
33	B	624	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	B	601	CLA	C15-C16-C17-C18
27	k	101	BCR	C19-C20-C21-C22
33	d	413	STE	C12-C13-C14-C15
25	c	511	CLA	C16-C17-C18-C19
29	d	411	LMG	C39-C40-C41-C42
30	A	616	SQD	C8-C7-O47-C45
30	A	613	SQD	C23-C24-C25-C26
29	C	518	LMG	C14-C15-C16-C17
29	c	522	LMG	C30-C31-C32-C33
30	B	622	SQD	C33-C34-C35-C36
31	d	407	LHG	C27-C28-C29-C30
33	T	102	STE	C5-C6-C7-C8
25	b	604	CLA	C15-C16-C17-C18
29	C	518	LMG	C30-C31-C32-C33
32	c	519	DGD	C1B-C2B-C3B-C4B
29	b	621	LMG	C13-C14-C15-C16
31	D	409	LHG	C28-C29-C30-C31
31	l	101	LHG	C14-C15-C16-C17
27	d	405	BCR	C7-C8-C9-C10
33	c	523	STE	C5-C6-C7-C8
25	B	601	CLA	C16-C17-C18-C19
25	C	513	CLA	C16-C17-C18-C20
25	C	508	CLA	CBD-CGD-O2D-CED
25	C	511	CLA	CBD-CGD-O2D-CED
29	c	524	LMG	C33-C34-C35-C36
30	A	613	SQD	C12-C13-C14-C15
30	F	101	SQD	C26-C27-C28-C29
32	H	102	DGD	C5A-C6A-C7A-C8A
28	a	611	PL9	C20-C19-C21-C22
29	c	524	LMG	C28-C29-C30-C31
33	C	521	STE	C5-C6-C7-C8
33	I	101	STE	C4-C5-C6-C7
33	j	101	STE	C4-C5-C6-C7
29	D	408	LMG	C12-C13-C14-C15
30	f	102	SQD	C24-C25-C26-C27
33	B	626	STE	C4-C5-C6-C7
33	c	521	STE	C2-C3-C4-C5
29	b	621	LMG	C23-C24-C25-C26
30	a	614	SQD	C11-C12-C13-C14
31	D	409	LHG	C17-C18-C19-C20
32	A	617	DGD	C8B-C9B-CAB-CBB
33	m	102	STE	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	b	601	CLA	C15-C16-C17-C18
25	b	603	CLA	C5-C6-C7-C8
25	b	608	CLA	C5-C6-C7-C8
30	a	613	SQD	C34-C35-C36-C37
31	A	614	LHG	C18-C19-C20-C21
32	a	615	DGD	C3A-C4A-C5A-C6A
32	c	517	DGD	C5A-C6A-C7A-C8A
32	c	517	DGD	O1B-C1B-O2G-C2G
29	d	410	LMG	C38-C39-C40-C41
29	d	410	LMG	C32-C33-C34-C35
33	d	413	STE	C9-C10-C11-C12
30	A	616	SQD	C10-C11-C12-C13
33	B	625	STE	C1-C2-C3-C4
29	c	524	LMG	C18-C19-C20-C21
32	c	517	DGD	C3B-C4B-C5B-C6B
33	x	102	STE	C4-C5-C6-C7
29	d	411	LMG	O6-C5-C6-O5
25	C	512	CLA	C3-C5-C6-C7
30	B	622	SQD	O6-C44-C45-O47
32	A	617	DGD	O2G-C2G-C3G-O3G
30	a	613	SQD	C19-C20-C21-C22
29	D	408	LMG	C32-C33-C34-C35
30	a	613	SQD	C13-C14-C15-C16
31	D	409	LHG	C30-C31-C32-C33
31	d	409	LHG	C27-C28-C29-C30
32	H	102	DGD	CCB-CDB-CEB-CFB
32	c	517	DGD	C8B-C9B-CAB-CBB
25	C	505	CLA	C5-C6-C7-C8
25	c	505	CLA	C5-C6-C7-C8
30	L	101	SQD	C29-C30-C31-C32
32	C	516	DGD	C6A-C7A-C8A-C9A
33	B	620	STE	C6-C7-C8-C9
33	T	103	STE	C3-C4-C5-C6
33	a	617	STE	C5-C6-C7-C8
33	c	521	STE	C11-C12-C13-C14
25	a	608	CLA	CBD-CGD-O2D-CED
31	d	408	LHG	C14-C15-C16-C17
32	a	615	DGD	CEB-CFB-CGB-CHB
32	c	519	DGD	C4A-C5A-C6A-C7A
33	b	620	STE	C6-C7-C8-C9
25	C	502	CLA	C16-C17-C18-C20
25	a	609	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	b	606	CLA	C10-C11-C12-C13
25	b	614	CLA	C5-C6-C7-C8
31	A	615	LHG	C13-C14-C15-C16
31	e	101	LHG	C11-C10-C9-C8
32	C	516	DGD	CAA-CBA-CCA-CDA
32	C	516	DGD	C6B-C7B-C8B-C9B
31	D	410	LHG	C14-C15-C16-C17
32	a	615	DGD	C7B-C8B-C9B-CAB
33	D	413	STE	C13-C14-C15-C16
25	b	604	CLA	C3-C5-C6-C7
29	C	518	LMG	O9-C10-O7-C8
31	d	408	LHG	O9-C7-O7-C5
32	c	519	DGD	C8B-C9B-CAB-CBB
29	A	612	LMG	C12-C13-C14-C15
30	L	101	SQD	C24-C25-C26-C27
35	f	101	HEM	C2A-CAA-CBA-CGA
25	D	404	CLA	O1D-CGD-O2D-CED
29	c	522	LMG	C35-C36-C37-C38
31	D	412	LHG	C26-C27-C28-C29
25	B	611	CLA	C13-C15-C16-C17
25	a	608	CLA	C13-C15-C16-C17
29	b	621	LMG	C18-C19-C20-C21
31	A	615	LHG	C30-C31-C32-C33
30	B	622	SQD	C13-C14-C15-C16
32	a	615	DGD	C6B-C7B-C8B-C9B
31	D	409	LHG	O1-C1-C2-O2
32	C	516	DGD	C9B-CAB-CBB-CCB
25	b	601	CLA	C1A-C2A-CAA-CBA
25	c	508	CLA	C1A-C2A-CAA-CBA
25	c	512	CLA	C1A-C2A-CAA-CBA
25	c	513	CLA	C1A-C2A-CAA-CBA
25	c	506	CLA	C5-C6-C7-C8
29	D	408	LMG	C39-C40-C41-C42
32	c	519	DGD	C2B-C3B-C4B-C5B
29	M	101	LMG	C35-C36-C37-C38
30	A	613	SQD	C27-C28-C29-C30
31	A	615	LHG	C11-C12-C13-C14
30	a	613	SQD	C15-C16-C17-C18
32	c	517	DGD	C8A-C9A-CAA-CBA
32	c	517	DGD	CCA-CDA-CEA-CFA
32	c	518	DGD	CCB-CDB-CEB-CFB
33	c	521	STE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
33	t	102	STE	C2-C3-C4-C5
30	A	616	SQD	O49-C7-O47-C45
29	A	612	LMG	C16-C17-C18-C19
29	c	520	LMG	C36-C37-C38-C39
25	B	601	CLA	C3-C5-C6-C7
25	B	601	CLA	C11-C10-C8-C7
25	B	602	CLA	C11-C12-C13-C15
25	B	604	CLA	C11-C10-C8-C7
25	B	604	CLA	C11-C12-C13-C15
25	B	604	CLA	C12-C13-C15-C16
25	B	608	CLA	C6-C7-C8-C10
25	B	613	CLA	C12-C13-C15-C16
25	B	615	CLA	C11-C12-C13-C15
25	B	616	CLA	C6-C7-C8-C10
25	C	503	CLA	C12-C13-C15-C16
25	C	506	CLA	C6-C7-C8-C10
25	C	507	CLA	C11-C10-C8-C7
25	C	512	CLA	C11-C10-C8-C7
25	b	602	CLA	C6-C7-C8-C10
25	b	604	CLA	C12-C13-C15-C16
25	b	614	CLA	C11-C12-C13-C15
25	b	615	CLA	C11-C10-C8-C7
25	c	504	CLA	C11-C10-C8-C7
25	c	509	CLA	C6-C7-C8-C10
31	A	614	LHG	C32-C33-C34-C35
32	a	615	DGD	C4A-C5A-C6A-C7A
33	T	103	STE	C10-C11-C12-C13
32	a	615	DGD	CEA-CFA-CGA-CHA
31	d	409	LHG	C31-C32-C33-C34
31	e	101	LHG	C16-C17-C18-C19
33	I	101	STE	C7-C8-C9-C10
28	D	407	PL9	C30-C29-C31-C32
25	C	505	CLA	C2-C3-C5-C6
25	c	505	CLA	C2-C3-C5-C6
29	c	520	LMG	C33-C34-C35-C36
31	D	409	LHG	C18-C19-C20-C21
32	c	519	DGD	C5A-C6A-C7A-C8A
30	a	613	SQD	C12-C13-C14-C15
32	c	518	DGD	C4A-C5A-C6A-C7A
25	b	602	CLA	C15-C16-C17-C18
32	H	102	DGD	C4E-C5E-C6E-O5E
25	c	501	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	B	602	CLA	C11-C12-C13-C14
25	B	604	CLA	C14-C13-C15-C16
25	C	503	CLA	C14-C13-C15-C16
25	C	506	CLA	C6-C7-C8-C9
25	C	508	CLA	C11-C10-C8-C9
25	C	512	CLA	C11-C12-C13-C14
25	b	602	CLA	C6-C7-C8-C9
25	b	615	CLA	C11-C10-C8-C9
25	c	504	CLA	C11-C10-C8-C9
25	c	505	CLA	C11-C10-C8-C9
25	c	506	CLA	C11-C10-C8-C9
25	C	504	CLA	C11-C12-C13-C14
29	b	621	LMG	C19-C20-C21-C22
33	M	102	STE	C11-C10-C9-C8
33	d	412	STE	C6-C7-C8-C9
33	l	102	STE	C13-C14-C15-C16
29	d	410	LMG	C31-C32-C33-C34
31	d	409	LHG	C33-C34-C35-C36
25	C	503	CLA	C15-C16-C17-C18
28	A	611	PL9	C32-C33-C34-C35
29	c	524	LMG	C35-C36-C37-C38
31	d	409	LHG	C30-C31-C32-C33
29	M	101	LMG	C2-C1-O1-C7
25	b	606	CLA	C15-C16-C17-C18
29	A	612	LMG	O1-C7-C8-C9
29	C	518	LMG	O1-C7-C8-C9
29	M	101	LMG	O1-C7-C8-C9
29	M	101	LMG	C7-C8-C9-O8
30	B	622	SQD	O6-C44-C45-C46
30	a	613	SQD	O6-C44-C45-C46
31	A	614	LHG	C4-C5-C6-O8
32	A	617	DGD	C1G-C2G-C3G-O3G
31	D	409	LHG	C29-C30-C31-C32
31	D	412	LHG	C12-C13-C14-C15
25	b	616	CLA	C10-C11-C12-C13
30	A	616	SQD	C30-C31-C32-C33
32	C	515	DGD	C8A-C9A-CAA-CBA
25	B	610	CLA	O1D-CGD-O2D-CED
29	c	522	LMG	C29-C28-O8-C9
25	c	506	CLA	C16-C17-C18-C19
29	c	522	LMG	C34-C35-C36-C37
32	C	515	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
25	B	615	CLA	C13-C15-C16-C17
31	A	614	LHG	C34-C35-C36-C37
25	A	606	CLA	C2C-C3C-CAC-CBC
32	h	101	DGD	O6E-C5E-C6E-O5E
32	a	615	DGD	C4B-C5B-C6B-C7B
28	d	406	PL9	C32-C33-C34-C36
27	c	514	BCR	C35-C13-C14-C15
27	c	515	BCR	C20-C21-C22-C37
25	C	513	CLA	C8-C10-C11-C12
25	b	613	CLA	C10-C11-C12-C13
29	m	101	LMG	C15-C16-C17-C18
32	c	518	DGD	O6E-C5E-C6E-O5E
32	C	515	DGD	CCB-CDB-CEB-CFB
32	C	517	DGD	C2A-C3A-C4A-C5A
32	h	101	DGD	CBA-CCA-CDA-CEA
33	B	620	STE	C11-C12-C13-C14
25	C	505	CLA	C4-C3-C5-C6
25	B	605	CLA	C8-C10-C11-C12
27	K	102	BCR	C37-C22-C23-C24
29	D	411	LMG	C35-C36-C37-C38
31	A	614	LHG	C27-C28-C29-C30
29	D	408	LMG	O6-C5-C6-O5
25	B	605	CLA	C13-C15-C16-C17
25	B	612	CLA	C13-C15-C16-C17
25	C	509	CLA	C13-C15-C16-C17
32	H	102	DGD	CBA-CCA-CDA-CEA
25	b	615	CLA	C13-C15-C16-C17
25	c	503	CLA	C15-C16-C17-C18
32	c	518	DGD	CAB-CBB-CCB-CDB
33	B	620	STE	C7-C8-C9-C10
29	B	621	LMG	C16-C17-C18-C19
31	A	614	LHG	C11-C10-C9-C8
25	C	501	CLA	O1D-CGD-O2D-CED
25	b	601	CLA	O2A-C1-C2-C3
29	A	612	LMG	C9-C8-O7-C10
30	A	613	SQD	C14-C15-C16-C17
31	l	101	LHG	C18-C19-C20-C21
27	K	102	BCR	C18-C19-C20-C21
27	c	515	BCR	C18-C19-C20-C21
29	D	411	LMG	C16-C17-C18-C19
29	d	411	LMG	C37-C38-C39-C40
32	h	101	DGD	CAB-CBB-CCB-CDB

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Mol	Chain	Res	Type	Atoms
33	C	519	STE	C3-C4-C5-C6
29	C	518	LMG	C11-C12-C13-C14
30	f	102	SQD	C28-C29-C30-C31
32	c	517	DGD	CAB-CBB-CCB-CDB
27	B	619	BCR	C11-C10-C9-C8
27	b	618	BCR	C20-C21-C22-C23
31	A	615	LHG	C31-C32-C33-C34
30	L	101	SQD	O5-C1-O6-C44
29	d	410	LMG	C39-C40-C41-C42
30	f	102	SQD	C34-C35-C36-C37
32	A	617	DGD	CEB-CFB-CGB-CHB
30	a	614	SQD	C15-C16-C17-C18
33	B	624	STE	C3-C4-C5-C6
30	L	101	SQD	C19-C20-C21-C22
25	B	616	CLA	C4-C3-C5-C6
25	C	510	CLA	C2-C3-C5-C6
29	c	520	LMG	C39-C40-C41-C42
29	c	522	LMG	C11-C12-C13-C14
30	L	101	SQD	C11-C12-C13-C14
32	a	615	DGD	CBA-CCA-CDA-CEA
33	C	521	STE	C7-C8-C9-C10
33	l	102	STE	C4-C5-C6-C7
25	a	607	CLA	C16-C17-C18-C20
29	b	621	LMG	C38-C39-C40-C41
30	a	613	SQD	C30-C31-C32-C33
32	A	617	DGD	CBB-CCB-CDB-CEB
33	B	620	STE	C4-C5-C6-C7
33	C	520	STE	C6-C7-C8-C9
29	B	621	LMG	C37-C38-C39-C40
30	A	613	SQD	C17-C18-C19-C20
32	C	516	DGD	CDA-CEA-CFA-CGA
33	M	103	STE	C1-C2-C3-C4
30	L	101	SQD	C7-C8-C9-C10
29	A	612	LMG	C14-C15-C16-C17
31	D	409	LHG	C11-C10-C9-C8
29	b	621	LMG	O1-C7-C8-O7
32	C	517	DGD	CDA-CEA-CFA-CGA
32	c	519	DGD	CDA-CEA-CFA-CGA
32	A	617	DGD	C8A-C9A-CAA-CBA
33	B	624	STE	C7-C8-C9-C10
33	b	620	STE	C13-C14-C15-C16
29	m	101	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
25	C	510	CLA	C3-C5-C6-C7
25	c	502	CLA	C3-C5-C6-C7
29	D	408	LMG	C38-C39-C40-C41
25	B	606	CLA	C15-C16-C17-C18
31	d	408	LHG	C35-C36-C37-C38
33	I	101	STE	C2-C3-C4-C5
32	c	517	DGD	C4D-C5D-C6D-O5D
30	A	616	SQD	C17-C18-C19-C20
32	C	515	DGD	C6B-C7B-C8B-C9B
29	D	411	LMG	C37-C38-C39-C40
29	C	518	LMG	C32-C33-C34-C35
31	l	101	LHG	C28-C29-C30-C31
30	A	616	SQD	C31-C32-C33-C34
32	H	102	DGD	C7B-C8B-C9B-CAB
32	A	617	DGD	C5B-C6B-C7B-C8B
29	b	621	LMG	C24-C25-C26-C27
25	C	513	CLA	C15-C16-C17-C18
28	A	611	PL9	C15-C14-C16-C17
33	c	523	STE	C6-C7-C8-C9
25	b	608	CLA	C13-C15-C16-C17
30	F	101	SQD	C30-C31-C32-C33
31	A	614	LHG	C24-C25-C26-C27
32	C	516	DGD	CCA-CDA-CEA-CFA
33	B	623	STE	C6-C7-C8-C9
33	B	626	STE	C6-C7-C8-C9
33	b	620	STE	C12-C13-C14-C15
33	T	103	STE	C6-C7-C8-C9
31	A	614	LHG	O9-C7-O7-C5
25	A	607	CLA	C11-C12-C13-C14
25	B	604	CLA	C11-C10-C8-C9
25	B	604	CLA	C11-C12-C13-C14
25	B	608	CLA	C6-C7-C8-C9
25	B	610	CLA	C14-C13-C15-C16
25	B	613	CLA	C14-C13-C15-C16
25	B	616	CLA	C6-C7-C8-C9
25	C	505	CLA	C14-C13-C15-C16
25	D	403	CLA	C11-C12-C13-C14
25	D	405	CLA	C6-C7-C8-C9
25	b	604	CLA	C14-C13-C15-C16
25	b	615	CLA	C11-C12-C13-C14
25	A	606	CLA	C13-C15-C16-C17
29	c	522	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
29	d	411	LMG	C34-C35-C36-C37
29	d	410	LMG	C37-C38-C39-C40
25	a	607	CLA	C16-C17-C18-C19
33	B	624	STE	C13-C14-C15-C16
29	d	411	LMG	C14-C15-C16-C17
29	m	101	LMG	C14-C15-C16-C17
29	m	101	LMG	C18-C19-C20-C21
25	b	613	CLA	C8-C10-C11-C12
31	D	409	LHG	C25-C26-C27-C28
31	e	101	LHG	O6-C4-C5-C6
29	D	411	LMG	C33-C34-C35-C36
25	A	607	CLA	C11-C12-C13-C15
25	B	607	CLA	C12-C13-C15-C16
25	C	503	CLA	C11-C10-C8-C7
25	C	505	CLA	C12-C13-C15-C16
25	C	512	CLA	C11-C12-C13-C15
25	D	403	CLA	C11-C12-C13-C15
25	D	405	CLA	C6-C7-C8-C10
25	b	607	CLA	C6-C7-C8-C10
25	b	607	CLA	C11-C12-C13-C15
25	b	616	CLA	C11-C10-C8-C7
25	c	505	CLA	C11-C10-C8-C7
25	c	506	CLA	C11-C10-C8-C7
25	c	510	CLA	C6-C7-C8-C10
25	c	511	CLA	C12-C13-C15-C16
25	c	512	CLA	C11-C10-C8-C7
25	B	605	CLA	C10-C11-C12-C13
33	b	623	STE	C7-C8-C9-C10
28	a	611	PL9	C47-C48-C49-C51
31	D	412	LHG	C9-C10-C11-C12
31	d	408	LHG	C11-C12-C13-C14
32	A	617	DGD	CFA-CGA-CHA-CIA
33	B	623	STE	C7-C8-C9-C10
33	T	102	STE	C13-C14-C15-C16
29	D	411	LMG	C32-C33-C34-C35
30	B	622	SQD	C29-C30-C31-C32
33	B	625	STE	C3-C4-C5-C6
33	D	413	STE	C12-C13-C14-C15
33	j	101	STE	C5-C6-C7-C8
32	a	615	DGD	CFA-CGA-CHA-CIA
25	C	510	CLA	C4-C3-C5-C6
25	c	505	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	d	402	PHO	C3A-C2A-CAA-CBA
33	b	623	STE	C3-C4-C5-C6
32	H	102	DGD	O2G-C1B-C2B-C3B
26	A	608	PHO	C2-C3-C5-C6
29	A	612	LMG	C17-C18-C19-C20
33	C	521	STE	C12-C13-C14-C15
30	a	614	SQD	C31-C32-C33-C34
31	l	101	LHG	C17-C18-C19-C20
29	C	518	LMG	O10-C28-O8-C9
25	C	508	CLA	C5-C6-C7-C8
31	D	410	LHG	C30-C31-C32-C33
25	B	612	CLA	C16-C17-C18-C19
25	C	502	CLA	C16-C17-C18-C19
27	B	619	BCR	C11-C12-C13-C35
31	d	407	LHG	C14-C15-C16-C17
30	a	613	SQD	C31-C32-C33-C34
32	c	518	DGD	CBA-CCA-CDA-CEA
33	b	623	STE	C4-C5-C6-C7
25	B	613	CLA	C10-C11-C12-C13
25	C	508	CLA	C8-C10-C11-C12
32	c	519	DGD	C2A-C3A-C4A-C5A
30	B	622	SQD	C19-C20-C21-C22
29	b	621	LMG	O1-C7-C8-C9
29	c	522	LMG	C7-C8-C9-O8
30	A	613	SQD	O6-C44-C45-C46
30	a	614	SQD	C44-C45-C46-O48
33	B	620	STE	C11-C10-C9-C8
33	B	624	STE	C10-C11-C12-C13
32	A	617	DGD	CCB-CDB-CEB-CFB
25	C	505	CLA	C16-C17-C18-C20
25	B	615	CLA	C5-C6-C7-C8
25	c	502	CLA	C13-C15-C16-C17
30	B	622	SQD	C27-C28-C29-C30
31	e	101	LHG	C14-C15-C16-C17
31	D	410	LHG	C11-C10-C9-C8
32	c	519	DGD	C7B-C8B-C9B-CAB
33	H	103	STE	C7-C8-C9-C10
32	C	516	DGD	C4A-C5A-C6A-C7A
33	C	519	STE	C2-C3-C4-C5
33	a	617	STE	C2-C3-C4-C5
25	b	609	CLA	C4-C3-C5-C6
26	A	608	PHO	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	A	616	SQD	C33-C34-C35-C36
30	a	613	SQD	C29-C30-C31-C32
31	d	407	LHG	C29-C30-C31-C32
32	a	615	DGD	CDA-CEA-CFA-CGA
28	d	406	PL9	C13-C14-C16-C17
25	C	502	CLA	C3-C5-C6-C7
25	b	601	CLA	C3-C5-C6-C7
25	c	502	CLA	CBD-CGD-O2D-CED
33	J	101	STE	C2-C3-C4-C5
30	A	616	SQD	O47-C45-C46-O48
25	C	505	CLA	C16-C17-C18-C19
25	D	405	CLA	C16-C17-C18-C19
29	D	411	LMG	C31-C32-C33-C34
30	A	616	SQD	C12-C13-C14-C15
32	c	519	DGD	C5B-C6B-C7B-C8B
27	H	101	BCR	C23-C24-C25-C30
27	K	102	BCR	C1-C6-C7-C8
27	b	617	BCR	C1-C6-C7-C8
27	d	405	BCR	C23-C24-C25-C30
29	M	101	LMG	C17-C18-C19-C20
29	c	520	LMG	C4-C5-C6-O5
32	C	516	DGD	C4B-C5B-C6B-C7B
30	B	622	SQD	C9-C10-C11-C12
33	H	103	STE	C13-C14-C15-C16
33	T	102	STE	C10-C11-C12-C13
25	D	405	CLA	C13-C15-C16-C17
30	F	101	SQD	C33-C34-C35-C36
33	a	616	STE	C5-C6-C7-C8
32	C	515	DGD	O1G-C1A-C2A-C3A
29	M	101	LMG	O7-C8-C9-O8
30	A	613	SQD	O6-C44-C45-O47
30	a	613	SQD	O47-C45-C46-O48
32	c	517	DGD	C6A-C7A-C8A-C9A
29	C	518	LMG	C15-C16-C17-C18
32	A	617	DGD	C7B-C8B-C9B-CAB
33	m	102	STE	C1-C2-C3-C4
28	d	406	PL9	C15-C14-C16-C17
29	A	612	LMG	C31-C32-C33-C34
29	b	621	LMG	C39-C40-C41-C42
30	A	613	SQD	C29-C30-C31-C32
31	l	101	LHG	C30-C31-C32-C33
27	C	514	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
25	A	606	CLA	C15-C16-C17-C18
32	H	102	DGD	C3A-C4A-C5A-C6A
32	h	101	DGD	CCA-CDA-CEA-CFA
31	D	409	LHG	C32-C33-C34-C35
31	e	101	LHG	C28-C29-C30-C31
25	C	510	CLA	C11-C10-C8-C9
25	b	607	CLA	C6-C7-C8-C9
25	b	607	CLA	C11-C12-C13-C14
25	b	609	CLA	C14-C13-C15-C16
25	c	510	CLA	C6-C7-C8-C9
25	c	510	CLA	C11-C12-C13-C14
25	c	502	CLA	O1D-CGD-O2D-CED
30	a	613	SQD	C35-C36-C37-C38
33	D	413	STE	C11-C12-C13-C14
33	M	102	STE	C4-C5-C6-C7
25	B	603	CLA	C10-C11-C12-C13
26	d	402	PHO	C5-C6-C7-C8
32	a	615	DGD	C9B-CAB-CBB-CCB
33	C	520	STE	C4-C5-C6-C7
32	C	516	DGD	O6D-C1D-O3G-C3G
32	c	517	DGD	O6E-C1E-O5D-C6D
30	B	622	SQD	C35-C36-C37-C38
28	A	611	PL9	C29-C31-C32-C33
28	d	406	PL9	C34-C36-C37-C38
31	A	614	LHG	C9-C10-C11-C12
30	a	614	SQD	O6-C44-C45-O47
31	A	614	LHG	C14-C15-C16-C17
30	a	613	SQD	C27-C28-C29-C30
29	C	518	LMG	C40-C41-C42-C43
25	b	615	CLA	C10-C11-C12-C13
31	d	409	LHG	O1-C1-C2-O2
32	H	102	DGD	CDA-CEA-CFA-CGA
25	b	609	CLA	C2-C3-C5-C6
25	B	610	CLA	C16-C17-C18-C19
25	D	403	CLA	C16-C17-C18-C19
33	B	626	STE	C2-C3-C4-C5
31	d	408	LHG	C15-C16-C17-C18
27	T	101	BCR	C11-C10-C9-C34
27	a	610	BCR	C35-C13-C14-C15
27	c	515	BCR	C16-C17-C18-C36
27	t	101	BCR	C11-C10-C9-C34
27	x	101	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
25	c	507	CLA	C5-C6-C7-C8
29	A	612	LMG	C40-C41-C42-C43
31	l	101	LHG	O6-C4-C5-C6
25	b	602	CLA	C10-C11-C12-C13
25	b	607	CLA	C13-C15-C16-C17
27	t	101	BCR	C11-C12-C13-C35
32	c	517	DGD	CDB-CEB-CFB-CGB
25	B	606	CLA	C11-C12-C13-C15
25	B	611	CLA	C11-C10-C8-C7
25	C	508	CLA	C11-C10-C8-C7
25	C	510	CLA	C6-C7-C8-C10
25	C	510	CLA	C11-C10-C8-C7
25	C	513	CLA	C6-C7-C8-C10
25	a	609	CLA	C12-C13-C15-C16
25	b	603	CLA	C11-C12-C13-C15
25	b	609	CLA	C12-C13-C15-C16
25	c	505	CLA	C6-C7-C8-C10
25	c	509	CLA	C11-C12-C13-C15
33	C	520	STE	C1-C2-C3-C4
33	c	521	STE	C1-C2-C3-C4
29	d	411	LMG	C36-C37-C38-C39
32	c	518	DGD	C7B-C8B-C9B-CAB
29	b	621	LMG	C22-C23-C24-C25
32	C	517	DGD	C3B-C4B-C5B-C6B
33	d	412	STE	C11-C10-C9-C8
33	m	102	STE	C4-C5-C6-C7
25	C	512	CLA	C10-C11-C12-C13
25	A	606	CLA	C4C-C3C-CAC-CBC
27	D	406	BCR	C7-C8-C9-C10
27	T	101	BCR	C21-C22-C23-C24
25	B	612	CLA	CBA-CGA-O2A-C1
32	A	617	DGD	C2A-C1A-O1G-C1G
29	M	101	LMG	C39-C40-C41-C42
30	A	613	SQD	C30-C31-C32-C33
32	c	518	DGD	C5D-C6D-O5D-C1E
30	A	613	SQD	C32-C33-C34-C35
25	c	509	CLA	C8-C10-C11-C12
25	b	610	CLA	C2A-CAA-CBA-CGA
33	I	101	STE	C12-C13-C14-C15
30	L	101	SQD	C26-C27-C28-C29
33	B	625	STE	C6-C7-C8-C9
25	B	606	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	D	405	CLA	C16-C17-C18-C20
25	a	612	CLA	CBD-CGD-O2D-CED
32	c	519	DGD	C4B-C5B-C6B-C7B
25	C	506	CLA	C4-C3-C5-C6
25	c	506	CLA	C4-C3-C5-C6
29	c	524	LMG	O8-C28-C29-C30
33	B	626	STE	C9-C10-C11-C12
30	B	622	SQD	C16-C17-C18-C19
25	B	601	CLA	C5-C6-C7-C8
25	b	605	CLA	C8-C10-C11-C12
29	D	411	LMG	C9-C8-O7-C10
32	a	615	DGD	C1G-C2G-O2G-C1B
32	a	615	DGD	C8A-C9A-CAA-CBA
27	H	101	BCR	C11-C10-C9-C8
31	l	101	LHG	O6-C4-C5-O7
29	D	411	LMG	C15-C16-C17-C18
31	d	407	LHG	C31-C32-C33-C34
25	A	609	CLA	C6-C7-C8-C9
28	a	611	PL9	C34-C36-C37-C38
29	c	524	LMG	C7-C8-C9-O8
30	a	613	SQD	C44-C45-C46-O48
31	D	410	LHG	O10-C23-O8-C6
25	c	512	CLA	C4-C3-C5-C6
25	b	601	CLA	C2A-CAA-CBA-CGA
29	b	621	LMG	C14-C15-C16-C17
33	C	520	STE	C5-C6-C7-C8
25	B	603	CLA	C5-C6-C7-C8
25	B	603	CLA	C13-C15-C16-C17
25	B	607	CLA	C15-C16-C17-C18
32	a	615	DGD	C5B-C6B-C7B-C8B
33	H	103	STE	C10-C11-C12-C13
29	C	518	LMG	O1-C7-C8-O7
29	M	101	LMG	O1-C7-C8-O7
29	c	524	LMG	O7-C8-C9-O8
32	C	515	DGD	O1G-C1G-C2G-O2G
32	c	517	DGD	O1G-C1G-C2G-O2G
25	B	603	CLA	C11-C12-C13-C14
25	B	605	CLA	C6-C7-C8-C9
25	B	606	CLA	C11-C12-C13-C14
25	C	513	CLA	C11-C12-C13-C14
25	b	603	CLA	C11-C12-C13-C14
25	b	607	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	b	616	CLA	C6-C7-C8-C9
25	B	611	CLA	C16-C17-C18-C20
25	b	609	CLA	C16-C17-C18-C20
29	D	408	LMG	C34-C35-C36-C37
29	b	621	LMG	C33-C34-C35-C36
29	b	621	LMG	C31-C32-C33-C34
32	C	516	DGD	C3A-C4A-C5A-C6A
32	C	517	DGD	C2B-C3B-C4B-C5B
33	x	102	STE	C11-C10-C9-C8
32	C	517	DGD	O1A-C1A-O1G-C1G
29	C	518	LMG	C18-C19-C20-C21
25	c	511	CLA	C8-C10-C11-C12
26	D	402	PHO	C2C-C3C-CAC-CBC
32	C	516	DGD	C7B-C8B-C9B-CAB
31	e	101	LHG	C7-C8-C9-C10
25	A	607	CLA	C16-C17-C18-C20
25	B	615	CLA	C16-C17-C18-C19
25	b	608	CLA	C16-C17-C18-C19
25	c	505	CLA	C16-C17-C18-C20
25	B	602	CLA	C15-C16-C17-C18
31	d	407	LHG	C17-C18-C19-C20
32	a	615	DGD	CAB-CBB-CCB-CDB
32	h	101	DGD	CAA-CBA-CCA-CDA
32	A	617	DGD	C4A-C5A-C6A-C7A
32	c	519	DGD	C7A-C8A-C9A-CAA
25	B	613	CLA	C4-C3-C5-C6
25	C	506	CLA	C2-C3-C5-C6
31	A	614	LHG	O2-C2-C3-O3
25	B	616	CLA	CBD-CGD-O2D-CED
26	d	401	PHO	CBD-CGD-O2D-CED
32	C	516	DGD	C8A-C9A-CAA-CBA
33	B	625	STE	C2-C3-C4-C5
29	M	101	LMG	O6-C5-C6-O5
25	c	501	CLA	CBD-CGD-O2D-CED
25	a	608	CLA	O1D-CGD-O2D-CED
31	A	615	LHG	C10-C11-C12-C13
32	h	101	DGD	C9A-CAA-CBA-CCA
32	h	101	DGD	CDB-CEB-CFB-CGB
25	B	604	CLA	C1A-C2A-CAA-CBA
25	c	511	CLA	C1A-C2A-CAA-CBA
25	B	616	CLA	O1D-CGD-O2D-CED
25	C	511	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	C	511	CLA	CBA-CGA-O2A-C1
29	A	612	LMG	C36-C37-C38-C39
31	l	101	LHG	C10-C11-C12-C13
25	B	610	CLA	C16-C17-C18-C20
33	c	523	STE	C2-C3-C4-C5
29	m	101	LMG	C32-C33-C34-C35
32	c	517	DGD	C7B-C8B-C9B-CAB
33	d	412	STE	C9-C10-C11-C12
33	x	102	STE	C9-C10-C11-C12
25	A	607	CLA	C6-C7-C8-C10
25	B	613	CLA	C6-C7-C8-C10
25	B	613	CLA	C11-C12-C13-C15
25	B	614	CLA	C12-C13-C15-C16
25	C	504	CLA	C11-C10-C8-C7
25	C	505	CLA	C6-C7-C8-C10
25	C	506	CLA	C12-C13-C15-C16
25	C	509	CLA	C11-C10-C8-C7
25	C	509	CLA	C12-C13-C15-C16
25	b	601	CLA	C12-C13-C15-C16
25	b	602	CLA	C11-C12-C13-C15
25	b	605	CLA	C12-C13-C15-C16
25	b	606	CLA	C11-C12-C13-C15
25	b	608	CLA	C11-C10-C8-C7
25	b	608	CLA	C11-C12-C13-C15
25	c	502	CLA	C6-C7-C8-C10
25	c	512	CLA	C6-C7-C8-C10
25	c	512	CLA	C12-C13-C15-C16
25	d	403	CLA	C11-C12-C13-C15
25	B	606	CLA	C16-C17-C18-C20
25	c	502	CLA	C16-C17-C18-C19
25	C	505	CLA	O1D-CGD-O2D-CED
26	d	401	PHO	O1D-CGD-O2D-CED
29	c	520	LMG	C35-C36-C37-C38
32	A	617	DGD	C7A-C8A-C9A-CAA
32	C	517	DGD	C9A-CAA-CBA-CCA
32	H	102	DGD	C4B-C5B-C6B-C7B
25	B	604	CLA	CBA-CGA-O2A-C1
30	B	622	SQD	C15-C16-C17-C18
33	b	620	STE	C4-C5-C6-C7
32	a	615	DGD	CFB-CGB-CHB-CIB
25	C	511	CLA	O1A-CGA-O2A-C1
29	B	621	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
32	A	617	DGD	CDB-CEB-CFB-CGB
33	l	102	STE	C10-C11-C12-C13
25	B	605	CLA	C16-C17-C18-C20
25	b	611	CLA	C16-C17-C18-C19
29	m	101	LMG	C37-C38-C39-C40
32	C	516	DGD	C3B-C4B-C5B-C6B
33	a	617	STE	C7-C8-C9-C10
25	B	614	CLA	C8-C10-C11-C12
31	D	412	LHG	C29-C30-C31-C32
32	h	101	DGD	C2B-C3B-C4B-C5B
33	d	412	STE	C3-C4-C5-C6
25	A	607	CLA	C6-C7-C8-C9
25	C	510	CLA	C6-C7-C8-C9
25	a	609	CLA	C14-C13-C15-C16
31	d	407	LHG	C33-C34-C35-C36
33	M	103	STE	C6-C7-C8-C9
25	C	508	CLA	O1D-CGD-O2D-CED
32	C	516	DGD	CBB-CCB-CDB-CEB
25	B	604	CLA	O1A-CGA-O2A-C1
25	B	612	CLA	O1A-CGA-O2A-C1
30	a	614	SQD	O47-C45-C46-O48
31	A	614	LHG	O7-C5-C6-O8
31	d	407	LHG	C25-C26-C27-C28
29	D	408	LMG	C30-C31-C32-C33
25	D	404	CLA	C2C-C3C-CAC-CBC
29	D	411	LMG	C7-C8-C9-O8
25	c	512	CLA	C2-C3-C5-C6
25	C	502	CLA	CAD-CBD-CGD-O2D
25	C	504	CLA	CAD-CBD-CGD-O2D
25	b	607	CLA	CAD-CBD-CGD-O2D
25	c	504	CLA	CAD-CBD-CGD-O2D
25	c	510	CLA	CAD-CBD-CGD-O2D
29	c	522	LMG	C31-C32-C33-C34
31	l	101	LHG	C25-C26-C27-C28
25	B	605	CLA	C16-C17-C18-C19
25	C	501	CLA	C16-C17-C18-C20
25	b	611	CLA	C16-C17-C18-C20
33	M	102	STE	C10-C11-C12-C13
25	B	616	CLA	O1A-CGA-O2A-C1
31	D	410	LHG	C12-C13-C14-C15
25	B	609	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	C	504	CLA	CAD-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O1D
25	C	509	CLA	CHA-CBD-CGD-O1D
25	C	509	CLA	CHA-CBD-CGD-O2D
25	b	607	CLA	CAD-CBD-CGD-O1D
25	c	504	CLA	CAD-CBD-CGD-O1D
25	c	510	CLA	CAD-CBD-CGD-O1D
26	d	402	PHO	CHA-CBD-CGD-O2D
27	K	102	BCR	C20-C21-C22-C37
31	D	409	LHG	C3-O3-P-O4
31	d	407	LHG	C3-O3-P-O5
33	b	622	STE	C2-C3-C4-C5
33	d	413	STE	C6-C7-C8-C9
28	a	611	PL9	C15-C14-C16-C17
32	a	615	DGD	C3B-C4B-C5B-C6B
25	c	509	CLA	CAA-CBA-CGA-O2A
28	A	611	PL9	C13-C14-C16-C17
32	c	519	DGD	CAB-CBB-CCB-CDB
33	t	102	STE	C3-C4-C5-C6
25	C	507	CLA	C5-C6-C7-C8
32	h	101	DGD	C7A-C8A-C9A-CAA
25	b	612	CLA	C16-C17-C18-C20
29	c	522	LMG	C41-C42-C43-C44
28	a	611	PL9	C4-C3-C7-C8
31	D	412	LHG	C19-C20-C21-C22
33	B	623	STE	C4-C5-C6-C7
25	c	504	CLA	C8-C10-C11-C12
29	b	621	LMG	C9-C8-O7-C10
31	D	409	LHG	C16-C17-C18-C19
31	D	412	LHG	C16-C17-C18-C19
33	b	620	STE	C3-C4-C5-C6
33	B	626	STE	C1-C2-C3-C4
31	D	412	LHG	C27-C28-C29-C30
27	x	101	BCR	C15-C16-C17-C18
25	B	611	CLA	C16-C17-C18-C19
31	d	409	LHG	C35-C36-C37-C38
30	A	616	SQD	C19-C20-C21-C22
25	B	606	CLA	C8-C10-C11-C12
25	C	510	CLA	C8-C10-C11-C12
25	B	601	CLA	C11-C10-C8-C9
25	B	607	CLA	C11-C10-C8-C9
25	B	615	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	B	616	CLA	C11-C10-C8-C9
25	C	507	CLA	C11-C10-C8-C9
25	a	608	CLA	C14-C13-C15-C16
25	b	608	CLA	C11-C12-C13-C14
25	c	505	CLA	C6-C7-C8-C9
25	c	512	CLA	C11-C12-C13-C14
33	C	519	STE	C7-C8-C9-C10
25	a	608	CLA	C11-C12-C13-C15
25	b	606	CLA	C12-C13-C15-C16
25	c	513	CLA	C6-C7-C8-C10
27	c	514	BCR	C20-C21-C22-C23
32	h	101	DGD	C1A-C2A-C3A-C4A
33	E	102	STE	C4-C5-C6-C7
25	C	505	CLA	O1A-CGA-O2A-C1
33	B	626	STE	C5-C6-C7-C8
31	A	615	LHG	O10-C23-O8-C6
32	C	515	DGD	C5B-C6B-C7B-C8B
29	D	411	LMG	C29-C30-C31-C32
30	a	613	SQD	C24-C23-O48-C46
25	A	606	CLA	C16-C17-C18-C20
25	b	610	CLA	C5-C6-C7-C8
32	A	617	DGD	C5A-C6A-C7A-C8A
25	b	615	CLA	C8-C10-C11-C12
30	F	101	SQD	O6-C44-C45-C46
27	a	610	BCR	C19-C20-C21-C22
27	c	516	BCR	C13-C14-C15-C16
33	l	102	STE	C1-C2-C3-C4
33	j	101	STE	C2-C3-C4-C5
30	f	102	SQD	C35-C36-C37-C38
25	c	513	CLA	C5-C6-C7-C8
30	a	613	SQD	C24-C25-C26-C27
25	b	616	CLA	C2-C1-O2A-CGA
33	d	412	STE	C7-C8-C9-C10
25	B	615	CLA	C16-C17-C18-C20
30	a	614	SQD	C30-C31-C32-C33
28	A	611	PL9	C9-C11-C12-C13
25	A	607	CLA	C16-C17-C18-C19
31	A	615	LHG	C14-C15-C16-C17
32	C	515	DGD	C5D-C6D-O5D-C1E
29	c	522	LMG	O10-C28-O8-C9
27	c	516	BCR	C19-C20-C21-C22
30	B	622	SQD	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
30	L	101	SQD	C16-C17-C18-C19
32	H	102	DGD	O6E-C5E-C6E-O5E
25	B	610	CLA	C15-C16-C17-C18
32	H	102	DGD	C3B-C4B-C5B-C6B
30	a	613	SQD	O10-C23-O48-C46
25	B	613	CLA	C6-C7-C8-C9
25	C	505	CLA	C6-C7-C8-C9
25	C	513	CLA	C11-C10-C8-C9
25	b	602	CLA	C11-C12-C13-C14
25	c	512	CLA	C11-C10-C8-C9
33	x	102	STE	C15-C16-C17-C18
25	b	611	CLA	C13-C15-C16-C17
31	A	615	LHG	C19-C20-C21-C22
25	B	608	CLA	C16-C17-C18-C19
25	B	609	CLA	C16-C17-C18-C19
25	c	502	CLA	C16-C17-C18-C20
25	c	513	CLA	C16-C17-C18-C19
25	B	616	CLA	CBA-CGA-O2A-C1
29	c	520	LMG	C29-C28-O8-C9
32	C	517	DGD	C5B-C6B-C7B-C8B
33	B	623	STE	C5-C6-C7-C8
25	B	616	CLA	C2-C3-C5-C6
25	C	513	CLA	C11-C10-C8-C7
25	c	504	CLA	O1D-CGD-O2D-CED
30	a	613	SQD	C23-C24-C25-C26
25	C	505	CLA	CBA-CGA-O2A-C1
25	C	508	CLA	C16-C17-C18-C19
29	B	621	LMG	C15-C16-C17-C18
31	l	101	LHG	C29-C30-C31-C32
25	b	609	CLA	C13-C15-C16-C17
25	c	504	CLA	CBD-CGD-O2D-CED
29	c	524	LMG	C13-C14-C15-C16
32	H	102	DGD	C9B-CAB-CBB-CCB
32	c	517	DGD	CBA-CCA-CDA-CEA
32	c	518	DGD	C8B-C9B-CAB-CBB
27	c	516	BCR	C20-C21-C22-C37
27	x	101	BCR	C35-C13-C14-C15
25	B	613	CLA	C2-C1-O2A-CGA
25	d	403	CLA	C2-C1-O2A-CGA
30	B	622	SQD	C34-C35-C36-C37
30	F	101	SQD	C27-C28-C29-C30
31	d	408	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
29	D	408	LMG	C13-C14-C15-C16
31	d	408	LHG	C1-C2-C3-O3
29	c	524	LMG	C38-C39-C40-C41
31	D	409	LHG	C15-C16-C17-C18
32	c	518	DGD	CBB-CCB-CDB-CEB
25	B	603	CLA	C11-C10-C8-C9
25	C	501	CLA	C14-C13-C15-C16
25	C	507	CLA	C6-C7-C8-C9
25	b	605	CLA	C6-C7-C8-C9
25	c	508	CLA	C11-C10-C8-C9
25	c	512	CLA	C14-C13-C15-C16
25	d	403	CLA	C11-C12-C13-C14
33	B	620	STE	C5-C6-C7-C8
33	T	103	STE	C5-C6-C7-C8
32	A	617	DGD	CFB-CGB-CHB-CIB
29	B	621	LMG	O7-C10-C11-C12
33	c	521	STE	O1-C1-C2-C3
26	d	402	PHO	C1A-C2A-CAA-CBA
29	D	411	LMG	O1-C7-C8-C9
30	a	613	SQD	C28-C29-C30-C31
29	d	411	LMG	C10-C11-C12-C13
29	B	621	LMG	O9-C10-C11-C12
33	B	623	STE	O2-C1-C2-C3
25	B	603	CLA	C2A-CAA-CBA-CGA
29	d	411	LMG	C11-C12-C13-C14
27	t	101	BCR	C20-C21-C22-C23
27	x	101	BCR	C20-C21-C22-C23
25	D	403	CLA	C2C-C3C-CAC-CBC
33	B	623	STE	O1-C1-C2-C3
33	c	521	STE	O2-C1-C2-C3
27	A	610	BCR	C1-C6-C7-C8
27	B	618	BCR	C23-C24-C25-C30
27	C	514	BCR	C23-C24-C25-C30
27	H	101	BCR	C23-C24-C25-C26
27	K	102	BCR	C5-C6-C7-C8
27	b	617	BCR	C5-C6-C7-C8
27	c	514	BCR	C23-C24-C25-C30
27	d	405	BCR	C23-C24-C25-C26
33	l	102	STE	C12-C13-C14-C15
29	d	411	LMG	C15-C16-C17-C18
25	c	510	CLA	C4-C3-C5-C6
25	d	404	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	A	616	SQD	C34-C35-C36-C37
31	d	408	LHG	C33-C34-C35-C36
32	A	617	DGD	CEA-CFA-CGA-CHA
33	b	620	STE	C5-C6-C7-C8
25	A	607	CLA	C11-C10-C8-C7
25	B	615	CLA	C12-C13-C15-C16
25	D	403	CLA	C12-C13-C15-C16
25	a	608	CLA	C6-C7-C8-C10
25	a	608	CLA	C12-C13-C15-C16
25	b	606	CLA	C6-C7-C8-C10
25	c	501	CLA	C11-C12-C13-C15
25	c	507	CLA	C11-C10-C8-C7
25	c	508	CLA	C11-C10-C8-C7
25	c	512	CLA	C11-C12-C13-C15
30	f	102	SQD	C32-C33-C34-C35
28	a	611	PL9	C19-C21-C22-C23
25	C	501	CLA	C2A-CAA-CBA-CGA
29	D	411	LMG	O7-C8-C9-O8
30	f	102	SQD	O6-C44-C45-O47
35	E	101	HEM	CAD-CBD-CGD-O1D
32	C	516	DGD	CCB-CDB-CEB-CFB
25	b	613	CLA	CBD-CGD-O2D-CED
29	d	410	LMG	O9-C10-C11-C12
33	b	622	STE	O2-C1-C2-C3
29	M	101	LMG	C12-C13-C14-C15
33	a	616	STE	C7-C8-C9-C10
25	B	603	CLA	C16-C17-C18-C19
29	d	411	LMG	C30-C31-C32-C33
33	b	620	STE	C7-C8-C9-C10
33	b	622	STE	O1-C1-C2-C3
31	A	615	LHG	C15-C16-C17-C18
33	M	103	STE	C4-C5-C6-C7
33	E	102	STE	C7-C8-C9-C10
33	D	413	STE	O2-C1-C2-C3
25	a	608	CLA	C6-C7-C8-C9
33	T	102	STE	C4-C5-C6-C7
25	b	611	CLA	C10-C11-C12-C13
33	H	103	STE	C6-C7-C8-C9
33	t	102	STE	C6-C7-C8-C9
27	K	101	BCR	C22-C23-C24-C25
29	m	101	LMG	C33-C34-C35-C36
31	l	101	LHG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
25	B	604	CLA	C2C-C3C-CAC-CBC
25	C	502	CLA	C4-C3-C5-C6
25	d	403	CLA	C4-C3-C5-C6
31	D	410	LHG	C2-C3-O3-P
31	d	409	LHG	C2-C3-O3-P
25	c	510	CLA	C2-C3-C5-C6
30	a	614	SQD	C29-C30-C31-C32
32	C	515	DGD	C2B-C3B-C4B-C5B
25	B	612	CLA	C10-C11-C12-C13
33	B	625	STE	O1-C1-C2-C3
29	C	518	LMG	C33-C34-C35-C36
29	d	410	LMG	C11-C12-C13-C14
32	c	519	DGD	O6D-C5D-C6D-O5D
29	A	612	LMG	C13-C14-C15-C16
29	B	621	LMG	C36-C37-C38-C39
32	C	515	DGD	O1G-C1G-C2G-C3G
35	E	101	HEM	CAD-CBD-CGD-O2D
35	f	101	HEM	CAD-CBD-CGD-O1D
29	D	411	LMG	O1-C7-C8-O7
25	B	614	CLA	C2A-CAA-CBA-CGA
36	V	201	HEC	CAD-CBD-CGD-O2D
30	B	622	SQD	C28-C29-C30-C31
30	A	616	SQD	C11-C12-C13-C14
33	b	622	STE	C5-C6-C7-C8
26	A	608	PHO	C10-C11-C12-C13
25	d	404	CLA	C16-C17-C18-C19
26	d	401	PHO	CHA-CBD-CGD-O1D
25	b	612	CLA	C8-C10-C11-C12
32	h	101	DGD	O2G-C1B-C2B-C3B
29	d	410	LMG	O7-C10-C11-C12
32	C	515	DGD	C4D-C5D-C6D-O5D
25	D	403	CLA	C4C-C3C-CAC-CBC
33	T	103	STE	C9-C10-C11-C12
25	C	506	CLA	C16-C17-C18-C20
29	M	101	LMG	C18-C19-C20-C21
25	C	502	CLA	C2-C3-C5-C6
25	A	607	CLA	C12-C13-C15-C16
25	b	607	CLA	C11-C10-C8-C7
29	C	518	LMG	C16-C17-C18-C19
33	D	413	STE	O1-C1-C2-C3
32	a	615	DGD	C2B-C3B-C4B-C5B
25	C	505	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	C	509	CLA	C14-C13-C15-C16
25	C	511	CLA	C6-C7-C8-C9
25	C	513	CLA	C14-C13-C15-C16
25	D	404	CLA	C14-C13-C15-C16
25	d	403	CLA	C6-C7-C8-C9
26	d	401	PHO	C14-C13-C15-C16
30	L	101	SQD	C10-C11-C12-C13
29	c	524	LMG	C11-C12-C13-C14
33	b	623	STE	C5-C6-C7-C8
33	l	102	STE	C15-C16-C17-C18
25	C	506	CLA	C2-C1-O2A-CGA
25	b	608	CLA	C2-C1-O2A-CGA
32	C	515	DGD	O6D-C5D-C6D-O5D
25	c	505	CLA	C16-C17-C18-C19
25	c	513	CLA	C16-C17-C18-C20
33	b	623	STE	C1-C2-C3-C4
25	B	610	CLA	C8-C10-C11-C12
25	c	512	CLA	C5-C6-C7-C8
29	B	621	LMG	C30-C31-C32-C33
31	D	409	LHG	C9-C10-C11-C12
36	v	201	HEC	CAD-CBD-CGD-O2D
25	B	613	CLA	C2-C3-C5-C6
36	V	201	HEC	CAD-CBD-CGD-O1D
33	t	102	STE	C4-C5-C6-C7
32	C	516	DGD	C2D-C1D-O3G-C3G
32	c	517	DGD	C2E-C1E-O5D-C6D
25	B	616	CLA	O2A-C1-C2-C3
31	D	409	LHG	C11-C12-C13-C14
27	H	101	BCR	C10-C11-C12-C13
27	T	101	BCR	C18-C19-C20-C21
25	b	602	CLA	CBD-CGD-O2D-CED
33	l	102	STE	C14-C15-C16-C17
30	a	613	SQD	C33-C34-C35-C36
36	v	201	HEC	CAD-CBD-CGD-O1D
25	c	503	CLA	CBA-CGA-O2A-C1
25	c	502	CLA	O1A-CGA-O2A-C1
26	d	402	PHO	C4C-C3C-CAC-CBC
33	b	622	STE	C6-C7-C8-C9
32	C	517	DGD	O6E-C5E-C6E-O5E
29	A	612	LMG	C39-C40-C41-C42
33	C	521	STE	C6-C7-C8-C9
29	A	612	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
32	A	617	DGD	O1G-C1G-C2G-C3G
32	c	517	DGD	O1G-C1G-C2G-C3G
32	C	515	DGD	CDB-CEB-CFB-CGB
25	c	503	CLA	O1A-CGA-O2A-C1
29	D	411	LMG	O10-C28-O8-C9
25	b	610	CLA	C3-C5-C6-C7
29	c	520	LMG	C29-C30-C31-C32
25	A	607	CLA	C10-C11-C12-C13
25	b	609	CLA	C15-C16-C17-C18
31	d	408	LHG	C31-C32-C33-C34
32	C	517	DGD	C3A-C4A-C5A-C6A
32	h	101	DGD	C7B-C8B-C9B-CAB
25	b	613	CLA	CAA-CBA-CGA-O2A
31	D	410	LHG	C17-C18-C19-C20
25	C	504	CLA	C11-C10-C8-C9
25	D	403	CLA	C14-C13-C15-C16
25	b	608	CLA	C11-C10-C8-C9
25	b	613	CLA	C11-C12-C13-C14
25	c	507	CLA	C11-C10-C8-C9
33	T	103	STE	C11-C12-C13-C14
25	B	613	CLA	CAA-CBA-CGA-O2A
31	A	614	LHG	O6-C4-C5-C6
33	B	625	STE	O2-C1-C2-C3
28	D	407	PL9	C32-C33-C34-C35
25	B	612	CLA	CAA-CBA-CGA-O2A
25	b	612	CLA	CAA-CBA-CGA-O2A
30	a	613	SQD	O47-C7-C8-C9
25	B	602	CLA	C12-C13-C15-C16
25	B	605	CLA	C11-C12-C13-C15
25	B	606	CLA	C11-C10-C8-C7
25	C	512	CLA	C6-C7-C8-C10
25	D	403	CLA	C6-C7-C8-C10
25	b	602	CLA	C12-C13-C15-C16
25	d	403	CLA	C6-C7-C8-C10
25	d	404	CLA	C11-C12-C13-C15
32	h	101	DGD	O1B-C1B-C2B-C3B
27	A	610	BCR	C5-C6-C7-C8
27	B	618	BCR	C23-C24-C25-C26
27	C	514	BCR	C1-C6-C7-C8
27	C	514	BCR	C23-C24-C25-C26
27	K	102	BCR	C23-C24-C25-C30
27	c	514	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	c	514	BCR	C5-C6-C7-C8
27	c	514	BCR	C23-C24-C25-C26
27	k	101	BCR	C23-C24-C25-C30
27	x	101	BCR	C23-C24-C25-C26
27	x	101	BCR	C23-C24-C25-C30
32	c	518	DGD	CDA-CEA-CFA-CGA
32	A	617	DGD	CBA-CCA-CDA-CEA
25	A	606	CLA	C2-C1-O2A-CGA
25	D	404	CLA	C2-C1-O2A-CGA
29	c	522	LMG	C42-C43-C44-C45
32	c	518	DGD	C5B-C6B-C7B-C8B
29	m	101	LMG	O8-C28-C29-C30
35	f	101	HEM	CAD-CBD-CGD-O2D
25	c	513	CLA	C8-C10-C11-C12
32	a	615	DGD	C9A-CAA-CBA-CCA
25	b	604	CLA	C13-C15-C16-C17
25	c	510	CLA	C5-C6-C7-C8
25	b	601	CLA	CAA-CBA-CGA-O2A
26	D	402	PHO	O1D-CGD-O2D-CED
31	d	407	LHG	C26-C27-C28-C29
33	B	623	STE	C3-C4-C5-C6
32	C	517	DGD	O6D-C5D-C6D-O5D
25	c	501	CLA	O1D-CGD-O2D-CED
29	D	408	LMG	C18-C19-C20-C21
32	c	519	DGD	C9B-CAB-CBB-CCB
30	B	622	SQD	C4-C5-C6-S
27	B	618	BCR	C18-C19-C20-C21
25	c	506	CLA	C2-C3-C5-C6
28	a	611	PL9	C23-C24-C26-C27
25	a	608	CLA	C3-C5-C6-C7
25	b	609	CLA	C16-C17-C18-C19
32	c	518	DGD	C5A-C6A-C7A-C8A
33	B	624	STE	C11-C12-C13-C14
33	c	521	STE	C7-C8-C9-C10
32	C	515	DGD	C4E-C5E-C6E-O5E
25	B	614	CLA	C6-C7-C8-C9
25	B	615	CLA	C14-C13-C15-C16
25	C	506	CLA	C14-C13-C15-C16
25	b	602	CLA	C11-C10-C8-C9
25	b	605	CLA	C14-C13-C15-C16
25	b	606	CLA	C6-C7-C8-C9
25	c	501	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
33	j	101	STE	C7-C8-C9-C10
29	A	612	LMG	C28-C29-C30-C31
26	D	402	PHO	CBD-CGD-O2D-CED
32	c	517	DGD	C1G-C2G-C3G-O3G
25	b	602	CLA	C8-C10-C11-C12
25	B	602	CLA	C1A-C2A-CAA-CBA
25	C	512	CLA	C1A-C2A-CAA-CBA
25	c	502	CLA	CBA-CGA-O2A-C1
31	A	614	LHG	O7-C7-C8-C9
27	K	102	BCR	C17-C18-C19-C20
35	f	101	HEM	CAA-CBA-CGA-O2A
32	A	617	DGD	O2G-C1B-C2B-C3B
25	b	610	CLA	C10-C11-C12-C13
29	c	522	LMG	C36-C37-C38-C39
32	C	517	DGD	C6A-C7A-C8A-C9A
25	a	612	CLA	O1D-CGD-O2D-CED
29	B	621	LMG	O8-C28-C29-C30
25	c	505	CLA	C15-C16-C17-C18
29	B	621	LMG	C29-C30-C31-C32
25	B	601	CLA	C11-C12-C13-C15
25	C	505	CLA	C11-C10-C8-C7
25	C	511	CLA	C6-C7-C8-C10
25	C	512	CLA	O2A-C1-C2-C3
26	d	401	PHO	O2A-C1-C2-C3
33	B	624	STE	C4-C5-C6-C7
33	I	101	STE	C11-C12-C13-C14
25	C	510	CLA	C10-C11-C12-C13
29	c	520	LMG	O6-C5-C6-O5
28	A	611	PL9	C44-C46-C47-C48
29	D	411	LMG	C29-C28-O8-C9
25	B	602	CLA	C3A-C2A-CAA-CBA
25	C	512	CLA	C3A-C2A-CAA-CBA
25	a	609	CLA	C15-C16-C17-C18
25	B	607	CLA	C16-C17-C18-C19
31	d	408	LHG	C7-C8-C9-C10
27	B	618	BCR	C20-C21-C22-C23
27	B	619	BCR	C12-C13-C14-C15
27	b	617	BCR	C12-C13-C14-C15
25	b	613	CLA	O1D-CGD-O2D-CED
25	b	601	CLA	CAA-CBA-CGA-O1A
29	m	101	LMG	O10-C28-O8-C9
32	H	102	DGD	C8A-C9A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	B	606	CLA	C5-C6-C7-C8
31	A	615	LHG	O7-C7-C8-C9
25	b	612	CLA	CAA-CBA-CGA-O1A
25	b	610	CLA	C13-C15-C16-C17
25	A	607	CLA	C11-C10-C8-C9
25	B	601	CLA	C11-C12-C13-C14
25	b	606	CLA	C11-C12-C13-C14
31	A	614	LHG	C10-C11-C12-C13
30	A	613	SQD	C9-C10-C11-C12
31	d	408	LHG	O2-C2-C3-O3
33	d	413	STE	O1-C1-C2-C3
35	f	101	HEM	CAA-CBA-CGA-O1A
31	e	101	LHG	O10-C23-C24-C25
27	K	102	BCR	C11-C12-C13-C14
25	b	613	CLA	CAA-CBA-CGA-O1A
29	c	524	LMG	C14-C15-C16-C17
32	C	516	DGD	C5D-C6D-O5D-C1E
32	c	517	DGD	C5D-C6D-O5D-C1E
32	c	518	DGD	C2D-C1D-O3G-C3G
25	B	613	CLA	CAA-CBA-CGA-O1A
30	a	613	SQD	O49-C7-C8-C9
31	A	614	LHG	O9-C7-C8-C9
32	A	617	DGD	O1B-C1B-C2B-C3B
31	d	407	LHG	O8-C23-C24-C25
32	c	517	DGD	O1G-C1A-C2A-C3A
25	B	602	CLA	C2A-CAA-CBA-CGA
25	b	602	CLA	C2A-CAA-CBA-CGA
33	C	521	STE	C11-C12-C13-C14
25	c	512	CLA	C15-C16-C17-C18
30	f	102	SQD	O6-C44-C45-C46
25	B	612	CLA	CAA-CBA-CGA-O1A
25	b	605	CLA	C15-C16-C17-C18
25	d	404	CLA	C2-C3-C5-C6
29	c	522	LMG	C37-C38-C39-C40
33	C	521	STE	C2-C3-C4-C5
30	F	101	SQD	C34-C35-C36-C37
25	B	607	CLA	CAD-CBD-CGD-O2D
25	a	607	CLA	CAD-CBD-CGD-O2D
25	c	513	CLA	CAD-CBD-CGD-O2D
26	A	608	PHO	CAD-CBD-CGD-O2D
26	d	401	PHO	CAD-CBD-CGD-O2D
25	b	604	CLA	C5-C6-C7-C8

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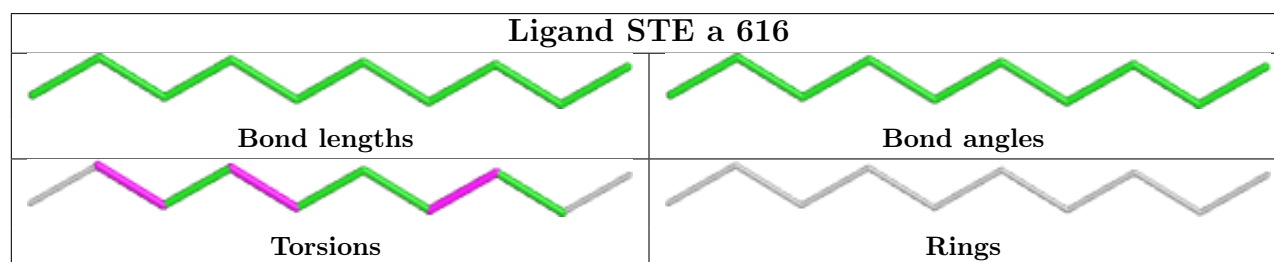
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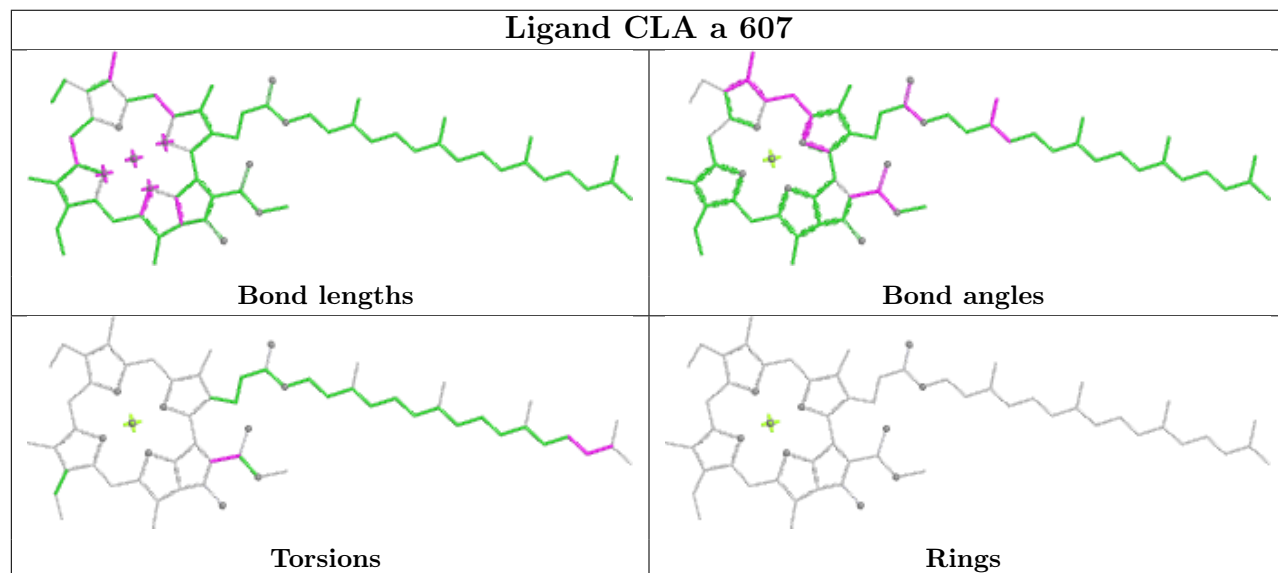
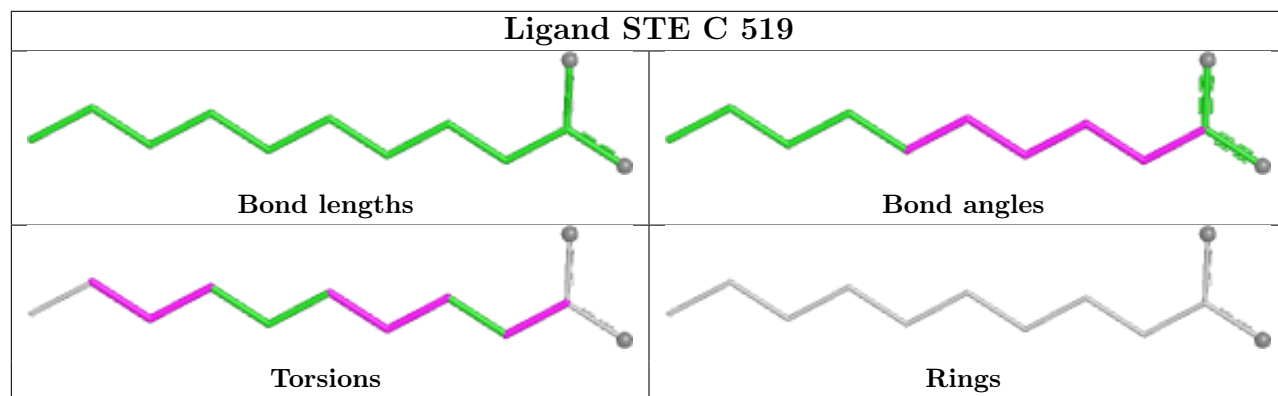
Mol	Chain	Res	Type	Atoms
30	A	613	SQD	O47-C7-C8-C9
32	C	515	DGD	O1B-C1B-C2B-C3B
33	T	102	STE	C1-C2-C3-C4
29	b	621	LMG	O6-C1-O1-C7
32	C	515	DGD	O6E-C1E-O5D-C6D
25	c	513	CLA	C2-C1-O2A-CGA
32	c	517	DGD	O1B-C1B-C2B-C3B
30	a	614	SQD	O6-C44-C45-C46
28	D	407	PL9	C46-C47-C48-C49
32	c	518	DGD	C3B-C4B-C5B-C6B
33	c	523	STE	O2-C1-C2-C3
33	C	519	STE	O2-C1-C2-C3
29	D	408	LMG	C28-C29-C30-C31
28	A	611	PL9	C2-C3-C7-C8
33	T	102	STE	C11-C10-C9-C8
29	D	408	LMG	C22-C23-C24-C25
33	M	102	STE	O2-C1-C2-C3

There are no ring outliers.

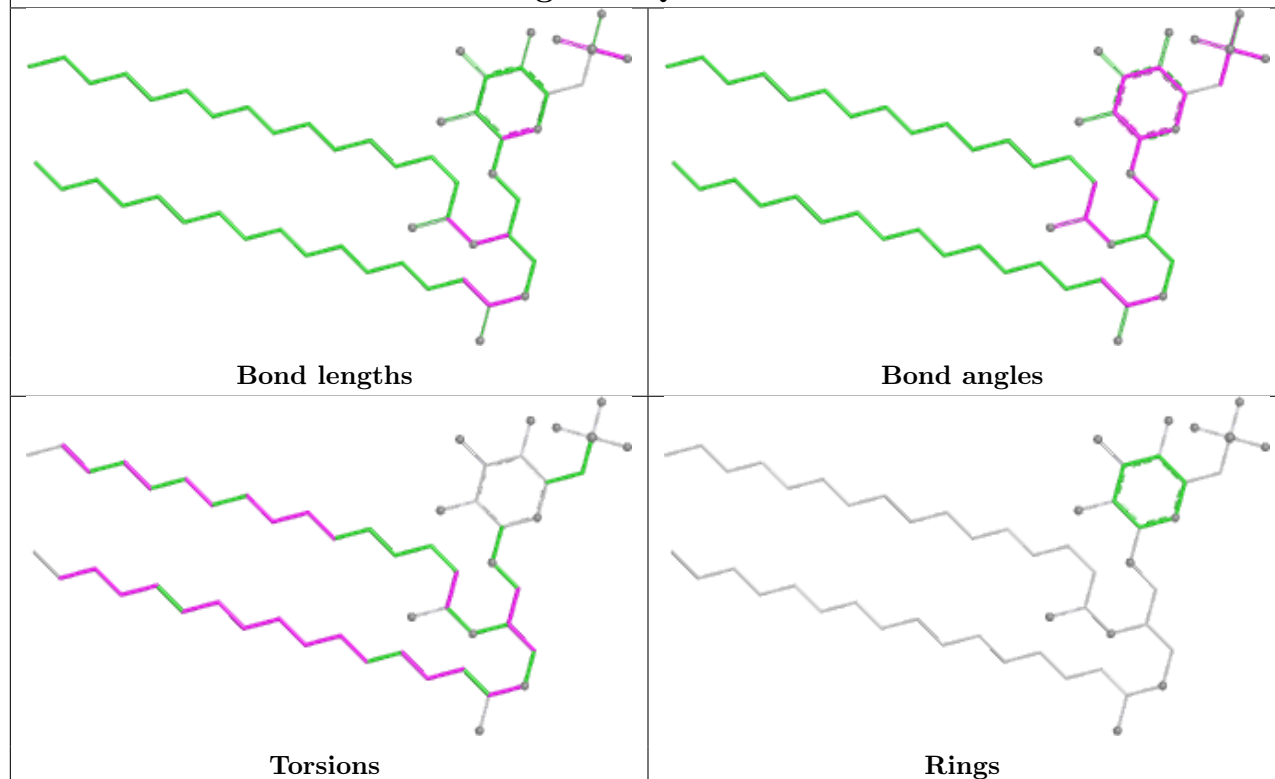
No monomer is involved in short contacts.

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.

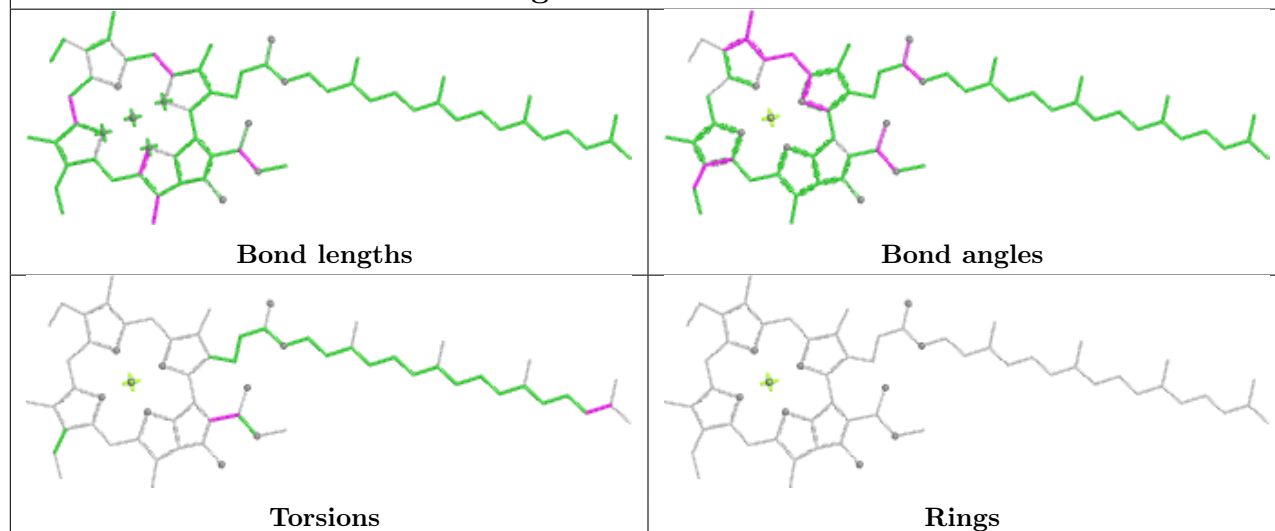


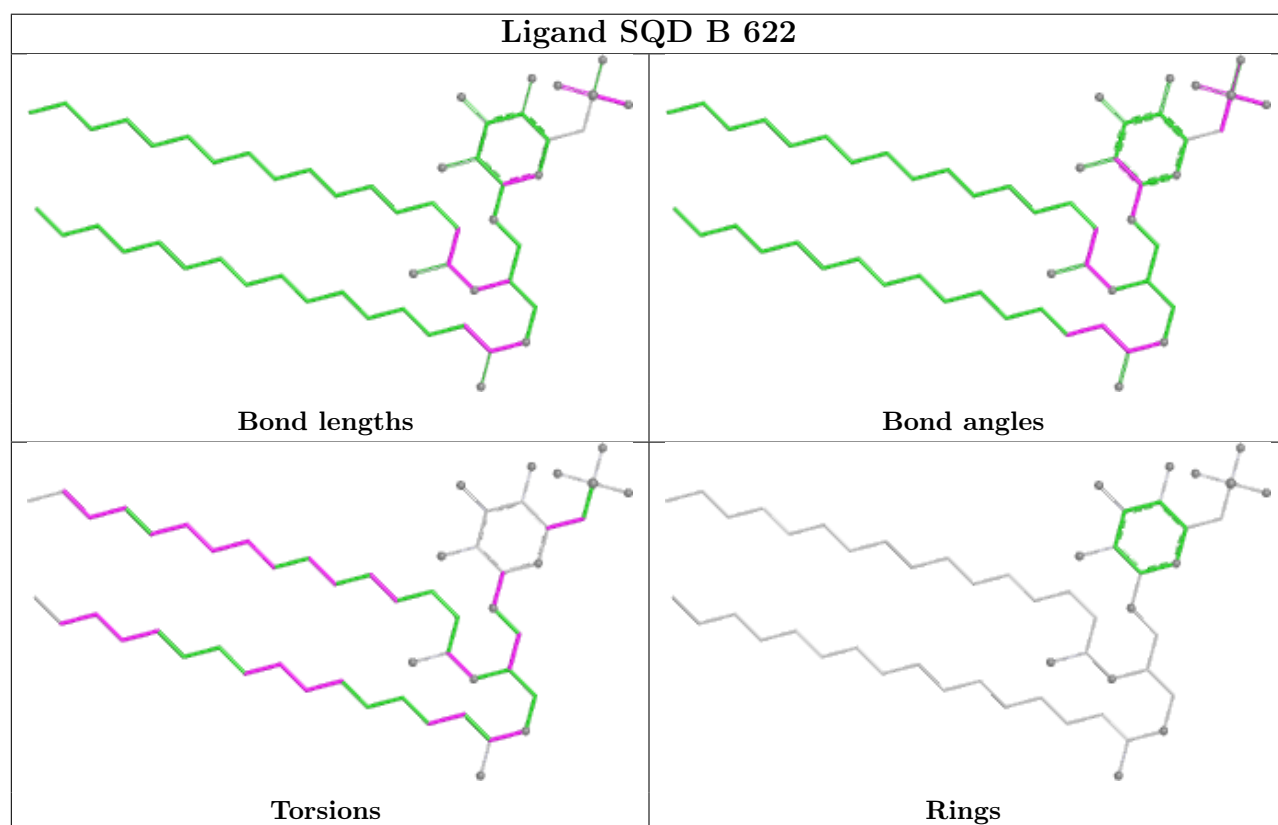
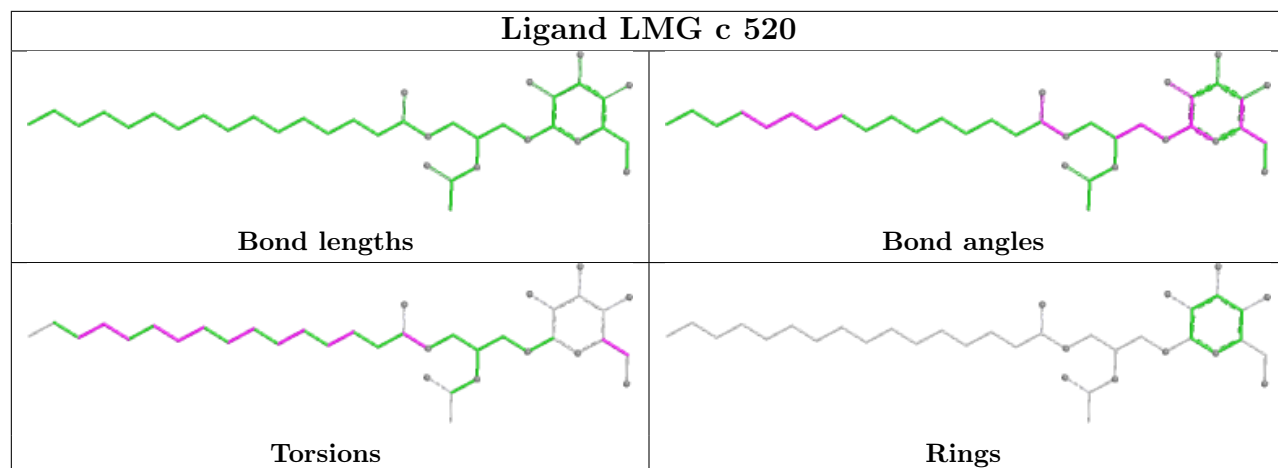


Ligand SQD a 613

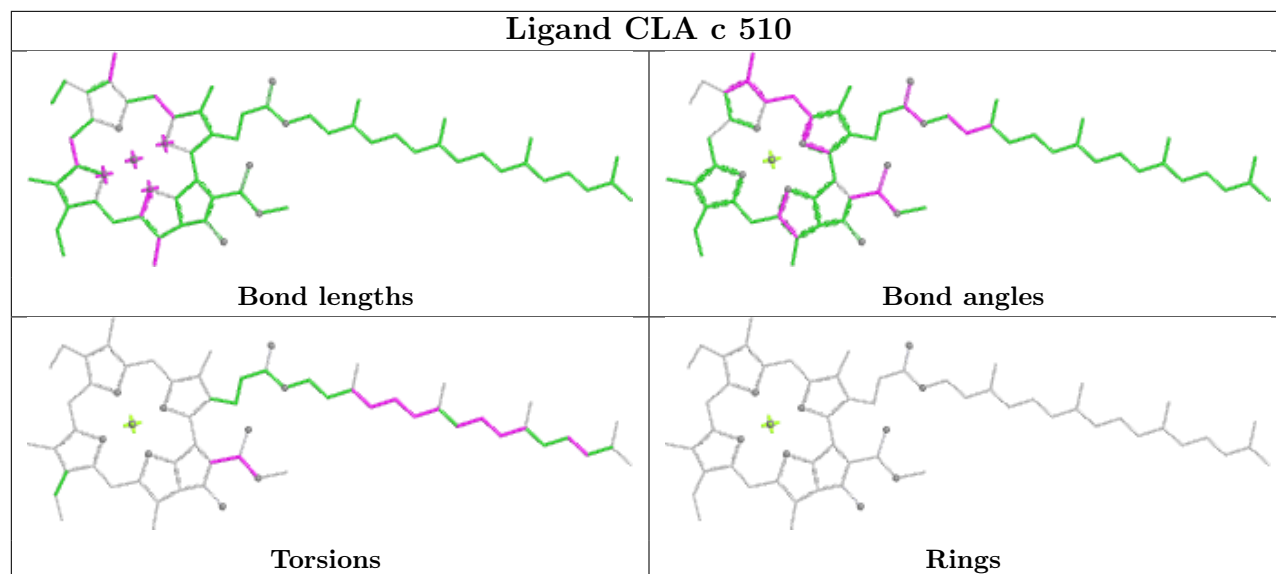


Ligand CLA B 609

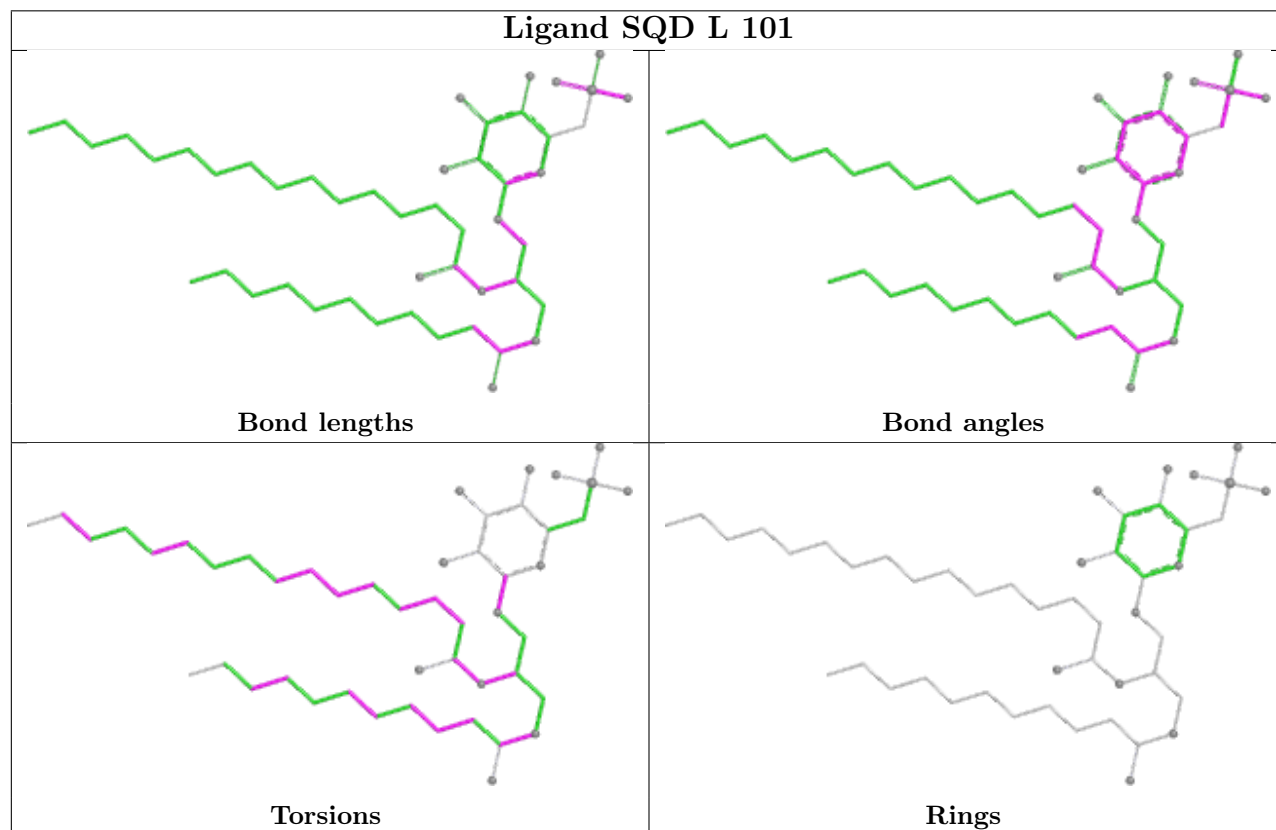


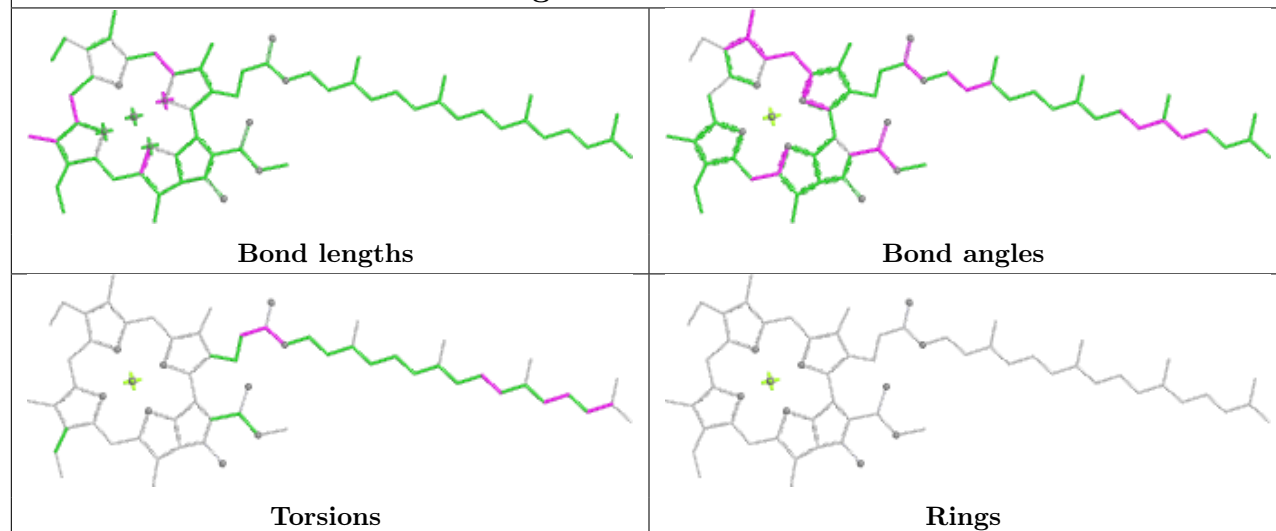
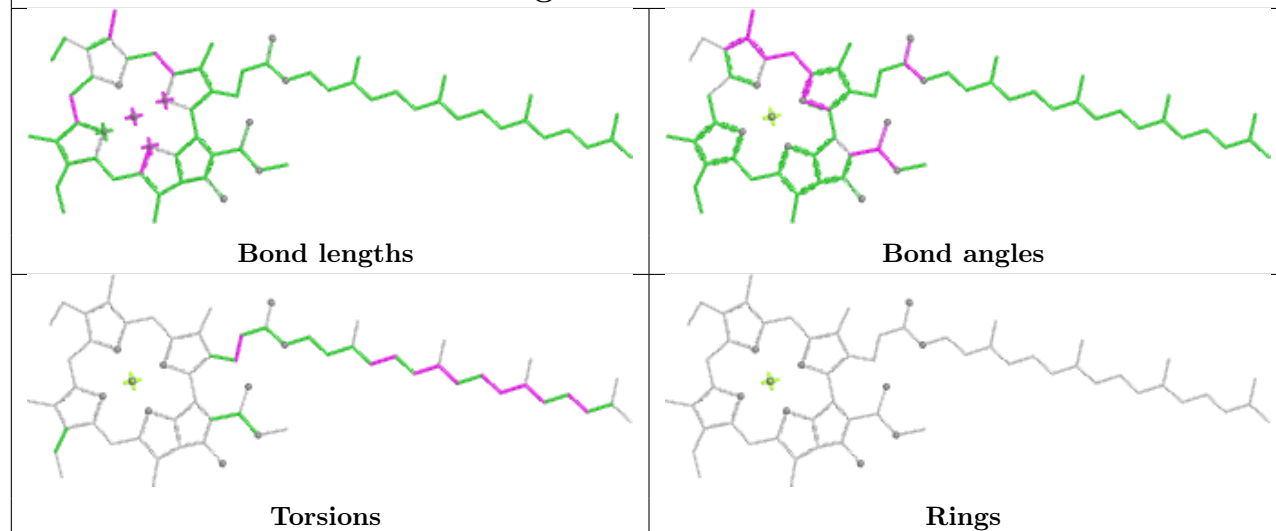
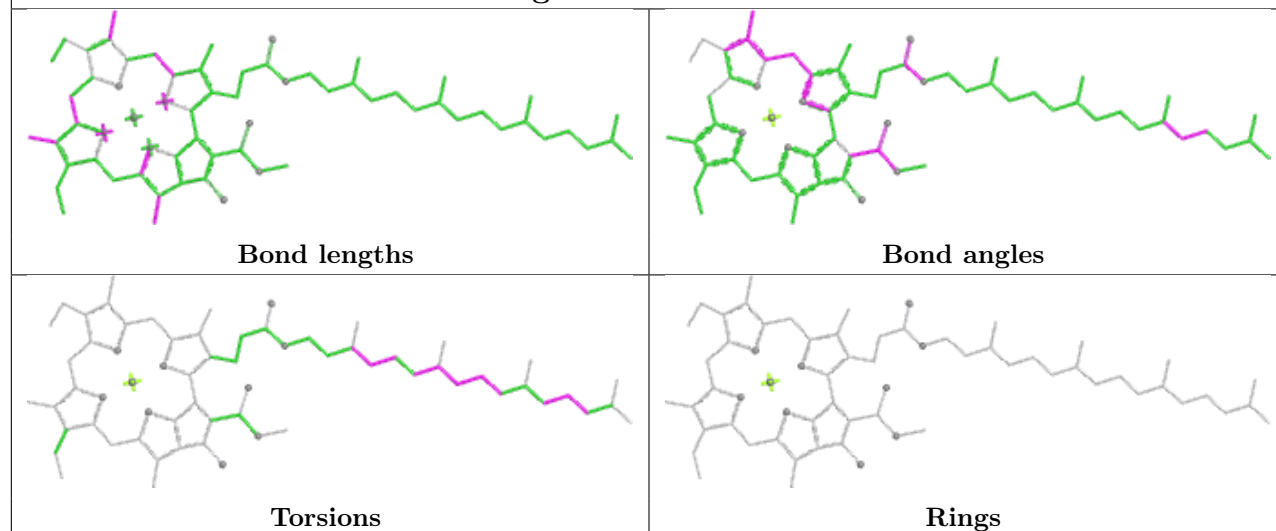


Ligand CLA c 510

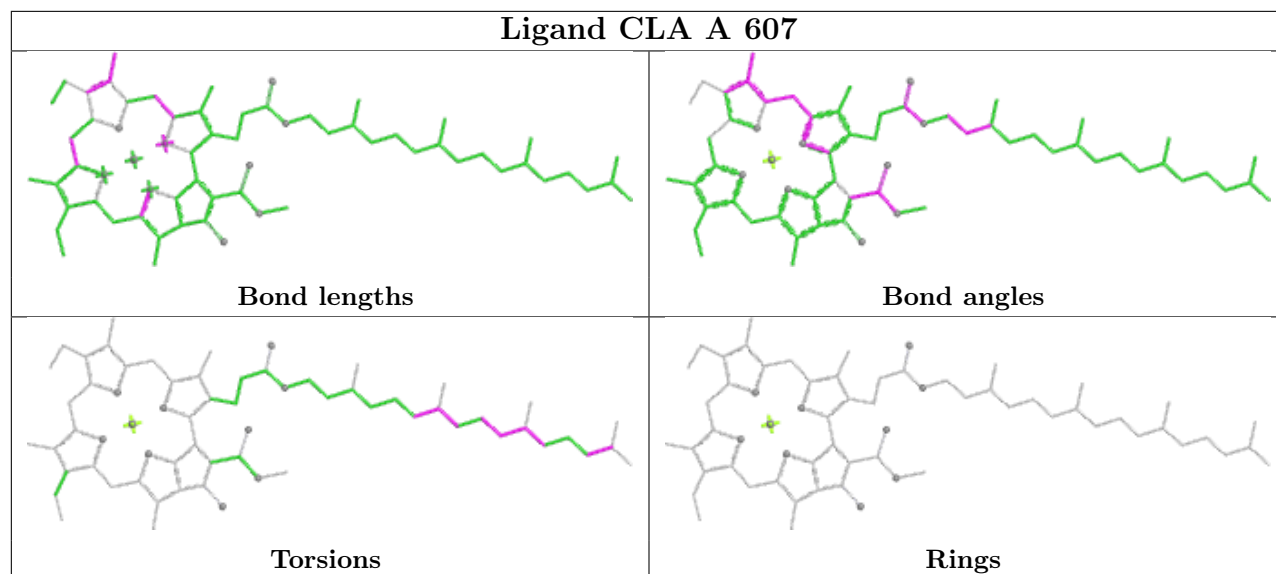


Ligand SQD L 101

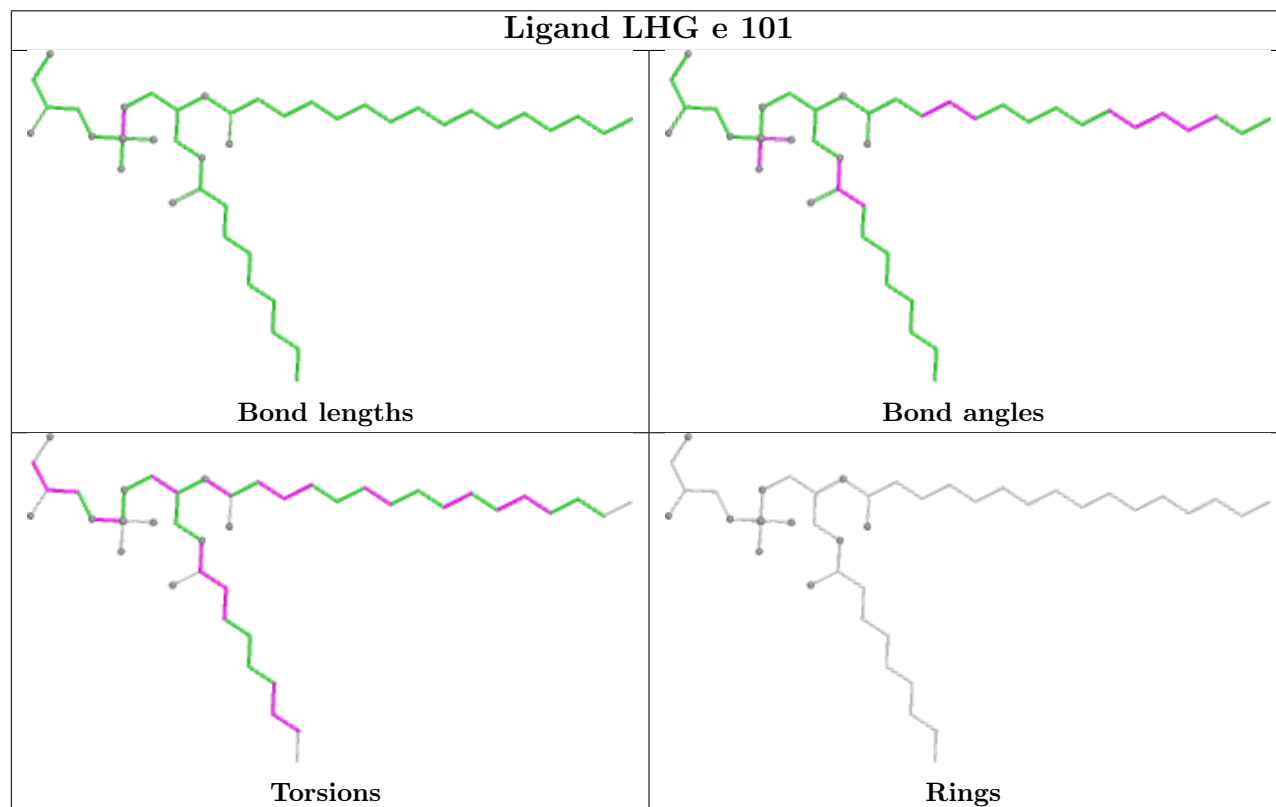


Ligand CLA B 612**Ligand CLA b 606****Ligand CLA C 510**

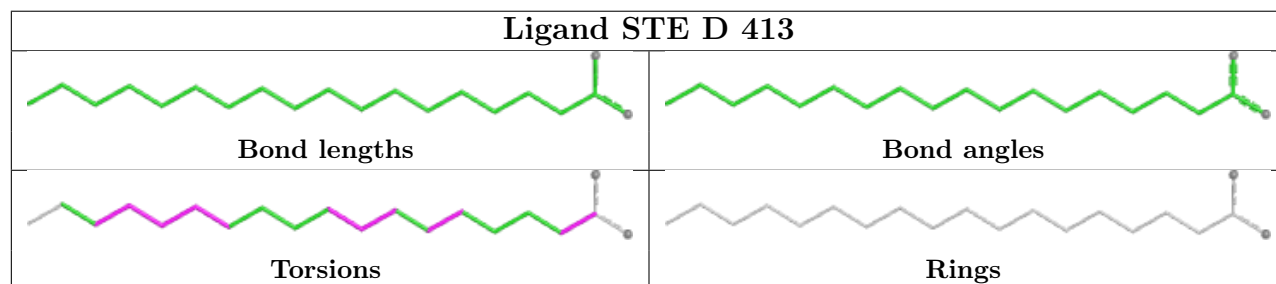
Ligand CLA A 607



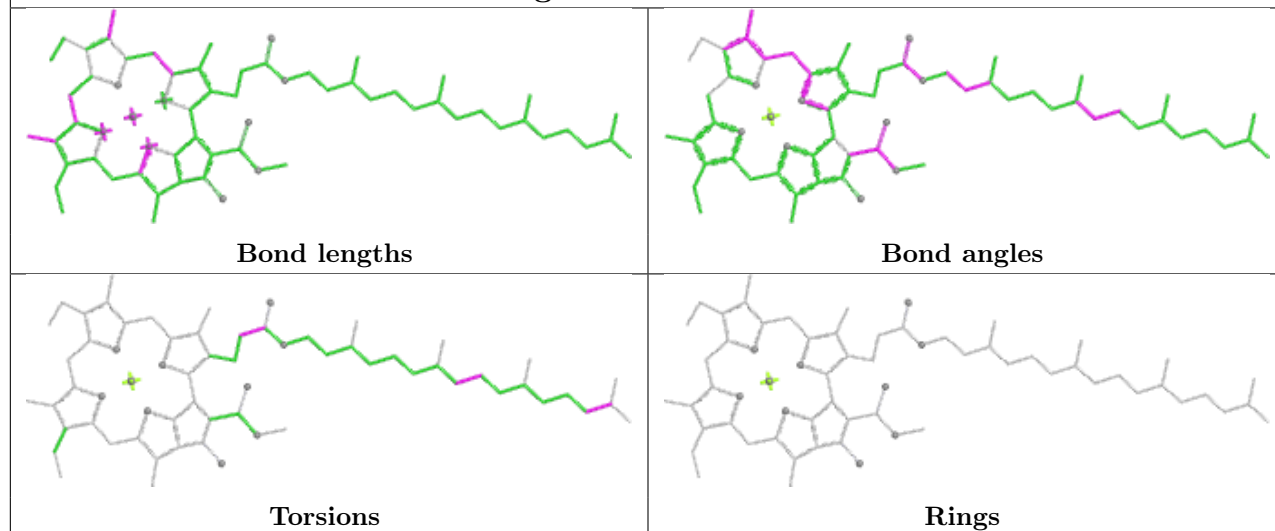
Ligand LHG e 101



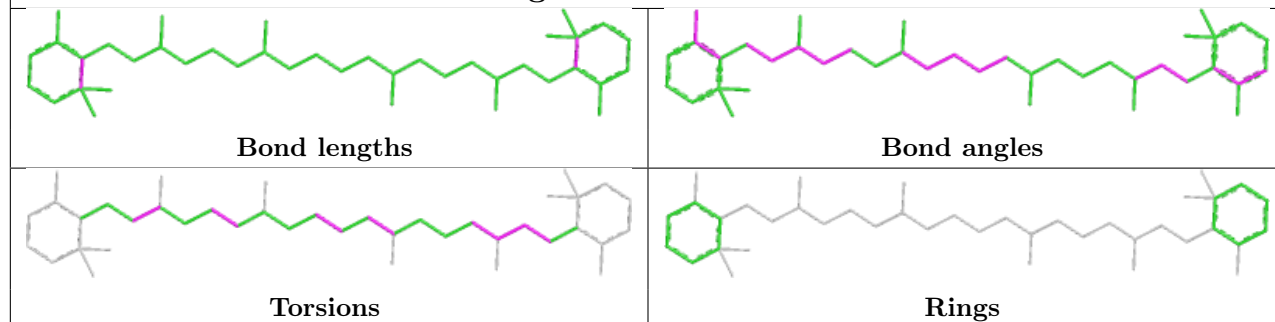
Ligand STE D 413



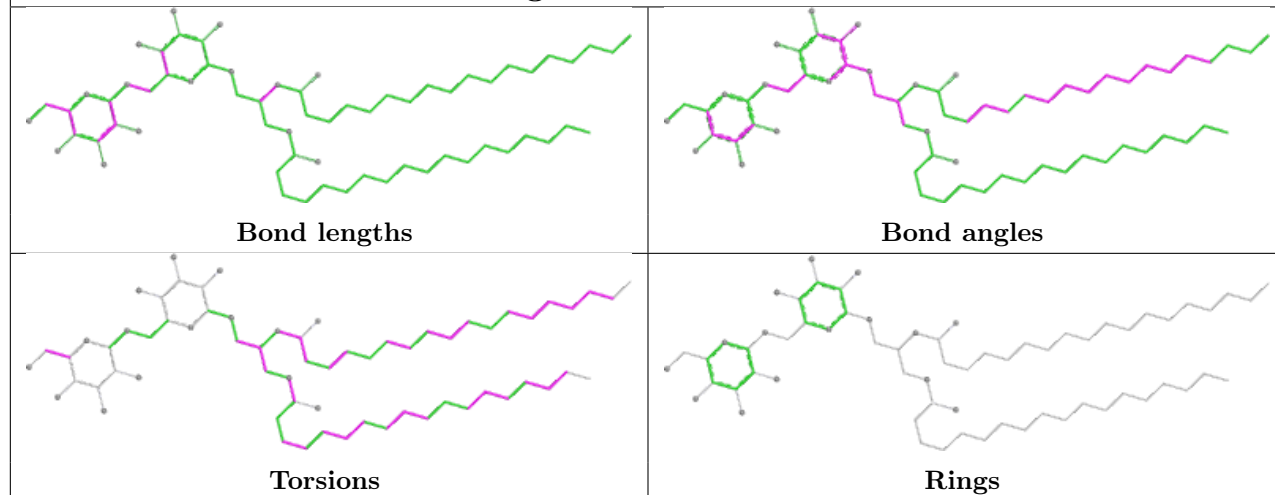
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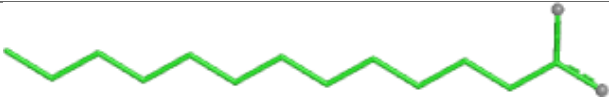
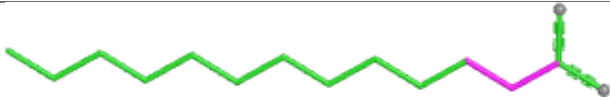
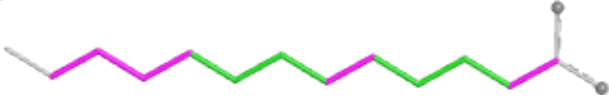
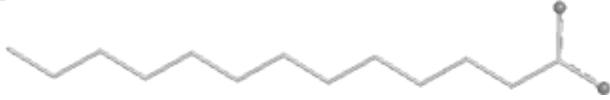


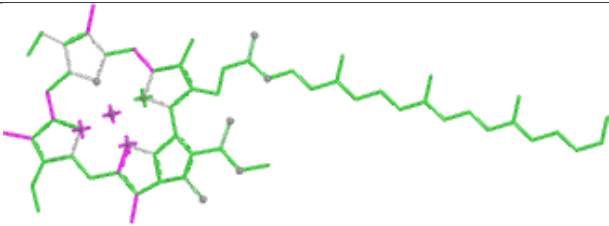
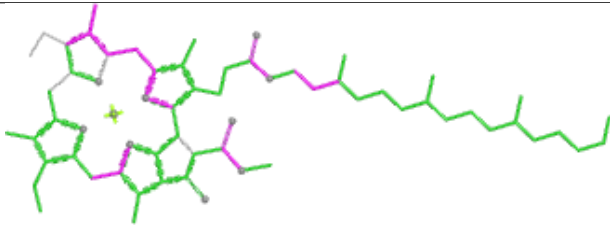
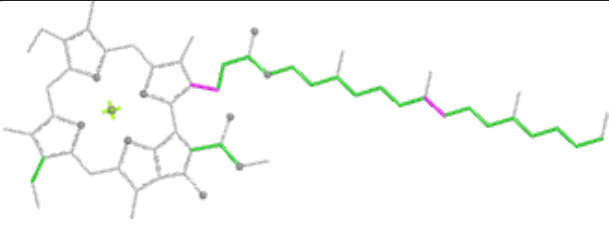
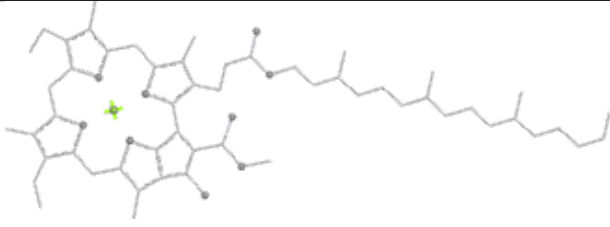
Ligand BCR K 101

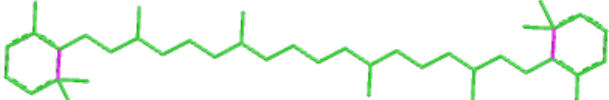
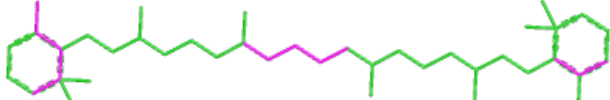
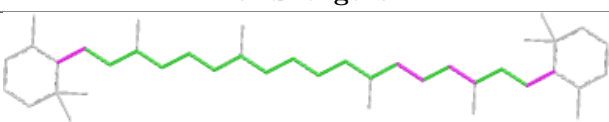
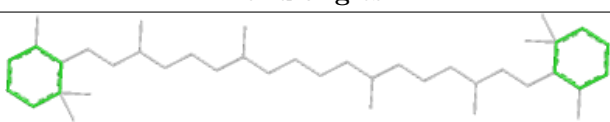


Ligand DGD A 617

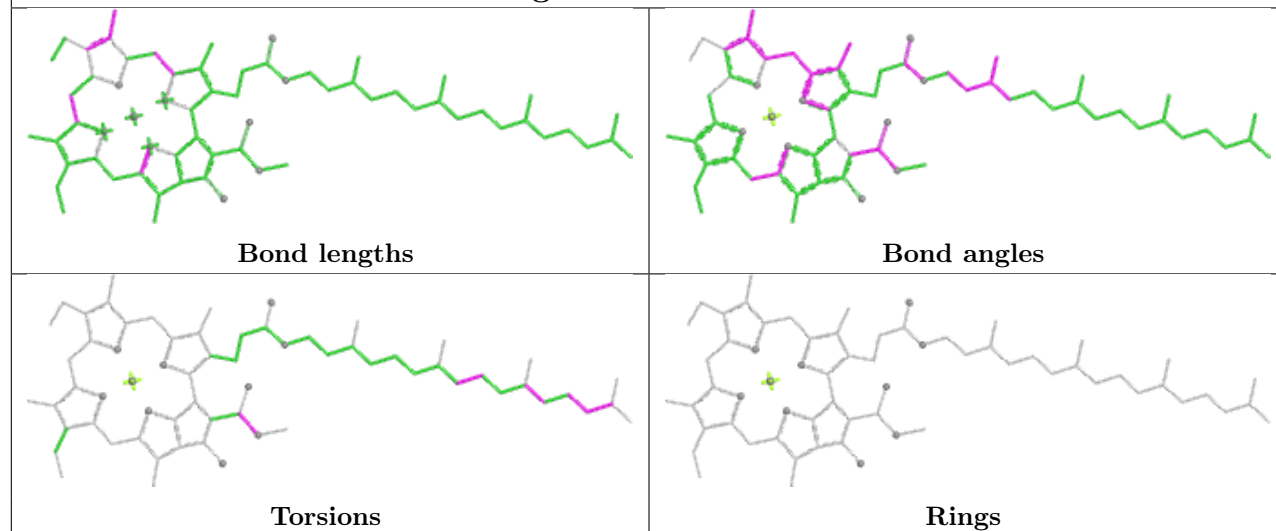


Ligand STE M 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

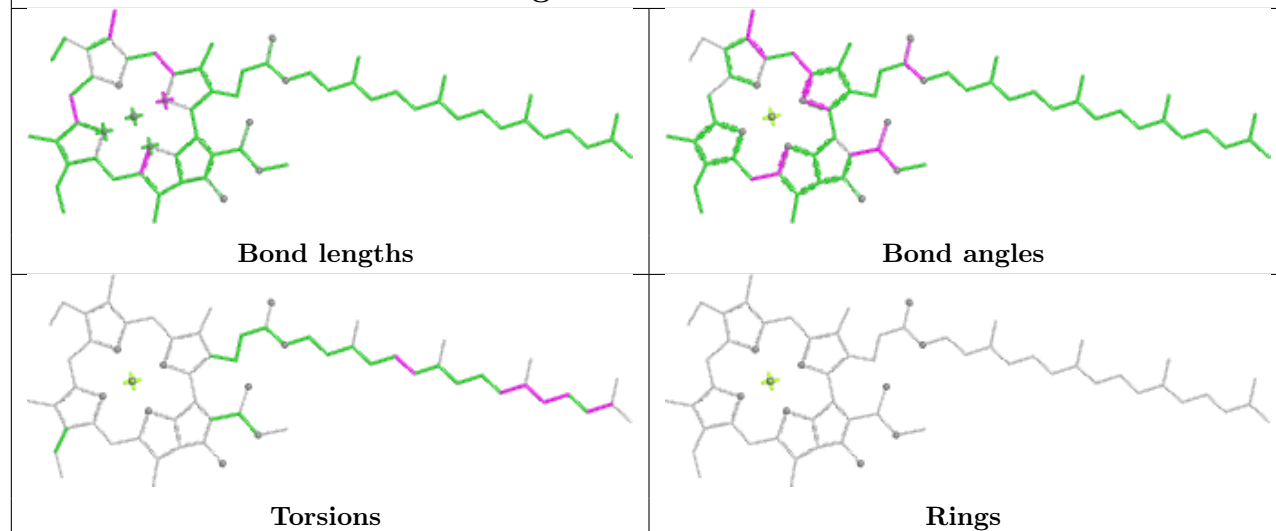
Ligand CLA c 508	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR C 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

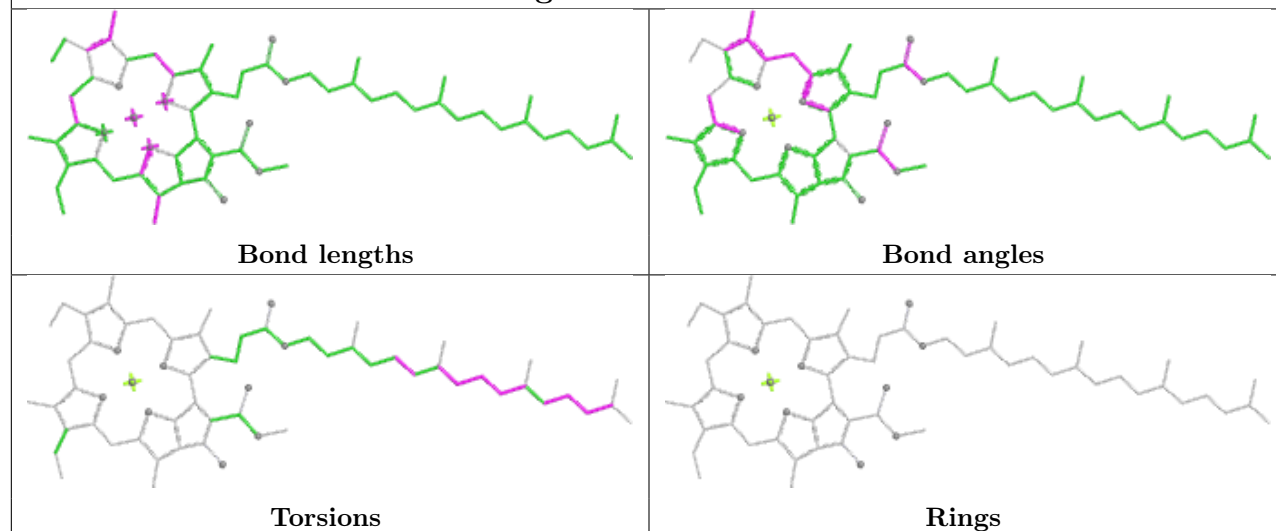
Ligand CLA B 610

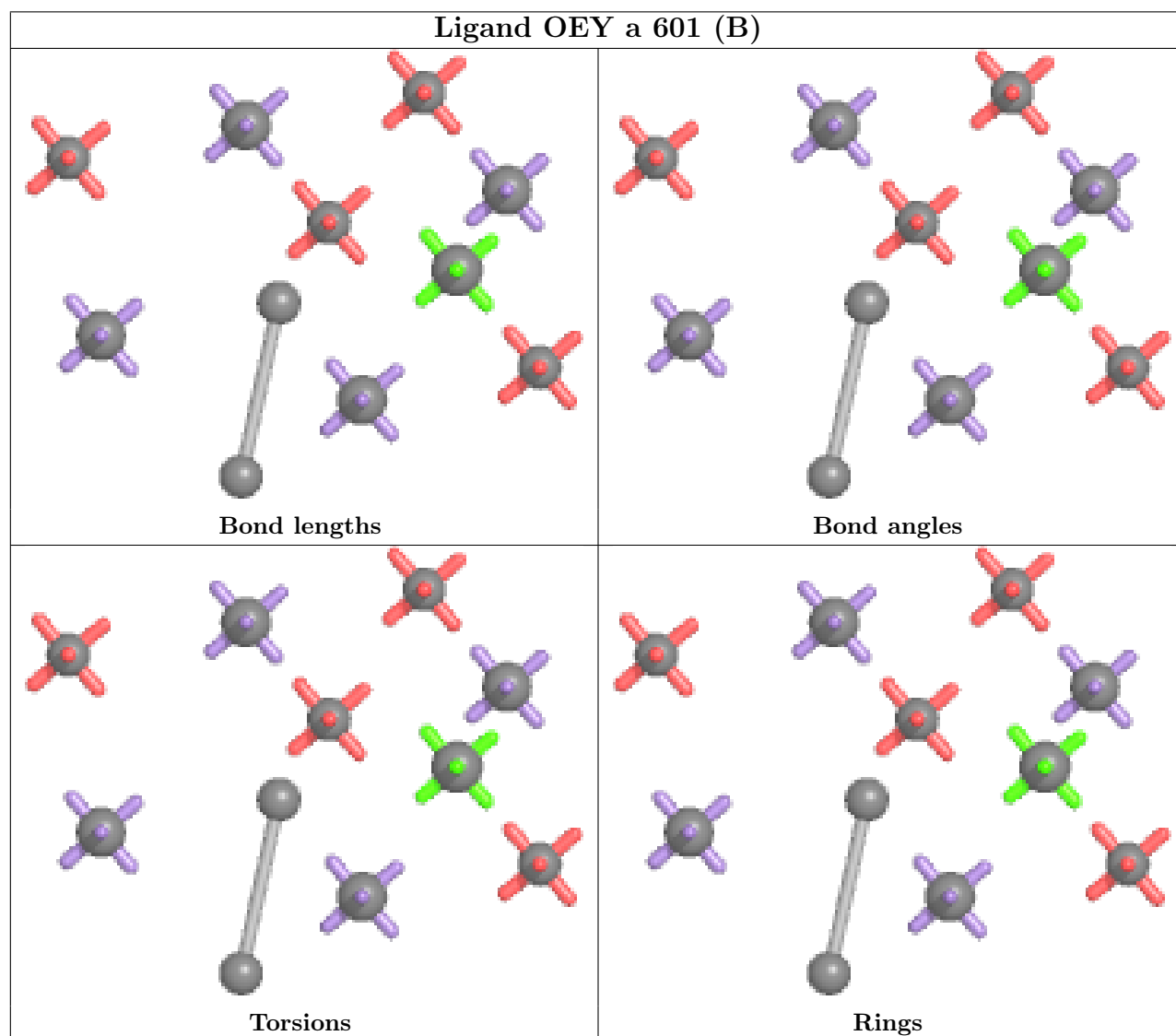
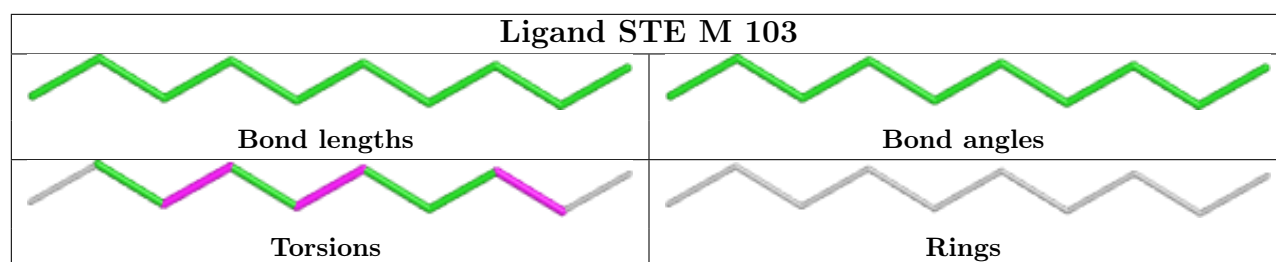


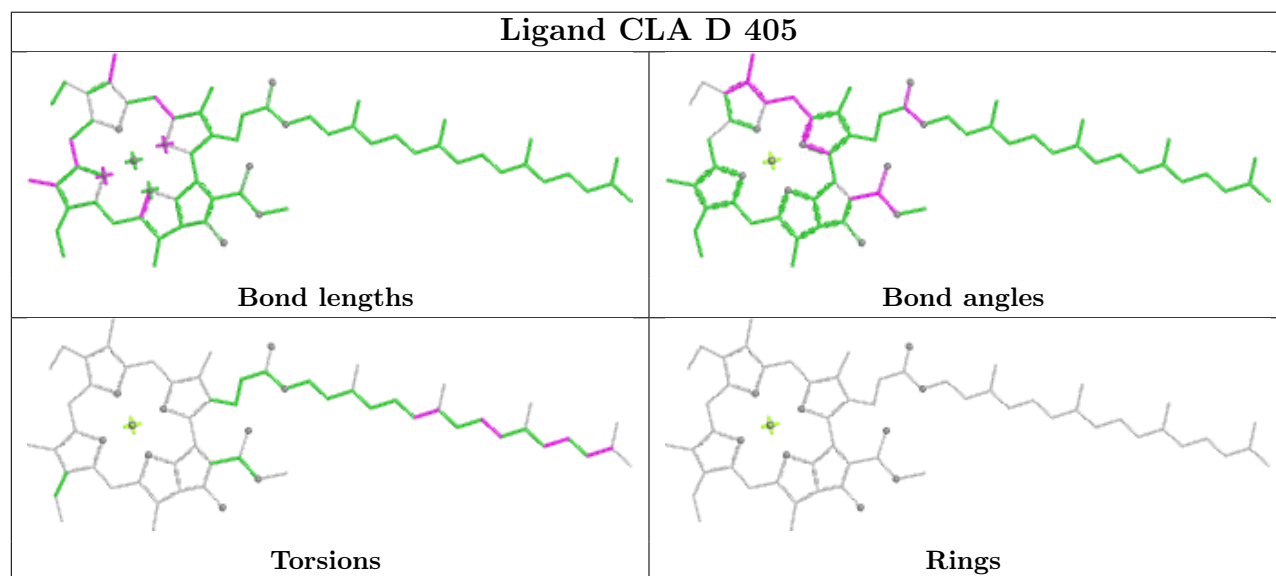
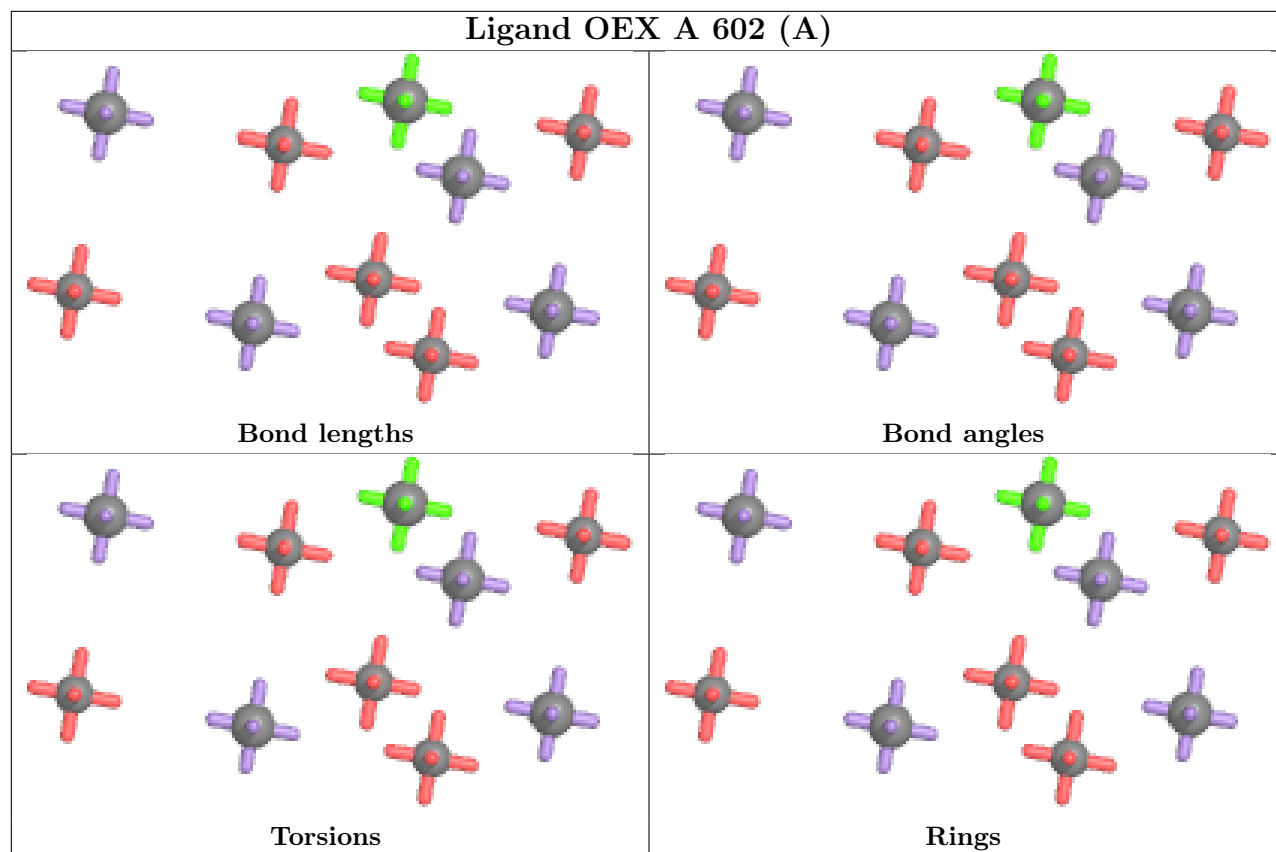
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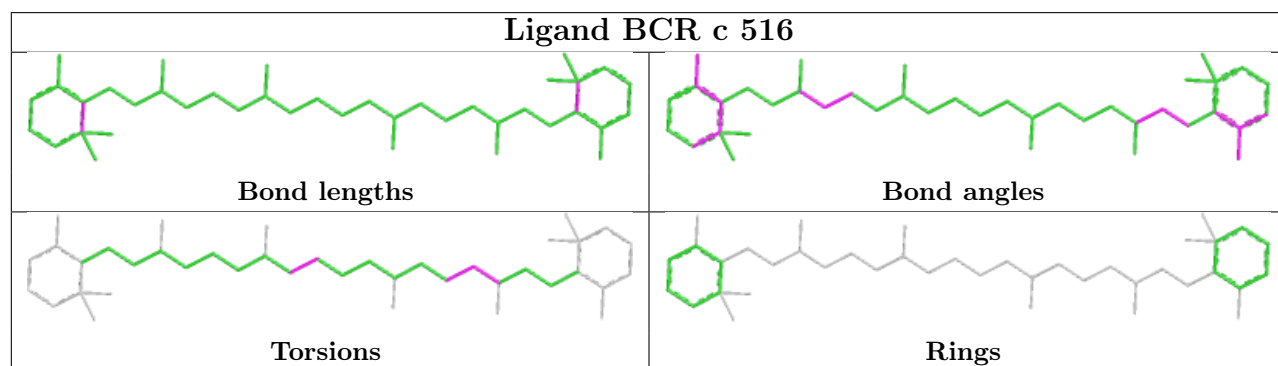
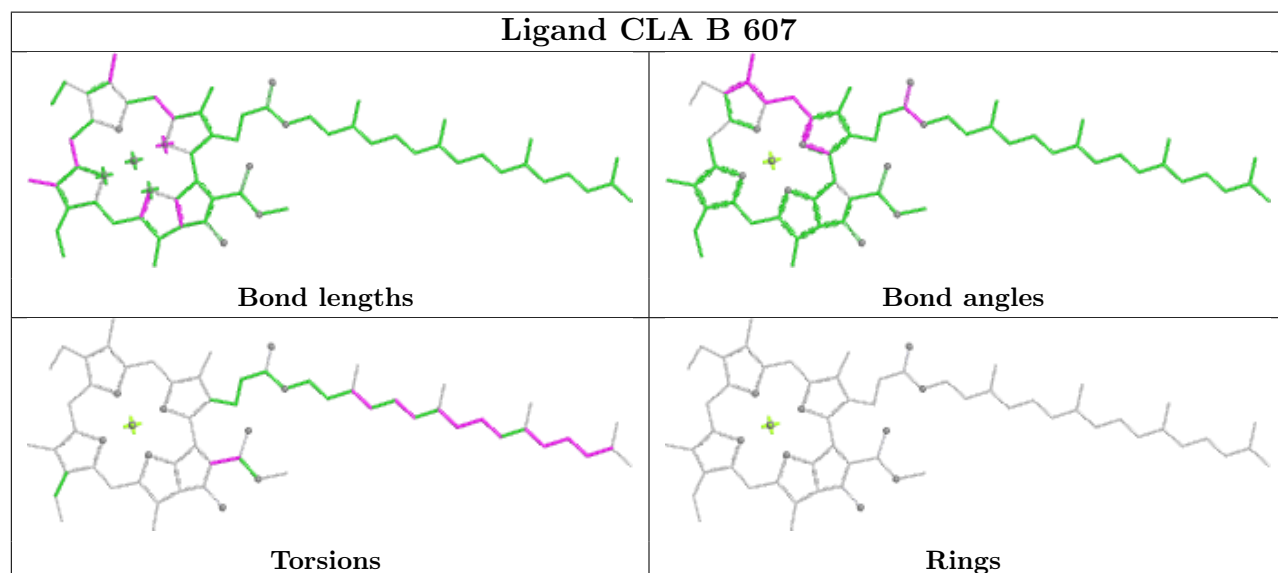
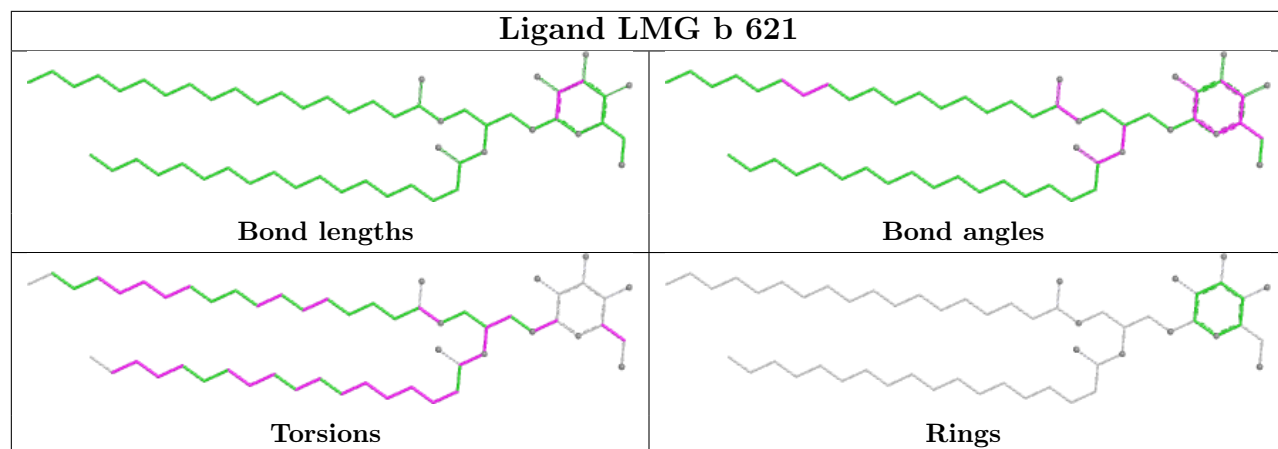


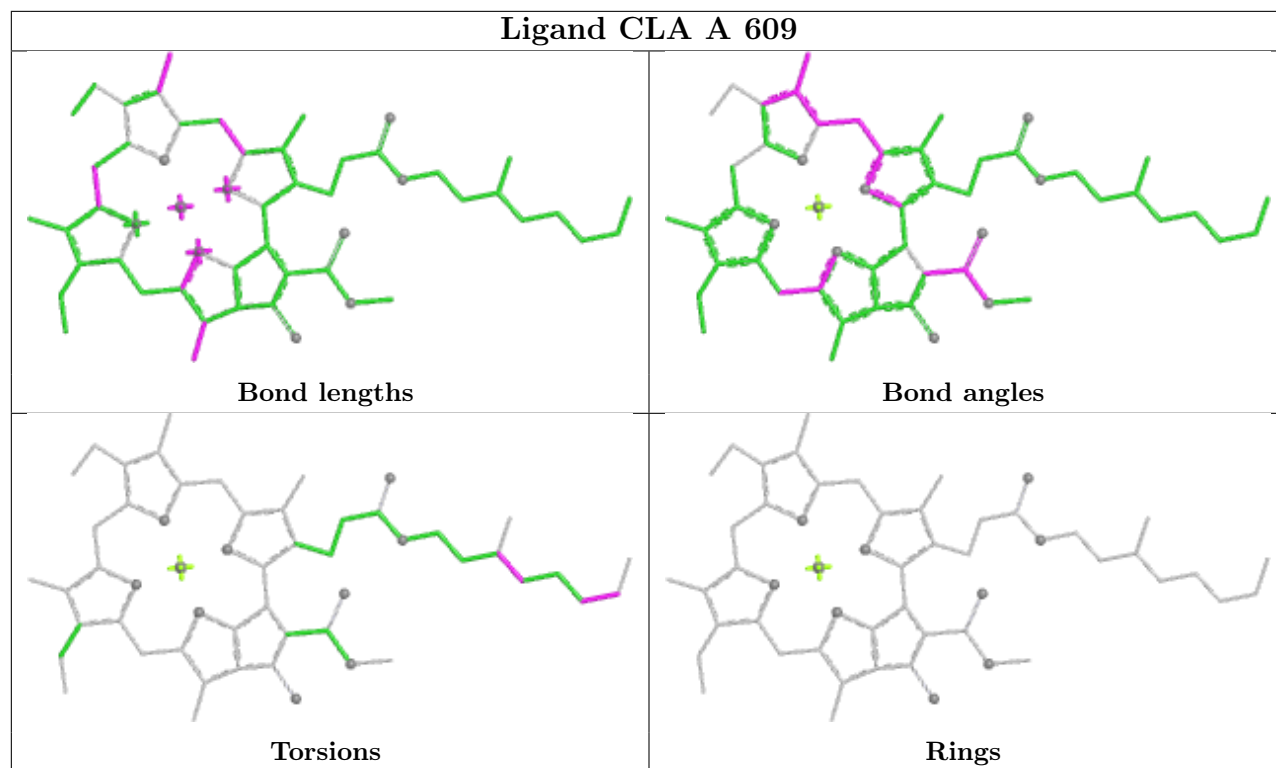
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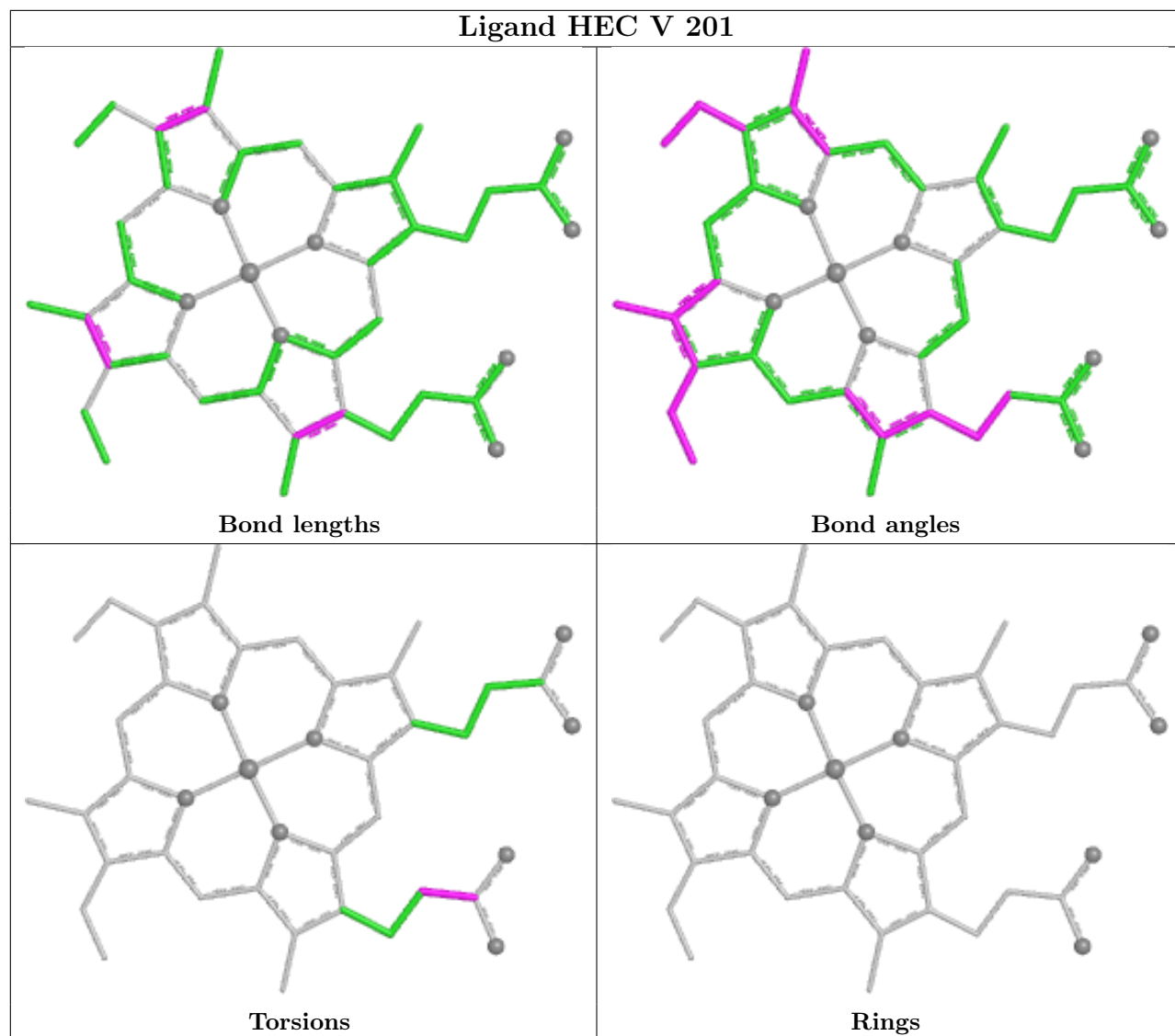




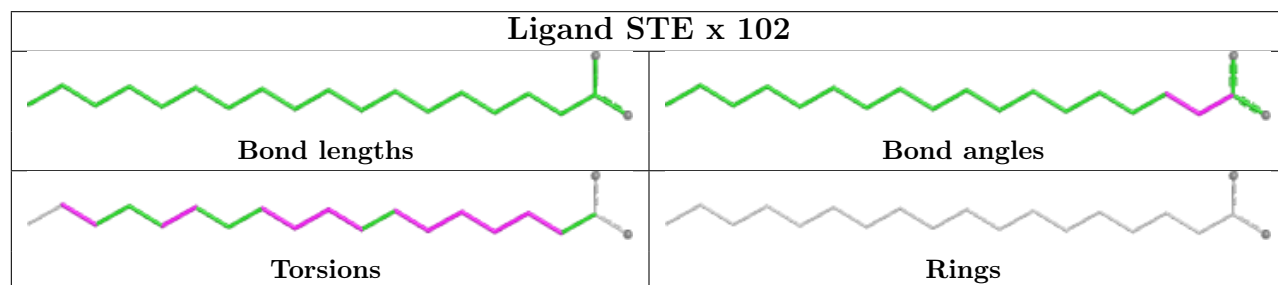


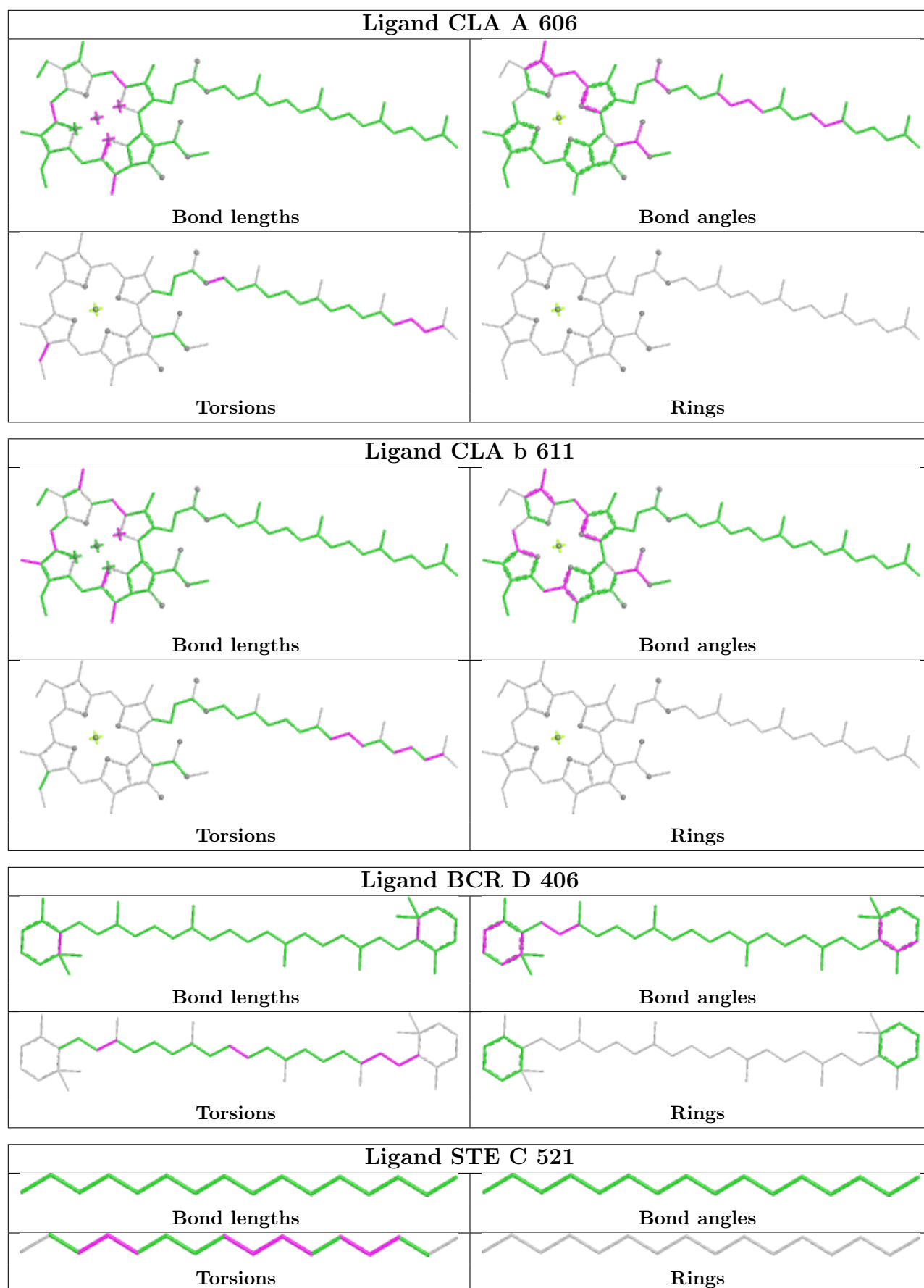


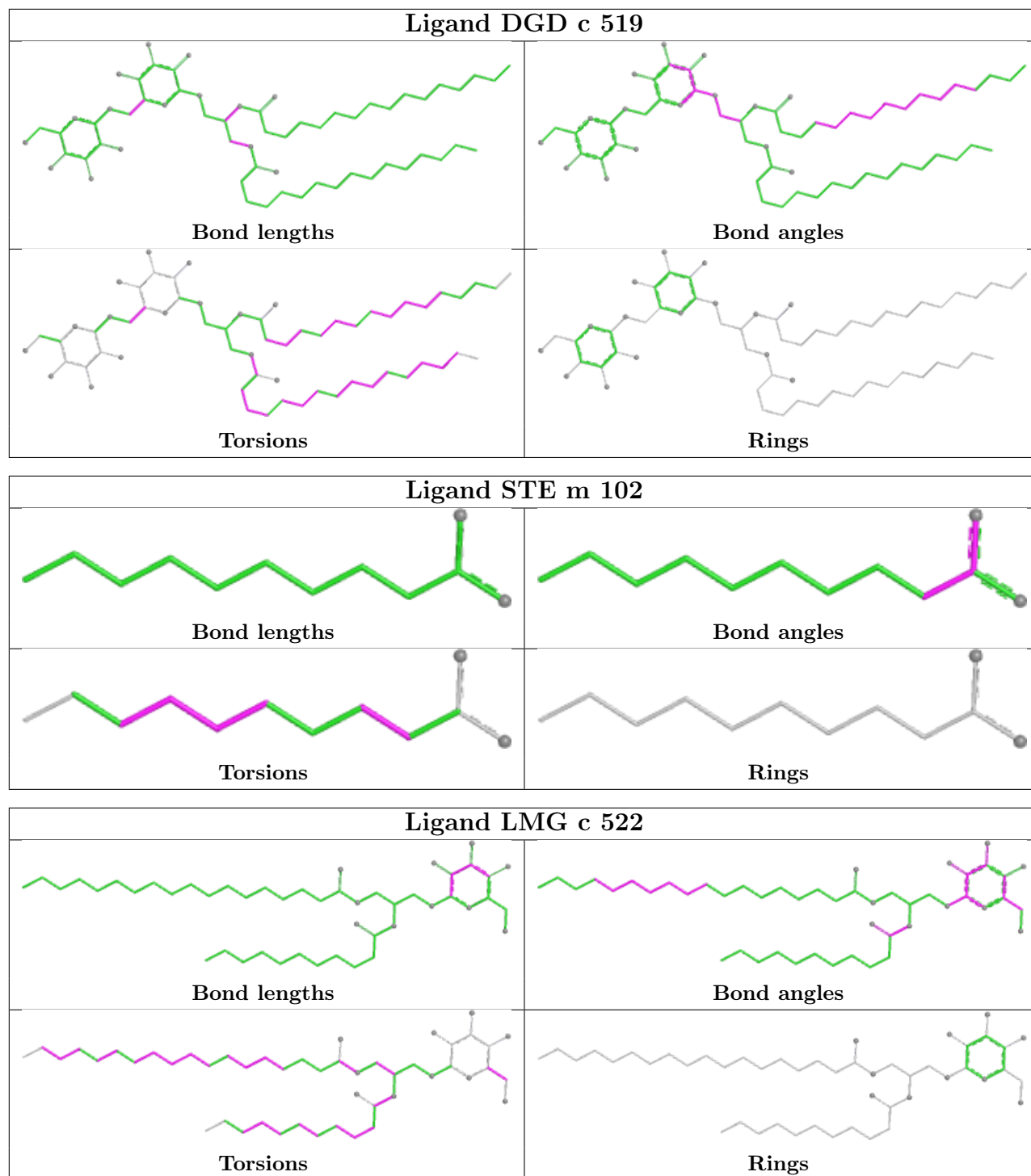
Ligand HEC V 201



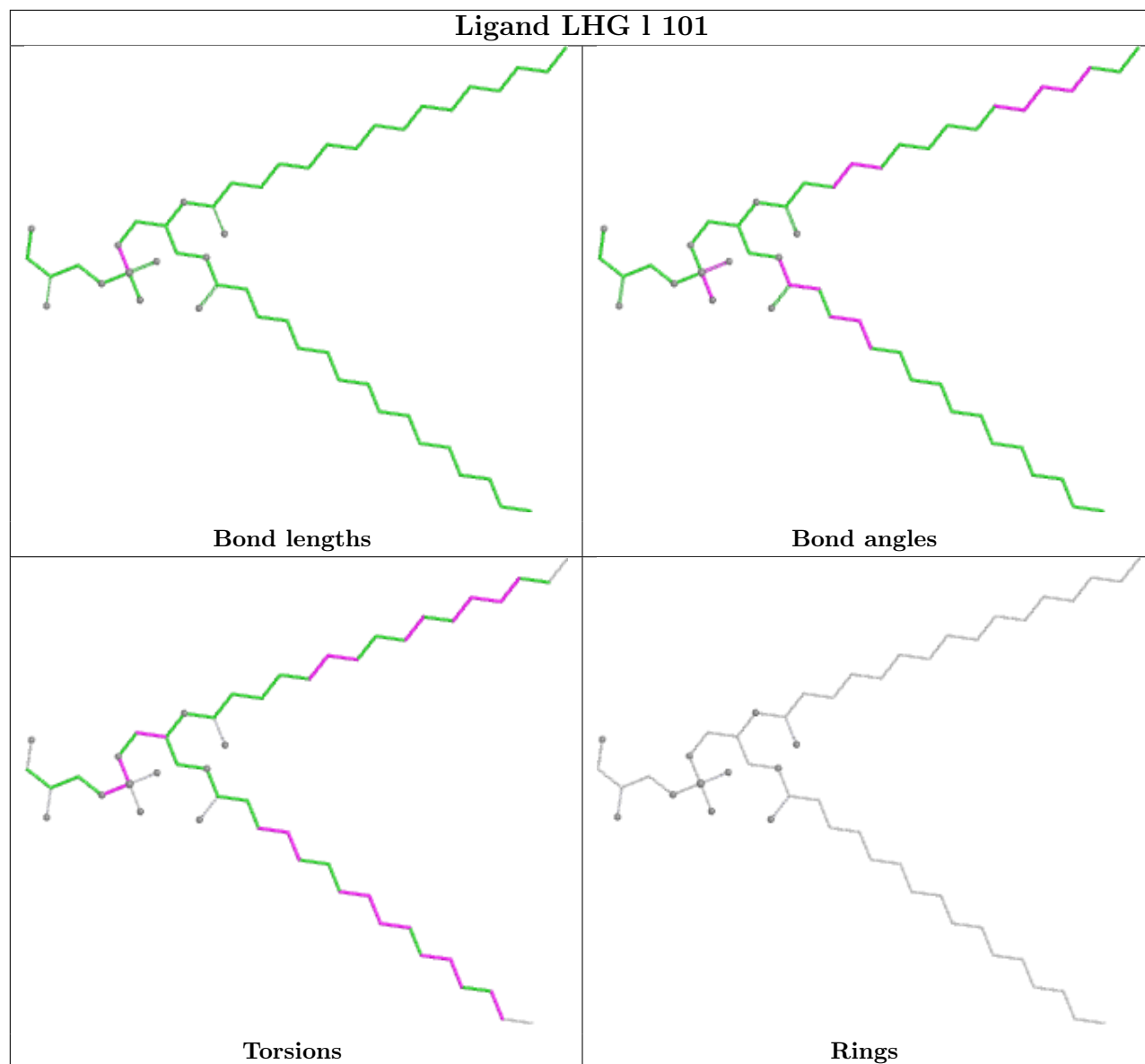
Ligand STE x 102



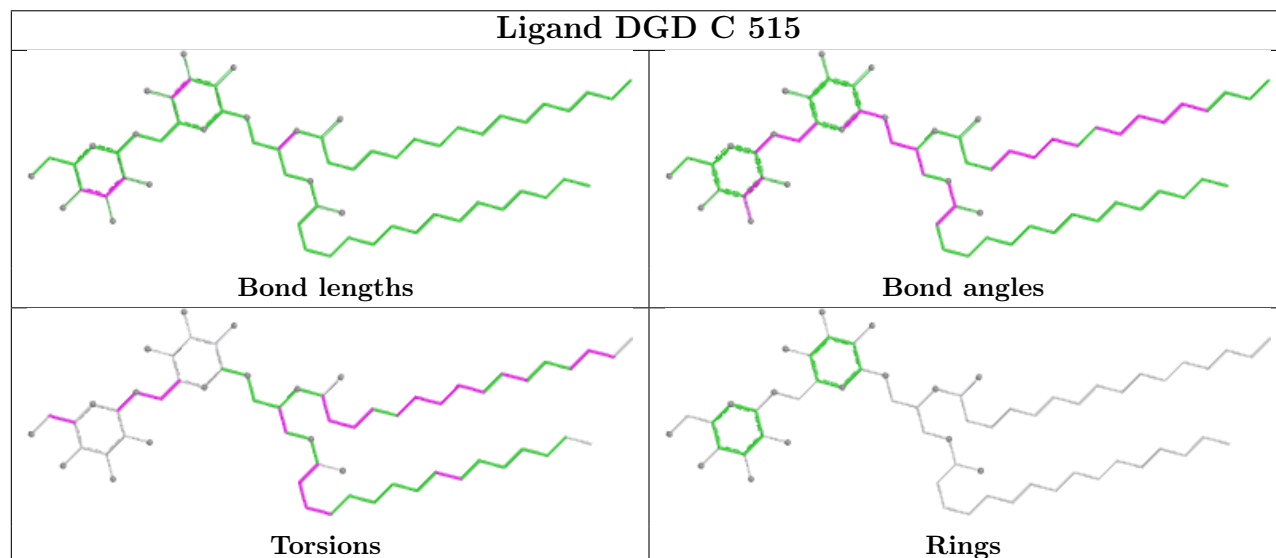








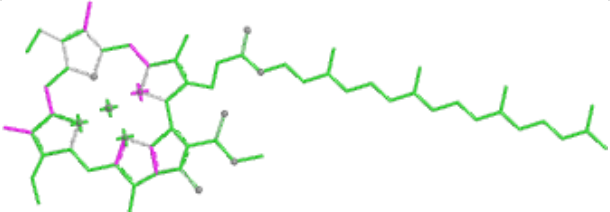
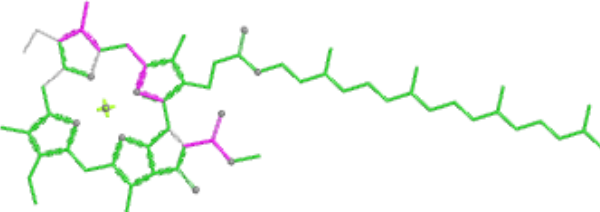
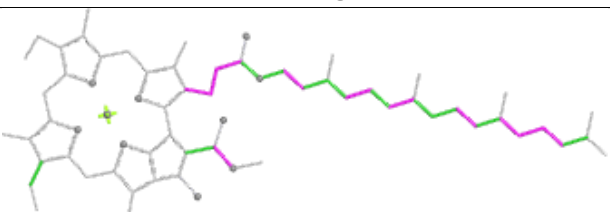
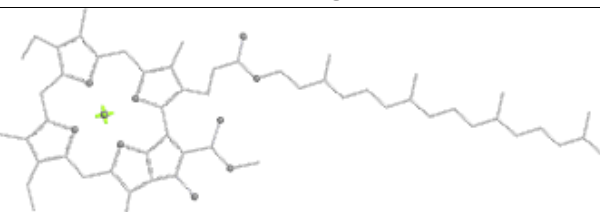
Ligand LHG 1 101



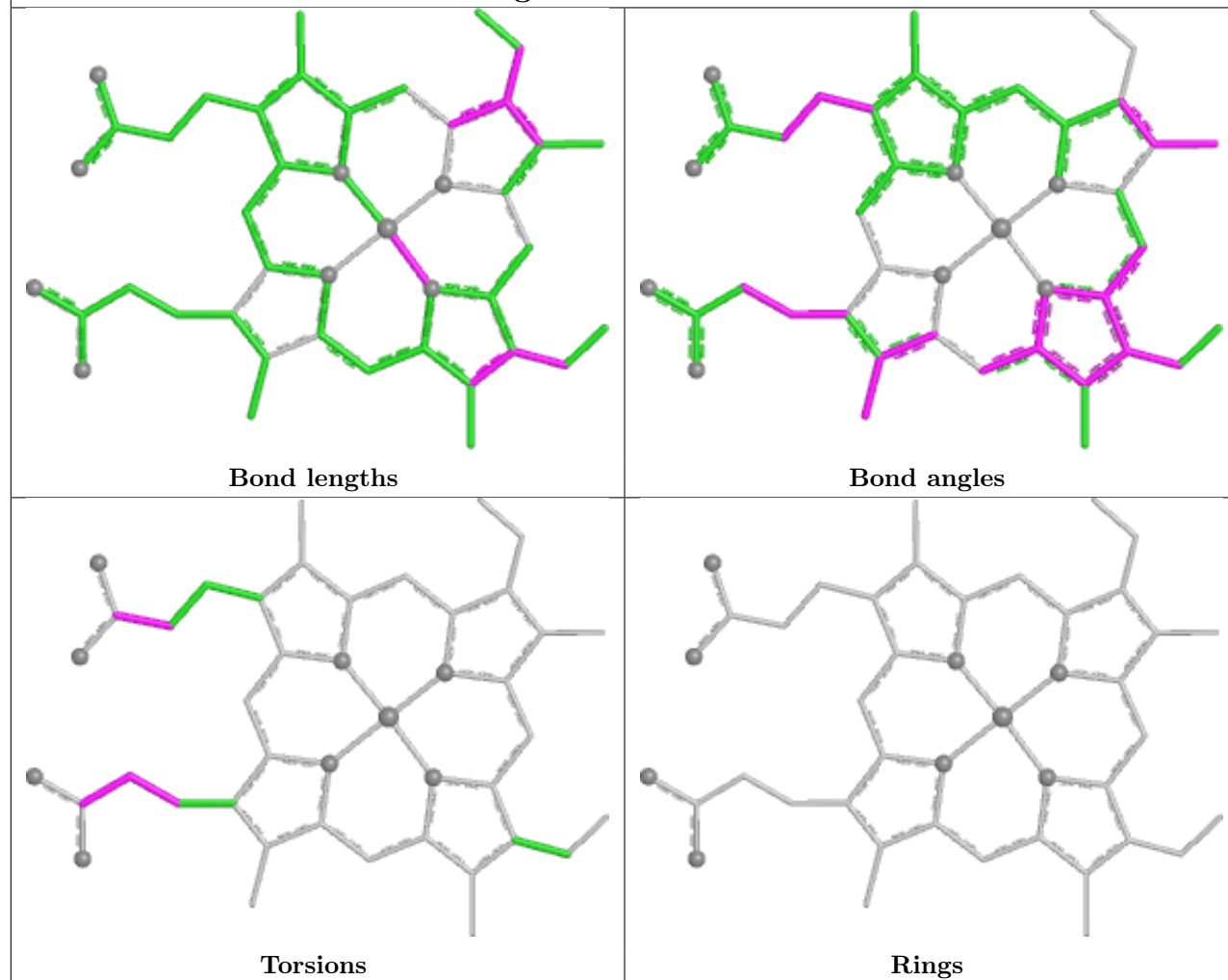
Ligand DGD C 515



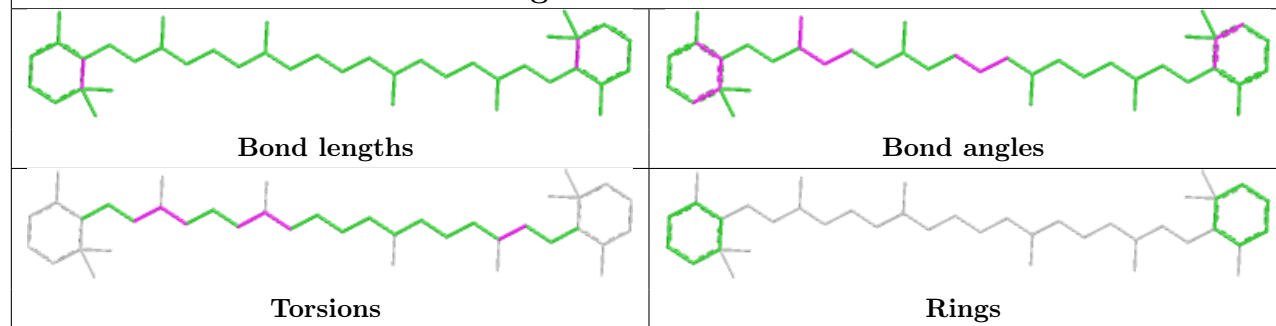
Ligand STE H 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

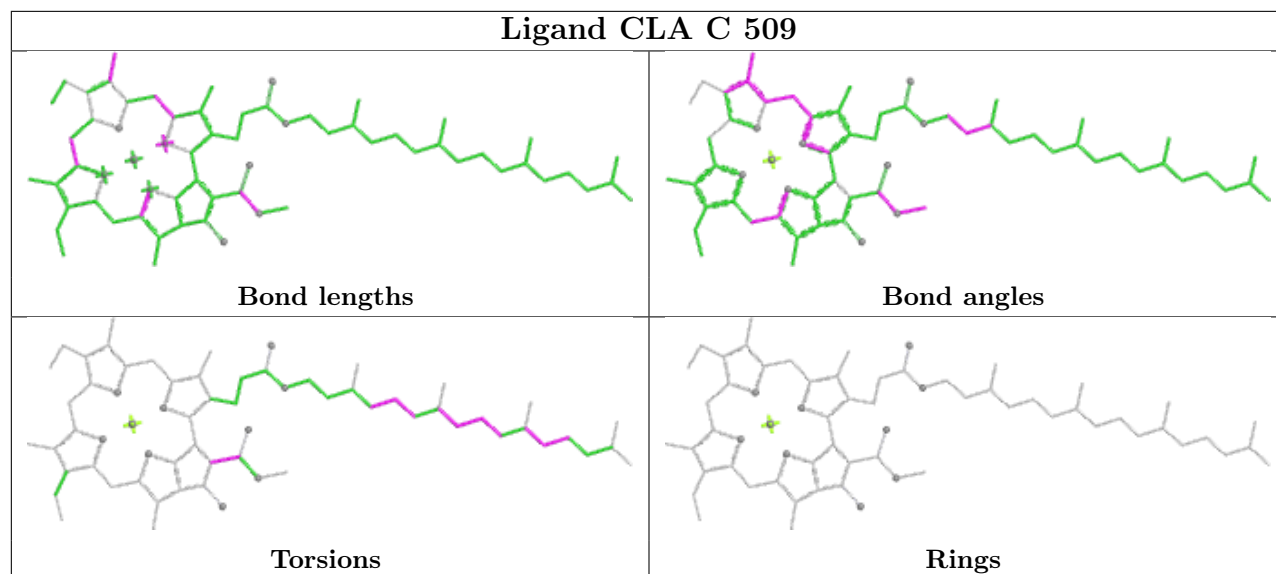
Ligand HEM f 101



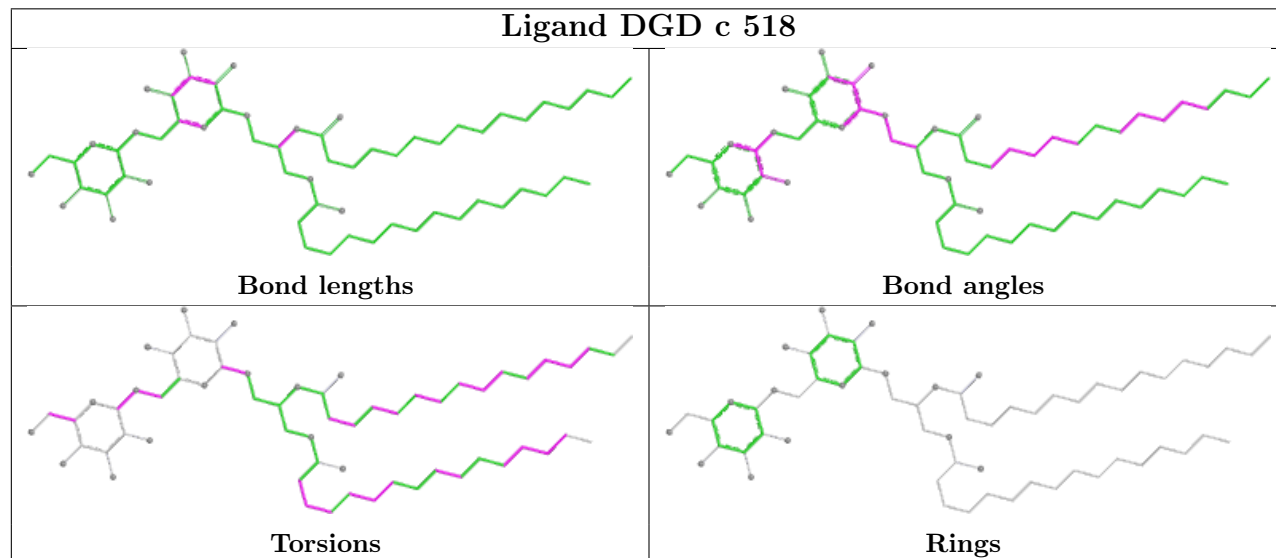
Ligand BCR B 619



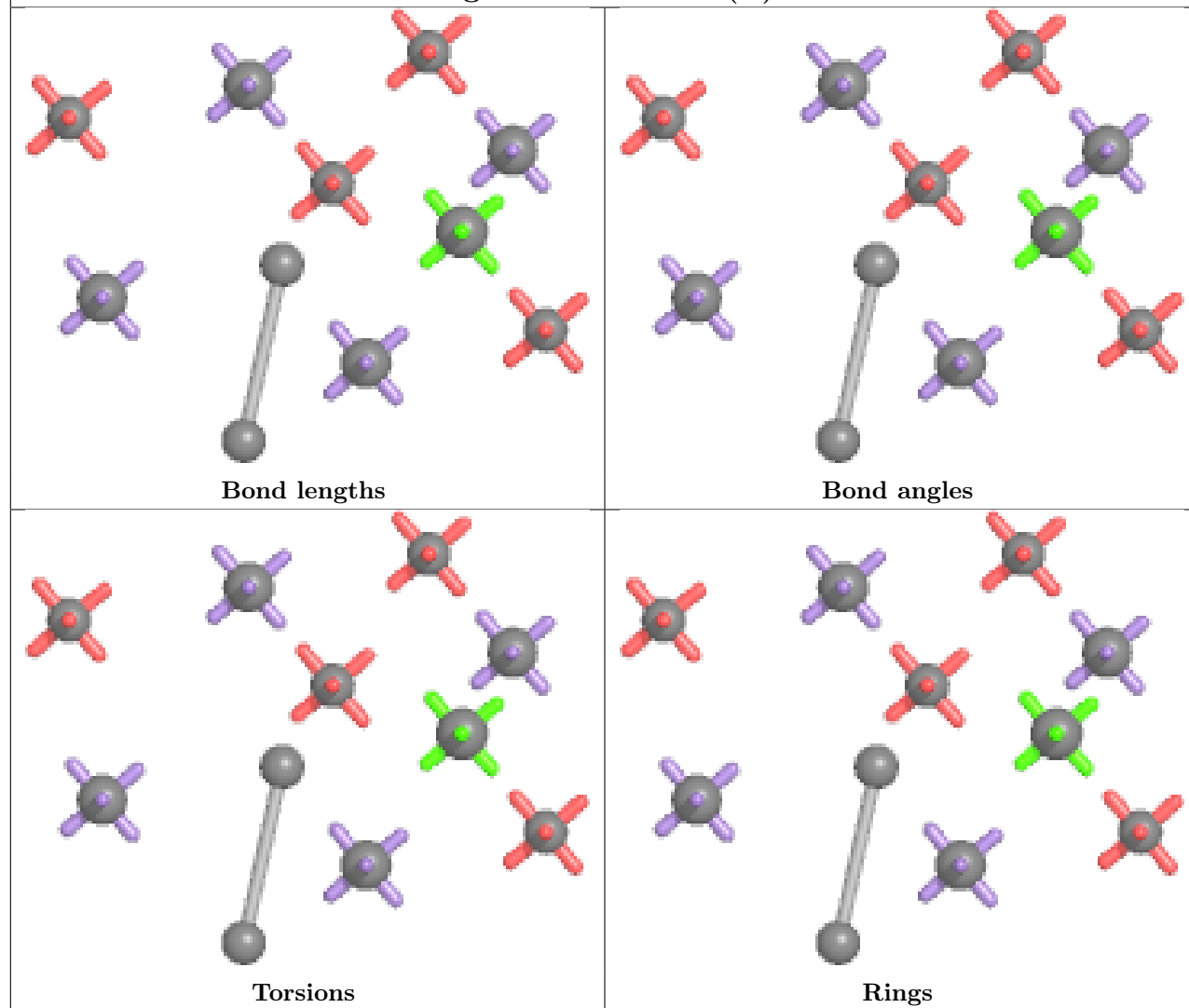
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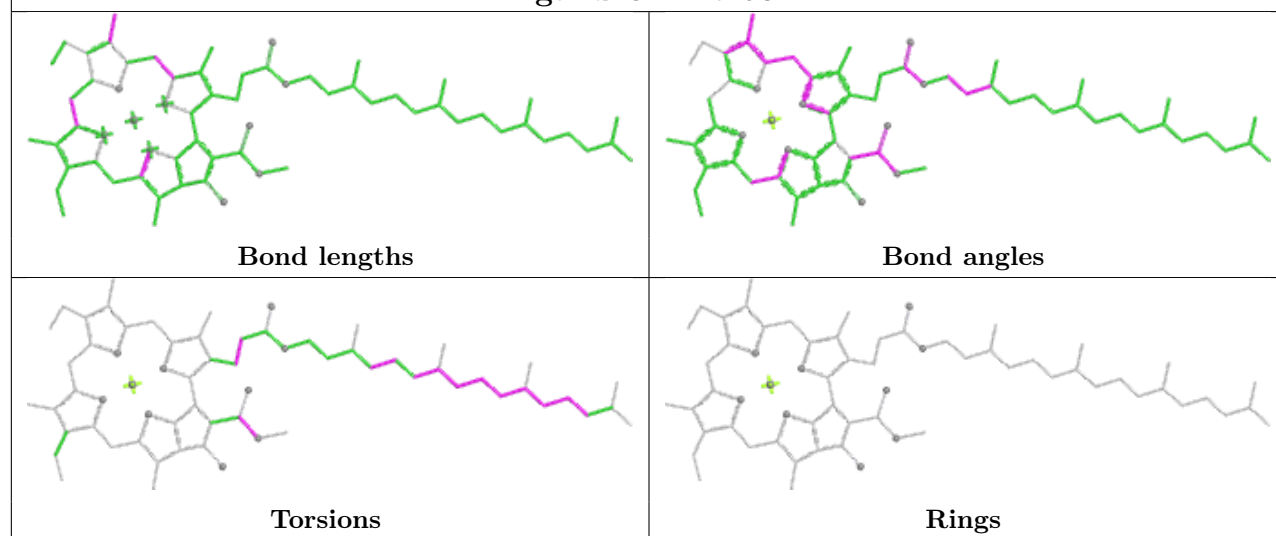
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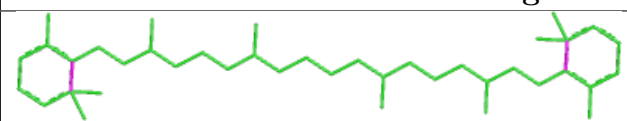
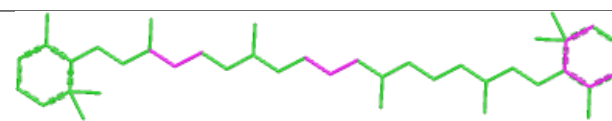
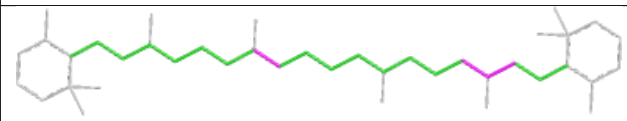
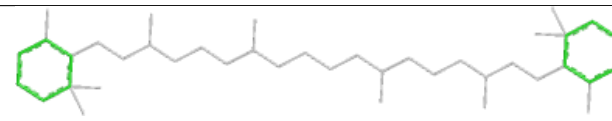


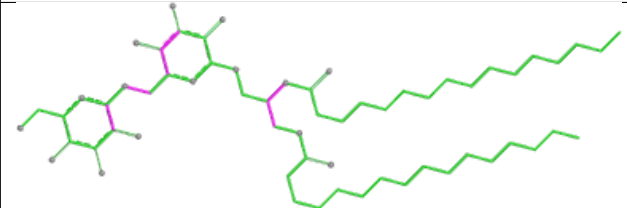
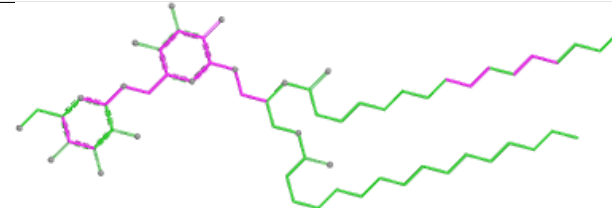
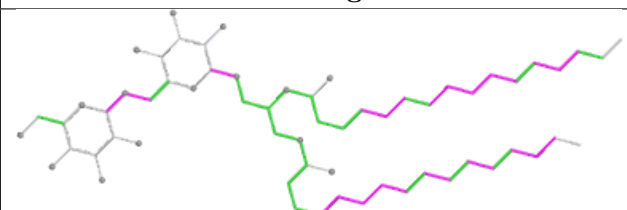
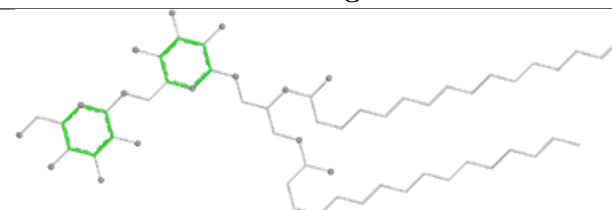
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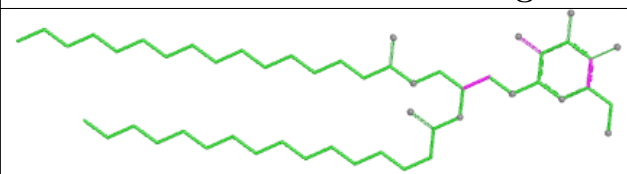
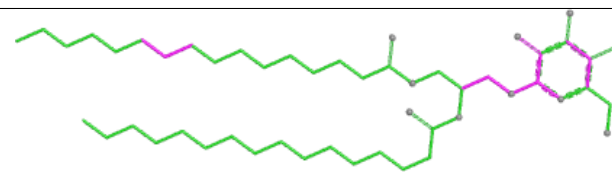
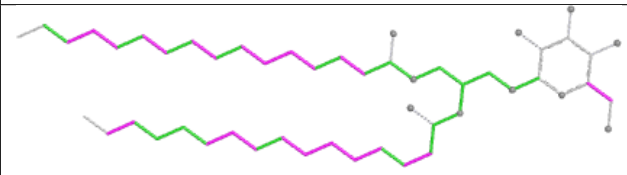
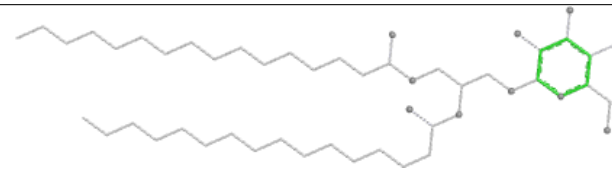




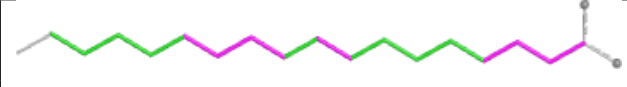
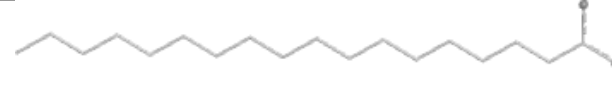
Ligand CLA b 602



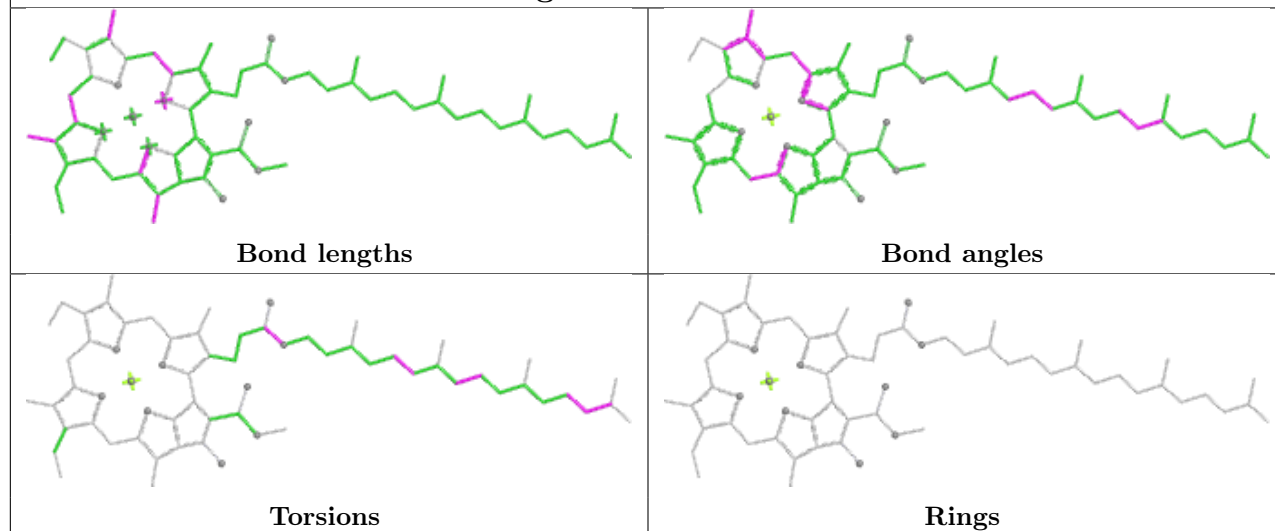
Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD C 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

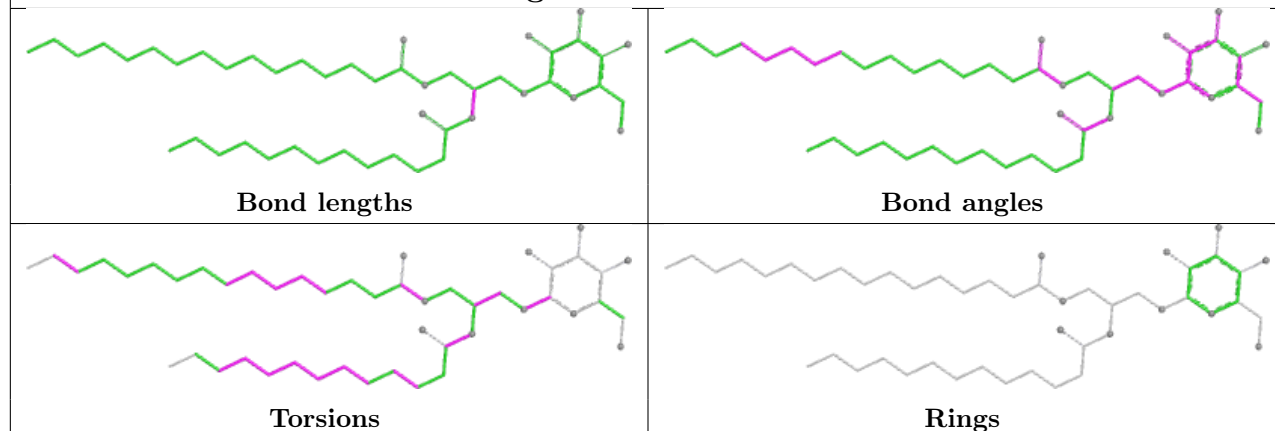
Ligand LMG D 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE c 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

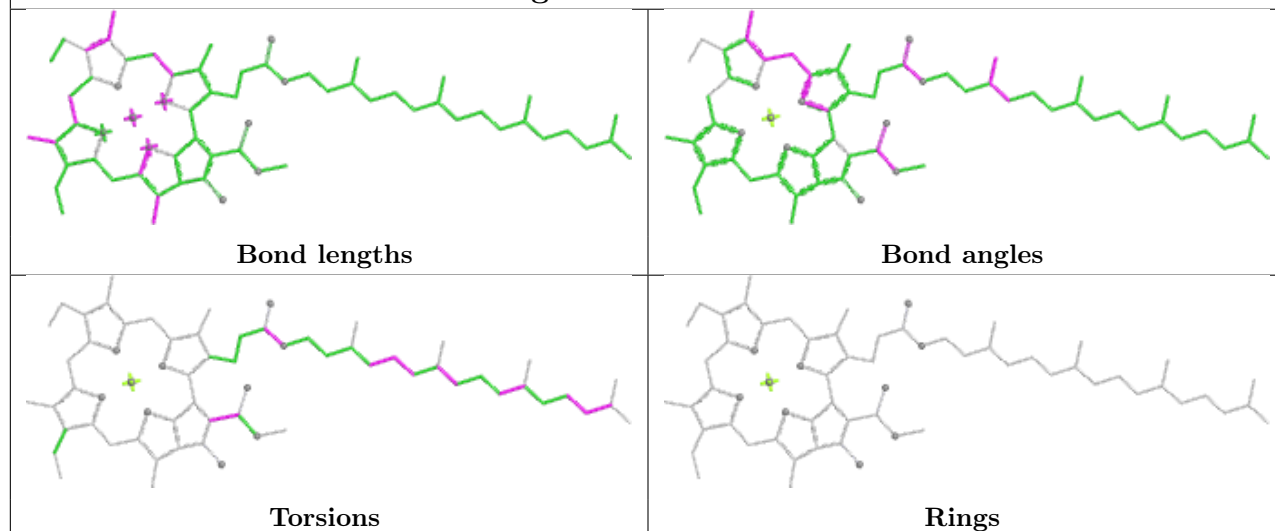
Ligand CLA c 503

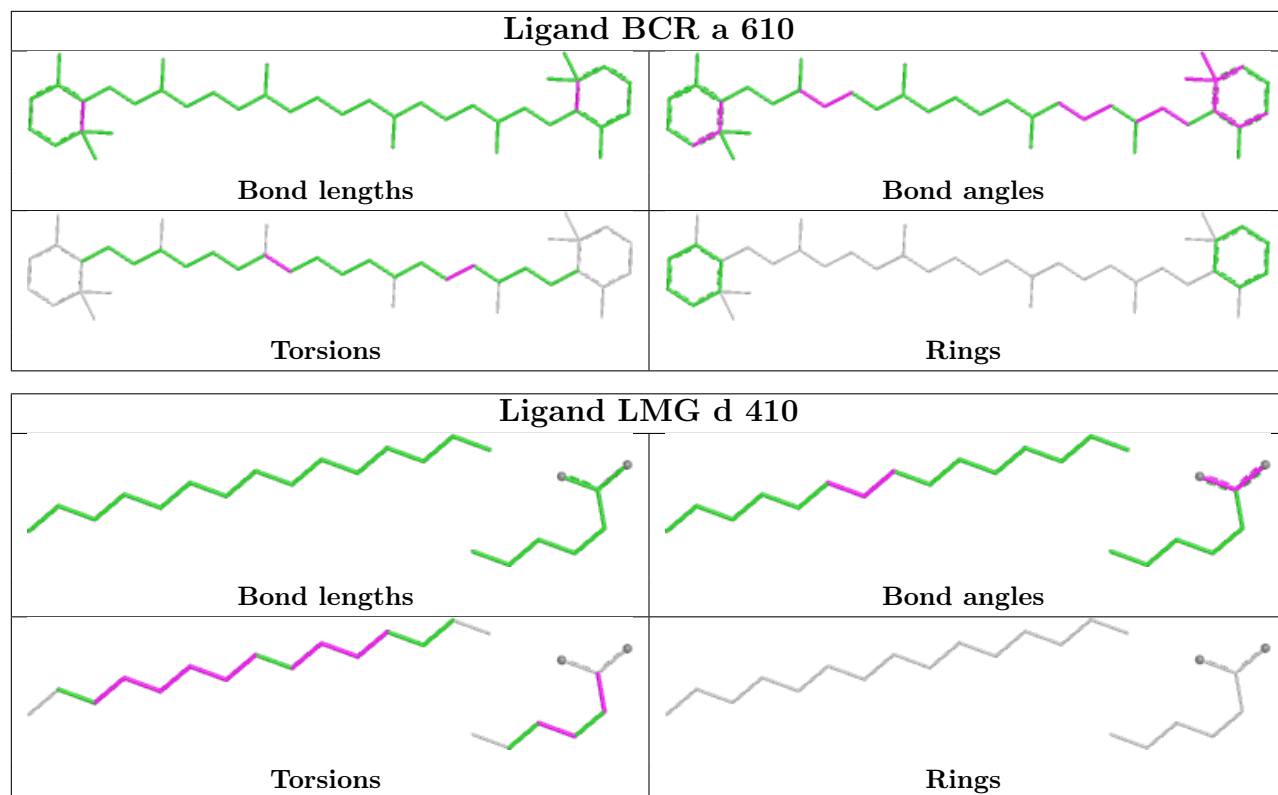


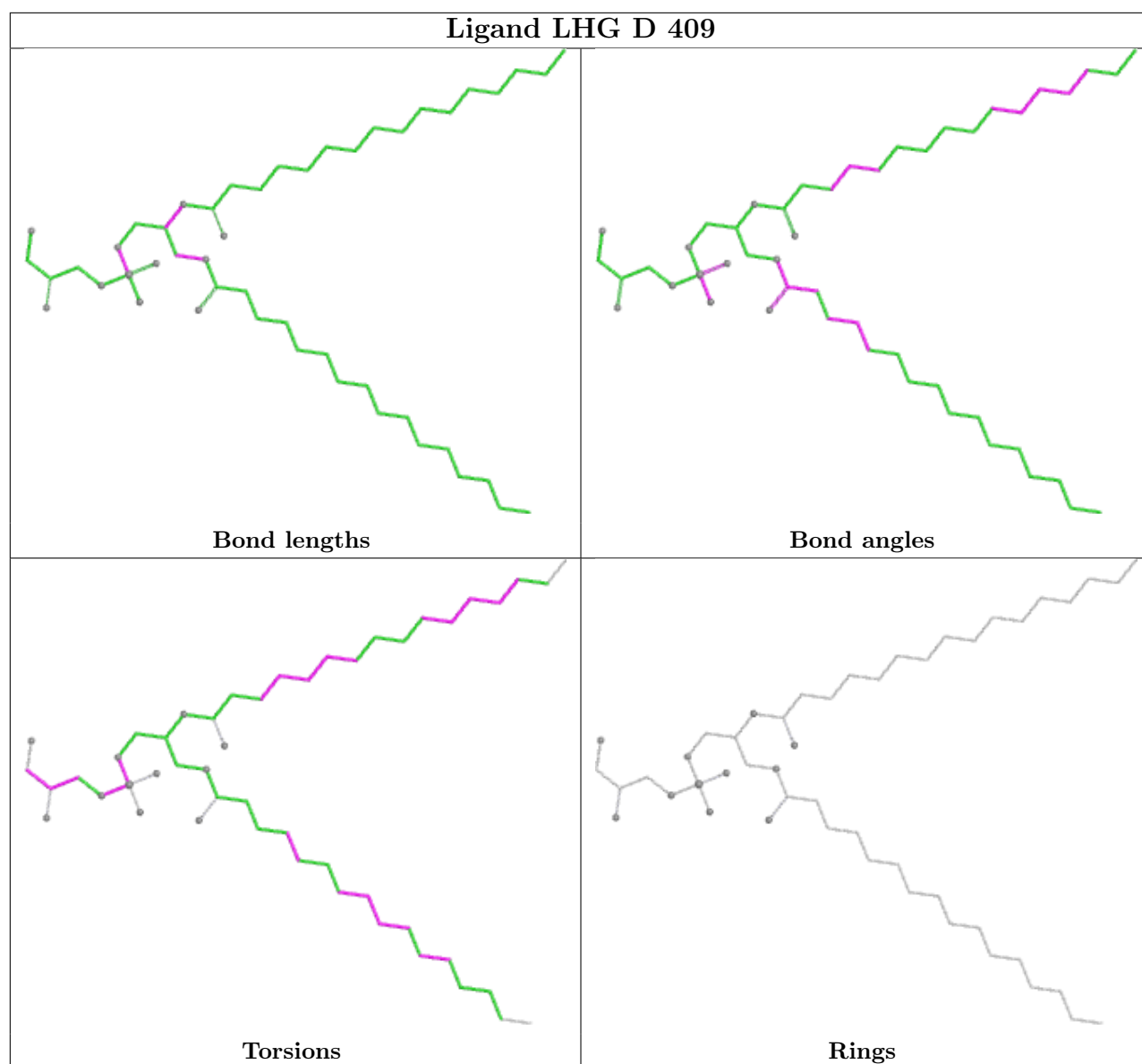
Ligand LMG C 518

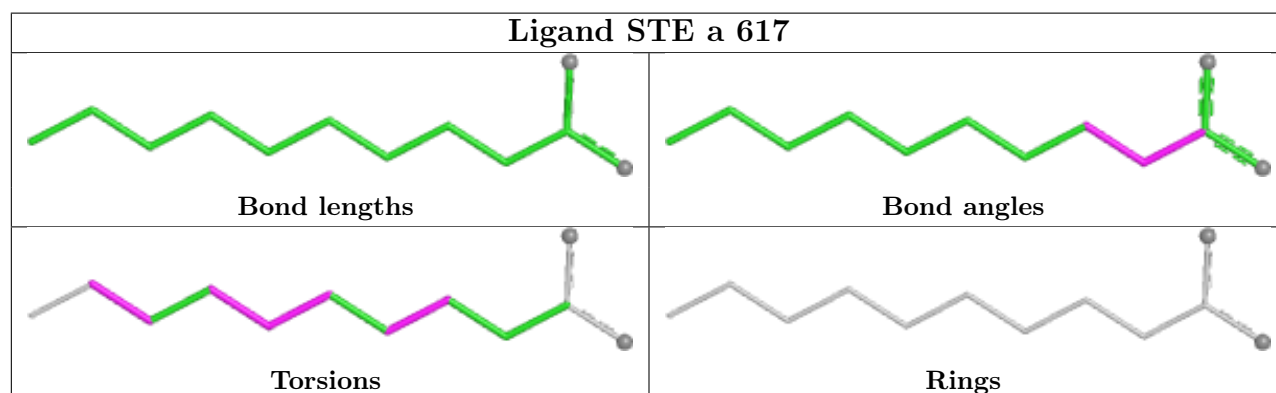
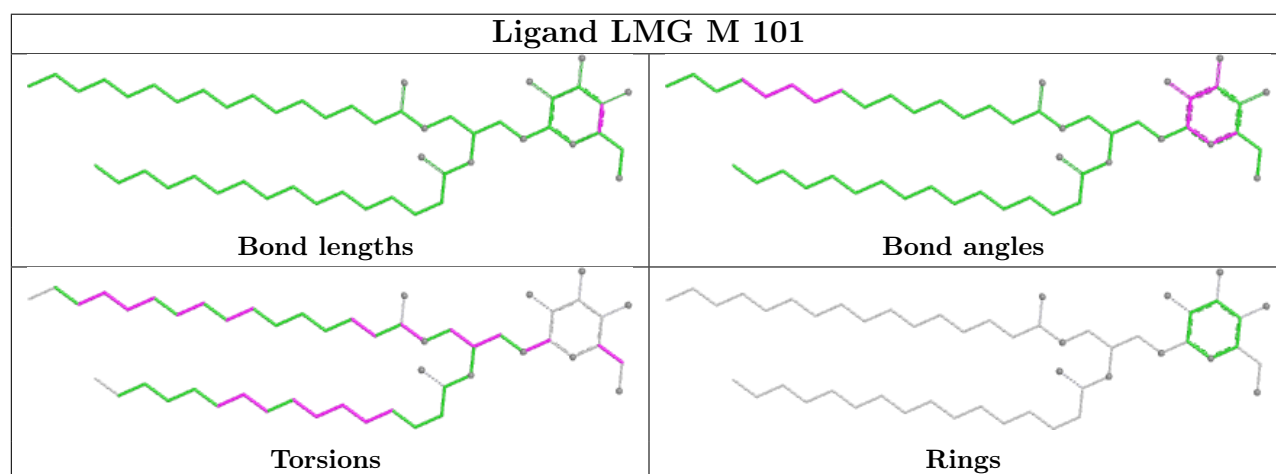
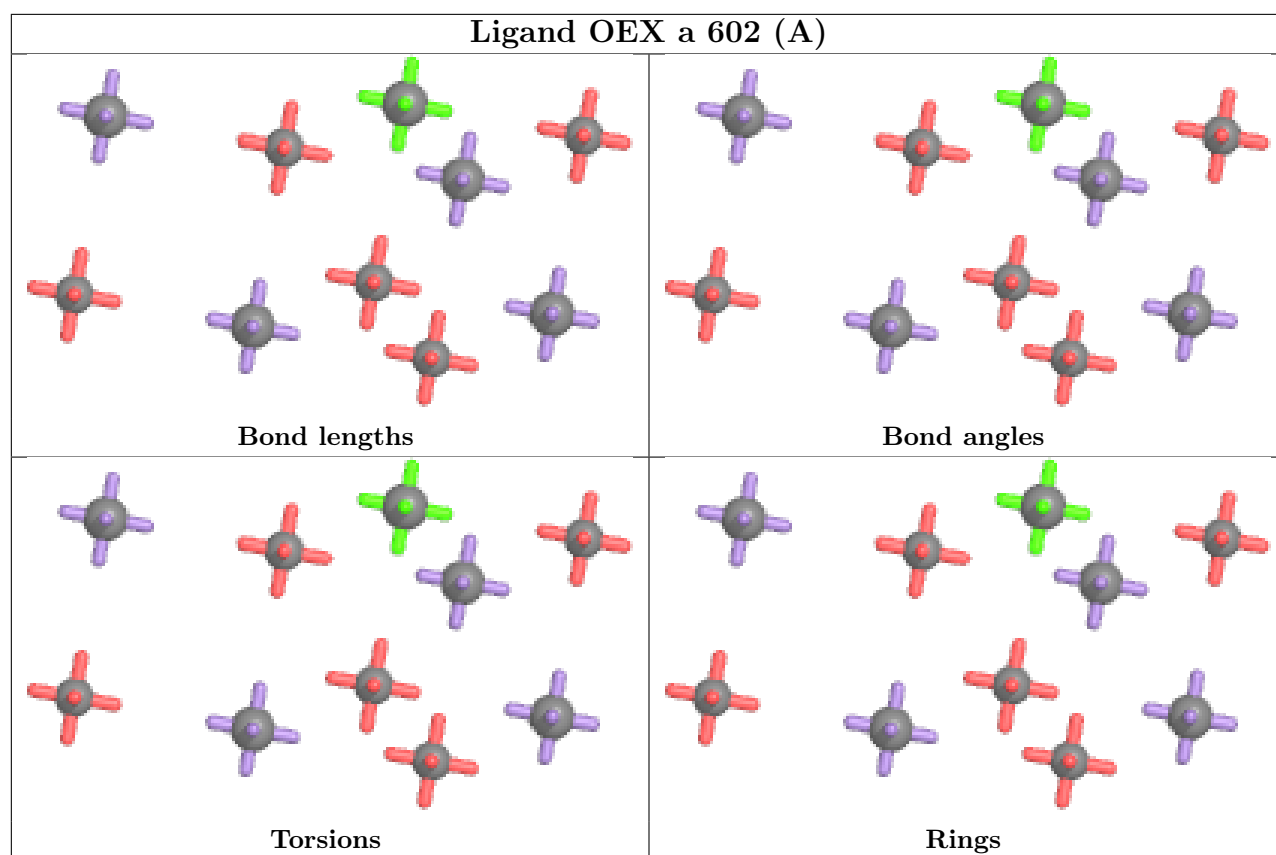


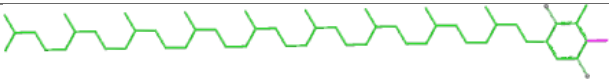
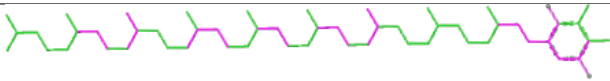
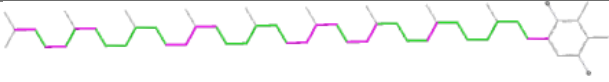
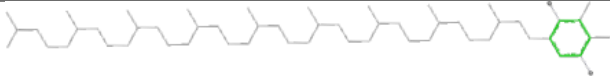
Ligand CLA B 601

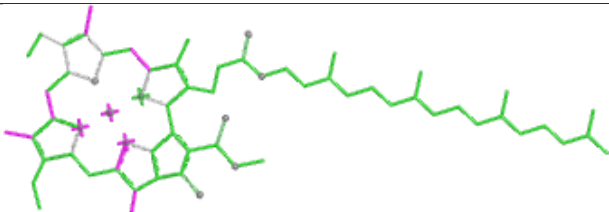
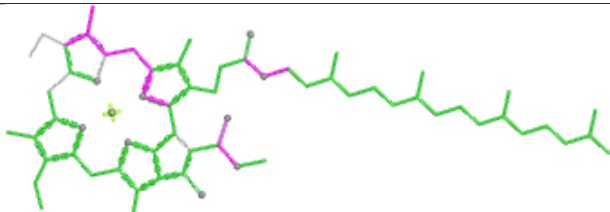
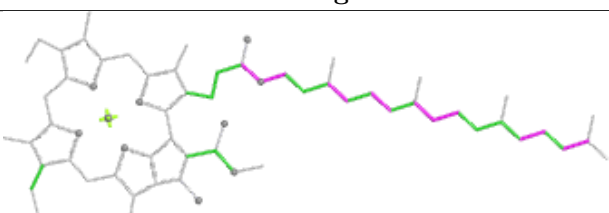
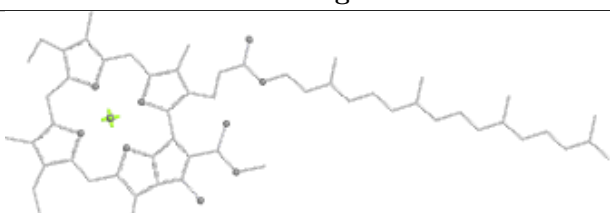


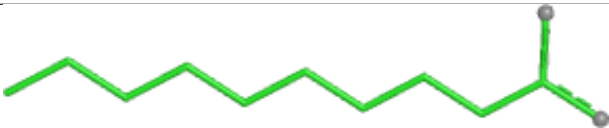
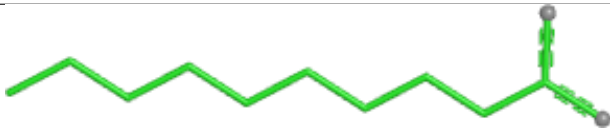
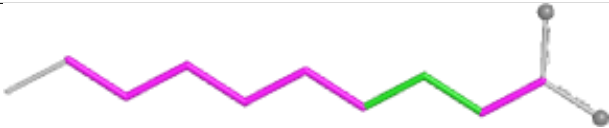
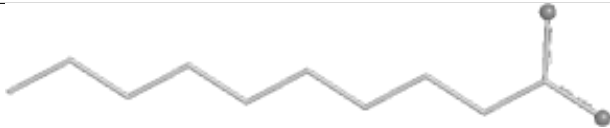


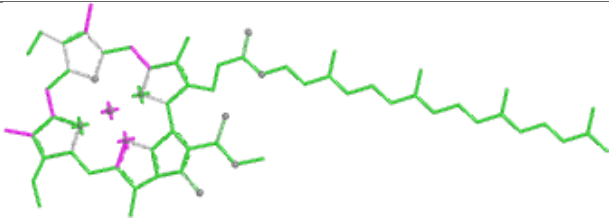
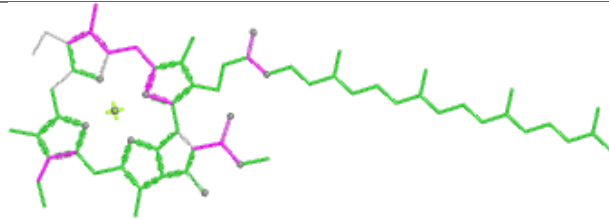
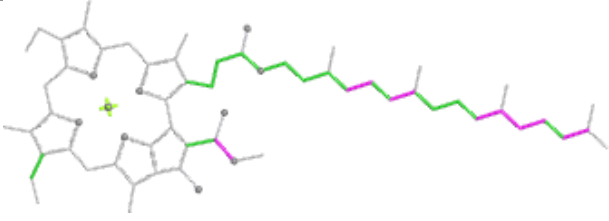
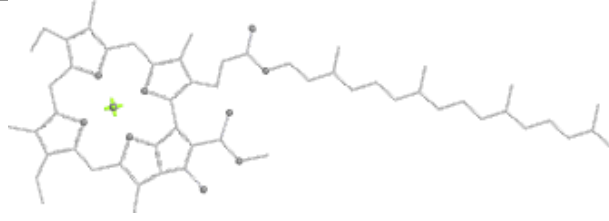


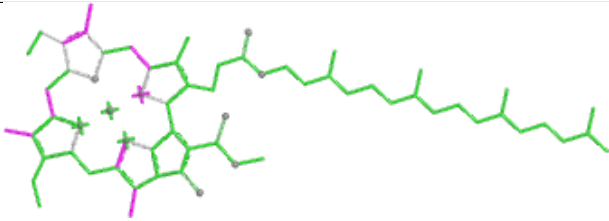
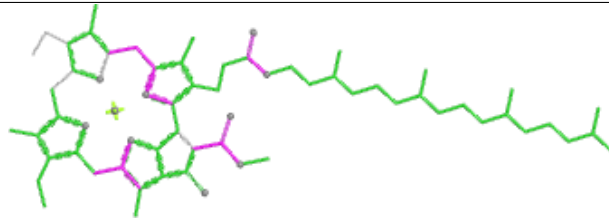
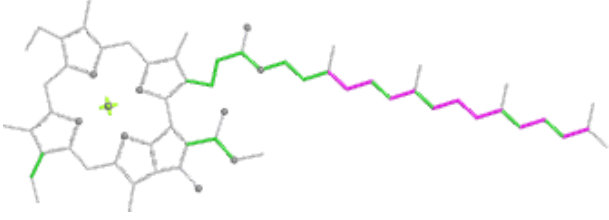
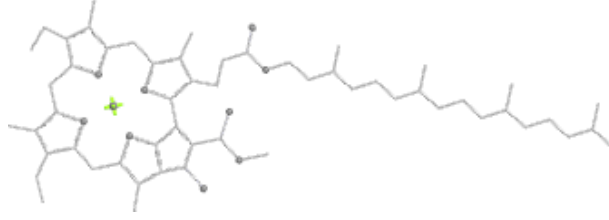


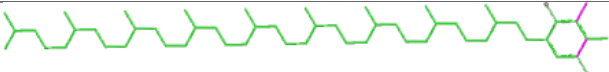
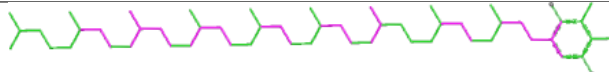
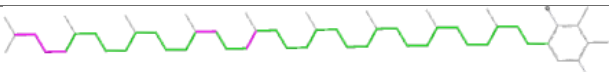
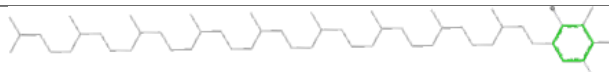
Ligand PL9 a 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

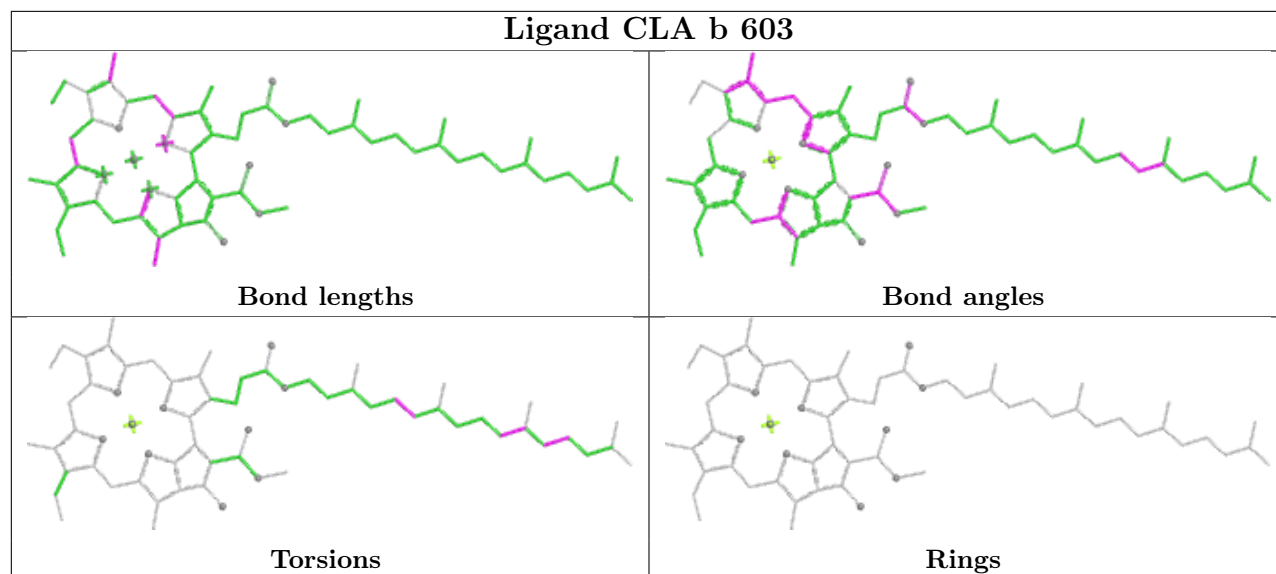
Ligand STE B 623	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

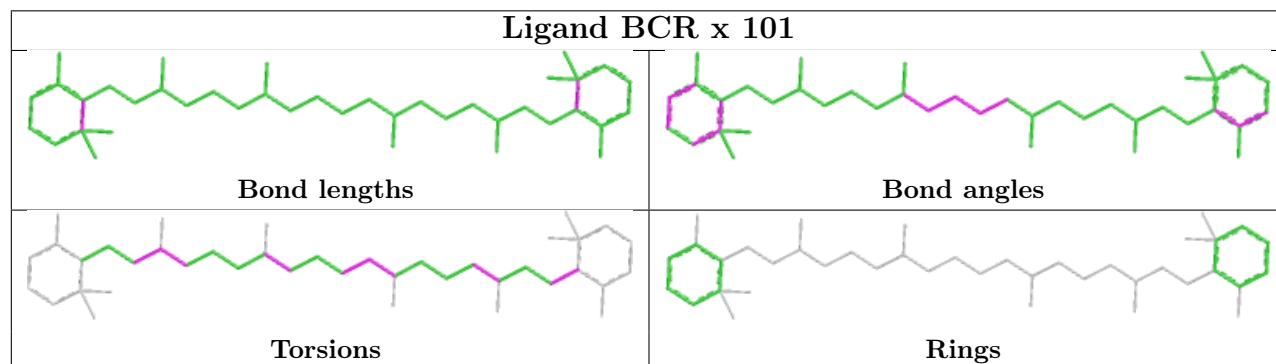
Ligand CLA B 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

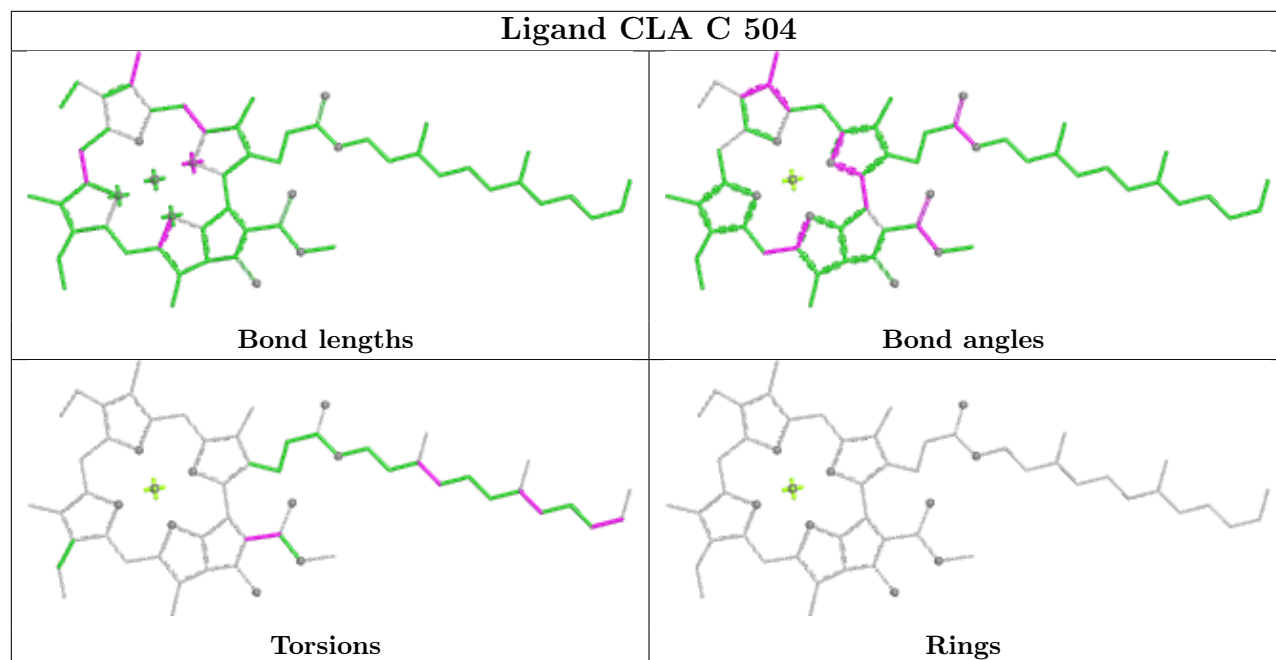
Ligand CLA b 603

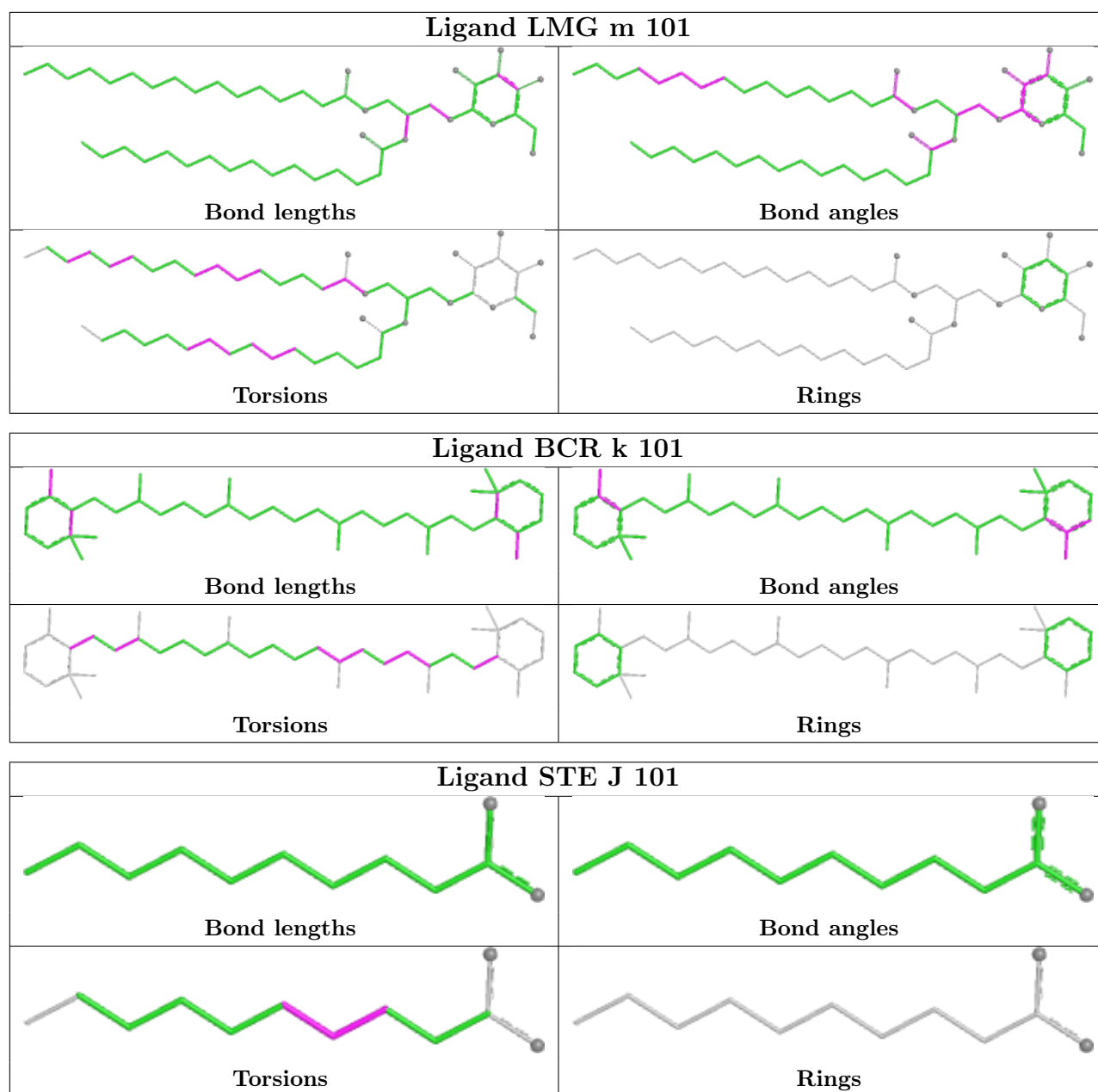


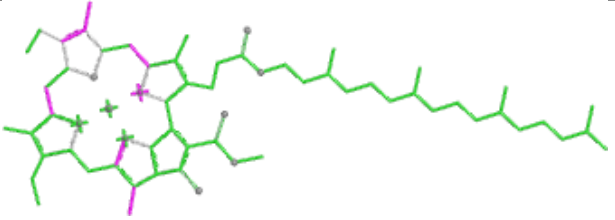
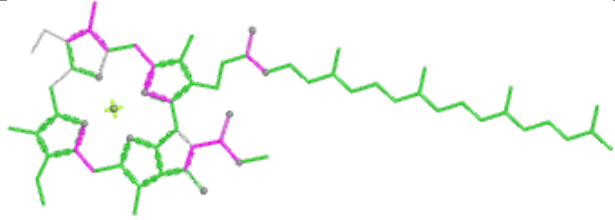
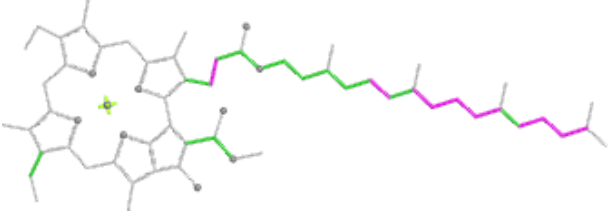
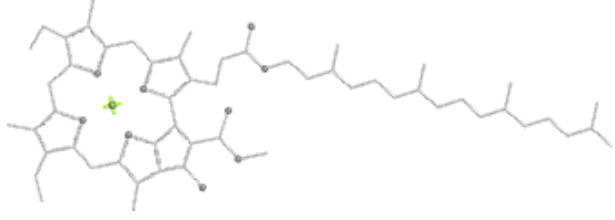
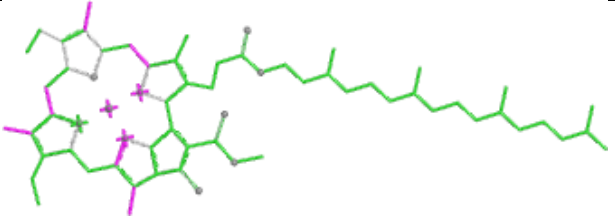
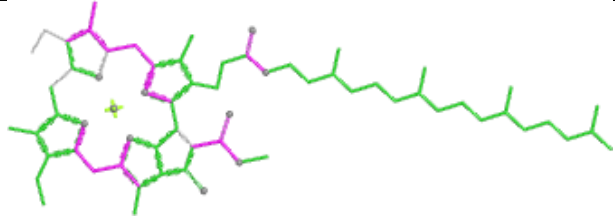
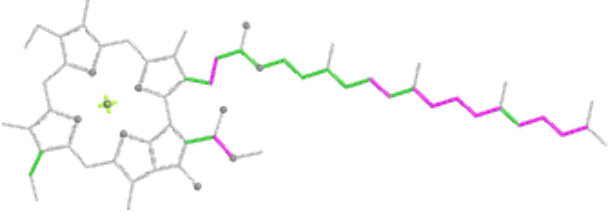
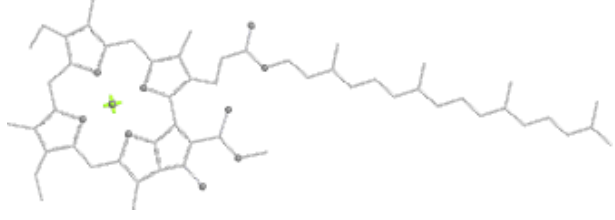




Ligand BCR x 101

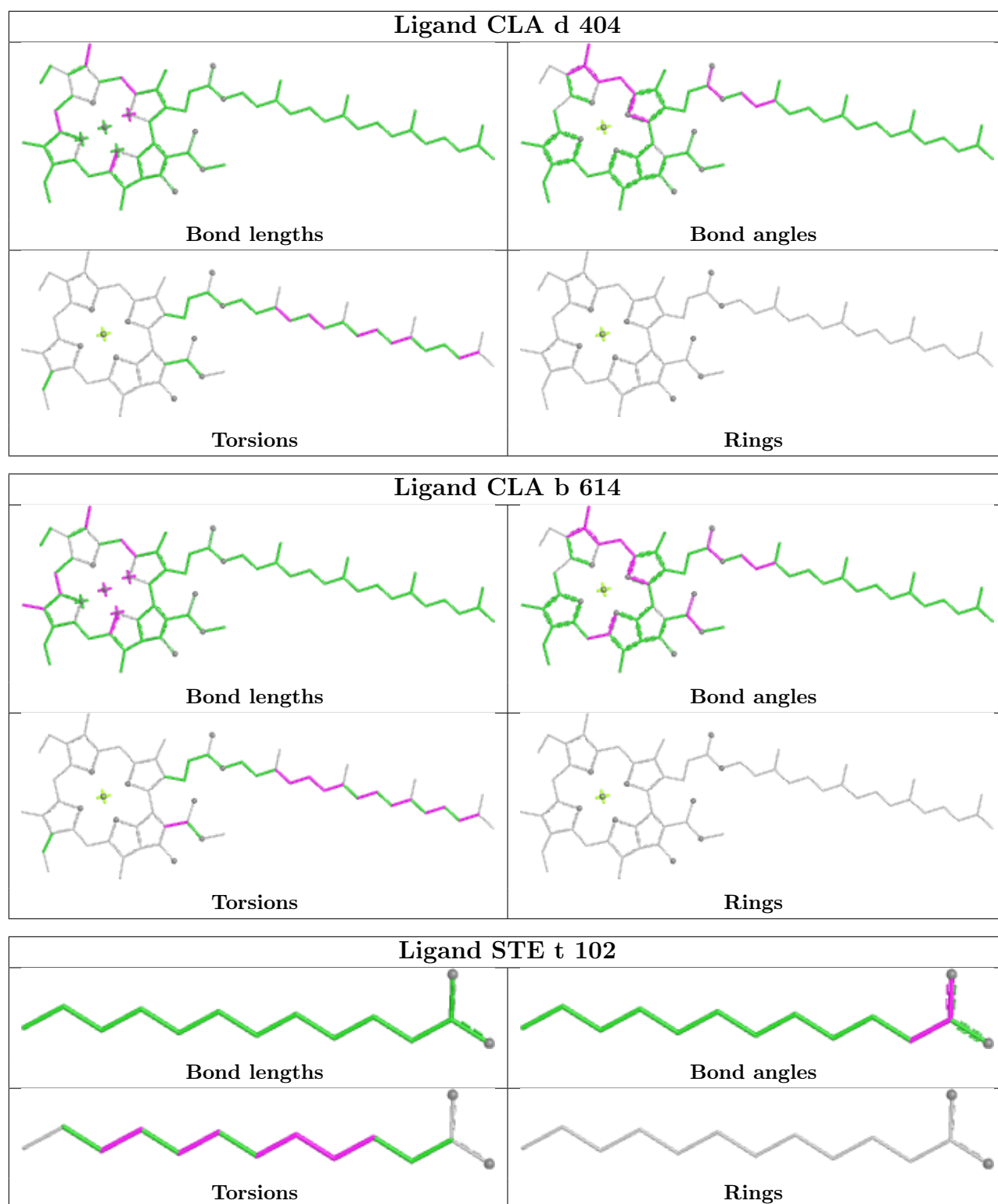


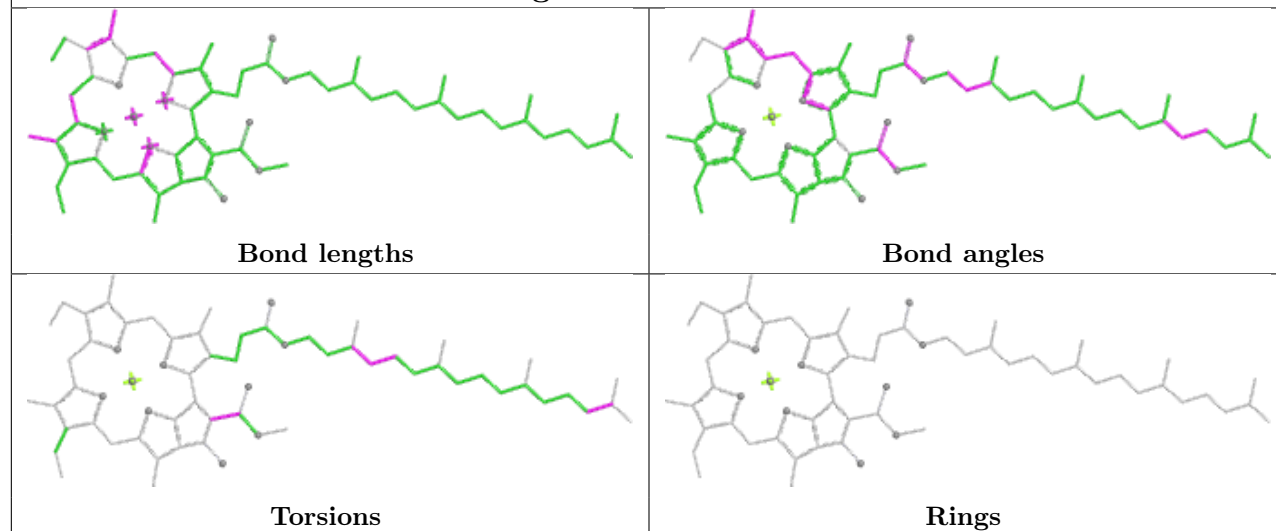
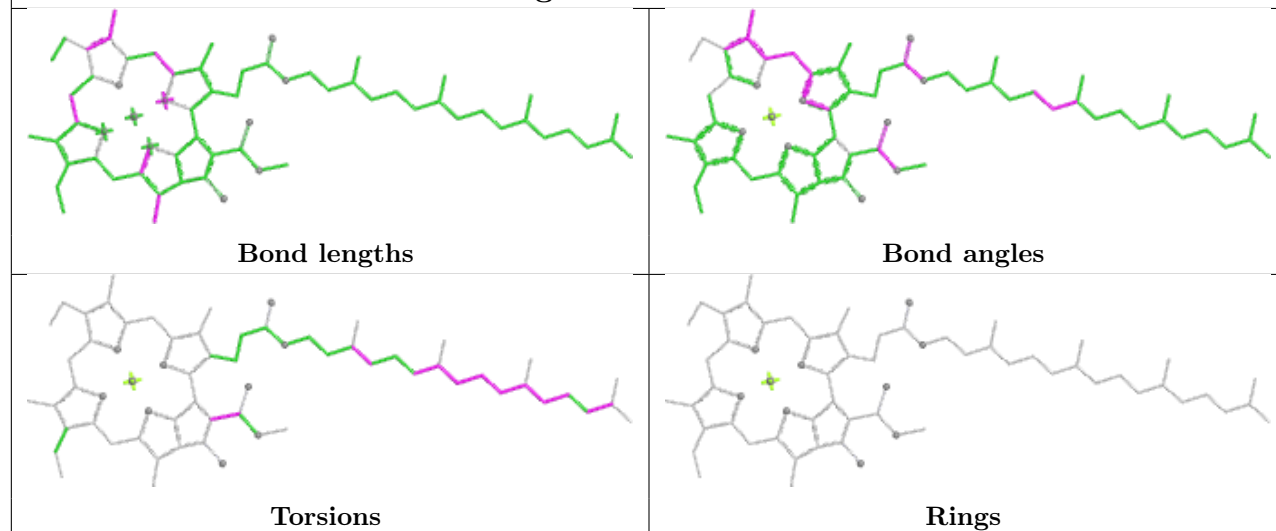
Ligand CLA C 504

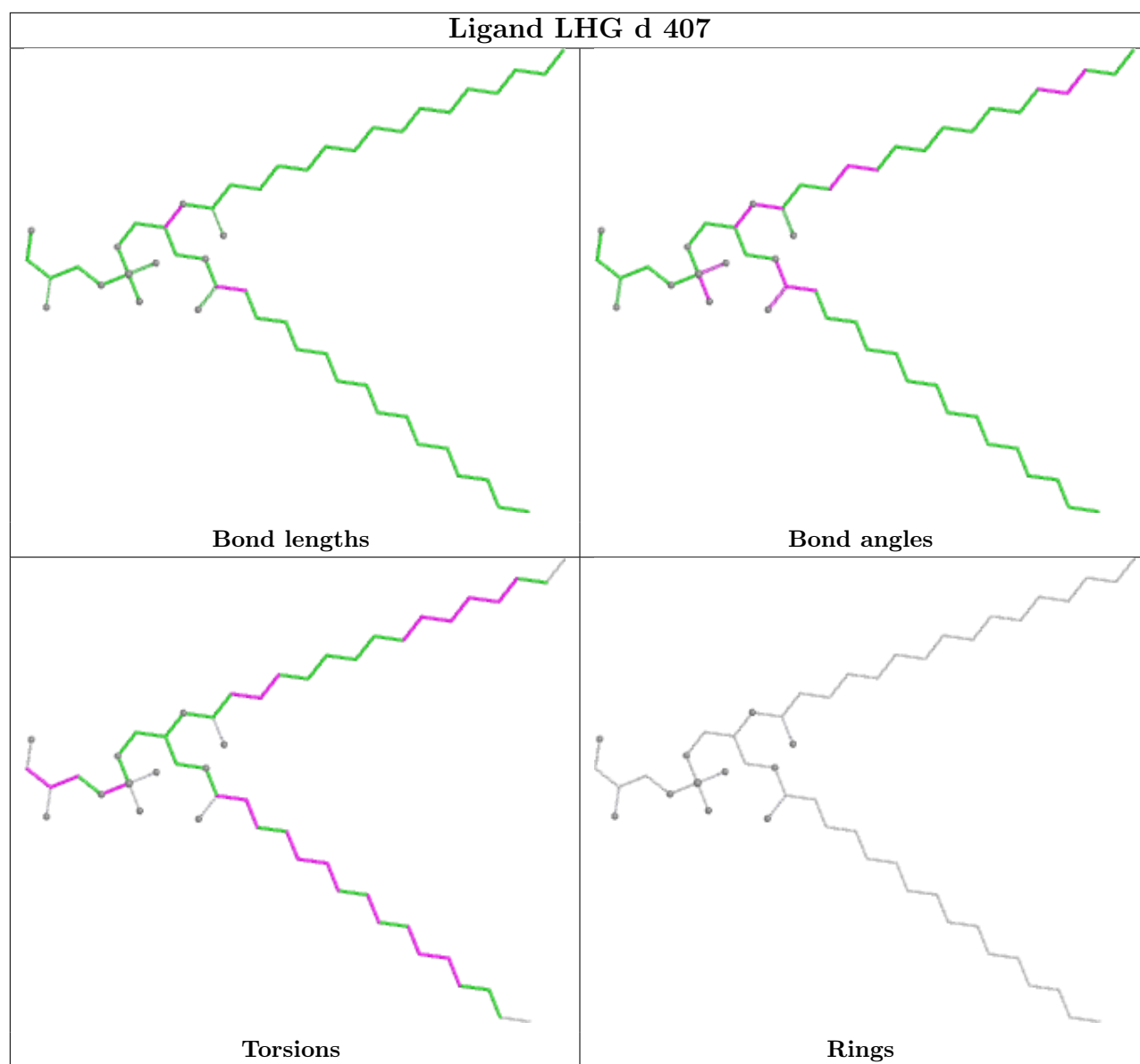


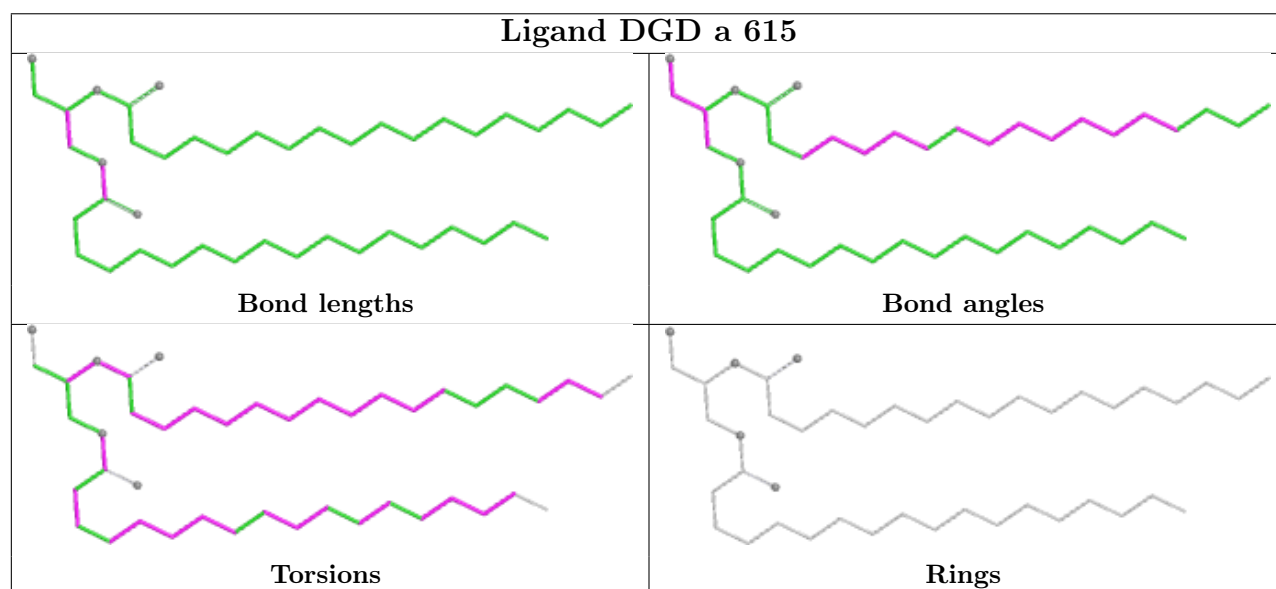
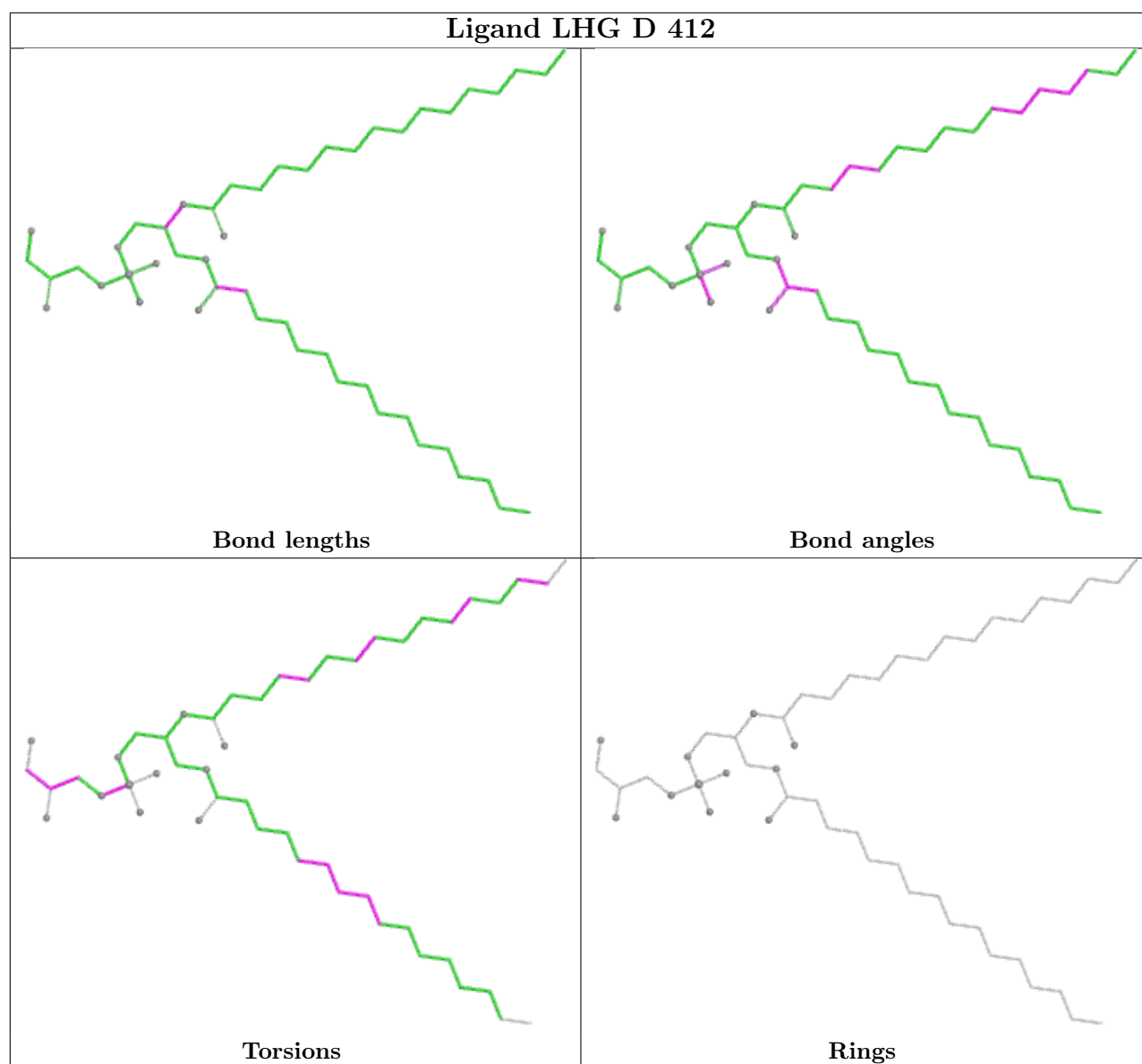


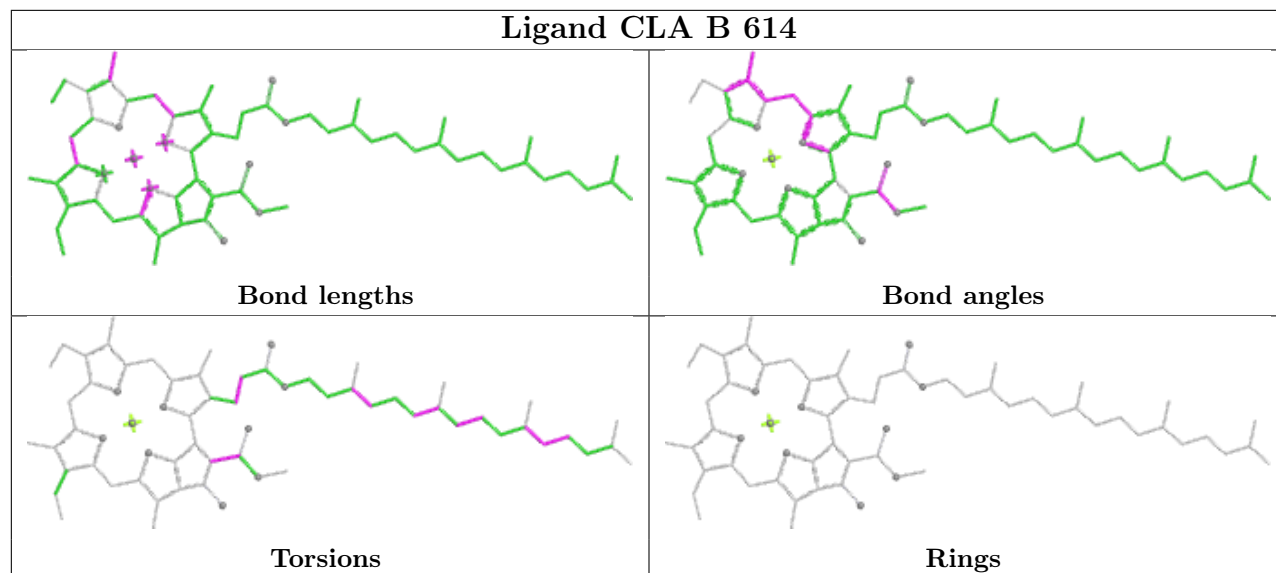
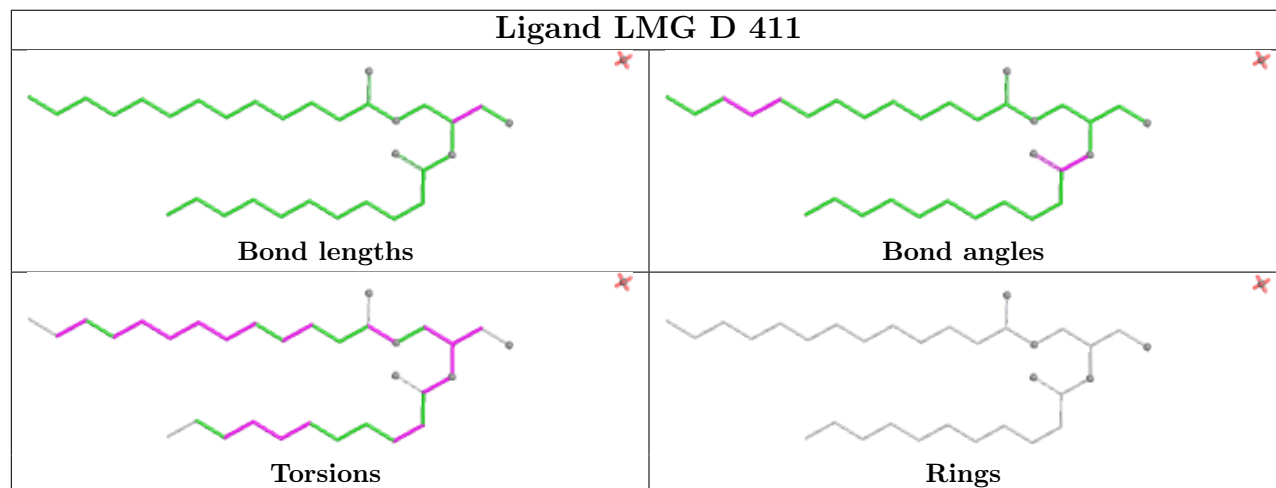
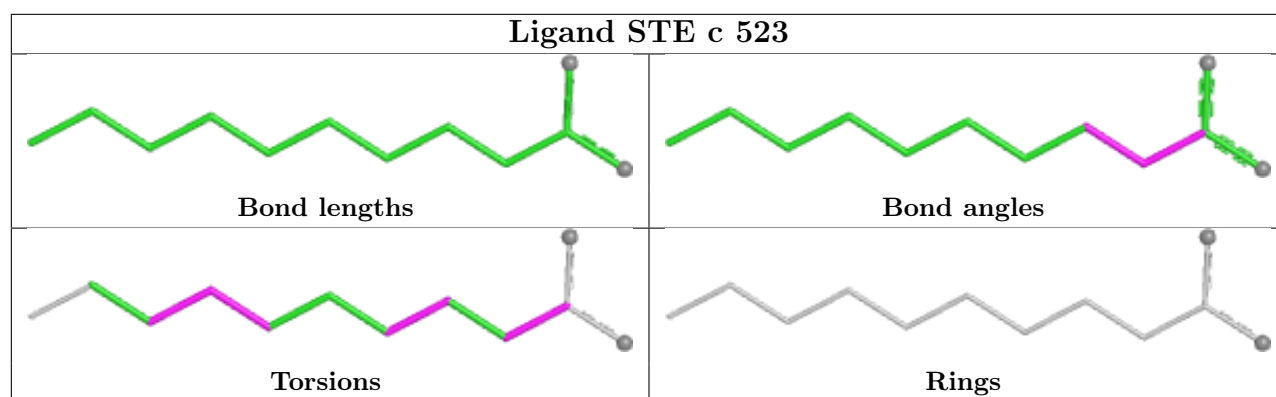
Ligand CLA B 606			
			
Bond lengths			
		Bond angles	
			
Torsions			
		Rings	
Ligand CLA B 603			
			
Bond lengths			
		Bond angles	
			
Torsions			
		Rings	
Ligand STE I 101			
			
Bond lengths			
		Bond angles	
			
Torsions			
		Rings	

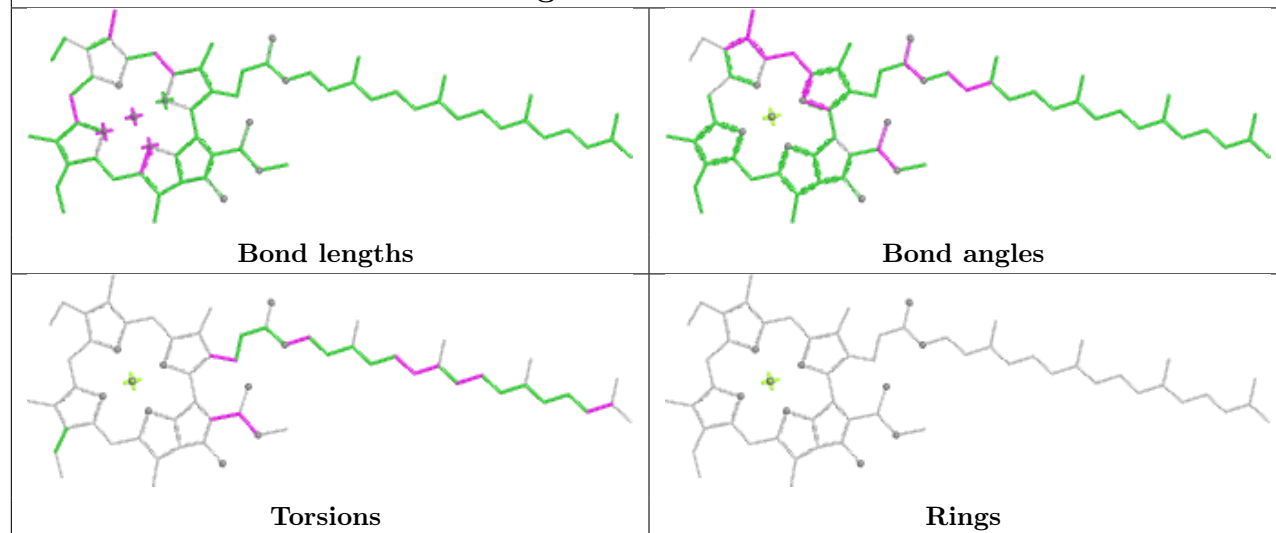
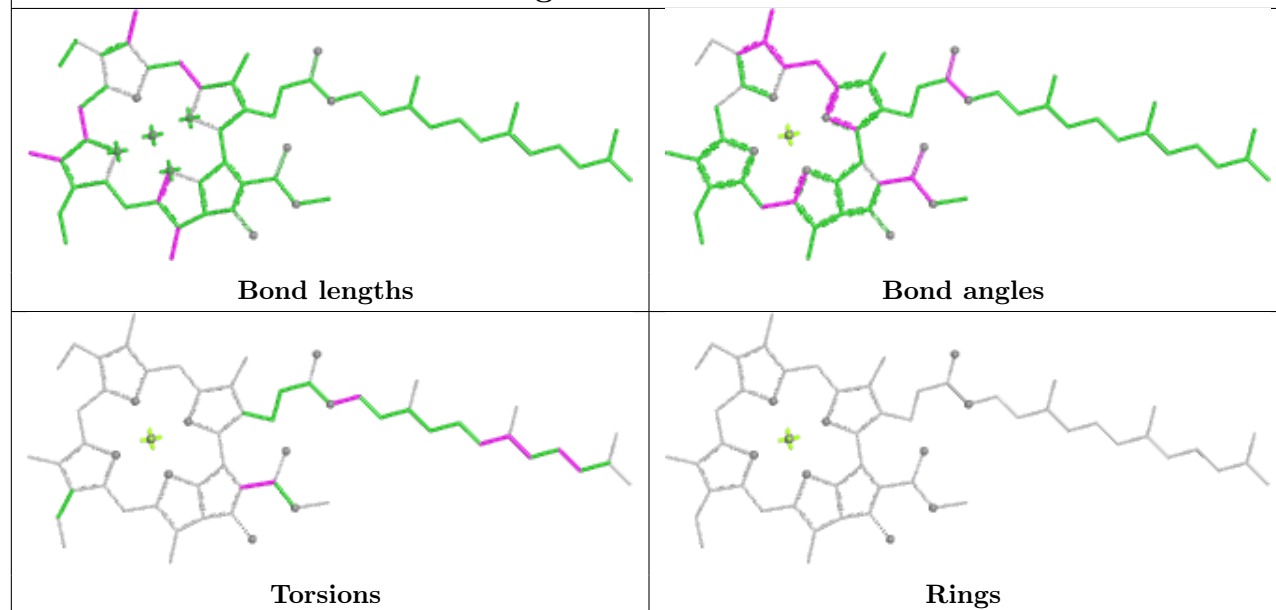


Ligand CLA C 502**Ligand CLA b 607**

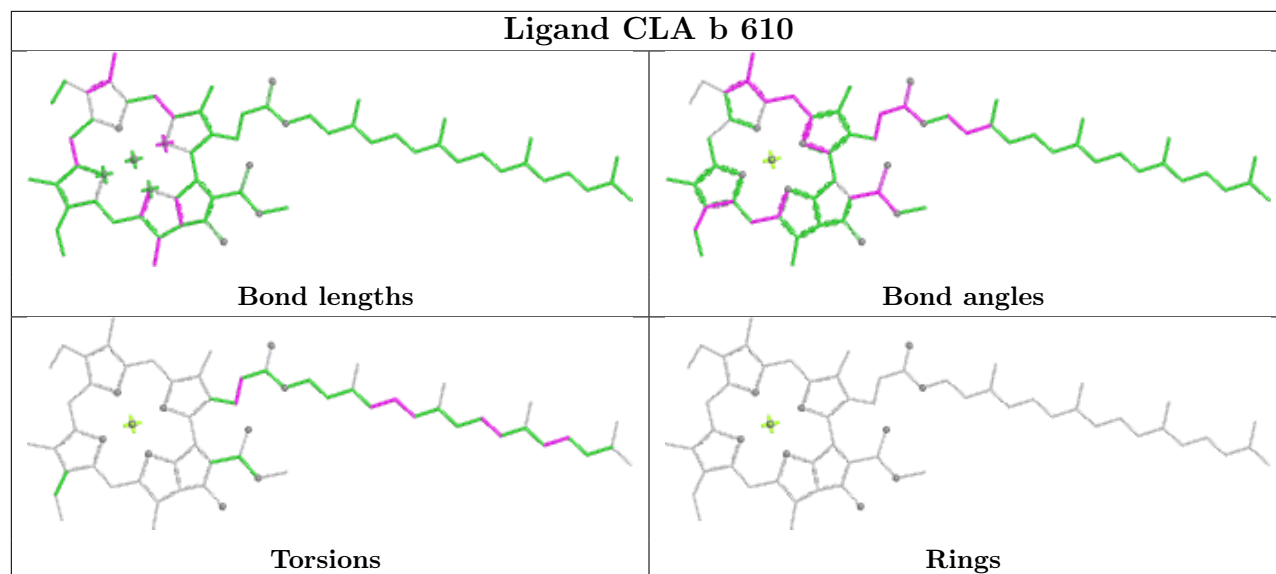




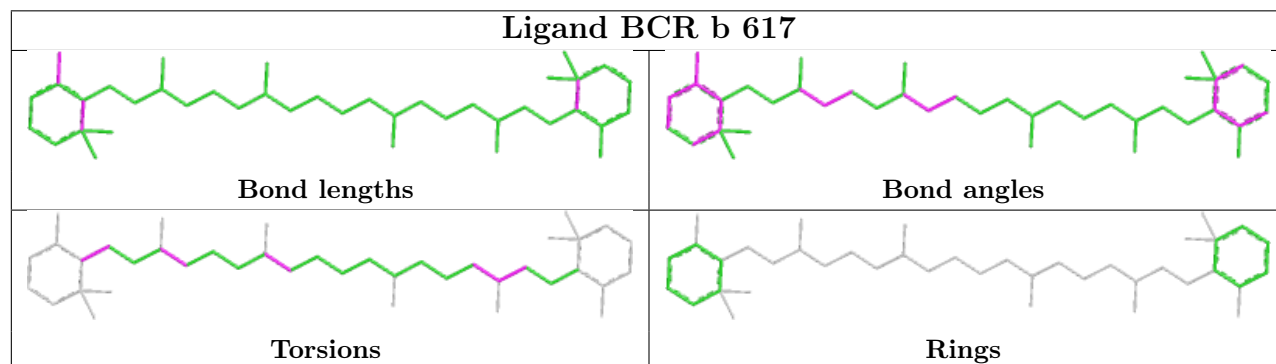


Ligand CLA c 513**Ligand CLA b 616**

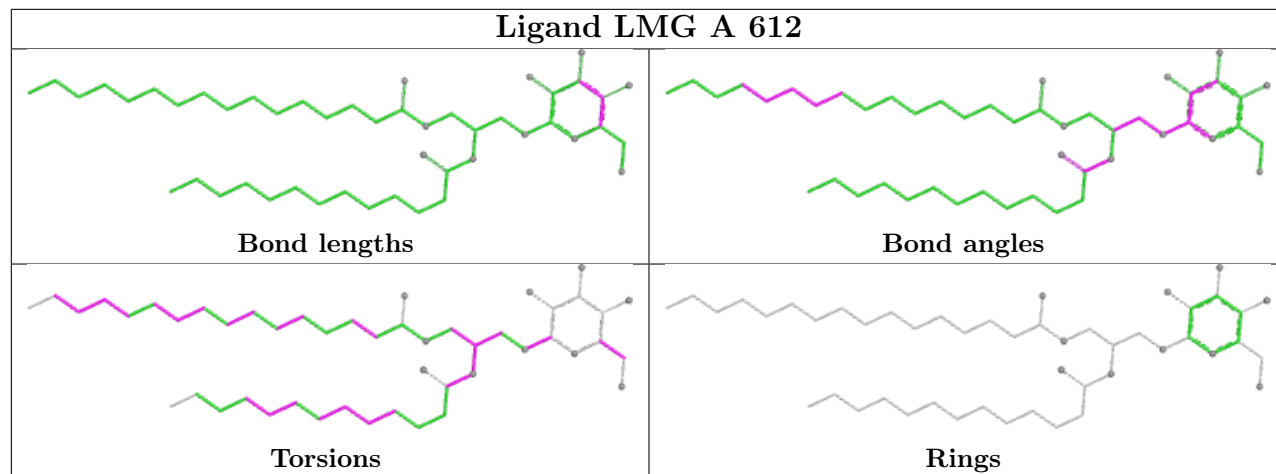
Ligand CLA b 610

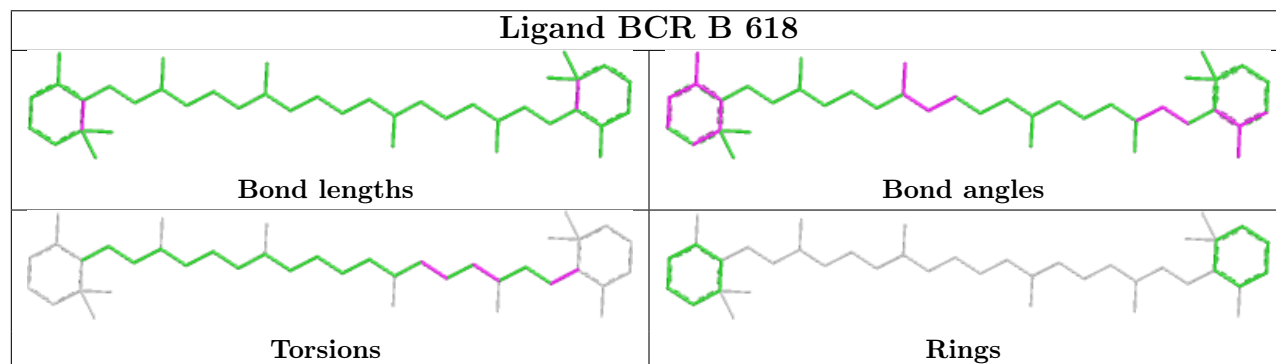
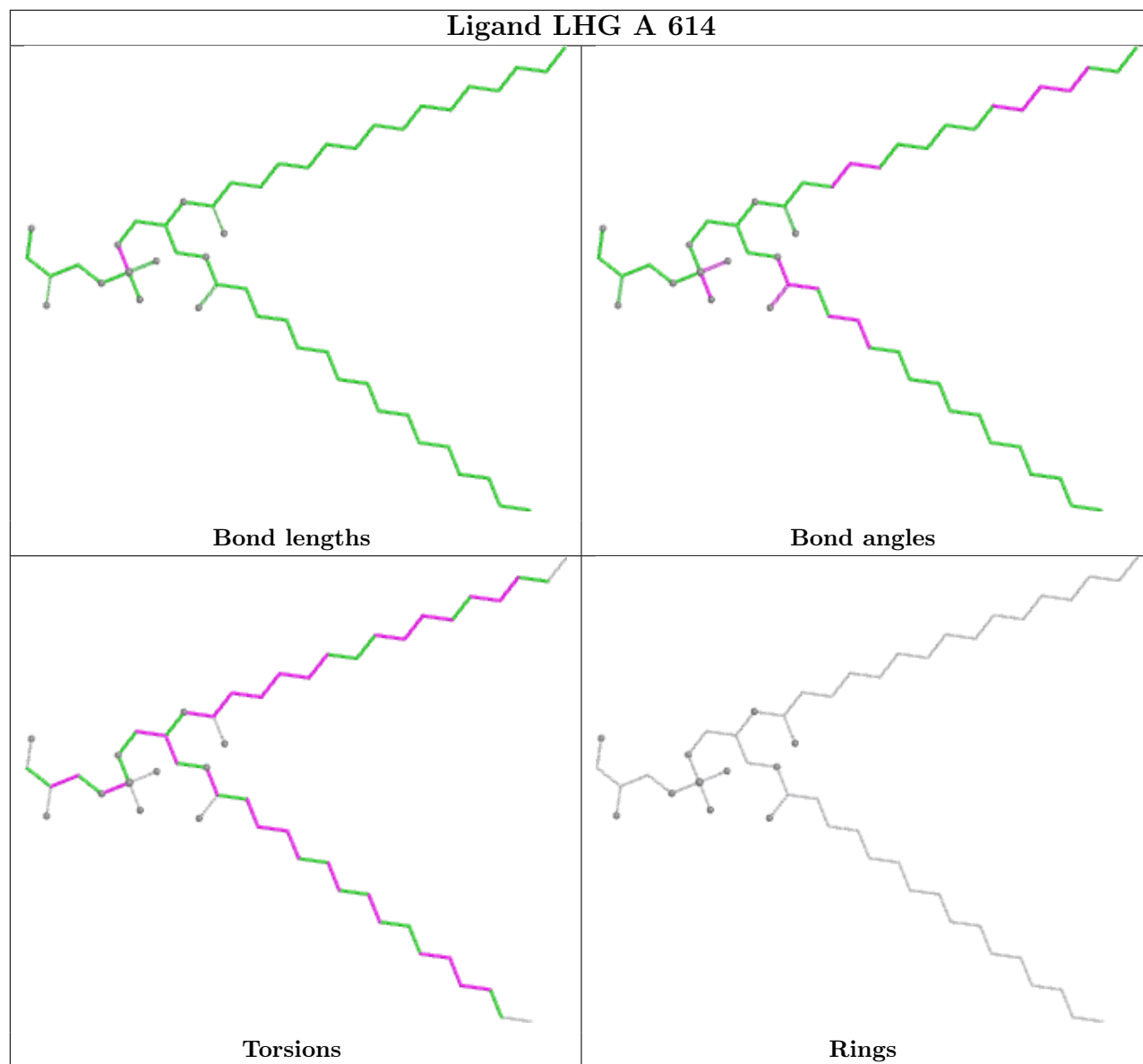


Ligand BCR b 617

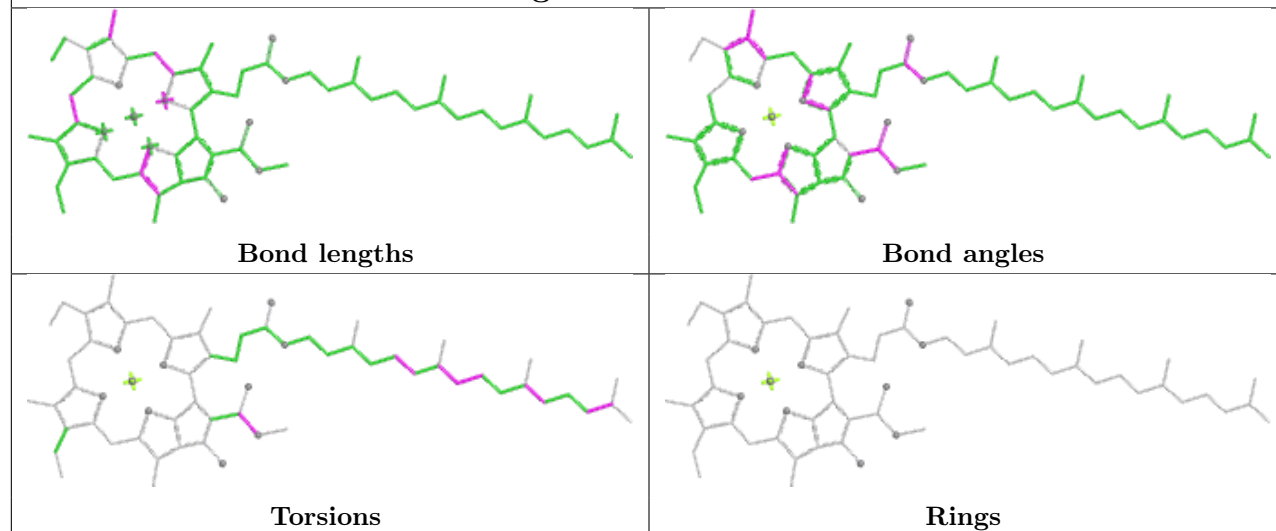


Ligand LMG A 612

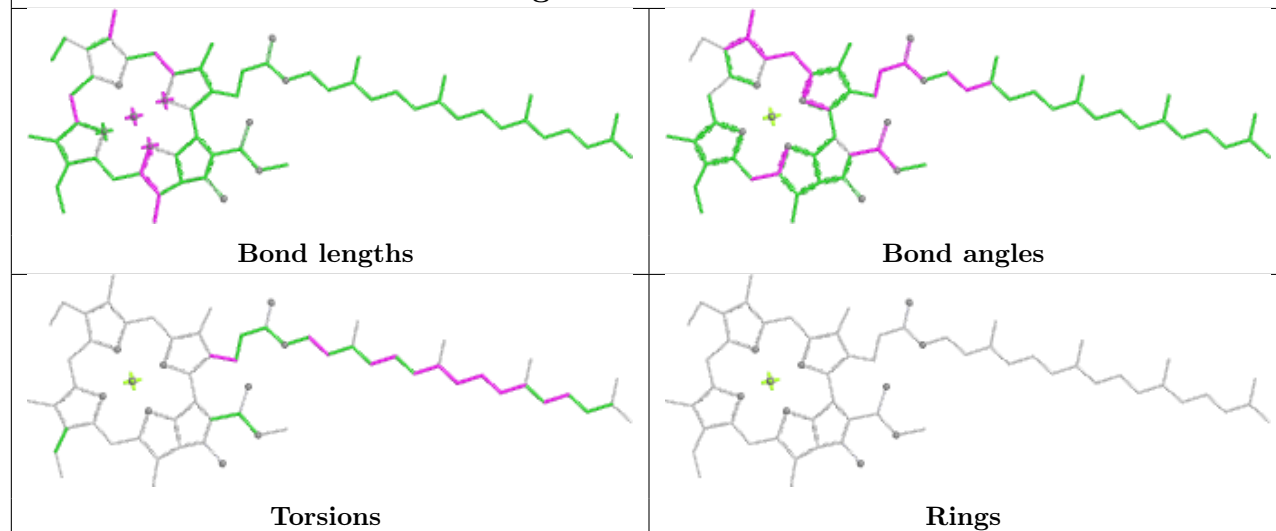




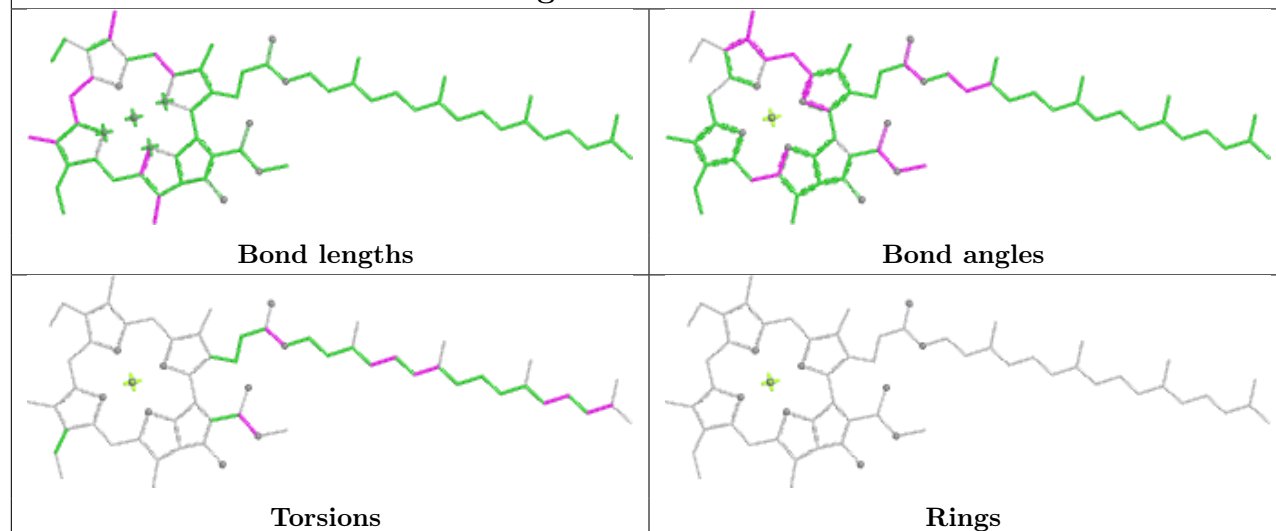
Ligand CLA C 508



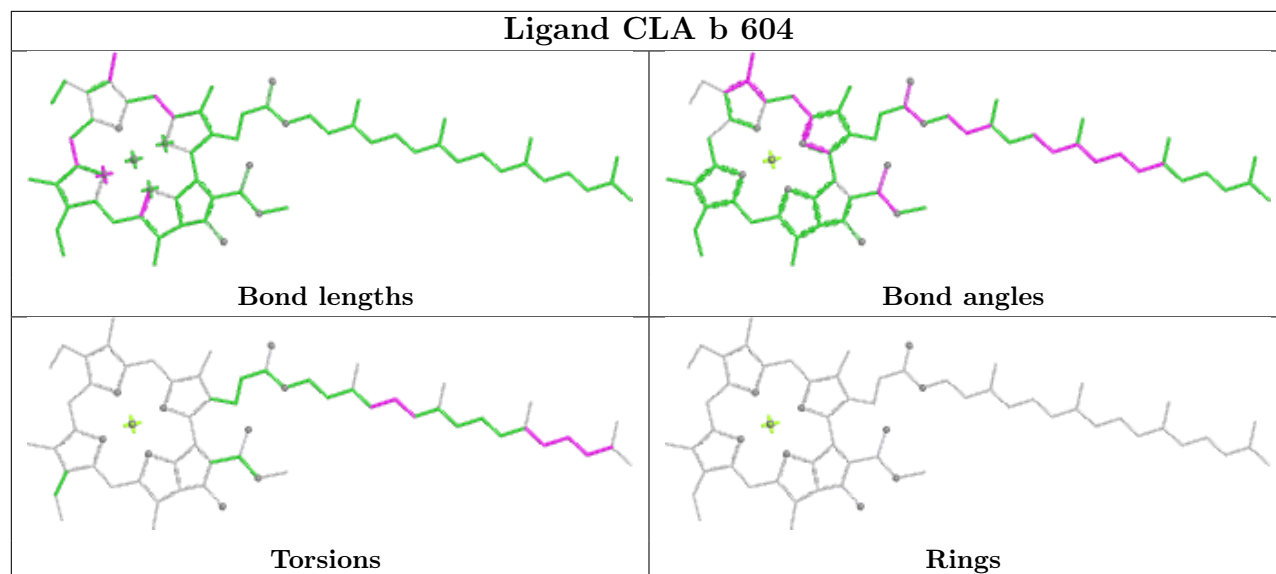
Ligand CLA C 512



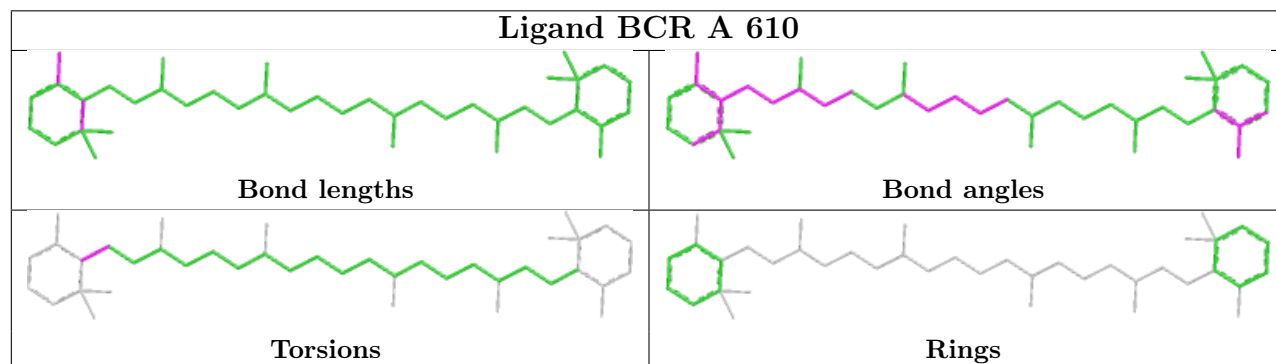
Ligand CLA c 502



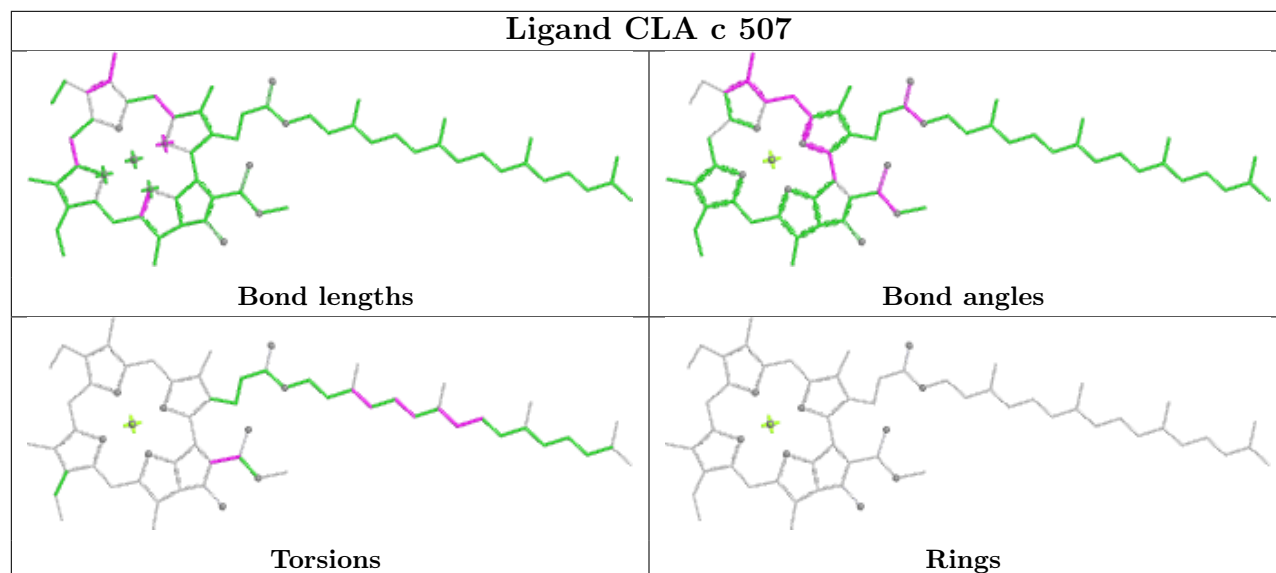
Ligand CLA b 604



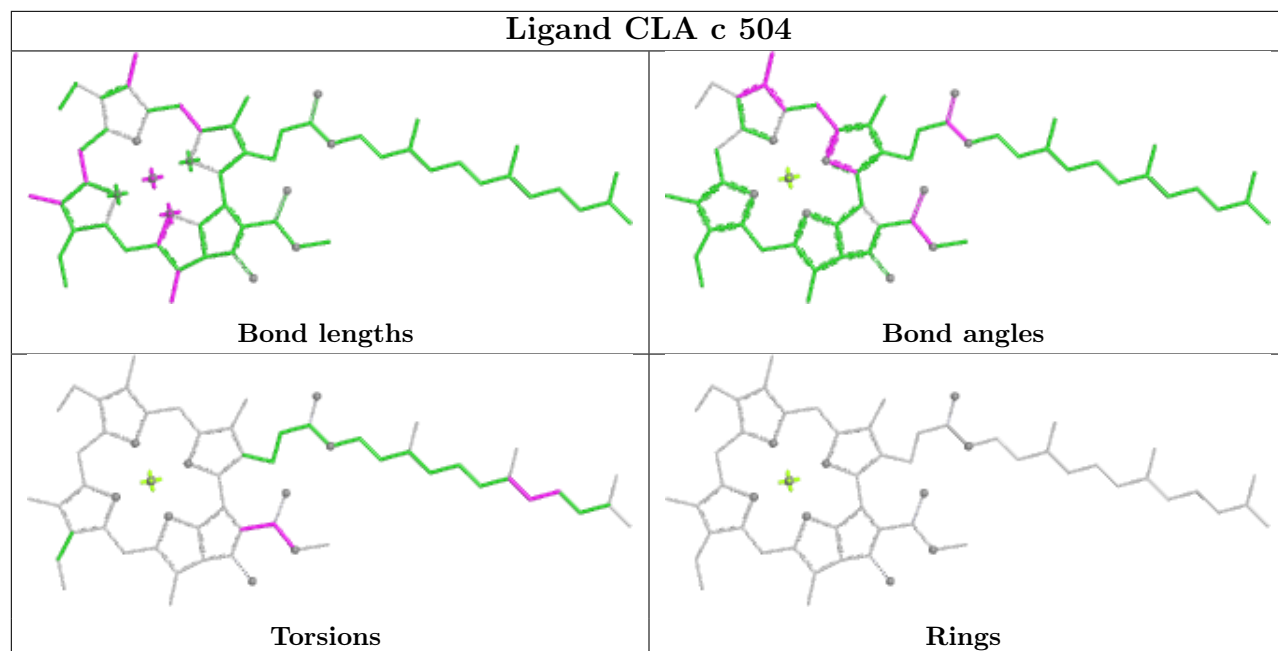
Ligand BCR A 610



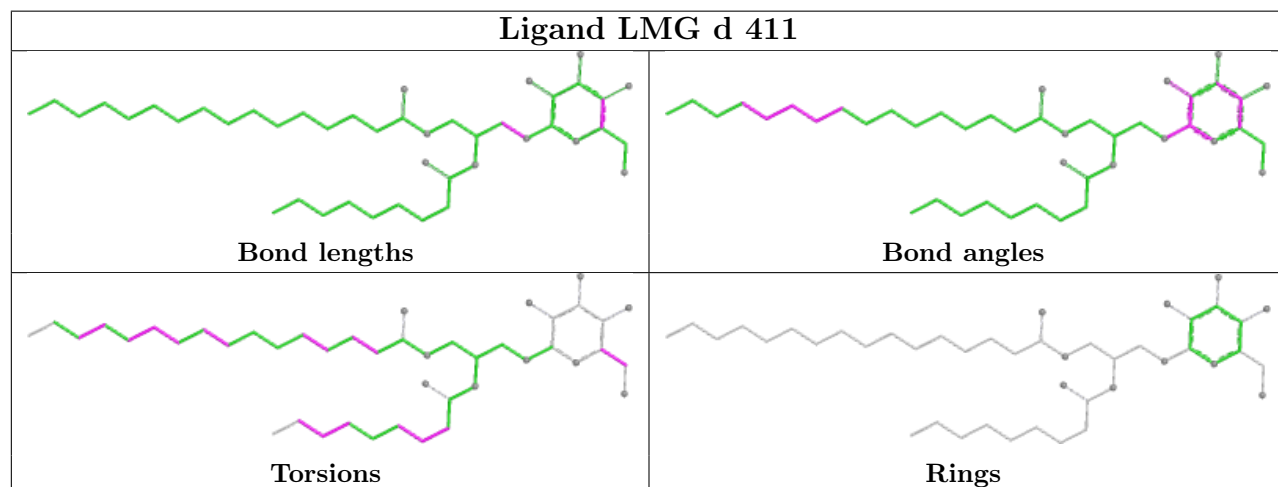
Ligand CLA c 507

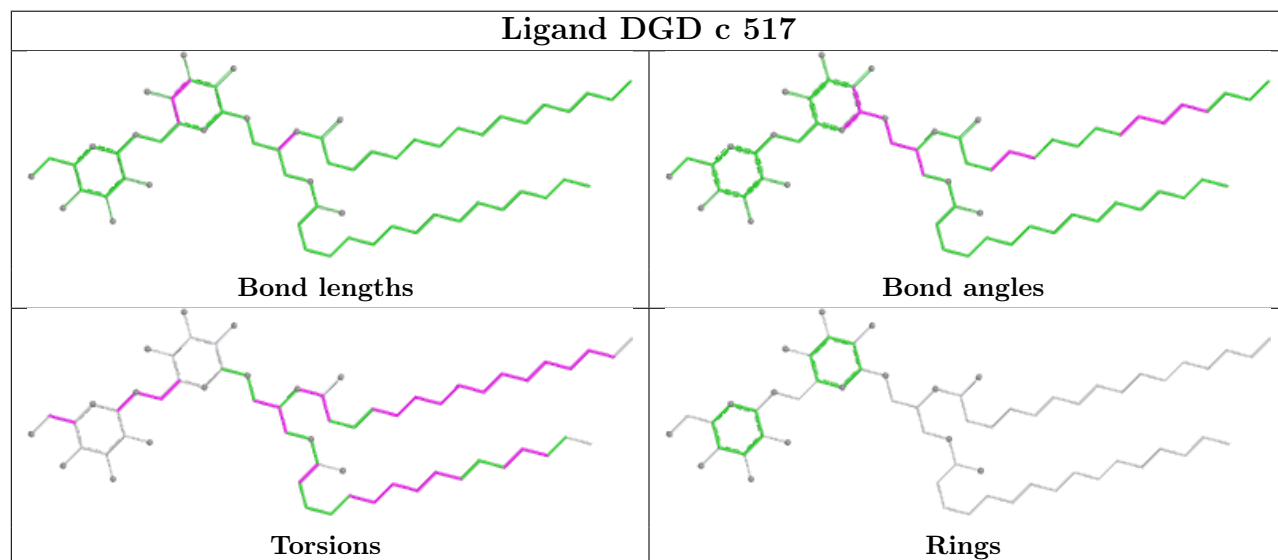
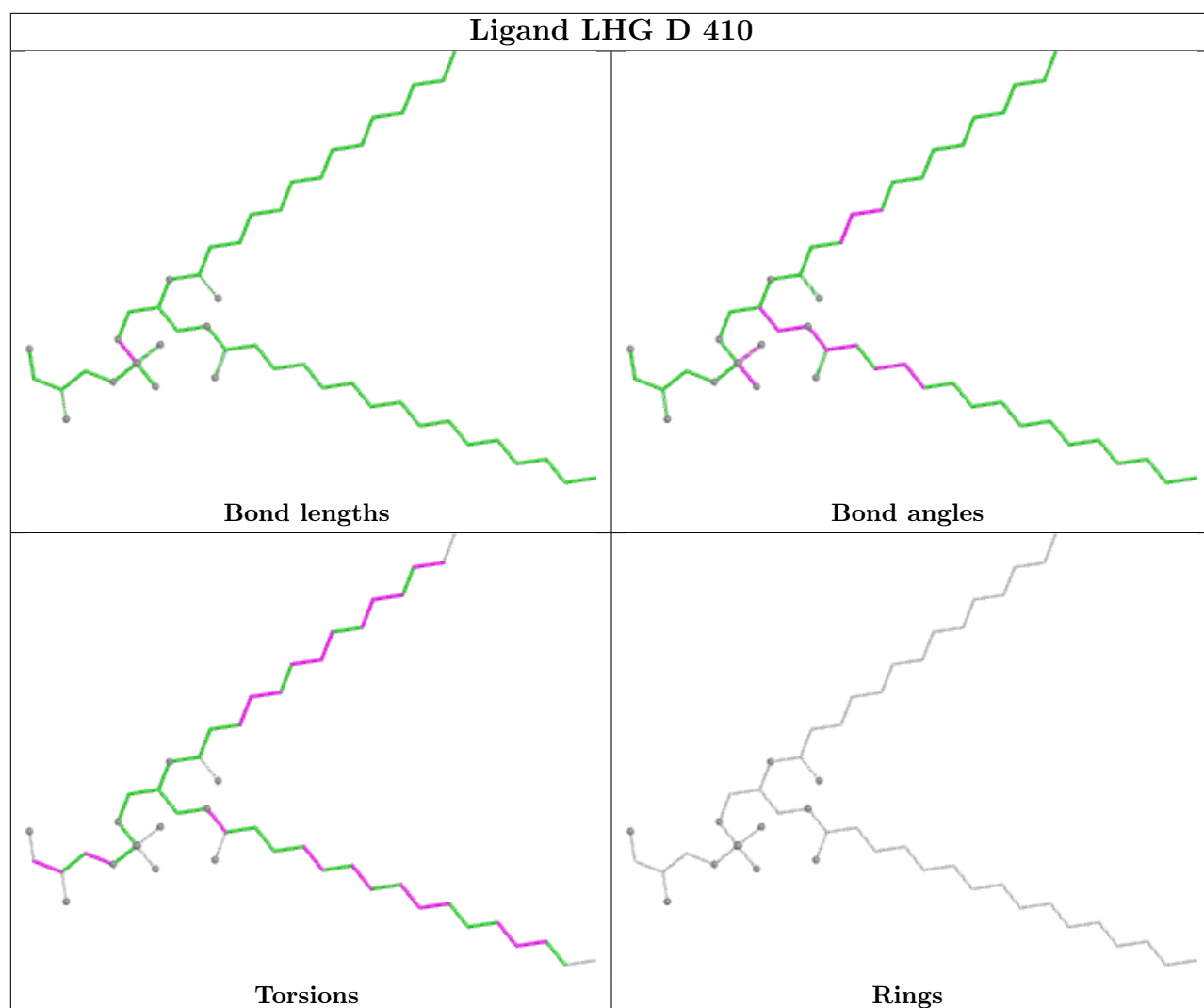


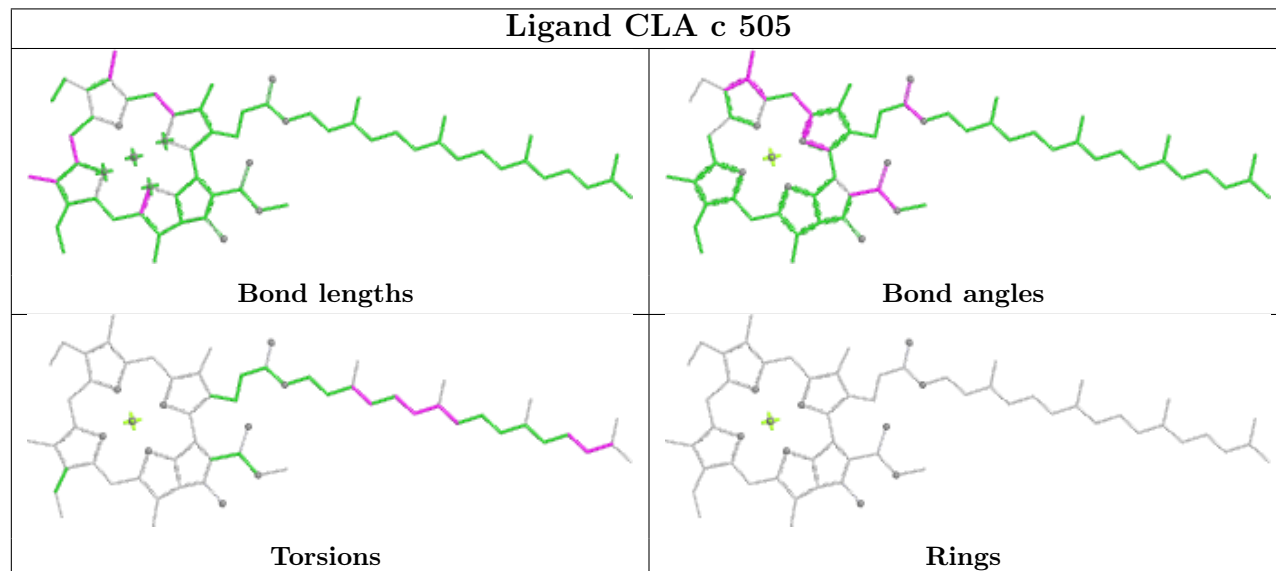
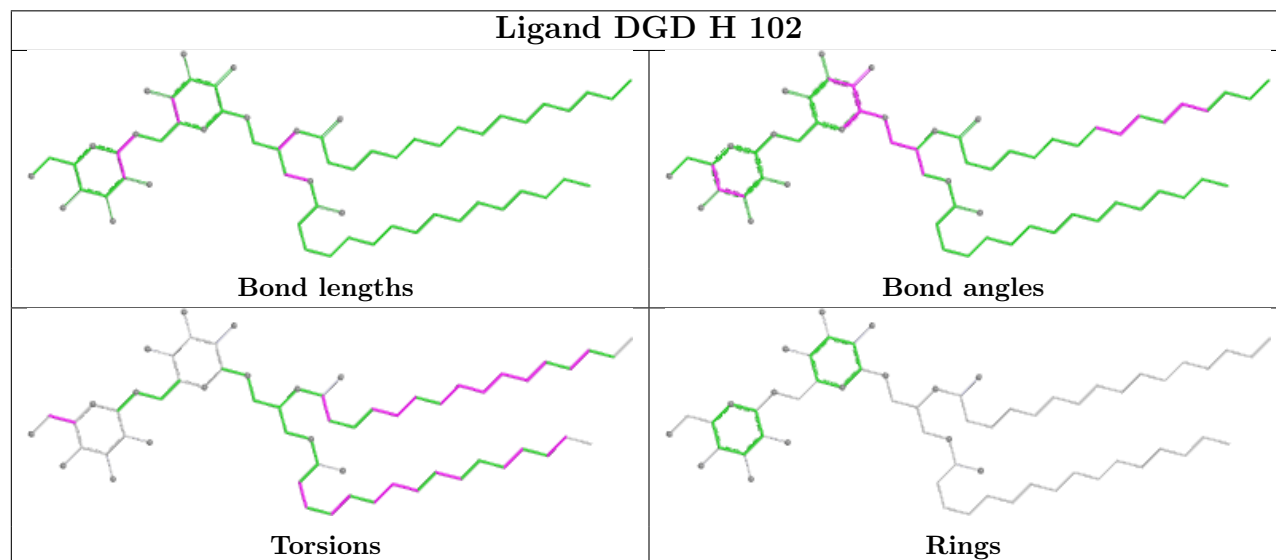
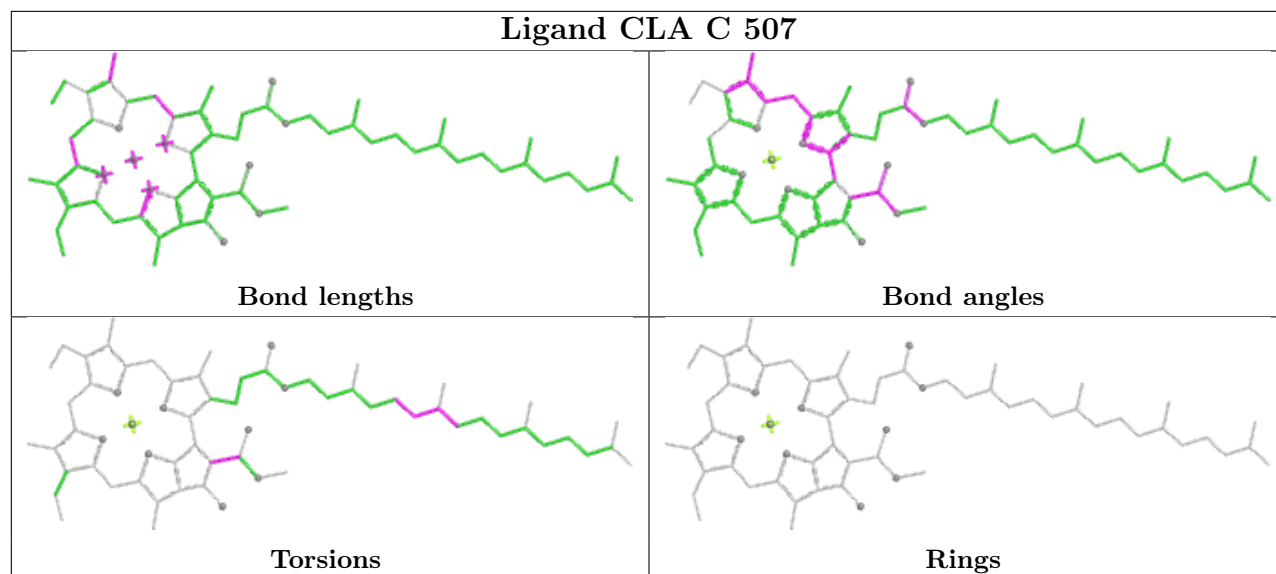
Ligand CLA c 504

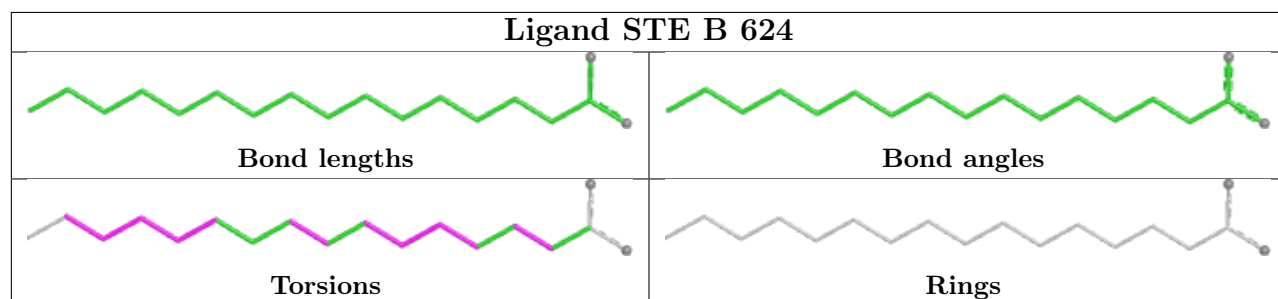
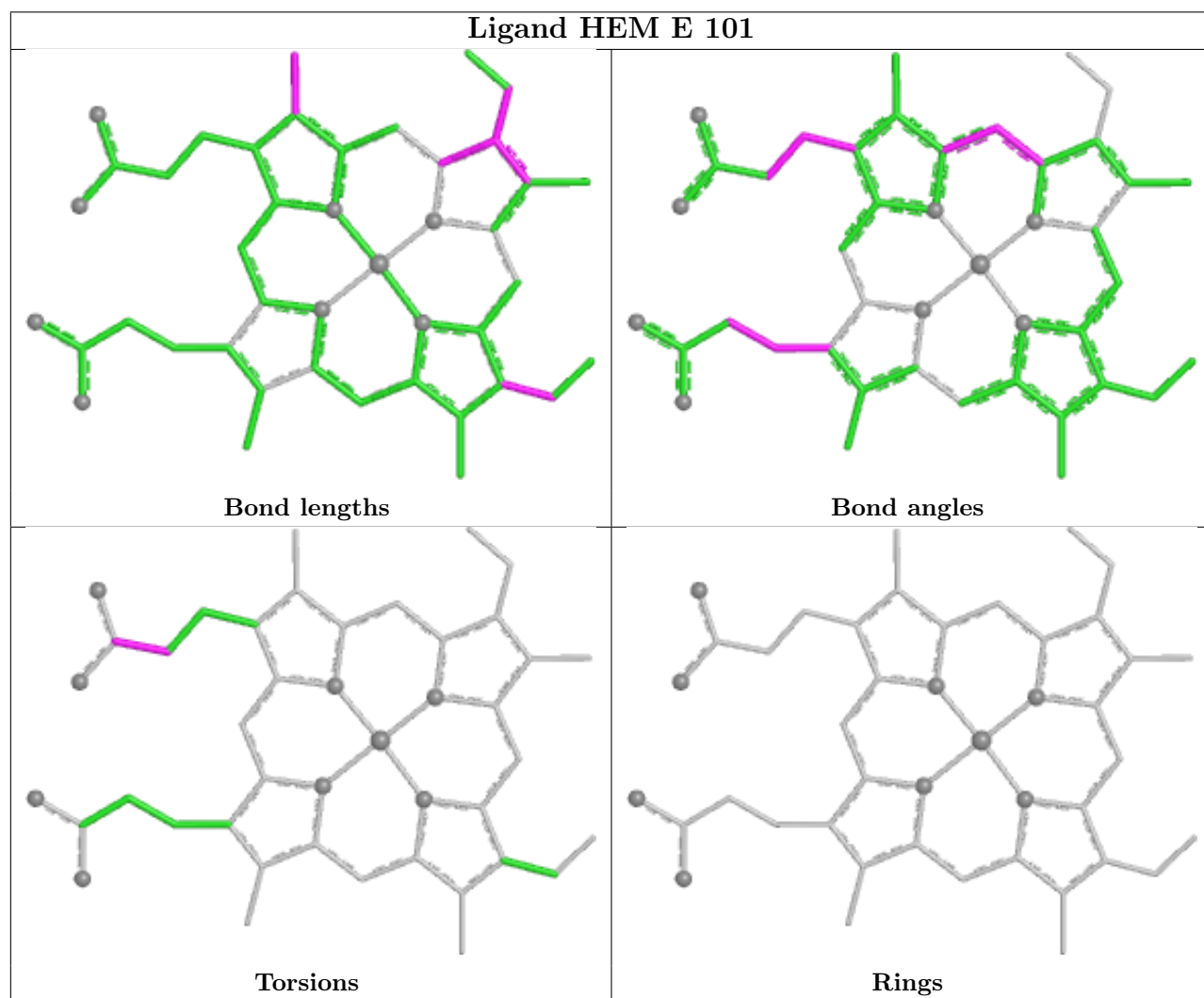
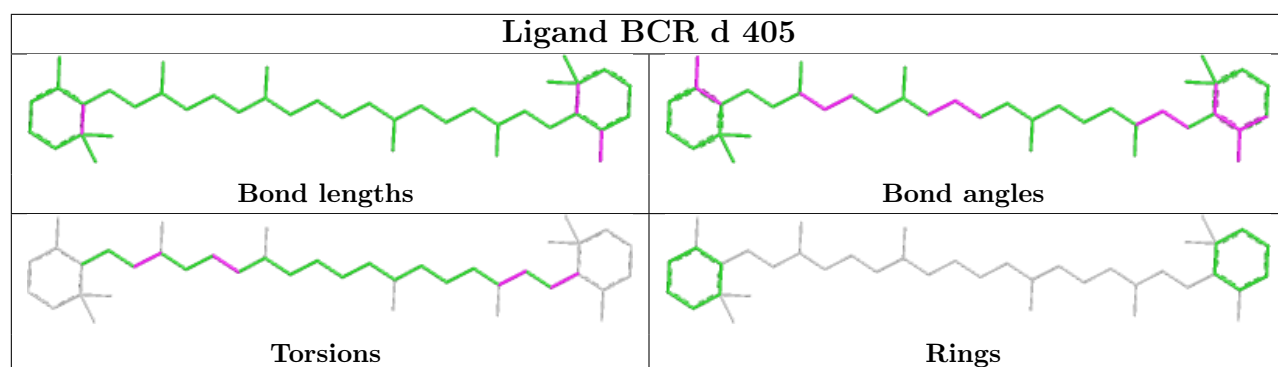


Ligand LMG d 411

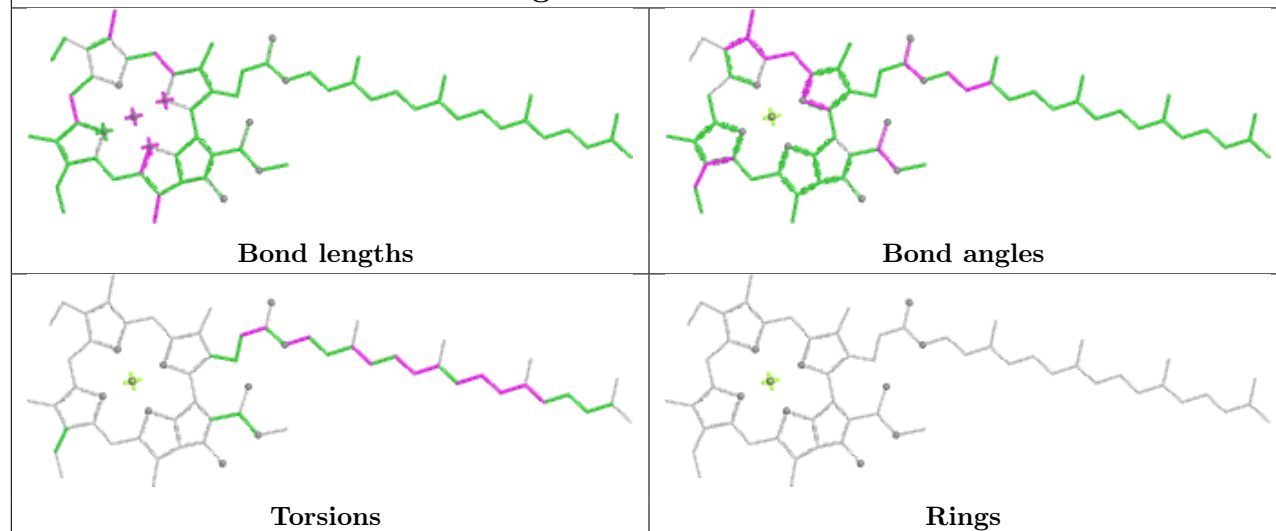




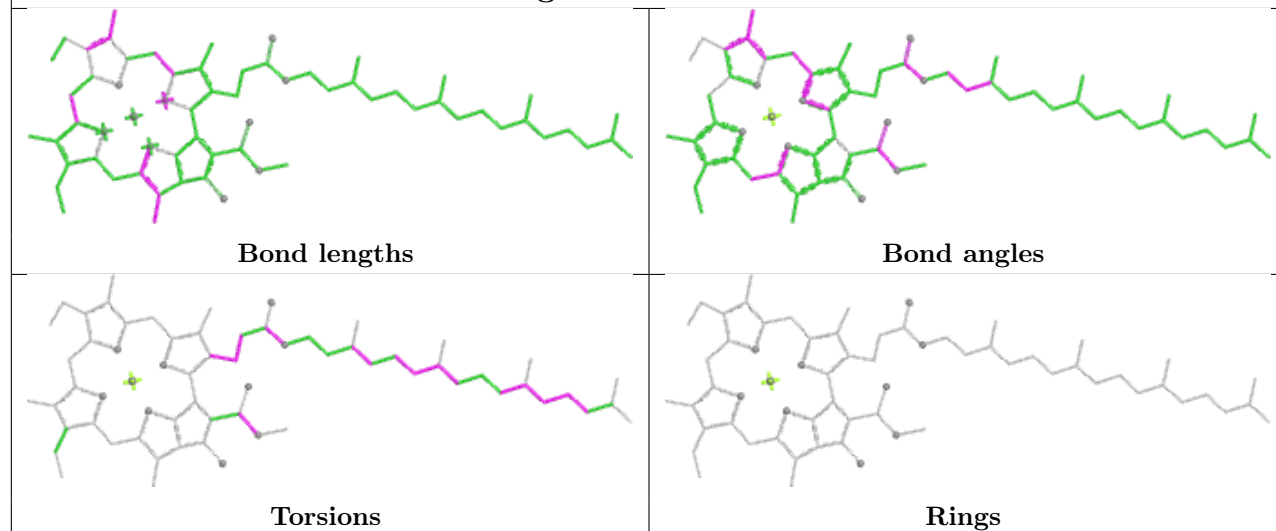




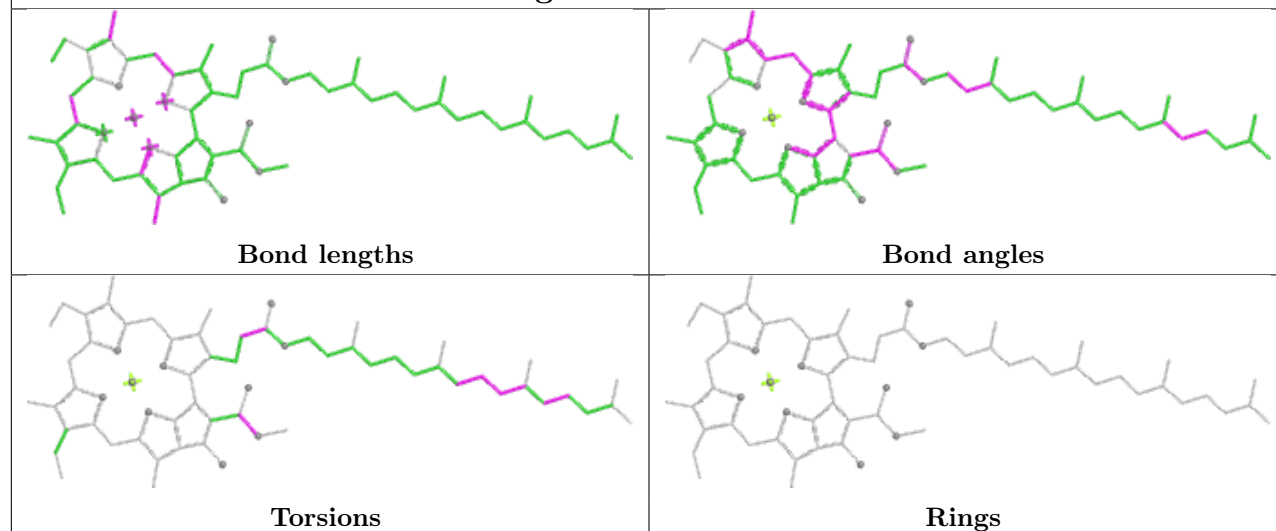
Ligand CLA B 613



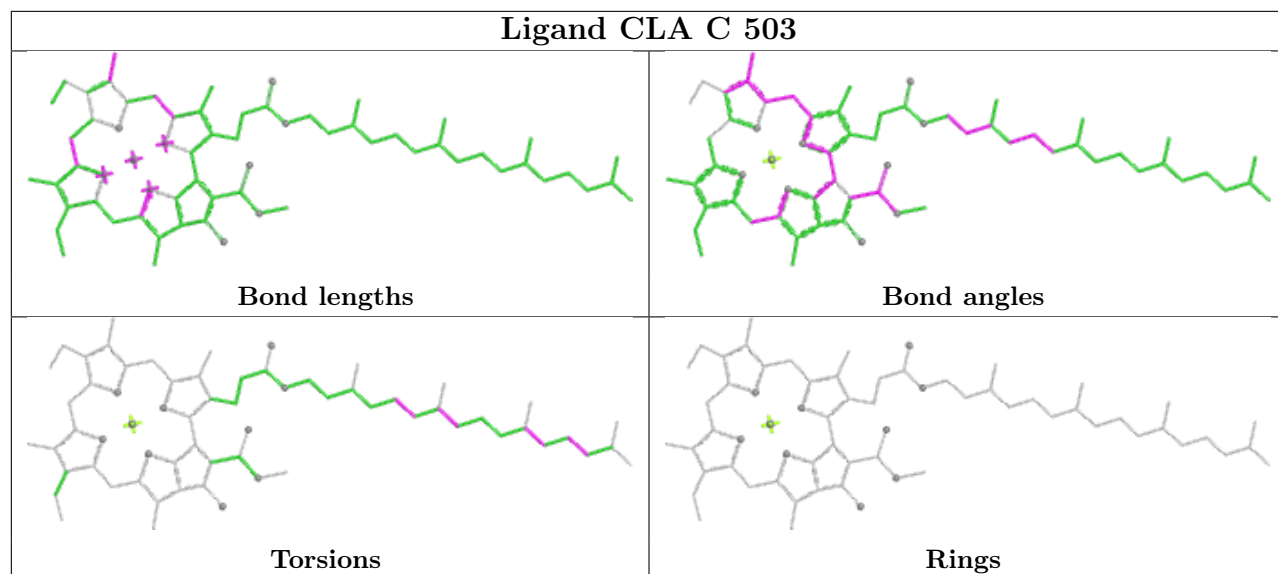
Ligand CLA c 512



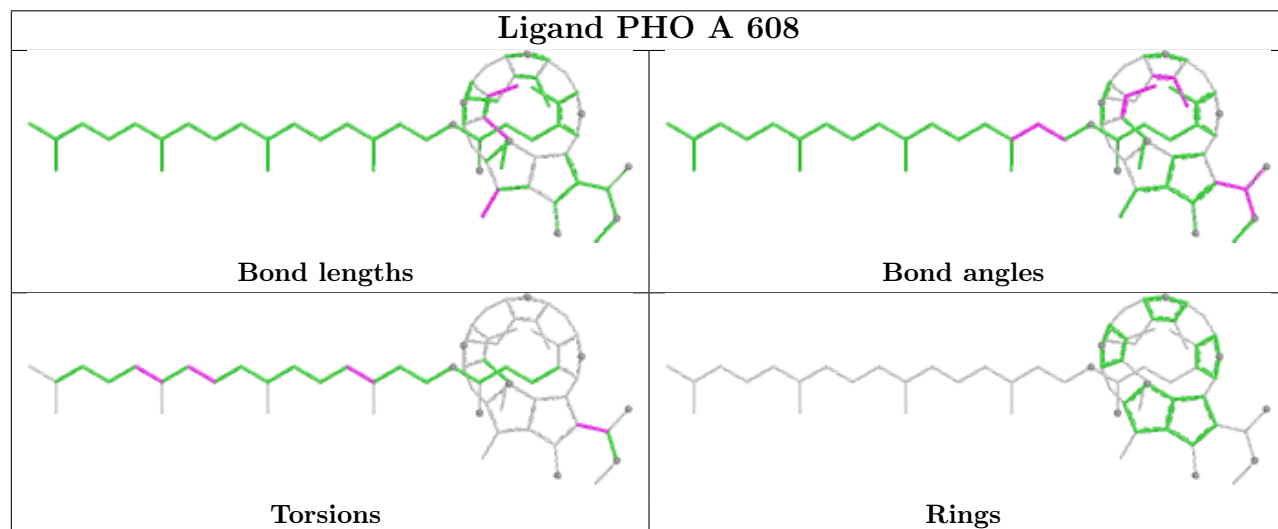
Ligand CLA b 613



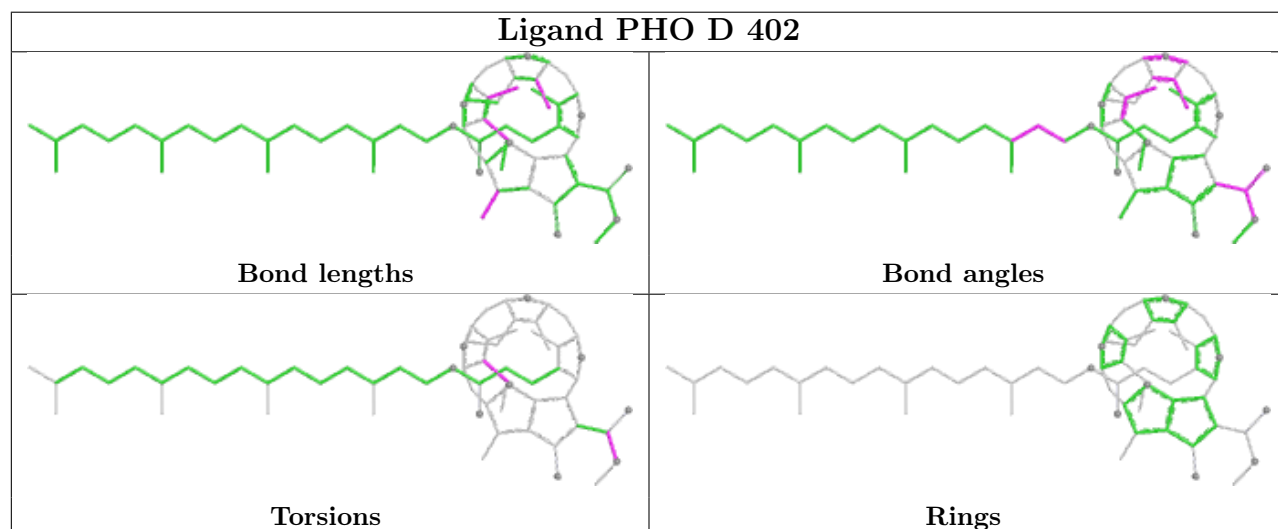
Ligand CLA C 503

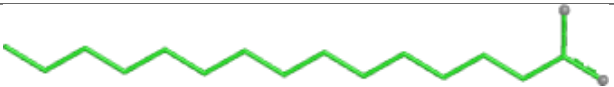
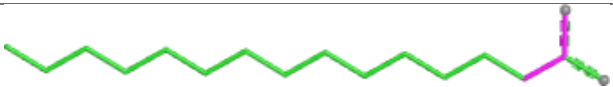
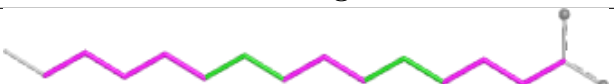



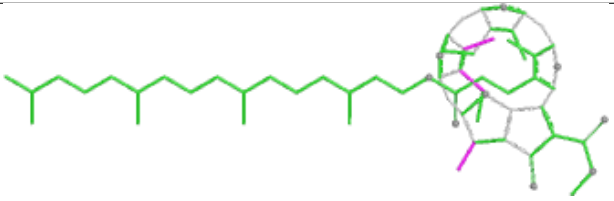
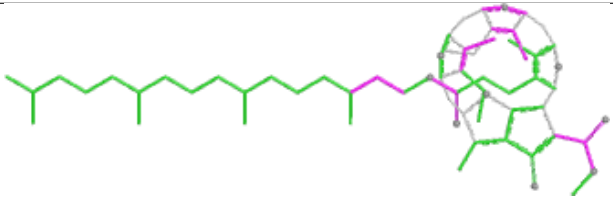
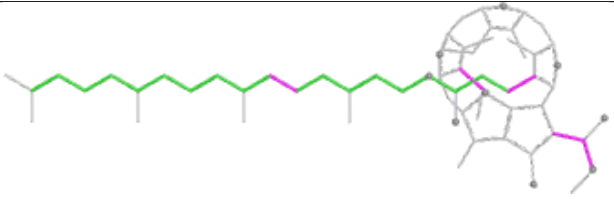
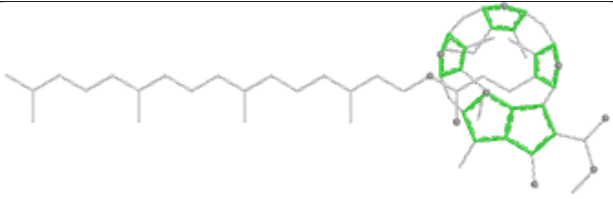
Ligand PHO A 608

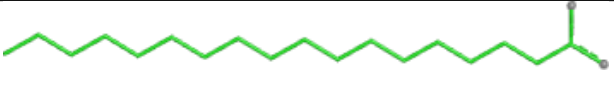
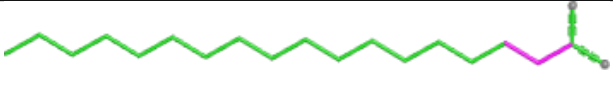
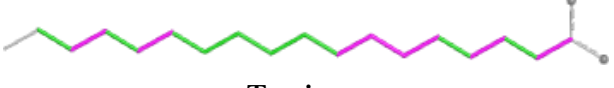
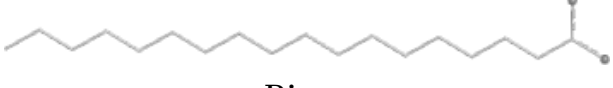


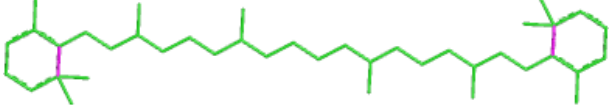
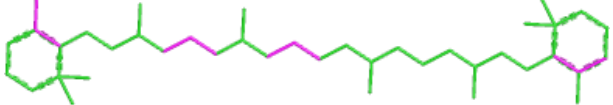
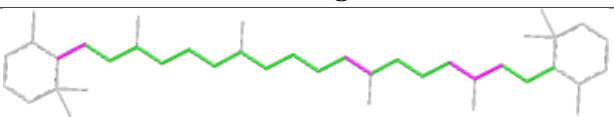
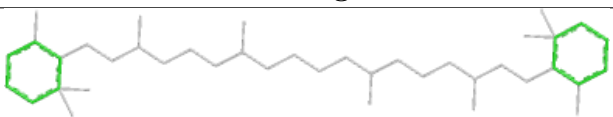
Ligand PHO D 402







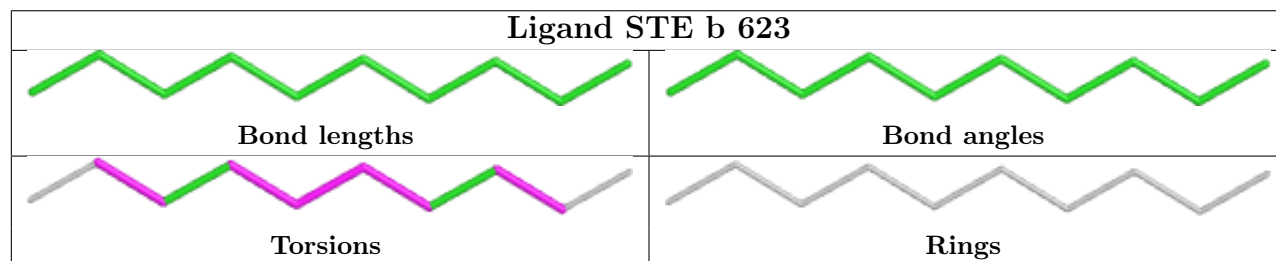
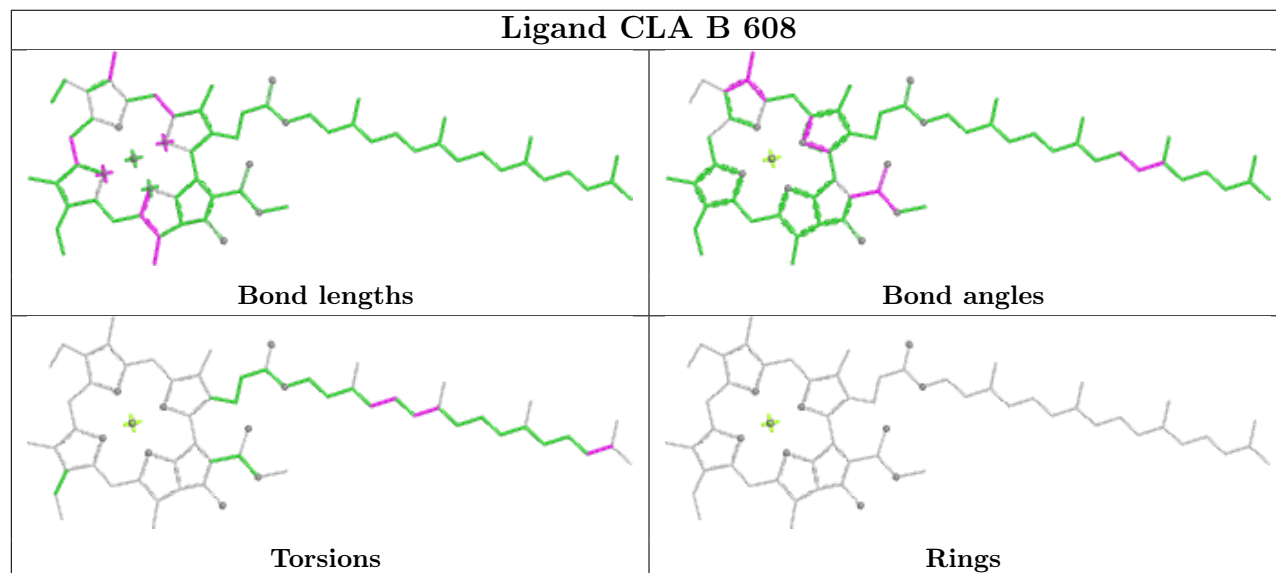
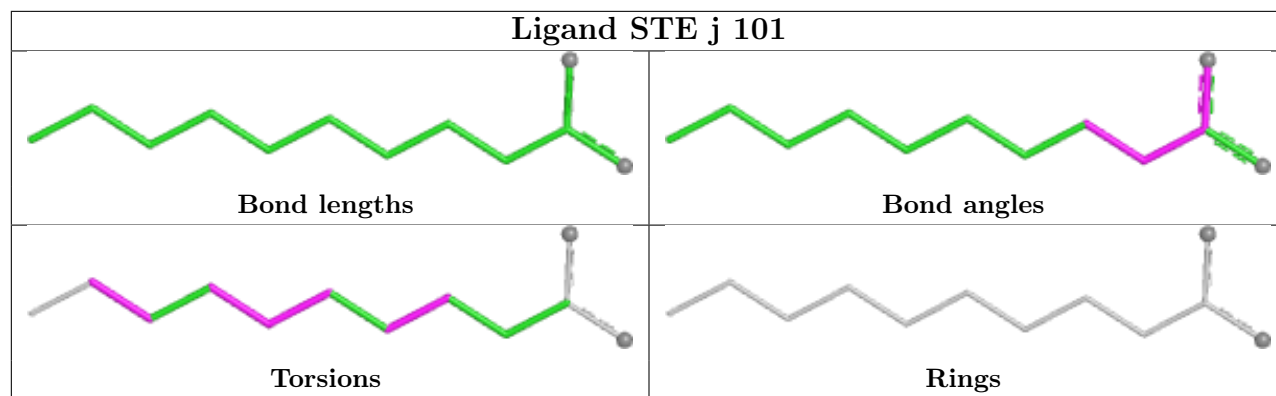
Ligand STE d 413	
 Bond lengths	 Bond angles
 Torsions	 Rings

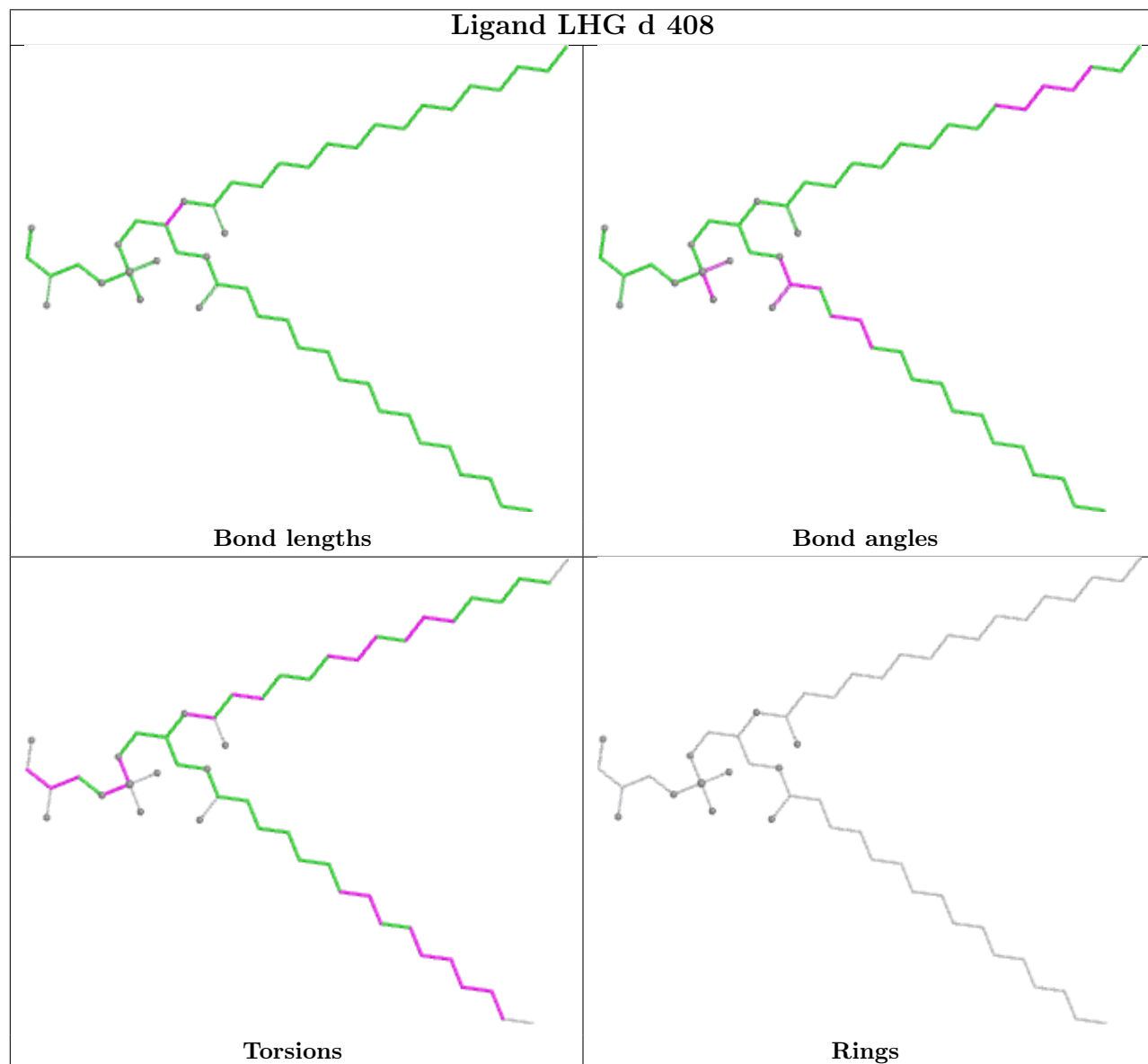
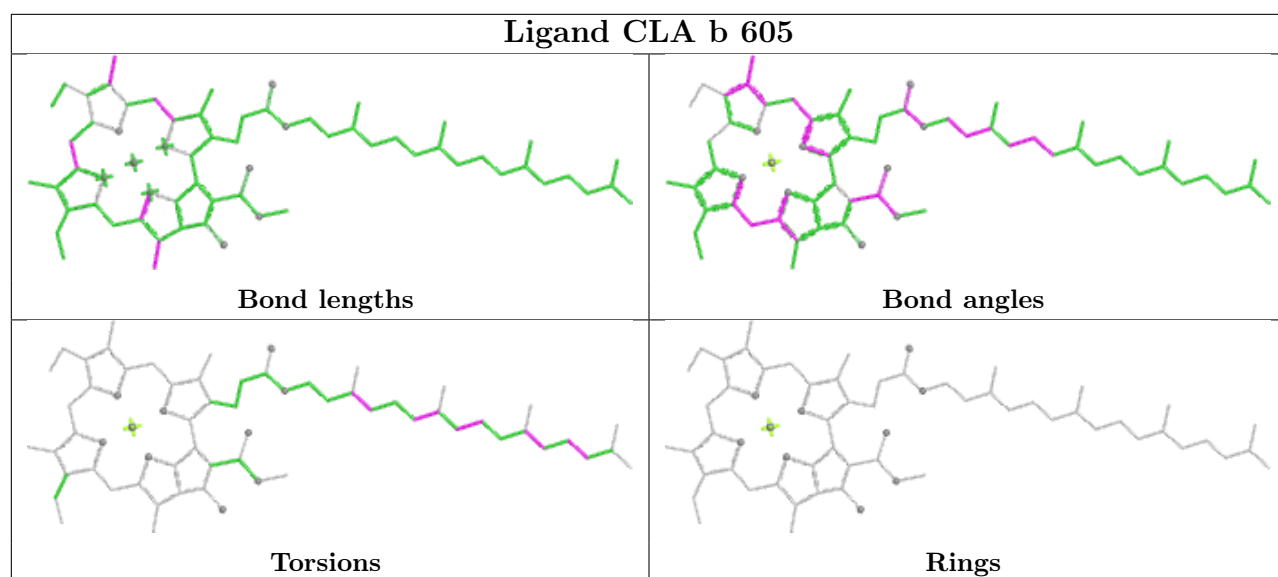
Ligand PHO d 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE b 622	
 Bond lengths	 Bond angles
 Torsions	 Rings

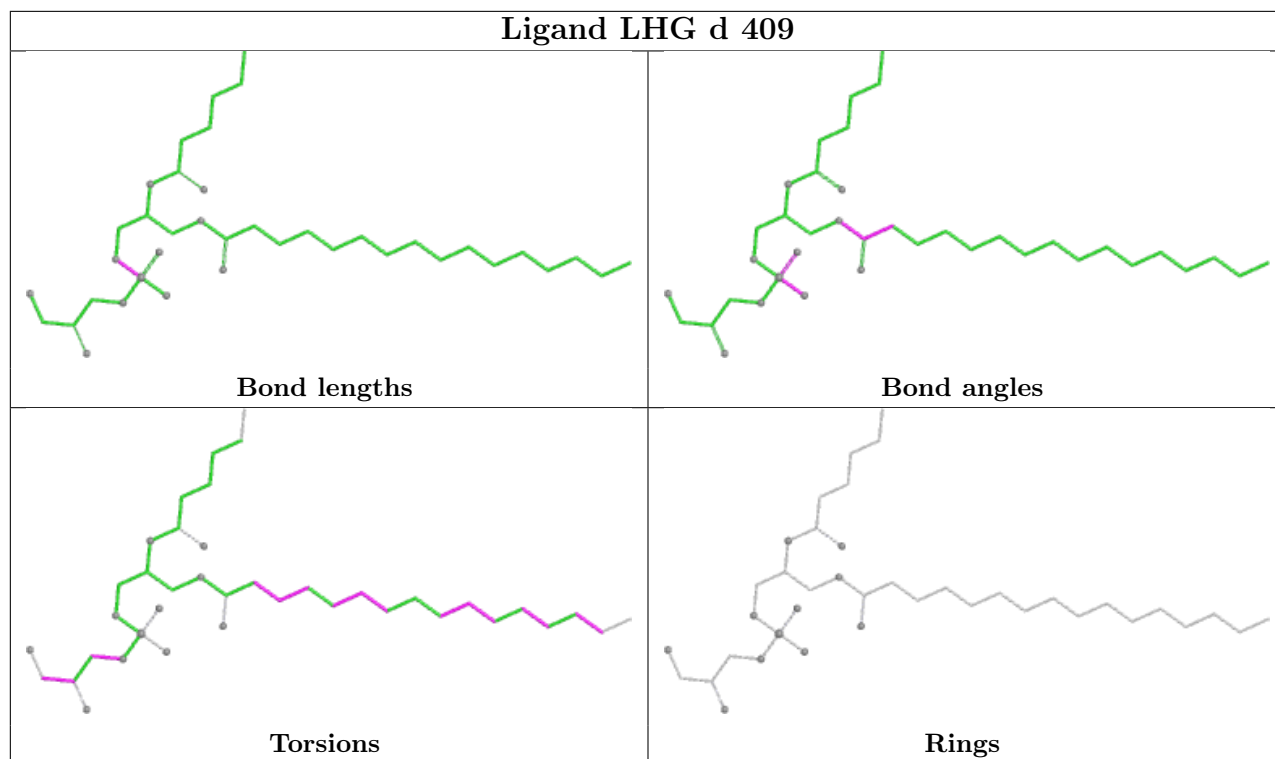
Ligand BCR Y 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE B 626	
 Bond lengths	 Bond angles
 Torsions	 Rings

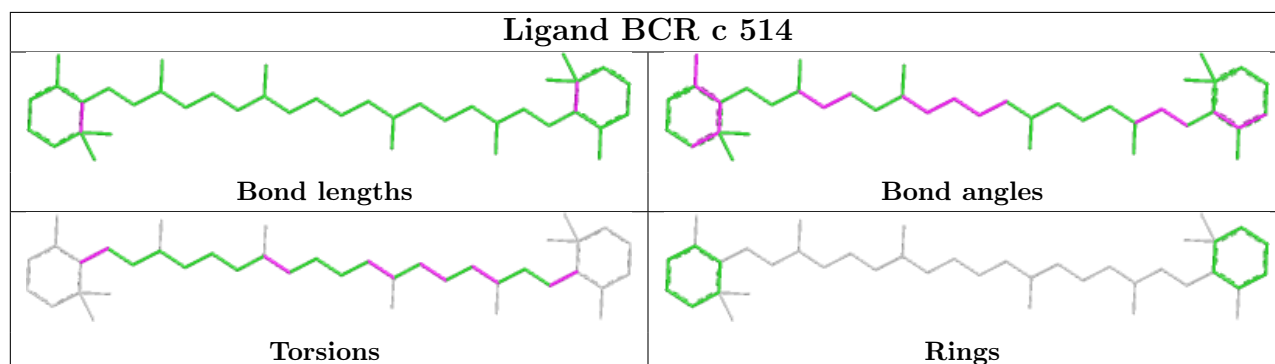




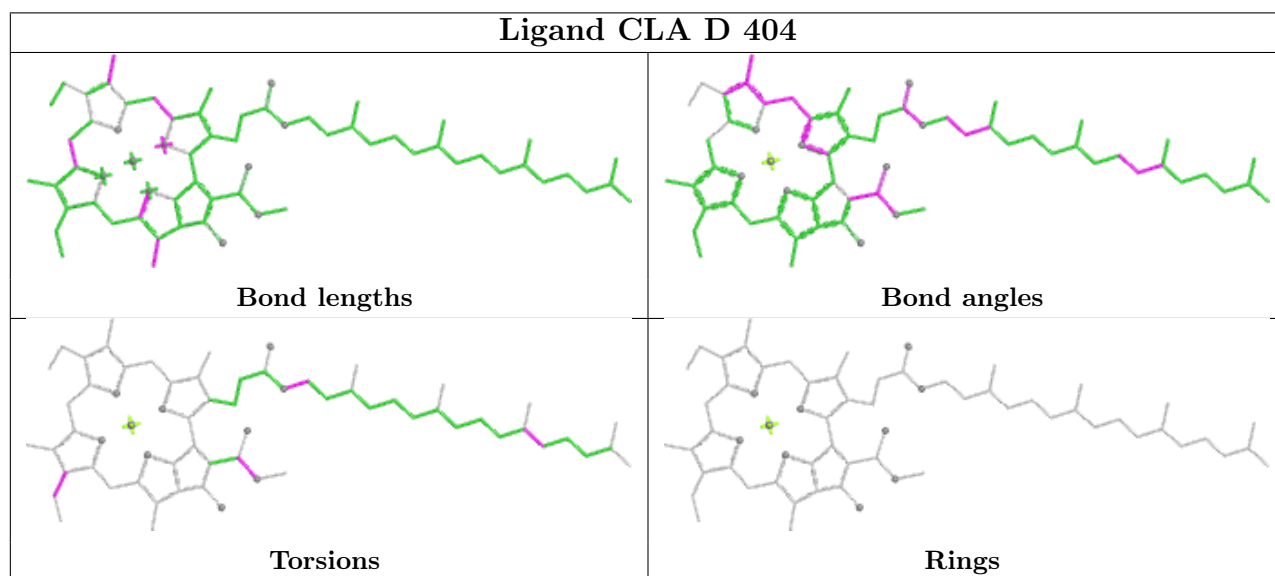
Ligand LHG d 409

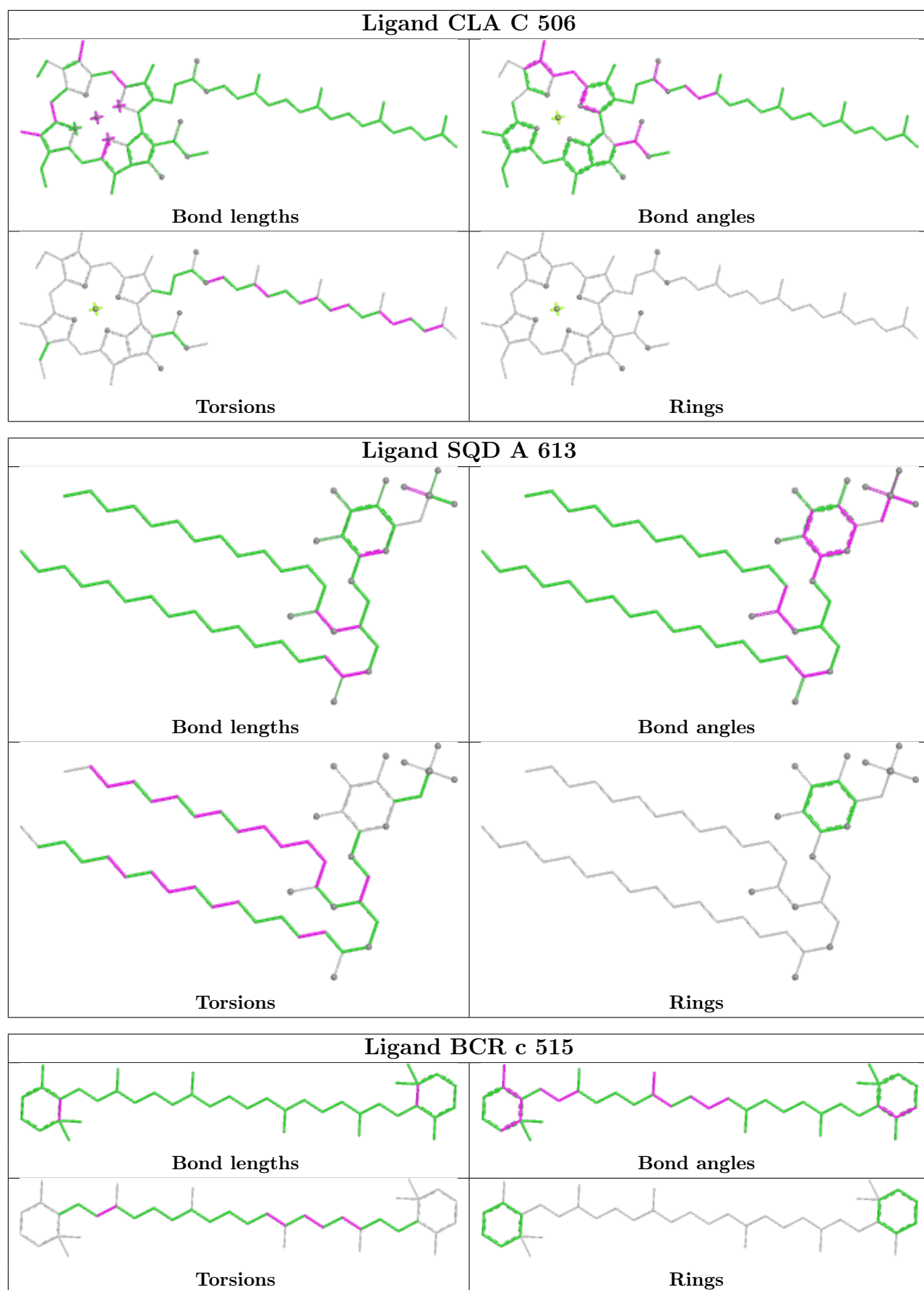


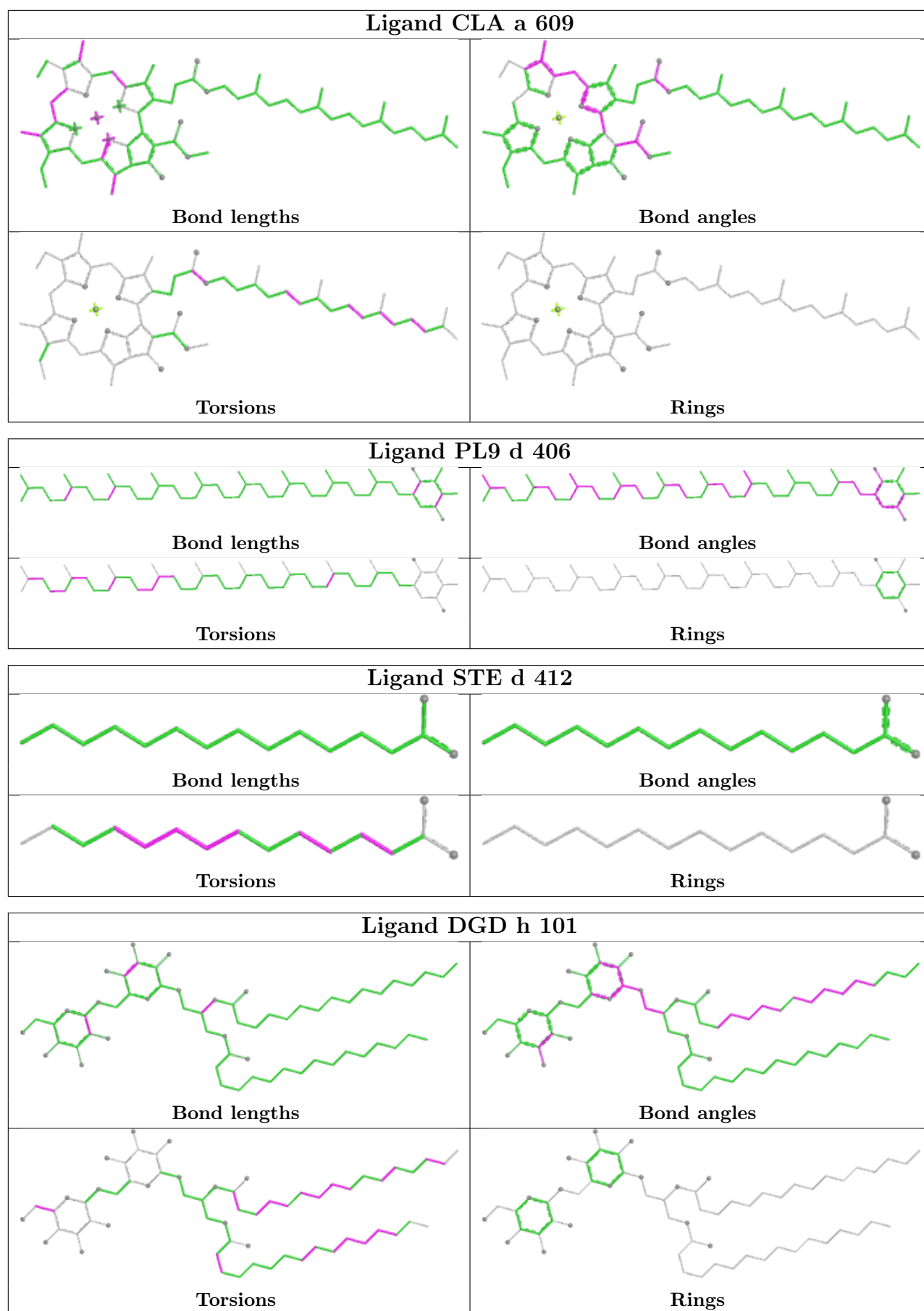
Ligand BCR c 514

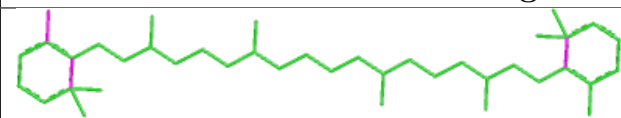
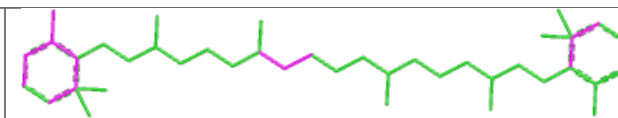
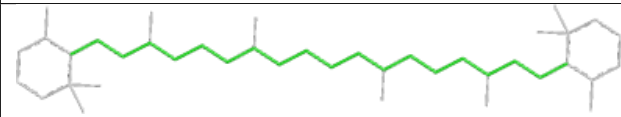
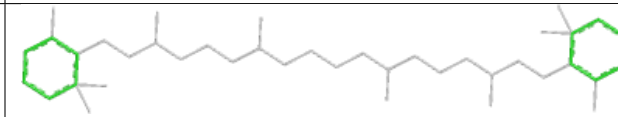


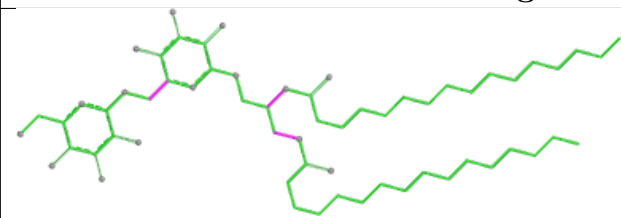
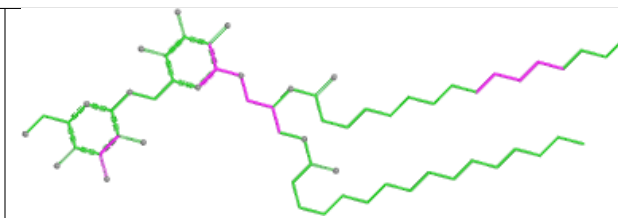
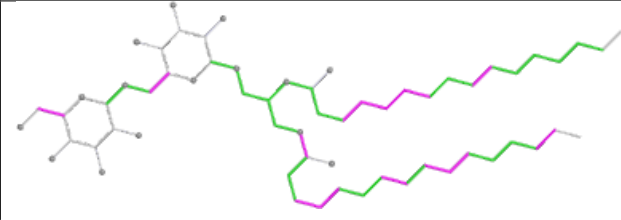
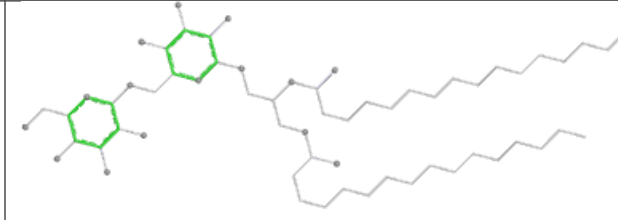
Ligand CLA D 404

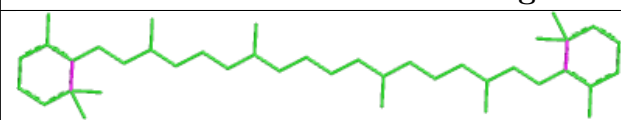
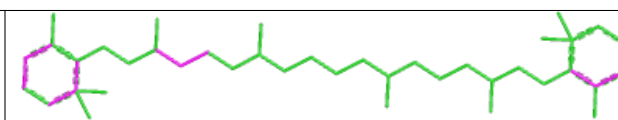
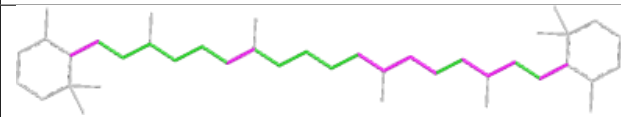
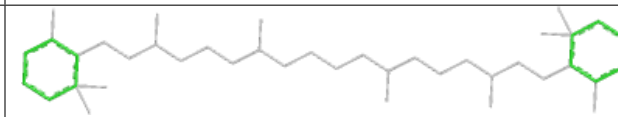


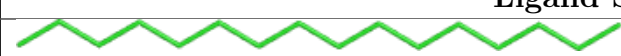
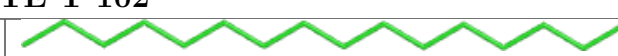

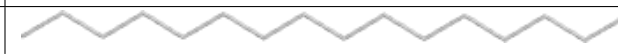


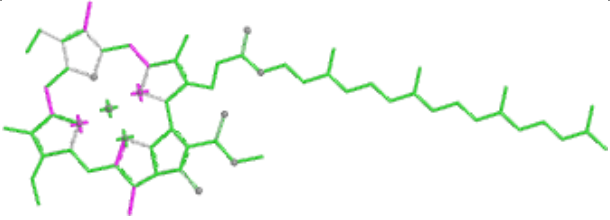
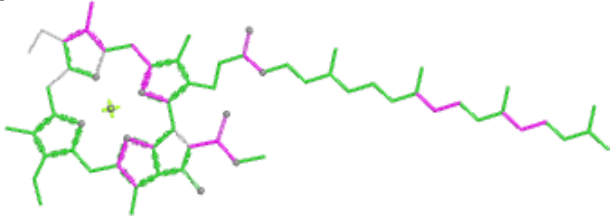
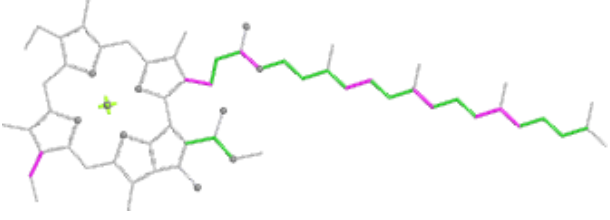
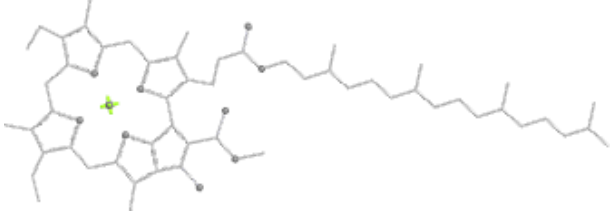
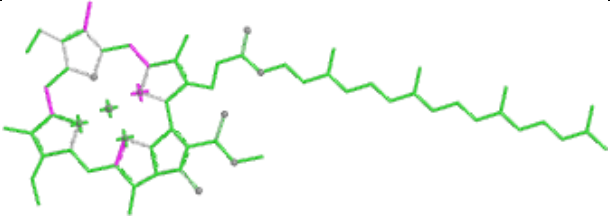
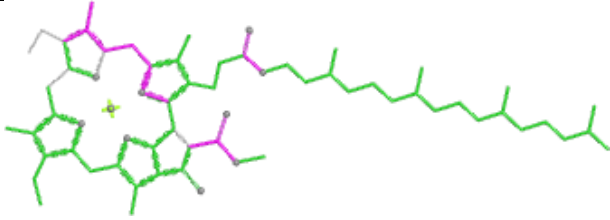
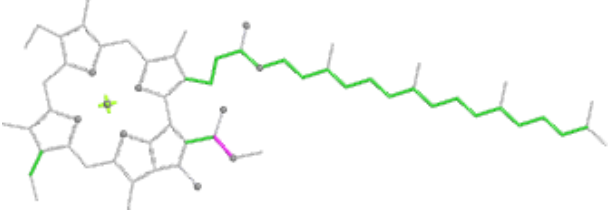
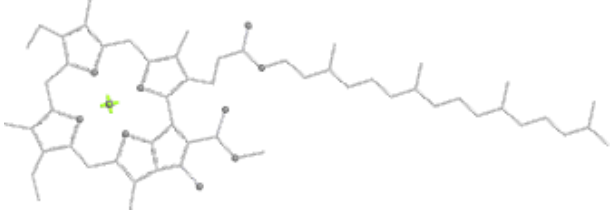






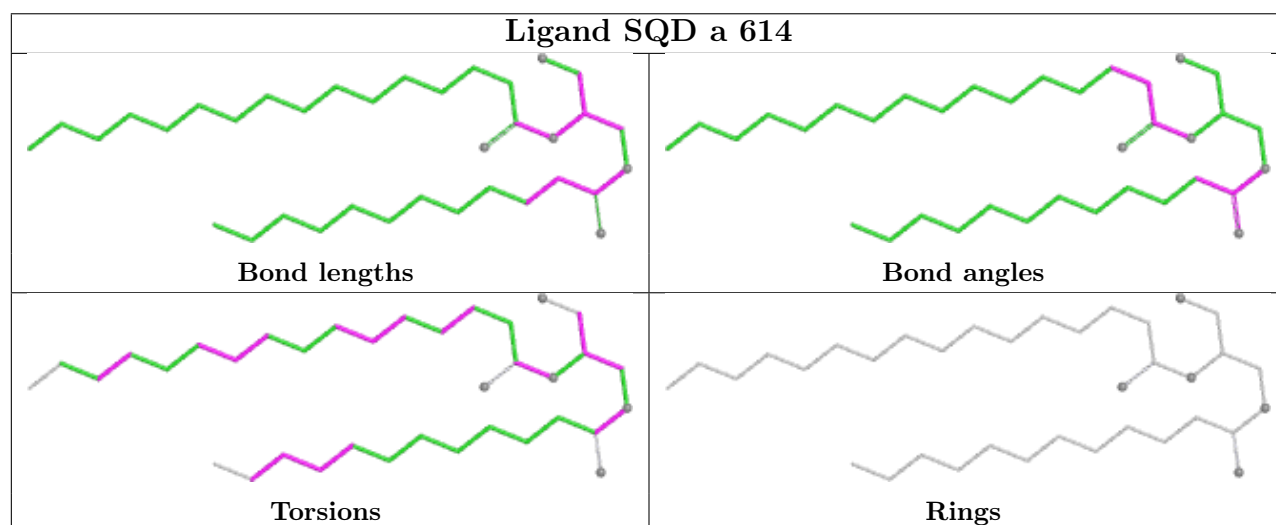
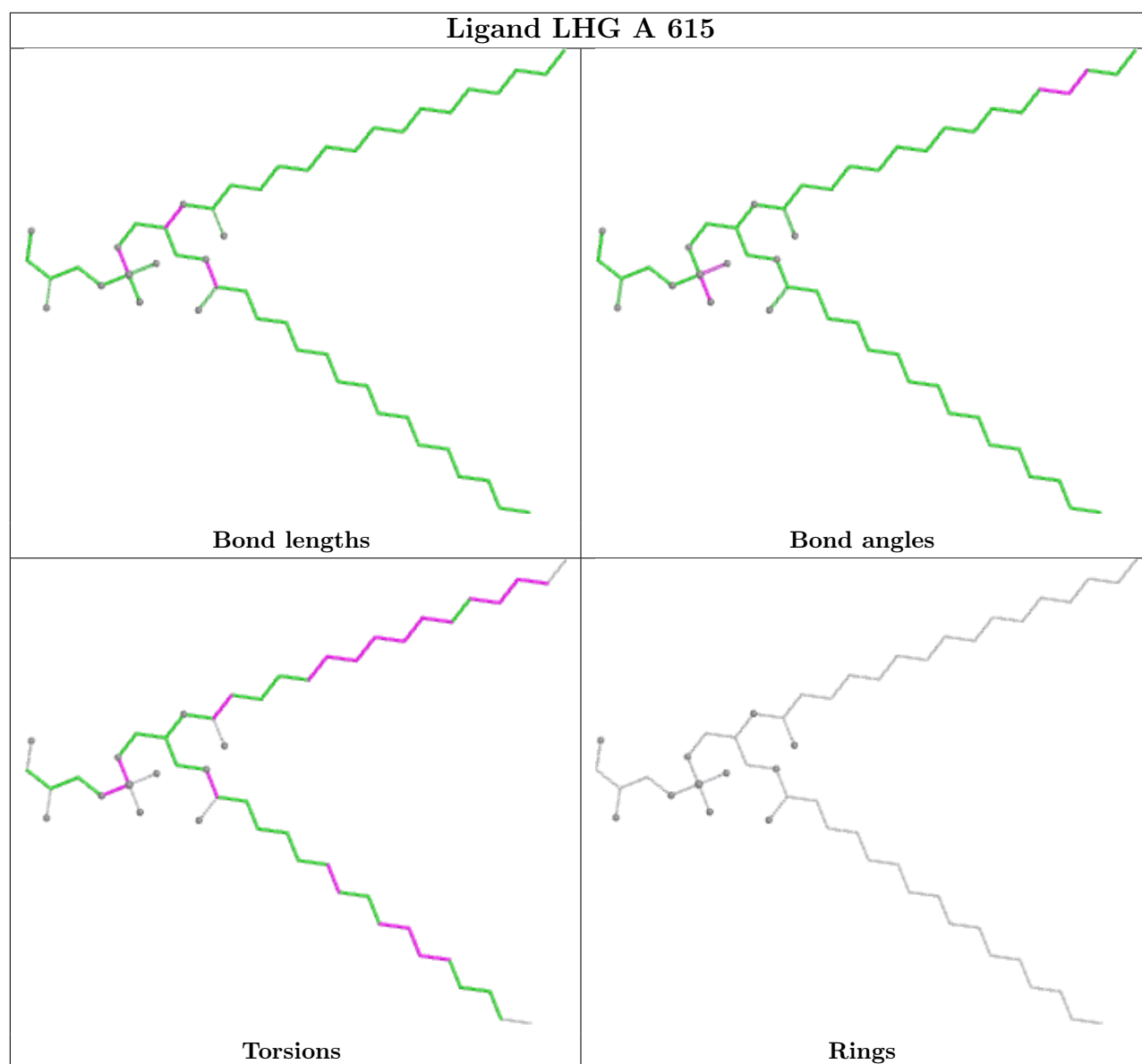
Ligand BCR B 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD C 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

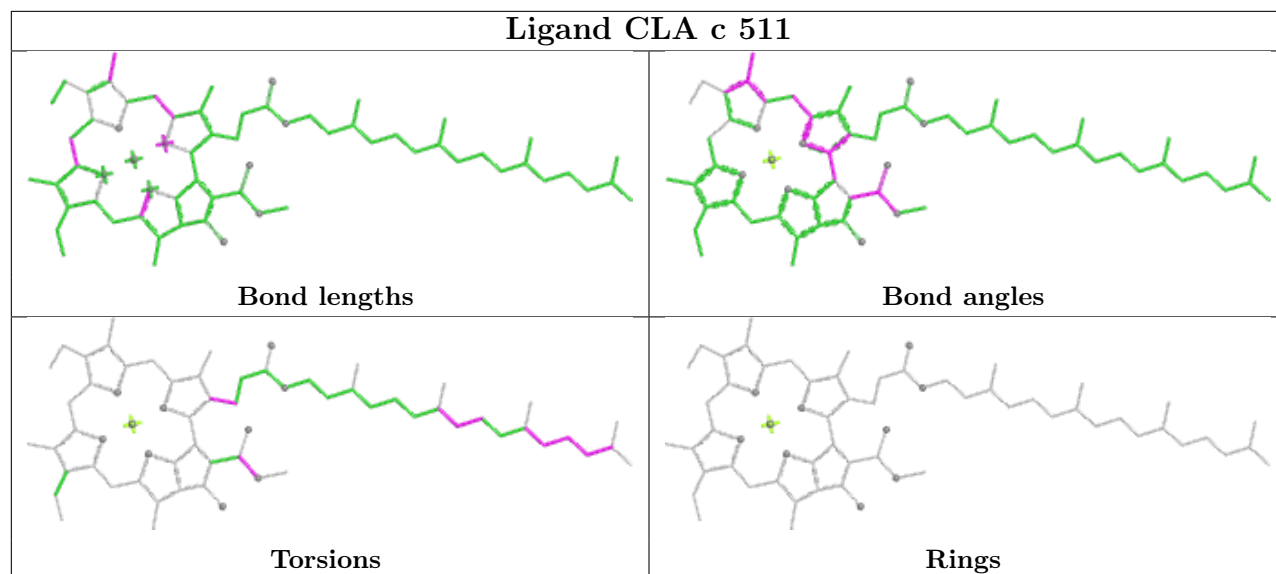
Ligand BCR K 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE T 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

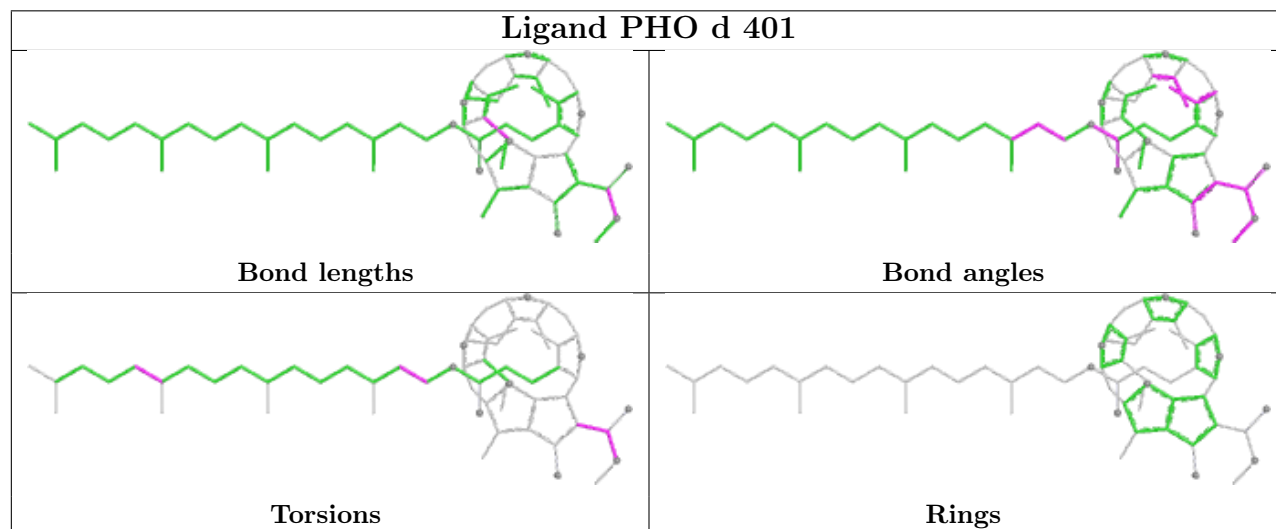
Ligand CLA B 604			
			
Bond lengths			
		Bond angles	
			
Torsions			
		Rings	
Ligand CLA a 612			
			
Bond lengths			
		Bond angles	
			
Torsions			
		Rings	
Ligand STE T 103			
			
Bond lengths			
		Bond angles	
			
Torsions			
		Rings	



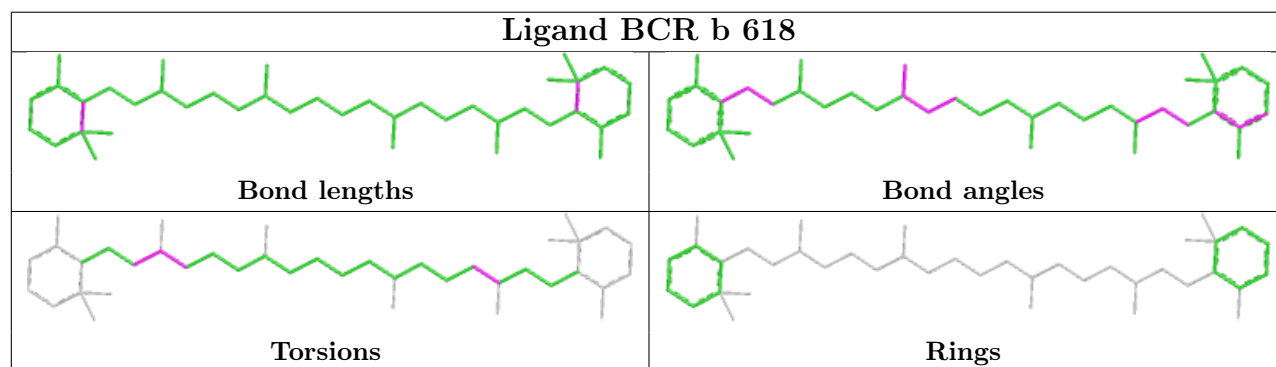
Ligand CLA c 511

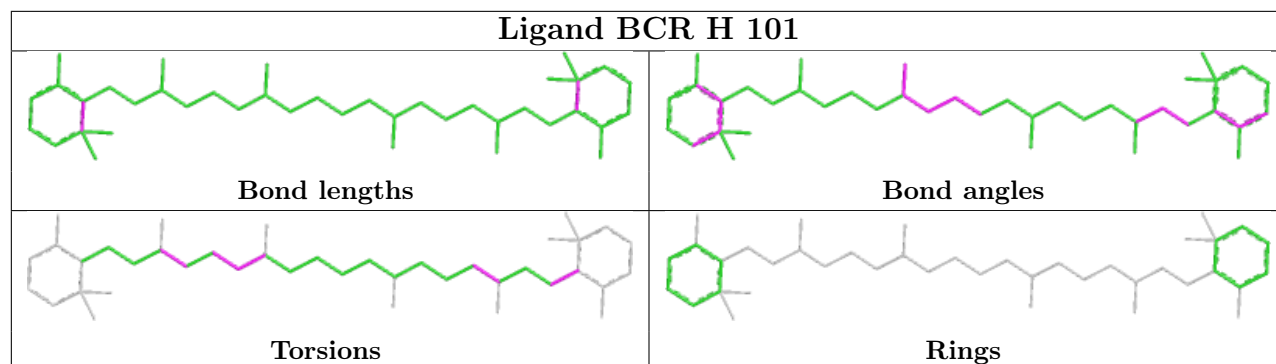
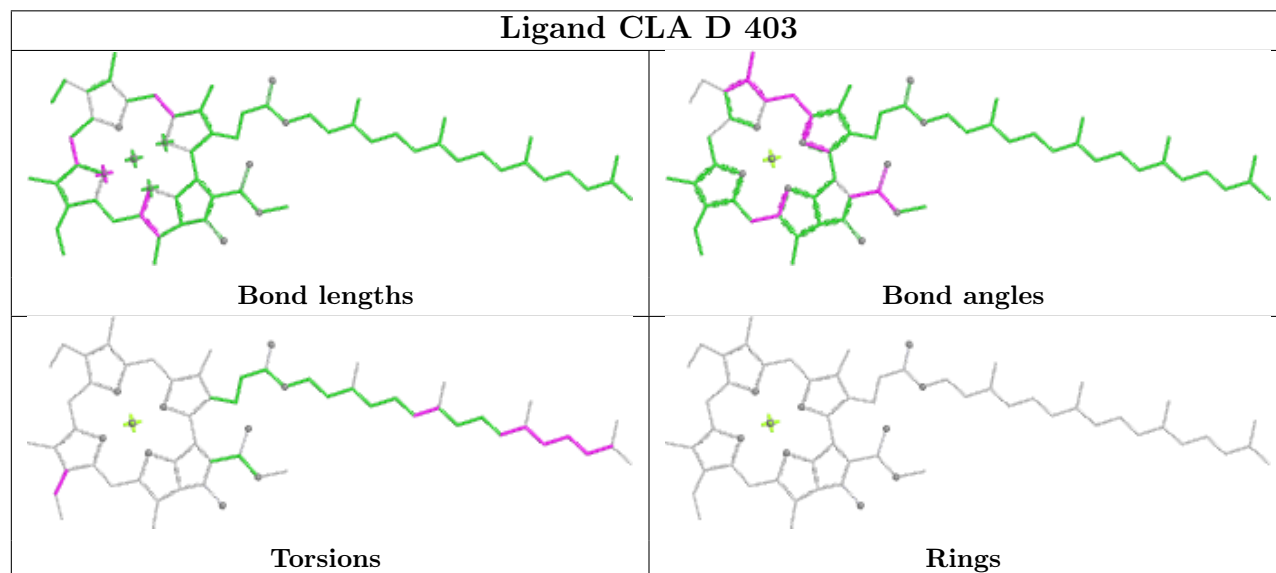
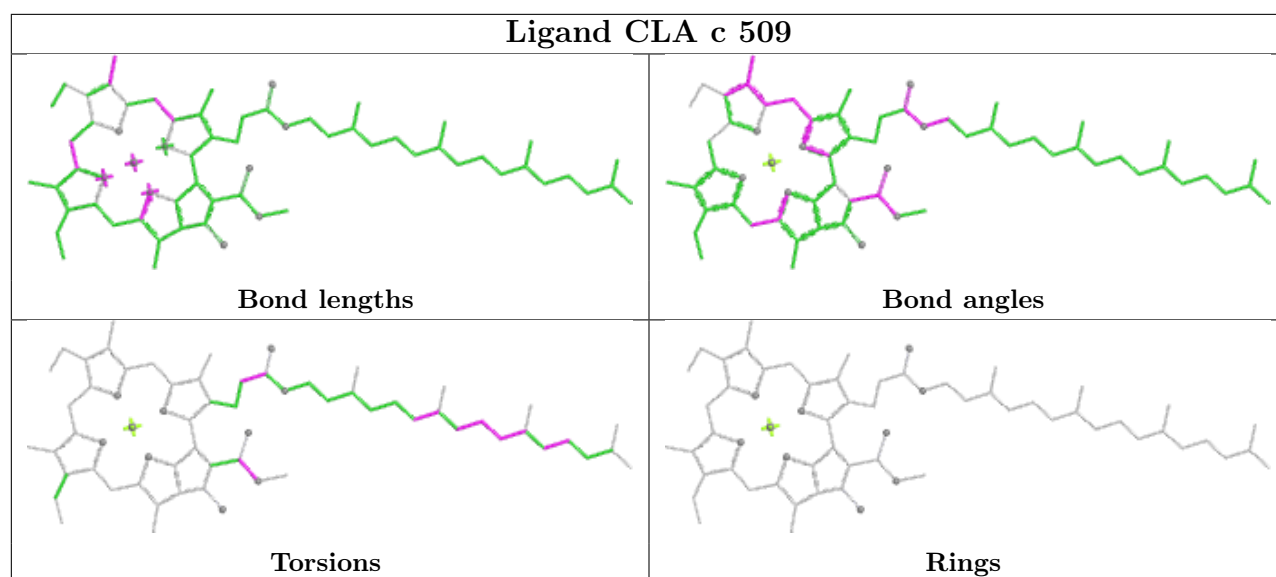


Ligand PHO d 401

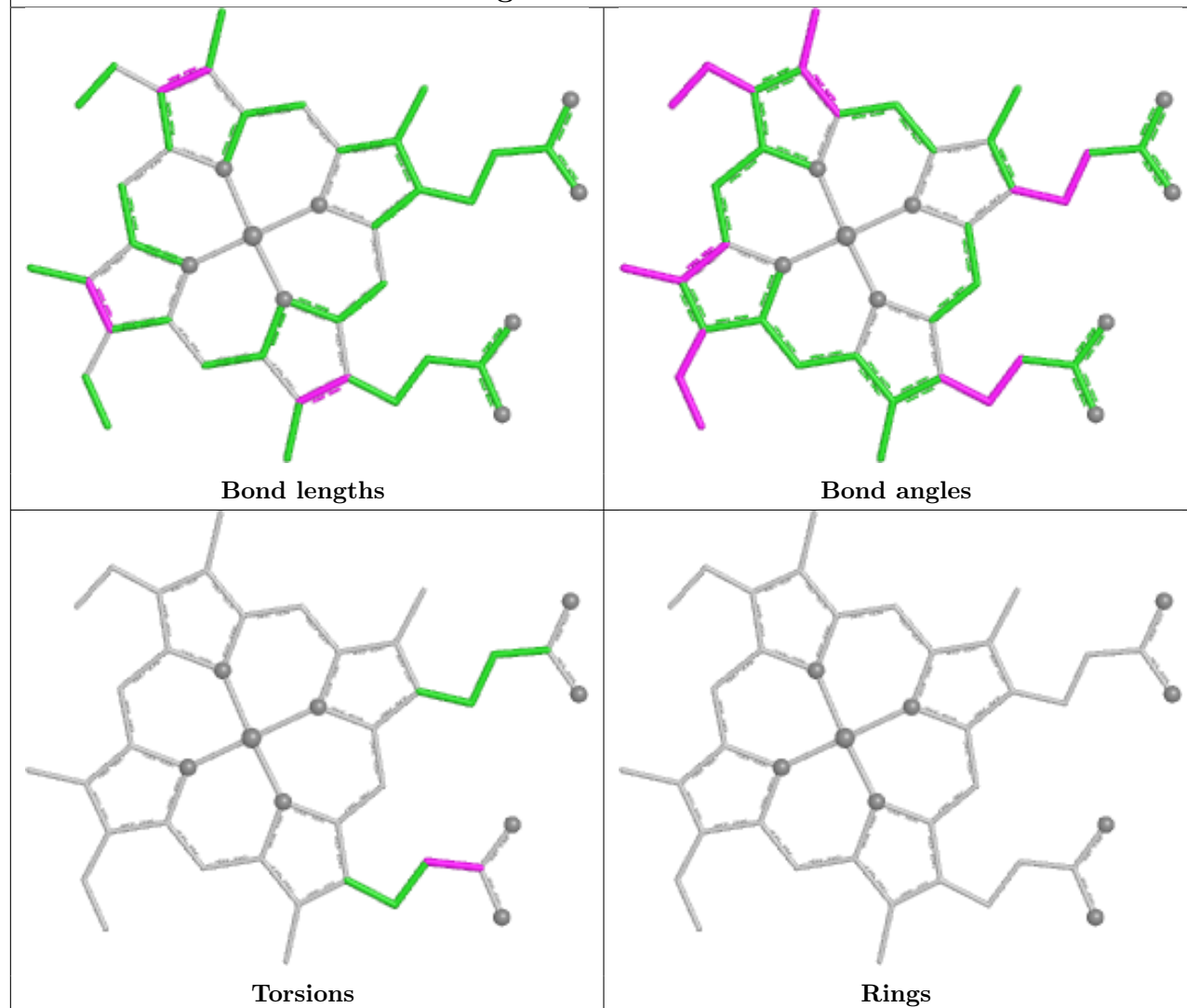


Ligand BCR b 618

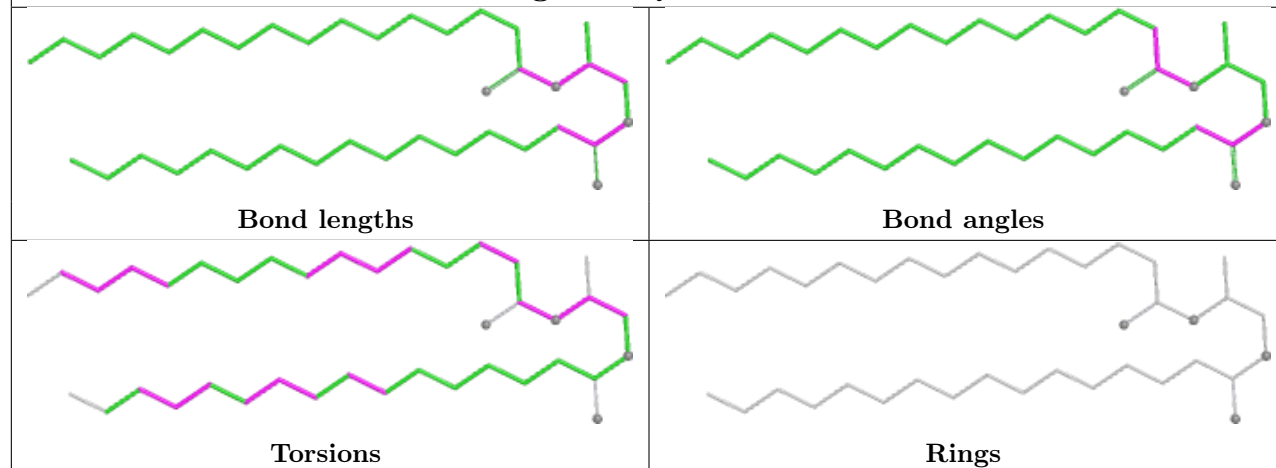


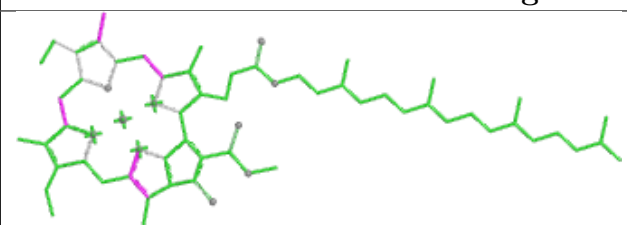
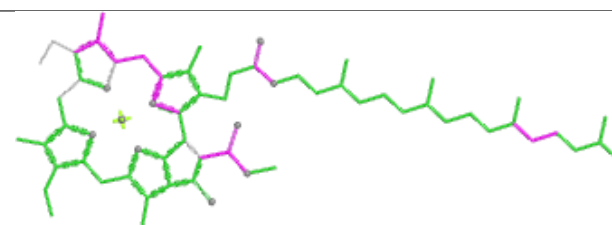
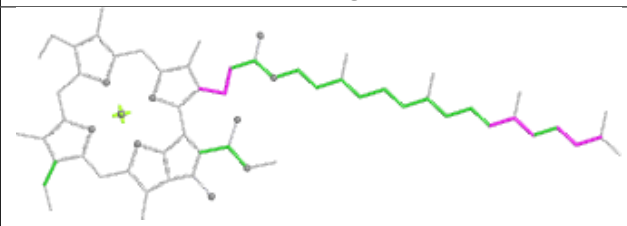
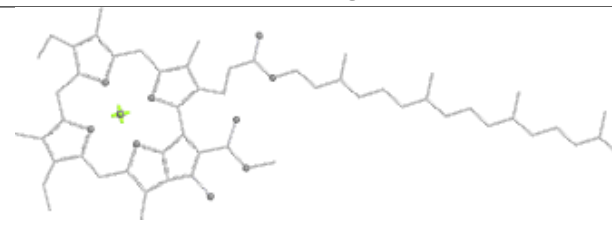


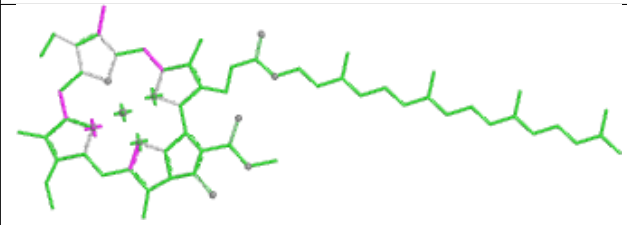
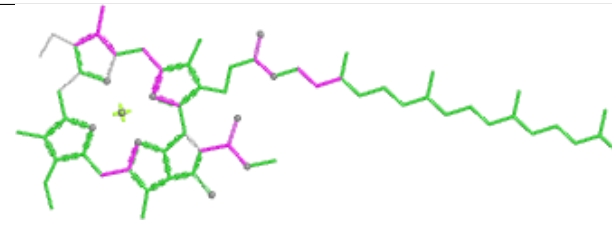
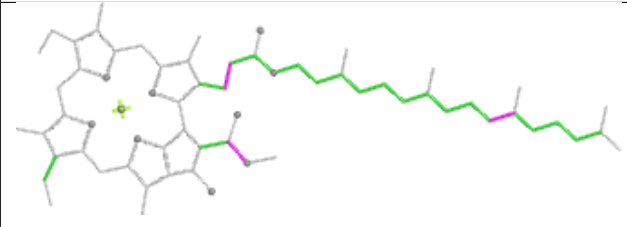
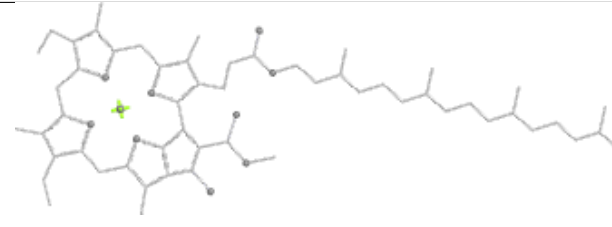
Ligand HEC v 201

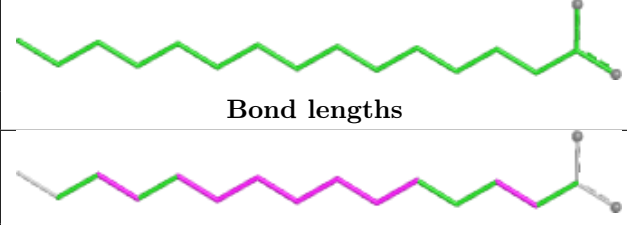
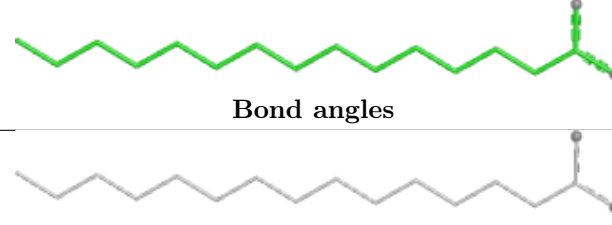
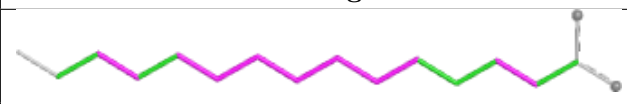
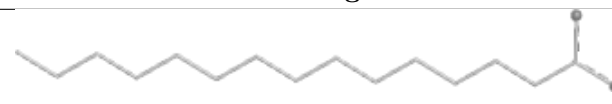


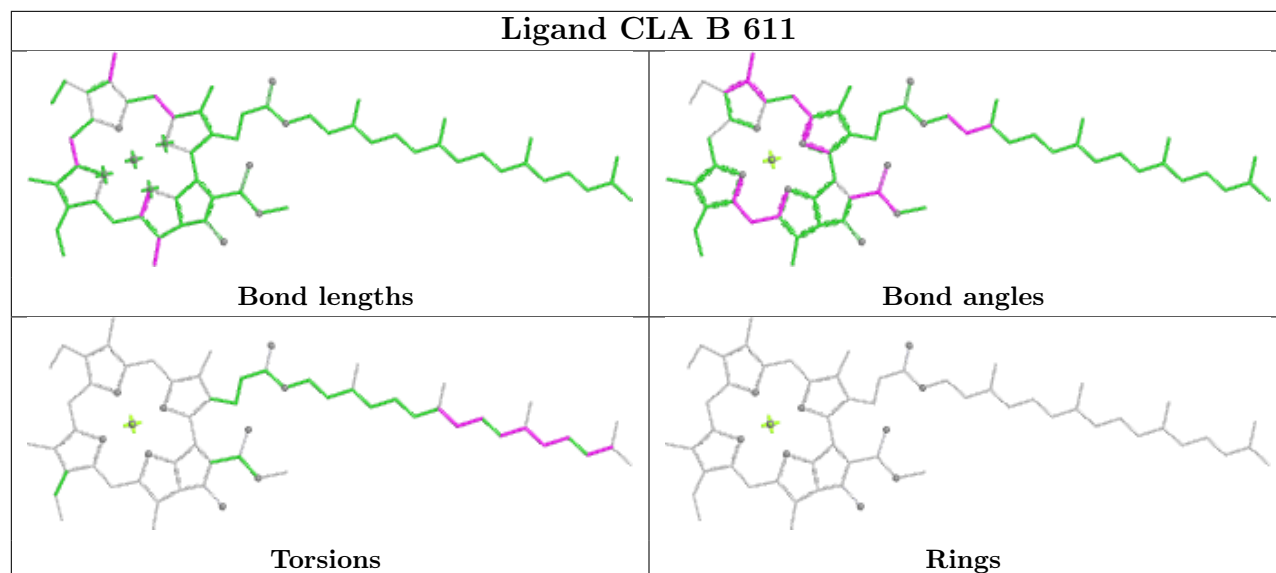
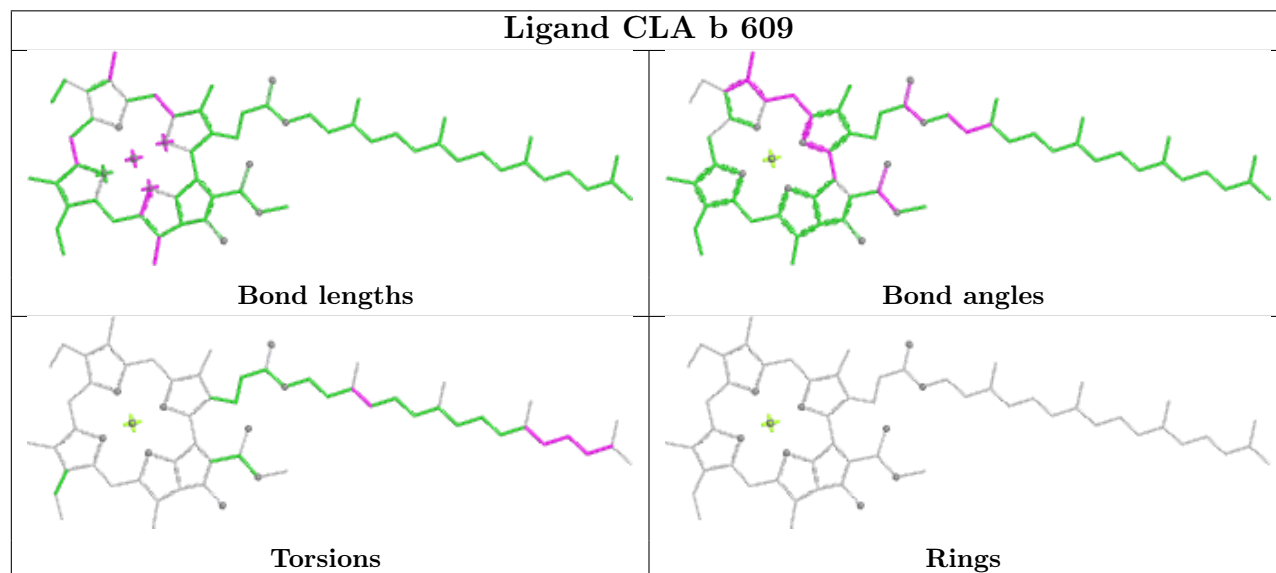
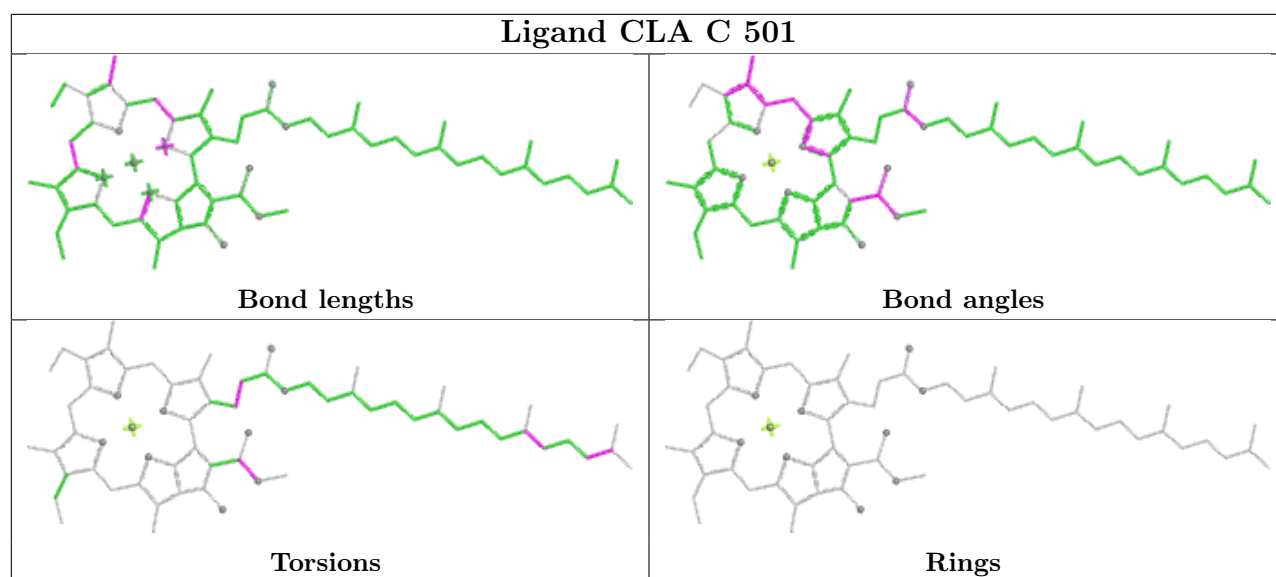
Ligand SQD A 616

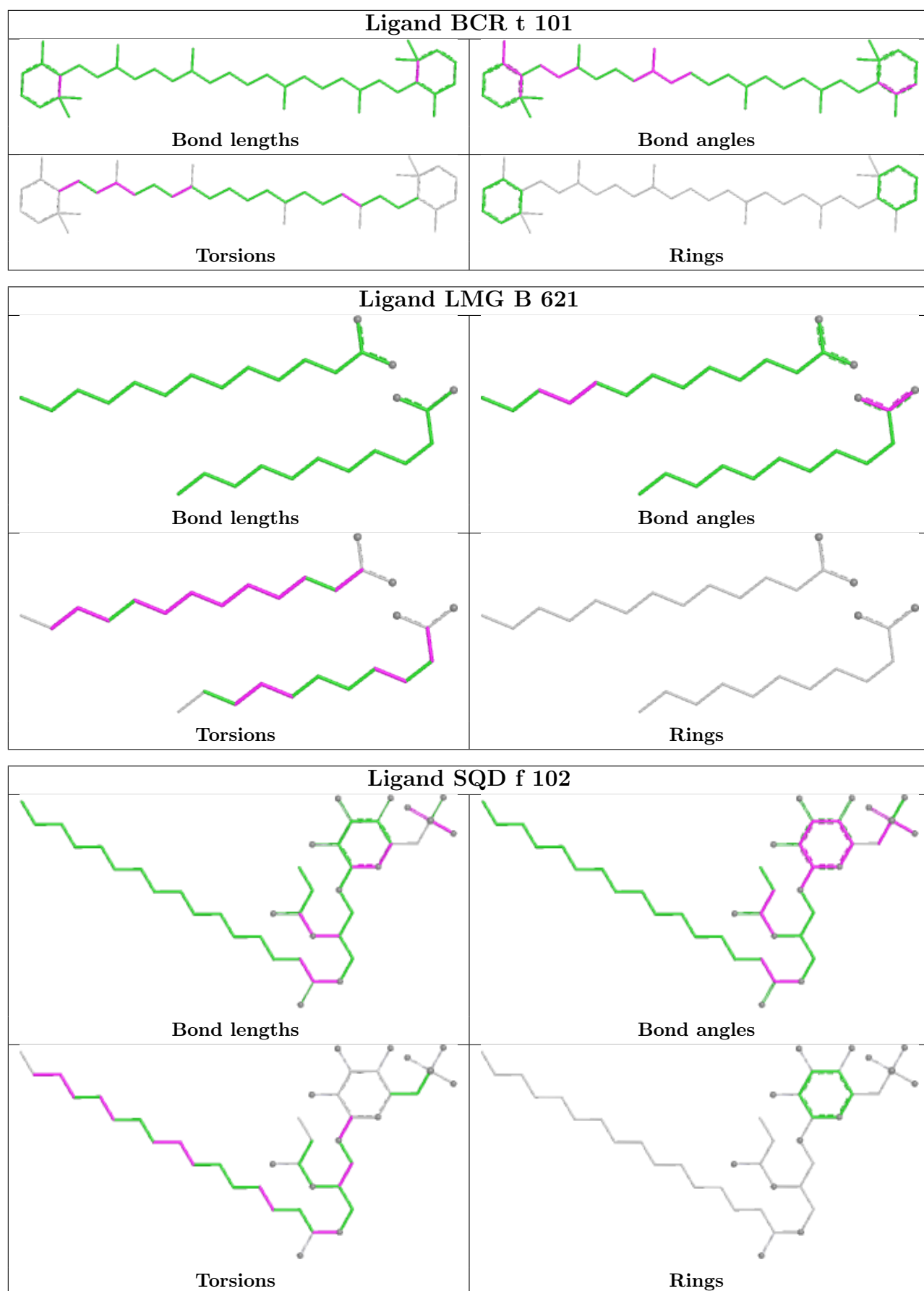


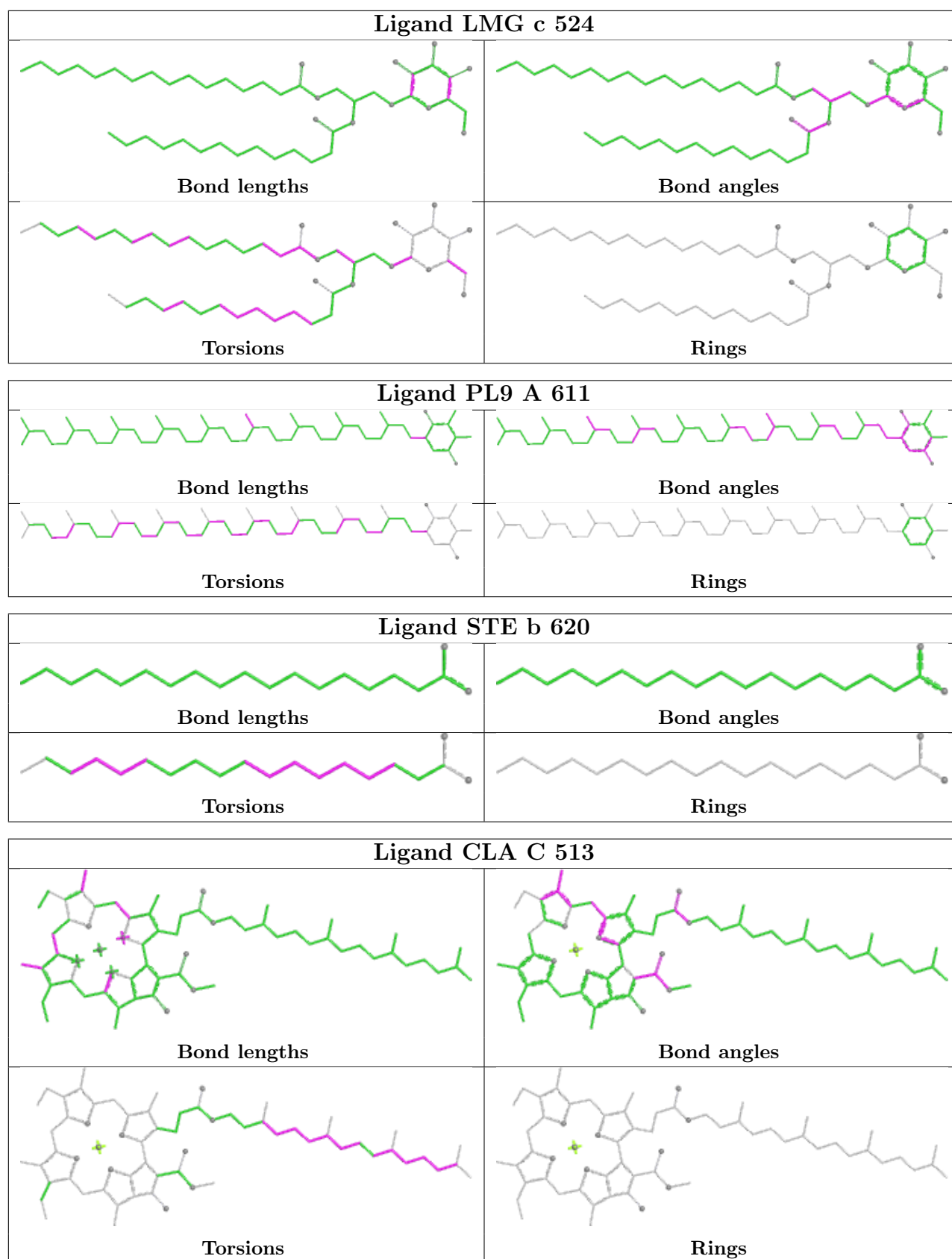
Ligand CLA B 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

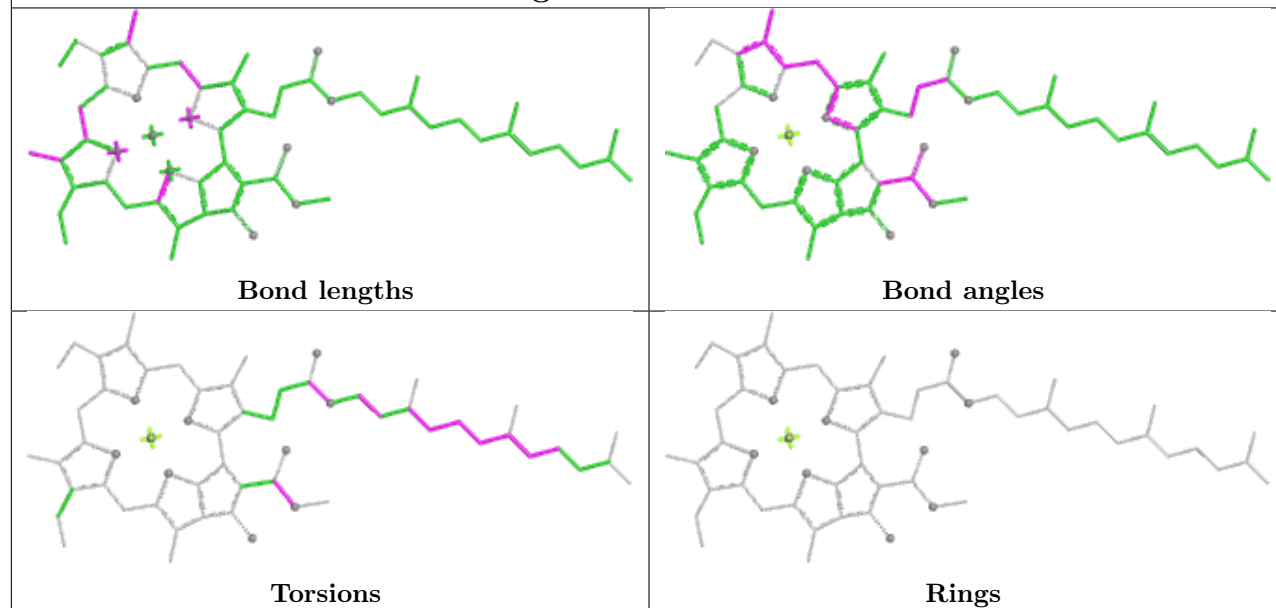
Ligand STE B 620	
	
Bond lengths	Bond angles
	
Torsions	Rings



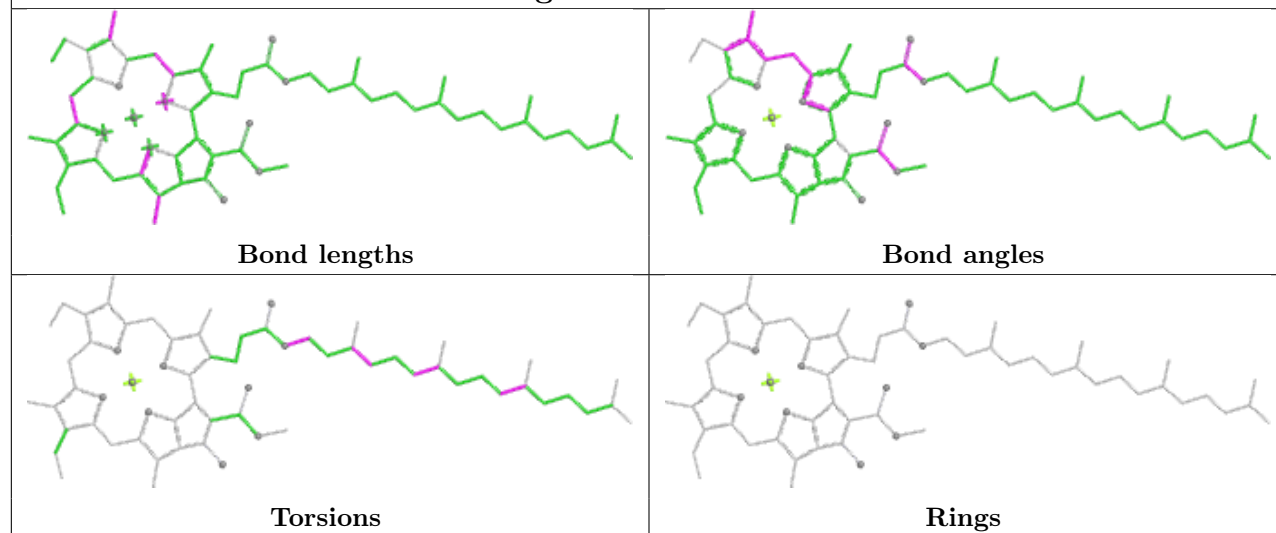


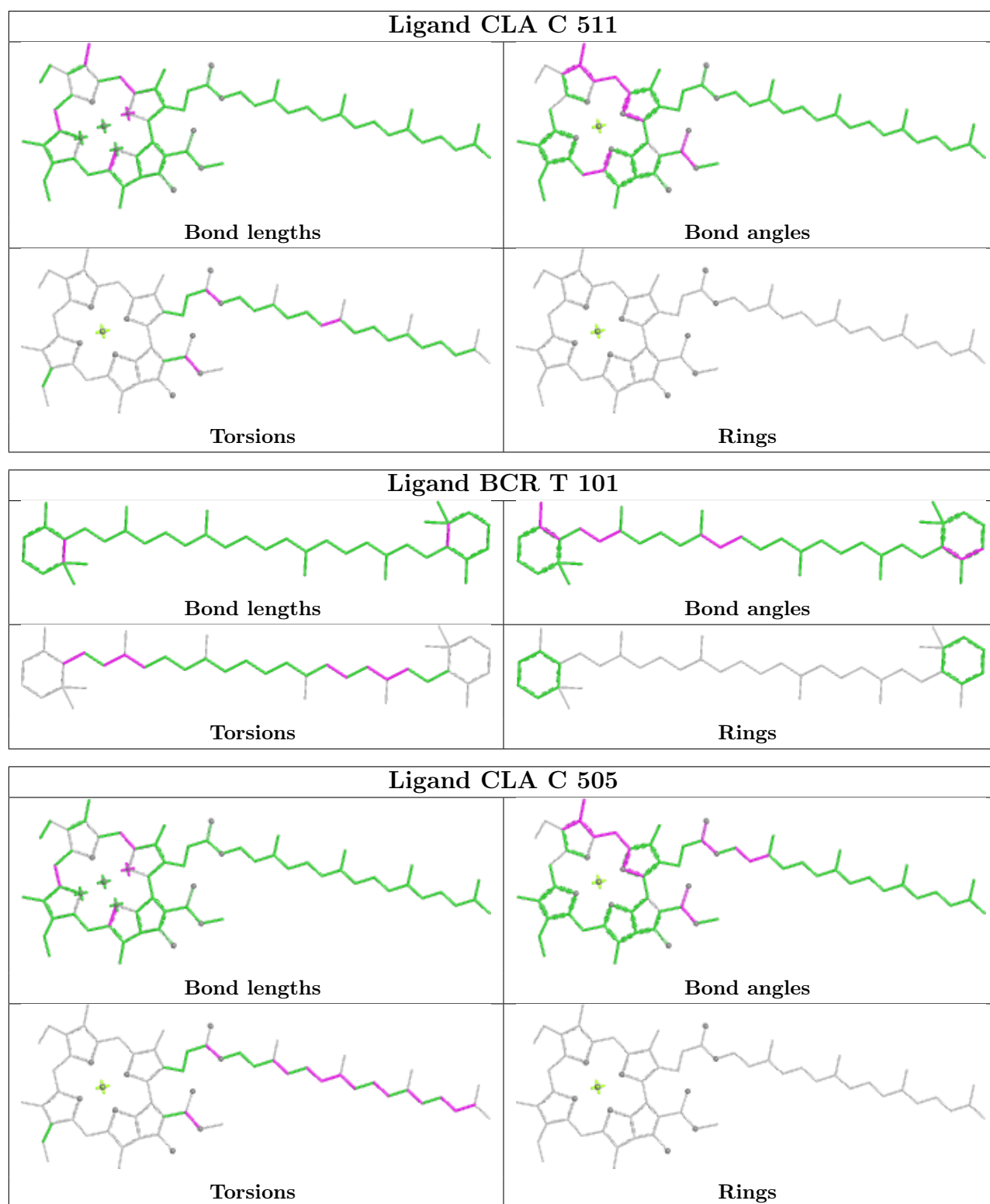


Ligand CLA B 616

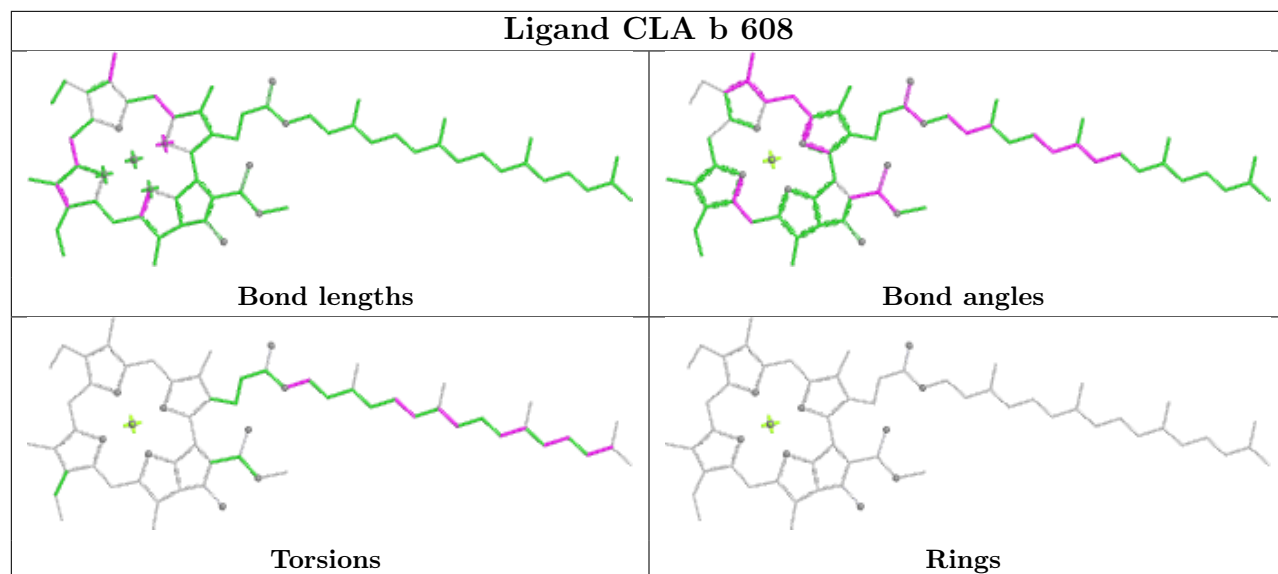


Ligand CLA d 403

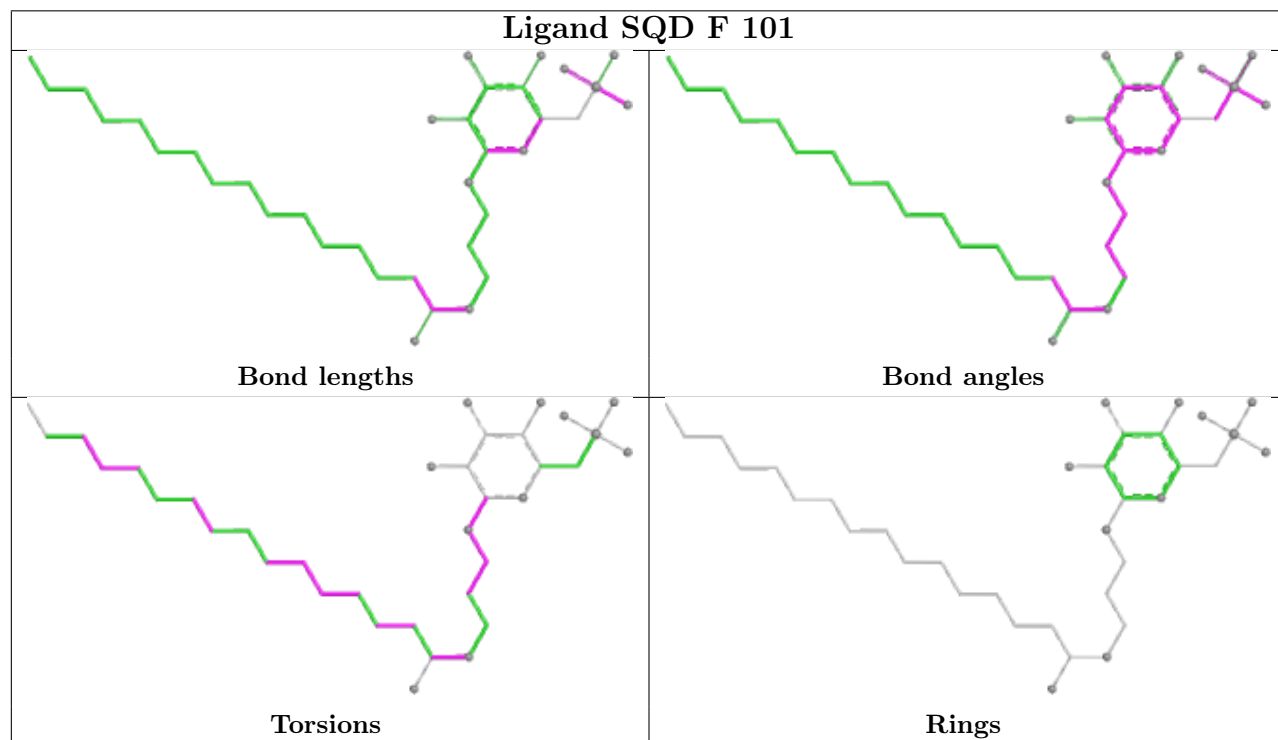




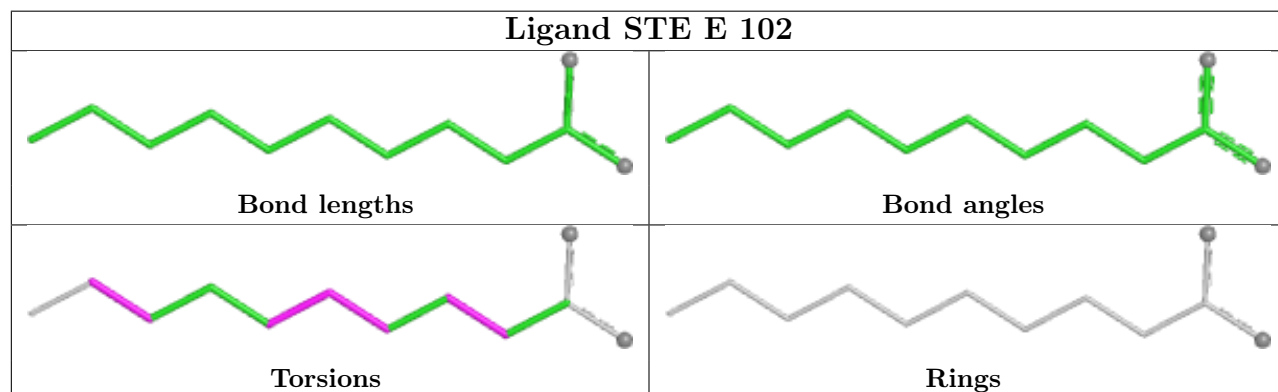
Ligand CLA b 608

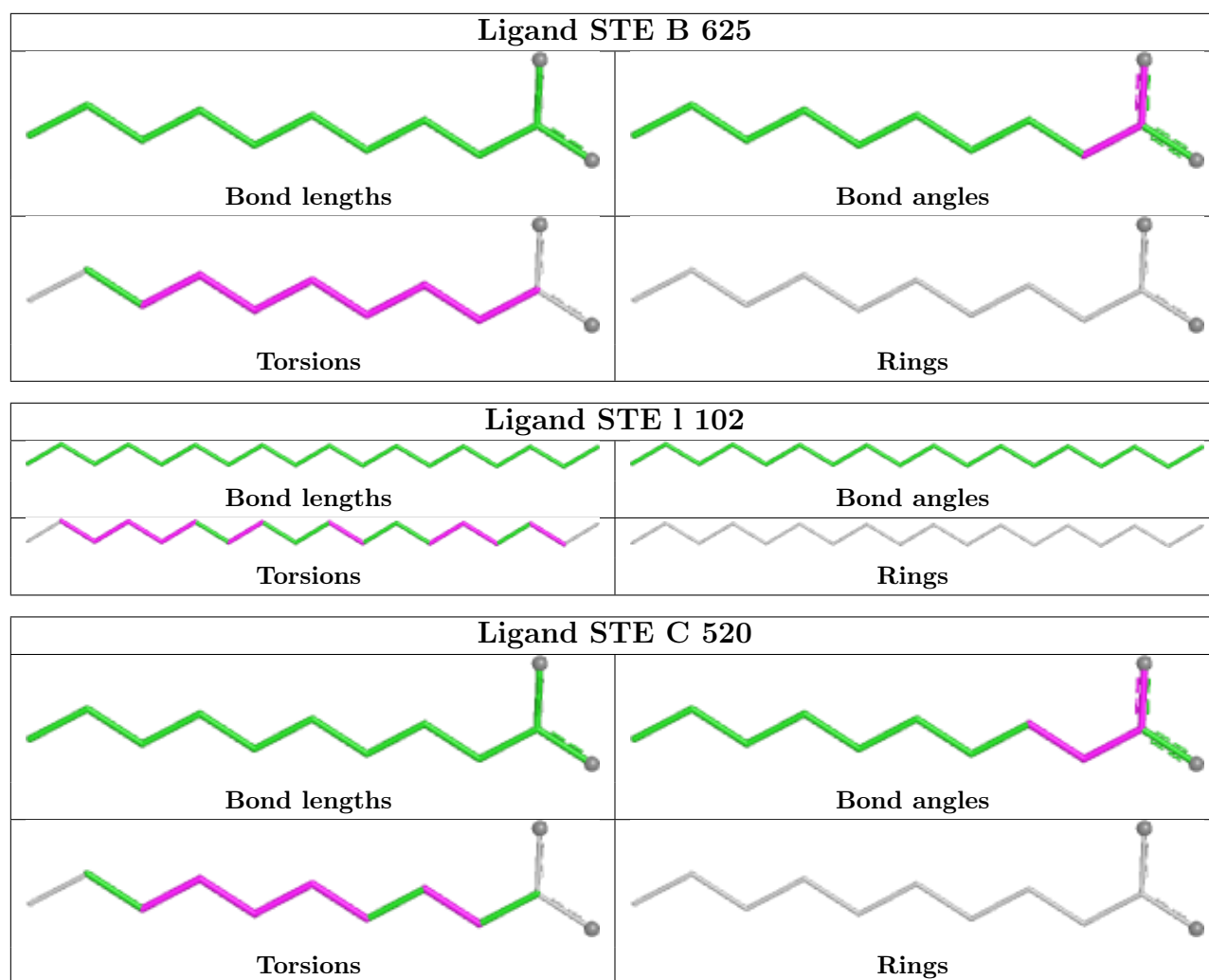


Ligand SQD F 101



Ligand STE E 102





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.50	0 100 100	13, 31, 52, 80	64 (19%)
1	a	334/344 (97%)	-0.40	1 (0%) 90 91	13, 33, 58, 76	64 (19%)
2	B	505/510 (99%)	-0.43	0 100 100	19, 35, 62, 88	4 (0%)
2	b	505/510 (99%)	-0.28	2 (0%) 89 90	27, 38, 71, 111	0
3	C	442/461 (95%)	-0.35	0 100 100	15, 38, 54, 79	11 (2%)
3	c	451/461 (97%)	-0.24	1 (0%) 92 92	15, 41, 62, 97	12 (2%)
4	D	341/352 (96%)	-0.50	1 (0%) 90 91	15, 33, 50, 78	2 (0%)
4	d	341/352 (96%)	-0.39	0 100 100	16, 36, 59, 81	3 (0%)
5	E	82/84 (97%)	0.33	3 (3%) 45 48	36, 53, 69, 85	1 (1%)
5	e	82/84 (97%)	0.32	1 (1%) 76 77	41, 59, 79, 85	0
6	F	34/45 (75%)	-0.03	1 (2%) 54 55	41, 47, 63, 85	0
6	f	34/45 (75%)	0.13	0 100 100	44, 52, 78, 94	0
7	H	65/66 (98%)	-0.19	2 (3%) 51 53	36, 42, 58, 75	0
7	h	63/66 (95%)	0.11	1 (1%) 70 71	41, 50, 61, 64	0
8	I	35/38 (92%)	-0.32	0 100 100	34, 40, 67, 83	0
8	i	35/38 (92%)	-0.20	0 100 100	33, 42, 72, 80	0
9	J	36/40 (90%)	-0.10	0 100 100	36, 51, 78, 88	0
9	j	36/40 (90%)	0.28	1 (2%) 55 57	42, 53, 86, 98	0
10	K	37/46 (80%)	0.06	0 100 100	46, 54, 71, 83	0
10	k	37/46 (80%)	0.23	0 100 100	49, 56, 70, 83	0
11	L	37/37 (100%)	-0.52	0 100 100	27, 32, 63, 68	0
11	l	36/37 (97%)	-0.61	0 100 100	28, 33, 66, 88	0
12	M	32/36 (88%)	-0.50	0 100 100	30, 36, 58, 70	0
12	m	31/36 (86%)	-0.51	0 100 100	28, 35, 52, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.19	2 (0%) 82 83	29, 43, 79, 132	1 (0%)
13	o	244/272 (89%)	-0.18	1 (0%) 89 90	29, 42, 82, 123	0
14	T	29/32 (90%)	-0.50	1 (3%) 48 50	29, 34, 60, 72	0
14	t	29/32 (90%)	-0.46	1 (3%) 48 50	29, 34, 73, 89	0
15	U	97/134 (72%)	-0.16	0 100 100	33, 45, 69, 86	0
15	u	97/134 (72%)	-0.26	1 (1%) 79 80	32, 42, 58, 87	0
16	V	137/163 (84%)	-0.29	0 100 100	32, 42, 55, 80	0
16	v	137/163 (84%)	-0.12	0 100 100	35, 48, 67, 85	0
17	Y	27/46 (58%)	0.84	2 (7%) 22 24	55, 72, 92, 96	0
17	y	30/46 (65%)	0.65	0 100 100	62, 75, 88, 94	0
18	X	38/41 (92%)	-0.04	1 (2%) 57 59	42, 52, 69, 78	0
18	x	39/41 (95%)	0.22	1 (2%) 57 59	51, 61, 87, 99	0
19	Z	62/62 (100%)	0.74	3 (4%) 36 38	55, 69, 108, 124	0
19	z	62/62 (100%)	0.62	3 (4%) 36 38	61, 71, 112, 117	0
20	R	34/41 (82%)	0.84	2 (5%) 29 31	64, 75, 84, 93	0
20	r	31/41 (75%)	1.23	4 (12%) 9 9	75, 94, 112, 117	0
All	All	5302/5700 (93%)	-0.24	36 (0%) 84 85	13, 40, 74, 132	162 (3%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	35	LEU	4.2
9	j	6	GLY	3.7
14	t	30	THR	3.4
19	Z	62	VAL	3.3
13	O	60	ARG	3.1
20	r	14	LEU	3.0
13	o	58	ASN	2.9
5	e	79	PHE	2.9
7	H	41	PHE	2.7
19	z	27	TYR	2.7
3	c	23	ALA	2.7
19	Z	33	TRP	2.6
17	Y	25	ILE	2.6
7	H	65	LEU	2.6
13	O	59	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
19	z	33	TRP	2.6
6	F	12	SER	2.5
5	E	3	GLY	2.4
17	Y	22	LEU	2.4
20	r	3	TRP	2.4
18	X	2	THR	2.3
20	r	18	TRP	2.3
7	h	64	ALA	2.3
1	a	250	ALA	2.3
15	u	53	ALA	2.3
2	b	499	VAL	2.2
4	D	227	GLU	2.2
18	x	40	SER	2.2
2	b	495	PHE	2.2
19	z	40	ILE	2.2
14	T	30	THR	2.2
19	Z	30	PRO	2.1
5	E	4	THR	2.1
20	R	6	LEU	2.1
5	E	79	PHE	2.1
20	r	28	VAL	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
14	FME	t	1	10/11	0.92	0.09	33,40,56,70	0
14	FME	T	1	10/11	0.94	0.09	29,41,54,64	0
8	FME	I	1	10/11	0.94	0.09	38,46,49,50	0
12	FME	M	1	10/11	0.95	0.09	39,47,62,64	0
12	FME	m	1	10/11	0.96	0.09	30,46,64,66	0
8	FME	i	1	10/11	0.96	0.08	36,49,53,53	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

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
33	STE	b	622	20/20	0.74	0.17	47,58,69,70	0
33	STE	H	103	18/20	0.75	0.19	47,63,69,73	0
31	LHG	A	614	49/49	0.76	0.16	54,76,98,103	0
29	LMG	b	621	55/55	0.78	0.17	53,65,77,85	0
33	STE	x	102	20/20	0.78	0.15	45,53,60,64	0
29	LMG	c	522	48/55	0.80	0.15	45,69,89,93	0
33	STE	m	102	12/20	0.80	0.18	50,56,67,69	0
33	STE	a	616	10/20	0.80	0.15	37,55,60,62	0
32	DGD	a	615	44/66	0.81	0.14	36,51,70,72	0
33	STE	B	626	16/20	0.81	0.15	42,59,71,72	0
28	PL9	A	611	55/55	0.81	0.17	42,61,74,85	0
33	STE	I	101	15/20	0.81	0.16	39,48,61,65	0
29	LMG	d	410	23/55	0.82	0.17	41,59,69,72	0
33	STE	E	102	12/20	0.82	0.15	60,67,83,84	0
33	STE	b	623	10/20	0.82	0.13	43,50,62,63	0
33	STE	c	521	20/20	0.82	0.13	42,54,83,83	0
33	STE	c	523	12/20	0.82	0.12	54,62,72,77	0
31	LHG	e	101	42/49	0.82	0.14	57,77,97,102	0
30	SQD	a	614	36/54	0.82	0.14	35,55,66,72	0
29	LMG	A	612	48/55	0.83	0.12	45,57,68,75	0
33	STE	J	101	12/20	0.83	0.14	46,54,61,64	0
33	STE	T	102	16/20	0.83	0.14	36,47,61,66	0
33	STE	d	412	16/20	0.83	0.14	48,54,75,77	0
29	LMG	D	411	33/55	0.83	0.14	41,52,69,74	0
28	PL9	a	611	55/55	0.83	0.16	43,64,79,85	0
32	DGD	A	617	66/66	0.84	0.12	45,57,67,74	0
33	STE	a	617	12/20	0.84	0.12	52,58,64,66	0
25	CLA	b	601	65/65	0.84	0.12	49,64,78,89	0
33	STE	B	620	17/20	0.85	0.12	38,47,64,66	0
30	SQD	A	616	39/54	0.86	0.13	39,49,72,77	0
30	SQD	f	102	41/54	0.86	0.14	63,78,89,92	0
33	STE	j	101	12/20	0.86	0.13	49,55,61,67	0
33	STE	T	103	15/20	0.86	0.14	44,53,64,66	0
33	STE	C	521	16/20	0.86	0.13	37,49,64,65	0
33	STE	D	413	20/20	0.87	0.12	37,46,70,81	0
33	STE	b	620	20/20	0.87	0.11	38,52,71,73	0
29	LMG	c	520	37/55	0.87	0.12	45,64,74,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	STE	C	519	12/20	0.87	0.12	34,42,52,53	0
33	STE	B	624	18/20	0.87	0.12	40,49,78,85	0
33	STE	C	520	12/20	0.88	0.11	43,49,57,58	0
29	LMG	c	524	49/55	0.88	0.10	40,56,68,73	0
33	STE	B	625	12/20	0.88	0.12	44,59,64,67	0
30	SQD	B	622	54/54	0.88	0.11	40,57,82,93	0
25	CLA	B	601	65/65	0.88	0.11	37,53,75,87	0
29	LMG	M	101	51/55	0.89	0.10	31,46,62,65	0
29	LMG	B	621	28/55	0.89	0.12	38,48,58,70	0
29	LMG	m	101	51/55	0.89	0.10	34,49,64,70	0
29	LMG	C	518	48/55	0.89	0.12	45,63,73,78	0
27	BCR	d	405	40/40	0.89	0.12	39,49,78,87	0
30	SQD	F	101	36/54	0.89	0.12	49,66,74,77	0
30	SQD	L	101	49/54	0.89	0.10	37,55,73,77	0
33	STE	t	102	14/20	0.89	0.11	36,49,54,61	0
33	STE	B	623	12/20	0.89	0.12	41,51,60,68	0
27	BCR	x	101	40/40	0.90	0.11	42,54,65,71	0
33	STE	l	102	18/20	0.90	0.12	36,44,63,66	0
33	STE	M	103	10/20	0.90	0.11	41,44,50,50	0
30	SQD	a	613	54/54	0.90	0.10	40,57,71,73	0
33	STE	d	413	17/20	0.90	0.12	46,51,62,65	0
27	BCR	Y	101	40/40	0.91	0.10	46,52,61,64	0
32	DGD	h	101	62/66	0.91	0.09	38,45,53,53	0
27	BCR	c	514	40/40	0.91	0.10	44,55,64,66	0
25	CLA	C	513	65/65	0.91	0.10	44,56,83,89	0
27	BCR	k	101	40/40	0.91	0.11	47,57,64,68	0
27	BCR	B	618	40/40	0.91	0.09	29,36,47,50	0
27	BCR	D	406	40/40	0.91	0.10	34,41,66,70	0
27	BCR	H	101	40/40	0.91	0.09	35,43,50,55	0
32	DGD	c	518	62/66	0.92	0.09	37,48,74,80	0
27	BCR	K	102	40/40	0.92	0.11	39,49,63,65	0
27	BCR	C	514	40/40	0.92	0.09	32,39,47,47	0
33	STE	M	102	15/20	0.92	0.10	37,46,62,67	0
32	DGD	C	516	62/66	0.92	0.10	38,47,83,95	0
32	DGD	H	102	62/66	0.92	0.09	34,42,49,53	0
27	BCR	K	101	40/40	0.92	0.11	49,56,60,61	0
25	CLA	c	513	65/65	0.93	0.10	47,61,81,86	0
27	BCR	A	610	40/40	0.93	0.08	27,34,40,43	0
32	DGD	C	515	62/66	0.93	0.10	27,37,65,71	0
27	BCR	T	101	40/40	0.93	0.07	31,37,49,53	0
30	SQD	A	613	52/54	0.93	0.10	32,53,75,79	0
25	CLA	C	503	65/65	0.93	0.08	33,42,47,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
27	BCR	b	618	40/40	0.93	0.07	28,38,48,53	0
29	LMG	D	408	51/55	0.93	0.10	33,47,64,71	0
27	BCR	B	619	40/40	0.93	0.08	32,40,46,49	0
27	BCR	c	516	40/40	0.93	0.11	45,53,58,66	0
25	CLA	C	512	65/65	0.93	0.09	35,51,68,77	0
25	CLA	c	509	65/65	0.93	0.10	38,45,55,58	0
25	CLA	c	512	65/65	0.93	0.10	45,53,76,81	0
34	BCT	a	606	4/4	0.93	0.08	34,40,44,49	0
27	BCR	t	101	40/40	0.94	0.07	28,36,46,47	0
25	CLA	c	508	64/65	0.94	0.09	32,43,73,90	0
31	LHG	d	407	49/49	0.94	0.10	32,46,58,65	0
31	LHG	d	409	39/49	0.94	0.09	32,43,54,58	0
25	CLA	B	606	65/65	0.94	0.08	26,36,57,62	0
28	PL9	D	407	55/55	0.94	0.07	23,32,38,45	0
27	BCR	b	617	40/40	0.94	0.07	30,38,43,43	0
25	CLA	c	511	65/65	0.94	0.09	40,52,61,64	0
32	DGD	C	517	62/66	0.94	0.08	34,43,66,71	0
27	BCR	b	619	40/40	0.94	0.08	33,42,57,60	0
25	CLA	C	510	65/65	0.94	0.08	32,42,51,54	0
27	BCR	c	515	40/40	0.94	0.08	34,41,48,55	0
25	CLA	C	511	65/65	0.94	0.09	36,48,57,65	0
25	CLA	c	506	65/65	0.94	0.08	36,44,74,78	0
27	BCR	B	617	40/40	0.94	0.07	32,38,49,50	0
25	CLA	a	608	65/65	0.95	0.09	31,38,79,85	0
25	CLA	B	604	65/65	0.95	0.07	23,31,58,61	0
25	CLA	b	606	65/65	0.95	0.07	28,38,58,64	0
25	CLA	b	608	65/65	0.95	0.07	33,41,51,53	0
25	CLA	b	614	65/65	0.95	0.08	25,37,60,65	0
25	CLA	b	615	65/65	0.95	0.08	29,40,50,51	0
25	CLA	b	616	60/65	0.95	0.08	32,40,70,73	0
29	LMG	d	411	44/55	0.95	0.08	39,45,71,76	0
25	CLA	c	501	65/65	0.95	0.07	30,38,45,50	0
27	BCR	a	610	40/40	0.95	0.06	24,31,40,44	0
25	CLA	c	502	65/65	0.95	0.07	32,41,53,60	0
25	CLA	c	503	65/65	0.95	0.07	33,44,49,53	0
25	CLA	c	504	60/65	0.95	0.07	35,42,72,73	0
25	CLA	c	505	65/65	0.95	0.07	29,39,54,58	0
25	CLA	C	506	65/65	0.95	0.08	29,42,72,76	0
25	CLA	c	507	65/65	0.95	0.08	30,40,50,56	0
25	CLA	C	507	65/65	0.95	0.07	28,36,48,51	0
25	CLA	C	508	65/65	0.95	0.08	30,39,82,89	0
31	LHG	D	410	47/49	0.95	0.09	28,39,66,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	LHG	D	412	49/49	0.95	0.09	30,40,54,58	0
25	CLA	c	510	65/65	0.95	0.08	37,47,53,61	0
25	CLA	C	509	65/65	0.95	0.08	31,39,52,58	0
25	CLA	B	610	65/65	0.95	0.07	23,30,38,41	0
31	LHG	l	101	49/49	0.95	0.08	31,42,48,53	0
25	CLA	B	616	60/65	0.95	0.09	26,36,74,85	0
25	CLA	d	404	65/65	0.95	0.08	32,41,75,81	0
28	PL9	d	406	55/55	0.95	0.07	27,33,37,41	0
26	PHO	d	401	64/64	0.95	0.06	24,31,36,38	0
25	CLA	C	501	65/65	0.95	0.07	25,33,44,48	0
25	CLA	C	502	65/65	0.95	0.07	32,39,48,53	0
32	DGD	c	517	62/66	0.95	0.08	29,38,60,66	0
25	CLA	a	607	65/65	0.95	0.07	23,30,38,50	0
34	BCT	D	401	4/4	0.95	0.08	34,39,39,40	0
32	DGD	c	519	62/66	0.95	0.08	32,45,68,76	0
25	CLA	b	610	65/65	0.96	0.07	29,37,42,46	0
25	CLA	b	611	65/65	0.96	0.06	26,33,46,53	0
25	CLA	b	612	65/65	0.96	0.07	27,33,43,51	0
25	CLA	b	613	65/65	0.96	0.07	23,31,61,67	0
25	CLA	C	505	65/65	0.96	0.08	27,36,59,61	0
25	CLA	B	608	65/65	0.96	0.06	24,31,45,50	0
25	CLA	B	609	65/65	0.96	0.07	28,37,43,48	0
25	CLA	B	602	65/65	0.96	0.07	29,37,48,53	0
25	CLA	B	611	65/65	0.96	0.06	22,29,41,46	0
25	CLA	B	612	65/65	0.96	0.07	24,31,39,44	0
25	CLA	B	613	65/65	0.96	0.06	22,30,55,60	0
25	CLA	B	614	65/65	0.96	0.07	27,35,61,74	0
25	CLA	B	615	65/65	0.96	0.07	29,36,53,63	0
25	CLA	D	405	65/65	0.96	0.07	28,36,81,92	0
31	LHG	A	615	49/49	0.96	0.07	30,37,47,57	0
31	LHG	D	409	49/49	0.96	0.07	27,36,44,52	0
25	CLA	B	603	65/65	0.96	0.07	24,31,49,53	0
25	CLA	A	607	65/65	0.96	0.09	26,32,83,88	0
25	CLA	a	609	65/65	0.96	0.08	23,30,63,67	0
31	LHG	d	408	49/49	0.96	0.07	30,40,47,57	0
25	CLA	a	612	65/65	0.96	0.06	22,30,36,42	0
25	CLA	B	605	65/65	0.96	0.06	23,31,40,42	0
25	CLA	b	602	65/65	0.96	0.07	30,39,51,55	0
25	CLA	d	403	65/65	0.96	0.07	25,33,46,55	0
25	CLA	b	603	65/65	0.96	0.07	25,33,55,62	0
26	PHO	A	608	64/64	0.96	0.05	20,28,33,39	0
26	PHO	D	402	64/64	0.96	0.06	25,32,38,42	0

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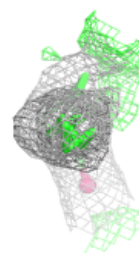
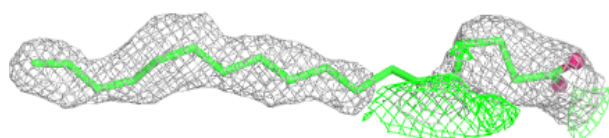
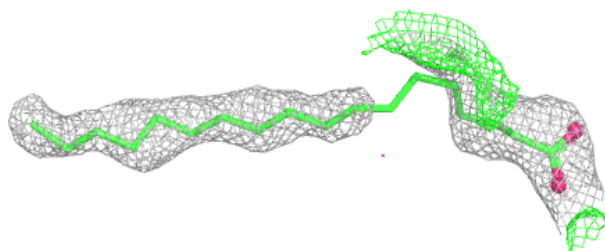
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	CLA	b	604	65/65	0.96	0.08	25,33,63,76	0
26	PHO	d	402	64/64	0.96	0.06	29,38,43,49	0
25	CLA	b	605	65/65	0.96	0.07	22,35,43,46	0
25	CLA	A	606	65/65	0.96	0.06	22,27,37,43	0
25	CLA	C	504	59/65	0.96	0.07	32,39,66,71	0
25	CLA	b	609	65/65	0.96	0.07	33,41,55,63	0
35	HEM	f	101	43/43	0.96	0.09	47,59,75,85	0
25	CLA	b	607	65/65	0.97	0.07	22,32,50,58	0
25	CLA	D	404	65/65	0.97	0.06	21,29,45,48	0
25	CLA	A	609	54/65	0.97	0.06	21,28,58,62	0
25	CLA	B	607	65/65	0.97	0.07	20,29,52,58	0
35	HEM	E	101	43/43	0.97	0.08	44,50,62,68	0
25	CLA	D	403	65/65	0.97	0.05	21,27,38,44	0
24	CL	a	604	1/1	0.98	0.05	32,32,32,32	0
36	HEC	V	201	43/43	0.98	0.07	27,34,41,45	0
36	HEC	v	201	43/43	0.98	0.07	31,38,43,50	0
22	OEX	a	602[A]	10/10	0.99	0.03	29,32,36,37	10
23	FE2	a	603	1/1	0.99	0.02	38,38,38,38	0
24	CL	A	604	1/1	0.99	0.04	33,33,33,33	0
24	CL	A	605	1/1	0.99	0.08	34,34,34,34	0
21	OEY	A	601[B]	11/11	0.99	0.03	26,29,33,34	11
24	CL	a	605	1/1	0.99	0.08	33,33,33,33	0
21	OEY	a	601[B]	11/11	0.99	0.03	27,30,33,38	11
22	OEX	A	602[A]	10/10	0.99	0.03	31,32,36,38	10
23	FE2	A	603	1/1	1.00	0.01	32,32,32,32	0

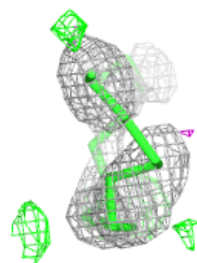
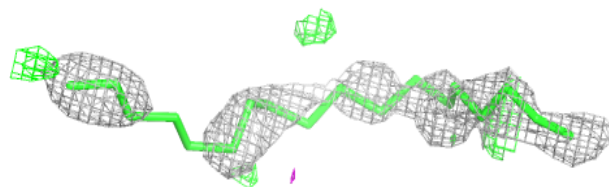
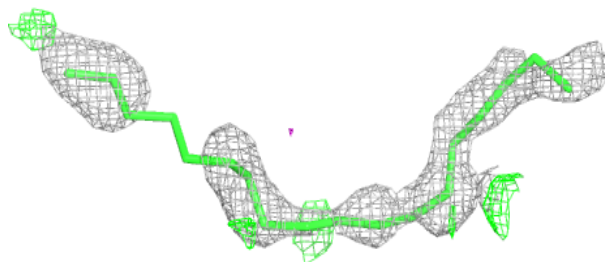
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE 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)

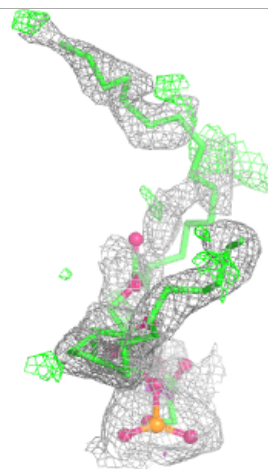
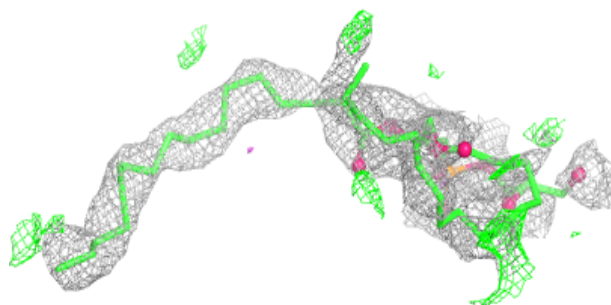
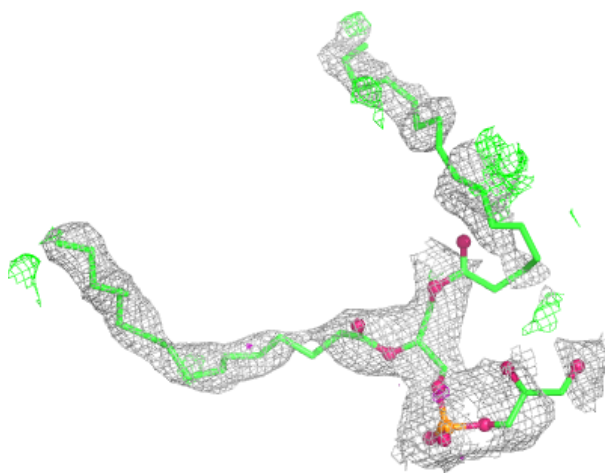
**Electron density around STE H 103:**

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



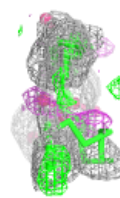
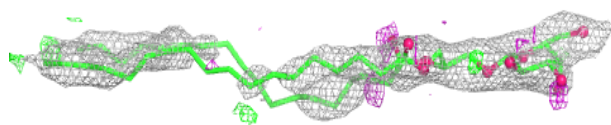
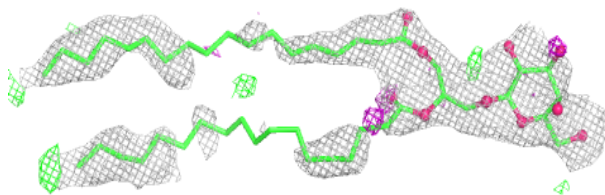
Electron density around LHG A 614:

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

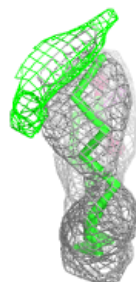
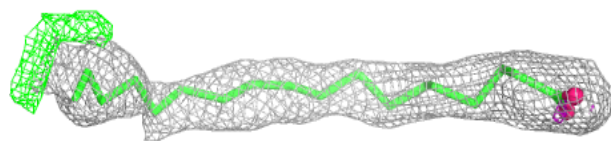
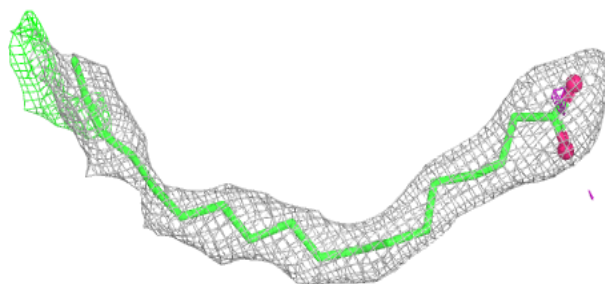


Electron density around LMG b 621:

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

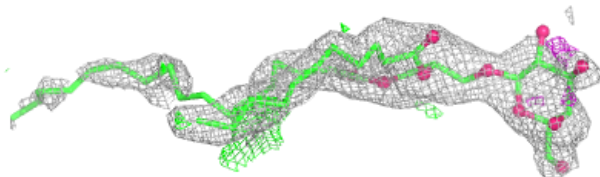
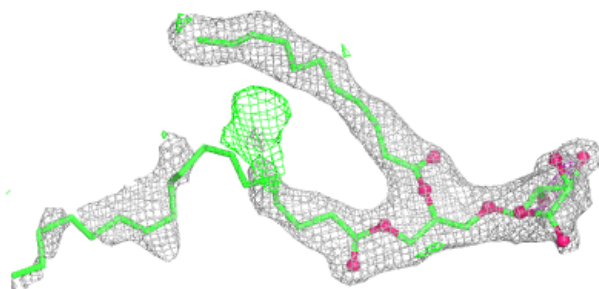
**Electron density around STE x 102:**

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

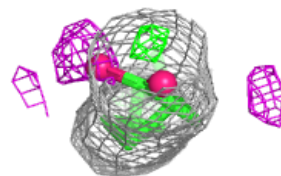
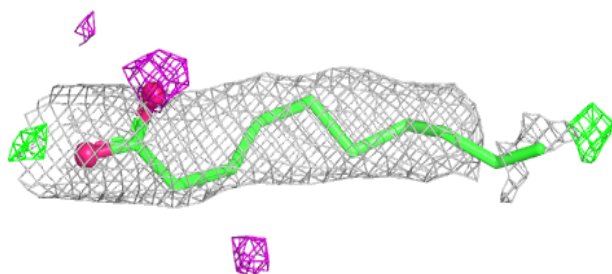
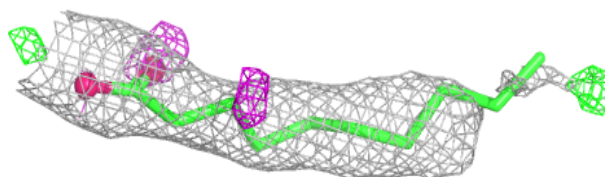


Electron density around LMG c 522:

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

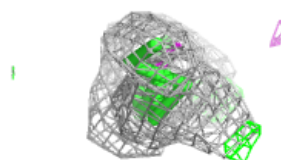
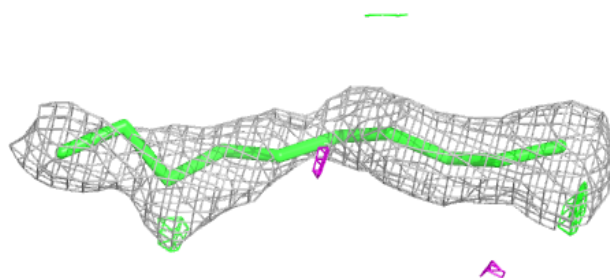
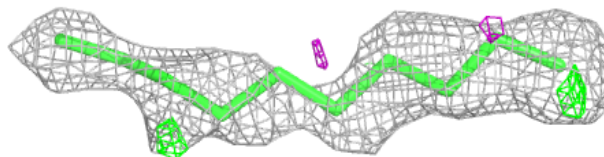
**Electron density around STE m 102:**

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

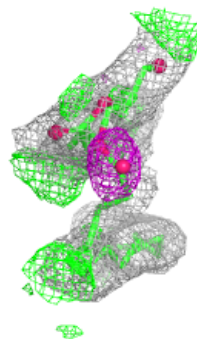
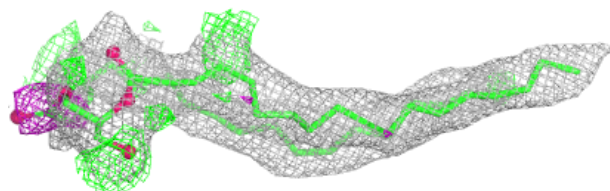
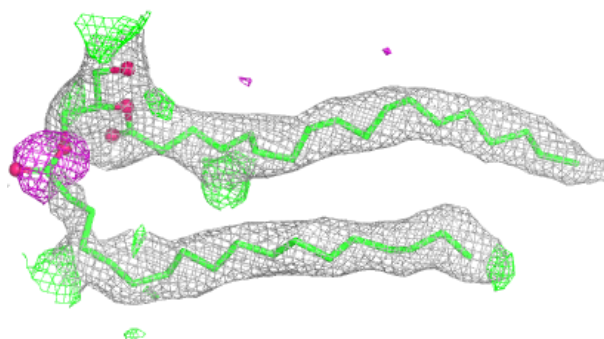


Electron density around STE a 616:

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

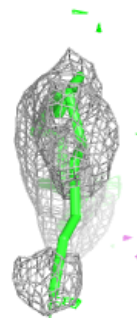
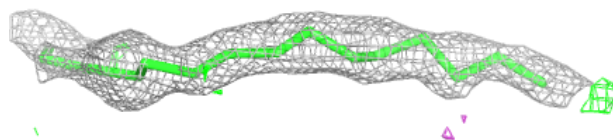
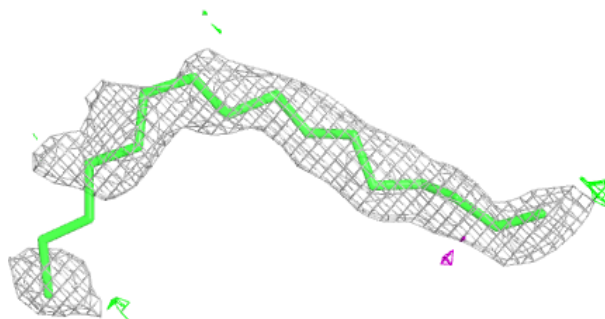
**Electron density around DGD a 615:**

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

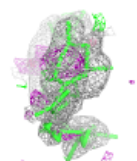
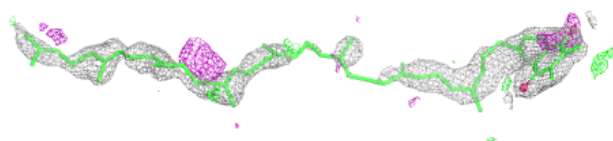
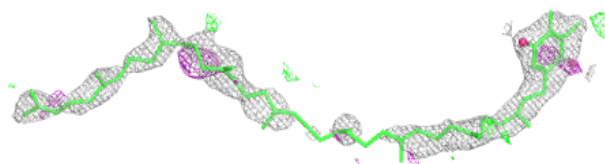


Electron density around STE B 626:

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

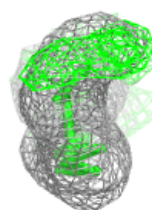
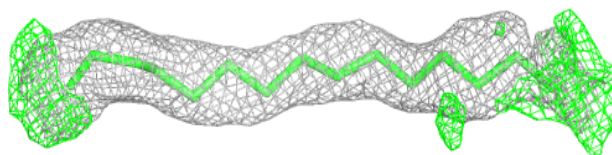
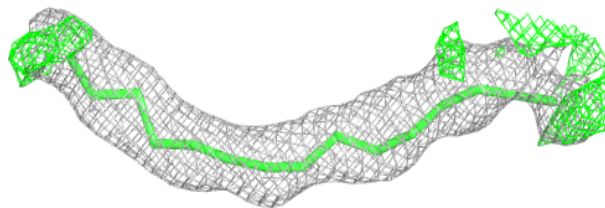
**Electron density around PL9 A 611:**

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

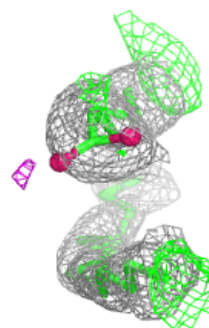
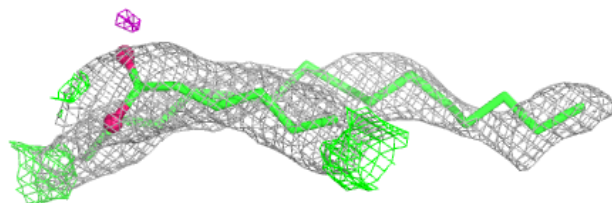
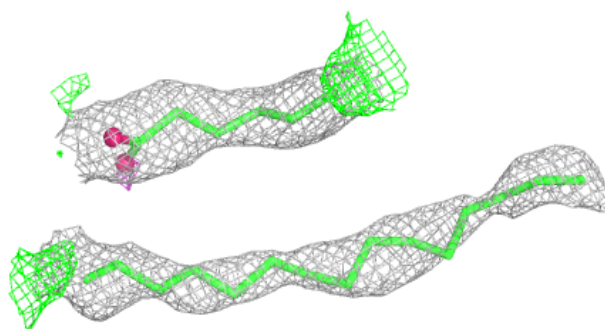


Electron density around STE I 101:

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

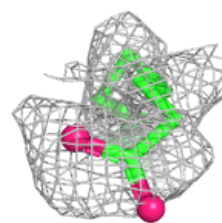
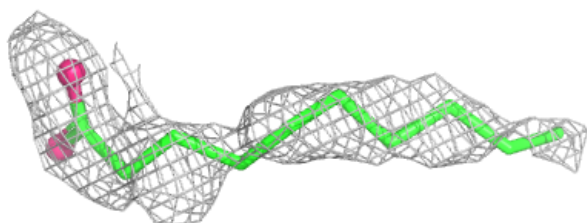
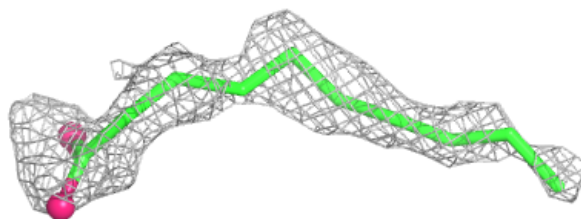
**Electron density around LMG d 410:**

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

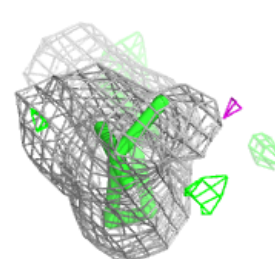
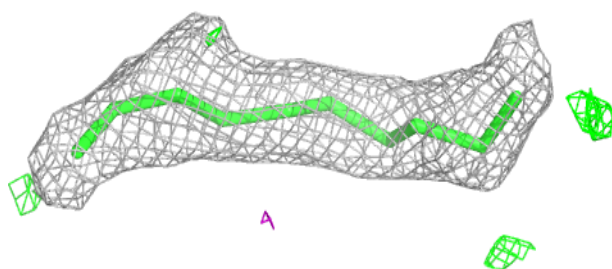
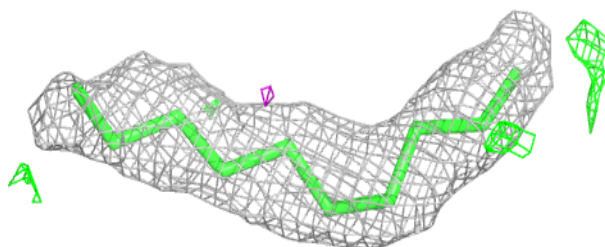


Electron density around STE E 102:

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

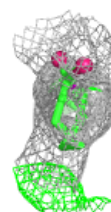
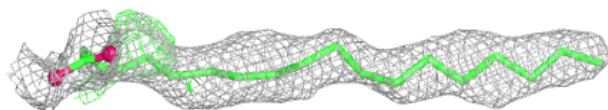
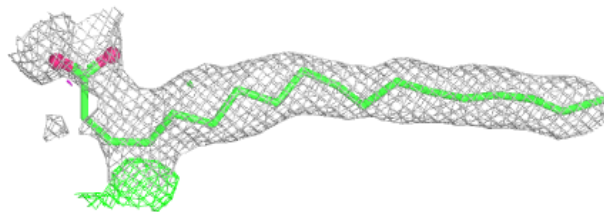
**Electron density around STE b 623:**

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

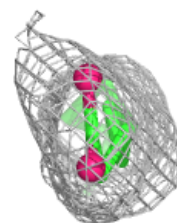
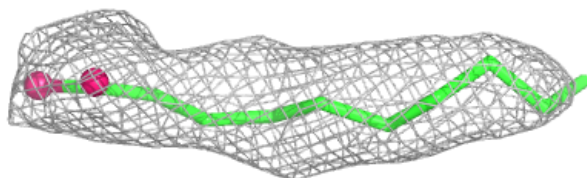
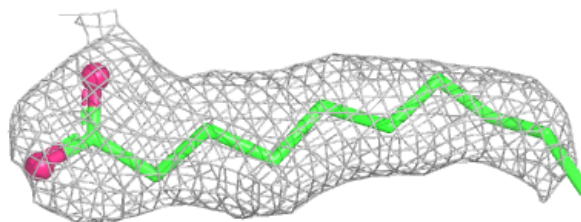


Electron density around STE c 521:

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

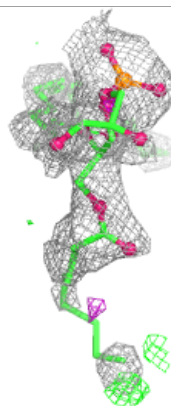
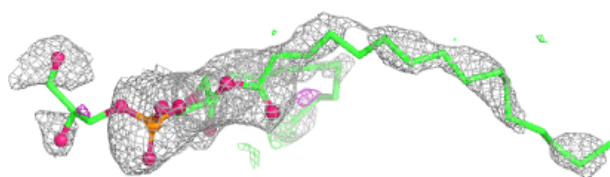
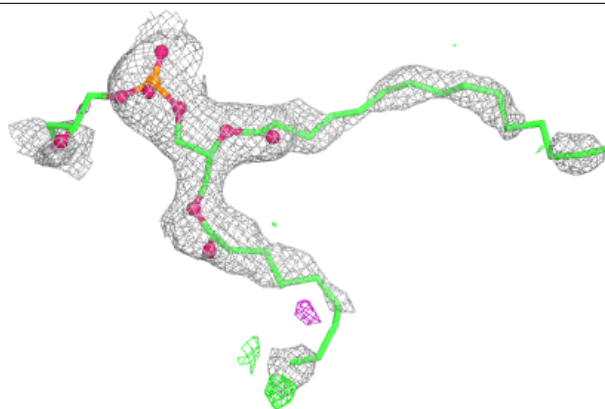
**Electron density around STE c 523:**

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



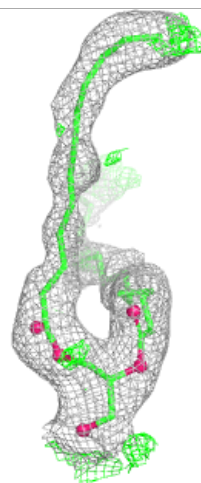
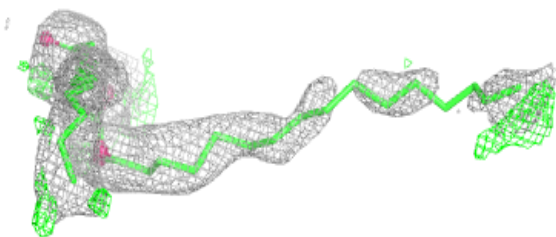
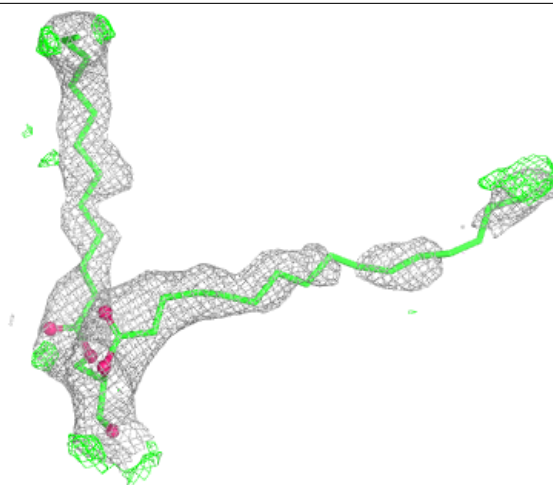
Electron density around LHG e 101:

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



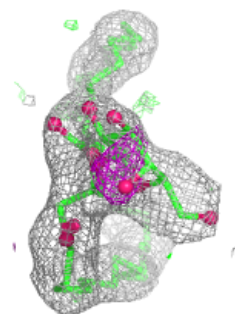
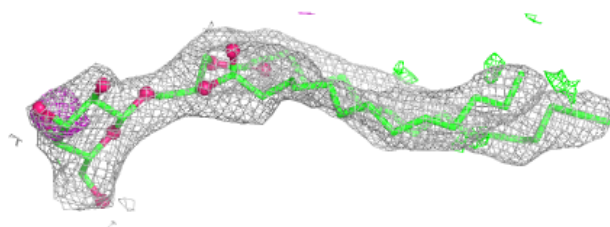
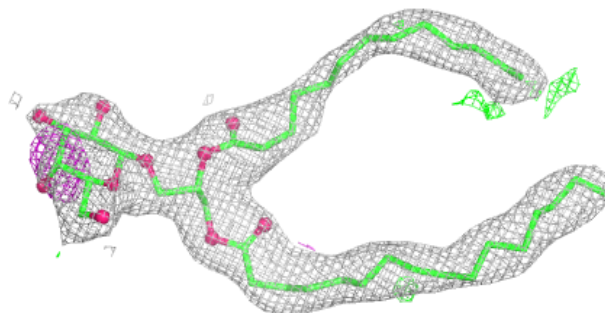
Electron density around SQD a 614:

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

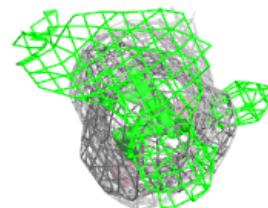
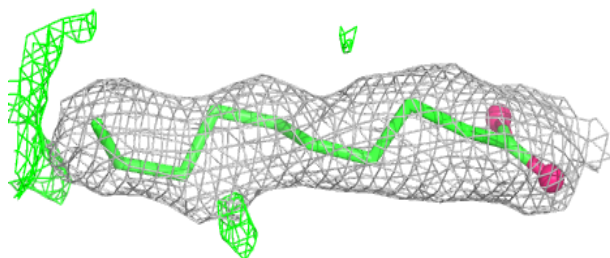
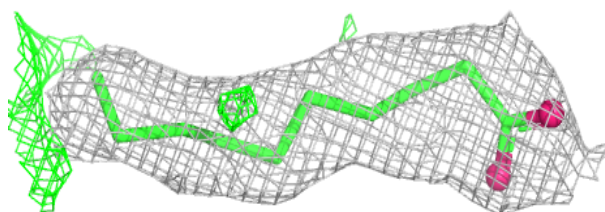


Electron density around LMG A 612:

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

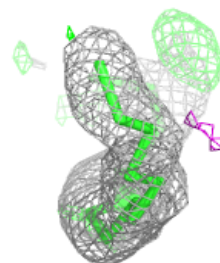
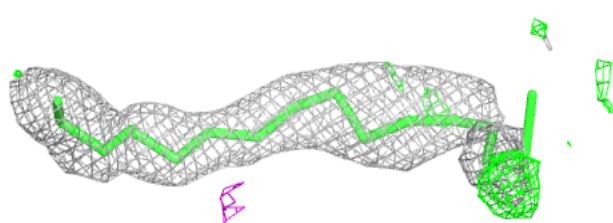
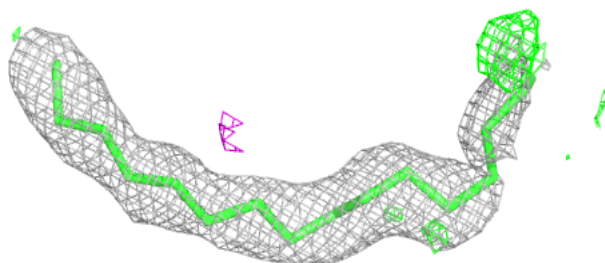
**Electron density around STE J 101:**

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

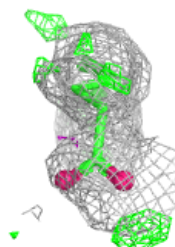
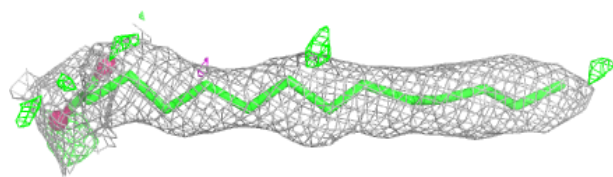
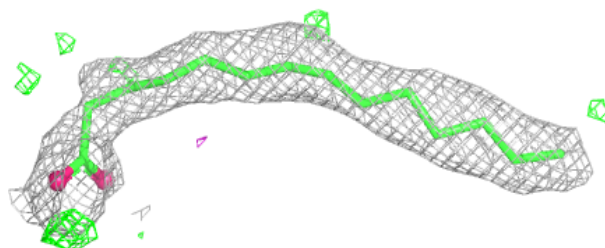


Electron density around STE T 102:

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

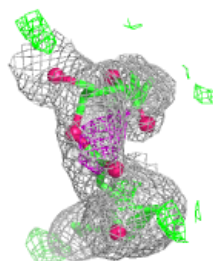
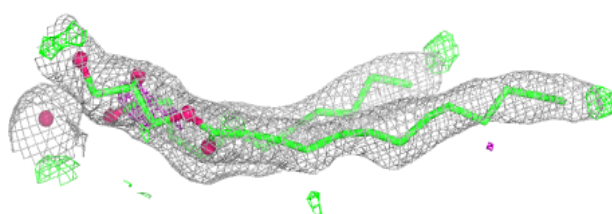
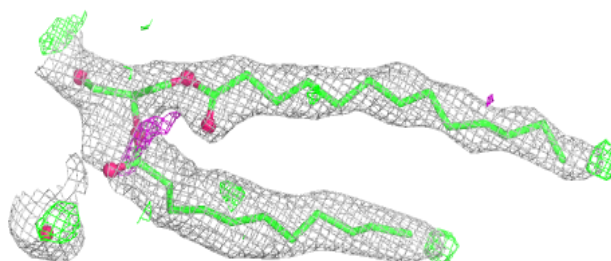
**Electron density around STE d 412:**

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

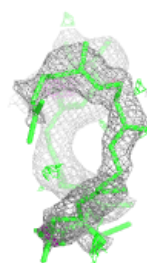
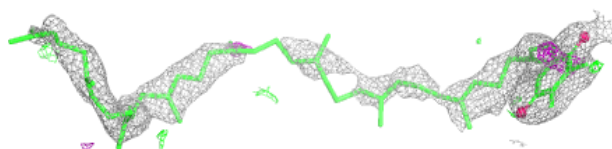
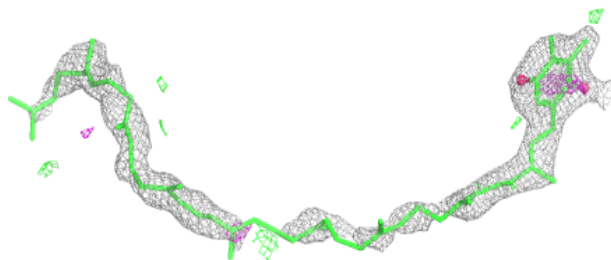


Electron density around LMG D 411:

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

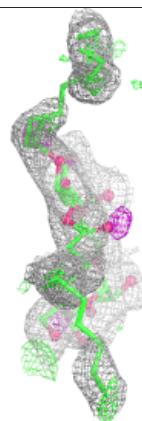
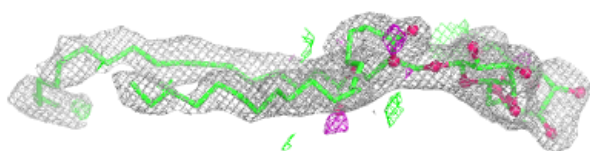
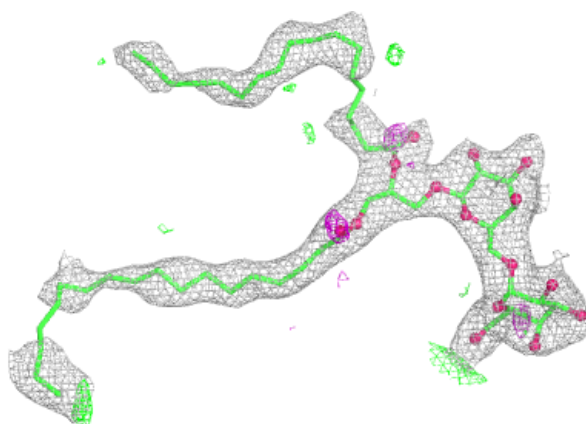
**Electron density around PL9 a 611:**

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

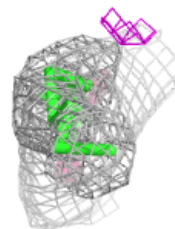
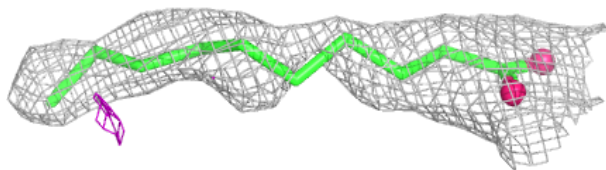
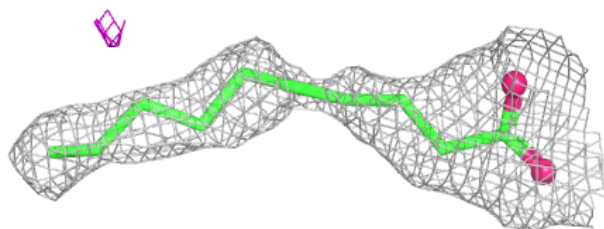


Electron density around DGD A 617:

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

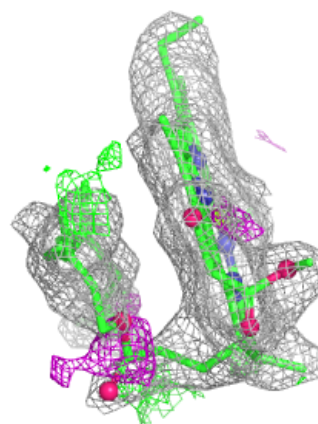
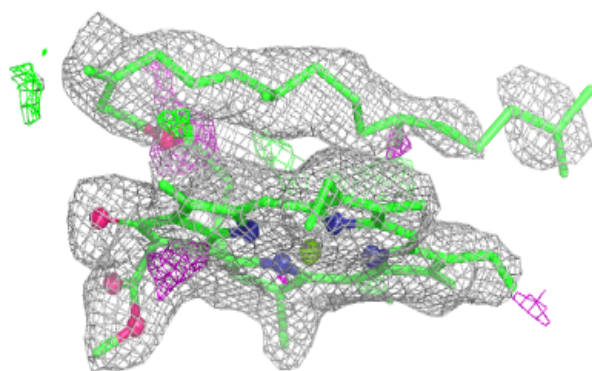
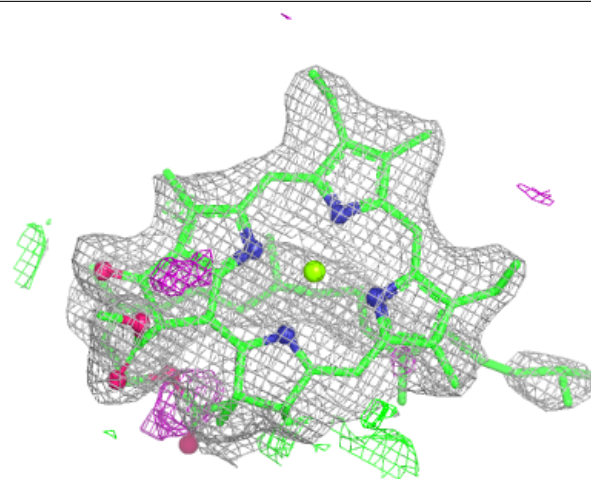
**Electron density around STE a 617:**

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



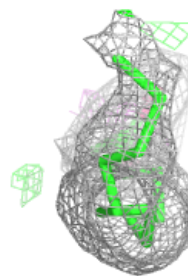
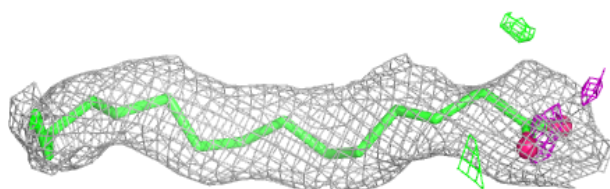
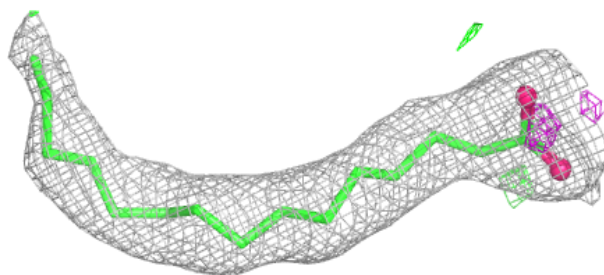
Electron density around CLA b 601:

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



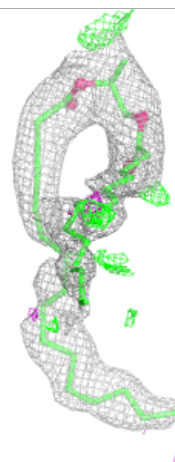
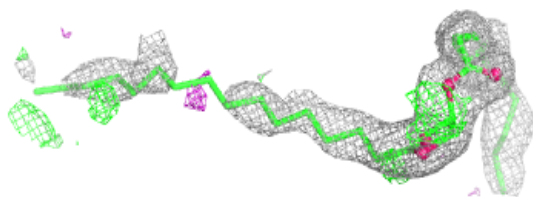
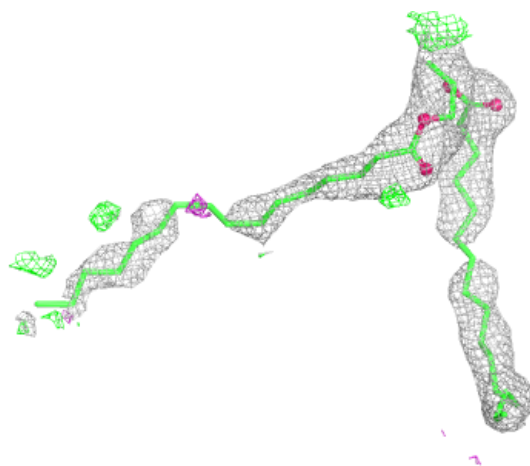
Electron density around STE B 620:

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



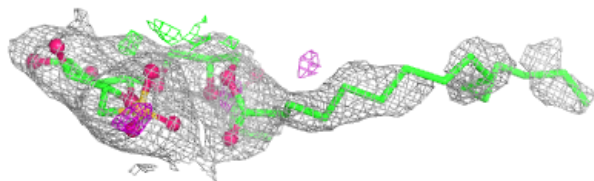
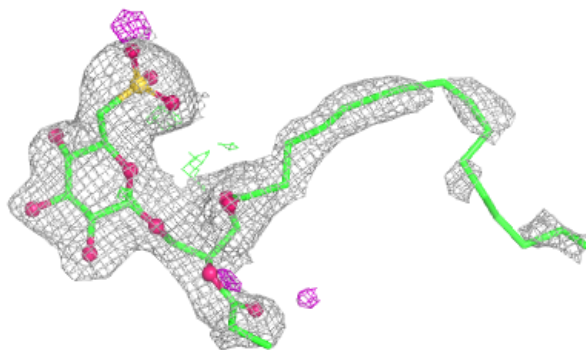
Electron density around SQD A 616:

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

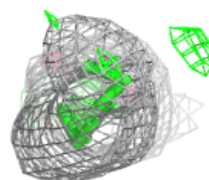
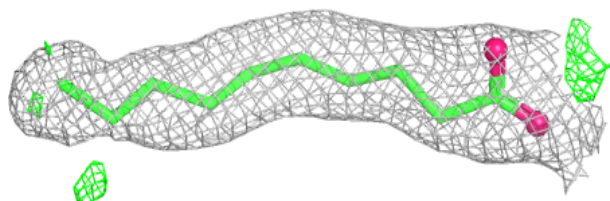
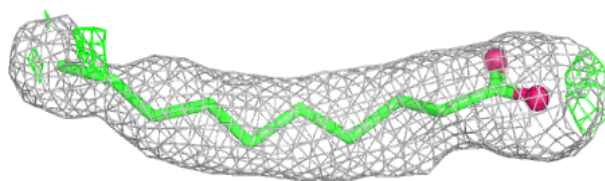


Electron density around SQD f 102:

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

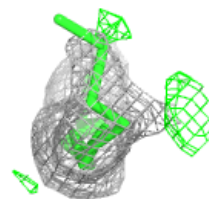
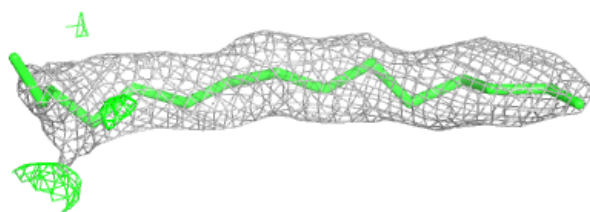
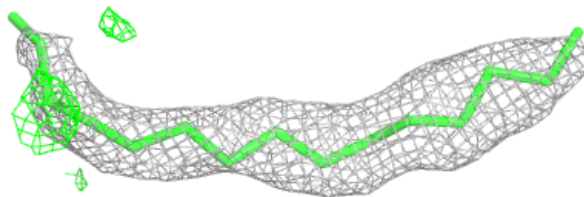
**Electron density around STE j 101:**

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

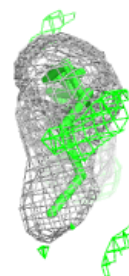
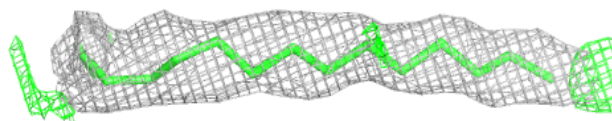
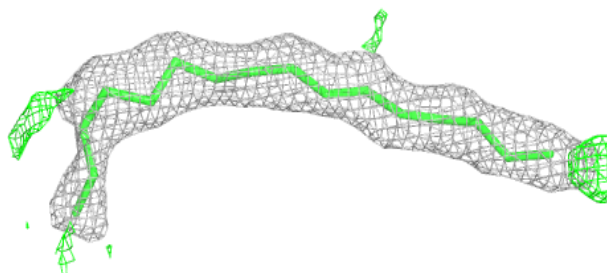


Electron density around STE T 103:

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

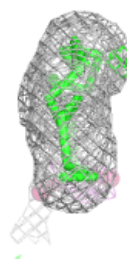
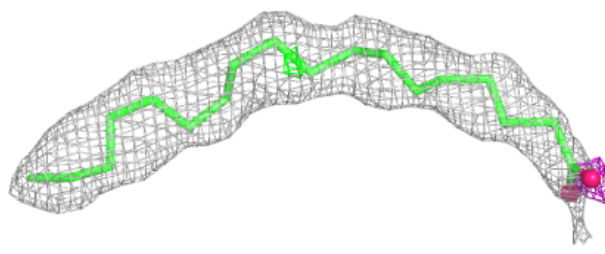
**Electron density around STE C 521:**

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

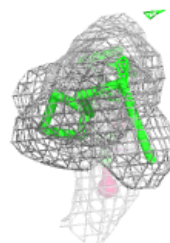
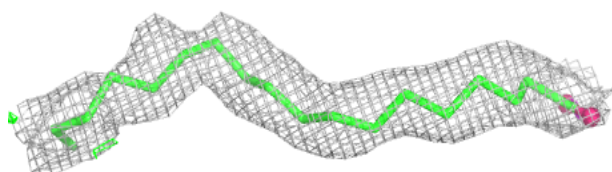
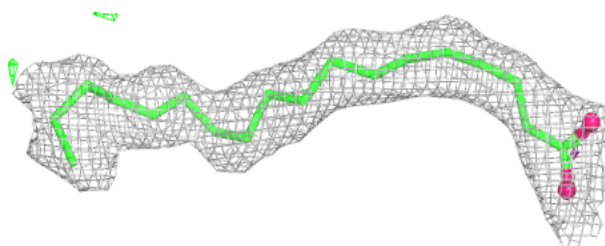


Electron density around STE D 413:

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

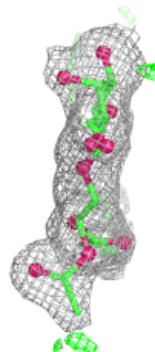
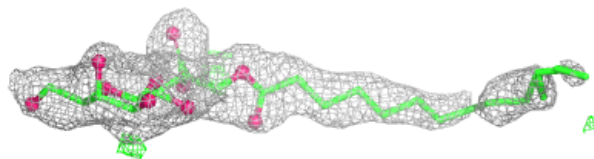
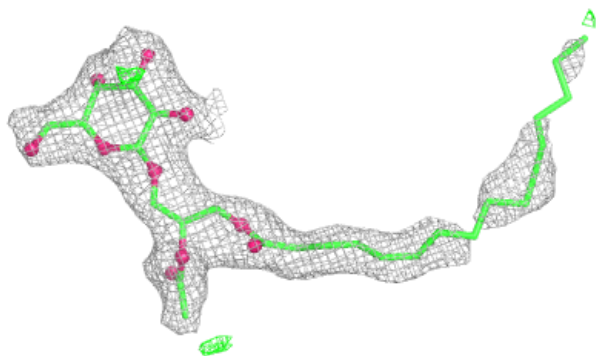
**Electron density around STE b 620:**

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

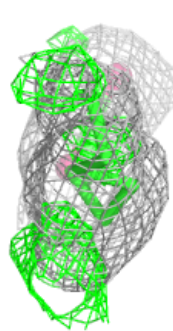
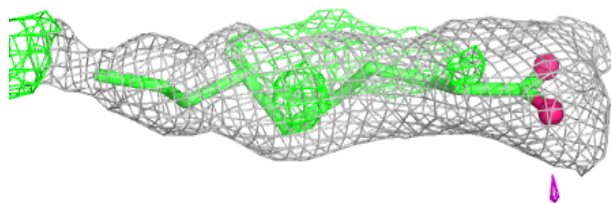
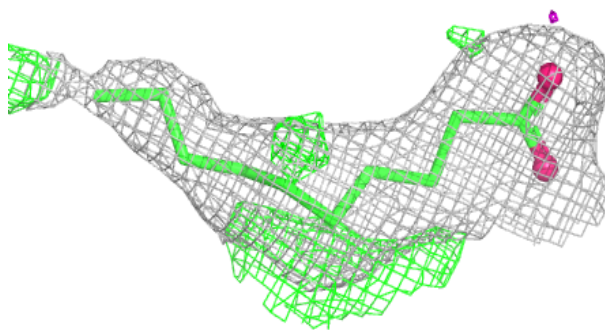


Electron density around LMG c 520:

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

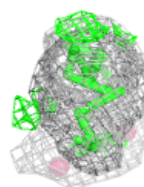
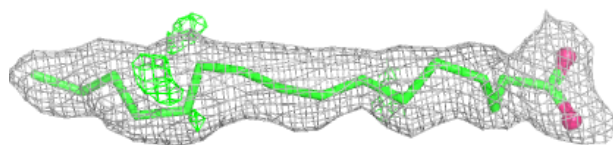
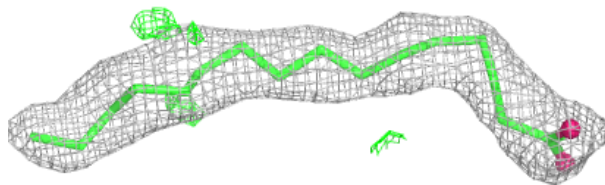
**Electron density around STE C 519:**

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

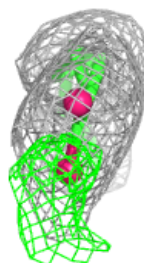
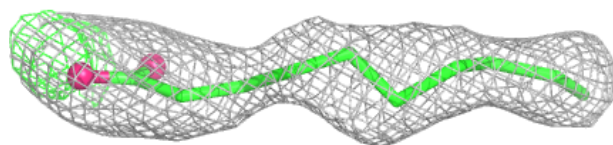
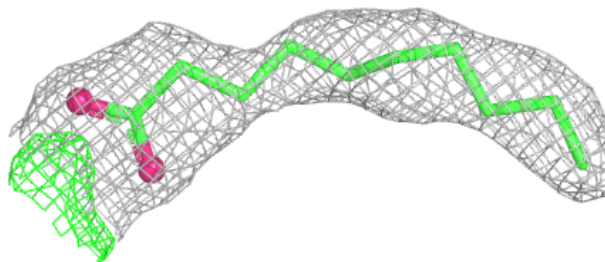


Electron density around STE B 624:

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

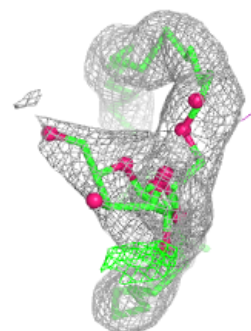
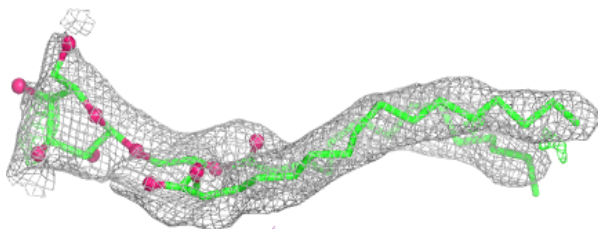
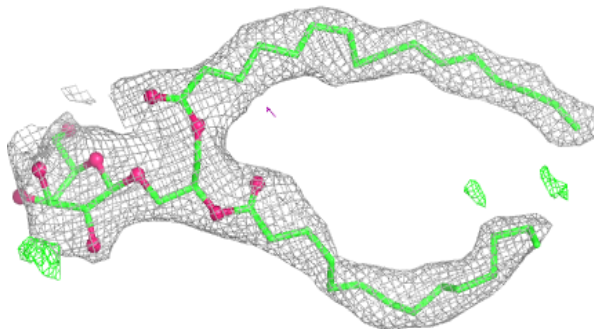
**Electron density around STE C 520:**

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

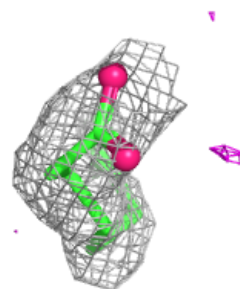
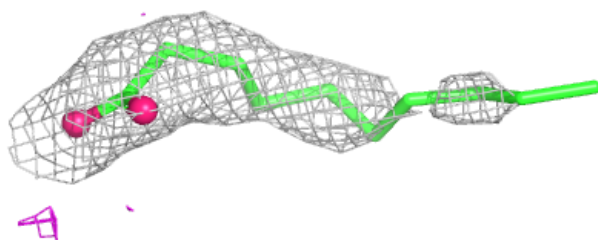


Electron density around LMG c 524:

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

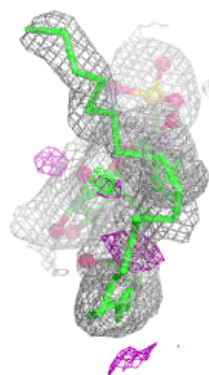
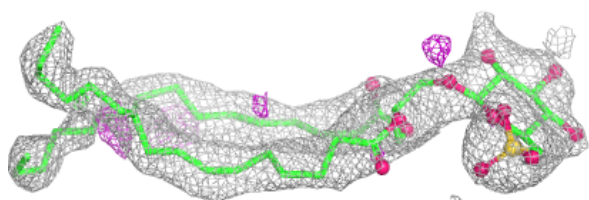
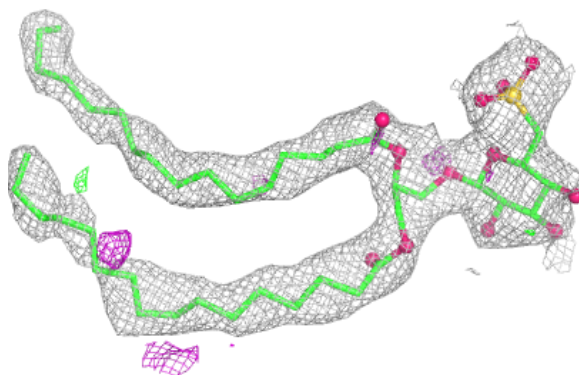
**Electron density around STE B 625:**

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

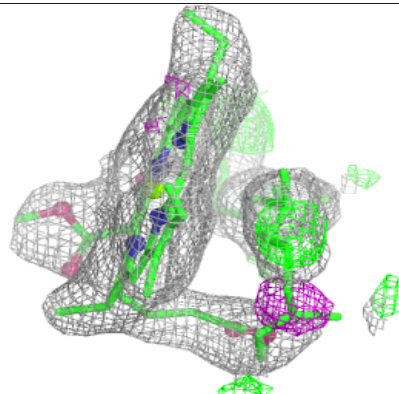
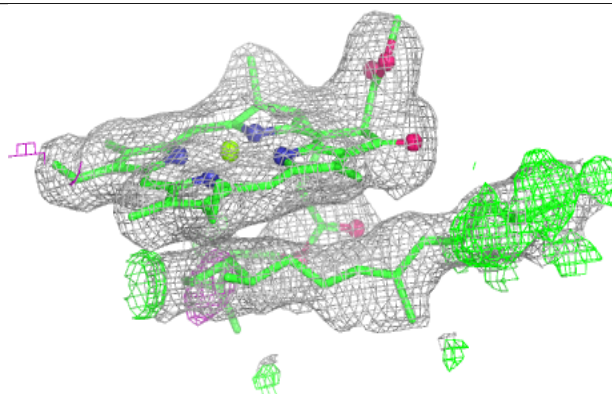
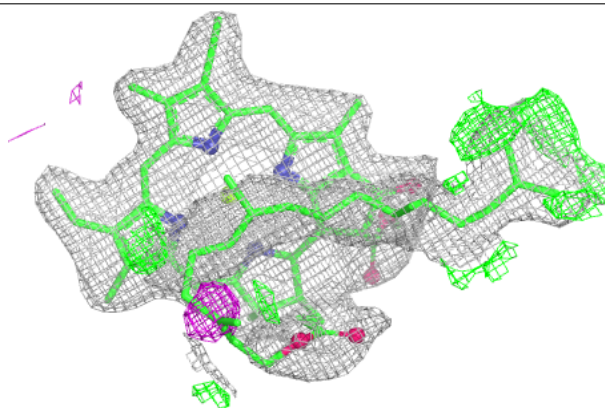


Electron density around SQD B 622:

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

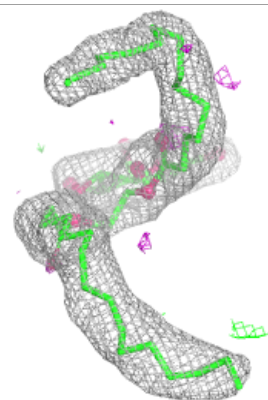
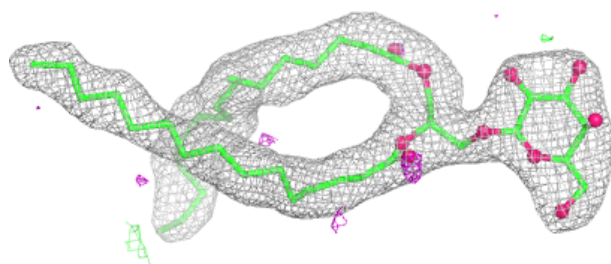
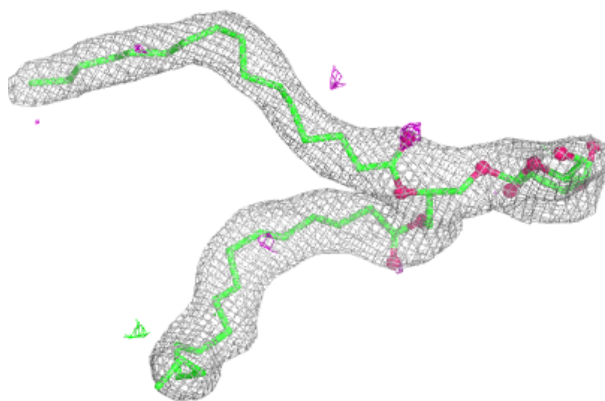
**Electron density around CLA B 601:**

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

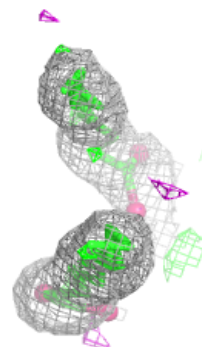
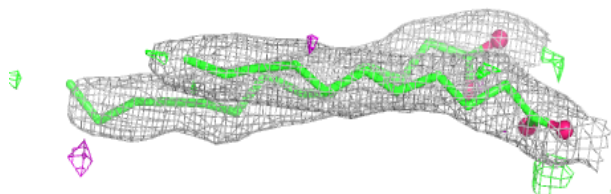
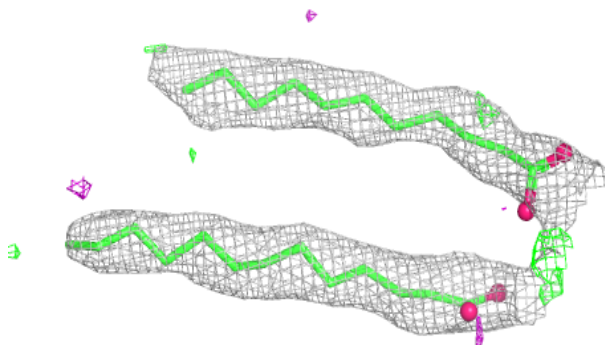


Electron density around LMG M 101:

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

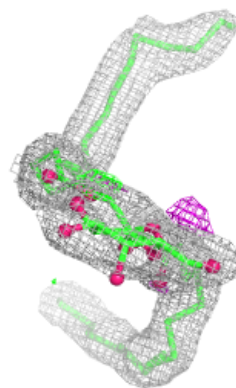
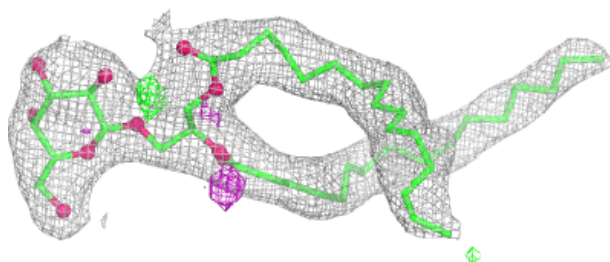
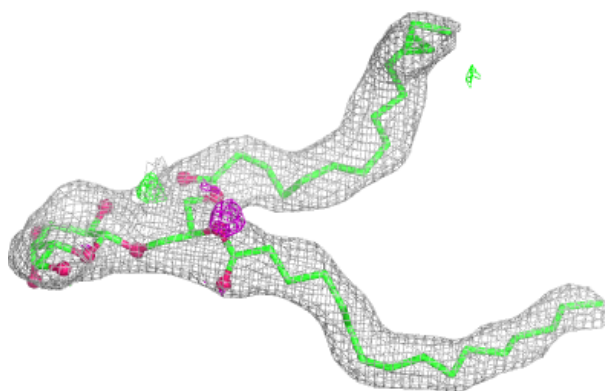
**Electron density around LMG B 621:**

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

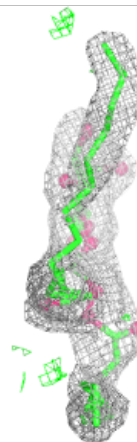
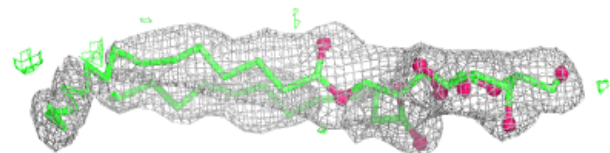
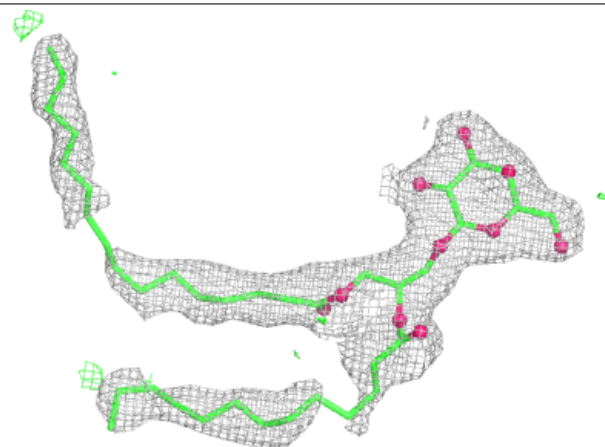


Electron density around LMG m 101:

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

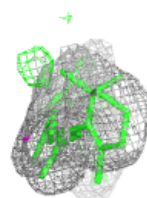
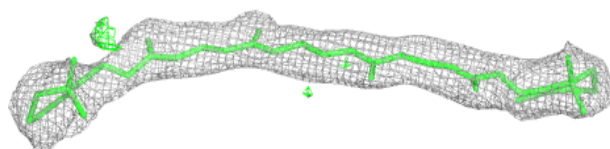
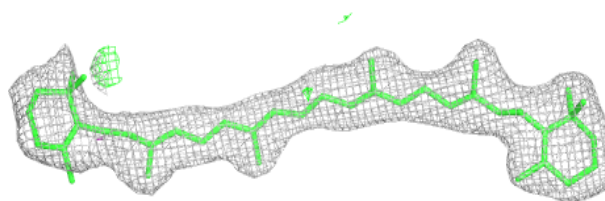
**Electron density around LMG C 518:**

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

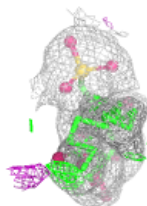
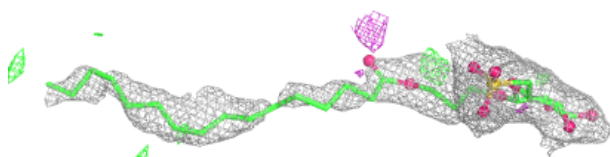
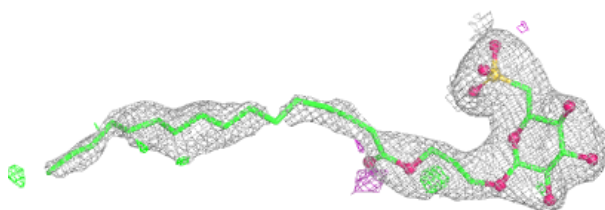


Electron density around BCR d 405:

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

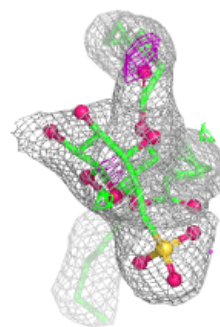
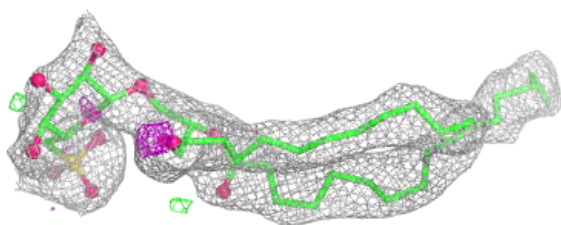
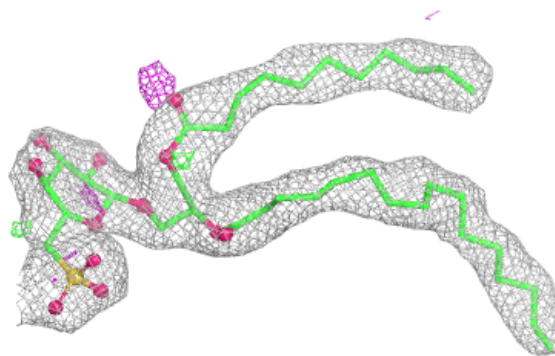
**Electron density around SQD F 101:**

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

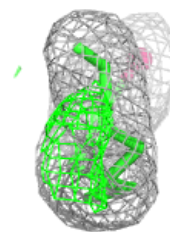
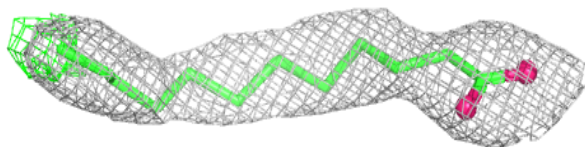
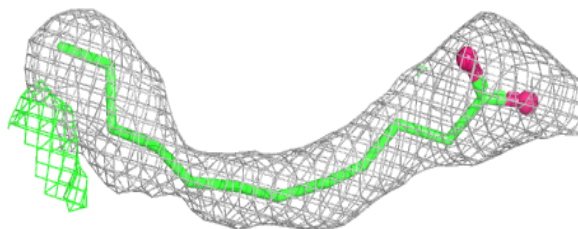


Electron density around SQD L 101:

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

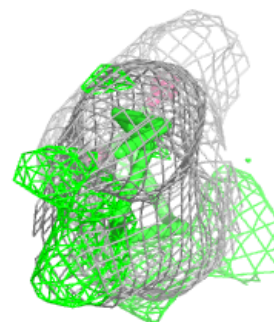
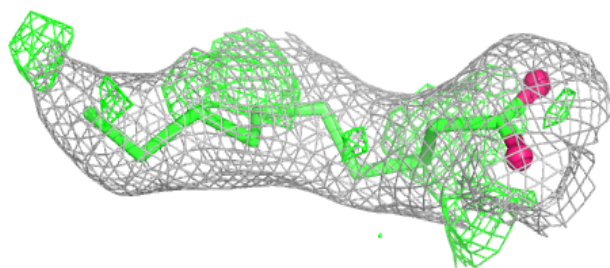
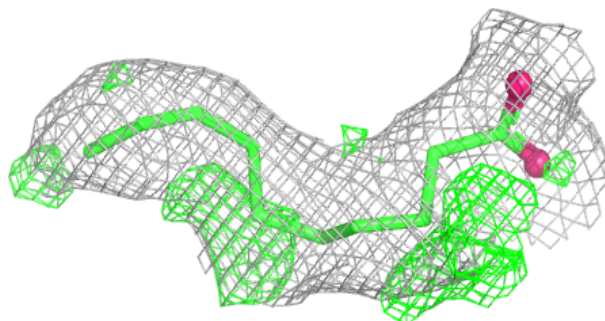
**Electron density around STE t 102:**

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

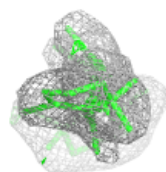
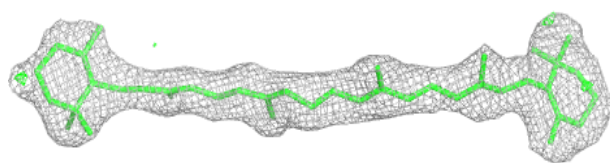
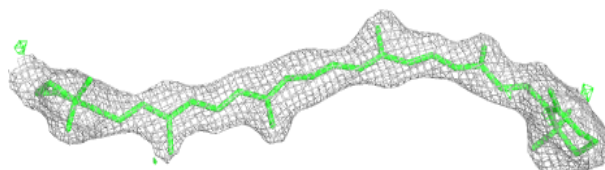


Electron density around STE B 623:

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

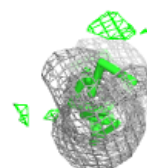
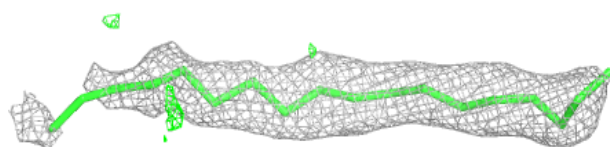
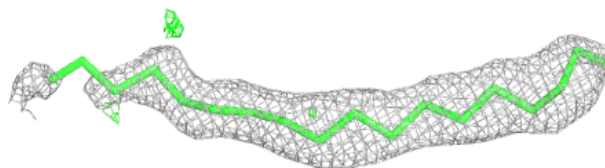
**Electron density around BCR x 101:**

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

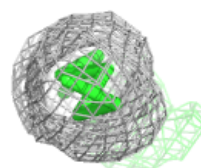
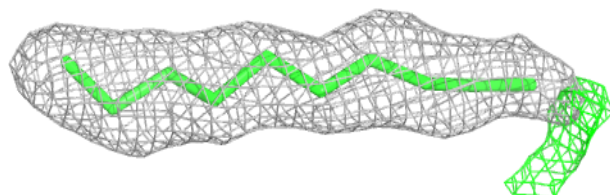
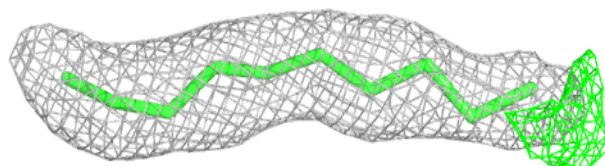


Electron density around STE I 102:

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

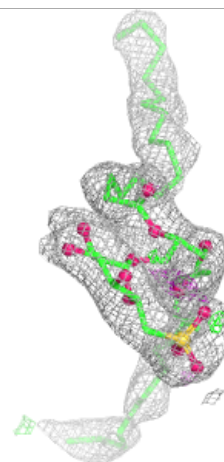
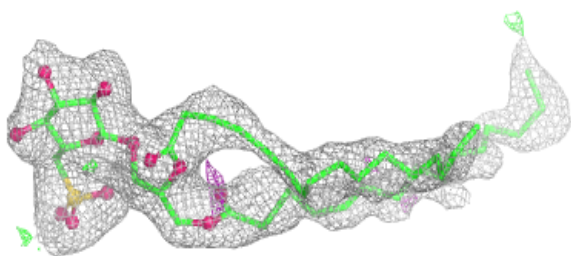
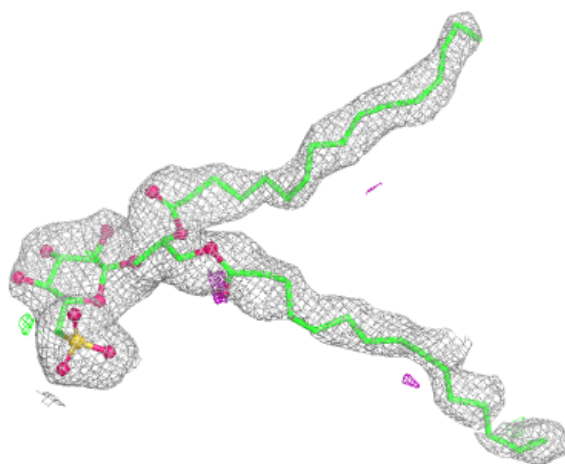
**Electron density around STE M 103:**

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



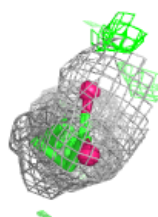
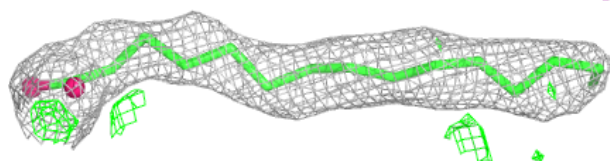
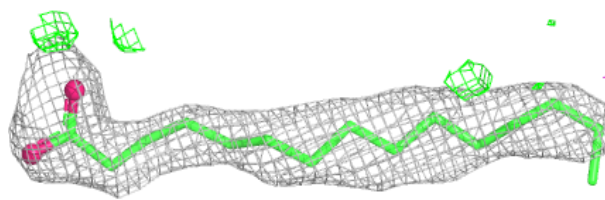
Electron density around SQD a 613:

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

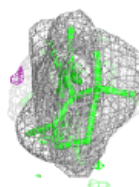
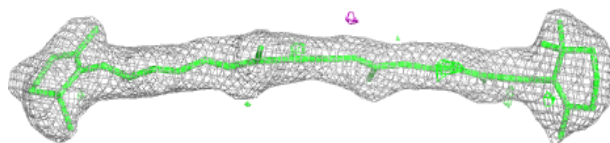
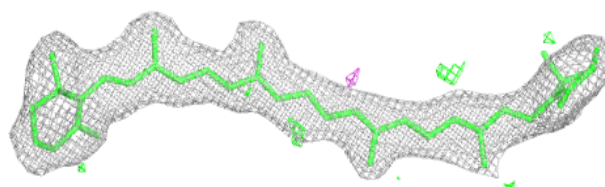


Electron density around STE d 413:

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

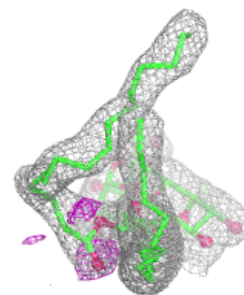
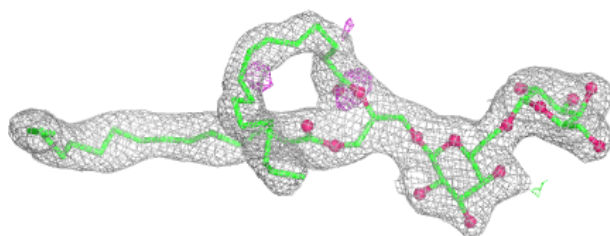
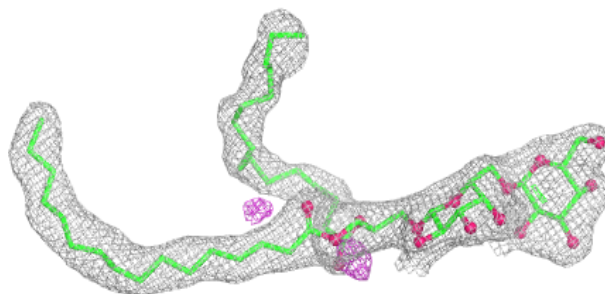
**Electron density around BCR Y 101:**

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

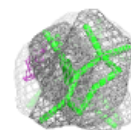
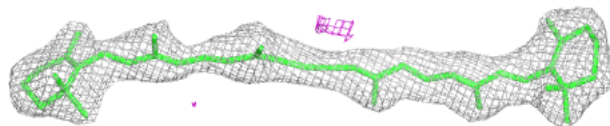


Electron density around DGD h 101:

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

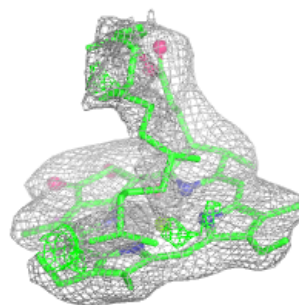
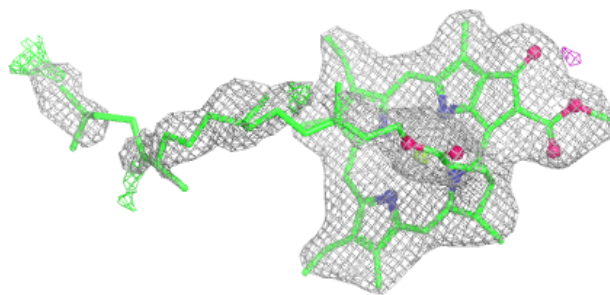
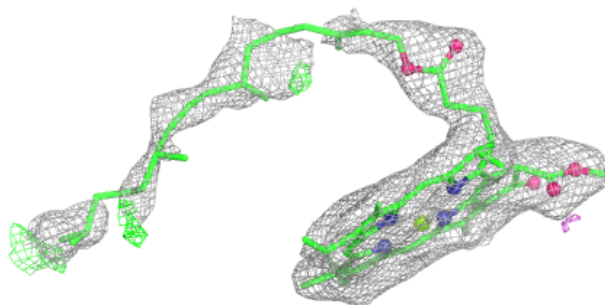
**Electron density around BCR c 514:**

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

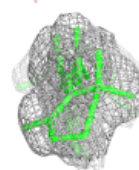
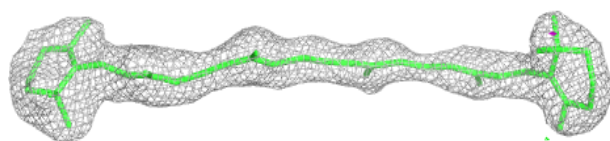
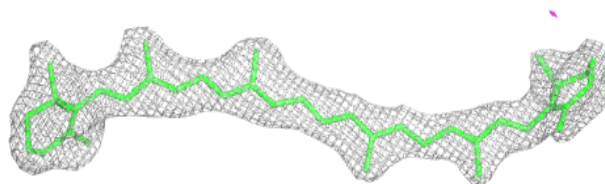


Electron density around CLA C 513:

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

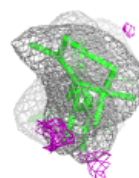
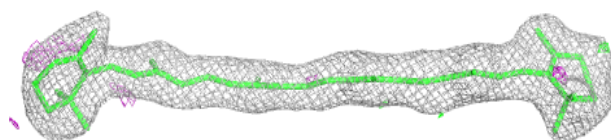
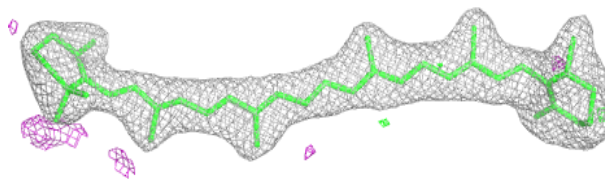
**Electron density around BCR k 101:**

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

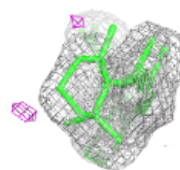
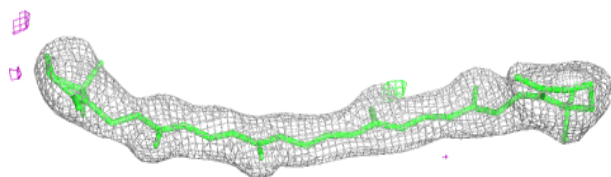
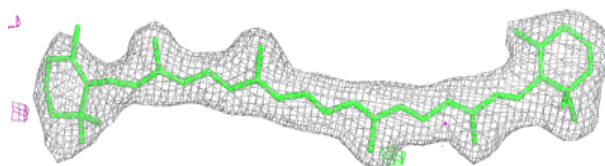


Electron density around BCR B 618:

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

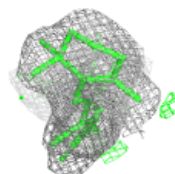
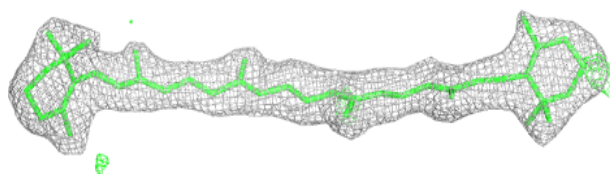
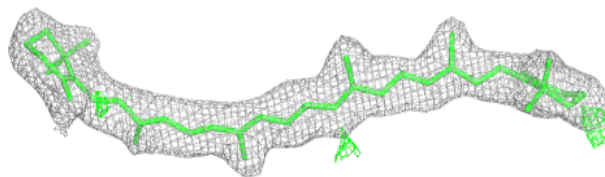
**Electron density around BCR D 406:**

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

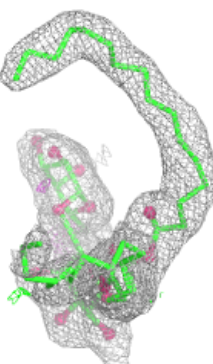
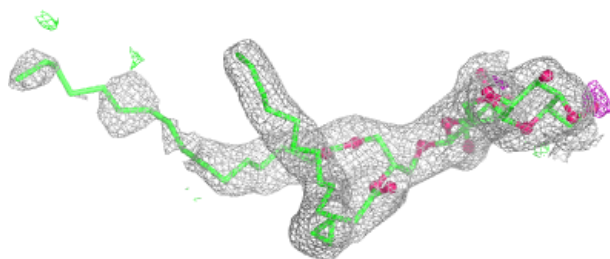
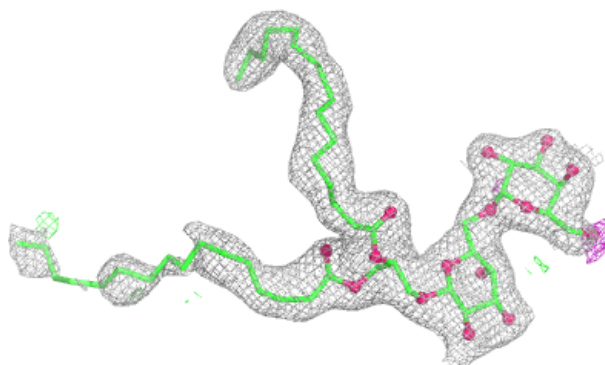


Electron density around BCR H 101:

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

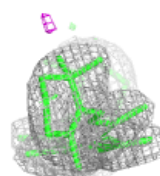
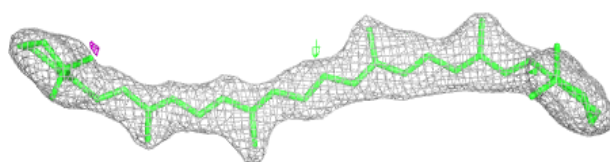
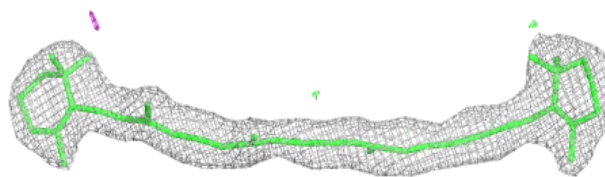
**Electron density around DGD c 518:**

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

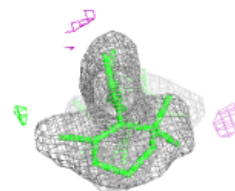
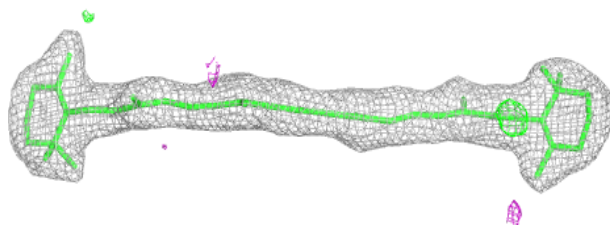
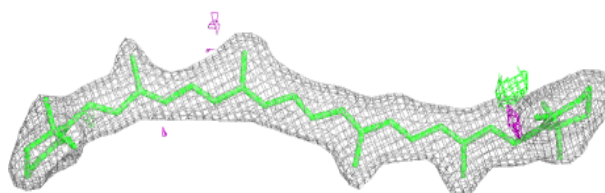


Electron density around BCR K 102:

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

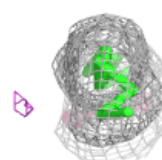
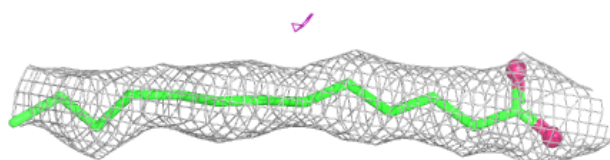
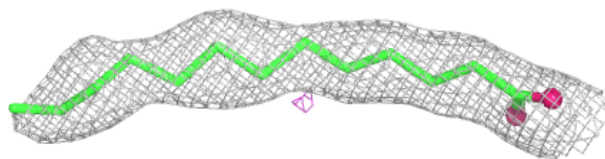
**Electron density around BCR C 514:**

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

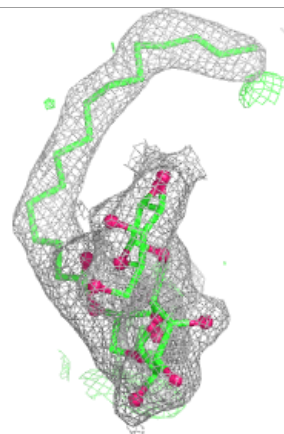
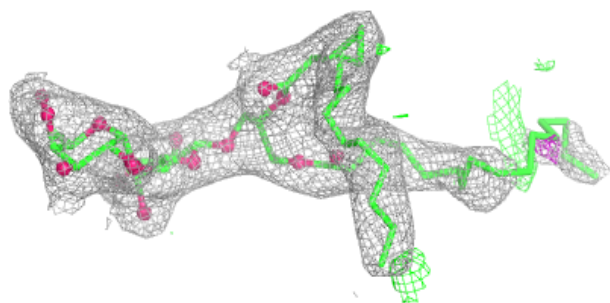
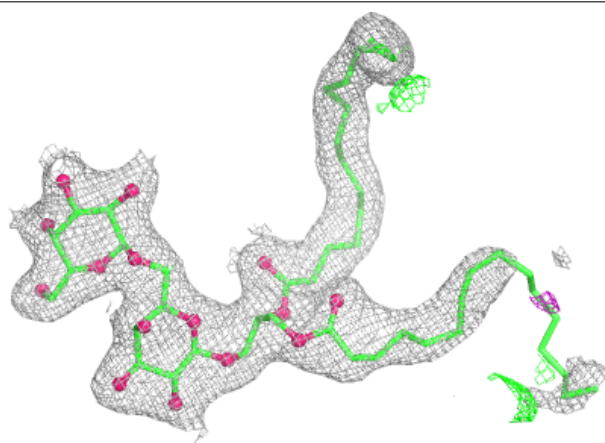


Electron density around STE M 102:

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

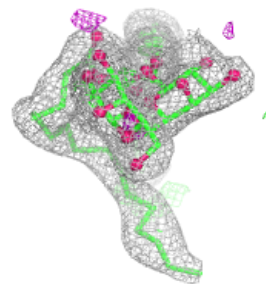
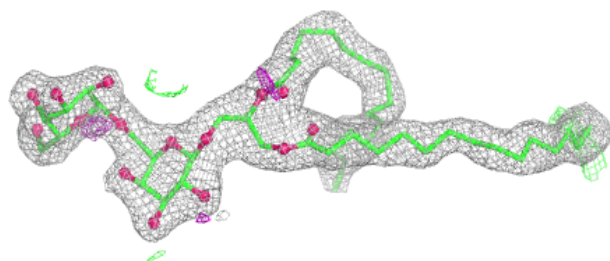
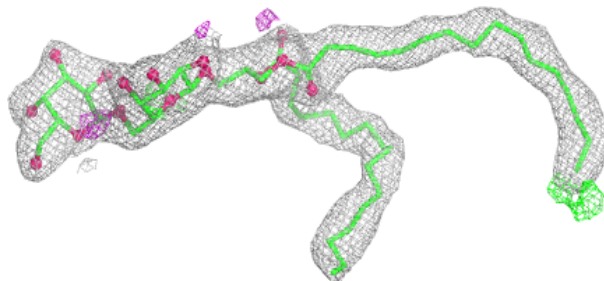
**Electron density around DGD C 516:**

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

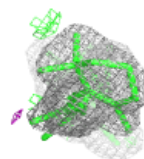
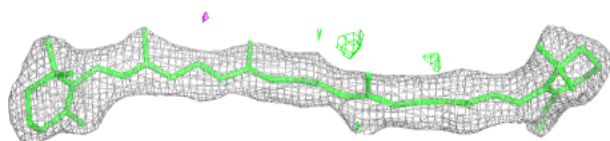
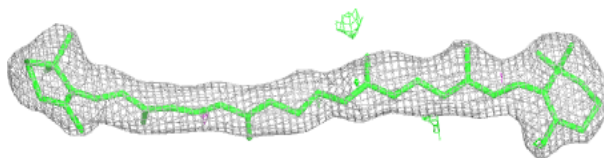


Electron density around DGD H 102:

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

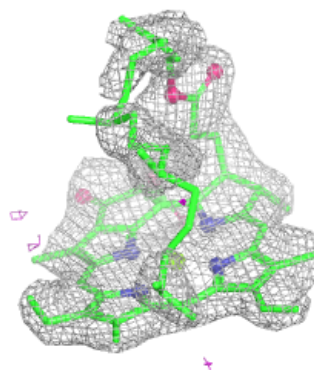
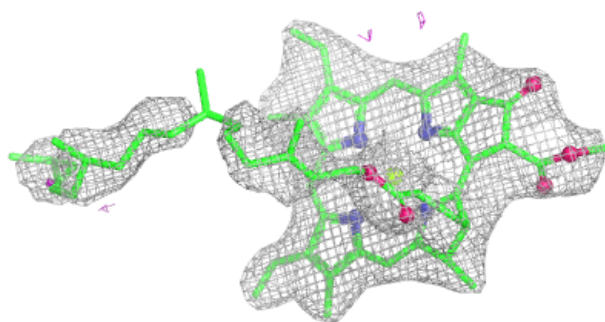
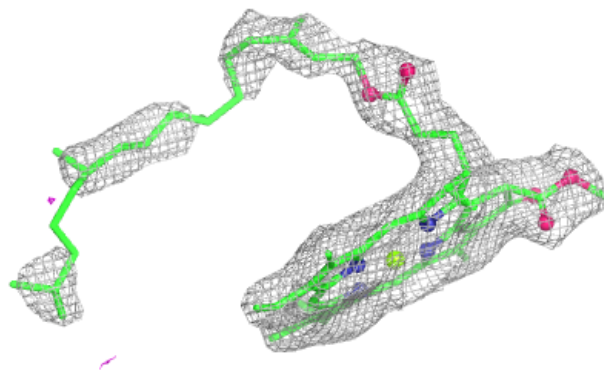
**Electron density around BCR K 101:**

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

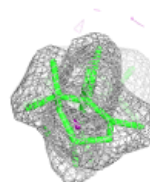
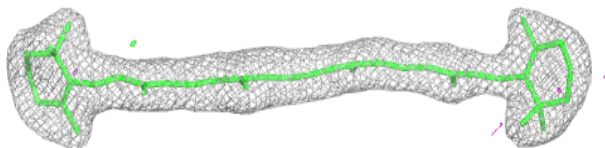
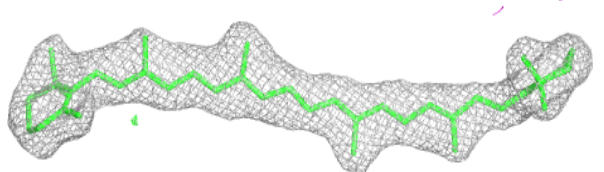


Electron density around CLA c 513:

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

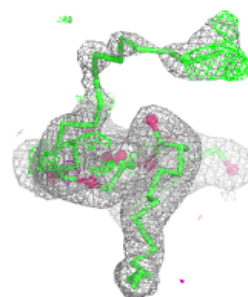
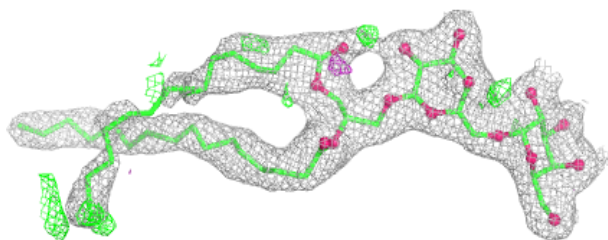
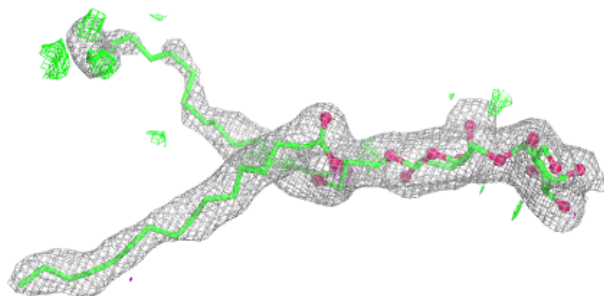
**Electron density around BCR A 610:**

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

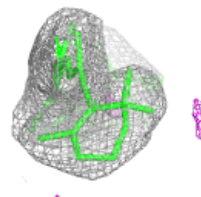
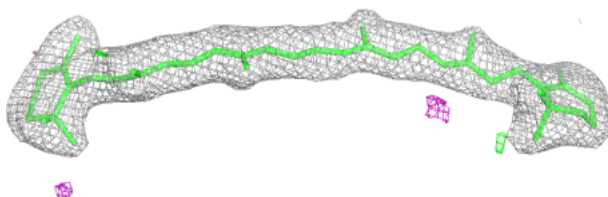
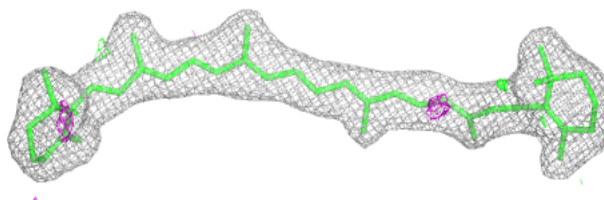


Electron density around DGD C 515:

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

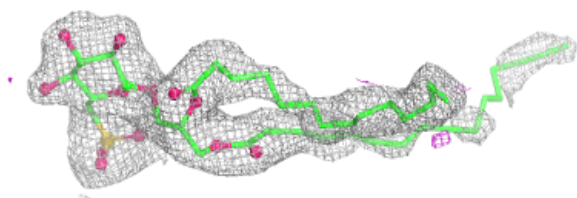
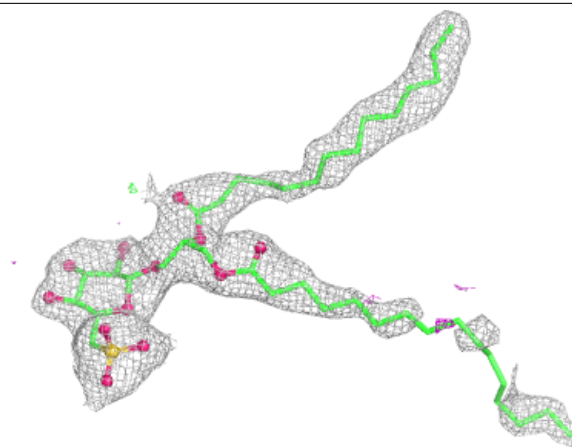
**Electron density around BCR T 101:**

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



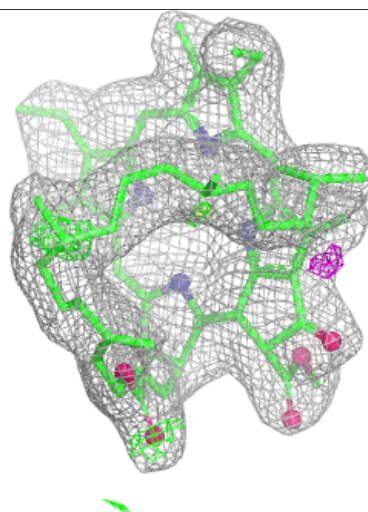
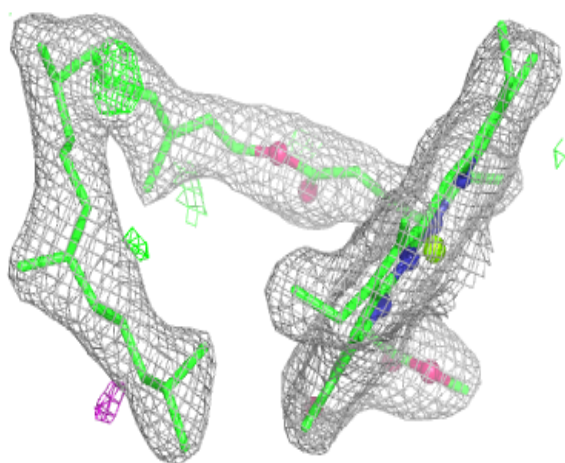
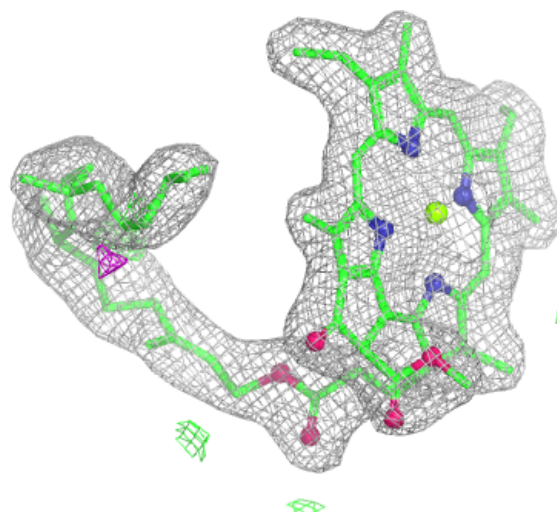
Electron density around SQD A 613:

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



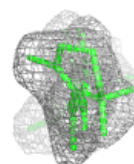
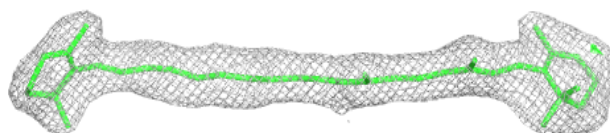
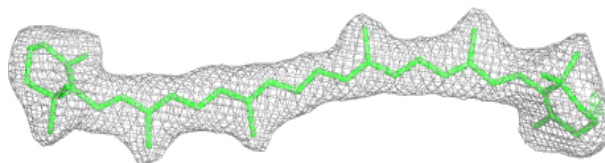
Electron density around CLA C 503:

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

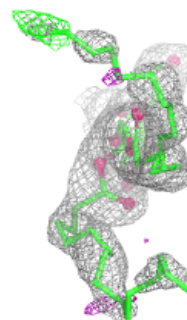
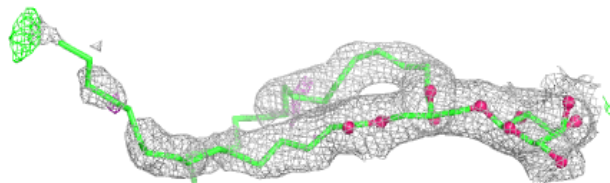
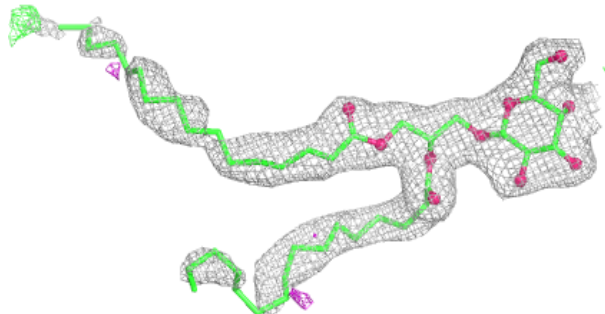


Electron density around BCR b 618:

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

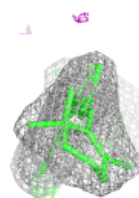
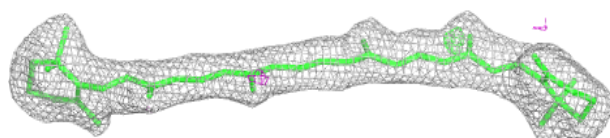
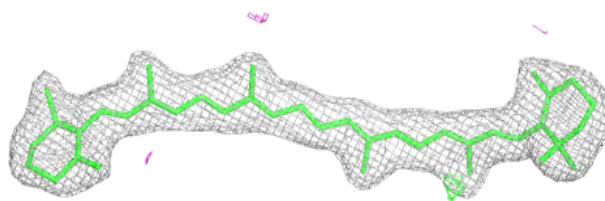
**Electron density around LMG D 408:**

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

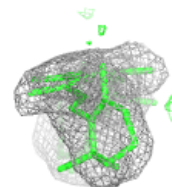
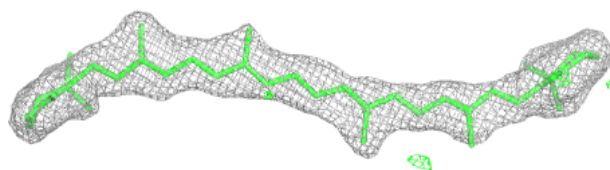
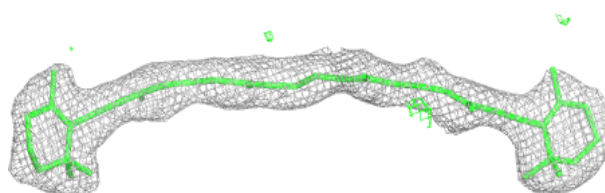


Electron density around BCR B 619:

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

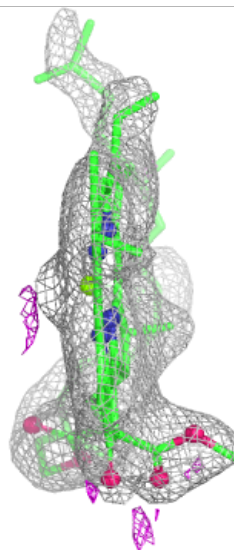
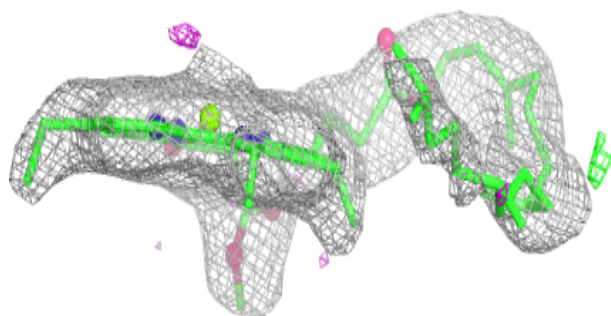
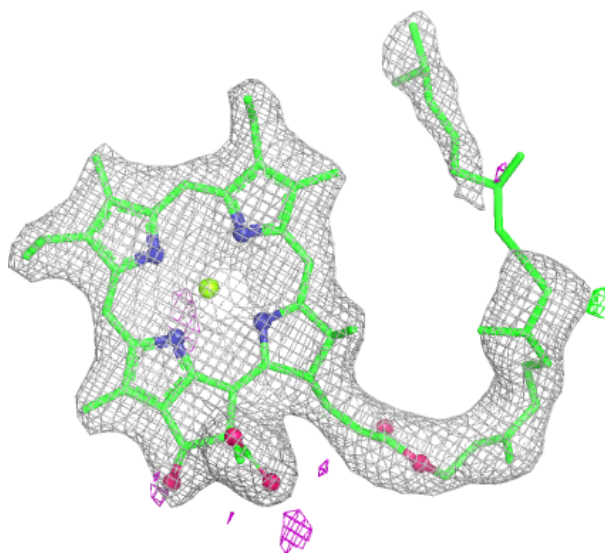
**Electron density around BCR c 516:**

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



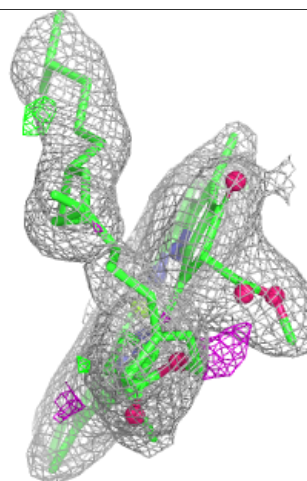
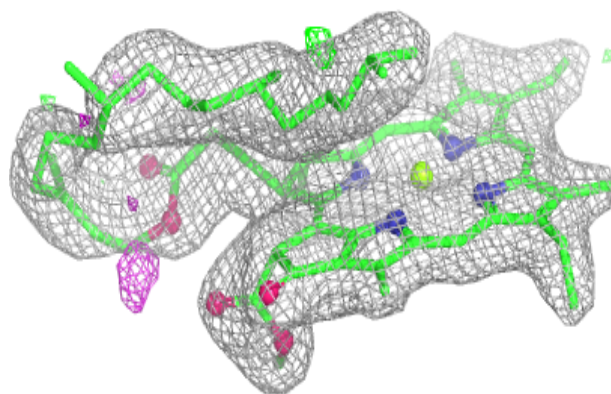
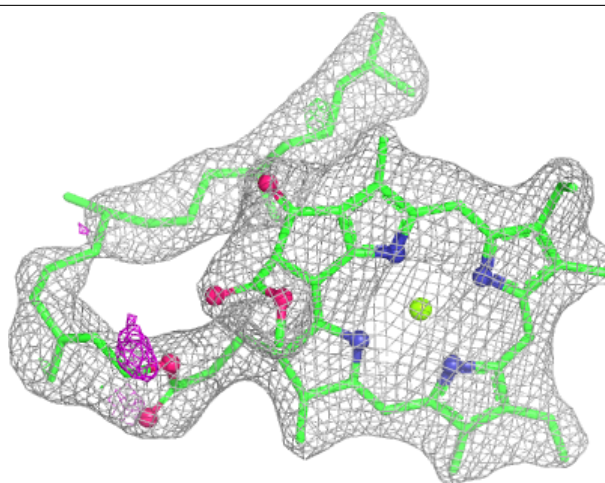
Electron density around CLA C 512:

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



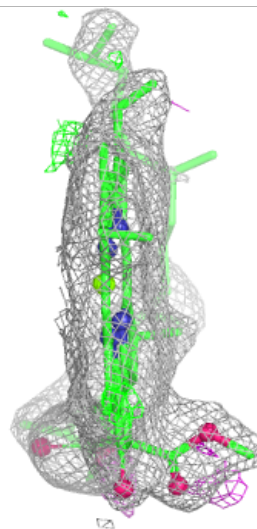
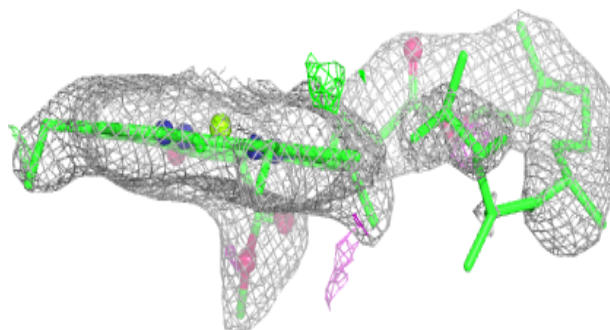
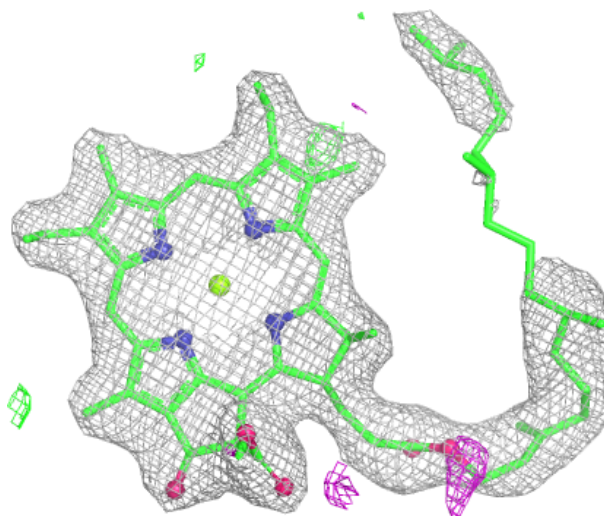
Electron density around CLA c 509:

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



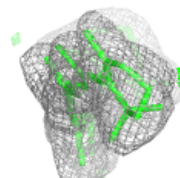
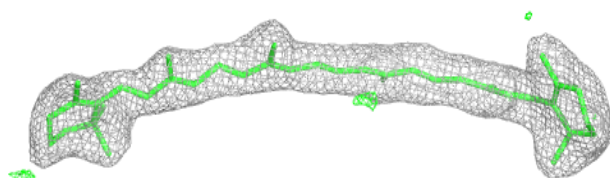
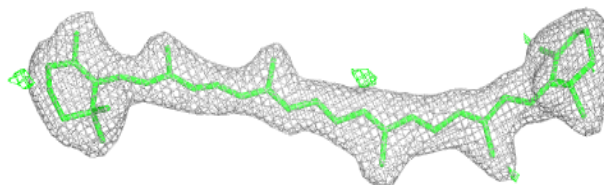
Electron density around CLA c 512:

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

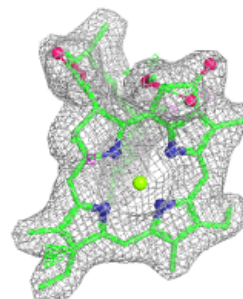
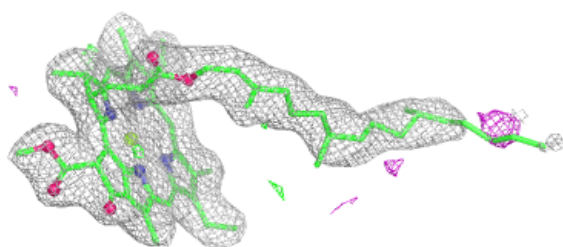
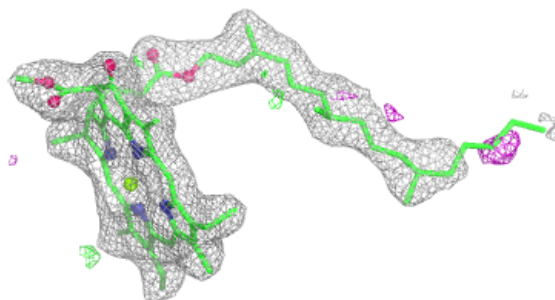


Electron density around BCR t 101:

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

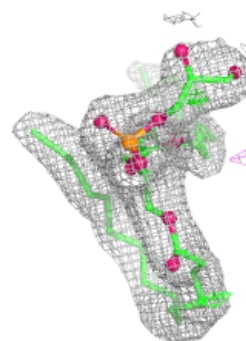
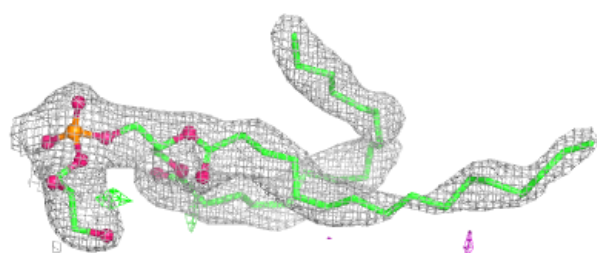
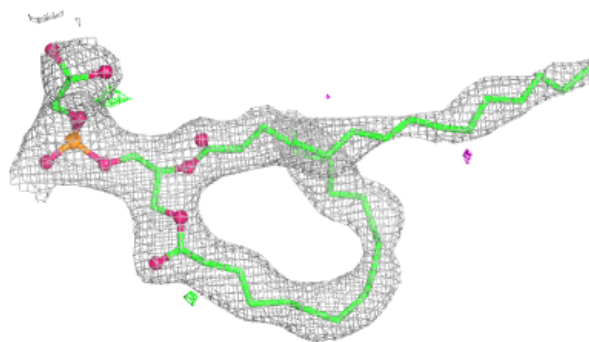
**Electron density around CLA c 508:**

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

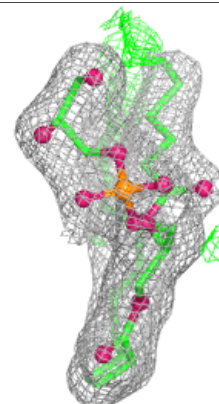
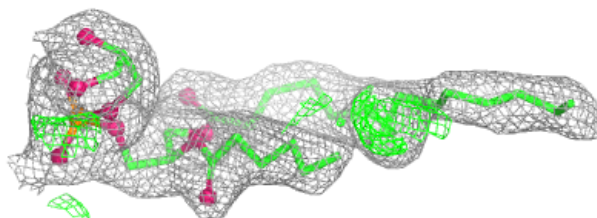
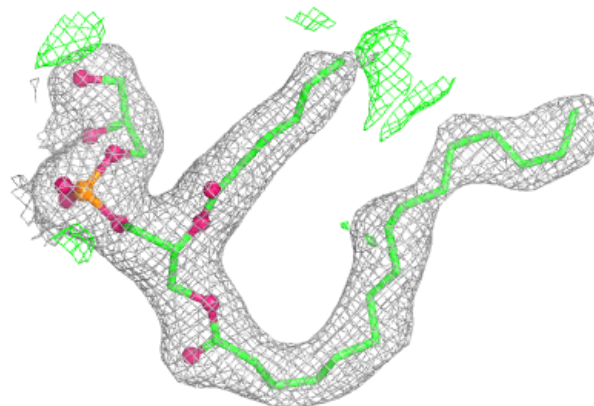


Electron density around LHG d 407:

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

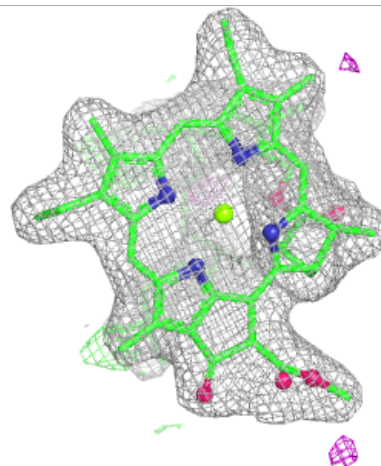
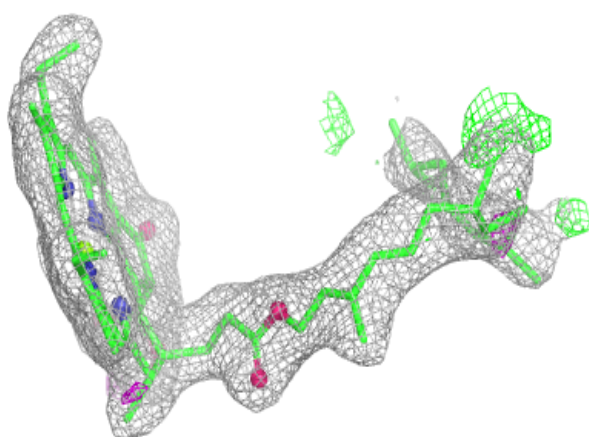
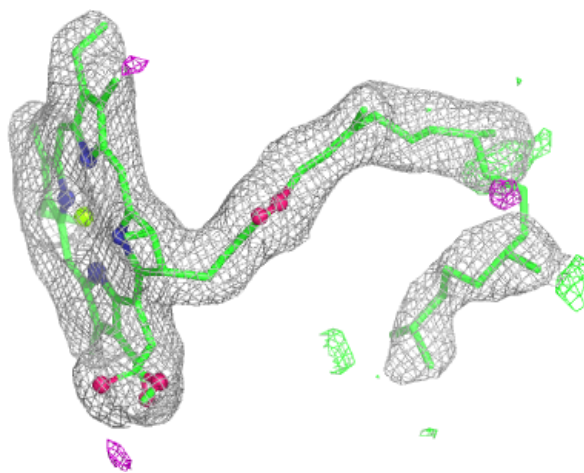
**Electron density around LHG d 409:**

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



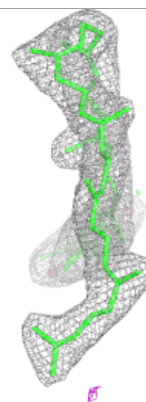
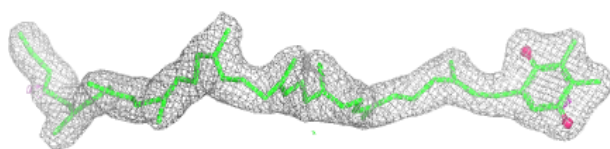
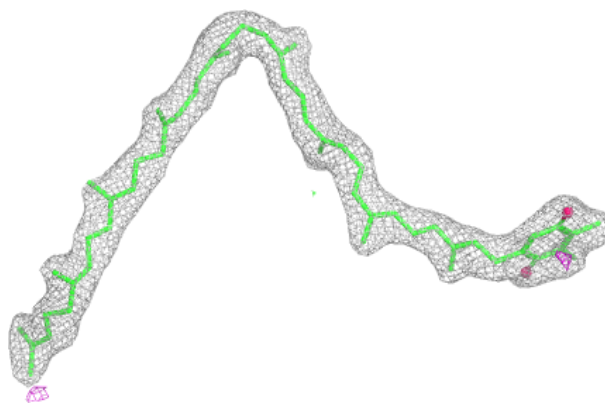
Electron density around CLA B 606:

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

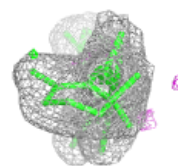
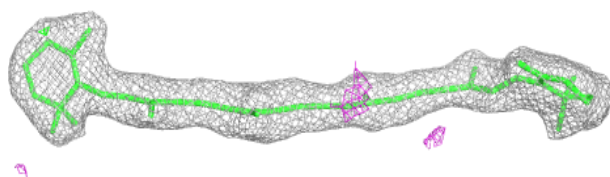
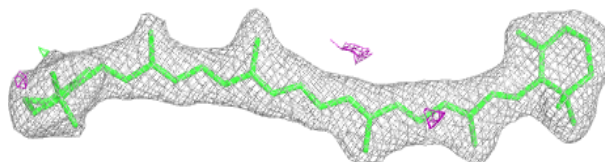


Electron density around PL9 D 407:

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

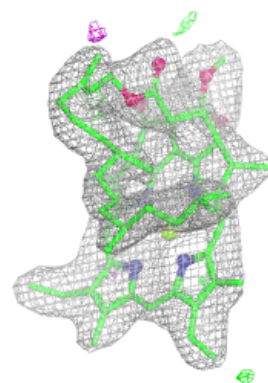
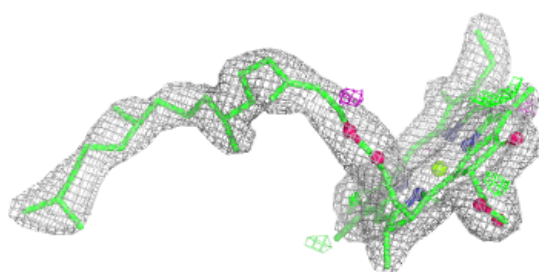
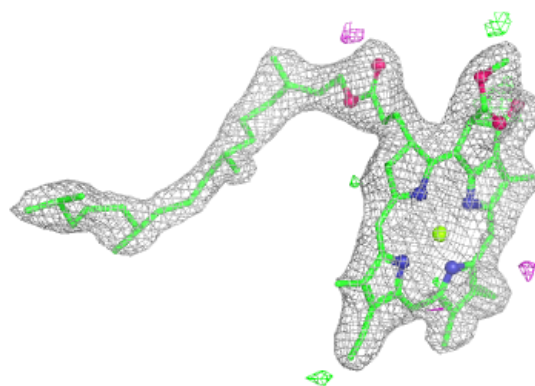
**Electron density around BCR b 617:**

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

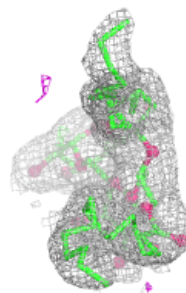
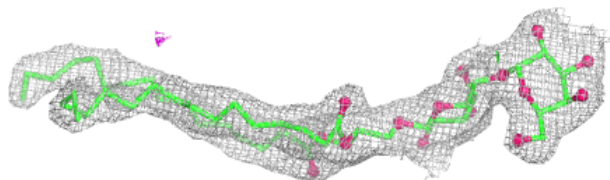
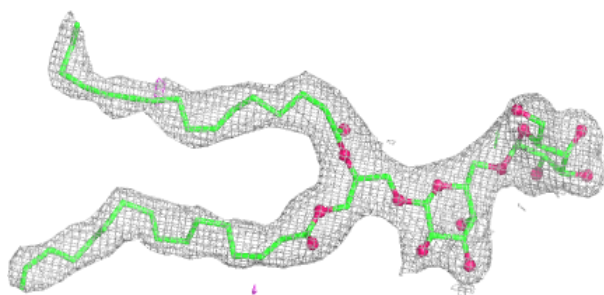


Electron density around CLA c 511:

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

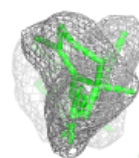
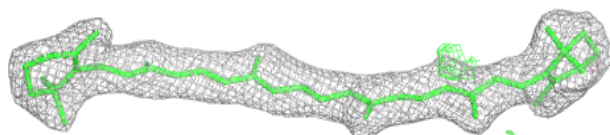
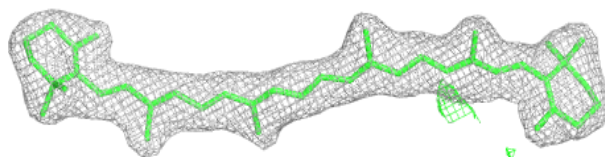
**Electron density around DGD C 517:**

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

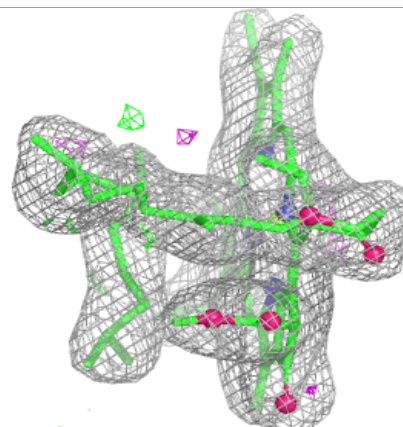
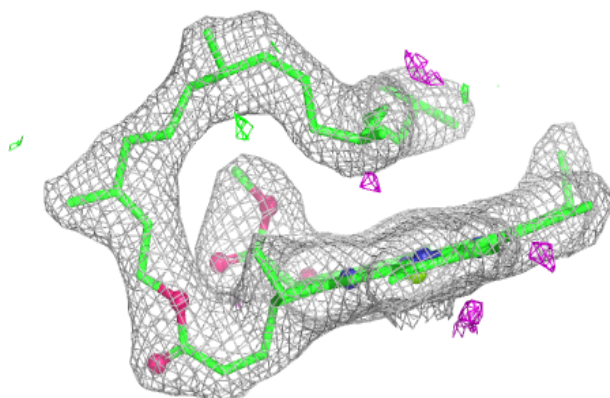
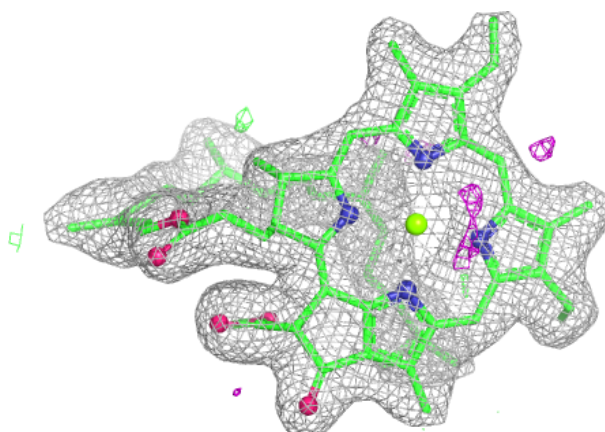


Electron density around BCR b 619:

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

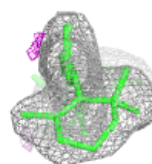
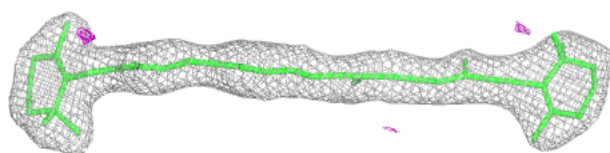
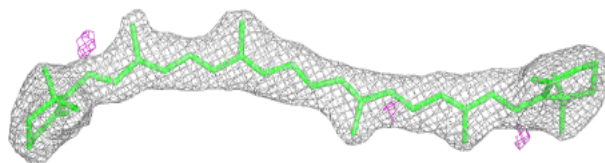
**Electron density around CLA C 510:**

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

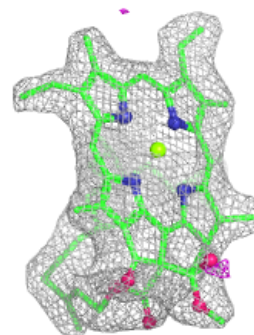
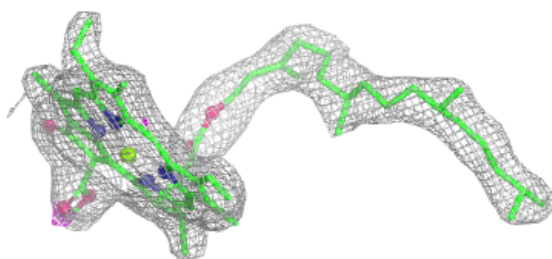
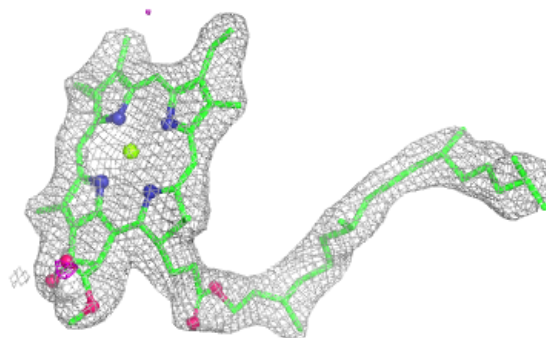


Electron density around BCR c 515:

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

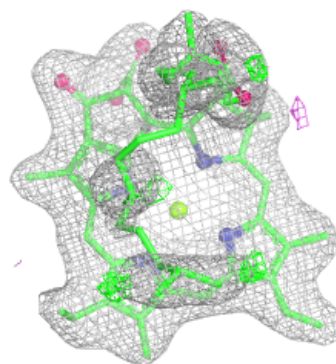
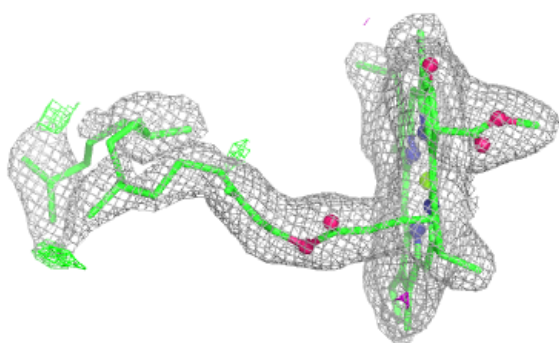
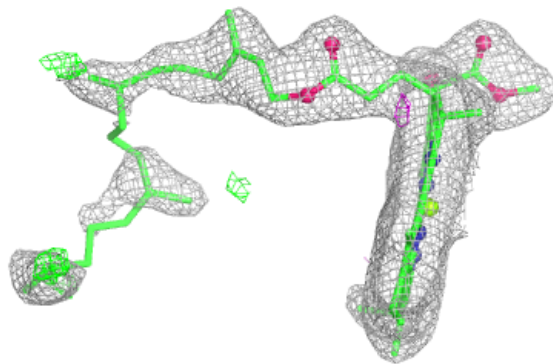
**Electron density around CLA C 511:**

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

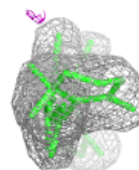
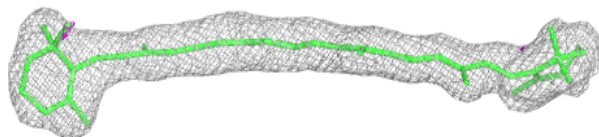
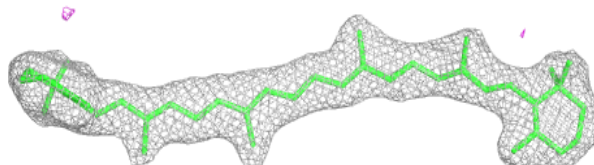


Electron density around CLA c 506:

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

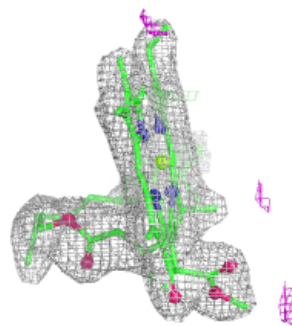
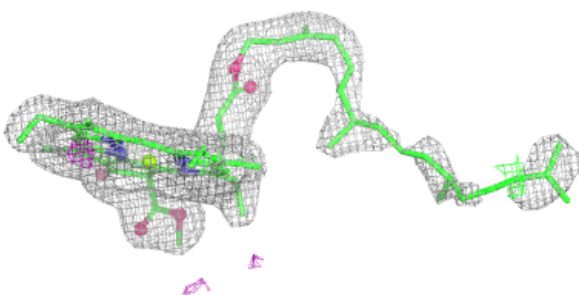
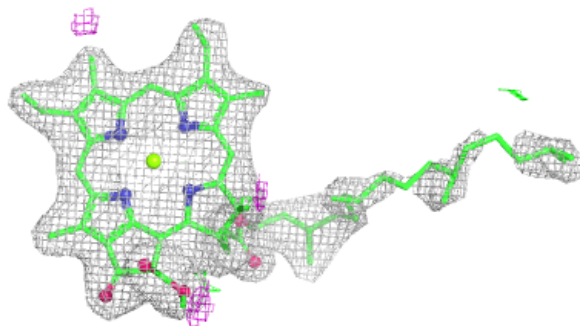
**Electron density around BCR B 617:**

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

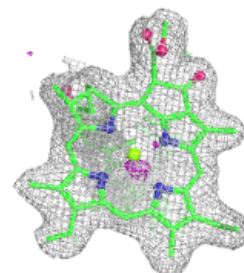
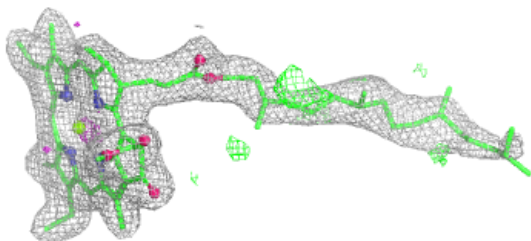
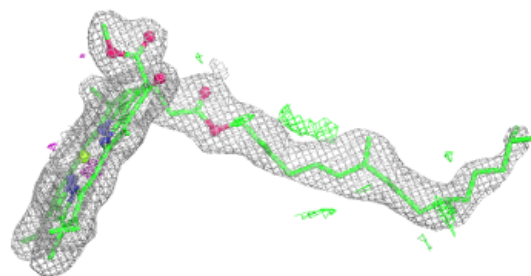


Electron density around CLA a 608:

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

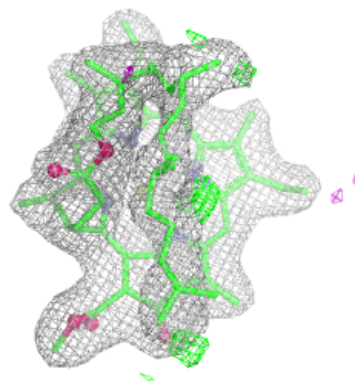
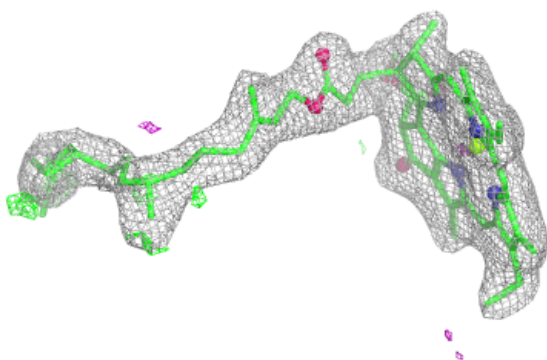
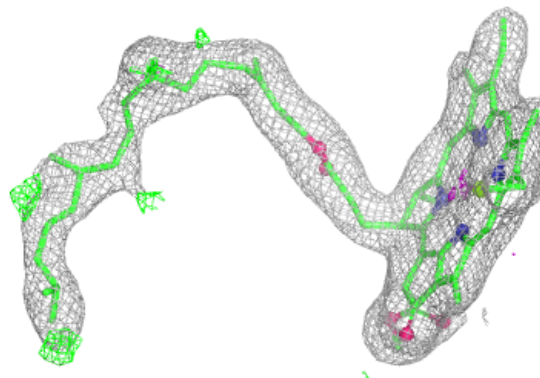
**Electron density around CLA B 604:**

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

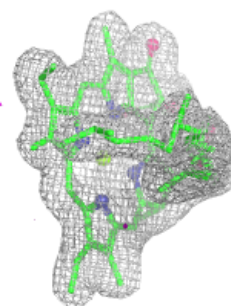
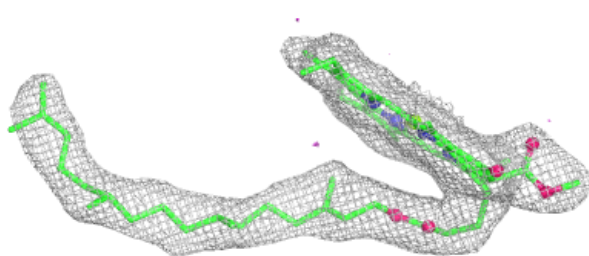
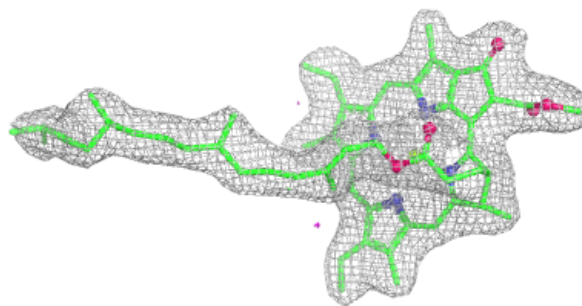


Electron density around CLA b 606:

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

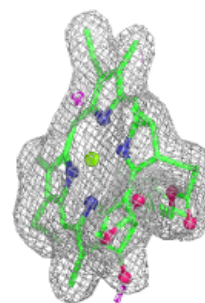
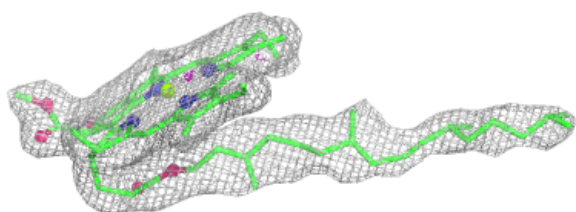
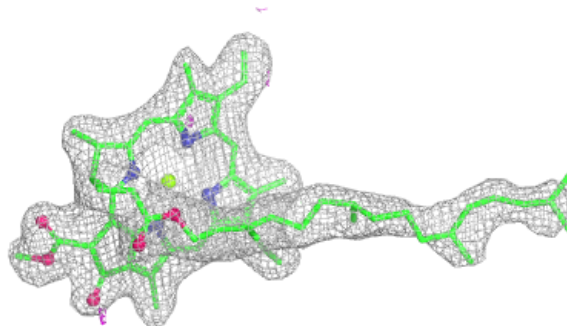
**Electron density around CLA b 608:**

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



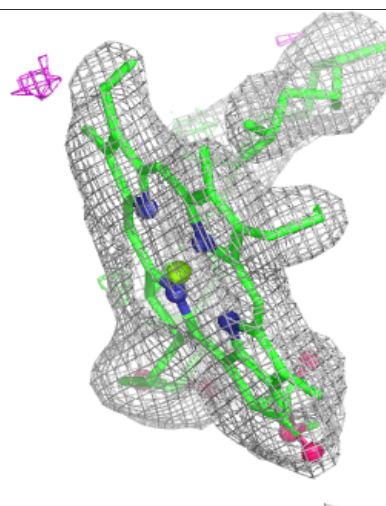
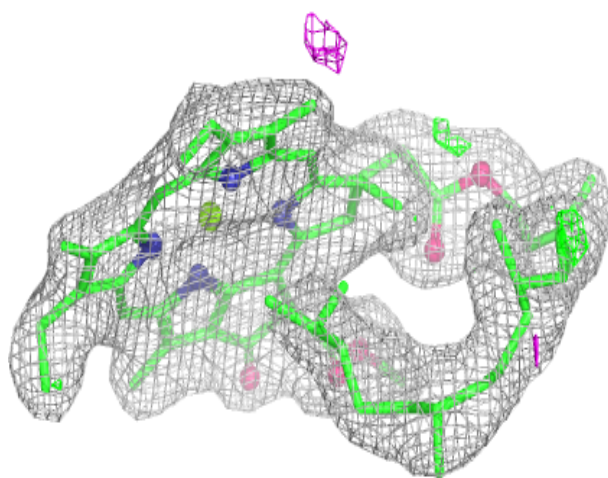
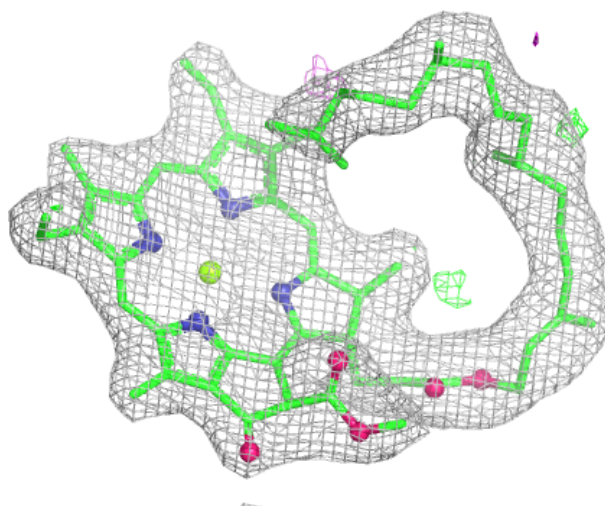
Electron density around CLA b 614:

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



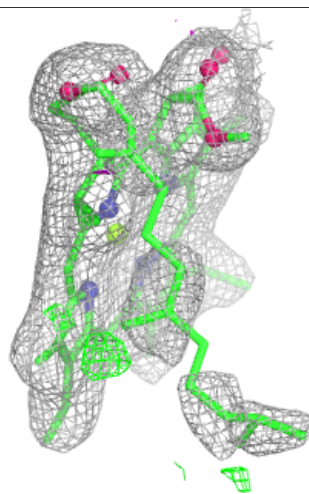
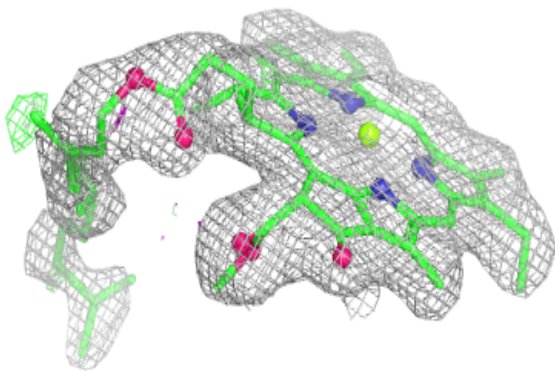
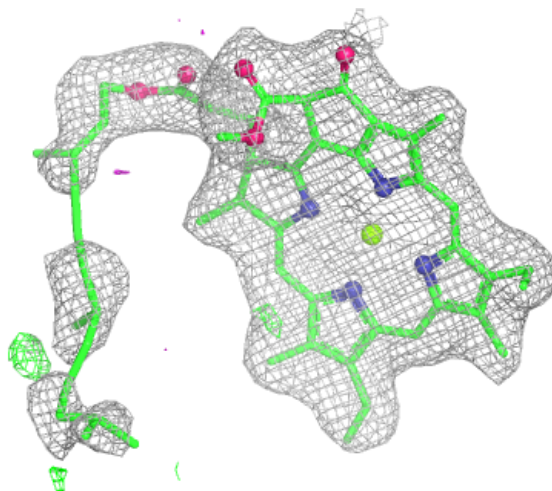
Electron density around CLA b 615:

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



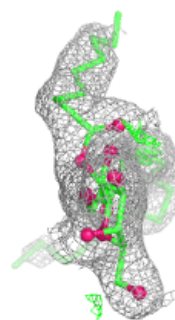
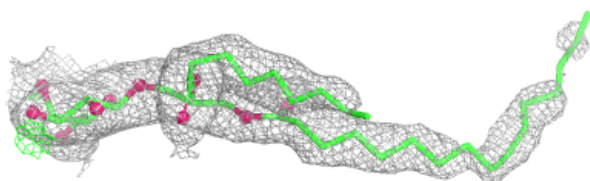
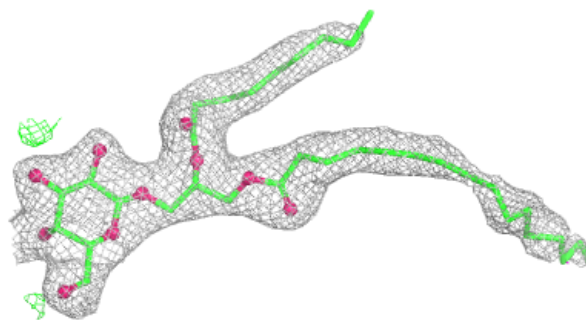
Electron density around CLA b 616:

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

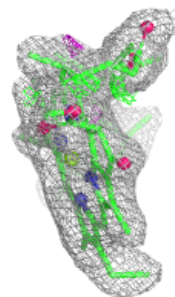
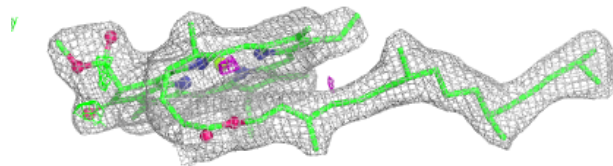
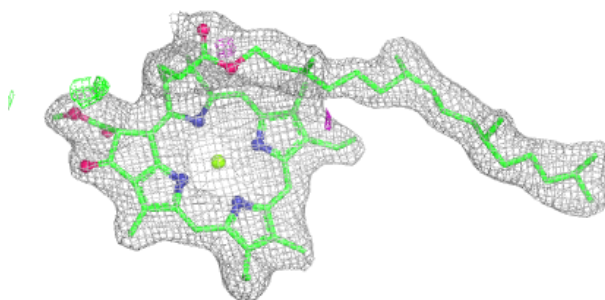


Electron density around LMG d 411:

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

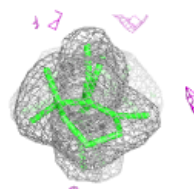
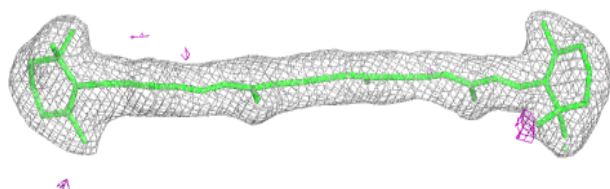
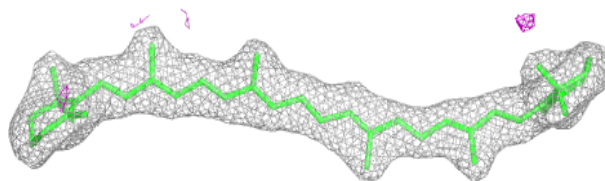
**Electron density around CLA c 501:**

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

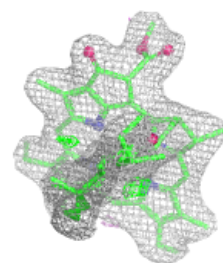
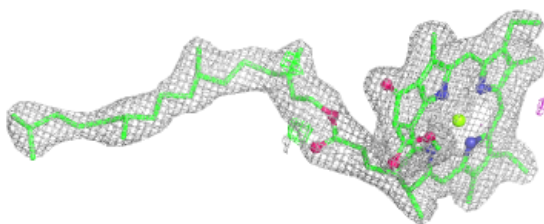
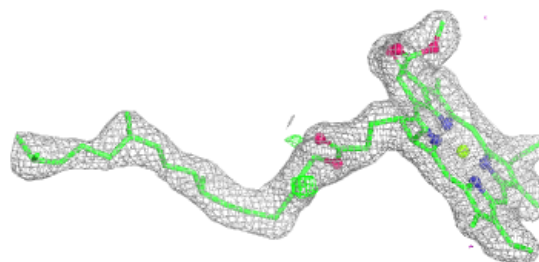


Electron density around BCR a 610:

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

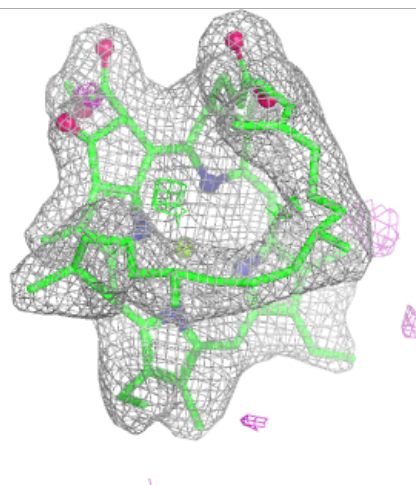
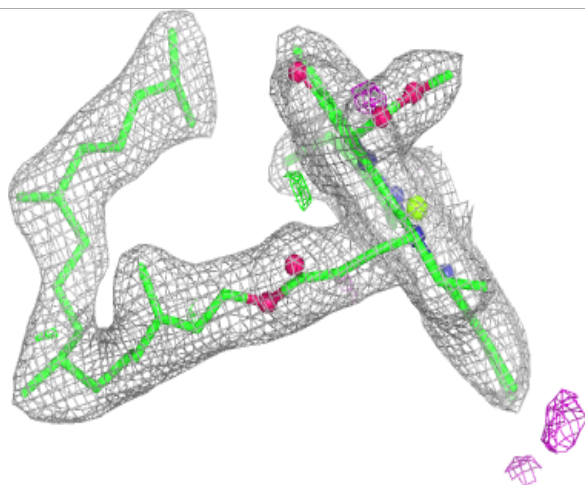
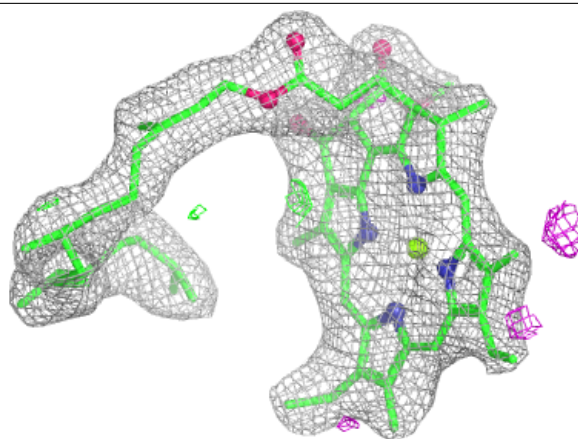
**Electron density around CLA c 502:**

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



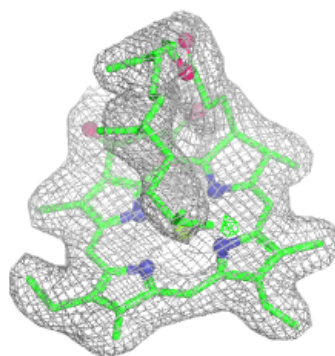
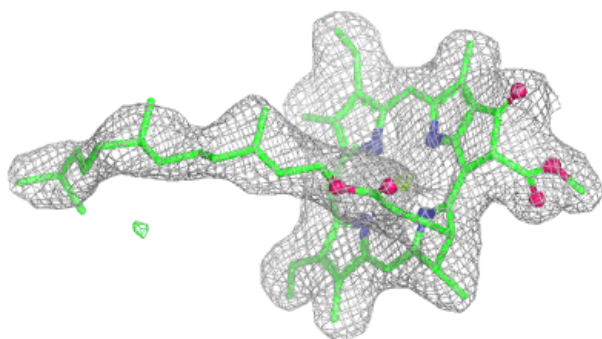
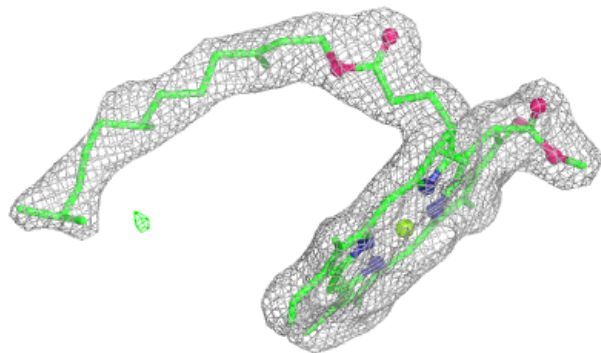
Electron density around CLA c 503:

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

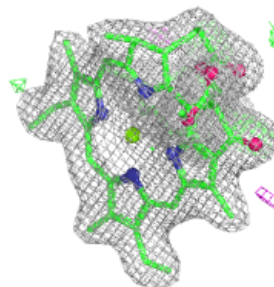
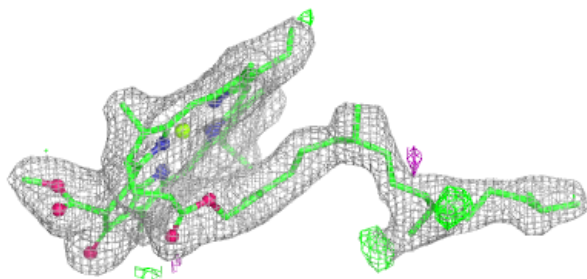
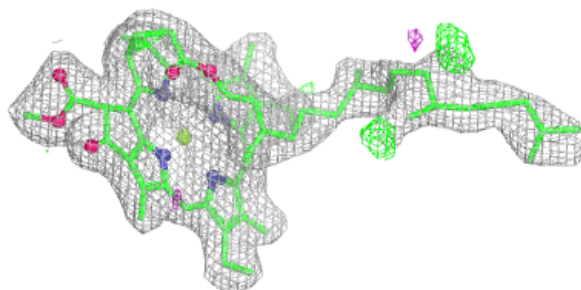


Electron density around CLA c 504:

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

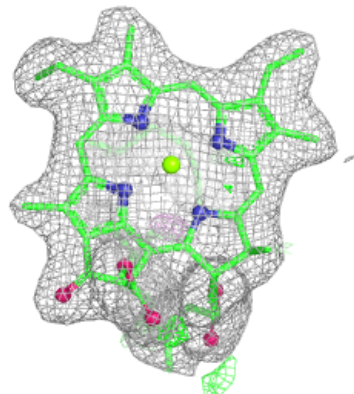
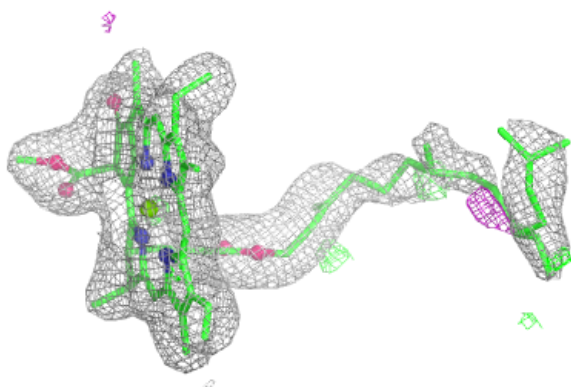
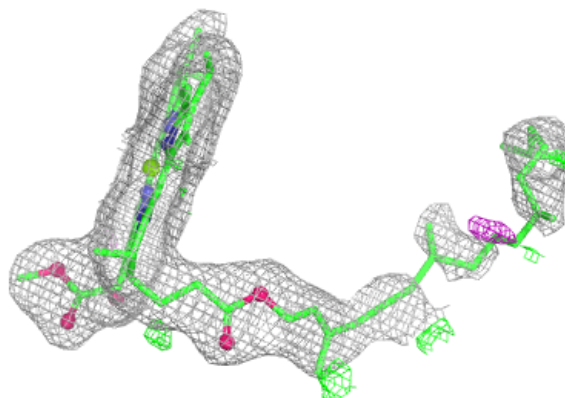
**Electron density around CLA c 505:**

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



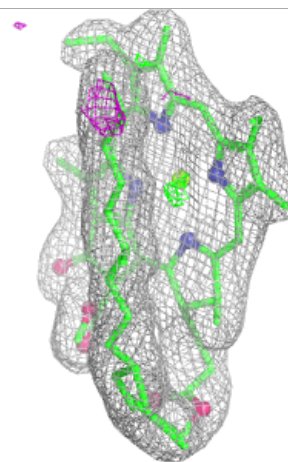
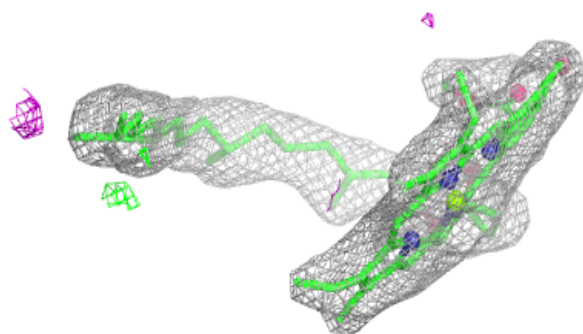
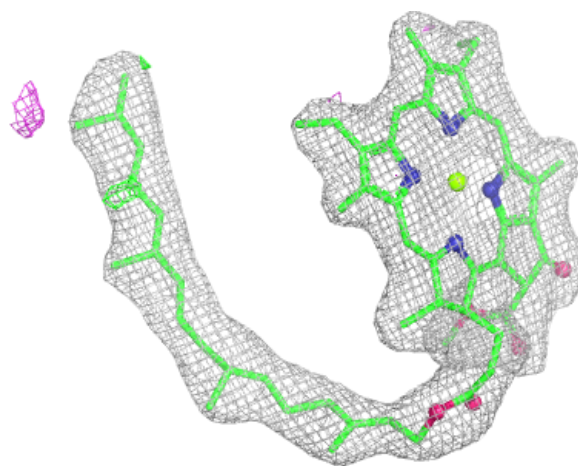
Electron density around CLA C 506:

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



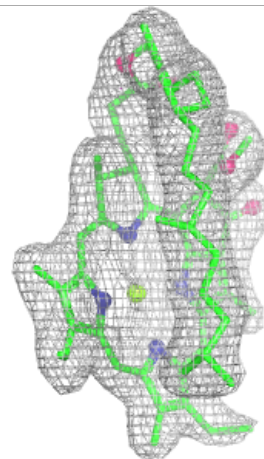
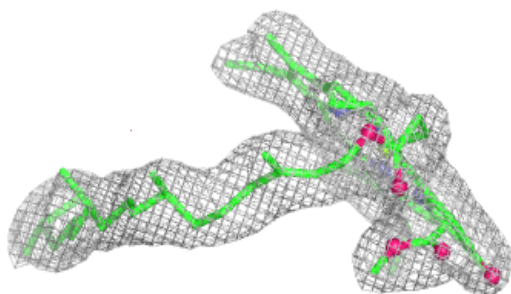
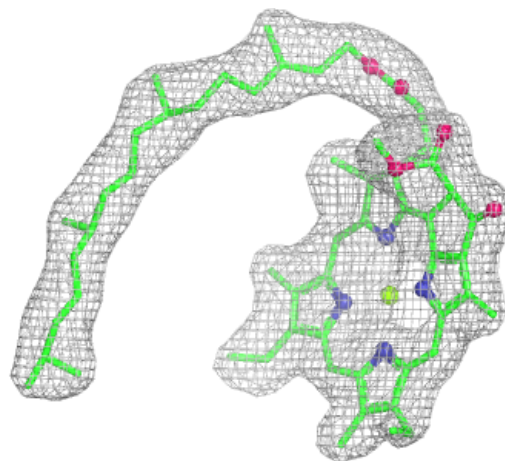
Electron density around CLA c 507:

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



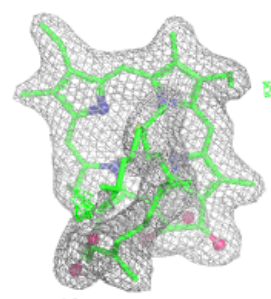
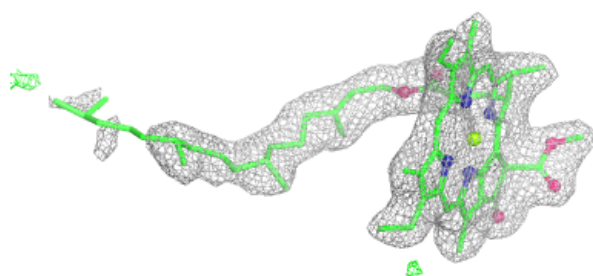
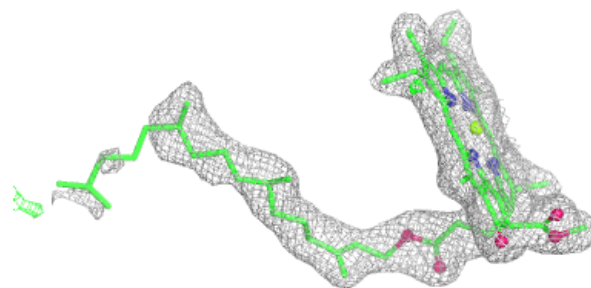
Electron density around CLA C 507:

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

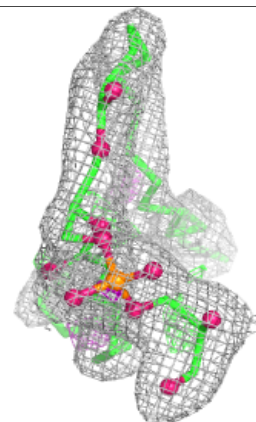
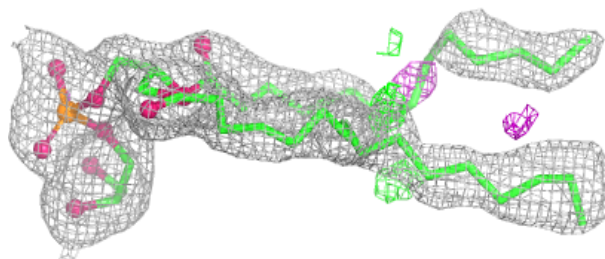
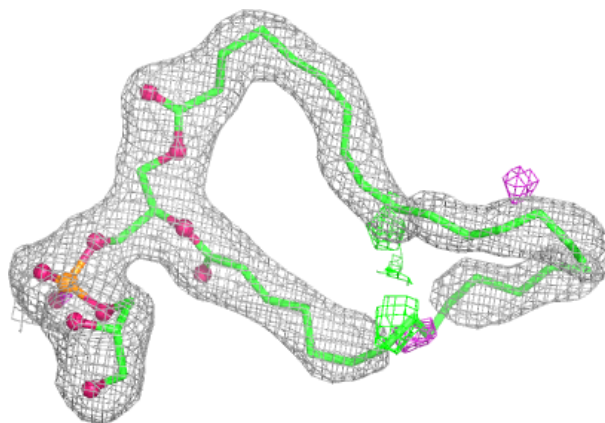


Electron density around CLA C 508:

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

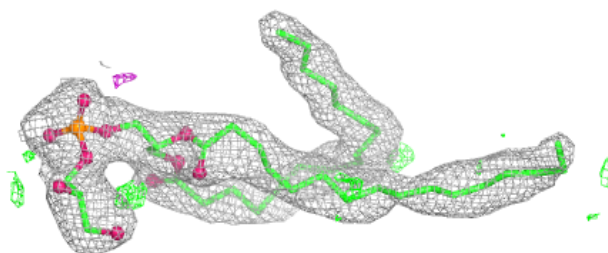
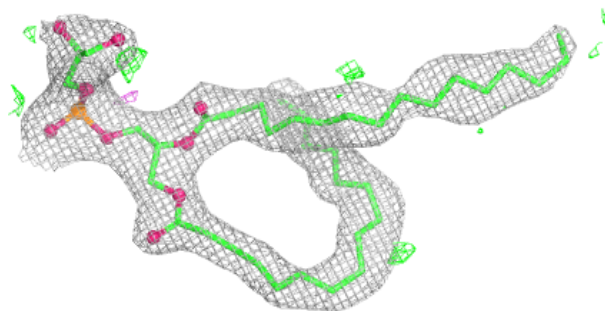
**Electron density around LHG D 410:**

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

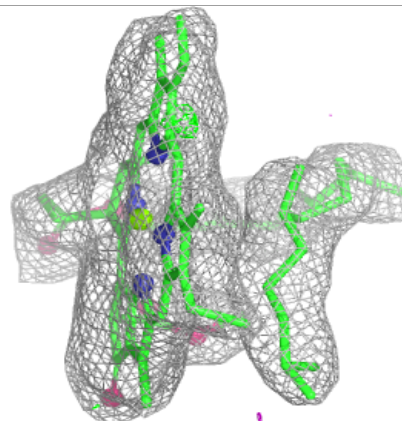
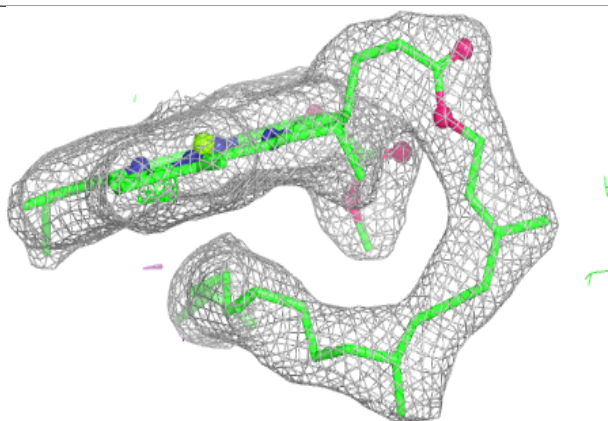
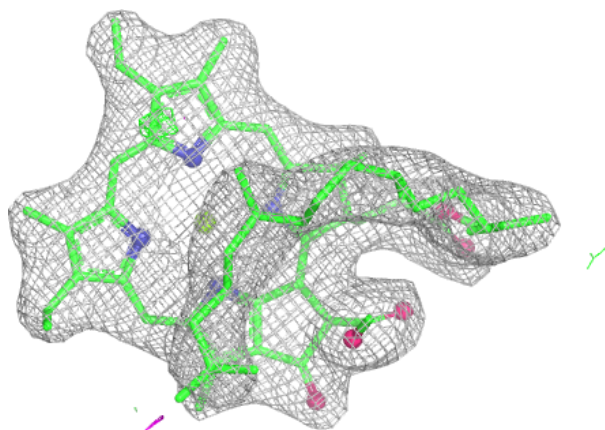


Electron density around LHG D 412:

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

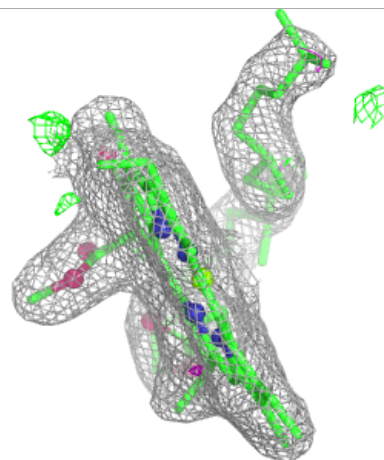
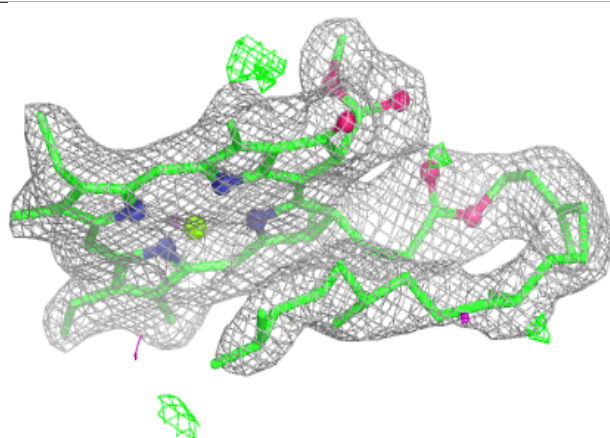
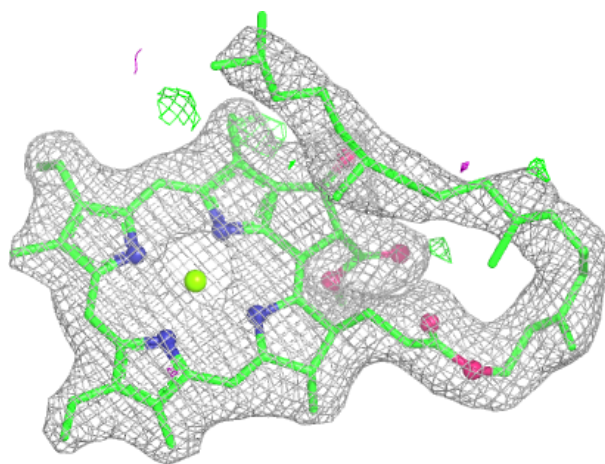
**Electron density around CLA c 510:**

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



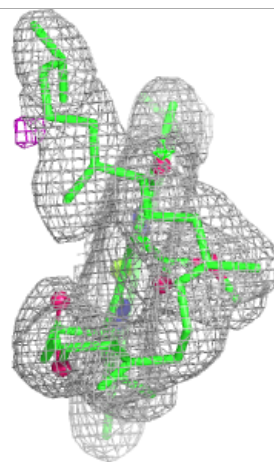
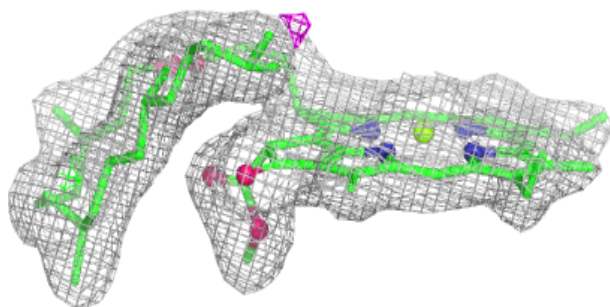
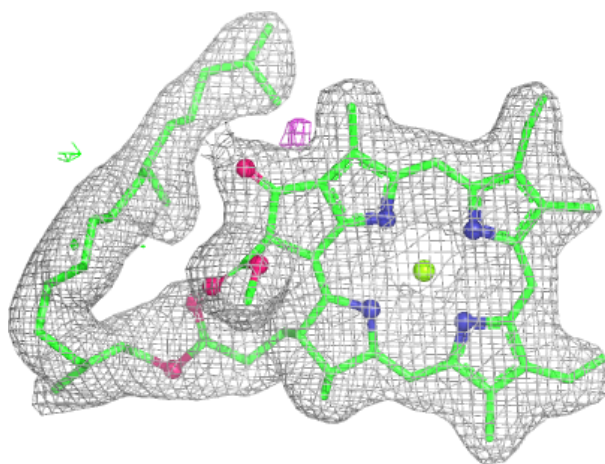
Electron density around CLA C 509:

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



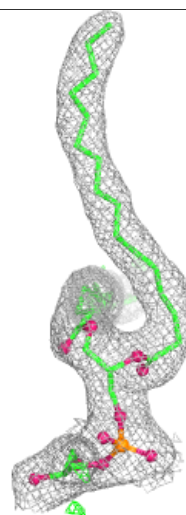
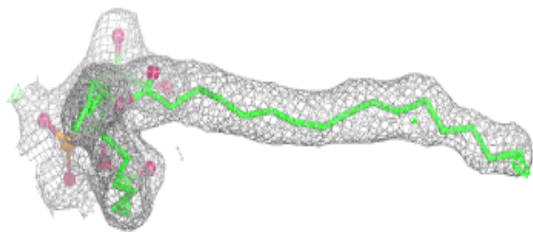
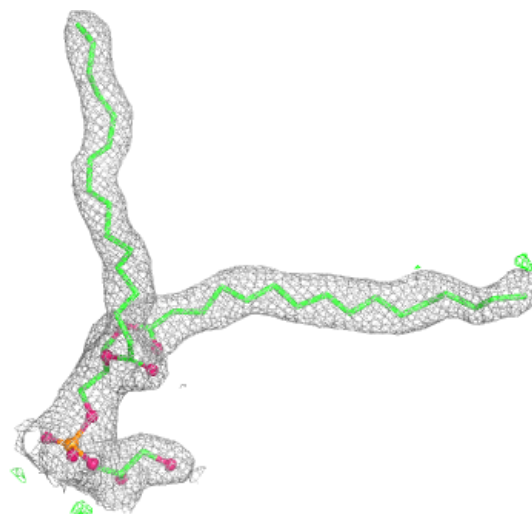
Electron density around CLA B 610:

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



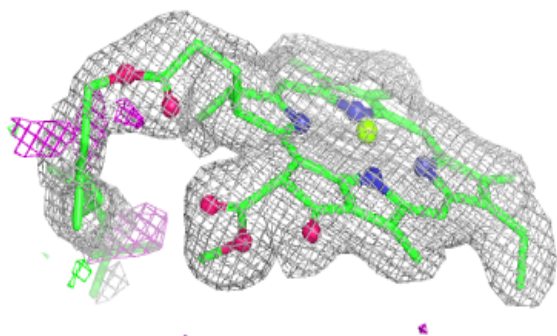
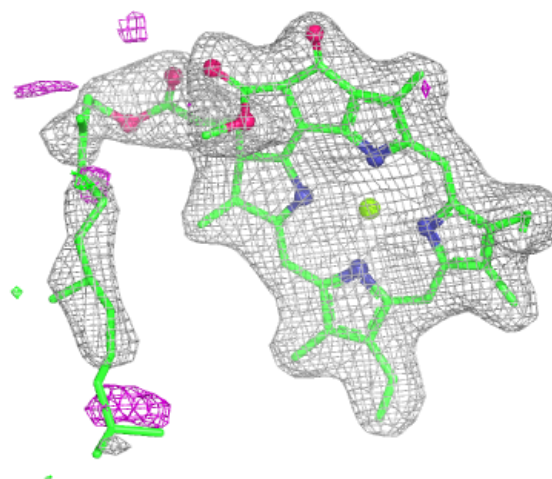
Electron density around LHG 1 101:

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



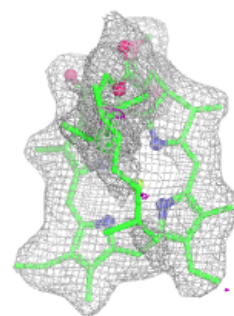
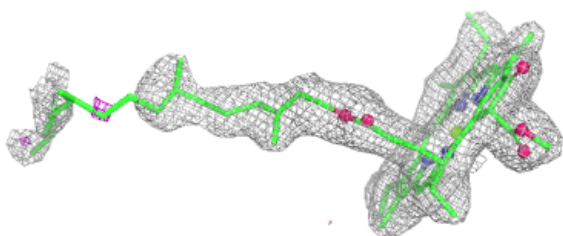
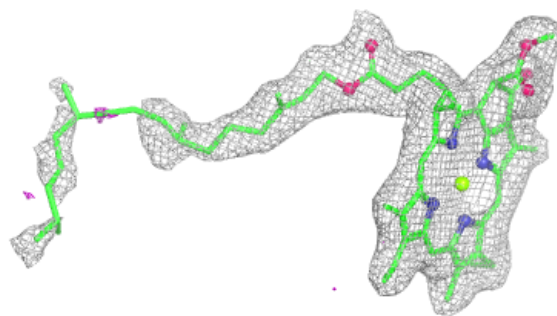
Electron density around CLA B 616:

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

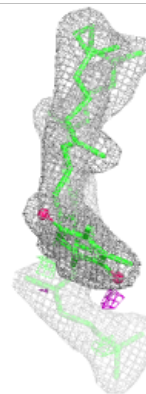
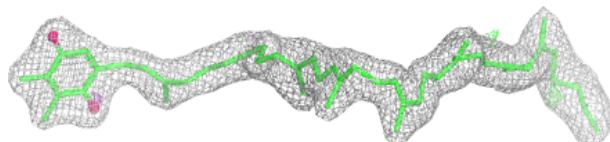
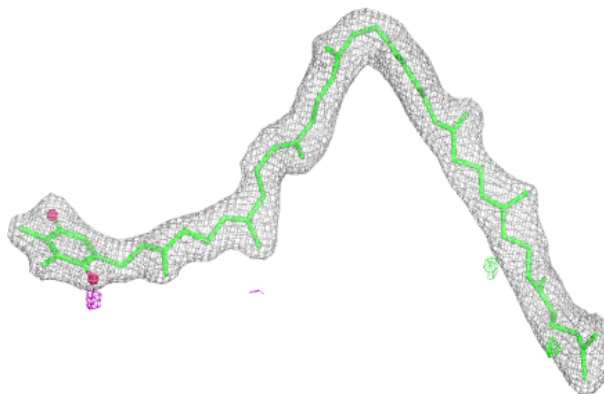


Electron density around CLA d 404:

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

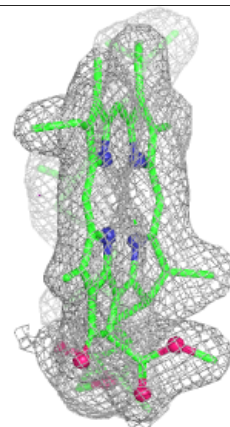
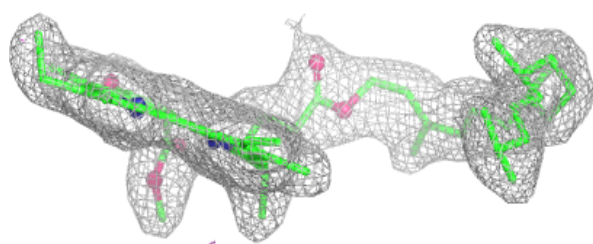
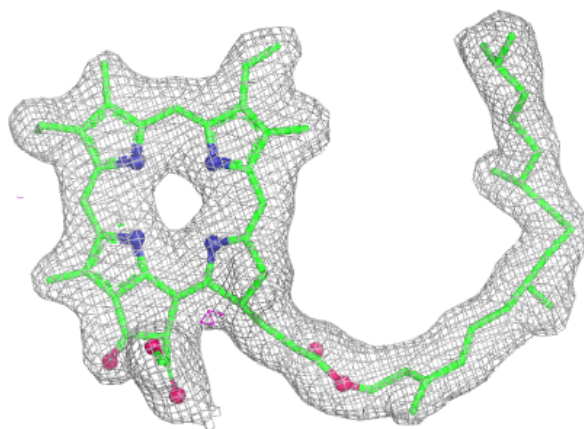
**Electron density around PL9 d 406:**

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

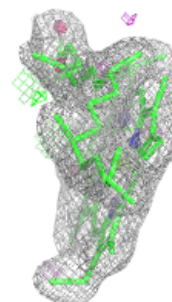
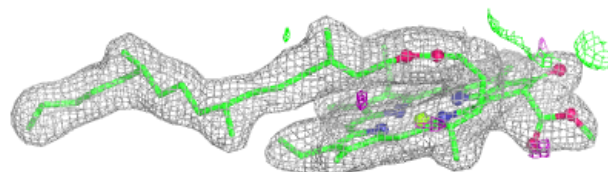
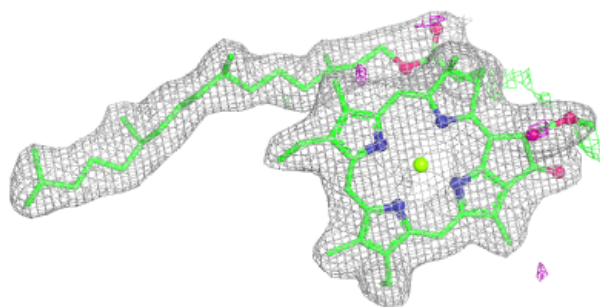


Electron density around PHO d 401:

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

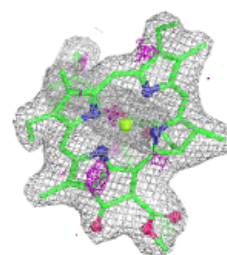
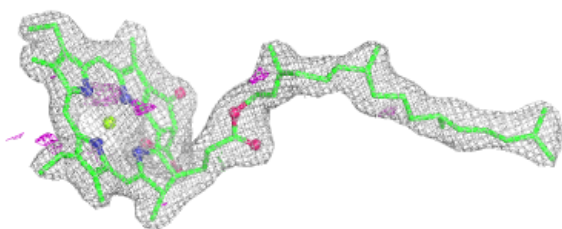
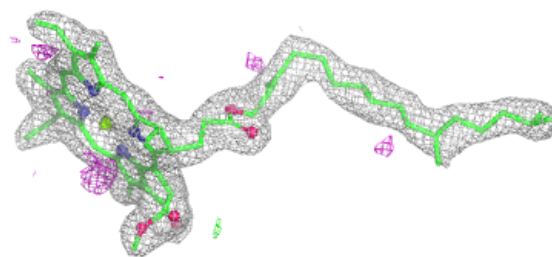
**Electron density around CLA C 501:**

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

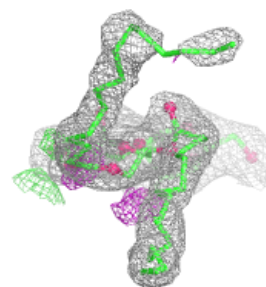
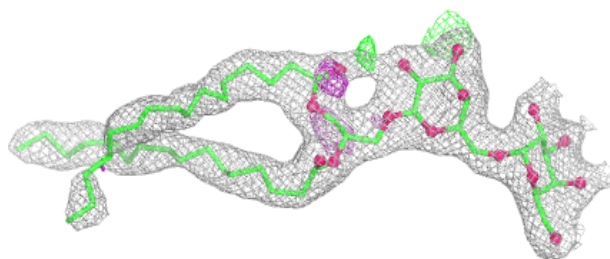
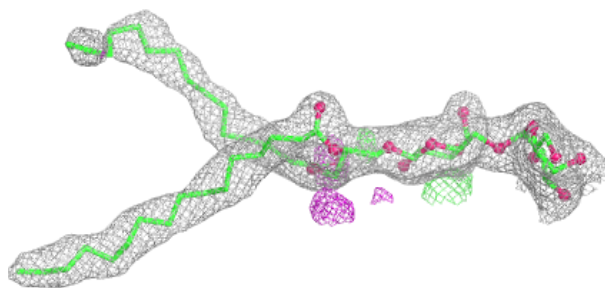


Electron density around CLA C 502:

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

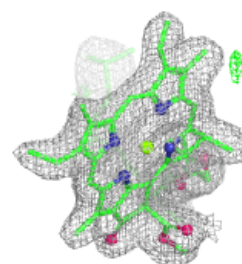
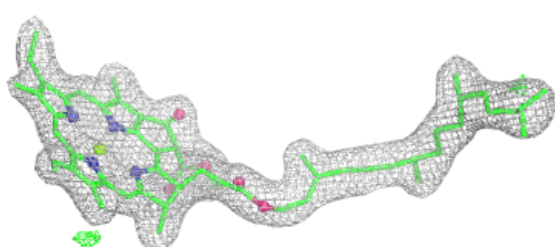
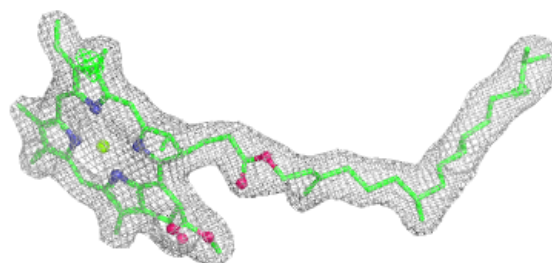
**Electron density around DGD c 517:**

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

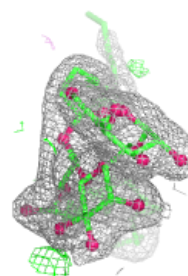
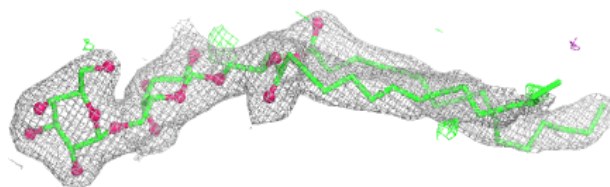
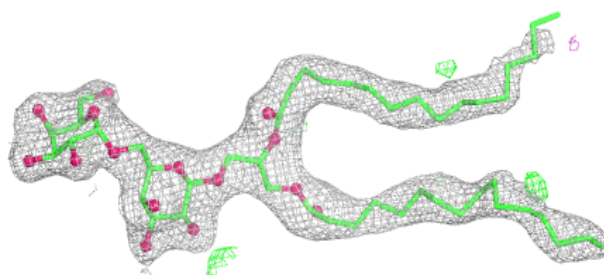


Electron density around CLA a 607:

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

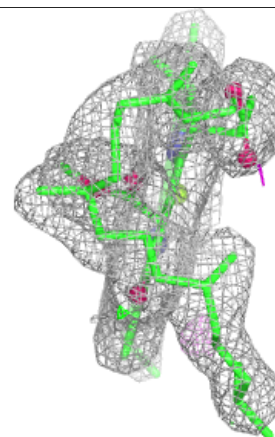
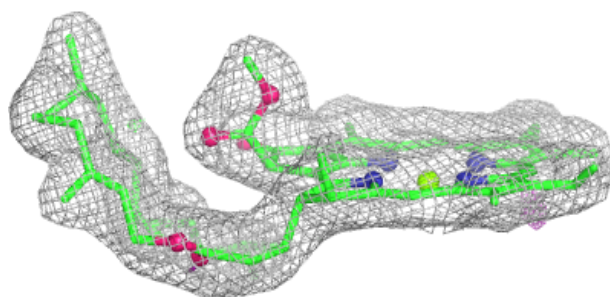
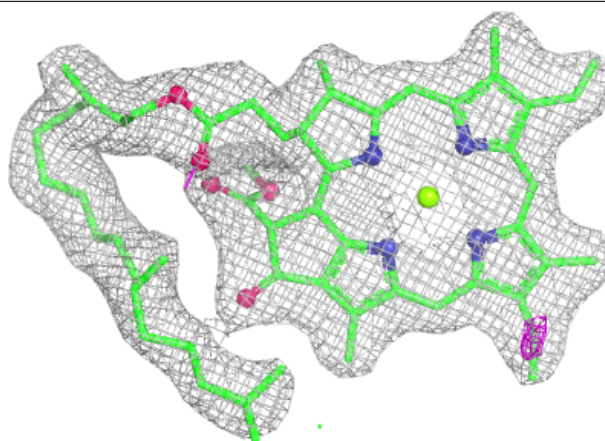
**Electron density around DGD c 519:**

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



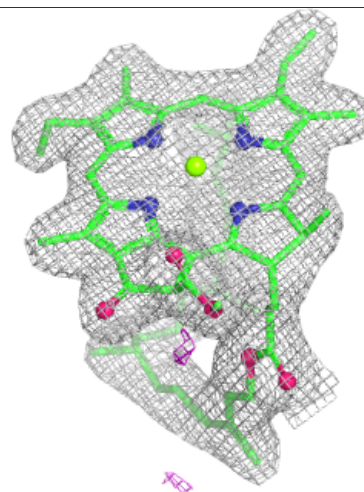
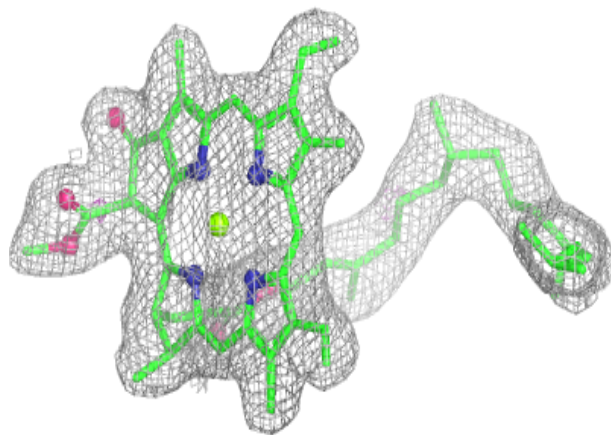
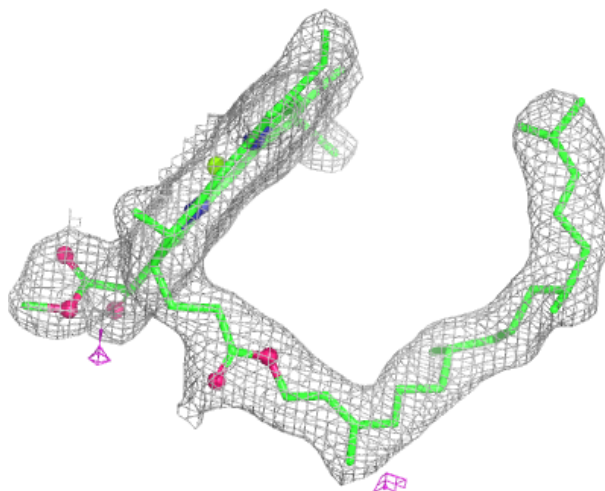
Electron density around CLA b 610:

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



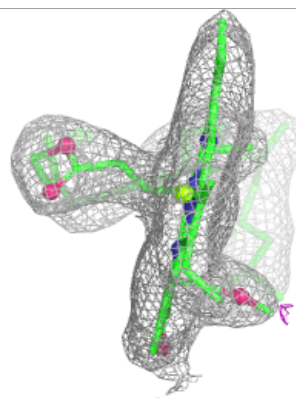
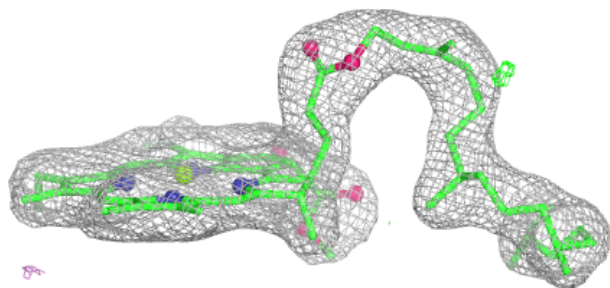
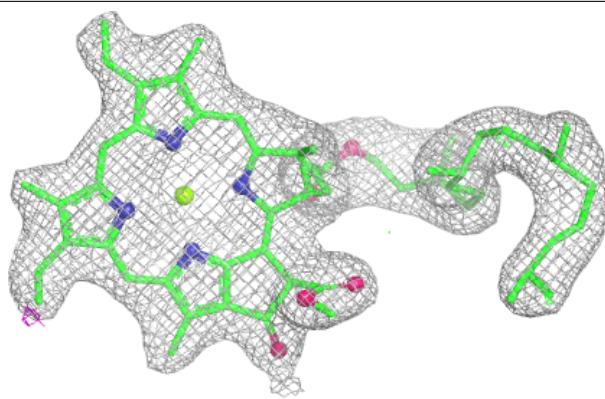
Electron density around CLA b 611:

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



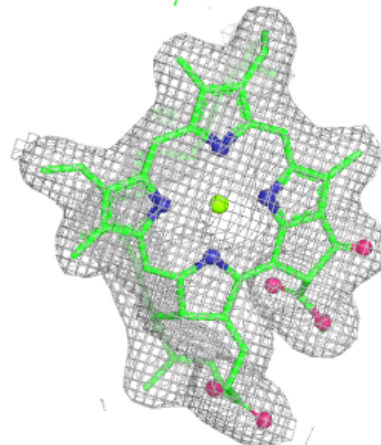
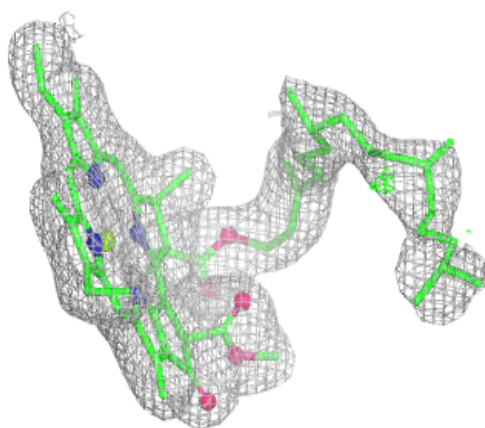
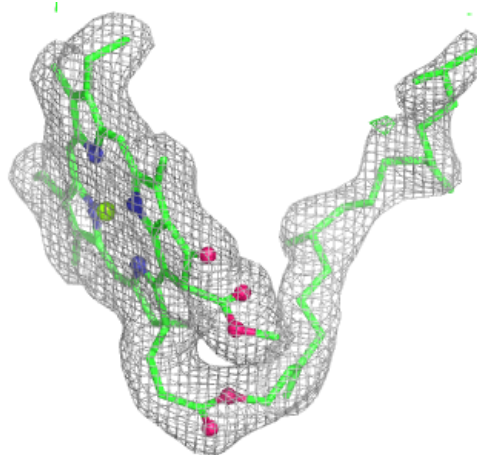
Electron density around CLA b 612:

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



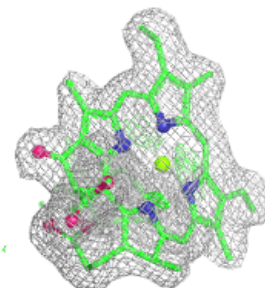
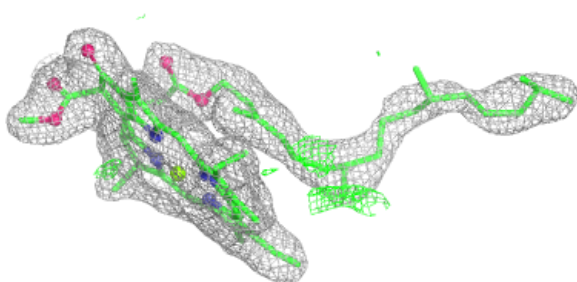
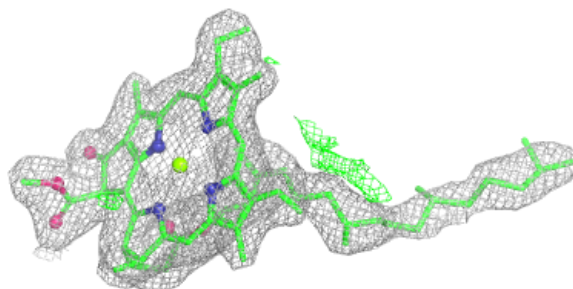
Electron density around CLA b 613:

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

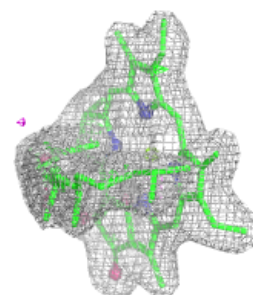
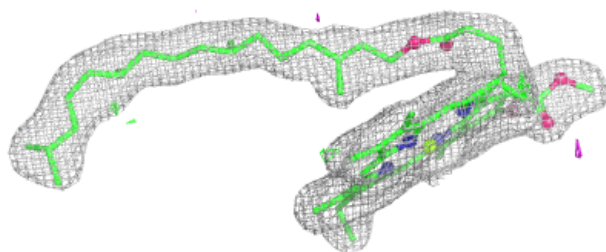
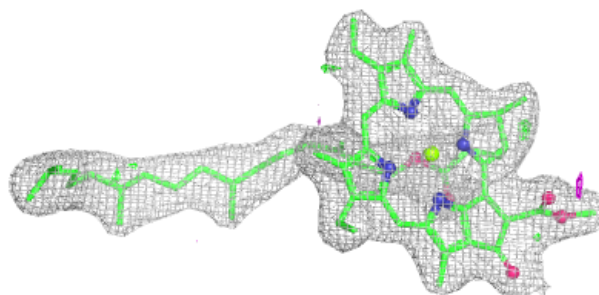


Electron density around CLA C 505:

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

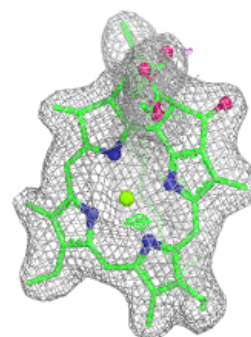
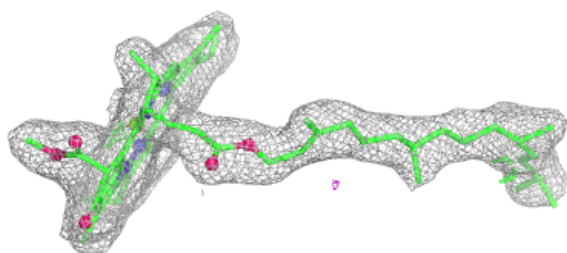
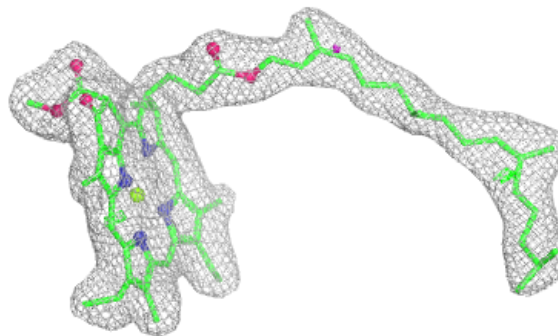
**Electron density around CLA B 608:**

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

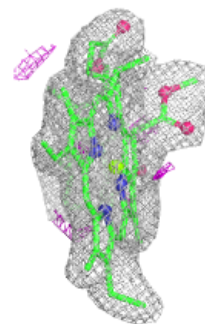
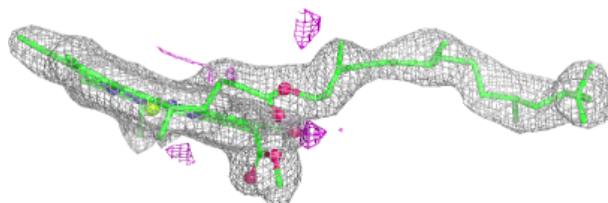
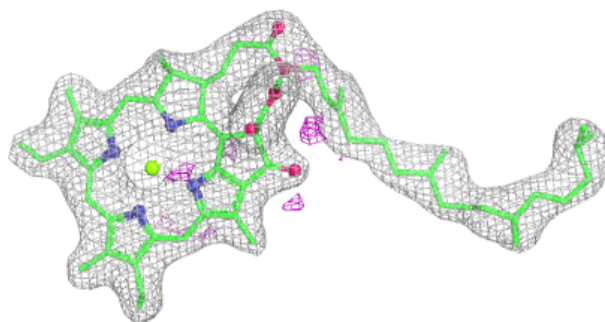


Electron density around CLA B 609:

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

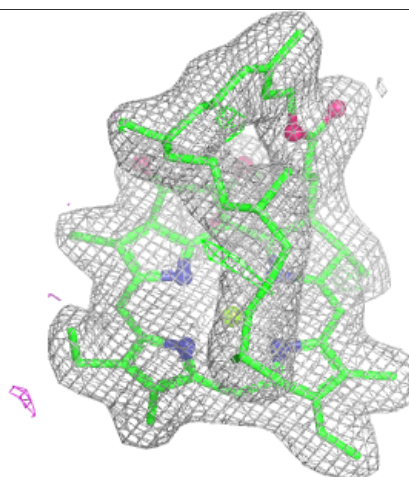
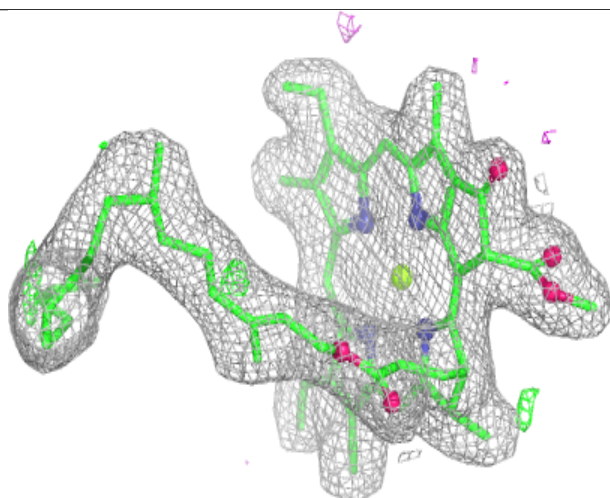
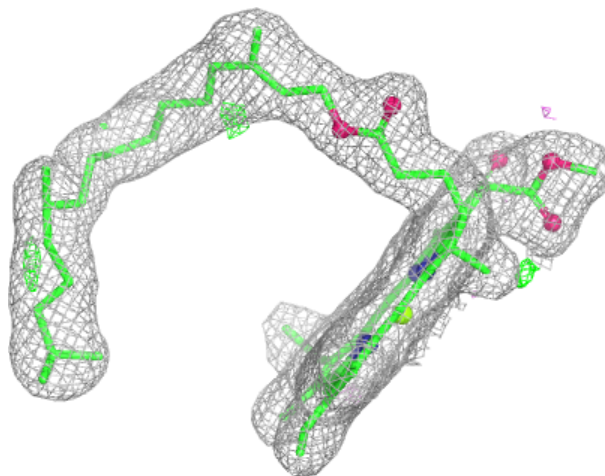
**Electron density around CLA B 602:**

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



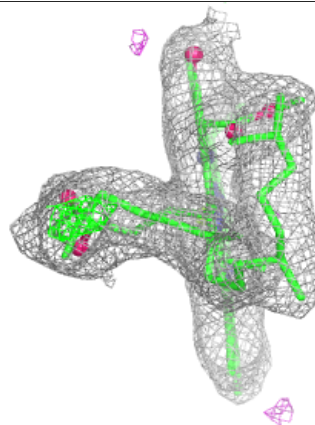
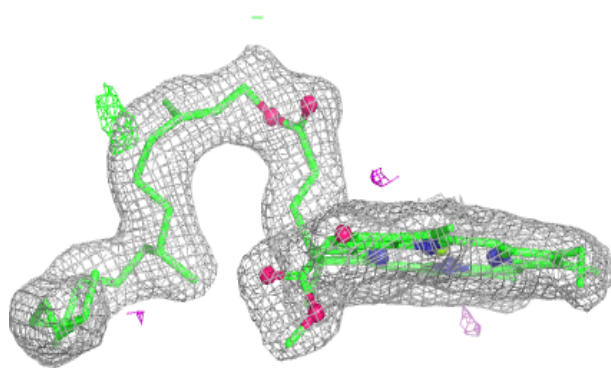
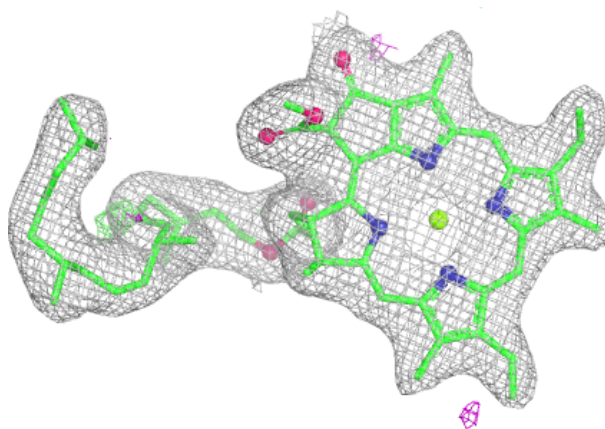
Electron density around CLA B 611:

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



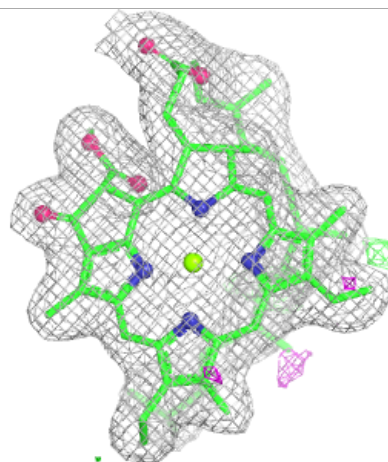
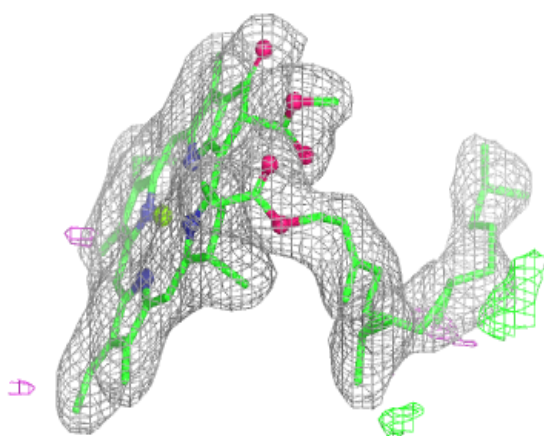
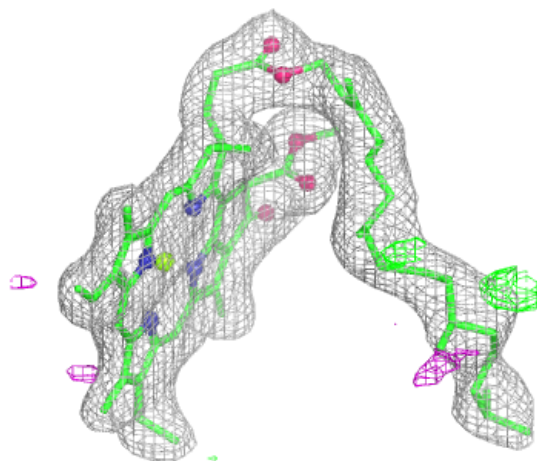
Electron density around CLA B 612:

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



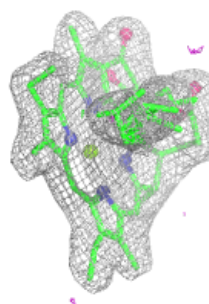
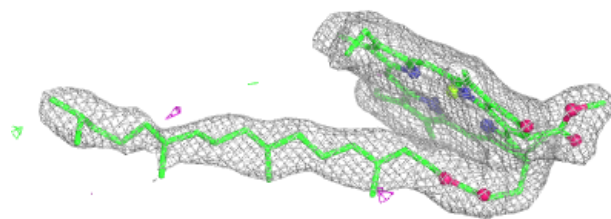
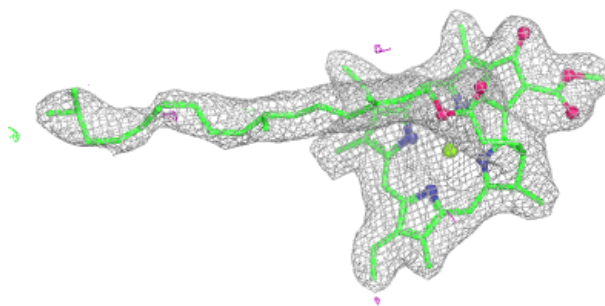
Electron density around CLA B 613:

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



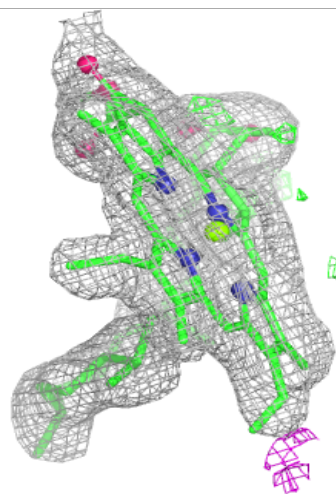
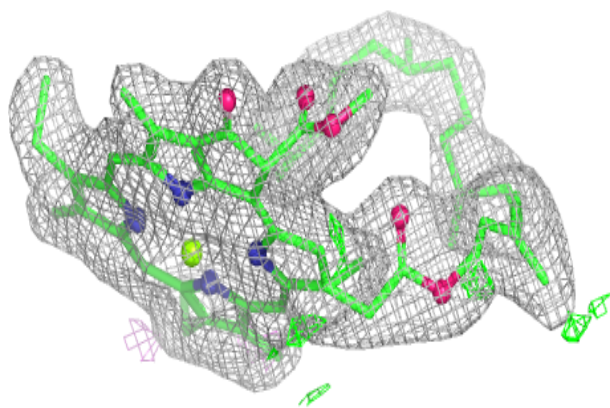
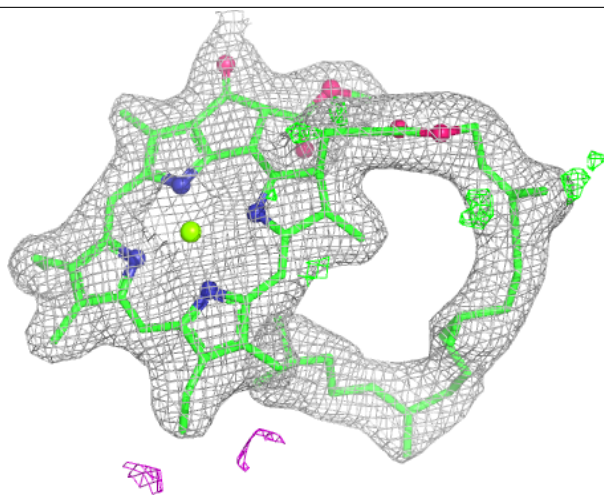
Electron density around CLA B 614:

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



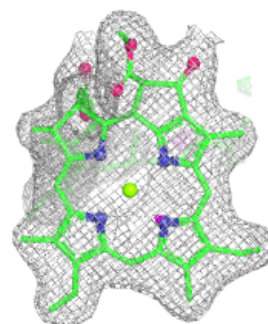
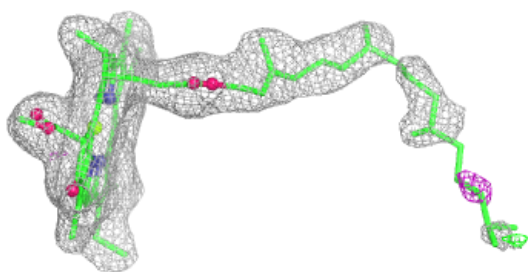
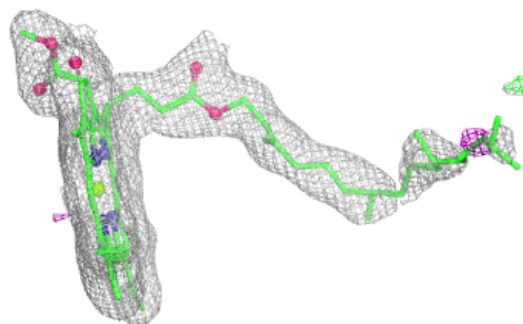
Electron density around CLA B 615:

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



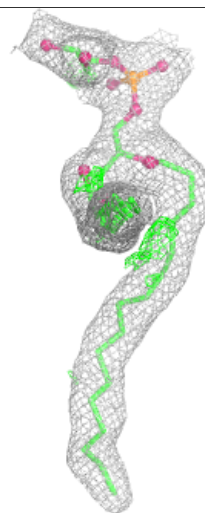
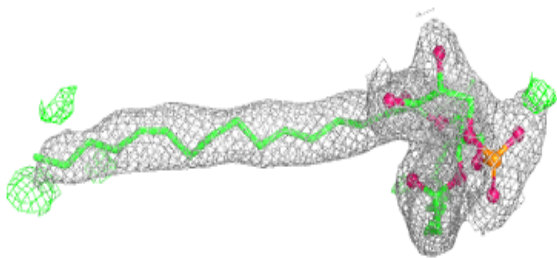
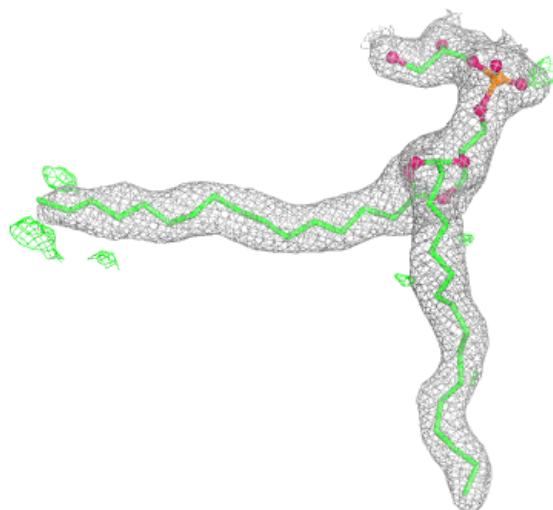
Electron density around CLA D 405:

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



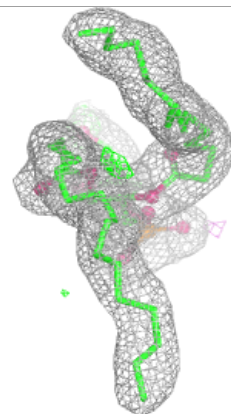
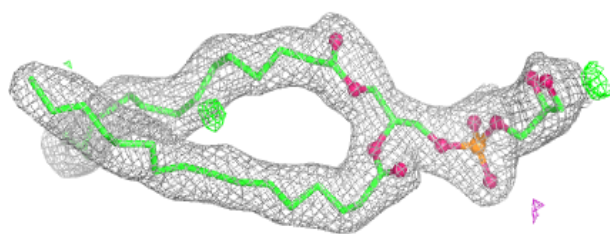
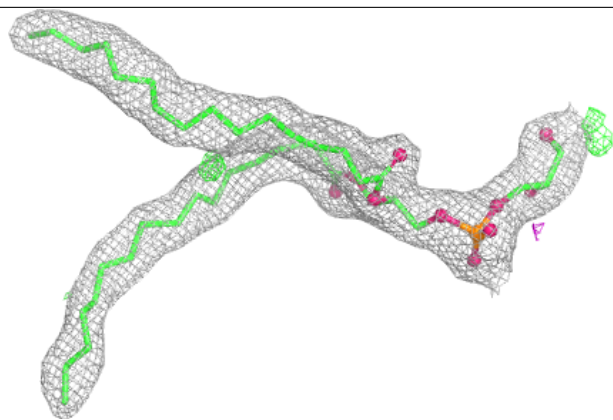
Electron density around LHG A 615:

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

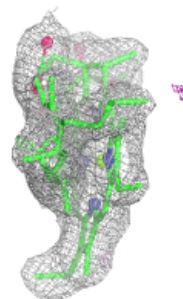
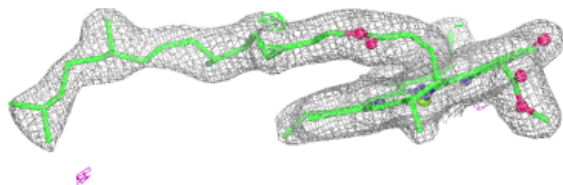
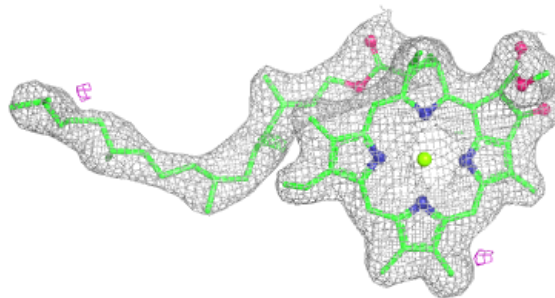


Electron density around LHG D 409:

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

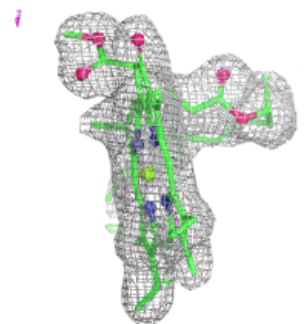
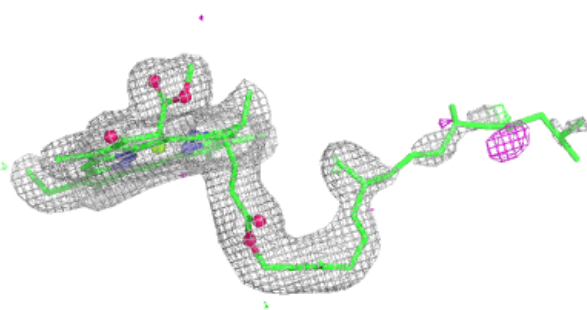
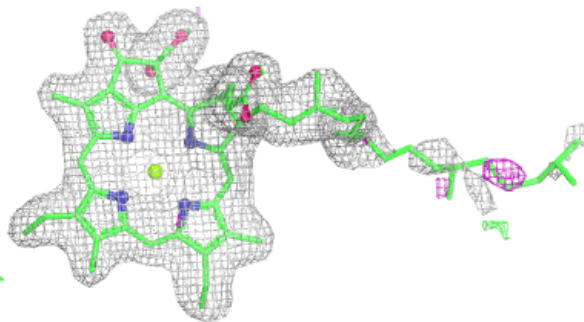
**Electron density around CLA B 603:**

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

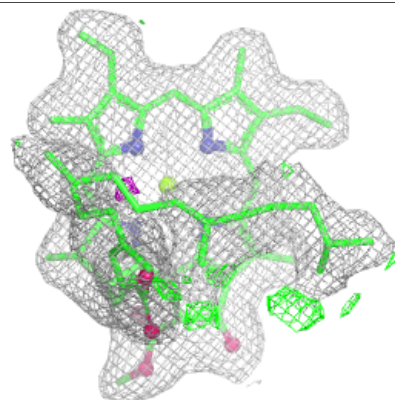
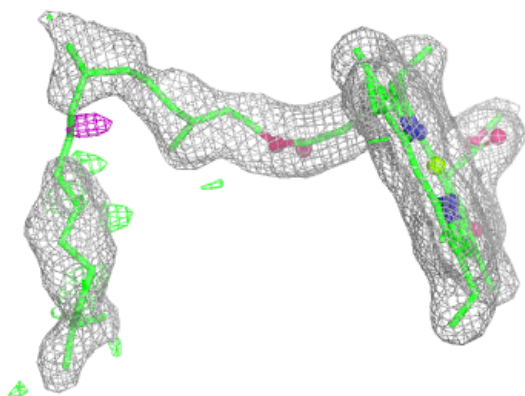
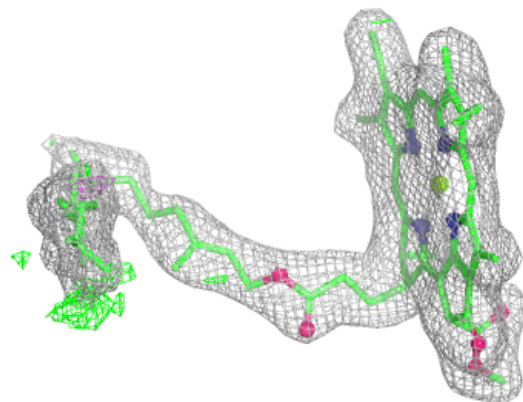


Electron density around CLA A 607:

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

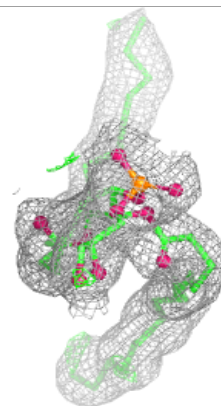
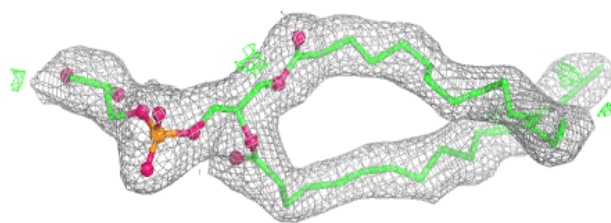
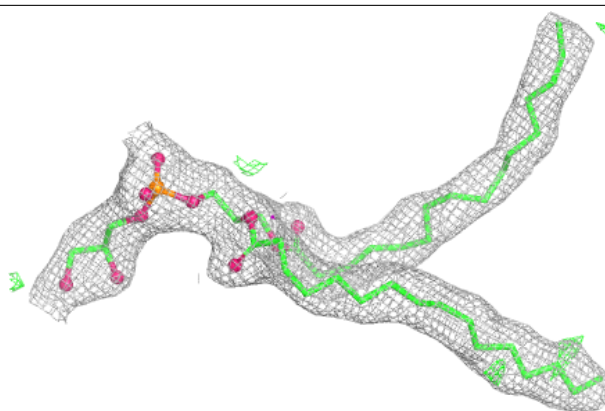
**Electron density around CLA a 609:**

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

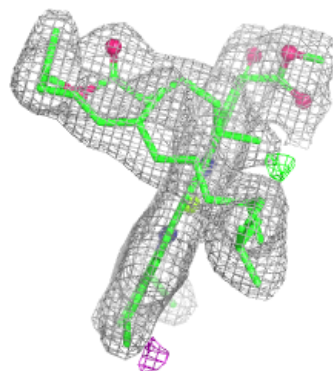
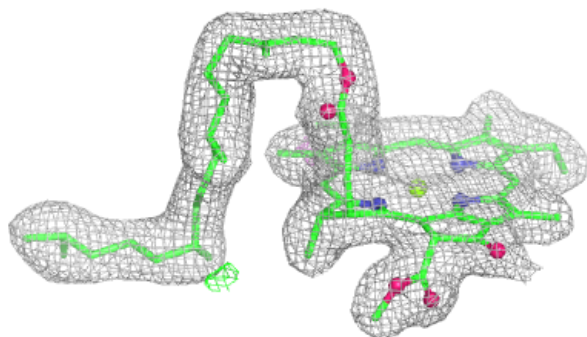
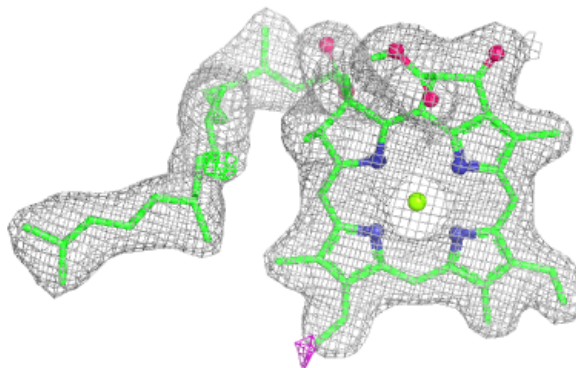


Electron density around LHG d 408:

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

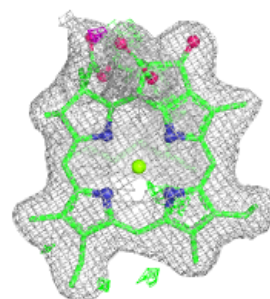
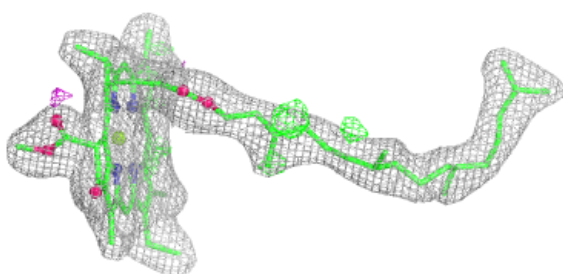
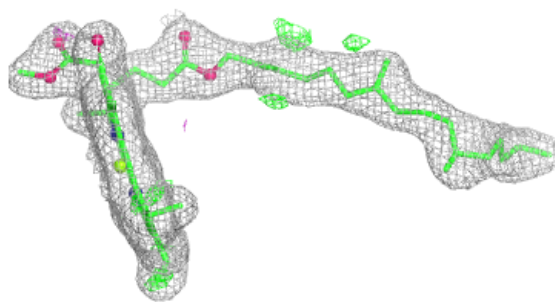
**Electron density around CLA a 612:**

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

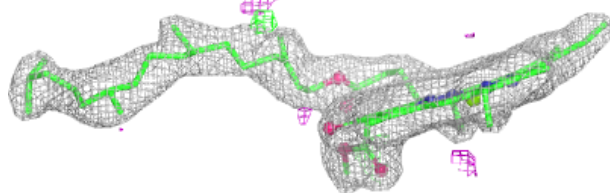
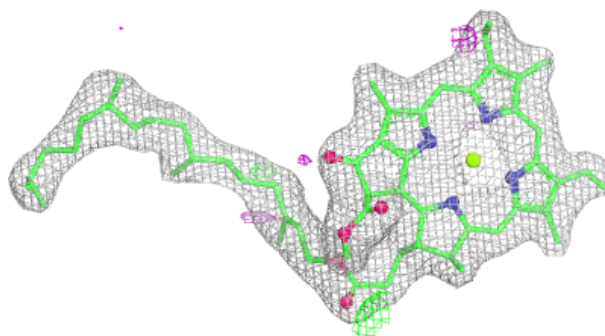


Electron density around CLA B 605:

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

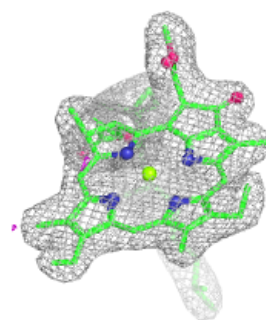
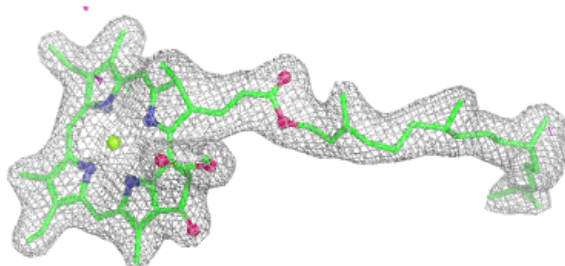
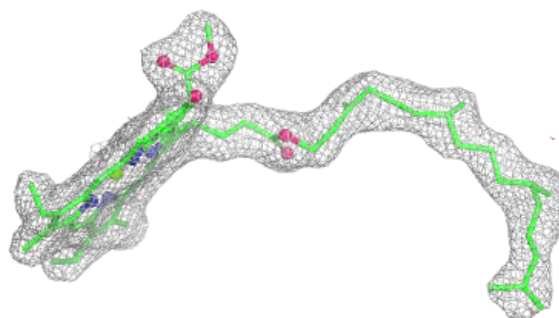
**Electron density around CLA b 602:**

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

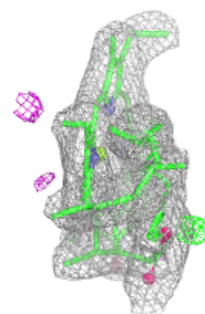
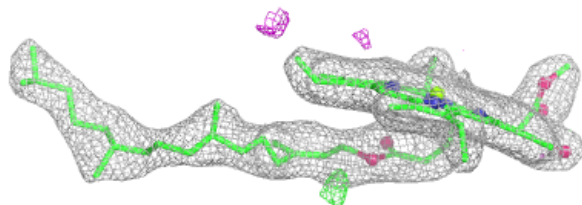
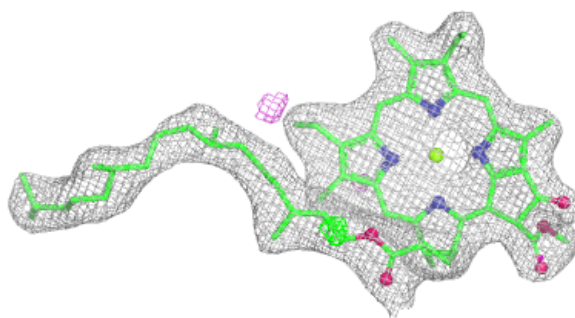


Electron density around CLA d 403:

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

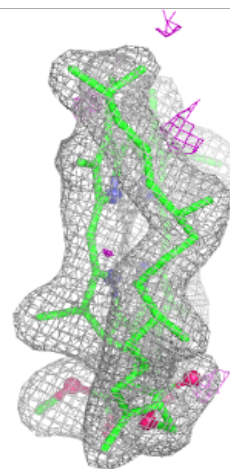
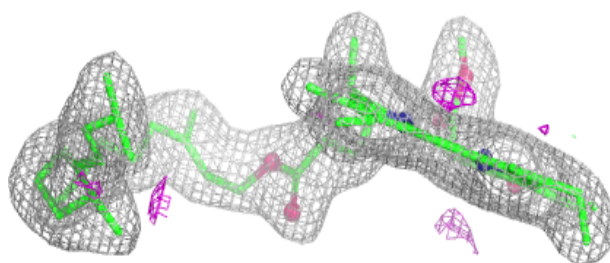
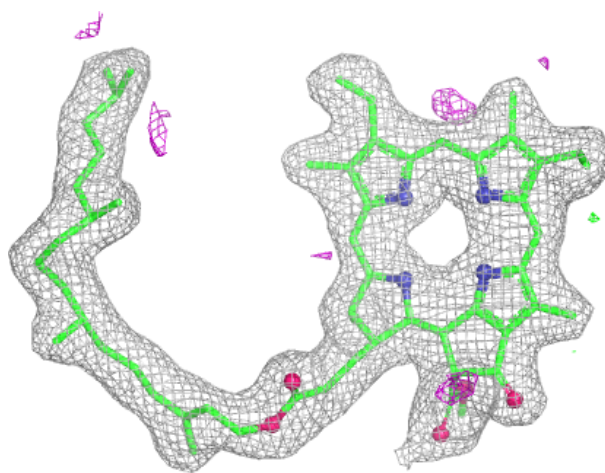
**Electron density around CLA b 603:**

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



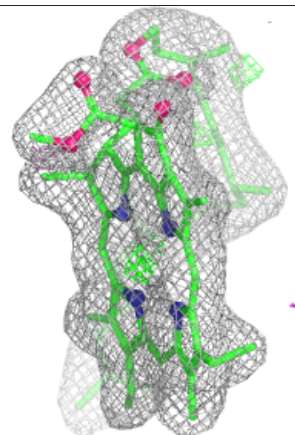
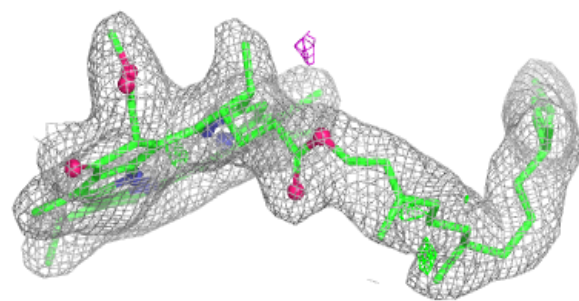
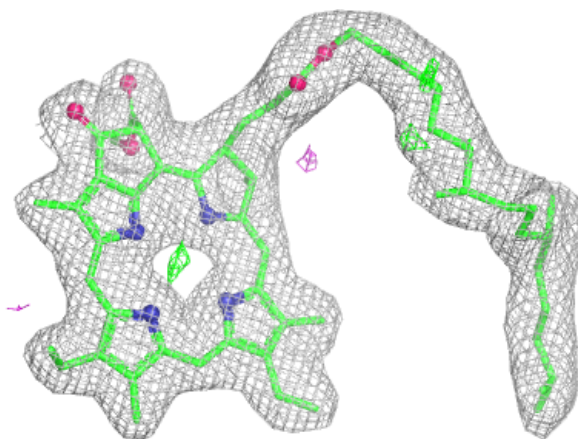
Electron density around PHO A 608:

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



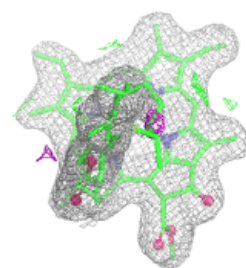
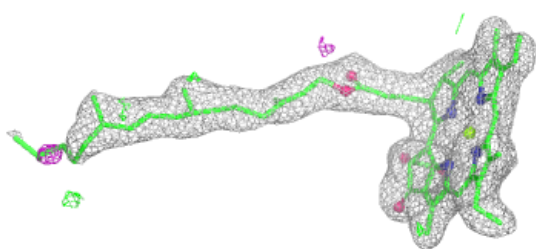
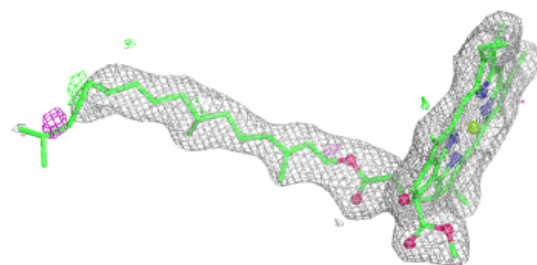
Electron density around PHO D 402:

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



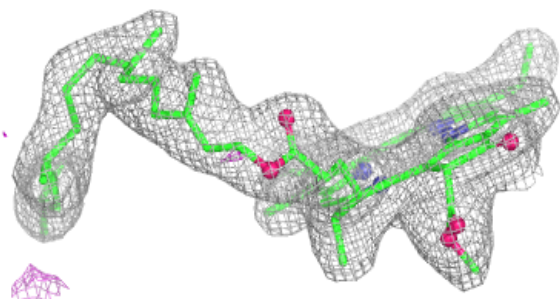
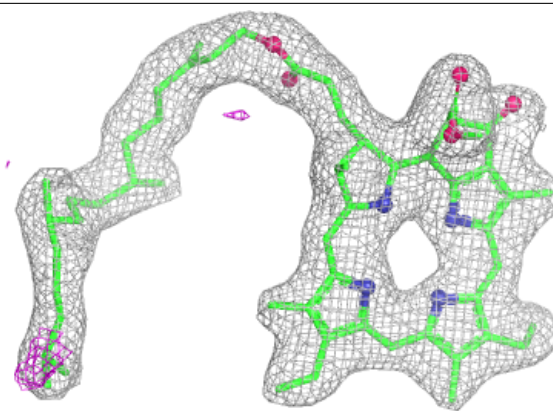
Electron density around CLA b 604:

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



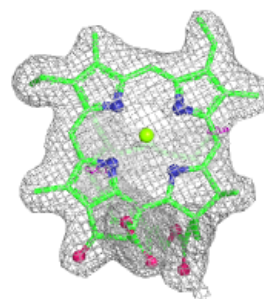
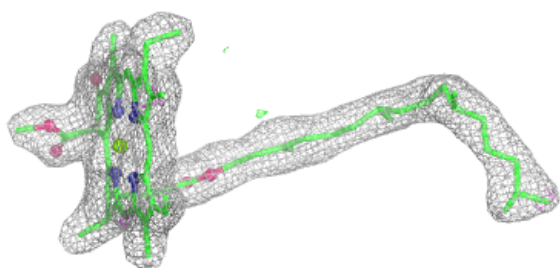
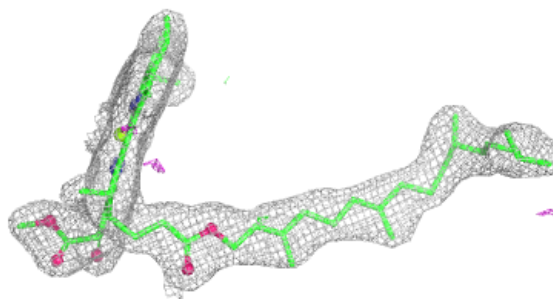
Electron density around PHO d 402:

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

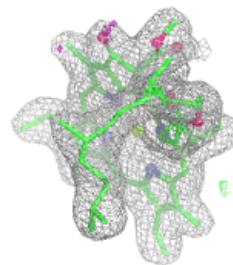
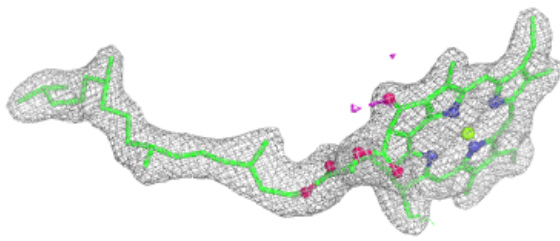
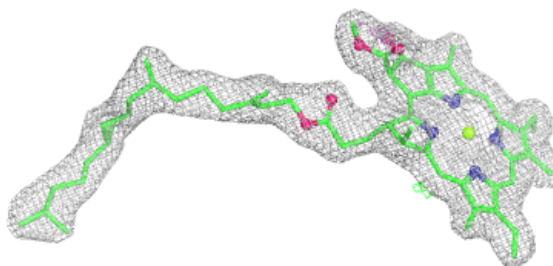


Electron density around CLA b 605:

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

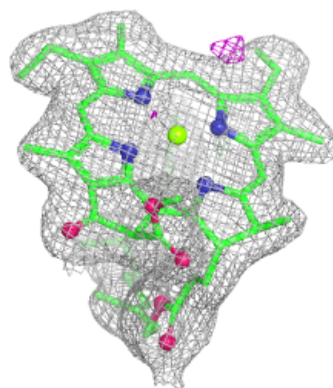
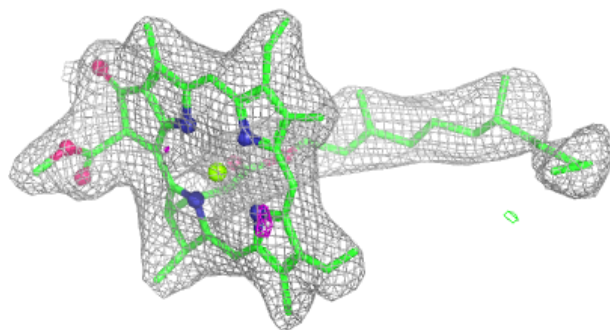
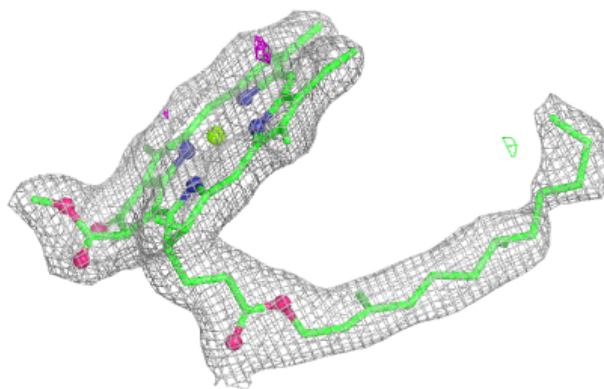
**Electron density around CLA A 606:**

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

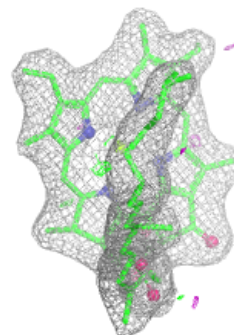
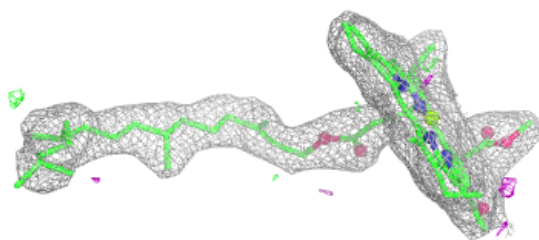
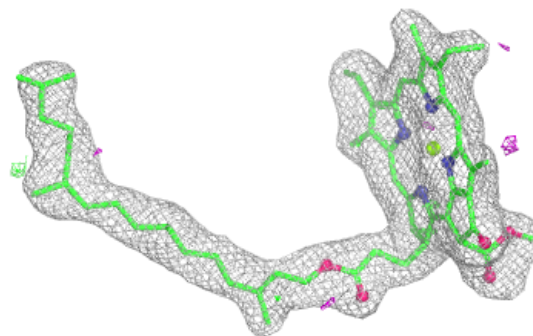


Electron density around CLA C 504:

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

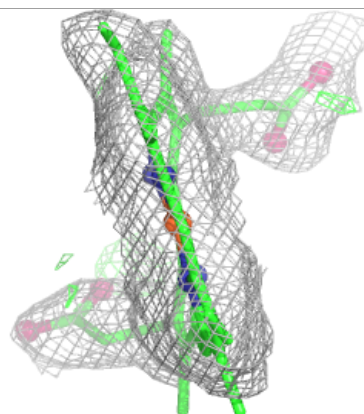
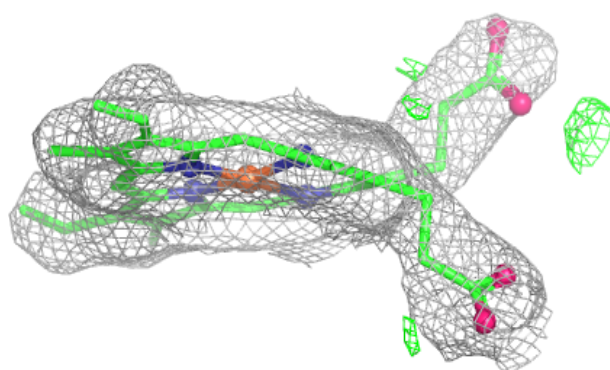
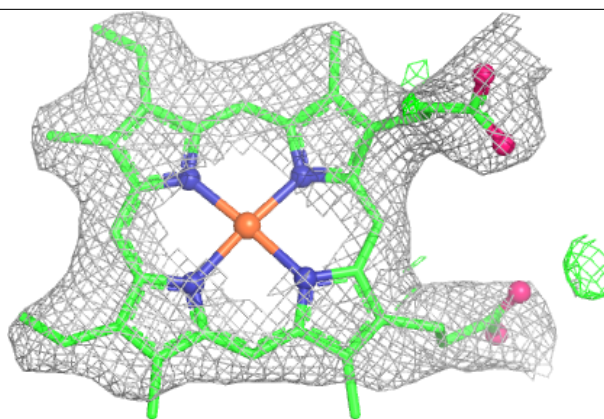
**Electron density around CLA b 609:**

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

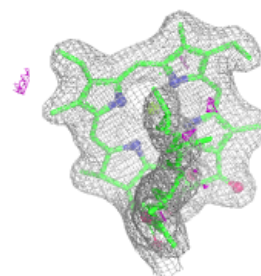
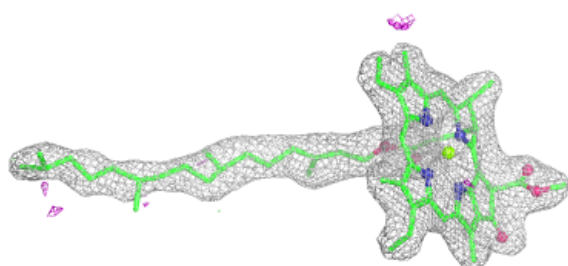
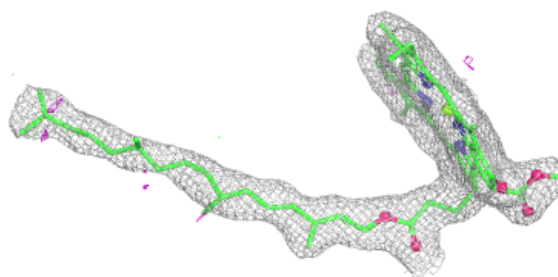


Electron density around HEM f 101:

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

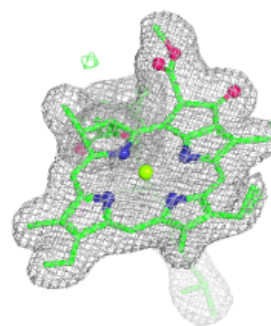
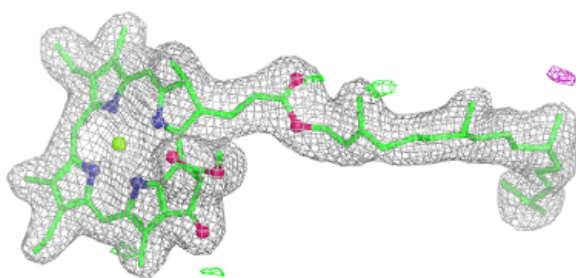
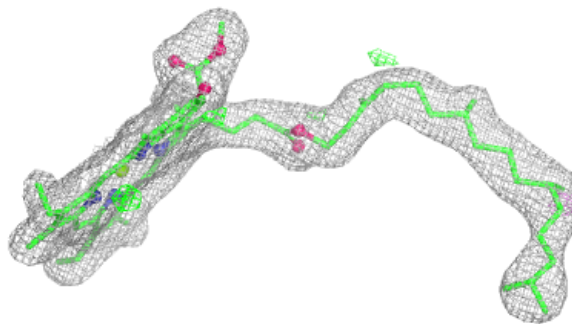
**Electron density around CLA b 607:**

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

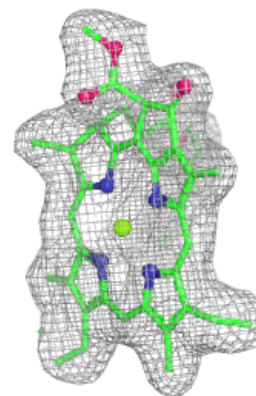
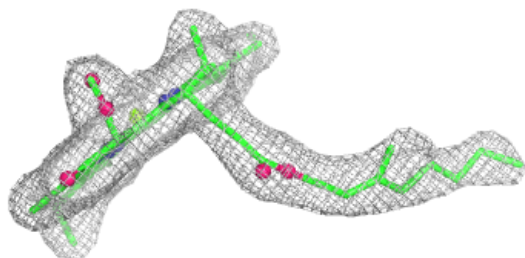
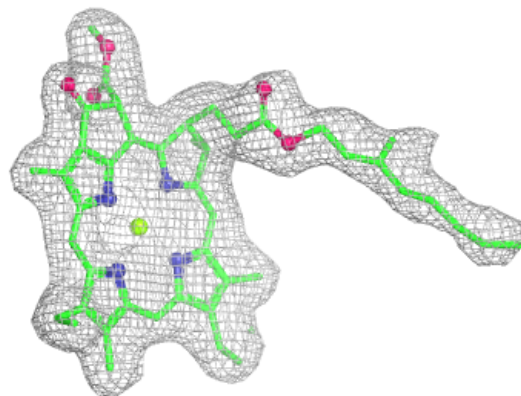


Electron density around CLA D 404:

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

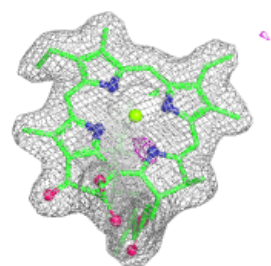
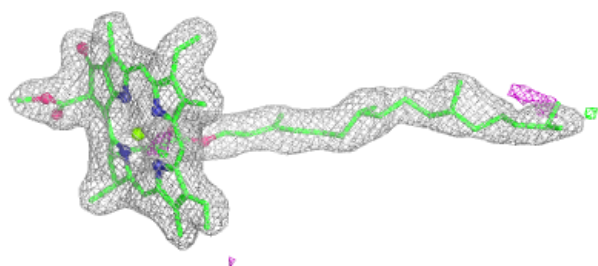
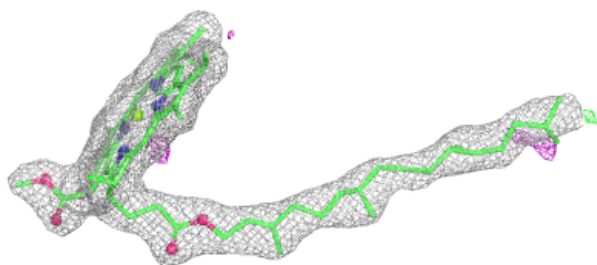
**Electron density around CLA A 609:**

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



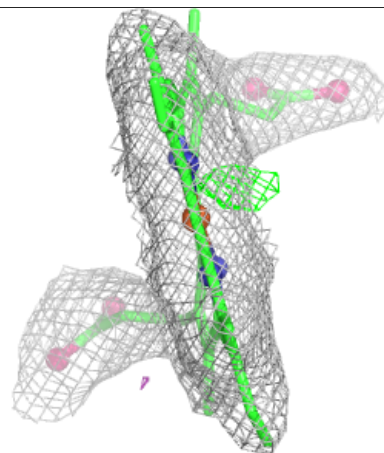
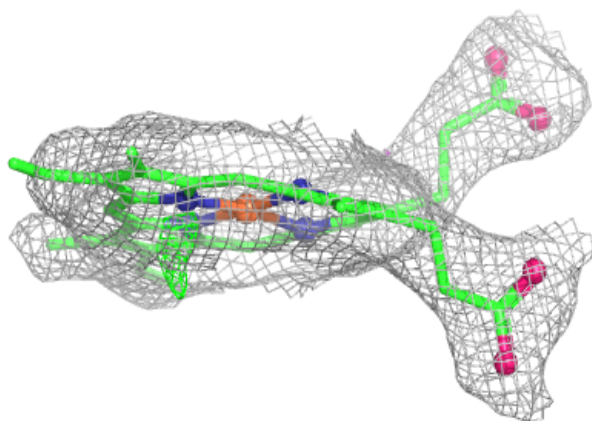
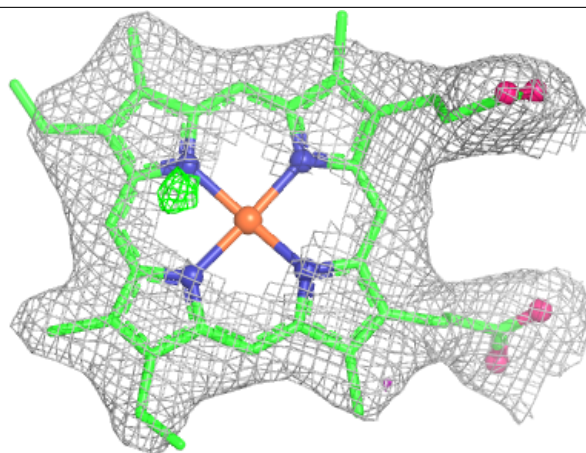
Electron density around CLA B 607:

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



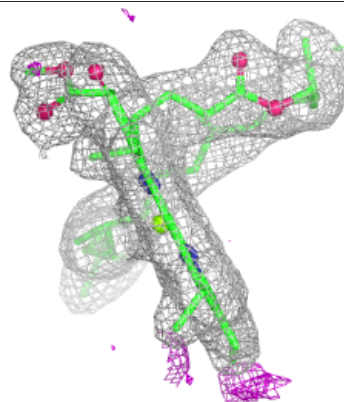
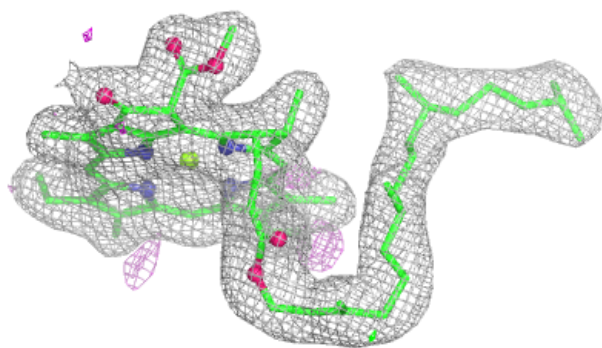
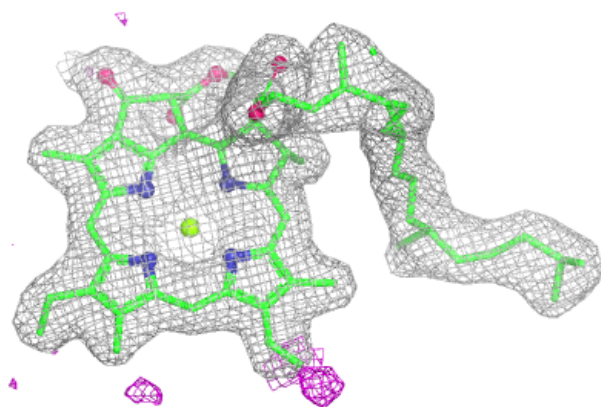
Electron density around HEM E 101:

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



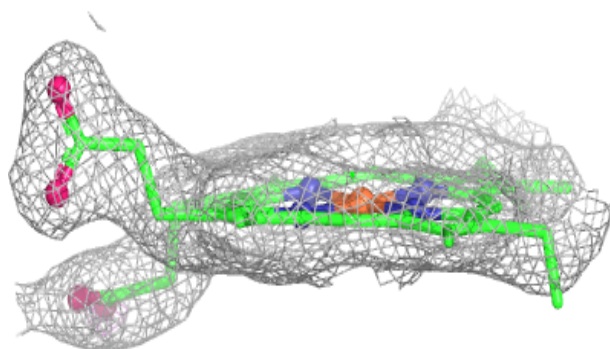
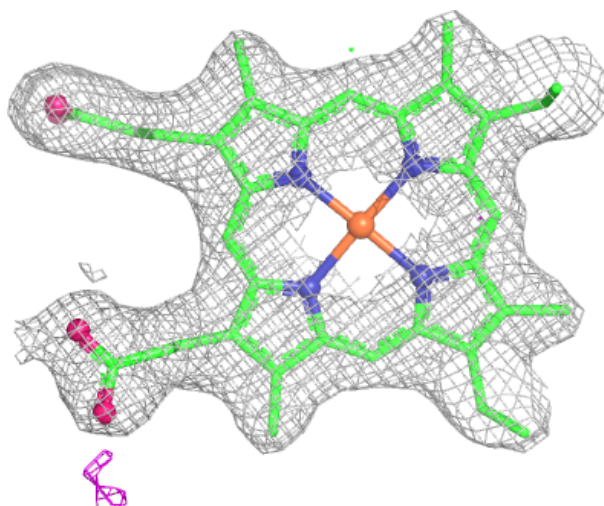
Electron density around CLA D 403:

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



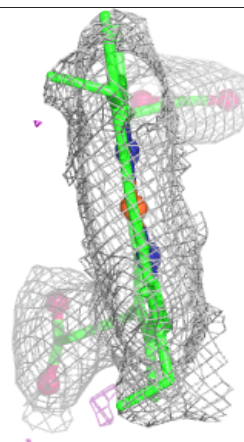
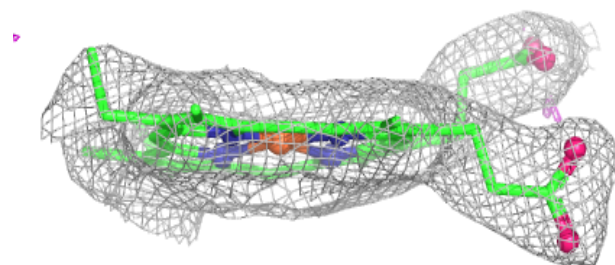
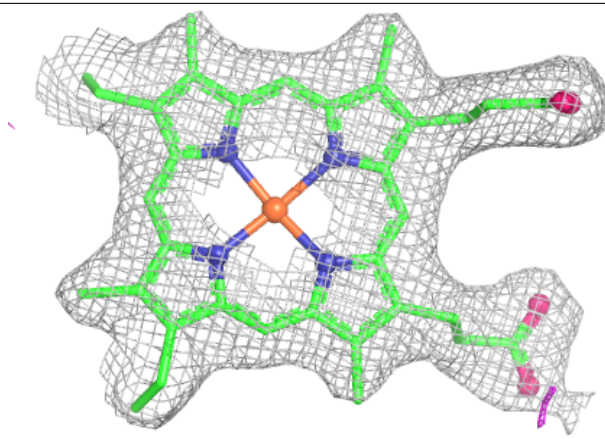
Electron density around HEC V 201:

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



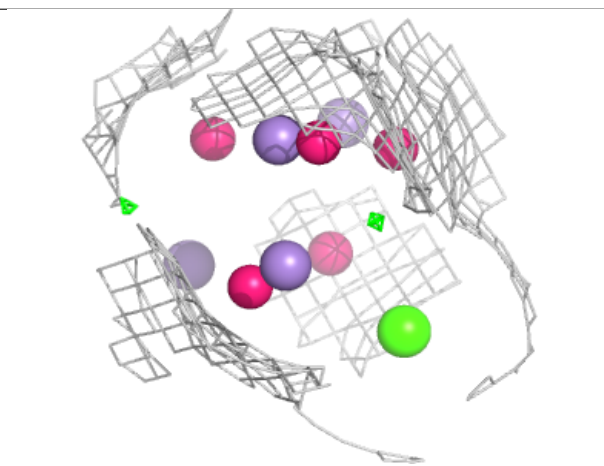
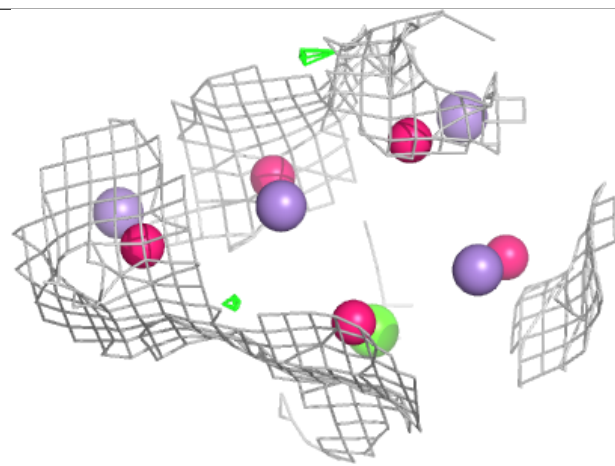
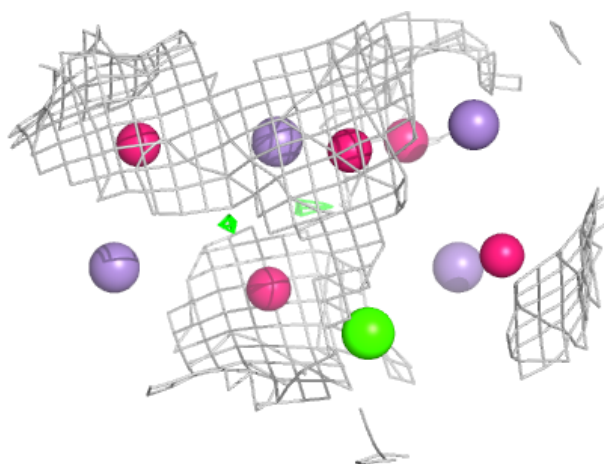
Electron density around HEC v 201:

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



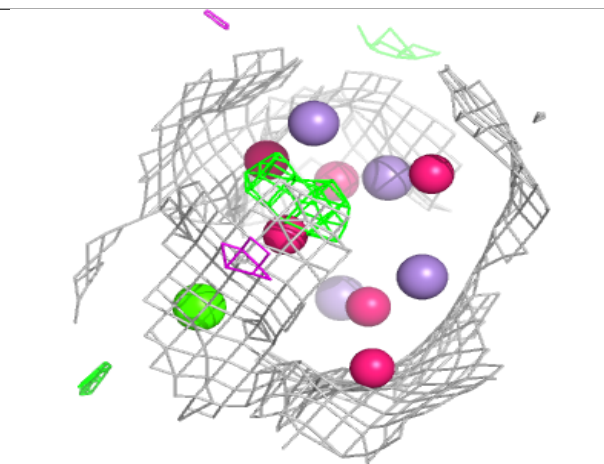
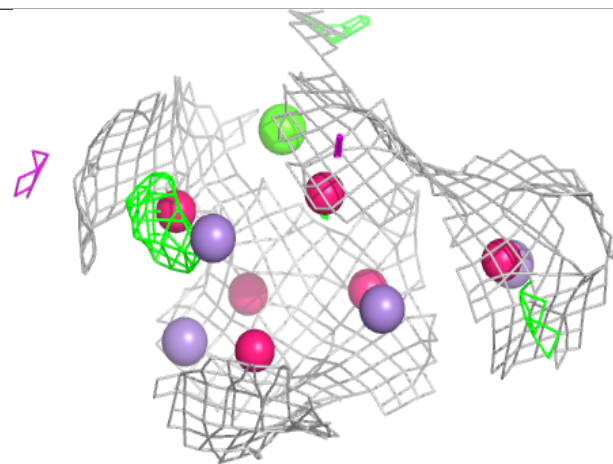
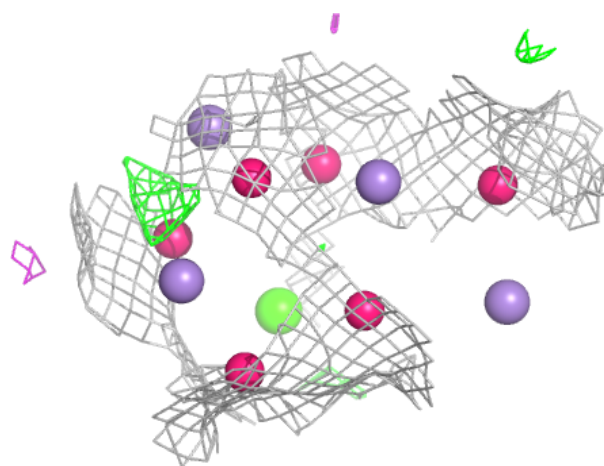
Electron density around OEX a 602 (Å):

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



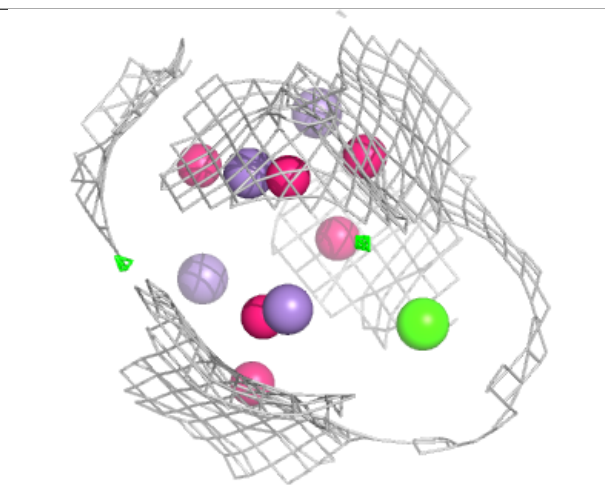
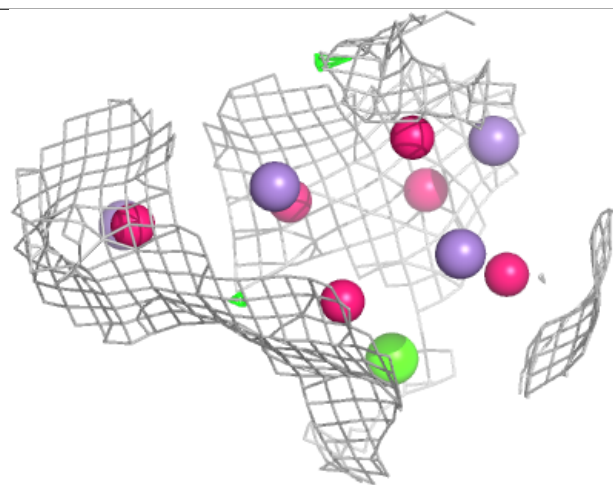
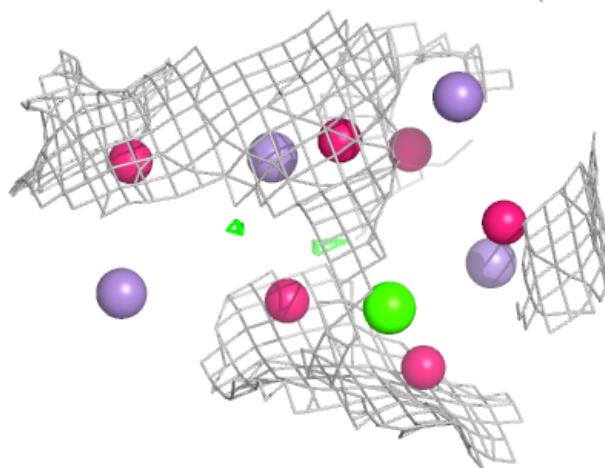
Electron density around OEY A 601 (B):

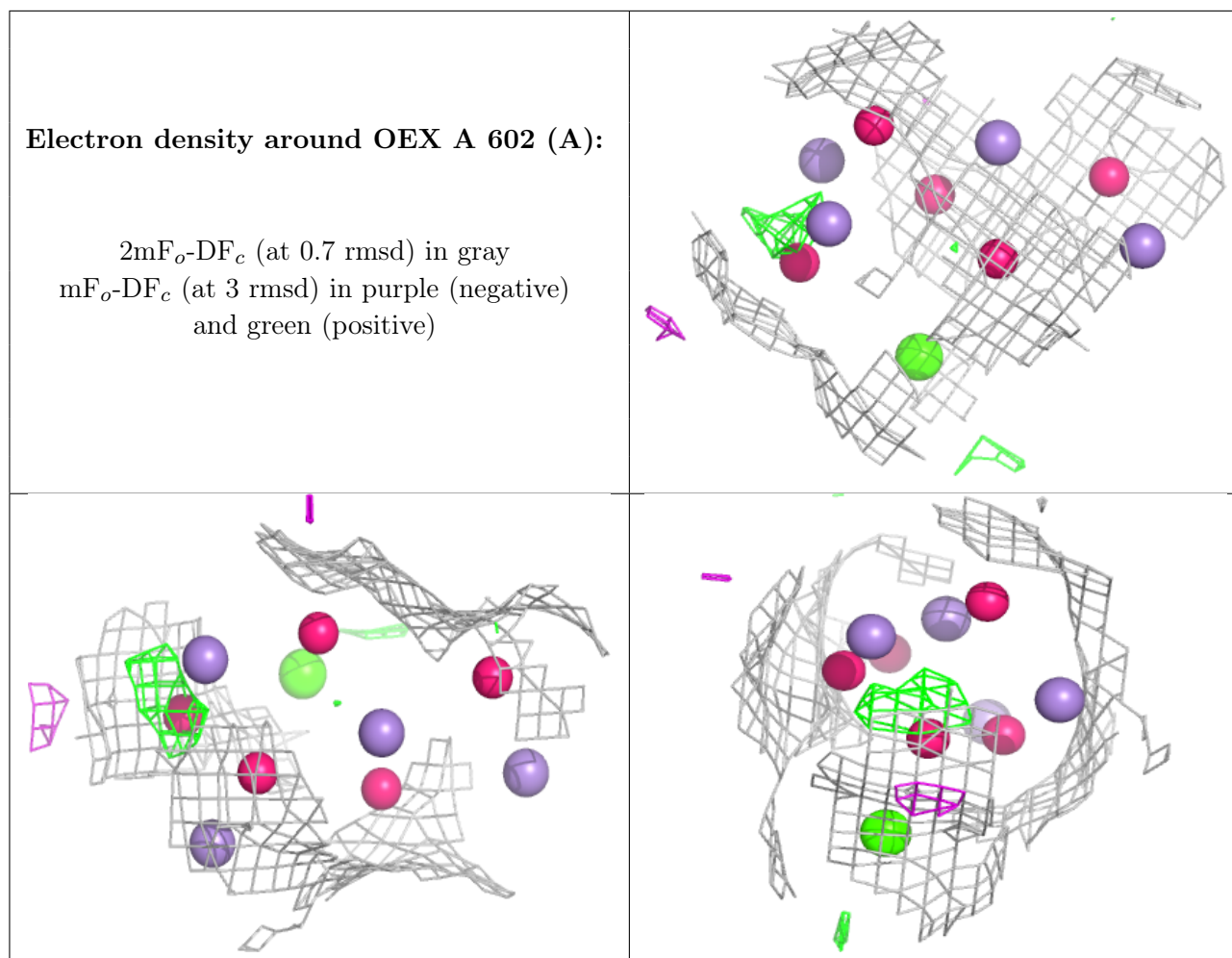
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OEY a 601 (B):

$2mF_o-DF_c$ (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.