



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 05:22 PM EDT

PDB ID : 8F4H / pdb_00008f4h
Title : RT XFEL structure of Photosystem II 1200 microseconds after the third illumination at 2.10 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 : 2022-11-10
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0

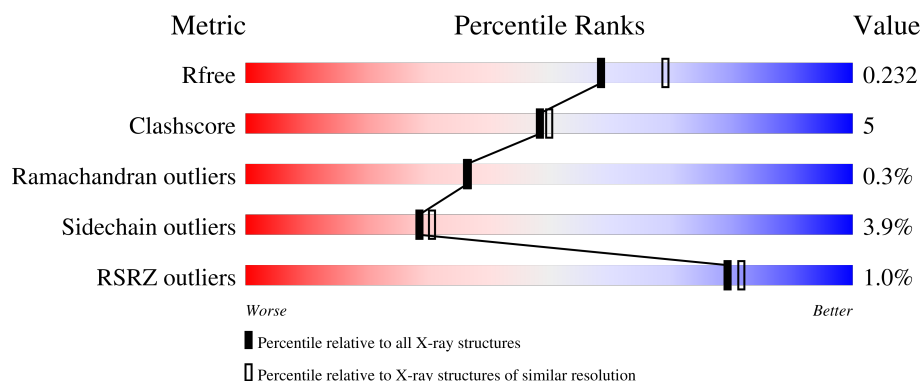
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

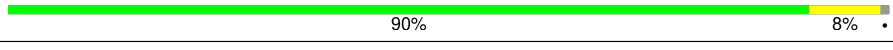
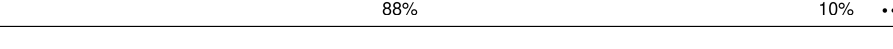
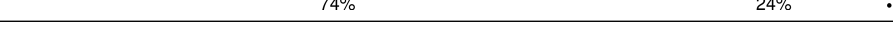
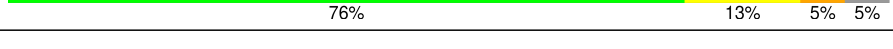
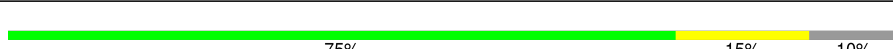
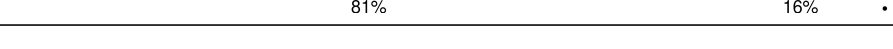
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	

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Buster-report : wwPDB partial adaption of 1.1.7 (2018)
 Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
 CCP4 : 9.0.015 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.50

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Mol	Chain	Length	Quality of chain
1	a	344	% 
2	B	510	
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	% 
5	e	84	4% 
6	F	45	
6	f	45	
7	H	66	3% 
7	h	66	3% 
8	I	38	
8	i	38	
9	J	40	2% 
9	j	40	
10	K	46	
10	k	46	
11	L	37	3% 
11	l	37	
12	M	36	
12	m	36	
13	O	272	% 
13	o	272	%

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Mol	Chain	Length	Quality of chain
14	T	32	
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
36	HEC	V	201	X	-	-	-
36	HEC	v	201	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 54161 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
			3604	2343	595	643	23			
1	a	334	Total	C	N	O	S	0	64	0
			3601	2340	595	643	23			

- 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
			3592	2355	601	621	15			
3	c	451	Total	C	N	O	S	0	12	0
			3666	2396	617	638	15			

- 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
			2745	1818	448	467	12			
4	d	341	Total	C	N	O	S	0	3	0
			2751	1822	448	469	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				

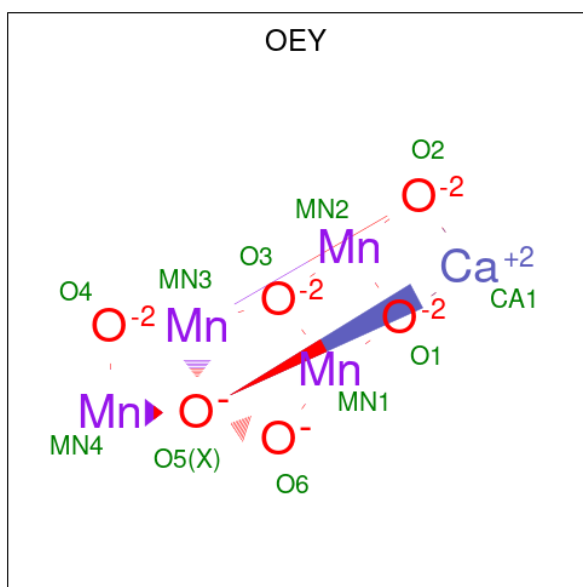
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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.

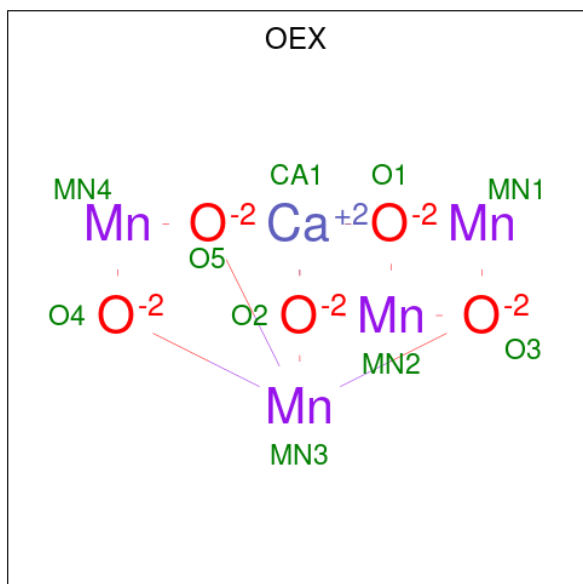
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O		0	0	0
			271	184	47	40				
20	r	31	Total	C	N	O		0	0	0
			246	166	43	37				

- 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
			22	2	8	12		
21	a	1	Total	Ca	Mn	O	0	1
			22	2	8	12		

- 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		

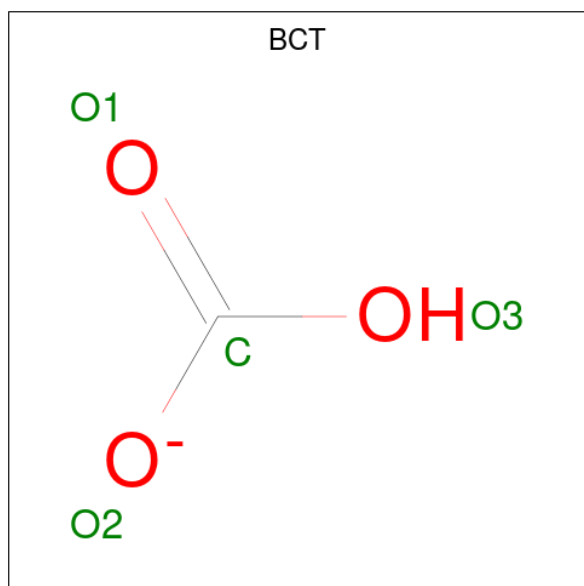
- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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).

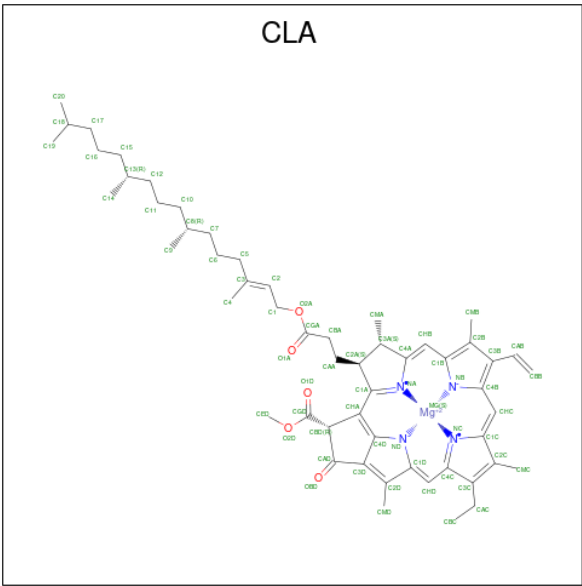
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	2	Total	Cl	0	0
			2	2		
24	a	2	Total	Cl	0	0
			2	2		

- Molecule 25 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



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

- Molecule 26 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
26	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	C	1	Total 59	C 49	Mg 1	N 4	O 5	0	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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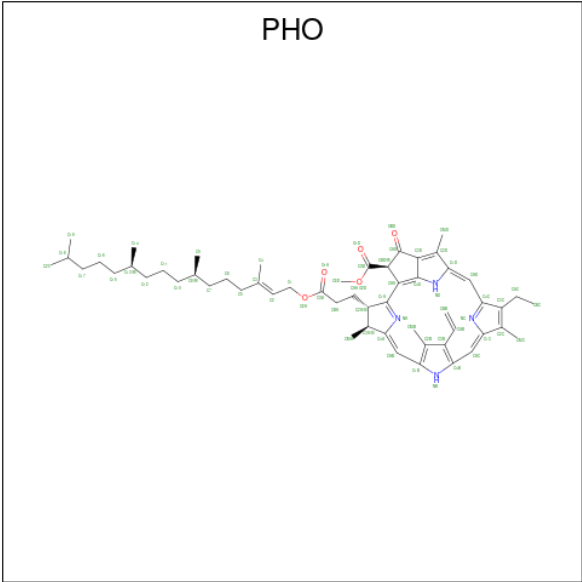
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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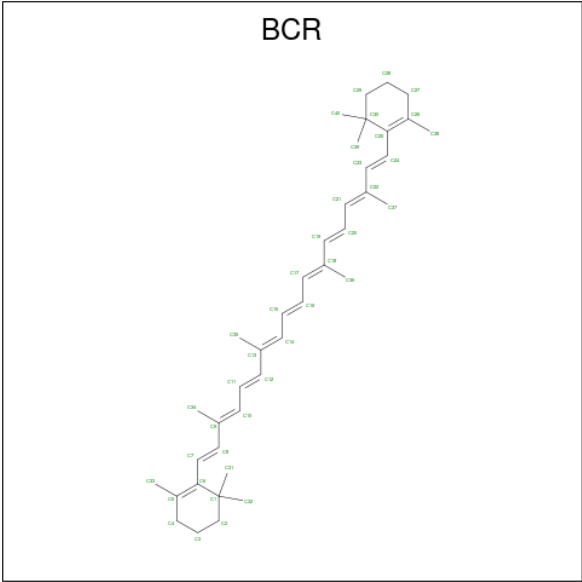
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
26	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 27 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



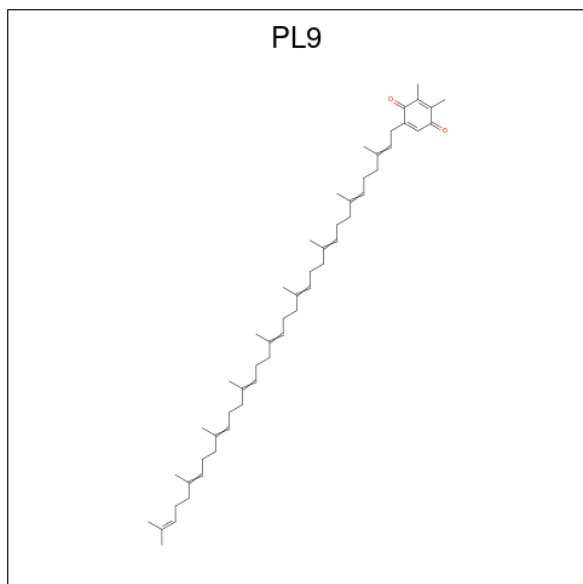
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	N	O	0	0
			64	55	4	5		
27	D	1	Total	C	N	O	0	0
			64	55	4	5		
27	a	1	Total	C	N	O	0	0
			64	55	4	5		
27	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 28 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



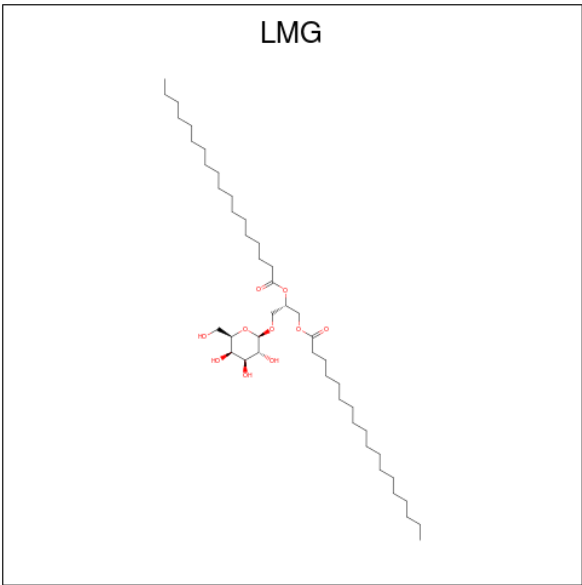
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C 40 40	0	0
28	B	1	Total C 40 40	0	0
28	B	1	Total C 40 40	0	0
28	B	1	Total C 40 40	0	0
28	C	1	Total C 40 40	0	0
28	D	1	Total C 40 40	0	0
28	K	1	Total C 40 40	0	0
28	K	1	Total C 40 40	0	0
28	T	1	Total C 40 40	0	0
28	X	1	Total C 40 40	0	0
28	Z	1	Total C 40 40	0	0
28	a	1	Total C 40 40	0	0
28	b	1	Total C 40 40	0	0
28	b	1	Total C 40 40	0	0
28	b	1	Total C 40 40	0	0
28	c	1	Total C 40 40	0	0
28	c	1	Total C 40 40	0	0
28	c	1	Total C 40 40	0	0
28	d	1	Total C 40 40	0	0
28	h	1	Total C 40 40	0	0
28	k	1	Total C 40 40	0	0
28	t	1	Total C 40 40	0	0

- Molecule 29 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: $C_{53}H_{80}O_2$).



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

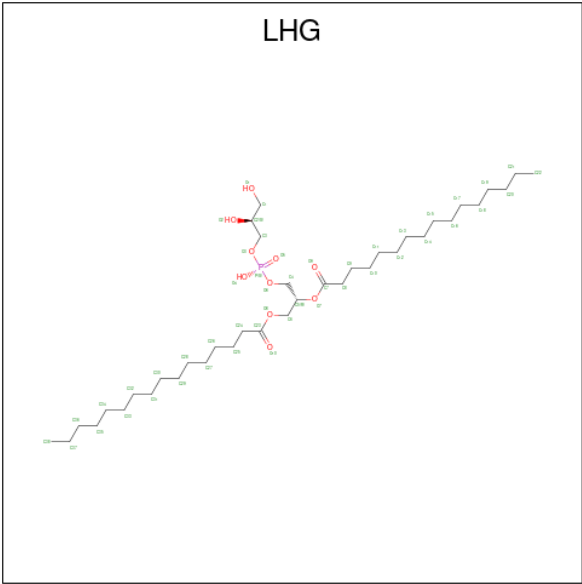
- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			48	38	10		
30	B	1	Total	C	O	0	0
			28	24	4		
30	C	1	Total	C	O	0	0
			48	38	10		
30	D	1	Total	C	O	0	0
			51	41	10		
30	D	1	Total	C	O	0	0
			33	27	6		
30	M	1	Total	C	O	0	0
			51	41	10		
30	b	1	Total	C	O	0	0
			55	45	10		
30	c	1	Total	C	O	0	0
			37	27	10		
30	c	1	Total	C	O	0	0
			48	38	10		
30	c	1	Total	C	O	0	0
			49	39	10		
30	d	1	Total	C	O	0	0
			23	21	2		
30	d	1	Total	C	O	0	0
			44	34	10		
30	m	1	Total	C	O	0	0
			51	41	10		

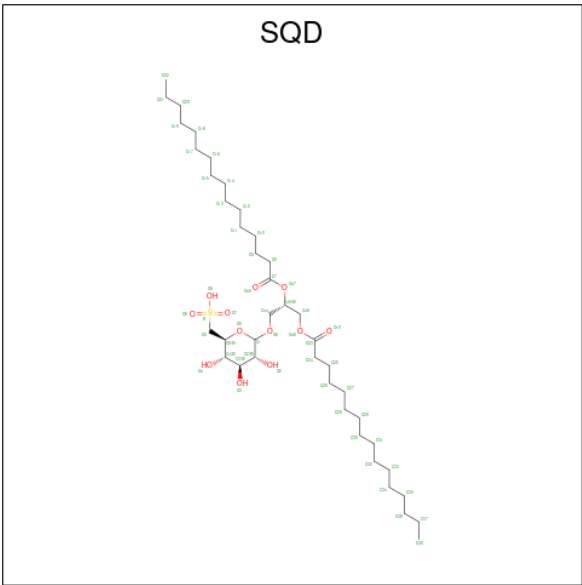
- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG)

(formula: C₃₈H₇₅O₁₀P).



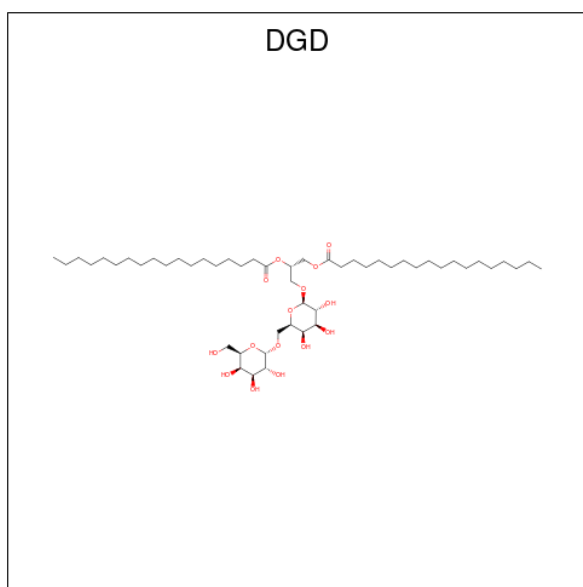
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			47	36	10	1		
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	L	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			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 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



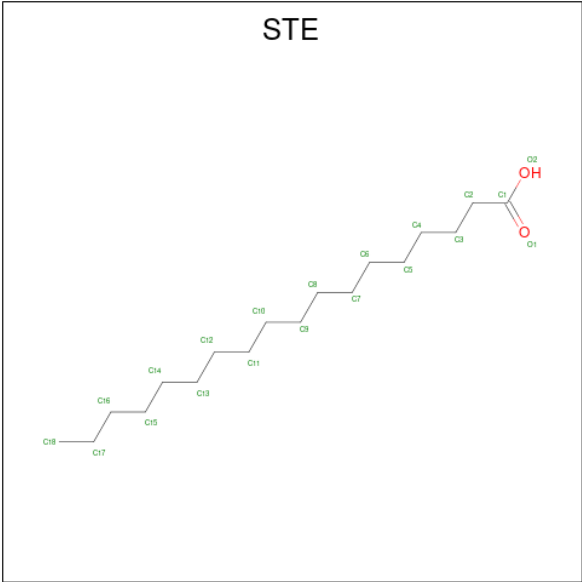
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	O	S	0	0
			52	39	12	1		
32	A	1	Total	C	O		0	0
			39	35	4			
32	B	1	Total	C	O	S	0	0
			54	41	12	1		
32	F	1	Total	C	O	S	0	0
			36	25	10	1		
32	a	1	Total	C	O	S	0	0
			54	41	12	1		
32	b	1	Total	C	O	S	0	0
			49	36	12	1		
32	f	1	Total	C	O	S	0	0
			41	28	12	1		
32	t	1	Total	C	O		0	0
			36	31	5			

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



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

- Molecule 34 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



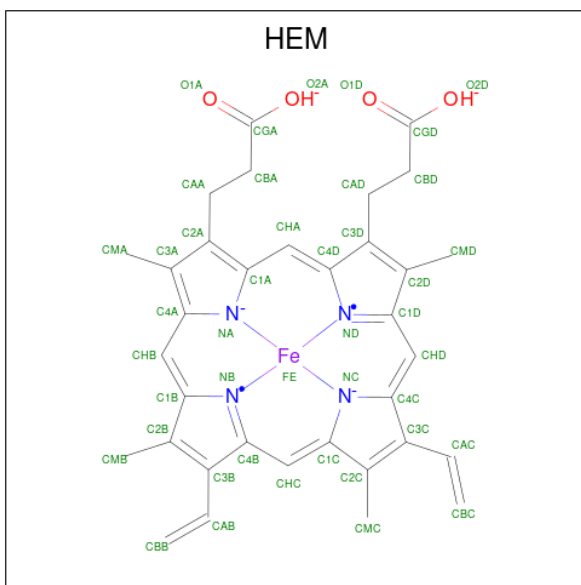
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	B	1	Total C O 17 15 2	0	0
34	B	1	Total C O 12 10 2	0	0
34	B	1	Total C O 12 10 2	0	0
34	B	1	Total C 16 16	0	0
34	C	1	Total C O 12 10 2	0	0
34	C	1	Total C O 12 10 2	0	0
34	C	1	Total C 16 16	0	0
34	F	1	Total C O 12 10 2	0	0
34	H	1	Total C 18 18	0	0
34	I	1	Total C 15 15	0	0
34	J	1	Total C O 12 10 2	0	0
34	L	1	Total C O 12 10 2	0	0
34	M	1	Total C O 15 13 2	0	0
34	M	1	Total C 10 10	0	0

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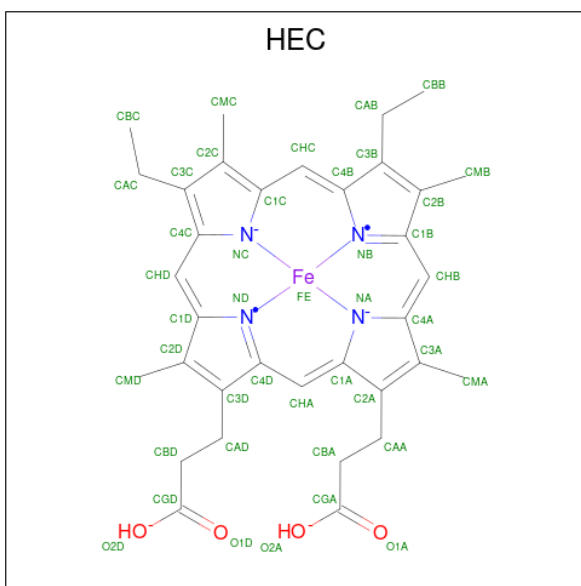
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	T	1	Total C 16 16	0	0
34	T	1	Total C 15 15	0	0
34	X	1	Total C O 20 18 2	0	0
34	a	1	Total C O 12 10 2	0	0
34	b	1	Total C O 20 18 2	0	0
34	b	1	Total C O 20 18 2	0	0
34	b	1	Total C 10 10	0	0
34	c	1	Total C O 20 18 2	0	0
34	d	1	Total C O 16 14 2	0	0
34	d	1	Total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

- 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	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
35	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 36 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	121	Total O 129 129	0	4
37	B	171	Total O 171 171	0	0
37	C	149	Total O 149 149	0	0
37	D	105	Total O 105 105	0	0
37	E	16	Total O 16 16	0	0
37	F	8	Total O 8 8	0	0
37	H	26	Total O 26 26	0	0
37	I	13	Total O 13 13	0	0
37	J	11	Total O 11 11	0	0
37	K	4	Total O 4 4	0	0
37	L	10	Total O 10 10	0	0
37	M	3	Total O 3 3	0	0
37	O	68	Total O 68 68	0	0
37	T	6	Total O 6 6	0	0
37	U	33	Total O 33 33	0	0
37	V	54	Total O 54 54	0	0
37	X	7	Total O 7 7	0	0
37	Z	5	Total O 5 5	0	0
37	a	109	Total O 117 117	0	4
37	b	142	Total O 142 142	0	0
37	c	132	Total O 132 132	0	0

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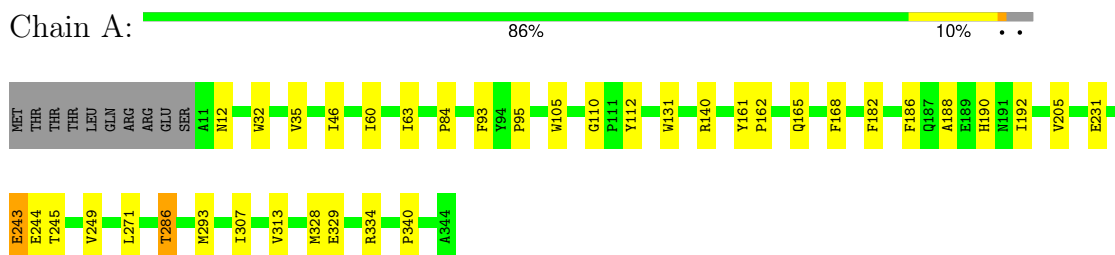
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	d	92	Total 92	O 92	0	0
37	e	13	Total 13	O 13	0	0
37	f	4	Total 4	O 4	0	0
37	h	16	Total 16	O 16	0	0
37	i	12	Total 12	O 12	0	0
37	j	9	Total 9	O 9	0	0
37	k	6	Total 6	O 6	0	0
37	l	8	Total 8	O 8	0	0
37	m	7	Total 7	O 7	0	0
37	o	77	Total 77	O 77	0	0
37	t	10	Total 10	O 10	0	0
37	u	38	Total 38	O 38	0	0
37	v	39	Total 39	O 39	0	0
37	x	4	Total 4	O 4	0	0
37	z	5	Total 5	O 5	0	0
37	r	7	Total 7	O 7	0	0

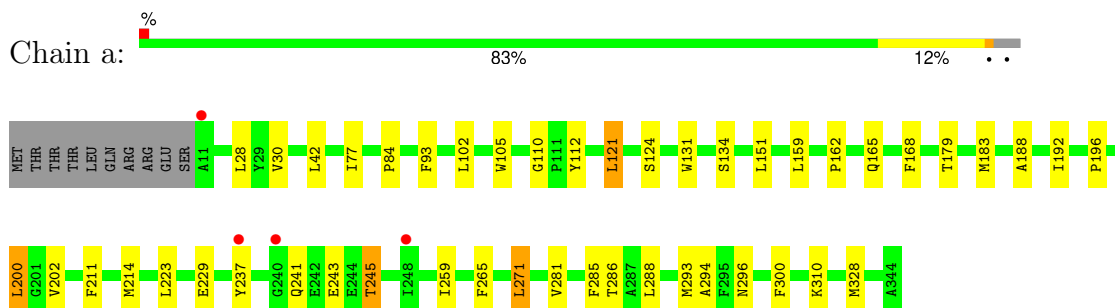
3 Residue-property plots

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

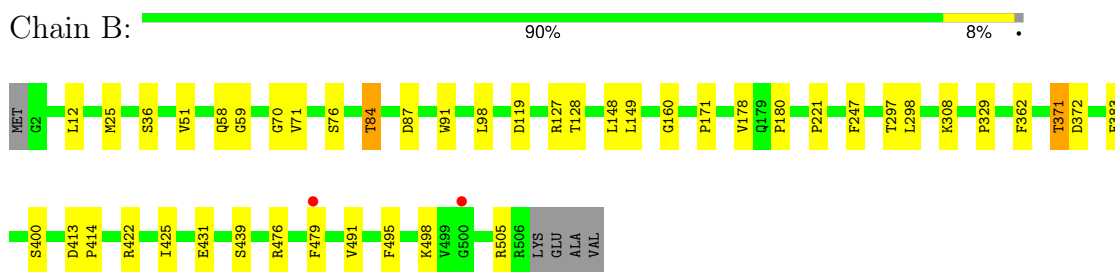
- Molecule 1: Photosystem II protein D1 1



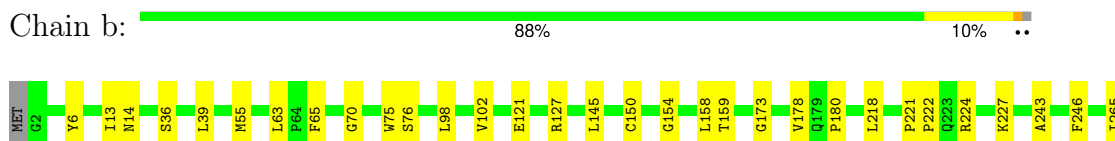
- Molecule 1: Photosystem II protein D1 1



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein





- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 86% 9% .



- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 88% 10% ..



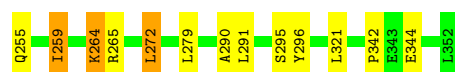
- Molecule 4: Photosystem II D2 protein

Chain D: 87% 10% ..



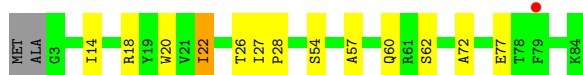
- Molecule 4: Photosystem II D2 protein

Chain d: 86% 10% ..

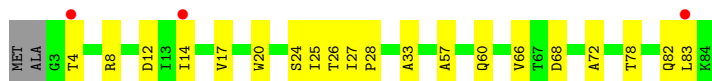
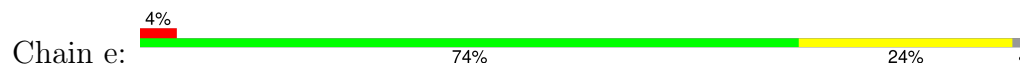


- Molecule 5: Cytochrome b559 subunit alpha

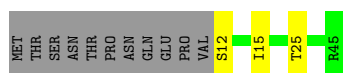
Chain E: 82% 14% ..



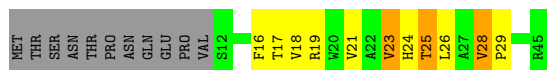
- Molecule 5: Cytochrome b559 subunit alpha



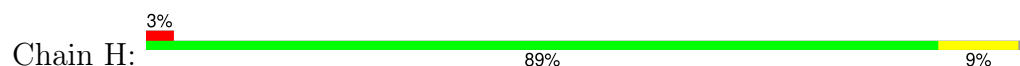
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 6: Cytochrome b559 subunit beta



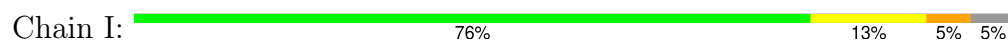
- Molecule 7: Photosystem II reaction center protein H



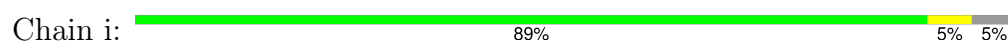
- Molecule 7: Photosystem II reaction center protein H

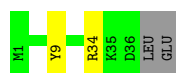


- Molecule 8: Photosystem II reaction center protein I

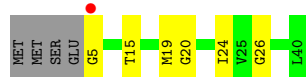
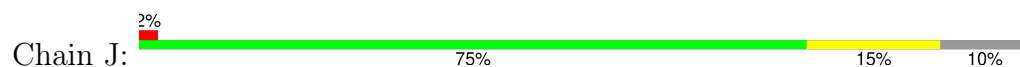


- Molecule 8: Photosystem II reaction center protein I





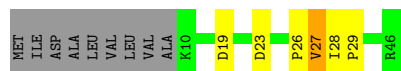
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



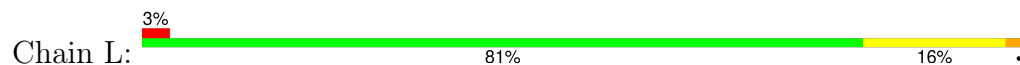
- Molecule 10: Photosystem II reaction center protein K



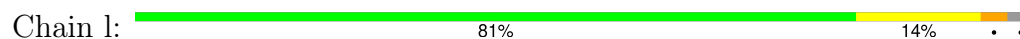
- Molecule 10: Photosystem II reaction center protein K



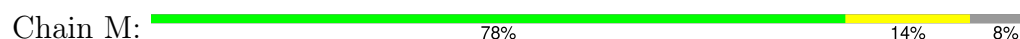
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



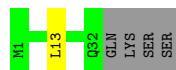
- Molecule 12: Photosystem II reaction center protein M





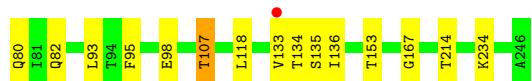
- Molecule 12: Photosystem II reaction center protein M

Chain m: 86% 11%



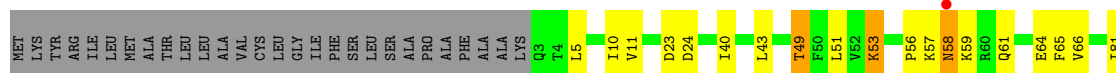
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 78% 11% 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 76% 12% 10%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 81% 12% 6%



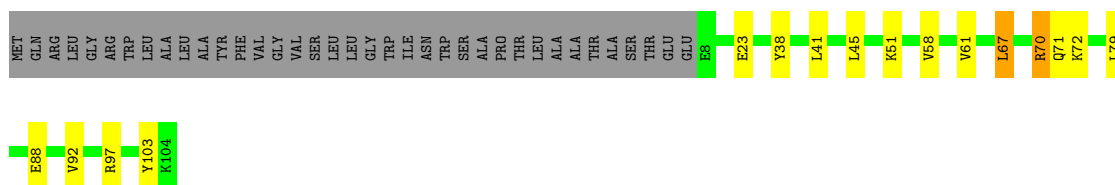
- Molecule 14: Photosystem II reaction center protein T

Chain t: 6% 78% 16% 6%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

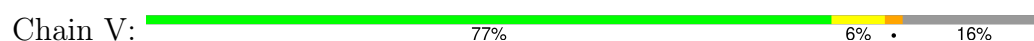
Chain U: 60% 10% 28%



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Cytochrome c-550



- Molecule 16: Cytochrome c-550



- Molecule 17: Photosystem II reaction center protein Ycf12

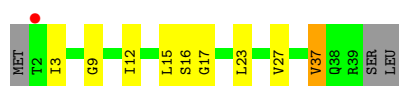


- Molecule 17: Photosystem II reaction center protein Ycf12

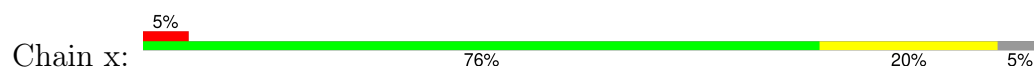


- Molecule 18: Photosystem II reaction center X protein

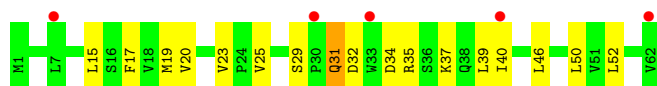




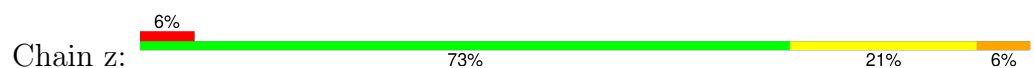
- Molecule 18: Photosystem II reaction center X protein



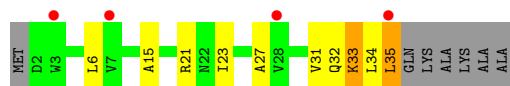
- Molecule 19: Photosystem II reaction center protein Z



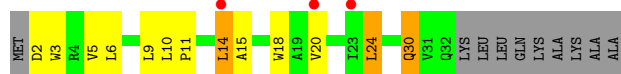
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.56Å 223.17Å 310.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.48 – 2.10 29.48 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.48-2.10) 82.6 (29.48-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.34 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.188 , 0.232 0.188 , 0.232	Depositor DCC
R_{free} test set	4187 reflections (0.67%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	54161	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: CL, DGD, CLA, SQD, PHO, OEY, BCR, HEM, LHG, FE2, LMG, BCT, FME, PL9, HEC, STE, OEX

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	0.29	0/3717	0.44	0/5060
1	a	0.27	0/3714	0.43	0/5056
2	B	0.32	0/4155	0.48	0/5661
2	b	0.32	0/4118	0.48	0/5611
3	C	0.30	0/3711	0.46	0/5051
3	c	0.28	0/3791	0.45	0/5158
4	D	0.34	0/2838	0.50	0/3862
4	d	0.34	0/2847	0.48	0/3874
5	E	0.25	0/688	0.43	0/940
5	e	0.23	0/683	0.41	0/932
6	F	0.28	0/284	0.39	0/387
6	f	0.23	0/284	0.41	0/387
7	H	0.32	0/523	0.48	0/713
7	h	0.28	0/511	0.45	0/697
8	I	0.49	1/293 (0.3%)	0.53	0/396
8	i	0.31	0/293	0.44	0/396
9	J	0.28	0/263	0.38	0/356
9	j	0.25	0/263	0.42	0/356
10	K	0.25	0/303	0.46	0/416
10	k	0.26	0/303	0.49	0/416
11	L	0.35	0/311	0.45	0/422
11	l	0.36	0/303	0.44	0/412
12	M	0.33	0/249	0.49	0/341
12	m	0.34	0/244	0.52	0/334
13	O	0.31	0/1904	0.50	0/2585
13	o	0.32	0/1905	0.50	0/2583
14	T	0.34	0/257	0.57	0/349
14	t	0.31	0/255	0.46	0/346
15	U	0.28	0/785	0.46	0/1064
15	u	0.30	0/785	0.48	0/1064
16	V	0.31	0/1085	0.49	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.26	0/1085	0.43	0/1473
17	Y	0.19	0/197	0.32	0/264
17	y	0.19	0/219	0.38	0/294
18	X	0.25	0/284	0.37	0/384
18	x	0.23	0/289	0.31	0/391
19	Z	0.31	0/490	0.45	0/669
19	z	0.19	0/488	0.29	0/666
20	R	0.24	0/277	0.38	0/380
20	r	0.29	0/252	0.40	0/347
All	All	0.30	1/45246 (0.0%)	0.46	0/61566

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	33	LYS	CA-C	5.85	1.55	1.52

There are no bond angle outliers.

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](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3604	0	3445	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	3601	0	3436	34	0
2	B	4005	0	3871	31	0
2	b	3978	0	3836	40	0
3	C	3592	0	3501	30	0
3	c	3666	0	3574	31	0
4	D	2745	0	2653	29	0
4	d	2751	0	2659	27	0
5	E	666	0	651	9	0
5	e	664	0	648	13	0
6	F	275	0	282	4	0
6	f	275	0	282	10	0
7	H	510	0	532	4	0
7	h	498	0	518	9	0
8	I	296	0	311	3	0
8	i	296	0	311	2	0
9	J	257	0	268	4	0
9	j	257	0	268	3	0
10	K	293	0	305	4	0
10	k	293	0	305	4	0
11	L	304	0	316	6	0
11	l	296	0	304	4	0
12	M	256	0	269	3	0
12	m	251	0	267	0	0
13	O	1870	0	1830	21	0
13	o	1874	0	1846	20	0
14	T	258	0	261	2	0
14	t	256	0	256	4	0
15	U	774	0	773	9	0
15	u	774	0	773	5	0
16	V	1064	0	1073	8	0
16	v	1064	0	1073	14	0
17	Y	196	0	217	5	0
17	y	218	0	241	5	0
18	X	281	0	312	8	0
18	x	286	0	314	6	0
19	Z	479	0	516	7	0
19	z	477	0	509	13	0
20	R	271	0	298	7	0
20	r	246	0	263	9	0
21	A	22	0	0	2	0
21	a	22	0	0	2	0
22	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	a	10	0	0	0	0
23	A	1	0	0	0	0
23	a	1	0	0	0	0
24	A	2	0	0	0	0
24	a	2	0	0	0	0
25	A	4	0	1	0	0
25	d	4	0	1	0	0
26	A	249	0	264	5	0
26	B	1035	0	1139	29	0
26	C	839	0	922	21	0
26	D	130	0	144	7	0
26	a	260	0	288	8	0
26	b	970	0	1067	34	0
26	c	839	0	919	19	0
26	d	130	0	144	1	0
26	h	65	0	72	5	0
27	A	64	0	74	0	0
27	D	64	0	74	2	0
27	a	64	0	74	0	0
27	d	64	0	74	2	0
28	A	40	0	56	2	0
28	B	120	0	168	5	0
28	C	40	0	56	3	0
28	D	40	0	56	1	0
28	K	80	0	112	1	0
28	T	40	0	56	4	0
28	X	40	0	56	1	0
28	Z	40	0	56	3	0
28	a	40	0	56	1	0
28	b	120	0	168	6	0
28	c	120	0	168	9	0
28	d	40	0	56	3	0
28	h	40	0	56	4	0
28	k	40	0	56	1	0
28	t	40	0	56	2	0
29	A	55	0	80	8	0
29	D	55	0	80	1	0
29	a	55	0	80	6	0
29	d	55	0	80	1	0
30	A	48	0	66	2	0
30	B	28	0	40	0	0
30	C	48	0	66	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	D	84	0	117	2	0
30	M	51	0	72	2	0
30	b	55	0	86	0	0
30	c	134	0	181	4	0
30	d	67	0	92	0	0
30	m	51	0	72	2	0
31	A	96	0	141	2	0
31	D	98	0	148	6	0
31	L	49	0	74	3	0
31	d	137	0	199	8	0
31	e	42	0	57	2	0
31	l	49	0	74	3	0
32	A	91	0	136	2	0
32	B	54	0	78	5	0
32	F	36	0	46	2	0
32	a	54	0	78	2	0
32	b	49	0	65	4	0
32	f	41	0	49	4	0
32	t	36	0	56	0	0
33	A	66	0	96	4	0
33	C	186	0	246	3	0
33	H	62	0	82	1	0
33	a	44	0	75	3	0
33	c	186	0	246	3	0
33	h	62	0	82	0	0
34	B	57	0	89	2	0
34	C	40	0	63	2	0
34	F	12	0	16	0	0
34	H	18	0	35	2	0
34	I	15	0	26	1	0
34	J	12	0	16	1	0
34	L	12	0	16	0	0
34	M	25	0	38	0	0
34	T	31	0	60	1	0
34	X	20	0	35	5	0
34	a	12	0	16	0	0
34	b	50	0	86	2	0
34	c	20	0	35	2	0
34	d	53	0	85	6	0
34	j	12	0	16	1	0
34	k	12	0	16	1	0
34	l	18	0	35	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	t	42	0	64	3	0
35	F	43	0	30	1	0
35	e	43	0	30	2	0
36	V	43	0	30	0	0
36	v	43	0	30	2	0
37	A	129	0	0	2	0
37	B	171	0	0	1	0
37	C	149	0	0	1	0
37	D	105	0	0	0	0
37	E	16	0	0	0	0
37	F	8	0	0	1	0
37	H	26	0	0	1	0
37	I	13	0	0	0	0
37	J	11	0	0	1	0
37	K	4	0	0	0	0
37	L	10	0	0	0	0
37	M	3	0	0	0	0
37	O	68	0	0	4	0
37	T	6	0	0	0	0
37	U	33	0	0	1	0
37	V	54	0	0	0	0
37	X	7	0	0	0	0
37	Z	5	0	0	0	0
37	a	117	0	0	0	0
37	b	142	0	0	0	0
37	c	132	0	0	0	0
37	d	92	0	0	0	0
37	e	13	0	0	0	0
37	f	4	0	0	0	0
37	h	16	0	0	0	0
37	i	12	0	0	0	0
37	j	9	0	0	0	0
37	k	6	0	0	0	0
37	l	8	0	0	1	0
37	m	7	0	0	0	0
37	o	77	0	0	1	0
37	r	7	0	0	1	0
37	t	10	0	0	0	0
37	u	38	0	0	1	0
37	v	39	0	0	0	0
37	x	4	0	0	0	0
37	z	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	54161	0	53863	580	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (580) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161[C]:TYR:HH	1:A:190[C]:HIS:HE2	0.96	0.91
21:A:601[C]:OEY:O5	21:A:601[C]:OEY:O6	1.92	0.86
21:a:601[C]:OEY:O5	21:a:601[C]:OEY:O6	1.99	0.79
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.47	0.78
21:a:601[A]:OEY:O5	21:a:601[A]:OEY:O6	2.04	0.75
4:D:24:ARG:HD3	18:X:37:VAL:HG12	1.66	0.75
21:A:601[A]:OEY:O6	21:A:601[A]:OEY:O5	2.04	0.74
4:d:246:MET:HE3	4:d:264:LYS:HD2	1.69	0.74
34:d:414:STE:H31	18:x:17:GLY:HA2	1.70	0.73
32:A:618:SQD:H342	26:b:615:CLA:H93	1.72	0.72
3:C:389:GLU:OE1	37:C:601:HOH:O	2.08	0.71
26:C:502:CLA:H61	26:C:512:CLA:H42	1.70	0.71
26:B:606:CLA:H72	28:B:619:BCR:H311	1.71	0.71
1:a:102:LEU:HD12	33:a:614:DGD:HB22	1.71	0.70
13:O:27:ARG:NH1	37:O:301:HOH:O	2.17	0.70
26:h:101:CLA:H193	26:h:101:CLA:HAB	1.71	0.69
28:t:101:BCR:HC8	28:t:101:BCR:H311	1.74	0.69
6:F:12:SER:N	37:F:201:HOH:O	2.25	0.69
30:c:522:LMG:H112	30:c:522:LMG:H292	1.75	0.69
26:C:513:CLA:H201	34:C:521:STE:H171	1.76	0.68
26:b:603:CLA:H42	26:b:604:CLA:H2	1.76	0.68
20:r:30:GLN:O	37:r:101:HOH:O	2.12	0.67
18:X:17:GLY:HA2	34:X:102:STE:H142	1.76	0.67
2:B:127:ARG:HG3	2:B:128:THR:HG23	1.76	0.67
4:d:42:TYR:CZ	6:f:25:THR:HG22	2.29	0.67
3:C:148:GLY:O	3:C:156:LYS:NZ	2.28	0.67
2:b:102:VAL:HG11	26:b:605:CLA:H142	1.77	0.67
3:c:217:PRO:HG3	33:c:517:DGD:HA81	1.77	0.67
1:A:188[C]:ALA:HB2	1:A:328[C]:MET:HB2	1.77	0.67
9:J:15:THR:HG22	9:J:19:MET:HE2	1.75	0.67
5:e:8:ARG:NH1	5:e:12:ASP:OD2	2.27	0.67
2:B:91:TRP:HE1	34:B:620:STE:H32	1.60	0.66
15:U:88:GLU:OE2	37:U:201:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.59	0.66
26:b:614:CLA:H2	26:b:615:CLA:HBB2	1.77	0.66
13:o:49:THR:HG23	13:o:236:GLN:HB2	1.77	0.66
28:b:616:BCR:H322	30:m:101:LMG:H112	1.78	0.65
15:u:53:ALA:HB1	15:u:54:PRO:HD2	1.79	0.65
1:a:188[C]:ALA:HB2	1:a:328[C]:MET:HB2	1.79	0.64
26:b:602:CLA:HMD3	26:b:605:CLA:HBB1	1.80	0.64
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.79	0.64
1:a:200:LEU:HD12	33:c:519:DGD:HAW2	1.79	0.64
13:O:58:ASN:ND2	13:O:61:GLN:OE1	2.29	0.63
2:b:498:LYS:HE3	4:d:20:ASP:HA	1.78	0.63
35:e:101:HEM:HHC	35:e:101:HEM:HBB2	1.80	0.63
9:J:5:GLY:N	37:J:202:HOH:O	2.30	0.63
13:O:57:LYS:HE3	13:O:58:ASN:HB3	1.81	0.63
31:D:409:LHG:H152	31:L:101:LHG:H281	1.81	0.63
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.35	0.61
26:b:613:CLA:H122	34:l:102:STE:H182	1.80	0.61
1:a:165[C]:GLN:NE2	1:a:294:ALA:O	2.33	0.61
26:b:613:CLA:H192	26:b:613:CLA:H141	1.83	0.61
4:D:141:TYR:OH	31:D:409:LHG:O4	2.13	0.61
29:A:612:PL9:H33	4:D:42:TYR:HB2	1.81	0.61
6:f:24:HIS:O	6:f:28:VAL:HG13	2.01	0.61
13:o:57:LYS:O	13:o:59:LYS:N	2.29	0.61
26:B:615:CLA:H2	26:B:616:CLA:HBB2	1.82	0.60
4:D:246:MET:HE3	4:D:264:LYS:HE2	1.82	0.60
29:a:611:PL9:H151	31:e:102:LHG:H292	1.84	0.60
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.36	0.60
4:d:279:LEU:HD22	27:d:402:PHO:HBC3	1.84	0.60
13:o:83:GLY:HA2	13:o:98:GLU:HG3	1.84	0.60
4:D:186:GLN:HB2	26:D:402:CLA:HBC1	1.84	0.60
1:a:300:PHE:HZ	33:c:519:DGD:HB62	1.66	0.60
20:r:2:ASP:HB3	20:r:5:VAL:HG23	1.84	0.59
26:c:512:CLA:H142	26:c:513:CLA:H143	1.83	0.59
14:T:7:VAL:HG12	34:T:102:STE:H183	1.84	0.59
15:U:58:VAL:O	15:U:61:VAL:HG22	2.03	0.59
2:B:371:THR:OG1	2:B:372:ASP:O	2.19	0.59
26:B:603:CLA:C3D	26:B:605:CLA:H2	2.33	0.59
3:c:42:LEU:HD21	26:c:511:CLA:H2A	1.83	0.59
26:b:612:CLA:H172	31:d:407:LHG:H212	1.85	0.59
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.67	0.59
35:e:101:HEM:HBC2	35:e:101:HEM:HMC2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:a:609:CLA:H172	8:i:9:TYR:HB3	1.85	0.58
17:y:22:LEU:HA	17:y:25:ILE:HG22	1.84	0.58
19:Z:31:GLN:CD	19:Z:32:ASP:H	2.11	0.58
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	1.86	0.58
7:h:12:ARG:NH2	7:h:15:ASN:O	2.35	0.57
13:O:56:PRO:O	13:O:58:ASN:N	2.35	0.57
16:v:6:GLU:OE1	16:v:6:GLU:N	2.35	0.57
26:c:504:CLA:H91	26:c:508:CLA:H171	1.86	0.57
26:B:613:CLA:H172	31:D:409:LHG:H202	1.87	0.56
4:d:93:TRP:CZ3	34:d:414:STE:H62	2.40	0.56
32:a:613:SQD:H311	34:k:102:STE:H82	1.86	0.56
19:Z:29:SER:HB3	19:Z:31:GLN:HE21	1.71	0.56
4:d:36:LEU:HB2	34:d:413:STE:H121	1.88	0.56
29:A:612:PL9:H152	31:A:617:LHG:H361	1.87	0.56
5:E:57:ALA:HB3	5:E:60:GLN:HB2	1.88	0.56
3:C:137:PRO:HD3	26:C:513:CLA:HED2	1.86	0.56
26:c:512:CLA:H121	26:c:513:CLA:H151	1.88	0.56
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.88	0.55
28:T:101:BCR:H311	28:T:101:BCR:HC8	1.88	0.55
3:c:117:VAL:HG12	34:c:521:STE:H141	1.88	0.55
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.88	0.55
3:c:75:PHE:O	10:k:10:LYS:NZ	2.36	0.55
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.87	0.55
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.87	0.55
3:C:455:PHE:HD2	8:I:33:LYS:HG3	1.70	0.55
1:a:241:GLN:NE2	1:a:245:THR:HG23	2.22	0.55
11:l:2:GLU:N	37:l:202:HOH:O	2.39	0.55
16:V:28:GLU:OE2	16:V:31:ARG:NH1	2.40	0.55
16:v:76:MET:HE2	16:v:112:LEU:HD22	1.88	0.55
2:B:171:PRO:HA	7:H:65:LEU:HD12	1.89	0.55
31:d:407:LHG:H351	31:d:407:LHG:H101	1.89	0.54
17:y:20:ALA:O	17:y:24:MET:HG2	2.07	0.54
3:c:461:ARG:HG2	4:d:223:PHE:CD1	2.42	0.54
5:E:26:THR:HA	20:R:15:ALA:HB1	1.90	0.54
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.08	0.54
4:d:126:MET:HE3	4:d:143:ALA:O	2.07	0.54
1:A:63[B]:ILE:HB	3:C:335:THR:HG21	1.90	0.53
5:e:14:ILE:O	5:e:20:TRP:NE1	2.40	0.53
31:l:101:LHG:H241	31:l:101:LHG:H101	1.89	0.53
4:D:85:MET:HE1	5:E:72:ALA:HB2	1.90	0.53
30:M:101:LMG:HC5	34:t:105:STE:H22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:F:101:HEM:HBC2	35:F:101:HEM:HHH	1.90	0.53
1:A:165[C]:GLN:O	3:C:357[C]:ARG:NH1	2.37	0.53
1:a:84:PRO:HA	1:a:112:TYR:CG	2.44	0.53
2:b:413:ASP:OD1	2:b:415:PRO:HD2	2.08	0.53
1:a:77:ILE:HD11	14:t:6:TYR:HB3	1.90	0.53
26:C:503:CLA:HBB1	26:C:512:CLA:H41	1.91	0.53
2:b:36:SER:OG	28:b:617:BCR:H362	2.08	0.53
4:D:150:ILE:O	4:D:154:VAL:HG13	2.10	0.52
16:v:76:MET:HE3	36:v:201:HEC:HBB3	1.91	0.52
3:c:180:MET:HE1	30:c:522:LMG:HC72	1.91	0.52
4:D:266:TRP:CD1	31:D:407:LHG:HC31	2.43	0.52
15:U:58:VAL:HG12	15:U:79:LEU:HD22	1.92	0.52
29:a:611:PL9:H251	31:e:102:LHG:H223	1.92	0.52
9:j:26:GLY:HA2	34:j:101:STE:H81	1.91	0.52
3:C:406:SER:HA	3:C:420:VAL:HG23	1.91	0.52
4:d:259:ILE:HD12	31:d:408:LHG:H291	1.90	0.52
26:B:614:CLA:H91	32:B:622:SQD:H382	1.91	0.51
4:D:279:LEU:HD22	27:D:401:PHO:HBC3	1.92	0.51
9:J:20:GLY:O	9:J:24:ILE:HG13	2.10	0.51
1:A:286:THR:HG23	26:A:607:CLA:HED3	1.91	0.51
10:k:18:PHE:HE2	19:z:13:VAL:HG21	1.76	0.51
26:B:614:CLA:H112	32:B:622:SQD:H382	1.92	0.51
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.92	0.51
4:d:49:LEU:HD13	28:d:405:BCR:C15	2.41	0.51
16:v:41:HIS:HA	16:v:45:ILE:O	2.11	0.51
26:D:403:CLA:H141	18:X:15:LEU:HD22	1.93	0.50
2:B:36:SER:OG	28:B:618:BCR:H362	2.11	0.50
26:C:505:CLA:HBC2	28:C:514:BCR:H341	1.93	0.50
3:C:141:GLU:H	3:C:141:GLU:CD	2.18	0.50
15:U:45:LEU:HD21	15:U:71:GLN:HB3	1.94	0.50
2:B:479[A]:PHE:O	4:D:139:ARG:NH2	2.32	0.50
13:O:9:ASP:OD1	37:O:302:HOH:O	2.20	0.50
3:C:180:MET:HG2	3:C:199:ILE:O	2.12	0.50
26:C:503:CLA:HBB2	26:C:512:CLA:H92	1.94	0.50
2:b:39:LEU:HD22	34:b:622:STE:H41	1.93	0.50
26:c:511:CLA:H172	19:z:20:VAL:HG22	1.93	0.50
4:d:241:GLU:CD	4:d:241:GLU:H	2.18	0.50
15:u:53:ALA:O	37:u:201:HOH:O	2.19	0.50
19:z:40:ILE:O	19:z:44:SER:OG	2.18	0.50
26:B:604:CLA:H93	26:B:605:CLA:HAB	1.93	0.50
2:b:283:GLU:O	2:b:287:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:614:LMG:HC72	3:C:216:SER:HB2	1.94	0.50
12:M:6:LEU:HD12	30:M:101:LMG:HC91	1.93	0.50
1:a:93:PHE:HZ	26:a:609:CLA:HAA1	1.77	0.50
1:a:237:TYR:CE1	4:d:264:LYS:HD3	2.47	0.50
26:c:501:CLA:C3D	26:c:503:CLA:H2	2.41	0.50
26:h:101:CLA:H171	28:h:102:BCR:C16	2.42	0.50
3:c:131:TYR:OH	26:c:513:CLA:HED2	2.12	0.50
3:c:391[B]:ARG:HH21	3:c:394:GLU:HG2	1.77	0.50
3:C:71:GLU:HB3	3:C:89:ILE:HD12	1.94	0.49
3:c:45:LEU:HA	3:c:139:THR:HG22	1.95	0.49
3:c:472:LEU:HD11	4:d:255:GLN:HG3	1.95	0.49
3:C:45:LEU:HA	3:C:139:THR:HG22	1.93	0.49
13:o:56:PRO:HB2	13:o:61:GLN:HB2	1.93	0.49
5:e:68:ASP:O	5:e:72:ALA:HB2	2.12	0.49
19:z:31:GLN:HG3	19:z:32:ASP:H	1.76	0.49
2:B:498:LYS:NZ	4:D:19:ASP:OD2	2.46	0.49
26:B:614:CLA:H191	34:t:105:STE:H112	1.94	0.49
3:C:67:MET:HB3	3:C:88:LEU:HD12	1.95	0.49
26:C:504:CLA:H143	26:C:508:CLA:H141	1.93	0.49
13:O:133:VAL:C	13:O:135:SER:H	2.20	0.49
26:C:506:CLA:H8	28:C:514:BCR:H14C	1.95	0.49
4:d:85:MET:HE3	4:d:107:LEU:HB3	1.95	0.49
26:b:602:CLA:H141	26:b:602:CLA:H161	1.63	0.49
33:A:619:DGD:HE4	2:b:76:SER:HB3	1.94	0.48
32:B:622:SQD:O8	11:L:7:ARG:NH1	2.46	0.48
26:h:101:CLA:CHA	26:h:101:CLA:HBA2	2.43	0.48
13:o:57:LYS:C	13:o:59:LYS:H	2.19	0.48
3:C:334:PRO:HA	13:O:153:THR:OG1	2.12	0.48
13:o:216:GLU:OE2	13:o:234:LYS:HD2	2.13	0.48
3:C:38:GLY:HA3	26:C:511:CLA:HMD2	1.95	0.48
19:Z:34:ASP:O	19:Z:37:LYS:HG2	2.13	0.48
13:o:53:LYS:NZ	13:o:232:GLU:OE1	2.45	0.48
5:E:18:ARG:HE	20:R:23:ILE:HD12	1.79	0.48
28:b:616:BCR:H383	32:b:619:SQD:H112	1.94	0.48
5:e:57:ALA:HB3	5:e:60:GLN:HG2	1.95	0.48
2:B:119:ASP:H	11:L:1:MET:CE	2.27	0.48
26:B:601:CLA:H2	26:B:601:CLA:HAA2	1.95	0.48
19:Z:29:SER:HB3	19:Z:31:GLN:HG3	1.96	0.48
3:c:406:SER:HA	3:c:420:VAL:HG23	1.95	0.48
2:B:59:GLY:O	26:B:607:CLA:HED2	2.13	0.48
2:B:221:PRO:HA	26:B:609:CLA:HED3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:13:ILE:HG12	26:b:611:CLA:HAC2	1.96	0.48
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.95	0.48
13:O:133:VAL:O	13:O:135:SER:N	2.46	0.48
2:b:505:ARG:HG3	2:b:506:ARG:N	2.28	0.48
33:A:619:DGD:HD5	2:b:75:TRP:HB3	1.95	0.48
15:U:70:ARG:NH1	16:V:85:GLU:OE2	2.47	0.48
26:a:609:CLA:H41	26:a:609:CLA:H142	1.95	0.48
4:D:42:TYR:CE1	6:F:25:THR:HG22	2.48	0.47
4:D:146:PHE:O	4:D:149:PRO:HD2	2.14	0.47
2:b:504:THR:HG22	18:x:39:ARG:HG2	1.96	0.47
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.49	0.47
6:f:19:ARG:O	6:f:23:VAL:HG13	2.14	0.47
6:f:26:LEU:O	6:f:29:PRO:HD2	2.12	0.47
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.96	0.47
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.50	0.47
31:D:407:LHG:H312	31:D:407:LHG:H341	1.75	0.47
28:T:101:BCR:H15C	32:b:619:SQD:H202	1.95	0.47
3:c:121:SER:HB3	34:c:521:STE:H182	1.95	0.47
6:f:21:VAL:O	6:f:25:THR:OG1	2.31	0.47
31:A:615:LHG:H151	32:A:616:SQD:H282	1.96	0.47
7:H:2:ALA:N	37:H:202:HOH:O	2.47	0.47
1:a:102:LEU:H	33:a:614:DGD:C2A	2.27	0.47
26:b:611:CLA:HBB1	26:b:611:CLA:HMB1	1.96	0.47
1:A:271:LEU:HD11	29:A:612:PL9:HC71	1.94	0.47
11:L:20:GLY:O	11:L:24:ILE:HD12	2.15	0.47
16:V:63:THR:HG22	16:V:64:PRO:CD	2.45	0.47
26:c:503:CLA:H203	26:c:510:CLA:HAB	1.96	0.47
5:e:57:ALA:H	5:e:60:GLN:HE21	1.62	0.47
16:v:104:MET:HA	16:v:107:LEU:HD22	1.95	0.47
4:D:218:VAL:HG13	4:D:244:TYR:CD1	2.50	0.47
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	1.97	0.47
1:a:200:LEU:HD23	1:a:285:PHE:CG	2.49	0.47
33:A:619:DGD:HB41	34:I:101:STE:H62	1.96	0.47
2:B:12:LEU:HB2	26:B:612:CLA:HMC2	1.97	0.47
4:D:241:GLU:CD	4:D:241:GLU:H	2.22	0.47
29:D:405:PL9:H412	11:L:29:LEU:HD23	1.97	0.47
3:c:165:LEU:HD13	26:c:507:CLA:HED1	1.96	0.47
13:o:51:LEU:HB3	13:o:65:PHE:HB3	1.96	0.47
13:o:130:GLN:HB2	37:o:307:HOH:O	2.14	0.47
1:A:63[C]:ILE:HB	3:C:335:THR:HG21	1.96	0.47
3:C:79:LYS:HB3	3:C:79:LYS:HE2	1.70	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:218:LEU:HD12	34:b:623:STE:H62	1.96	0.47
5:e:33:ALA:HB2	20:r:11:PRO:HG2	1.97	0.47
13:O:6:THR:HG22	13:O:9:ASP:CG	2.40	0.47
20:R:27:ALA:O	20:R:31:VAL:HG23	2.15	0.47
32:f:101:SQD:H331	32:f:101:SQD:H282	1.97	0.47
10:k:17:ILE:HG13	10:k:18:PHE:CD1	2.50	0.47
15:u:86:GLU:H	15:u:86:GLU:CD	2.22	0.47
20:r:11:PRO:HA	20:r:14:LEU:HD23	1.96	0.47
2:B:495:PHE:HD2	2:B:505:ARG:HH22	1.61	0.47
4:D:266:TRP:CG	31:D:407:LHG:HC31	2.50	0.47
26:b:614:CLA:H2	26:b:615:CLA:CBB	2.43	0.47
26:B:606:CLA:H101	26:B:606:CLA:H13	1.76	0.46
13:O:32:ILE:HG21	13:O:93:LEU:HD21	1.97	0.46
13:o:5:LEU:HB3	13:o:10:ILE:HD11	1.97	0.46
29:A:612:PL9:H272	29:A:612:PL9:H251	1.48	0.46
3:C:79:LYS:HB2	3:C:84:GLN:NE2	2.29	0.46
32:f:101:SQD:H332	32:f:101:SQD:H301	1.85	0.46
13:o:23:ASP:OD1	13:o:24:ASP:N	2.48	0.46
17:Y:39:LEU:HD21	19:Z:25:VAL:HA	1.96	0.46
1:a:179[B]:THR:O	1:a:183[B]:MET:HG3	2.16	0.46
26:b:612:CLA:H51	31:d:407:LHG:H361	1.98	0.46
4:D:23:LYS:NZ	30:D:408:LMG:H122	2.30	0.46
4:d:79:SER:HA	4:d:172:SER:HB3	1.96	0.46
19:z:1:MET:SD	19:z:1:MET:N	2.85	0.46
26:A:613:CLA:H161	26:A:613:CLA:H141	1.61	0.46
33:A:619:DGD:HB42	33:A:619:DGD:HB91	1.97	0.46
5:E:14:ILE:O	5:E:20:TRP:NE1	2.48	0.46
3:c:257:PHE:O	3:c:261:ARG:HG3	2.15	0.46
11:l:14:ARG:HB3	14:t:25:GLU:HG2	1.96	0.46
16:V:87:GLU:CD	16:V:96:ARG:HH12	2.22	0.46
1:a:265:PHE:CD1	1:a:271:LEU:HD23	2.51	0.46
28:a:610:BCR:H20C	28:a:610:BCR:H361	1.82	0.46
1:A:243:GLU:H	1:A:243:GLU:CD	2.23	0.46
3:C:154:LYS:HE3	3:C:266:TRP:CD2	2.51	0.46
33:C:517:DGD:HA82	33:C:517:DGD:HAE2	1.78	0.46
5:e:17:VAL:HG23	9:j:7:ARG:HB2	1.98	0.46
26:h:101:CLA:H92	28:h:102:BCR:H402	1.98	0.46
2:B:495:PHE:HD2	2:B:505:ARG:NH2	2.13	0.46
16:V:3:LEU:HD23	16:V:3:LEU:HA	1.75	0.46
1:a:214:MET:SD	27:d:402:PHO:HED3	2.55	0.46
13:o:43:LEU:HB3	13:o:81:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:126:LEU:HB3	16:v:129:LYS:HB2	1.98	0.46
26:C:507:CLA:H61	26:C:507:CLA:H92	1.70	0.46
29:a:611:PL9:H322	29:a:611:PL9:H301	1.74	0.46
6:f:16:PHE:H	20:r:30:GLN:HE22	1.63	0.46
16:v:26:TYR:OH	16:v:122:GLU:OE1	2.28	0.46
1:A:334[A]:ARG:HD3	4:D:320:LEU:HD13	1.97	0.46
2:B:439:SER:O	37:B:701:HOH:O	2.21	0.46
4:D:194:ASN:HA	4:D:295:SER:OG	2.16	0.45
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.99	0.45
2:b:121:GLU:OE2	7:h:12:ARG:NH1	2.35	0.45
26:b:608:CLA:H202	26:b:608:CLA:H161	1.72	0.45
34:d:414:STE:H152	18:x:12:ILE:HD13	1.98	0.45
2:B:58:GLN:C	2:B:329:PRO:HB3	2.42	0.45
26:B:605:CLA:H61	26:B:605:CLA:H41	1.57	0.45
13:O:57:LYS:HE2	13:O:57:LYS:HB3	1.75	0.45
18:X:12:ILE:HG21	34:X:102:STE:H22	1.99	0.45
31:d:409:LHG:H242	31:d:409:LHG:H272	1.58	0.45
26:B:605:CLA:H92	26:B:605:CLA:H62	1.80	0.45
26:B:612:CLA:H162	26:B:612:CLA:H122	1.77	0.45
3:C:178:LYS:NZ	3:C:184:GLY:O	2.46	0.45
3:c:334:PRO:HA	13:o:153:THR:OG1	2.17	0.45
34:d:414:STE:H41	18:x:20:VAL:HG21	1.98	0.45
28:T:101:BCR:H20C	28:T:101:BCR:H361	1.86	0.45
26:a:606:CLA:HBD	26:a:612:CLA:HAC2	1.99	0.45
26:a:607:CLA:H202	29:a:611:PL9:H222	1.99	0.45
26:b:611:CLA:H8	26:b:611:CLA:H122	1.64	0.45
2:B:149[B]:LEU:HG	26:B:604:CLA:H18	1.97	0.45
2:b:292:LEU:C	2:b:294:SER:H	2.25	0.45
13:o:40:ILE:HD13	13:o:243:ILE:HG12	1.98	0.45
2:b:458:PHE:HB3	26:b:603:CLA:HBC2	1.99	0.45
3:c:75:PHE:CZ	3:c:105:VAL:HG21	2.48	0.45
4:d:190:ASN:HB2	4:d:296:TYR:CD1	2.52	0.45
5:e:26:THR:HA	20:r:15:ALA:HB1	1.99	0.45
32:f:101:SQD:H371	32:f:101:SQD:H342	1.76	0.45
3:C:94:THR:HG22	26:C:501:CLA:HED1	1.98	0.45
3:C:203:THR:O	3:C:235:GLY:HA3	2.17	0.45
30:D:406:LMG:H182	30:D:406:LMG:H212	1.43	0.45
2:b:224:ARG:HG3	7:h:25:TRP:CD2	2.52	0.45
31:d:408:LHG:H321	14:t:21:ILE:HD11	1.97	0.45
13:O:64:GLU:OE1	13:O:64:GLU:N	2.50	0.45
2:b:159:THR:O	2:b:180:PRO:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:90:LEU:HD12	4:d:90:LEU:HA	1.74	0.45
1:a:328[C]:MET:HE1	4:d:183:LEU:HD22	2.00	0.44
2:b:478:VAL:O	4:d:139:ARG:HG2	2.17	0.44
16:v:13:ASN:HD21	16:v:17:LYS:HB3	1.80	0.44
19:z:32:ASP:OD1	19:z:32:ASP:N	2.50	0.44
14:T:18:PHE:HB2	28:T:101:BCR:HC8	1.98	0.44
28:Z:101:BCR:H11C	28:Z:101:BCR:H341	1.86	0.44
2:b:400:SER:OG	2:b:410:THR:OG1	2.16	0.44
26:b:613:CLA:H43	32:b:619:SQD:H102	1.99	0.44
3:c:352:GLY:O	3:c:355[A]:THR:HG22	2.17	0.44
2:B:148:LEU:HD23	2:B:148:LEU:HA	1.80	0.44
2:b:127:ARG:NH2	7:h:18:TYR:O	2.50	0.44
1:A:307:ILE:HG22	1:A:313:VAL:HA	1.99	0.44
29:A:612:PL9:H361	6:F:25:THR:HG21	1.99	0.44
2:B:495:PHE:HB3	2:B:505:ARG:NH1	2.32	0.44
26:B:601:CLA:H51	34:H:102:STE:H152	1.98	0.44
13:O:72:THR:CG2	13:O:107:THR:HG23	2.47	0.44
1:a:131:TRP:CH2	26:c:505:CLA:HAA2	2.52	0.44
2:b:55:MET:HE2	2:b:63:LEU:HD23	2.00	0.44
6:f:17:THR:HG22	32:f:101:SQD:H61	2.00	0.44
9:j:16:VAL:HA	9:j:19:MET:HE2	2.00	0.44
19:z:46:LEU:HD22	19:z:46:LEU:HA	1.87	0.44
2:B:413:ASP:HA	2:B:414:PRO:HD3	1.86	0.44
26:B:603:CLA:C2D	26:B:605:CLA:H2	2.48	0.44
30:C:518:LMG:H191	10:K:27:VAL:HG11	1.99	0.44
18:X:9:GLY:HA2	18:X:12:ILE:HD12	2.00	0.44
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.53	0.44
3:c:348:GLU:OE2	13:o:11:VAL:HA	2.18	0.44
26:c:505:CLA:CMD	26:c:507:CLA:HAB	2.47	0.44
26:A:608:CLA:HAB	26:D:402:CLA:H72	1.98	0.44
2:b:299:GLU:H	2:b:299:GLU:HG2	1.56	0.44
29:d:406:PL9:H401	29:d:406:PL9:H421	1.62	0.44
34:d:414:STE:H71	18:x:16:SER:HB3	2.00	0.44
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.99	0.44
32:F:102:SQD:H302	18:X:27:VAL:HG11	1.99	0.44
32:F:102:SQD:H441	20:R:34:LEU:HD11	2.00	0.44
16:V:6:GLU:CD	16:V:6:GLU:H	2.26	0.44
17:y:39:LEU:O	17:y:44:GLY:N	2.46	0.44
20:r:20:VAL:O	20:r:24:LEU:HB2	2.17	0.44
4:D:127:LEU:HD23	4:D:127:LEU:HA	1.83	0.44
1:a:237:TYR:HB2	1:a:245:THR:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:619:SQD:H151	32:b:619:SQD:H122	1.91	0.44
19:z:31:GLN:HG3	19:z:32:ASP:OD1	2.18	0.44
20:R:33:LYS:HE2	20:R:33:LYS:HB2	1.83	0.44
26:c:501:CLA:HBB1	28:c:515:BCR:H21C	1.99	0.44
1:A:162[C]:PRO:HB3	1:A:168[C]:PHE:HA	1.99	0.43
3:C:415:ASN:O	3:C:416:SER:HB2	2.17	0.43
28:C:514:BCR:H20C	28:C:514:BCR:H361	1.82	0.43
33:H:101:DGD:HB51	33:H:101:DGD:HB21	1.57	0.43
2:b:65:PHE:HE2	26:b:603:CLA:HED2	1.83	0.43
26:c:511:CLA:H143	26:c:511:CLA:H161	1.85	0.43
30:m:101:LMG:H181	30:m:101:LMG:H152	1.64	0.43
2:B:160:GLY:HA3	2:B:180:PRO:HB3	2.01	0.43
6:F:15:ILE:HD13	20:R:23:ILE:HD11	1.99	0.43
8:I:4:LEU:O	8:I:8:VAL:HG23	2.18	0.43
16:V:126:LEU:HB3	16:V:129:LYS:HB2	2.00	0.43
3:c:240:ILE:HA	3:c:240:ILE:HD13	1.70	0.43
7:h:41:PHE:CZ	7:h:45:ILE:HD11	2.53	0.43
3:C:143:TYR:CE2	26:C:513:CLA:HED3	2.53	0.43
33:C:516:DGD:HB22	30:C:518:LMG:H302	2.00	0.43
28:D:404:BCR:H20C	28:D:404:BCR:H361	1.85	0.43
13:O:27:ARG:O	13:O:27:ARG:HG2	2.18	0.43
1:a:192:ILE:HG13	1:a:293:MET:HE1	2.00	0.43
12:M:6:LEU:HD11	34:t:105:STE:H41	2.01	0.43
28:c:514:BCR:H15C	28:c:514:BCR:H351	1.90	0.43
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.99	0.43
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.99	0.43
2:B:422:ARG:O	2:B:425:ILE:HG12	2.19	0.43
26:b:606:CLA:H142	26:b:612:CLA:H203	2.01	0.43
28:c:515:BCR:H15C	28:c:515:BCR:H351	1.87	0.43
11:l:26:VAL:HG11	31:l:101:LHG:H192	2.00	0.43
32:B:622:SQD:H442	14:t:23:PHE:CD1	2.53	0.43
5:e:57:ALA:H	5:e:60:GLN:NE2	2.17	0.43
2:B:25:MET:HE3	28:B:617:BCR:H23C	2.00	0.43
19:Z:23:VAL:HG22	19:Z:40:ILE:HD12	2.00	0.43
2:b:397:VAL:HG12	2:b:417:VAL:HG11	2.00	0.43
26:b:614:CLA:H203	26:b:614:CLA:H161	1.76	0.43
26:c:504:CLA:H92	26:c:504:CLA:H62	1.68	0.43
28:Z:101:BCR:H20C	28:Z:101:BCR:H361	1.88	0.43
2:b:227:LYS:HB3	2:b:227:LYS:HE2	1.85	0.43
18:x:27:VAL:O	18:x:31:ILE:HG13	2.18	0.43
19:z:32:ASP:HB2	19:z:35:ARG:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:161:PRO:HG3	4:D:170:ALA:HB2	2.01	0.43
26:D:402:CLA:H142	26:D:402:CLA:H112	1.78	0.43
1:a:202:VAL:HG11	26:a:607:CLA:C3D	2.49	0.43
1:A:249:VAL:HG12	2:B:491:VAL:CG2	2.48	0.43
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.54	0.43
26:b:606:CLA:H93	26:b:606:CLA:H111	1.88	0.43
26:b:615:CLA:H61	26:b:615:CLA:H92	1.76	0.43
28:b:617:BCR:H15C	28:b:617:BCR:H351	1.88	0.43
19:z:1:MET:HB2	19:z:4:LEU:HB3	2.01	0.43
1:A:340[A]:PRO:HD3	15:U:103:TYR:CZ	2.54	0.42
30:A:614:LMG:HC91	30:A:614:LMG:H291	1.82	0.42
26:C:508:CLA:H192	26:C:508:CLA:H162	1.90	0.42
26:C:509:CLA:H91	26:C:509:CLA:H112	1.62	0.42
13:o:178:LYS:HD3	13:o:178:LYS:HA	1.78	0.42
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.54	0.42
26:A:613:CLA:HBB1	26:A:613:CLA:HMB3	2.01	0.42
26:C:506:CLA:H91	26:C:506:CLA:H203	2.01	0.42
7:H:37:LEU:HD22	28:X:101:BCR:H16C	2.01	0.42
29:A:612:PL9:H471	29:A:612:PL9:H451	1.51	0.42
15:U:92:VAL:HG12	15:U:97:ARG:HD2	2.00	0.42
1:a:296:ASN:HB2	3:c:400:PRO:O	2.18	0.42
26:b:613:CLA:H121	26:b:613:CLA:H91	2.02	0.42
5:e:25:ILE:HD13	20:r:18:TRP:NE1	2.34	0.42
28:A:611:BCR:H24C	28:A:611:BCR:H371	1.84	0.42
2:B:84:THR:HG21	13:o:66:VAL:HB	2.02	0.42
26:C:503:CLA:CHC	34:C:521:STE:H183	2.49	0.42
1:a:162[B]:PRO:HB3	1:a:168[B]:PHE:HA	2.00	0.42
1:a:310:LYS:HD2	16:v:1:ALA:HB1	2.01	0.42
2:B:247:PHE:CE1	26:B:602:CLA:H102	2.55	0.42
1:a:196:PRO:O	1:a:200:LEU:HD13	2.19	0.42
2:b:224:ARG:HA	2:b:224:ARG:HD2	1.89	0.42
26:b:612:CLA:H143	26:b:612:CLA:H111	1.90	0.42
10:k:26:PRO:O	10:k:29:PRO:HD2	2.19	0.42
3:C:42:LEU:HD21	26:C:511:CLA:H2A	2.01	0.42
3:C:467:LEU:HD23	3:C:467:LEU:HA	1.74	0.42
27:D:401:PHO:H3A	27:D:401:PHO:HBA2	1.76	0.42
9:J:26:GLY:HA2	34:J:101:STE:H71	2.00	0.42
1:a:121:LEU:HD21	26:c:505:CLA:H172	2.00	0.42
26:b:609:CLA:H203	26:b:609:CLA:H162	1.69	0.42
30:c:523:LMG:HC2	8:i:9:TYR:OH	2.20	0.42
3:C:168:LEU:HD23	3:C:168:LEU:HA	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:23:ASP:OD2	17:Y:21:GLN:NE2	2.53	0.42
28:Z:101:BCR:H24C	28:Z:101:BCR:H371	1.88	0.42
26:c:513:CLA:H2	28:c:514:BCR:H271	2.02	0.42
11:l:26:VAL:HG11	31:l:101:LHG:H212	2.02	0.42
1:A:63[A]:ILE:HB	3:C:335:THR:HG21	2.01	0.42
29:A:612:PL9:H422	29:A:612:PL9:H401	1.88	0.42
2:B:71:VAL:HG23	26:B:606:CLA:HMA2	2.01	0.42
26:a:609:CLA:H18	26:a:609:CLA:H151	1.73	0.42
26:b:613:CLA:H93	26:b:613:CLA:H61	1.65	0.42
17:y:41:VAL:C	17:y:43:ARG:H	2.28	0.42
1:A:182[A]:PHE:O	1:A:186[A]:PHE:HB2	2.20	0.42
8:I:2:GLU:O	8:I:6:ILE:HG12	2.20	0.42
1:a:281:VAL:HG11	32:a:613:SQD:H181	2.02	0.42
16:v:93:PRO:HA	16:v:101:PHE:CD2	2.55	0.42
4:D:78:VAL:HG11	4:D:114:ILE:HD12	2.02	0.42
15:U:67:LEU:HD23	15:U:72:LYS:HG2	2.02	0.42
17:Y:23:THR:HG22	17:Y:27:MET:HE3	2.02	0.42
2:b:334:ASP:OD1	2:b:334:ASP:N	2.52	0.42
19:z:36:SER:O	19:z:39:LEU:N	2.52	0.42
2:b:6:TYR:OH	31:d:407:LHG:HC2	2.19	0.41
2:b:222:PRO:HB3	7:h:26:GLY:HA3	2.02	0.41
26:b:607:CLA:H161	26:b:607:CLA:H141	1.89	0.41
4:d:12:ARG:HA	4:d:12:ARG:HD3	1.88	0.41
28:k:101:BCR:H24C	28:k:101:BCR:H371	1.85	0.41
26:B:612:CLA:H61	26:B:612:CLA:H102	1.91	0.41
33:C:516:DGD:HG32	30:C:518:LMG:HC92	2.02	0.41
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.55	0.41
15:U:38:TYR:HB2	15:U:41:LEU:HD12	2.01	0.41
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	2.02	0.41
2:b:383:PHE:N	4:d:344:GLU:O	2.51	0.41
5:e:78:THR:O	5:e:82:GLN:HG3	2.19	0.41
29:A:612:PL9:H252	26:D:402:CLA:H141	2.02	0.41
18:X:16:SER:HB3	34:X:102:STE:H82	2.02	0.41
29:a:611:PL9:H371	29:a:611:PL9:H351	1.70	0.41
2:b:145:LEU:HD23	2:b:145:LEU:HA	1.86	0.41
26:b:604:CLA:H62	26:b:604:CLA:H41	1.73	0.41
3:c:146:PHE:HZ	26:c:512:CLA:HBB2	1.86	0.41
28:d:405:BCR:H20C	28:d:405:BCR:H361	1.92	0.41
6:f:16:PHE:H	20:r:30:GLN:NE2	2.18	0.41
16:v:41:HIS:CD2	36:v:201:HEC:NB	2.88	0.41
3:C:409:GLY:HA3	3:C:413[B]:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:L:101:LHG:H311	12:M:18:PRO:HB3	2.01	0.41
13:O:80:GLN:HG3	37:O:305:HOH:O	2.19	0.41
26:b:606:CLA:H193	26:b:606:CLA:H161	1.87	0.41
3:c:95:LEU:HD21	26:c:501:CLA:OBD	2.20	0.41
28:h:102:BCR:H20C	28:h:102:BCR:H361	1.76	0.41
1:A:334[B]:ARG:HD3	37:A:767:HOH:O	2.20	0.41
26:B:603:CLA:H202	7:H:42:LEU:HD12	2.02	0.41
26:B:608:CLA:H162	26:B:608:CLA:H193	1.75	0.41
13:O:27:ARG:HG3	37:O:301:HOH:O	2.20	0.41
20:R:32:GLN:O	20:R:35:LEU:N	2.54	0.41
2:b:173:GLY:HA3	2:b:265:ILE:HD11	2.01	0.41
3:c:93:ALA:HB1	3:c:99:VAL:HG21	2.03	0.41
3:c:157:MET:HE2	3:c:157:MET:HA	2.02	0.41
26:h:101:CLA:H111	26:h:101:CLA:H91	1.65	0.41
15:u:103:TYR:CD1	16:v:50:PRO:HG2	2.56	0.41
26:B:601:CLA:H41	34:H:102:STE:H171	2.02	0.41
28:B:618:BCR:H20C	28:B:618:BCR:H361	1.91	0.41
10:K:26:PRO:O	10:K:29:PRO:HD2	2.20	0.41
18:X:17:GLY:HA2	34:X:102:STE:H121	2.01	0.41
3:c:113:VAL:O	3:c:117:VAL:HG23	2.21	0.41
28:c:516:BCR:H20C	28:c:516:BCR:H361	1.87	0.41
16:v:57:GLU:H	16:v:57:GLU:CD	2.28	0.41
26:A:607:CLA:CBD	26:A:613:CLA:HAC2	2.51	0.41
26:D:403:CLA:H43	34:X:102:STE:H182	2.03	0.41
26:a:606:CLA:CBD	26:a:612:CLA:HAC2	2.51	0.41
2:b:154:GLY:HA2	2:b:158:LEU:HD12	2.03	0.41
28:h:102:BCR:H24C	28:h:102:BCR:H371	1.83	0.41
5:E:18:ARG:O	5:E:22[A]:ILE:HG22	2.20	0.41
5:E:60:GLN:HG2	5:E:62:SER:H	1.86	0.41
1:a:102:LEU:H	33:a:614:DGD:HA22	1.86	0.41
1:a:105:TRP:CE2	1:a:110:GLY:HA3	2.56	0.41
5:e:20:TRP:O	5:e:24:SER:OG	2.26	0.41
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.53	0.41
1:A:46:ILE:HD12	28:A:611:BCR:H15C	2.01	0.41
1:A:84:PRO:HA	1:A:112:TYR:CG	2.56	0.41
1:A:131:TRP:CH2	26:C:505:CLA:HAA2	2.56	0.41
1:A:329[C]:GLU:HG3	37:A:807:HOH:O	2.20	0.41
2:B:149[B]:LEU:HD11	26:B:604:CLA:H112	2.03	0.41
26:B:604:CLA:H142	34:B:620:STE:H142	2.03	0.41
28:K:102:BCR:H15C	28:K:102:BCR:H351	1.90	0.41
11:L:27:LEU:HD23	11:L:27:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:234:LYS:HE2	13:O:234:LYS:HB2	1.87	0.41
2:b:477:ASP:OD2	2:b:478:VAL:HG13	2.20	0.41
28:b:618:BCR:H371	28:b:618:BCR:H24C	1.88	0.41
3:c:26:ARG:HA	26:c:511:CLA:OBD	2.21	0.41
3:c:327[C]:ASN:N	3:c:327[C]:ASN:HD22	2.19	0.41
3:c:391[A]:ARG:HD2	3:c:395:TYR:CZ	2.56	0.41
28:c:516:BCR:H24C	28:c:516:BCR:H371	1.84	0.41
6:f:26:LEU:C	6:f:29:PRO:HD2	2.45	0.41
7:h:29:PRO:O	7:h:33:VAL:HG23	2.20	0.41
19:z:38:GLN:O	19:z:42:LEU:HD22	2.21	0.41
2:B:119:ASP:H	11:L:1:MET:HE1	1.86	0.41
26:B:614:CLA:H91	26:B:614:CLA:H112	1.79	0.41
26:C:502:CLA:H161	26:C:502:CLA:H141	1.71	0.41
4:D:146:PHE:C	4:D:149:PRO:HD2	2.46	0.41
13:O:51:LEU:HD23	13:O:67:PRO:HA	2.03	0.41
1:a:245:THR:HB	4:d:265:ARG:HE	1.86	0.41
26:b:601:CLA:H92	7:h:46:LEU:HD22	2.03	0.41
4:d:160:TYR:HA	4:d:290:ALA:HB2	2.03	0.41
26:B:610:CLA:HHC	26:B:610:CLA:HBB1	2.03	0.40
28:B:619:BCR:H11C	28:B:619:BCR:H341	1.92	0.40
3:C:139:THR:HB	3:C:141:GLU:OE2	2.21	0.40
31:L:101:LHG:H383	31:L:101:LHG:H351	1.83	0.40
16:V:78:ASN:OD1	16:V:96:ARG:NH1	2.51	0.40
19:Z:31:GLN:NE2	19:Z:32:ASP:HB2	2.36	0.40
30:c:523:LMG:H182	30:c:523:LMG:H152	1.97	0.40
26:d:404:CLA:H93	26:d:404:CLA:H61	1.81	0.40
13:o:5:LEU:HA	13:o:5:LEU:HD23	1.66	0.40
13:o:92:SER:HB3	13:o:131:PRO:HA	2.02	0.40
32:B:622:SQD:H322	32:B:622:SQD:H292	1.92	0.40
4:D:110:LEU:HD23	4:D:110:LEU:HA	1.94	0.40
26:D:403:CLA:H142	26:D:403:CLA:H111	1.84	0.40
1:a:124:SER:HA	1:a:151:LEU:HD21	2.04	0.40
2:b:150:CYS:HB2	26:b:602:CLA:CMC	2.50	0.40
26:b:612:CLA:H192	31:d:407:LHG:H221	2.03	0.40
3:c:142:GLU:CD	3:c:142:GLU:H	2.29	0.40
28:c:515:BCR:H24C	28:c:515:BCR:H371	1.91	0.40
7:h:33:VAL:O	7:h:37:LEU:HD12	2.21	0.40
1:A:32:TRP:O	1:A:35:VAL:HB	2.21	0.40
1:A:105:TRP:CE2	1:A:110:GLY:HA3	2.56	0.40
1:A:140:ARG:HB2	4:D:220:ASN:HA	2.02	0.40
26:C:511:CLA:H151	26:C:511:CLA:H111	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:28:ILE:HD11	17:Y:28:ILE:HD13	2.04	0.40
1:a:211:PHE:CD1	29:a:611:PL9:H111	2.57	0.40
2:b:377:VAL:HG11	4:d:342:PRO:HG3	2.04	0.40
4:d:194:ASN:HA	4:d:295:SER:OG	2.21	0.40
4:d:272:LEU:C	4:d:272:LEU:HD23	2.46	0.40
28:t:101:BCR:H24C	28:t:101:BCR:H371	1.96	0.40
17:y:17:GLU:O	17:y:20:ALA:HB3	2.22	0.40
28:b:617:BCR:H24C	28:b:617:BCR:H371	1.82	0.40
28:c:514:BCR:H24C	28:c:514:BCR:H371	1.84	0.40
28:d:405:BCR:H23C	28:d:405:BCR:H392	2.03	0.40
26:C:504:CLA:H62	26:C:504:CLA:H41	1.88	0.40
2:b:221:PRO:HA	26:b:608:CLA:HED3	2.02	0.40
26:b:609:CLA:H122	26:b:614:CLA:HAA1	2.02	0.40
28:c:514:BCR:H11C	28:c:514:BCR:H341	1.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	458/344 (133%)	449 (98%)	9 (2%)	0	100	100
1	a	458/344 (133%)	448 (98%)	8 (2%)	2 (0%)	30	28
2	B	507/510 (99%)	499 (98%)	8 (2%)	0	100	100
2	b	503/510 (99%)	491 (98%)	11 (2%)	1 (0%)	43	44
3	C	461/461 (100%)	451 (98%)	9 (2%)	1 (0%)	43	44
3	c	471/461 (102%)	457 (97%)	13 (3%)	1 (0%)	43	44
4	D	341/352 (97%)	333 (98%)	8 (2%)	0	100	100
4	d	342/352 (97%)	331 (97%)	11 (3%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	e	80/84 (95%)	80 (100%)	0	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%)	61 (97%)	2 (3%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
9	J	34/40 (85%)	31 (91%)	3 (9%)	0	100	100
9	j	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	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%)	30 (97%)	1 (3%)	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	227 (93%)	12 (5%)	4 (2%)	7	4
13	o	242/272 (89%)	236 (98%)	5 (2%)	1 (0%)	30	28
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
15	u	95/134 (71%)	90 (95%)	4 (4%)	1 (1%)	11	8
16	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	15
16	v	135/163 (83%)	130 (96%)	5 (4%)	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%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	7	3
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	R	32/41 (78%)	31 (97%)	1 (3%)	0	100	100
20	r	29/41 (71%)	28 (97%)	0	1 (3%)	3	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5534/5700 (97%)	5381 (97%)	139 (2%)	14 (0%)	36	36

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	59	LYS
16	V	64	PRO
13	o	58	ASN
3	C	416	SER
19	Z	31	GLN
3	c	416	SER
15	u	53	ALA
13	O	57	LYS
13	O	62	GLU
13	O	134	THR
2	b	293	ALA
20	r	30	GLN
1	a	259	ILE
1	a	30	VAL

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	374/280 (134%)	364 (97%)	10 (3%)	39	45
1	a	373/280 (133%)	358 (96%)	15 (4%)	28	29
2	B	407/407 (100%)	396 (97%)	11 (3%)	39	45
2	b	402/407 (99%)	395 (98%)	7 (2%)	53	62
3	C	361/362 (100%)	350 (97%)	11 (3%)	36	41
3	c	370/362 (102%)	357 (96%)	13 (4%)	32	35
4	D	278/283 (98%)	275 (99%)	3 (1%)	65	74
4	d	279/283 (99%)	273 (98%)	6 (2%)	45	53
5	E	72/73 (99%)	69 (96%)	3 (4%)	26	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	71/73 (97%)	68 (96%)	3 (4%)	26	28
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	24 (86%)	4 (14%)	3	1
7	H	54/55 (98%)	52 (96%)	2 (4%)	30	33
7	h	53/55 (96%)	49 (92%)	4 (8%)	12	10
8	I	32/34 (94%)	30 (94%)	2 (6%)	16	14
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%)	22 (92%)	2 (8%)	10	8
10	K	30/37 (81%)	28 (93%)	2 (7%)	15	12
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	2
11	L	35/35 (100%)	33 (94%)	2 (6%)	18	17
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	3
12	M	28/32 (88%)	26 (93%)	2 (7%)	13	11
12	m	28/32 (88%)	27 (96%)	1 (4%)	31	34
13	O	206/228 (90%)	198 (96%)	8 (4%)	28	31
13	o	207/228 (91%)	197 (95%)	10 (5%)	23	23
14	T	26/28 (93%)	25 (96%)	1 (4%)	29	32
14	t	25/28 (89%)	25 (100%)	0	100	100
15	U	84/112 (75%)	80 (95%)	4 (5%)	23	23
15	u	84/112 (75%)	83 (99%)	1 (1%)	63	72
16	V	117/138 (85%)	116 (99%)	1 (1%)	70	78
16	v	117/138 (85%)	109 (93%)	8 (7%)	14	12
17	Y	19/37 (51%)	19 (100%)	0	100	100
17	y	22/37 (60%)	20 (91%)	2 (9%)	9	6
18	X	31/34 (91%)	28 (90%)	3 (10%)	8	5
18	x	31/34 (91%)	30 (97%)	1 (3%)	34	38
19	Z	52/52 (100%)	43 (83%)	9 (17%)	2	1
19	z	51/52 (98%)	46 (90%)	5 (10%)	7	5
20	R	28/33 (85%)	24 (86%)	4 (14%)	3	1
20	r	25/33 (76%)	19 (76%)	6 (24%)	1	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4572/4654 (98%)	4397 (96%)	175 (4%)	28	32

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	60[A]	ILE
1	A	60[B]	ILE
1	A	60[C]	ILE
1	A	205	VAL
1	A	231	GLU
1	A	243	GLU
1	A	244	GLU
1	A	245	THR
1	A	286	THR
2	B	76	SER
2	B	84	THR
2	B	87	ASP
2	B	98	LEU
2	B	297	THR
2	B	298	LEU
2	B	362	PHE
2	B	371	THR
2	B	400	SER
2	B	431	GLU
2	B	476	ARG
3	C	106	VAL
3	C	141	GLU
3	C	144	SER
3	C	240	ILE
3	C	279	LEU
3	C	289	PHE
3	C	315	MET
3	C	355[A]	THR
3	C	355[B]	THR
3	C	355[C]	THR
3	C	416	SER
4	D	43	LEU
4	D	150	ILE
4	D	154	VAL
5	E	22[A]	ILE
5	E	22[B]	ILE

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Mol	Chain	Res	Type
5	E	54	SER
7	H	20	LYS
7	H	56	ASP
8	I	4	LEU
8	I	34	ARG
10	K	19	ASP
10	K	27	VAL
11	L	10	VAL
11	L	24	ILE
12	M	16	LEU
12	M	25	LEU
13	O	23	ASP
13	O	78	LEU
13	O	82	GLN
13	O	98	GLU
13	O	107	THR
13	O	118	LEU
13	O	136	ILE
13	O	214	THR
14	T	25	GLU
15	U	23	GLU
15	U	51	LYS
15	U	67	LEU
15	U	70	ARG
16	V	3	LEU
18	X	3	ILE
18	X	23	LEU
18	X	37	VAL
19	Z	15	LEU
19	Z	17	PHE
19	Z	19	MET
19	Z	20	VAL
19	Z	35	ARG
19	Z	39	LEU
19	Z	46	LEU
19	Z	50	LEU
19	Z	52	LEU
20	R	6	LEU
20	R	21	ARG
20	R	33	LYS
20	R	35	LEU
1	a	28	LEU

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Mol	Chain	Res	Type
1	a	42	LEU
1	a	121	LEU
1	a	134	SER
1	a	159[A]	LEU
1	a	159[B]	LEU
1	a	159[C]	LEU
1	a	200	LEU
1	a	223	LEU
1	a	229	GLU
1	a	243	GLU
1	a	245	THR
1	a	271	LEU
1	a	286	THR
1	a	288	LEU
2	b	14	ASN
2	b	98	LEU
2	b	299	GLU
2	b	362	PHE
2	b	413	ASP
2	b	505	ARG
2	b	506	ARG
3	c	24	THR
3	c	29	GLU
3	c	30	SER
3	c	72	LEU
3	c	124	VAL
3	c	125	LEU
3	c	142	GLU
3	c	165	LEU
3	c	240	ILE
3	c	315	MET
3	c	396	MET
3	c	413[A]	GLU
3	c	413[B]	GLU
4	d	233	ARG
4	d	259	ILE
4	d	264	LYS
4	d	272	LEU
4	d	291	LEU
4	d	321	LEU
5	e	4	THR
5	e	66	VAL

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Mol	Chain	Res	Type
5	e	83	LEU
6	f	18	VAL
6	f	23	VAL
6	f	25	THR
6	f	28	VAL
7	h	7	LEU
7	h	27	THR
7	h	37	LEU
7	h	56	ASP
8	i	34	ARG
9	j	13	VAL
9	j	21	VAL
10	k	10	LYS
10	k	19	ASP
10	k	30	VAL
10	k	35	LEU
11	l	2	GLU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
13	o	49	THR
13	o	53	LYS
13	o	58	ASN
13	o	64	GLU
13	o	87	VAL
13	o	118	LEU
13	o	130	GLN
13	o	134	THR
13	o	143	LYS
13	o	199	LEU
15	u	23	GLU
16	v	19	ILE
16	v	22	THR
16	v	52	LEU
16	v	61	LEU
16	v	69	ILE
16	v	90	GLU
16	v	106	ASN
16	v	107	LEU
17	y	19	ILE
17	y	30	ILE

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Mol	Chain	Res	Type
18	x	15	LEU
19	z	1	MET
19	z	20	VAL
19	z	27	TYR
19	z	42	LEU
19	z	46	LEU
20	r	3	TRP
20	r	6	LEU
20	r	9	LEU
20	r	10	LEU
20	r	14	LEU
20	r	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	394	GLN
3	C	311	GLN
3	C	385	GLN
4	D	61	HIS
4	D	250	ASN
7	H	59	ASN
13	O	130	GLN
13	O	155	ASN
13	O	231	HIS
15	U	71	GLN
15	U	78	ASN
16	V	86	GLN
16	V	106	ASN
17	Y	21	GLN
18	X	38	GLN
19	Z	31	GLN
1	a	234	ASN
1	a	325	ASN
2	b	14	ASN
2	b	338	GLN
2	b	409	GLN
2	b	497	GLN
3	c	311	GLN
3	c	322	GLN
3	c	378	ASN
3	c	382	ASN

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Mol	Chain	Res	Type
4	d	236	ASN
5	e	60	GLN
5	e	82	GLN
12	m	5	GLN
13	o	155	ASN
15	u	78	ASN
16	v	106	ASN
18	x	33	GLN
19	z	31	GLN
19	z	58	ASN
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	$\# Z > 2$
12	FME	M	1	12	8,9,10	1.12	1 (12%)	8,9,11	1.83	2 (25%)
8	FME	i	1	8	8,9,10	1.04	0	8,9,11	0.84	0
12	FME	m	1	12	8,9,10	0.97	0	8,9,11	0.71	0
8	FME	I	1	8	8,9,10	1.07	1 (12%)	8,9,11	1.45	1 (12%)
14	FME	T	1	14	8,9,10	1.12	1 (12%)	8,9,11	0.96	0
14	FME	t	1	14	8,9,10	1.23	1 (12%)	8,9,11	0.72	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
12	FME	M	1	12	-	1/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-
14	FME	t	1	14	-	4/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-2.73	1.42	1.46
14	T	1	FME	CA-N	-2.46	1.43	1.46
12	M	1	FME	CA-N	-2.44	1.43	1.46
8	I	1	FME	CA-N	-2.25	1.43	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	1	FME	CA-N-CN	-3.88	116.86	122.82
8	I	1	FME	CA-N-CN	-3.32	117.71	122.82
12	M	1	FME	CB-CA-N	2.36	114.82	110.52

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

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 190 ligands modelled in this entry, 6 are monoatomic - leaving 184 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
26	CLA	c	502	3	69,73,73	1.30	8 (11%)	82,113,113	1.43	8 (9%)
28	BCR	A	611	-	41,41,41	0.99	2 (4%)	56,56,56	1.26	5 (8%)
28	BCR	B	617	-	41,41,41	0.95	1 (2%)	56,56,56	1.32	5 (8%)
26	CLA	B	605	2	69,73,73	1.23	6 (8%)	82,113,113	1.27	6 (7%)
29	PL9	d	406	-	55,55,55	1.03	3 (5%)	68,69,69	1.57	14 (20%)
33	DGD	c	518	-	63,63,67	0.98	2 (3%)	77,77,81	1.46	12 (15%)
33	DGD	C	515	-	63,63,67	1.04	5 (7%)	77,77,81	1.31	9 (11%)
26	CLA	c	511	3	69,73,73	1.40	8 (11%)	82,113,113	1.56	7 (8%)
34	STE	F	103	-	11,11,19	0.75	0	11,11,19	1.16	1 (9%)
26	CLA	b	613	2	69,73,73	1.32	7 (10%)	82,113,113	1.31	9 (10%)
26	CLA	A	608	37	69,73,73	1.26	9 (13%)	82,113,113	1.40	10 (12%)
26	CLA	B	609	2	69,73,73	1.26	6 (8%)	82,113,113	1.28	6 (7%)
30	LMG	d	410	-	21,21,55	0.53	0	20,20,63	1.15	2 (10%)
26	CLA	B	603	2	69,73,73	1.47	8 (11%)	82,113,113	1.38	9 (10%)
34	STE	B	624	-	11,11,19	0.71	0	11,11,19	1.17	0
34	STE	t	103	-	13,13,19	0.66	0	13,13,19	1.22	1 (7%)
28	BCR	b	618	-	41,41,41	0.97	2 (4%)	56,56,56	1.09	4 (7%)
28	BCR	B	618	-	41,41,41	1.00	2 (4%)	56,56,56	1.24	6 (10%)
26	CLA	C	506	3	69,73,73	1.28	7 (10%)	82,113,113	1.30	6 (7%)
28	BCR	K	101	-	41,41,41	1.07	3 (7%)	56,56,56	1.12	2 (3%)
34	STE	k	102	-	11,11,19	0.74	0	11,11,19	1.14	0
34	STE	T	102	-	15,15,19	0.41	0	14,14,19	0.71	0
35	HEM	F	101	5,6	50,50,50	1.50	6 (12%)	67,82,82	1.12	3 (4%)
32	SQD	F	102	-	34,36,54	1.53	5 (14%)	42,45,65	1.80	9 (21%)
26	CLA	a	607	37	69,73,73	1.25	8 (11%)	82,113,113	1.39	8 (9%)
30	LMG	d	411	-	44,44,55	0.90	2 (4%)	52,52,63	1.31	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LMG	c	522	-	48,48,55	0.91	3 (6%)	56,56,63	1.29	9 (16%)
26	CLA	c	503	3	69,73,73	1.38	9 (13%)	82,113,113	1.44	6 (7%)
26	CLA	B	604	2	69,73,73	1.23	7 (10%)	82,113,113	1.40	8 (9%)
34	STE	B	623	-	11,11,19	0.73	0	11,11,19	1.37	2 (18%)
33	DGD	a	614	-	43,43,67	0.89	3 (6%)	45,45,81	1.42	6 (13%)
30	LMG	B	621	-	26,26,55	0.63	0	26,26,63	1.21	1 (3%)
26	CLA	B	610	37	69,73,73	1.29	8 (11%)	82,113,113	1.41	10 (12%)
34	STE	d	414	-	19,19,19	0.63	0	19,19,19	1.02	1 (5%)
28	BCR	h	102	-	41,41,41	0.95	2 (4%)	56,56,56	1.14	3 (5%)
34	STE	t	104	-	9,9,19	0.39	0	8,8,19	0.70	0
26	CLA	b	614	2	69,73,73	1.41	10 (14%)	82,113,113	1.29	6 (7%)
34	STE	d	412	-	15,15,19	0.78	0	15,15,19	0.98	1 (6%)
26	CLA	b	603	2	69,73,73	1.22	8 (11%)	82,113,113	1.56	10 (12%)
28	BCR	c	515	-	41,41,41	1.13	2 (4%)	56,56,56	1.27	8 (14%)
33	DGD	C	516	-	63,63,67	1.02	5 (7%)	77,77,81	1.41	9 (11%)
32	SQD	t	102	-	35,35,54	1.78	6 (17%)	37,37,65	1.39	4 (10%)
26	CLA	b	612	2	69,73,73	1.28	8 (11%)	82,113,113	1.39	9 (10%)
22	OEX	A	602[B]	3,1,37	0,14,14	-	-	-	-	-
26	CLA	b	615	2	64,68,73	1.19	6 (9%)	76,107,113	1.50	7 (9%)
31	LHG	d	408	-	48,48,48	0.60	0	51,54,54	1.28	6 (11%)
26	CLA	C	510	3	69,73,73	1.41	8 (11%)	82,113,113	1.44	9 (10%)
30	LMG	M	101	-	51,51,55	0.82	3 (5%)	59,59,63	1.42	7 (11%)
26	CLA	b	606	37	69,73,73	1.07	6 (8%)	82,113,113	1.25	8 (9%)
32	SQD	a	613	-	52,54,54	1.57	7 (13%)	62,65,65	1.88	9 (14%)
34	STE	B	625	-	15,15,19	0.39	0	14,14,19	0.75	0
32	SQD	b	619	-	47,49,54	1.69	10 (21%)	57,60,65	1.82	13 (22%)
28	BCR	c	516	-	41,41,41	1.08	2 (4%)	56,56,56	1.10	2 (3%)
34	STE	M	102	-	14,14,19	0.73	0	14,14,19	1.23	1 (7%)
26	CLA	c	504	37	64,68,73	1.31	6 (9%)	76,107,113	1.34	9 (11%)
28	BCR	Z	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	7 (12%)
34	STE	T	103	-	14,14,19	0.31	0	13,13,19	0.97	0
28	BCR	t	101	-	41,41,41	0.93	1 (2%)	56,56,56	1.29	7 (12%)
26	CLA	B	606	2	69,73,73	1.49	5 (7%)	82,113,113	1.42	10 (12%)
28	BCR	T	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.28	6 (10%)
33	DGD	h	103	-	63,63,67	0.96	2 (3%)	77,77,81	1.48	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LMG	D	408	-	31,31,55	0.74	2 (6%)	33,33,63	1.20	3 (9%)
34	STE	c	521	-	19,19,19	0.63	0	19,19,19	0.97	0
26	CLA	C	507	37	69,73,73	1.27	6 (8%)	82,113,113	1.42	7 (8%)
28	BCR	k	101	-	41,41,41	1.05	3 (7%)	56,56,56	1.10	3 (5%)
26	CLA	C	503	3	69,73,73	1.54	9 (13%)	82,113,113	1.54	10 (12%)
26	CLA	b	605	2	69,73,73	1.36	7 (10%)	82,113,113	1.50	7 (8%)
26	CLA	C	508	3	69,73,73	1.29	7 (10%)	82,113,113	1.40	5 (6%)
21	OEY	a	601[C]	3,1,37	0,16,16	-	-	-	-	-
27	PHO	d	402	-	58,69,69	2.11	10 (17%)	55,99,99	1.60	8 (14%)
22	OEX	a	602[B]	3,1,37	0,14,14	-	-	-	-	-
26	CLA	B	613	2	69,73,73	1.32	8 (11%)	82,113,113	1.44	12 (14%)
25	BCT	A	606	23	3,3,3	1.18	0	2,3,3	2.85	1 (50%)
28	BCR	B	619	-	41,41,41	0.97	1 (2%)	56,56,56	1.22	5 (8%)
21	OEY	A	601[C]	3,1,37	0,16,16	-	-	-	-	-
25	BCT	d	401	23	3,3,3	1.11	0	2,3,3	2.94	1 (50%)
26	CLA	b	609	37	69,73,73	1.43	7 (10%)	82,113,113	1.33	9 (10%)
21	OEY	a	601[A]	3,1,37	0,16,16	-	-	-	-	-
31	LHG	D	407	-	48,48,48	0.73	1 (2%)	51,54,54	1.22	5 (9%)
32	SQD	A	616	-	50,52,54	1.56	8 (16%)	60,63,65	1.85	12 (20%)
34	STE	H	102	-	17,17,19	0.42	0	16,16,19	0.69	0
30	LMG	c	523	-	49,49,55	1.04	4 (8%)	57,57,63	1.28	4 (7%)
26	CLA	d	404	4	69,73,73	1.15	8 (11%)	82,113,113	1.21	6 (7%)
26	CLA	c	508	3	68,72,73	1.59	11 (16%)	80,111,113	1.48	10 (12%)
30	LMG	m	101	-	51,51,55	0.76	1 (1%)	59,59,63	1.45	8 (13%)
26	CLA	C	505	3	69,73,73	1.22	6 (8%)	82,113,113	1.32	9 (10%)
26	CLA	c	505	3	69,73,73	1.17	6 (8%)	82,113,113	1.34	7 (8%)
26	CLA	B	611	2	69,73,73	1.32	6 (8%)	82,113,113	1.57	6 (7%)
34	STE	J	101	-	11,11,19	0.70	0	11,11,19	1.30	2 (18%)
34	STE	C	520	-	11,11,19	0.74	0	11,11,19	1.16	1 (9%)
32	SQD	A	618	-	38,38,54	1.78	5 (13%)	40,40,65	1.12	2 (5%)
27	PHO	a	608	-	58,69,69	2.08	11 (18%)	55,99,99	1.48	7 (12%)
34	STE	l	102	-	17,17,19	0.30	0	16,16,19	0.97	0
26	CLA	B	608	2	69,73,73	1.23	7 (10%)	82,113,113	1.34	9 (10%)
26	CLA	b	611	2	69,73,73	1.19	6 (8%)	82,113,113	1.28	10 (12%)
34	STE	L	102	-	11,11,19	0.73	0	11,11,19	1.20	1 (9%)
35	HEM	e	101	5,6	50,50,50	1.59	8 (16%)	67,82,82	1.39	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	DGD	c	517	-	63,63,67	0.94	2 (3%)	77,77,81	1.43	13 (16%)
26	CLA	b	604	2	69,73,73	1.40	7 (10%)	82,113,113	1.48	10 (12%)
28	BCR	K	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.11	3 (5%)
29	PL9	A	612	-	55,55,55	0.88	2 (3%)	68,69,69	1.41	12 (17%)
34	STE	t	105	-	17,17,19	0.61	0	17,17,19	1.09	0
26	CLA	C	502	3	69,73,73	1.38	7 (10%)	82,113,113	1.23	7 (8%)
26	CLA	a	612	37	69,73,73	1.24	7 (10%)	82,113,113	1.31	6 (7%)
26	CLA	c	509	3	69,73,73	1.21	8 (11%)	82,113,113	1.42	6 (7%)
30	LMG	b	621	-	55,55,55	0.93	5 (9%)	63,63,63	1.33	7 (11%)
26	CLA	C	504	37	63,67,73	1.40	9 (14%)	74,105,113	1.33	9 (12%)
26	CLA	c	510	3	69,73,73	1.48	11 (15%)	82,113,113	1.27	6 (7%)
33	DGD	c	519	-	63,63,67	0.90	3 (4%)	77,77,81	1.39	6 (7%)
34	STE	B	620	-	16,16,19	0.66	0	16,16,19	1.04	0
26	CLA	B	601	37	69,73,73	1.36	8 (11%)	82,113,113	1.32	7 (8%)
26	CLA	c	507	37	69,73,73	1.32	8 (11%)	82,113,113	1.33	9 (10%)
32	SQD	f	101	-	39,41,54	1.68	8 (20%)	49,52,65	1.58	10 (20%)
26	CLA	h	101	37	69,73,73	1.31	9 (13%)	82,113,113	1.40	7 (8%)
34	STE	C	519	-	11,11,19	0.61	0	11,11,19	1.84	3 (27%)
28	BCR	a	610	-	41,41,41	0.98	3 (7%)	56,56,56	1.19	5 (8%)
28	BCR	C	514	-	41,41,41	1.10	3 (7%)	56,56,56	1.08	4 (7%)
26	CLA	A	613	37	69,73,73	1.40	9 (13%)	82,113,113	1.37	7 (8%)
28	BCR	c	514	-	41,41,41	1.06	2 (4%)	56,56,56	1.18	4 (7%)
26	CLA	b	607	2	69,73,73	1.40	8 (11%)	82,113,113	1.34	9 (10%)
31	LHG	e	102	-	41,41,48	0.79	1 (2%)	44,47,54	1.30	6 (13%)
33	DGD	A	619	-	67,67,67	1.09	5 (7%)	81,81,81	1.33	11 (13%)
26	CLA	B	612	2	69,73,73	1.21	6 (8%)	82,113,113	1.51	9 (10%)
30	LMG	A	614	-	48,48,55	0.95	5 (10%)	56,56,63	1.26	6 (10%)
26	CLA	B	616	2	64,68,73	1.37	10 (15%)	76,107,113	1.48	6 (7%)
26	CLA	b	608	2	69,73,73	1.38	10 (14%)	82,113,113	1.25	7 (8%)
26	CLA	b	601	2	69,73,73	1.24	9 (13%)	82,113,113	1.36	8 (9%)
26	CLA	c	506	3	69,73,73	1.35	6 (8%)	82,113,113	1.32	7 (8%)
34	STE	M	103	-	9,9,19	0.35	0	8,8,19	0.79	0
34	STE	b	622	-	19,19,19	0.64	0	19,19,19	1.01	1 (5%)
26	CLA	A	610	1	58,62,73	1.28	6 (10%)	68,99,113	1.37	7 (10%)
26	CLA	B	615	2	69,73,73	1.42	9 (13%)	82,113,113	1.25	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	d	403	4	69,73,73	1.29	8 (11%)	82,113,113	1.25	5 (6%)
32	SQD	B	622	-	52,54,54	1.57	8 (15%)	62,65,65	1.80	13 (20%)
34	STE	b	623	-	9,9,19	0.40	0	8,8,19	0.64	0
28	BCR	b	616	-	41,41,41	1.01	2 (4%)	56,56,56	1.35	6 (10%)
36	HEC	V	201	16	50,50,50	1.75	7 (14%)	68,82,82	1.43	9 (13%)
26	CLA	b	602	2	69,73,73	1.42	9 (13%)	82,113,113	1.36	8 (9%)
26	CLA	A	607	1	69,73,73	1.37	8 (11%)	82,113,113	1.29	8 (9%)
30	LMG	C	518	-	48,48,55	0.84	2 (4%)	56,56,63	1.34	7 (12%)
26	CLA	c	512	3	69,73,73	1.21	9 (13%)	82,113,113	1.37	9 (10%)
21	OEY	A	601[A]	3,1,37	0,16,16	-	-	-	-	-
26	CLA	C	501	3	69,73,73	1.25	10 (14%)	82,113,113	1.43	8 (9%)
28	BCR	D	404	-	41,41,41	1.06	3 (7%)	56,56,56	1.28	7 (12%)
34	STE	b	620	-	19,19,19	0.59	0	19,19,19	1.15	0
36	HEC	v	201	16	50,50,50	1.68	7 (14%)	68,82,82	1.51	10 (14%)
26	CLA	a	609	1	69,73,73	1.17	7 (10%)	82,113,113	1.23	6 (7%)
26	CLA	B	607	37	69,73,73	1.12	7 (10%)	82,113,113	1.24	5 (6%)
26	CLA	C	511	3	69,73,73	1.24	7 (10%)	82,113,113	1.40	4 (4%)
26	CLA	C	513	3	69,73,73	1.34	8 (11%)	82,113,113	1.41	7 (8%)
26	CLA	a	606	1	69,73,73	1.43	11 (15%)	82,113,113	1.29	6 (7%)
26	CLA	C	512	3	69,73,73	1.27	9 (13%)	82,113,113	1.45	8 (9%)
26	CLA	c	513	3	69,73,73	1.36	7 (10%)	82,113,113	1.19	7 (8%)
31	LHG	l	101	-	48,48,48	0.65	0	51,54,54	1.25	8 (15%)
26	CLA	B	602	2	69,73,73	1.30	6 (8%)	82,113,113	1.39	11 (13%)
29	PL9	D	405	-	55,55,55	1.08	1 (1%)	68,69,69	1.55	13 (19%)
34	STE	a	615	-	11,11,19	0.81	0	11,11,19	1.03	1 (9%)
26	CLA	B	614	2	69,73,73	1.30	6 (8%)	82,113,113	1.37	8 (9%)
30	LMG	D	406	-	51,51,55	0.78	0	59,59,63	1.34	8 (13%)
33	DGD	H	101	-	63,63,67	1.17	6 (9%)	77,77,81	1.36	10 (12%)
28	BCR	d	405	-	41,41,41	1.02	2 (4%)	56,56,56	1.23	9 (16%)
26	CLA	C	509	3	69,73,73	1.34	8 (11%)	82,113,113	1.43	8 (9%)
31	LHG	L	101	-	48,48,48	0.74	1 (2%)	51,54,54	1.23	5 (9%)
33	DGD	C	517	-	63,63,67	0.98	3 (4%)	77,77,81	1.35	6 (7%)
34	STE	C	521	-	15,15,19	0.39	0	14,14,19	0.70	0
34	STE	X	102	-	19,19,19	0.61	0	19,19,19	1.14	0
26	CLA	D	402	4	69,73,73	1.29	8 (11%)	82,113,113	1.36	7 (8%)
31	LHG	d	409	-	38,38,48	0.79	1 (2%)	41,44,54	1.13	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	D	403	4	69,73,73	1.29	9 (13%)	82,113,113	1.20	7 (8%)
28	BCR	X	101	-	41,41,41	0.95	2 (4%)	56,56,56	1.28	8 (14%)
28	BCR	b	617	-	41,41,41	1.01	2 (4%)	56,56,56	1.15	4 (7%)
26	CLA	c	501	3	69,73,73	1.26	6 (8%)	82,113,113	1.47	7 (8%)
27	PHO	D	401	-	58,69,69	2.17	10 (17%)	55,99,99	1.68	10 (18%)
31	LHG	A	615	-	46,46,48	0.81	1 (2%)	49,52,54	1.22	4 (8%)
26	CLA	b	610	2	69,73,73	1.27	6 (8%)	82,113,113	1.40	5 (6%)
29	PL9	a	611	-	55,55,55	0.78	1 (1%)	68,69,69	1.47	11 (16%)
27	PHO	A	609	-	58,69,69	2.05	12 (20%)	55,99,99	1.47	4 (7%)
34	STE	I	101	-	14,14,19	0.39	0	13,13,19	0.79	0
34	STE	j	101	-	11,11,19	0.84	0	11,11,19	1.11	2 (18%)
34	STE	d	413	-	16,16,19	0.63	0	16,16,19	1.12	1 (6%)
31	LHG	D	409	-	48,48,48	0.94	2 (4%)	51,54,54	1.35	7 (13%)
30	LMG	c	520	-	37,37,55	0.97	1 (2%)	45,45,63	1.30	4 (8%)
31	LHG	A	617	-	48,48,48	0.84	3 (6%)	51,54,54	1.20	6 (11%)
31	LHG	d	407	-	48,48,48	0.75	2 (4%)	51,54,54	1.41	7 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	c	502	3	-	10/39/115/115	-
28	BCR	A	611	-	-	4/29/63/63	0/2/2/2
28	BCR	B	617	-	-	5/29/63/63	0/2/2/2
26	CLA	B	605	2	-	11/39/115/115	-
29	PL9	d	406	-	-	12/53/73/73	0/1/1/1
33	DGD	c	518	-	-	22/51/91/95	0/2/2/2
33	DGD	C	515	-	-	18/51/91/95	0/2/2/2
26	CLA	c	511	3	-	6/39/115/115	-
34	STE	F	103	-	-	7/9/9/17	-
26	CLA	b	613	2	-	18/39/115/115	-
26	CLA	A	608	37	-	8/39/115/115	-
26	CLA	B	609	2	-	7/39/115/115	-
30	LMG	d	410	-	-	11/17/17/70	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	B	603	2	-	13/39/115/115	-
34	STE	B	624	-	-	1/9/9/17	-
34	STE	t	103	-	-	3/11/11/17	-
28	BCR	b	618	-	-	4/29/63/63	0/2/2/2
28	BCR	B	618	-	-	4/29/63/63	0/2/2/2
26	CLA	C	506	3	-	9/39/115/115	-
28	BCR	K	101	-	-	7/29/63/63	0/2/2/2
34	STE	k	102	-	-	3/9/9/17	-
34	STE	T	102	-	-	7/13/13/17	-
35	HEM	F	101	5,6	-	2/14/54/54	-
32	SQD	F	102	-	-	16/28/48/69	0/1/1/1
26	CLA	a	607	37	-	10/39/115/115	-
30	LMG	d	411	-	-	10/39/59/70	0/1/1/1
30	LMG	c	522	-	-	22/43/63/70	0/1/1/1
26	CLA	c	503	3	-	10/39/115/115	-
26	CLA	B	604	2	-	14/39/115/115	-
34	STE	B	623	-	-	7/9/9/17	-
33	DGD	a	614	-	-	18/45/45/95	-
30	LMG	B	621	-	-	8/22/22/70	-
26	CLA	B	610	37	-	7/39/115/115	-
34	STE	d	414	-	-	7/17/17/17	-
28	BCR	h	102	-	-	6/29/63/63	0/2/2/2
34	STE	t	104	-	-	3/7/7/17	-
26	CLA	b	614	2	-	9/39/115/115	-
34	STE	d	412	-	-	4/13/13/17	-
26	CLA	b	603	2	-	8/39/115/115	-
28	BCR	c	515	-	-	3/29/63/63	0/2/2/2
33	DGD	C	516	-	-	19/51/91/95	0/2/2/2
32	SQD	t	102	-	-	19/37/37/69	-
26	CLA	b	612	2	-	8/39/115/115	-
26	CLA	b	615	2	-	8/33/109/115	-
31	LHG	d	408	-	-	22/53/53/53	-
26	CLA	C	510	3	-	8/39/115/115	-
30	LMG	M	101	-	-	24/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	b	606	37	-	12/39/115/115	-
32	SQD	a	613	-	-	27/49/69/69	0/1/1/1
34	STE	B	625	-	-	5/13/13/17	-
32	SQD	b	619	-	-	23/44/64/69	0/1/1/1
28	BCR	c	516	-	-	5/29/63/63	0/2/2/2
34	STE	M	102	-	-	6/12/12/17	-
26	CLA	c	504	37	-	8/33/109/115	-
28	BCR	Z	101	-	-	6/29/63/63	0/2/2/2
34	STE	T	103	-	-	9/12/12/17	-
28	BCR	t	101	-	-	5/29/63/63	0/2/2/2
26	CLA	B	606	2	-	13/39/115/115	-
28	BCR	T	101	-	-	7/29/63/63	0/2/2/2
33	DGD	h	103	-	-	15/51/91/95	0/2/2/2
30	LMG	D	408	-	-	18/33/33/70	-
34	STE	c	521	-	-	8/17/17/17	-
26	CLA	C	507	37	-	7/39/115/115	-
28	BCR	k	101	-	-	6/29/63/63	0/2/2/2
26	CLA	C	503	3	-	4/39/115/115	-
26	CLA	b	605	2	-	6/39/115/115	-
26	CLA	C	508	3	-	6/39/115/115	-
27	PHO	d	402	-	-	4/37/103/103	0/5/6/6
26	CLA	B	613	2	-	8/39/115/115	-
28	BCR	B	619	-	-	2/29/63/63	0/2/2/2
26	CLA	b	609	37	-	8/39/115/115	-
32	SQD	A	616	-	-	23/47/67/69	0/1/1/1
31	LHG	D	407	-	-	25/53/53/53	-
34	STE	H	102	-	-	7/15/15/17	-
30	LMG	c	523	-	-	22/44/64/70	0/1/1/1
26	CLA	d	404	4	-	10/39/115/115	-
26	CLA	c	508	3	-	6/38/114/115	-
30	LMG	m	101	-	-	22/46/66/70	0/1/1/1
26	CLA	C	505	3	-	9/39/115/115	-
26	CLA	c	505	3	-	11/39/115/115	-
26	CLA	B	611	2	-	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	STE	J	101	-	-	6/9/9/17	-
34	STE	C	520	-	-	5/9/9/17	-
32	SQD	A	618	-	-	16/39/39/69	-
27	PHO	a	608	-	-	2/37/103/103	0/5/6/6
34	STE	l	102	-	-	9/15/15/17	-
26	CLA	B	608	2	-	5/39/115/115	-
26	CLA	b	611	2	-	14/39/115/115	-
34	STE	L	102	-	-	7/9/9/17	-
35	HEM	e	101	5,6	-	3/14/54/54	-
33	DGD	c	517	-	-	24/51/91/95	0/2/2/2
26	CLA	b	604	2	-	9/39/115/115	-
28	BCR	K	102	-	-	4/29/63/63	0/2/2/2
29	PL9	A	612	-	-	23/53/73/73	0/1/1/1
34	STE	t	105	-	-	8/15/15/17	-
26	CLA	C	502	3	-	8/39/115/115	-
26	CLA	a	612	37	-	5/39/115/115	-
26	CLA	c	509	3	-	10/39/115/115	-
30	LMG	b	621	-	-	27/50/70/70	0/1/1/1
26	CLA	C	504	37	-	7/32/108/115	-
26	CLA	c	510	3	-	8/39/115/115	-
33	DGD	c	519	-	-	17/51/91/95	0/2/2/2
34	STE	B	620	-	-	7/14/14/17	-
26	CLA	B	601	37	-	13/39/115/115	-
26	CLA	c	507	37	-	9/39/115/115	-
32	SQD	f	101	-	-	18/36/56/69	0/1/1/1
26	CLA	h	101	37	-	16/39/115/115	-
34	STE	C	519	-	-	4/9/9/17	-
28	BCR	a	610	-	-	2/29/63/63	0/2/2/2
28	BCR	C	514	-	-	7/29/63/63	0/2/2/2
26	CLA	A	613	37	-	4/39/115/115	-
28	BCR	c	514	-	-	0/29/63/63	0/2/2/2
26	CLA	b	607	2	-	7/39/115/115	-
31	LHG	e	102	-	-	23/46/46/53	-
33	DGD	A	619	-	-	25/55/95/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	B	612	2	-	5/39/115/115	-
30	LMG	A	614	-	-	19/43/63/70	0/1/1/1
26	CLA	B	616	2	-	14/33/109/115	-
26	CLA	b	608	2	-	9/39/115/115	-
26	CLA	b	601	2	-	10/39/115/115	-
26	CLA	c	506	3	-	13/39/115/115	-
34	STE	M	103	-	-	2/7/7/17	-
34	STE	b	622	-	-	12/17/17/17	-
26	CLA	A	610	1	-	5/26/102/115	-
26	CLA	B	615	2	-	12/39/115/115	-
26	CLA	d	403	4	-	5/39/115/115	-
32	SQD	B	622	-	-	25/49/69/69	0/1/1/1
34	STE	b	623	-	-	6/7/7/17	-
28	BCR	b	616	-	-	6/29/63/63	0/2/2/2
36	HEC	V	201	16	1/1/3/7	5/14/54/54	-
26	CLA	b	602	2	-	9/39/115/115	-
26	CLA	A	607	1	-	4/39/115/115	-
30	LMG	C	518	-	-	18/43/63/70	0/1/1/1
26	CLA	c	512	3	-	16/39/115/115	-
28	BCR	D	404	-	-	7/29/63/63	0/2/2/2
26	CLA	C	501	3	-	5/39/115/115	-
34	STE	b	620	-	-	6/17/17/17	-
36	HEC	v	201	16	1/1/3/7	5/14/54/54	-
26	CLA	a	609	1	-	11/39/115/115	-
26	CLA	B	607	37	-	18/39/115/115	-
26	CLA	C	511	3	-	5/39/115/115	-
26	CLA	C	513	3	-	13/39/115/115	-
26	CLA	a	606	1	-	6/39/115/115	-
26	CLA	C	512	3	-	12/39/115/115	-
26	CLA	c	513	3	-	13/39/115/115	-
31	LHG	l	101	-	-	15/53/53/53	-
26	CLA	B	602	2	-	7/39/115/115	-
29	PL9	D	405	-	-	8/53/73/73	0/1/1/1
34	STE	a	615	-	-	7/9/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	B	614	2	-	8/39/115/115	-
30	LMG	D	406	-	-	18/46/66/70	0/1/1/1
33	DGD	H	101	-	-	18/51/91/95	0/2/2/2
28	BCR	d	405	-	-	4/29/63/63	0/2/2/2
26	CLA	C	509	3	-	10/39/115/115	-
31	LHG	L	101	-	-	21/53/53/53	-
33	DGD	C	517	-	-	15/51/91/95	0/2/2/2
34	STE	C	521	-	-	10/13/13/17	-
34	STE	X	102	-	-	11/17/17/17	-
26	CLA	D	402	4	-	7/39/115/115	-
31	LHG	d	409	-	-	9/43/43/53	-
26	CLA	D	403	4	-	8/39/115/115	-
28	BCR	X	101	-	-	5/29/63/63	0/2/2/2
28	BCR	b	617	-	-	1/29/63/63	0/2/2/2
26	CLA	c	501	3	-	6/39/115/115	-
27	PHO	D	401	-	-	4/37/103/103	0/5/6/6
31	LHG	A	615	-	-	24/51/51/53	-
26	CLA	b	610	2	-	5/39/115/115	-
29	PL9	a	611	-	-	21/53/73/73	0/1/1/1
27	PHO	A	609	-	-	4/37/103/103	0/5/6/6
34	STE	I	101	-	-	4/12/12/17	-
34	STE	j	101	-	-	5/9/9/17	-
34	STE	d	413	-	-	8/14/14/17	-
31	LHG	D	409	-	-	18/53/53/53	-
30	LMG	c	520	-	-	13/31/51/70	0/1/1/1
31	LHG	A	617	-	-	24/53/53/53	-
31	LHG	d	407	-	-	18/53/53/53	-

All (795) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	401	PHO	C1B-C2B	9.32	1.49	1.39
27	d	402	PHO	C1B-C2B	9.28	1.49	1.39
27	a	608	PHO	C1B-C2B	9.25	1.49	1.39
27	D	401	PHO	C3B-C4B	9.03	1.50	1.41
27	d	402	PHO	C3B-C4B	8.43	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	609	PHO	C1B-C2B	8.35	1.48	1.39
26	B	606	CLA	MG-NA	8.29	2.26	2.06
27	A	609	PHO	C3B-C4B	8.28	1.49	1.41
27	a	608	PHO	C3B-C4B	8.17	1.49	1.41
36	V	201	HEC	C3D-C2D	7.53	1.53	1.36
26	C	503	CLA	MG-NA	7.33	2.23	2.06
36	v	201	HEC	C3D-C2D	7.07	1.52	1.36
26	b	609	CLA	MG-NB	-6.93	1.92	2.05
26	b	607	CLA	MG-NA	6.47	2.21	2.06
26	C	510	CLA	MG-NA	6.38	2.21	2.06
26	b	602	CLA	MG-NA	6.18	2.21	2.06
26	b	604	CLA	MG-NA	6.17	2.20	2.06
26	B	615	CLA	MG-NA	6.16	2.20	2.06
26	c	511	CLA	MG-NA	6.14	2.20	2.06
26	B	611	CLA	MG-NA	6.06	2.20	2.06
35	e	101	HEM	FE-NA	6.03	2.15	1.95
26	B	603	CLA	MG-NA	5.90	2.20	2.06
26	c	508	CLA	MG-ND	5.77	2.17	2.05
26	C	509	CLA	MG-NA	5.56	2.19	2.06
32	A	618	SQD	O47-C45	-5.45	1.37	1.47
26	b	605	CLA	MG-NA	5.43	2.19	2.06
26	b	608	CLA	MG-NA	5.41	2.19	2.06
26	c	503	CLA	MG-NA	5.41	2.19	2.06
26	C	513	CLA	MG-NA	5.41	2.19	2.06
26	C	506	CLA	MG-NA	5.18	2.18	2.06
35	F	101	HEM	FE-NB	5.18	2.10	1.94
26	B	602	CLA	MG-NA	5.10	2.18	2.06
32	F	102	SQD	O48-C23	5.03	1.48	1.33
32	B	622	SQD	O48-C23	4.93	1.47	1.33
32	a	613	SQD	O48-C23	4.89	1.47	1.33
26	C	508	CLA	MG-NA	4.88	2.17	2.06
26	B	603	CLA	MG-NB	4.88	2.15	2.05
32	t	102	SQD	O48-C23	4.88	1.47	1.33
32	A	618	SQD	O48-C23	4.87	1.47	1.33
26	B	612	CLA	MG-NA	4.84	2.17	2.06
26	c	513	CLA	MG-ND	-4.79	1.96	2.05
26	c	502	CLA	MG-NA	4.76	2.17	2.06
26	C	512	CLA	MG-NA	4.72	2.17	2.06
26	b	614	CLA	MG-NB	4.70	2.15	2.05
26	c	507	CLA	MG-NA	4.70	2.17	2.06
32	f	101	SQD	O48-C23	4.69	1.47	1.33
26	B	601	CLA	MG-NA	4.69	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	502	CLA	MG-NA	4.69	2.17	2.06
26	B	609	CLA	MG-NA	4.68	2.17	2.06
27	D	401	PHO	C1D-C2D	4.67	1.44	1.39
32	b	619	SQD	O48-C23	4.64	1.46	1.33
26	c	510	CLA	MG-ND	-4.58	1.96	2.05
32	A	616	SQD	O48-C23	4.57	1.46	1.33
26	c	508	CLA	MG-NA	4.54	2.17	2.06
35	e	101	HEM	FE-NB	4.54	2.08	1.94
26	b	613	CLA	MG-NA	4.53	2.17	2.06
26	C	507	CLA	MG-NA	4.51	2.17	2.06
26	d	403	CLA	MG-NC	4.49	2.16	2.06
26	c	510	CLA	MG-NA	4.47	2.16	2.06
27	d	402	PHO	C1D-C2D	4.46	1.44	1.39
26	c	501	CLA	MG-NA	4.46	2.16	2.06
26	B	614	CLA	MG-NC	4.46	2.16	2.06
26	a	606	CLA	MG-NB	4.45	2.14	2.05
26	c	506	CLA	MG-ND	-4.44	1.97	2.05
26	A	607	CLA	MG-NB	4.44	2.14	2.05
26	b	612	CLA	MG-NA	4.43	2.16	2.06
26	B	610	CLA	MG-NA	4.43	2.16	2.06
36	V	201	HEC	FE-ND	4.42	2.08	1.94
26	B	613	CLA	MG-NA	4.41	2.16	2.06
26	D	402	CLA	MG-NA	4.39	2.16	2.06
26	b	613	CLA	C1D-ND	4.39	1.43	1.37
26	A	607	CLA	MG-NA	4.37	2.16	2.06
26	a	612	CLA	MG-NA	4.32	2.16	2.06
26	b	610	CLA	MG-NA	4.31	2.16	2.06
26	A	613	CLA	C1D-ND	4.28	1.43	1.37
36	v	201	HEC	FE-ND	4.27	2.08	1.94
26	b	614	CLA	MG-NA	4.27	2.16	2.06
26	C	504	CLA	MG-NA	4.25	2.16	2.06
26	a	606	CLA	MG-NA	4.25	2.16	2.06
26	b	605	CLA	MG-ND	4.24	2.14	2.05
26	c	504	CLA	MG-NB	-4.24	1.97	2.05
26	C	503	CLA	MG-NB	4.22	2.14	2.05
26	B	605	CLA	MG-NA	4.12	2.16	2.06
26	b	601	CLA	C1D-ND	4.11	1.43	1.37
26	B	616	CLA	C1D-ND	4.09	1.43	1.37
26	B	613	CLA	MG-NB	4.06	2.13	2.05
28	C	514	BCR	C1-C6	-4.05	1.48	1.53
26	A	613	CLA	MG-NA	4.05	2.15	2.06
35	F	101	HEM	FE-NC	4.04	2.08	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	h	101	CLA	MG-NA	4.03	2.15	2.06
26	d	403	CLA	C1D-ND	4.01	1.43	1.37
32	b	619	SQD	O47-C7	3.98	1.45	1.34
31	D	409	LHG	O7-C5	-3.97	1.37	1.46
26	c	506	CLA	MG-NA	3.97	2.15	2.06
26	A	608	CLA	MG-NA	3.97	2.15	2.06
36	V	201	HEC	FE-NC	3.97	2.08	1.95
26	A	613	CLA	MG-NC	3.93	2.15	2.06
26	c	510	CLA	MG-NB	3.89	2.13	2.05
28	c	515	BCR	C1-C6	-3.89	1.48	1.53
26	c	508	CLA	C1D-ND	3.87	1.42	1.37
29	D	405	PL9	C6-C1	-3.87	1.42	1.48
26	C	502	CLA	C1D-ND	3.86	1.42	1.37
26	b	611	CLA	C1D-ND	3.86	1.42	1.37
36	V	201	HEC	FE-NB	3.85	2.06	1.94
36	v	201	HEC	FE-NA	3.85	2.07	1.95
32	B	622	SQD	O47-C7	3.83	1.45	1.34
26	B	604	CLA	MG-NA	3.79	2.15	2.06
26	A	610	CLA	C1D-ND	3.78	1.42	1.37
26	c	513	CLA	C1D-ND	3.76	1.42	1.37
26	B	608	CLA	MG-NA	3.76	2.15	2.06
26	C	505	CLA	MG-NA	3.76	2.15	2.06
32	t	102	SQD	O47-C7	3.73	1.44	1.34
26	b	608	CLA	MG-NB	-3.72	1.98	2.05
26	D	403	CLA	C1D-ND	3.71	1.42	1.37
26	A	608	CLA	C1D-ND	3.70	1.42	1.37
26	b	609	CLA	MG-ND	3.70	2.13	2.05
28	b	616	BCR	C1-C6	-3.70	1.49	1.53
26	c	503	CLA	C1D-ND	3.68	1.42	1.37
26	B	614	CLA	C1D-ND	3.66	1.42	1.37
26	c	511	CLA	C1D-ND	3.64	1.42	1.37
30	c	523	LMG	C3-C2	3.64	1.61	1.52
26	B	601	CLA	C4B-NB	3.64	1.42	1.37
32	A	616	SQD	O47-C45	-3.64	1.38	1.46
27	A	609	PHO	C4D-CHA	3.62	1.45	1.39
26	c	504	CLA	C4B-NB	3.62	1.42	1.37
26	c	505	CLA	MG-NA	3.61	2.14	2.06
26	B	610	CLA	C4B-NB	3.61	1.42	1.37
26	b	604	CLA	C4B-NB	3.61	1.42	1.37
26	C	513	CLA	C1D-ND	3.60	1.42	1.37
26	c	509	CLA	MG-NA	3.60	2.14	2.06
26	c	510	CLA	C1D-ND	3.57	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	605	CLA	C1D-ND	3.57	1.42	1.37
32	a	613	SQD	O47-C45	-3.56	1.38	1.46
26	B	606	CLA	C1D-ND	3.55	1.42	1.37
26	D	402	CLA	C1D-ND	3.54	1.42	1.37
26	C	511	CLA	C1D-ND	3.52	1.42	1.37
32	t	102	SQD	C24-C23	3.52	1.60	1.50
28	c	514	BCR	C1-C6	-3.52	1.49	1.53
26	a	609	CLA	C1D-ND	3.51	1.42	1.37
32	f	101	SQD	O47-C7	3.51	1.44	1.34
26	B	604	CLA	C1D-ND	3.51	1.42	1.37
26	h	101	CLA	C1D-ND	3.51	1.42	1.37
26	c	502	CLA	C1D-ND	3.51	1.42	1.37
26	B	601	CLA	C1D-ND	3.50	1.42	1.37
26	b	603	CLA	MG-NA	3.49	2.14	2.06
26	c	508	CLA	MG-NC	3.48	2.14	2.06
26	a	606	CLA	C1D-ND	3.48	1.42	1.37
32	b	619	SQD	O5-C1	3.47	1.50	1.41
26	A	607	CLA	MG-ND	-3.47	1.98	2.05
33	H	101	DGD	O5D-C1E	3.47	1.46	1.40
26	h	101	CLA	C4B-NB	3.47	1.42	1.37
26	B	613	CLA	C1D-ND	3.46	1.42	1.37
28	K	101	BCR	C1-C6	-3.46	1.49	1.53
32	a	613	SQD	O47-C7	3.46	1.44	1.34
26	C	507	CLA	C4B-NB	3.46	1.42	1.37
26	B	616	CLA	MG-NB	3.46	2.12	2.05
26	b	603	CLA	C1D-ND	3.45	1.42	1.37
28	Z	101	BCR	C1-C6	-3.44	1.49	1.53
28	c	516	BCR	C1-C6	-3.44	1.49	1.53
26	C	512	CLA	C1D-ND	3.43	1.42	1.37
27	a	608	PHO	C1D-C2D	3.42	1.43	1.39
26	C	501	CLA	C1D-ND	3.42	1.42	1.37
26	C	507	CLA	C1D-ND	3.42	1.42	1.37
26	B	609	CLA	C1D-ND	3.41	1.42	1.37
32	A	618	SQD	O47-C7	3.41	1.43	1.34
26	B	611	CLA	C1D-ND	3.40	1.42	1.37
26	A	607	CLA	C1D-ND	3.39	1.42	1.37
27	A	609	PHO	C1D-C2D	3.39	1.43	1.39
26	b	604	CLA	C1B-C2B	3.39	1.51	1.43
27	d	402	PHO	C4D-CHA	3.37	1.44	1.39
26	C	509	CLA	C1D-ND	3.37	1.42	1.37
26	C	504	CLA	C4B-NB	3.37	1.42	1.37
26	C	510	CLA	C1D-ND	3.36	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	602	CLA	C1D-ND	3.35	1.42	1.37
26	b	614	CLA	C1D-ND	3.35	1.42	1.37
26	C	502	CLA	C1B-C2B	3.35	1.51	1.43
26	C	505	CLA	C1D-ND	3.35	1.42	1.37
26	A	613	CLA	C1B-C2B	3.35	1.51	1.43
26	b	607	CLA	C1D-ND	3.33	1.42	1.37
26	c	506	CLA	C1D-ND	3.32	1.42	1.37
32	f	101	SQD	O47-C45	-3.32	1.38	1.46
26	B	602	CLA	C4B-NB	3.31	1.42	1.37
26	C	504	CLA	C1D-ND	3.31	1.42	1.37
26	b	611	CLA	C4B-NB	3.30	1.42	1.37
26	A	610	CLA	C4B-NB	3.30	1.42	1.37
28	k	101	BCR	C1-C6	-3.29	1.49	1.53
26	B	610	CLA	C1D-ND	3.29	1.42	1.37
26	a	606	CLA	MG-ND	-3.28	1.99	2.05
32	A	618	SQD	C24-C23	3.28	1.60	1.50
26	c	513	CLA	MG-NA	3.28	2.14	2.06
26	a	612	CLA	C1D-ND	3.28	1.42	1.37
32	F	102	SQD	C24-C23	3.27	1.60	1.50
26	b	612	CLA	C1D-ND	3.27	1.42	1.37
26	b	602	CLA	MG-NB	-3.27	1.99	2.05
26	B	603	CLA	C1D-ND	3.26	1.42	1.37
27	a	608	PHO	C4D-CHA	3.26	1.44	1.39
28	K	102	BCR	C1-C6	-3.26	1.49	1.53
28	T	101	BCR	C30-C25	-3.23	1.49	1.53
26	C	508	CLA	C1B-C2B	3.22	1.50	1.43
28	B	618	BCR	C30-C25	-3.22	1.49	1.53
26	c	509	CLA	C1D-ND	3.21	1.42	1.37
28	b	617	BCR	C30-C25	-3.21	1.49	1.53
26	C	511	CLA	MG-NC	3.21	2.13	2.06
26	a	607	CLA	C1D-ND	3.20	1.42	1.37
28	c	516	BCR	C30-C25	-3.20	1.49	1.53
26	D	402	CLA	MG-NC	3.20	2.13	2.06
26	c	507	CLA	C4B-NB	3.18	1.42	1.37
26	c	508	CLA	C4B-NB	3.18	1.42	1.37
26	b	602	CLA	C1D-ND	3.18	1.42	1.37
27	A	609	PHO	C3D-C4D	3.18	1.45	1.41
26	b	610	CLA	C1B-C2B	3.18	1.50	1.43
28	T	101	BCR	C1-C6	-3.18	1.49	1.53
26	B	607	CLA	C1D-ND	3.18	1.42	1.37
26	a	607	CLA	MG-NA	3.16	2.13	2.06
26	b	614	CLA	MG-ND	-3.16	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	621	LMG	C4-C3	3.16	1.60	1.52
31	A	615	LHG	P-O6	3.15	1.71	1.59
26	b	602	CLA	C1B-C2B	3.15	1.50	1.43
26	b	602	CLA	C4B-NB	3.14	1.42	1.37
26	c	501	CLA	C1B-C2B	3.14	1.50	1.43
26	c	509	CLA	C1B-C2B	3.14	1.50	1.43
26	C	511	CLA	C1B-C2B	3.14	1.50	1.43
26	b	610	CLA	C1D-ND	3.14	1.42	1.37
33	C	516	DGD	O2G-C2G	-3.13	1.39	1.46
26	b	609	CLA	C1D-ND	3.12	1.42	1.37
26	B	614	CLA	C4B-NB	3.12	1.42	1.37
32	t	102	SQD	O47-C45	-3.11	1.39	1.46
32	A	616	SQD	C24-C23	3.11	1.59	1.50
28	A	611	BCR	C1-C6	-3.11	1.49	1.53
26	B	608	CLA	C1D-ND	3.11	1.41	1.37
33	c	517	DGD	O2G-C2G	-3.11	1.39	1.46
26	c	501	CLA	C1D-ND	3.11	1.41	1.37
26	a	609	CLA	C4B-NB	3.11	1.41	1.37
28	Z	101	BCR	C30-C25	-3.10	1.49	1.53
26	D	403	CLA	MG-NB	-3.10	1.99	2.05
26	a	612	CLA	C1B-C2B	3.09	1.50	1.43
26	B	611	CLA	C1B-C2B	3.09	1.50	1.43
32	a	613	SQD	C24-C23	3.09	1.59	1.50
26	B	609	CLA	C4B-NB	3.09	1.41	1.37
26	b	603	CLA	C1B-C2B	3.08	1.50	1.43
26	c	507	CLA	CHC-C1C	3.08	1.44	1.38
35	F	101	HEM	CAB-C3B	3.08	1.55	1.47
32	A	616	SQD	O47-C7	3.08	1.43	1.34
26	B	616	CLA	MG-NC	3.08	2.13	2.06
26	b	613	CLA	C4B-NB	3.07	1.41	1.37
26	h	101	CLA	C1B-C2B	3.07	1.50	1.43
26	c	512	CLA	C1D-ND	3.07	1.41	1.37
32	b	619	SQD	C24-C23	3.07	1.59	1.50
26	c	511	CLA	C1B-C2B	3.07	1.50	1.43
26	b	608	CLA	C1D-ND	3.07	1.41	1.37
26	B	615	CLA	MG-NB	3.07	2.11	2.05
26	b	604	CLA	C1D-ND	3.07	1.41	1.37
32	B	622	SQD	C24-C23	3.06	1.59	1.50
33	C	517	DGD	C6D-C5D	3.06	1.60	1.51
26	b	615	CLA	C1B-C2B	3.06	1.50	1.43
26	B	601	CLA	C1B-C2B	3.06	1.50	1.43
33	A	619	DGD	C4D-C5D	3.06	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	407	LHG	O7-C5	-3.05	1.39	1.46
26	c	507	CLA	C1D-ND	3.05	1.41	1.37
28	K	102	BCR	C30-C25	-3.05	1.49	1.53
26	c	508	CLA	C1B-C2B	3.05	1.50	1.43
26	A	607	CLA	C1B-C2B	3.05	1.50	1.43
32	B	622	SQD	O47-C45	-3.04	1.39	1.46
32	f	101	SQD	C24-C23	3.04	1.59	1.50
26	C	506	CLA	C1D-ND	3.04	1.41	1.37
26	C	502	CLA	C4B-NB	3.04	1.41	1.37
32	B	622	SQD	O5-C1	3.03	1.49	1.41
28	d	405	BCR	C30-C25	-3.03	1.49	1.53
26	C	503	CLA	C1D-ND	3.03	1.41	1.37
26	C	503	CLA	C1B-C2B	3.03	1.50	1.43
29	d	406	PL9	C6-C1	-3.03	1.43	1.48
26	B	605	CLA	C1B-C2B	3.02	1.50	1.43
28	D	404	BCR	C30-C25	-3.01	1.49	1.53
26	D	402	CLA	C1B-C2B	3.01	1.50	1.43
26	B	608	CLA	C4B-NB	3.01	1.41	1.37
26	C	501	CLA	CHC-C1C	3.01	1.44	1.38
31	A	617	LHG	P-O6	3.00	1.71	1.59
26	B	615	CLA	C1D-ND	3.00	1.41	1.37
32	a	613	SQD	O5-C1	3.00	1.49	1.41
26	c	510	CLA	C1B-C2B	2.99	1.50	1.43
35	e	101	HEM	CAC-C3C	2.99	1.55	1.47
26	B	614	CLA	MG-NA	2.98	2.13	2.06
26	C	501	CLA	MG-NA	2.98	2.13	2.06
26	B	612	CLA	C1B-C2B	2.97	1.50	1.43
28	K	101	BCR	C30-C25	-2.97	1.50	1.53
26	a	606	CLA	C1B-C2B	2.97	1.50	1.43
26	c	513	CLA	C4B-NB	2.97	1.41	1.37
26	b	615	CLA	C1D-ND	2.96	1.41	1.37
26	B	603	CLA	C1B-C2B	2.96	1.50	1.43
28	X	101	BCR	C30-C25	-2.96	1.50	1.53
26	d	404	CLA	C4B-NB	2.95	1.41	1.37
26	c	512	CLA	C4B-NB	2.95	1.41	1.37
33	H	101	DGD	C1E-C2E	2.95	1.61	1.52
26	A	608	CLA	C4B-NB	2.95	1.41	1.37
26	C	506	CLA	C4B-NB	2.95	1.41	1.37
26	c	512	CLA	C1B-C2B	2.95	1.50	1.43
26	c	508	CLA	CHC-C1C	2.95	1.44	1.38
26	C	507	CLA	C1B-C2B	2.94	1.50	1.43
26	c	504	CLA	C1D-ND	2.94	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	612	PL9	C3-C4	-2.94	1.45	1.49
26	b	601	CLA	C4B-NB	2.94	1.41	1.37
26	C	513	CLA	C1B-C2B	2.93	1.50	1.43
26	B	609	CLA	C1B-C2B	2.93	1.50	1.43
26	b	605	CLA	C1D-ND	2.92	1.41	1.37
26	c	504	CLA	C1B-C2B	2.92	1.50	1.43
26	A	610	CLA	C1B-C2B	2.92	1.50	1.43
28	D	404	BCR	C1-C6	-2.92	1.50	1.53
26	b	603	CLA	C4B-NB	2.92	1.41	1.37
26	B	602	CLA	C1B-C2B	2.91	1.50	1.43
26	C	510	CLA	C1B-C2B	2.90	1.49	1.43
26	c	511	CLA	C4B-NB	2.90	1.41	1.37
26	C	510	CLA	C4B-NB	2.90	1.41	1.37
26	b	607	CLA	C4B-NB	2.90	1.41	1.37
35	F	101	HEM	CAC-C3C	2.89	1.55	1.47
26	c	509	CLA	C4B-NB	2.89	1.41	1.37
33	a	614	DGD	O2G-C1B	2.89	1.42	1.34
26	b	604	CLA	MG-NB	2.89	2.11	2.05
26	b	605	CLA	C1B-C2B	2.88	1.49	1.43
26	b	603	CLA	MG-NC	2.88	2.13	2.06
26	b	608	CLA	C4B-NB	2.88	1.41	1.37
26	a	607	CLA	C4B-NB	2.87	1.41	1.37
26	C	513	CLA	C4B-NB	2.87	1.41	1.37
26	B	610	CLA	C1B-C2B	2.86	1.49	1.43
32	F	102	SQD	O5-C1	2.86	1.49	1.41
36	v	201	HEC	FE-NC	2.85	2.04	1.95
26	b	612	CLA	C4B-NB	2.85	1.41	1.37
26	a	606	CLA	CHC-C1C	2.85	1.44	1.38
32	f	101	SQD	O5-C1	2.85	1.49	1.41
26	B	607	CLA	C1B-C2B	2.85	1.49	1.43
33	a	614	DGD	O1G-C1A	2.85	1.41	1.33
27	a	608	PHO	CMC-C2C	-2.85	1.46	1.50
33	H	101	DGD	C4D-C5D	2.85	1.59	1.53
26	b	608	CLA	MG-ND	2.84	2.11	2.05
26	b	605	CLA	CHC-C1C	2.84	1.44	1.38
30	c	522	LMG	C3-C2	2.84	1.59	1.52
28	c	514	BCR	C30-C25	-2.84	1.50	1.53
26	b	601	CLA	C1B-C2B	2.84	1.49	1.43
27	D	401	PHO	CMB-C2B	-2.84	1.45	1.51
27	D	401	PHO	C4D-CHA	2.84	1.43	1.39
26	D	403	CLA	C1B-C2B	2.84	1.49	1.43
26	d	404	CLA	C1B-C2B	2.83	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	504	CLA	MG-NB	2.83	2.11	2.05
26	D	403	CLA	MG-NA	2.83	2.13	2.06
26	D	402	CLA	C4B-NB	2.83	1.41	1.37
26	c	506	CLA	C4B-NB	2.83	1.41	1.37
28	B	617	BCR	C1-C6	-2.83	1.50	1.53
28	c	515	BCR	C30-C25	-2.82	1.50	1.53
26	a	609	CLA	MG-NB	-2.82	2.00	2.05
26	C	508	CLA	C4B-NB	2.82	1.41	1.37
31	d	409	LHG	P-O6	2.82	1.70	1.59
26	b	612	CLA	C1B-C2B	2.80	1.49	1.43
29	d	406	PL9	C53-C6	-2.80	1.45	1.50
26	B	601	CLA	CHC-C1C	2.80	1.44	1.38
33	c	519	DGD	C6D-C5D	2.80	1.60	1.51
26	C	504	CLA	C3B-C4B	2.79	1.50	1.42
32	A	616	SQD	O5-C1	2.79	1.49	1.41
28	B	619	BCR	C1-C6	-2.79	1.50	1.53
26	B	616	CLA	MG-NA	2.78	2.12	2.06
26	B	601	CLA	C3B-C4B	2.78	1.50	1.42
26	c	502	CLA	C4B-NB	2.77	1.41	1.37
26	c	505	CLA	C1D-ND	2.77	1.41	1.37
26	a	607	CLA	CHC-C1C	2.77	1.44	1.38
26	B	616	CLA	C1B-C2B	2.77	1.49	1.43
26	b	606	CLA	CHC-C1C	2.77	1.44	1.38
26	C	504	CLA	CHC-C1C	2.77	1.44	1.38
26	c	512	CLA	CHC-C1C	2.76	1.44	1.38
26	B	616	CLA	C4B-NB	2.76	1.41	1.37
26	B	606	CLA	C1B-C2B	2.76	1.49	1.43
26	b	615	CLA	MG-NA	2.76	2.12	2.06
28	h	102	BCR	C30-C25	-2.76	1.50	1.53
30	A	614	LMG	C4-C5	2.75	1.58	1.53
26	C	505	CLA	C1B-C2B	2.75	1.49	1.43
26	B	615	CLA	C4B-NB	2.75	1.41	1.37
26	c	513	CLA	C1B-C2B	2.75	1.49	1.43
35	F	101	HEM	FE-NA	2.75	2.04	1.95
28	t	101	BCR	C30-C25	-2.74	1.50	1.53
26	c	507	CLA	C1B-C2B	2.74	1.49	1.43
32	b	619	SQD	O47-C45	-2.74	1.40	1.46
26	b	614	CLA	C4B-NB	2.74	1.41	1.37
27	a	608	PHO	C3D-C4D	2.74	1.45	1.41
31	d	407	LHG	O7-C5	-2.74	1.40	1.46
26	c	502	CLA	C1B-C2B	2.73	1.49	1.43
26	b	608	CLA	C1B-C2B	2.73	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	607	CLA	MG-ND	-2.73	2.00	2.05
26	c	503	CLA	C1B-C2B	2.73	1.49	1.43
26	C	510	CLA	CHC-C1C	2.73	1.43	1.38
26	b	613	CLA	CHC-C1C	2.73	1.43	1.38
26	b	613	CLA	C3B-C4B	2.72	1.50	1.42
26	c	505	CLA	CHC-C1C	2.72	1.43	1.38
26	B	606	CLA	C4B-NB	2.72	1.41	1.37
33	a	614	DGD	C1G-C2G	2.72	1.59	1.50
26	c	505	CLA	C3B-C4B	2.71	1.50	1.42
26	c	503	CLA	MG-NC	2.71	2.12	2.06
26	b	615	CLA	C4B-NB	2.71	1.41	1.37
28	a	610	BCR	C1-C6	-2.71	1.50	1.53
26	b	607	CLA	CHC-C1C	2.70	1.43	1.38
33	H	101	DGD	C6D-C5D	2.70	1.59	1.51
26	B	602	CLA	CHC-C1C	2.70	1.43	1.38
26	c	505	CLA	C4B-NB	2.70	1.41	1.37
26	B	610	CLA	C3B-C4B	2.70	1.50	1.42
26	B	603	CLA	C3B-C4B	2.70	1.50	1.42
26	c	508	CLA	C3B-C4B	2.69	1.50	1.42
26	C	501	CLA	C4B-NB	2.69	1.41	1.37
26	c	503	CLA	C4B-NB	2.69	1.41	1.37
26	d	403	CLA	MG-ND	-2.69	2.00	2.05
26	C	502	CLA	MG-ND	-2.69	2.00	2.05
33	A	619	DGD	O2G-C2G	-2.69	1.40	1.46
26	b	614	CLA	C3B-C4B	2.68	1.50	1.42
26	C	511	CLA	MG-NA	2.68	2.12	2.06
26	C	509	CLA	CHC-C1C	2.68	1.43	1.38
33	C	515	DGD	C4E-C3E	2.68	1.59	1.52
26	A	613	CLA	MG-ND	-2.68	2.00	2.05
26	C	506	CLA	CHC-C1C	2.68	1.43	1.38
26	C	505	CLA	C4B-NB	2.68	1.41	1.37
26	C	503	CLA	C4B-NB	2.68	1.41	1.37
26	a	607	CLA	C3B-C4B	2.67	1.50	1.42
26	B	615	CLA	CHC-C1C	2.66	1.43	1.38
26	b	611	CLA	C1B-C2B	2.66	1.49	1.43
26	c	512	CLA	C3B-C4B	2.66	1.50	1.42
26	B	615	CLA	C1B-C2B	2.66	1.49	1.43
26	b	610	CLA	C4B-NB	2.66	1.41	1.37
27	d	402	PHO	CMC-C2C	-2.65	1.46	1.50
26	A	613	CLA	C4B-NB	2.65	1.41	1.37
26	B	605	CLA	CHC-C1C	2.65	1.43	1.38
28	k	101	BCR	C30-C25	-2.65	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	606	CLA	C4B-NB	2.65	1.41	1.37
26	h	101	CLA	CHC-C1C	2.64	1.43	1.38
26	B	604	CLA	C1B-C2B	2.64	1.49	1.43
26	c	510	CLA	C4B-NB	2.64	1.41	1.37
28	d	405	BCR	C1-C6	-2.63	1.50	1.53
33	C	515	DGD	O2G-C2G	-2.63	1.40	1.46
26	B	612	CLA	C1D-ND	2.62	1.41	1.37
26	C	504	CLA	C1B-C2B	2.62	1.49	1.43
26	C	501	CLA	C3B-C4B	2.62	1.50	1.42
28	b	618	BCR	C1-C6	-2.62	1.50	1.53
26	C	503	CLA	C3B-C4B	2.62	1.50	1.42
26	b	614	CLA	C1B-C2B	2.62	1.49	1.43
26	A	608	CLA	C1B-C2B	2.61	1.49	1.43
26	B	604	CLA	MG-ND	2.61	2.11	2.05
26	C	507	CLA	CHC-C1C	2.61	1.43	1.38
33	C	516	DGD	C1G-C2G	2.61	1.59	1.50
26	C	509	CLA	C1B-C2B	2.60	1.49	1.43
30	b	621	LMG	C4-C5	2.60	1.58	1.53
26	c	513	CLA	C3B-C4B	2.60	1.50	1.42
26	B	608	CLA	C1B-C2B	2.60	1.49	1.43
26	C	502	CLA	C3B-C4B	2.60	1.50	1.42
26	b	613	CLA	C1B-C2B	2.60	1.49	1.43
26	c	513	CLA	CHC-C1C	2.60	1.43	1.38
26	c	507	CLA	C3B-C4B	2.59	1.50	1.42
30	b	621	LMG	C9-C8	2.59	1.58	1.50
30	d	411	LMG	C4-C5	2.58	1.58	1.53
26	B	610	CLA	CHC-C1C	2.58	1.43	1.38
26	b	611	CLA	C3B-C4B	2.58	1.50	1.42
26	c	505	CLA	C1B-C2B	2.58	1.49	1.43
31	L	101	LHG	O7-C5	-2.58	1.40	1.46
27	D	401	PHO	CMD-C2D	-2.57	1.46	1.51
26	b	604	CLA	C3B-C4B	2.57	1.50	1.42
26	C	509	CLA	C3B-C4B	2.57	1.50	1.42
26	C	508	CLA	MG-NC	2.57	2.12	2.06
26	a	609	CLA	C1B-C2B	2.56	1.49	1.43
30	c	523	LMG	C1-C2	2.55	1.60	1.52
26	c	504	CLA	CHC-C1C	2.55	1.43	1.38
32	b	619	SQD	O9-S	2.55	1.52	1.45
30	C	518	LMG	O7-C8	-2.55	1.40	1.46
26	C	508	CLA	C1D-ND	2.55	1.41	1.37
26	a	606	CLA	MG-NC	2.55	2.12	2.06
26	B	613	CLA	MG-ND	-2.54	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	511	CLA	CHC-C1C	2.54	1.43	1.38
26	b	604	CLA	CHC-C1C	2.53	1.43	1.38
26	C	511	CLA	C4B-NB	2.53	1.41	1.37
26	B	613	CLA	C1B-C2B	2.53	1.49	1.43
26	b	611	CLA	CHC-C1C	2.53	1.43	1.38
33	h	103	DGD	C4D-C3D	2.52	1.58	1.52
26	C	509	CLA	MG-NC	-2.52	2.00	2.06
26	b	602	CLA	CMD-C2D	-2.52	1.45	1.50
26	b	607	CLA	C1B-C2B	2.52	1.49	1.43
26	C	509	CLA	C4B-NB	2.51	1.41	1.37
26	c	501	CLA	C4B-NB	2.51	1.41	1.37
26	B	614	CLA	C1B-C2B	2.51	1.49	1.43
26	C	512	CLA	C1B-C2B	2.51	1.49	1.43
26	a	607	CLA	C1B-C2B	2.51	1.49	1.43
27	a	608	PHO	CMB-C2B	-2.51	1.46	1.51
27	a	608	PHO	C4D-ND	-2.50	1.34	1.38
35	e	101	HEM	CAB-C3B	2.50	1.54	1.47
26	b	606	CLA	C1D-ND	2.50	1.41	1.37
26	B	616	CLA	CHC-C1C	2.50	1.43	1.38
26	A	608	CLA	CHC-C1C	2.50	1.43	1.38
27	A	609	PHO	CMC-C2C	-2.50	1.46	1.50
27	A	609	PHO	C4D-ND	-2.50	1.34	1.38
26	C	503	CLA	CHC-C1C	2.49	1.43	1.38
26	C	506	CLA	C1B-C2B	2.49	1.49	1.43
26	C	510	CLA	C3B-C4B	2.49	1.50	1.42
26	C	506	CLA	C3B-C4B	2.49	1.50	1.42
32	f	101	SQD	O7-S	2.49	1.52	1.45
26	h	101	CLA	C3B-C4B	2.48	1.50	1.42
26	b	606	CLA	C3B-C4B	2.48	1.50	1.42
30	A	614	LMG	C7-C8	2.48	1.58	1.50
26	a	612	CLA	C4B-NB	2.48	1.41	1.37
27	D	401	PHO	C4D-ND	-2.47	1.34	1.38
26	b	609	CLA	C1B-C2B	2.47	1.48	1.43
26	B	607	CLA	C4B-NB	2.46	1.41	1.37
26	B	616	CLA	CMC-C2C	-2.46	1.45	1.50
26	B	614	CLA	CHC-C1C	2.45	1.43	1.38
26	D	403	CLA	MG-ND	-2.45	2.00	2.05
26	B	608	CLA	CHC-C1C	2.44	1.43	1.38
26	C	505	CLA	CHC-C1C	2.44	1.43	1.38
26	d	404	CLA	CHC-C1C	2.44	1.43	1.38
31	e	102	LHG	P-O6	2.44	1.69	1.59
26	b	606	CLA	C1B-C2B	2.44	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	401	PHO	C3D-C4D	2.43	1.44	1.41
26	a	607	CLA	MG-NB	2.42	2.10	2.05
26	C	512	CLA	C3B-C4B	2.42	1.49	1.42
26	b	614	CLA	CHC-C1C	2.42	1.43	1.38
33	A	619	DGD	C4D-C3D	2.42	1.58	1.52
26	b	605	CLA	C3B-C4B	2.42	1.49	1.42
26	b	607	CLA	C3B-C4B	2.42	1.49	1.42
26	C	511	CLA	C3B-C4B	2.42	1.49	1.42
30	D	408	LMG	C9-C8	2.42	1.58	1.50
26	d	403	CLA	C1B-C2B	2.41	1.48	1.43
26	d	404	CLA	C1D-ND	2.41	1.41	1.37
26	D	403	CLA	MG-NC	2.41	2.12	2.06
28	C	514	BCR	C30-C25	-2.41	1.50	1.53
26	a	606	CLA	C4B-NB	2.40	1.41	1.37
30	c	523	LMG	C4-C3	2.40	1.58	1.52
26	A	607	CLA	C4B-NB	2.40	1.41	1.37
26	C	512	CLA	C4B-NB	2.40	1.41	1.37
29	d	406	PL9	C31-C29	-2.40	1.46	1.51
26	B	604	CLA	CHC-C1C	2.40	1.43	1.38
31	D	409	LHG	C24-C23	2.40	1.57	1.50
26	A	607	CLA	C3B-C4B	2.39	1.49	1.42
33	c	519	DGD	O2G-C2G	-2.39	1.41	1.46
33	A	619	DGD	C1E-C2E	2.39	1.59	1.52
26	B	615	CLA	C3B-C4B	2.39	1.49	1.42
26	B	605	CLA	C4B-NB	2.39	1.41	1.37
26	B	611	CLA	C4B-NB	2.39	1.41	1.37
26	c	512	CLA	MG-NC	2.39	2.11	2.06
36	V	201	HEC	CMB-C2B	2.38	1.55	1.50
26	B	612	CLA	C3B-C4B	2.38	1.49	1.42
33	A	619	DGD	C3G-C2G	2.38	1.58	1.50
26	c	501	CLA	MG-NB	-2.38	2.01	2.05
26	B	601	CLA	MG-NC	2.38	2.11	2.06
26	C	508	CLA	C3B-C4B	2.37	1.49	1.42
26	B	607	CLA	MG-ND	-2.37	2.01	2.05
26	a	609	CLA	C3B-C4B	2.37	1.49	1.42
26	c	502	CLA	MG-NB	-2.37	2.01	2.05
32	A	618	SQD	C46-C45	2.37	1.55	1.50
26	c	510	CLA	C3B-C4B	2.36	1.49	1.42
30	b	621	LMG	C3-C2	2.36	1.58	1.52
26	b	609	CLA	C4B-NB	2.36	1.41	1.37
26	c	503	CLA	MG-NB	2.35	2.10	2.05
26	B	611	CLA	CHC-C1C	2.35	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	511	CLA	MG-NC	2.35	2.11	2.06
26	b	609	CLA	C3B-C4B	2.35	1.49	1.42
32	f	101	SQD	O9-S	2.35	1.51	1.45
26	c	506	CLA	CHC-C1C	2.35	1.43	1.38
28	X	101	BCR	C1-C6	-2.34	1.50	1.53
26	C	505	CLA	C3B-C4B	2.34	1.49	1.42
27	a	608	PHO	CMD-C2D	-2.34	1.46	1.51
28	b	618	BCR	C30-C25	-2.34	1.50	1.53
27	A	609	PHO	CMD-C2D	-2.34	1.46	1.51
26	C	501	CLA	CMC-C2C	-2.34	1.46	1.50
33	C	515	DGD	O1G-C1A	2.34	1.40	1.33
26	B	604	CLA	C3B-C4B	2.34	1.49	1.42
26	B	616	CLA	C3B-C4B	2.34	1.49	1.42
32	b	619	SQD	O5-C5	2.33	1.50	1.44
26	c	503	CLA	CHC-C1C	2.33	1.43	1.38
35	e	101	HEM	C3B-C2B	-2.33	1.32	1.37
26	d	404	CLA	C3B-C4B	2.33	1.49	1.42
26	b	601	CLA	MG-NA	2.33	2.11	2.06
26	C	512	CLA	CHC-C1C	2.33	1.43	1.38
28	a	610	BCR	C30-C25	-2.32	1.50	1.53
26	B	605	CLA	C3B-C4B	2.32	1.49	1.42
26	d	404	CLA	C1D-C2D	2.32	1.49	1.45
26	C	507	CLA	C3B-C4B	2.32	1.49	1.42
26	C	513	CLA	C3B-C4B	2.32	1.49	1.42
26	c	501	CLA	CHC-C1C	2.32	1.43	1.38
26	d	403	CLA	CMD-C2D	-2.31	1.46	1.50
26	b	612	CLA	C3B-C4B	2.30	1.49	1.42
35	e	101	HEM	FE-ND	2.30	2.02	1.94
26	c	510	CLA	CMB-C2B	-2.30	1.46	1.50
32	A	616	SQD	O9-S	2.30	1.51	1.45
26	c	506	CLA	C1B-C2B	2.30	1.48	1.43
26	D	402	CLA	C3B-C4B	2.30	1.49	1.42
26	D	403	CLA	C4B-NB	2.30	1.40	1.37
26	c	504	CLA	C3B-C4B	2.29	1.49	1.42
26	B	603	CLA	C4B-NB	2.29	1.40	1.37
32	b	619	SQD	O7-S	2.29	1.51	1.45
26	b	611	CLA	CMC-C2C	-2.29	1.46	1.50
32	t	102	SQD	C44-C45	2.29	1.56	1.51
26	C	509	CLA	CMD-C2D	-2.29	1.46	1.50
26	B	613	CLA	C4B-NB	2.29	1.40	1.37
26	c	510	CLA	CMD-C2D	-2.29	1.46	1.50
26	b	610	CLA	C3B-C4B	2.28	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	517	DGD	C4D-C5D	2.28	1.57	1.53
33	C	516	DGD	O6D-C5D	-2.28	1.38	1.44
32	B	622	SQD	O9-S	2.28	1.51	1.45
26	A	613	CLA	CHC-C1C	2.28	1.43	1.38
30	c	520	LMG	C4-C5	2.27	1.57	1.53
26	B	612	CLA	CHC-C1C	2.27	1.43	1.38
26	b	602	CLA	CMB-C2B	-2.27	1.46	1.50
26	c	509	CLA	MG-NB	-2.27	2.01	2.05
26	b	601	CLA	MG-NB	-2.27	2.01	2.05
26	D	403	CLA	C3B-C4B	2.27	1.49	1.42
26	b	609	CLA	CMD-C2D	-2.27	1.46	1.50
36	V	201	HEC	CAC-C3C	2.27	1.56	1.51
26	B	612	CLA	C4B-NB	2.27	1.40	1.37
30	m	101	LMG	C4-C3	2.27	1.58	1.52
30	M	101	LMG	C4-C3	2.27	1.58	1.52
32	F	102	SQD	O9-S	2.27	1.51	1.45
26	b	602	CLA	C3B-C4B	2.26	1.49	1.42
30	A	614	LMG	C4-C3	2.26	1.58	1.52
28	h	102	BCR	C1-C6	-2.26	1.50	1.53
26	b	601	CLA	C1D-C2D	2.26	1.49	1.45
30	C	518	LMG	C4-C5	2.26	1.57	1.53
26	C	501	CLA	C1B-C2B	2.26	1.48	1.43
26	B	613	CLA	C3B-C4B	2.26	1.49	1.42
26	d	403	CLA	C4B-NB	2.26	1.40	1.37
26	B	615	CLA	CMB-C2B	-2.26	1.46	1.50
26	c	512	CLA	MG-NB	2.26	2.10	2.05
28	K	101	BCR	C38-C26	-2.26	1.47	1.50
26	B	602	CLA	C3B-C4B	2.25	1.49	1.42
26	C	513	CLA	MG-ND	2.25	2.10	2.05
26	A	608	CLA	C3B-C4B	2.25	1.49	1.42
33	c	518	DGD	O2G-C2G	-2.25	1.41	1.46
26	B	616	CLA	C1D-C2D	2.25	1.49	1.45
33	H	101	DGD	O2G-C2G	-2.25	1.41	1.46
28	b	617	BCR	C1-C6	-2.24	1.50	1.53
26	c	509	CLA	CMB-C2B	-2.24	1.46	1.50
26	b	614	CLA	CMB-C2B	-2.24	1.46	1.50
26	b	605	CLA	C4B-NB	2.24	1.40	1.37
26	b	612	CLA	CHC-C1C	2.24	1.43	1.38
26	C	503	CLA	MG-ND	2.24	2.10	2.05
26	b	612	CLA	MG-ND	2.23	2.10	2.05
27	d	402	PHO	C4D-ND	-2.23	1.35	1.38
26	a	606	CLA	C3B-C4B	2.23	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	402	PHO	CMB-C2B	-2.23	1.47	1.51
26	c	510	CLA	CHC-C1C	2.23	1.43	1.38
26	C	510	CLA	MG-NB	2.23	2.10	2.05
30	c	523	LMG	O6-C5	-2.23	1.38	1.44
26	C	512	CLA	CMD-C2D	-2.23	1.46	1.50
27	d	402	PHO	CMD-C2D	-2.22	1.47	1.51
33	c	518	DGD	C1G-C2G	2.22	1.57	1.50
33	c	519	DGD	O2E-C2E	-2.22	1.37	1.43
33	C	515	DGD	C3D-C2D	2.21	1.58	1.52
26	C	511	CLA	CHC-C1C	2.21	1.42	1.38
26	B	609	CLA	C3B-C4B	2.21	1.49	1.42
26	B	608	CLA	C3B-C4B	2.21	1.49	1.42
26	c	508	CLA	MG-NB	2.21	2.10	2.05
26	A	613	CLA	C3B-C4B	2.21	1.49	1.42
30	A	614	LMG	C1-C2	2.21	1.59	1.52
26	c	509	CLA	C3B-C4B	2.20	1.49	1.42
26	b	603	CLA	CHC-C1C	2.20	1.42	1.38
32	A	616	SQD	O7-S	2.20	1.51	1.45
26	c	507	CLA	MG-NC	-2.20	2.01	2.06
26	A	608	CLA	MG-NB	-2.20	2.01	2.05
26	c	502	CLA	CMC-C2C	-2.19	1.46	1.50
26	C	501	CLA	C1D-C2D	2.19	1.49	1.45
36	v	201	HEC	FE-NB	2.19	2.01	1.94
30	c	522	LMG	O7-C8	-2.19	1.41	1.46
26	B	603	CLA	CMC-C2C	-2.19	1.46	1.50
26	c	512	CLA	C1D-C2D	2.18	1.49	1.45
32	b	619	SQD	C44-C45	2.18	1.57	1.50
32	a	613	SQD	O7-S	2.18	1.51	1.45
26	b	601	CLA	C3B-C4B	2.18	1.49	1.42
27	d	402	PHO	CAC-C3C	-2.18	1.47	1.51
26	h	101	CLA	C3D-C4D	2.18	1.49	1.44
26	c	507	CLA	C3D-C4D	2.18	1.49	1.44
26	B	613	CLA	CHC-C1C	2.17	1.42	1.38
27	D	401	PHO	CAC-C3C	-2.17	1.47	1.51
27	A	609	PHO	O2D-CGD	2.17	1.38	1.33
26	B	611	CLA	MG-ND	2.17	2.10	2.05
30	b	621	LMG	C7-C8	2.17	1.57	1.50
26	c	503	CLA	C3B-C4B	2.17	1.49	1.42
33	C	515	DGD	C4D-C3D	2.17	1.58	1.52
26	A	613	CLA	C1D-C2D	2.17	1.49	1.45
26	B	615	CLA	CMD-C2D	-2.17	1.46	1.50
26	b	601	CLA	CMD-C2D	-2.17	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	610	CLA	MG-NC	-2.16	2.01	2.06
28	A	611	BCR	C33-C5	-2.16	1.47	1.50
26	c	502	CLA	C3B-C4B	2.16	1.49	1.42
30	A	614	LMG	O8-C9	-2.16	1.40	1.45
32	A	616	SQD	C8-C7	2.16	1.57	1.50
26	B	606	CLA	CHC-C1C	2.16	1.42	1.38
33	C	517	DGD	O2G-C2G	-2.15	1.41	1.46
26	A	610	CLA	C1D-C2D	2.15	1.49	1.45
30	M	101	LMG	C9-C8	2.15	1.57	1.50
27	A	609	PHO	CMB-C2B	-2.15	1.47	1.51
29	a	611	PL9	C53-C6	-2.15	1.46	1.50
26	c	509	CLA	CHC-C1C	2.14	1.42	1.38
26	b	610	CLA	CHC-C1C	2.14	1.42	1.38
26	B	603	CLA	CHC-C1C	2.14	1.42	1.38
26	B	610	CLA	CMB-C2B	-2.14	1.46	1.50
26	c	508	CLA	CMC-C2C	-2.14	1.46	1.50
26	C	512	CLA	MG-NB	2.14	2.10	2.05
33	C	516	DGD	C1E-C2E	2.14	1.58	1.52
36	v	201	HEC	CMA-C3A	2.14	1.55	1.50
31	A	617	LHG	C24-C23	2.14	1.56	1.50
26	c	502	CLA	CHC-C1C	2.14	1.42	1.38
26	a	609	CLA	CMC-C2C	-2.14	1.46	1.50
26	A	607	CLA	CHC-C1C	2.13	1.42	1.38
26	b	615	CLA	C3B-C4B	2.13	1.48	1.42
32	B	622	SQD	O7-S	2.12	1.51	1.45
26	C	501	CLA	MG-NB	2.12	2.10	2.05
26	a	612	CLA	C1D-C2D	2.12	1.49	1.45
26	c	510	CLA	CMC-C2C	-2.12	1.46	1.50
32	b	619	SQD	O6-C44	2.12	1.47	1.43
26	C	513	CLA	CHC-C1C	2.12	1.42	1.38
26	B	609	CLA	CMD-C2D	-2.11	1.46	1.50
26	c	511	CLA	C3B-C4B	2.11	1.48	1.42
26	b	603	CLA	C3B-C4B	2.11	1.48	1.42
33	c	517	DGD	O4D-C4D	-2.11	1.37	1.43
32	t	102	SQD	C46-C45	2.11	1.57	1.50
35	e	101	HEM	CMC-C2C	2.11	1.55	1.50
27	a	608	PHO	CAC-C3C	-2.11	1.48	1.51
26	a	612	CLA	C3B-C4B	2.10	1.48	1.42
26	h	101	CLA	CMC-C2C	-2.10	1.46	1.50
26	c	511	CLA	CMD-C2D	-2.10	1.46	1.50
30	D	408	LMG	C7-C8	2.10	1.56	1.51
35	F	101	HEM	CMA-C3A	2.10	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	610	CLA	CMD-C2D	-2.10	1.46	1.50
26	b	607	CLA	C3C-C2C	2.10	1.41	1.36
31	A	617	LHG	O8-C23	2.10	1.39	1.33
26	b	613	CLA	CMC-C2C	-2.10	1.46	1.50
26	C	502	CLA	CMB-C2B	-2.10	1.46	1.50
26	d	404	CLA	CMD-C2D	-2.09	1.46	1.50
26	C	504	CLA	CMB-C2B	-2.09	1.46	1.50
28	C	514	BCR	C33-C5	-2.09	1.47	1.50
26	C	512	CLA	CMB-C2B	-2.09	1.46	1.50
26	d	403	CLA	C3B-C4B	2.09	1.48	1.42
26	C	513	CLA	CMC-C2C	-2.09	1.46	1.50
26	B	607	CLA	O2D-CGD	2.09	1.38	1.33
26	B	607	CLA	CMB-C2B	-2.09	1.46	1.50
28	a	610	BCR	C38-C26	-2.09	1.47	1.50
26	a	609	CLA	CHC-C1C	2.09	1.42	1.38
28	k	101	BCR	C33-C5	-2.09	1.47	1.50
26	c	512	CLA	CMB-C2B	-2.09	1.46	1.50
26	b	602	CLA	C1D-C2D	2.08	1.49	1.45
26	b	601	CLA	MG-NC	2.08	2.11	2.06
33	h	103	DGD	O2G-C1B	2.08	1.40	1.34
26	C	503	CLA	CMC-C2C	-2.08	1.46	1.50
26	A	608	CLA	CMB-C2B	-2.08	1.46	1.50
36	v	201	HEC	CMC-C2C	2.07	1.55	1.50
26	a	606	CLA	C3D-C4D	2.07	1.48	1.44
27	a	608	PHO	O2D-CGD	2.07	1.38	1.33
26	b	615	CLA	CHC-C1C	2.07	1.42	1.38
35	e	101	HEM	C2A-C3A	-2.07	1.33	1.38
26	b	607	CLA	MG-NB	2.06	2.09	2.05
30	c	522	LMG	C1-C2	2.06	1.58	1.52
26	b	606	CLA	CMD-C2D	-2.06	1.46	1.50
26	C	510	CLA	CMD-C2D	-2.06	1.46	1.50
30	d	411	LMG	O7-C8	-2.06	1.41	1.46
26	C	508	CLA	CHC-C1C	2.06	1.42	1.38
26	d	404	CLA	CMB-C2B	-2.06	1.46	1.50
27	A	609	PHO	C1D-ND	2.06	1.42	1.38
29	A	612	PL9	C35-C34	-2.06	1.45	1.50
26	b	614	CLA	CMD-C2D	-2.06	1.46	1.50
26	b	612	CLA	CMC-C2C	-2.05	1.46	1.50
26	C	504	CLA	O2D-CGD	2.05	1.38	1.33
26	B	604	CLA	C4B-NB	2.05	1.40	1.37
26	D	402	CLA	CMD-C2D	-2.05	1.46	1.50
26	B	608	CLA	C1B-NB	-2.05	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	M	101	LMG	C4-C5	2.05	1.57	1.53
33	C	516	DGD	C4D-C5D	2.05	1.57	1.53
32	a	613	SQD	O9-S	2.04	1.50	1.45
27	A	609	PHO	CAC-C3C	-2.04	1.48	1.51
26	B	607	CLA	C3B-C4B	2.04	1.48	1.42
32	B	622	SQD	C46-C45	2.04	1.57	1.50
26	d	403	CLA	CHC-C1C	2.04	1.42	1.38
26	b	608	CLA	C3B-C4B	2.03	1.48	1.42
28	B	618	BCR	C1-C6	-2.03	1.51	1.53
26	c	503	CLA	CMB-C2B	-2.03	1.46	1.50
28	b	616	BCR	C30-C25	-2.03	1.51	1.53
26	a	606	CLA	CMD-C2D	-2.03	1.46	1.50
26	c	508	CLA	C3C-C2C	2.03	1.41	1.36
33	H	101	DGD	C4E-C5E	2.02	1.57	1.53
26	b	603	CLA	CMD-C2D	-2.02	1.46	1.50
26	A	610	CLA	CMC-C2C	-2.02	1.46	1.50
26	C	501	CLA	C1B-NB	-2.02	1.35	1.37
28	D	404	BCR	C38-C26	-2.02	1.47	1.50
26	b	608	CLA	CMB-C2B	-2.02	1.46	1.50
26	a	612	CLA	CMB-C2B	-2.02	1.46	1.50
26	b	608	CLA	CMD-C2D	-2.02	1.46	1.50
26	h	101	CLA	C1D-C2D	2.02	1.49	1.45
26	A	608	CLA	CMD-C2D	-2.01	1.46	1.50
26	B	601	CLA	CMB-C2B	-2.01	1.46	1.50
26	b	608	CLA	CMC-C2C	-2.01	1.46	1.50
26	C	506	CLA	CMC-C2C	-2.01	1.46	1.50
27	D	401	PHO	CMC-C2C	-2.01	1.47	1.50
32	f	101	SQD	O5-C5	2.01	1.49	1.44
32	F	102	SQD	O7-S	2.01	1.50	1.45
26	D	403	CLA	C1D-C2D	2.01	1.49	1.45
31	d	407	LHG	P-O6	2.01	1.67	1.59
36	V	201	HEC	CMD-C2D	2.01	1.54	1.50
26	D	402	CLA	CHC-C1C	2.00	1.42	1.38
27	d	402	PHO	C3D-C4D	2.00	1.44	1.41

All (1072) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	511	CLA	C4A-NA-C1A	10.05	111.27	106.68
26	C	511	CLA	C4A-NA-C1A	8.85	110.72	106.68
26	b	603	CLA	C4A-NA-C1A	8.75	110.67	106.68
26	B	611	CLA	C4A-NA-C1A	8.52	110.57	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	503	CLA	C4A-NA-C1A	8.34	110.48	106.68
26	b	615	CLA	C4A-NA-C1A	8.09	110.37	106.68
26	c	503	CLA	C4A-NA-C1A	8.03	110.34	106.68
26	b	610	CLA	C4A-NA-C1A	7.97	110.31	106.68
26	B	612	CLA	C4A-NA-C1A	7.86	110.26	106.68
26	C	508	CLA	C4A-NA-C1A	7.85	110.26	106.68
26	c	509	CLA	C4A-NA-C1A	7.85	110.26	106.68
32	a	613	SQD	O6-C1-C2	7.84	120.17	108.27
26	c	501	CLA	C4A-NA-C1A	7.77	110.22	106.68
26	C	510	CLA	C4A-NA-C1A	7.66	110.17	106.68
26	c	508	CLA	C4A-NA-C1A	7.62	110.16	106.68
26	C	507	CLA	C4A-NA-C1A	7.57	110.13	106.68
26	C	513	CLA	C4A-NA-C1A	7.43	110.07	106.68
26	B	616	CLA	C4A-NA-C1A	7.42	110.06	106.68
26	b	612	CLA	C4A-NA-C1A	7.14	109.94	106.68
26	C	509	CLA	C4A-NA-C1A	7.09	109.91	106.68
26	A	613	CLA	C4A-NA-C1A	6.99	109.87	106.68
26	b	605	CLA	C4A-NA-C1A	6.97	109.86	106.68
26	h	101	CLA	C4A-NA-C1A	6.97	109.86	106.68
26	c	505	CLA	C4A-NA-C1A	6.92	109.83	106.68
26	B	606	CLA	C4A-NA-C1A	6.90	109.83	106.68
26	c	502	CLA	C4A-NA-C1A	6.72	109.75	106.68
26	C	505	CLA	C4A-NA-C1A	6.68	109.73	106.68
27	a	608	PHO	C4D-CHA-CBD	-6.55	105.31	108.45
26	b	604	CLA	C4A-NA-C1A	6.53	109.66	106.68
26	c	510	CLA	C4A-NA-C1A	6.52	109.66	106.68
27	A	609	PHO	C4D-CHA-CBD	-6.45	105.36	108.45
26	C	501	CLA	C4A-NA-C1A	6.40	109.60	106.68
26	B	614	CLA	C4A-NA-C1A	6.39	109.59	106.68
26	b	614	CLA	C4A-NA-C1A	6.37	109.58	106.68
26	B	601	CLA	C4A-NA-C1A	6.26	109.53	106.68
26	D	402	CLA	C4A-NA-C1A	6.25	109.53	106.68
26	B	603	CLA	C4A-NA-C1A	6.23	109.52	106.68
32	F	102	SQD	O6-C1-C2	6.21	117.70	108.27
26	A	610	CLA	C4A-NA-C1A	6.19	109.50	106.68
26	B	615	CLA	C4A-NA-C1A	6.16	109.49	106.68
26	c	507	CLA	C4A-NA-C1A	6.14	109.48	106.68
26	B	604	CLA	C4A-NA-C1A	6.05	109.44	106.68
26	C	512	CLA	C4A-NA-C1A	6.03	109.43	106.68
26	C	506	CLA	C4A-NA-C1A	6.03	109.43	106.68
26	b	601	CLA	C4A-NA-C1A	6.02	109.43	106.68
26	B	613	CLA	C1-C2-C3	-6.00	116.36	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	b	619	SQD	O47-C7-C8	5.86	124.16	111.48
26	B	609	CLA	C4A-NA-C1A	5.80	109.32	106.68
26	c	504	CLA	C4A-NA-C1A	5.77	109.31	106.68
26	a	606	CLA	C4A-NA-C1A	5.77	109.31	106.68
26	d	403	CLA	C4A-NA-C1A	5.63	109.25	106.68
32	a	613	SQD	C1-O5-C5	-5.63	102.73	113.72
26	c	506	CLA	C4A-NA-C1A	5.59	109.23	106.68
26	A	607	CLA	C4A-NA-C1A	5.56	109.22	106.68
26	b	608	CLA	C4A-NA-C1A	5.54	109.21	106.68
36	v	201	HEC	C1D-ND-C4D	5.53	111.76	105.21
32	A	616	SQD	O6-C1-C2	5.48	116.59	108.27
26	B	608	CLA	C4A-NA-C1A	5.44	109.16	106.68
36	V	201	HEC	C1D-ND-C4D	5.40	111.60	105.21
26	B	610	CLA	C4A-NA-C1A	5.38	109.14	106.68
27	D	401	PHO	C1-C2-C3	-5.25	117.60	126.20
26	C	502	CLA	C4A-NA-C1A	5.25	109.07	106.68
32	B	622	SQD	O47-C7-C8	5.18	122.68	111.48
26	B	602	CLA	C4A-NA-C1A	5.15	109.03	106.68
29	d	406	PL9	C7-C3-C4	5.12	121.13	116.91
26	a	607	CLA	C4A-NA-C1A	5.11	109.01	106.68
26	A	608	CLA	C4A-NA-C1A	5.08	109.00	106.68
32	t	102	SQD	O47-C7-C8	5.05	122.39	111.48
26	c	512	CLA	C4A-NA-C1A	5.04	108.98	106.68
26	d	404	CLA	C4A-NA-C1A	4.97	108.95	106.68
27	D	401	PHO	C4D-CHA-CBD	-4.93	106.09	108.45
29	D	405	PL9	C7-C3-C4	4.91	120.96	116.91
33	c	518	DGD	O3G-C3G-C2G	-4.88	98.95	110.82
26	b	602	CLA	C4A-NA-C1A	4.82	108.88	106.68
26	B	605	CLA	C4A-NA-C1A	4.79	108.87	106.68
26	c	501	CLA	O2D-CGD-O1D	-4.77	114.55	123.85
26	b	613	CLA	C1-C2-C3	-4.72	118.47	126.20
26	b	609	CLA	C4A-NA-C1A	4.71	108.83	106.68
26	a	612	CLA	C4A-NA-C1A	4.69	108.82	106.68
26	B	611	CLA	O2D-CGD-O1D	-4.64	114.82	123.85
32	b	619	SQD	O5-C5-C4	4.61	118.01	109.70
26	b	605	CLA	O2D-CGD-O1D	-4.61	114.88	123.85
32	B	622	SQD	O6-C1-C2	4.58	115.23	108.27
26	c	512	CLA	C1-C2-C3	-4.57	118.71	126.20
26	b	604	CLA	O2D-CGD-O1D	-4.56	114.97	123.85
26	c	513	CLA	C4A-NA-C1A	4.55	108.76	106.68
28	b	616	BCR	C2-C1-C6	4.53	117.02	110.44
26	B	613	CLA	C4A-NA-C1A	4.52	108.74	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	613	CLA	C4A-NA-C1A	4.52	108.74	106.68
27	d	402	PHO	C4D-CHA-CBD	-4.50	106.30	108.45
26	C	504	CLA	C4A-NA-C1A	4.48	108.72	106.68
26	b	611	CLA	C4A-NA-C1A	4.47	108.72	106.68
27	d	402	PHO	C1-C2-C3	-4.45	118.91	126.20
31	D	409	LHG	O4-P-O5	4.40	132.92	112.44
32	A	616	SQD	C1-C2-C3	-4.38	100.80	110.01
26	B	610	CLA	O2D-CGD-O1D	-4.37	115.34	123.85
26	C	501	CLA	C3B-C4B-NB	-4.37	106.63	110.53
31	A	615	LHG	O4-P-O5	4.36	132.74	112.44
31	d	408	LHG	O4-P-O5	4.35	132.70	112.44
32	B	622	SQD	O7-S-C6	4.34	113.23	106.76
31	e	102	LHG	O4-P-O5	4.33	132.61	112.44
32	A	616	SQD	O47-C7-C8	4.33	120.85	111.48
33	C	516	DGD	O3G-C3G-C2G	-4.31	100.34	110.82
26	C	513	CLA	O2D-CGD-O1D	-4.30	115.47	123.85
26	b	615	CLA	O2D-CGD-O1D	-4.24	115.59	123.85
31	d	407	LHG	O4-P-O5	4.23	132.14	112.44
31	A	617	LHG	O4-P-O5	4.22	132.09	112.44
26	b	605	CLA	O2D-CGD-CBD	4.21	118.59	111.23
31	l	101	LHG	O4-P-O5	4.21	132.01	112.44
32	A	616	SQD	C1-O5-C5	-4.20	105.52	113.72
31	D	407	LHG	O4-P-O5	4.19	131.93	112.44
26	A	608	CLA	O2D-CGD-O1D	-4.18	115.70	123.85
26	C	506	CLA	C3B-C4B-NB	-4.18	106.80	110.53
26	D	402	CLA	O2D-CGD-O1D	-4.18	115.72	123.85
32	b	619	SQD	O6-C1-C2	4.17	114.61	108.27
31	L	101	LHG	O4-P-O5	4.15	131.75	112.44
26	c	505	CLA	C3B-C4B-NB	-4.15	106.83	110.53
29	a	611	PL9	C7-C3-C4	4.14	120.32	116.91
32	A	616	SQD	O9-S-O7	-4.14	100.36	113.82
31	d	409	LHG	O4-P-O5	4.12	131.62	112.44
26	B	611	CLA	O2D-CGD-CBD	4.12	118.43	111.23
26	B	602	CLA	O2D-CGD-CBD	4.04	118.30	111.23
26	b	607	CLA	C4A-NA-C1A	4.03	108.52	106.68
27	D	401	PHO	C2B-C1B-NB	-4.01	106.53	109.43
33	h	103	DGD	O3G-C3G-C2G	-3.99	101.11	110.82
26	c	508	CLA	C3B-C4B-NB	-3.97	106.99	110.53
33	H	101	DGD	O3G-C3G-C2G	-3.97	101.17	110.82
26	a	609	CLA	O2D-CGD-O1D	-3.96	116.14	123.85
26	C	512	CLA	O2D-CGD-O1D	-3.95	116.15	123.85
30	b	621	LMG	C1-O6-C5	-3.95	106.01	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	608	PHO	C2B-C1B-NB	-3.93	106.59	109.43
26	b	607	CLA	O2D-CGD-O1D	-3.93	116.20	123.85
26	c	502	CLA	C1-C2-C3	-3.93	119.76	126.20
36	v	201	HEC	CMD-C2D-C1D	3.92	131.16	125.03
32	f	101	SQD	O5-C5-C4	3.91	116.75	109.70
26	D	403	CLA	C4A-NA-C1A	3.90	108.46	106.68
26	b	602	CLA	O2D-CGD-O1D	-3.90	116.25	123.85
32	A	616	SQD	O7-S-C6	3.90	112.58	106.76
25	d	401	BCT	O2-C-O1	3.90	129.65	119.68
26	b	607	CLA	C3B-C4B-NB	-3.89	107.05	110.53
27	d	402	PHO	C2B-C1B-NB	-3.89	106.62	109.43
32	f	101	SQD	O9-S-O7	-3.88	101.19	113.82
26	B	605	CLA	O2D-CGD-O1D	-3.85	116.36	123.85
25	A	606	BCT	O2-C-O1	3.83	129.46	119.68
29	d	406	PL9	C22-C23-C24	-3.83	118.87	127.62
26	B	610	CLA	C3B-C4B-NB	-3.82	107.12	110.53
26	c	502	CLA	O2D-CGD-O1D	-3.81	116.43	123.85
26	b	605	CLA	C3B-C4B-NB	-3.81	107.13	110.53
26	B	607	CLA	C4A-NA-C1A	3.79	108.41	106.68
26	C	512	CLA	C1-C2-C3	-3.78	120.00	126.20
26	b	606	CLA	C3B-C4B-NB	-3.78	107.16	110.53
33	C	517	DGD	O3G-C3G-C2G	-3.77	101.64	110.82
28	T	101	BCR	C2-C1-C6	3.76	115.90	110.44
33	c	519	DGD	O6D-C1D-O3G	-3.76	101.17	110.04
30	M	101	LMG	C1-C2-C3	-3.73	102.16	110.01
26	B	604	CLA	C1-C2-C3	-3.72	120.11	126.20
33	c	517	DGD	O3G-C3G-C2G	-3.71	101.79	110.82
32	a	613	SQD	C1-C2-C3	-3.71	102.21	110.01
28	D	404	BCR	C2-C1-C6	3.70	115.82	110.44
28	T	101	BCR	C3-C4-C5	-3.70	107.45	114.06
26	b	606	CLA	C4A-NA-C1A	3.70	108.37	106.68
26	B	602	CLA	O2D-CGD-O1D	-3.69	116.66	123.85
32	t	102	SQD	O48-C23-C24	3.69	123.08	111.83
26	c	507	CLA	C3B-C4B-NB	-3.69	107.24	110.53
26	C	501	CLA	O2D-CGD-O1D	-3.69	116.67	123.85
26	d	404	CLA	C3B-C4B-NB	-3.67	107.26	110.53
26	A	608	CLA	O2D-CGD-CBD	3.65	117.61	111.23
26	c	512	CLA	C3B-C4B-NB	-3.64	107.28	110.53
26	b	613	CLA	O2D-CGD-O1D	-3.64	116.77	123.85
26	D	402	CLA	O2D-CGD-CBD	3.62	117.55	111.23
26	B	601	CLA	C3B-C4B-NB	-3.60	107.31	110.53
26	B	612	CLA	O2D-CGD-O1D	-3.59	116.86	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	608	CLA	O2D-CGD-O1D	-3.59	116.87	123.85
26	b	614	CLA	C3B-C4B-NB	-3.58	107.33	110.53
26	c	509	CLA	O2A-CGA-O1A	-3.58	114.66	123.63
34	C	519	STE	C3-C2-C1	-3.58	105.16	114.51
26	c	512	CLA	O2D-CGD-O1D	-3.56	116.91	123.85
29	A	612	PL9	O1-C4-C3	-3.56	116.97	120.73
27	A	609	PHO	CMB-C2B-C3B	3.56	131.79	124.68
26	a	609	CLA	O2D-CGD-CBD	3.56	117.45	111.23
26	b	609	CLA	O2D-CGD-O1D	-3.56	116.93	123.85
33	h	103	DGD	C4E-C3E-C2E	-3.55	104.60	110.83
32	a	613	SQD	O47-C7-C8	3.54	119.14	111.48
26	a	606	CLA	C3B-C4B-NB	-3.53	107.38	110.53
35	e	101	HEM	C3B-C4B-NB	-3.52	106.94	109.47
26	B	615	CLA	C3B-C4B-NB	-3.52	107.39	110.53
32	B	622	SQD	C3-C4-C5	3.51	116.59	110.23
33	c	519	DGD	O3G-C3G-C2G	-3.51	102.29	110.82
26	a	607	CLA	C3B-C4B-NB	-3.50	107.41	110.53
26	h	101	CLA	O2D-CGD-O1D	-3.49	117.05	123.85
26	b	602	CLA	O2D-CGD-CBD	3.49	117.33	111.23
29	a	611	PL9	C7-C3-C2	-3.49	119.27	123.39
26	B	614	CLA	C3B-C4B-NB	-3.48	107.42	110.53
26	C	503	CLA	O2D-CGD-O1D	-3.48	117.07	123.85
26	A	610	CLA	O2D-CGD-O1D	-3.48	117.08	123.85
26	B	604	CLA	O2D-CGD-O1D	-3.48	117.08	123.85
28	B	617	BCR	C2-C1-C6	3.46	115.47	110.44
26	C	507	CLA	C3B-C4B-NB	-3.45	107.45	110.53
32	A	618	SQD	O47-C7-C8	3.45	118.94	111.48
26	b	601	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
26	B	603	CLA	O2D-CGD-O1D	-3.44	117.15	123.85
32	a	613	SQD	O48-C23-C24	3.44	122.32	111.83
29	d	406	PL9	C7-C3-C2	-3.42	119.36	123.39
26	b	606	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
32	a	613	SQD	O9-S-O7	-3.41	102.72	113.82
32	B	622	SQD	O48-C23-C24	3.41	122.23	111.83
26	C	512	CLA	C3B-C4B-NB	-3.41	107.49	110.53
26	B	606	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
26	C	504	CLA	C3B-C4B-NB	-3.40	107.49	110.53
26	c	508	CLA	C1-C2-C3	-3.40	120.63	126.20
29	A	612	PL9	C7-C8-C9	-3.39	120.99	126.83
26	C	508	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
32	a	613	SQD	O8-S-C6	3.39	112.51	105.97
26	B	605	CLA	C3B-C4B-NB	-3.39	107.51	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	C	515	DGD	O3G-C3G-C2G	-3.39	102.58	110.82
26	B	612	CLA	C1-C2-C3	-3.37	120.67	126.20
26	d	403	CLA	O2D-CGD-O1D	-3.37	117.30	123.85
26	B	611	CLA	C1-C2-C3	-3.36	120.68	126.20
26	h	101	CLA	C3B-C4B-NB	-3.36	107.53	110.53
26	b	601	CLA	O2D-CGD-CBD	3.36	117.10	111.23
26	D	402	CLA	C3B-C4B-NB	-3.36	107.53	110.53
28	t	101	BCR	C2-C1-C6	3.35	115.31	110.44
26	b	603	CLA	C1-C2-C3	-3.35	120.70	126.20
26	B	612	CLA	O2A-CGA-O1A	-3.35	115.24	123.63
26	C	505	CLA	C3B-C4B-NB	-3.35	107.54	110.53
26	b	609	CLA	CAA-CBA-CGA	-3.33	103.75	113.21
35	F	101	HEM	CBD-CAD-C3D	-3.33	103.33	112.53
33	h	103	DGD	C1D-C2D-C3D	-3.33	103.01	110.01
26	B	603	CLA	C3B-C4B-NB	-3.31	107.57	110.53
26	A	613	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
26	C	510	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
26	b	613	CLA	C3B-C4B-NB	-3.30	107.59	110.53
29	D	405	PL9	C37-C38-C39	-3.29	120.08	127.62
26	b	611	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
26	A	607	CLA	CHB-C4A-NA	3.29	129.14	124.40
33	c	518	DGD	O6D-C1D-O3G	-3.28	102.28	110.04
26	a	609	CLA	C4A-NA-C1A	3.28	108.17	106.68
32	B	622	SQD	O9-S-O7	-3.27	103.17	113.82
29	D	405	PL9	C8-C7-C3	3.27	120.49	112.03
27	d	402	PHO	CMB-C2B-C3B	3.26	131.20	124.68
29	a	611	PL9	C22-C23-C24	-3.26	120.17	127.62
26	b	607	CLA	O2D-CGD-CBD	3.25	116.91	111.23
33	a	614	DGD	O3G-C3G-C2G	-3.24	103.43	111.77
26	b	615	CLA	O2D-CGD-CBD	3.24	116.90	111.23
26	c	501	CLA	O2D-CGD-CBD	3.24	116.90	111.23
26	a	607	CLA	O2D-CGD-CBD	3.24	116.90	111.23
32	F	102	SQD	O8-S-C6	3.24	112.23	105.97
28	B	617	BCR	C11-C10-C9	-3.24	122.74	127.28
29	a	611	PL9	C7-C8-C9	-3.24	121.26	126.83
26	B	614	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
36	V	201	HEC	CBD-CAD-C3D	-3.23	103.60	112.53
30	b	621	LMG	C1-C2-C3	-3.22	103.23	110.01
26	B	616	CLA	C3B-C4B-NB	-3.22	107.66	110.53
31	d	407	LHG	O8-C23-C24	3.21	121.62	111.83
28	c	515	BCR	C27-C26-C25	3.21	127.04	122.70
26	c	512	CLA	CHB-C4A-NA	3.21	129.03	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	401	PHO	O1D-CGD-CBD	3.20	129.58	124.72
29	a	611	PL9	O1-C4-C3	-3.20	117.35	120.73
29	D	405	PL9	C20-C19-C21	3.20	120.78	115.23
26	A	608	CLA	C3B-C4B-NB	-3.19	107.68	110.53
32	f	101	SQD	O7-S-C6	3.19	111.52	106.76
26	B	602	CLA	C3B-C4B-NB	-3.19	107.69	110.53
32	B	622	SQD	C46-C45-C44	-3.18	104.37	111.78
26	A	607	CLA	O2A-CGA-O1A	-3.17	115.69	123.63
26	B	611	CLA	C3B-C4B-NB	-3.17	107.70	110.53
26	d	403	CLA	C3B-C4B-NB	-3.17	107.70	110.53
35	e	101	HEM	CBD-CAD-C3D	-3.17	103.78	112.53
28	D	404	BCR	C3-C4-C5	-3.16	108.42	114.06
31	D	409	LHG	O8-C23-C24	3.16	121.47	111.83
33	C	516	DGD	O6D-C1D-O3G	-3.16	102.58	110.04
26	A	608	CLA	C1-C2-C3	-3.16	121.02	126.20
26	C	510	CLA	C3B-C4B-NB	-3.15	107.71	110.53
30	m	101	LMG	O1-C7-C8	-3.15	103.15	110.82
26	B	608	CLA	CMB-C2B-C1B	-3.15	120.62	125.42
26	c	510	CLA	C3B-C4B-NB	-3.15	107.72	110.53
26	B	603	CLA	O2D-CGD-CBD	3.15	116.73	111.23
26	C	507	CLA	CHB-C4A-NA	3.14	128.93	124.40
28	K	101	BCR	C27-C26-C25	3.13	126.93	122.70
26	a	606	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
33	C	517	DGD	O6D-C1D-O3G	-3.12	102.67	110.04
26	a	607	CLA	O2A-CGA-O1A	-3.11	115.84	123.63
28	t	101	BCR	C3-C4-C5	-3.11	108.51	114.06
26	B	610	CLA	CHB-C4A-NA	3.11	128.89	124.40
31	d	407	LHG	C11-C10-C9	-3.11	98.66	114.37
26	B	609	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
29	d	406	PL9	C7-C8-C9	-3.11	121.48	126.83
32	F	102	SQD	O9-S-O7	-3.09	103.77	113.82
30	c	523	LMG	O6-C1-O1	-3.09	102.74	110.04
28	A	611	BCR	C2-C1-C6	3.07	114.90	110.44
32	b	619	SQD	O8-S-C6	3.06	111.88	105.97
29	d	406	PL9	C40-C39-C41	3.06	120.53	115.23
26	c	506	CLA	C3B-C4B-NB	-3.05	107.81	110.53
31	d	408	LHG	O8-C23-C24	3.05	121.12	111.83
26	d	404	CLA	CHB-C4A-NA	3.05	128.80	124.40
31	D	407	LHG	O8-C23-C24	3.04	121.11	111.83
26	b	601	CLA	CHB-C4A-NA	3.04	128.79	124.40
26	a	612	CLA	C1-C2-C3	-3.04	121.22	126.20
32	b	619	SQD	O9-S-O7	-3.04	103.95	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	511	CLA	C3B-C4B-NB	-3.03	107.82	110.53
26	b	607	CLA	CHB-C4A-NA	3.03	128.78	124.40
26	a	607	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
26	c	503	CLA	C3B-C4B-NB	-3.02	107.83	110.53
28	B	617	BCR	C29-C30-C25	3.02	114.83	110.44
30	c	520	LMG	O6-C1-O1	-3.02	102.92	110.04
26	C	504	CLA	C1-C2-C3	-3.02	121.25	126.20
26	c	511	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
27	d	402	PHO	O2D-CGD-O1D	-3.01	117.98	123.85
33	A	619	DGD	C3G-C2G-C1G	-3.01	104.76	111.78
26	C	503	CLA	C3B-C4B-NB	-3.01	107.84	110.53
30	D	406	LMG	O2-C2-C1	-3.01	102.90	110.08
26	C	511	CLA	CHB-C4A-NA	3.00	128.73	124.40
26	B	607	CLA	CED-O2D-CGD	3.00	122.71	115.92
33	c	517	DGD	C3G-C2G-C1G	-2.99	104.80	111.78
29	D	405	PL9	C27-C28-C29	-2.99	120.77	127.62
26	c	504	CLA	CMB-C2B-C1B	-2.99	120.86	125.42
26	a	612	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
28	d	405	BCR	C27-C26-C25	2.98	126.73	122.70
26	B	614	CLA	O2D-CGD-CBD	2.98	116.44	111.23
26	b	609	CLA	CHB-C4A-NA	2.98	128.70	124.40
33	c	519	DGD	CDB-CCB-CBB	-2.98	99.32	114.37
28	b	617	BCR	C2-C1-C6	2.98	114.76	110.44
26	B	604	CLA	CHB-C4A-NA	2.98	128.69	124.40
33	h	103	DGD	C1E-O6E-C5E	2.97	119.53	113.72
26	b	605	CLA	C1-C2-C3	-2.97	121.33	126.20
26	c	513	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
26	B	616	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
26	C	507	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
26	C	509	CLA	C1-C2-C3	-2.95	121.36	126.20
26	a	609	CLA	CHB-C4A-NA	2.95	128.66	124.40
26	C	509	CLA	CMB-C2B-C1B	-2.95	120.92	125.42
35	e	101	HEM	C3B-C2B-C1B	2.95	108.63	106.41
33	C	515	DGD	O6D-C1D-O3G	-2.95	103.08	110.04
31	e	102	LHG	O8-C23-C24	2.95	120.82	111.83
33	a	614	DGD	C1G-C2G-C3G	-2.94	105.01	111.80
32	F	102	SQD	O5-C1-C2	-2.94	104.33	110.37
32	B	622	SQD	O5-C5-C4	2.94	115.00	109.70
26	b	610	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
26	c	503	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
26	A	608	CLA	O2A-CGA-O1A	-2.94	116.28	123.63
26	c	508	CLA	O2A-CGA-O1A	-2.93	116.29	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	K	102	BCR	C27-C26-C25	2.93	126.66	122.70
26	B	607	CLA	C4-C3-C5	2.93	120.31	115.23
26	b	604	CLA	O2A-CGA-O1A	-2.92	116.31	123.63
29	D	405	PL9	C42-C43-C44	-2.92	120.94	127.62
28	A	611	BCR	C11-C10-C9	-2.92	123.19	127.28
32	F	102	SQD	O9-S-C6	2.91	111.11	106.76
27	d	402	PHO	O1D-CGD-CBD	2.90	129.13	124.72
26	C	512	CLA	CHB-C4A-NA	2.90	128.59	124.40
26	c	502	CLA	C3B-C4B-NB	-2.89	107.95	110.53
33	c	518	DGD	C3D-C4D-C5D	-2.89	104.99	110.23
28	D	404	BCR	C27-C26-C25	2.89	126.61	122.70
29	A	612	PL9	C7-C3-C4	2.89	119.29	116.91
28	b	616	BCR	C27-C26-C25	2.89	126.61	122.70
26	B	602	CLA	CHB-C4A-NA	2.89	128.56	124.40
26	B	610	CLA	C1-C2-C3	-2.88	121.48	126.20
36	v	201	HEC	CAD-CBD-CGD	-2.88	106.03	113.67
26	a	606	CLA	O2A-CGA-O1A	-2.88	116.44	123.63
26	B	610	CLA	O2A-CGA-O1A	-2.87	116.44	123.63
32	F	102	SQD	C1-O5-C5	-2.87	108.11	113.72
28	B	618	BCR	C2-C1-C6	2.87	114.61	110.44
26	h	101	CLA	CHB-C4A-NA	2.87	128.54	124.40
28	X	101	BCR	C2-C1-C6	2.87	114.61	110.44
26	B	609	CLA	O2A-CGA-O1A	-2.87	116.45	123.63
26	C	509	CLA	CHB-C4A-NA	2.87	128.54	124.40
26	A	613	CLA	O2D-CGD-CBD	2.86	116.24	111.23
28	Z	101	BCR	C11-C10-C9	-2.86	123.26	127.28
28	a	610	BCR	C2-C1-C6	2.86	114.60	110.44
29	A	612	PL9	C22-C23-C24	-2.86	121.07	127.62
26	c	507	CLA	CHB-C4A-NA	2.86	128.53	124.40
26	c	507	CLA	CHD-C4C-NC	2.86	128.66	124.23
26	c	504	CLA	O2A-CGA-O1A	-2.84	116.51	123.63
33	c	517	DGD	O6D-C1D-O3G	-2.84	103.32	110.04
26	c	509	CLA	CHB-C4A-NA	2.84	128.50	124.40
28	c	515	BCR	C7-C8-C9	-2.84	122.03	126.23
31	A	617	LHG	O8-C23-C24	2.84	120.49	111.83
26	c	504	CLA	C1-C2-C3	-2.84	121.55	126.20
33	C	516	DGD	O3G-C1D-C2D	-2.84	103.97	108.27
27	D	401	PHO	CMB-C2B-C3B	2.83	130.34	124.68
36	v	201	HEC	CAD-C3D-C4D	2.83	129.63	124.70
32	b	619	SQD	O7-S-C6	2.83	110.98	106.76
26	D	403	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
26	A	613	CLA	CHB-C4A-NA	2.83	128.48	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	616	SQD	O5-C1-C2	-2.82	104.57	110.37
28	d	405	BCR	C24-C23-C22	-2.82	122.07	126.23
26	c	508	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
28	k	101	BCR	C33-C5-C6	-2.81	121.42	124.48
32	b	619	SQD	O48-C23-C24	2.81	120.40	111.83
26	b	615	CLA	CHB-C4A-NA	2.81	128.45	124.40
26	B	606	CLA	C3B-C4B-NB	-2.81	108.02	110.53
26	D	402	CLA	O2A-CGA-O1A	-2.81	116.60	123.63
28	B	619	BCR	C2-C1-C6	2.81	114.52	110.44
29	D	405	PL9	C7-C8-C9	-2.81	122.00	126.83
30	m	101	LMG	O3-C3-C2	-2.80	103.77	110.38
27	A	609	PHO	C1-C2-C3	-2.80	121.61	126.20
32	A	616	SQD	O9-S-C6	2.80	110.93	106.76
26	c	513	CLA	C3B-C4B-NB	-2.80	108.03	110.53
26	C	512	CLA	O2D-CGD-CBD	2.79	116.11	111.23
26	B	601	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
27	D	401	PHO	O2D-CGD-O1D	-2.79	118.42	123.85
26	h	101	CLA	O2D-CGD-CBD	2.78	116.09	111.23
26	B	610	CLA	O2D-CGD-CBD	2.78	116.09	111.23
26	A	608	CLA	CHB-C4A-NA	2.78	128.41	124.40
26	b	611	CLA	C1-C2-C3	-2.78	121.64	126.20
32	f	101	SQD	O6-C1-C2	2.78	112.49	108.27
30	C	518	LMG	O6-C1-O1	-2.77	103.49	110.04
26	B	616	CLA	CHB-C4A-NA	2.77	128.40	124.40
28	b	618	BCR	C27-C26-C25	2.77	126.45	122.70
26	b	606	CLA	CHB-C4A-NA	2.77	128.39	124.40
26	c	505	CLA	O2D-CGD-CBD	2.76	116.06	111.23
28	Z	101	BCR	C27-C26-C25	2.76	126.43	122.70
28	A	611	BCR	C27-C26-C25	2.76	126.43	122.70
28	c	516	BCR	C27-C26-C25	2.75	126.42	122.70
26	b	604	CLA	C3B-C4B-NB	-2.75	108.07	110.53
26	C	503	CLA	O1D-CGD-CBD	2.75	129.94	124.52
26	c	506	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
26	b	611	CLA	CHB-C4A-NA	2.74	128.36	124.40
32	f	101	SQD	O48-C23-C24	2.74	120.20	111.83
26	C	512	CLA	O2A-CGA-O1A	-2.74	116.77	123.63
26	B	601	CLA	CAA-C2A-C3A	-2.74	105.60	113.00
26	B	602	CLA	CMB-C2B-C1B	-2.74	121.25	125.42
36	v	201	HEC	CHB-C1B-NB	2.74	127.37	124.42
33	C	515	DGD	CDB-CCB-CBB	-2.74	100.53	114.37
30	d	411	LMG	O7-C10-O9	-2.74	117.31	123.70
29	D	405	PL9	C7-C3-C2	-2.73	120.16	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	506	CLA	O2A-CGA-O1A	-2.73	116.79	123.63
30	c	522	LMG	O7-C10-O9	-2.73	117.32	123.70
28	X	101	BCR	C27-C26-C25	2.73	126.39	122.70
26	A	610	CLA	CHB-C4A-NA	2.72	128.33	124.40
26	C	501	CLA	C1-C2-C3	-2.72	121.74	126.20
30	c	522	LMG	O6-C1-O1	-2.72	103.62	110.04
26	a	606	CLA	CHB-C4A-NA	2.72	128.32	124.40
31	L	101	LHG	O8-C23-C24	2.71	120.11	111.83
28	h	102	BCR	C27-C26-C25	2.71	126.37	122.70
32	F	102	SQD	O48-C23-C24	2.71	120.11	111.83
26	C	502	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
26	C	509	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
32	A	616	SQD	O48-C23-C24	2.70	120.08	111.83
33	A	619	DGD	C4E-C3E-C2E	-2.70	106.09	110.83
26	b	610	CLA	O2D-CGD-CBD	2.69	115.94	111.23
31	d	407	LHG	C20-C19-C18	-2.69	100.76	114.37
26	b	611	CLA	C3B-C4B-NB	-2.69	108.13	110.53
29	d	406	PL9	C37-C38-C39	-2.69	121.47	127.62
30	m	101	LMG	O1-C1-C2	-2.69	104.19	108.27
33	H	101	DGD	C1D-C2D-C3D	-2.68	104.37	110.01
26	b	611	CLA	O2A-CGA-O1A	-2.68	116.93	123.63
28	A	611	BCR	C3-C4-C5	-2.68	109.28	114.06
26	c	509	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
26	B	606	CLA	O2A-CGA-O1A	-2.67	116.94	123.63
29	A	612	PL9	C7-C3-C2	-2.67	120.24	123.39
30	m	101	LMG	O8-C28-O10	-2.67	116.95	123.63
33	A	619	DGD	CDB-CCB-CBB	-2.67	100.89	114.37
36	v	201	HEC	CHA-C4D-ND	2.67	127.29	124.42
26	B	614	CLA	CHC-C4B-NB	2.67	128.05	124.05
26	C	504	CLA	O2A-CGA-O1A	-2.67	116.96	123.63
29	d	406	PL9	C27-C28-C29	-2.66	121.53	127.62
28	c	514	BCR	C27-C26-C25	2.66	126.30	122.70
26	c	504	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
32	b	619	SQD	O9-S-C6	2.66	110.72	106.76
33	A	619	DGD	O5D-C1E-C2E	2.66	112.31	108.27
33	C	516	DGD	O2D-C2D-C1D	-2.66	103.75	110.08
26	b	612	CLA	CMB-C2B-C1B	-2.65	121.38	125.42
28	b	618	BCR	C2-C1-C6	2.65	114.29	110.44
26	C	509	CLA	C3B-C4B-NB	-2.65	108.17	110.53
26	A	613	CLA	C1-C2-C3	-2.65	121.86	126.20
26	b	603	CLA	C3B-C4B-NB	-2.64	108.17	110.53
26	B	608	CLA	O2D-CGD-CBD	2.64	115.85	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	d	411	LMG	O6-C1-O1	-2.64	103.81	110.04
33	c	517	DGD	O5D-C6D-C5D	-2.64	103.47	109.42
32	f	101	SQD	C3-C4-C5	2.64	115.01	110.23
29	D	405	PL9	C22-C23-C24	-2.64	121.59	127.62
26	h	101	CLA	O2A-CGA-O1A	-2.64	117.03	123.63
26	c	511	CLA	O2A-CGA-O1A	-2.64	117.04	123.63
26	c	513	CLA	CHB-C4A-NA	2.63	128.20	124.40
26	B	609	CLA	C1-C2-C3	-2.63	121.89	126.20
26	d	404	CLA	CHD-C1D-ND	-2.63	121.10	124.80
26	a	612	CLA	CHB-C4A-NA	2.63	128.19	124.40
26	b	603	CLA	CHB-C4A-NA	2.63	128.19	124.40
28	d	405	BCR	C2-C1-C6	2.62	114.25	110.44
29	d	406	PL9	C8-C7-C3	2.62	118.81	112.03
26	b	604	CLA	O1D-CGD-CBD	2.62	129.68	124.52
26	B	601	CLA	CHB-C4A-NA	2.62	128.18	124.40
31	D	409	LHG	O8-C23-O10	-2.61	117.10	123.63
26	C	513	CLA	O2A-CGA-O1A	-2.61	117.10	123.63
26	b	610	CLA	CHB-C4A-NA	2.61	128.16	124.40
28	B	618	BCR	C3-C4-C5	-2.61	109.41	114.06
32	f	101	SQD	C1-O5-C5	-2.60	108.64	113.72
28	K	101	BCR	C33-C5-C6	-2.60	121.64	124.48
26	b	613	CLA	O2A-CGA-O1A	-2.60	117.12	123.63
26	b	611	CLA	O1D-CGD-CBD	2.60	129.65	124.52
26	a	607	CLA	C1-C2-C3	-2.60	121.94	126.20
26	b	603	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
28	a	610	BCR	C27-C26-C25	2.59	126.20	122.70
33	h	103	DGD	C3G-C2G-C1G	-2.59	105.75	111.78
26	b	607	CLA	C1D-ND-C4D	2.59	108.13	106.31
29	d	406	PL9	C20-C19-C21	2.58	119.72	115.23
26	a	607	CLA	CHB-C4A-NA	2.58	128.13	124.40
26	B	613	CLA	CED-O2D-CGD	2.58	121.78	115.92
26	C	511	CLA	C3B-C4B-NB	-2.58	108.22	110.53
26	C	511	CLA	O2A-CGA-O1A	-2.58	117.17	123.63
26	B	603	CLA	O2A-CGA-O1A	-2.58	117.17	123.63
26	b	612	CLA	C7-C6-C5	-2.58	106.39	113.26
31	d	409	LHG	O8-C23-C24	2.58	119.70	111.83
31	D	407	LHG	O8-C23-O10	-2.58	117.18	123.63
26	c	505	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
32	A	616	SQD	O8-S-C6	2.58	110.95	105.97
33	a	614	DGD	CDB-CCB-CBB	-2.57	101.38	114.37
34	b	622	STE	C3-C2-C1	-2.57	107.81	114.51
34	C	519	STE	O2-C1-C2	2.57	122.11	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	509	CLA	CMB-C2B-C3B	2.57	132.59	126.55
26	c	509	CLA	C3B-C4B-NB	-2.57	108.24	110.53
36	V	201	HEC	C2A-C1A-NA	-2.56	107.85	110.32
26	B	612	CLA	CHB-C4A-NA	2.56	128.10	124.40
26	B	612	CLA	C3B-C4B-NB	-2.56	108.24	110.53
26	a	607	CLA	C1D-ND-C4D	2.56	108.11	106.31
26	B	608	CLA	CMB-C2B-C3B	2.56	132.57	126.55
33	c	518	DGD	CDB-CCB-CBB	-2.56	101.44	114.37
30	m	101	LMG	C38-C37-C36	-2.56	101.45	114.37
26	C	501	CLA	O2A-CGA-O1A	-2.55	117.24	123.63
28	C	514	BCR	C27-C26-C25	2.55	126.15	122.70
26	C	502	CLA	O1D-CGD-CBD	2.55	129.54	124.52
28	c	516	BCR	C33-C5-C6	-2.54	121.71	124.48
33	c	517	DGD	CDB-CCB-CBB	-2.54	101.51	114.37
26	c	511	CLA	O2D-CGD-CBD	2.54	115.67	111.23
34	B	623	STE	C3-C2-C1	-2.54	107.88	114.51
29	a	611	PL9	C12-C13-C14	-2.54	121.81	127.62
29	D	405	PL9	C12-C13-C14	-2.54	121.81	127.62
33	C	516	DGD	CDB-CCB-CBB	-2.54	101.54	114.37
31	D	409	LHG	C11-C10-C9	-2.53	101.56	114.37
28	a	610	BCR	C7-C8-C9	-2.53	122.49	126.23
33	C	517	DGD	CDB-CCB-CBB	-2.53	101.57	114.37
26	a	612	CLA	O2D-CGD-CBD	2.53	115.65	111.23
30	D	408	LMG	O1-C7-C8	-2.53	105.27	111.77
32	f	101	SQD	O47-C7-C8	2.53	120.21	110.93
28	c	515	BCR	C2-C1-C6	2.53	114.11	110.44
31	e	102	LHG	C11-C10-C9	-2.52	101.61	114.37
32	b	619	SQD	C3-C4-C5	2.52	114.81	110.23
26	d	403	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
32	A	616	SQD	O47-C7-O49	-2.52	117.81	123.70
26	b	604	CLA	C1-C2-C3	-2.52	122.07	126.20
26	c	503	CLA	CHB-C4A-NA	2.52	128.04	124.40
28	B	617	BCR	C33-C5-C6	-2.52	121.73	124.48
32	b	619	SQD	C1-C2-C3	-2.52	104.71	110.01
26	b	605	CLA	CHB-C4A-NA	2.52	128.03	124.40
26	b	606	CLA	CMB-C2B-C1B	-2.52	121.59	125.42
26	B	612	CLA	O1D-CGD-CBD	2.51	129.47	124.52
28	B	619	BCR	C29-C30-C25	2.51	114.09	110.44
28	X	101	BCR	C16-C17-C18	-2.51	123.76	127.28
26	b	606	CLA	CMB-C2B-C3B	2.51	132.44	126.55
30	m	101	LMG	O7-C10-O9	-2.50	117.85	123.70
26	C	508	CLA	C3B-C4B-NB	-2.50	108.30	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	C	516	DGD	C1D-C2D-C3D	-2.50	104.75	110.01
26	c	505	CLA	O2A-CGA-O1A	-2.50	117.38	123.63
26	C	502	CLA	CHD-C1D-ND	-2.50	121.29	124.80
35	e	101	HEM	CHB-C1B-NB	2.50	127.45	124.37
26	C	513	CLA	O2D-CGD-CBD	2.50	115.59	111.23
26	C	502	CLA	O2A-CGA-O1A	-2.49	117.39	123.63
27	a	608	PHO	OBD-CAD-CBD	-2.49	122.17	125.82
30	M	101	LMG	O1-C7-C8	-2.49	104.76	110.82
30	c	522	LMG	C3-C4-C5	-2.49	105.72	110.23
26	b	603	CLA	O2D-CGD-CBD	2.49	115.58	111.23
30	M	101	LMG	C40-C39-C38	-2.49	101.79	114.37
27	d	402	PHO	C3B-C4B-NB	-2.49	105.84	107.46
30	m	101	LMG	C1-O6-C5	-2.48	108.87	113.72
33	H	101	DGD	O6D-C1D-O3G	-2.48	104.18	110.04
29	a	611	PL9	C37-C38-C39	-2.48	121.95	127.62
28	X	101	BCR	C35-C13-C14	-2.48	118.80	122.82
26	c	508	CLA	CHB-C4A-NA	2.48	127.98	124.40
26	C	510	CLA	CMB-C2B-C1B	-2.48	121.65	125.42
36	V	201	HEC	CMD-C2D-C1D	2.48	128.90	125.03
26	B	608	CLA	C1-O2A-CGA	2.47	122.64	116.65
35	e	101	HEM	C1B-NB-C4B	2.47	108.14	105.21
30	C	518	LMG	O1-C7-C8	-2.47	104.80	110.82
28	c	514	BCR	C33-C5-C6	-2.47	121.79	124.48
33	H	101	DGD	C4E-C3E-C2E	-2.47	106.49	110.83
26	B	604	CLA	C3B-C4B-NB	-2.47	108.32	110.53
27	A	609	PHO	C2B-C1B-NB	-2.47	107.64	109.43
26	b	603	CLA	O2A-CGA-O1A	-2.47	117.45	123.63
26	b	615	CLA	C3B-C4B-NB	-2.47	108.33	110.53
35	e	101	HEM	CAB-C3B-C2B	-2.46	120.42	128.43
26	b	601	CLA	C3B-C4B-NB	-2.46	108.33	110.53
26	d	404	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
26	b	604	CLA	CHB-C4A-NA	2.46	127.96	124.40
26	B	605	CLA	O1D-CGD-CBD	2.46	129.38	124.52
28	a	610	BCR	C30-C25-C26	-2.46	119.27	122.64
36	v	201	HEC	C2A-C1A-NA	-2.46	107.95	110.32
26	B	606	CLA	CGD-CBD-CAD	-2.46	102.88	110.85
26	c	505	CLA	CHB-C4A-NA	2.46	127.95	124.40
26	b	612	CLA	C3B-C4B-NB	-2.46	108.34	110.53
26	B	615	CLA	CHB-C4A-NA	2.46	127.94	124.40
32	f	101	SQD	O5-C1-C2	-2.46	105.32	110.37
26	c	508	CLA	CHD-C4C-NC	2.46	128.04	124.23
30	M	101	LMG	O6-C1-O1	-2.46	104.24	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	406	LMG	C38-C37-C36	-2.46	101.96	114.37
31	d	407	LHG	C18-C17-C16	-2.45	101.97	114.37
31	d	407	LHG	O8-C23-O10	-2.45	117.49	123.63
26	B	607	CLA	CHB-C4A-NA	2.45	127.94	124.40
30	c	522	LMG	O2-C2-C1	-2.45	104.23	110.08
30	M	101	LMG	C38-C37-C36	-2.45	101.98	114.37
26	C	507	CLA	C1-C2-C3	-2.45	122.18	126.20
26	B	602	CLA	C16-C15-C13	-2.45	107.82	115.97
26	c	507	CLA	CHD-C1D-ND	-2.45	121.36	124.80
26	B	605	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
26	c	501	CLA	C3B-C4B-NB	-2.45	108.34	110.53
31	d	408	LHG	C18-C17-C16	-2.45	102.00	114.37
26	A	610	CLA	O2D-CGD-CBD	2.43	115.49	111.23
33	a	614	DGD	C5B-C4B-C3B	-2.43	102.07	114.37
26	B	613	CLA	CMB-C2B-C1B	-2.43	121.72	125.42
26	B	608	CLA	CHB-C4A-NA	2.43	127.91	124.40
26	B	601	CLA	CAA-CBA-CGA	-2.43	106.31	113.21
34	d	414	STE	O2-C1-C2	2.43	121.67	114.00
32	A	618	SQD	O48-C23-C24	2.43	119.24	111.83
27	D	401	PHO	OBD-CAD-CBD	-2.43	122.27	125.82
30	d	411	LMG	O1-C7-C8	-2.42	104.92	110.82
26	A	613	CLA	C3B-C4B-NB	-2.42	108.37	110.53
33	h	103	DGD	C1D-O6D-C5D	-2.42	108.99	113.72
30	A	614	LMG	C38-C37-C36	-2.42	102.13	114.37
26	b	608	CLA	C3B-C4B-NB	-2.42	108.37	110.53
26	B	606	CLA	CMB-C2B-C1B	-2.42	121.73	125.42
29	A	612	PL9	C27-C28-C29	-2.42	122.09	127.62
32	B	622	SQD	C9-C8-C7	-2.42	104.83	113.69
26	b	612	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
30	c	523	LMG	C1-O6-C5	-2.42	109.00	113.72
28	B	618	BCR	C27-C26-C25	2.41	125.96	122.70
31	l	101	LHG	C5-O7-C7	-2.41	112.03	117.80
26	b	609	CLA	C3B-C4B-NB	-2.41	108.38	110.53
26	b	612	CLA	CHB-C4A-NA	2.41	127.88	124.40
26	c	512	CLA	CHD-C1D-ND	-2.41	121.41	124.80
31	A	615	LHG	O8-C6-C5	-2.41	101.45	108.40
28	b	617	BCR	C27-C26-C25	2.41	125.96	122.70
27	a	608	PHO	O2A-CGA-O1A	-2.41	117.61	123.63
26	B	604	CLA	C6-C7-C8	-2.41	107.97	115.97
26	B	615	CLA	O2D-CGD-O1D	-2.41	119.17	123.85
34	C	520	STE	C3-C2-C1	-2.40	108.23	114.51
33	h	103	DGD	CDB-CCB-CBB	-2.40	102.22	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	406	LMG	C40-C39-C38	-2.40	102.22	114.37
31	A	617	LHG	C11-C10-C9	-2.40	102.22	114.37
26	b	612	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
27	D	401	PHO	C3D-C4D-ND	2.40	110.78	107.71
32	a	613	SQD	O9-S-C6	2.40	110.34	106.76
33	C	515	DGD	C6D-O5D-C1E	2.40	118.94	113.80
34	M	102	STE	C3-C2-C1	-2.39	108.26	114.51
26	B	614	CLA	CHB-C4A-NA	2.39	127.85	124.40
26	C	504	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
33	A	619	DGD	O6D-C1D-O3G	-2.39	104.40	110.04
26	b	602	CLA	CHD-C1D-ND	-2.39	121.44	124.80
28	T	101	BCR	C29-C30-C25	2.39	113.91	110.44
26	c	504	CLA	CMB-C2B-C3B	2.39	132.17	126.55
28	b	616	BCR	C3-C4-C5	-2.39	109.80	114.06
26	B	602	CLA	CMB-C2B-C3B	2.38	132.16	126.55
28	C	514	BCR	C2-C1-C6	2.38	113.90	110.44
26	C	504	CLA	CHB-C4A-NA	2.38	127.83	124.40
34	J	101	STE	C3-C2-C1	-2.38	108.30	114.51
26	C	506	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
33	h	103	DGD	O6E-C5E-C4E	2.37	113.97	109.70
33	A	619	DGD	CBB-CAB-C9B	-2.37	102.37	114.37
32	a	613	SQD	O5-C1-C2	-2.37	105.50	110.37
26	c	513	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
26	B	602	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
36	v	201	HEC	C3D-C4D-ND	-2.37	108.06	110.35
32	A	616	SQD	O5-C5-C4	2.37	113.97	109.70
26	b	608	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
26	B	606	CLA	CHB-C1B-NB	2.36	127.59	124.05
26	b	606	CLA	CHD-C1D-ND	-2.36	121.48	124.80
30	d	411	LMG	C40-C39-C38	-2.36	102.44	114.37
28	b	616	BCR	C15-C14-C13	-2.36	123.97	127.28
26	C	503	CLA	C7-C6-C5	-2.36	106.98	113.26
31	A	615	LHG	C11-C10-C9	-2.36	102.46	114.37
26	b	609	CLA	C1-C2-C3	-2.36	122.34	126.20
26	a	606	CLA	C1-C2-C3	-2.35	122.34	126.20
31	d	408	LHG	C20-C19-C18	-2.35	102.47	114.37
33	c	517	DGD	O3G-C1D-C2D	-2.35	104.70	108.27
29	A	612	PL9	O2-C1-C2	-2.35	116.48	121.83
26	C	513	CLA	C3B-C4B-NB	-2.35	108.43	110.53
33	c	519	DGD	CBB-CAB-C9B	-2.35	102.49	114.37
26	b	604	CLA	O2D-CGD-CBD	2.35	115.34	111.23
33	h	103	DGD	CBB-CAB-C9B	-2.35	102.49	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	l	101	LHG	C11-C10-C9	-2.35	102.50	114.37
29	d	406	PL9	C42-C43-C44	-2.35	122.25	127.62
33	c	518	DGD	C6D-C5D-C4D	2.35	116.99	112.07
26	b	611	CLA	CMB-C2B-C1B	-2.35	121.85	125.42
26	B	603	CLA	C7-C6-C5	-2.34	107.02	113.26
28	Z	101	BCR	C7-C8-C9	-2.34	122.77	126.23
26	c	512	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
34	j	101	STE	O2-C1-O1	-2.34	117.31	123.33
29	D	405	PL9	C32-C33-C34	-2.34	122.27	127.62
26	c	507	CLA	CHB-C1B-NB	2.34	127.56	124.05
28	b	617	BCR	C15-C14-C13	-2.34	124.00	127.28
26	A	610	CLA	CHD-C1D-ND	-2.34	121.51	124.80
26	c	506	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
35	e	101	HEM	C4D-ND-C1D	2.34	107.97	105.21
32	f	101	SQD	O9-S-C6	2.34	110.24	106.76
26	b	611	CLA	CMB-C2B-C3B	2.33	132.03	126.55
33	c	518	DGD	O2D-C2D-C1D	-2.33	104.52	110.08
26	c	508	CLA	CHD-C1D-ND	-2.33	121.53	124.80
26	C	502	CLA	C1-C2-C3	-2.33	122.39	126.20
33	c	517	DGD	C4E-C3E-C2E	-2.32	106.75	110.83
28	b	618	BCR	C29-C30-C25	2.32	113.81	110.44
26	B	608	CLA	C3B-C4B-NB	-2.32	108.46	110.53
31	d	408	LHG	C11-C10-C9	-2.32	102.64	114.37
32	B	622	SQD	O8-S-C6	2.32	110.45	105.97
28	c	514	BCR	C2-C1-C6	2.32	113.81	110.44
26	b	604	CLA	CHD-C1D-ND	-2.32	121.54	124.80
27	d	402	PHO	O2A-CGA-O1A	-2.32	117.83	123.63
26	c	501	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
34	C	519	STE	O1-C1-C2	-2.31	115.76	123.09
26	B	612	CLA	CHD-C1D-ND	-2.31	121.55	124.80
26	D	403	CLA	C1-C2-C3	-2.31	122.41	126.20
32	B	622	SQD	O5-C1-C2	-2.31	105.62	110.37
26	c	511	CLA	CHB-C4A-NA	2.31	127.73	124.40
28	b	616	BCR	C11-C10-C9	-2.31	124.04	127.28
30	C	518	LMG	C40-C39-C38	-2.31	102.72	114.37
26	C	504	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
36	V	201	HEC	CMC-C2C-C1C	-2.30	121.91	125.42
28	X	101	BCR	C15-C14-C13	-2.30	124.05	127.28
29	a	611	PL9	C40-C39-C41	2.30	119.22	115.23
28	C	514	BCR	C33-C5-C6	-2.30	121.97	124.48
26	B	610	CLA	CAA-C2A-C3A	-2.30	106.78	113.00
26	b	602	CLA	CHD-C1D-C2D	2.30	130.26	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	509	CLA	O1D-CGD-CBD	2.30	129.05	124.52
26	C	505	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
31	L	101	LHG	C11-C10-C9	-2.30	102.76	114.37
33	h	103	DGD	O6D-C1D-O3G	-2.29	104.62	110.04
31	D	407	LHG	C27-C26-C25	-2.29	102.77	114.37
26	C	503	CLA	CHB-C4A-NA	2.29	127.71	124.40
36	V	201	HEC	CHA-C4D-ND	2.29	126.89	124.42
33	C	516	DGD	O5D-C6D-C5D	-2.29	104.25	109.42
26	c	507	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
26	C	507	CLA	C2A-C1A-CHA	2.29	127.84	123.87
26	C	508	CLA	O2D-CGD-CBD	2.29	115.23	111.23
30	b	621	LMG	C40-C39-C38	-2.29	102.80	114.37
28	K	102	BCR	C24-C23-C22	-2.29	122.85	126.23
28	T	101	BCR	C27-C26-C25	2.29	125.79	122.70
28	t	101	BCR	C11-C10-C9	-2.29	124.07	127.28
26	B	601	CLA	C2A-C1A-CHA	2.28	127.83	123.87
28	Z	101	BCR	C15-C14-C13	-2.28	124.07	127.28
32	b	619	SQD	C9-C8-C7	-2.28	105.33	113.69
26	c	508	CLA	O2D-CGD-CBD	2.28	115.22	111.23
31	d	407	LHG	C27-C26-C25	-2.28	102.84	114.37
26	C	505	CLA	CHB-C4A-NA	2.28	127.69	124.40
26	A	607	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
26	A	607	CLA	C3B-C4B-NB	-2.28	108.50	110.53
32	t	102	SQD	O48-C23-O10	-2.27	117.94	123.63
32	F	102	SQD	O7-S-C6	2.27	110.15	106.76
28	c	514	BCR	C15-C16-C17	-2.27	118.87	123.52
26	b	602	CLA	CHB-C1B-NB	2.27	127.46	124.05
28	A	611	BCR	C7-C8-C9	-2.27	122.87	126.23
27	D	401	PHO	O2A-CGA-O1A	-2.27	117.95	123.63
26	b	615	CLA	CHC-C4B-NB	2.27	127.45	124.05
28	B	618	BCR	C11-C10-C9	-2.27	124.10	127.28
28	t	101	BCR	C28-C27-C26	-2.27	110.02	114.06
32	B	622	SQD	C1-O5-C5	-2.26	109.30	113.72
29	a	611	PL9	O2-C1-C2	-2.26	116.68	121.83
30	c	522	LMG	C40-C39-C38	-2.26	102.92	114.37
28	T	101	BCR	C15-C14-C13	-2.26	124.10	127.28
27	a	608	PHO	CMB-C2B-C3B	2.26	129.21	124.68
26	C	503	CLA	C1-O2A-CGA	2.26	122.13	116.65
26	A	607	CLA	CED-O2D-CGD	2.26	121.04	115.92
26	B	606	CLA	CHA-C4D-ND	2.26	137.21	132.55
26	C	510	CLA	C11-C10-C8	-2.26	108.46	115.97
26	D	403	CLA	CHB-C4A-NA	2.26	127.66	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	h	102	BCR	C2-C1-C6	2.26	113.72	110.44
34	j	101	STE	O2-C1-C2	2.25	121.11	114.00
30	D	406	LMG	O6-C1-O1	-2.25	104.73	110.04
32	b	619	SQD	C1-O5-C5	2.25	118.11	113.72
28	B	617	BCR	C15-C16-C17	-2.25	118.92	123.52
29	A	612	PL9	C20-C19-C21	2.25	119.13	115.23
30	m	101	LMG	C9-C8-C7	-2.25	106.55	111.78
26	b	602	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
28	X	101	BCR	C16-C15-C14	-2.25	118.92	123.52
30	D	406	LMG	O1-C1-C2	-2.24	104.86	108.27
33	C	515	DGD	O5D-C6D-C5D	-2.24	104.36	109.42
33	H	101	DGD	C1D-O6D-C5D	-2.24	109.34	113.72
33	H	101	DGD	C6D-C5D-C4D	2.24	116.77	112.07
26	C	513	CLA	O1D-CGD-CBD	2.24	128.94	124.52
30	c	523	LMG	C38-C37-C36	-2.24	103.05	114.37
35	F	101	HEM	C4D-ND-C1D	2.24	107.86	105.21
29	A	612	PL9	C40-C39-C41	2.24	119.11	115.23
30	C	518	LMG	C38-C37-C36	-2.24	103.06	114.37
26	c	501	CLA	CHB-C4A-NA	2.24	127.63	124.40
33	c	518	DGD	CBB-CAB-C9B	-2.24	103.07	114.37
33	h	103	DGD	C3D-C4D-C5D	-2.24	106.18	110.23
30	c	523	LMG	C40-C39-C38	-2.23	103.07	114.37
26	C	509	CLA	CHD-C1D-ND	-2.23	121.66	124.80
31	L	101	LHG	C27-C26-C25	-2.23	103.08	114.37
29	A	612	PL9	C12-C13-C14	-2.23	122.51	127.62
29	A	612	PL9	O2-C1-C6	2.23	124.03	120.48
31	l	101	LHG	C20-C19-C18	-2.23	103.09	114.37
26	h	101	CLA	CHD-C1D-ND	-2.23	121.66	124.80
26	c	502	CLA	CHB-C1B-NB	2.23	127.39	124.05
26	B	606	CLA	O2D-CGD-CBD	2.23	115.13	111.23
30	d	411	LMG	C38-C37-C36	-2.23	103.11	114.37
29	D	405	PL9	C50-C49-C48	-2.23	115.98	122.66
26	c	504	CLA	C3B-C4B-NB	-2.22	108.54	110.53
33	h	103	DGD	C6D-C5D-C4D	2.22	116.73	112.07
30	b	621	LMG	C8-O7-C10	2.22	123.11	117.80
28	c	515	BCR	C11-C10-C9	-2.22	124.16	127.28
26	b	603	CLA	CHC-C4B-NB	2.22	127.38	124.05
33	c	517	DGD	O3E-C3E-C2E	-2.22	105.15	110.38
26	c	502	CLA	O1D-CGD-CBD	2.22	128.89	124.52
26	B	603	CLA	CHD-C1D-ND	-2.22	121.68	124.80
30	A	614	LMG	C40-C39-C38	-2.22	103.16	114.37
26	B	613	CLA	CMB-C2B-C3B	2.21	131.75	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	621	LMG	C38-C37-C36	-2.21	103.19	114.37
33	a	614	DGD	C2G-O2G-C1B	2.21	123.09	117.80
33	c	518	DGD	C2G-O2G-C1B	-2.21	112.51	117.80
28	t	101	BCR	C27-C26-C25	2.21	125.69	122.70
28	k	101	BCR	C24-C23-C22	-2.21	122.97	126.23
30	D	408	LMG	C38-C37-C36	-2.21	103.20	114.37
33	c	517	DGD	CBB-CAB-C9B	-2.21	103.20	114.37
26	B	609	CLA	CHA-C1A-NA	-2.21	121.39	126.39
26	b	607	CLA	CHB-C1B-NB	2.21	127.36	124.05
31	D	409	LHG	C20-C19-C18	-2.21	103.21	114.37
26	C	505	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
26	b	614	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
28	Z	101	BCR	C15-C16-C17	-2.20	119.01	123.52
26	B	613	CLA	C16-C15-C13	-2.20	108.64	115.97
26	A	610	CLA	CMB-C2B-C1B	-2.20	122.06	125.42
26	d	404	CLA	CHD-C1D-C2D	2.20	130.07	125.49
28	Z	101	BCR	C2-C1-C6	2.20	113.64	110.44
26	b	605	CLA	C11-C12-C13	-2.20	108.66	115.97
26	c	512	CLA	O1D-CGD-CBD	2.20	128.85	124.52
26	a	609	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
26	c	504	CLA	CHB-C4A-NA	2.20	127.57	124.40
28	B	618	BCR	C35-C13-C14	-2.20	119.26	122.82
26	D	402	CLA	CHB-C4A-NA	2.19	127.56	124.40
26	B	604	CLA	O2D-CGD-CBD	2.19	115.06	111.23
28	t	101	BCR	C33-C5-C6	-2.19	122.09	124.48
28	B	619	BCR	C27-C26-C25	2.19	125.67	122.70
26	A	608	CLA	C1D-ND-C4D	2.19	107.85	106.31
26	b	608	CLA	C1-C2-C3	-2.19	122.61	126.20
28	X	101	BCR	C24-C23-C22	-2.19	123.00	126.23
30	c	520	LMG	C40-C39-C38	-2.19	103.31	114.37
26	B	614	CLA	C2A-C1A-CHA	2.19	127.66	123.87
34	t	103	STE	O2-C1-C2	2.19	120.91	114.00
26	c	511	CLA	C2A-C1A-CHA	2.18	127.66	123.87
33	A	619	DGD	O3G-C3G-C2G	-2.18	105.51	110.82
26	C	506	CLA	CHB-C1B-NB	2.18	127.32	124.05
28	D	404	BCR	C38-C26-C25	-2.18	122.11	124.48
28	b	616	BCR	C30-C25-C26	-2.18	119.66	122.64
30	c	520	LMG	C38-C37-C36	-2.18	103.36	114.37
26	A	613	CLA	CHC-C4B-NB	2.18	127.31	124.05
26	b	608	CLA	C7-C6-C5	-2.18	107.46	113.26
26	b	601	CLA	C1-C2-C3	-2.18	122.63	126.20
30	A	614	LMG	C1-C2-C3	-2.18	105.43	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	501	CLA	CHD-C1D-ND	-2.17	121.74	124.80
26	B	609	CLA	CHC-C4B-NB	2.17	127.31	124.05
29	d	406	PL9	C36-C34-C33	-2.17	116.29	121.17
26	b	603	CLA	C11-C10-C8	-2.17	108.75	115.97
28	t	101	BCR	C7-C8-C9	-2.17	123.02	126.23
28	d	405	BCR	C30-C25-C26	-2.17	119.67	122.64
28	h	102	BCR	C7-C8-C9	-2.17	123.03	126.23
26	B	615	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
33	H	101	DGD	CDB-CCB-CBB	-2.16	103.42	114.37
26	c	510	CLA	C16-C15-C13	-2.16	108.77	115.97
30	c	520	LMG	O3-C3-C2	-2.16	105.28	110.38
33	c	517	DGD	C6D-O5D-C1E	2.16	118.43	113.80
33	c	518	DGD	O2G-C1B-O1B	-2.16	118.65	123.70
31	l	101	LHG	C18-C17-C16	-2.16	103.44	114.37
26	C	502	CLA	C3B-C4B-NB	-2.16	108.60	110.53
31	l	101	LHG	O8-C23-C24	2.16	118.42	111.83
28	K	102	BCR	C15-C16-C17	-2.16	119.10	123.52
26	c	502	CLA	CHB-C4A-NA	2.16	127.51	124.40
36	v	201	HEC	CAD-C3D-C2D	-2.15	123.83	127.87
26	B	608	CLA	CHD-C1D-ND	-2.15	121.77	124.80
26	C	501	CLA	CHB-C4A-NA	2.15	127.51	124.40
34	J	101	STE	O2-C1-C2	2.15	120.80	114.00
33	c	518	DGD	O6E-C1E-O5D	-2.15	104.96	110.04
33	c	518	DGD	C1D-C2D-C3D	-2.15	105.48	110.01
26	C	501	CLA	O2D-CGD-CBD	2.15	114.99	111.23
31	d	408	LHG	O8-C23-O10	-2.15	118.25	123.63
32	F	102	SQD	O4-C4-C3	-2.15	105.31	110.38
26	c	503	CLA	C11-C12-C13	-2.15	108.82	115.97
33	A	619	DGD	C8B-C7B-C6B	-2.15	103.50	114.37
26	B	610	CLA	CHD-C1D-ND	-2.15	121.78	124.80
30	c	522	LMG	C38-C37-C36	-2.15	103.51	114.37
26	D	403	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
26	c	503	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
34	d	412	STE	O2-C1-C2	2.14	120.77	114.00
26	b	614	CLA	C1-C2-C3	-2.14	122.69	126.20
30	d	410	LMG	C38-C37-C36	-2.14	103.56	114.37
26	A	607	CLA	O1D-CGD-CBD	2.14	128.73	124.52
26	C	505	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
27	a	608	PHO	CMD-C2D-C3D	2.13	128.95	124.68
28	D	404	BCR	C24-C23-C22	-2.13	123.08	126.23
26	C	506	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
26	B	613	CLA	CHB-C4A-NA	2.13	127.48	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	614	LMG	O6-C1-O1	-2.13	105.01	110.04
26	b	608	CLA	CHC-C4B-NB	2.13	127.25	124.05
26	B	602	CLA	C1-C2-C3	-2.13	122.71	126.20
28	B	619	BCR	C33-C5-C6	-2.13	122.16	124.48
33	C	517	DGD	C8B-C7B-C6B	-2.13	103.61	114.37
31	e	102	LHG	C20-C19-C18	-2.13	103.61	114.37
26	b	615	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
26	B	602	CLA	C11-C12-C13	-2.13	108.89	115.97
36	V	201	HEC	C4B-NB-C1B	2.13	107.73	105.21
31	l	101	LHG	C29-C28-C27	-2.12	103.63	114.37
36	V	201	HEC	C3D-C4D-ND	-2.12	108.30	110.35
28	k	101	BCR	C27-C26-C25	2.12	125.57	122.70
31	d	409	LHG	C27-C26-C25	-2.12	103.64	114.37
33	C	517	DGD	CAB-C9B-C8B	-2.12	103.64	114.37
26	b	612	CLA	C1-C2-C3	-2.12	122.72	126.20
28	d	405	BCR	C33-C5-C6	-2.12	122.17	124.48
33	H	101	DGD	CAB-C9B-C8B	-2.12	103.66	114.37
26	c	510	CLA	C7-C6-C5	-2.12	107.62	113.26
26	b	610	CLA	C7-C6-C5	-2.12	107.62	113.26
26	D	403	CLA	CAC-C3C-C4C	2.12	127.54	124.79
26	B	603	CLA	C2A-C1A-CHA	2.12	127.54	123.87
30	M	101	LMG	O5-C6-C5	-2.11	104.14	111.33
29	a	611	PL9	C42-C43-C44	-2.11	122.80	127.62
26	b	601	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
33	c	517	DGD	O5E-C6E-C5E	-2.11	104.16	111.33
26	d	403	CLA	CHB-C4A-NA	2.11	127.44	124.40
26	B	604	CLA	C1D-ND-C4D	2.11	107.79	106.31
33	a	614	DGD	CBB-CAB-C9B	-2.11	103.72	114.37
28	c	515	BCR	C15-C16-C17	-2.10	119.21	123.52
31	A	617	LHG	C20-C19-C18	-2.10	103.74	114.37
26	C	510	CLA	CHB-C1B-NB	2.10	127.20	124.05
26	B	605	CLA	CHD-C1D-ND	-2.10	121.84	124.80
28	B	619	BCR	C11-C10-C9	-2.10	124.33	127.28
34	L	102	STE	O2-C1-C2	2.10	120.64	114.00
26	c	513	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
26	b	614	CLA	CHB-C4A-NA	2.10	127.43	124.40
33	c	519	DGD	C6D-O5D-C1E	2.10	118.29	113.80
30	B	621	LMG	C38-C37-C36	-2.09	103.78	114.37
35	F	101	HEM	CHC-C4B-NB	2.09	126.68	124.42
30	D	408	LMG	O7-C10-O9	-2.09	118.81	123.70
28	c	515	BCR	C33-C5-C6	-2.09	122.20	124.48
26	C	510	CLA	CMB-C2B-C3B	2.09	131.47	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	V	201	HEC	C1D-C2D-C3D	-2.09	104.78	106.98
26	C	512	CLA	C6-C5-C3	-2.09	108.38	113.47
26	C	513	CLA	CHB-C4A-NA	2.09	127.41	124.40
30	b	621	LMG	O2-C2-C1	-2.09	105.10	110.08
26	A	608	CLA	CAC-C3C-C4C	2.09	127.51	124.79
26	B	616	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
26	b	606	CLA	CHB-C1B-NB	2.09	127.18	124.05
26	B	613	CLA	CHC-C1C-NC	2.09	127.45	124.31
29	D	405	PL9	O1-C4-C3	-2.09	118.53	120.73
33	C	516	DGD	C3E-C4E-C5E	-2.09	106.45	110.23
30	D	406	LMG	O1-C7-C8	-2.09	105.75	110.82
29	d	406	PL9	O1-C4-C3	-2.08	118.53	120.73
28	b	618	BCR	C30-C25-C26	-2.08	119.79	122.64
33	C	515	DGD	CBB-CAB-C9B	-2.08	103.84	114.37
26	c	507	CLA	O2D-CGD-O1D	-2.08	119.79	123.85
26	c	510	CLA	CHB-C4A-NA	2.08	127.40	124.40
30	M	101	LMG	O7-C10-O9	-2.08	118.84	123.70
26	B	613	CLA	C3B-C4B-NB	-2.08	108.67	110.53
26	b	607	CLA	CMB-C2B-C3B	2.08	131.44	126.55
26	C	505	CLA	C1D-ND-C4D	2.08	107.77	106.31
28	B	618	BCR	C15-C14-C13	-2.08	124.36	127.28
30	C	518	LMG	O7-C10-O9	-2.08	118.85	123.70
28	D	404	BCR	C33-C5-C6	-2.08	122.22	124.48
29	d	406	PL9	O2-C1-C6	2.08	123.78	120.48
26	c	506	CLA	C1-O2A-CGA	2.07	121.67	116.65
26	C	504	CLA	CHB-C1B-NB	2.07	127.16	124.05
26	b	611	CLA	CAC-C3C-C4C	2.07	127.49	124.79
28	d	405	BCR	C1-C6-C5	-2.07	119.81	122.64
26	c	506	CLA	CHB-C4A-NA	2.07	127.39	124.40
26	b	614	CLA	CHB-C1B-NB	2.07	127.16	124.05
26	c	506	CLA	CHB-C1B-NB	2.07	127.16	124.05
26	A	608	CLA	C2D-C1D-ND	-2.07	108.08	110.13
31	A	615	LHG	C27-C26-C25	-2.07	103.90	114.37
26	B	613	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
33	C	515	DGD	C8B-C7B-C6B	-2.07	103.91	114.37
32	B	622	SQD	O9-S-C6	2.07	109.84	106.76
33	c	519	DGD	C1D-C2D-C3D	-2.07	105.66	110.01
34	d	413	STE	O2-C1-C2	2.07	120.53	114.00
31	e	102	LHG	C5-O7-C7	-2.07	112.85	117.80
28	Z	101	BCR	C33-C5-C6	-2.07	122.23	124.48
26	B	603	CLA	CHB-C4A-NA	2.07	127.38	124.40
33	c	517	DGD	C5B-C4B-C3B	-2.07	103.93	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	503	CLA	C1D-ND-C4D	2.07	107.76	106.31
26	C	505	CLA	C2D-C1D-ND	-2.06	108.08	110.13
36	v	201	HEC	CBA-CAA-C2A	-2.06	106.83	112.53
26	c	510	CLA	CHA-C1A-NA	-2.06	121.72	126.39
33	C	515	DGD	CAB-C9B-C8B	-2.06	103.95	114.37
26	a	609	CLA	C3B-C4B-NB	-2.06	108.69	110.53
26	b	604	CLA	C4-C3-C5	2.06	118.80	115.23
26	A	610	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
26	B	616	CLA	CHC-C1C-NC	2.06	127.41	124.31
26	c	505	CLA	C1-C2-C3	-2.06	122.82	126.20
30	c	522	LMG	C9-C8-C7	-2.06	106.99	111.78
28	D	404	BCR	C21-C20-C19	-2.06	117.24	123.20
26	C	505	CLA	CMB-C2B-C3B	2.06	131.38	126.55
26	A	607	CLA	C7-C6-C5	-2.06	107.78	113.26
29	d	406	PL9	O2-C1-C2	-2.06	117.16	121.83
28	b	617	BCR	C35-C13-C14	-2.05	119.49	122.82
33	c	518	DGD	C7B-C6B-C5B	-2.05	103.98	114.37
26	B	606	CLA	CMB-C2B-C3B	2.05	131.38	126.55
28	C	514	BCR	C1-C6-C5	-2.05	119.83	122.64
26	B	614	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
26	b	609	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
29	A	612	PL9	C32-C33-C34	-2.05	122.93	127.62
32	b	619	SQD	O49-C7-C8	-2.05	115.76	123.78
33	c	517	DGD	O2G-C1B-O1B	-2.05	118.91	123.70
26	b	608	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
26	B	610	CLA	O1D-CGD-CBD	2.05	128.56	124.52
33	C	515	DGD	C6B-C5B-C4B	-2.05	104.01	114.37
31	A	617	LHG	C18-C17-C16	-2.05	104.01	114.37
26	D	403	CLA	CHA-C1A-NA	-2.05	121.75	126.39
26	b	603	CLA	C11-C12-C13	-2.05	109.16	115.97
30	c	522	LMG	O8-C28-O10	-2.05	118.51	123.63
30	D	406	LMG	O8-C28-O10	-2.05	118.51	123.63
26	D	402	CLA	CHA-C4D-ND	2.05	136.77	132.55
31	D	407	LHG	C11-C10-C9	-2.05	104.03	114.37
30	C	518	LMG	C6-C5-C4	-2.04	108.00	113.02
33	A	619	DGD	CFB-CEB-CDB	-2.04	104.04	114.37
29	a	611	PL9	O2-C1-C6	2.04	123.72	120.48
33	H	101	DGD	C3G-C2G-C1G	-2.04	107.03	111.78
26	B	613	CLA	CHA-C1A-NA	-2.04	121.78	126.39
31	A	617	LHG	C27-C26-C25	-2.04	104.07	114.37
33	H	101	DGD	C3E-C4E-C5E	-2.04	106.54	110.23
34	F	103	STE	C3-C2-C1	-2.04	109.19	114.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	602	CLA	C3B-C4B-NB	-2.04	108.71	110.53
26	c	507	CLA	C2A-C1A-CHA	2.03	127.40	123.87
28	c	515	BCR	C35-C13-C14	-2.03	119.52	122.82
26	C	503	CLA	C4-C3-C5	2.03	118.76	115.23
26	B	607	CLA	CMB-C2B-C1B	-2.03	122.32	125.42
31	l	101	LHG	O8-C23-O10	-2.03	118.54	123.63
26	c	508	CLA	CHD-C1D-C2D	2.03	129.72	125.49
26	c	501	CLA	O1D-CGD-CBD	2.03	128.53	124.52
26	a	612	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
26	b	609	CLA	CMB-C2B-C3B	2.03	131.33	126.55
31	L	101	LHG	C5-O7-C7	-2.03	112.94	117.80
26	b	613	CLA	CHB-C4A-NA	2.03	127.33	124.40
32	t	102	SQD	C9-C8-C7	-2.03	106.26	113.69
26	C	508	CLA	CHD-C1D-ND	-2.03	121.95	124.80
26	b	607	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
33	C	516	DGD	CBB-CAB-C9B	-2.03	104.12	114.37
26	C	510	CLA	CHB-C4A-NA	2.03	127.33	124.40
28	a	610	BCR	C11-C10-C9	-2.03	124.44	127.28
34	a	615	STE	O2-C1-C2	2.03	120.40	114.00
28	d	405	BCR	C11-C10-C9	-2.03	124.44	127.28
28	c	515	BCR	C30-C25-C26	-2.02	119.87	122.64
26	B	611	CLA	CHB-C4A-NA	2.02	127.32	124.40
26	C	504	CLA	C2D-C1D-ND	-2.02	108.12	110.13
26	b	613	CLA	CHA-C4D-ND	2.02	136.72	132.55
28	d	405	BCR	C38-C26-C25	-2.02	122.28	124.48
26	c	504	CLA	CHD-C1D-ND	-2.02	121.96	124.80
26	C	503	CLA	CHD-C1D-C2D	2.02	129.68	125.49
26	b	601	CLA	CAC-C3C-C4C	2.02	127.42	124.79
28	X	101	BCR	C29-C30-C25	2.02	113.37	110.44
26	B	613	CLA	O2D-CGD-O1D	-2.02	119.92	123.85
27	a	608	PHO	OBD-CAD-C3D	2.02	131.04	127.89
26	b	613	CLA	O1D-CGD-CBD	2.01	128.49	124.52
30	C	518	LMG	O2-C2-C1	-2.01	105.28	110.08
26	c	512	CLA	CHD-C1D-C2D	2.01	129.67	125.49
31	e	102	LHG	C18-C17-C16	-2.01	104.20	114.37
31	D	409	LHG	C27-C26-C25	-2.01	104.21	114.37
26	c	513	CLA	CMB-C2B-C3B	2.01	131.28	126.55
26	b	613	CLA	O2D-CGD-CBD	2.01	114.74	111.23
26	b	609	CLA	O1D-CGD-CBD	2.01	128.48	124.52
30	D	406	LMG	C1-C2-C3	-2.01	105.78	110.01
30	A	614	LMG	O8-C28-O10	-2.01	118.60	123.63
33	A	619	DGD	C1D-C2D-C3D	-2.01	105.78	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	507	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
31	D	409	LHG	C18-C17-C16	-2.01	104.22	114.37
30	d	410	LMG	O7-C10-O9	-2.01	118.17	123.33
27	D	401	PHO	OBD-CAD-C3D	2.01	131.02	127.89
34	B	623	STE	O2-C1-C2	2.01	120.34	114.00
26	C	510	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
26	b	612	CLA	CHB-C1B-NB	2.01	127.06	124.05
33	A	619	DGD	CAB-C9B-C8B	-2.00	104.23	114.37
33	C	517	DGD	CBB-CAB-C9B	-2.00	104.24	114.37
30	d	411	LMG	O5-C6-C5	-2.00	104.51	111.33
28	T	101	BCR	C1-C6-C5	-2.00	119.90	122.64
30	c	522	LMG	C42-C41-C40	-2.00	104.24	114.37
35	e	101	HEM	C2D-C1D-ND	-2.00	107.59	109.90
30	b	621	LMG	C42-C41-C40	-2.00	104.25	114.37
26	c	502	CLA	CHD-C1D-ND	-2.00	121.98	124.80
26	B	612	CLA	C11-C12-C13	-2.00	109.31	115.97
30	A	614	LMG	O3-C3-C2	-2.00	105.66	110.38
28	d	405	BCR	C7-C8-C9	-2.00	123.28	126.23

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
36	V	201	HEC	NA
36	v	201	HEC	NA

All (1804) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A	608	CLA	C2B-C3B-CAB-CBB
26	A	608	CLA	C4B-C3B-CAB-CBB
26	B	602	CLA	C6-C7-C8-C9
26	B	614	CLA	CAD-CBD-CGD-O1D
26	B	614	CLA	CAD-CBD-CGD-O2D
26	B	615	CLA	C2B-C3B-CAB-CBB
26	B	615	CLA	C4B-C3B-CAB-CBB
26	C	503	CLA	C2B-C3B-CAB-CBB
26	C	503	CLA	C4B-C3B-CAB-CBB
26	C	507	CLA	CHA-CBD-CGD-O2D
26	C	512	CLA	C2B-C3B-CAB-CBB
26	C	512	CLA	C4B-C3B-CAB-CBB
26	D	403	CLA	C4-C3-C5-C6
26	a	612	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
26	b	605	CLA	C14-C13-C15-C16
26	b	613	CLA	CAD-CBD-CGD-O1D
26	b	613	CLA	CAD-CBD-CGD-O2D
26	b	613	CLA	C11-C12-C13-C15
26	c	505	CLA	C2B-C3B-CAB-CBB
26	c	505	CLA	C4B-C3B-CAB-CBB
26	c	512	CLA	C2B-C3B-CAB-CBB
26	c	512	CLA	C4B-C3B-CAB-CBB
26	d	404	CLA	C2B-C3B-CAB-CBB
26	d	404	CLA	C4B-C3B-CAB-CBB
26	h	101	CLA	C1A-C2A-CAA-CBA
28	A	611	BCR	C12-C13-C14-C15
28	A	611	BCR	C35-C13-C14-C15
28	D	404	BCR	C7-C8-C9-C34
28	D	404	BCR	C23-C24-C25-C26
28	K	101	BCR	C5-C6-C7-C8
28	K	101	BCR	C21-C22-C23-C24
28	K	101	BCR	C37-C22-C23-C24
28	T	101	BCR	C5-C6-C7-C8
28	T	101	BCR	C6-C7-C8-C9
28	T	101	BCR	C7-C8-C9-C10
28	Z	101	BCR	C16-C17-C18-C19
28	Z	101	BCR	C16-C17-C18-C36
28	d	405	BCR	C23-C24-C25-C26
28	d	405	BCR	C23-C24-C25-C30
28	h	102	BCR	C11-C10-C9-C8
29	A	612	PL9	C12-C13-C14-C16
29	A	612	PL9	C34-C36-C37-C38
29	A	612	PL9	C37-C38-C39-C40
29	D	405	PL9	C32-C33-C34-C36
29	D	405	PL9	C42-C43-C44-C46
29	a	611	PL9	C22-C23-C24-C26
29	a	611	PL9	C39-C41-C42-C43
29	a	611	PL9	C47-C48-C49-C50
29	d	406	PL9	C32-C33-C34-C36
29	d	406	PL9	C40-C39-C41-C42
30	A	614	LMG	O9-C10-O7-C8
30	A	614	LMG	C11-C10-O7-C8
30	C	518	LMG	C11-C10-O7-C8
30	D	408	LMG	O1-C7-C8-O7
30	c	523	LMG	O6-C1-O1-C7
31	A	615	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
31	A	615	LHG	O1-C1-C2-C3
31	A	615	LHG	C3-O3-P-O6
31	D	407	LHG	C1-C2-C3-O3
31	D	407	LHG	C3-O3-P-O4
31	D	407	LHG	C3-O3-P-O5
31	D	407	LHG	C3-O3-P-O6
31	D	407	LHG	C4-O6-P-O3
31	D	407	LHG	C4-O6-P-O4
31	D	407	LHG	C4-O6-P-O5
31	D	409	LHG	C1-C2-C3-O3
31	D	409	LHG	C3-O3-P-O5
31	D	409	LHG	C3-O3-P-O6
31	L	101	LHG	C4-O6-P-O3
31	d	408	LHG	C1-C2-C3-O3
31	d	408	LHG	C3-O3-P-O5
31	d	408	LHG	C4-O6-P-O3
31	d	408	LHG	C4-O6-P-O4
31	e	102	LHG	O1-C1-C2-C3
31	e	102	LHG	C4-O6-P-O3
31	e	102	LHG	C4-O6-P-O4
31	l	101	LHG	C4-O6-P-O3
32	B	622	SQD	C2-C1-O6-C44
32	B	622	SQD	O5-C1-O6-C44
32	B	622	SQD	O49-C7-O47-C45
32	B	622	SQD	C8-C7-O47-C45
32	F	102	SQD	O5-C1-O6-C44
32	a	613	SQD	O6-C44-C45-O47
32	b	619	SQD	O5-C1-O6-C44
32	b	619	SQD	O49-C7-O47-C45
32	b	619	SQD	C5-C6-S-O7
32	b	619	SQD	C5-C6-S-O8
32	b	619	SQD	C5-C6-S-O9
32	f	101	SQD	O5-C1-O6-C44
32	t	102	SQD	O6-C44-C45-C46
32	t	102	SQD	O6-C44-C45-O47
32	t	102	SQD	O49-C7-O47-C45
32	t	102	SQD	C8-C7-O47-C45
33	A	619	DGD	C2B-C1B-O2G-C2G
33	A	619	DGD	O1B-C1B-O2G-C2G
33	A	619	DGD	O2G-C2G-C3G-O3G
26	h	101	CLA	O1D-CGD-O2D-CED
26	c	513	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	h	101	CLA	CBD-CGD-O2D-CED
30	A	614	LMG	O10-C28-O8-C9
30	c	522	LMG	O10-C28-O8-C9
30	c	523	LMG	O10-C28-O8-C9
29	a	611	PL9	C47-C48-C49-C51
31	A	617	LHG	O10-C23-O8-C6
31	e	102	LHG	O10-C23-O8-C6
32	f	101	SQD	O10-C23-O48-C46
30	D	408	LMG	O9-C10-O7-C8
30	c	522	LMG	O9-C10-O7-C8
26	A	610	CLA	C3-C5-C6-C7
26	B	616	CLA	C3-C5-C6-C7
26	C	512	CLA	C3-C5-C6-C7
26	b	613	CLA	C3-C5-C6-C7
30	A	614	LMG	C29-C28-O8-C9
30	c	523	LMG	C29-C28-O8-C9
31	A	617	LHG	C24-C23-O8-C6
31	e	102	LHG	C24-C23-O8-C6
36	V	201	HEC	C4C-C3C-CAC-CBC
26	C	501	CLA	CBD-CGD-O2D-CED
26	b	606	CLA	CBD-CGD-O2D-CED
27	d	402	PHO	CBD-CGD-O2D-CED
30	D	408	LMG	C11-C10-O7-C8
32	b	619	SQD	C8-C7-O47-C45
26	B	604	CLA	C4-C3-C5-C6
26	B	605	CLA	C4-C3-C5-C6
26	B	607	CLA	C4-C3-C5-C6
26	C	504	CLA	C4-C3-C5-C6
26	b	602	CLA	C4-C3-C5-C6
26	c	507	CLA	C4-C3-C5-C6
29	A	612	PL9	C25-C24-C26-C27
29	A	612	PL9	C40-C39-C41-C42
29	A	612	PL9	C45-C44-C46-C47
26	B	605	CLA	C2-C3-C5-C6
26	B	607	CLA	C2-C3-C5-C6
26	D	403	CLA	C2-C3-C5-C6
26	b	602	CLA	C2-C3-C5-C6
26	c	507	CLA	C2-C3-C5-C6
29	A	612	PL9	C18-C19-C21-C22
29	d	406	PL9	C38-C39-C41-C42
32	F	102	SQD	C24-C23-O48-C46
32	f	101	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
29	D	405	PL9	C32-C33-C34-C35
29	a	611	PL9	C22-C23-C24-C25
29	A	612	PL9	C32-C33-C34-C36
29	A	612	PL9	C37-C38-C39-C41
29	a	611	PL9	C42-C43-C44-C46
30	C	518	LMG	O9-C10-O7-C8
26	b	603	CLA	C3-C5-C6-C7
26	h	101	CLA	C3-C5-C6-C7
26	c	503	CLA	CBD-CGD-O2D-CED
31	D	407	LHG	O2-C2-C3-O3
26	B	601	CLA	CBA-CGA-O2A-C1
30	c	522	LMG	C29-C28-O8-C9
32	F	102	SQD	O10-C23-O48-C46
30	c	522	LMG	C11-C10-O7-C8
26	c	513	CLA	O1D-CGD-O2D-CED
30	c	520	LMG	C4-C5-C6-O5
26	B	614	CLA	C4-C3-C5-C6
26	b	613	CLA	C4-C3-C5-C6
26	B	614	CLA	C2-C3-C5-C6
26	b	604	CLA	C2-C3-C5-C6
29	A	612	PL9	C23-C24-C26-C27
26	B	601	CLA	O1A-CGA-O2A-C1
29	A	612	PL9	C9-C11-C12-C13
29	A	612	PL9	C24-C26-C27-C28
29	A	612	PL9	C29-C31-C32-C33
29	a	611	PL9	C19-C21-C22-C23
29	a	611	PL9	C24-C26-C27-C28
36	V	201	HEC	C2C-C3C-CAC-CBC
26	b	611	CLA	C8-C10-C11-C12
30	c	520	LMG	O6-C5-C6-O5
30	A	614	LMG	O6-C1-O1-C7
30	b	621	LMG	O6-C1-O1-C7
29	a	611	PL9	C42-C43-C44-C45
26	B	615	CLA	CBD-CGD-O2D-CED
31	d	409	LHG	C24-C25-C26-C27
31	e	102	LHG	C1-C2-C3-O3
26	c	506	CLA	CBA-CGA-O2A-C1
32	b	619	SQD	C24-C23-O48-C46
32	B	622	SQD	C29-C30-C31-C32
26	b	604	CLA	C4-C3-C5-C6
29	a	611	PL9	C30-C29-C31-C32
29	a	611	PL9	C35-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
26	C	504	CLA	C2-C3-C5-C6
29	A	612	PL9	C43-C44-C46-C47
29	a	611	PL9	C33-C34-C36-C37
26	A	608	CLA	C14-C13-C15-C16
26	B	606	CLA	C11-C10-C8-C9
26	B	607	CLA	C6-C7-C8-C9
26	C	503	CLA	C11-C10-C8-C9
26	C	509	CLA	C11-C10-C8-C9
26	C	512	CLA	C6-C7-C8-C9
26	D	403	CLA	C11-C12-C13-C14
26	b	601	CLA	C11-C10-C8-C9
26	b	603	CLA	C6-C7-C8-C9
26	b	604	CLA	C11-C10-C8-C9
26	b	609	CLA	C14-C13-C15-C16
26	b	615	CLA	C6-C7-C8-C9
26	c	502	CLA	C6-C7-C8-C9
26	c	509	CLA	C6-C7-C8-C9
26	c	512	CLA	C6-C7-C8-C9
26	h	101	CLA	C11-C10-C8-C9
30	b	621	LMG	C2-C1-O1-C7
32	f	101	SQD	C2-C1-O6-C44
31	D	409	LHG	O2-C2-C3-O3
31	d	408	LHG	O2-C2-C3-O3
31	e	102	LHG	O2-C2-C3-O3
33	c	519	DGD	O1A-C1A-O1G-C1G
28	B	619	BCR	C37-C22-C23-C24
28	K	101	BCR	C7-C8-C9-C34
28	X	101	BCR	C11-C12-C13-C35
28	Z	101	BCR	C7-C8-C9-C34
28	k	101	BCR	C7-C8-C9-C34
28	t	101	BCR	C7-C8-C9-C34
31	d	407	LHG	C23-C24-C25-C26
34	B	620	STE	C1-C2-C3-C4
32	A	618	SQD	C9-C10-C11-C12
29	D	405	PL9	C47-C48-C49-C51
30	M	101	LMG	O10-C28-O8-C9
26	b	611	CLA	CBD-CGD-O2D-CED
26	c	512	CLA	CBD-CGD-O2D-CED
32	B	622	SQD	O6-C44-C45-O47
26	c	506	CLA	O1A-CGA-O2A-C1
26	b	606	CLA	O1D-CGD-O2D-CED
26	B	614	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	d	406	PL9	C37-C38-C39-C40
26	A	613	CLA	C13-C15-C16-C17
26	C	503	CLA	C5-C6-C7-C8
26	C	505	CLA	C15-C16-C17-C18
26	b	614	CLA	C15-C16-C17-C18
26	c	511	CLA	C13-C15-C16-C17
31	e	102	LHG	O1-C1-C2-O2
30	B	621	LMG	C10-C11-C12-C13
30	b	621	LMG	O6-C5-C6-O5
26	C	511	CLA	C11-C12-C13-C15
26	C	512	CLA	C11-C10-C8-C7
26	b	614	CLA	C11-C12-C13-C15
26	c	510	CLA	C11-C12-C13-C15
27	d	402	PHO	O1D-CGD-O2D-CED
33	C	515	DGD	O6E-C5E-C6E-O5E
32	f	101	SQD	C23-C24-C25-C26
33	a	614	DGD	O1B-C1B-O2G-C2G
26	h	101	CLA	C15-C16-C17-C18
30	c	522	LMG	C10-C11-C12-C13
32	A	616	SQD	C23-C24-C25-C26
33	c	519	DGD	C1A-C2A-C3A-C4A
34	C	520	STE	C1-C2-C3-C4
26	B	613	CLA	C15-C16-C17-C18
26	B	615	CLA	C5-C6-C7-C8
26	b	608	CLA	C15-C16-C17-C18
26	c	513	CLA	C10-C11-C12-C13
26	b	605	CLA	C2A-CAA-CBA-CGA
26	h	101	CLA	C2A-CAA-CBA-CGA
26	B	601	CLA	C13-C15-C16-C17
26	B	603	CLA	C15-C16-C17-C18
26	a	606	CLA	C15-C16-C17-C18
26	b	610	CLA	C8-C10-C11-C12
26	b	614	CLA	C10-C11-C12-C13
26	c	503	CLA	C5-C6-C7-C8
26	c	508	CLA	C13-C15-C16-C17
26	c	511	CLA	C15-C16-C17-C18
30	D	408	LMG	C28-C29-C30-C31
30	M	101	LMG	C28-C29-C30-C31
32	A	618	SQD	C23-C24-C25-C26
34	d	412	STE	C1-C2-C3-C4
32	b	619	SQD	O10-C23-O48-C46
26	c	503	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	B	607	CLA	C8-C10-C11-C12
26	C	505	CLA	C10-C11-C12-C13
26	C	506	CLA	C15-C16-C17-C18
26	C	512	CLA	C13-C15-C16-C17
26	b	601	CLA	C10-C11-C12-C13
26	c	502	CLA	C13-C15-C16-C17
31	A	617	LHG	O2-C2-C3-O3
34	c	521	STE	C1-C2-C3-C4
26	C	509	CLA	C5-C6-C7-C8
26	b	607	CLA	C5-C6-C7-C8
26	b	613	CLA	C5-C6-C7-C8
29	A	612	PL9	C12-C13-C14-C15
26	C	512	CLA	C15-C16-C17-C18
26	b	606	CLA	C5-C6-C7-C8
26	b	610	CLA	C13-C15-C16-C17
26	C	502	CLA	CBD-CGD-O2D-CED
26	B	604	CLA	C2-C3-C5-C6
32	A	616	SQD	C7-C8-C9-C10
32	F	102	SQD	C23-C24-C25-C26
26	A	613	CLA	C15-C16-C17-C18
26	B	613	CLA	C8-C10-C11-C12
26	C	504	CLA	C8-C10-C11-C12
26	C	509	CLA	C8-C10-C11-C12
26	h	101	CLA	C10-C11-C12-C13
30	M	101	LMG	C29-C28-O8-C9
32	t	102	SQD	C24-C23-O48-C46
32	f	101	SQD	C8-C7-O47-C45
26	C	502	CLA	C13-C15-C16-C17
34	b	620	STE	C14-C15-C16-C17
34	C	519	STE	C1-C2-C3-C4
32	f	101	SQD	O49-C7-O47-C45
31	A	617	LHG	C1-C2-C3-O3
26	B	606	CLA	C2A-CAA-CBA-CGA
26	B	611	CLA	C8-C10-C11-C12
26	b	606	CLA	C8-C10-C11-C12
26	b	609	CLA	C15-C16-C17-C18
26	b	613	CLA	C15-C16-C17-C18
26	c	503	CLA	C10-C11-C12-C13
26	c	503	CLA	C15-C16-C17-C18
26	c	507	CLA	C5-C6-C7-C8
29	A	612	PL9	C47-C48-C49-C51
26	C	501	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	D	406	LMG	C10-C11-C12-C13
26	B	606	CLA	C15-C16-C17-C18
26	C	507	CLA	C5-C6-C7-C8
26	c	509	CLA	C13-C15-C16-C17
32	F	102	SQD	C45-C46-O48-C23
26	B	605	CLA	C13-C15-C16-C17
26	B	616	CLA	C5-C6-C7-C8
26	B	616	CLA	C8-C10-C11-C12
26	C	507	CLA	C13-C15-C16-C17
26	a	609	CLA	C13-C15-C16-C17
26	b	611	CLA	C10-C11-C12-C13
32	b	619	SQD	C7-C8-C9-C10
29	a	611	PL9	C23-C24-C26-C27
33	a	614	DGD	C2B-C1B-O2G-C2G
26	C	512	CLA	C14-C13-C15-C16
30	C	518	LMG	C2-C1-O1-C7
30	c	523	LMG	C2-C1-O1-C7
32	F	102	SQD	C2-C1-O6-C44
33	c	518	DGD	C2E-C1E-O5D-C6D
26	b	612	CLA	C16-C17-C18-C20
26	C	508	CLA	C13-C15-C16-C17
36	v	201	HEC	C2C-C3C-CAC-CBC
28	B	617	BCR	C35-C13-C14-C15
28	C	514	BCR	C35-C13-C14-C15
28	D	404	BCR	C20-C21-C22-C37
28	T	101	BCR	C20-C21-C22-C37
28	a	610	BCR	C16-C17-C18-C36
28	b	616	BCR	C20-C21-C22-C37
28	b	617	BCR	C20-C21-C22-C37
28	b	618	BCR	C20-C21-C22-C37
28	c	515	BCR	C16-C17-C18-C36
28	c	515	BCR	C20-C21-C22-C37
28	C	514	BCR	C11-C12-C13-C35
28	T	101	BCR	C7-C8-C9-C34
34	t	105	STE	C11-C12-C13-C14
26	B	604	CLA	C10-C11-C12-C13
31	d	407	LHG	O1-C1-C2-C3
31	d	409	LHG	O1-C1-C2-C3
34	j	101	STE	C1-C2-C3-C4
26	A	608	CLA	C16-C17-C18-C20
26	B	601	CLA	C16-C17-C18-C19
26	b	613	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
28	B	617	BCR	C20-C21-C22-C23
28	C	514	BCR	C11-C10-C9-C8
28	C	514	BCR	C12-C13-C14-C15
30	C	518	LMG	O6-C1-O1-C7
30	c	520	LMG	O6-C1-O1-C7
33	c	518	DGD	O6E-C1E-O5D-C6D
26	c	506	CLA	C13-C15-C16-C17
29	d	406	PL9	C33-C34-C36-C37
32	A	618	SQD	C11-C12-C13-C14
30	c	520	LMG	C29-C28-O8-C9
26	C	508	CLA	C10-C11-C12-C13
26	b	612	CLA	C10-C11-C12-C13
26	B	606	CLA	CBD-CGD-O2D-CED
27	D	401	PHO	CBD-CGD-O2D-CED
26	A	608	CLA	C16-C17-C18-C19
26	B	603	CLA	C16-C17-C18-C19
26	B	605	CLA	C16-C17-C18-C20
26	B	611	CLA	C16-C17-C18-C19
26	B	611	CLA	C16-C17-C18-C20
26	B	615	CLA	C16-C17-C18-C20
26	b	610	CLA	C16-C17-C18-C20
26	c	503	CLA	C16-C17-C18-C20
33	C	517	DGD	O1A-C1A-O1G-C1G
30	D	406	LMG	C16-C17-C18-C19
30	m	101	LMG	C32-C33-C34-C35
31	L	101	LHG	C31-C32-C33-C34
31	d	409	LHG	C30-C31-C32-C33
32	a	613	SQD	C10-C11-C12-C13
33	c	519	DGD	C9B-CAB-CBB-CCB
34	T	103	STE	C13-C14-C15-C16
34	b	620	STE	C3-C4-C5-C6
34	b	622	STE	C2-C3-C4-C5
34	c	521	STE	C9-C10-C11-C12
28	b	618	BCR	C14-C15-C16-C17
30	c	523	LMG	C33-C34-C35-C36
30	d	410	LMG	C35-C36-C37-C38
31	D	407	LHG	C18-C19-C20-C21
31	e	102	LHG	C11-C10-C9-C8
32	t	102	SQD	C16-C17-C18-C19
33	A	619	DGD	C7A-C8A-C9A-CAA
33	c	517	DGD	C4B-C5B-C6B-C7B
33	c	517	DGD	CAB-CBB-CCB-CDB

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Mol	Chain	Res	Type	Atoms
33	c	518	DGD	CBB-CCB-CDB-CEB
33	h	103	DGD	C7B-C8B-C9B-CAB
26	b	614	CLA	C5-C6-C7-C8
30	M	101	LMG	C33-C34-C35-C36
30	d	411	LMG	C11-C12-C13-C14
31	D	407	LHG	C12-C13-C14-C15
31	D	409	LHG	C27-C28-C29-C30
32	t	102	SQD	C11-C12-C13-C14
33	c	519	DGD	C2B-C3B-C4B-C5B
33	h	103	DGD	C9B-CAB-CBB-CCB
34	H	102	STE	C11-C12-C13-C14
34	k	102	STE	C2-C3-C4-C5
33	c	519	DGD	C2A-C1A-O1G-C1G
30	C	518	LMG	C11-C12-C13-C14
30	c	522	LMG	C30-C31-C32-C33
31	A	617	LHG	C16-C17-C18-C19
31	A	617	LHG	C26-C27-C28-C29
31	A	617	LHG	C28-C29-C30-C31
31	D	407	LHG	C28-C29-C30-C31
31	d	409	LHG	C27-C28-C29-C30
31	e	102	LHG	C16-C17-C18-C19
31	e	102	LHG	C27-C28-C29-C30
32	A	618	SQD	C28-C29-C30-C31
32	a	613	SQD	C12-C13-C14-C15
33	A	619	DGD	C4B-C5B-C6B-C7B
33	C	515	DGD	CCB-CDB-CEB-CFB
33	a	614	DGD	C2B-C3B-C4B-C5B
34	T	102	STE	C5-C6-C7-C8
34	a	615	STE	C2-C3-C4-C5
34	d	414	STE	C12-C13-C14-C15
32	F	102	SQD	C45-C44-O6-C1
26	B	601	CLA	C3-C5-C6-C7
30	C	518	LMG	C31-C32-C33-C34
33	H	101	DGD	C7B-C8B-C9B-CAB
26	h	101	CLA	C4B-C3B-CAB-CBB
30	b	621	LMG	C40-C41-C42-C43
33	C	517	DGD	C5A-C6A-C7A-C8A
34	C	521	STE	C5-C6-C7-C8
26	A	607	CLA	C16-C17-C18-C19
26	B	601	CLA	C16-C17-C18-C20
26	B	603	CLA	C16-C17-C18-C20
26	B	605	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
26	C	505	CLA	C16-C17-C18-C20
26	a	609	CLA	C16-C17-C18-C19
26	a	609	CLA	C16-C17-C18-C20
26	b	610	CLA	C16-C17-C18-C19
26	b	612	CLA	C16-C17-C18-C19
26	b	613	CLA	C16-C17-C18-C19
33	a	614	DGD	O1A-C1A-O1G-C1G
30	D	406	LMG	C20-C21-C22-C23
26	c	509	CLA	C8-C10-C11-C12
30	C	518	LMG	C17-C18-C19-C20
34	I	101	STE	C11-C10-C9-C8
30	C	518	LMG	C30-C31-C32-C33
31	d	407	LHG	C30-C31-C32-C33
31	d	408	LHG	C30-C31-C32-C33
32	f	101	SQD	C27-C28-C29-C30
31	A	615	LHG	C7-C8-C9-C10
30	m	101	LMG	C29-C28-O8-C9
26	B	613	CLA	C5-C6-C7-C8
26	D	403	CLA	C10-C11-C12-C13
26	a	609	CLA	C5-C6-C7-C8
26	b	615	CLA	C5-C6-C7-C8
26	c	512	CLA	C13-C15-C16-C17
30	D	406	LMG	C15-C16-C17-C18
30	c	523	LMG	C14-C15-C16-C17
30	m	101	LMG	C34-C35-C36-C37
32	B	622	SQD	C13-C14-C15-C16
32	f	101	SQD	C24-C25-C26-C27
33	a	614	DGD	C3B-C4B-C5B-C6B
34	C	521	STE	C6-C7-C8-C9
34	d	412	STE	C5-C6-C7-C8
34	j	101	STE	C2-C3-C4-C5
26	h	101	CLA	C3A-C2A-CAA-CBA
30	c	520	LMG	C31-C32-C33-C34
32	t	102	SQD	C14-C15-C16-C17
33	c	519	DGD	C3B-C4B-C5B-C6B
26	b	613	CLA	C2-C3-C5-C6
31	A	615	LHG	C11-C12-C13-C14
31	L	101	LHG	C30-C31-C32-C33
26	C	506	CLA	C8-C10-C11-C12
26	b	615	CLA	C10-C11-C12-C13
26	d	404	CLA	C5-C6-C7-C8
26	B	606	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
26	c	504	CLA	C11-C12-C13-C14
32	t	102	SQD	O10-C23-O48-C46
32	t	102	SQD	C13-C14-C15-C16
33	A	619	DGD	CCB-CDB-CEB-CFB
26	a	609	CLA	C15-C16-C17-C18
31	A	617	LHG	C18-C19-C20-C21
31	D	409	LHG	C18-C19-C20-C21
33	A	619	DGD	CCA-CDA-CEA-CFA
34	T	102	STE	C7-C8-C9-C10
30	D	406	LMG	C21-C22-C23-C24
30	d	410	LMG	C31-C32-C33-C34
31	L	101	LHG	C26-C27-C28-C29
31	d	407	LHG	C27-C28-C29-C30
32	a	613	SQD	C11-C10-C9-C8
32	t	102	SQD	C10-C11-C12-C13
32	t	102	SQD	C18-C19-C20-C21
33	C	517	DGD	C7B-C8B-C9B-CAB
33	c	519	DGD	C5A-C6A-C7A-C8A
33	h	103	DGD	CBA-CCA-CDA-CEA
33	h	103	DGD	C5B-C6B-C7B-C8B
34	B	623	STE	C5-C6-C7-C8
34	d	413	STE	C3-C4-C5-C6
26	C	509	CLA	C3-C5-C6-C7
30	d	411	LMG	C28-C29-C30-C31
32	A	618	SQD	C7-C8-C9-C10
26	b	608	CLA	C13-C15-C16-C17
31	A	617	LHG	C29-C30-C31-C32
31	d	408	LHG	C12-C13-C14-C15
31	d	408	LHG	C18-C19-C20-C21
31	d	409	LHG	C26-C27-C28-C29
33	h	103	DGD	C2B-C3B-C4B-C5B
34	T	102	STE	C12-C13-C14-C15
34	b	622	STE	C3-C4-C5-C6
34	d	414	STE	C6-C7-C8-C9
30	D	406	LMG	C18-C19-C20-C21
30	d	410	LMG	C32-C33-C34-C35
30	m	101	LMG	C38-C39-C40-C41
31	L	101	LHG	C17-C18-C19-C20
31	L	101	LHG	C32-C33-C34-C35
33	a	614	DGD	CDB-CEB-CFB-CGB
33	c	519	DGD	C6A-C7A-C8A-C9A
34	B	620	STE	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
34	j	101	STE	C5-C6-C7-C8
34	t	103	STE	C6-C7-C8-C9
30	M	101	LMG	C13-C14-C15-C16
34	C	520	STE	C6-C7-C8-C9
34	F	103	STE	C3-C4-C5-C6
30	m	101	LMG	C18-C19-C20-C21
32	a	613	SQD	C18-C19-C20-C21
32	b	619	SQD	C26-C27-C28-C29
34	C	520	STE	C5-C6-C7-C8
34	C	521	STE	C7-C8-C9-C10
26	B	609	CLA	C16-C17-C18-C20
32	a	613	SQD	C23-C24-C25-C26
28	D	404	BCR	C23-C24-C25-C30
28	K	101	BCR	C1-C6-C7-C8
28	T	101	BCR	C1-C6-C7-C8
28	k	101	BCR	C1-C6-C7-C8
28	k	101	BCR	C5-C6-C7-C8
26	B	616	CLA	CBD-CGD-O2D-CED
26	C	509	CLA	C13-C15-C16-C17
26	b	613	CLA	C13-C15-C16-C17
30	c	522	LMG	C33-C34-C35-C36
33	A	619	DGD	C2B-C3B-C4B-C5B
33	C	516	DGD	C4A-C5A-C6A-C7A
30	b	621	LMG	C16-C17-C18-C19
34	d	413	STE	C5-C6-C7-C8
34	B	623	STE	C1-C2-C3-C4
32	A	616	SQD	C16-C17-C18-C19
34	C	519	STE	C5-C6-C7-C8
34	c	521	STE	C11-C12-C13-C14
31	A	615	LHG	C30-C31-C32-C33
32	F	102	SQD	C34-C35-C36-C37
34	T	102	STE	C14-C15-C16-C17
34	d	413	STE	C10-C11-C12-C13
29	A	612	PL9	C20-C19-C21-C22
30	A	614	LMG	C35-C36-C37-C38
30	D	406	LMG	C37-C38-C39-C40
30	b	621	LMG	C17-C18-C19-C20
30	c	523	LMG	C18-C19-C20-C21
31	D	407	LHG	C15-C16-C17-C18
32	a	613	SQD	C29-C30-C31-C32
28	c	516	BCR	C10-C11-C12-C13
28	t	101	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
30	c	523	LMG	C36-C37-C38-C39
30	d	411	LMG	C38-C39-C40-C41
32	a	613	SQD	C32-C33-C34-C35
33	H	101	DGD	C3B-C4B-C5B-C6B
34	T	103	STE	C9-C10-C11-C12
26	b	606	CLA	CBA-CGA-O2A-C1
26	d	404	CLA	C6-C7-C8-C9
30	c	523	LMG	C17-C18-C19-C20
31	D	409	LHG	C14-C15-C16-C17
32	B	622	SQD	C11-C12-C13-C14
33	A	619	DGD	C2A-C3A-C4A-C5A
34	B	625	STE	C11-C12-C13-C14
34	C	521	STE	C10-C11-C12-C13
30	M	101	LMG	C15-C16-C17-C18
30	c	523	LMG	C32-C33-C34-C35
31	A	615	LHG	C34-C35-C36-C37
33	C	516	DGD	CCA-CDA-CEA-CFA
33	c	517	DGD	C7A-C8A-C9A-CAA
33	c	518	DGD	O6D-C1D-O3G-C3G
31	A	615	LHG	C25-C26-C27-C28
31	D	409	LHG	C29-C30-C31-C32
32	F	102	SQD	C25-C26-C27-C28
34	a	615	STE	C4-C5-C6-C7
26	C	513	CLA	C15-C16-C17-C18
30	D	406	LMG	C36-C37-C38-C39
30	m	101	LMG	C16-C17-C18-C19
32	a	613	SQD	C16-C17-C18-C19
33	c	519	DGD	C4A-C5A-C6A-C7A
34	L	102	STE	C6-C7-C8-C9
34	b	620	STE	C12-C13-C14-C15
30	D	408	LMG	C11-C12-C13-C14
30	d	411	LMG	C39-C40-C41-C42
31	A	615	LHG	C13-C14-C15-C16
31	d	407	LHG	C16-C17-C18-C19
32	B	622	SQD	C25-C26-C27-C28
33	a	614	DGD	C5A-C6A-C7A-C8A
33	h	103	DGD	C7A-C8A-C9A-CAA
26	B	604	CLA	C3-C5-C6-C7
33	a	614	DGD	C2A-C1A-O1G-C1G
33	c	518	DGD	O6E-C5E-C6E-O5E
30	b	621	LMG	C11-C10-O7-C8
31	d	408	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
32	A	616	SQD	C8-C7-O47-C45
32	a	613	SQD	C8-C7-O47-C45
30	c	523	LMG	C10-C11-C12-C13
33	C	515	DGD	C5A-C6A-C7A-C8A
33	C	516	DGD	CCB-CDB-CEB-CFB
26	d	404	CLA	C10-C11-C12-C13
31	d	408	LHG	O9-C7-O7-C5
30	B	621	LMG	C31-C32-C33-C34
30	b	621	LMG	C15-C16-C17-C18
30	c	520	LMG	C34-C35-C36-C37
32	t	102	SQD	C15-C16-C17-C18
31	e	102	LHG	C17-C18-C19-C20
32	b	619	SQD	C11-C12-C13-C14
26	D	403	CLA	C15-C16-C17-C18
32	t	102	SQD	C17-C18-C19-C20
31	A	617	LHG	C23-C24-C25-C26
31	d	407	LHG	C32-C33-C34-C35
34	H	102	STE	C2-C3-C4-C5
30	A	614	LMG	C12-C13-C14-C15
31	L	101	LHG	C15-C16-C17-C18
31	l	101	LHG	C32-C33-C34-C35
32	F	102	SQD	C31-C32-C33-C34
31	l	101	LHG	C34-C35-C36-C37
33	a	614	DGD	C8A-C9A-CAA-CBA
31	A	615	LHG	C9-C10-C11-C12
33	C	516	DGD	C7A-C8A-C9A-CAA
33	c	517	DGD	CBB-CCB-CDB-CEB
34	X	102	STE	C7-C8-C9-C10
26	A	610	CLA	C5-C6-C7-C8
32	t	102	SQD	C19-C20-C21-C22
26	b	609	CLA	C2C-C3C-CAC-CBC
32	A	616	SQD	C30-C31-C32-C33
33	A	619	DGD	C5B-C6B-C7B-C8B
33	A	619	DGD	O6E-C5E-C6E-O5E
26	C	513	CLA	C10-C11-C12-C13
26	b	612	CLA	C13-C15-C16-C17
26	c	502	CLA	C15-C16-C17-C18
30	D	406	LMG	C19-C20-C21-C22
30	M	101	LMG	C34-C35-C36-C37
32	A	616	SQD	C29-C30-C31-C32
33	H	101	DGD	C6B-C7B-C8B-C9B
33	h	103	DGD	CCA-CDA-CEA-CFA

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Mol	Chain	Res	Type	Atoms
33	c	518	DGD	C8B-C9B-CAB-CBB
34	c	521	STE	C12-C13-C14-C15
29	A	612	PL9	C44-C46-C47-C48
26	C	505	CLA	C16-C17-C18-C19
31	L	101	LHG	C18-C19-C20-C21
31	L	101	LHG	C29-C30-C31-C32
33	h	103	DGD	CAB-CBB-CCB-CDB
30	c	522	LMG	C31-C32-C33-C34
30	m	101	LMG	C28-C29-C30-C31
33	H	101	DGD	C1A-C2A-C3A-C4A
30	m	101	LMG	C13-C14-C15-C16
31	A	615	LHG	C27-C28-C29-C30
31	D	407	LHG	C16-C17-C18-C19
30	d	411	LMG	O6-C5-C6-O5
32	A	616	SQD	O6-C44-C45-O47
33	C	516	DGD	C6A-C7A-C8A-C9A
34	H	102	STE	C9-C10-C11-C12
34	I	101	STE	C11-C12-C13-C14
34	X	102	STE	C2-C3-C4-C5
30	D	406	LMG	C31-C32-C33-C34
31	A	615	LHG	C32-C33-C34-C35
31	d	408	LHG	C15-C16-C17-C18
32	B	622	SQD	C15-C16-C17-C18
32	B	622	SQD	C18-C19-C20-C21
33	C	517	DGD	C3A-C4A-C5A-C6A
26	B	601	CLA	C5-C6-C7-C8
36	v	201	HEC	C4C-C3C-CAC-CBC
30	D	408	LMG	C31-C32-C33-C34
31	d	407	LHG	C10-C11-C12-C13
33	c	517	DGD	C6B-C7B-C8B-C9B
34	t	105	STE	C7-C8-C9-C10
30	c	522	LMG	C12-C13-C14-C15
26	B	606	CLA	O1D-CGD-O2D-CED
30	D	406	LMG	C17-C18-C19-C20
31	A	617	LHG	C25-C26-C27-C28
32	b	619	SQD	C9-C10-C11-C12
34	T	103	STE	C6-C7-C8-C9
34	T	103	STE	C12-C13-C14-C15
30	m	101	LMG	O6-C5-C6-O5
30	c	522	LMG	C41-C42-C43-C44
26	C	506	CLA	C4-C3-C5-C6
31	D	409	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
33	c	519	DGD	C1B-C2B-C3B-C4B
29	D	405	PL9	C28-C29-C31-C32
26	c	513	CLA	C8-C10-C11-C12
30	c	522	LMG	C36-C37-C38-C39
31	L	101	LHG	C14-C15-C16-C17
33	c	519	DGD	C2A-C3A-C4A-C5A
34	C	519	STE	C6-C7-C8-C9
34	d	414	STE	C14-C15-C16-C17
26	b	609	CLA	C2A-CAA-CBA-CGA
26	B	607	CLA	CBD-CGD-O2D-CED
26	c	509	CLA	CBD-CGD-O2D-CED
30	D	406	LMG	C30-C31-C32-C33
30	d	410	LMG	C30-C31-C32-C33
31	A	617	LHG	C33-C34-C35-C36
31	d	407	LHG	C26-C27-C28-C29
33	C	515	DGD	C4B-C5B-C6B-C7B
33	H	101	DGD	C5A-C6A-C7A-C8A
34	X	102	STE	C5-C6-C7-C8
26	B	614	CLA	O1D-CGD-O2D-CED
26	c	512	CLA	O1D-CGD-O2D-CED
30	M	101	LMG	C39-C40-C41-C42
30	d	411	LMG	C32-C33-C34-C35
34	L	102	STE	C5-C6-C7-C8
30	b	621	LMG	C32-C33-C34-C35
30	m	101	LMG	C17-C18-C19-C20
34	C	521	STE	C11-C10-C9-C8
31	d	407	LHG	O1-C1-C2-O2
26	b	606	CLA	O1A-CGA-O2A-C1
31	d	408	LHG	C29-C30-C31-C32
30	b	621	LMG	C29-C30-C31-C32
33	C	517	DGD	C4B-C5B-C6B-C7B
26	a	609	CLA	C1A-C2A-CAA-CBA
26	c	508	CLA	C1A-C2A-CAA-CBA
26	c	513	CLA	C1A-C2A-CAA-CBA
26	b	606	CLA	C10-C11-C12-C13
26	b	610	CLA	C15-C16-C17-C18
26	c	503	CLA	C8-C10-C11-C12
26	c	507	CLA	C10-C11-C12-C13
30	D	408	LMG	C30-C31-C32-C33
31	A	615	LHG	C10-C11-C12-C13
33	H	101	DGD	C9B-CAB-CBB-CCB
33	c	517	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
33	c	517	DGD	C2A-C3A-C4A-C5A
34	C	521	STE	C11-C12-C13-C14
31	L	101	LHG	O6-C4-C5-C6
30	D	406	LMG	O6-C5-C6-O5
30	D	406	LMG	C35-C36-C37-C38
32	A	616	SQD	C10-C11-C12-C13
26	b	611	CLA	O1D-CGD-O2D-CED
26	B	604	CLA	C11-C10-C8-C7
26	B	615	CLA	C12-C13-C15-C16
26	C	507	CLA	C11-C10-C8-C7
26	C	508	CLA	C11-C10-C8-C7
26	C	510	CLA	C6-C7-C8-C10
26	C	511	CLA	C6-C7-C8-C10
26	C	512	CLA	C11-C12-C13-C15
26	a	607	CLA	C11-C10-C8-C7
26	b	601	CLA	C6-C7-C8-C10
26	b	601	CLA	C12-C13-C15-C16
26	b	603	CLA	C6-C7-C8-C10
26	b	605	CLA	C12-C13-C15-C16
26	b	606	CLA	C6-C7-C8-C10
26	b	614	CLA	C11-C10-C8-C7
26	c	506	CLA	C11-C12-C13-C15
26	c	508	CLA	C12-C13-C15-C16
26	c	513	CLA	C12-C13-C15-C16
30	c	522	LMG	C35-C36-C37-C38
30	d	410	LMG	C33-C34-C35-C36
33	c	518	DGD	C5A-C6A-C7A-C8A
32	A	618	SQD	C12-C13-C14-C15
34	d	413	STE	C9-C10-C11-C12
30	m	101	LMG	C10-C11-C12-C13
31	e	102	LHG	C14-C15-C16-C17
33	c	518	DGD	C4E-C5E-C6E-O5E
26	C	510	CLA	C2-C3-C5-C6
29	a	611	PL9	C13-C14-C16-C17
30	b	621	LMG	C22-C23-C24-C25
31	L	101	LHG	C10-C11-C12-C13
32	a	613	SQD	C26-C27-C28-C29
33	c	518	DGD	CBA-CCA-CDA-CEA
34	T	103	STE	C11-C12-C13-C14
26	C	501	CLA	C2A-CAA-CBA-CGA
26	B	604	CLA	C14-C13-C15-C16
26	B	605	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
26	B	616	CLA	C11-C10-C8-C9
26	C	508	CLA	C11-C10-C8-C9
26	C	511	CLA	C6-C7-C8-C9
26	b	601	CLA	C6-C7-C8-C9
26	b	602	CLA	C11-C10-C8-C9
26	c	505	CLA	C6-C7-C8-C9
26	c	508	CLA	C14-C13-C15-C16
26	c	511	CLA	C14-C13-C15-C16
26	c	513	CLA	C14-C13-C15-C16
32	a	613	SQD	C31-C32-C33-C34
33	C	517	DGD	C6A-C7A-C8A-C9A
33	c	517	DGD	C5B-C6B-C7B-C8B
34	j	101	STE	C4-C5-C6-C7
30	A	614	LMG	C36-C37-C38-C39
32	B	622	SQD	C24-C23-O48-C46
26	B	615	CLA	O1D-CGD-O2D-CED
30	m	101	LMG	C31-C32-C33-C34
31	L	101	LHG	C9-C10-C11-C12
33	C	516	DGD	C2E-C1E-O5D-C6D
34	B	623	STE	C3-C4-C5-C6
33	c	517	DGD	O6E-C5E-C6E-O5E
30	b	621	LMG	O1-C7-C8-C9
31	e	102	LHG	C4-C5-C6-O8
32	B	622	SQD	O6-C44-C45-C46
32	a	613	SQD	O6-C44-C45-C46
33	A	619	DGD	O1G-C1G-C2G-C3G
33	c	517	DGD	O6D-C5D-C6D-O5D
30	c	520	LMG	C35-C36-C37-C38
34	F	103	STE	C5-C6-C7-C8
34	l	102	STE	C14-C15-C16-C17
26	B	606	CLA	C16-C17-C18-C20
26	c	503	CLA	C16-C17-C18-C19
33	C	516	DGD	C3A-C4A-C5A-C6A
33	H	101	DGD	C7A-C8A-C9A-CAA
34	d	412	STE	C3-C4-C5-C6
30	D	408	LMG	C16-C17-C18-C19
30	b	621	LMG	C38-C39-C40-C41
31	D	407	LHG	C11-C12-C13-C14
28	A	611	BCR	C16-C17-C18-C36
28	b	618	BCR	C16-C17-C18-C36
26	D	402	CLA	C13-C15-C16-C17
30	m	101	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
33	H	101	DGD	CCB-CDB-CEB-CFB
31	d	408	LHG	C7-C8-C9-C10
26	C	510	CLA	C4-C3-C5-C6
26	C	506	CLA	C2-C3-C5-C6
29	d	406	PL9	C13-C14-C16-C17
28	d	405	BCR	C37-C22-C23-C24
33	c	517	DGD	C3B-C4B-C5B-C6B
32	A	618	SQD	C24-C25-C26-C27
34	X	102	STE	C11-C10-C9-C8
28	D	404	BCR	C7-C8-C9-C10
26	C	506	CLA	C13-C15-C16-C17
26	C	513	CLA	C8-C10-C11-C12
26	b	607	CLA	C13-C15-C16-C17
30	M	101	LMG	C37-C38-C39-C40
32	b	619	SQD	C18-C19-C20-C21
26	b	602	CLA	C13-C15-C16-C17
30	m	101	LMG	C29-C30-C31-C32
31	L	101	LHG	C28-C29-C30-C31
31	l	101	LHG	C15-C16-C17-C18
32	A	618	SQD	C18-C19-C20-C21
32	t	102	SQD	C30-C31-C32-C33
34	b	623	STE	C5-C6-C7-C8
30	D	408	LMG	C9-C8-O7-C10
32	b	619	SQD	C46-C45-O47-C7
33	a	614	DGD	C1G-C2G-O2G-C1B
30	c	522	LMG	C29-C30-C31-C32
31	l	101	LHG	C13-C14-C15-C16
34	I	101	STE	C6-C7-C8-C9
30	M	101	LMG	C18-C19-C20-C21
30	c	523	LMG	C12-C13-C14-C15
30	d	410	LMG	C37-C38-C39-C40
32	B	622	SQD	C17-C18-C19-C20
34	H	102	STE	C7-C8-C9-C10
34	t	105	STE	C11-C10-C9-C8
26	B	602	CLA	C16-C17-C18-C20
34	J	101	STE	C2-C3-C4-C5
32	a	613	SQD	C14-C15-C16-C17
28	a	610	BCR	C16-C17-C18-C19
28	b	616	BCR	C20-C21-C22-C23
28	k	101	BCR	C20-C21-C22-C23
33	C	516	DGD	O6E-C1E-O5D-C6D
33	A	619	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
30	d	410	LMG	C29-C30-C31-C32
33	C	517	DGD	C9A-CAA-CBA-CCA
32	B	622	SQD	C31-C32-C33-C34
32	b	619	SQD	C11-C10-C9-C8
34	X	102	STE	C14-C15-C16-C17
30	M	101	LMG	C35-C36-C37-C38
32	A	616	SQD	C11-C10-C9-C8
33	c	518	DGD	CCB-CDB-CEB-CFB
26	B	607	CLA	C16-C17-C18-C20
34	L	102	STE	C3-C4-C5-C6
30	d	411	LMG	C35-C36-C37-C38
31	A	615	LHG	C11-C10-C9-C8
32	f	101	SQD	C26-C27-C28-C29
32	f	101	SQD	C29-C30-C31-C32
33	C	517	DGD	C3B-C4B-C5B-C6B
30	b	621	LMG	O7-C8-C9-O8
33	H	101	DGD	C6A-C7A-C8A-C9A
30	C	518	LMG	C29-C28-O8-C9
31	l	101	LHG	C19-C20-C21-C22
33	C	516	DGD	CDA-CEA-CFA-CGA
34	l	102	STE	C15-C16-C17-C18
30	A	614	LMG	C29-C30-C31-C32
30	D	408	LMG	C34-C35-C36-C37
31	A	615	LHG	C29-C30-C31-C32
33	C	515	DGD	C5B-C6B-C7B-C8B
33	C	516	DGD	C3B-C4B-C5B-C6B
34	J	101	STE	C7-C8-C9-C10
33	C	515	DGD	CAB-CBB-CCB-CDB
33	c	518	DGD	CAB-CBB-CCB-CDB
26	b	601	CLA	C5-C6-C7-C8
30	B	621	LMG	C13-C14-C15-C16
33	h	103	DGD	C3B-C4B-C5B-C6B
29	a	611	PL9	C34-C36-C37-C38
34	L	102	STE	C7-C8-C9-C10
30	c	522	LMG	C39-C40-C41-C42
33	H	101	DGD	C8B-C9B-CAB-CBB
34	t	105	STE	C5-C6-C7-C8
26	B	616	CLA	O1D-CGD-O2D-CED
31	A	615	LHG	C17-C18-C19-C20
33	c	519	DGD	C7B-C8B-C9B-CAB
30	c	520	LMG	C32-C33-C34-C35
30	c	522	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
31	d	407	LHG	C12-C13-C14-C15
26	C	508	CLA	C5-C6-C7-C8
33	H	101	DGD	C9A-CAA-CBA-CCA
33	A	619	DGD	CFA-CGA-CHA-CIA
34	t	105	STE	C13-C14-C15-C16
26	a	607	CLA	C13-C15-C16-C17
26	c	512	CLA	C15-C16-C17-C18
26	C	502	CLA	O1D-CGD-O2D-CED
27	D	401	PHO	O1D-CGD-O2D-CED
26	B	616	CLA	C11-C12-C13-C14
29	A	612	PL9	C12-C11-C9-C10
31	D	409	LHG	C7-C8-C9-C10
32	f	101	SQD	C32-C33-C34-C35
33	c	518	DGD	CAA-CBA-CCA-CDA
34	l	102	STE	C4-C5-C6-C7
31	D	407	LHG	C10-C11-C12-C13
31	d	409	LHG	C32-C33-C34-C35
32	B	622	SQD	C26-C27-C28-C29
32	A	616	SQD	O49-C7-O47-C45
32	a	613	SQD	O49-C7-O47-C45
31	D	407	LHG	O1-C1-C2-O2
26	B	604	CLA	C11-C10-C8-C9
26	B	606	CLA	C14-C13-C15-C16
26	B	615	CLA	C14-C13-C15-C16
26	C	504	CLA	C11-C10-C8-C9
26	C	510	CLA	C6-C7-C8-C9
26	C	510	CLA	C11-C10-C8-C9
26	C	512	CLA	C11-C12-C13-C14
26	a	607	CLA	C11-C10-C8-C9
26	b	602	CLA	C6-C7-C8-C9
26	b	603	CLA	C14-C13-C15-C16
26	b	606	CLA	C6-C7-C8-C9
26	b	606	CLA	C11-C10-C8-C9
26	b	613	CLA	C6-C7-C8-C9
26	b	614	CLA	C11-C10-C8-C9
26	b	614	CLA	C11-C12-C13-C14
26	c	504	CLA	C11-C10-C8-C9
26	c	506	CLA	C11-C12-C13-C14
26	c	508	CLA	C11-C12-C13-C14
26	c	510	CLA	C11-C12-C13-C14
34	C	519	STE	C2-C3-C4-C5
26	a	609	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
32	B	622	SQD	O10-C23-O48-C46
26	c	502	CLA	C4B-C3B-CAB-CBB
26	c	503	CLA	C4B-C3B-CAB-CBB
30	A	614	LMG	C38-C39-C40-C41
31	D	407	LHG	C11-C10-C9-C8
32	F	102	SQD	C27-C28-C29-C30
34	X	102	STE	C10-C11-C12-C13
34	T	103	STE	C15-C16-C17-C18
34	F	103	STE	C7-C8-C9-C10
33	c	518	DGD	C5B-C6B-C7B-C8B
31	d	407	LHG	C9-C10-C11-C12
34	M	103	STE	C4-C5-C6-C7
34	t	105	STE	C12-C13-C14-C15
30	c	520	LMG	C2-C1-O1-C7
33	H	101	DGD	CBB-CCB-CDB-CEB
33	c	518	DGD	C3A-C4A-C5A-C6A
34	F	103	STE	C2-C3-C4-C5
31	l	101	LHG	O6-C4-C5-C6
34	T	103	STE	C4-C5-C6-C7
33	H	101	DGD	O2G-C1B-C2B-C3B
26	B	602	CLA	C11-C12-C13-C15
26	B	603	CLA	C11-C10-C8-C7
26	B	604	CLA	C11-C12-C13-C15
26	B	604	CLA	C12-C13-C15-C16
26	B	605	CLA	C11-C10-C8-C7
26	B	606	CLA	C11-C12-C13-C15
26	B	606	CLA	C12-C13-C15-C16
26	B	616	CLA	C6-C7-C8-C10
26	C	505	CLA	C12-C13-C15-C16
26	C	509	CLA	C12-C13-C15-C16
26	C	510	CLA	C11-C10-C8-C7
26	D	403	CLA	C11-C12-C13-C15
26	a	607	CLA	C12-C13-C15-C16
26	a	612	CLA	C12-C13-C15-C16
26	b	602	CLA	C6-C7-C8-C10
26	b	602	CLA	C11-C10-C8-C7
26	b	603	CLA	C12-C13-C15-C16
26	b	605	CLA	C11-C10-C8-C7
26	b	608	CLA	C12-C13-C15-C16
26	b	609	CLA	C12-C13-C15-C16
26	c	504	CLA	C11-C10-C8-C7
26	c	505	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
26	c	512	CLA	C11-C10-C8-C7
26	c	513	CLA	C11-C12-C13-C15
26	h	101	CLA	C11-C10-C8-C7
26	B	601	CLA	C15-C16-C17-C18
26	B	608	CLA	C15-C16-C17-C18
32	A	618	SQD	C19-C20-C21-C22
32	a	613	SQD	C34-C35-C36-C37
26	B	616	CLA	C10-C11-C12-C13
32	A	616	SQD	C17-C18-C19-C20
30	D	408	LMG	C33-C34-C35-C36
33	c	519	DGD	C6B-C7B-C8B-C9B
34	C	521	STE	C4-C5-C6-C7
26	B	607	CLA	O1D-CGD-O2D-CED
34	b	623	STE	C7-C8-C9-C10
30	d	410	LMG	C34-C35-C36-C37
26	C	509	CLA	C10-C11-C12-C13
26	h	101	CLA	C8-C10-C11-C12
26	B	603	CLA	C8-C10-C11-C12
31	A	617	LHG	C10-C11-C12-C13
34	j	101	STE	C3-C4-C5-C6
33	c	519	DGD	CCA-CDA-CEA-CFA
34	F	103	STE	C4-C5-C6-C7
31	L	101	LHG	C19-C20-C21-C22
34	b	623	STE	C1-C2-C3-C4
32	f	101	SQD	C30-C31-C32-C33
30	D	408	LMG	C29-C28-O8-C9
31	D	409	LHG	C28-C29-C30-C31
26	c	513	CLA	C2C-C3C-CAC-CBC
26	B	605	CLA	C10-C11-C12-C13
30	c	522	LMG	C7-C8-C9-O8
32	A	616	SQD	O6-C44-C45-C46
28	A	611	BCR	C14-C15-C16-C17
31	d	407	LHG	C19-C20-C21-C22
32	b	619	SQD	C12-C13-C14-C15
34	l	102	STE	C7-C8-C9-C10
26	A	607	CLA	C15-C16-C17-C18
30	d	410	LMG	C36-C37-C38-C39
33	c	517	DGD	C8A-C9A-CAA-CBA
34	B	625	STE	C11-C10-C9-C8
34	X	102	STE	C4-C5-C6-C7
34	k	102	STE	C4-C5-C6-C7
30	D	408	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
30	B	621	LMG	C30-C31-C32-C33
30	D	406	LMG	C14-C15-C16-C17
31	A	617	LHG	C17-C18-C19-C20
32	b	619	SQD	C27-C28-C29-C30
26	b	609	CLA	C4C-C3C-CAC-CBC
31	D	407	LHG	C25-C26-C27-C28
32	A	616	SQD	C25-C26-C27-C28
30	B	621	LMG	C35-C36-C37-C38
26	B	607	CLA	C16-C17-C18-C19
26	C	510	CLA	C16-C17-C18-C20
34	l	102	STE	C9-C10-C11-C12
26	h	101	CLA	C2B-C3B-CAB-CBB
28	t	101	BCR	C1-C6-C7-C8
28	t	101	BCR	C5-C6-C7-C8
30	d	411	LMG	C10-C11-C12-C13
34	k	102	STE	C1-C2-C3-C4
34	d	413	STE	C2-C3-C4-C5
30	d	411	LMG	C30-C31-C32-C33
31	D	409	LHG	C24-C25-C26-C27
33	a	614	DGD	CCA-CDA-CEA-CFA
34	J	101	STE	C6-C7-C8-C9
30	c	520	LMG	C40-C41-C42-C43
32	A	618	SQD	C16-C17-C18-C19
26	c	504	CLA	C11-C12-C13-C15
26	B	612	CLA	C8-C10-C11-C12
31	A	617	LHG	O7-C5-C6-O8
31	e	102	LHG	O7-C5-C6-O8
32	a	613	SQD	O47-C45-C46-O48
29	a	611	PL9	C4-C3-C7-C8
31	A	617	LHG	C27-C28-C29-C30
32	F	102	SQD	C30-C31-C32-C33
27	A	609	PHO	C4-C3-C5-C6
29	D	405	PL9	C30-C29-C31-C32
34	B	620	STE	C5-C6-C7-C8
28	B	617	BCR	C10-C11-C12-C13
26	b	613	CLA	C8-C10-C11-C12
30	M	101	LMG	C11-C12-C13-C14
32	A	618	SQD	C27-C28-C29-C30
31	A	615	LHG	C28-C29-C30-C31
30	D	406	LMG	C28-C29-C30-C31
31	e	102	LHG	C7-C8-C9-C10
26	B	608	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	B	603	CLA	C11-C10-C8-C9
26	B	604	CLA	C11-C12-C13-C14
26	C	513	CLA	C11-C10-C8-C9
26	a	607	CLA	C14-C13-C15-C16
26	b	601	CLA	C11-C12-C13-C14
26	b	601	CLA	C14-C13-C15-C16
26	b	606	CLA	C11-C12-C13-C14
26	b	613	CLA	C11-C12-C13-C14
26	c	506	CLA	C11-C10-C8-C9
34	M	102	STE	C11-C10-C9-C8
32	t	102	SQD	C31-C32-C33-C34
30	D	408	LMG	C35-C36-C37-C38
28	D	404	BCR	C14-C15-C16-C17
33	C	516	DGD	C6B-C7B-C8B-C9B
26	A	607	CLA	C16-C17-C18-C20
26	B	609	CLA	C16-C17-C18-C19
26	B	615	CLA	C16-C17-C18-C19
33	A	619	DGD	CEB-CFB-CGB-CHB
34	b	622	STE	C6-C7-C8-C9
34	l	102	STE	C5-C6-C7-C8
26	c	512	CLA	C2A-CAA-CBA-CGA
34	B	623	STE	C2-C3-C4-C5
30	C	518	LMG	C12-C13-C14-C15
31	d	407	LHG	C29-C30-C31-C32
31	d	408	LHG	O1-C1-C2-O2
26	A	610	CLA	CBA-CGA-O2A-C1
33	C	517	DGD	C2A-C1A-O1G-C1G
29	a	611	PL9	C28-C29-C31-C32
29	d	406	PL9	C28-C29-C31-C32
26	B	602	CLA	C16-C17-C18-C19
26	B	616	CLA	C11-C12-C13-C15
26	C	510	CLA	C16-C17-C18-C19
26	a	606	CLA	C16-C17-C18-C19
30	D	406	LMG	C38-C39-C40-C41
32	a	613	SQD	C30-C31-C32-C33
30	b	621	LMG	C13-C14-C15-C16
26	B	607	CLA	C10-C11-C12-C13
31	d	407	LHG	C1-C2-C3-O3
28	B	617	BCR	C20-C21-C22-C37
28	B	619	BCR	C35-C13-C14-C15
28	C	514	BCR	C16-C17-C18-C36
28	h	102	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
30	c	520	LMG	O10-C28-O8-C9
26	B	616	CLA	CBA-CGA-O2A-C1
34	b	622	STE	C1-C2-C3-C4
26	b	605	CLA	C15-C16-C17-C18
33	C	516	DGD	CBB-CCB-CDB-CEB
34	X	102	STE	C11-C12-C13-C14
26	d	404	CLA	C16-C17-C18-C19
26	B	609	CLA	C15-C16-C17-C18
34	J	101	STE	C5-C6-C7-C8
26	B	606	CLA	C11-C10-C8-C7
26	B	616	CLA	C11-C10-C8-C7
26	C	504	CLA	C11-C10-C8-C7
26	C	513	CLA	C11-C10-C8-C7
26	b	601	CLA	C11-C12-C13-C15
26	b	603	CLA	C11-C12-C13-C15
26	b	604	CLA	C12-C13-C15-C16
26	b	606	CLA	C11-C12-C13-C15
26	b	607	CLA	C11-C12-C13-C15
26	c	501	CLA	C11-C12-C13-C15
26	c	502	CLA	C6-C7-C8-C10
26	c	506	CLA	C6-C7-C8-C10
26	c	506	CLA	C11-C10-C8-C7
26	h	101	CLA	C11-C12-C13-C15
30	C	518	LMG	C32-C33-C34-C35
33	a	614	DGD	C6B-C7B-C8B-C9B
33	C	515	DGD	C2A-C3A-C4A-C5A
33	C	516	DGD	C2A-C3A-C4A-C5A
33	a	614	DGD	CAA-CBA-CCA-CDA
34	t	104	STE	C4-C5-C6-C7
28	k	101	BCR	C17-C18-C19-C20
32	A	618	SQD	C14-C15-C16-C17
32	a	613	SQD	C25-C26-C27-C28
33	C	516	DGD	C5D-C6D-O5D-C1E
33	c	518	DGD	C5D-C6D-O5D-C1E
31	l	101	LHG	C18-C19-C20-C21
34	T	102	STE	C11-C12-C13-C14
26	a	607	CLA	C8-C10-C11-C12
26	b	607	CLA	C4-C3-C5-C6
33	h	103	DGD	O2G-C1B-C2B-C3B
26	A	610	CLA	O1A-CGA-O2A-C1
27	A	609	PHO	C2-C3-C5-C6
26	B	610	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
30	D	408	LMG	C36-C37-C38-C39
32	B	622	SQD	C9-C10-C11-C12
31	d	408	LHG	O1-C1-C2-C3
31	A	617	LHG	C19-C20-C21-C22
30	c	522	LMG	C38-C39-C40-C41
34	B	624	STE	C2-C3-C4-C5
26	c	504	CLA	C8-C10-C11-C12
26	C	513	CLA	O2A-C1-C2-C3
26	B	616	CLA	O1A-CGA-O2A-C1
26	c	513	CLA	C4C-C3C-CAC-CBC
30	A	614	LMG	C18-C19-C20-C21
33	C	515	DGD	CBB-CCB-CDB-CEB
34	b	622	STE	C9-C10-C11-C12
26	B	608	CLA	C16-C17-C18-C19
26	B	608	CLA	O1A-CGA-O2A-C1
31	A	617	LHG	C11-C12-C13-C14
32	t	102	SQD	C12-C13-C14-C15
26	b	604	CLA	C15-C16-C17-C18
33	C	515	DGD	O1G-C1A-C2A-C3A
31	L	101	LHG	O6-C4-C5-O7
31	l	101	LHG	O6-C4-C5-O7
30	C	518	LMG	C14-C15-C16-C17
31	l	101	LHG	C9-C10-C11-C12
30	c	522	LMG	O6-C1-O1-C7
30	C	518	LMG	O1-C7-C8-C9
30	M	101	LMG	O1-C7-C8-C9
30	b	621	LMG	C7-C8-C9-O8
31	A	617	LHG	C4-C5-C6-O8
33	A	619	DGD	C1G-C2G-C3G-O3G
33	C	515	DGD	O1G-C1G-C2G-C3G
35	e	101	HEM	C4B-C3B-CAB-CBB
33	c	517	DGD	C4D-C5D-C6D-O5D
31	A	615	LHG	C14-C15-C16-C17
32	A	618	SQD	C17-C18-C19-C20
26	c	505	CLA	C15-C16-C17-C18
30	b	621	LMG	O1-C7-C8-O7
26	C	505	CLA	C14-C13-C15-C16
26	b	604	CLA	C14-C13-C15-C16
26	h	101	CLA	C11-C12-C13-C14
33	c	517	DGD	C1B-C2B-C3B-C4B
26	C	513	CLA	C16-C17-C18-C19
26	b	609	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
31	L	101	LHG	C24-C25-C26-C27
31	d	407	LHG	C11-C10-C9-C8
32	a	613	SQD	C9-C10-C11-C12
33	H	101	DGD	CBA-CCA-CDA-CEA
34	B	620	STE	C7-C8-C9-C10
29	A	612	PL9	C47-C48-C49-C50
31	D	409	LHG	C19-C20-C21-C22
31	l	101	LHG	C16-C17-C18-C19
34	L	102	STE	C4-C5-C6-C7
31	D	407	LHG	C31-C32-C33-C34
33	H	101	DGD	C8A-C9A-CAA-CBA
34	B	620	STE	C11-C12-C13-C14
33	C	516	DGD	C8B-C9B-CAB-CBB
34	l	102	STE	C2-C3-C4-C5
34	t	103	STE	C3-C4-C5-C6
26	c	506	CLA	C2-C1-O2A-CGA
26	c	505	CLA	C16-C17-C18-C20
26	C	513	CLA	C13-C15-C16-C17
31	D	409	LHG	C32-C33-C34-C35
34	d	414	STE	C9-C10-C11-C12
31	e	102	LHG	C28-C29-C30-C31
31	d	409	LHG	C23-C24-C25-C26
33	C	517	DGD	C5B-C6B-C7B-C8B
26	b	611	CLA	C15-C16-C17-C18
31	d	408	LHG	C32-C33-C34-C35
34	t	103	STE	C9-C10-C11-C12
26	a	606	CLA	C16-C17-C18-C20
33	A	619	DGD	CDB-CEB-CFB-CGB
32	A	616	SQD	C28-C29-C30-C31
34	J	101	STE	C3-C4-C5-C6
34	b	622	STE	C7-C8-C9-C10
30	M	101	LMG	C36-C37-C38-C39
33	H	101	DGD	C2B-C3B-C4B-C5B
26	c	502	CLA	C3-C5-C6-C7
26	a	607	CLA	C4B-C3B-CAB-CBB
26	c	509	CLA	O1D-CGD-O2D-CED
31	A	615	LHG	C16-C17-C18-C19
30	c	523	LMG	C16-C17-C18-C19
30	m	101	LMG	C14-C15-C16-C17
33	c	518	DGD	CDB-CEB-CFB-CGB
29	A	612	PL9	C22-C23-C24-C26
33	a	614	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
33	C	517	DGD	CBB-CCB-CDB-CEB
33	C	515	DGD	O1B-C1B-O2G-C2G
26	A	608	CLA	C11-C12-C13-C15
26	B	603	CLA	C6-C7-C8-C10
26	B	607	CLA	C6-C7-C8-C10
26	B	607	CLA	C11-C10-C8-C7
26	B	607	CLA	C12-C13-C15-C16
26	B	613	CLA	C6-C7-C8-C10
26	c	507	CLA	C11-C12-C13-C15
26	c	509	CLA	C16-C17-C18-C19
32	a	613	SQD	C19-C20-C21-C22
34	C	521	STE	C9-C10-C11-C12
34	T	102	STE	C13-C14-C15-C16
30	c	523	LMG	C37-C38-C39-C40
31	d	408	LHG	C26-C27-C28-C29
30	A	614	LMG	C19-C20-C21-C22
31	D	409	LHG	C31-C32-C33-C34
34	b	622	STE	C4-C5-C6-C7
26	b	608	CLA	C4-C3-C5-C6
26	d	404	CLA	C16-C17-C18-C20
26	b	607	CLA	C2-C3-C5-C6
33	A	619	DGD	C6B-C7B-C8B-C9B
33	C	516	DGD	C2B-C3B-C4B-C5B
26	c	510	CLA	C3-C5-C6-C7
33	c	517	DGD	C6A-C7A-C8A-C9A
26	B	603	CLA	C14-C13-C15-C16
26	B	607	CLA	C11-C10-C8-C9
26	B	613	CLA	C6-C7-C8-C9
26	C	509	CLA	C14-C13-C15-C16
26	b	607	CLA	C11-C12-C13-C14
26	b	611	CLA	C11-C12-C13-C14
26	c	501	CLA	C11-C12-C13-C14
26	c	506	CLA	C6-C7-C8-C9
26	c	513	CLA	C11-C12-C13-C14
26	B	604	CLA	C13-C15-C16-C17
30	d	411	LMG	C36-C37-C38-C39
33	C	517	DGD	O6D-C5D-C6D-O5D
34	B	625	STE	C7-C8-C9-C10
32	B	622	SQD	C27-C28-C29-C30
30	c	522	LMG	C11-C12-C13-C14
30	A	614	LMG	O1-C7-C8-O7
30	C	518	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
30	M	101	LMG	O1-C7-C8-O7
30	c	522	LMG	O7-C8-C9-O8
32	b	619	SQD	O47-C45-C46-O48
33	C	515	DGD	O1G-C1G-C2G-O2G
26	c	510	CLA	C10-C11-C12-C13
26	b	614	CLA	C16-C17-C18-C20
31	D	407	LHG	C13-C14-C15-C16
30	C	518	LMG	C37-C38-C39-C40
26	c	505	CLA	C10-C11-C12-C13
30	C	518	LMG	C28-C29-C30-C31
32	B	622	SQD	C11-C10-C9-C8
26	B	605	CLA	CAD-CBD-CGD-O2D
26	B	607	CLA	CAD-CBD-CGD-O2D
26	B	612	CLA	CAD-CBD-CGD-O2D
26	C	502	CLA	CAD-CBD-CGD-O2D
26	C	513	CLA	CAD-CBD-CGD-O2D
26	c	502	CLA	CAD-CBD-CGD-O2D
31	D	407	LHG	C19-C20-C21-C22
34	b	622	STE	C11-C12-C13-C14
30	M	101	LMG	O6-C1-O1-C7
33	A	619	DGD	C1B-C2B-C3B-C4B
33	A	619	DGD	C5A-C6A-C7A-C8A
31	l	101	LHG	C12-C13-C14-C15
30	b	621	LMG	C35-C36-C37-C38
31	A	617	LHG	C11-C10-C9-C8
26	B	605	CLA	CAD-CBD-CGD-O1D
26	B	607	CLA	CAD-CBD-CGD-O1D
26	B	612	CLA	CAD-CBD-CGD-O1D
26	C	502	CLA	CAD-CBD-CGD-O1D
26	C	504	CLA	CAD-CBD-CGD-O1D
26	C	507	CLA	CHA-CBD-CGD-O1D
26	C	513	CLA	CAD-CBD-CGD-O1D
26	b	615	CLA	CHA-CBD-CGD-O1D
26	b	615	CLA	CHA-CBD-CGD-O2D
26	c	502	CLA	CAD-CBD-CGD-O1D
26	c	507	CLA	CHA-CBD-CGD-O1D
26	c	507	CLA	CHA-CBD-CGD-O2D
26	c	509	CLA	CHA-CBD-CGD-O1D
26	c	509	CLA	CHA-CBD-CGD-O2D
27	d	402	PHO	CHA-CBD-CGD-O2D
28	K	102	BCR	C11-C10-C9-C34
28	h	102	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
31	A	615	LHG	C3-O3-P-O5
31	L	101	LHG	C4-O6-P-O5
31	e	102	LHG	C3-O3-P-O5
31	e	102	LHG	C4-O6-P-O5
31	l	101	LHG	C4-O6-P-O5
33	c	517	DGD	C3A-C4A-C5A-C6A
33	a	614	DGD	CFA-CGA-CHA-CIA
26	c	508	CLA	C10-C11-C12-C13
33	C	515	DGD	CDA-CEA-CFA-CGA
26	a	607	CLA	C2B-C3B-CAB-CBB
26	c	502	CLA	C2B-C3B-CAB-CBB
28	B	617	BCR	C1-C6-C7-C8
28	K	102	BCR	C1-C6-C7-C8
26	b	608	CLA	C2-C3-C5-C6
28	h	102	BCR	C7-C8-C9-C34
26	A	610	CLA	C6-C7-C8-C9
30	c	520	LMG	C36-C37-C38-C39
34	T	102	STE	C3-C4-C5-C6
31	d	407	LHG	C15-C16-C17-C18
34	a	615	STE	C5-C6-C7-C8
26	c	512	CLA	C3-C5-C6-C7
34	H	102	STE	C1-C2-C3-C4
29	A	612	PL9	C4-C3-C7-C8
30	A	614	LMG	C9-C8-O7-C10
30	b	621	LMG	C9-C8-O7-C10
32	B	622	SQD	C44-C45-O47-C7
34	t	104	STE	C7-C8-C9-C10
30	A	614	LMG	C32-C33-C34-C35
31	D	409	LHG	C11-C12-C13-C14
33	c	519	DGD	CAB-CBB-CCB-CDB
33	h	103	DGD	CDB-CEB-CFB-CGB
26	B	606	CLA	C11-C12-C13-C14
26	B	611	CLA	C11-C12-C13-C14
26	B	615	CLA	C11-C10-C8-C9
26	B	616	CLA	C6-C7-C8-C9
26	C	506	CLA	C14-C13-C15-C16
26	C	507	CLA	C11-C10-C8-C9
26	C	512	CLA	C11-C10-C8-C9
26	D	402	CLA	C11-C12-C13-C14
26	a	609	CLA	C14-C13-C15-C16
26	b	605	CLA	C11-C10-C8-C9
26	b	608	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
26	c	512	CLA	C11-C10-C8-C9
31	D	407	LHG	C33-C34-C35-C36
26	d	403	CLA	C6-C7-C8-C10
28	X	101	BCR	C20-C21-C22-C23
30	A	614	LMG	C37-C38-C39-C40
28	Z	101	BCR	C6-C7-C8-C9
26	C	513	CLA	C16-C17-C18-C20
31	D	409	LHG	C11-C10-C9-C8
26	B	610	CLA	C4C-C3C-CAC-CBC
26	B	610	CLA	CBD-CGD-O2D-CED
30	M	101	LMG	C16-C17-C18-C19
30	D	408	LMG	C10-C11-C12-C13
30	M	101	LMG	C31-C32-C33-C34
31	D	407	LHG	C17-C18-C19-C20
31	l	101	LHG	C25-C26-C27-C28
31	d	408	LHG	C25-C26-C27-C28
31	d	409	LHG	C2-C3-O3-P
30	m	101	LMG	O7-C8-C9-O8
33	A	619	DGD	O1G-C1G-C2G-O2G
33	c	517	DGD	O1G-C1G-C2G-O2G
34	B	625	STE	C9-C10-C11-C12
30	D	408	LMG	C29-C30-C31-C32
30	c	523	LMG	C7-C8-C9-O8
26	B	614	CLA	C10-C11-C12-C13
34	C	521	STE	C12-C13-C14-C15
31	D	407	LHG	C30-C31-C32-C33
32	F	102	SQD	C29-C30-C31-C32
29	D	405	PL9	C12-C13-C14-C16
34	C	521	STE	C15-C16-C17-C18
32	A	618	SQD	C26-C27-C28-C29
26	c	501	CLA	C2A-CAA-CBA-CGA
28	K	102	BCR	C19-C20-C21-C22
28	k	101	BCR	C19-C20-C21-C22
34	J	101	STE	C1-C2-C3-C4
29	d	406	PL9	C43-C44-C46-C47
31	d	408	LHG	C11-C12-C13-C14
26	B	602	CLA	C11-C12-C13-C14
26	B	603	CLA	C6-C7-C8-C9
26	C	506	CLA	C11-C12-C13-C14
33	A	619	DGD	CEA-CFA-CGA-CHA
26	B	609	CLA	C4B-C3B-CAB-CBB
32	A	616	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
26	b	607	CLA	C16-C17-C18-C19
26	c	505	CLA	C16-C17-C18-C19
26	b	612	CLA	O1D-CGD-O2D-CED
26	B	610	CLA	C8-C10-C11-C12
32	A	616	SQD	C9-C10-C11-C12
32	B	622	SQD	C28-C29-C30-C31
31	d	408	LHG	C34-C35-C36-C37
32	b	619	SQD	C10-C11-C12-C13
30	B	621	LMG	C34-C35-C36-C37
33	c	518	DGD	C7B-C8B-C9B-CAB
26	B	611	CLA	C12-C13-C15-C16
26	C	506	CLA	C12-C13-C15-C16
26	b	601	CLA	C11-C10-C8-C7
26	c	509	CLA	C6-C7-C8-C10
26	d	404	CLA	C11-C12-C13-C15
33	C	517	DGD	C8A-C9A-CAA-CBA
30	c	522	LMG	C34-C35-C36-C37
31	L	101	LHG	C33-C34-C35-C36
32	f	101	SQD	C33-C34-C35-C36
33	A	619	DGD	CBB-CCB-CDB-CEB
26	B	604	CLA	C2C-C3C-CAC-CBC
31	A	617	LHG	C32-C33-C34-C35
26	c	510	CLA	C15-C16-C17-C18
26	a	606	CLA	C2C-C3C-CAC-CBC
30	M	101	LMG	O7-C8-C9-O8
28	D	404	BCR	C16-C17-C18-C36
33	a	614	DGD	C1B-C2B-C3B-C4B
26	c	505	CLA	C5-C6-C7-C8
32	a	613	SQD	C13-C14-C15-C16
26	d	403	CLA	C2-C1-O2A-CGA
28	c	516	BCR	C15-C16-C17-C18
32	A	618	SQD	C11-C10-C9-C8
26	c	501	CLA	C8-C10-C11-C12
33	c	518	DGD	C2A-C3A-C4A-C5A
29	d	406	PL9	C45-C44-C46-C47
26	B	610	CLA	O1D-CGD-O2D-CED
34	b	620	STE	O1-C1-C2-C3
31	A	617	LHG	C34-C35-C36-C37
30	M	101	LMG	C7-C8-C9-O8
32	a	613	SQD	C44-C45-C46-O48
33	h	103	DGD	C4B-C5B-C6B-C7B
32	A	616	SQD	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
34	b	623	STE	C2-C3-C4-C5
34	t	105	STE	C9-C10-C11-C12
26	B	614	CLA	C11-C10-C8-C9
26	C	511	CLA	C14-C13-C15-C16
26	c	504	CLA	C6-C7-C8-C9
26	c	505	CLA	C11-C10-C8-C9
26	c	511	CLA	C6-C7-C8-C9
26	d	403	CLA	C6-C7-C8-C9
26	d	404	CLA	C11-C12-C13-C14
33	h	103	DGD	C8A-C9A-CAA-CBA
34	B	625	STE	C6-C7-C8-C9
32	a	613	SQD	C24-C23-O48-C46
34	a	615	STE	C3-C4-C5-C6
32	B	622	SQD	C34-C35-C36-C37
26	D	402	CLA	C8-C10-C11-C12
33	a	614	DGD	C1G-C2G-C3G-O3G
36	v	201	HEC	CAD-CBD-CGD-O2D
29	A	612	PL9	C12-C11-C9-C8
33	c	518	DGD	C2D-C1D-O3G-C3G
34	b	620	STE	O2-C1-C2-C3
34	b	622	STE	O1-C1-C2-C3
34	d	413	STE	O1-C1-C2-C3
32	F	102	SQD	C24-C25-C26-C27
26	a	612	CLA	C1A-C2A-CAA-CBA
28	X	101	BCR	C11-C10-C9-C8
26	b	608	CLA	C16-C17-C18-C20
30	D	406	LMG	C29-C30-C31-C32
26	B	609	CLA	C2B-C3B-CAB-CBB
26	b	613	CLA	C2B-C3B-CAB-CBB
28	B	618	BCR	C23-C24-C25-C30
28	K	101	BCR	C23-C24-C25-C30
28	K	102	BCR	C5-C6-C7-C8
28	Z	101	BCR	C23-C24-C25-C30
28	b	616	BCR	C1-C6-C7-C8
28	c	516	BCR	C1-C6-C7-C8
28	h	102	BCR	C23-C24-C25-C30
30	M	101	LMG	C30-C31-C32-C33
31	e	102	LHG	C8-C7-O7-C5
34	d	413	STE	O2-C1-C2-C3
32	A	616	SQD	C24-C25-C26-C27
33	C	515	DGD	C2B-C3B-C4B-C5B
33	c	518	DGD	C9A-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
26	B	604	CLA	CBD-CGD-O2D-CED
30	d	410	LMG	O7-C10-C11-C12
34	M	102	STE	O2-C1-C2-C3
26	c	512	CLA	C4-C3-C5-C6
34	b	622	STE	O2-C1-C2-C3
26	A	608	CLA	C12-C13-C15-C16
26	C	506	CLA	C11-C12-C13-C15
26	a	609	CLA	C12-C13-C15-C16
26	b	611	CLA	C6-C7-C8-C10
26	b	613	CLA	C12-C13-C15-C16
27	a	608	PHO	C6-C7-C8-C10
32	f	101	SQD	O6-C44-C45-O47
29	d	406	PL9	C4-C3-C7-C8
34	X	102	STE	C9-C10-C11-C12
34	c	521	STE	C7-C8-C9-C10
29	d	406	PL9	C32-C33-C34-C35
34	B	623	STE	C7-C8-C9-C10
30	d	410	LMG	O9-C10-C11-C12
34	d	414	STE	O1-C1-C2-C3
26	B	603	CLA	C13-C15-C16-C17
28	B	618	BCR	C36-C18-C19-C20
28	B	618	BCR	C37-C22-C23-C24
28	c	515	BCR	C11-C12-C13-C35
28	d	405	BCR	C7-C8-C9-C34
34	a	615	STE	O2-C1-C2-C3
35	e	101	HEM	CAD-CBD-CGD-O1D
26	B	601	CLA	C4-C3-C5-C6
26	B	606	CLA	C10-C11-C12-C13
29	a	611	PL9	C38-C39-C41-C42
33	A	619	DGD	CBA-CCA-CDA-CEA
33	c	517	DGD	CDA-CEA-CFA-CGA
34	I	101	STE	C12-C13-C14-C15
31	A	615	LHG	C24-C25-C26-C27
32	b	619	SQD	C17-C18-C19-C20
34	M	103	STE	C6-C7-C8-C9
26	a	607	CLA	C6-C7-C8-C9
30	c	523	LMG	C19-C20-C21-C22
26	a	606	CLA	C4C-C3C-CAC-CBC
33	c	518	DGD	C9B-CAB-CBB-CCB
30	m	101	LMG	C33-C34-C35-C36
26	D	403	CLA	C5-C6-C7-C8
30	m	101	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
33	H	101	DGD	CAB-CBB-CCB-CDB
34	M	102	STE	O1-C1-C2-C3
26	D	402	CLA	C15-C16-C17-C18
36	V	201	HEC	C2B-C3B-CAB-CBB
31	d	409	LHG	C25-C26-C27-C28
32	a	613	SQD	O10-C23-O48-C46
33	c	517	DGD	O1G-C1A-C2A-C3A
31	D	407	LHG	C34-C35-C36-C37
33	C	516	DGD	C8A-C9A-CAA-CBA
33	C	516	DGD	C9A-CAA-CBA-CCA
29	D	405	PL9	C39-C41-C42-C43
30	c	520	LMG	O1-C7-C8-C9
30	m	101	LMG	C7-C8-C9-O8
36	v	201	HEC	CAD-CBD-CGD-O1D
33	a	614	DGD	O2G-C2G-C3G-O3G
26	B	603	CLA	C2A-CAA-CBA-CGA
32	F	102	SQD	O6-C44-C45-C46
26	B	609	CLA	C4-C3-C5-C6
26	B	608	CLA	C16-C17-C18-C20
32	b	619	SQD	C15-C16-C17-C18
33	h	103	DGD	CCB-CDB-CEB-CFB
30	C	518	LMG	C33-C34-C35-C36
30	m	101	LMG	C11-C12-C13-C14
32	A	618	SQD	C10-C11-C12-C13
26	b	613	CLA	C4B-C3B-CAB-CBB
26	c	502	CLA	C16-C17-C18-C20
27	D	401	PHO	CHA-CBD-CGD-O1D
27	D	401	PHO	CHA-CBD-CGD-O2D
27	d	402	PHO	CHA-CBD-CGD-O1D
34	a	615	STE	O1-C1-C2-C3
34	d	414	STE	O2-C1-C2-C3
35	e	101	HEM	CAD-CBD-CGD-O2D
26	d	403	CLA	C4-C3-C5-C6
31	d	408	LHG	C16-C17-C18-C19
30	c	523	LMG	O7-C8-C9-O8
34	B	623	STE	O2-C1-C2-C3
30	b	621	LMG	C39-C40-C41-C42
26	B	607	CLA	C13-C15-C16-C17
32	B	622	SQD	C33-C34-C35-C36
26	C	509	CLA	C11-C10-C8-C7
26	C	512	CLA	C6-C7-C8-C10
26	a	607	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
26	c	505	CLA	C11-C10-C8-C7
26	c	510	CLA	C12-C13-C15-C16
26	c	512	CLA	C6-C7-C8-C10
33	H	101	DGD	CDB-CEB-CFB-CGB
30	b	621	LMG	C28-C29-C30-C31
30	A	614	LMG	C30-C31-C32-C33
28	C	514	BCR	C11-C12-C13-C14
26	B	607	CLA	C11-C12-C13-C14
26	C	502	CLA	C11-C12-C13-C14
26	C	511	CLA	C11-C12-C13-C14
26	b	603	CLA	C11-C12-C13-C14
26	b	604	CLA	C11-C12-C13-C14
26	b	611	CLA	C6-C7-C8-C9
26	c	507	CLA	C11-C12-C13-C14
34	l	102	STE	C11-C10-C9-C8
31	A	617	LHG	C31-C32-C33-C34
34	H	102	STE	C13-C14-C15-C16
33	c	517	DGD	C5D-C6D-O5D-C1E
34	L	102	STE	O2-C1-C2-C3
26	c	513	CLA	C13-C15-C16-C17
26	a	612	CLA	C2C-C3C-CAC-CBC
26	b	615	CLA	C2-C1-O2A-CGA
26	d	404	CLA	C3A-C2A-CAA-CBA
34	B	620	STE	O2-C1-C2-C3
34	c	521	STE	O2-C1-C2-C3
30	b	621	LMG	C4-C5-C6-O5
26	c	504	CLA	O1D-CGD-O2D-CED
32	B	622	SQD	C46-C45-O47-C7
30	c	523	LMG	C31-C32-C33-C34
34	b	622	STE	C5-C6-C7-C8
28	C	514	BCR	C10-C11-C12-C13
28	T	101	BCR	C18-C19-C20-C21
34	t	105	STE	C6-C7-C8-C9
26	c	509	CLA	CAA-CBA-CGA-O2A
26	b	615	CLA	C11-C12-C13-C15
34	b	623	STE	C6-C7-C8-C9
26	C	507	CLA	C4-C3-C5-C6
26	B	605	CLA	C8-C10-C11-C12
28	b	618	BCR	C16-C17-C18-C19
32	t	102	SQD	C26-C27-C28-C29
34	B	620	STE	O1-C1-C2-C3
33	c	517	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
26	b	611	CLA	C3-C5-C6-C7
33	c	519	DGD	O6D-C1D-O3G-C3G
26	B	603	CLA	C10-C11-C12-C13
33	c	518	DGD	C6B-C7B-C8B-C9B
34	B	623	STE	O1-C1-C2-C3
34	C	520	STE	O1-C1-C2-C3
32	b	619	SQD	C44-C45-C46-O48
26	b	612	CLA	CBD-CGD-O2D-CED
34	b	622	STE	C10-C11-C12-C13
34	X	102	STE	O2-C1-C2-C3
34	c	521	STE	C4-C5-C6-C7
34	t	104	STE	C2-C3-C4-C5
26	a	612	CLA	C4C-C3C-CAC-CBC
34	X	102	STE	O1-C1-C2-C3
36	V	201	HEC	CAD-CBD-CGD-O1D
26	A	608	CLA	C11-C12-C13-C14
26	A	613	CLA	C14-C13-C15-C16
26	B	607	CLA	C14-C13-C15-C16
26	C	502	CLA	C6-C7-C8-C9
26	b	602	CLA	C14-C13-C15-C16
26	C	513	CLA	CBA-CGA-O2A-C1
34	L	102	STE	O1-C1-C2-C3
36	V	201	HEC	CAD-CBD-CGD-O2D
31	A	615	LHG	C15-C16-C17-C18
26	C	505	CLA	C4-C3-C5-C6
26	B	612	CLA	CAA-CBA-CGA-O2A
26	A	613	CLA	C16-C17-C18-C19
26	B	601	CLA	C2-C3-C5-C6
26	B	609	CLA	C2-C3-C5-C6
26	c	512	CLA	C2-C3-C5-C6
26	B	602	CLA	C6-C7-C8-C10
26	B	610	CLA	C11-C12-C13-C15
26	B	613	CLA	C12-C13-C15-C16
26	C	502	CLA	C11-C12-C13-C15
26	C	508	CLA	C12-C13-C15-C16
26	b	604	CLA	C11-C12-C13-C15
26	b	611	CLA	C11-C10-C8-C7
26	b	615	CLA	C6-C7-C8-C10
26	c	510	CLA	C11-C10-C8-C7
26	c	511	CLA	C6-C7-C8-C10
32	f	101	SQD	C34-C35-C36-C37
34	c	521	STE	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
26	b	602	CLA	C2B-C3B-CAB-CBB
26	b	611	CLA	C2B-C3B-CAB-CBB
26	c	503	CLA	C2B-C3B-CAB-CBB
28	B	618	BCR	C23-C24-C25-C26
28	K	101	BCR	C23-C24-C25-C26
28	Z	101	BCR	C23-C24-C25-C26
28	b	616	BCR	C5-C6-C7-C8
28	c	516	BCR	C23-C24-C25-C26
28	c	516	BCR	C23-C24-C25-C30
28	h	102	BCR	C23-C24-C25-C26
30	c	522	LMG	C15-C16-C17-C18
30	M	101	LMG	O8-C28-C29-C30
31	D	409	LHG	C30-C31-C32-C33
26	h	101	CLA	C16-C17-C18-C19
26	B	613	CLA	C13-C15-C16-C17
33	C	517	DGD	CBA-CCA-CDA-CEA
26	c	506	CLA	C8-C10-C11-C12
30	c	523	LMG	C13-C14-C15-C16
26	C	505	CLA	C2-C3-C5-C6
26	b	608	CLA	O1A-CGA-O2A-C1
31	d	407	LHG	C8-C7-O7-C5
34	d	414	STE	C15-C16-C17-C18
31	d	407	LHG	C33-C34-C35-C36
30	b	621	LMG	C41-C42-C43-C44
26	B	601	CLA	CAA-CBA-CGA-O2A
29	a	611	PL9	C15-C14-C16-C17
26	b	611	CLA	CAA-CBA-CGA-O2A
32	a	613	SQD	O47-C7-C8-C9
35	F	101	HEM	CAD-CBD-CGD-O1D
28	X	101	BCR	C20-C21-C22-C37
34	M	102	STE	C10-C11-C12-C13
26	c	506	CLA	C16-C17-C18-C20
34	a	615	STE	C6-C7-C8-C9
26	b	609	CLA	C5-C6-C7-C8
34	M	102	STE	C5-C6-C7-C8
33	c	519	DGD	CDB-CEB-CFB-CGB
26	B	615	CLA	C8-C10-C11-C12
34	M	102	STE	C1-C2-C3-C4
26	b	612	CLA	CAA-CBA-CGA-O2A
33	c	517	DGD	C1G-C2G-C3G-O3G
26	B	601	CLA	C4B-C3B-CAB-CBB
26	C	501	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	C	504	CLA	C4B-C3B-CAB-CBB
26	D	402	CLA	C4B-C3B-CAB-CBB
26	c	512	CLA	C1A-C2A-CAA-CBA
33	C	516	DGD	O6D-C1D-O3G-C3G
30	b	621	LMG	O7-C10-C11-C12
31	e	102	LHG	O8-C23-C24-C25
31	l	101	LHG	O7-C5-C6-O8
33	C	517	DGD	O1G-C1G-C2G-O2G
35	F	101	HEM	CAD-CBD-CGD-O2D
28	X	101	BCR	C11-C12-C13-C14
28	b	616	BCR	C21-C22-C23-C24
28	t	101	BCR	C7-C8-C9-C10
30	c	523	LMG	C39-C40-C41-C42
31	A	615	LHG	C33-C34-C35-C36
26	c	507	CLA	C2A-CAA-CBA-CGA
26	B	602	CLA	C3-C5-C6-C7
26	B	603	CLA	C5-C6-C7-C8
34	b	623	STE	C4-C5-C6-C7
32	f	101	SQD	C5-C6-S-O7
26	b	611	CLA	C13-C15-C16-C17
29	a	611	PL9	C40-C39-C41-C42
26	A	607	CLA	C2-C1-O2A-CGA
26	D	402	CLA	C2-C1-O2A-CGA
26	a	606	CLA	C2-C1-O2A-CGA
32	A	616	SQD	O47-C7-C8-C9
31	L	101	LHG	C34-C35-C36-C37
26	C	505	CLA	C6-C7-C8-C10
26	a	609	CLA	C11-C10-C8-C7
26	b	613	CLA	C11-C10-C8-C7
26	c	511	CLA	C12-C13-C15-C16
26	b	608	CLA	CBA-CGA-O2A-C1
33	A	619	DGD	O6D-C5D-C6D-O5D
31	d	408	LHG	C10-C11-C12-C13
26	C	513	CLA	O1A-CGA-O2A-C1
30	D	408	LMG	C14-C15-C16-C17
31	A	617	LHG	C13-C14-C15-C16
34	T	103	STE	C7-C8-C9-C10
32	A	616	SQD	C15-C16-C17-C18
30	c	523	LMG	O10-C28-C29-C30
30	M	101	LMG	C10-C11-C12-C13
34	l	102	STE	C13-C14-C15-C16
30	B	621	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	L	101	LHG	C7-C8-C9-C10
31	A	615	LHG	C2-C3-O3-P
34	C	520	STE	O2-C1-C2-C3
30	A	614	LMG	C31-C32-C33-C34
26	b	614	CLA	C8-C10-C11-C12
26	a	609	CLA	C11-C10-C8-C9
27	a	608	PHO	C6-C7-C8-C9
33	C	515	DGD	O1B-C1B-C2B-C3B
34	T	103	STE	C14-C15-C16-C17
32	A	616	SQD	C27-C28-C29-C30
26	D	402	CLA	C2C-C3C-CAC-CBC
33	c	517	DGD	O1B-C1B-C2B-C3B
33	C	515	DGD	C6B-C7B-C8B-C9B
29	d	406	PL9	C18-C19-C21-C22
30	C	518	LMG	O10-C28-O8-C9
34	H	102	STE	C3-C4-C5-C6
34	b	620	STE	C10-C11-C12-C13
26	B	613	CLA	CAA-CBA-CGA-O2A
30	c	523	LMG	O8-C28-C29-C30
32	f	101	SQD	O48-C23-C24-C25
26	B	601	CLA	CAA-CBA-CGA-O1A
26	B	612	CLA	CAA-CBA-CGA-O1A
26	b	611	CLA	CAA-CBA-CGA-O1A
26	b	612	CLA	CAA-CBA-CGA-O1A
30	b	621	LMG	C8-C7-O1-C1
30	m	101	LMG	C8-C7-O1-C1
33	C	515	DGD	C5D-C6D-O5D-C1E
31	e	102	LHG	C15-C16-C17-C18
30	B	621	LMG	O8-C28-C29-C30
30	b	621	LMG	C11-C12-C13-C14
32	F	102	SQD	O48-C23-C24-C25
26	B	604	CLA	C4C-C3C-CAC-CBC
34	d	413	STE	C6-C7-C8-C9
30	M	101	LMG	C14-C15-C16-C17
33	C	515	DGD	C1G-C2G-C3G-O3G
26	B	610	CLA	C5-C6-C7-C8
26	c	501	CLA	CAA-CBA-CGA-O2A
26	c	510	CLA	CAA-CBA-CGA-O2A
30	m	101	LMG	C4-C5-C6-O5
34	F	103	STE	O2-C1-C2-C3
26	d	403	CLA	C16-C17-C18-C19
26	C	501	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
26	C	509	CLA	CAD-CBD-CGD-O2D
26	D	403	CLA	CAD-CBD-CGD-O2D
26	c	501	CLA	CAD-CBD-CGD-O2D
26	c	506	CLA	CAD-CBD-CGD-O2D
27	A	609	PHO	CAD-CBD-CGD-O2D
34	F	103	STE	O1-C1-C2-C3
36	v	201	HEC	C2B-C3B-CAB-CBB
26	b	604	CLA	C10-C11-C12-C13
26	c	504	CLA	C5-C6-C7-C8
30	b	621	LMG	C34-C35-C36-C37
28	b	616	BCR	C6-C7-C8-C9
27	A	609	PHO	C8-C10-C11-C12
26	c	512	CLA	C2-C1-O2A-CGA
26	c	513	CLA	C2-C1-O2A-CGA
31	e	102	LHG	C24-C25-C26-C27
29	a	611	PL9	C21-C22-C23-C24
33	c	517	DGD	C9B-CAB-CBB-CCB
34	d	412	STE	C6-C7-C8-C9
32	a	613	SQD	O49-C7-C8-C9
26	B	615	CLA	C13-C15-C16-C17
30	A	614	LMG	C28-C29-C30-C31
32	b	619	SQD	O48-C23-C24-C25
32	A	616	SQD	C32-C33-C34-C35
33	h	103	DGD	CAA-CBA-CCA-CDA
26	b	603	CLA	C13-C15-C16-C17
32	A	616	SQD	C12-C13-C14-C15

There are no ring outliers.

144 monomers are involved in 267 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	A	611	BCR	2	0
28	B	617	BCR	1	0
26	B	605	CLA	5	0
29	d	406	PL9	1	0
26	c	511	CLA	4	0
26	b	613	CLA	5	0
26	A	608	CLA	1	0
26	B	609	CLA	1	0
26	B	603	CLA	3	0
28	b	618	BCR	1	0
28	B	618	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	C	506	CLA	2	0
34	k	102	STE	1	0
34	T	102	STE	1	0
35	F	101	HEM	1	0
32	F	102	SQD	2	0
26	a	607	CLA	2	0
30	c	522	LMG	2	0
26	c	503	CLA	2	0
26	B	604	CLA	4	0
33	a	614	DGD	3	0
26	B	610	CLA	1	0
34	d	414	STE	5	0
28	h	102	BCR	4	0
26	b	614	CLA	4	0
26	b	603	CLA	3	0
28	c	515	BCR	3	0
33	C	516	DGD	2	0
26	b	612	CLA	5	0
26	b	615	CLA	4	0
31	d	408	LHG	2	0
30	M	101	LMG	2	0
26	b	606	CLA	3	0
32	a	613	SQD	2	0
32	b	619	SQD	4	0
28	c	516	BCR	2	0
26	c	504	CLA	2	0
28	Z	101	BCR	3	0
28	t	101	BCR	2	0
26	B	606	CLA	3	0
28	T	101	BCR	4	0
30	D	408	LMG	1	0
34	c	521	STE	2	0
26	C	507	CLA	1	0
28	k	101	BCR	1	0
26	C	503	CLA	3	0
26	b	605	CLA	2	0
26	C	508	CLA	2	0
21	a	601[C]	OEY	1	0
27	d	402	PHO	2	0
26	B	613	CLA	1	0
28	B	619	BCR	2	0
21	A	601[C]	OEY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	b	609	CLA	2	0
21	a	601[A]	OEY	1	0
31	D	407	LHG	3	0
32	A	616	SQD	1	0
34	H	102	STE	2	0
30	c	523	LMG	2	0
26	d	404	CLA	1	0
26	c	508	CLA	1	0
30	m	101	LMG	2	0
26	C	505	CLA	2	0
26	c	505	CLA	3	0
34	J	101	STE	1	0
32	A	618	SQD	1	0
34	l	102	STE	1	0
26	B	608	CLA	1	0
26	b	611	CLA	3	0
35	e	101	HEM	2	0
33	c	517	DGD	1	0
26	b	604	CLA	2	0
28	K	102	BCR	1	0
29	A	612	PL9	8	0
34	t	105	STE	3	0
26	C	502	CLA	2	0
26	a	612	CLA	2	0
26	C	504	CLA	2	0
26	c	510	CLA	1	0
33	c	519	DGD	2	0
34	B	620	STE	2	0
26	B	601	CLA	3	0
26	c	507	CLA	2	0
32	f	101	SQD	4	0
26	h	101	CLA	5	0
28	a	610	BCR	1	0
28	C	514	BCR	3	0
26	A	613	CLA	3	0
28	c	514	BCR	4	0
26	b	607	CLA	1	0
31	e	102	LHG	2	0
33	A	619	DGD	4	0
26	B	612	CLA	3	0
30	A	614	LMG	2	0
26	B	616	CLA	1	0

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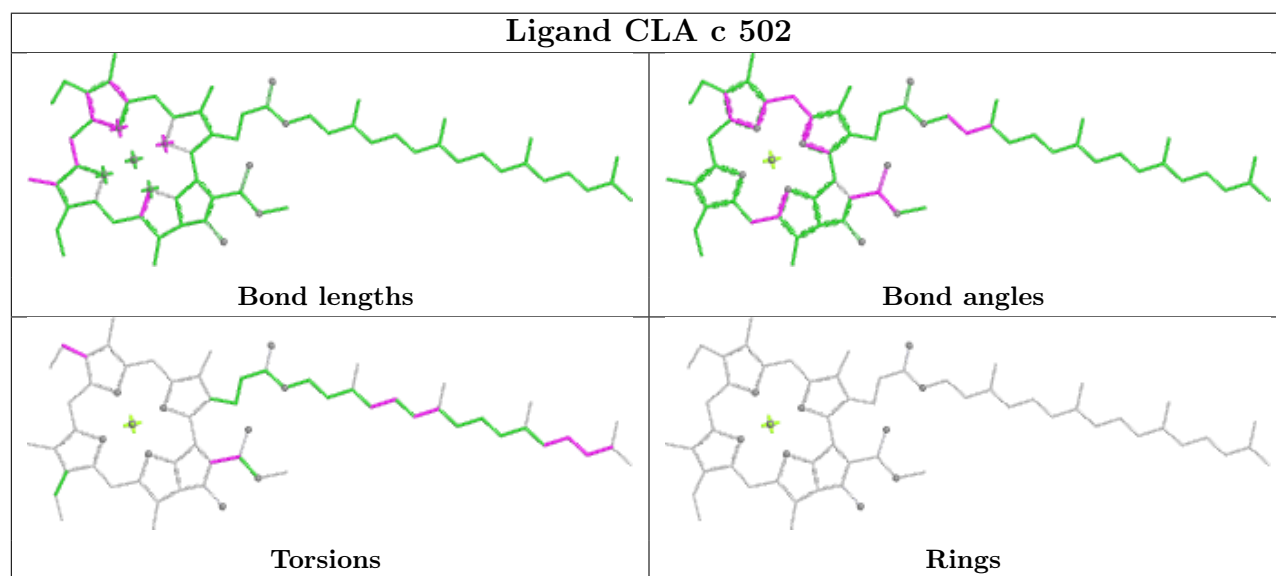
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	b	608	CLA	2	0
26	b	601	CLA	1	0
34	b	622	STE	1	0
26	B	615	CLA	1	0
32	B	622	SQD	5	0
34	b	623	STE	1	0
28	b	616	BCR	2	0
26	b	602	CLA	3	0
26	A	607	CLA	2	0
30	C	518	LMG	3	0
26	c	512	CLA	3	0
21	A	601[A]	OEY	1	0
26	C	501	CLA	1	0
28	D	404	BCR	1	0
36	v	201	HEC	2	0
26	a	609	CLA	4	0
26	B	607	CLA	1	0
26	C	511	CLA	3	0
26	C	513	CLA	3	0
26	a	606	CLA	2	0
26	C	512	CLA	3	0
26	c	513	CLA	4	0
31	l	101	LHG	3	0
26	B	602	CLA	1	0
29	D	405	PL9	1	0
26	B	614	CLA	4	0
30	D	406	LMG	1	0
33	H	101	DGD	1	0
28	d	405	BCR	3	0
26	C	509	CLA	1	0
31	L	101	LHG	3	0
33	C	517	DGD	1	0
34	C	521	STE	2	0
34	X	102	STE	5	0
26	D	402	CLA	4	0
31	d	409	LHG	1	0
26	D	403	CLA	3	0
28	X	101	BCR	1	0
28	b	617	BCR	3	0
26	c	501	CLA	3	0
27	D	401	PHO	2	0
31	A	615	LHG	1	0

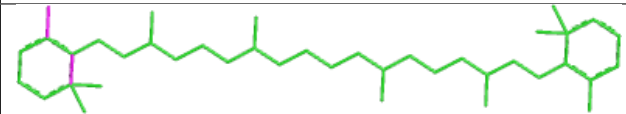
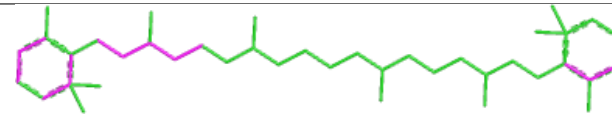
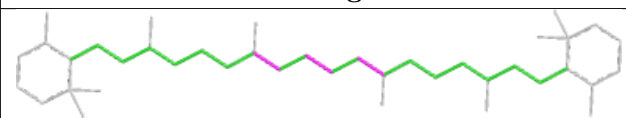
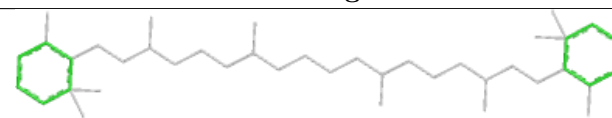
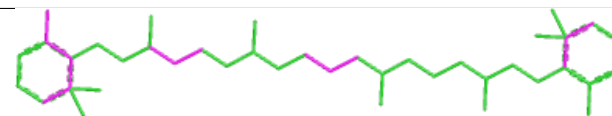
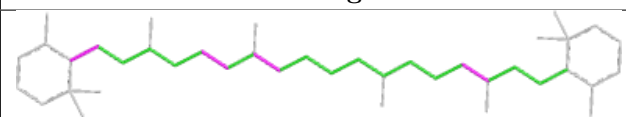
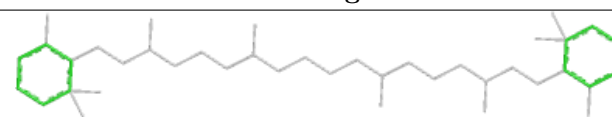
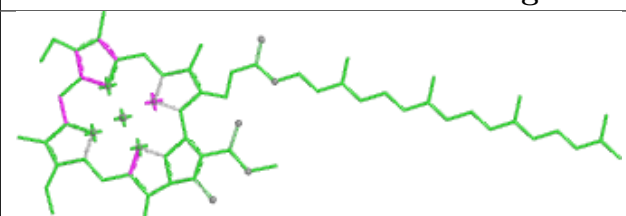
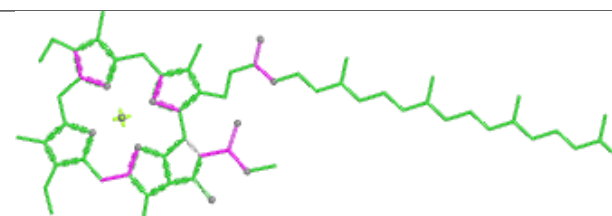
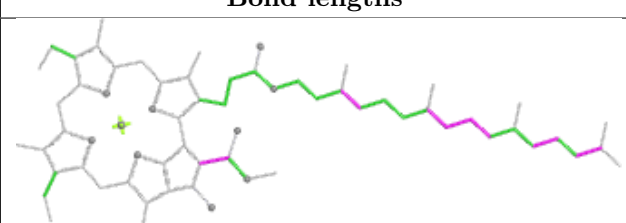
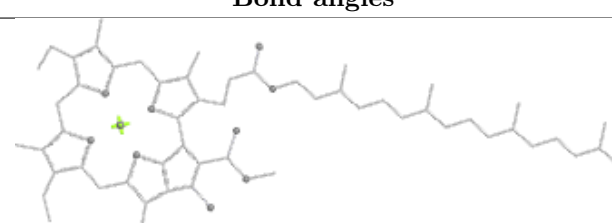
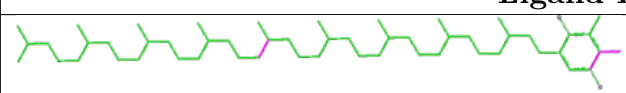
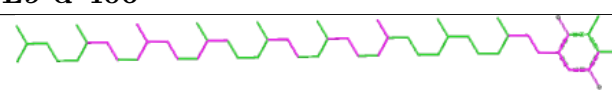
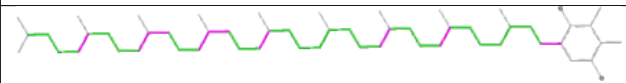
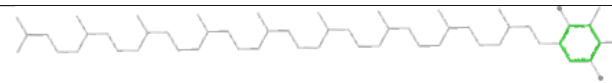
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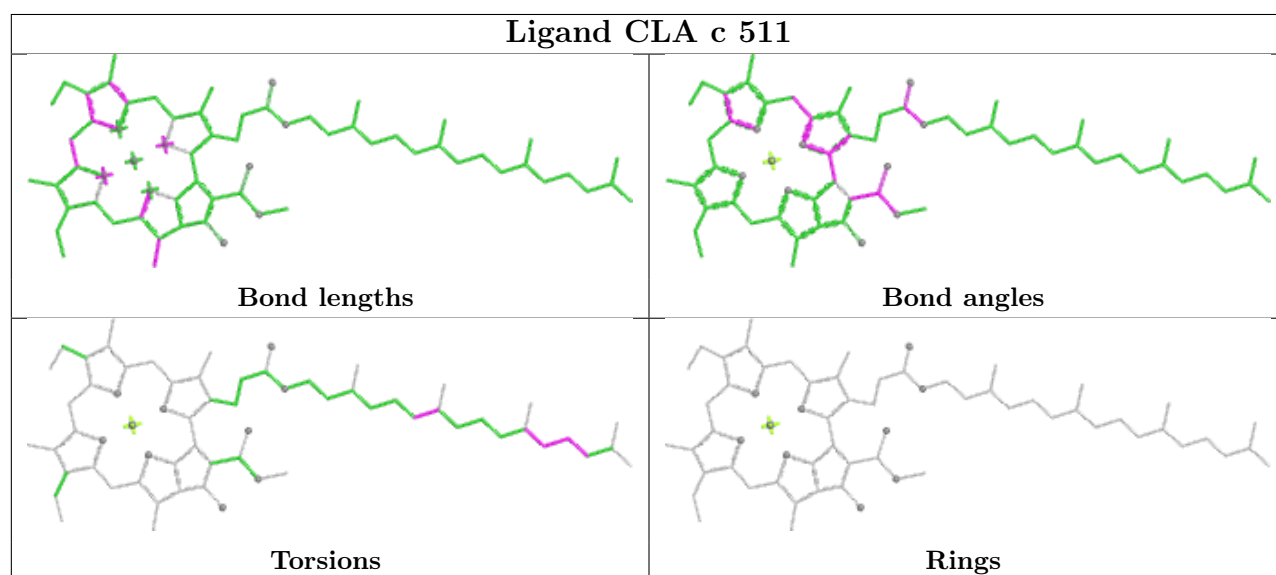
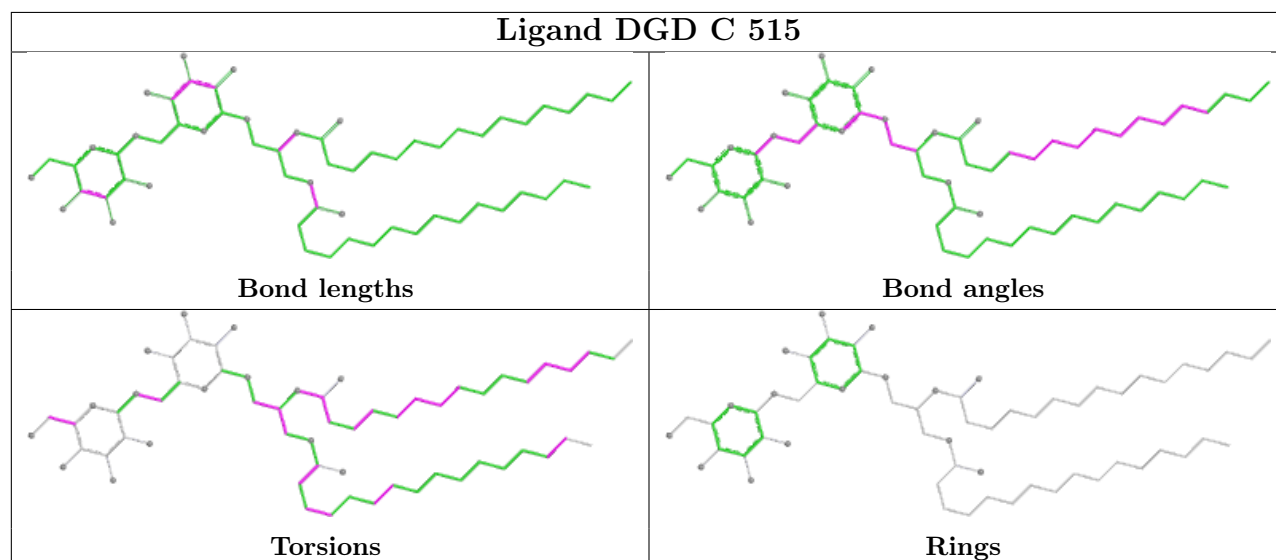
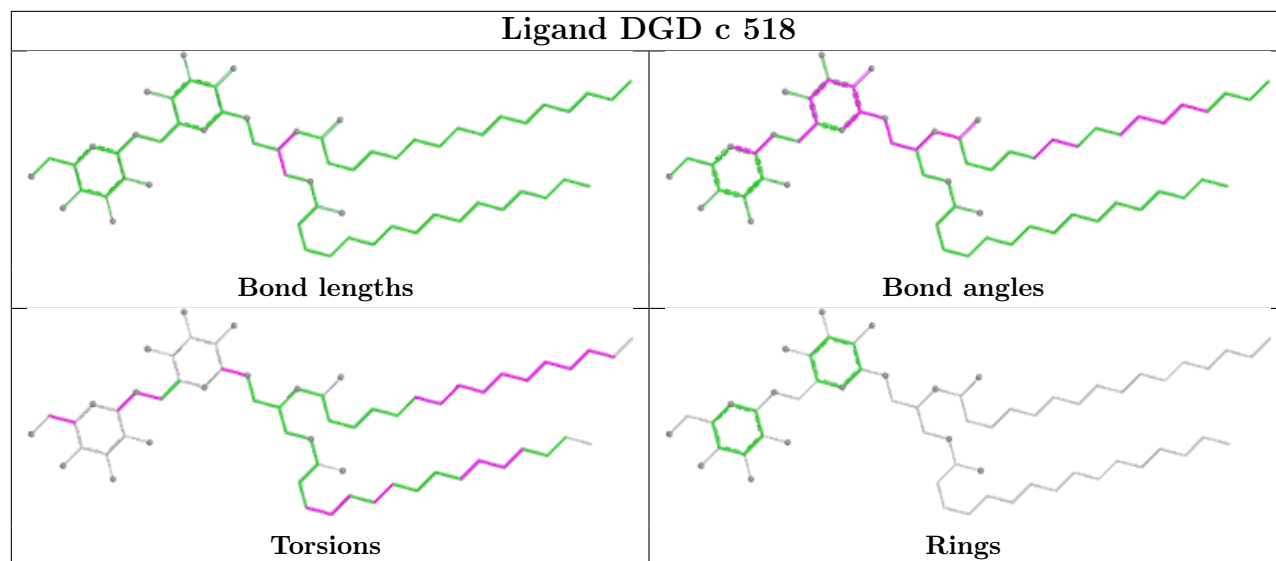
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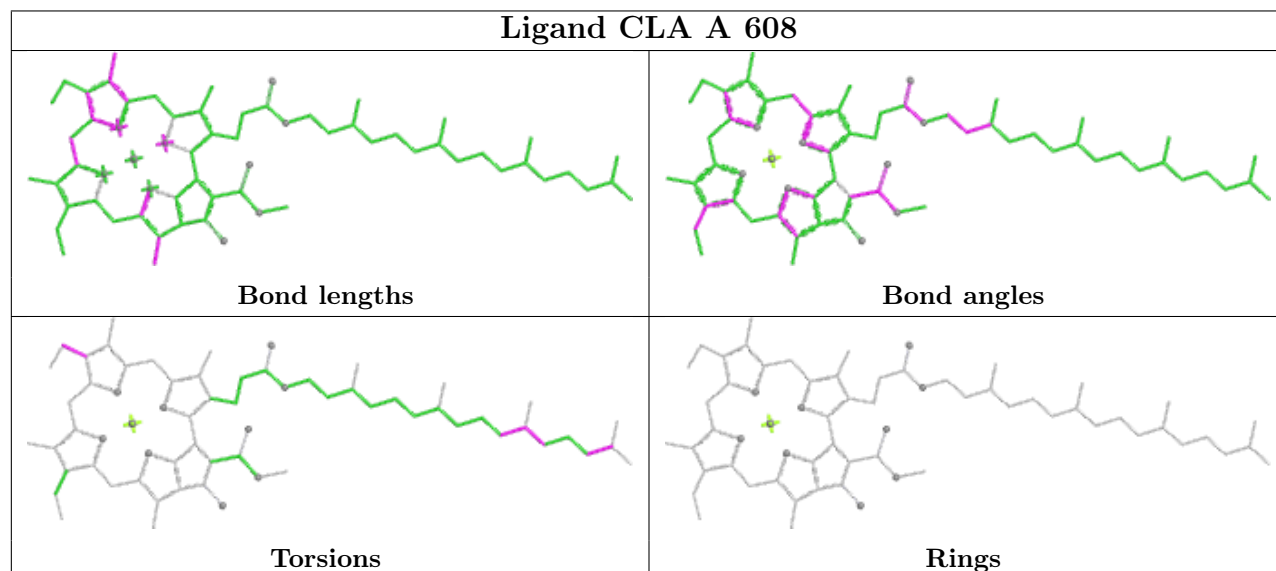
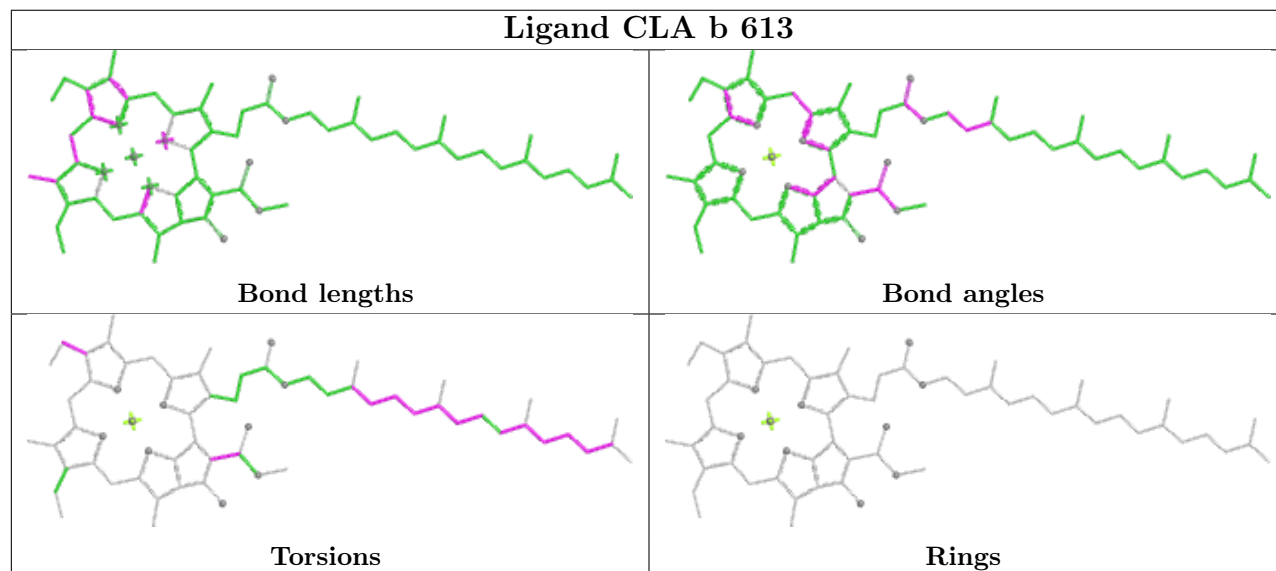
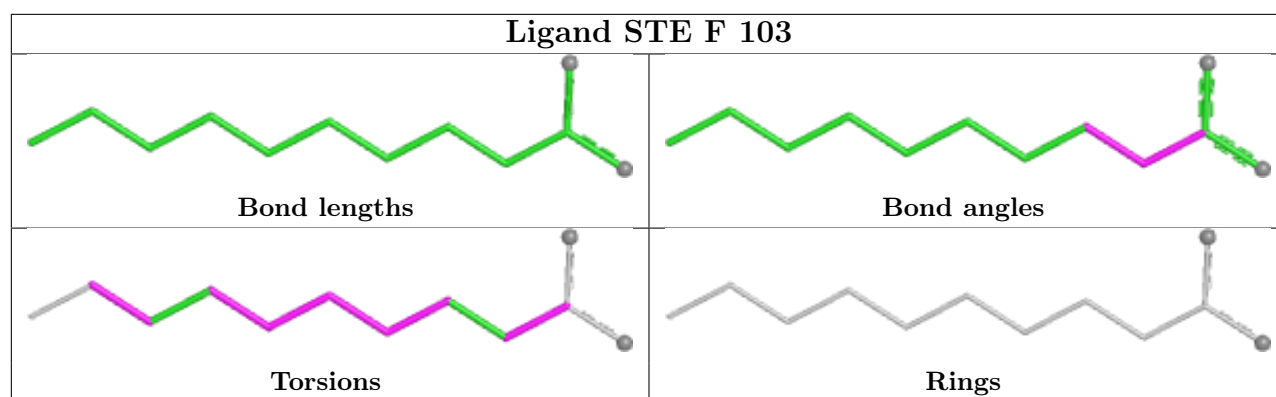
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	a	611	PL9	6	0
34	I	101	STE	1	0
34	j	101	STE	1	0
34	d	413	STE	1	0
31	D	409	LHG	3	0
31	A	617	LHG	1	0
31	d	407	LHG	5	0

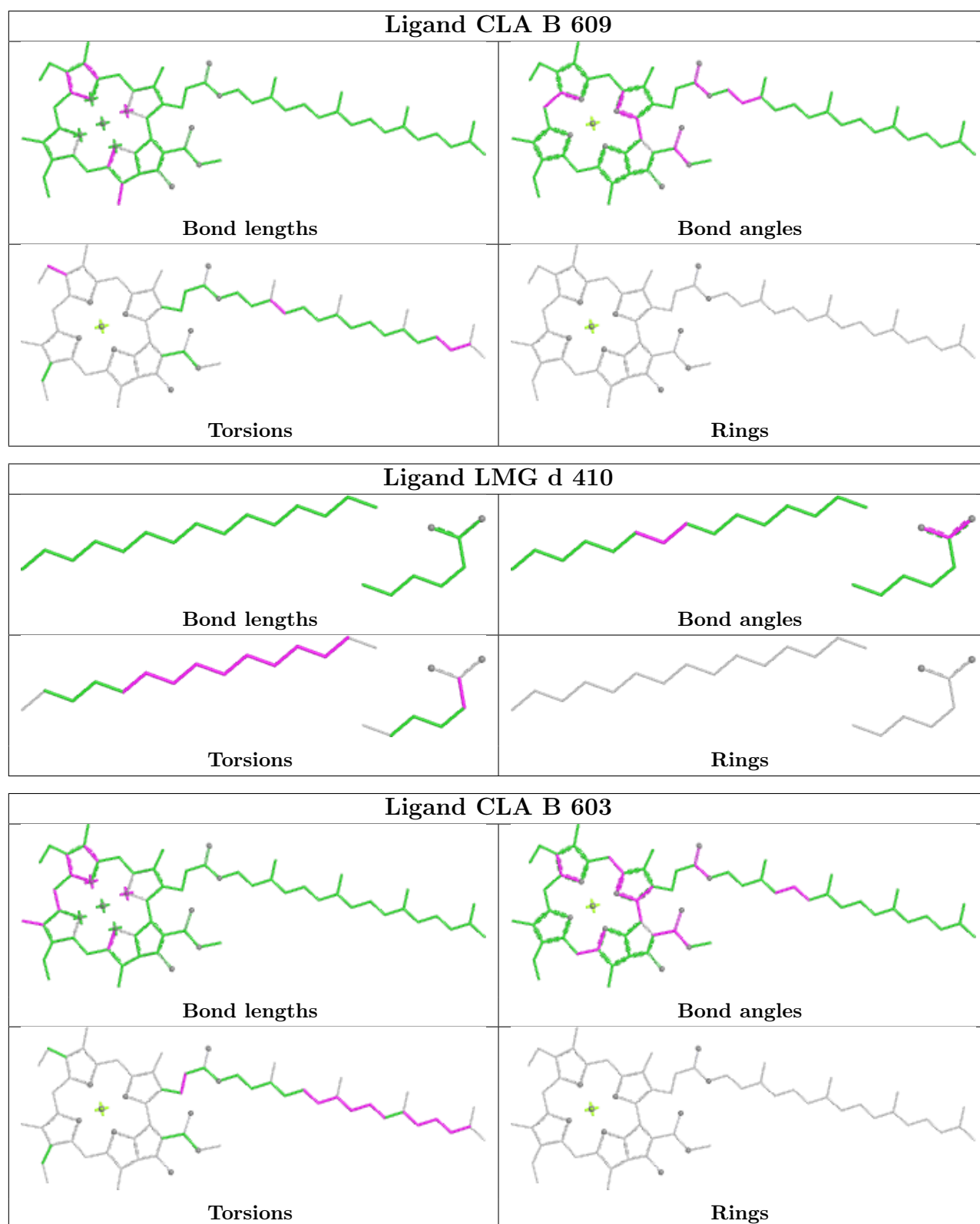
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

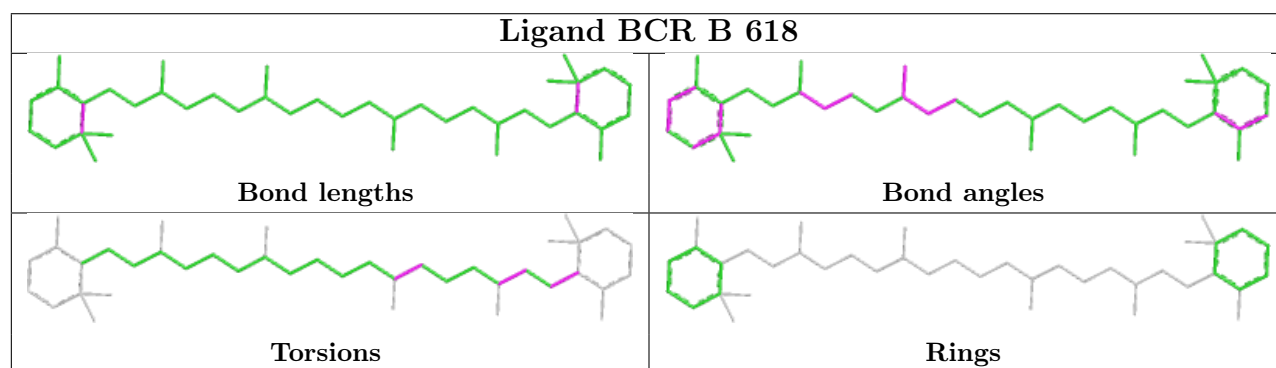
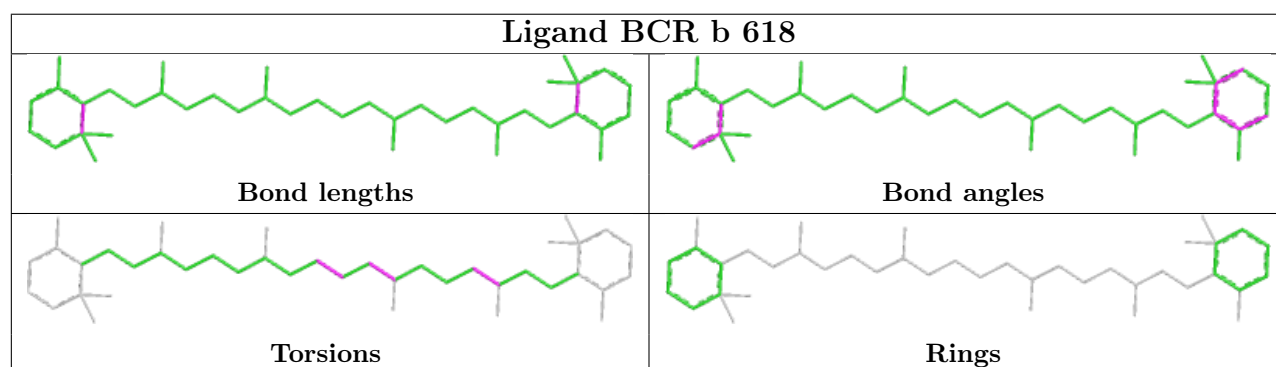
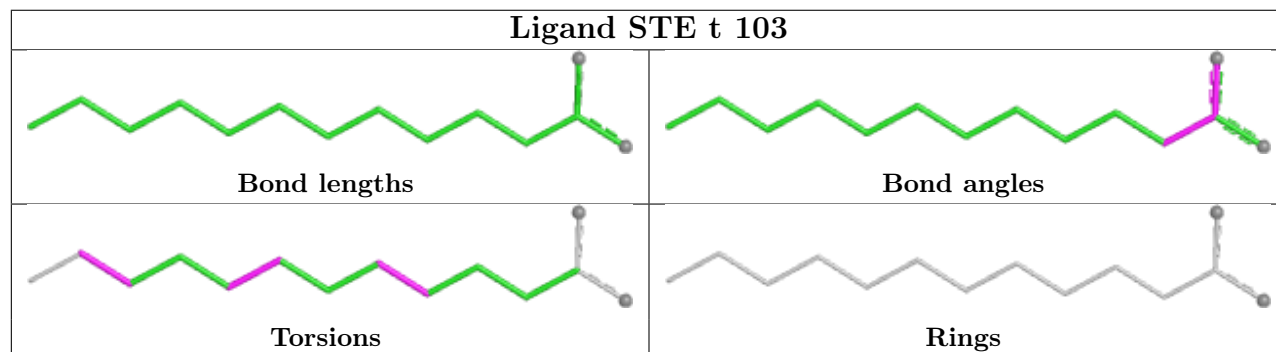
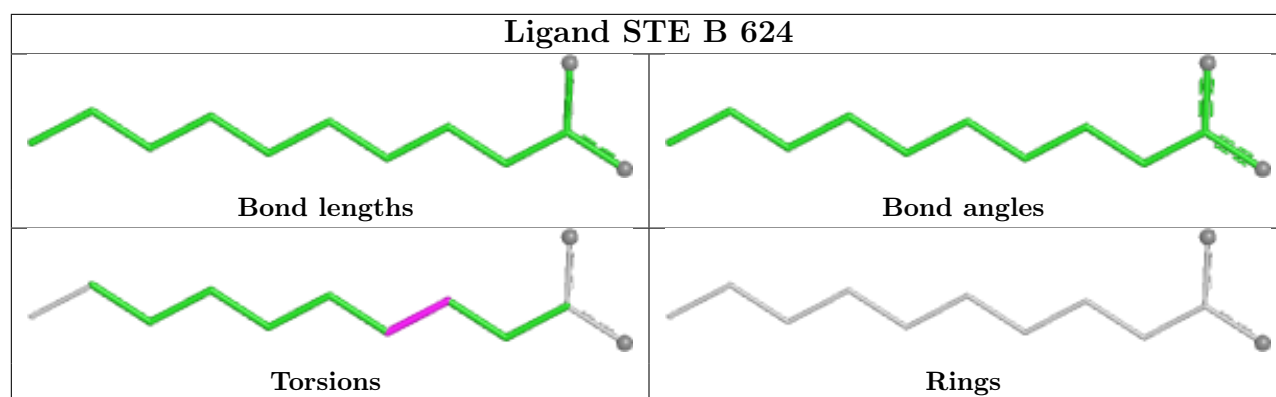


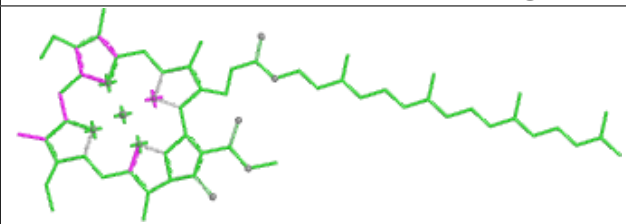
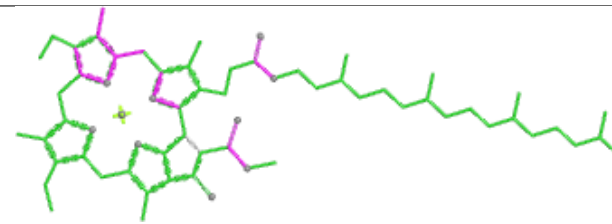
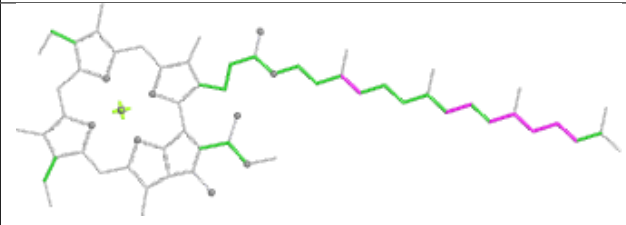
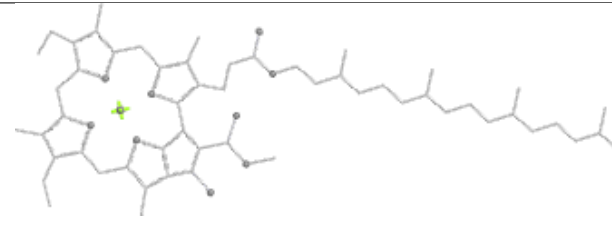
Ligand BCR A 611	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR B 617	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA B 605	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand PL9 d 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

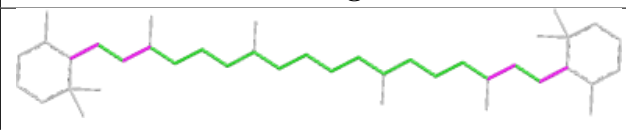
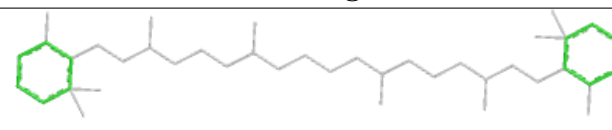


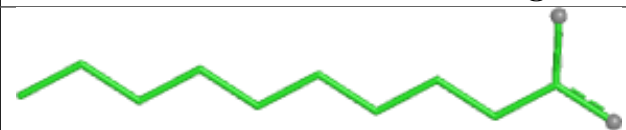
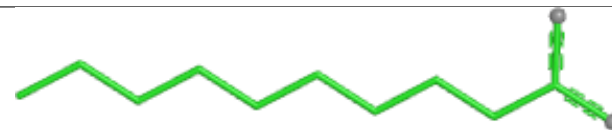
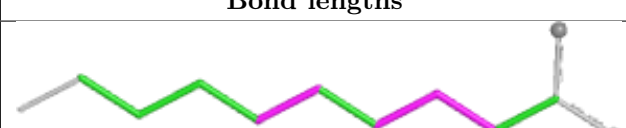
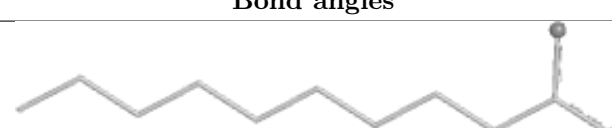


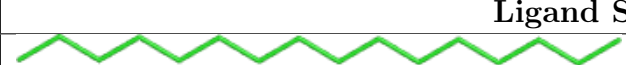
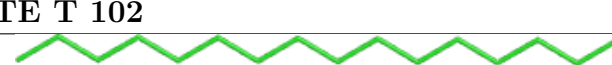
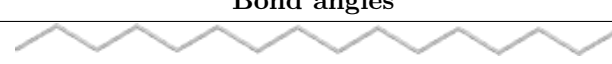


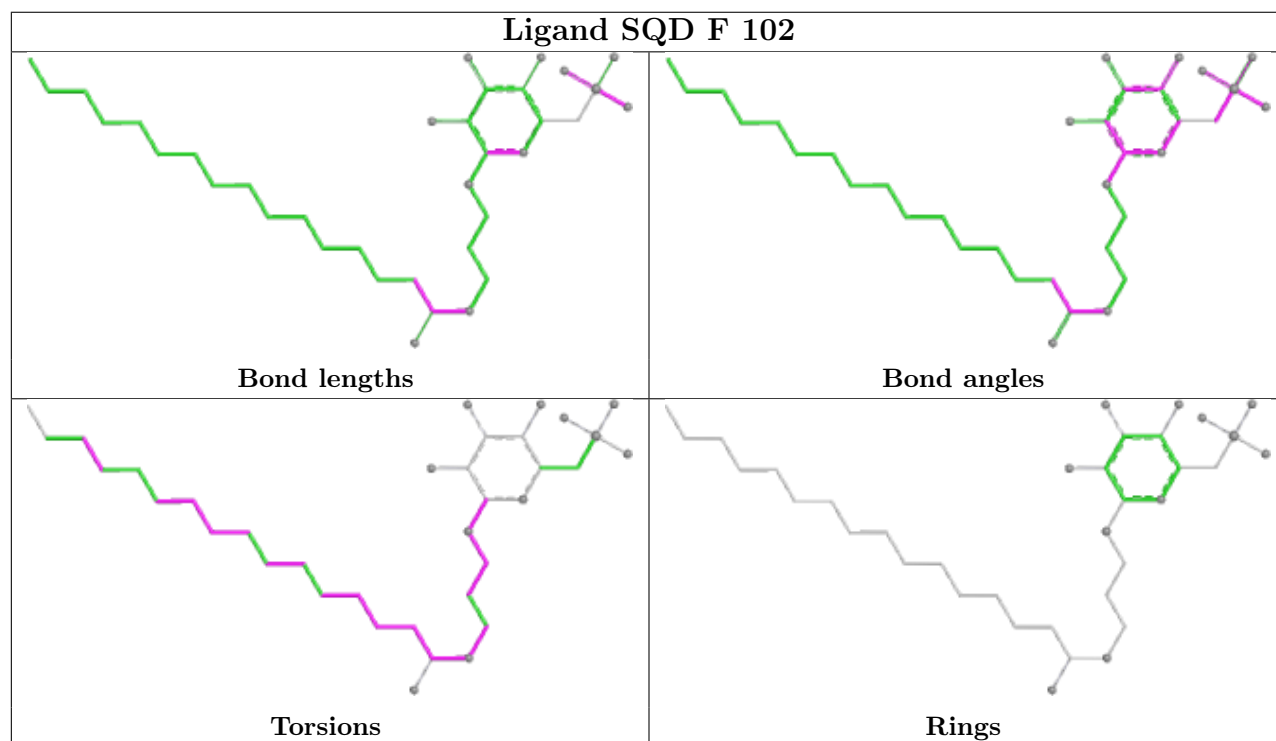
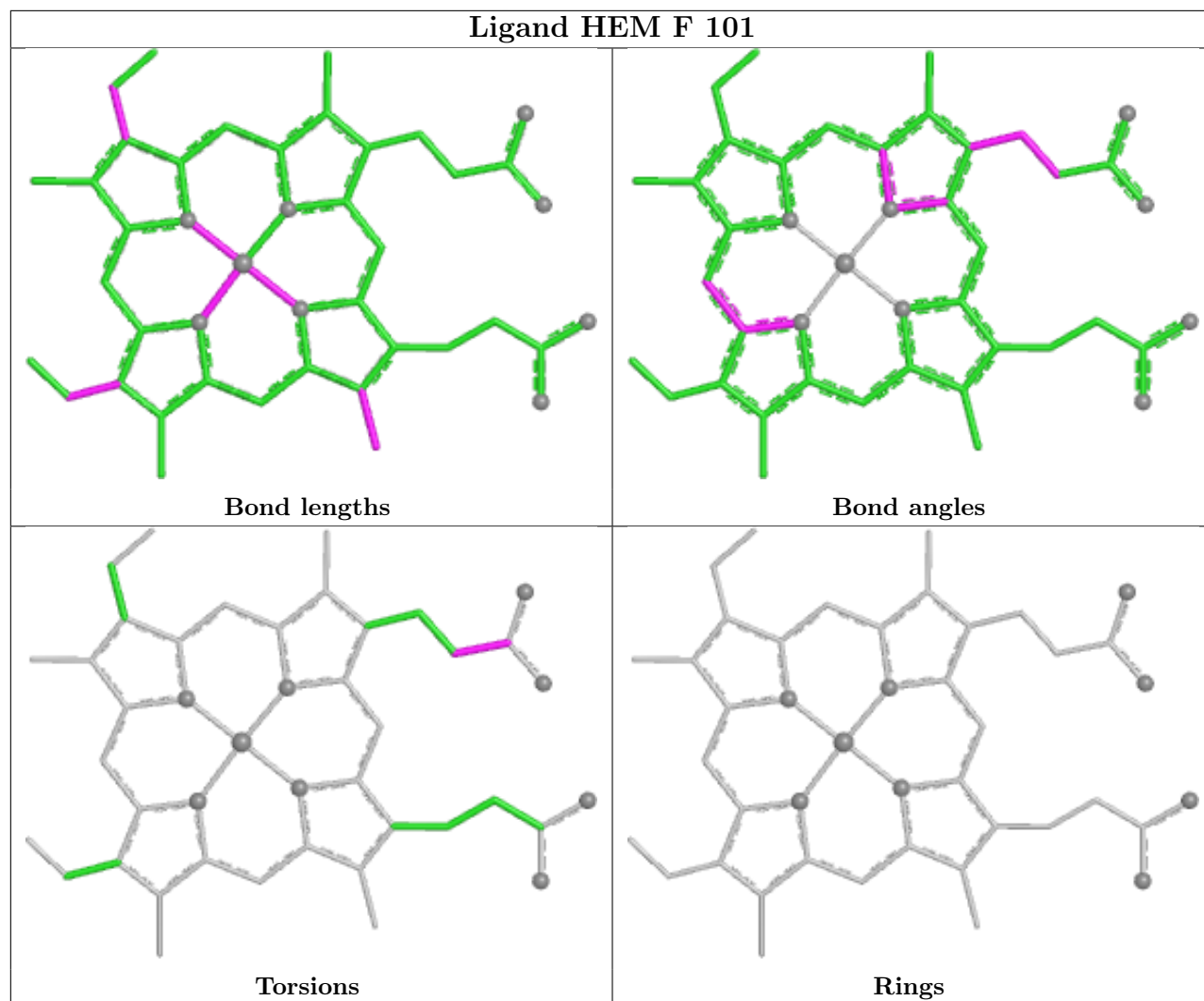


Ligand CLA C 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

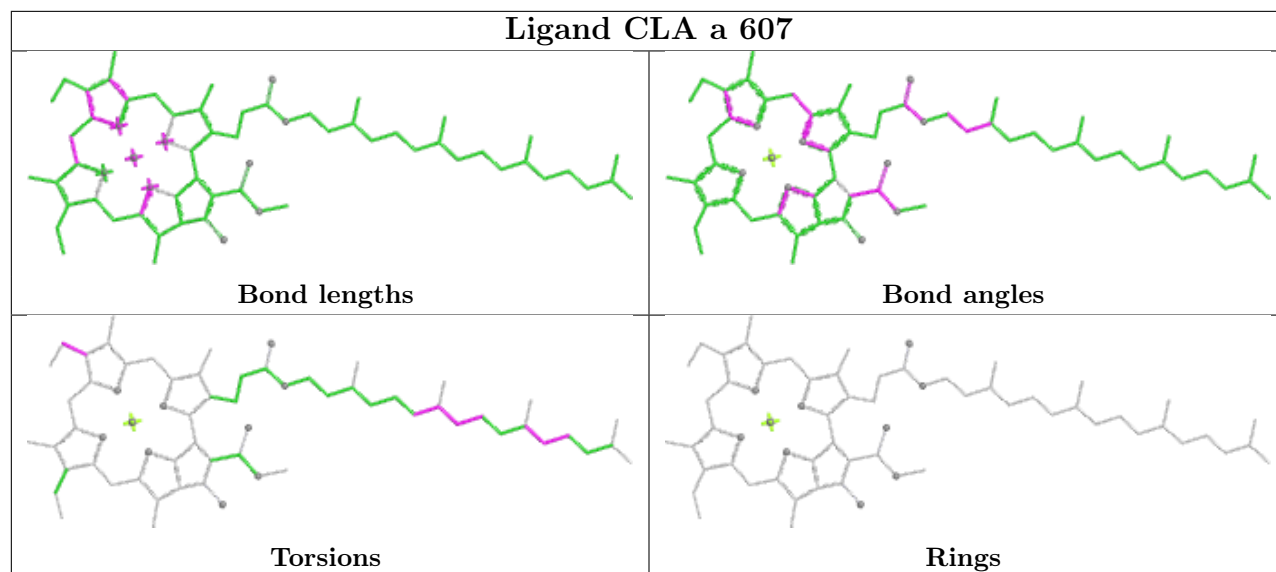
Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE k 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

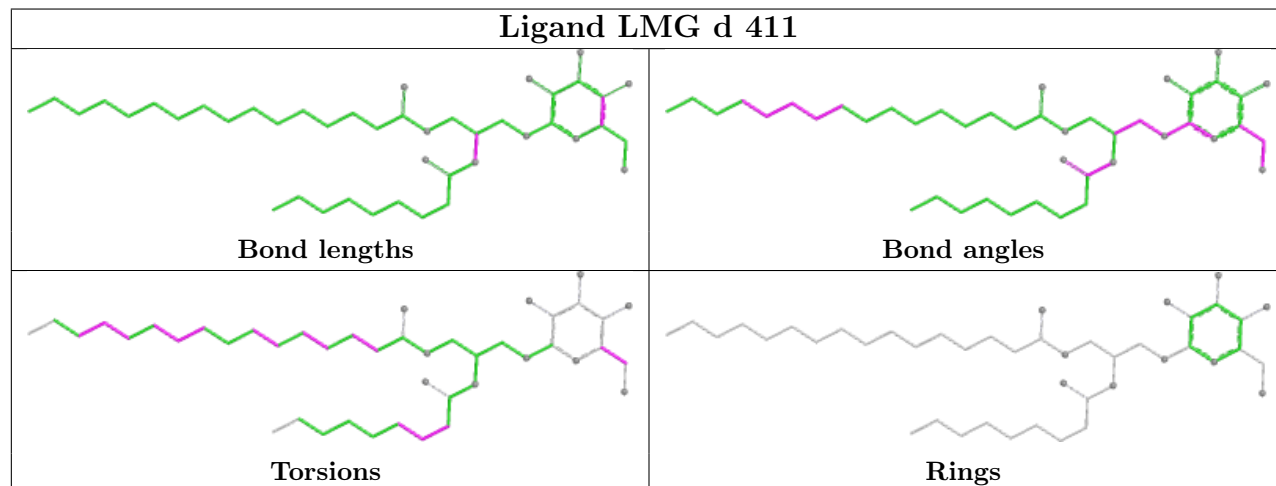
Ligand STE T 102	
	
Bond lengths	Bond angles
	
Torsions	Rings



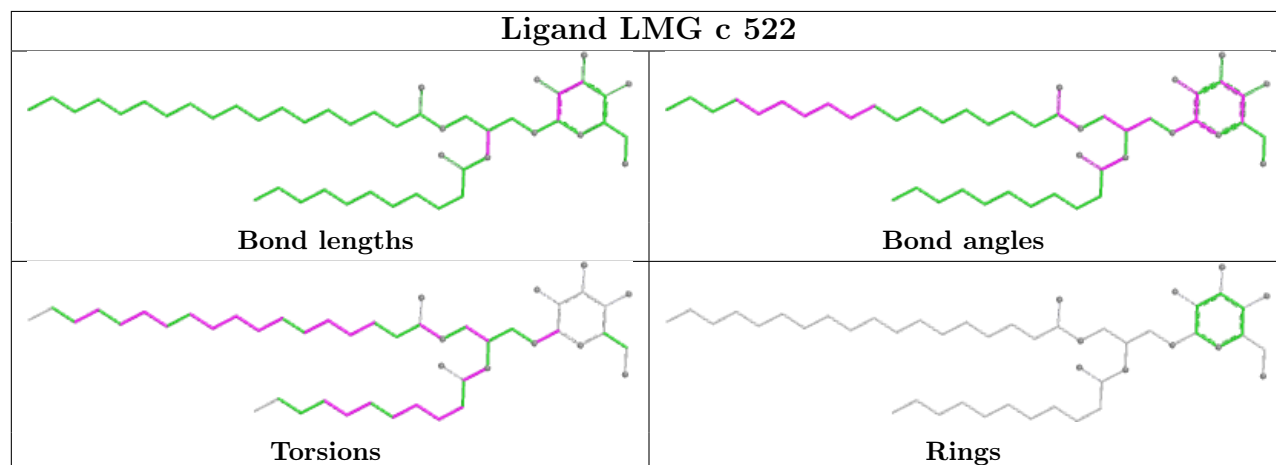
Ligand CLA a 607



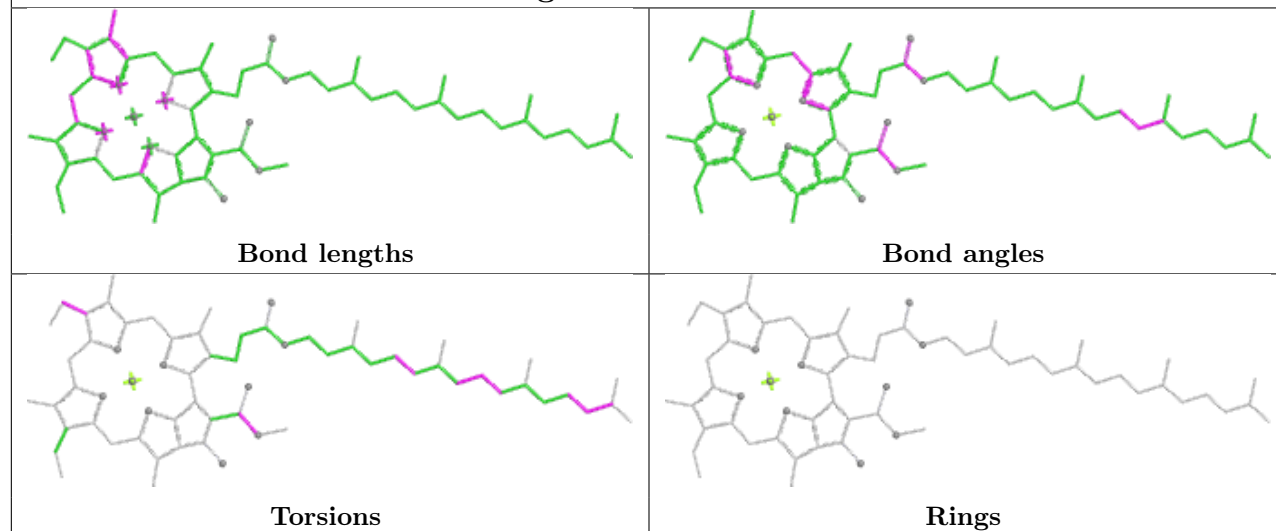
Ligand LMG d 411



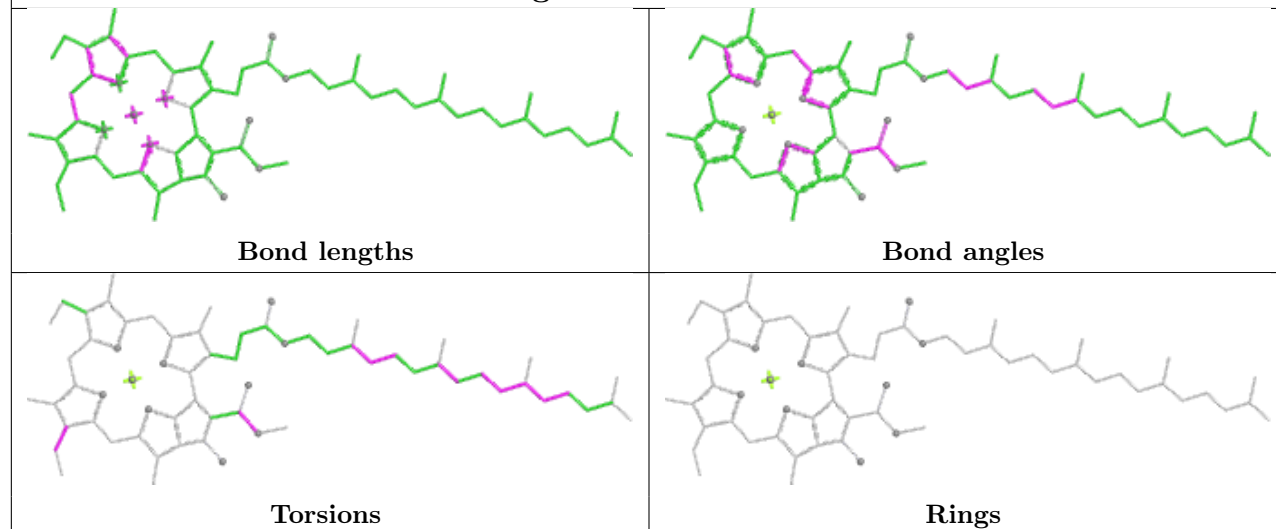
Ligand LMG c 522



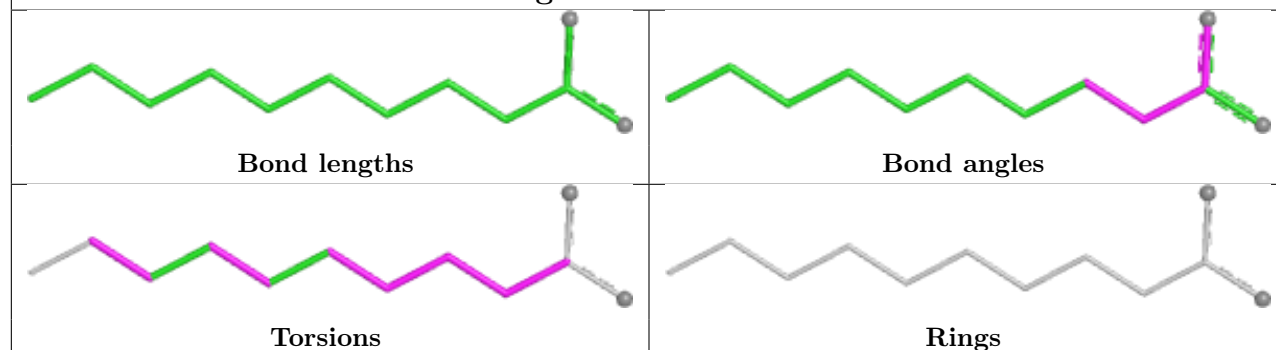
Ligand CLA c 503

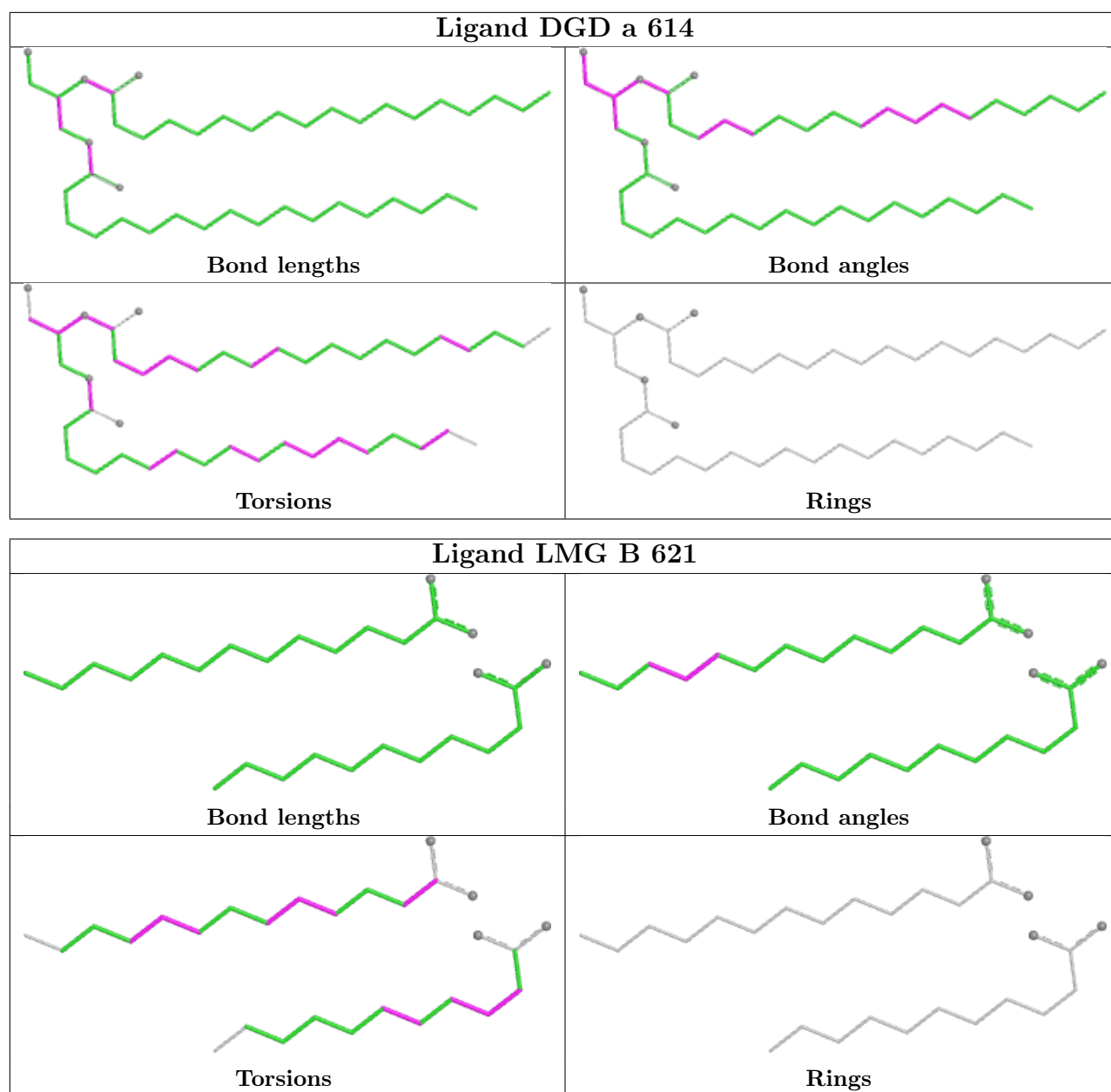


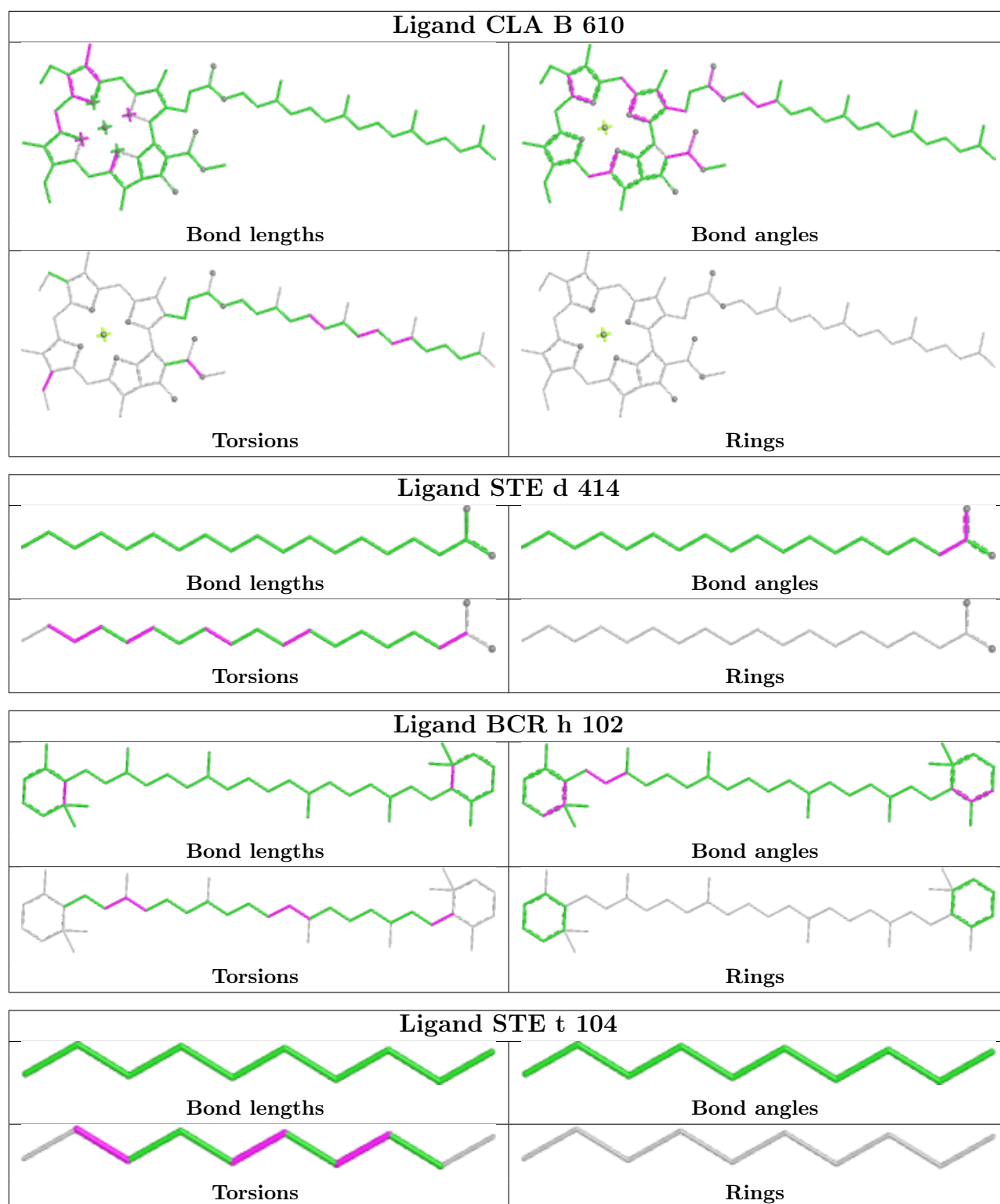
Ligand CLA B 604



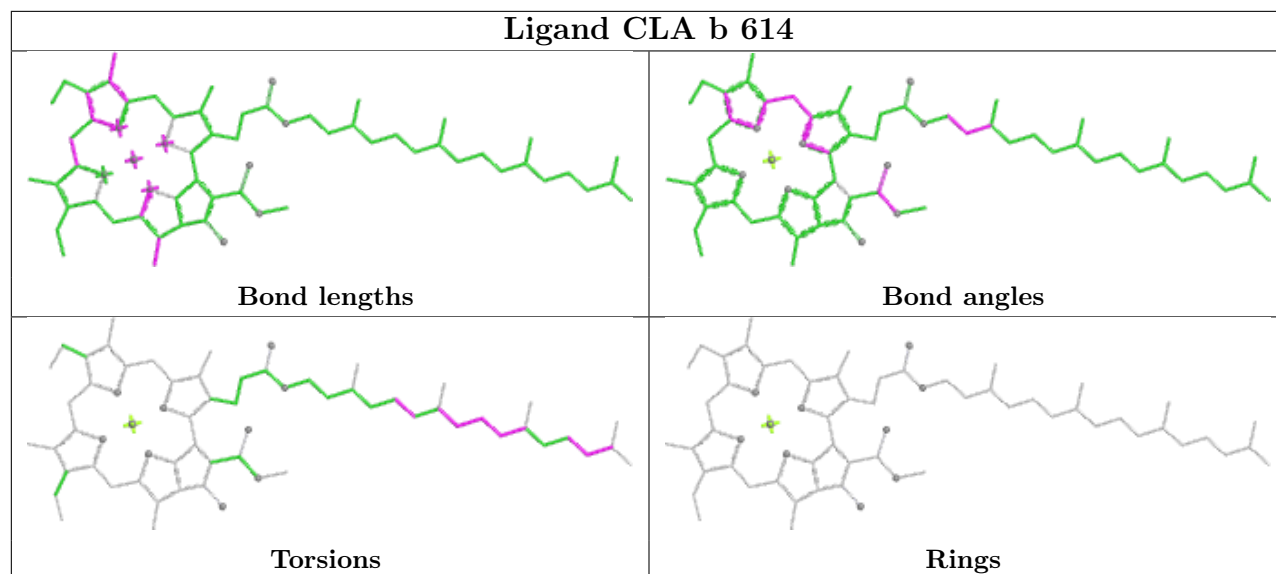
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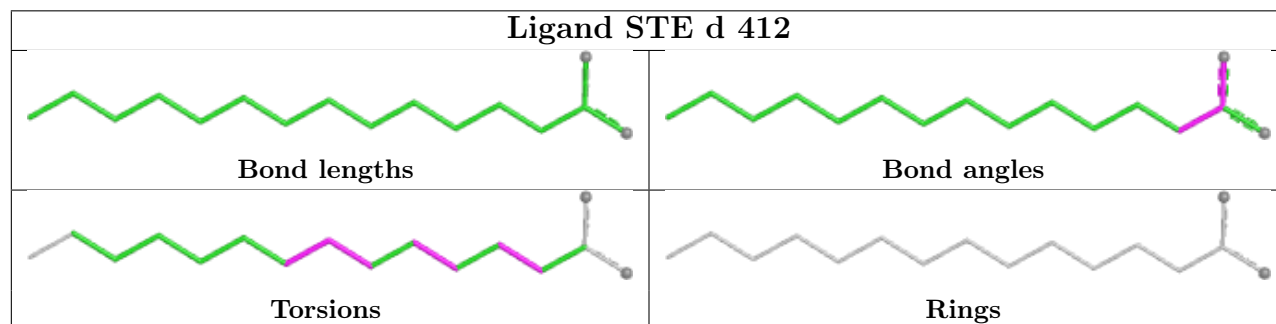




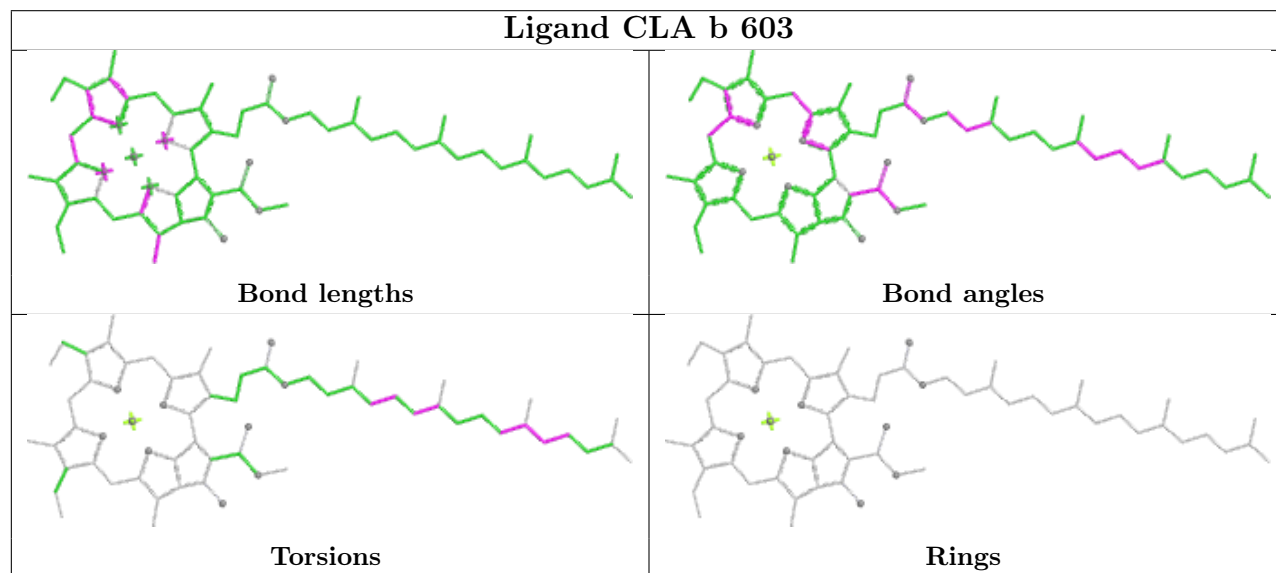
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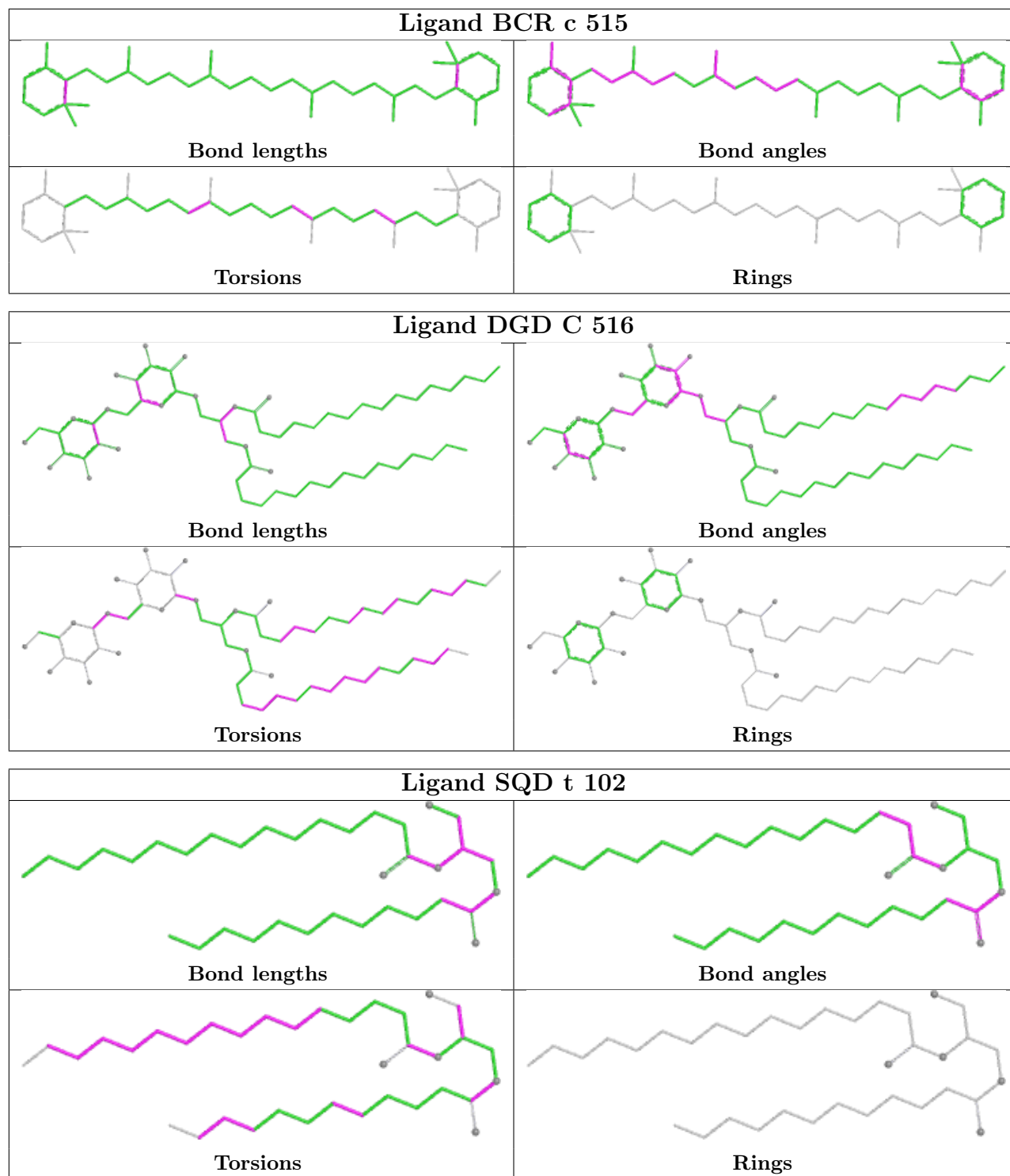


Ligand STE d 412

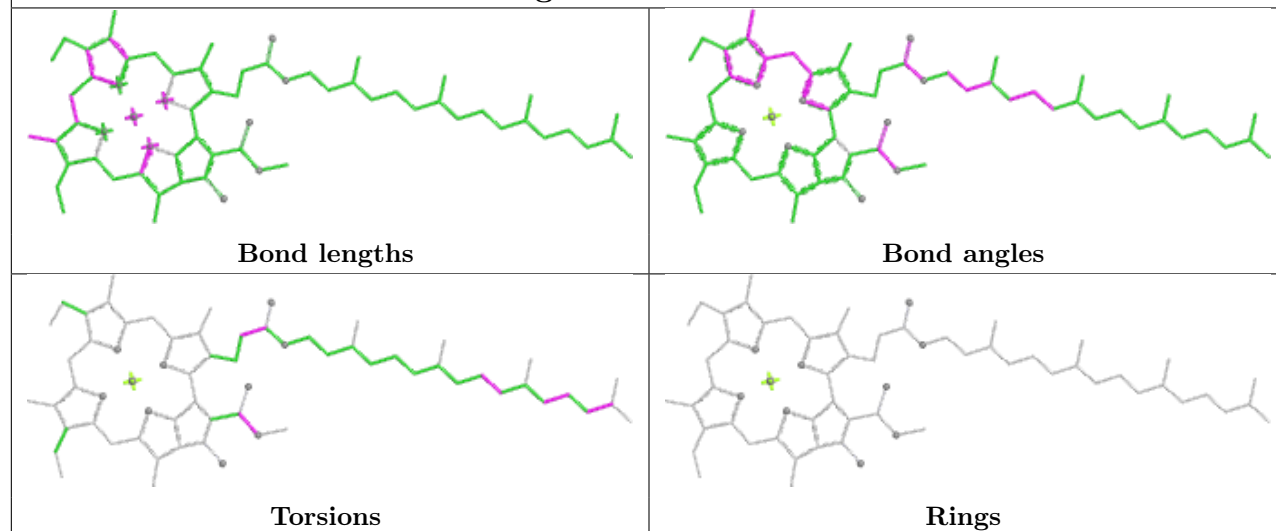


Ligand CLA b 603

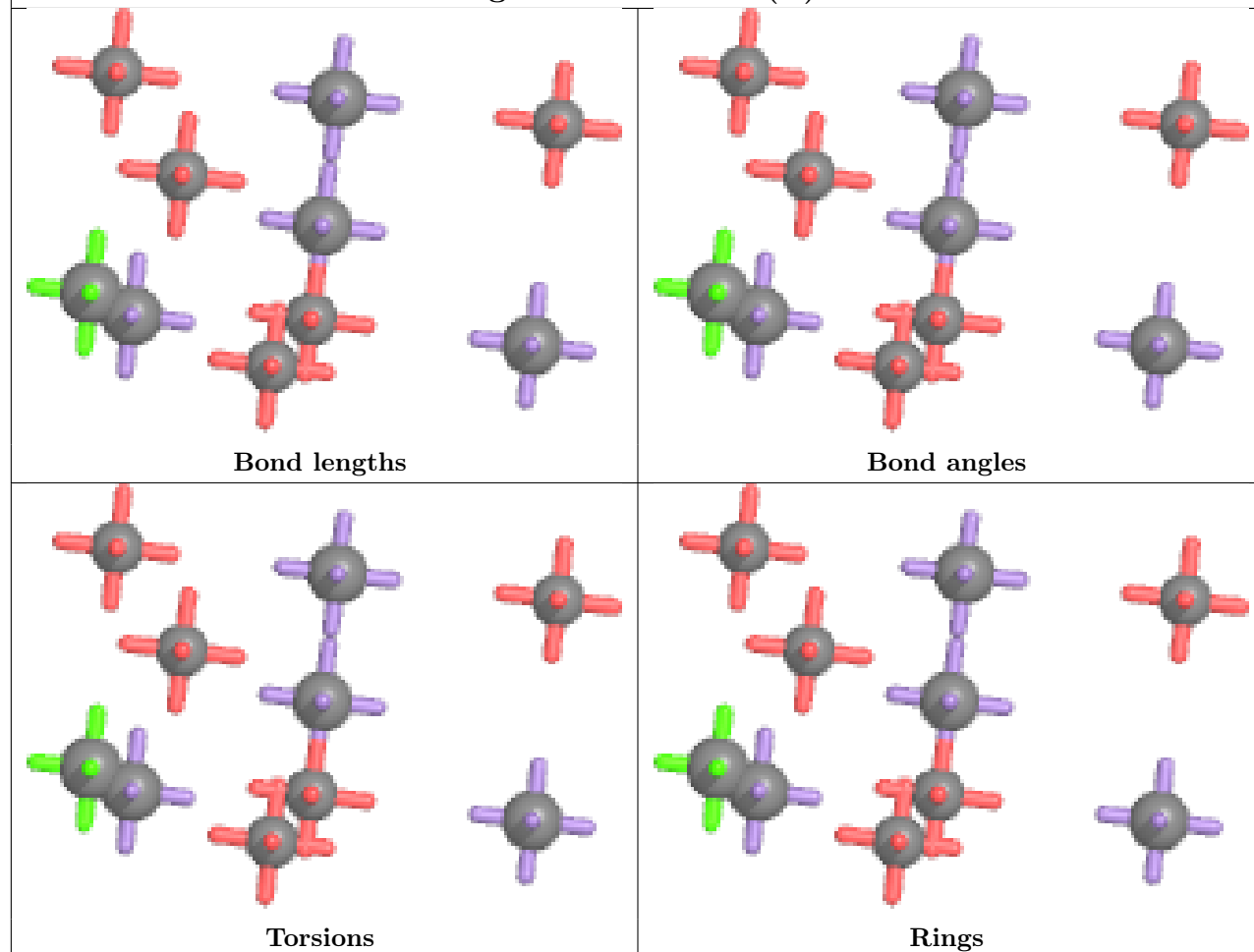


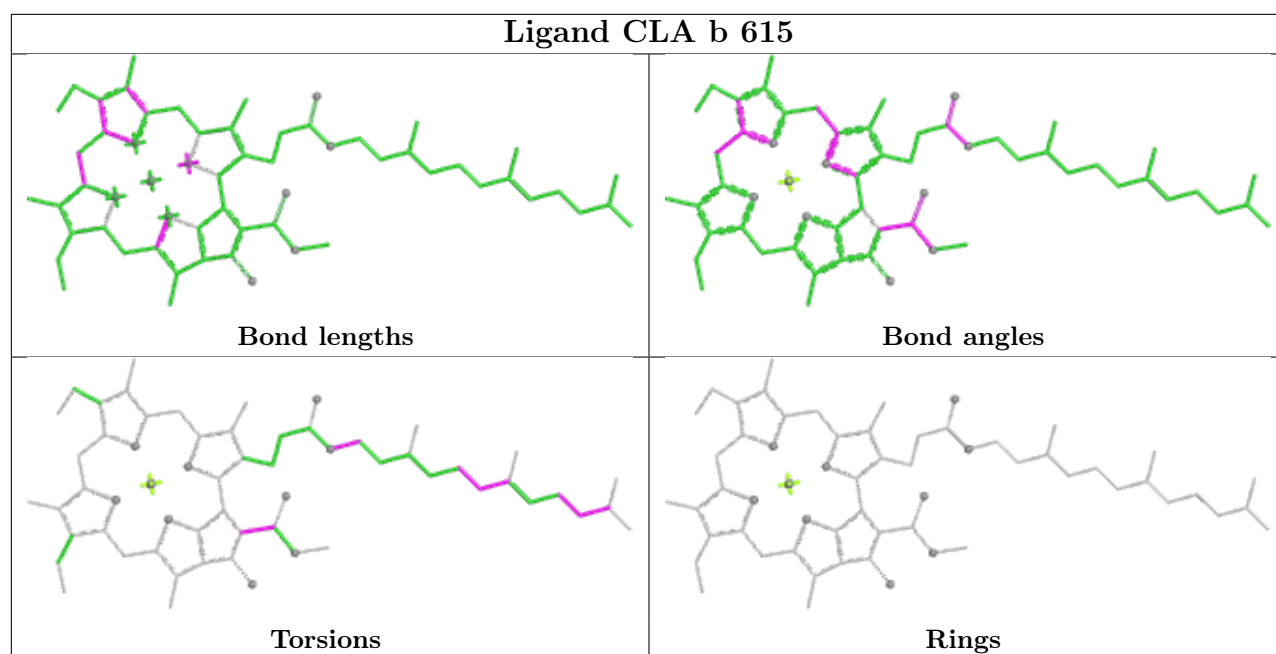


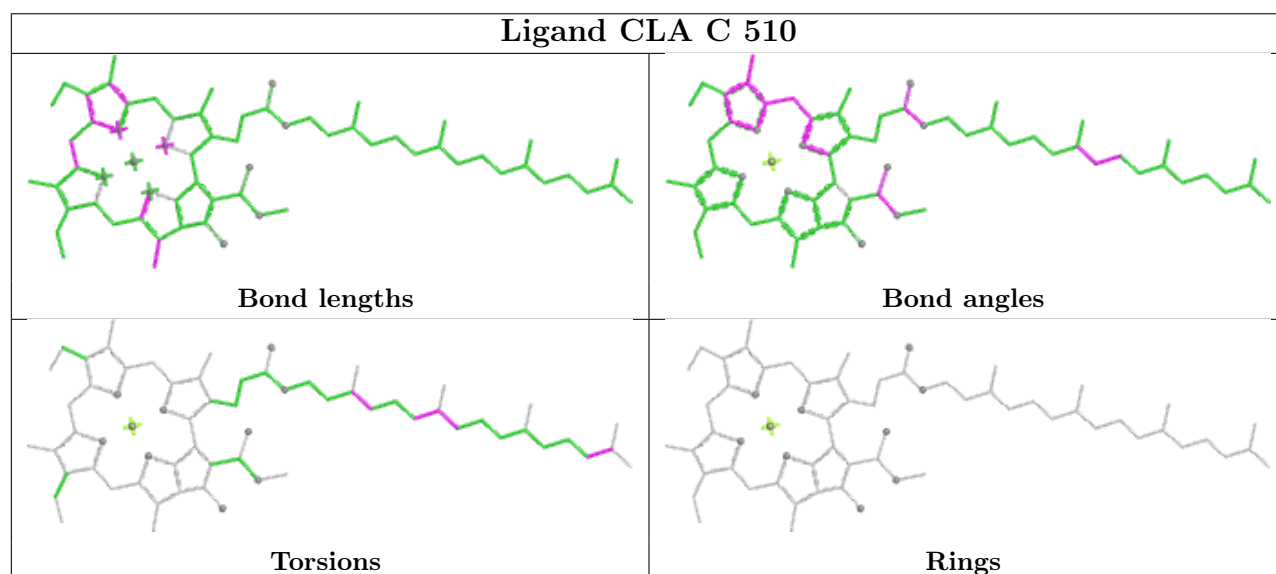
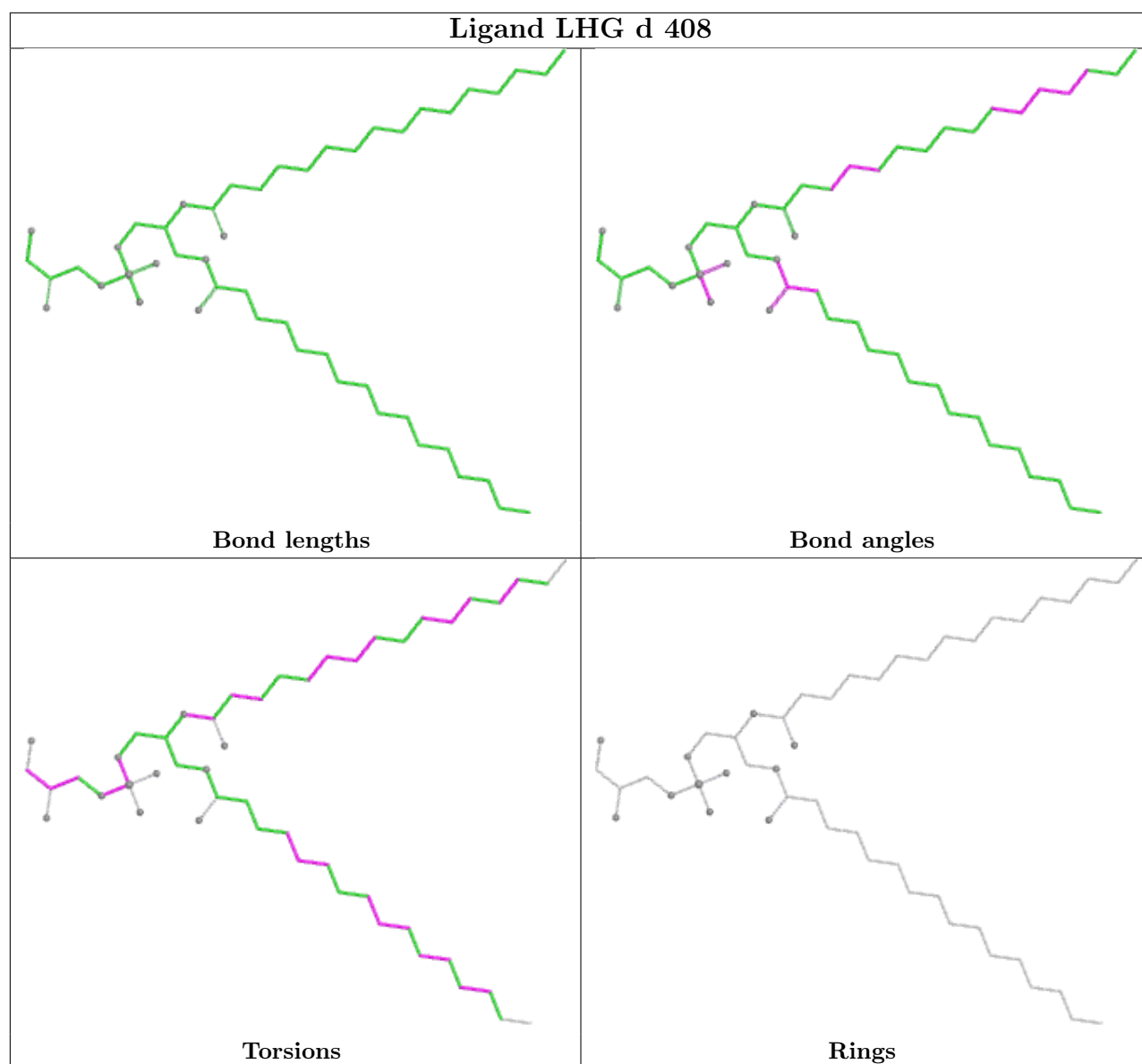
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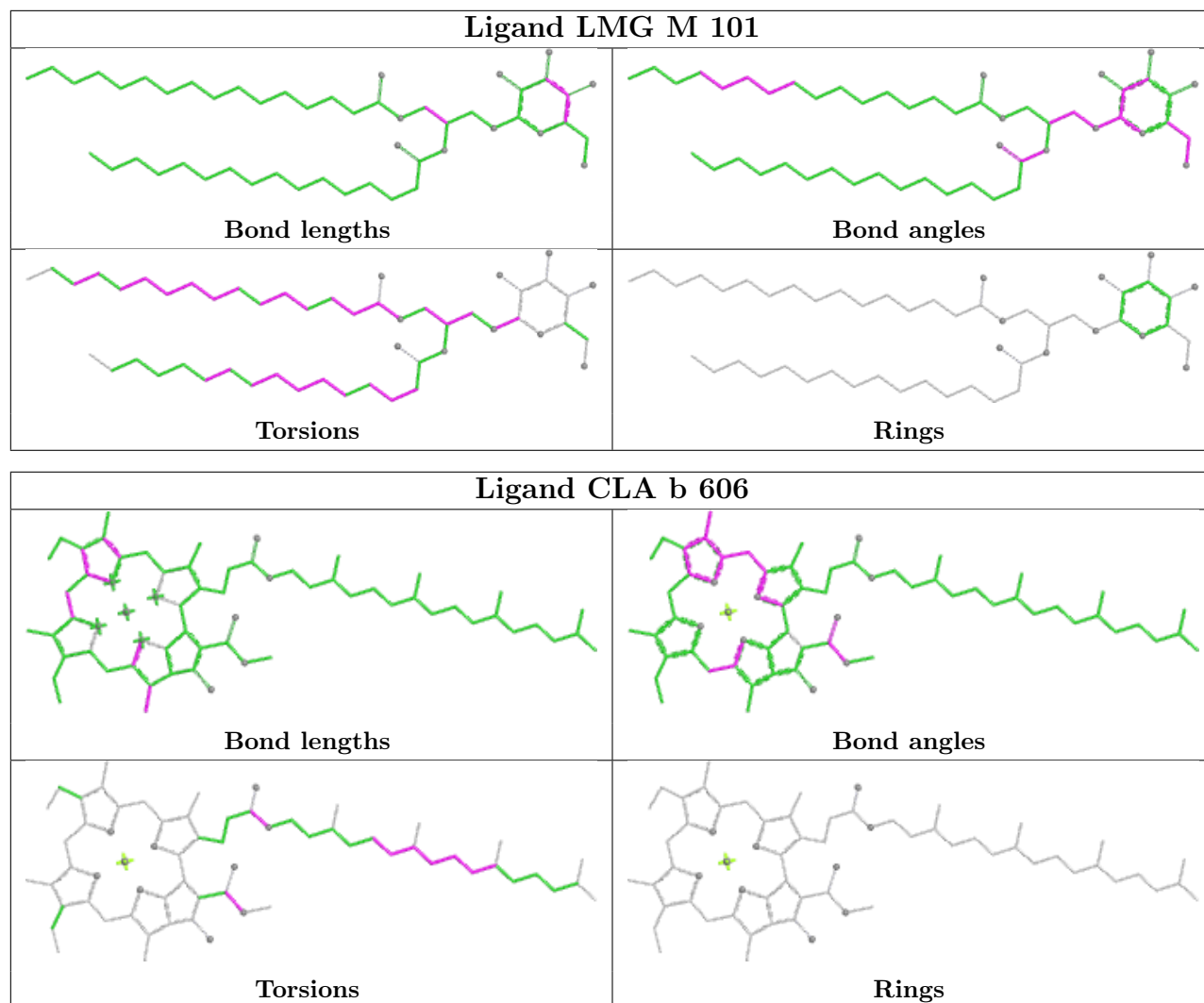


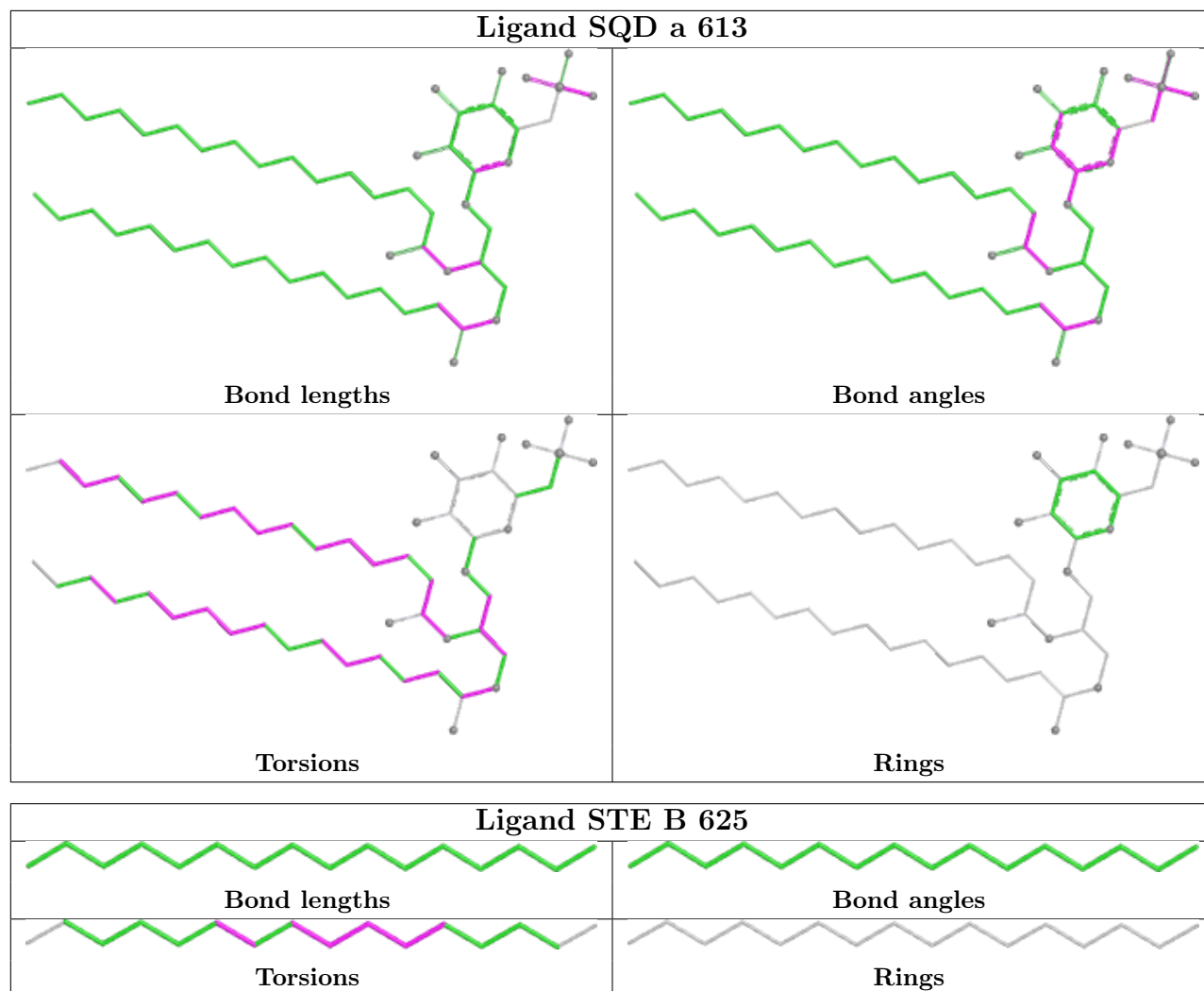
Ligand OEX A 602 (B)

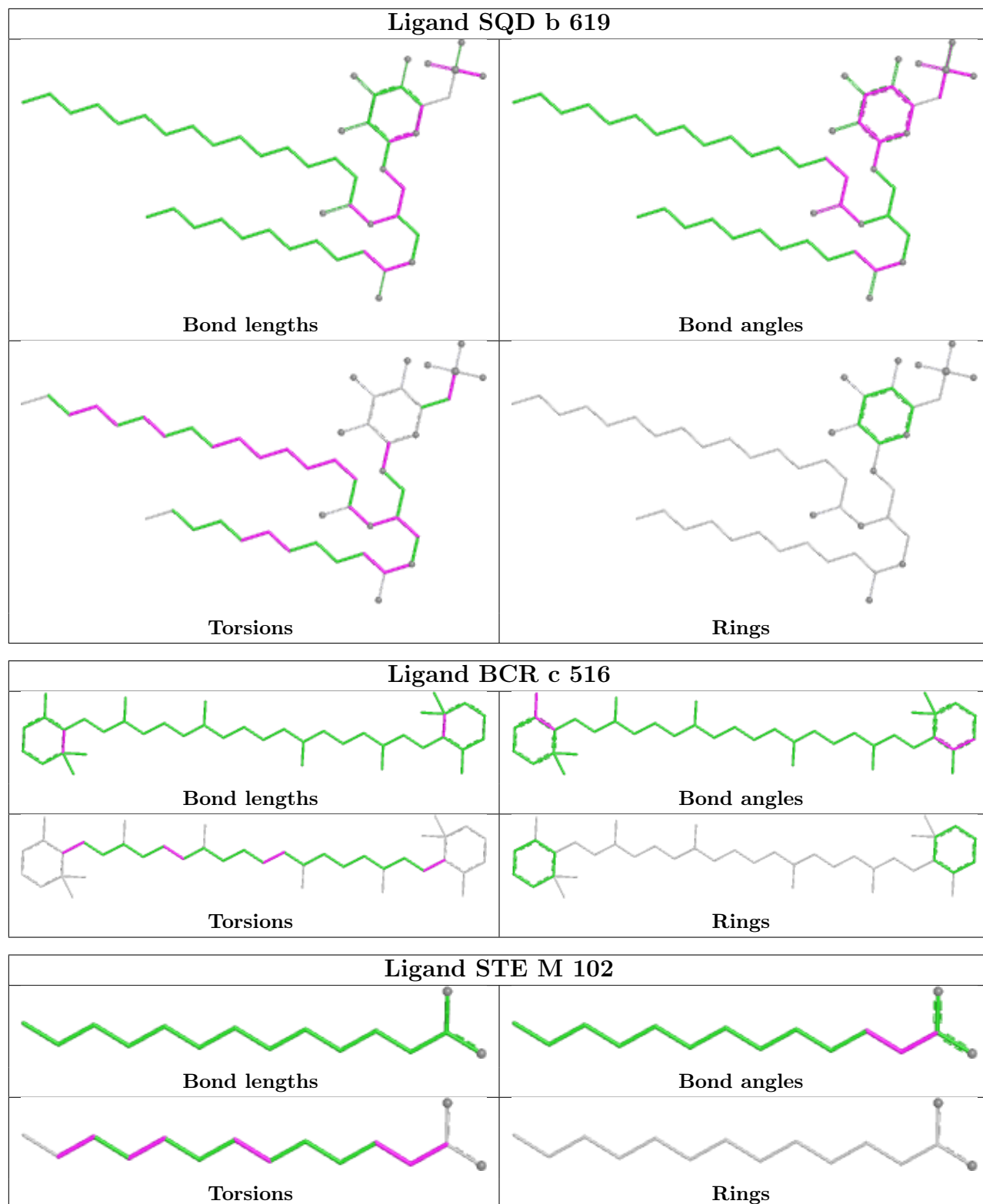


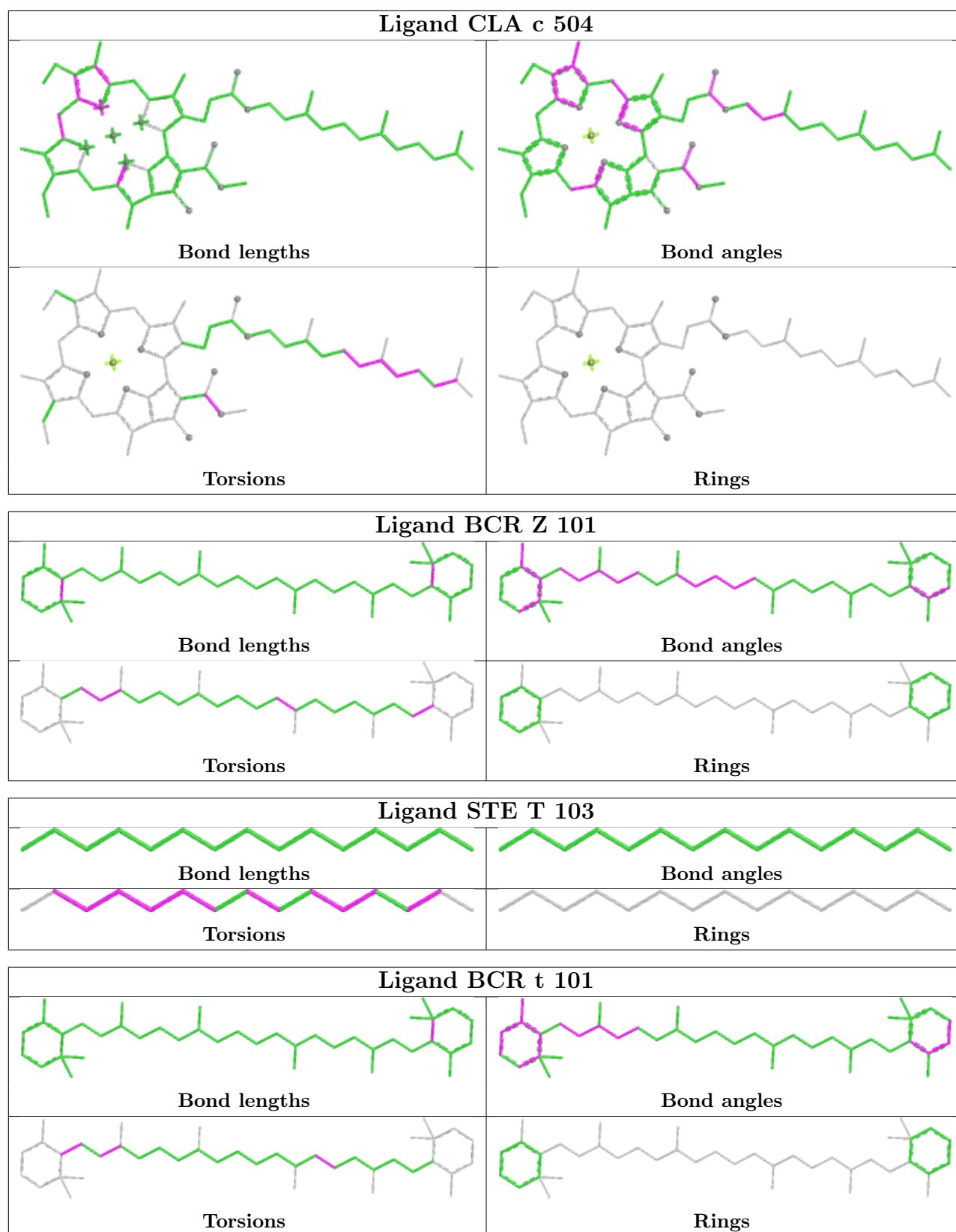


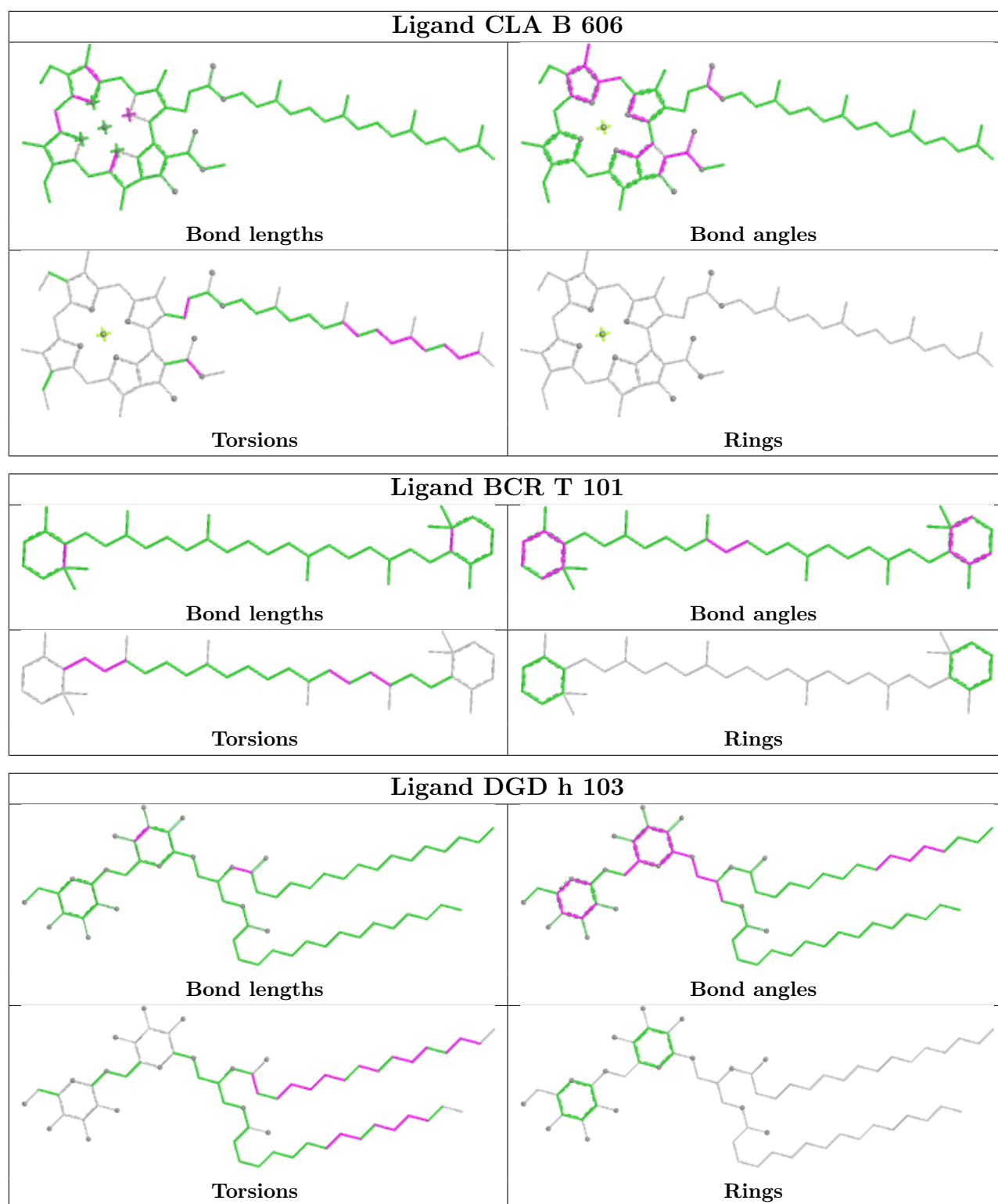


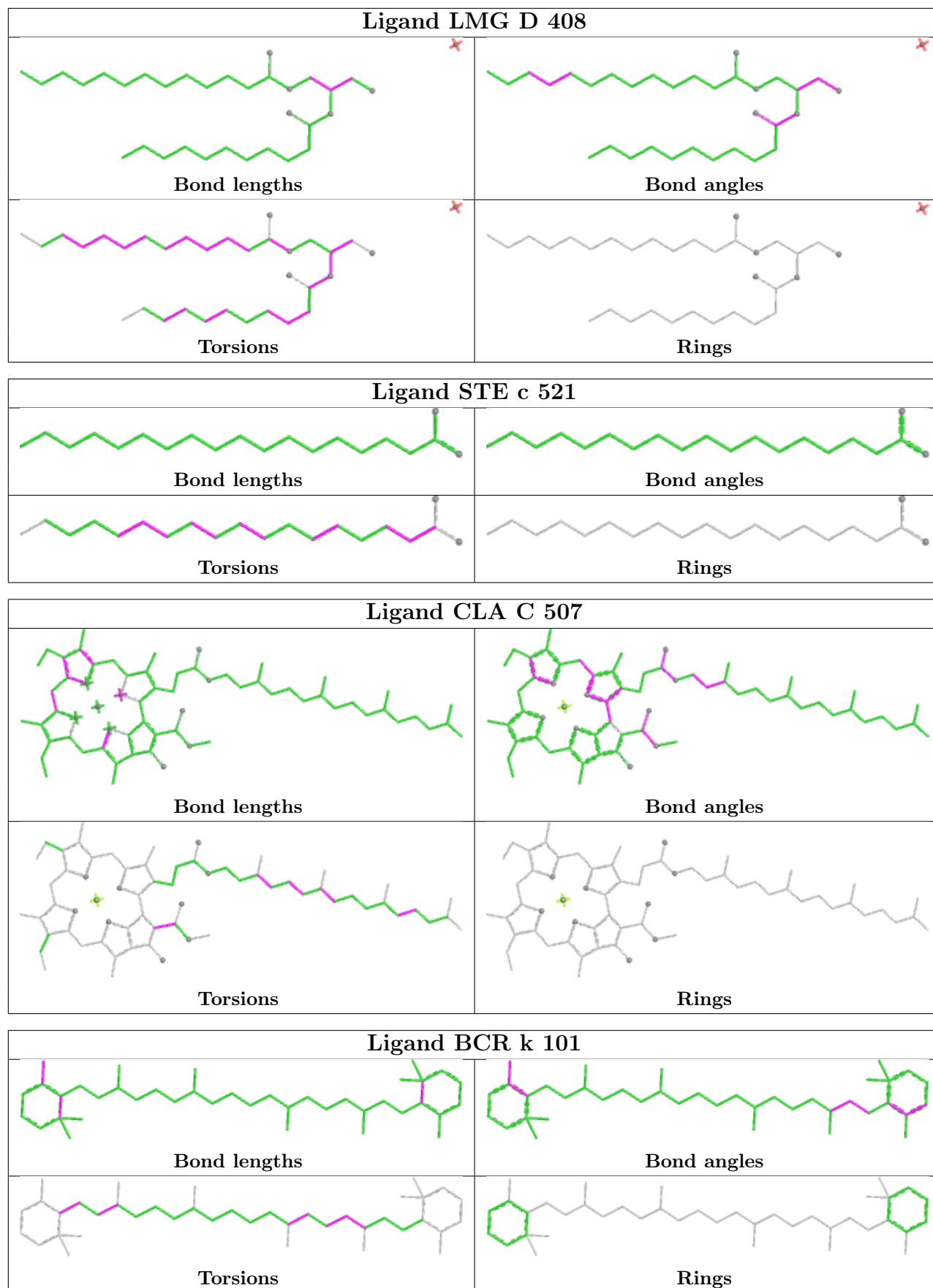




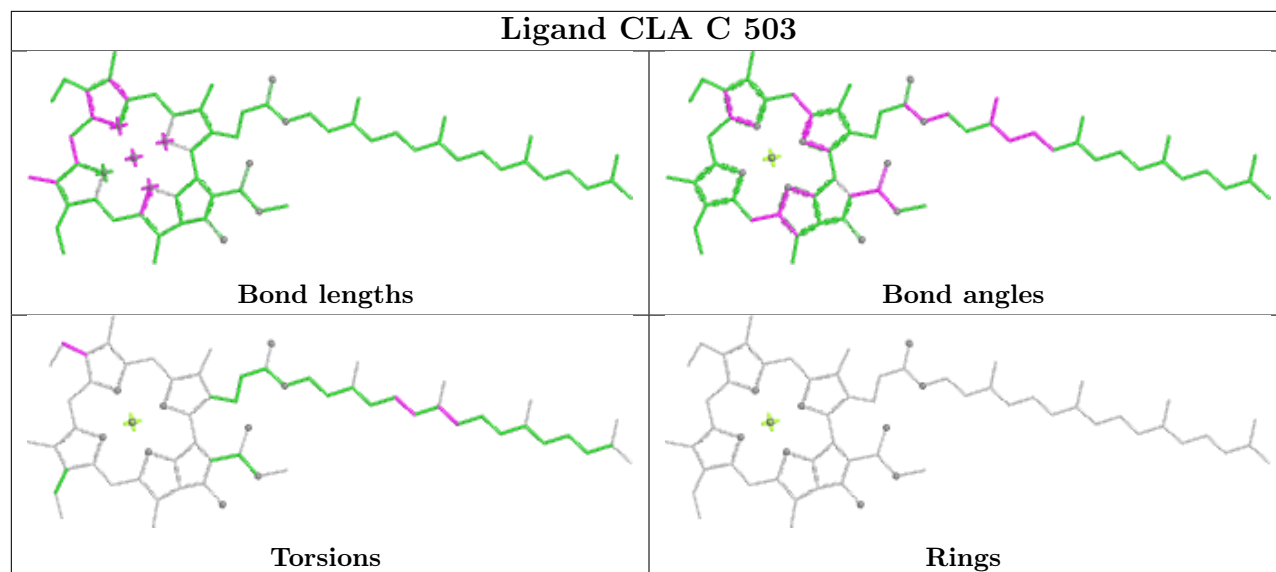




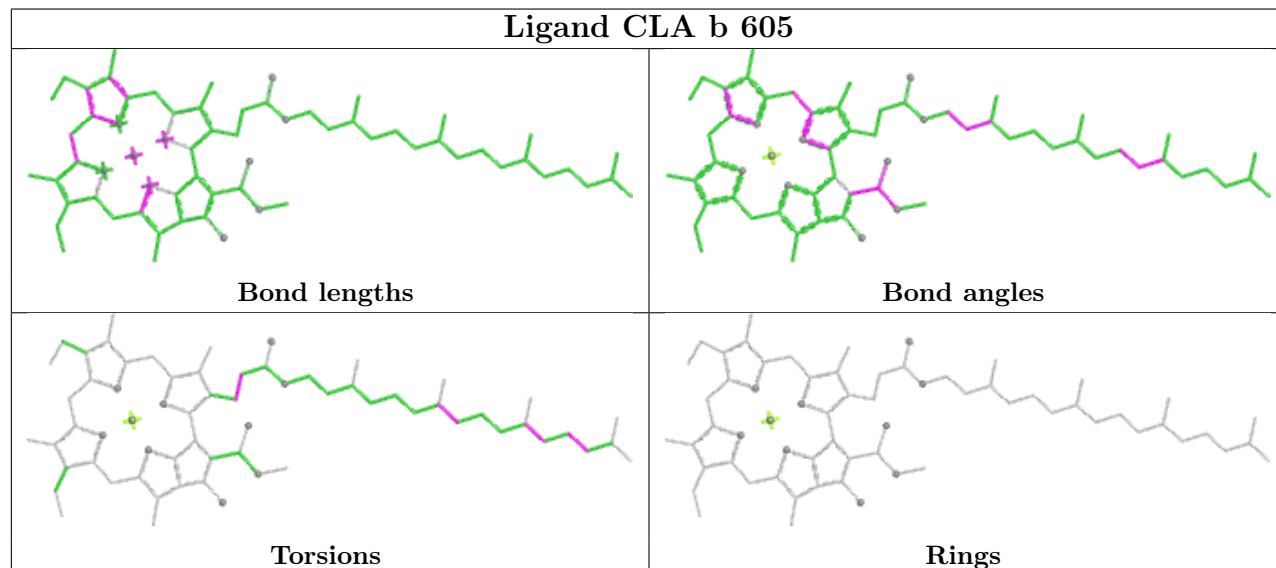




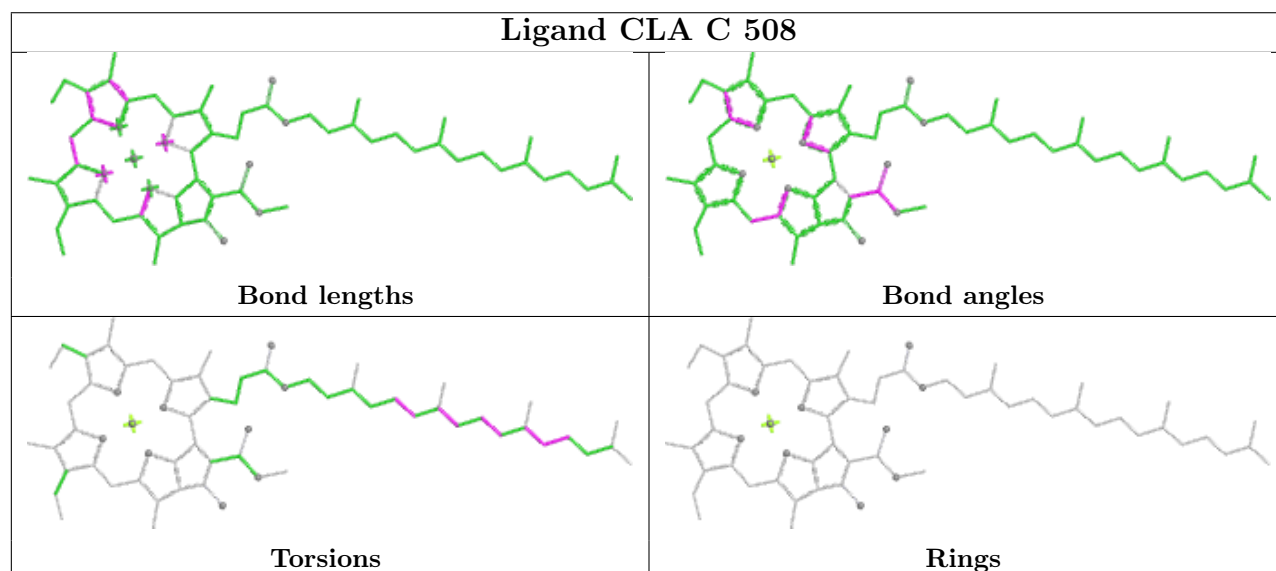
Ligand CLA C 503



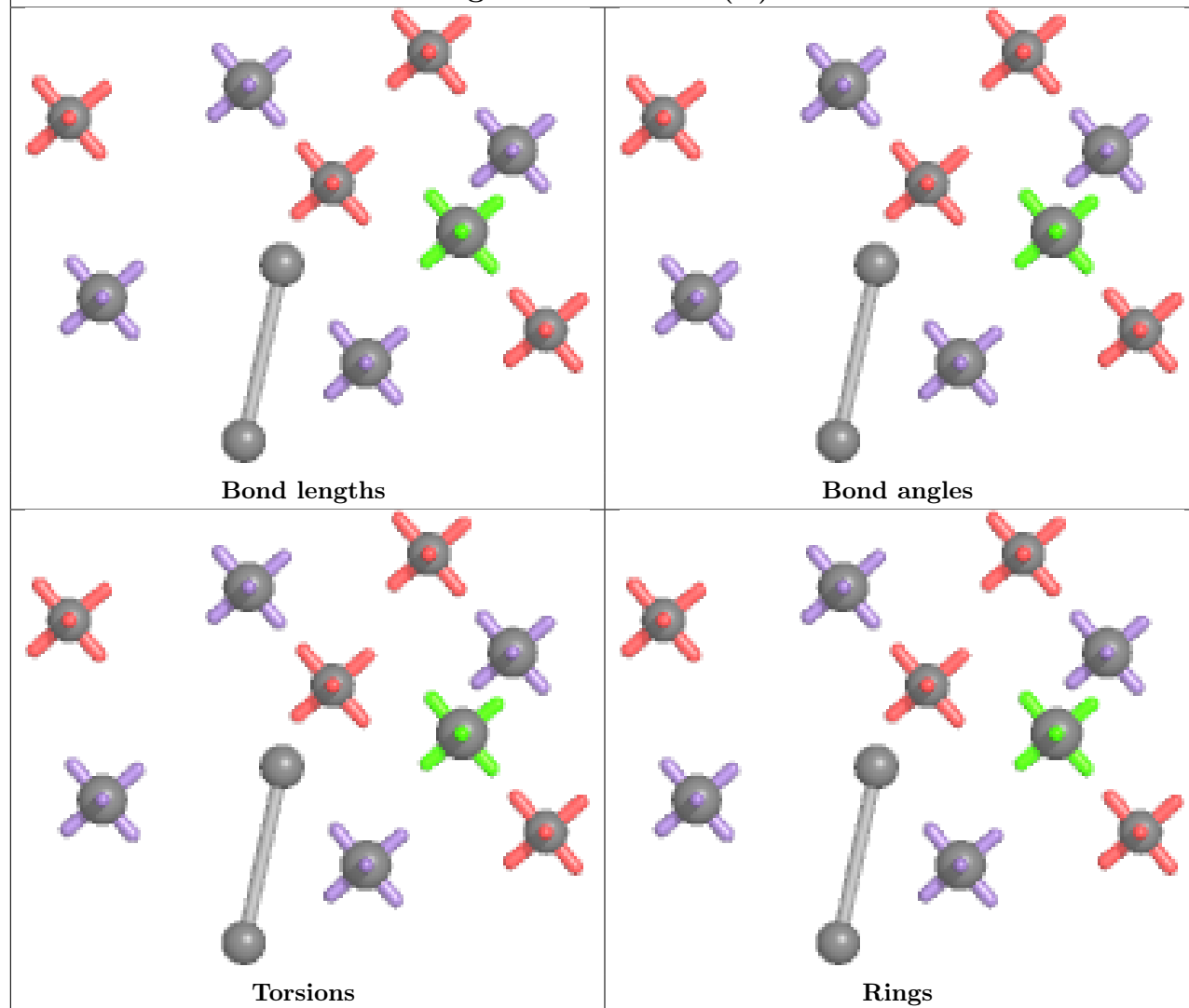
Ligand CLA b 605



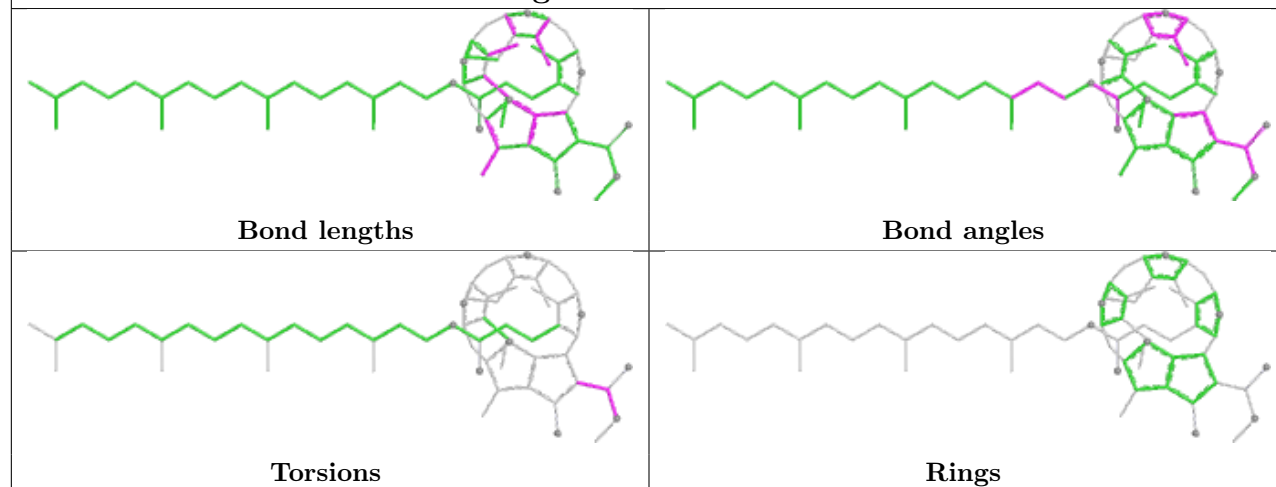
Ligand CLA C 508



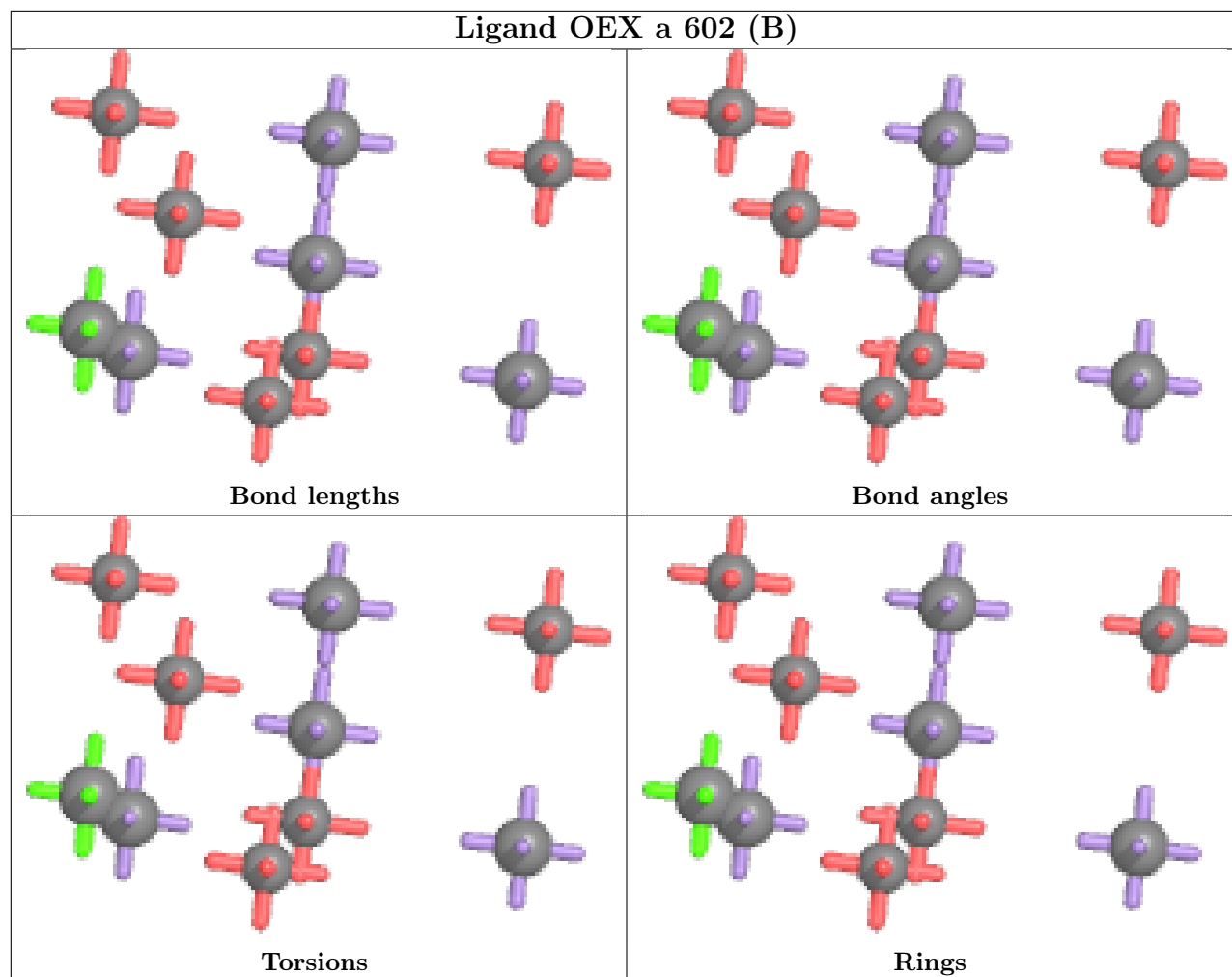
Ligand OEY a 601 (C)



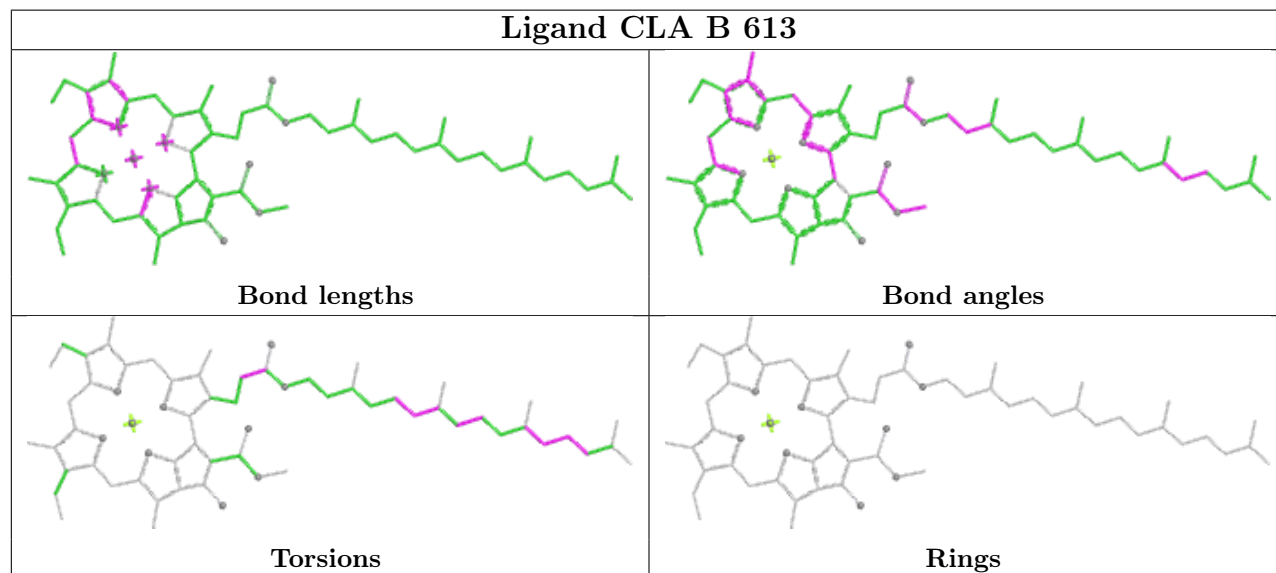
Ligand PHO d 402

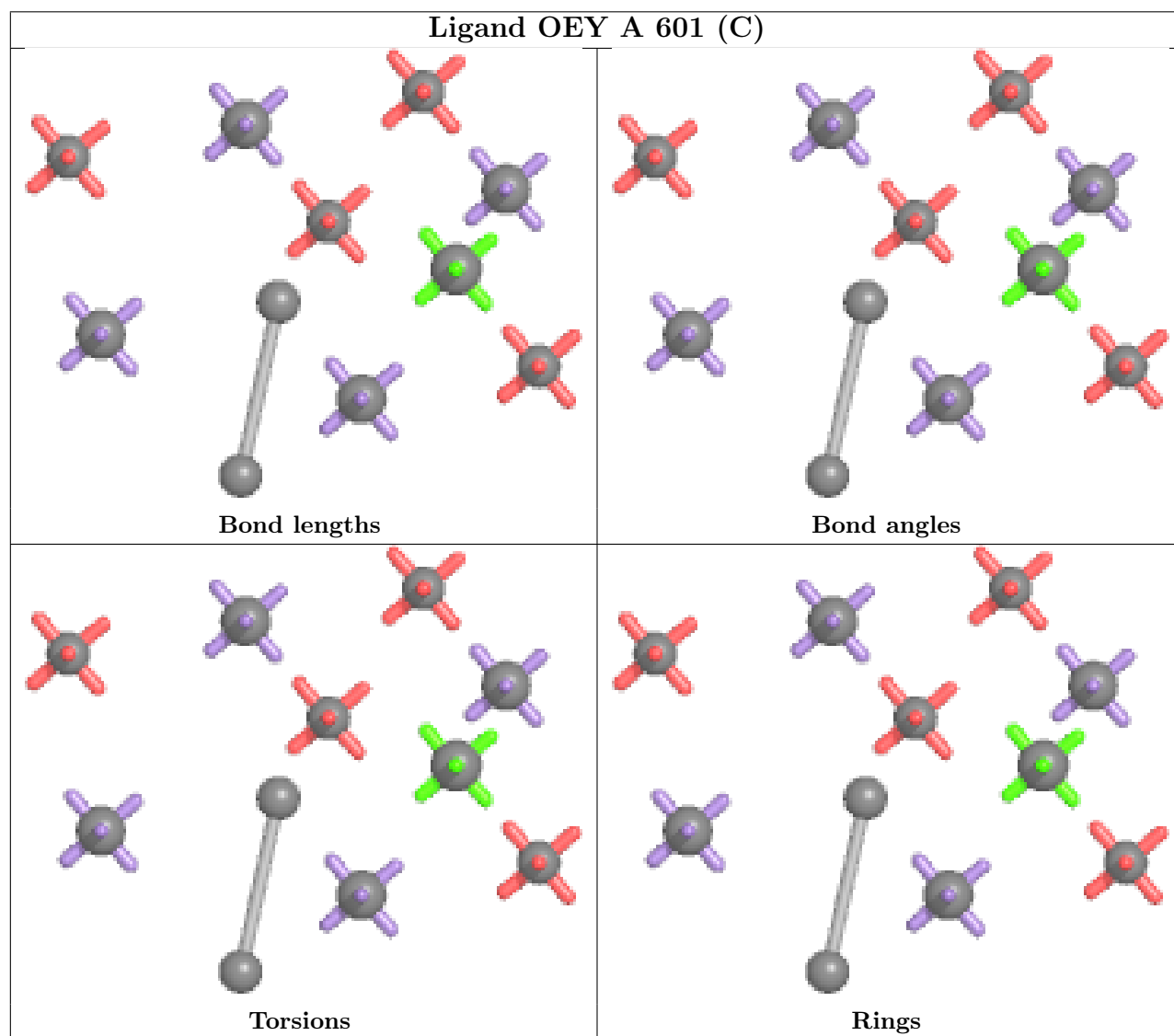
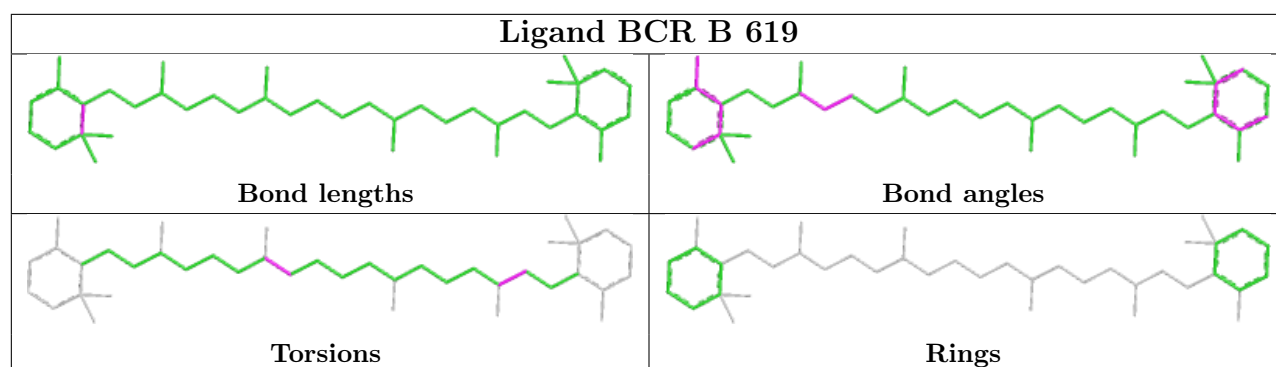


Ligand OEX a 602 (B)

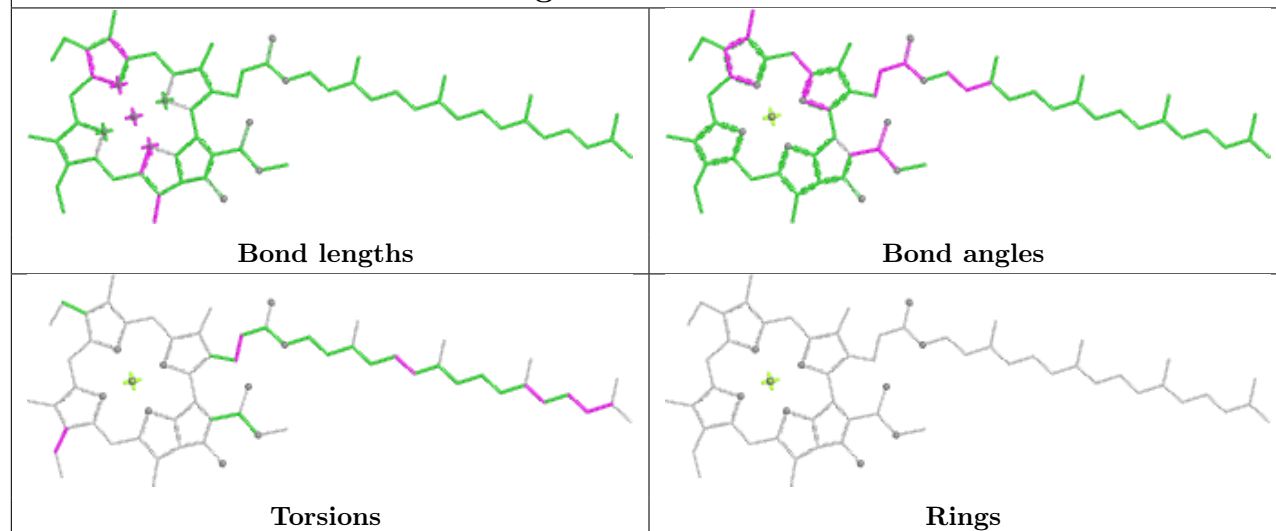


Ligand CLA B 613

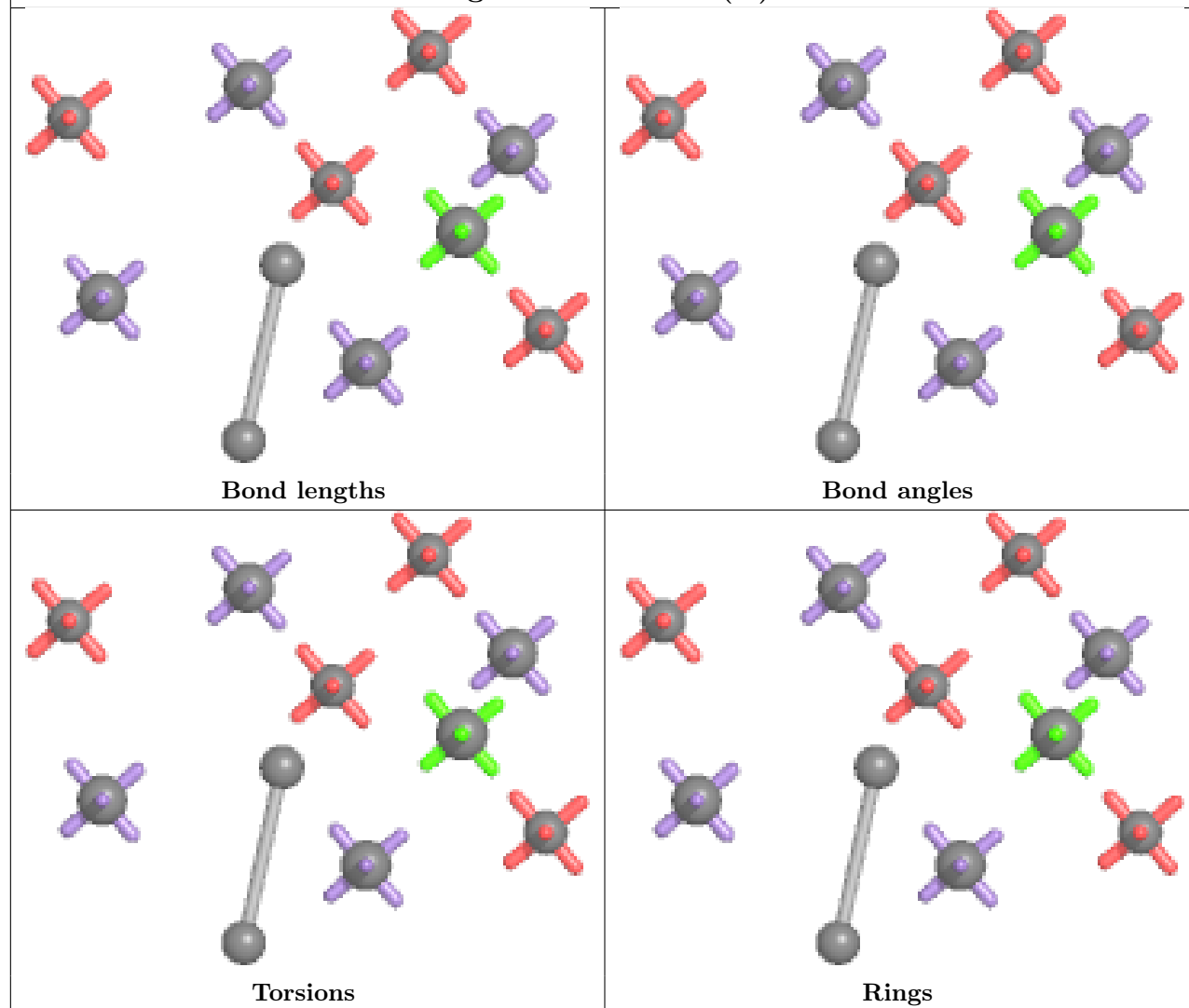


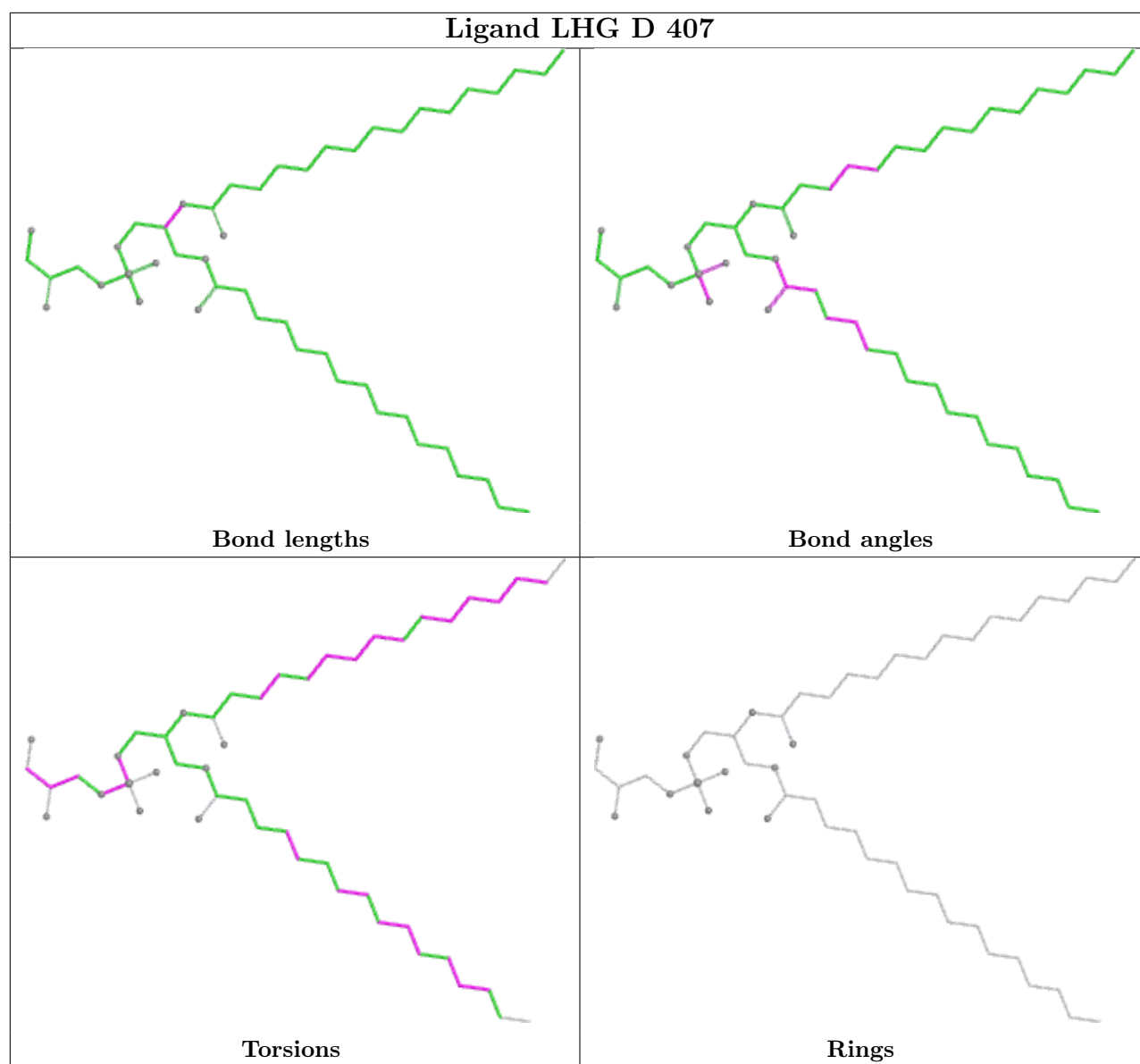


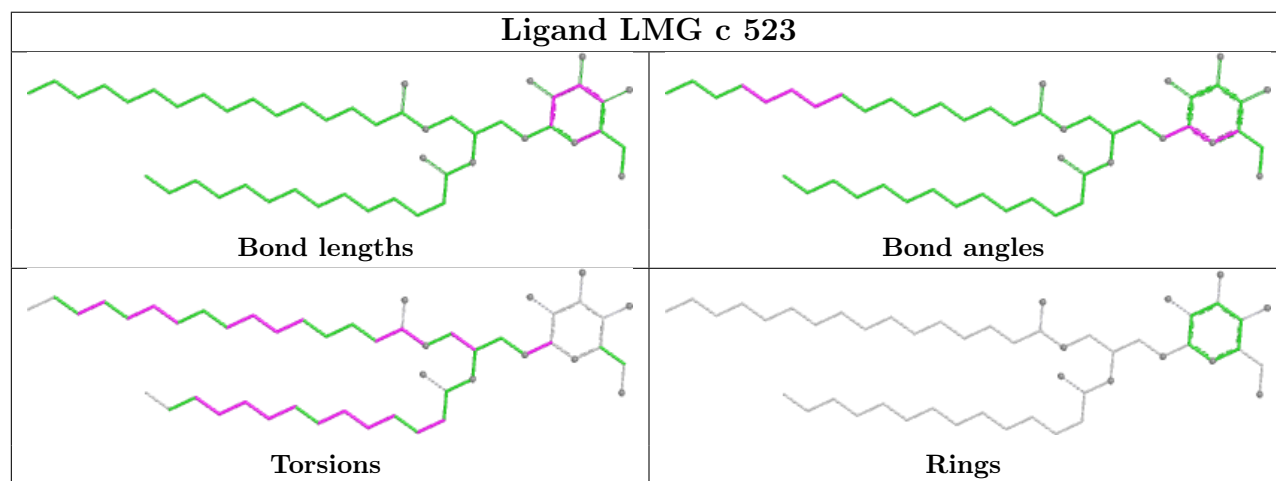
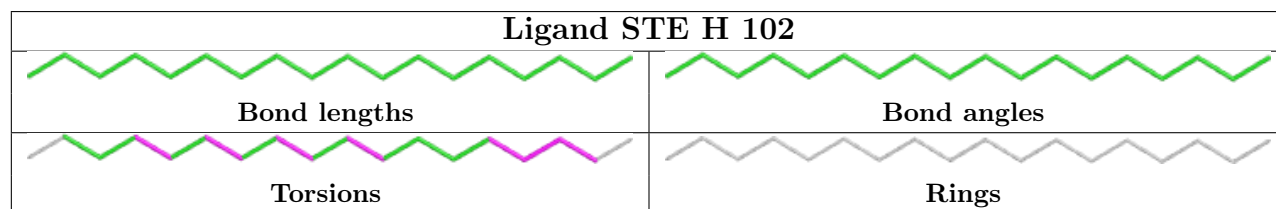
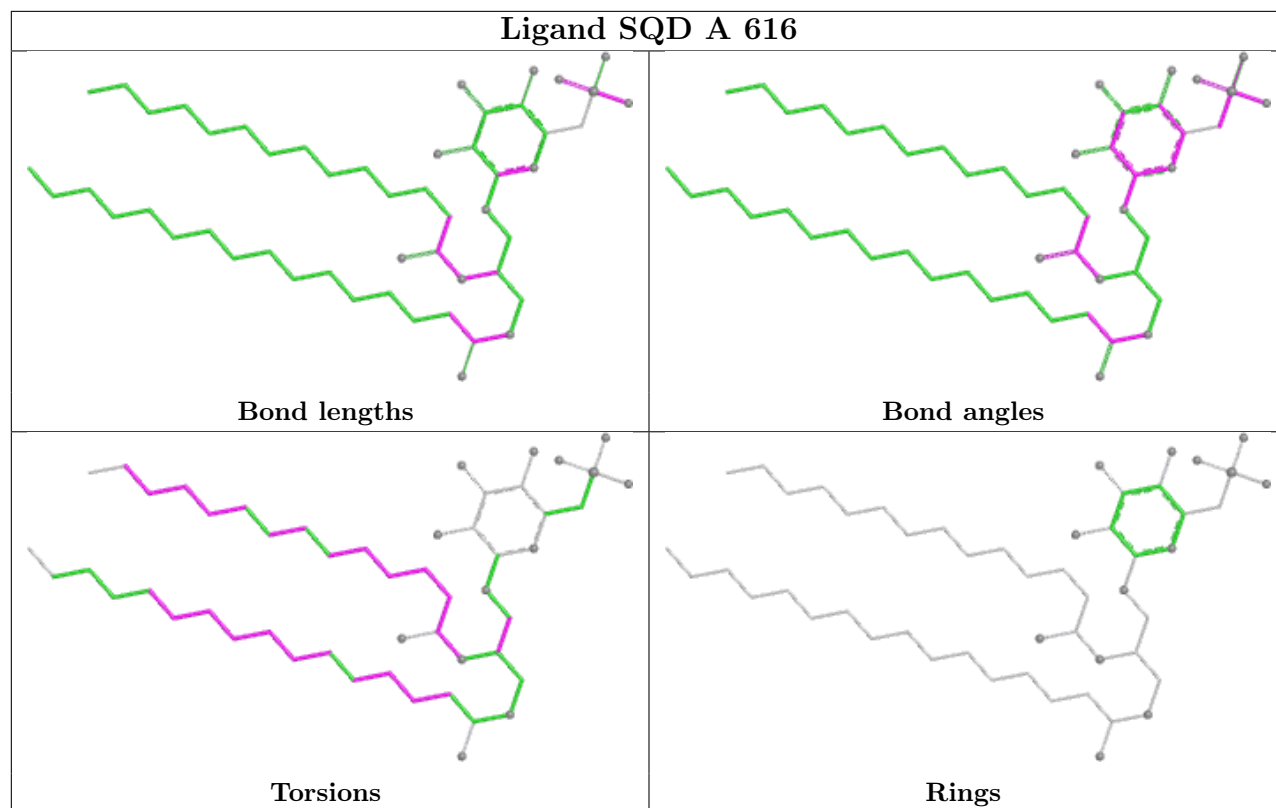
Ligand CLA b 609



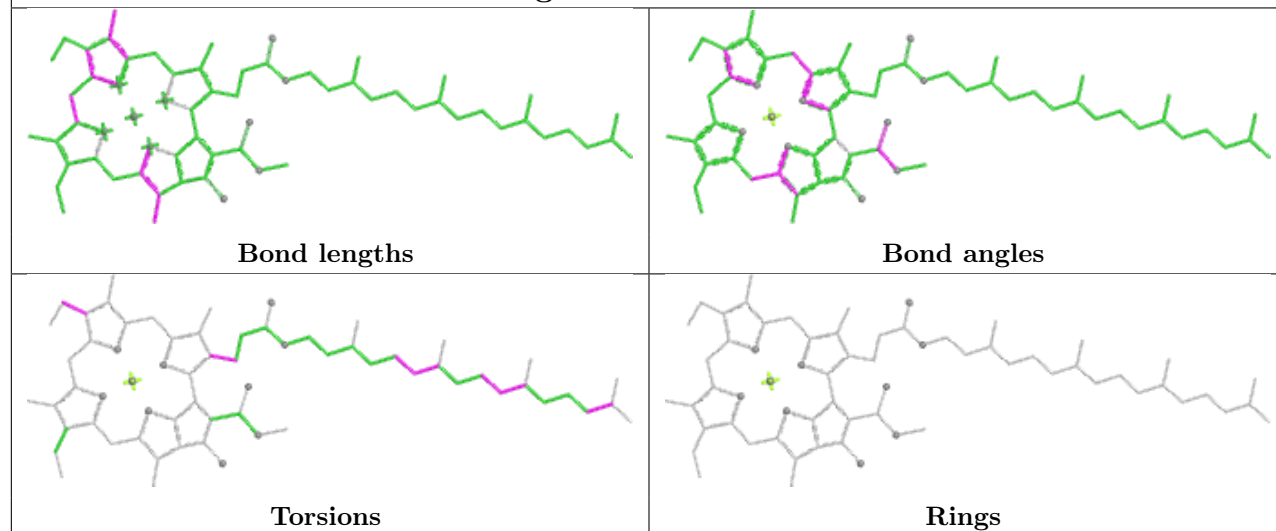
Ligand OEY a 601 (A)



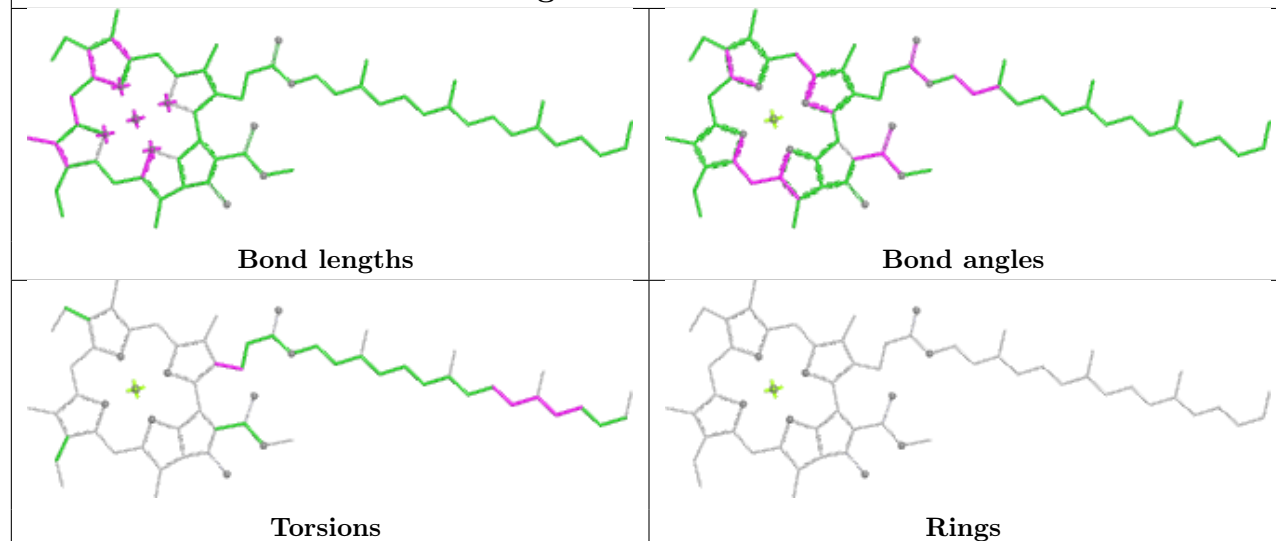




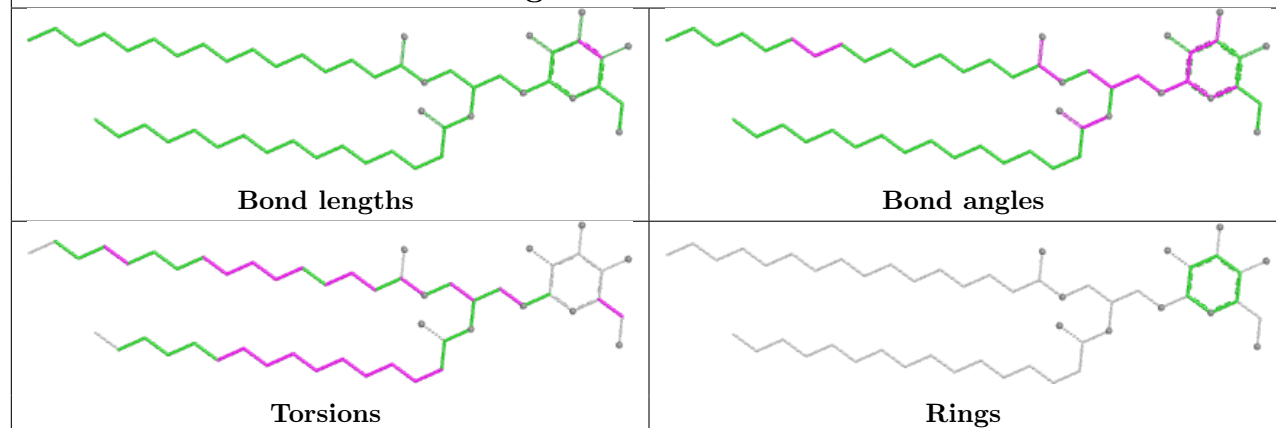
Ligand CLA d 404

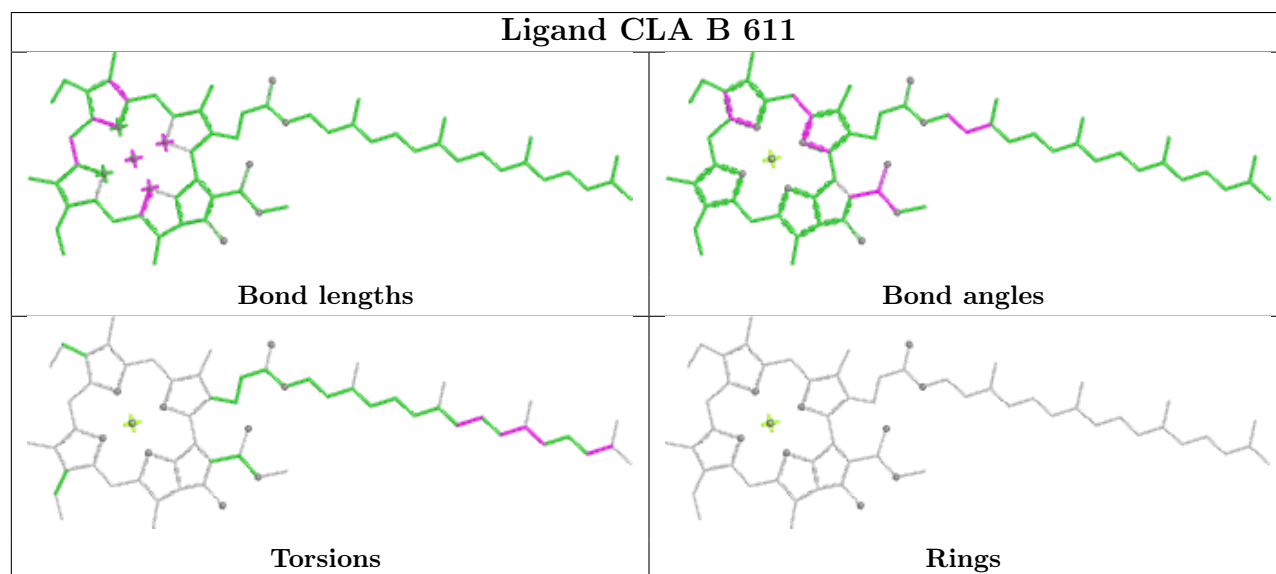
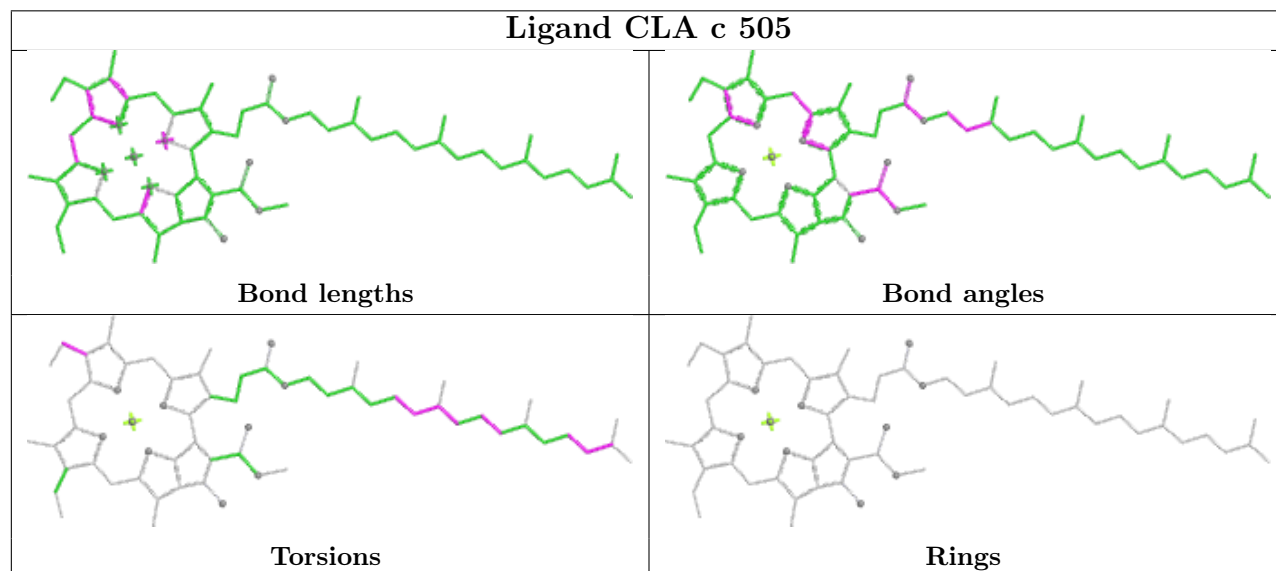
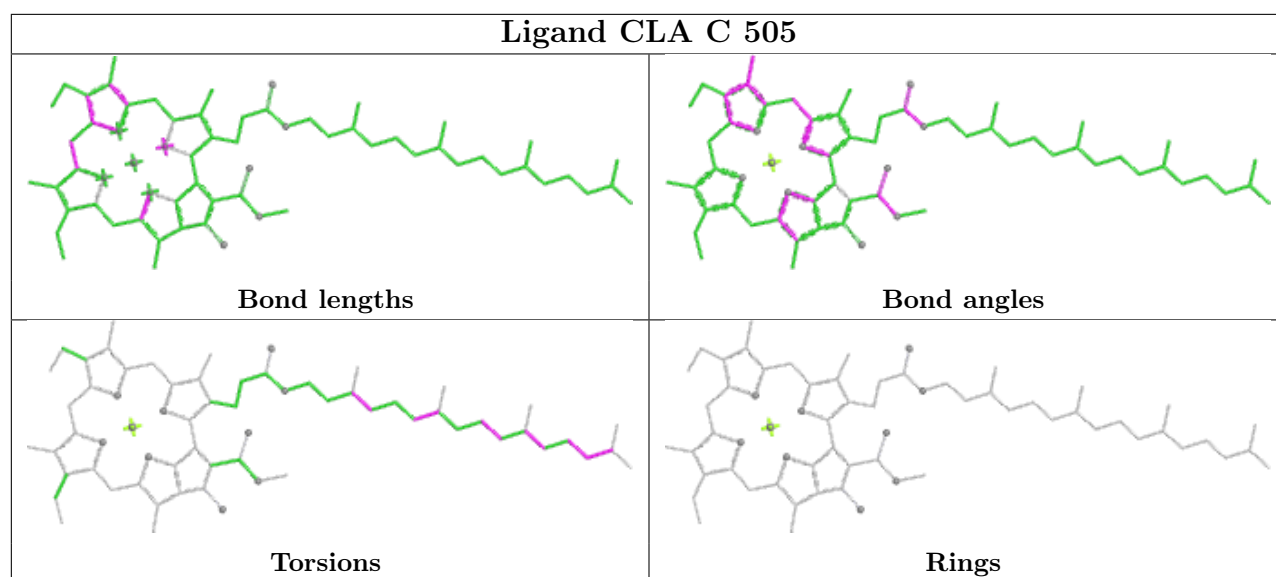


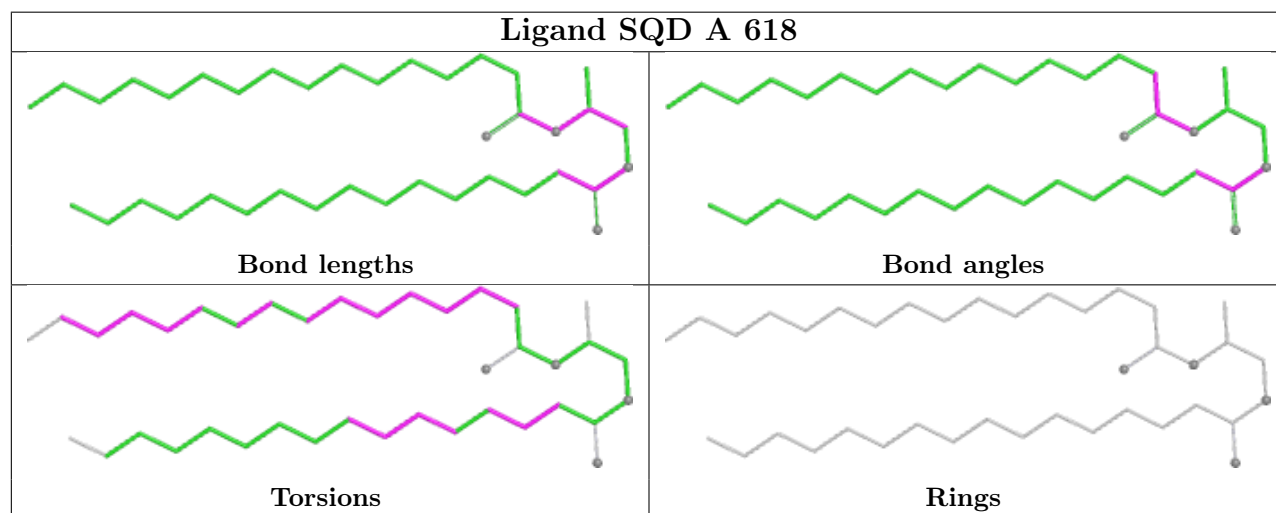
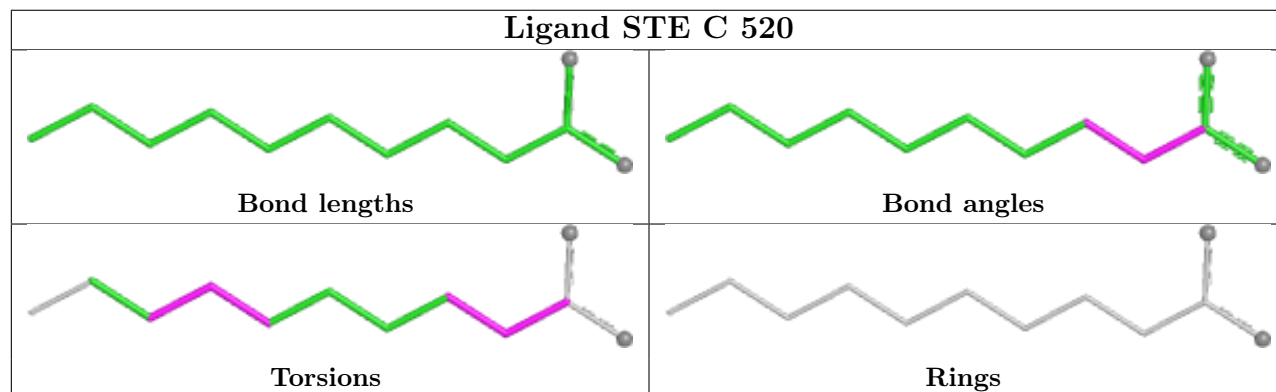
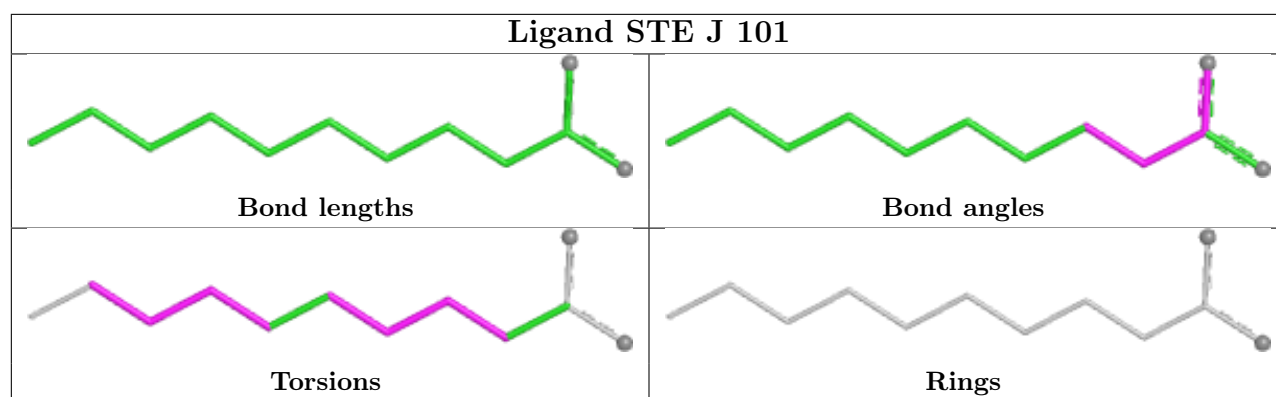
Ligand CLA c 508

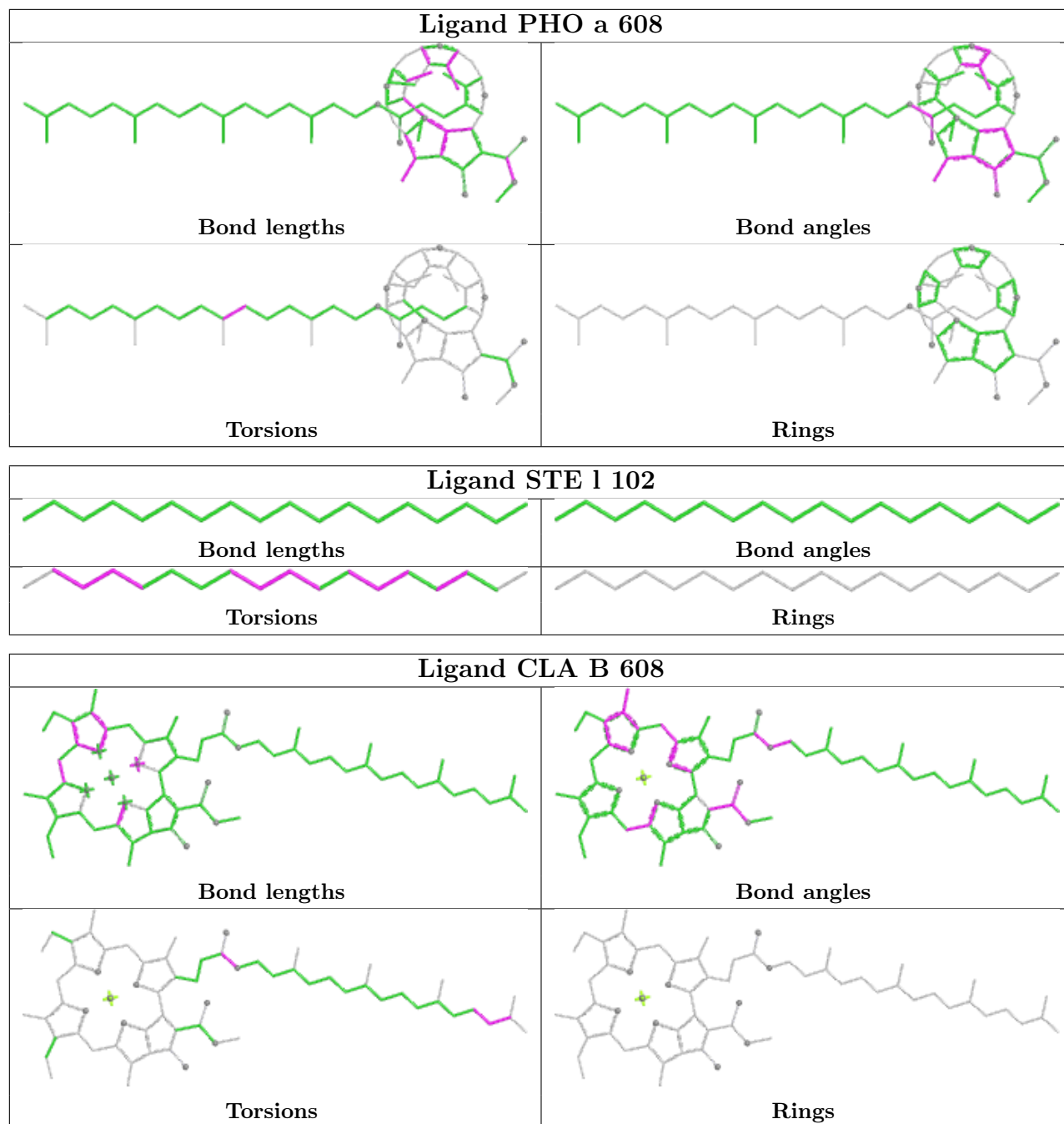


Ligand LMG m 101

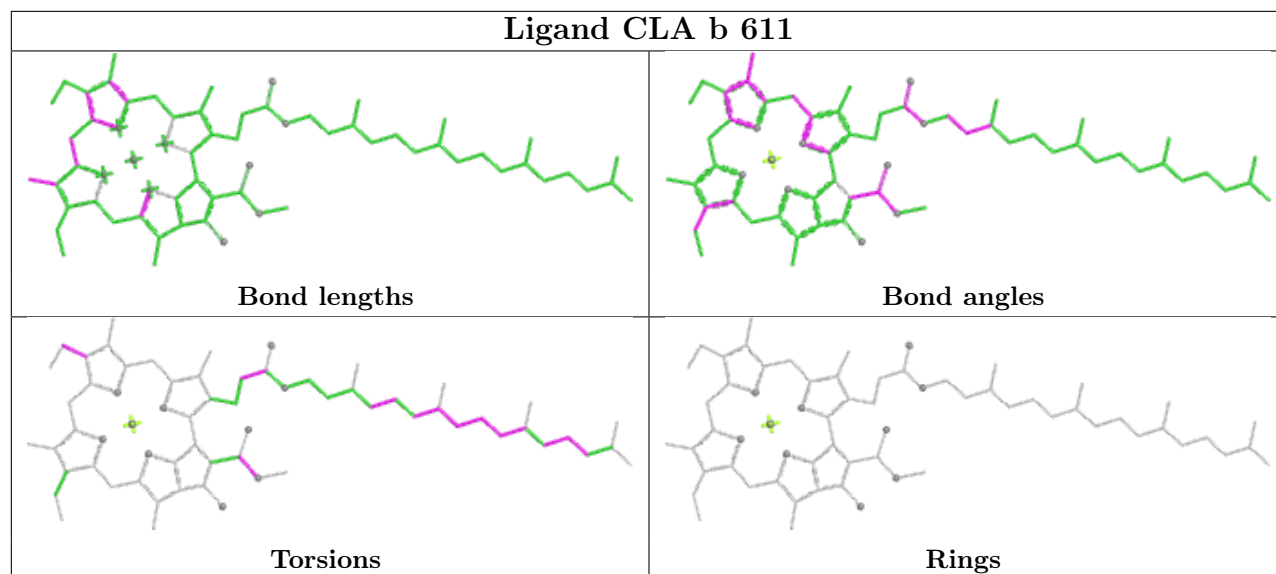




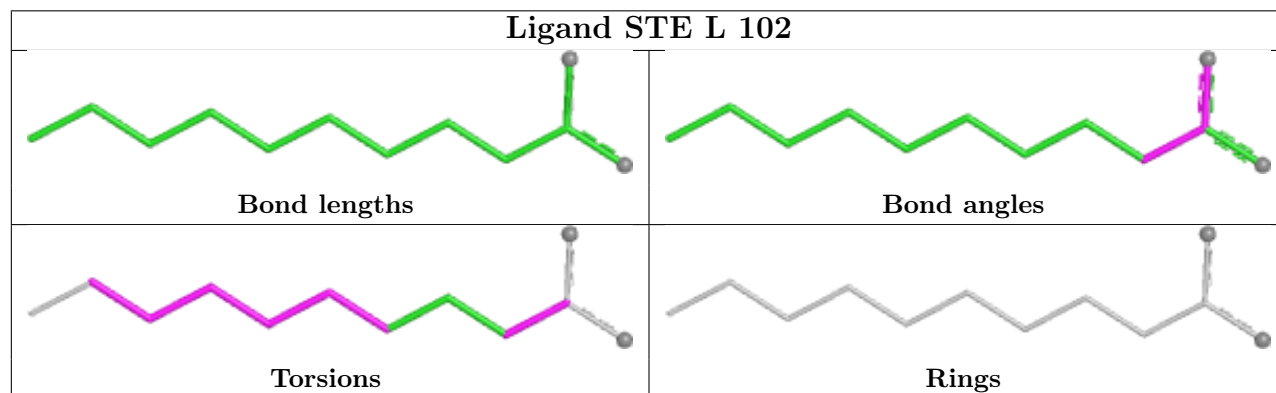




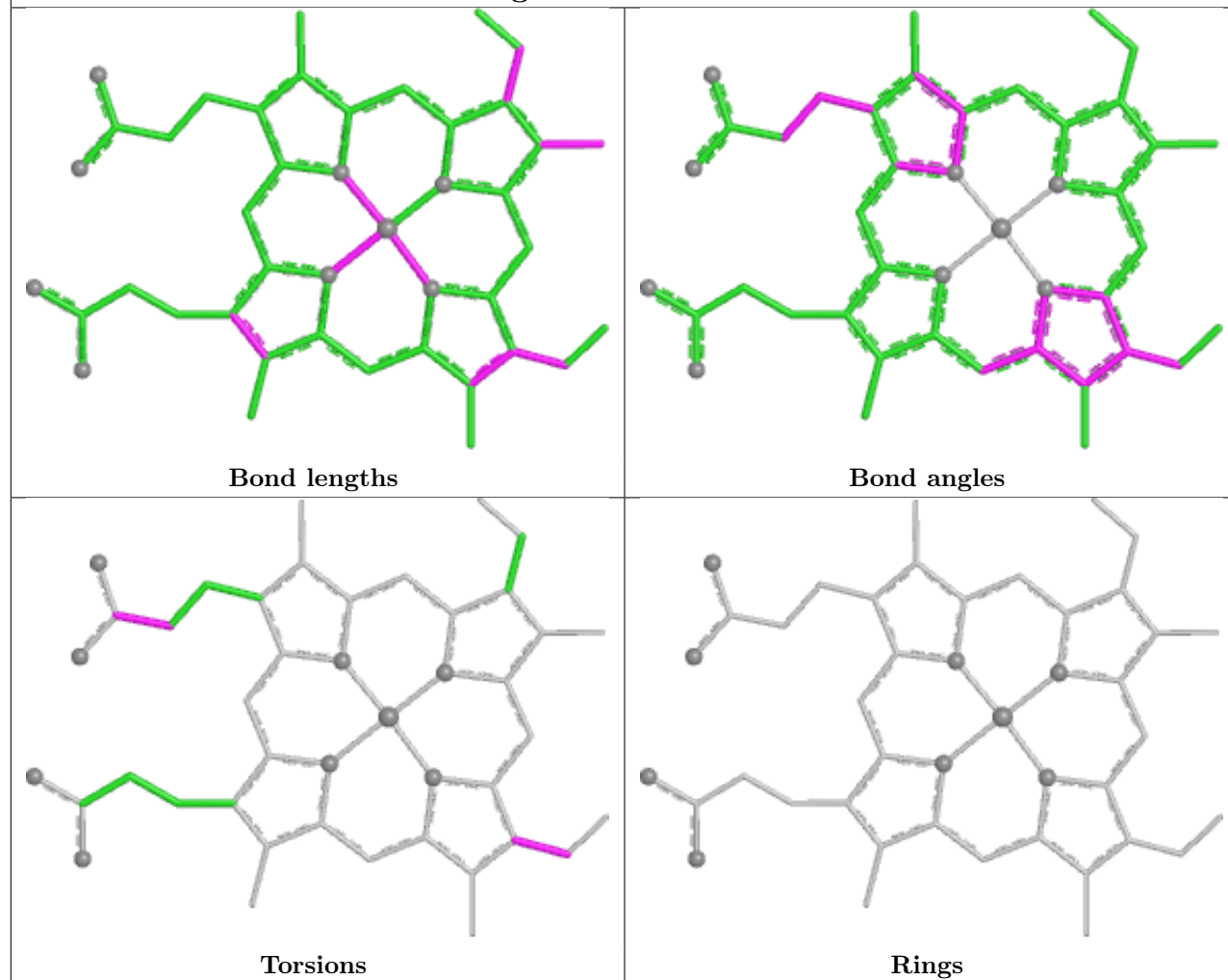
Ligand CLA b 611



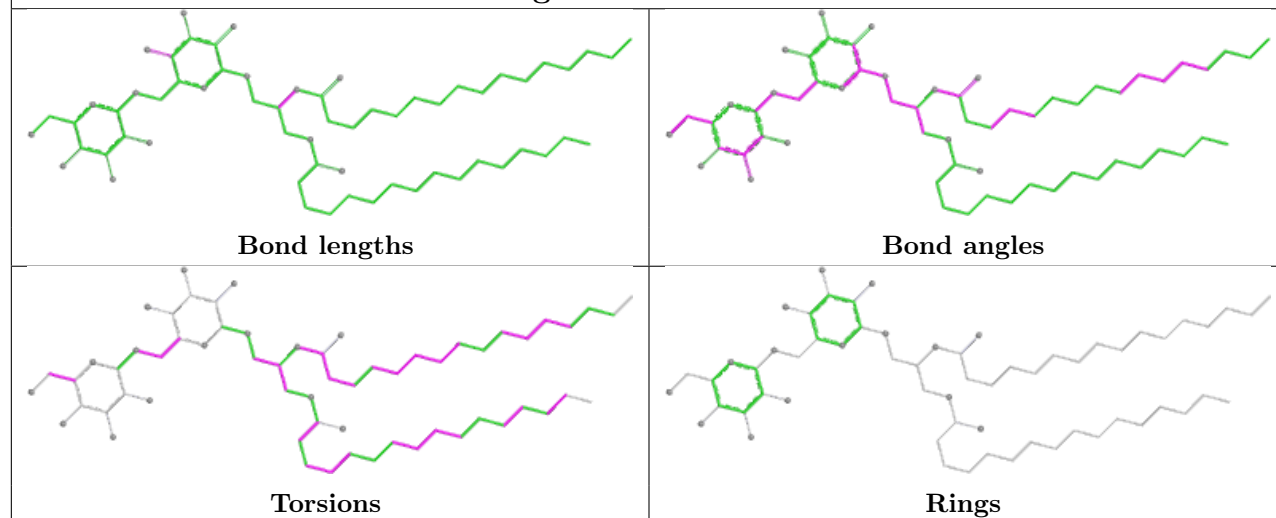
Ligand STE L 102

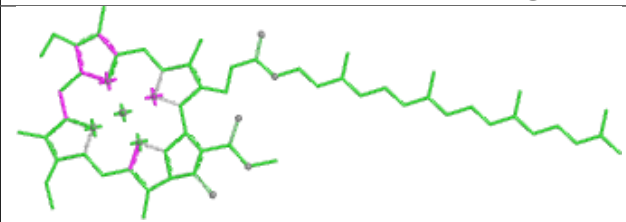
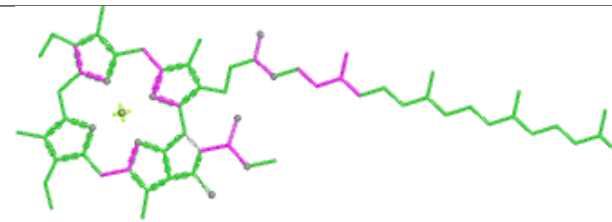
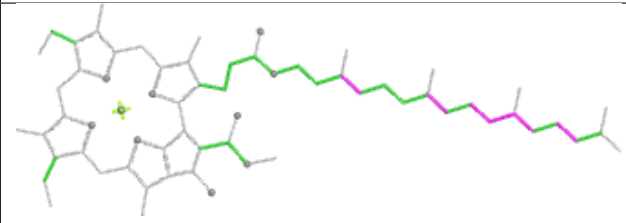
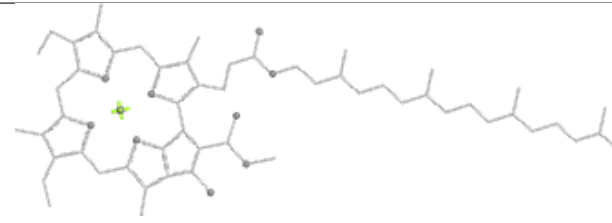


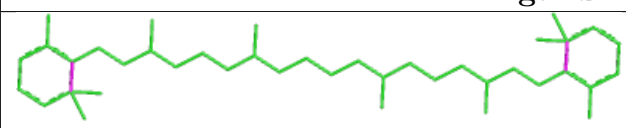
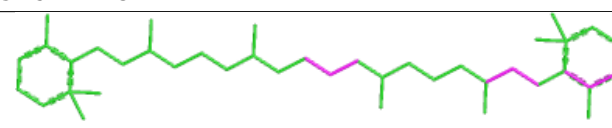
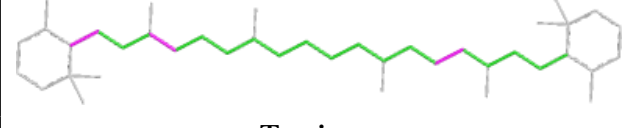
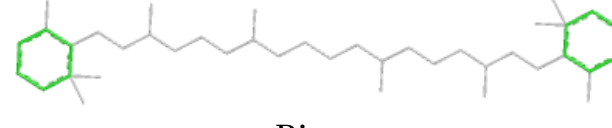
Ligand HEM e 101

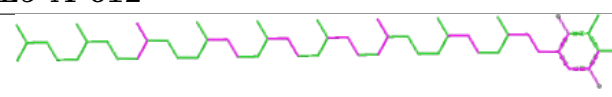
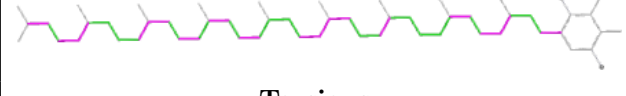
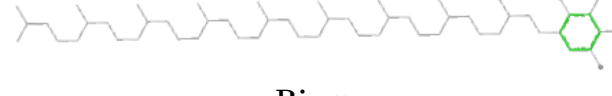


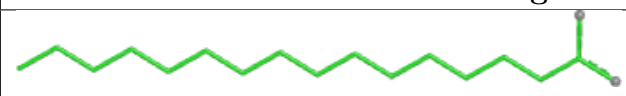
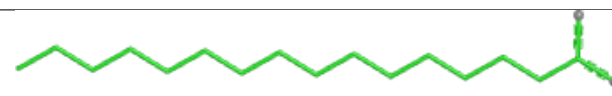
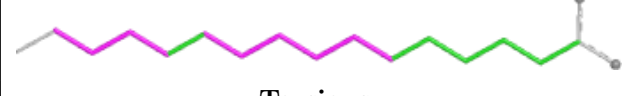
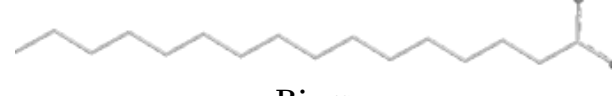
Ligand DGD c 517

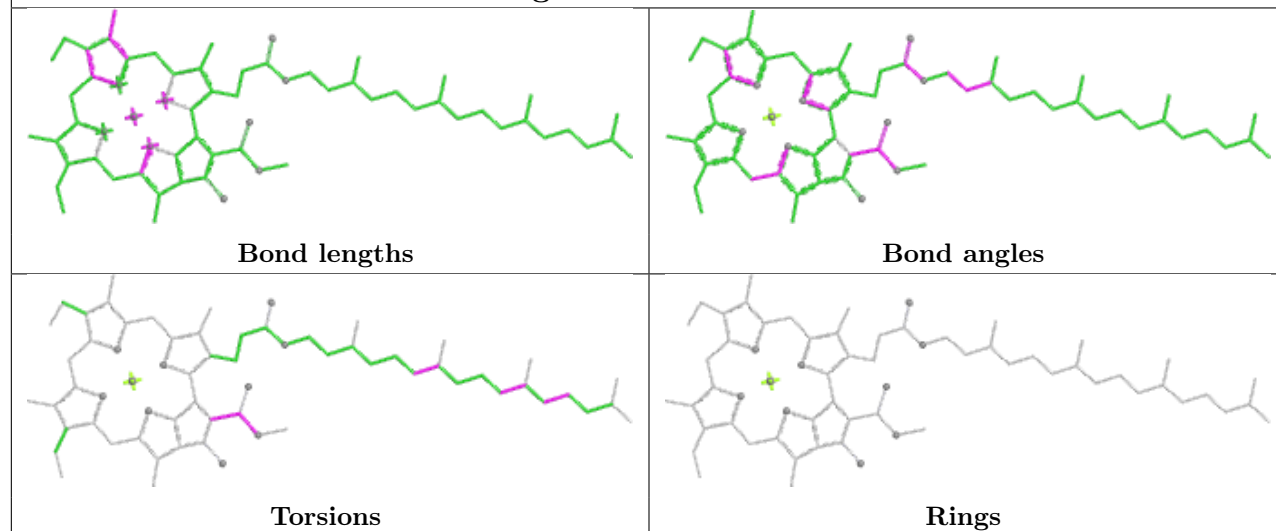
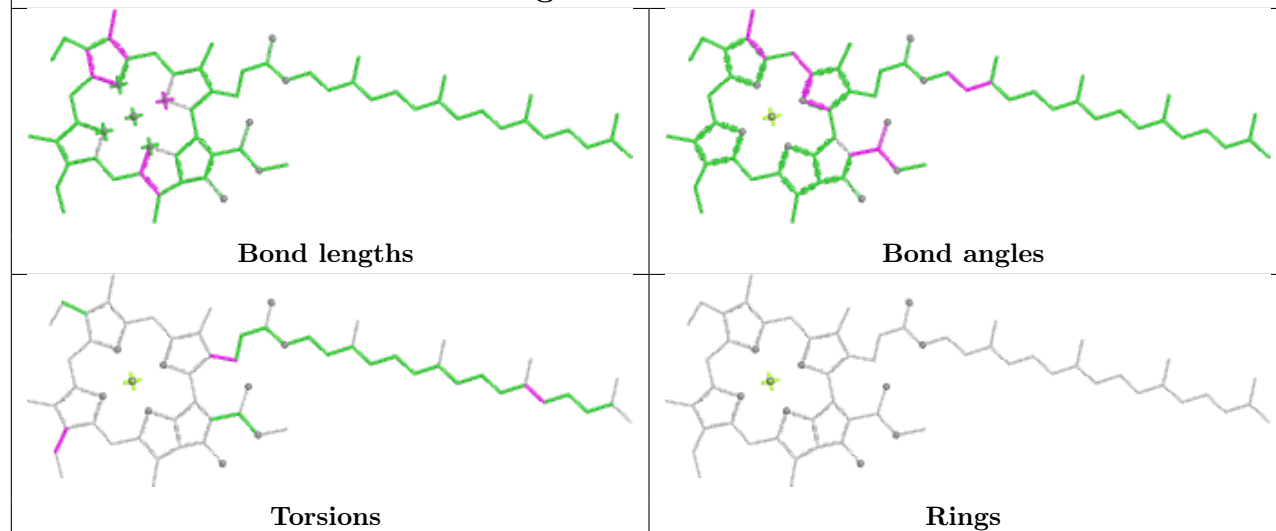
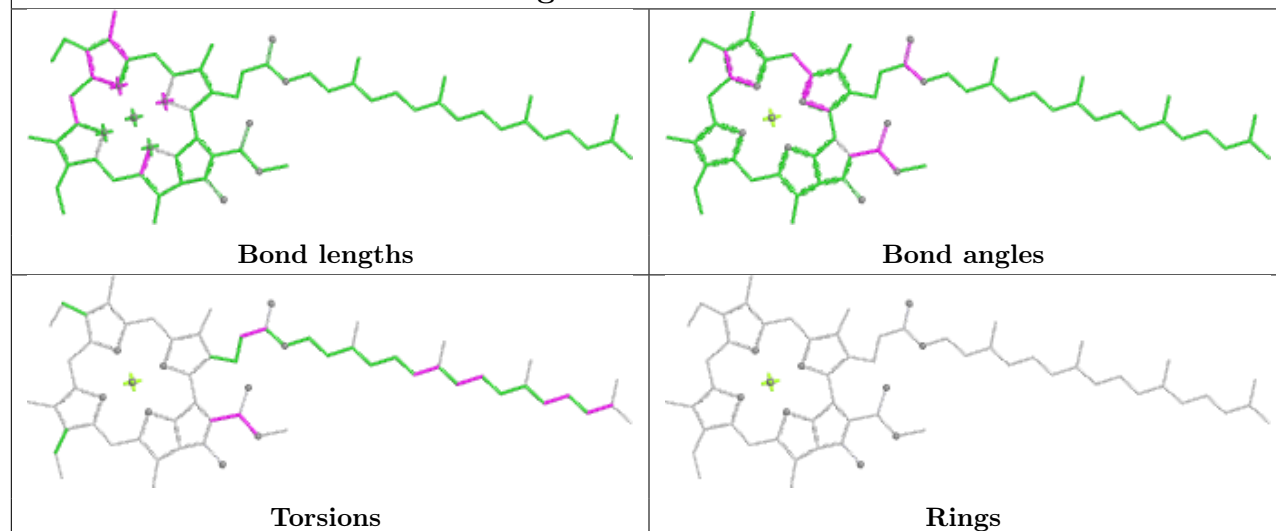


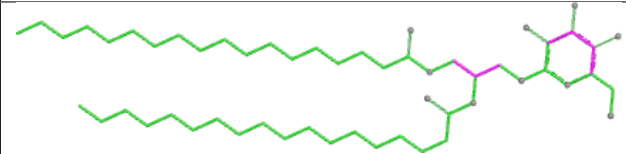
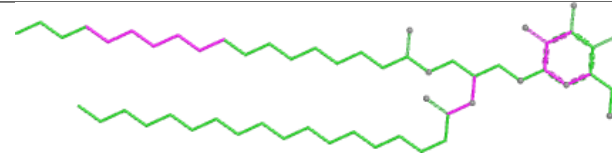
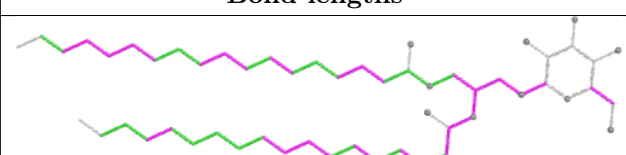
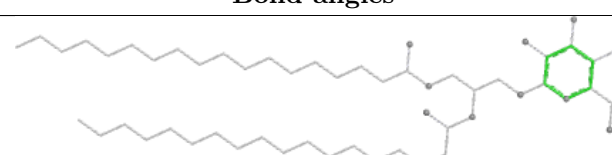
Ligand CLA b 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

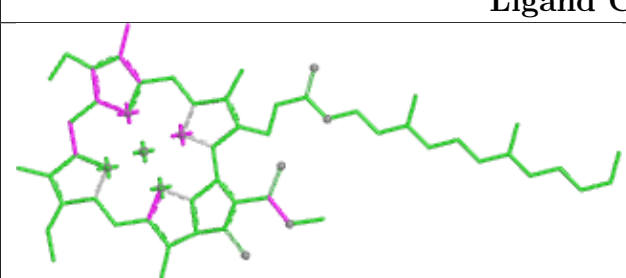
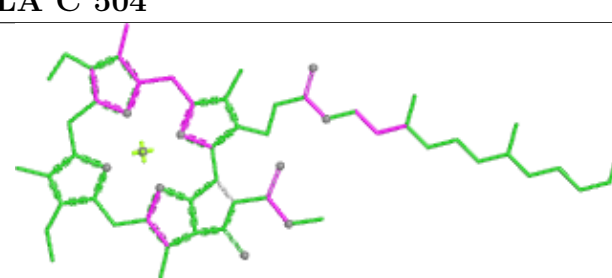
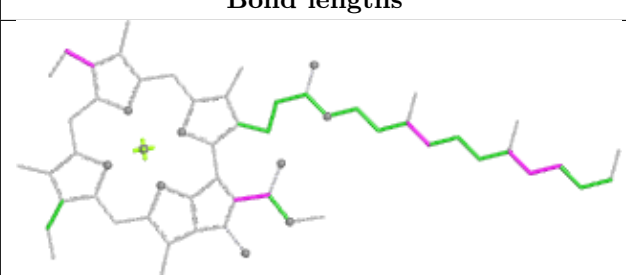
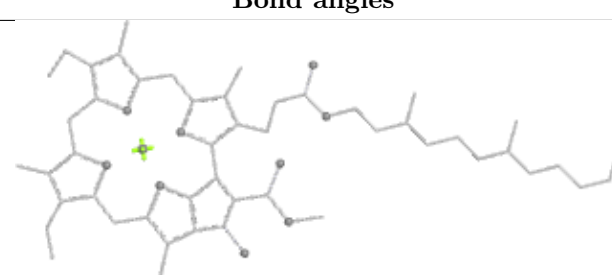
Ligand BCR K 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

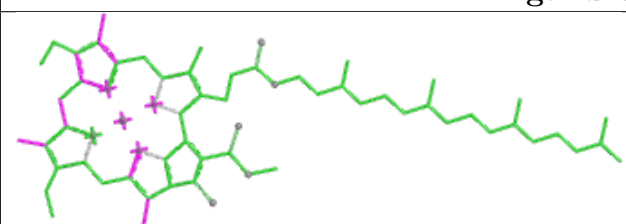
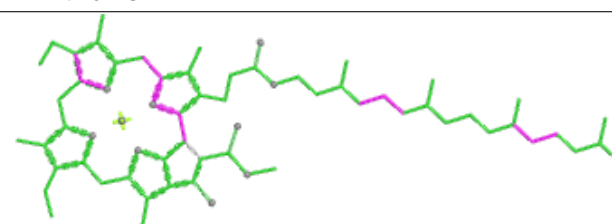
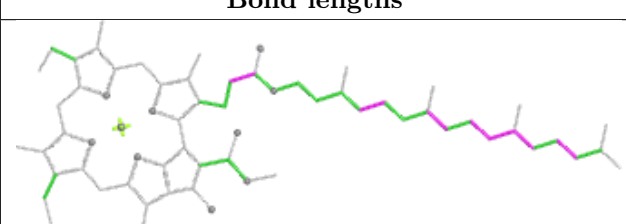
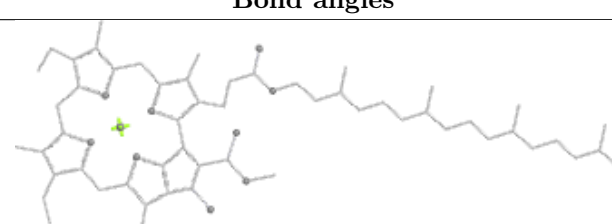
Ligand PL9 A 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

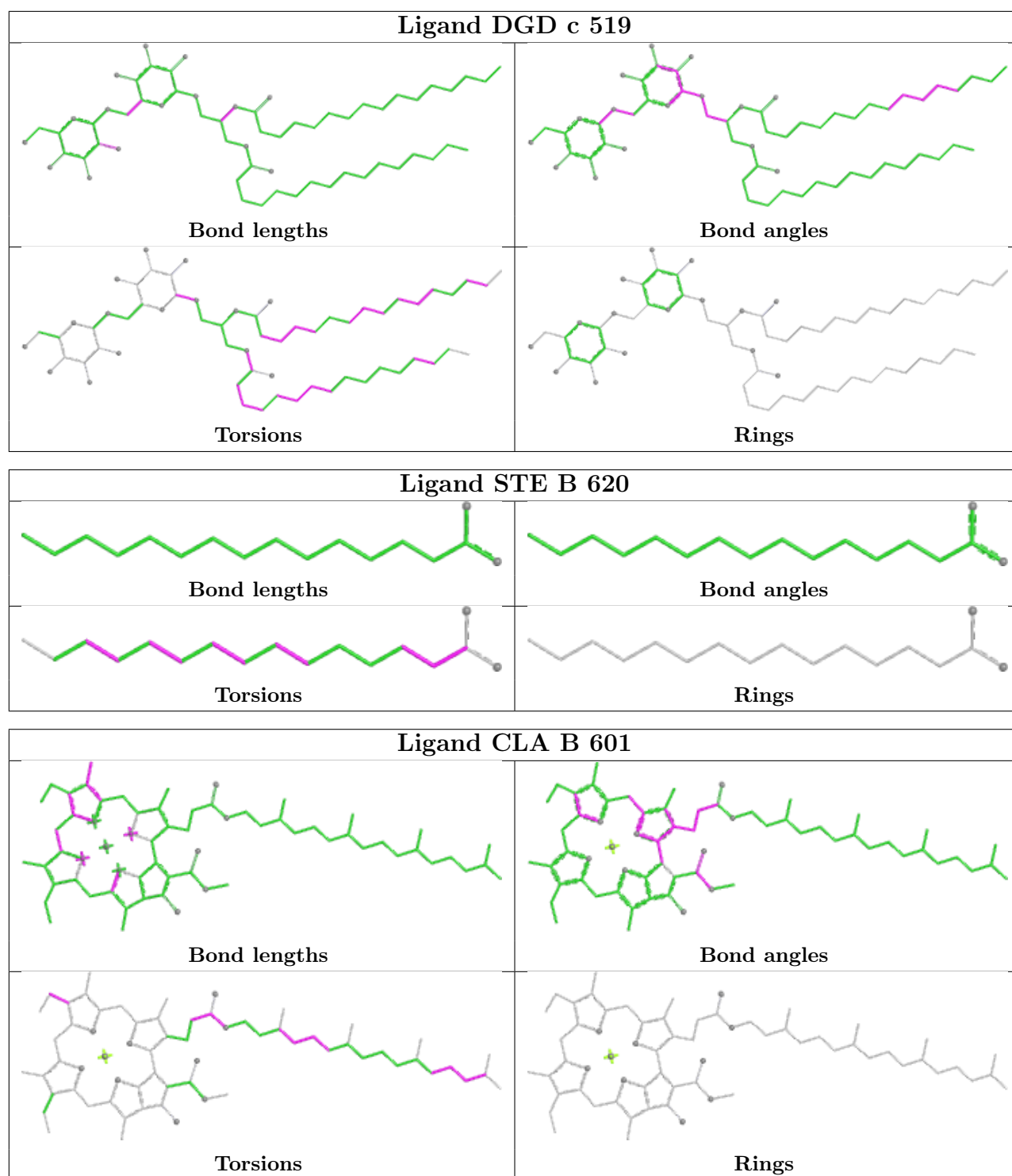
Ligand STE t 105	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 502**Ligand CLA a 612****Ligand CLA c 509**

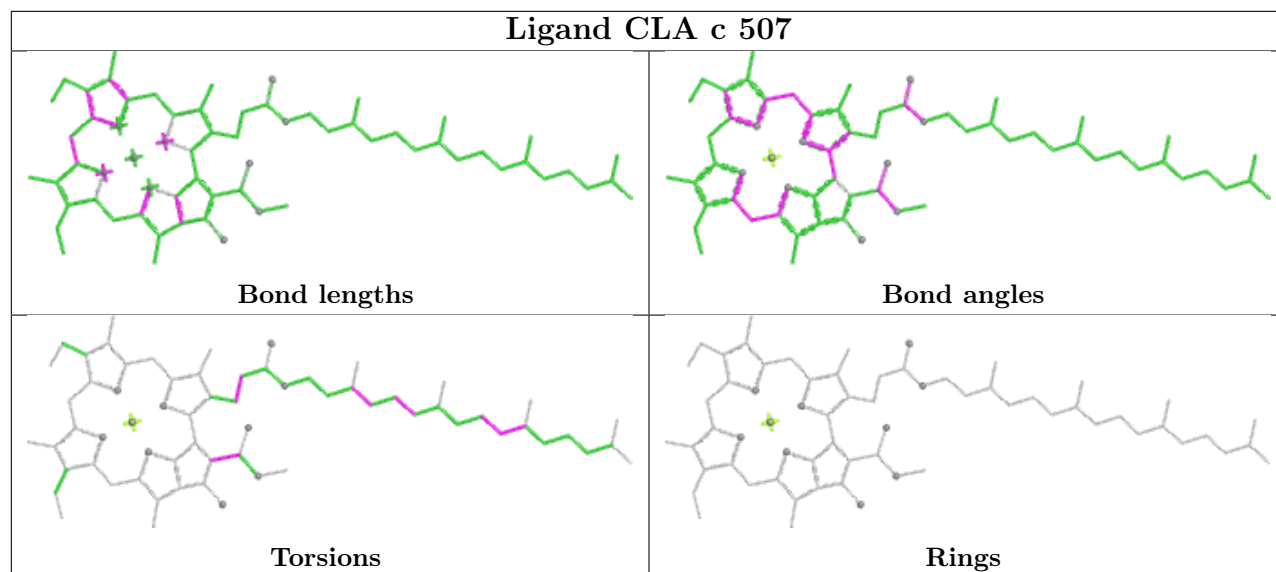
Ligand LMG b 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

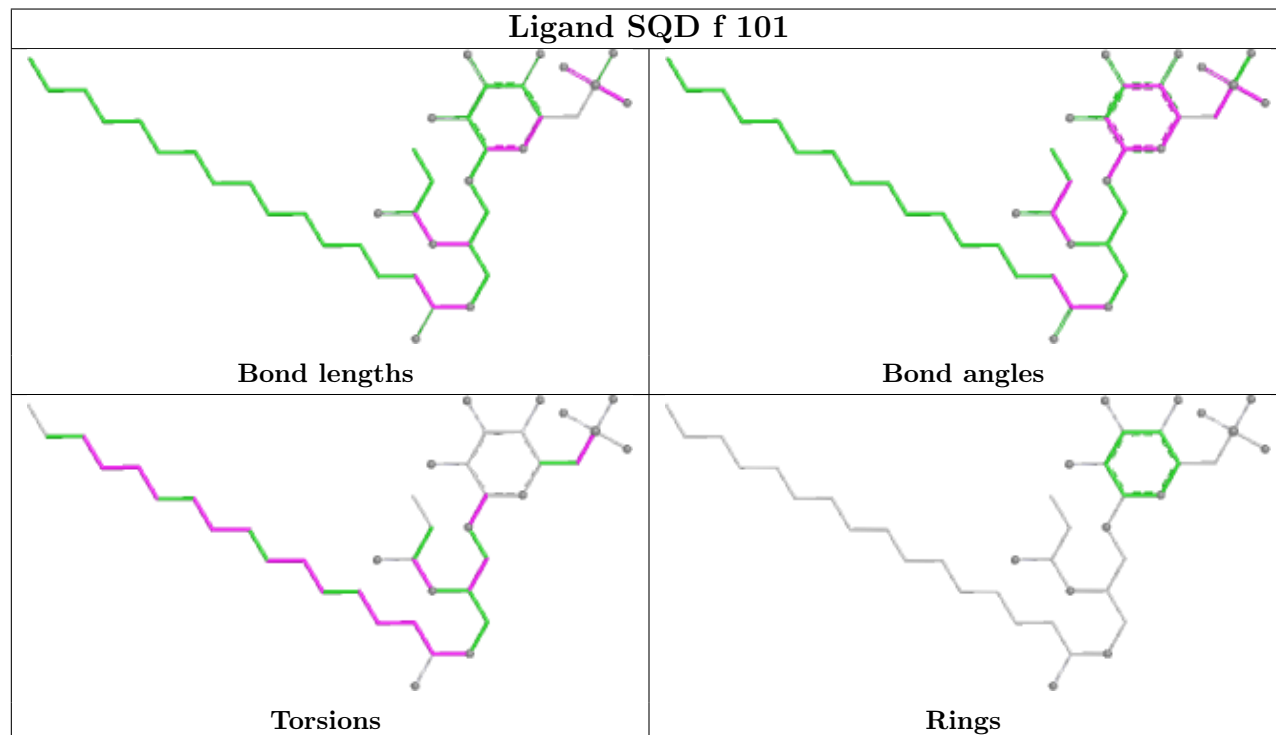
Ligand CLA c 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

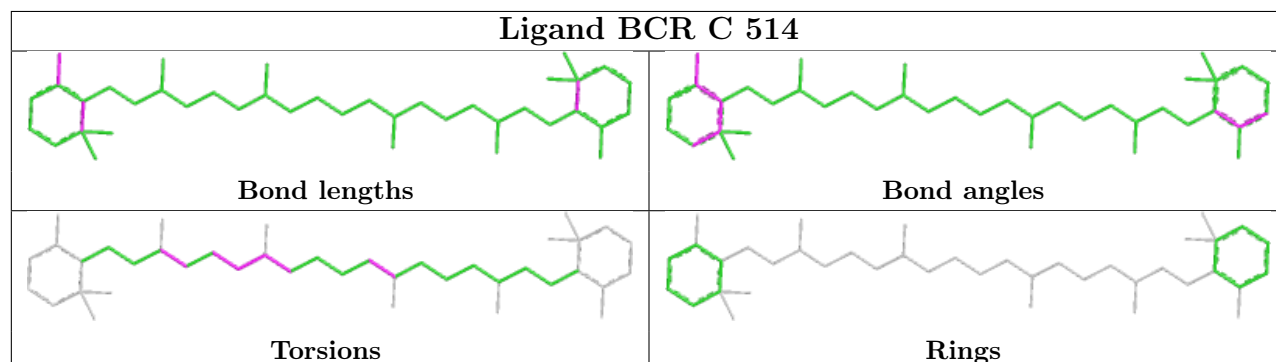
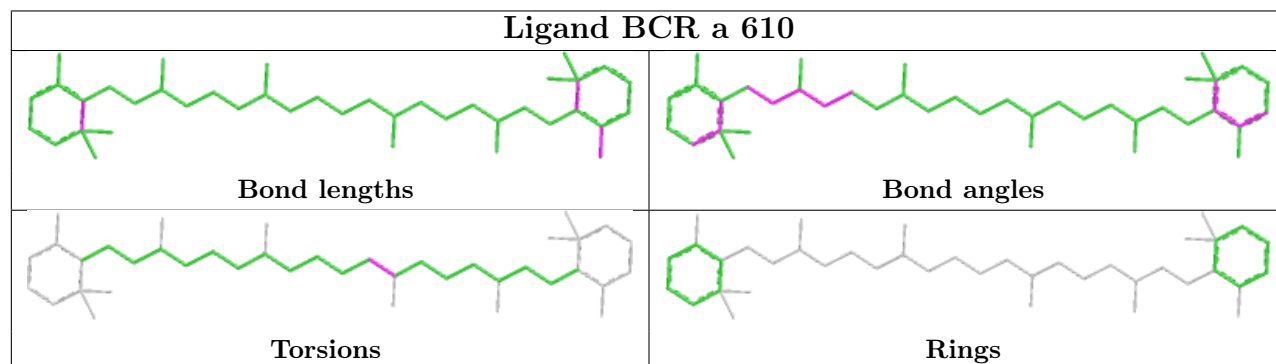
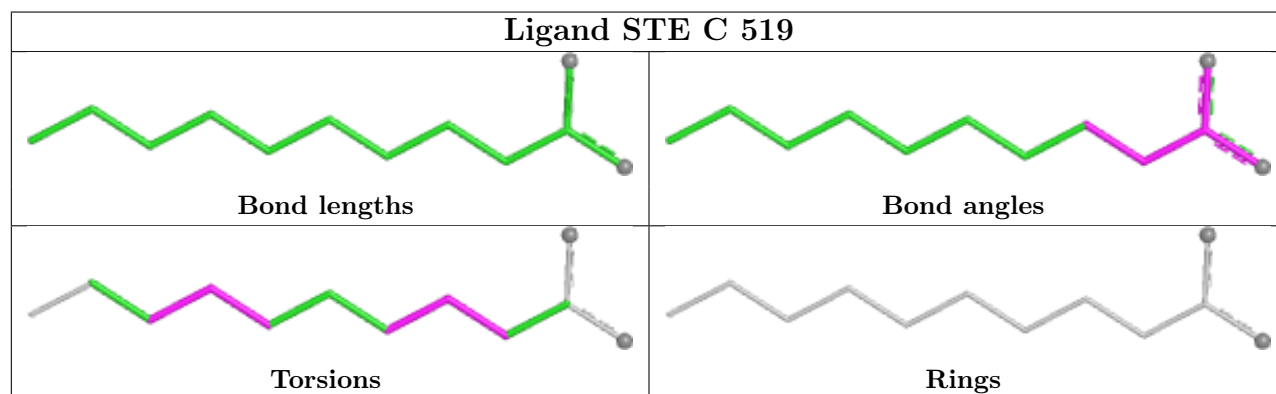
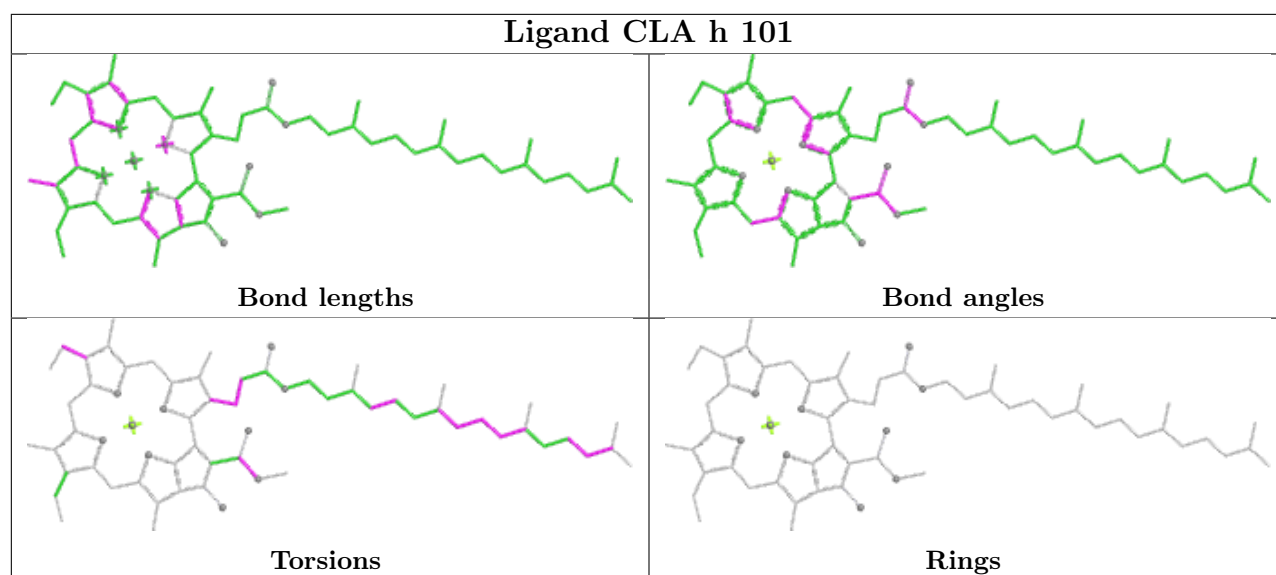


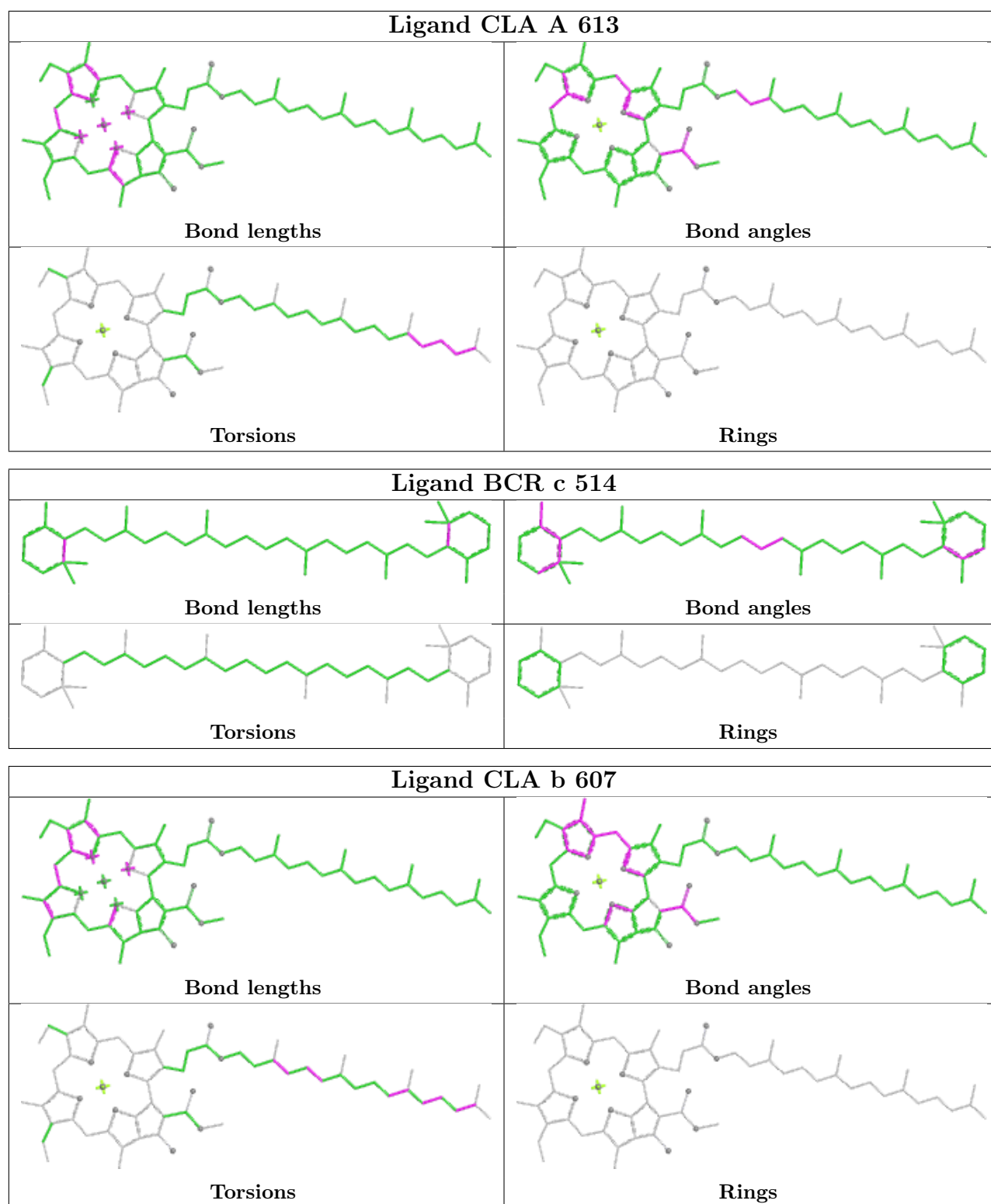
Ligand CLA c 507



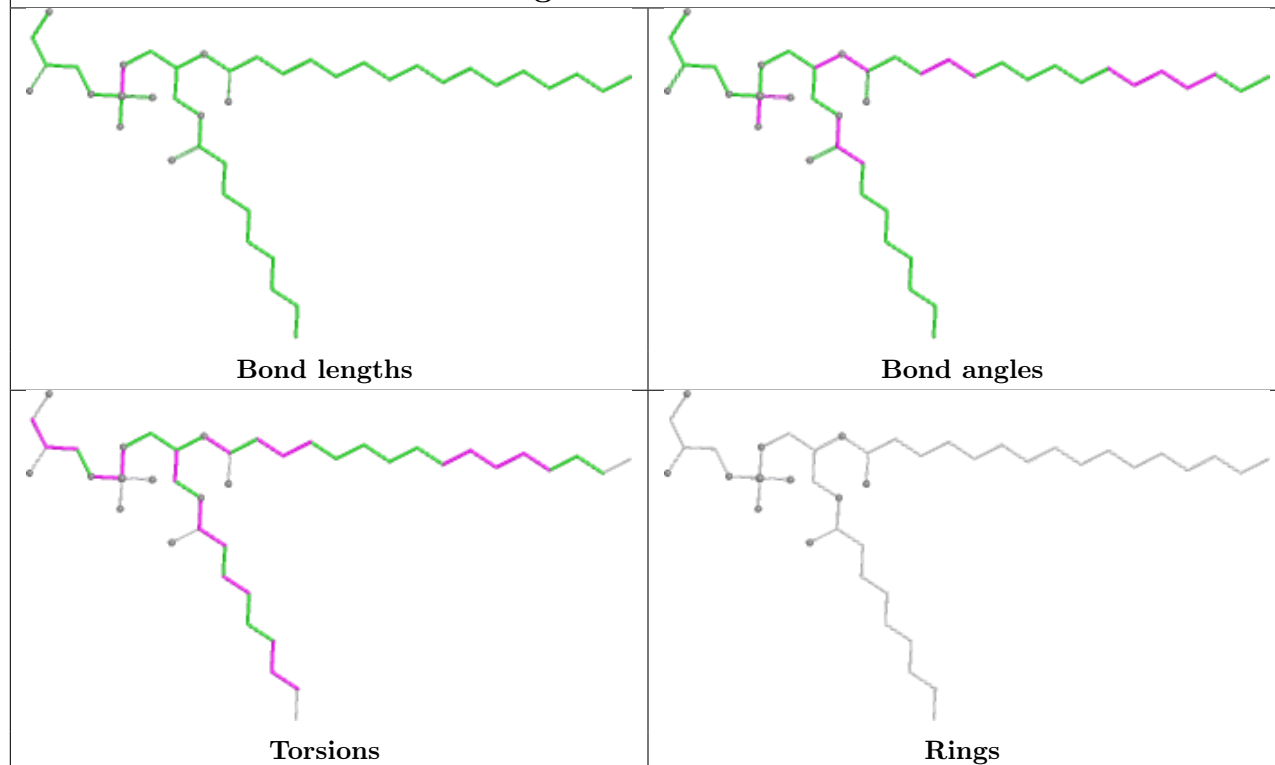
Ligand SQD f 101



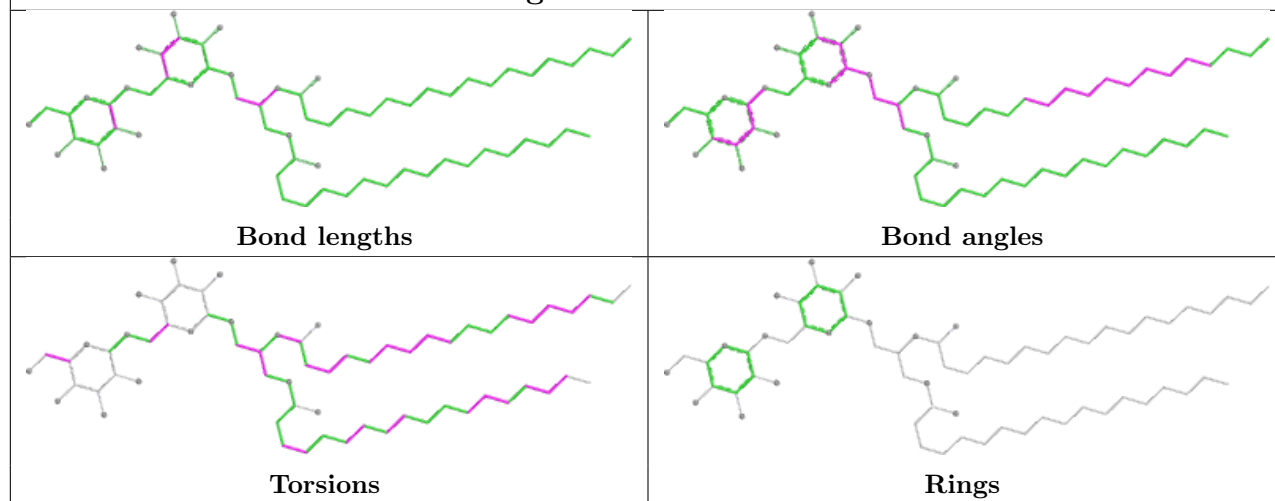




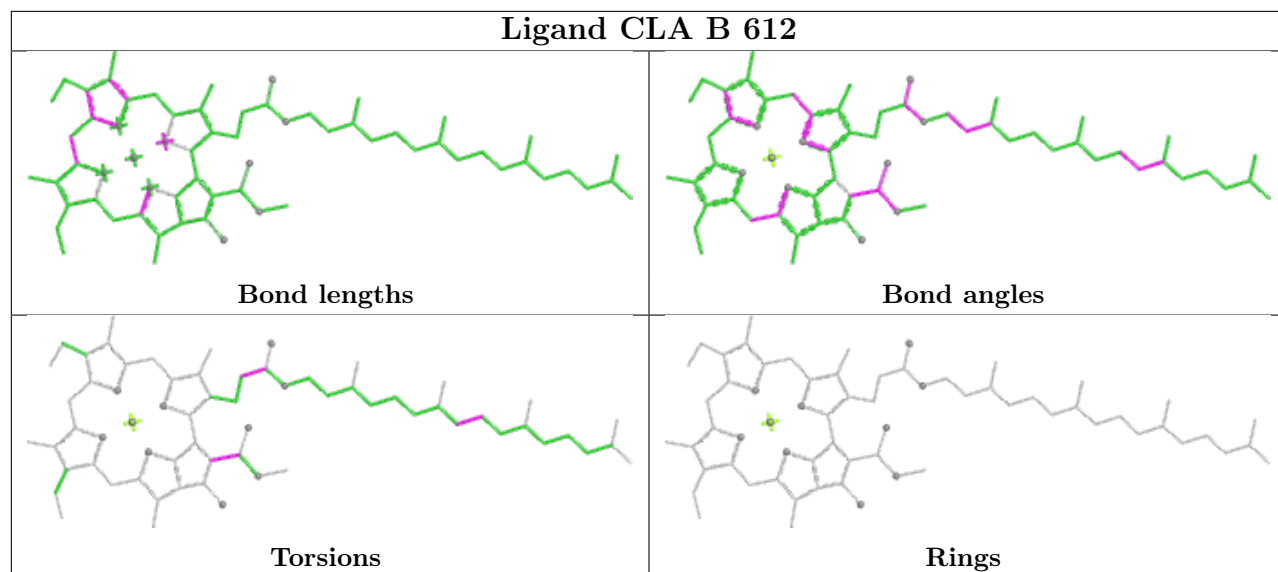
Ligand LHG e 102



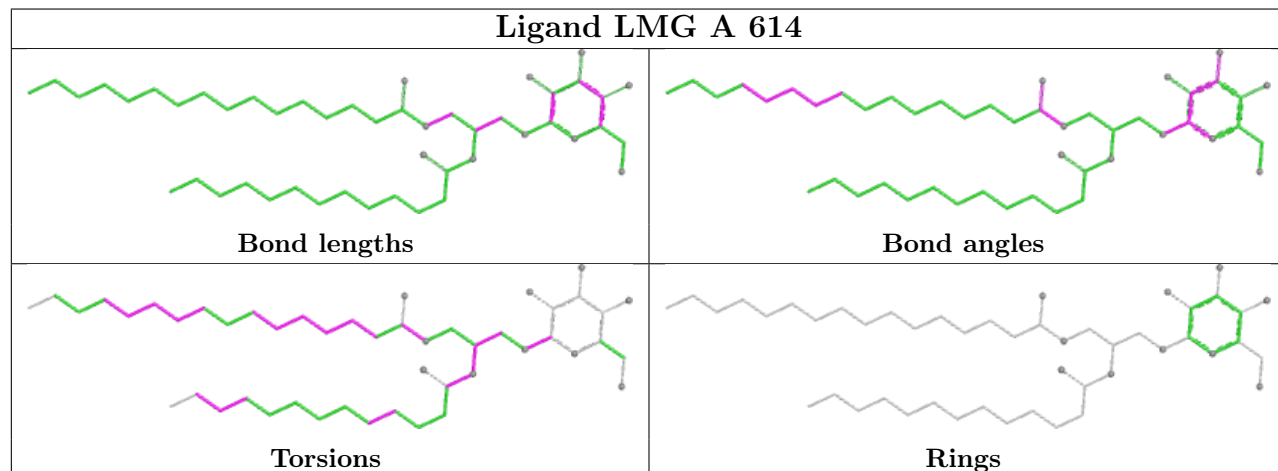
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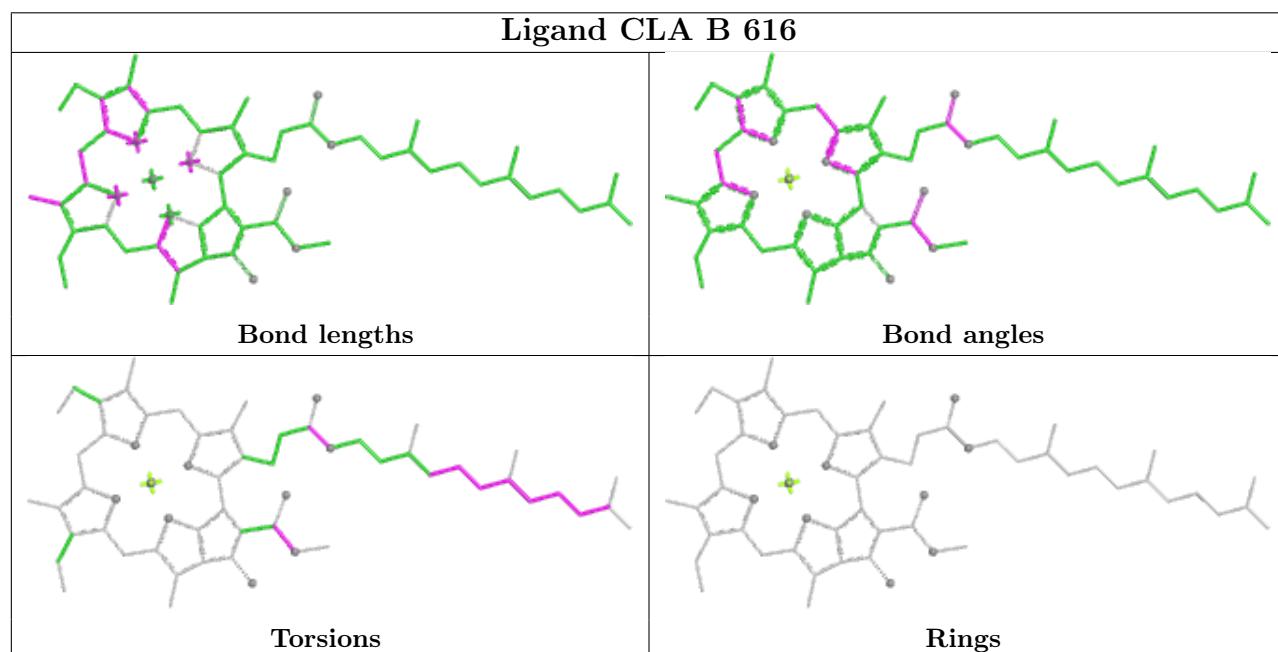
Ligand CLA B 612



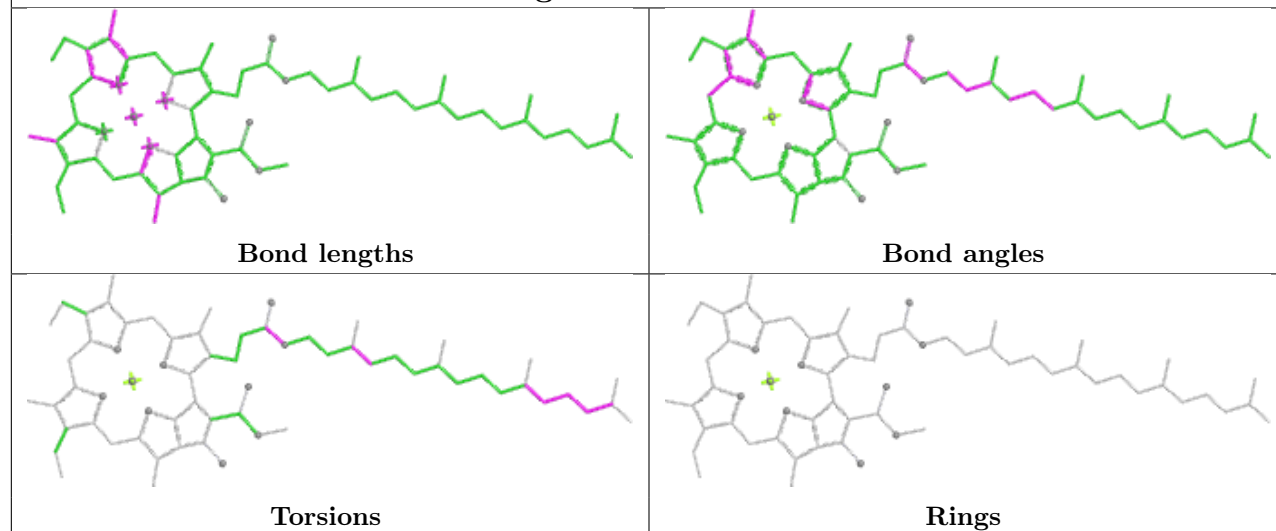
Ligand LMG A 614



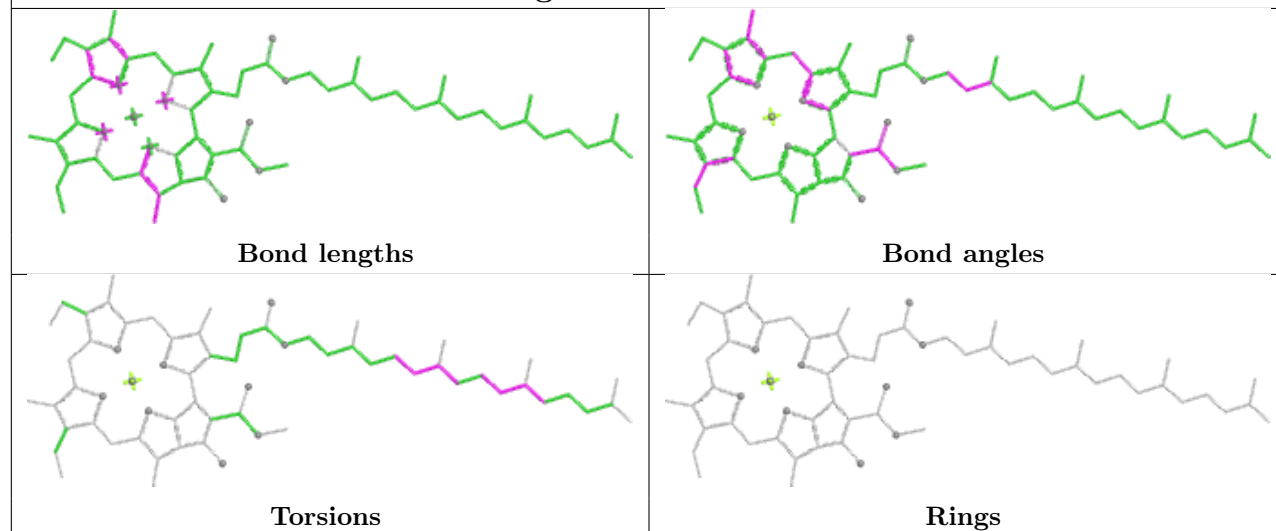
Ligand CLA B 616



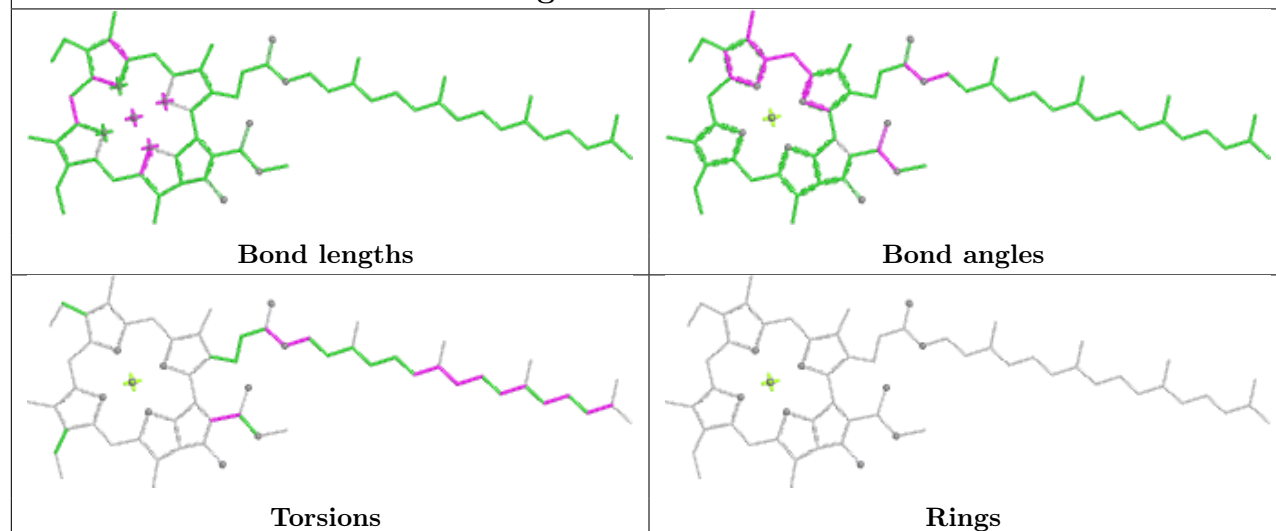
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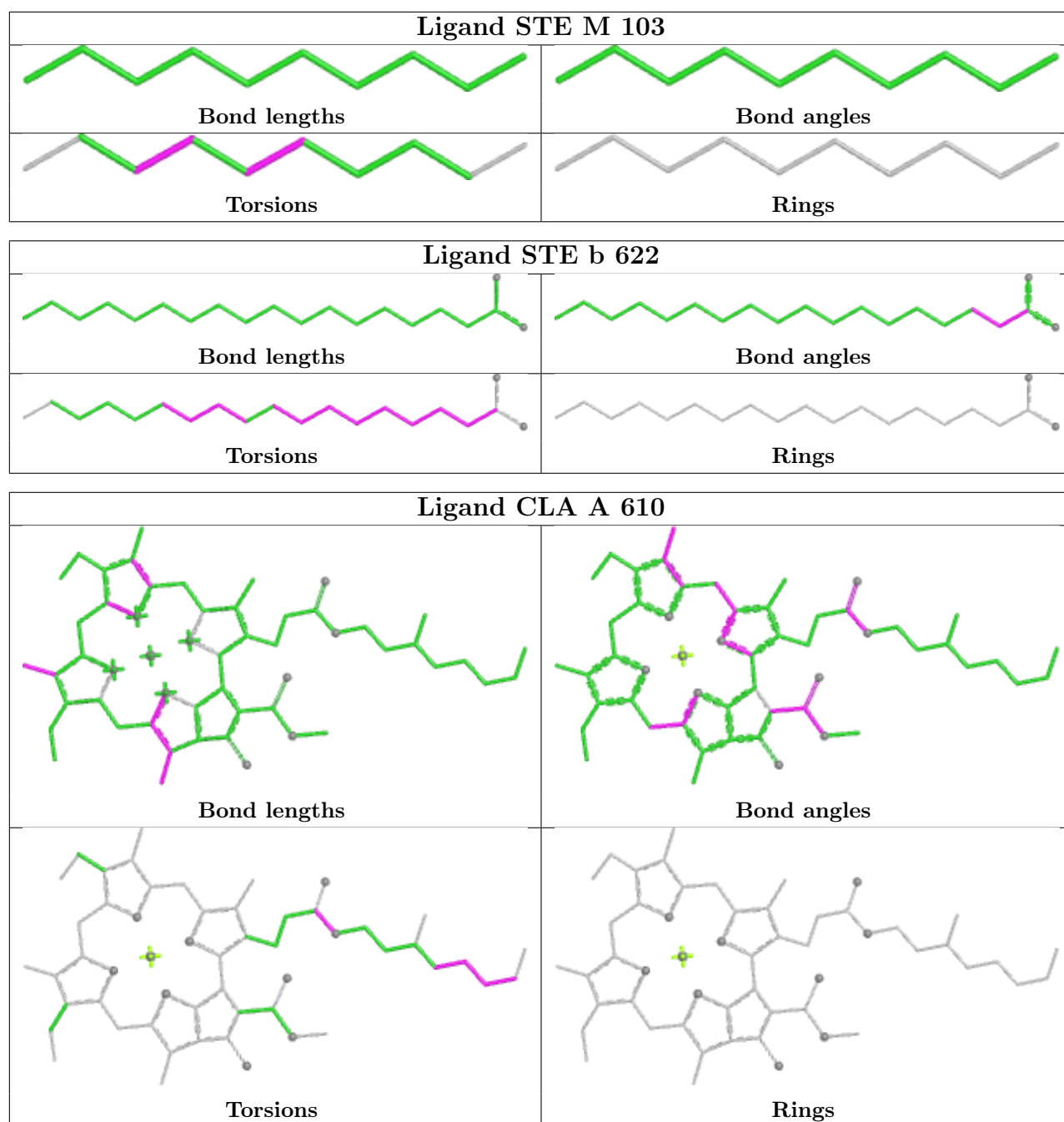


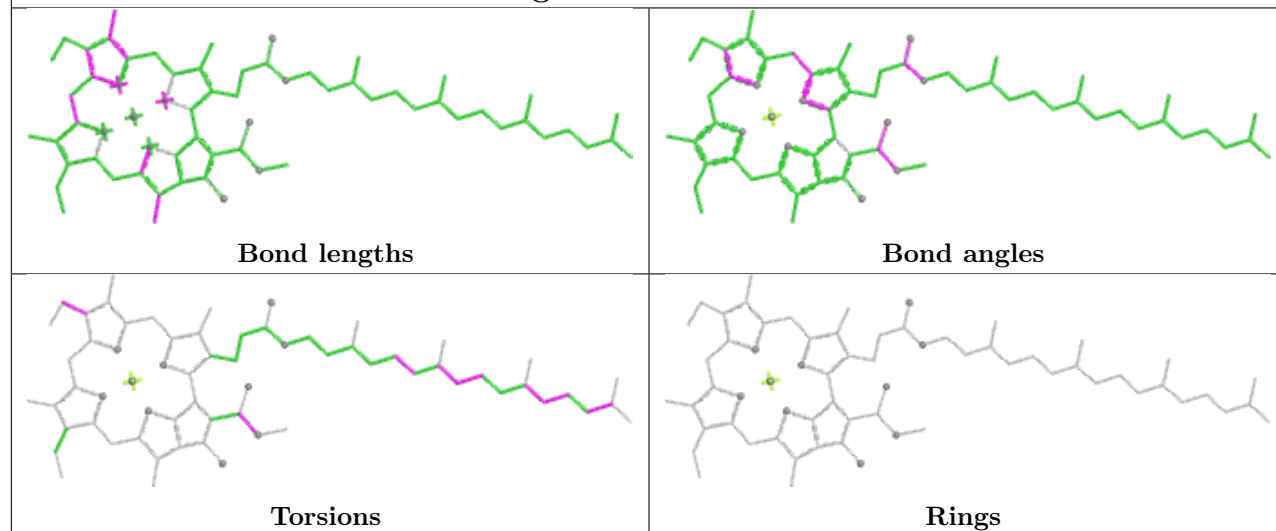
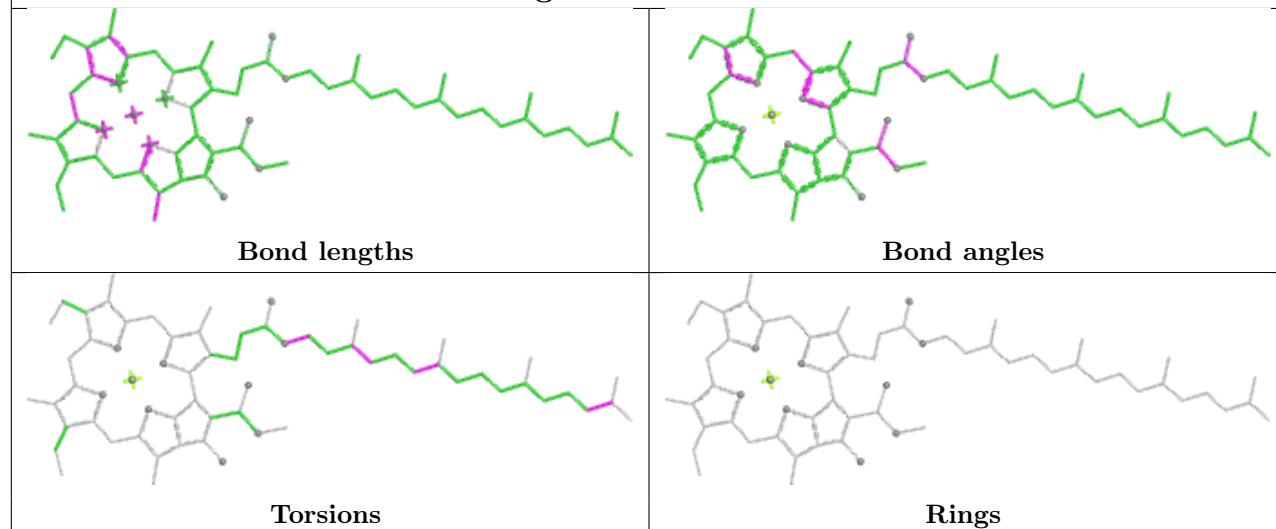
Ligand CLA b 601

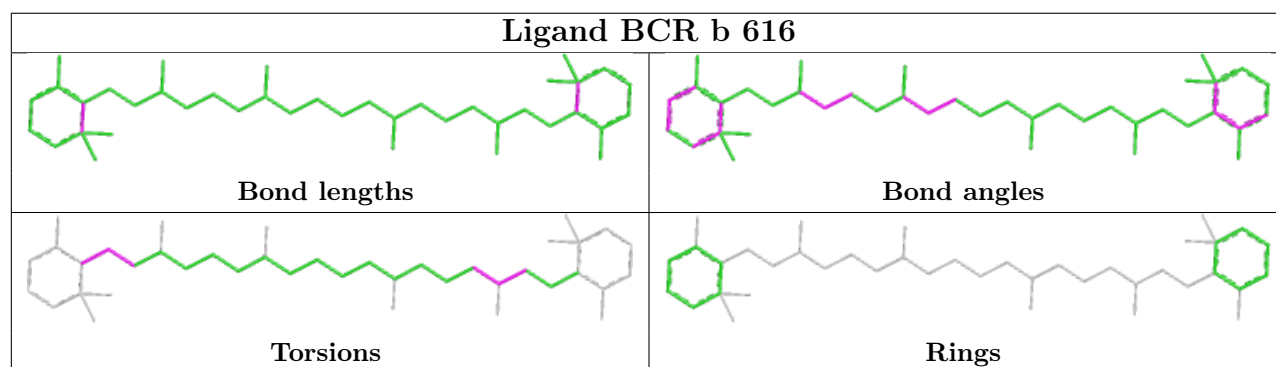
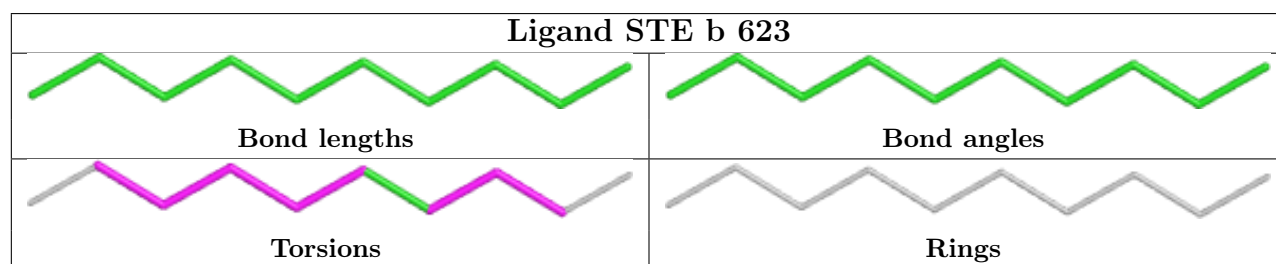
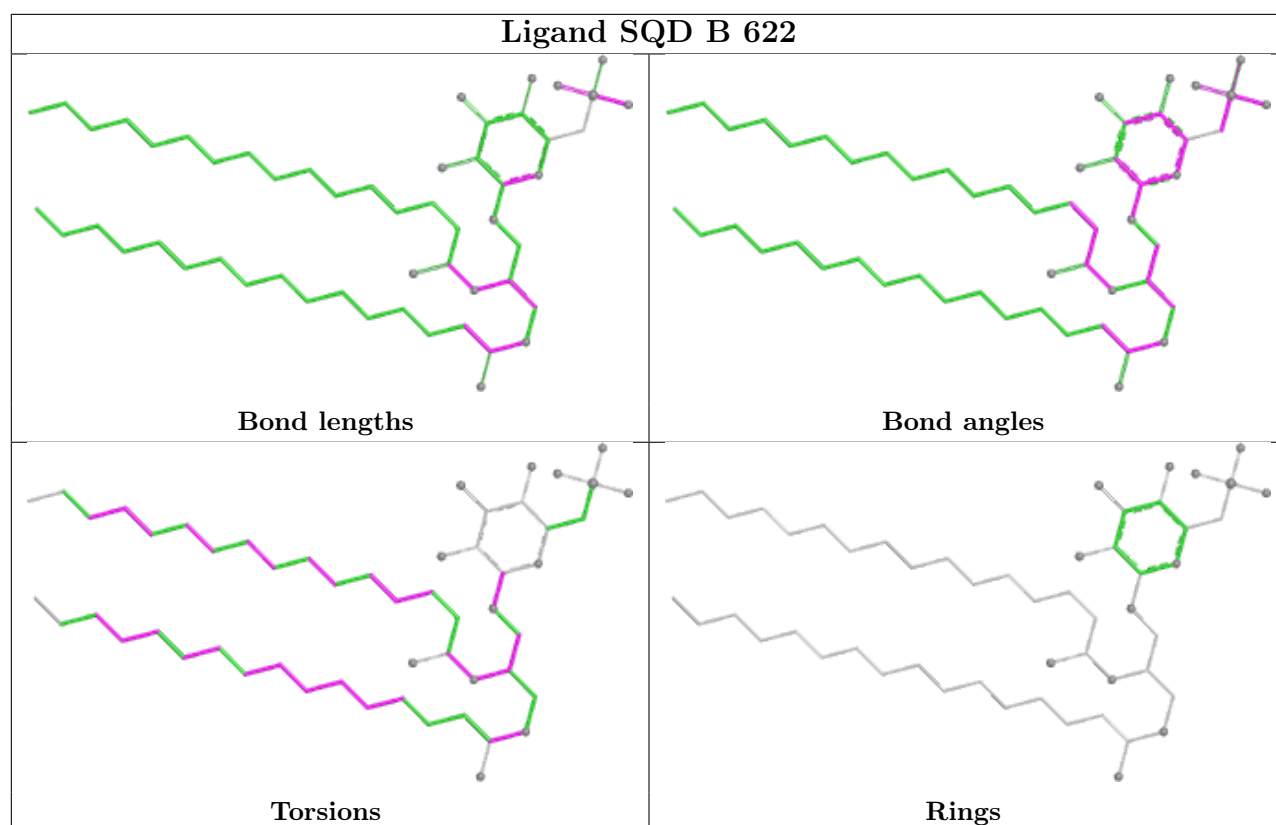


Ligand CLA c 506

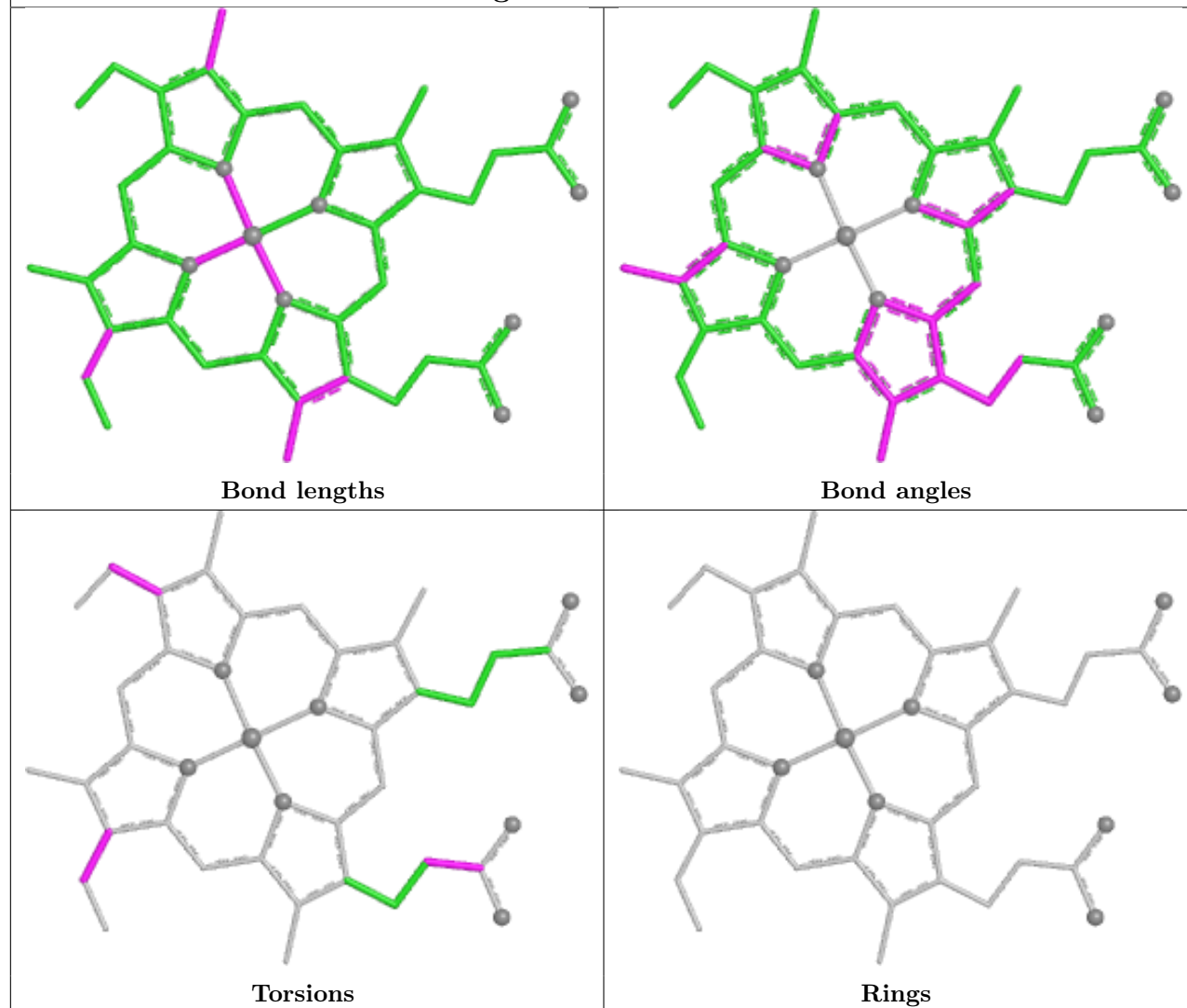




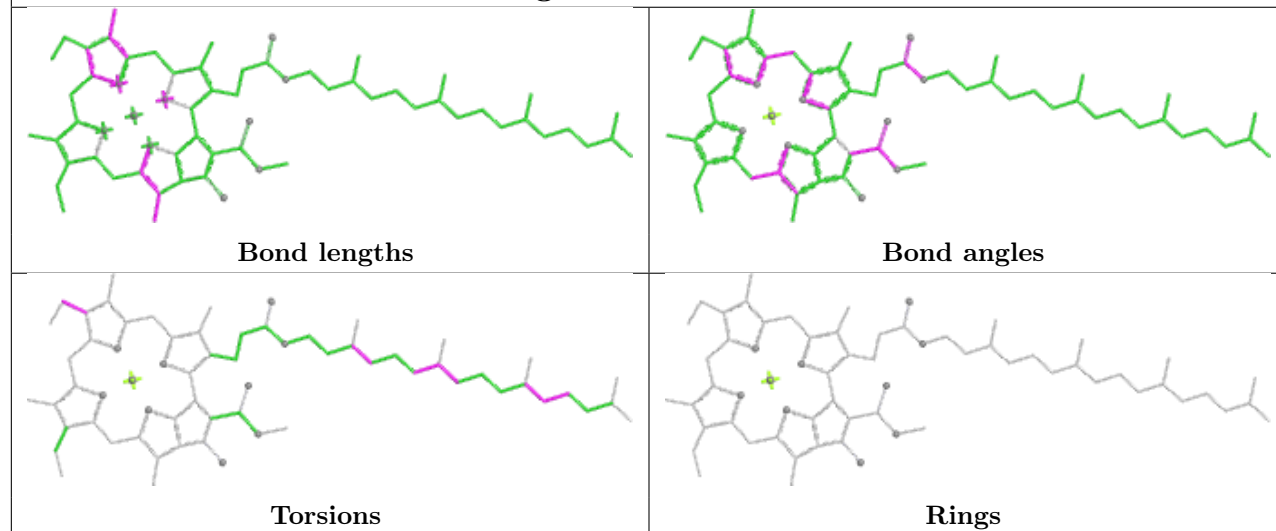
Ligand CLA B 615**Ligand CLA d 403**



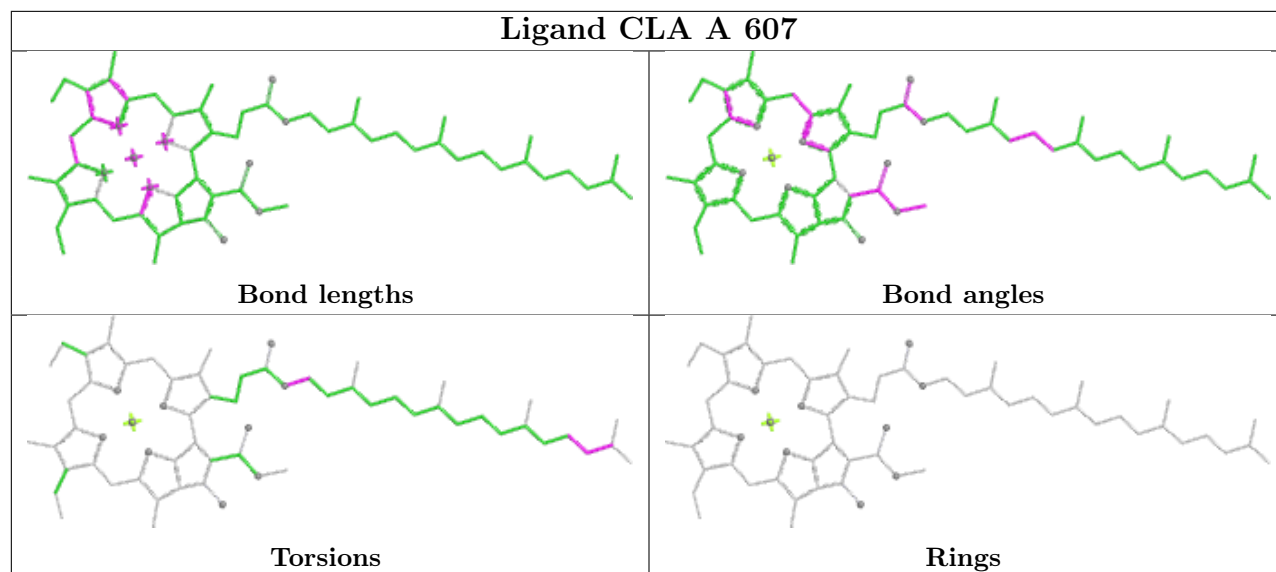
Ligand HEC V 201



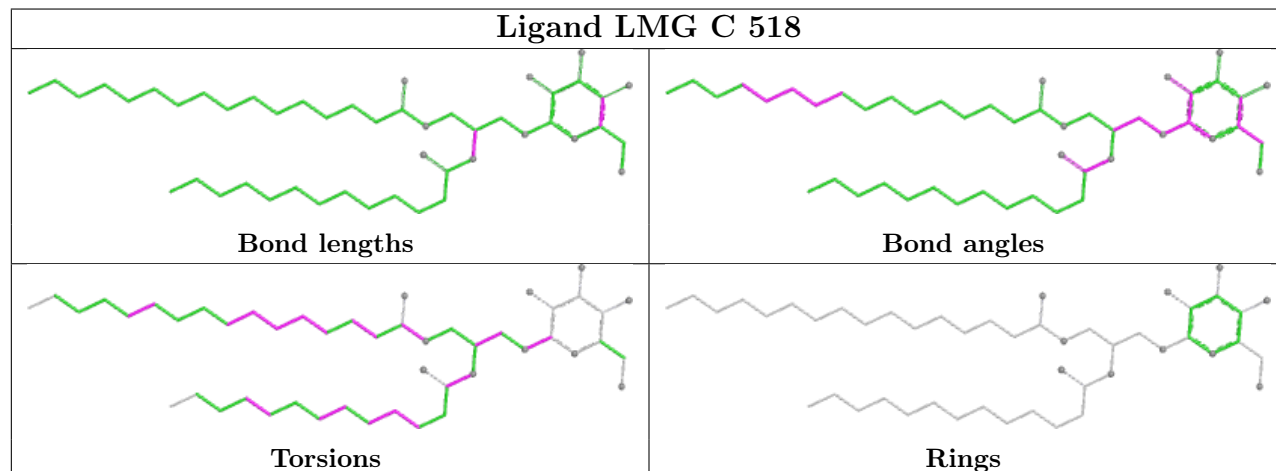
Ligand CLA b 602



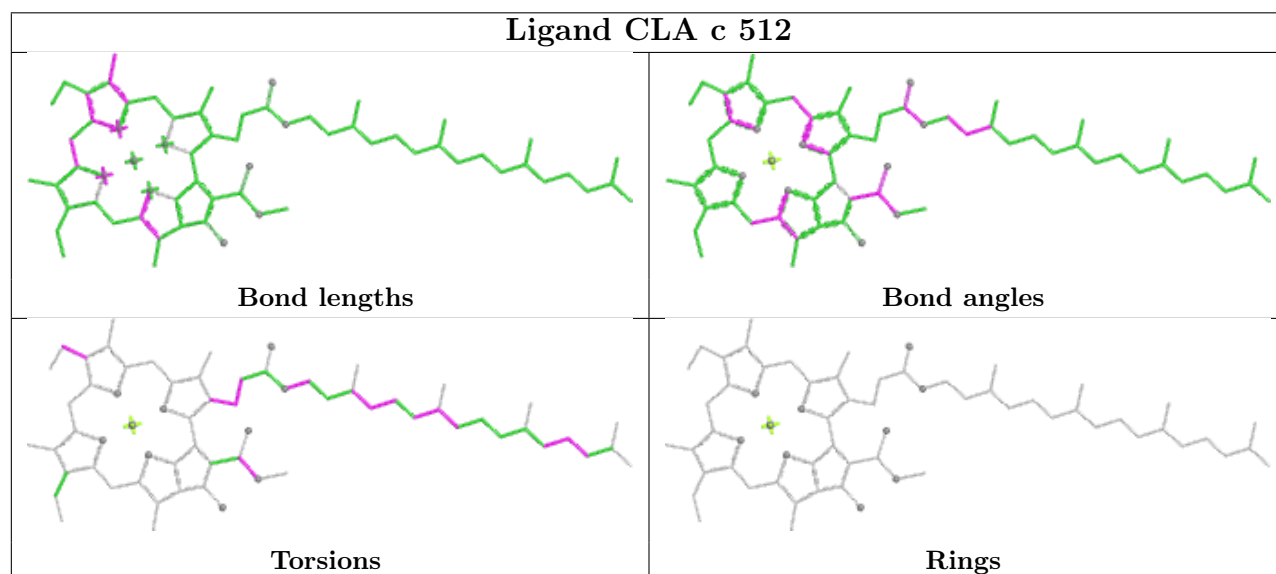
Ligand CLA A 607



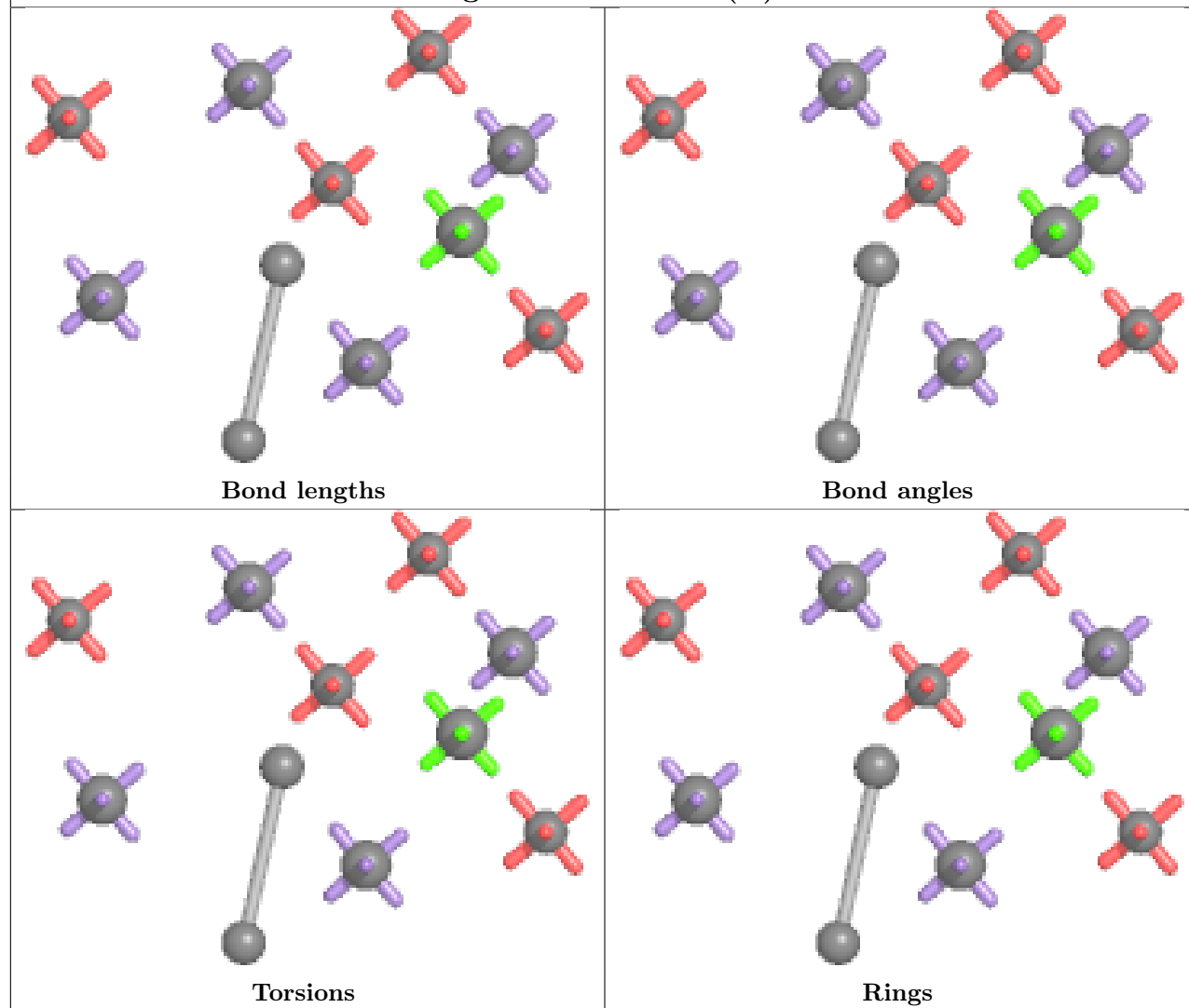
Ligand LMG C 518



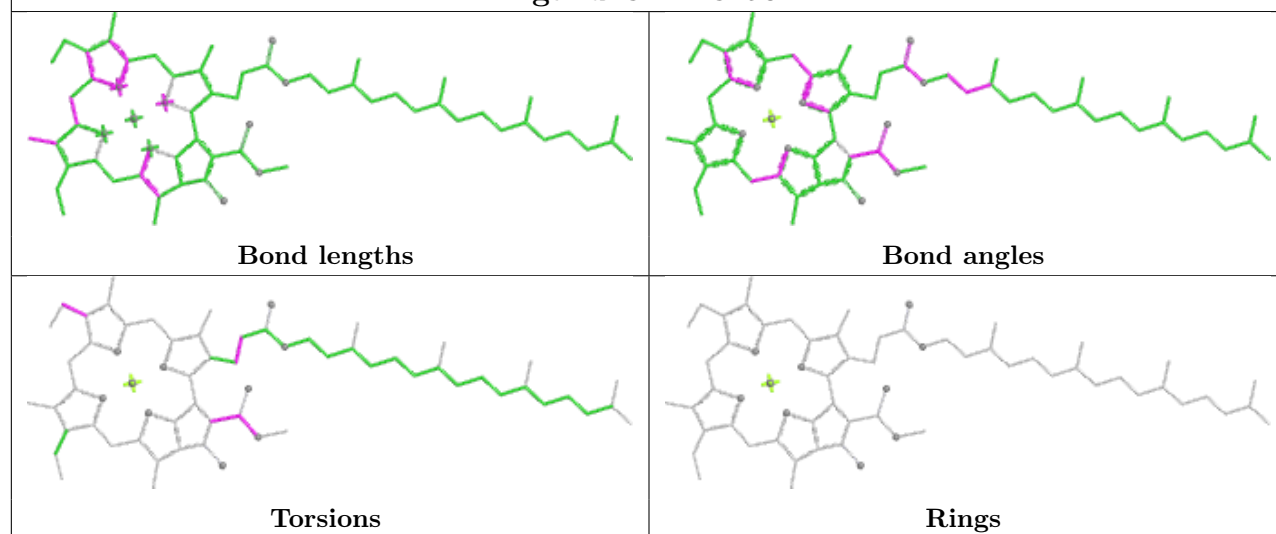
Ligand CLA c 512

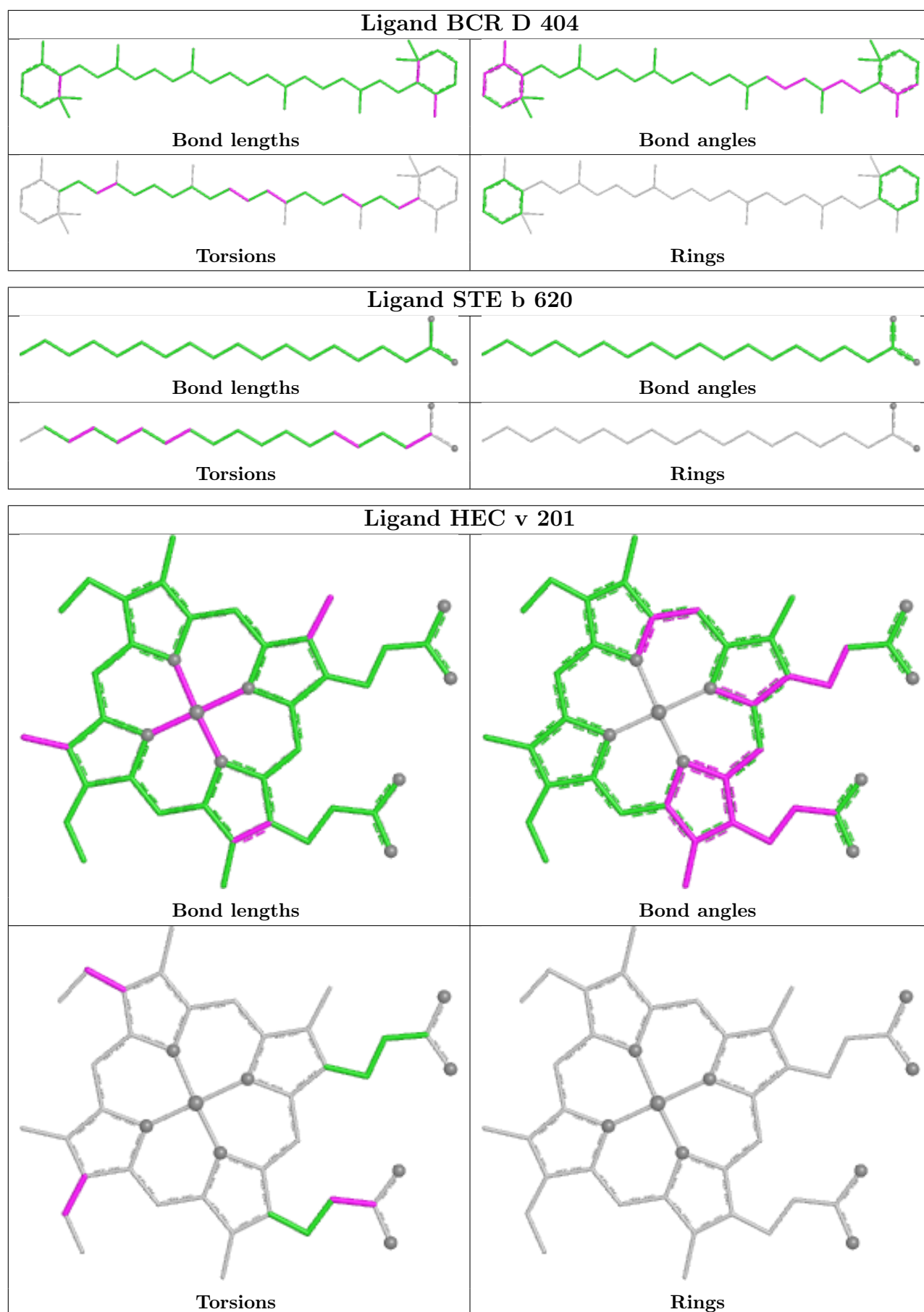


Ligand OEY A 601 (A)

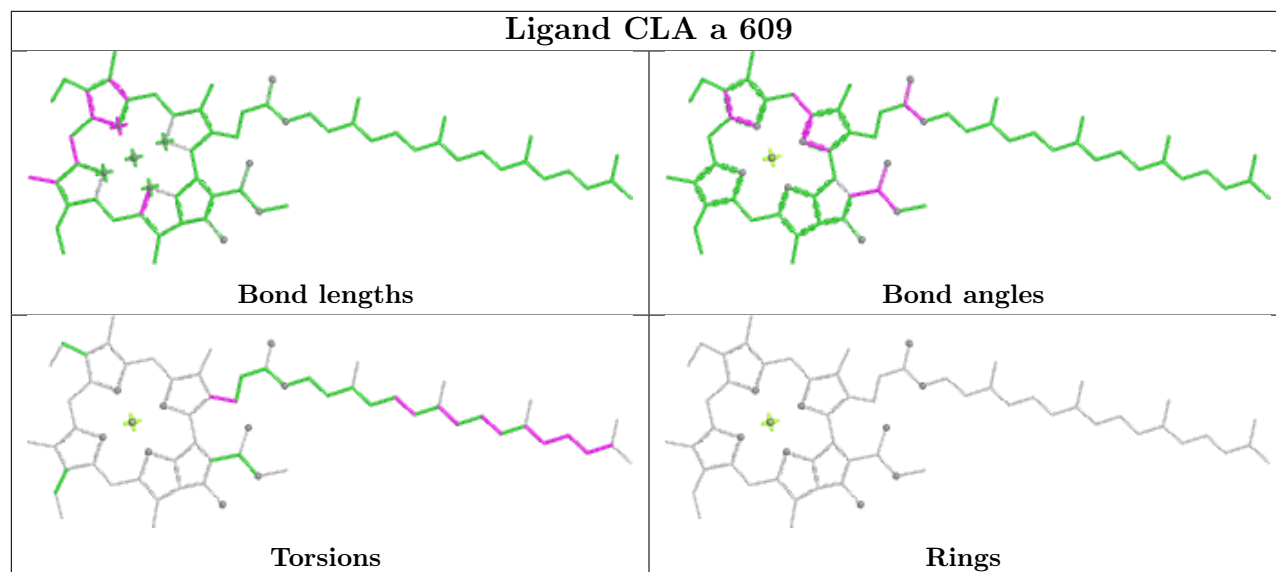


Ligand CLA C 501

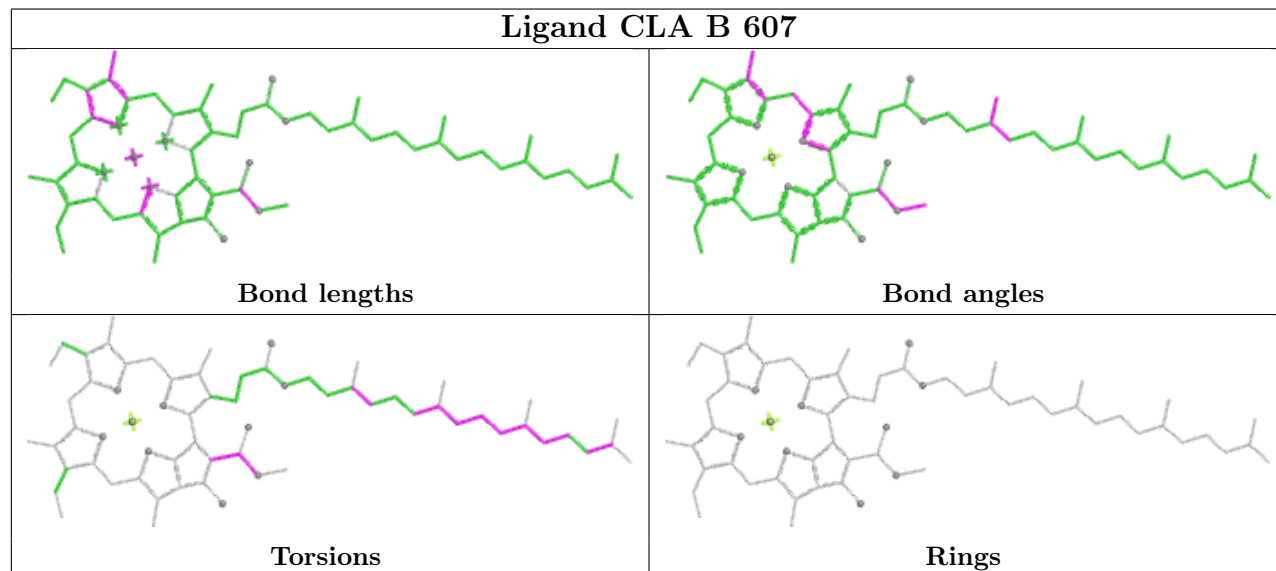




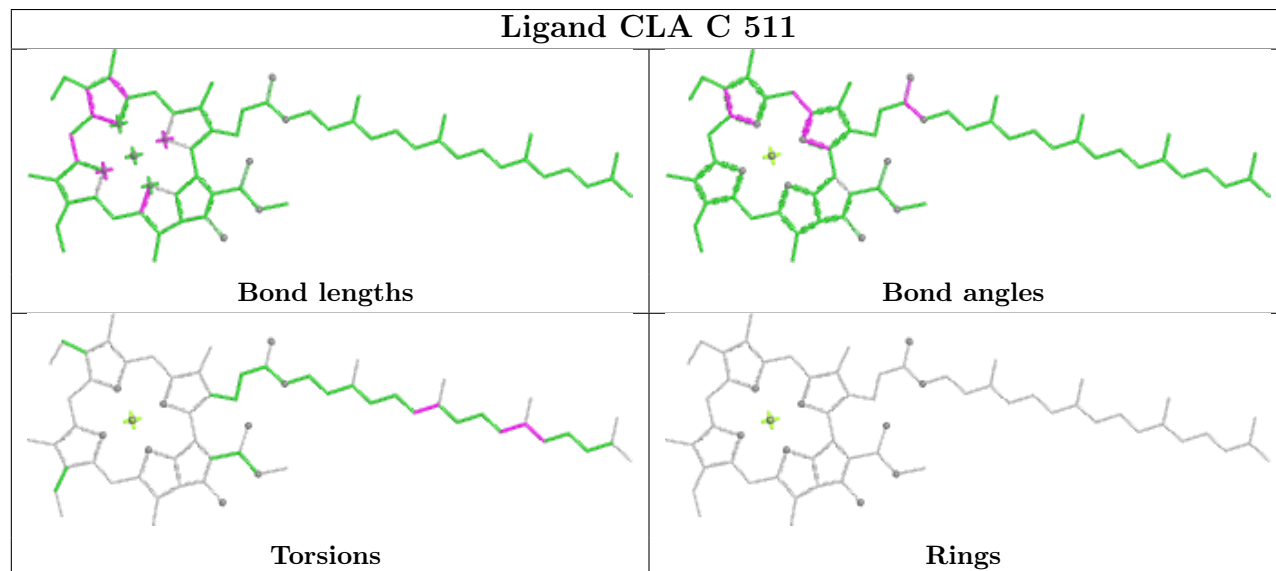
Ligand CLA a 609



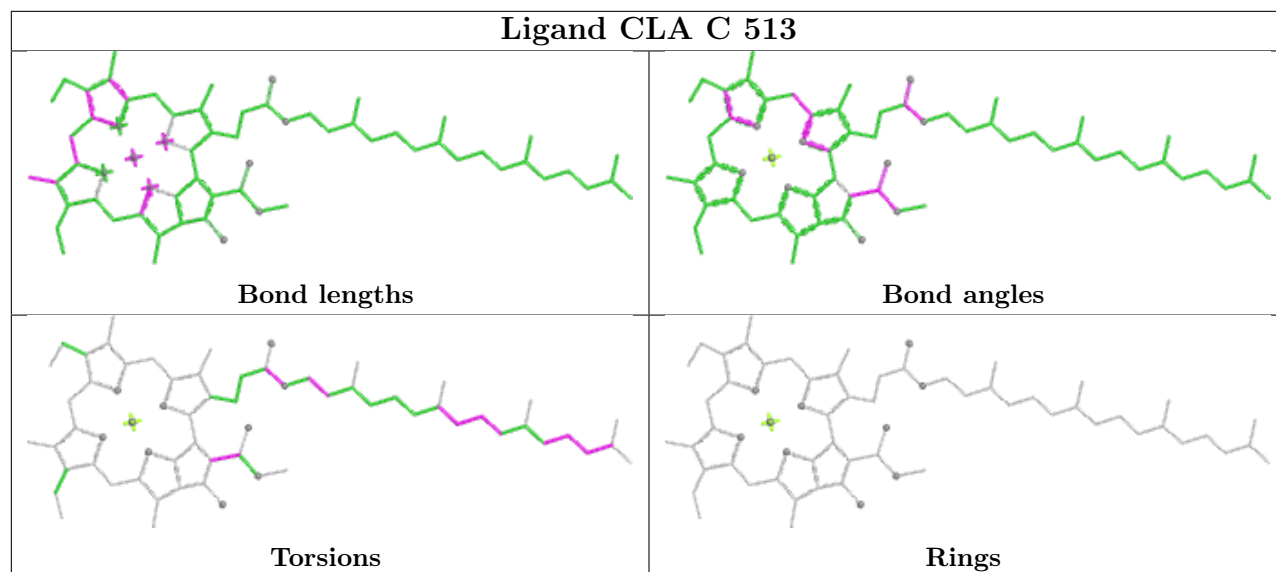
Ligand CLA B 607



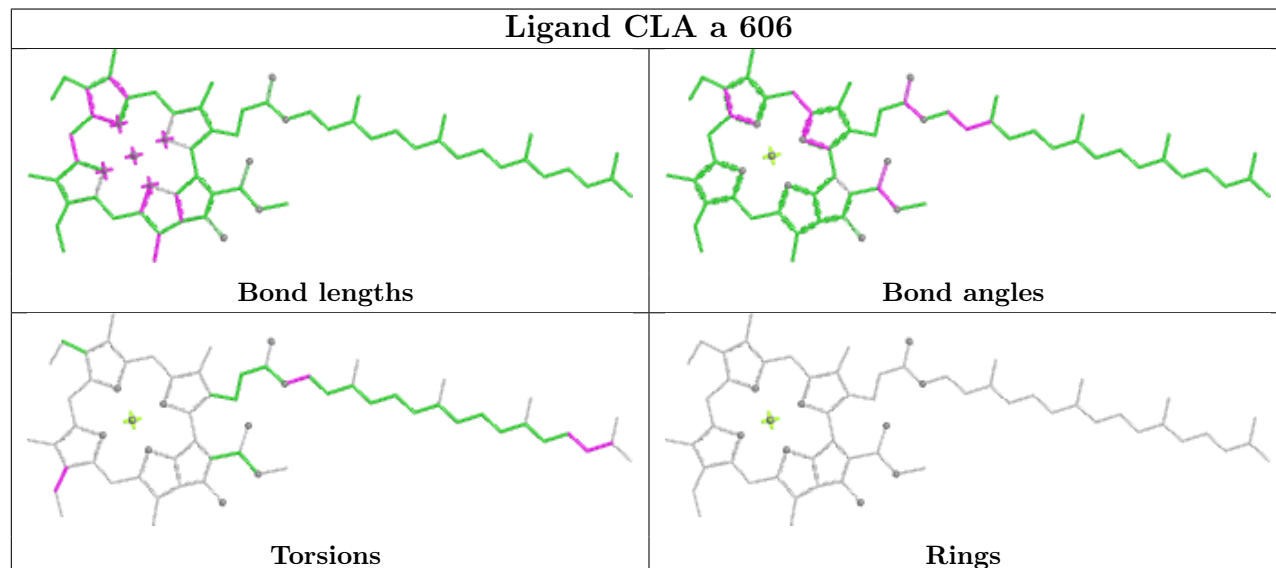
Ligand CLA C 511



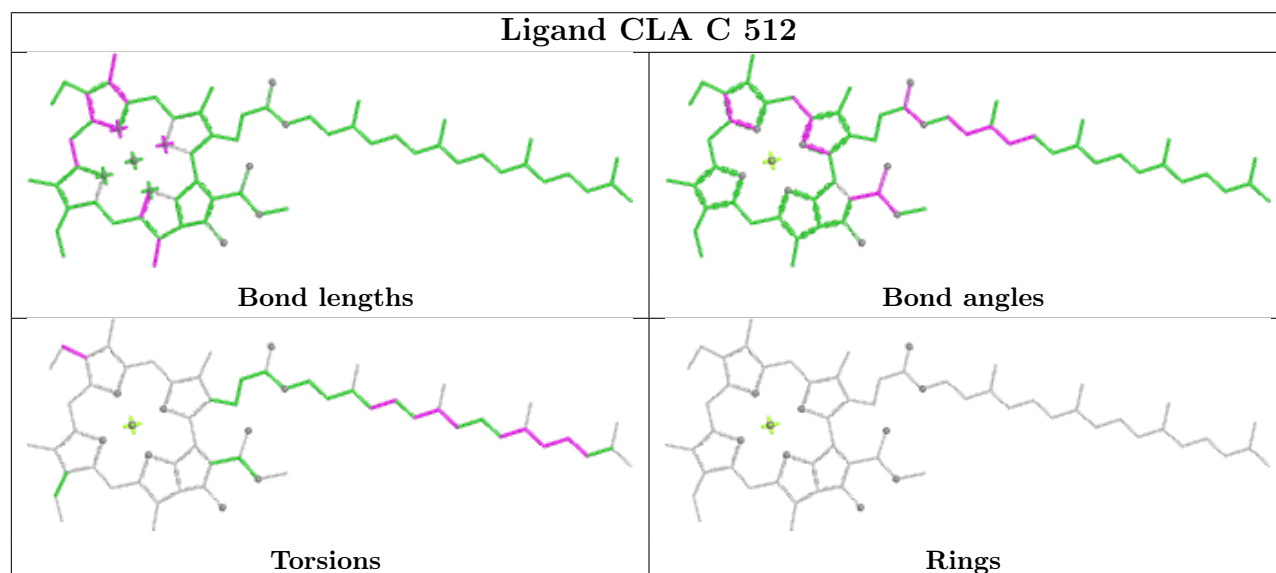
Ligand CLA C 513

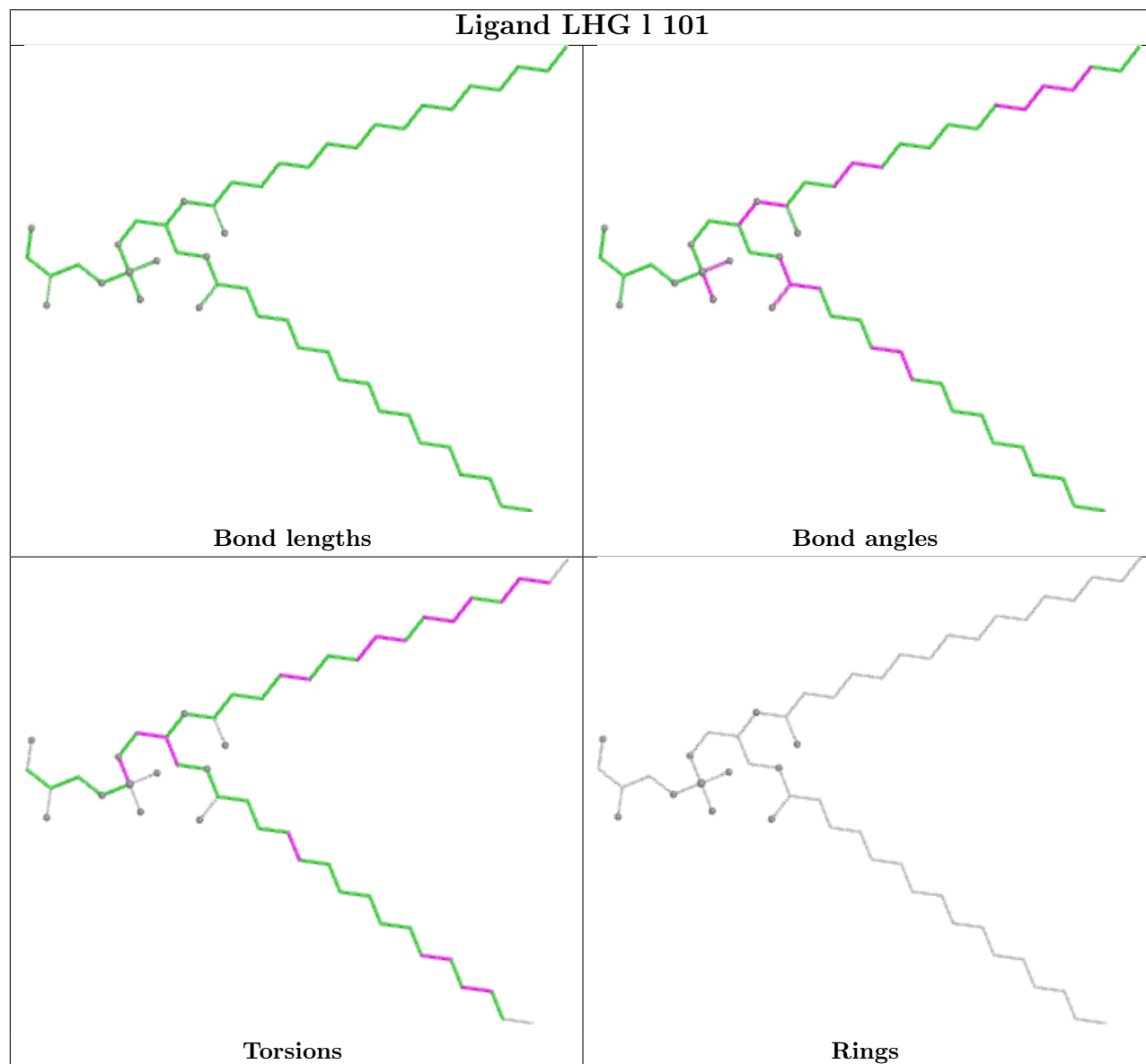
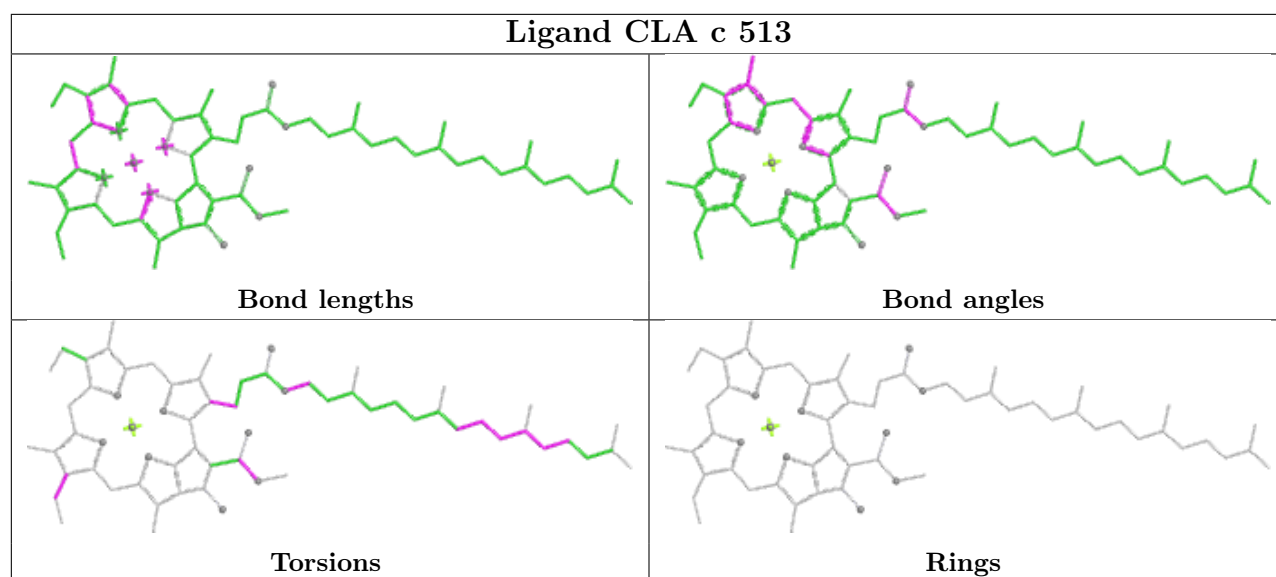


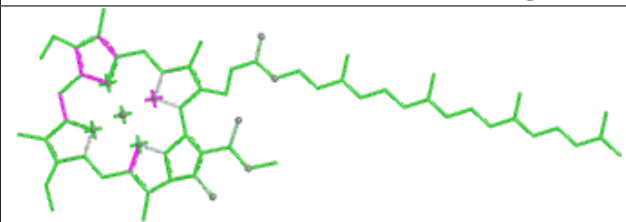
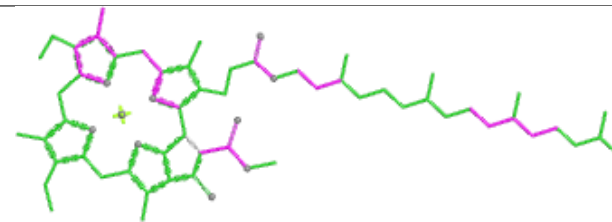
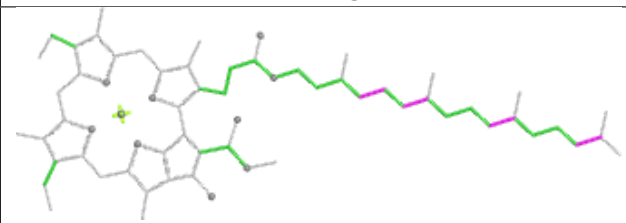
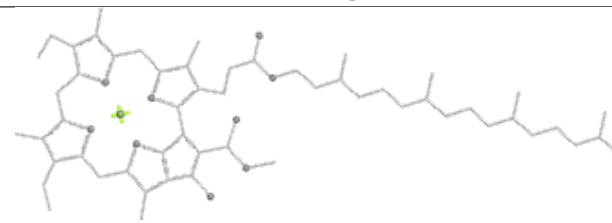
Ligand CLA a 606

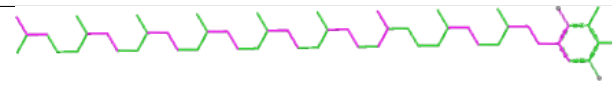
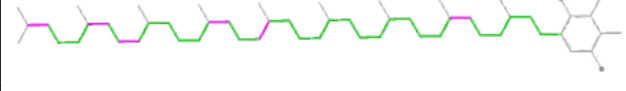
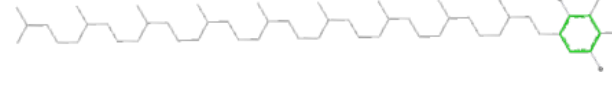


Ligand CLA C 512



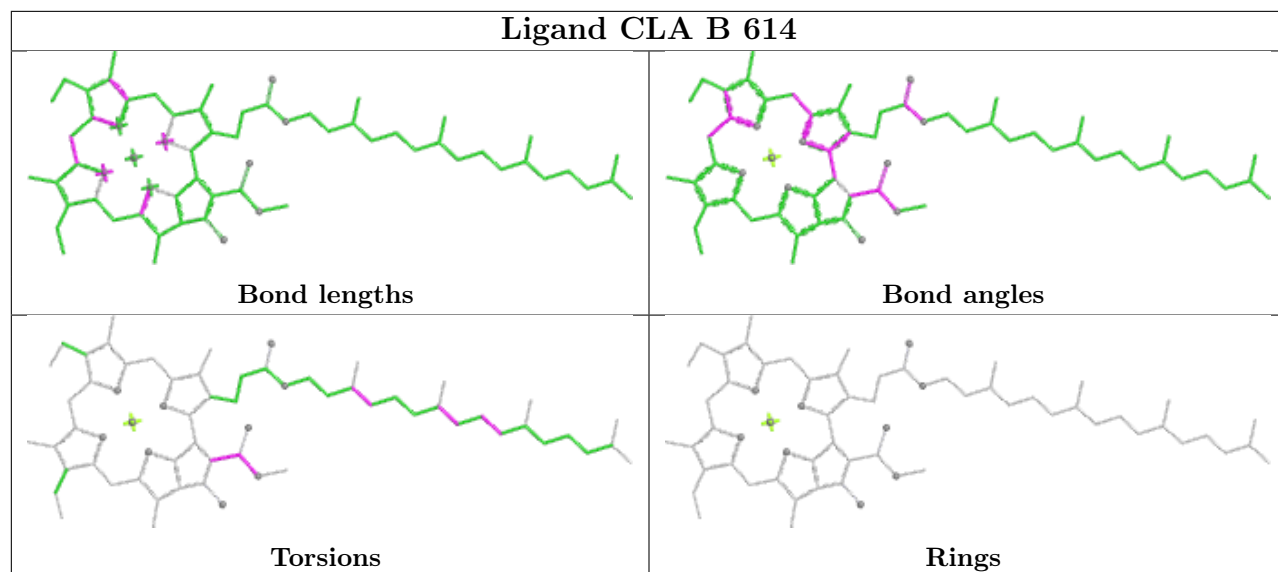


Ligand CLA B 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

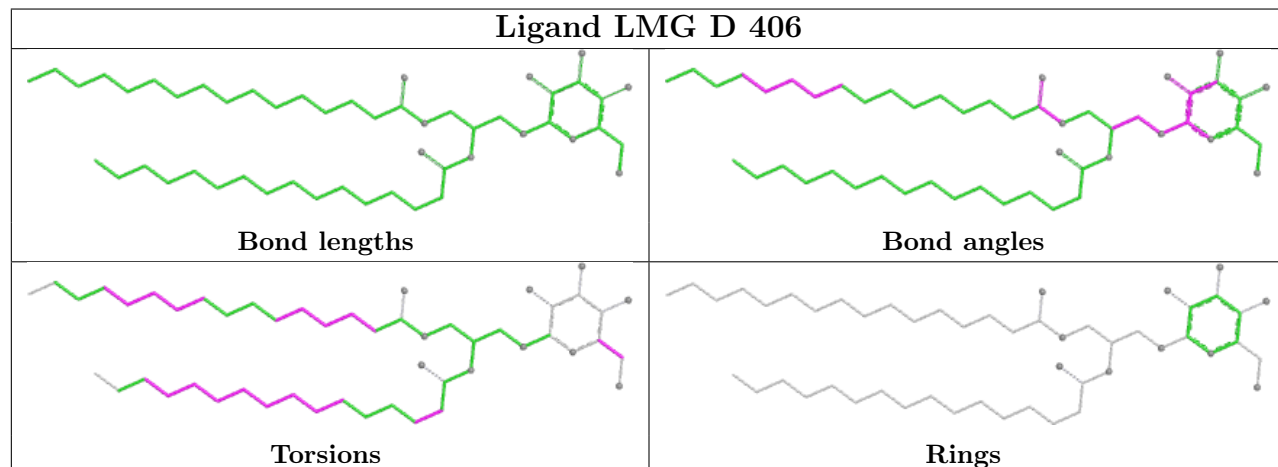
Ligand PL9 D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE a 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

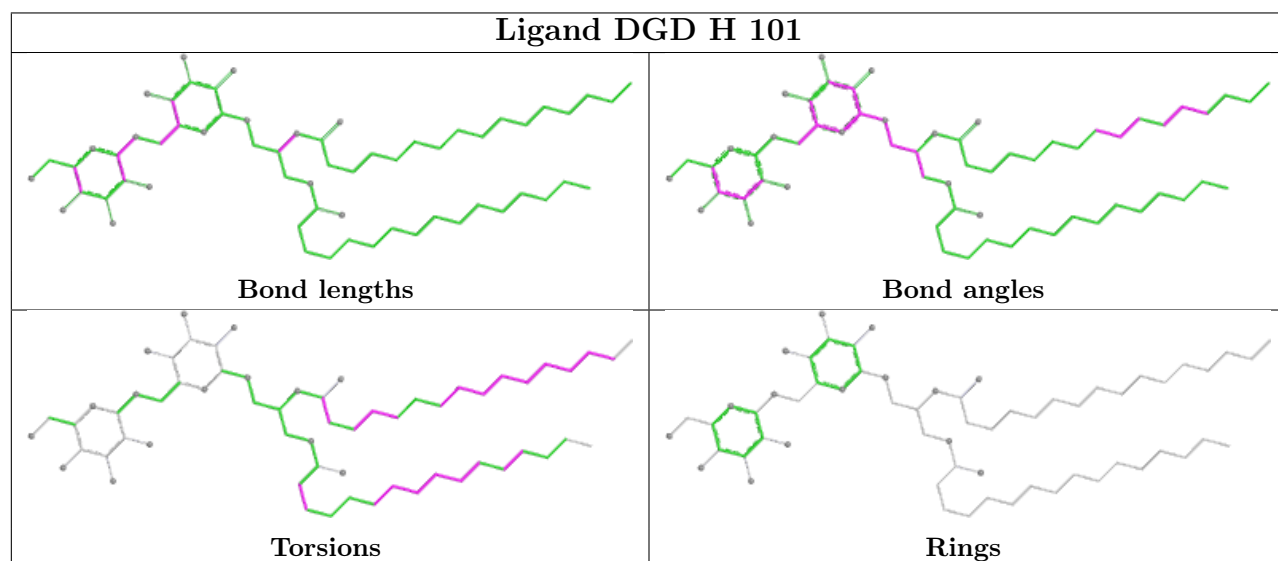
Ligand CLA B 614

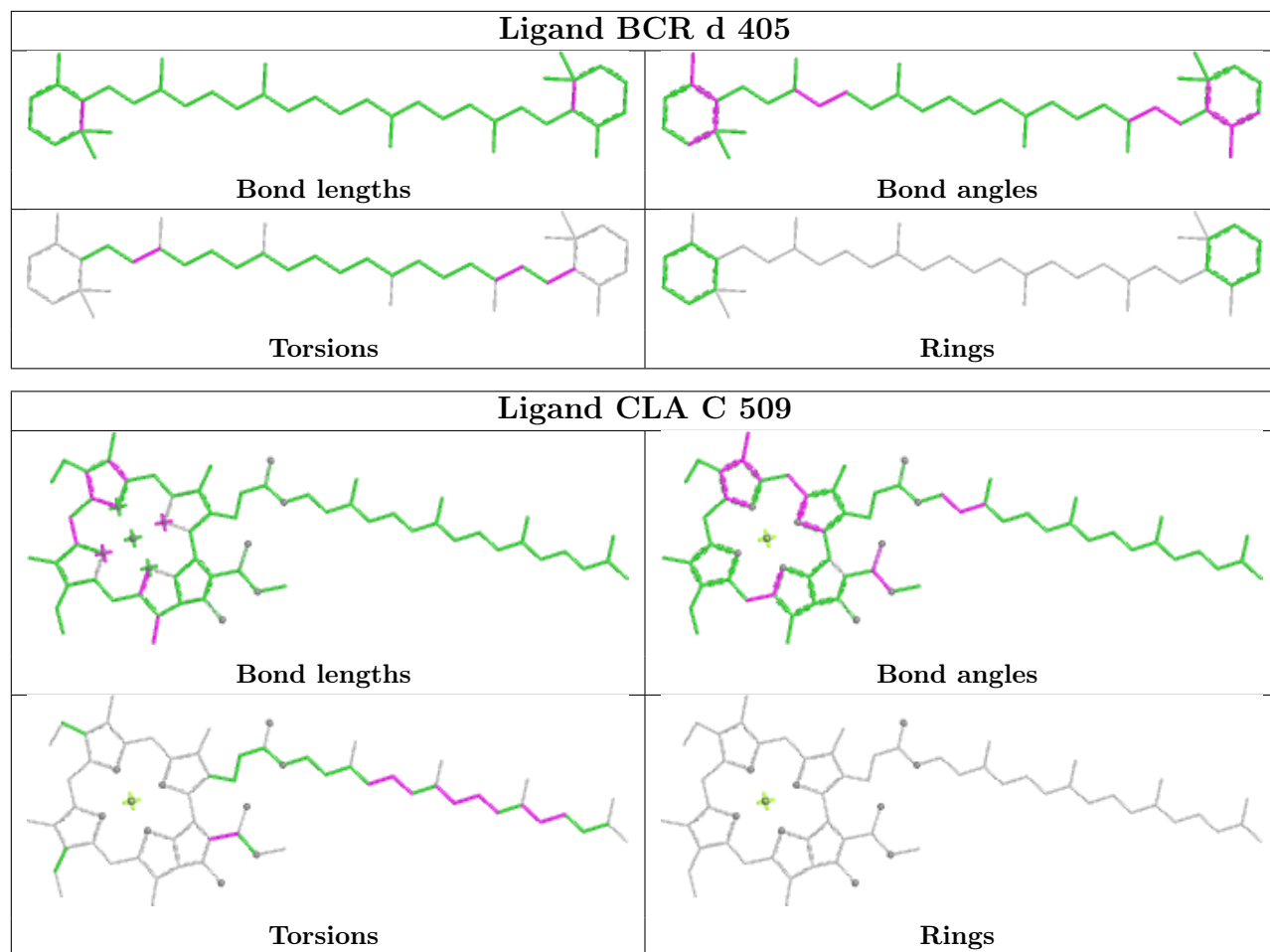


Ligand LMG D 406

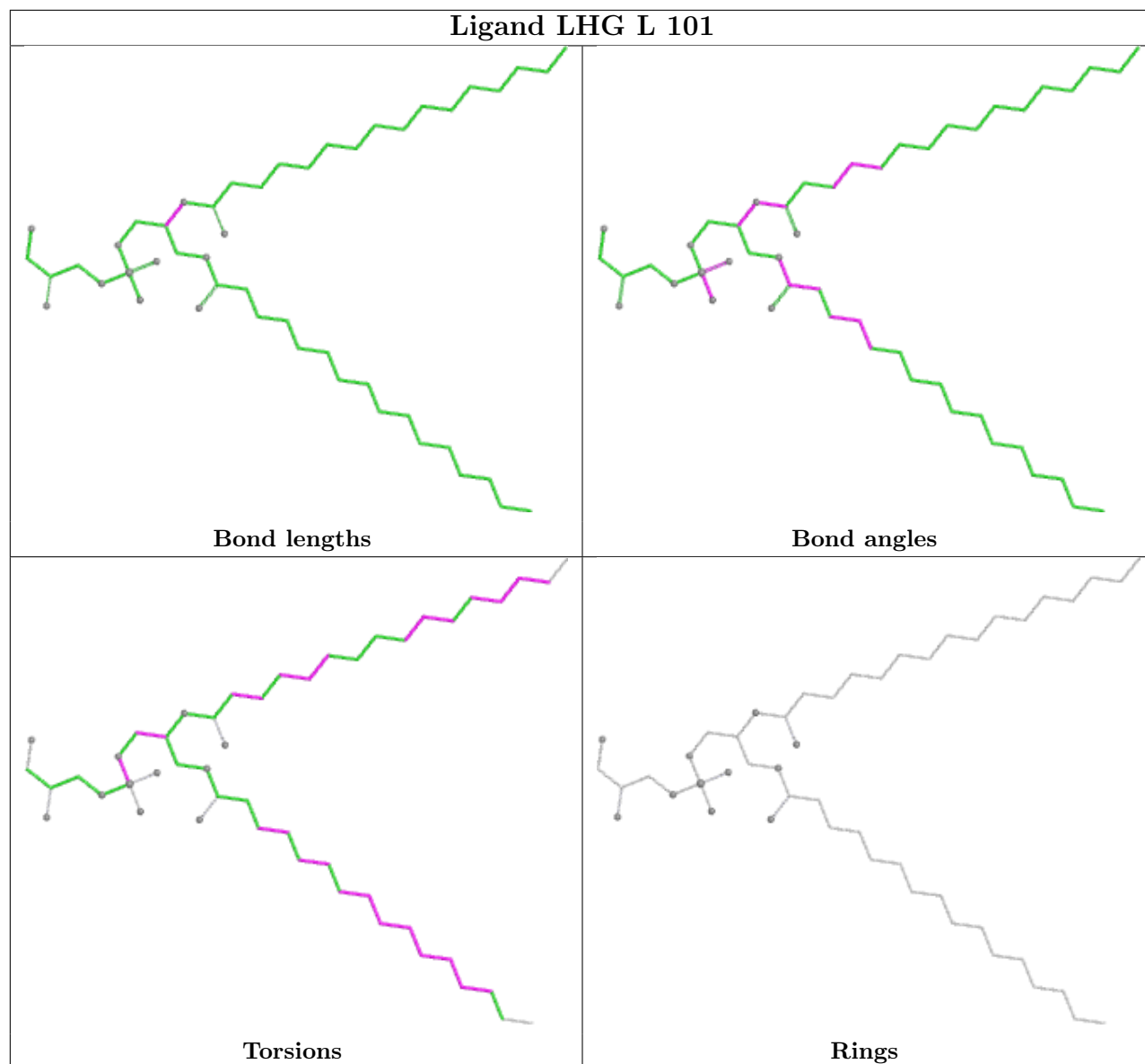


Ligand DGD H 101

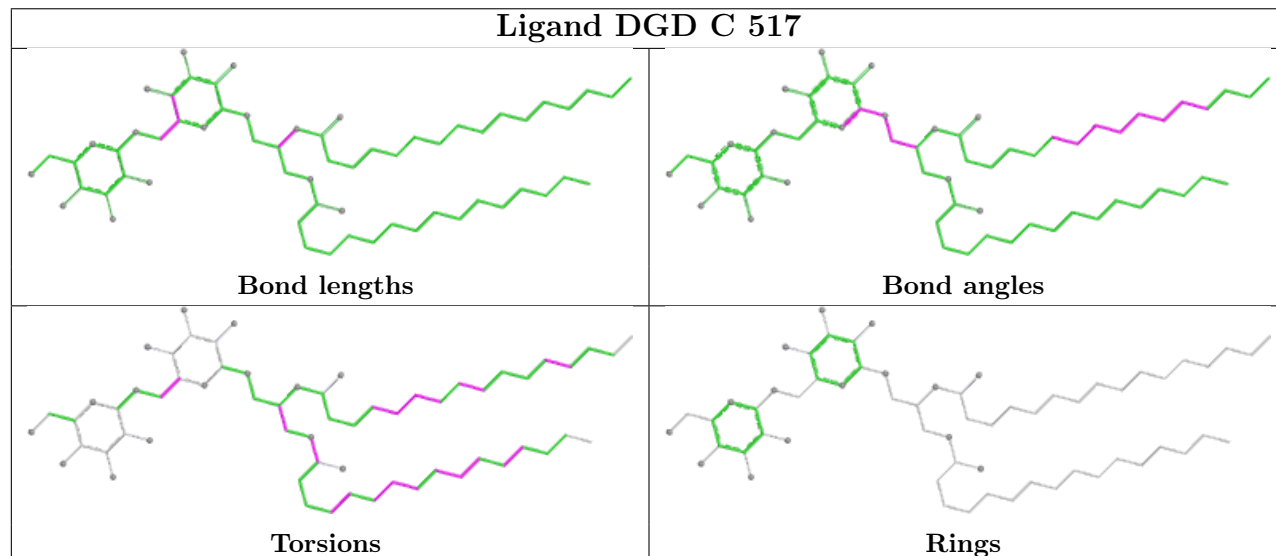


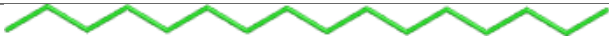
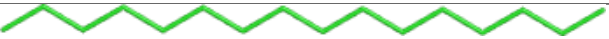
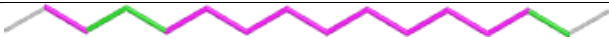


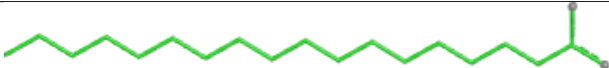
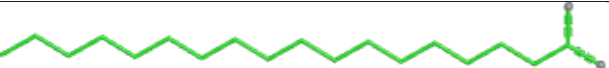
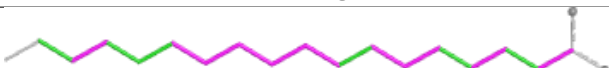
Ligand LHG L 101

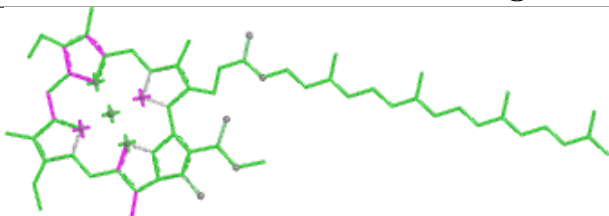
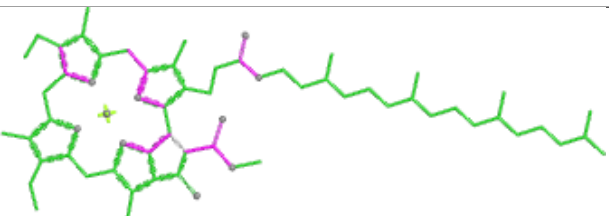
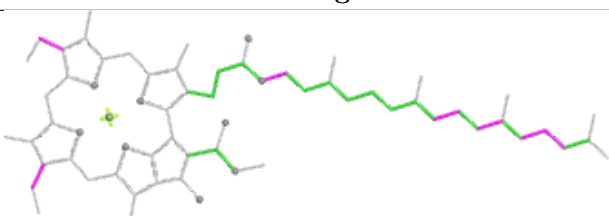
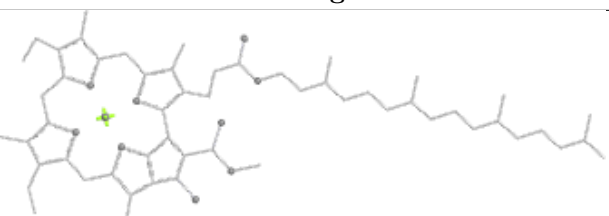


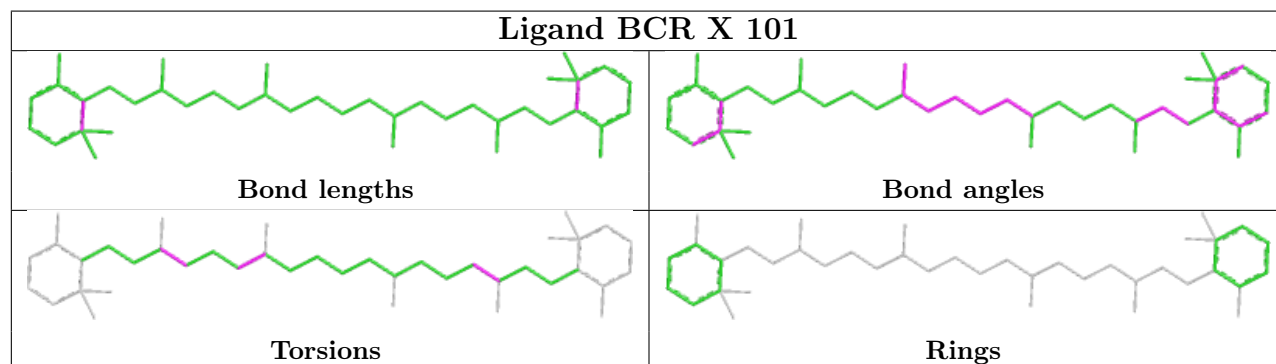
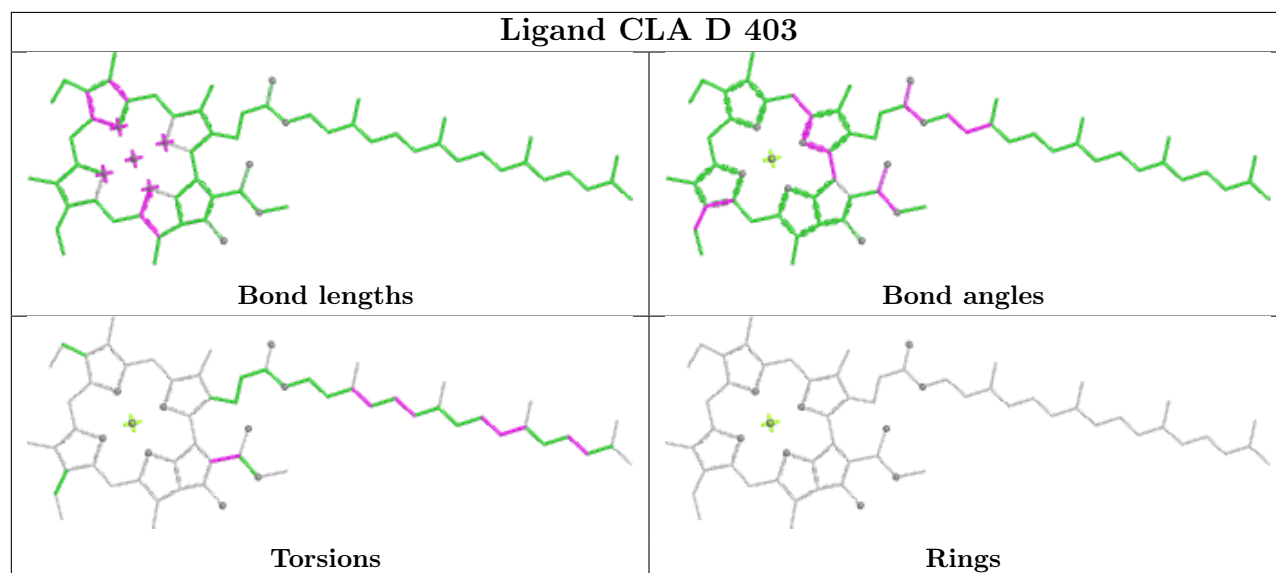
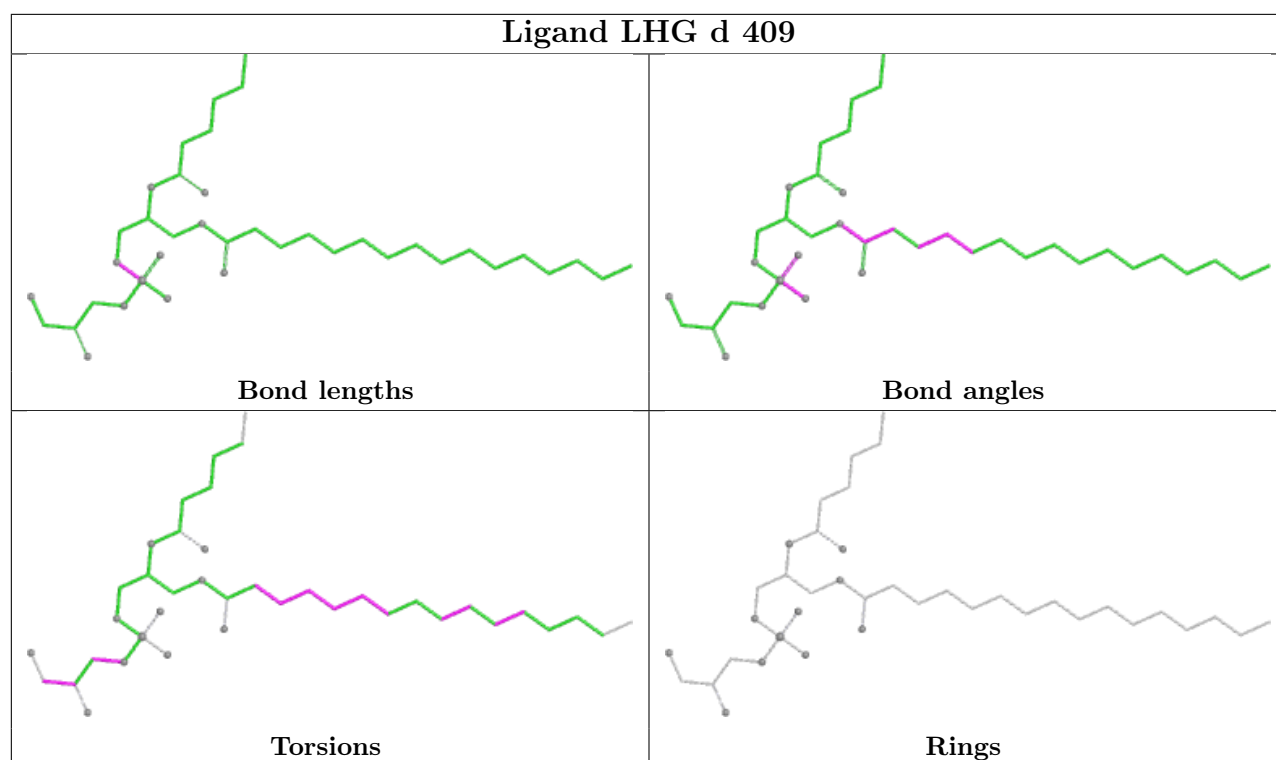
Ligand DGD C 517



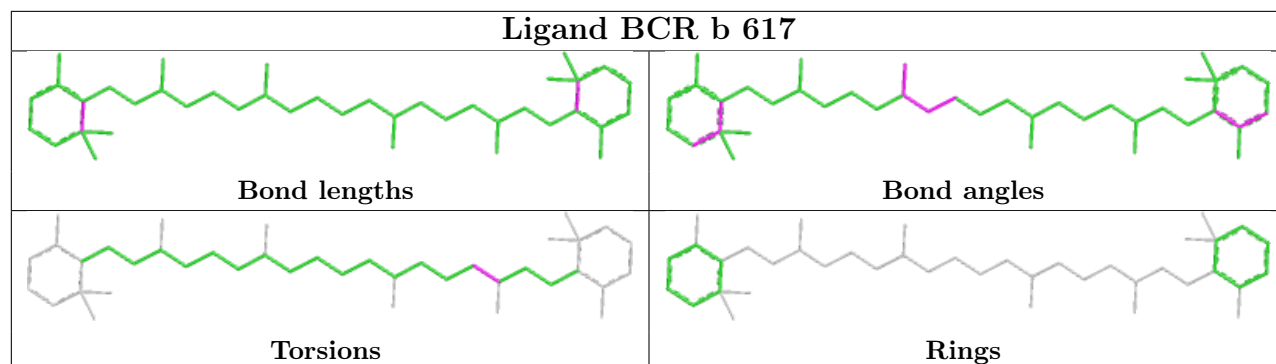
Ligand STE C 521	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE X 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

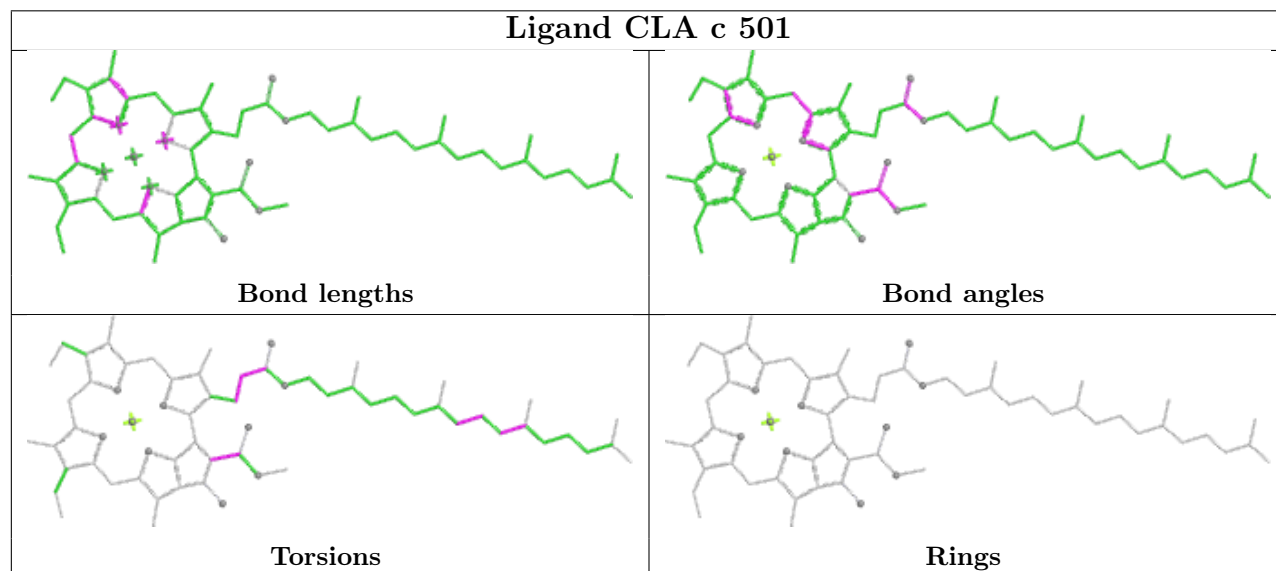
Ligand CLA D 402	
 Bond lengths	 Bond angles
 Torsions	 Rings



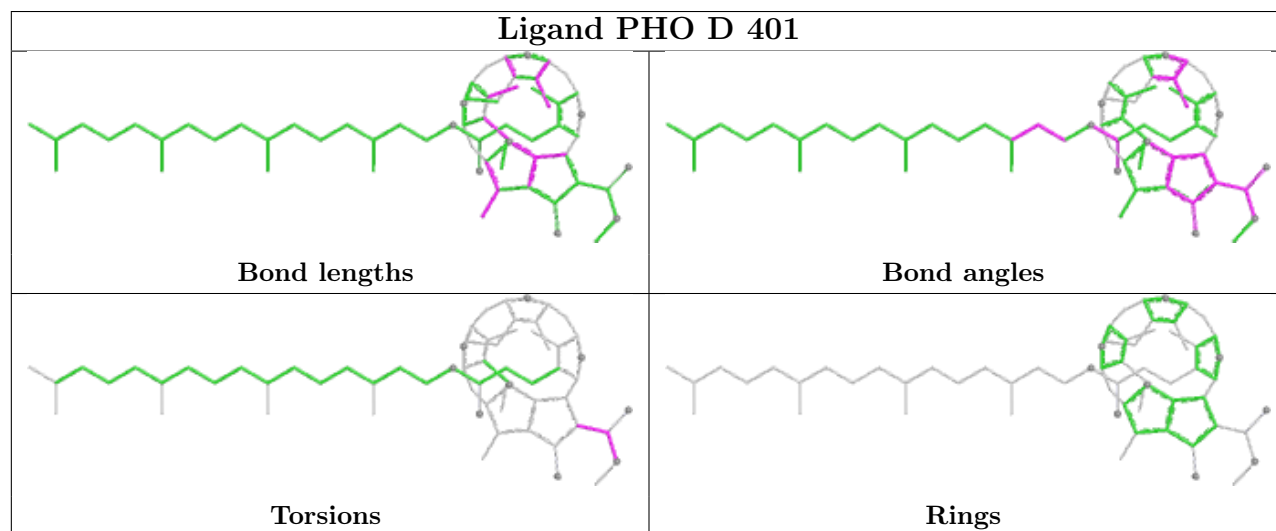
Ligand BCR b 617

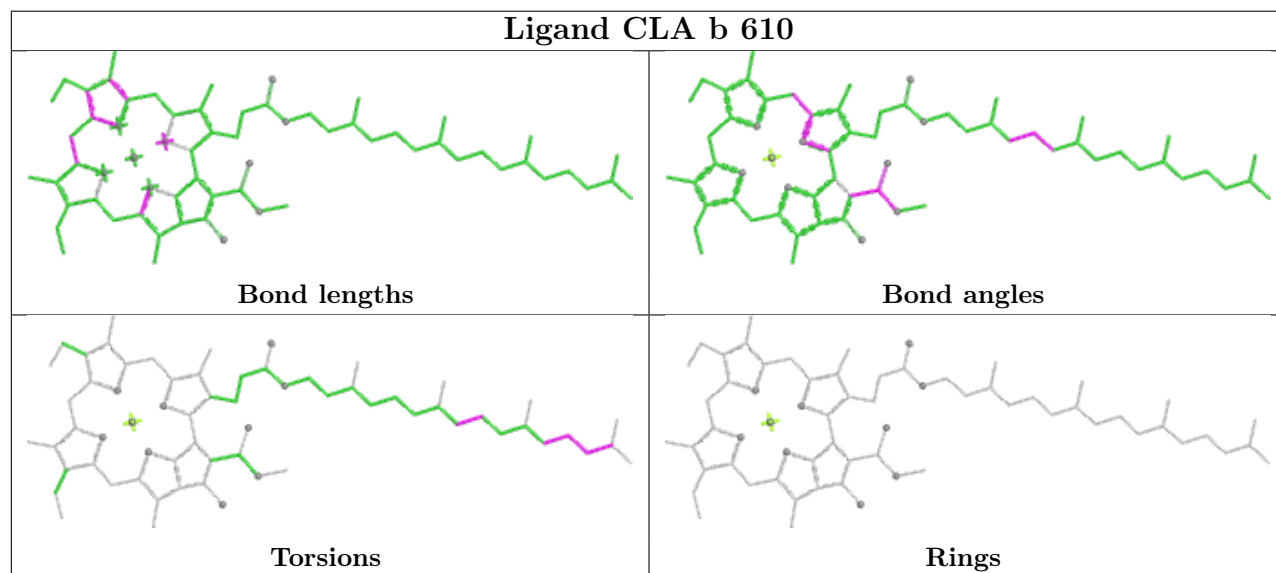
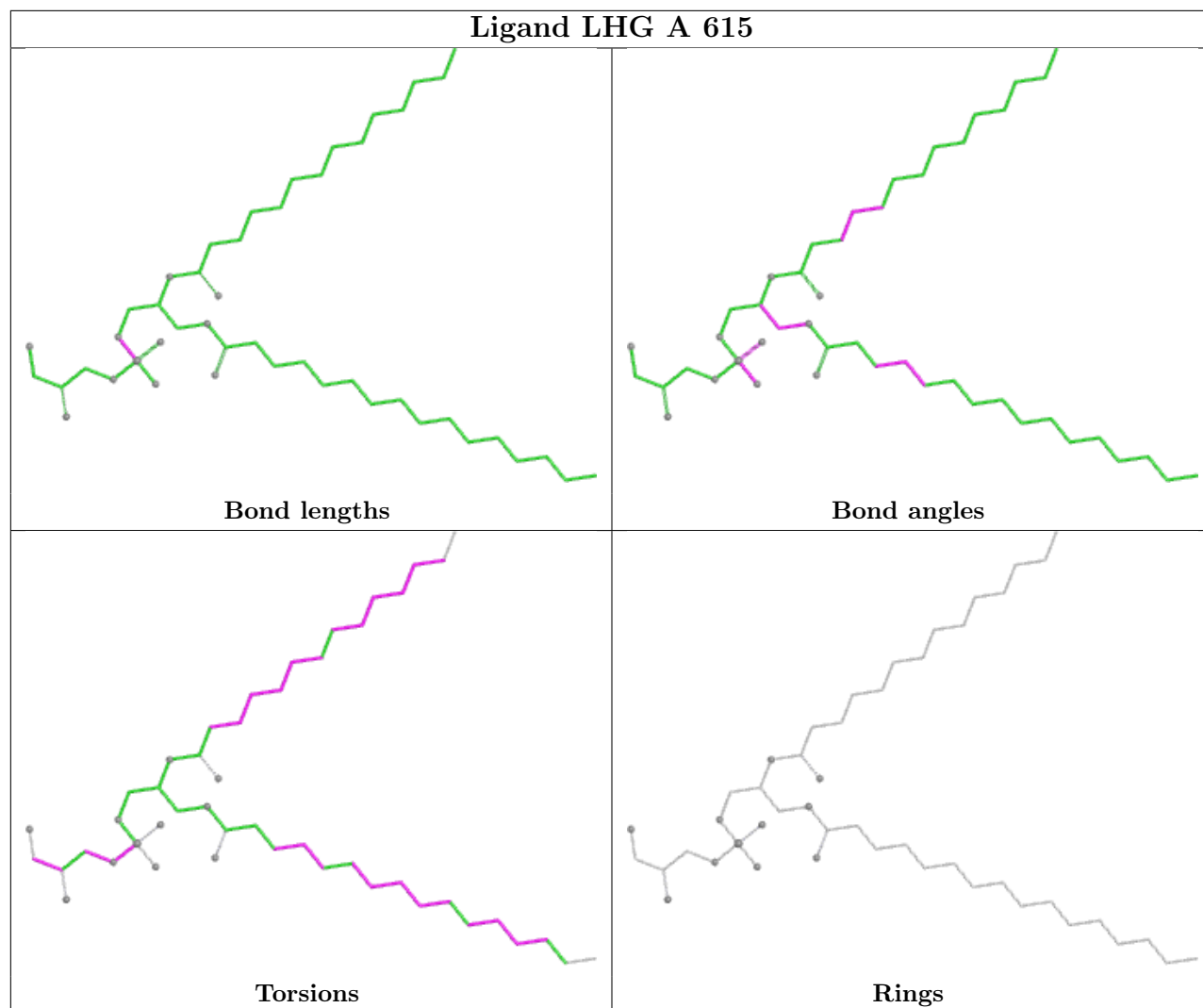


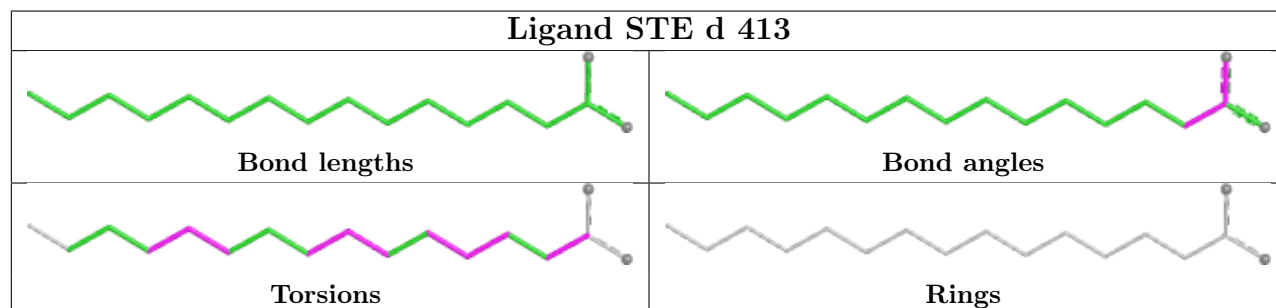
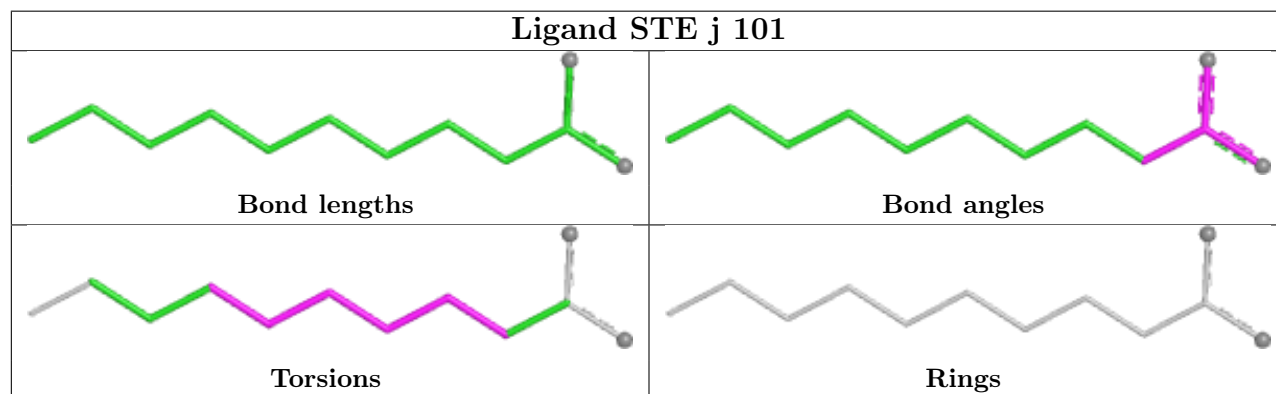
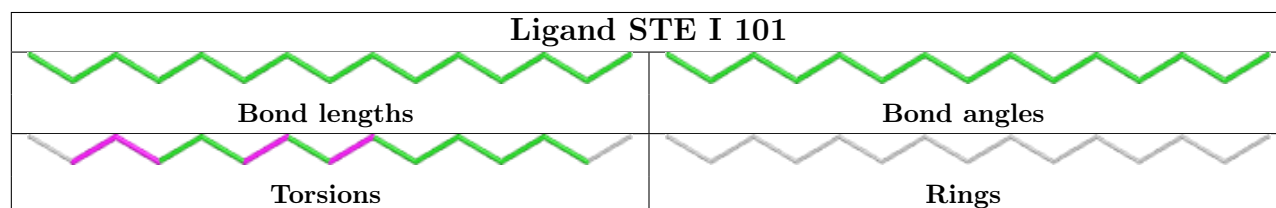
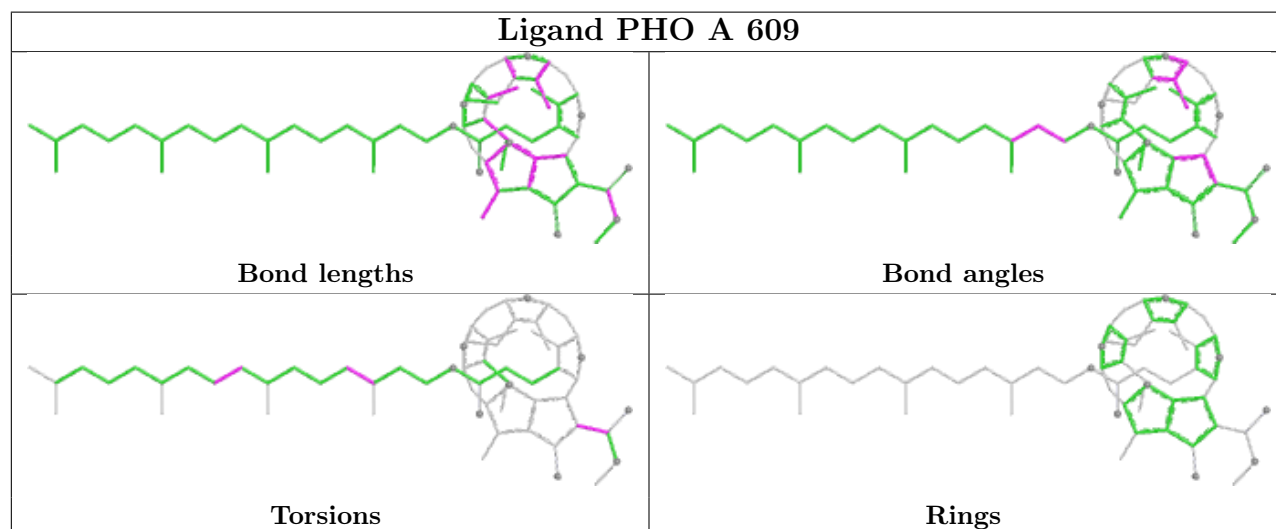
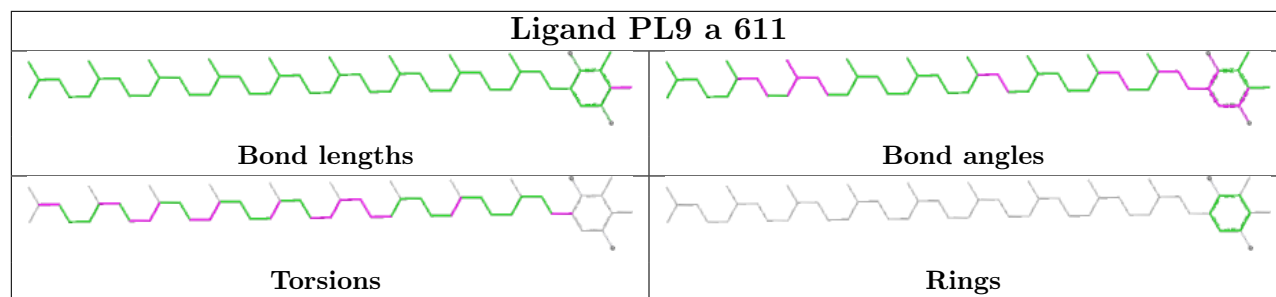
Ligand CLA c 501

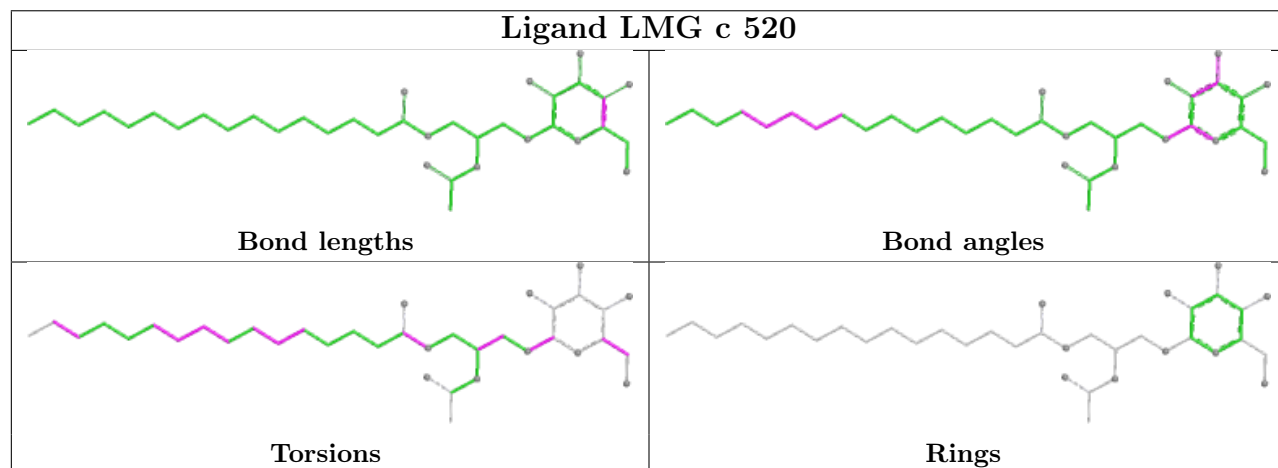
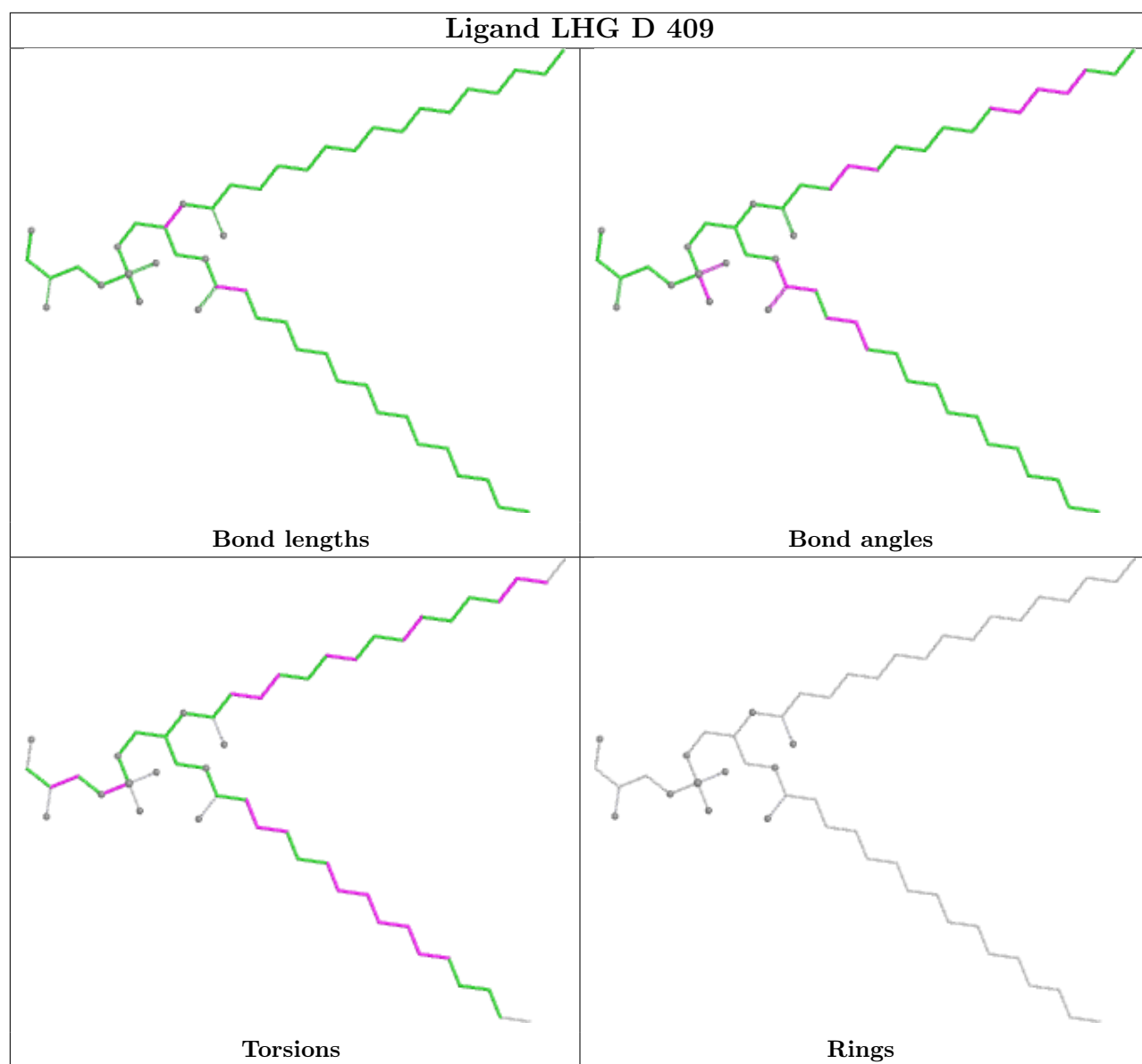


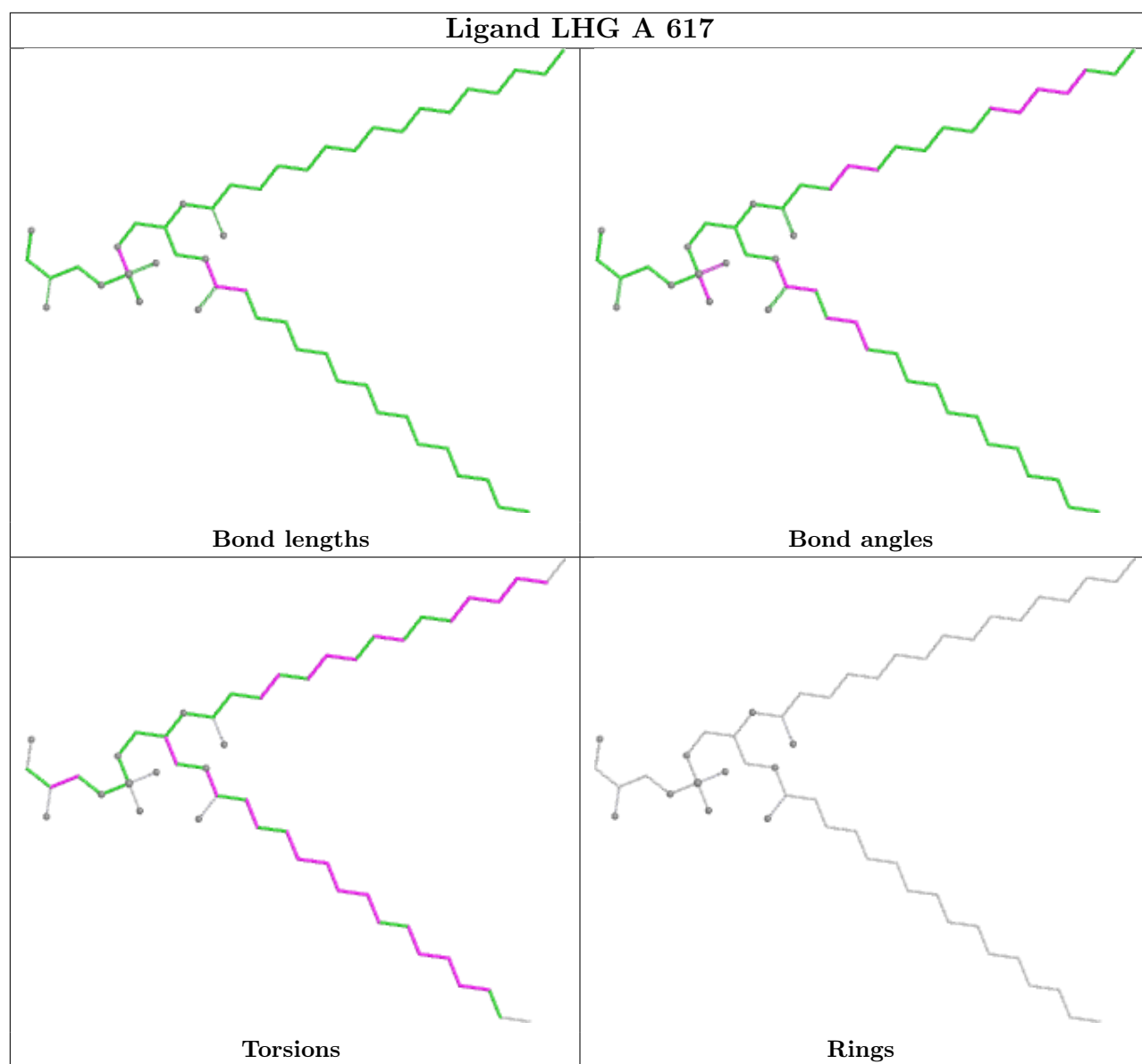
Ligand PHO D 401

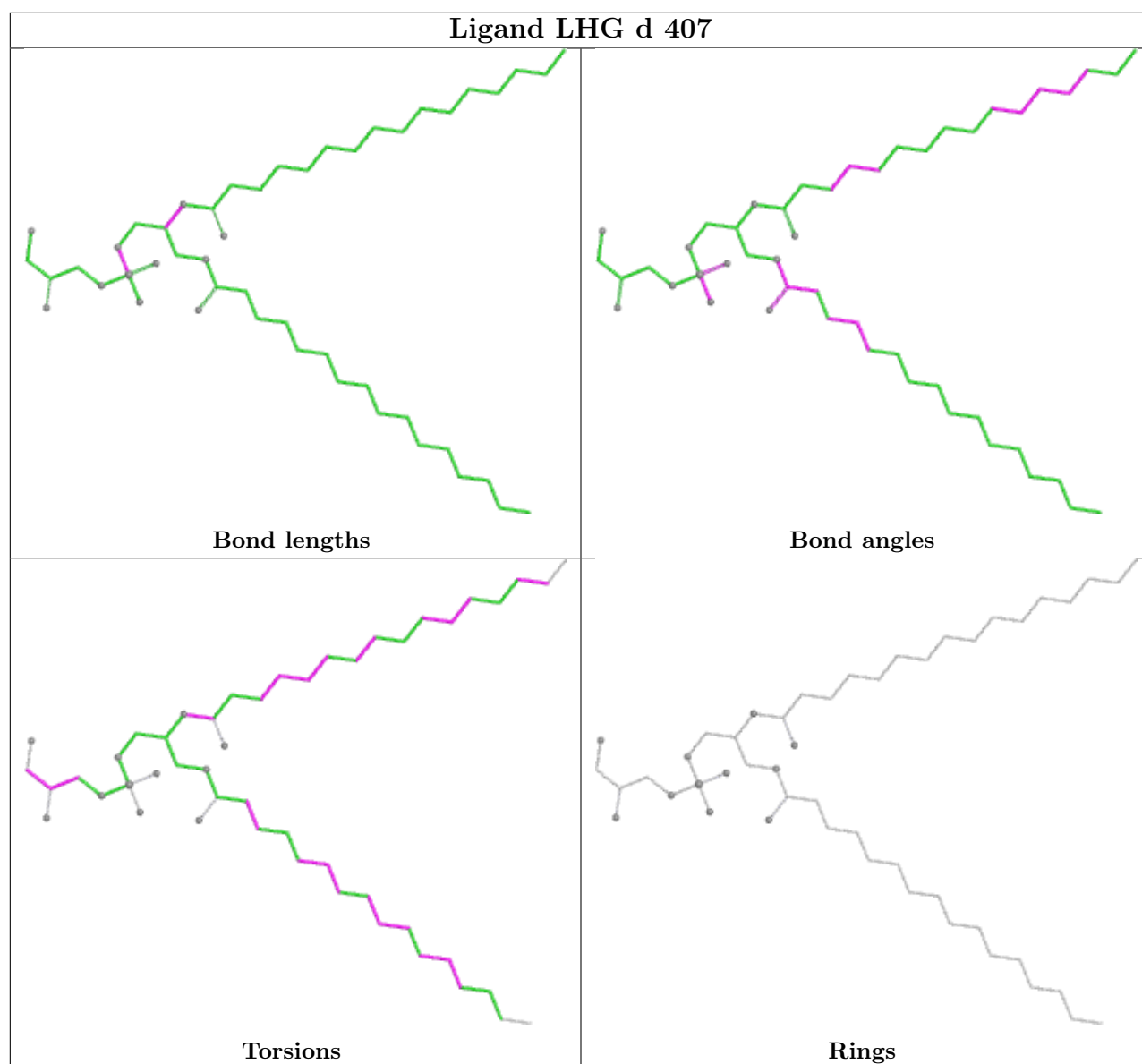












5.7 Other polymers [i](#)

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%)	-0.40	0 100 100	9, 31, 53, 81	64 (19%)
1	a	334/344 (97%)	-0.32	4 (1%) 76 78	9, 33, 64, 83	64 (19%)
2	B	505/510 (99%)	-0.33	2 (0%) 88 90	20, 35, 65, 96	4 (0%)
2	b	505/510 (99%)	-0.21	1 (0%) 91 92	27, 38, 78, 109	0
3	C	442/461 (95%)	-0.28	0 100 100	10, 39, 55, 78	11 (2%)
3	c	451/461 (97%)	-0.15	2 (0%) 88 90	10, 43, 63, 98	12 (2%)
4	D	341/352 (96%)	-0.45	0 100 100	11, 33, 52, 76	2 (0%)
4	d	341/352 (96%)	-0.33	1 (0%) 90 91	11, 37, 63, 86	3 (0%)
5	E	82/84 (97%)	0.35	1 (1%) 76 78	38, 57, 76, 87	1 (1%)
5	e	82/84 (97%)	0.58	3 (3%) 45 47	41, 65, 86, 97	0
6	F	34/45 (75%)	0.14	0 100 100	41, 49, 67, 88	0
6	f	34/45 (75%)	0.28	0 100 100	46, 55, 89, 108	0
7	H	65/66 (98%)	0.08	2 (3%) 51 54	37, 45, 62, 78	0
7	h	63/66 (95%)	0.38	2 (3%) 50 53	48, 56, 66, 72	0
8	I	35/38 (92%)	-0.16	0 100 100	32, 41, 65, 81	0
8	i	35/38 (92%)	-0.07	0 100 100	34, 43, 70, 86	0
9	J	36/40 (90%)	0.32	1 (2%) 55 57	40, 54, 84, 95	0
9	j	36/40 (90%)	0.43	0 100 100	41, 61, 97, 109	0
10	K	37/46 (80%)	0.16	0 100 100	48, 56, 70, 81	0
10	k	37/46 (80%)	0.33	0 100 100	53, 60, 77, 83	0
11	L	37/37 (100%)	-0.45	1 (2%) 56 59	27, 32, 63, 71	0
11	l	36/37 (97%)	-0.47	0 100 100	27, 33, 64, 79	0
12	M	32/36 (88%)	-0.36	0 100 100	29, 35, 61, 76	0
12	m	31/36 (86%)	-0.31	0 100 100	31, 36, 55, 66	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.06	4 (1%) 70 73	28, 44, 79, 137	1 (0%)
13	o	244/272 (89%)	-0.09	2 (0%) 82 84	28, 42, 78, 122	0
14	T	29/32 (90%)	-0.48	0 100 100	28, 33, 58, 77	0
14	t	29/32 (90%)	-0.26	2 (6%) 23 24	29, 35, 75, 90	0
15	U	97/134 (72%)	-0.12	0 100 100	35, 45, 68, 90	0
15	u	97/134 (72%)	-0.16	0 100 100	33, 43, 59, 85	0
16	V	137/163 (84%)	-0.22	0 100 100	33, 42, 58, 70	0
16	v	137/163 (84%)	0.00	0 100 100	38, 50, 69, 86	0
17	Y	27/46 (58%)	1.07	5 (18%) 3 3	58, 76, 110, 114	0
17	y	30/46 (65%)	0.94	0 100 100	68, 80, 98, 101	0
18	X	38/41 (92%)	0.23	1 (2%) 57 60	47, 59, 77, 83	0
18	x	39/41 (95%)	0.61	2 (5%) 33 35	59, 69, 92, 104	0
19	Z	62/62 (100%)	0.96	5 (8%) 18 19	59, 75, 112, 129	0
19	z	62/62 (100%)	0.90	4 (6%) 25 26	65, 76, 116, 122	0
20	R	34/41 (82%)	1.07	4 (11%) 9 9	68, 74, 87, 93	0
20	r	31/41 (75%)	1.29	3 (9%) 13 14	77, 89, 107, 110	0
All	All	5302/5700 (93%)	-0.13	52 (0%) 79 81	9, 41, 77, 137	162 (3%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Z	62	VAL	5.3
7	h	64	ALA	3.6
18	x	37	VAL	3.4
20	R	35	LEU	3.4
3	c	23	ALA	3.1
19	z	33	TRP	3.1
17	Y	25	ILE	3.0
19	z	29	SER	3.0
9	J	5	GLY	3.0
17	Y	20	ALA	2.9
13	O	60	ARG	2.9
14	t	30	THR	2.7
13	O	56	PRO	2.6
1	a	11	ALA	2.6
20	R	28	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
11	L	2	GLU	2.5
2	b	486	LEU	2.5
20	R	7	VAL	2.5
7	H	65	LEU	2.5
13	o	58	ASN	2.5
19	Z	40	ILE	2.5
19	z	26	ALA	2.4
20	r	14	LEU	2.4
13	o	246	ALA	2.4
17	Y	23	THR	2.4
20	r	23	ILE	2.4
14	t	29	ILE	2.3
13	O	59	LYS	2.3
17	Y	24	MET	2.3
1	a	237	TYR	2.3
4	d	27	PHE	2.2
7	h	41	PHE	2.2
2	B	500	GLY	2.2
19	Z	7	LEU	2.2
2	B	479[A]	PHE	2.2
5	E	79	PHE	2.2
5	e	14	ILE	2.2
18	X	2	THR	2.2
19	Z	30	PRO	2.2
20	r	20	VAL	2.2
17	Y	22	LEU	2.2
19	z	28	ALA	2.2
5	e	83	LEU	2.2
20	R	3	TRP	2.2
1	a	248	ILE	2.1
18	x	3	ILE	2.1
13	O	133	VAL	2.1
7	H	41	PHE	2.1
3	c	24	THR	2.1
5	e	4	THR	2.1
1	a	240	GLY	2.0
19	Z	33	TRP	2.0

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

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	0.91	0.10	33,37,56,68	0
12	FME	M	1	10/11	0.93	0.10	37,53,63,64	0
12	FME	m	1	10/11	0.95	0.09	30,49,65,66	0
14	FME	T	1	10/11	0.95	0.11	33,37,51,70	0
8	FME	I	1	10/11	0.97	0.07	37,48,53,55	0
8	FME	i	1	10/11	0.97	0.07	41,49,53,55	0

6.3 Carbohydrates

There are no oligosaccharides 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
34	STE	H	102	18/20	0.71	0.18	58,70,75,81	0
31	LHG	A	617	49/49	0.73	0.17	55,79,98,109	0
34	STE	a	615	12/20	0.73	0.14	54,63,79,81	0
30	LMG	b	621	55/55	0.74	0.19	57,69,86,89	0
30	LMG	c	522	48/55	0.76	0.15	60,73,85,89	0
33	DGD	a	614	44/66	0.78	0.15	38,54,67,71	0
30	LMG	d	410	23/55	0.78	0.19	52,65,73,74	0
26	CLA	h	101	65/65	0.78	0.14	55,72,92,97	0
31	LHG	e	102	42/49	0.79	0.14	60,86,104,113	0
29	PL9	A	612	55/55	0.79	0.16	44,63,82,88	0
34	STE	b	622	20/20	0.79	0.14	51,60,67,70	0
34	STE	d	414	20/20	0.79	0.16	46,52,62,65	0
34	STE	L	102	12/20	0.80	0.19	48,60,76,76	0
34	STE	k	102	12/20	0.80	0.12	60,70,74,75	0
29	PL9	a	611	55/55	0.82	0.15	50,66,78,86	0
32	SQD	t	102	36/54	0.82	0.14	40,59,75,76	0
30	LMG	D	408	33/55	0.82	0.14	44,59,81,83	0
34	STE	d	412	16/20	0.83	0.16	54,63,78,81	0
34	STE	J	101	12/20	0.83	0.15	57,62,72,72	0
33	DGD	A	619	66/66	0.83	0.12	47,59,67,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	STE	B	625	16/20	0.84	0.14	51,55,66,69	0
30	LMG	A	614	48/55	0.84	0.11	37,58,68,72	0
34	STE	b	623	10/20	0.84	0.15	46,56,62,65	0
30	LMG	c	520	37/55	0.84	0.12	52,68,80,83	0
26	CLA	B	601	65/65	0.84	0.12	41,63,87,94	0
34	STE	T	103	15/20	0.84	0.16	46,51,67,68	0
34	STE	F	103	12/20	0.85	0.13	58,75,86,89	0
34	STE	T	102	16/20	0.85	0.16	38,48,58,60	0
32	SQD	A	618	39/54	0.85	0.13	42,55,78,80	0
34	STE	C	520	12/20	0.85	0.13	48,55,59,63	0
34	STE	j	101	12/20	0.85	0.12	52,56,64,65	0
34	STE	b	620	20/20	0.85	0.13	42,56,76,78	0
34	STE	t	104	10/20	0.85	0.12	46,53,59,60	0
34	STE	B	624	12/20	0.86	0.12	50,52,71,73	0
32	SQD	f	101	41/54	0.86	0.14	62,81,91,95	0
30	LMG	C	518	48/55	0.86	0.13	48,68,82,86	0
30	LMG	c	523	49/55	0.86	0.10	41,56,78,83	0
30	LMG	B	621	28/55	0.86	0.13	40,50,64,67	0
34	STE	B	620	17/20	0.86	0.13	40,51,67,68	0
34	STE	C	519	12/20	0.87	0.14	39,47,51,53	0
34	STE	B	623	12/20	0.87	0.13	47,58,66,68	0
34	STE	C	521	16/20	0.87	0.11	39,49,64,64	0
34	STE	X	102	20/20	0.87	0.12	37,49,70,73	0
34	STE	c	521	20/20	0.87	0.13	50,56,82,82	0
34	STE	I	101	15/20	0.88	0.13	44,52,59,62	0
32	SQD	F	102	36/54	0.88	0.14	55,72,80,82	0
28	BCR	K	101	40/40	0.88	0.10	46,55,61,68	0
34	STE	t	103	14/20	0.88	0.11	38,49,60,60	0
34	STE	d	413	17/20	0.88	0.13	43,52,67,69	0
34	STE	t	105	18/20	0.88	0.12	44,57,86,87	0
28	BCR	d	405	40/40	0.89	0.10	42,50,79,84	0
28	BCR	h	102	40/40	0.89	0.11	42,58,68,68	0
33	DGD	C	516	62/66	0.89	0.11	36,49,88,96	0
32	SQD	B	622	54/54	0.89	0.11	39,60,80,86	0
30	LMG	m	101	51/55	0.89	0.10	33,48,64,66	0
32	SQD	a	613	54/54	0.89	0.11	45,60,75,81	0
32	SQD	b	619	49/54	0.89	0.10	37,56,72,77	0
30	LMG	M	101	51/55	0.89	0.10	31,48,67,68	0
33	DGD	H	101	62/66	0.90	0.10	38,47,56,61	0
26	CLA	C	513	65/65	0.90	0.10	50,57,77,85	0
33	DGD	h	103	62/66	0.90	0.10	38,50,59,62	0
34	STE	M	103	10/20	0.90	0.13	44,48,59,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	BCR	D	404	40/40	0.91	0.09	37,45,79,85	0
33	DGD	c	518	62/66	0.91	0.10	39,52,76,81	0
26	CLA	c	512	65/65	0.91	0.10	46,58,77,88	0
28	BCR	k	101	40/40	0.91	0.11	49,61,68,73	0
28	BCR	X	101	40/40	0.91	0.10	39,50,56,63	0
34	STE	l	102	18/20	0.91	0.12	36,41,68,73	0
28	BCR	Z	101	40/40	0.91	0.11	50,56,62,64	0
28	BCR	b	618	40/40	0.91	0.09	33,45,59,61	0
28	BCR	c	514	40/40	0.91	0.11	52,61,65,68	0
32	SQD	A	616	52/54	0.92	0.10	35,56,80,84	0
26	CLA	c	513	65/65	0.92	0.10	53,66,83,88	0
34	STE	M	102	15/20	0.92	0.10	37,44,53,64	0
26	CLA	C	503	65/65	0.92	0.09	36,42,49,54	0
28	BCR	B	618	40/40	0.92	0.07	26,37,46,48	0
28	BCR	c	516	40/40	0.92	0.12	52,59,63,68	0
30	LMG	D	406	51/55	0.92	0.09	36,52,71,74	0
28	BCR	t	101	40/40	0.93	0.07	29,38,48,51	0
28	BCR	b	616	40/40	0.93	0.08	30,40,48,48	0
28	BCR	b	617	40/40	0.93	0.07	27,36,46,47	0
26	CLA	C	512	65/65	0.93	0.10	40,51,75,81	0
26	CLA	c	508	64/65	0.93	0.09	36,43,81,96	0
28	BCR	K	102	40/40	0.93	0.10	38,51,62,64	0
31	LHG	A	615	47/49	0.93	0.11	30,45,70,80	0
28	BCR	T	101	40/40	0.93	0.07	33,39,47,52	0
31	LHG	d	409	39/49	0.93	0.09	37,43,51,54	0
28	BCR	B	619	40/40	0.93	0.08	33,41,54,60	0
28	BCR	C	514	40/40	0.93	0.09	31,41,51,54	0
26	CLA	c	511	65/65	0.94	0.10	44,56,70,72	0
31	LHG	D	409	49/49	0.94	0.09	29,40,53,59	0
31	LHG	d	407	49/49	0.94	0.09	32,45,61,66	0
25	BCT	d	401	4/4	0.94	0.08	32,36,43,48	0
26	CLA	C	506	65/65	0.94	0.09	32,42,74,77	0
26	CLA	C	508	65/65	0.94	0.09	34,41,87,91	0
28	BCR	A	611	40/40	0.94	0.07	25,33,38,41	0
28	BCR	B	617	40/40	0.94	0.08	30,38,48,53	0
26	CLA	C	510	65/65	0.94	0.08	30,43,57,73	0
26	CLA	C	511	65/65	0.94	0.10	33,48,60,63	0
26	CLA	B	606	65/65	0.94	0.08	27,35,61,69	0
26	CLA	B	616	60/65	0.94	0.08	26,36,76,89	0
26	CLA	a	607	65/65	0.94	0.09	29,37,86,95	0
26	CLA	b	605	65/65	0.94	0.08	31,39,60,71	0
33	DGD	C	515	62/66	0.94	0.09	25,36,63,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	CLA	b	613	65/65	0.94	0.09	28,37,66,71	0
33	DGD	C	517	62/66	0.94	0.08	30,44,69,75	0
26	CLA	c	503	65/65	0.94	0.08	37,45,51,53	0
26	CLA	c	504	60/65	0.94	0.08	31,45,69,74	0
33	DGD	c	517	62/66	0.94	0.08	30,38,60,67	0
26	CLA	c	506	65/65	0.94	0.09	39,46,72,76	0
33	DGD	c	519	62/66	0.94	0.09	33,48,71,80	0
26	CLA	c	507	65/65	0.94	0.08	33,41,50,53	0
26	CLA	C	502	65/65	0.94	0.08	30,39,51,56	0
30	LMG	d	411	44/55	0.94	0.09	41,52,72,76	0
26	CLA	c	510	65/65	0.94	0.08	34,44,56,63	0
28	BCR	c	515	40/40	0.94	0.09	33,47,53,56	0
26	CLA	c	502	65/65	0.95	0.07	34,41,53,58	0
26	CLA	C	501	65/65	0.95	0.07	25,35,49,53	0
25	BCT	A	606	4/4	0.95	0.09	35,35,39,40	0
26	CLA	c	505	65/65	0.95	0.07	33,41,56,64	0
26	CLA	a	606	65/65	0.95	0.07	23,31,37,47	0
29	PL9	D	405	55/55	0.95	0.07	24,31,38,39	0
26	CLA	C	509	65/65	0.95	0.09	34,42,57,59	0
29	PL9	d	406	55/55	0.95	0.07	25,33,38,41	0
26	CLA	a	609	65/65	0.95	0.09	24,30,68,76	0
26	CLA	c	509	65/65	0.95	0.09	38,45,57,61	0
26	CLA	b	601	65/65	0.95	0.08	34,42,54,60	0
26	CLA	B	602	65/65	0.95	0.07	28,37,55,57	0
28	BCR	a	610	40/40	0.95	0.06	20,34,43,45	0
26	CLA	b	607	65/65	0.95	0.07	33,41,59,66	0
26	CLA	C	504	59/65	0.95	0.08	35,43,75,82	0
26	CLA	d	404	65/65	0.95	0.08	34,43,83,86	0
26	CLA	b	614	65/65	0.95	0.07	31,40,53,58	0
27	PHO	d	402	64/64	0.95	0.06	30,39,45,49	0
26	CLA	b	615	60/65	0.95	0.08	31,41,84,91	0
26	CLA	b	611	65/65	0.96	0.07	26,32,40,42	0
26	CLA	b	612	65/65	0.96	0.07	25,32,62,72	0
26	CLA	C	507	65/65	0.96	0.07	31,38,51,52	0
26	CLA	B	610	65/65	0.96	0.07	24,31,40,42	0
26	CLA	B	611	65/65	0.96	0.06	20,30,38,46	0
26	CLA	c	501	65/65	0.96	0.07	28,38,47,53	0
26	CLA	B	612	65/65	0.96	0.06	22,28,35,42	0
26	CLA	B	614	65/65	0.96	0.08	23,35,64,75	0
26	CLA	B	615	65/65	0.96	0.07	25,37,51,61	0
31	LHG	L	101	49/49	0.96	0.07	31,38,51,54	0
26	CLA	A	613	65/65	0.96	0.06	24,29,38,46	0

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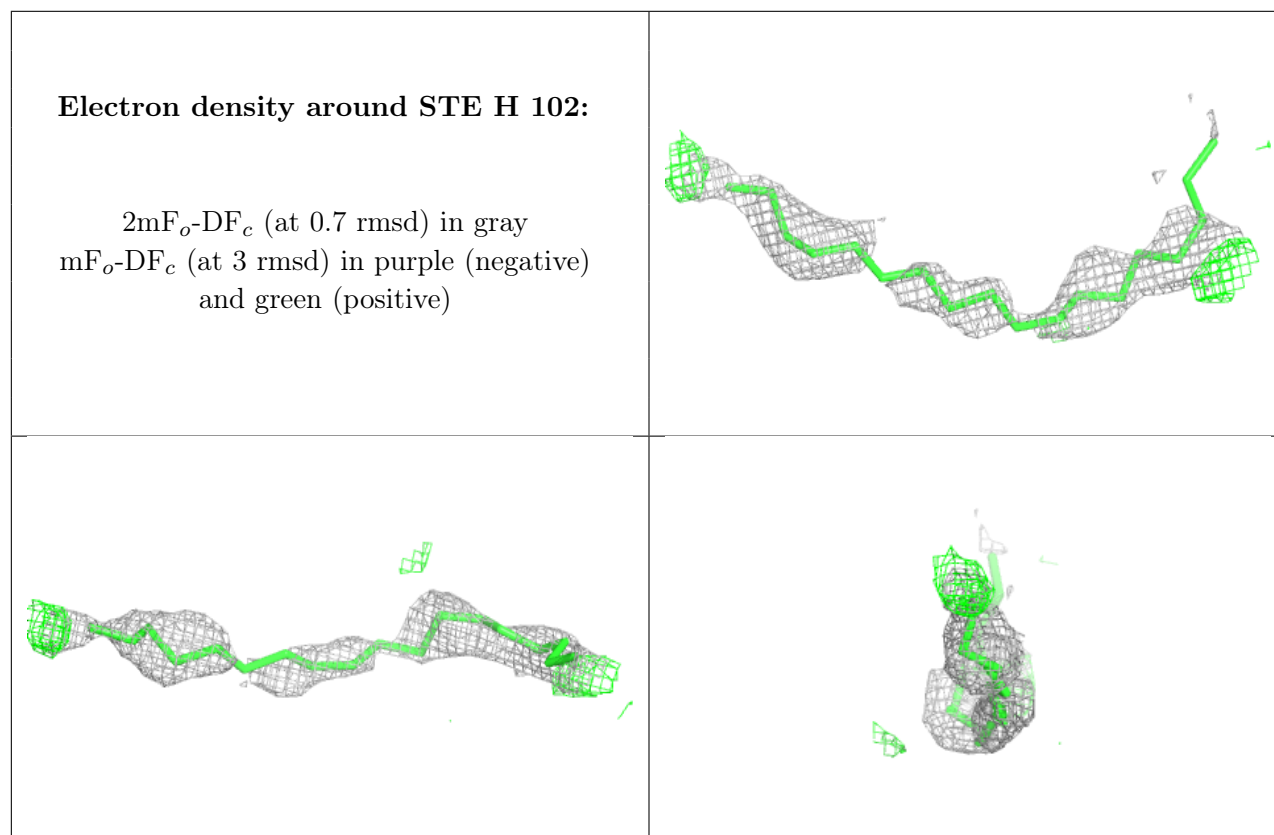
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	LHG	d	408	49/49	0.96	0.07	27,39,48,55	0
26	CLA	D	403	65/65	0.96	0.08	30,36,90,103	0
26	CLA	B	603	65/65	0.96	0.07	26,31,54,59	0
31	LHG	l	101	49/49	0.96	0.07	31,41,48,56	0
26	CLA	B	604	65/65	0.96	0.07	22,30,65,68	0
26	CLA	A	608	65/65	0.96	0.08	24,33,83,90	0
26	CLA	a	612	65/65	0.96	0.06	22,30,39,44	0
26	CLA	B	607	65/65	0.96	0.06	20,29,54,58	0
26	CLA	b	602	65/65	0.96	0.07	25,34,59,70	0
26	CLA	b	603	65/65	0.96	0.07	26,33,66,79	0
26	CLA	d	403	65/65	0.96	0.07	24,32,52,56	0
26	CLA	b	604	65/65	0.96	0.06	24,35,44,49	0
26	CLA	C	505	65/65	0.96	0.08	24,37,56,59	0
27	PHO	A	609	64/64	0.96	0.06	23,27,35,38	0
27	PHO	D	401	64/64	0.96	0.06	25,33,38,43	0
27	PHO	a	608	64/64	0.96	0.06	24,29,35,40	0
26	CLA	b	606	65/65	0.96	0.07	23,30,54,62	0
26	CLA	B	609	65/65	0.96	0.07	27,40,51,62	0
26	CLA	b	608	65/65	0.96	0.07	32,43,63,70	0
26	CLA	b	609	65/65	0.96	0.07	30,37,45,49	0
26	CLA	b	610	65/65	0.96	0.06	25,32,45,53	0
35	HEM	e	101	43/43	0.96	0.10	54,63,79,83	0
26	CLA	D	402	65/65	0.97	0.06	22,27,47,58	0
26	CLA	B	605	65/65	0.97	0.06	23,31,41,45	0
31	LHG	D	407	49/49	0.97	0.06	26,37,44,54	0
26	CLA	B	608	65/65	0.97	0.06	25,34,53,56	0
26	CLA	A	607	65/65	0.97	0.05	21,29,37,41	0
35	HEM	F	101	43/43	0.97	0.08	45,52,63,72	0
26	CLA	B	613	65/65	0.97	0.06	22,29,60,68	0
26	CLA	A	610	54/65	0.98	0.05	22,28,58,60	0
24	CL	A	604	1/1	0.98	0.04	34,34,34,34	0
36	HEC	V	201	43/43	0.98	0.05	26,33,40,47	0
36	HEC	v	201	43/43	0.98	0.07	32,38,46,50	0
24	CL	a	604	1/1	0.99	0.05	32,32,32,32	0
24	CL	a	605	1/1	0.99	0.12	30,30,30,30	0
21	OEY	A	601[C]	11/11	0.99	0.04	28,30,33,36	11
21	OEY	a	601[A]	11/11	0.99	0.03	31,35,39,39	11
21	OEY	a	601[C]	11/11	0.99	0.03	26,28,35,37	11
22	OEX	A	602[B]	10/10	0.99	0.03	27,31,34,34	10
22	OEX	a	602[B]	10/10	0.99	0.03	26,31,33,33	10
21	OEY	A	601[A]	11/11	0.99	0.04	31,34,38,38	11
24	CL	A	605	1/1	0.99	0.04	35,35,35,35	0

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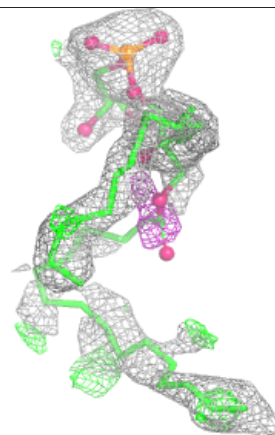
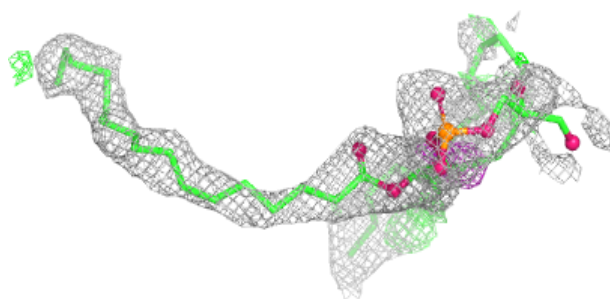
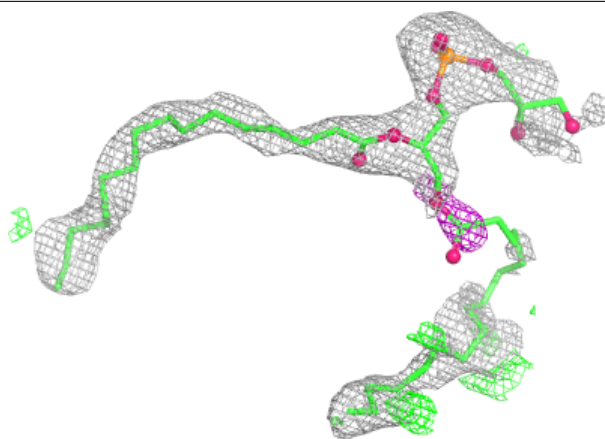
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	FE2	A	603	1/1	1.00	0.02	29,29,29,29	0
23	FE2	a	603	1/1	1.00	0.03	36,36,36,36	0

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.

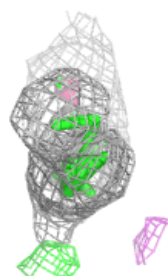
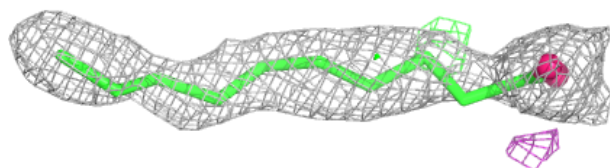
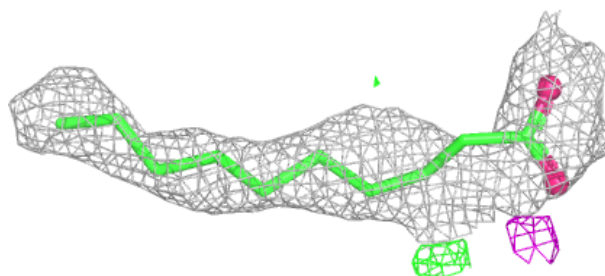


Electron density around LHG A 617:

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

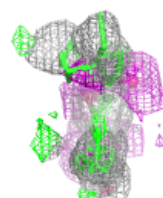
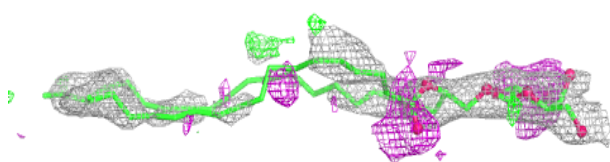
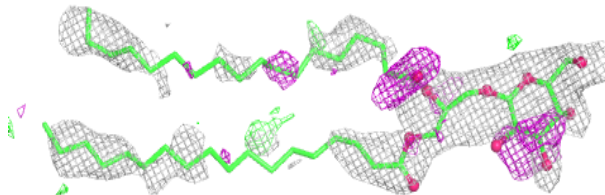
**Electron density around STE a 615:**

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

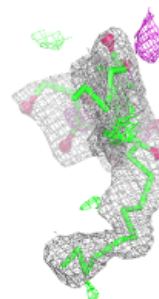
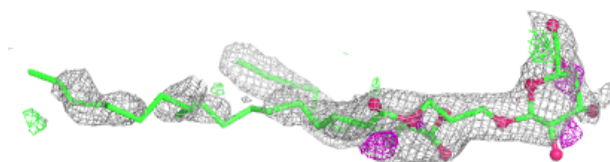
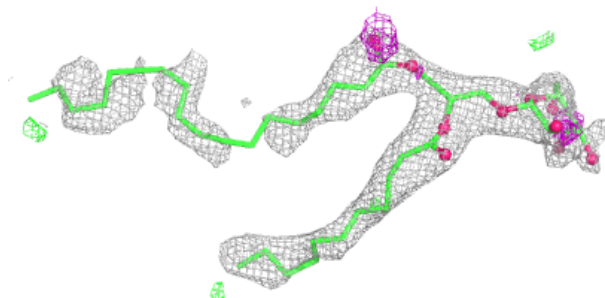


Electron density around LMG b 621:

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

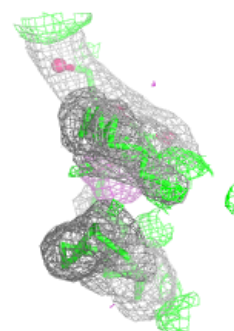
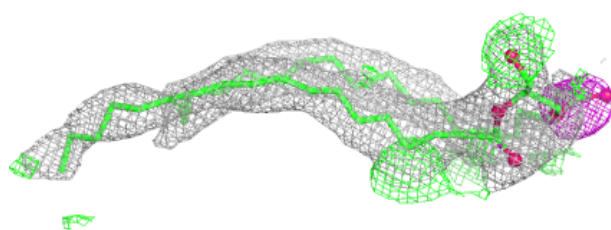
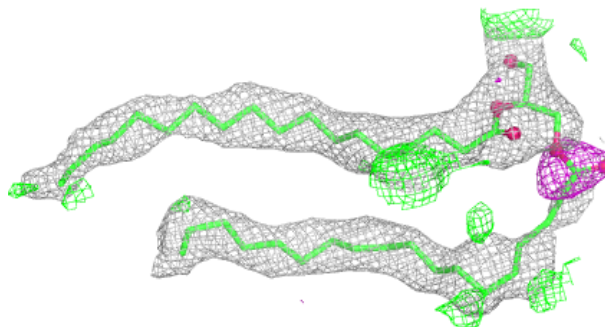
**Electron density around LMG c 522:**

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

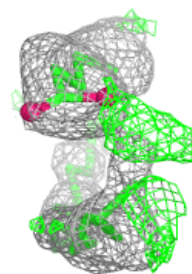
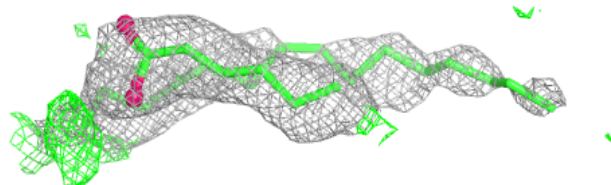
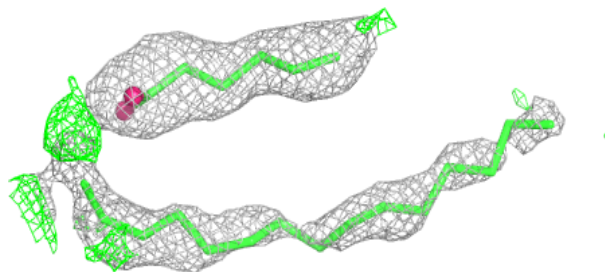


Electron density around DGD a 614:

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

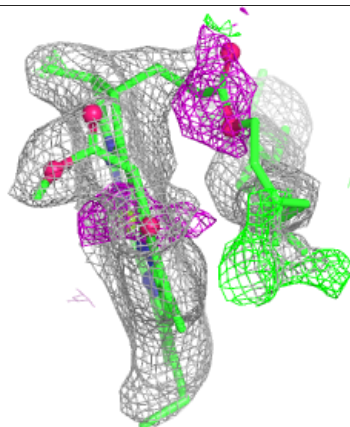
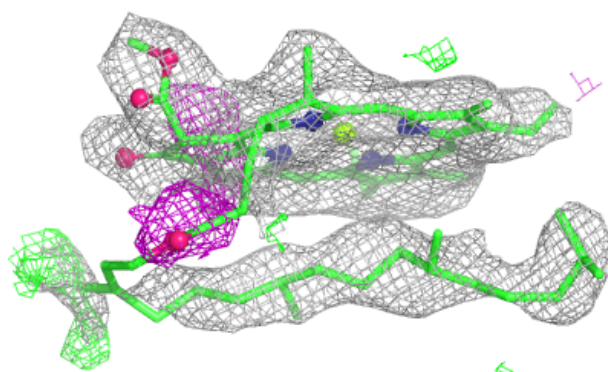
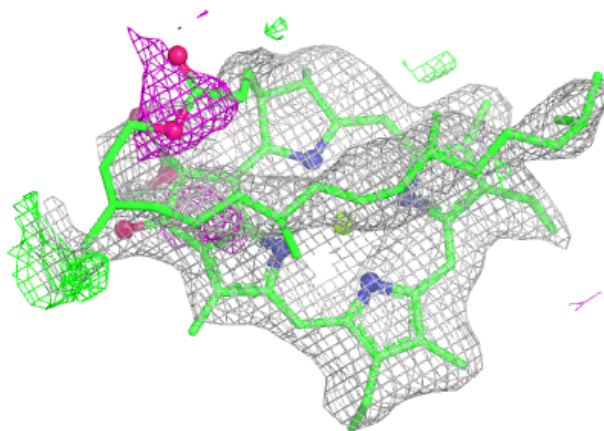
**Electron density around LMG d 410:**

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

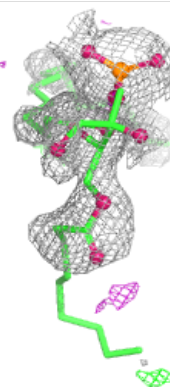
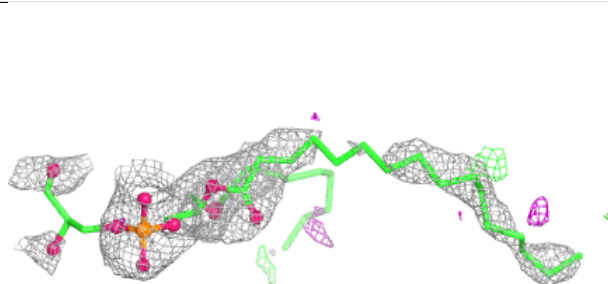
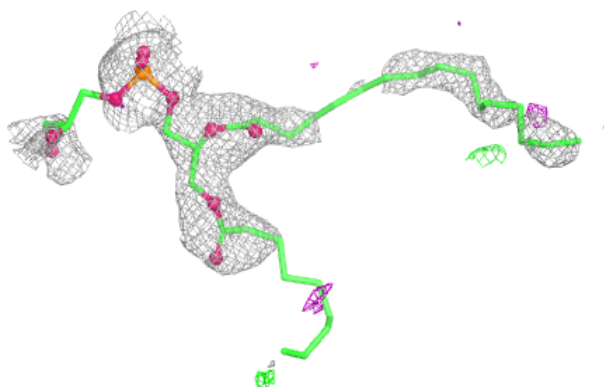


Electron density around CLA h 101:

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

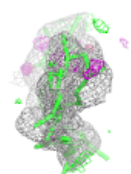
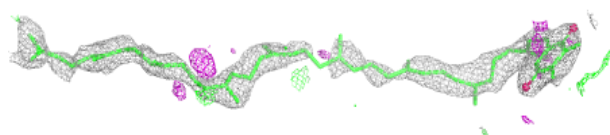
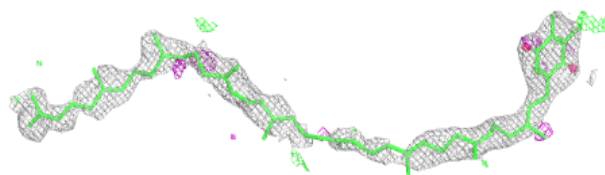
**Electron density around LHG e 102:**

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

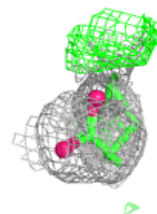
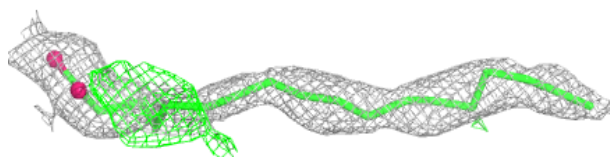
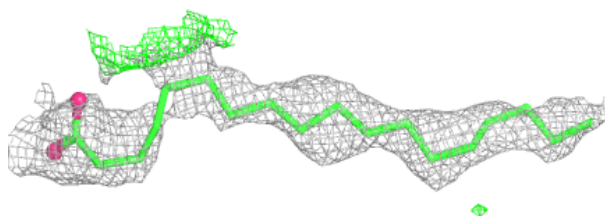


Electron density around PL9 A 612:

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

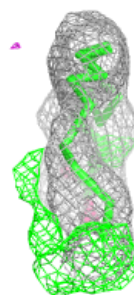
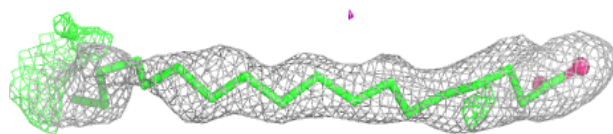
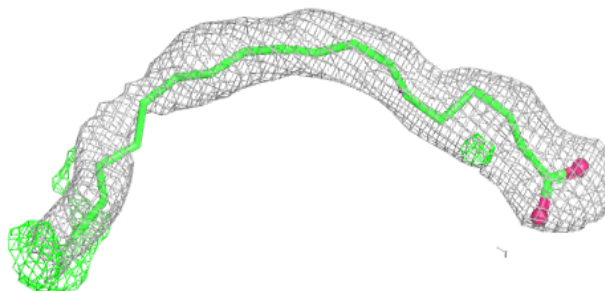
**Electron density around STE b 622:**

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

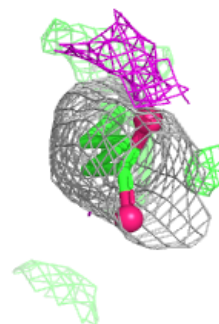
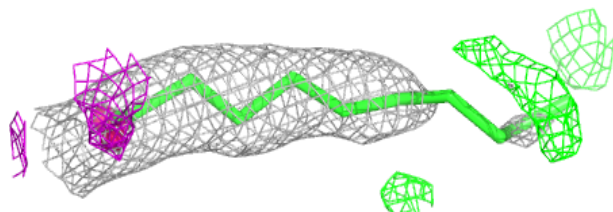
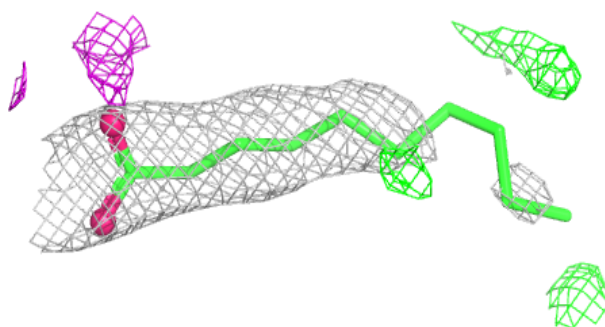


Electron density around STE d 414:

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

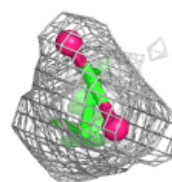
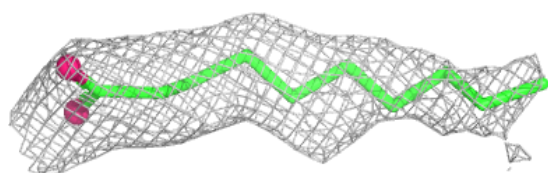
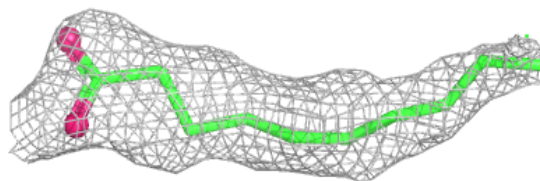
**Electron density around STE L 102:**

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

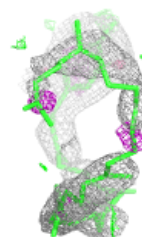
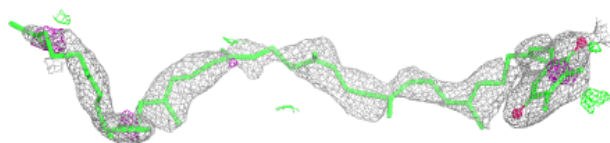
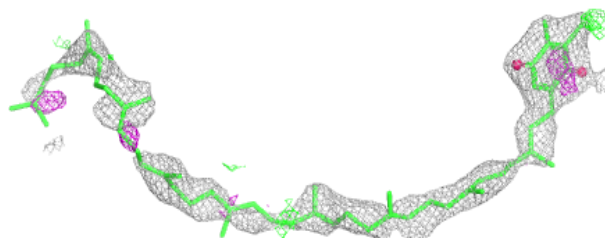


Electron density around STE k 102:

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

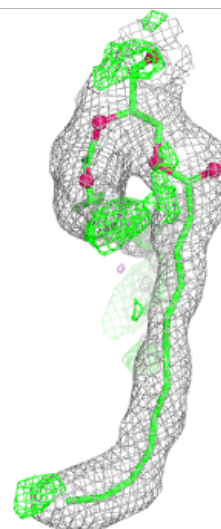
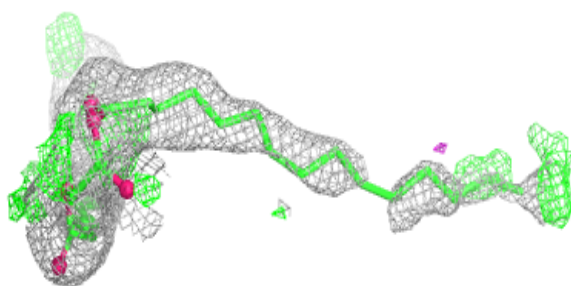
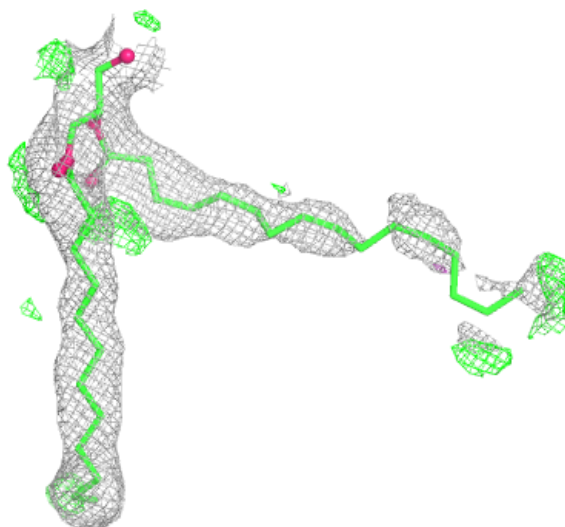
**Electron density around PL9 a 611:**

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



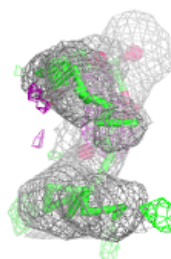
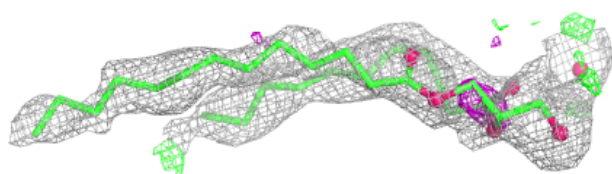
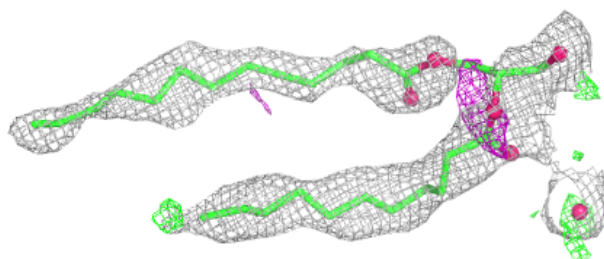
Electron density around SQD t 102:

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

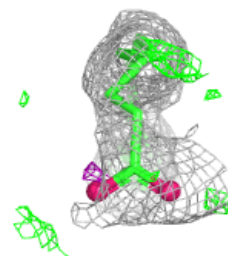
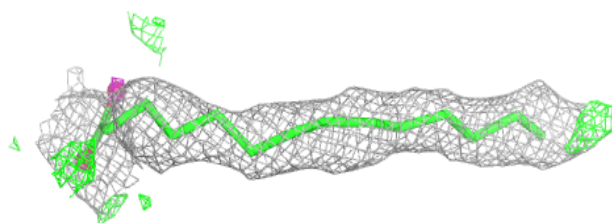
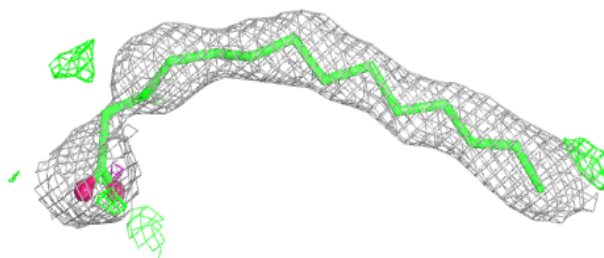


Electron density around LMG D 408:

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

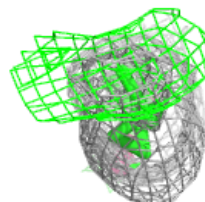
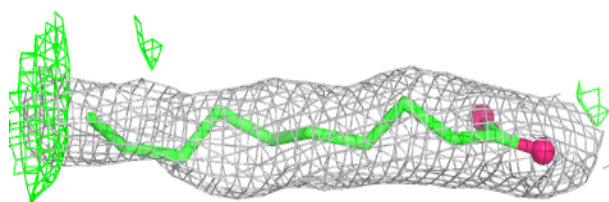
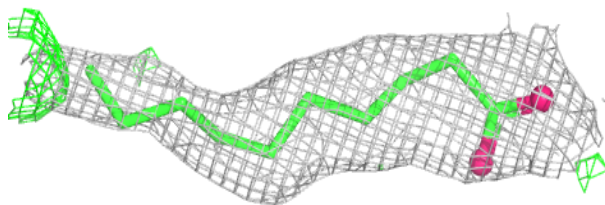
**Electron density around STE d 412:**

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and green (positive)

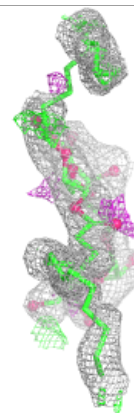
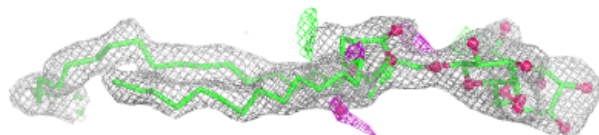
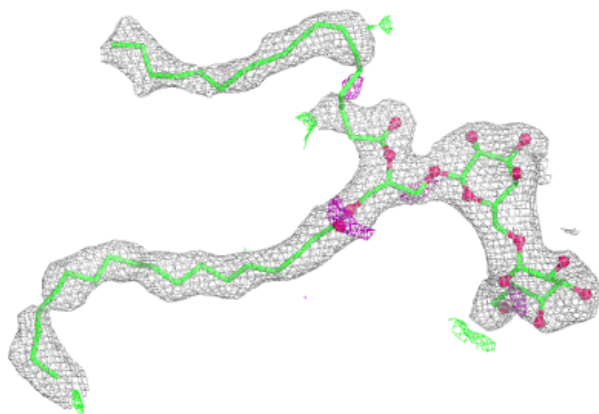


Electron density around STE J 101:

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

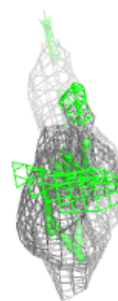
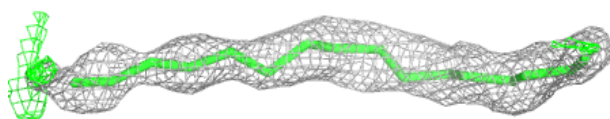
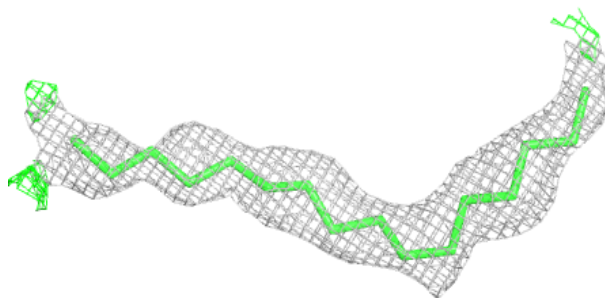
**Electron density around DGD A 619:**

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

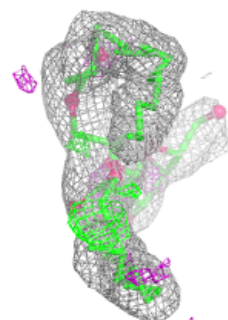
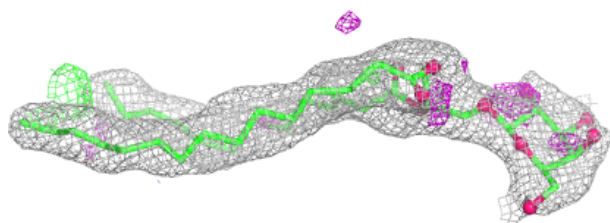
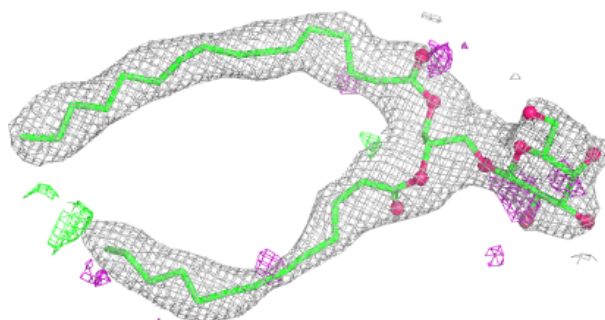


Electron density around STE B 625:

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

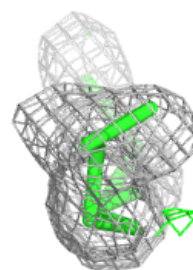
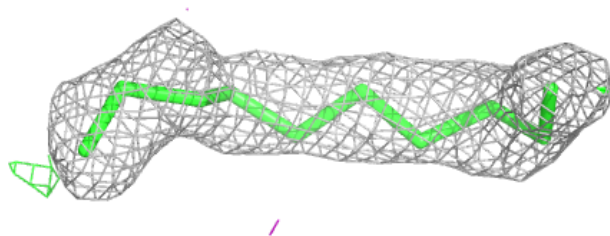
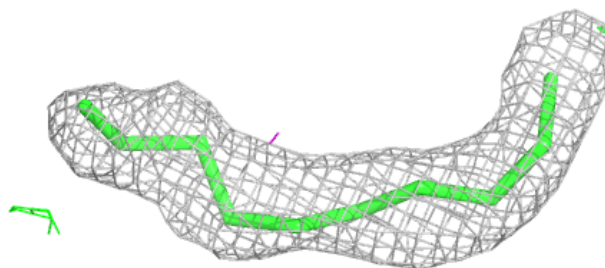
**Electron density around LMG A 614:**

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

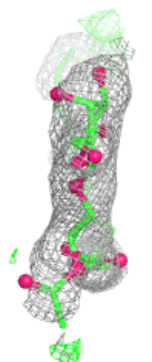
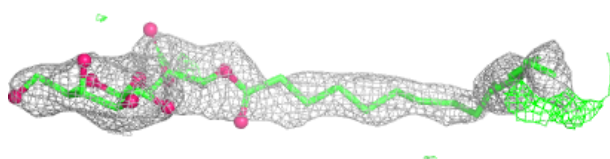
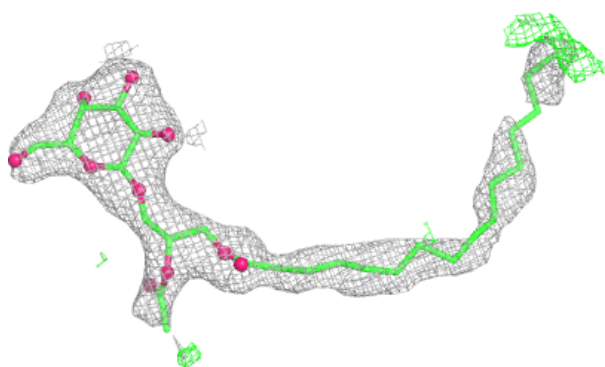


Electron density around STE b 623:

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

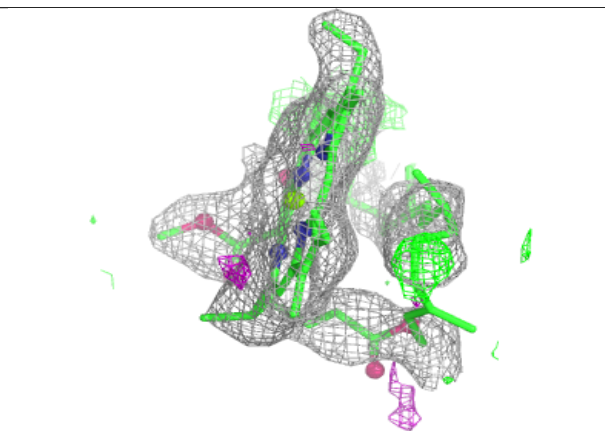
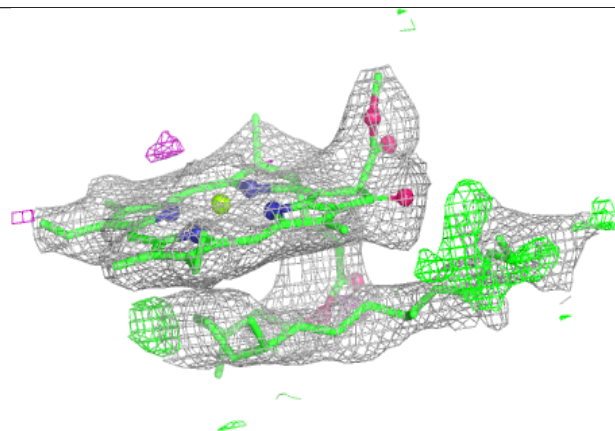
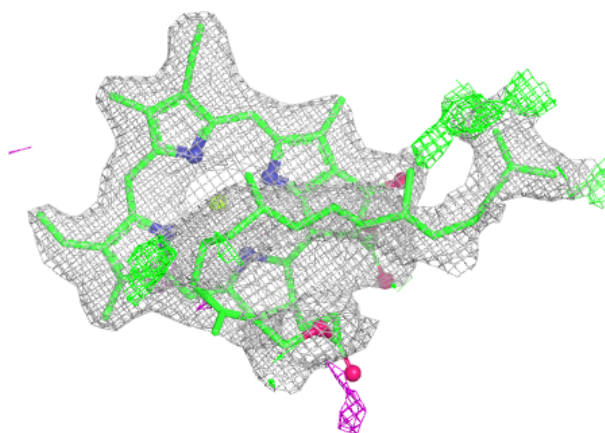
**Electron density around LMG c 520:**

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and green (positive)

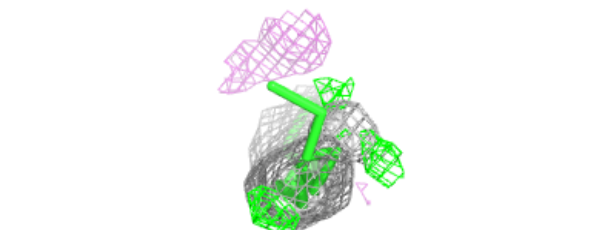
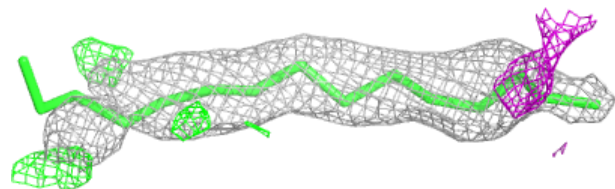
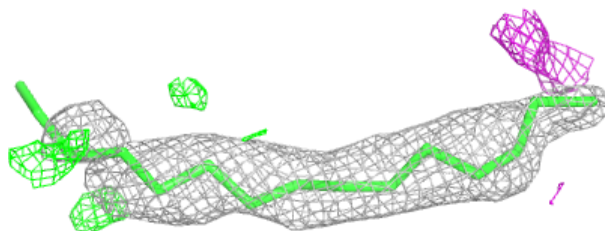


Electron density around CLA B 601:

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

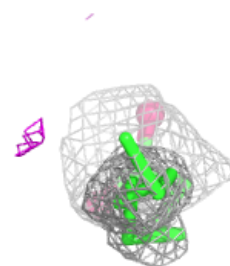
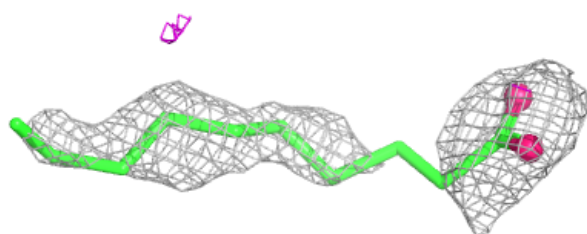
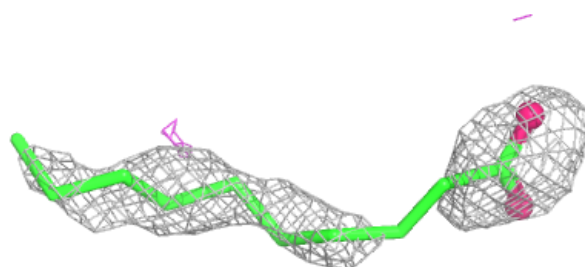
**Electron density around STE T 103:**

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

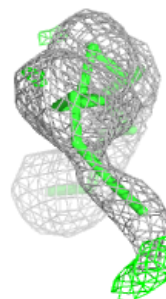
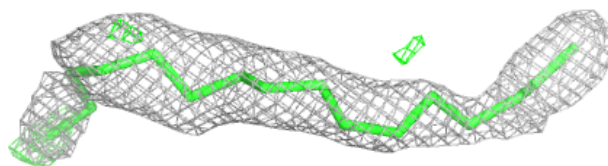
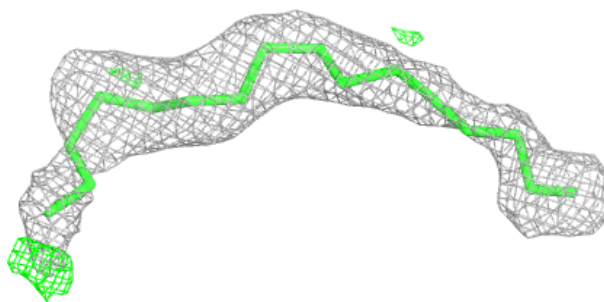


Electron density around STE F 103:

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

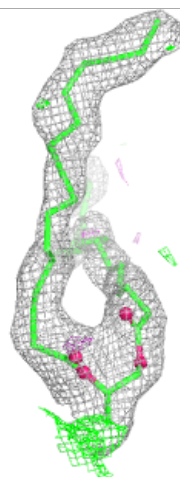
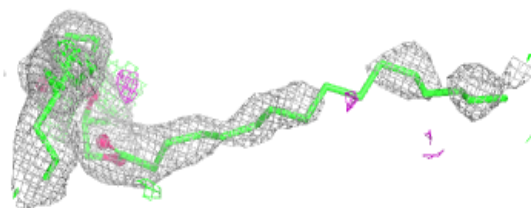
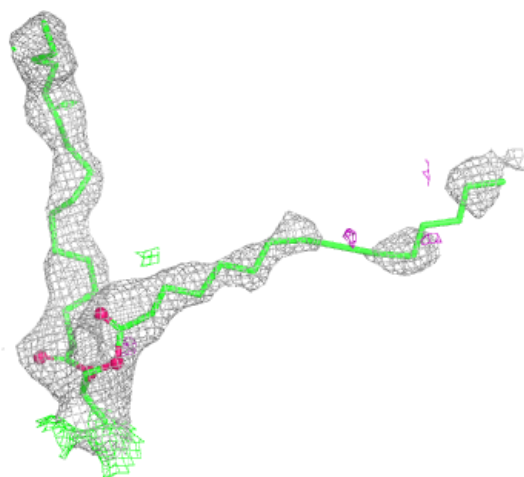
**Electron density around STE T 102:**

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



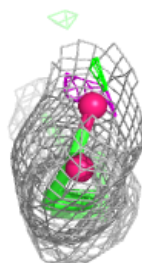
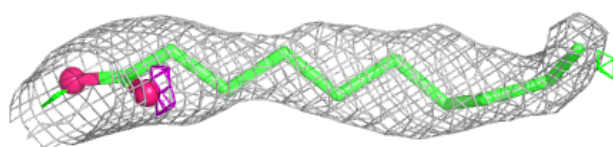
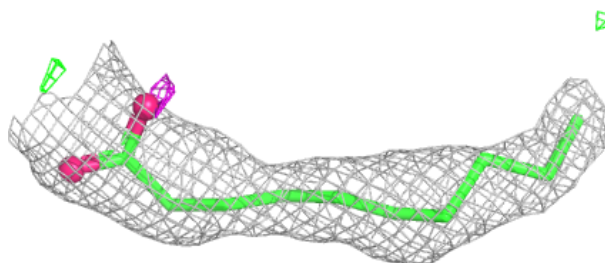
Electron density around SQD A 618:

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

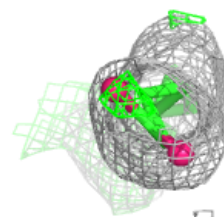
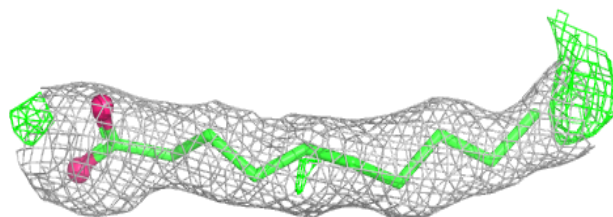
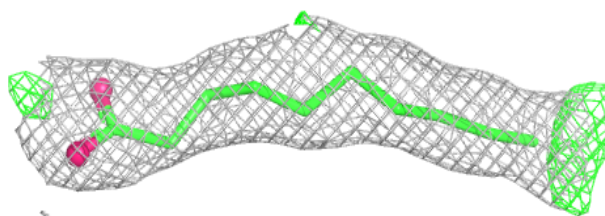


Electron density around STE C 520:

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

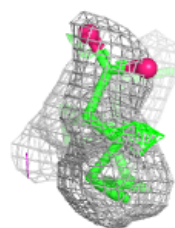
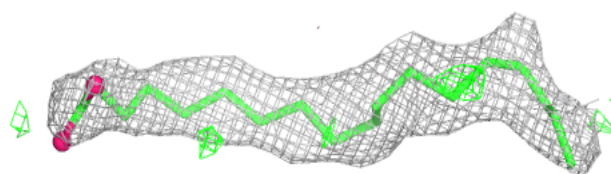
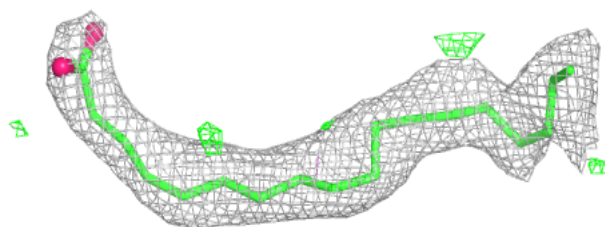
**Electron density around STE j 101:**

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

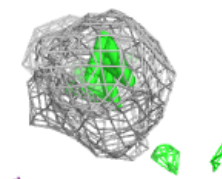
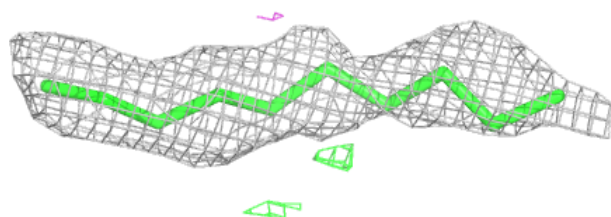
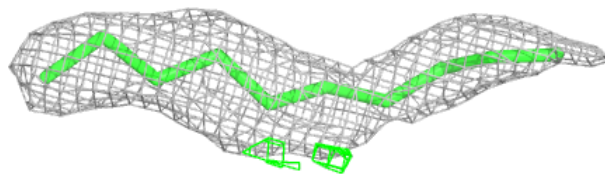


Electron density around STE b 620:

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

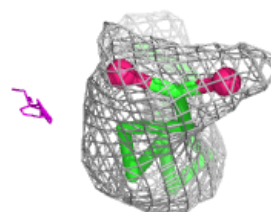
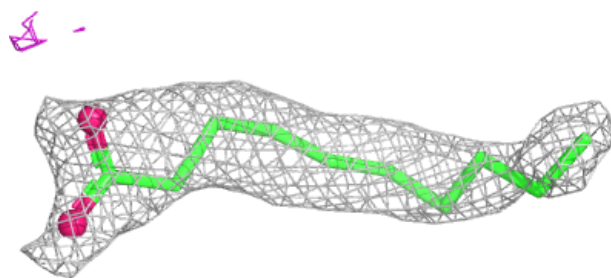
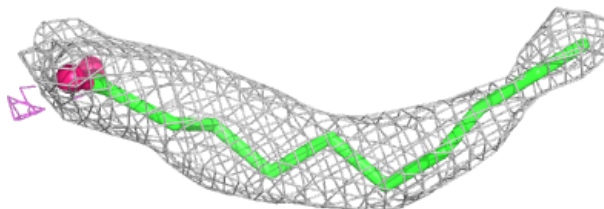
**Electron density around STE t 104:**

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

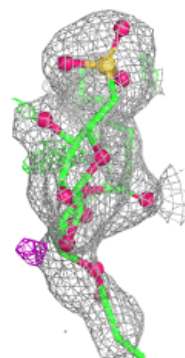
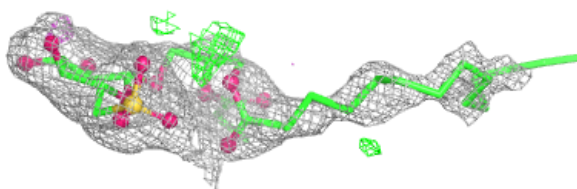
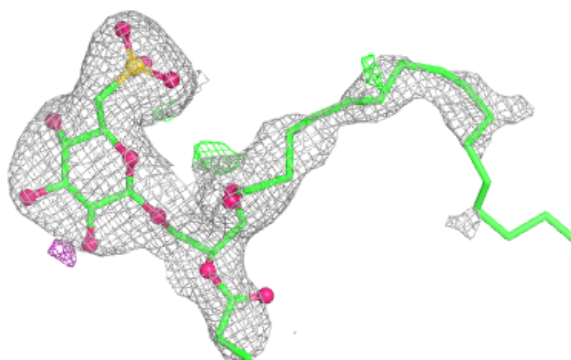


Electron density around STE B 624:

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

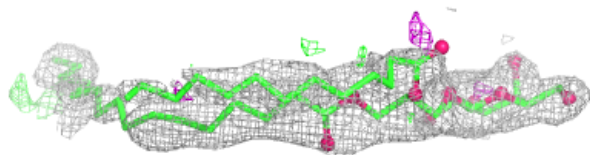
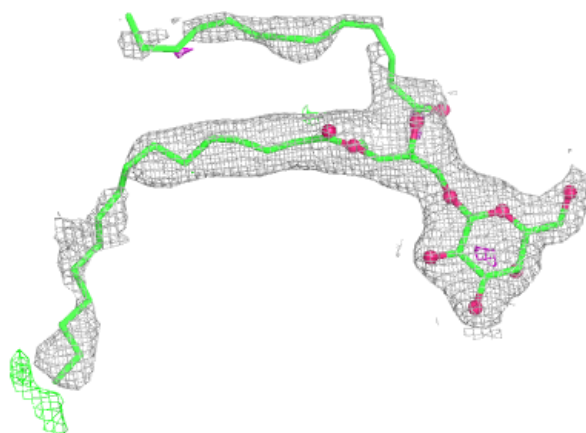
**Electron density around SQD f 101:**

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

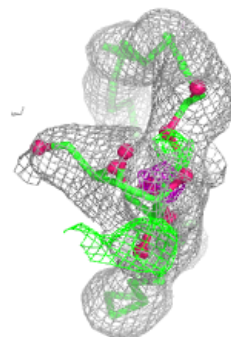
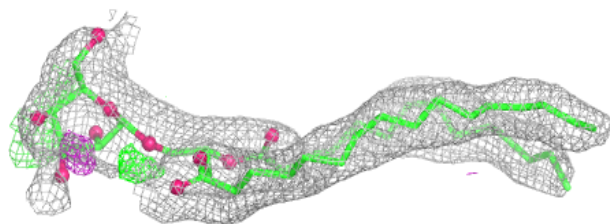
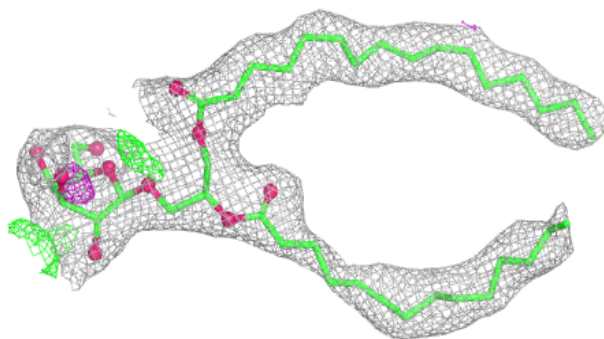


Electron density around LMG C 518:

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

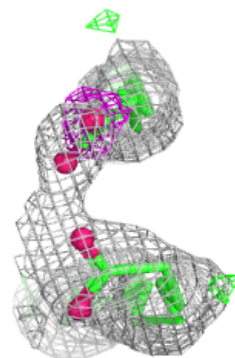
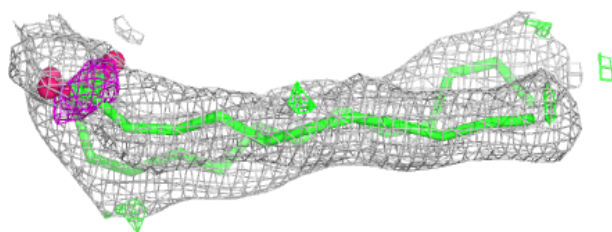
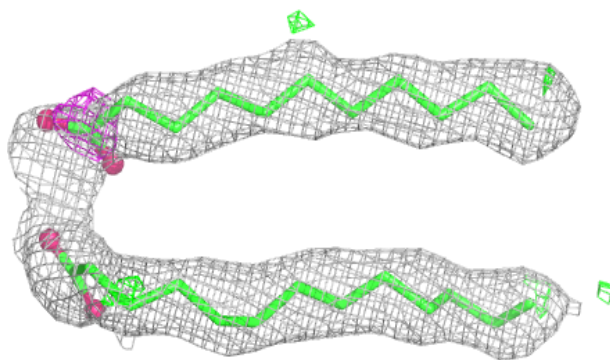
**Electron density around LMG c 523:**

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

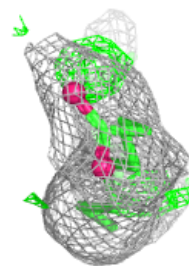
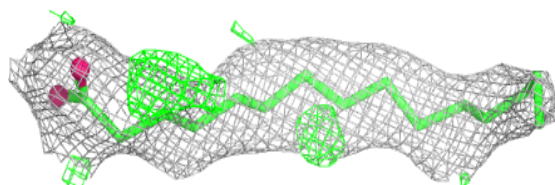
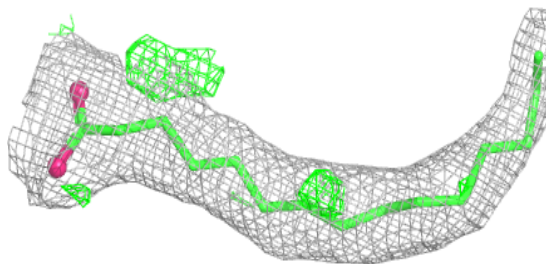


Electron density around LMG B 621:

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

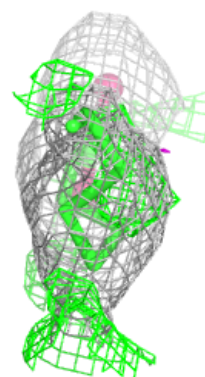
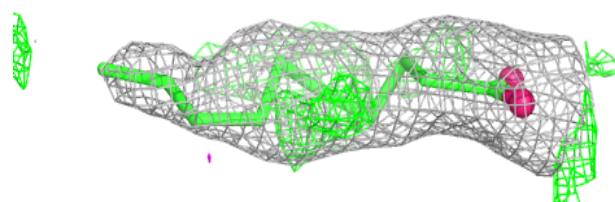
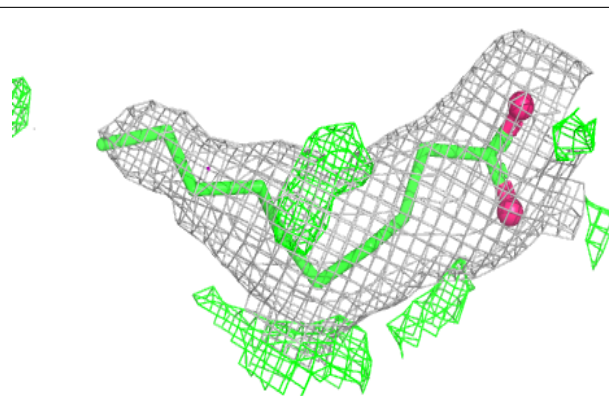
**Electron density around STE B 620:**

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

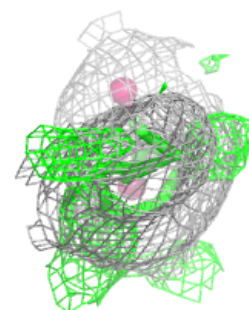
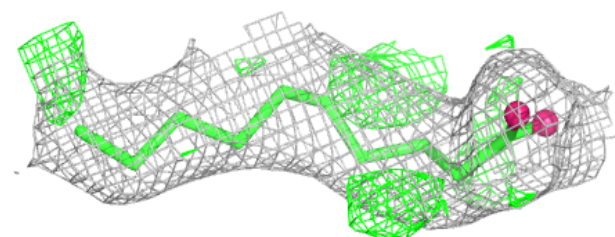
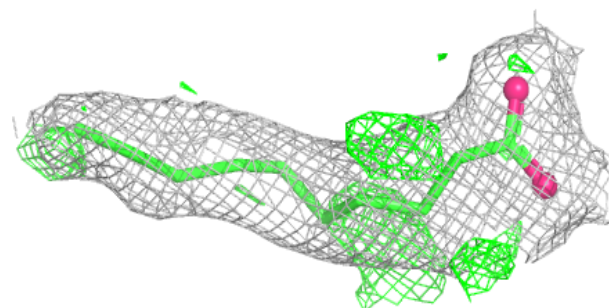


Electron density around STE C 519:

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

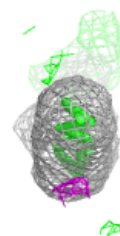
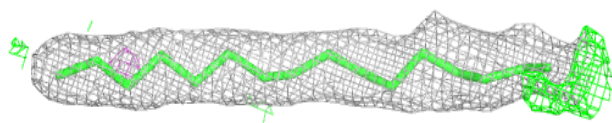
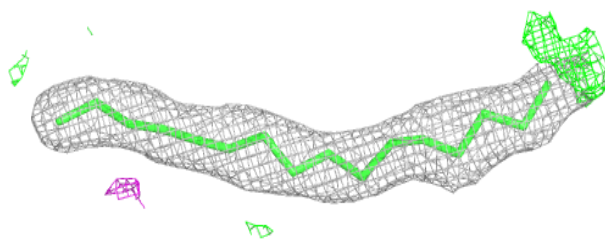
**Electron density around STE B 623:**

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

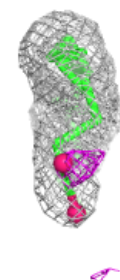
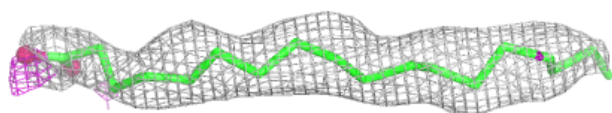
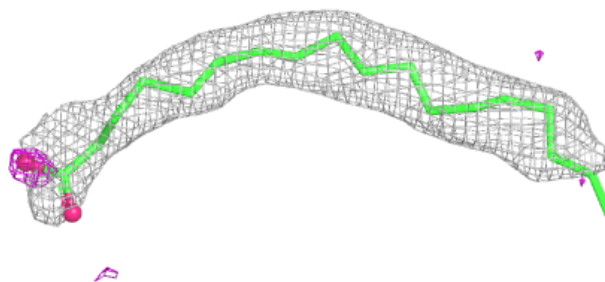


Electron density around STE C 521:

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

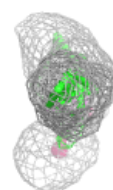
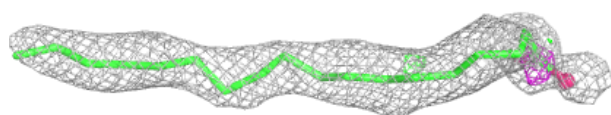
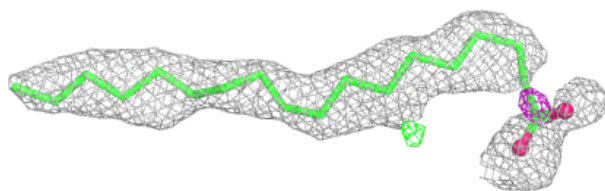
**Electron density around STE X 102:**

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

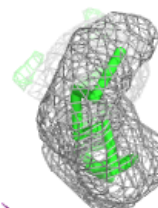
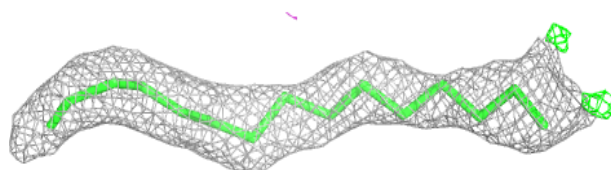
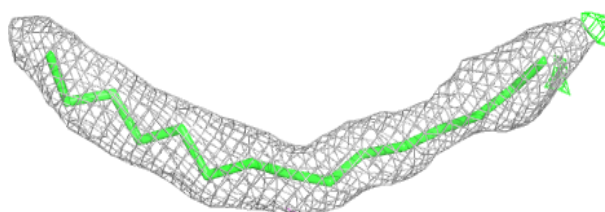


Electron density around STE c 521:

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

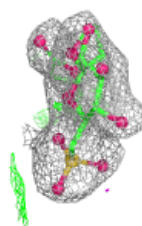
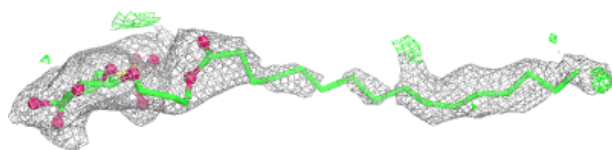
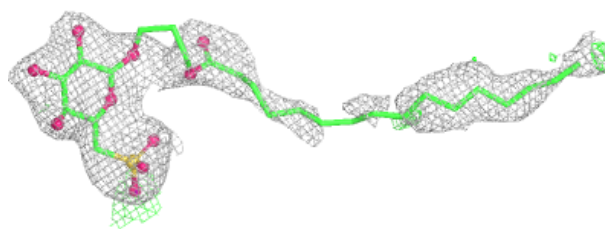
**Electron density around STE I 101:**

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

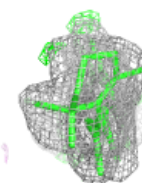
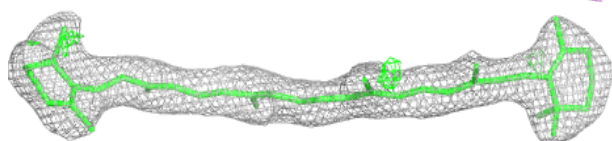
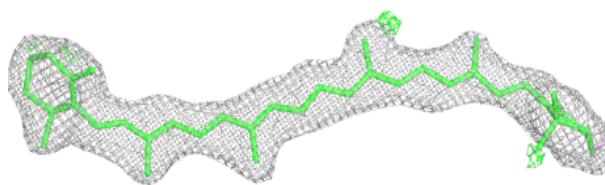


Electron density around SQD F 102:

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

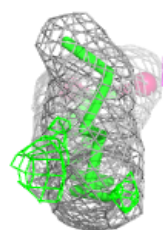
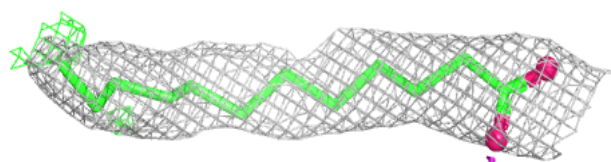
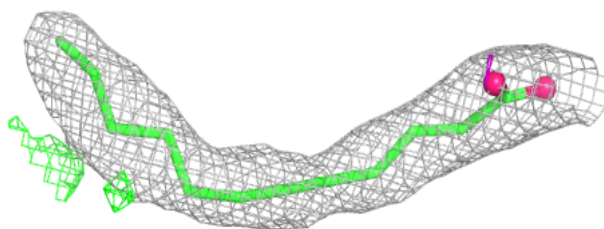
**Electron density around BCR K 101:**

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

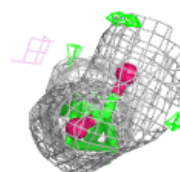
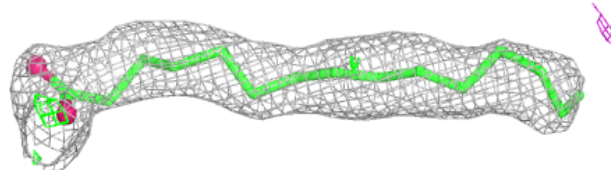
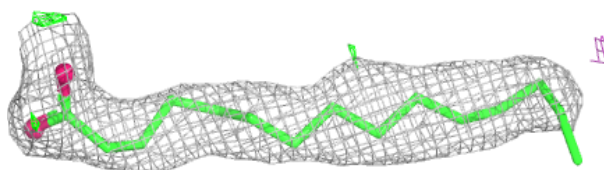


Electron density around STE t 103:

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

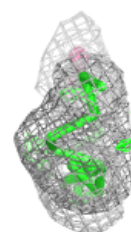
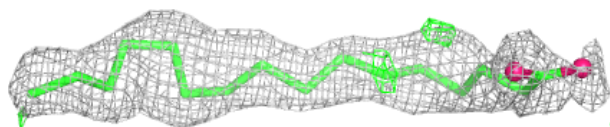
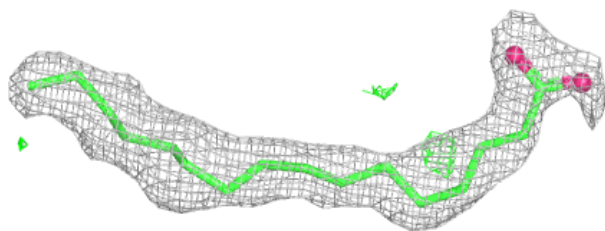
**Electron density around STE d 413:**

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

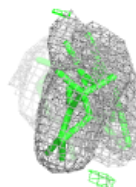
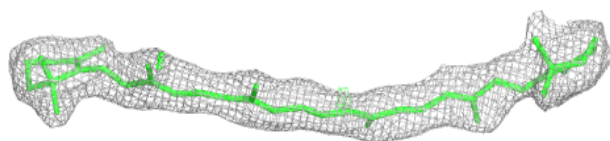
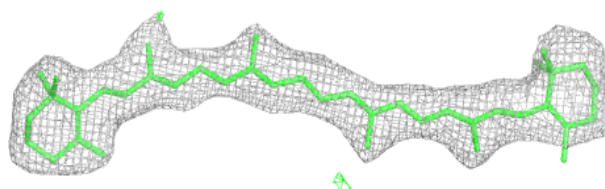


Electron density around STE t 105:

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

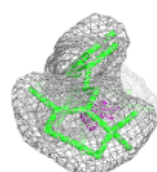
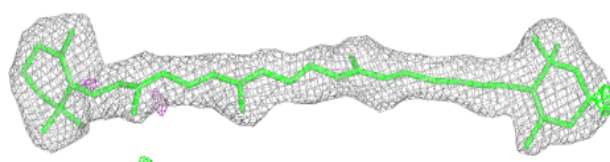
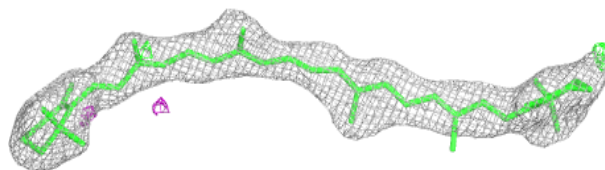
**Electron density around BCR d 405:**

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

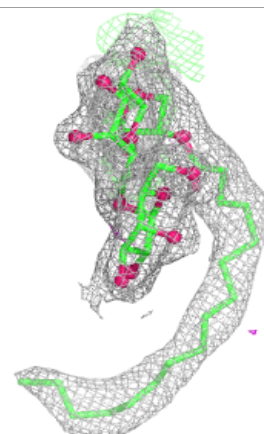
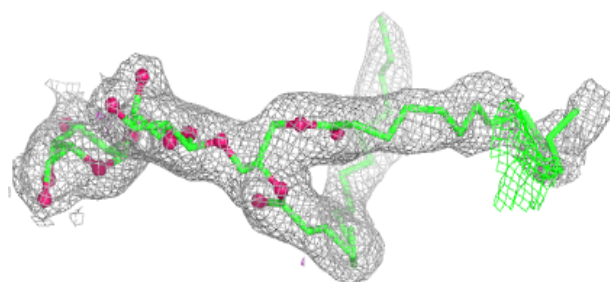
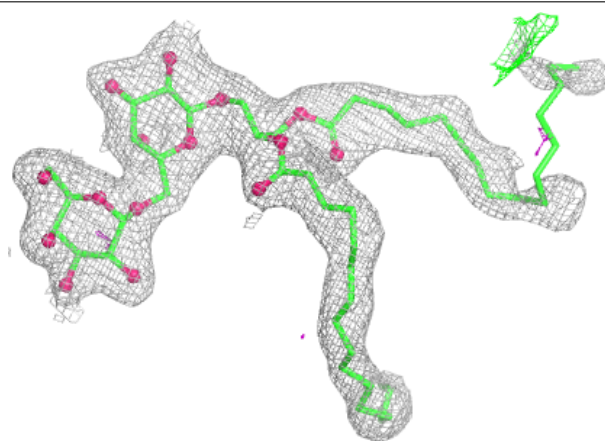


Electron density around BCR h 102:

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

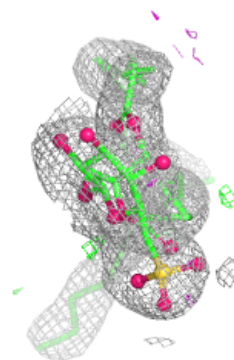
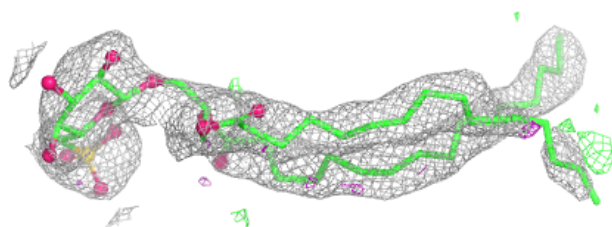
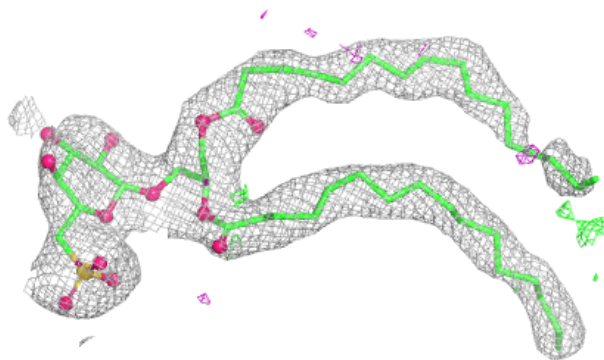
**Electron density around DGD C 516:**

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

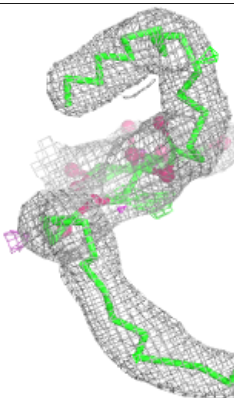
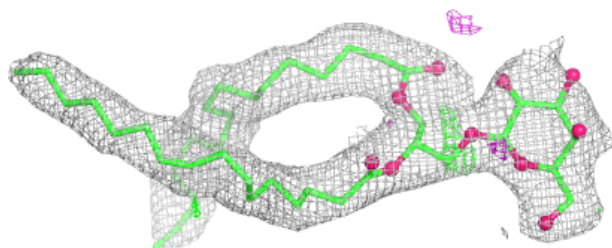
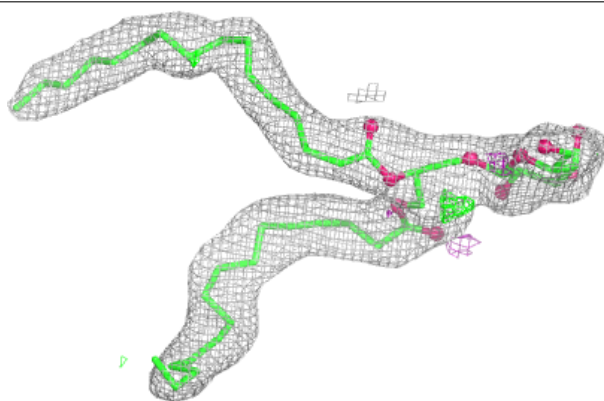


Electron density around SQD B 622:

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

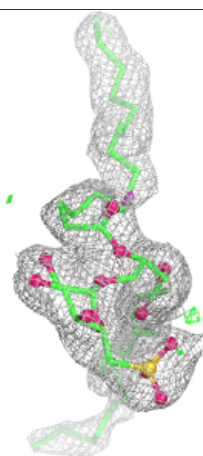
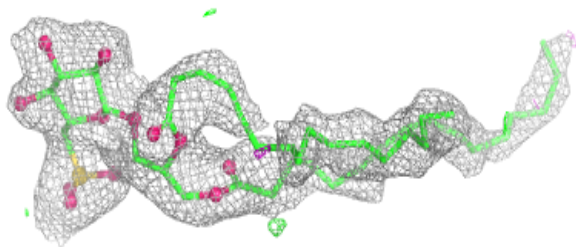
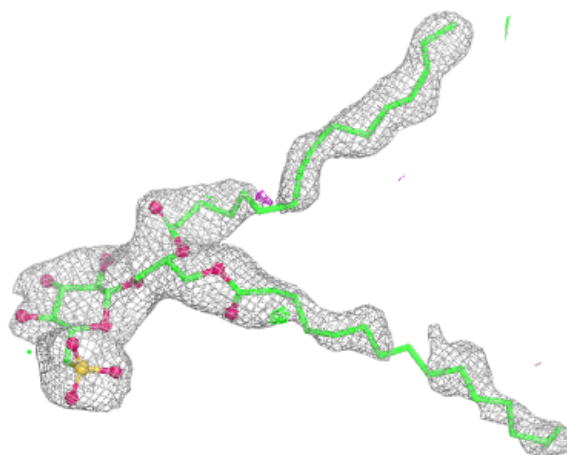
**Electron density around LMG m 101:**

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



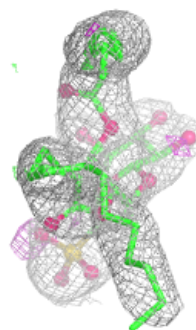
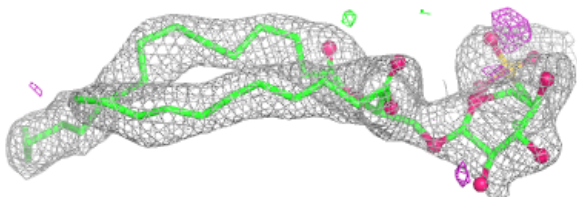
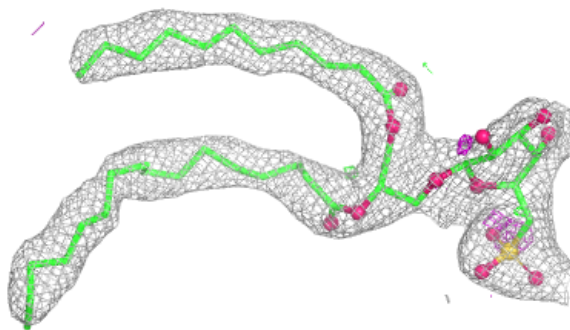
Electron density around SQD a 613:

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

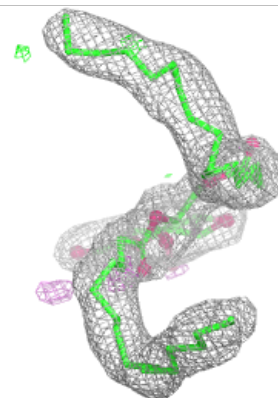
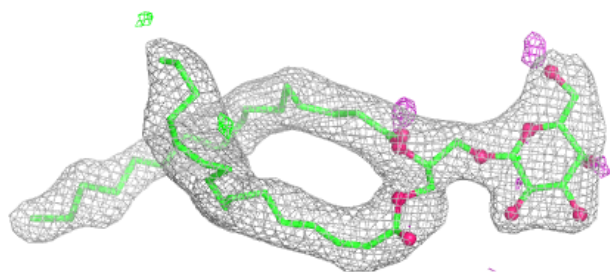
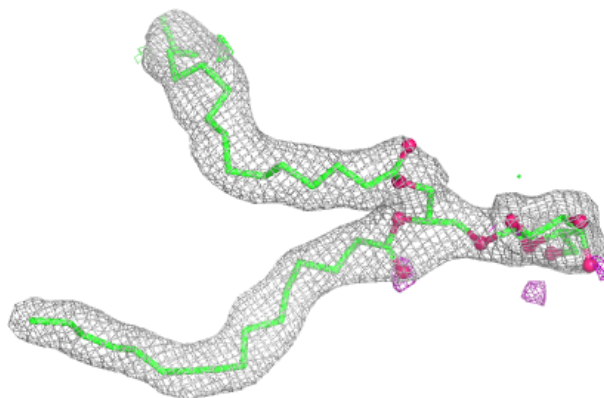


Electron density around SQD b 619:

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

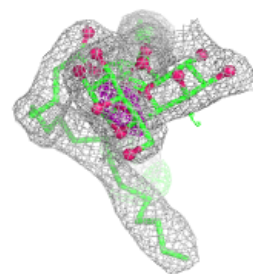
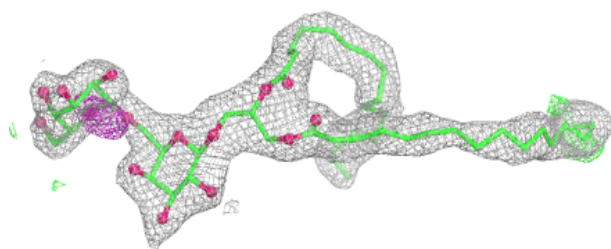
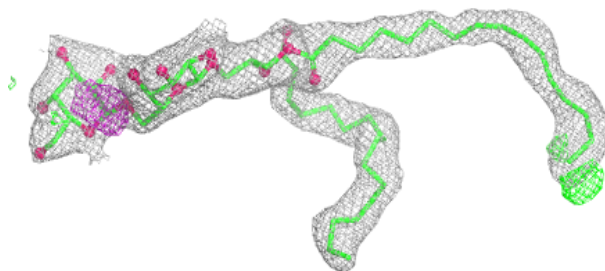
**Electron density around LMG M 101:**

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

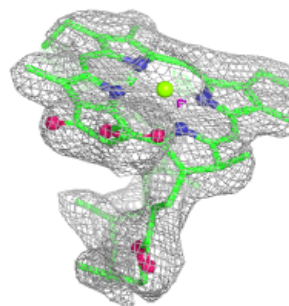
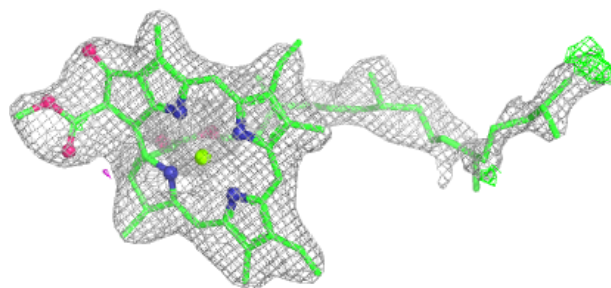
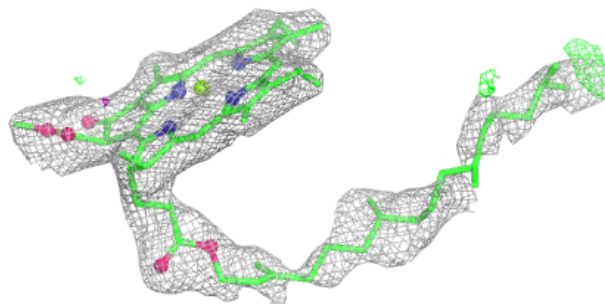


Electron density around DGD H 101:

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

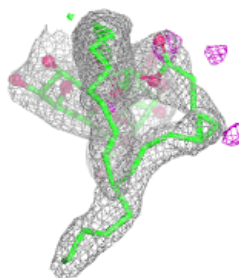
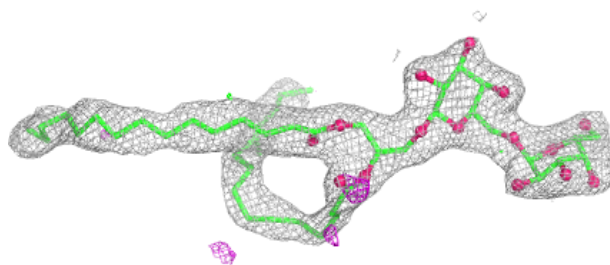
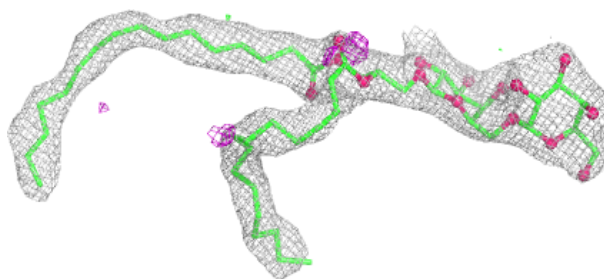
**Electron density around CLA C 513:**

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

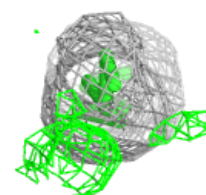
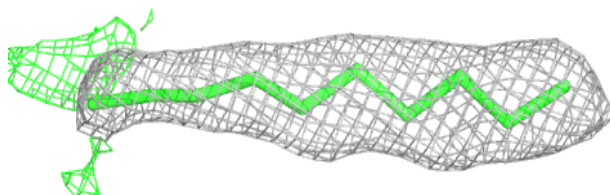
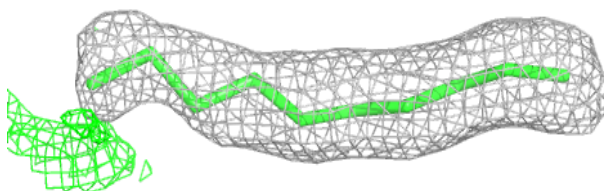


Electron density around DGD h 103:

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

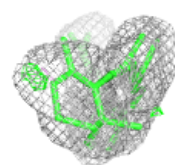
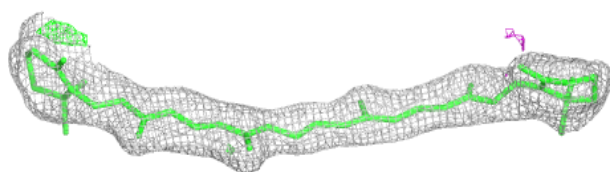
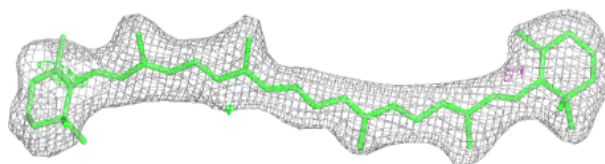
**Electron density around STE M 103:**

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

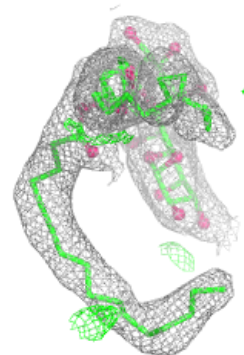
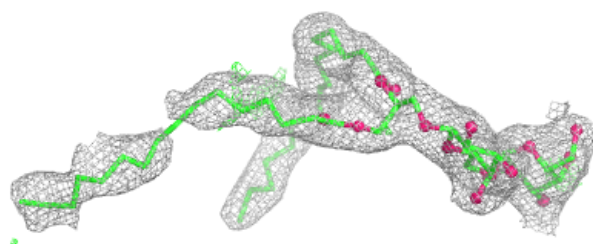
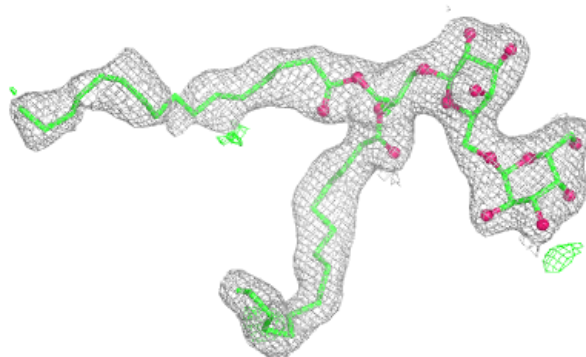


Electron density around BCR D 404:

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

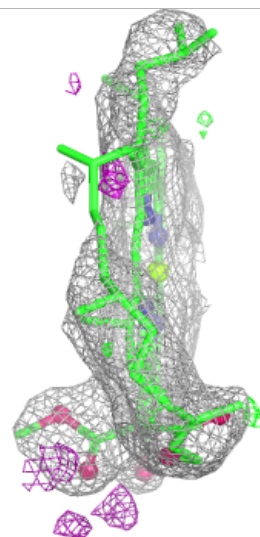
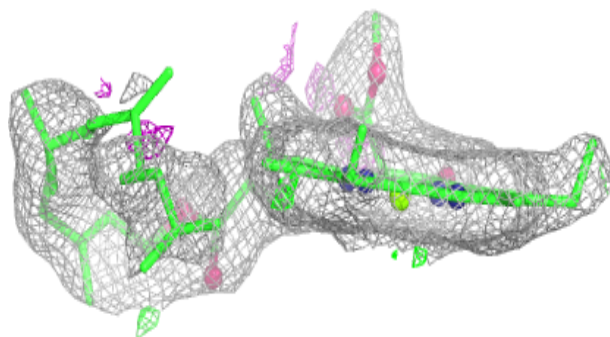
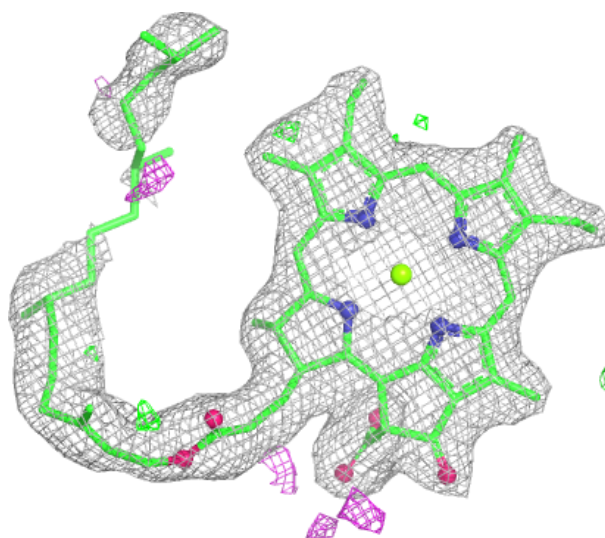
**Electron density around DGD c 518:**

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



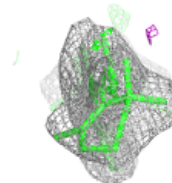
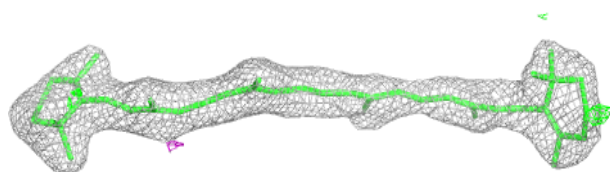
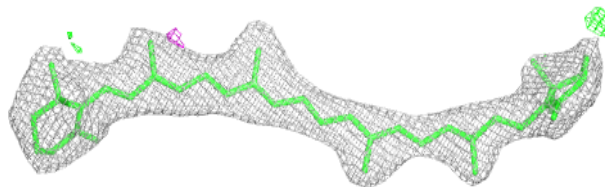
Electron density around CLA c 512:

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

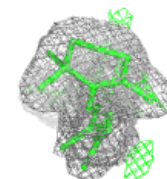
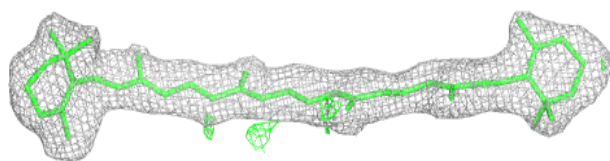
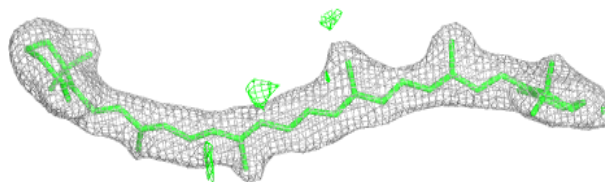


Electron density around BCR k 101:

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

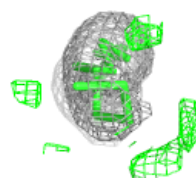
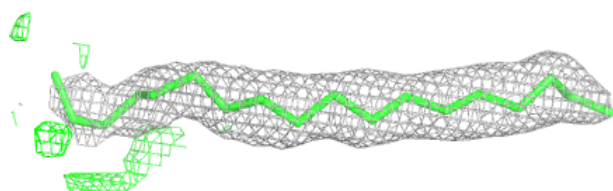
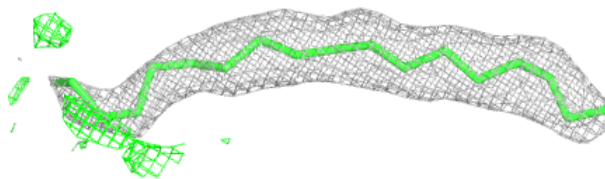
**Electron density around BCR X 101:**

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

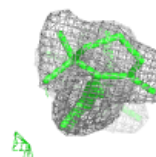
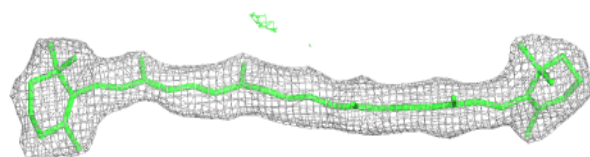
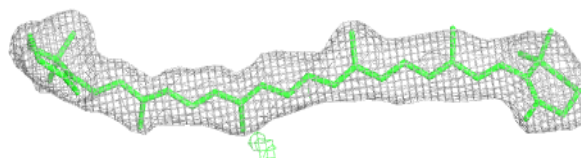


Electron density around STE I 102:

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

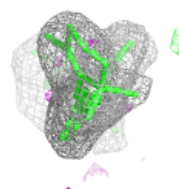
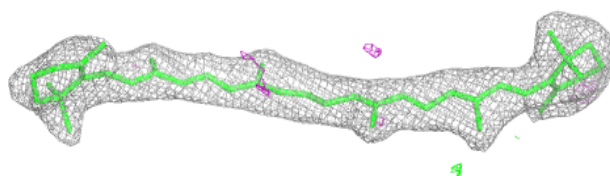
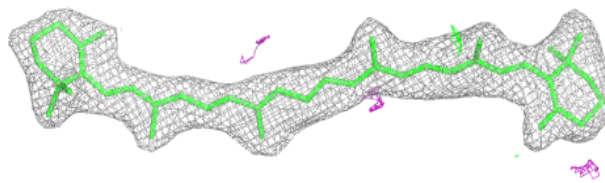
**Electron density around BCR Z 101:**

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

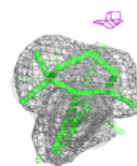
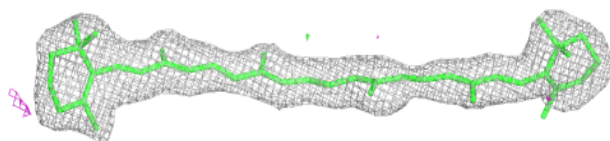
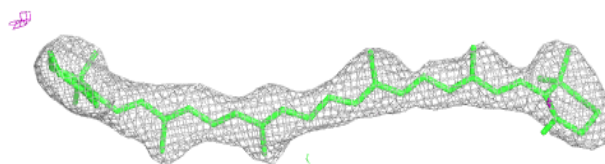


Electron density around BCR b 618:

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

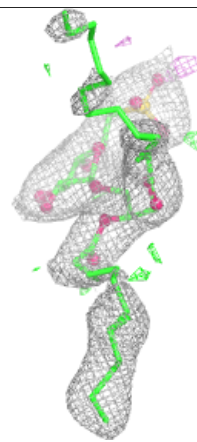
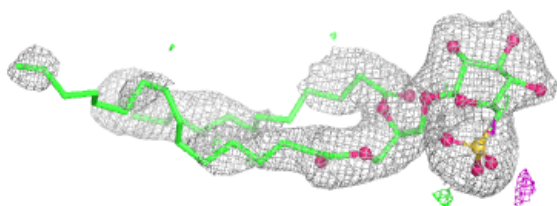
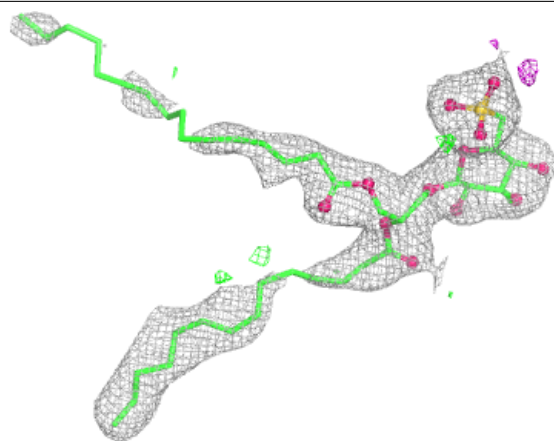
**Electron density around BCR c 514:**

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

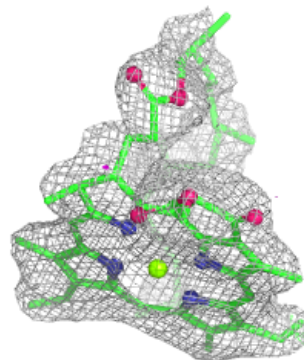
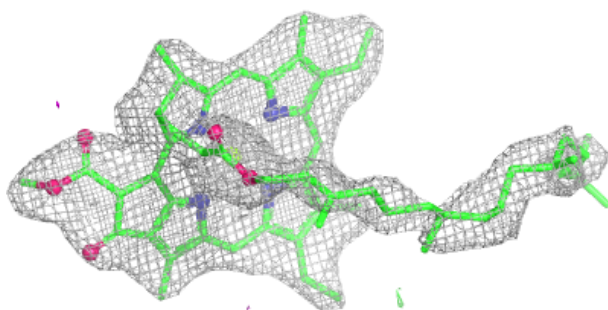
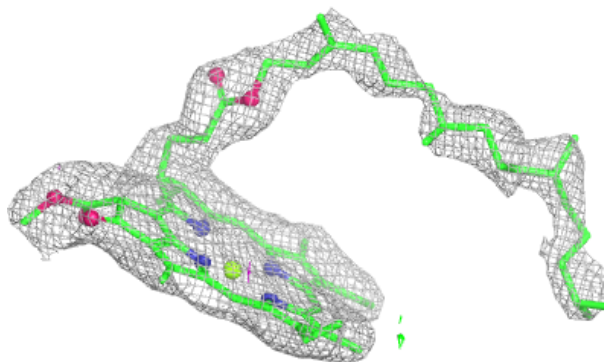


Electron density around SQD A 616:

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

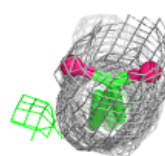
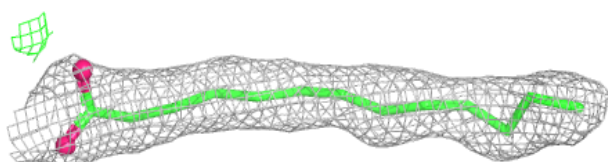
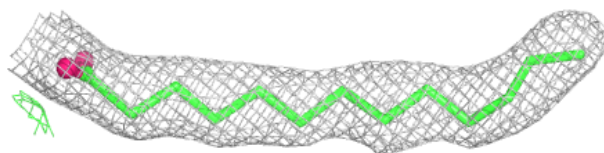
**Electron density around CLA c 513:**

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

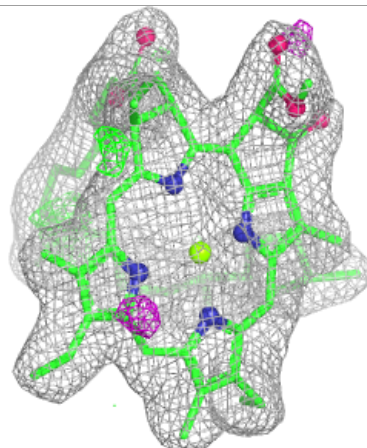
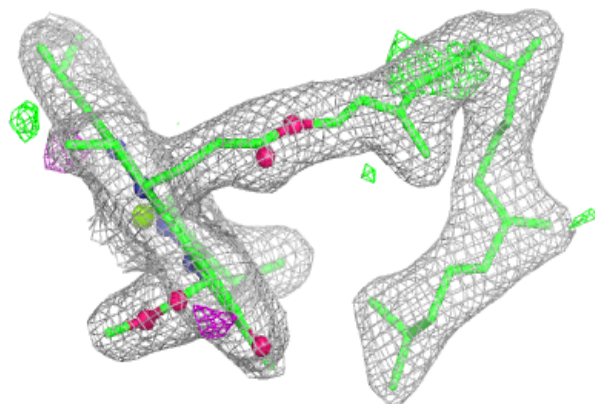
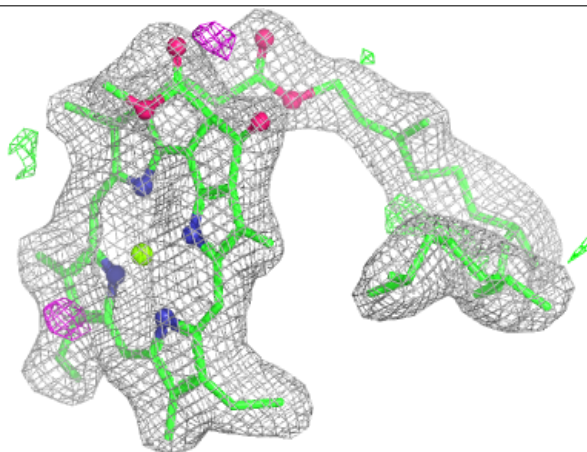


Electron density around STE M 102:

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

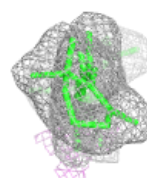
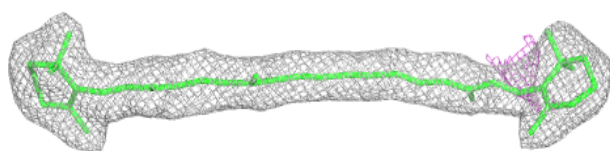
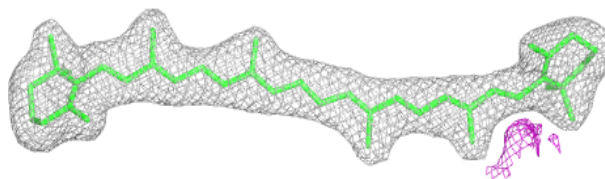
**Electron density around CLA C 503:**

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

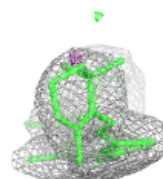
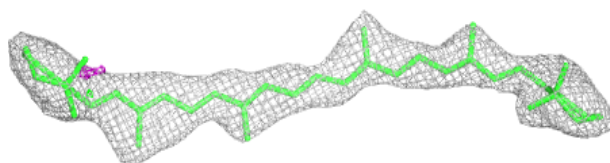
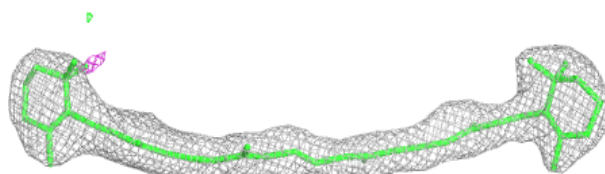


Electron density around BCR B 618:

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

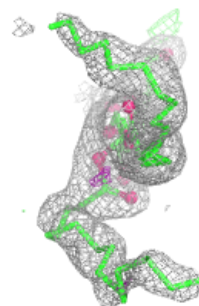
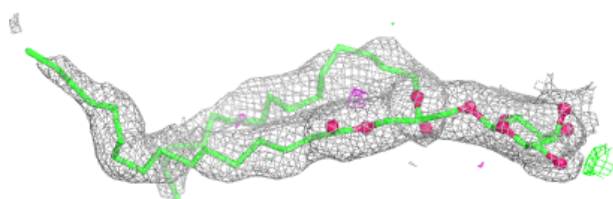
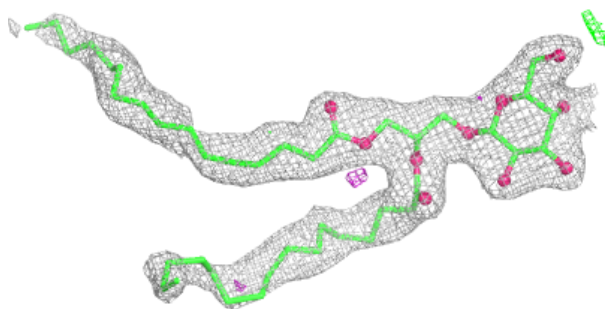
**Electron density around BCR c 516:**

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

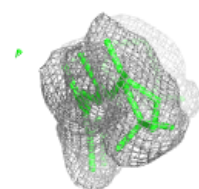
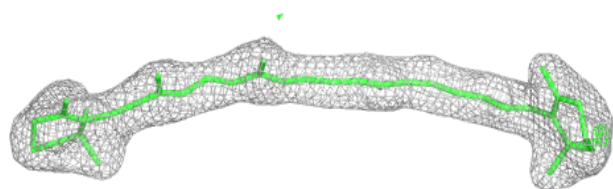
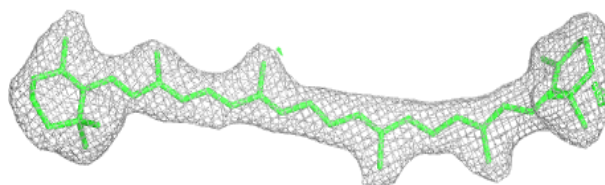


Electron density around LMG D 406:

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

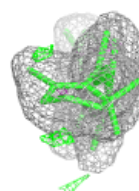
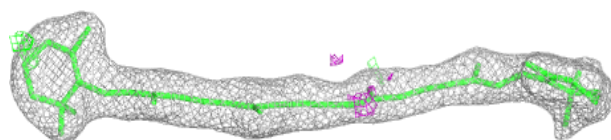
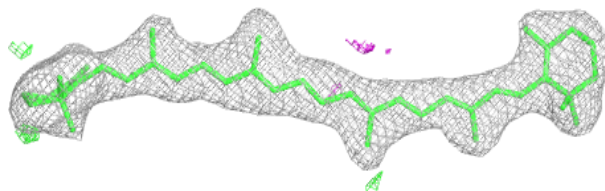
**Electron density around BCR t 101:**

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

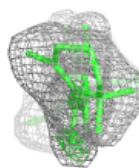
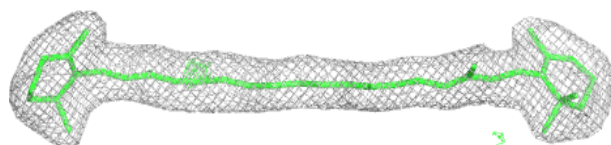
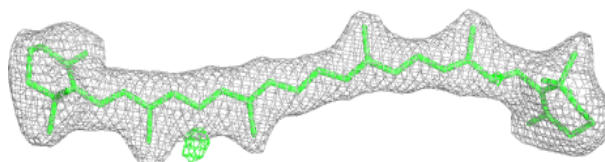


Electron density around BCR b 616:

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

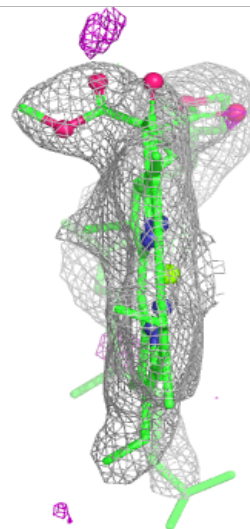
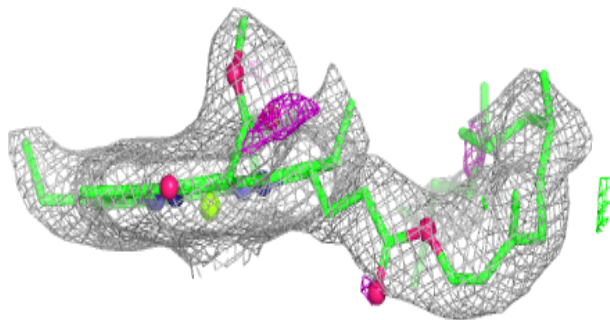
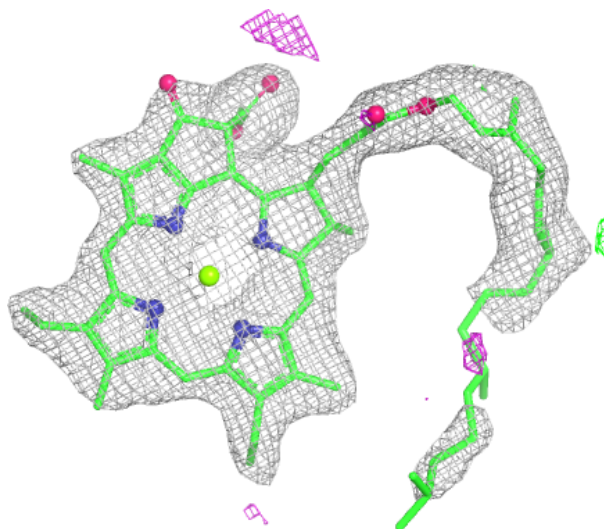
**Electron density around BCR b 617:**

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



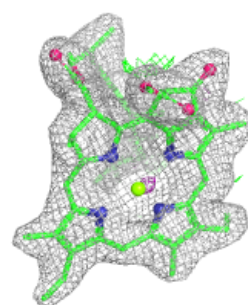
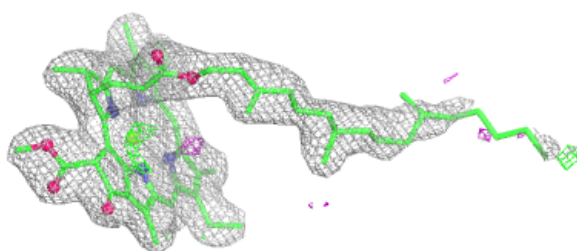
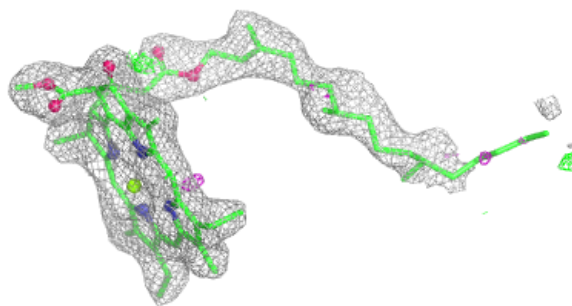
Electron density around CLA C 512:

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

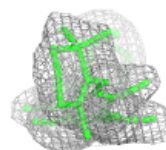
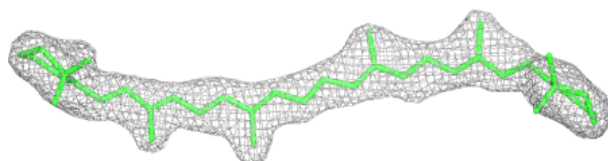
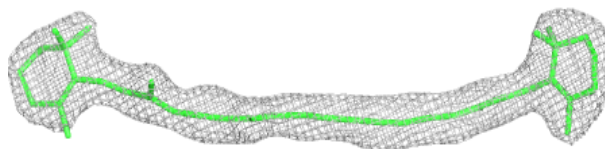


Electron density around CLA c 508:

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

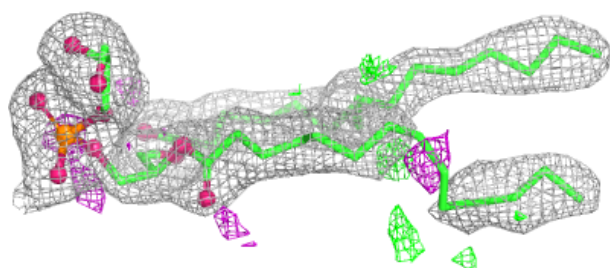
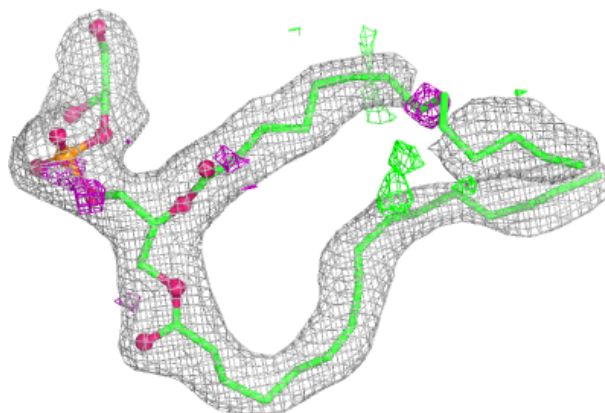
**Electron density around BCR K 102:**

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

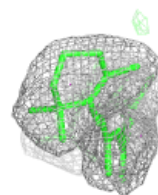
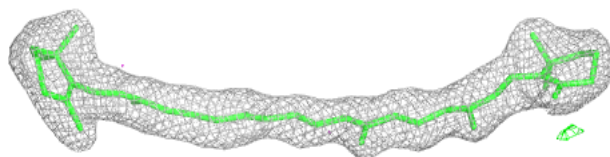
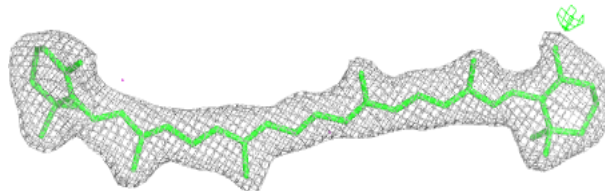


Electron density around LHG A 615:

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

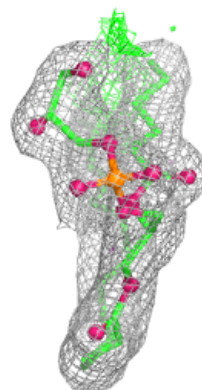
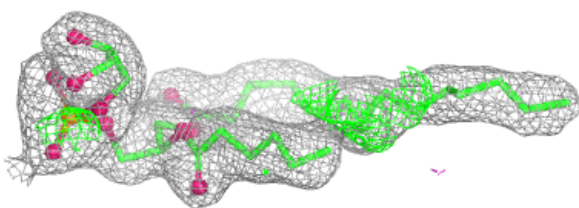
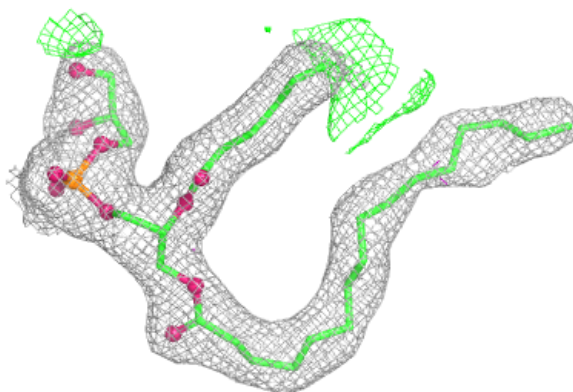
**Electron density around BCR T 101:**

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

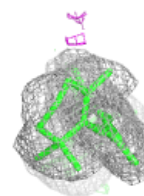
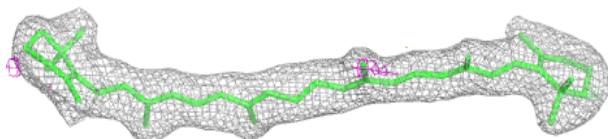
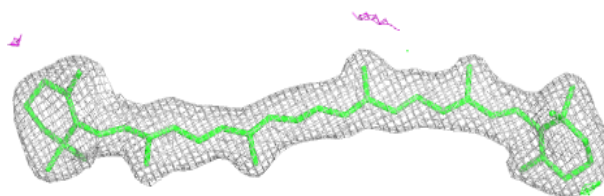


Electron density around LHG d 409:

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

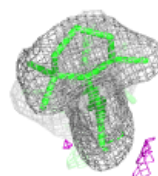
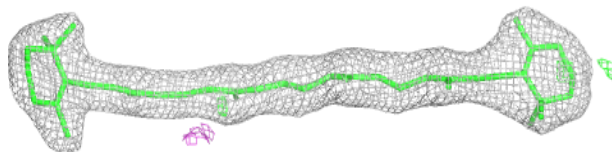
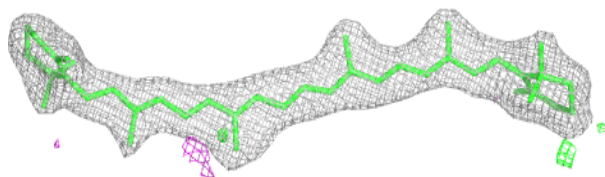
**Electron density around BCR B 619:**

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

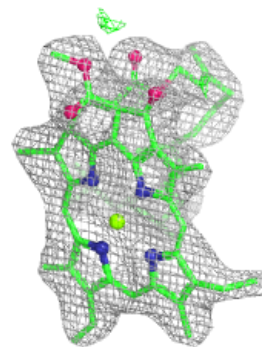
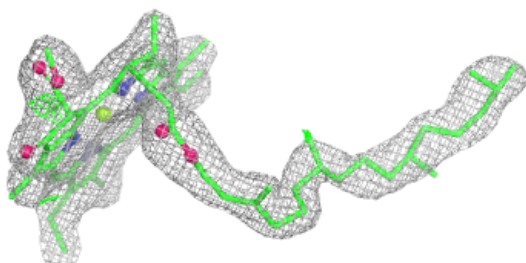
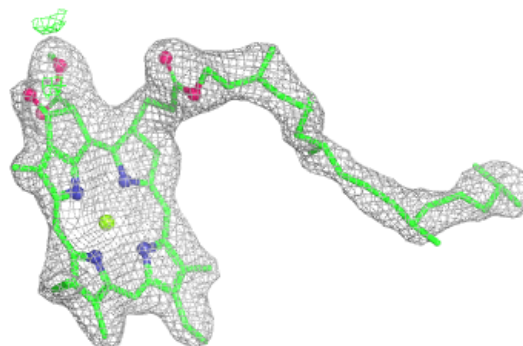


Electron density around BCR C 514:

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

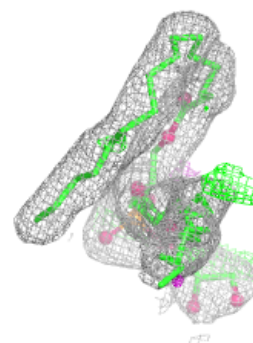
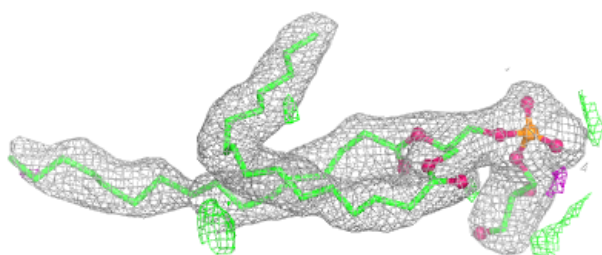
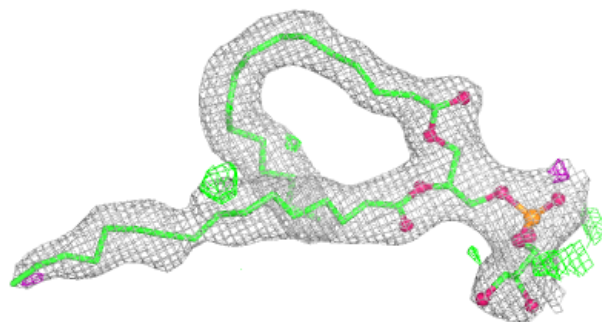
**Electron density around CLA c 511:**

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

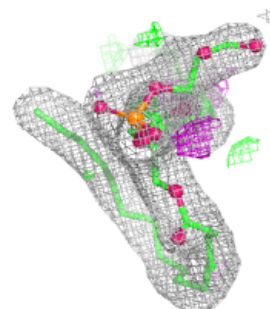
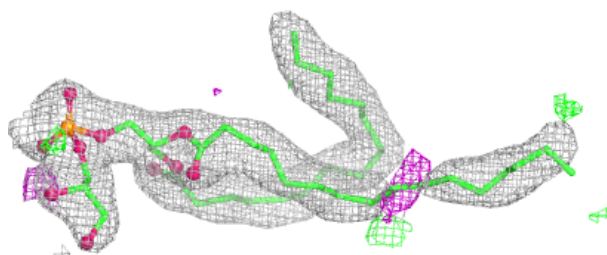
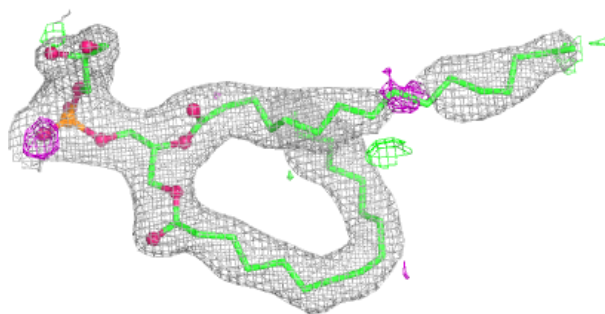


Electron density around LHG D 409:

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

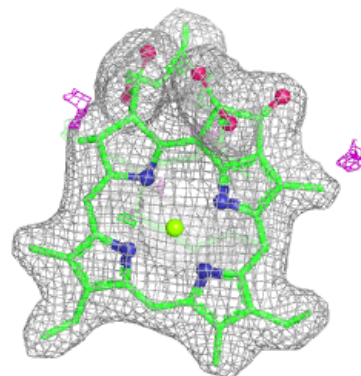
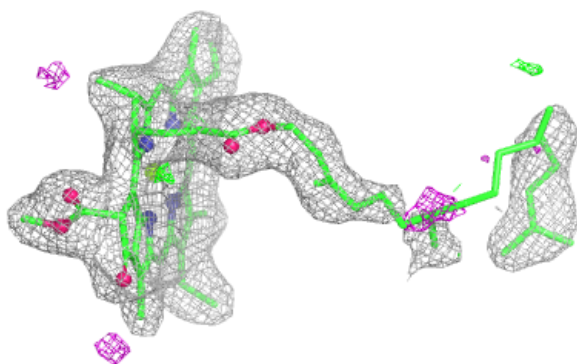
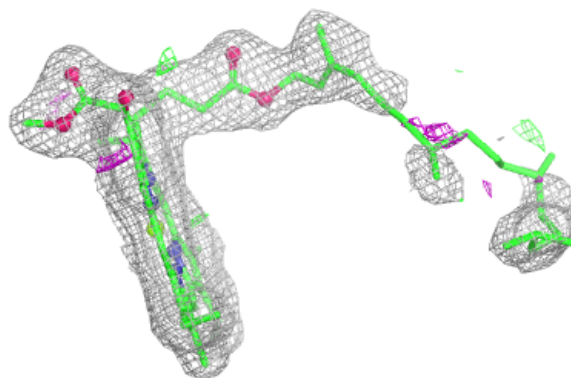
**Electron density around LHG d 407:**

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

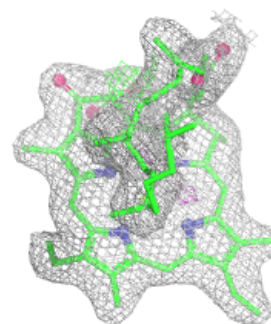
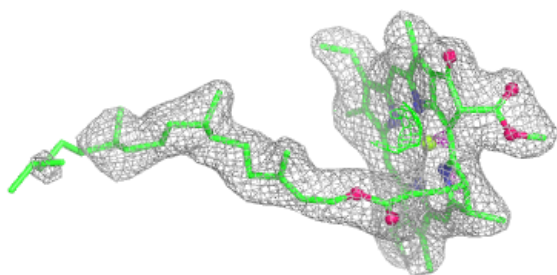
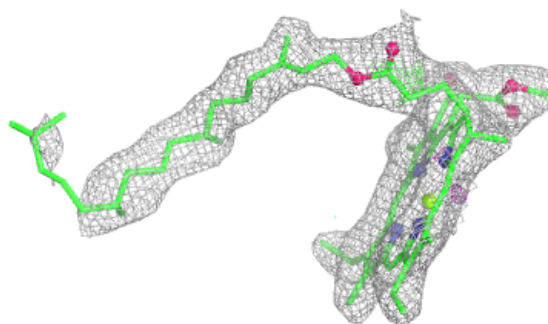


Electron density around CLA C 506:

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

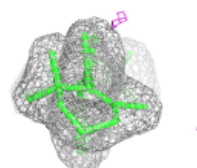
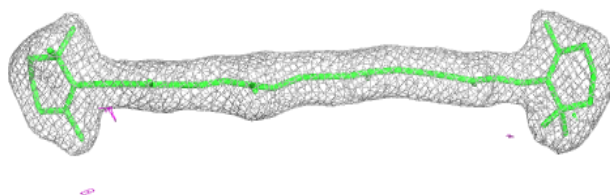
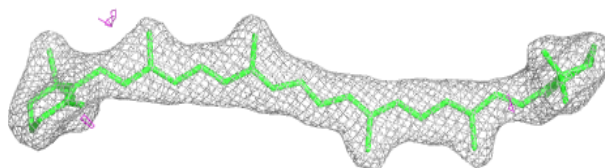
**Electron density around CLA C 508:**

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

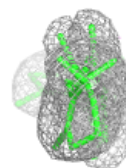
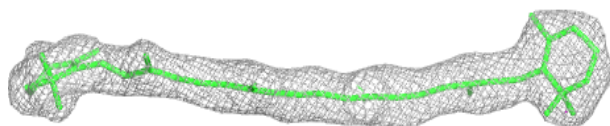
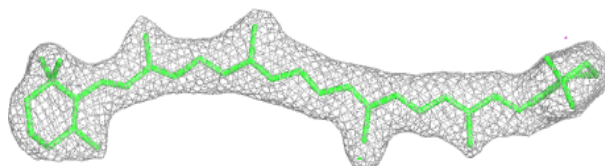


Electron density around BCR A 611:

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

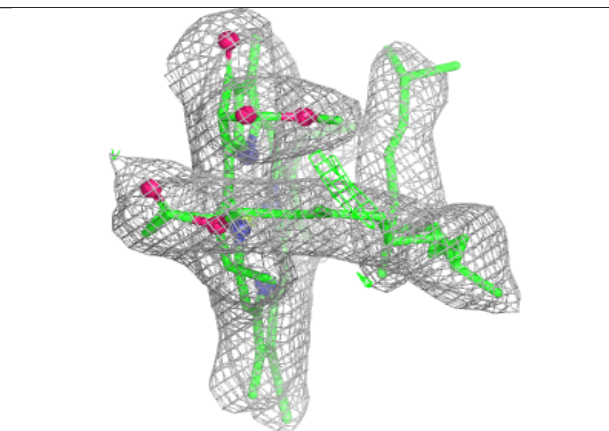
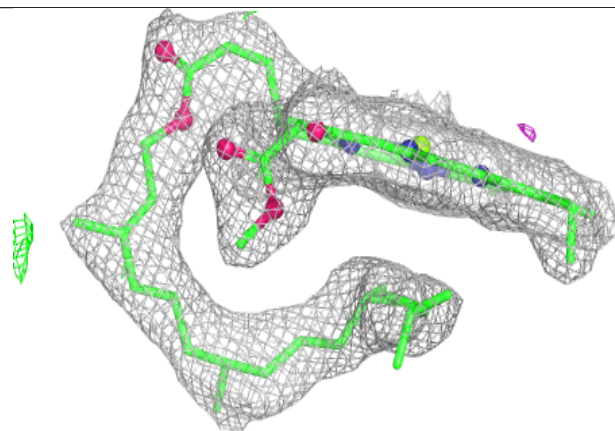
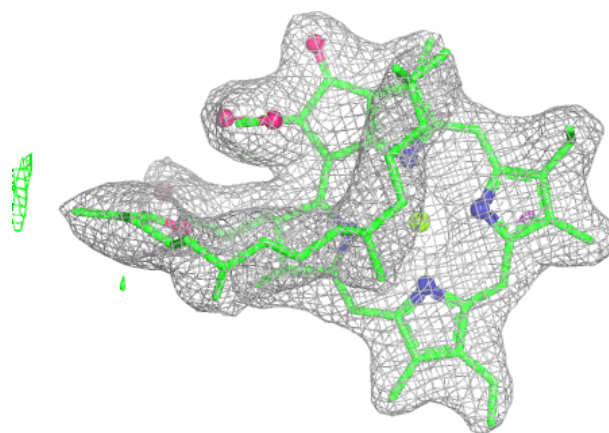
**Electron density around BCR B 617:**

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

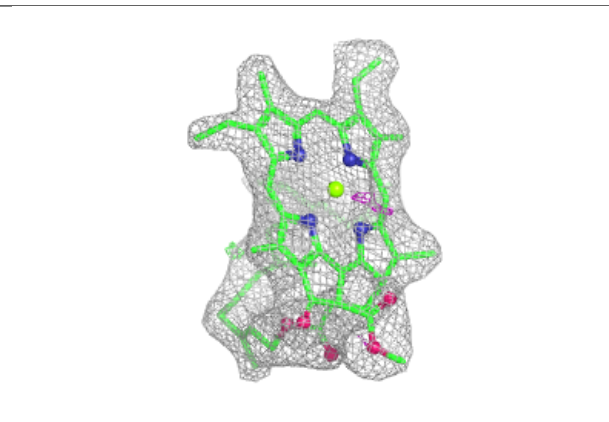
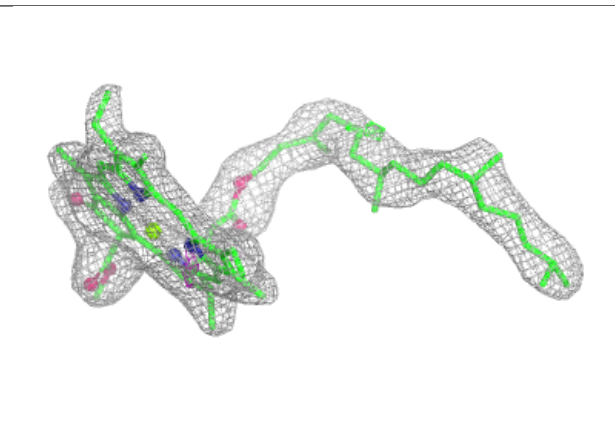
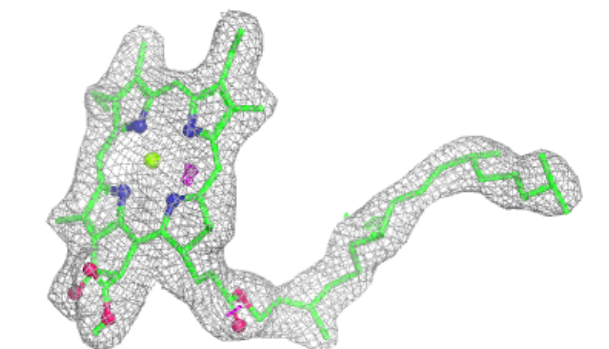


Electron density around CLA C 510:

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

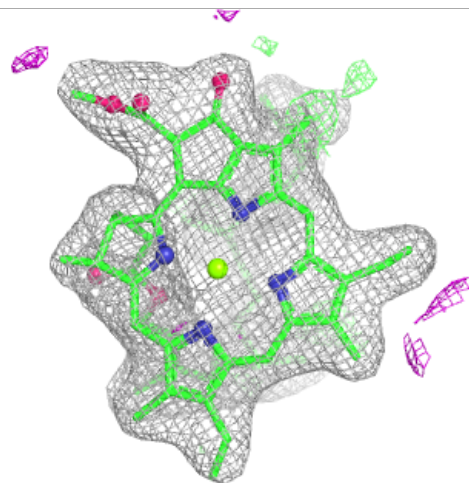
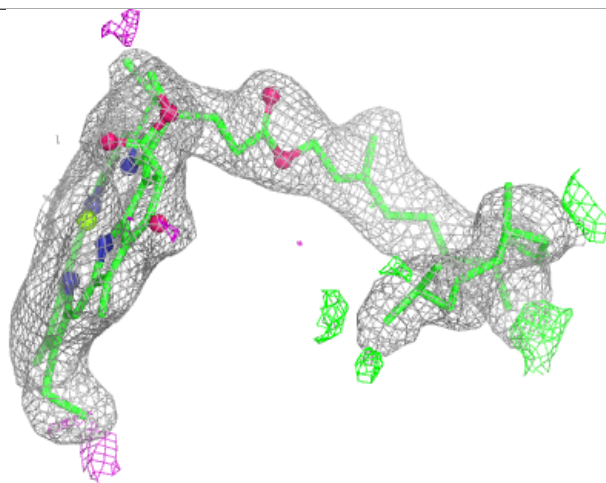
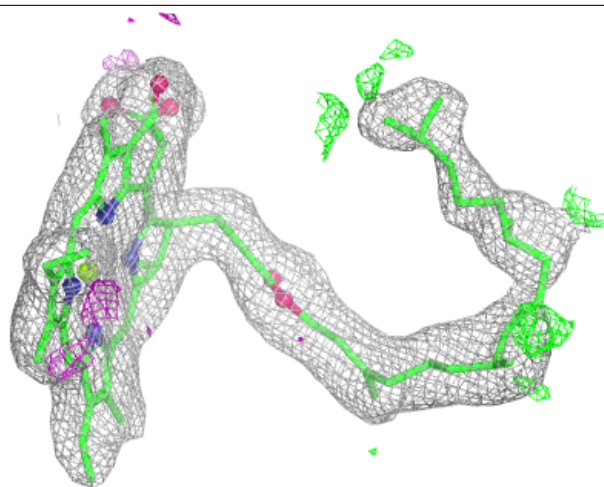
**Electron density around CLA C 511:**

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



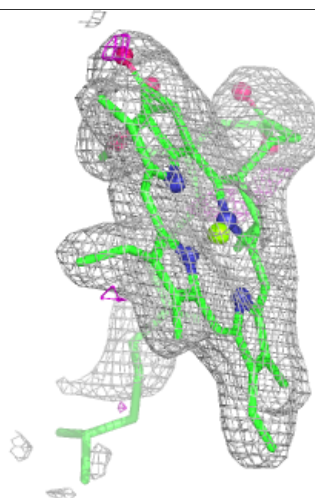
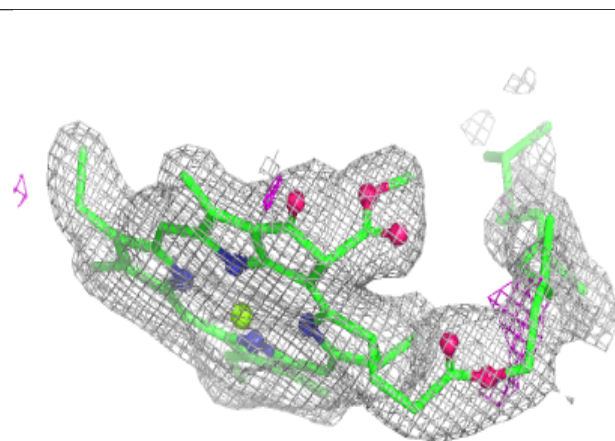
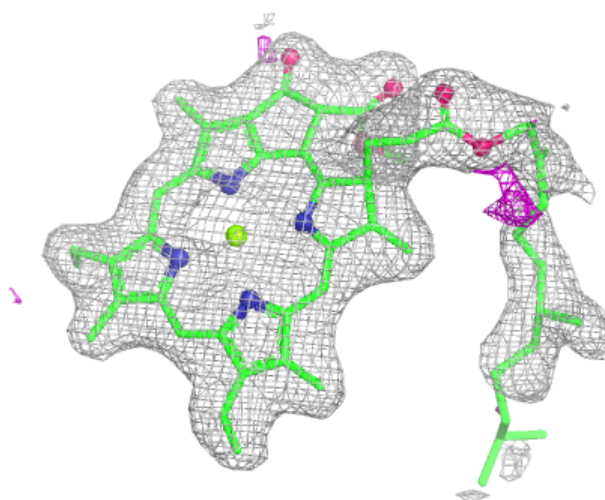
Electron density around CLA B 606:

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



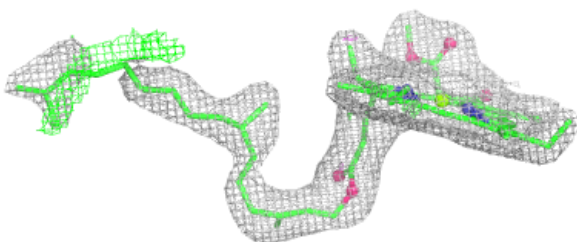
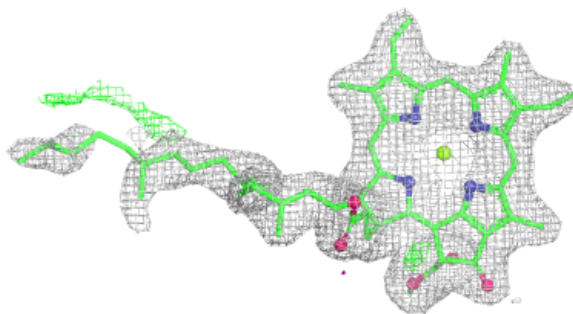
Electron density around CLA B 616:

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

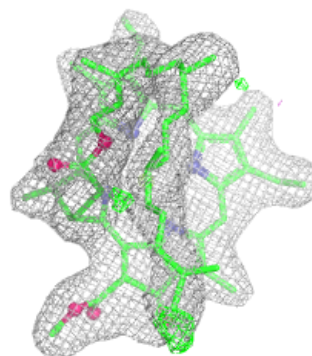
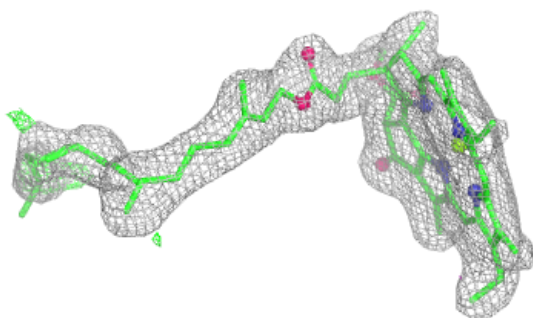
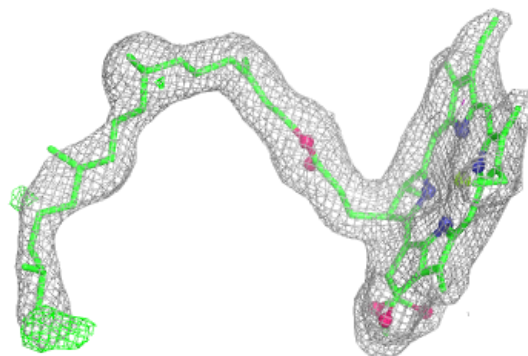


Electron density around CLA a 607:

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

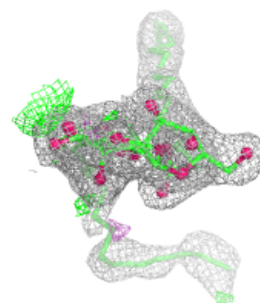
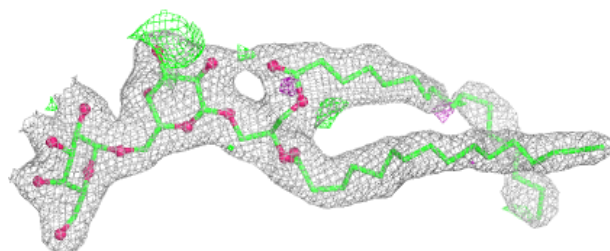
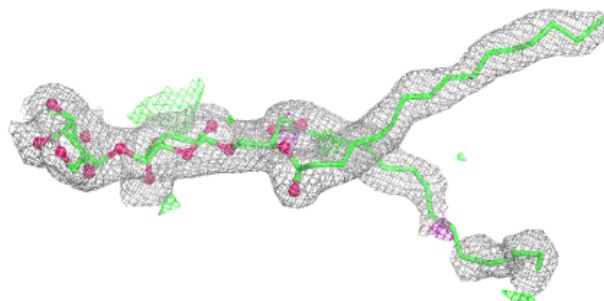
**Electron density around CLA b 605:**

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

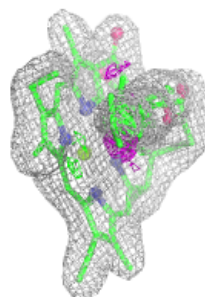
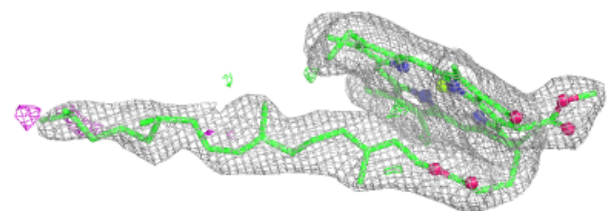
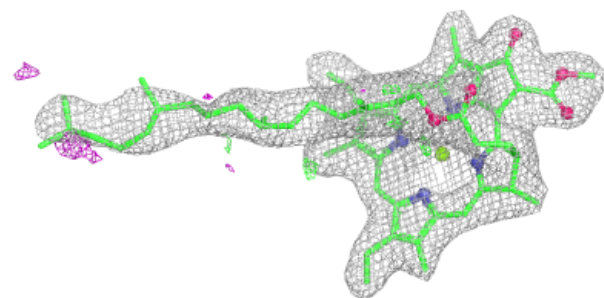


Electron density around DGD C 515:

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

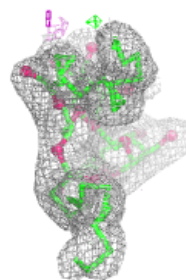
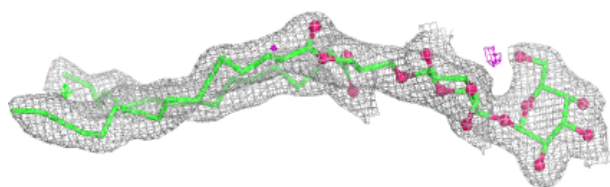
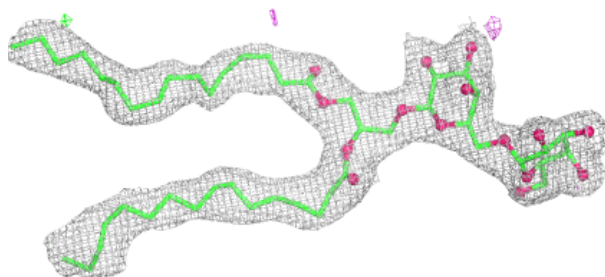
**Electron density around CLA b 613:**

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



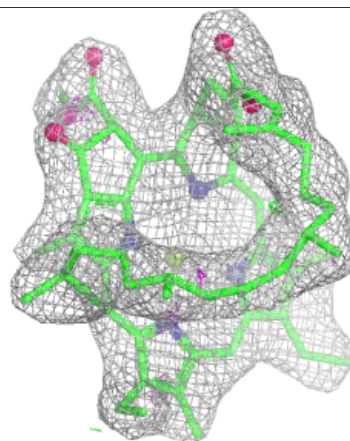
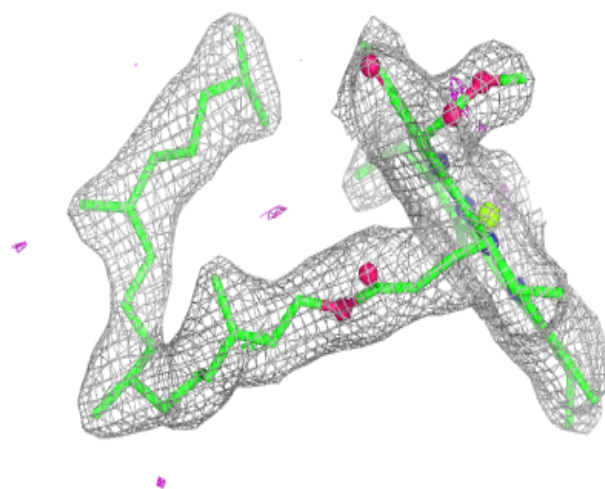
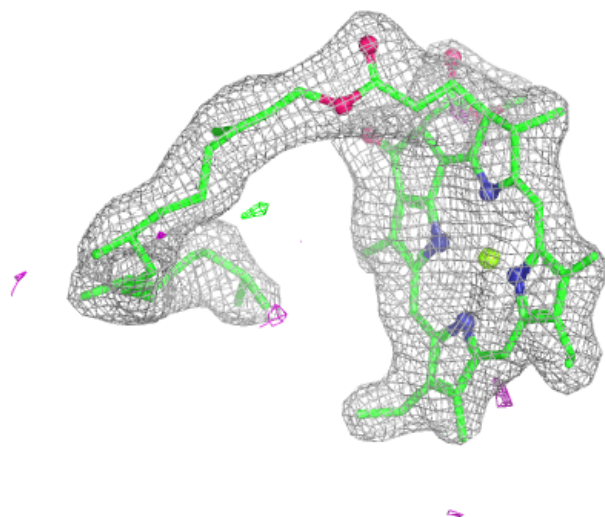
Electron density around DGD C 517:

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



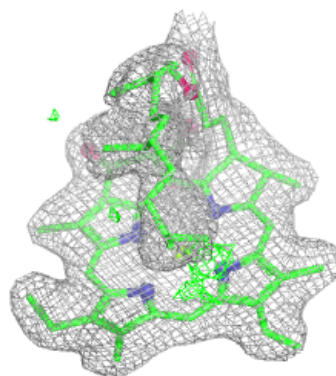
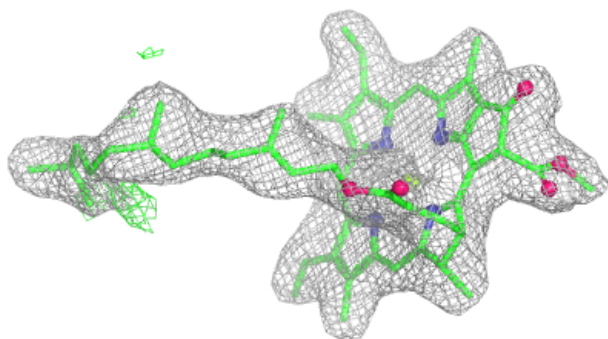
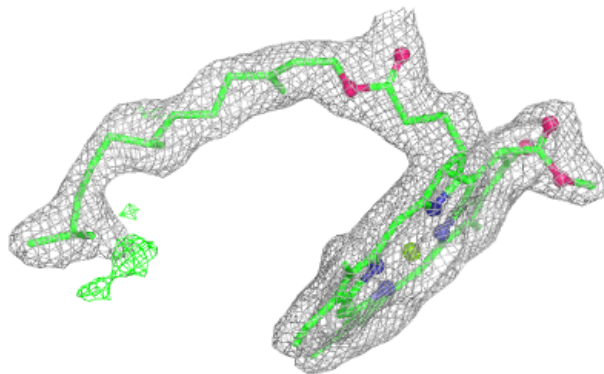
Electron density around CLA c 503:

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

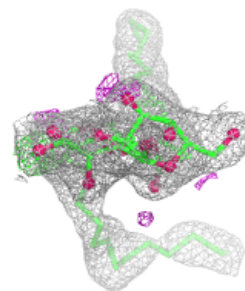
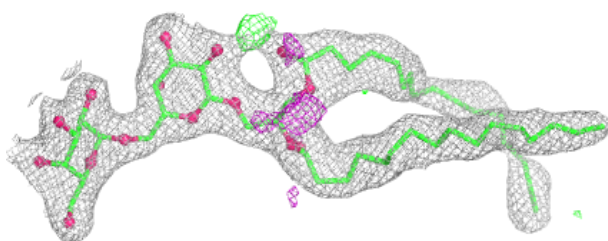
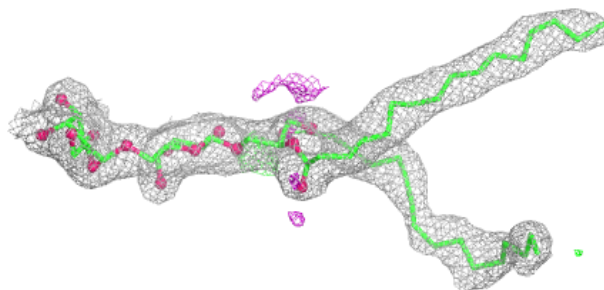


Electron density around CLA c 504:

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

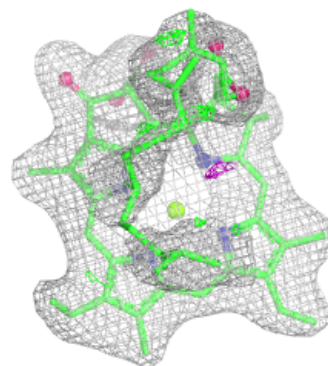
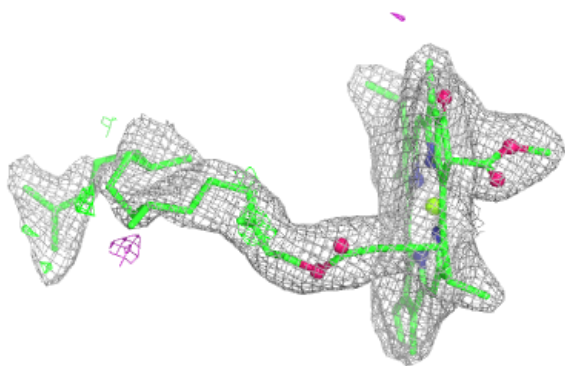
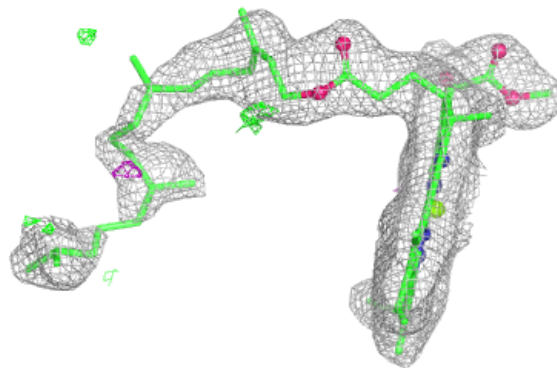
**Electron density around DGD c 517:**

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

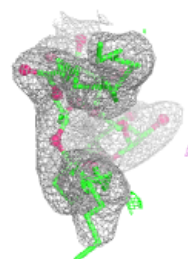
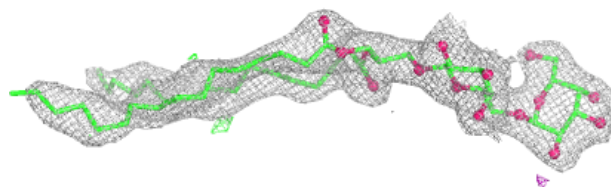
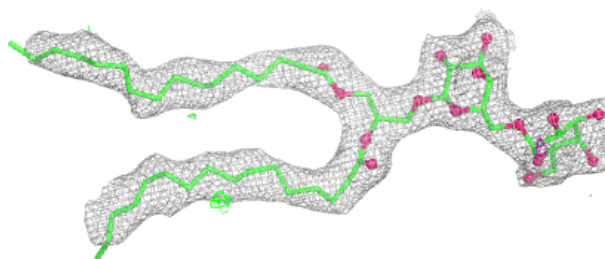


Electron density around CLA c 506:

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

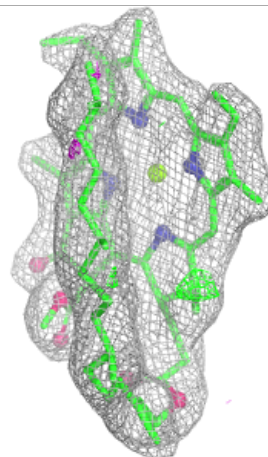
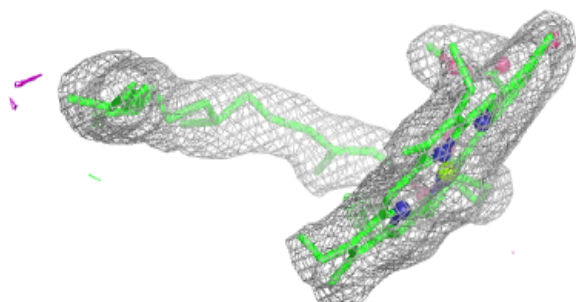
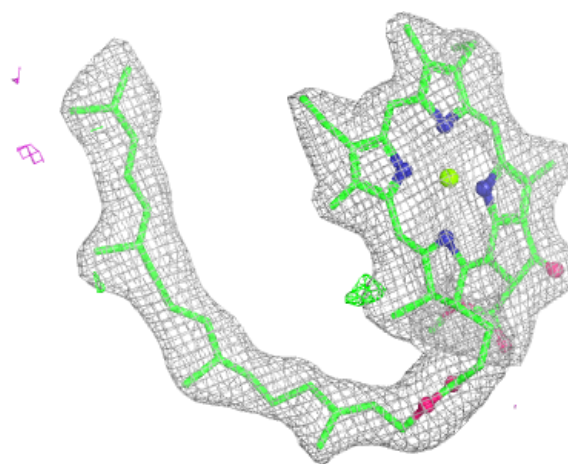
**Electron density around DGD c 519:**

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



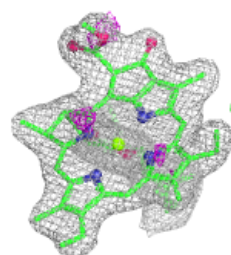
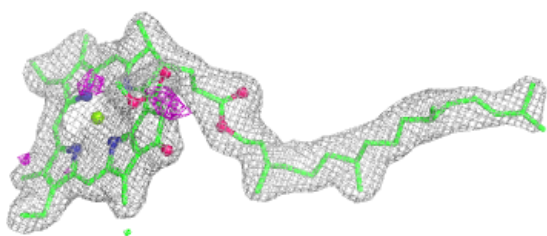
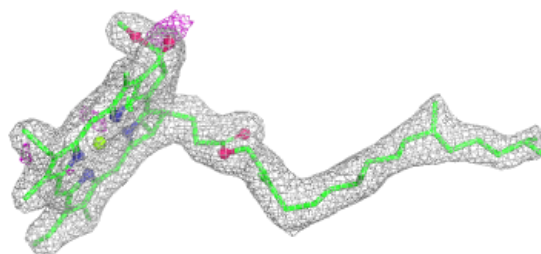
Electron density around CLA c 507:

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

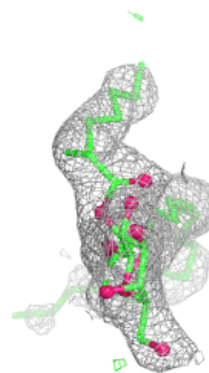
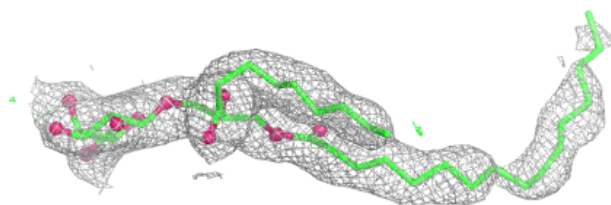
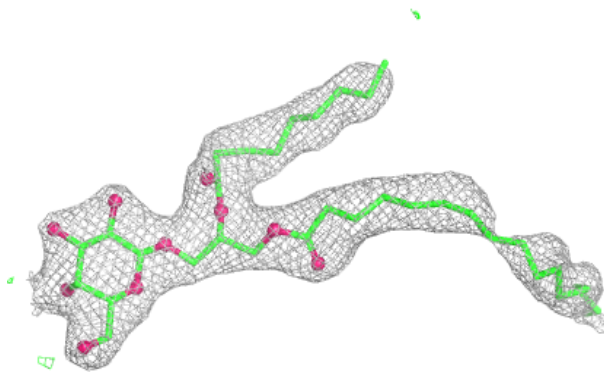


Electron density around CLA C 502:

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

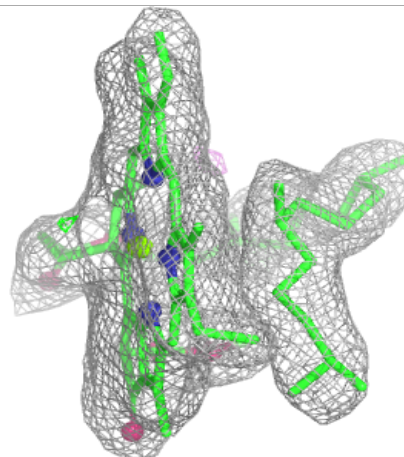
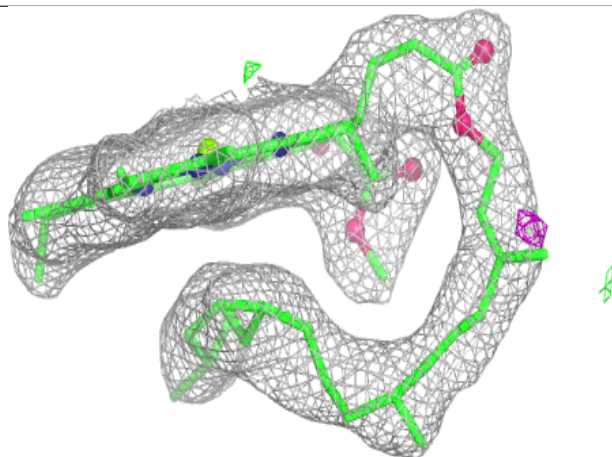
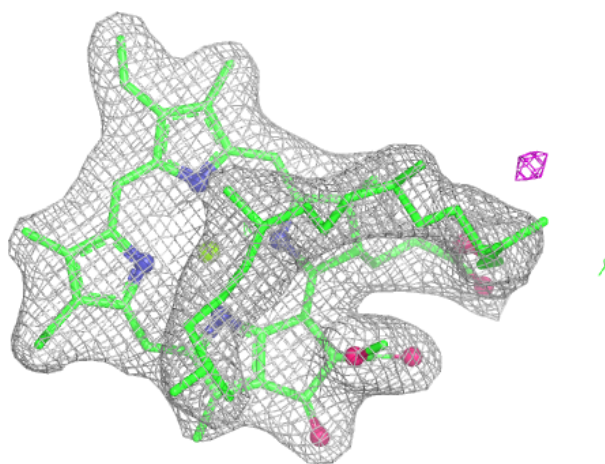
**Electron density around LMG d 411:**

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



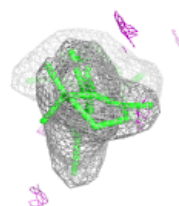
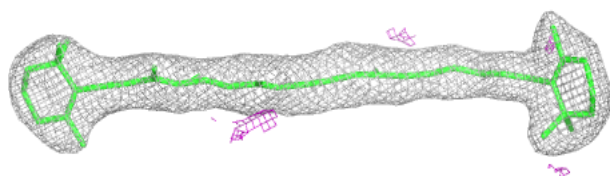
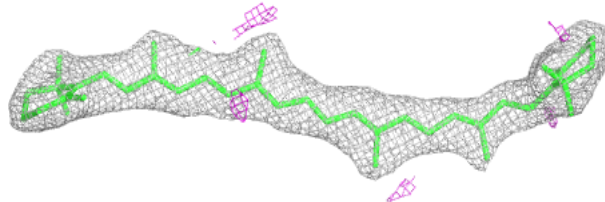
Electron density around CLA c 510:

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

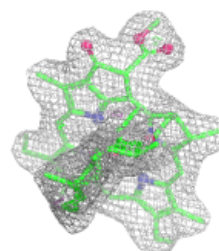
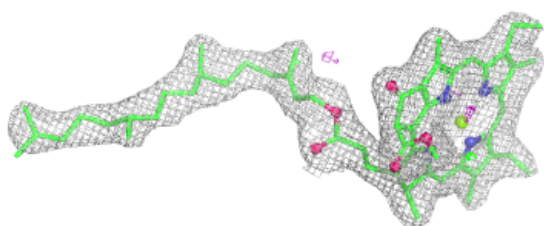
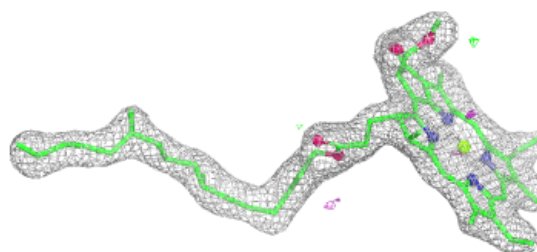


Electron density around BCR c 515:

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

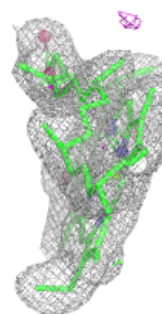
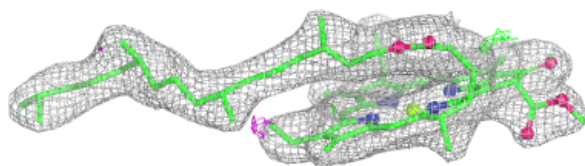
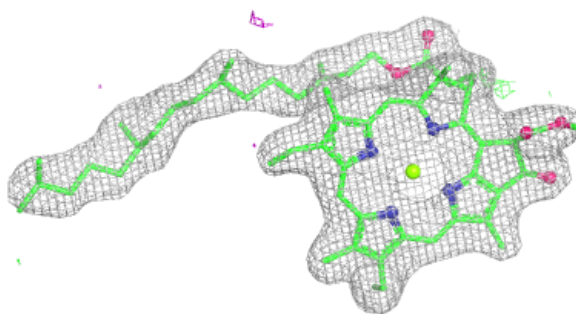
**Electron density around CLA c 502:**

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

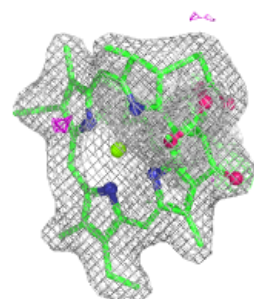
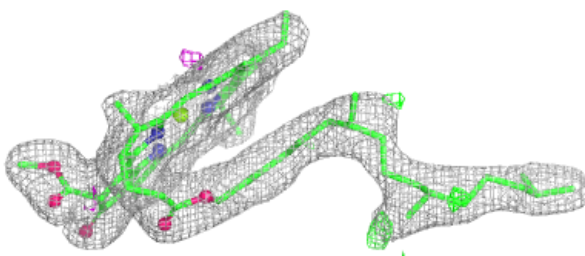
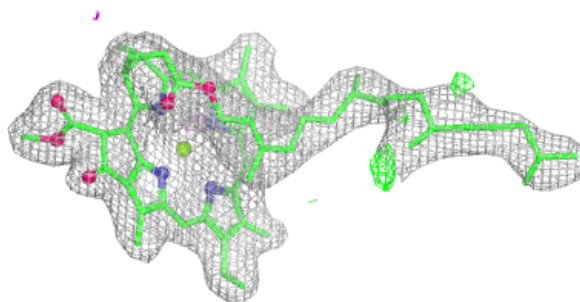


Electron density around CLA C 501:

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

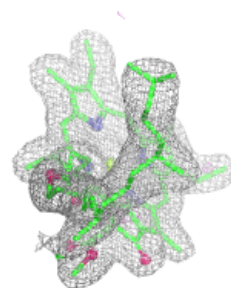
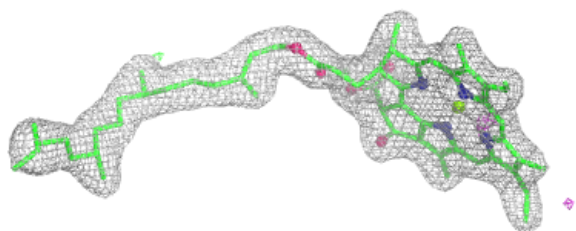
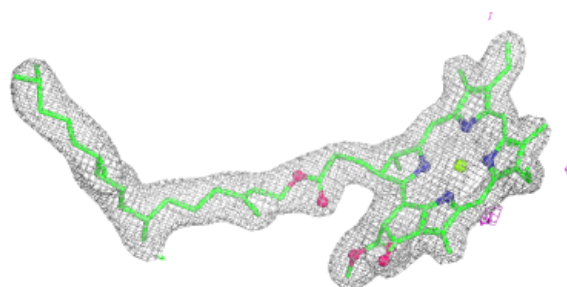
**Electron density around CLA c 505:**

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

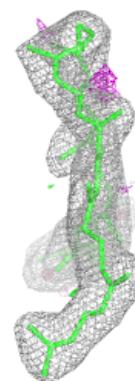
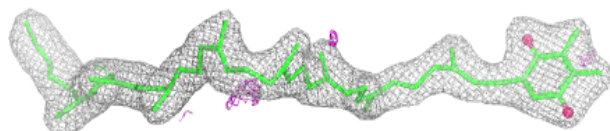
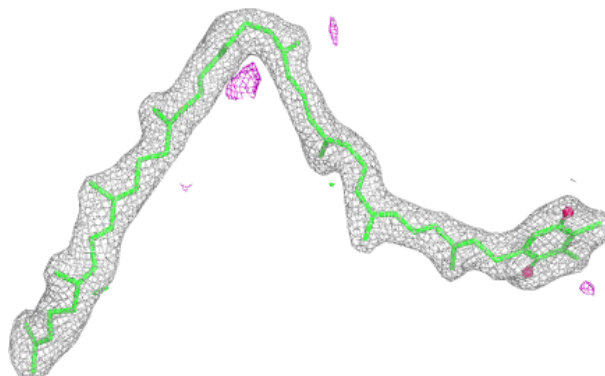


Electron density around CLA a 606:

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

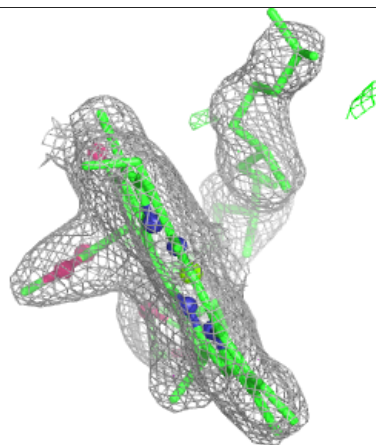
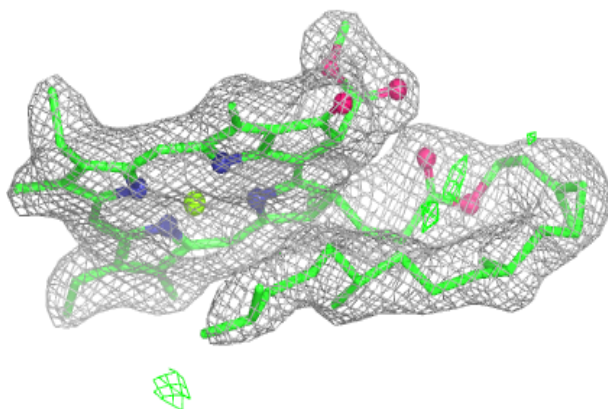
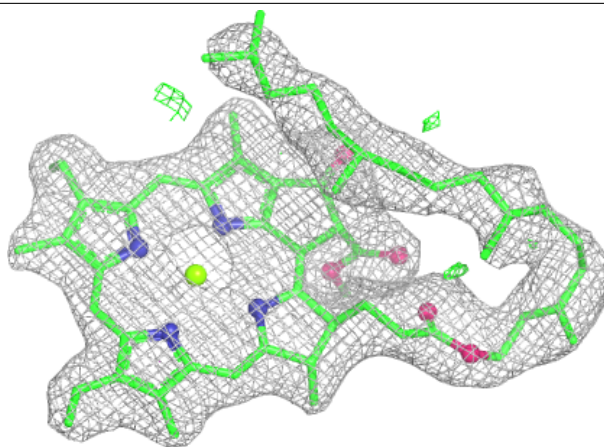
**Electron density around PL9 D 405:**

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

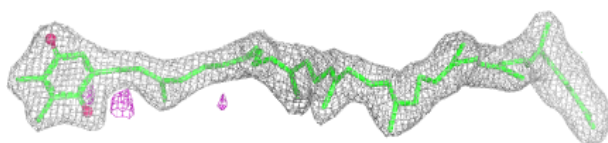
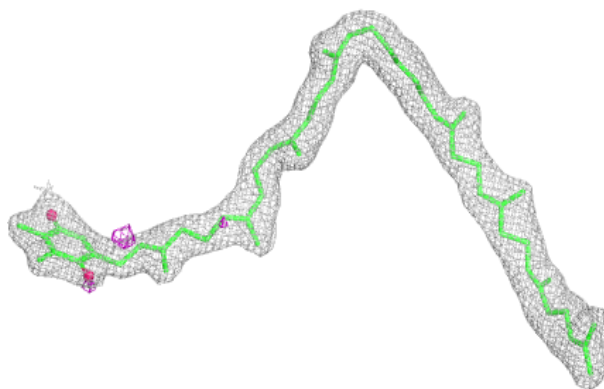


Electron density around CLA C 509:

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

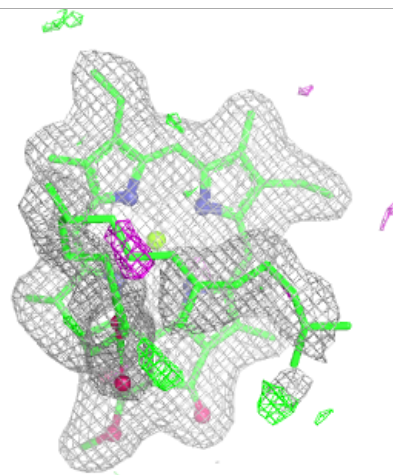
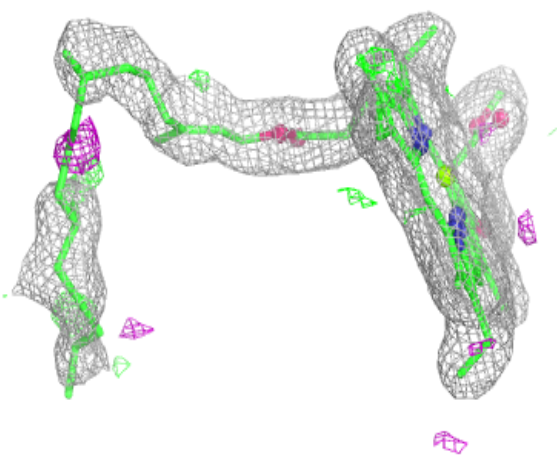
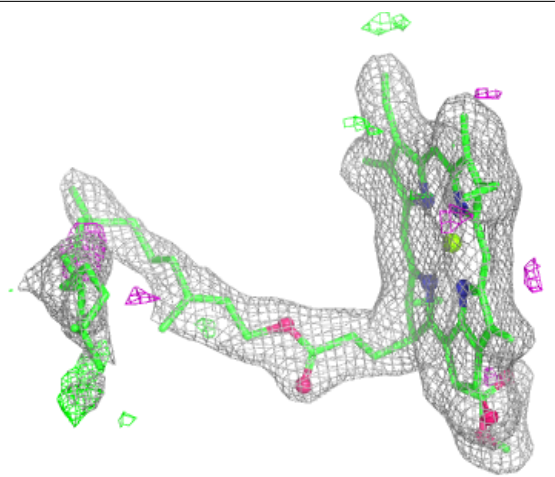
**Electron density around PL9 d 406:**

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



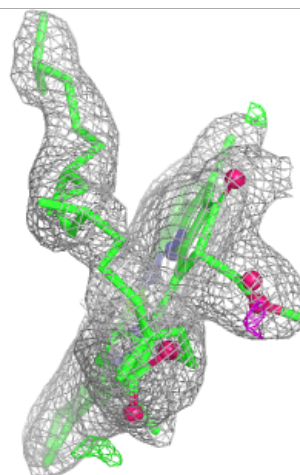
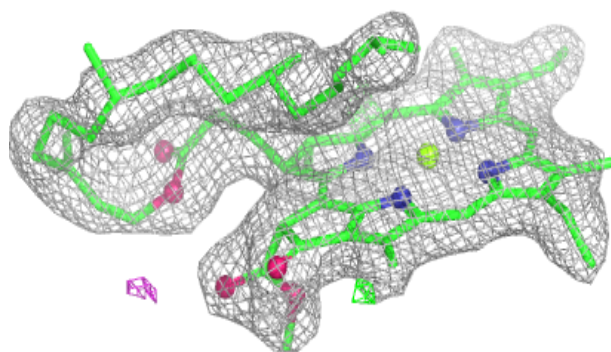
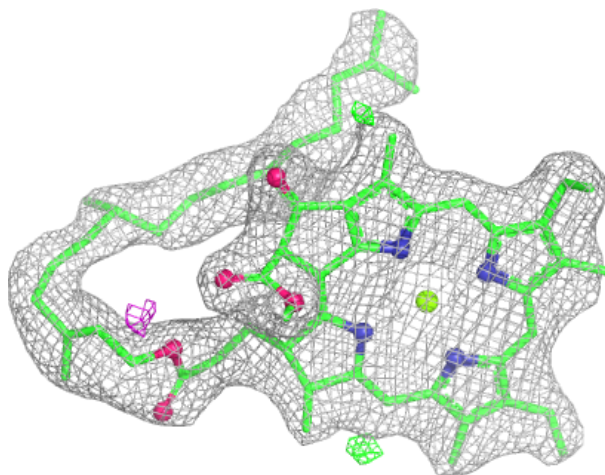
Electron density around CLA a 609:

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



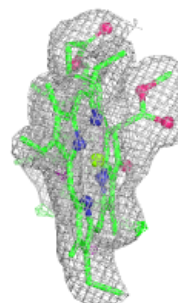
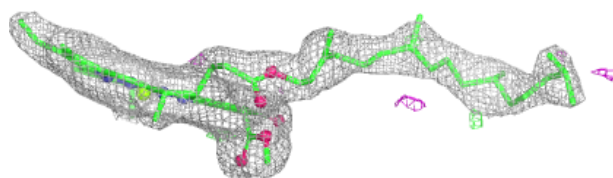
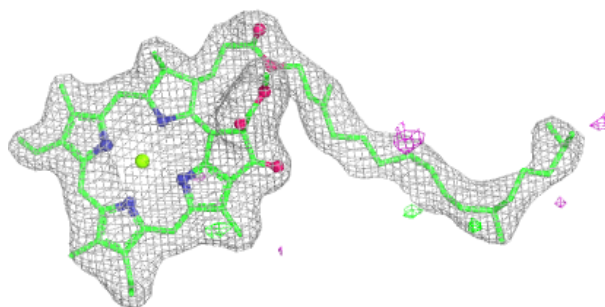
Electron density around CLA c 509:

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

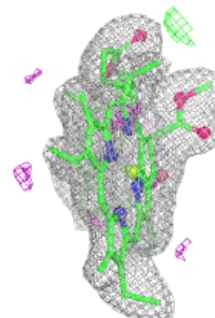
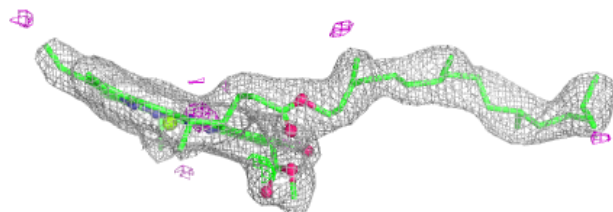
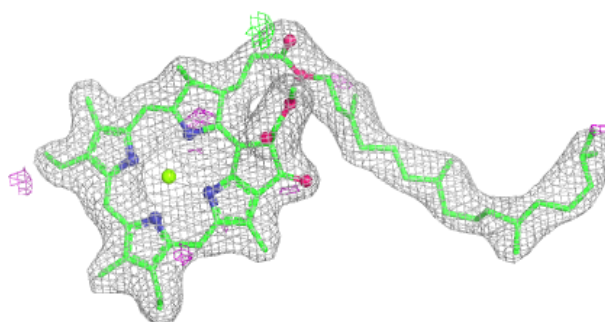


Electron density around CLA b 601:

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

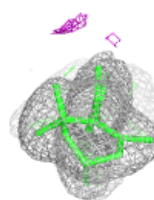
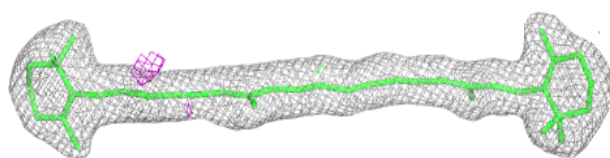
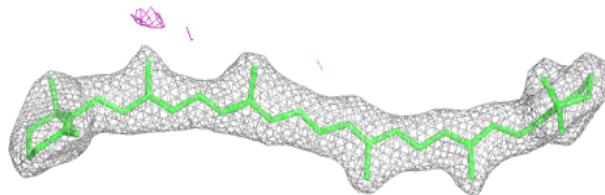
**Electron density around CLA B 602:**

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

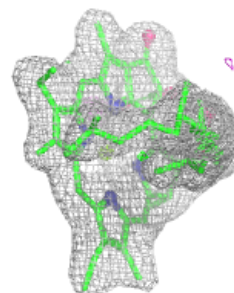
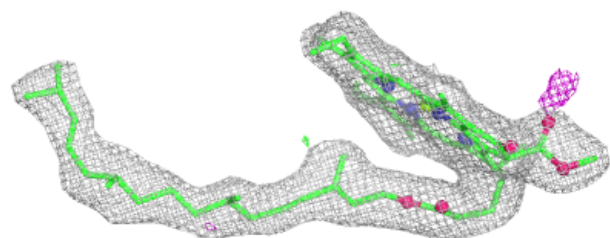
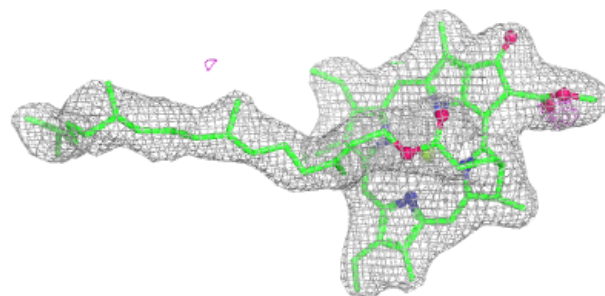


Electron density around BCR a 610:

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

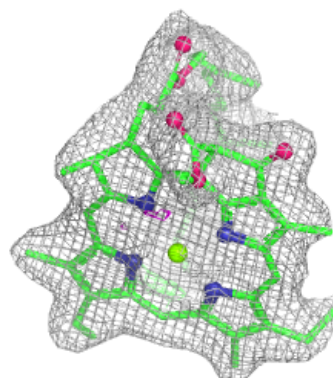
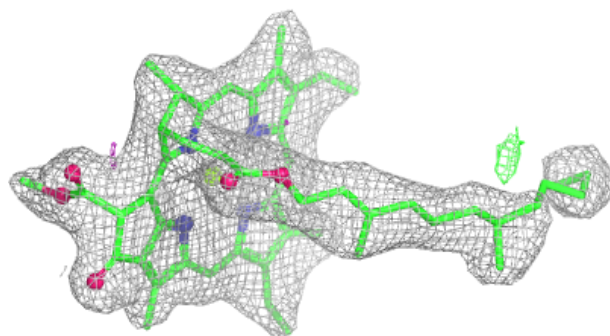
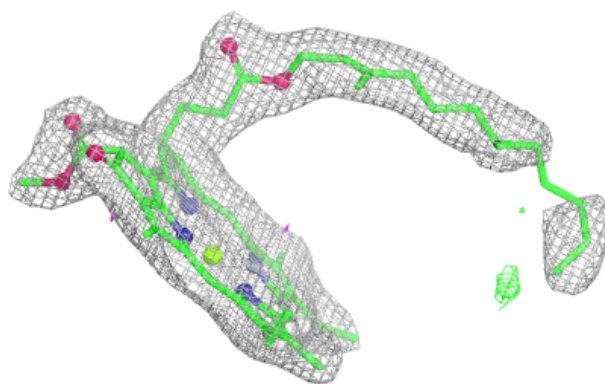
**Electron density around CLA b 607:**

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

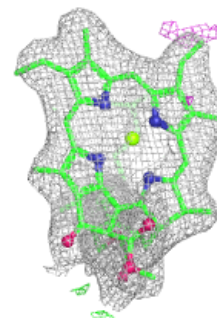
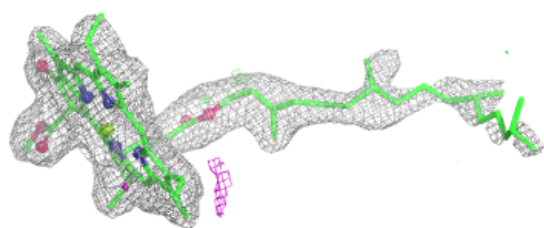
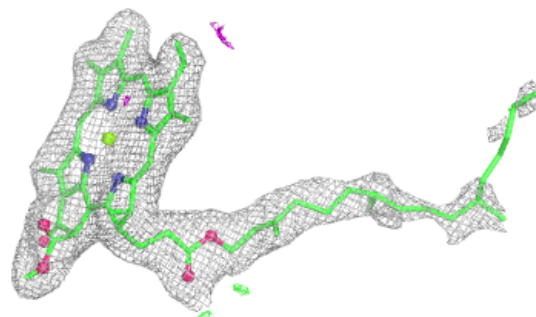


Electron density around CLA C 504:

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

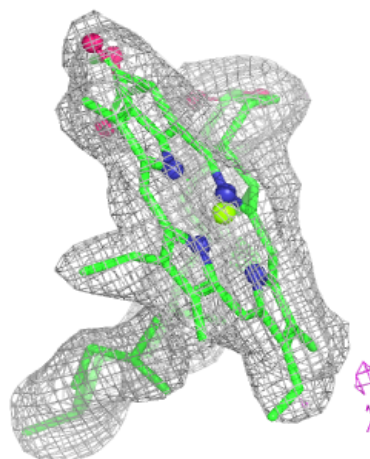
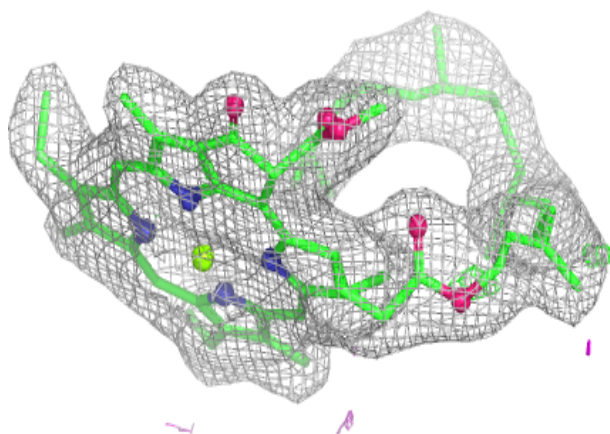
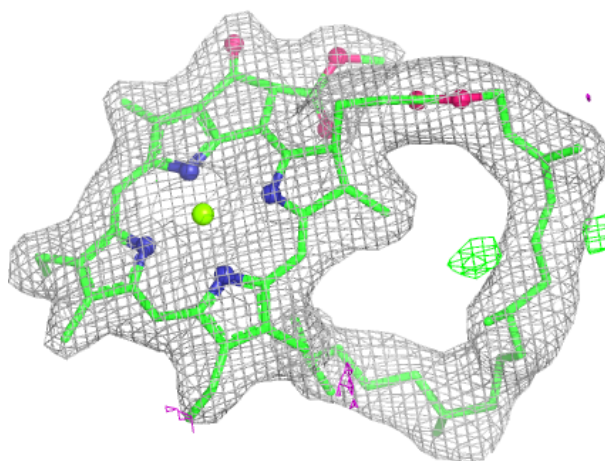
**Electron density around CLA d 404:**

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



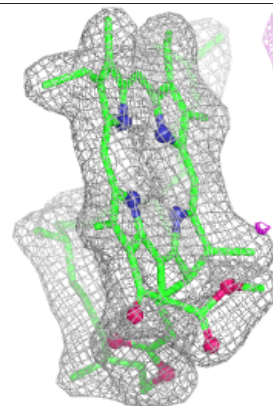
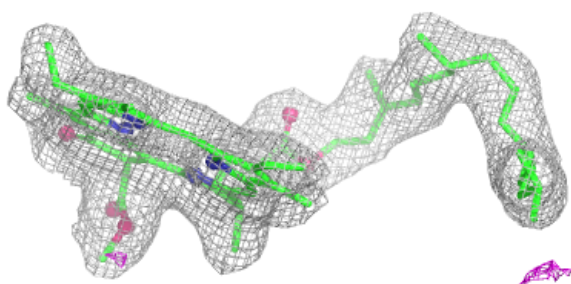
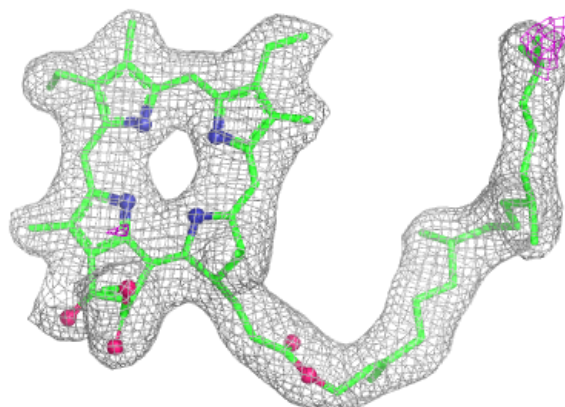
Electron density around CLA b 614:

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

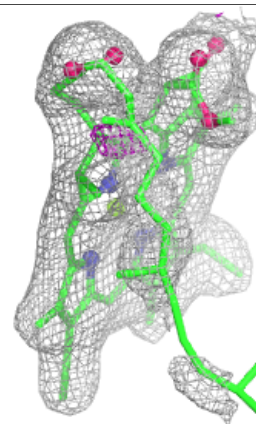
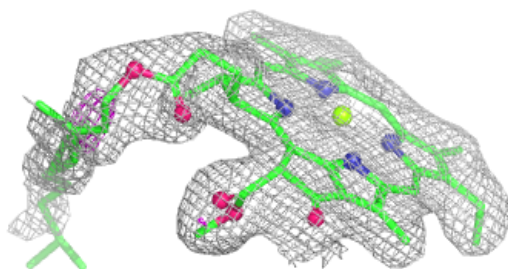
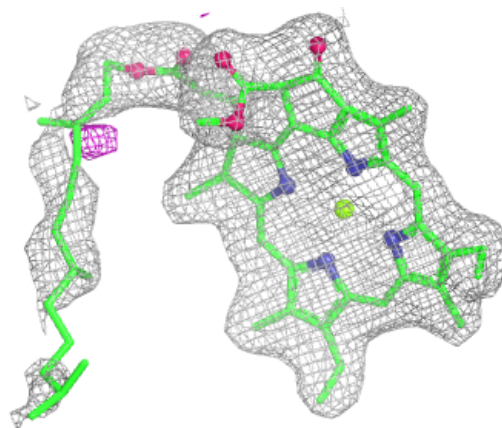


Electron density around PHO d 402:

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

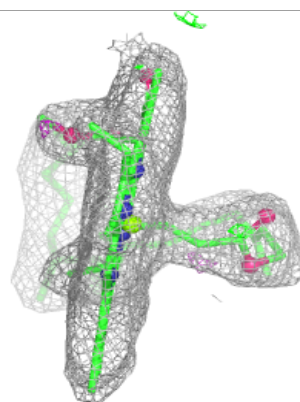
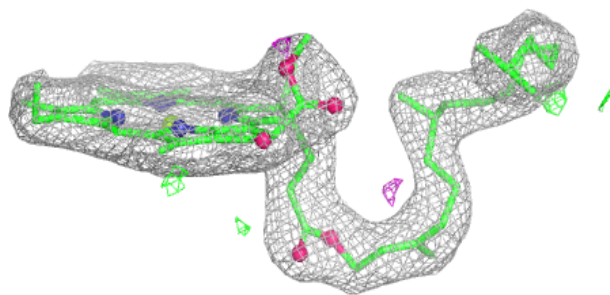
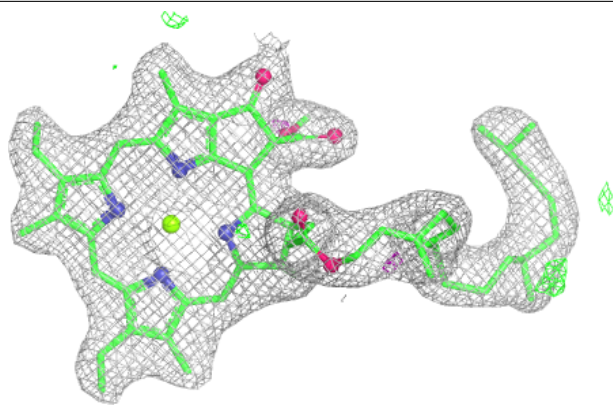
**Electron density around CLA b 615:**

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



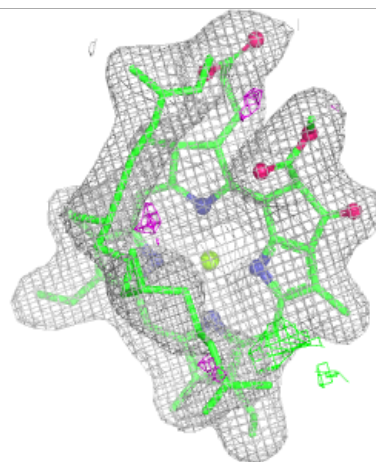
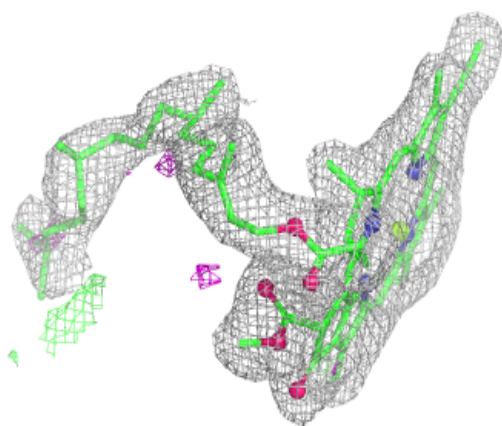
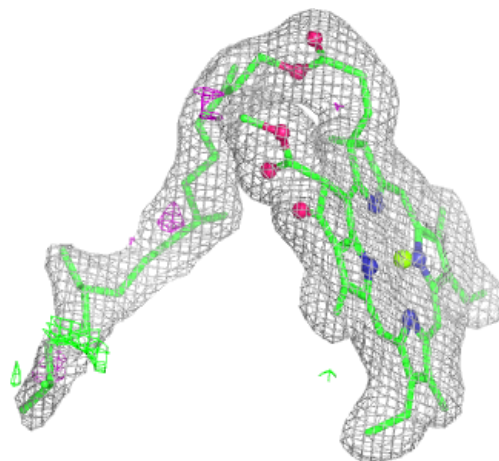
Electron density around CLA b 611:

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



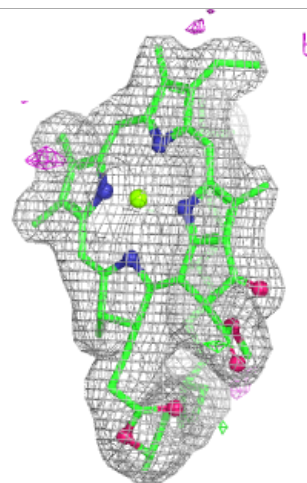
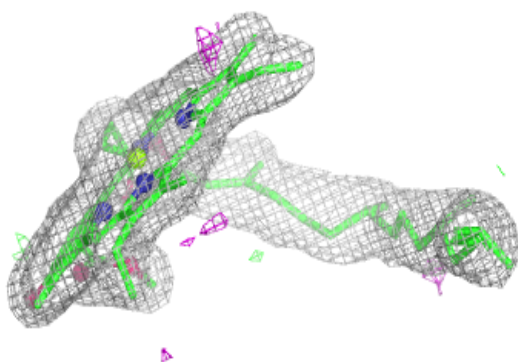
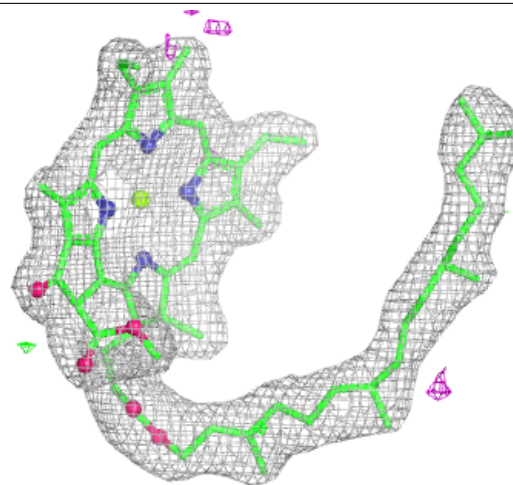
Electron density around CLA b 612:

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



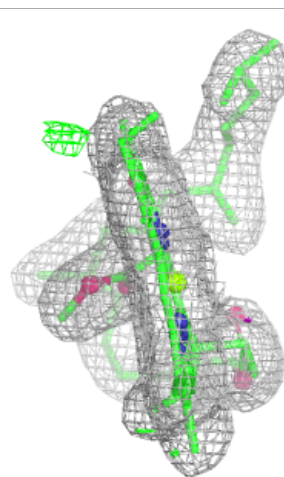
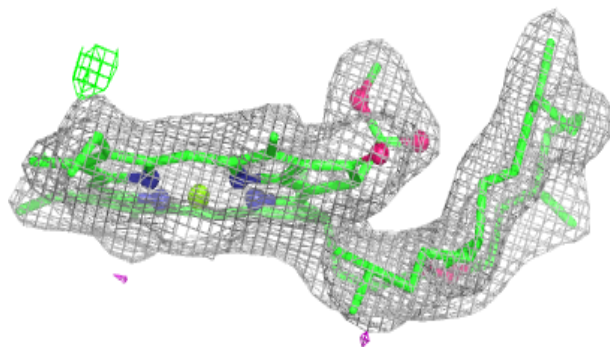
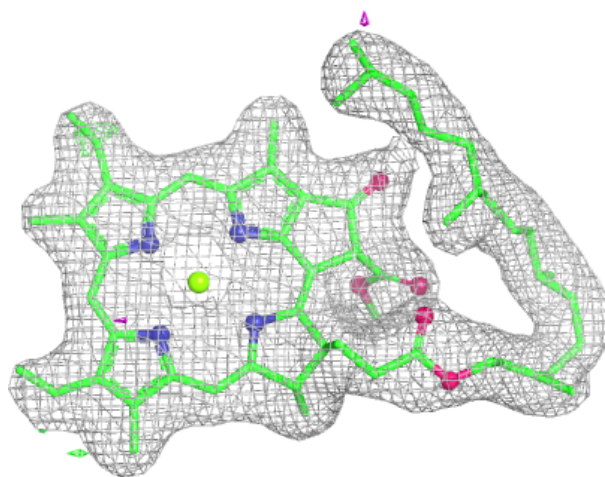
Electron density around CLA C 507:

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



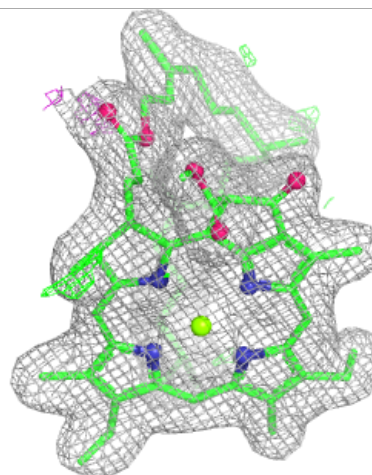
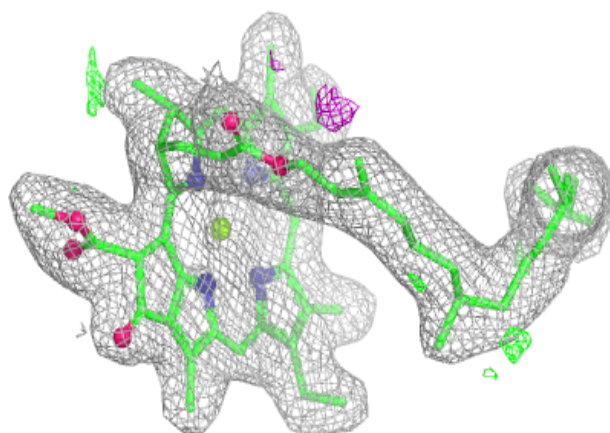
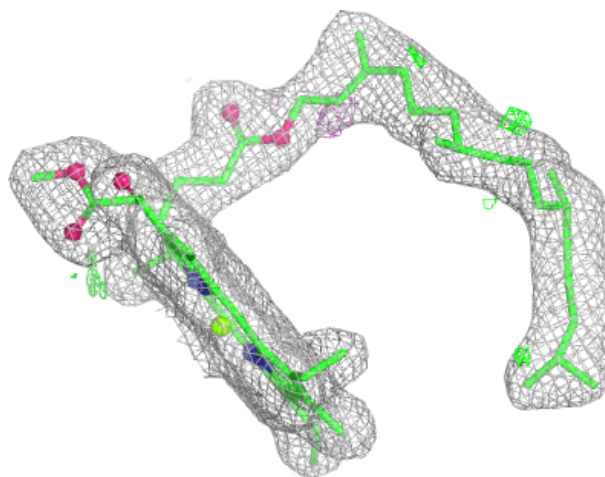
Electron density around CLA B 610:

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



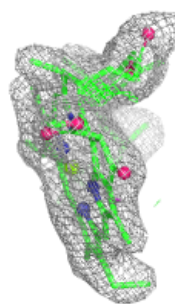
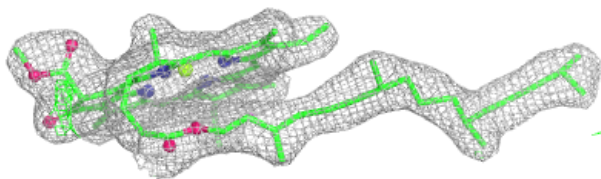
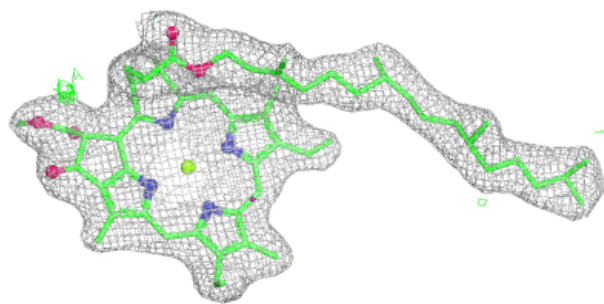
Electron density around CLA B 611:

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

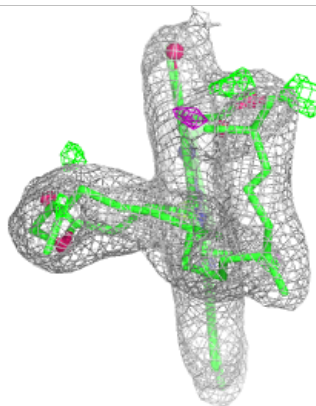
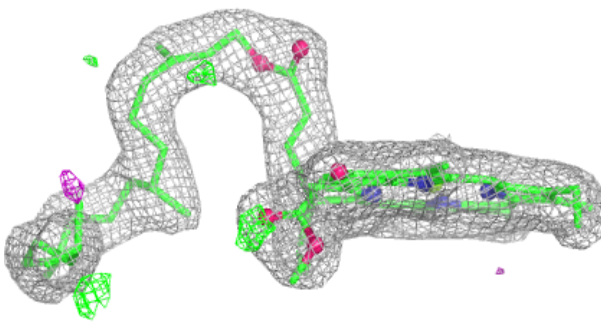
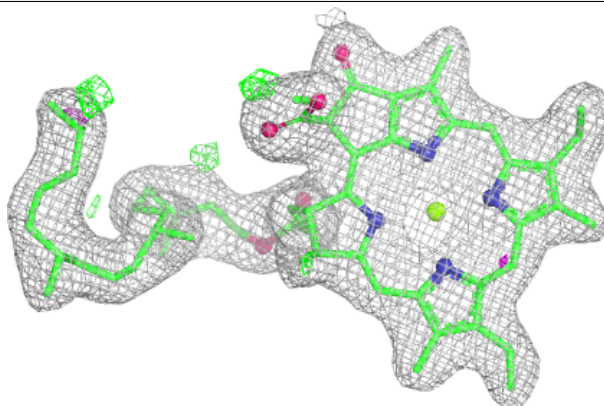


Electron density around CLA c 501:

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

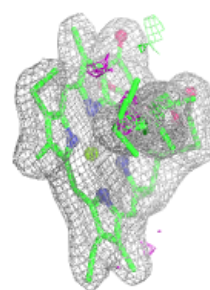
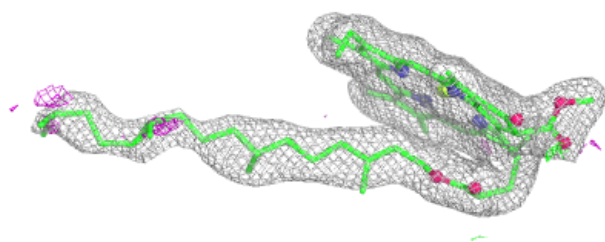
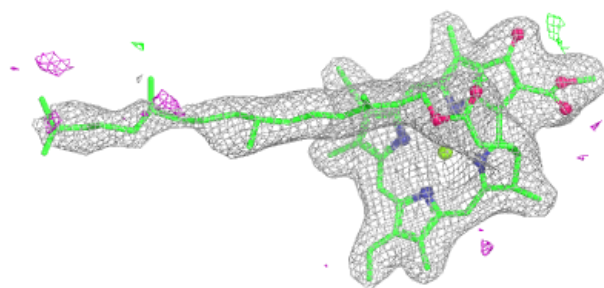
**Electron density around CLA B 612:**

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



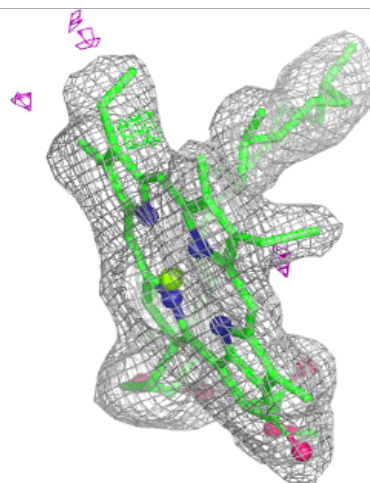
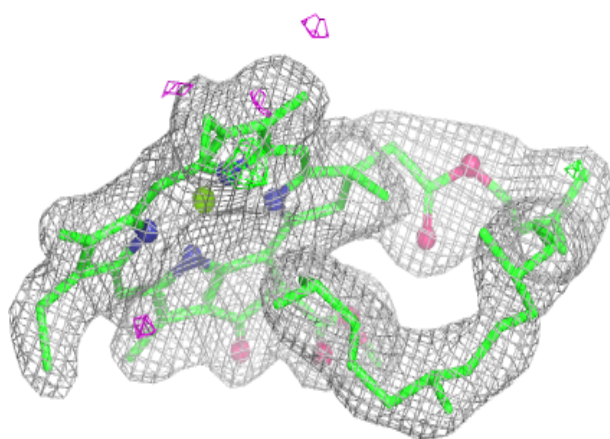
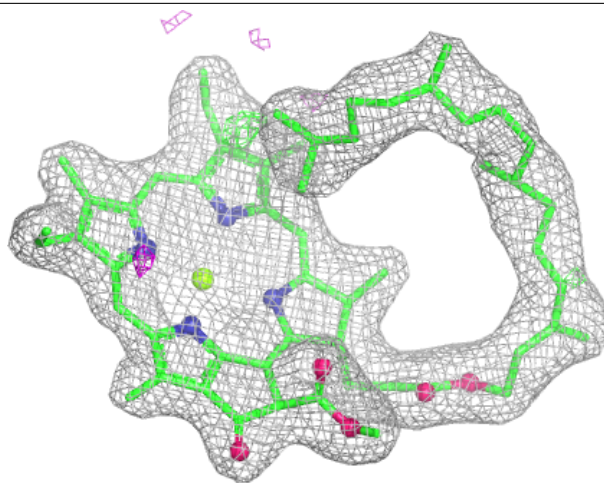
Electron density around CLA B 614:

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



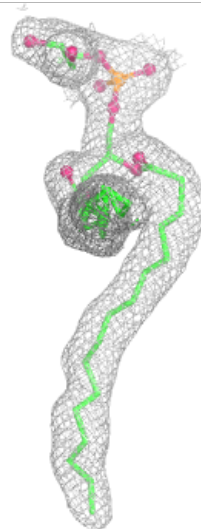
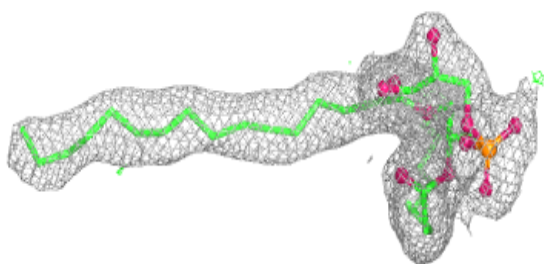
Electron density around CLA B 615:

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



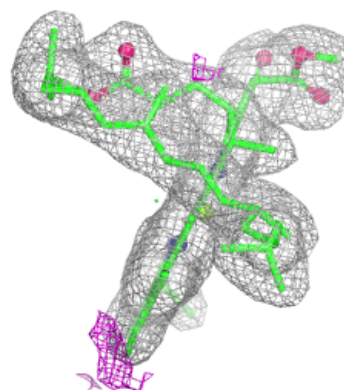
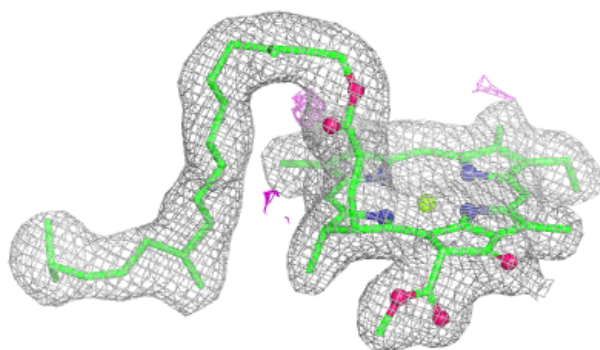
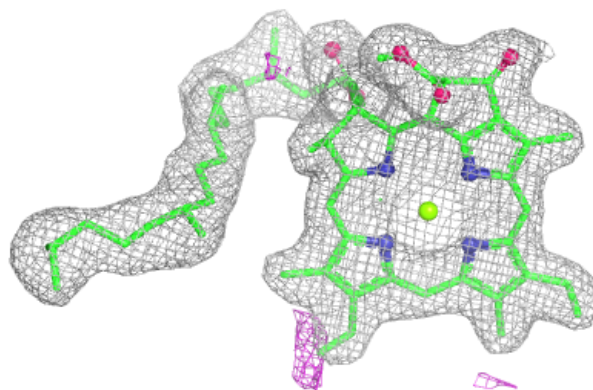
Electron density around LHG L 101:

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

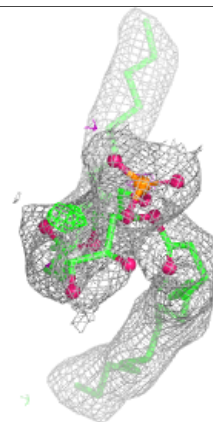
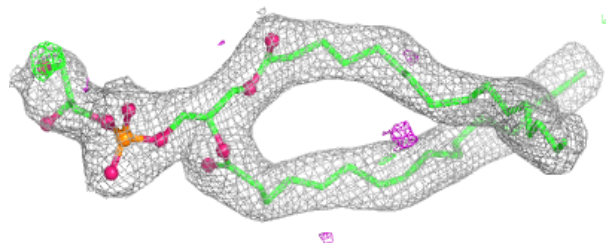
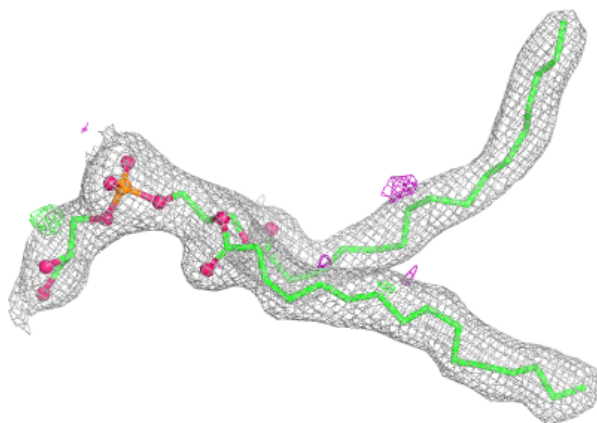


Electron density around CLA A 613:

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

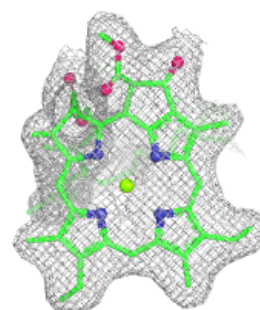
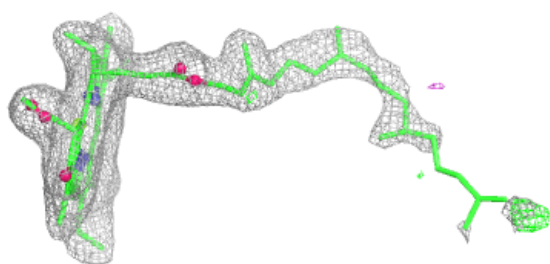
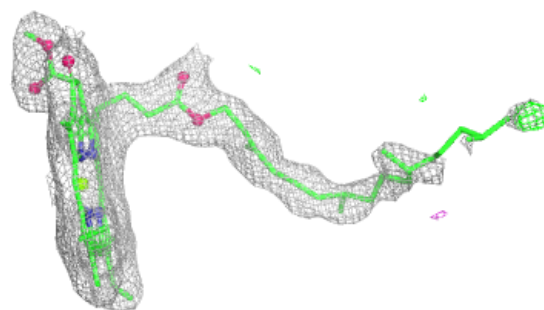
**Electron density around LHG d 408:**

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

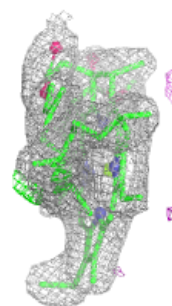
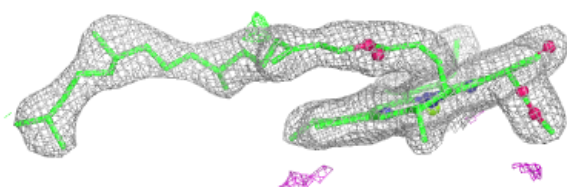
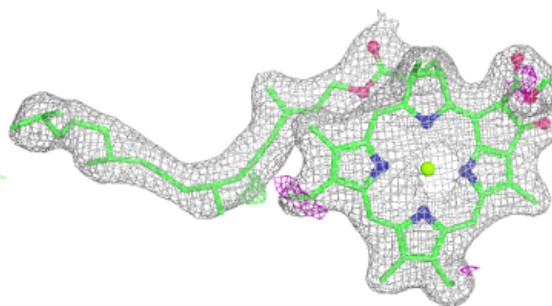


Electron density around CLA D 403:

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

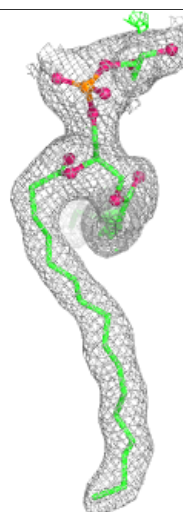
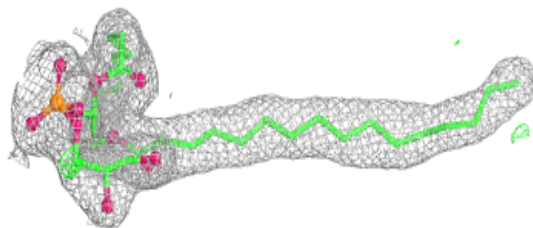
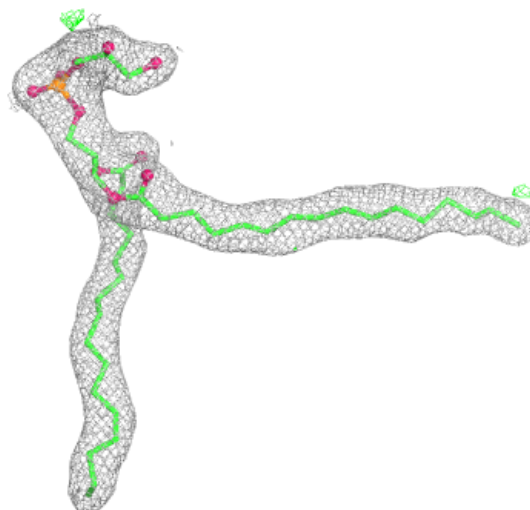
**Electron density around CLA B 603:**

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



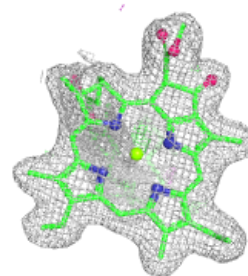
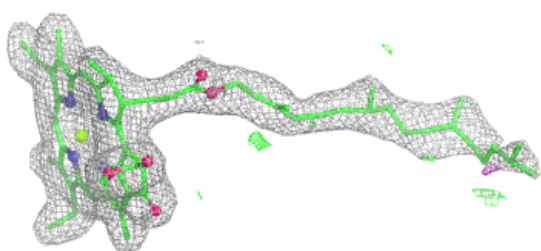
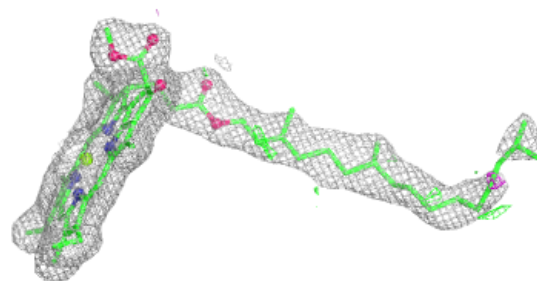
Electron density around LHG 1 101:

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

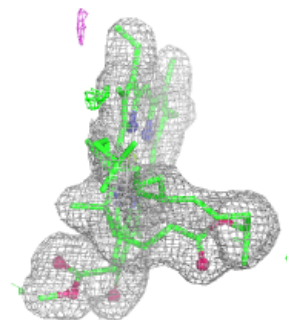
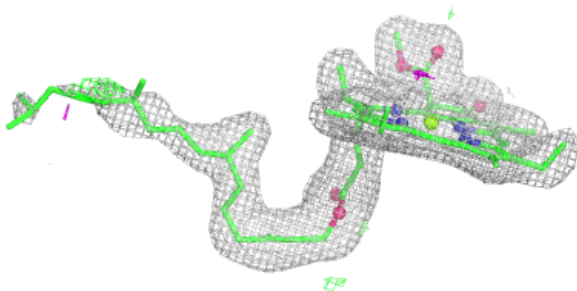
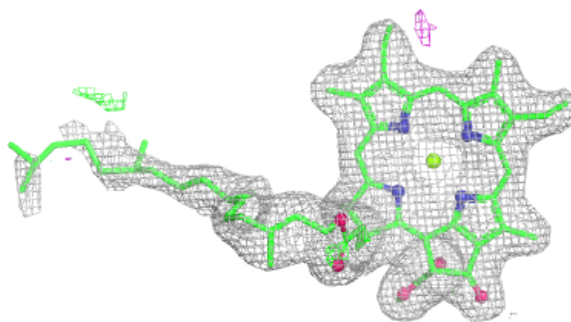


Electron density around CLA B 604:

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

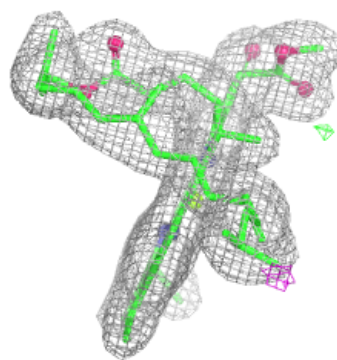
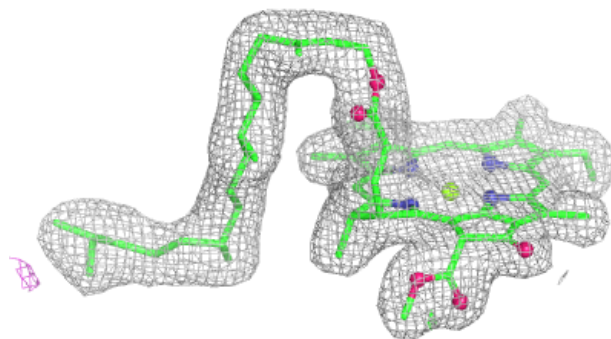
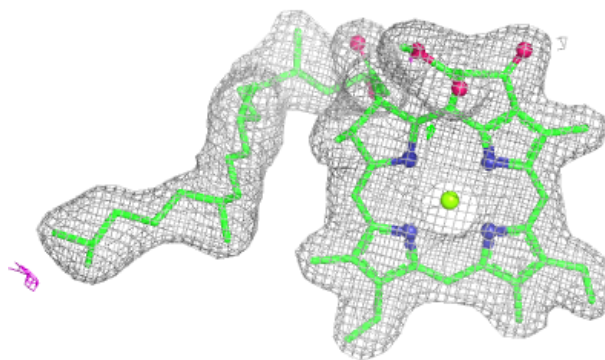
**Electron density around CLA A 608:**

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

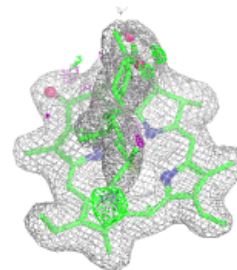
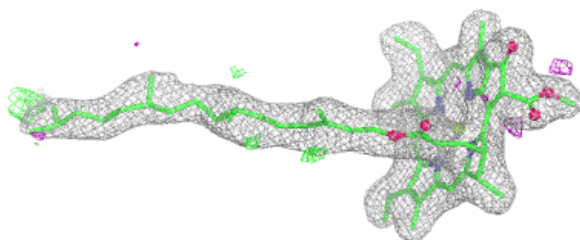
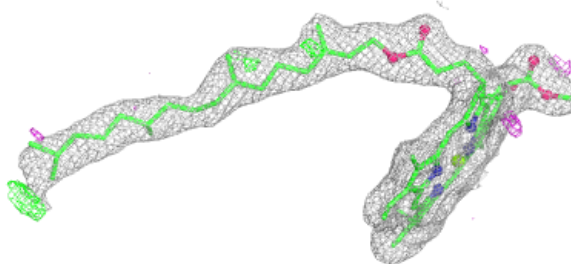


Electron density around CLA a 612:

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

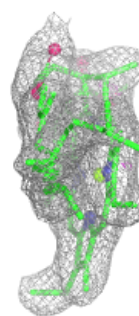
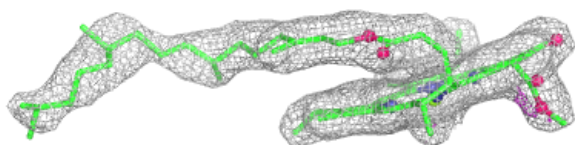
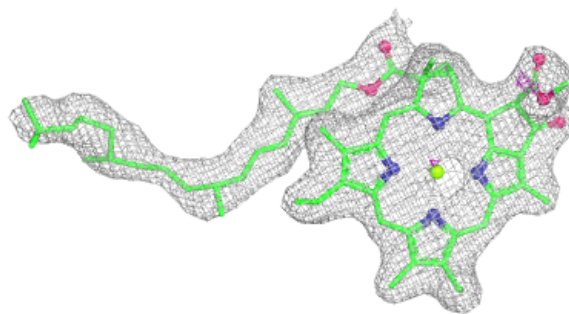
**Electron density around CLA B 607:**

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

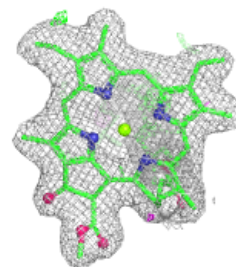
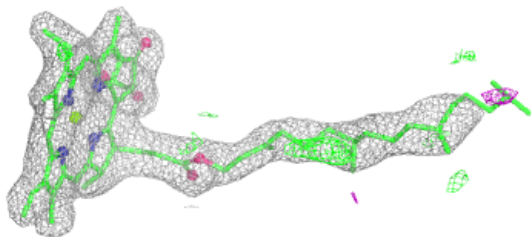
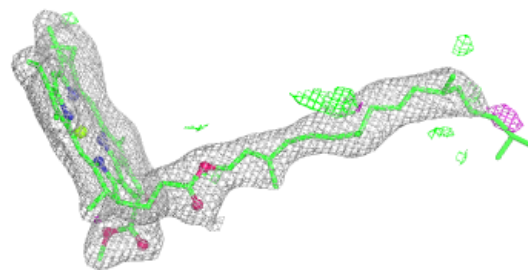


Electron density around CLA b 602:

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

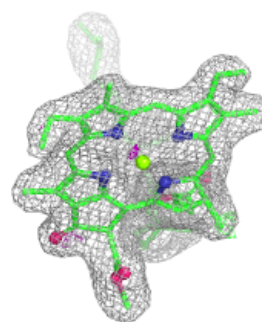
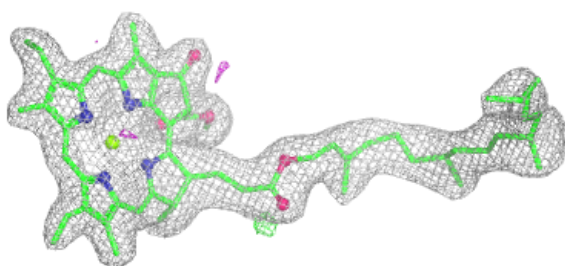
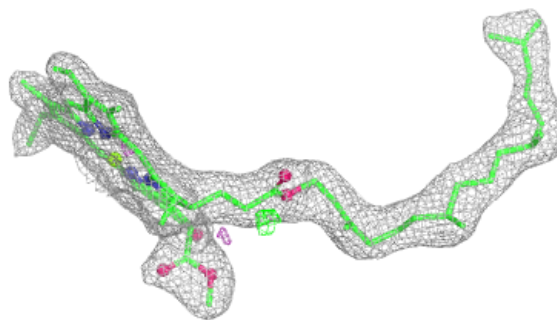
**Electron density around CLA b 603:**

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

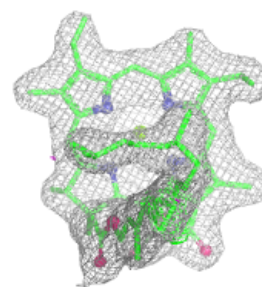
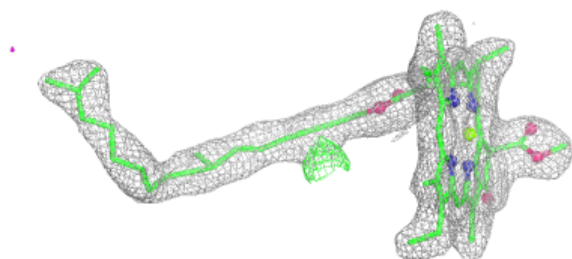
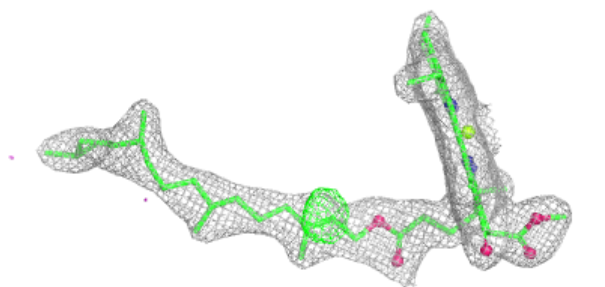


Electron density around CLA d 403:

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

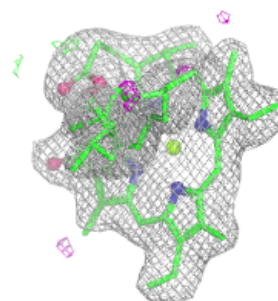
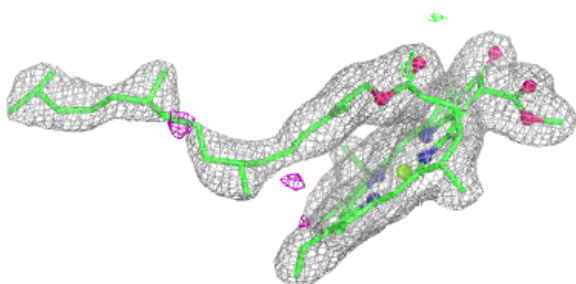
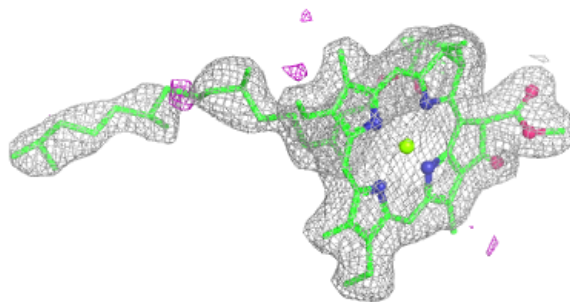
**Electron density around CLA b 604:**

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

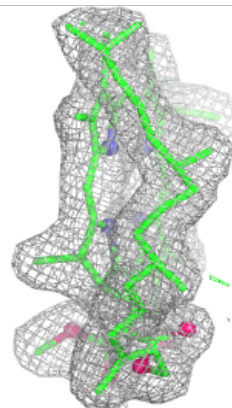
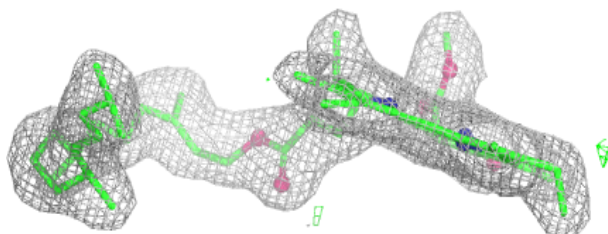
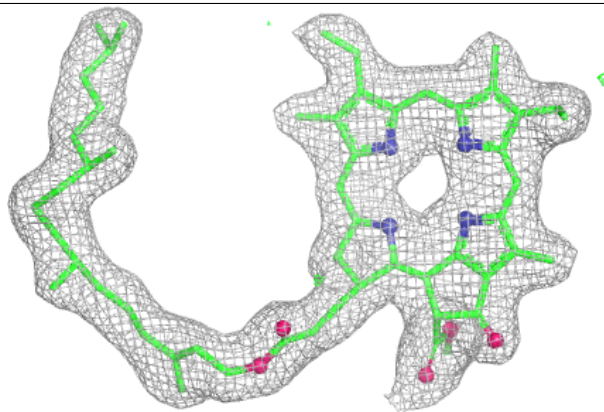


Electron density around CLA C 505:

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

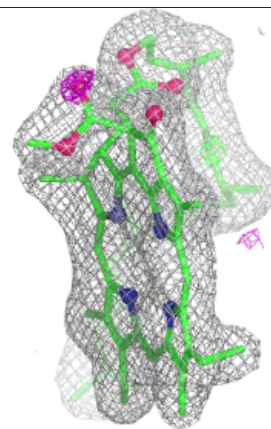
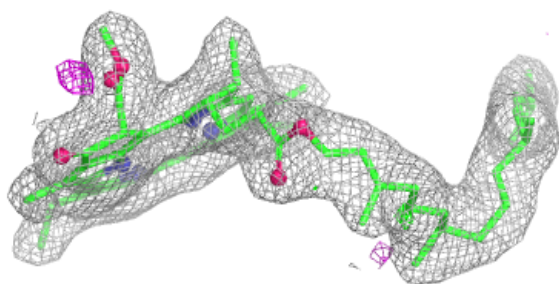
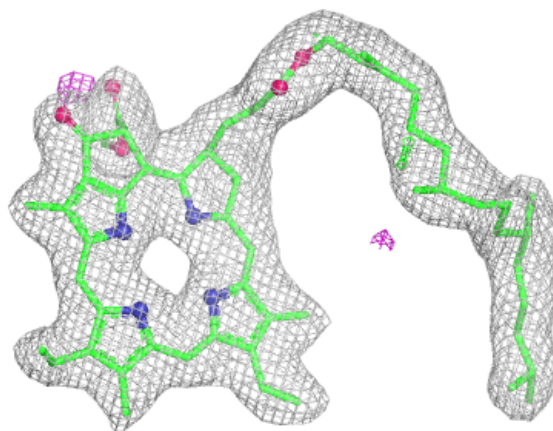
**Electron density around PHO A 609:**

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



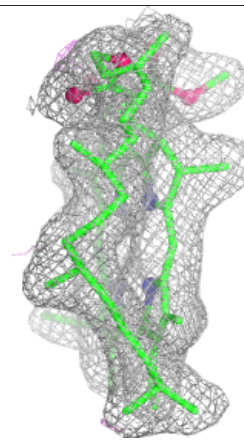
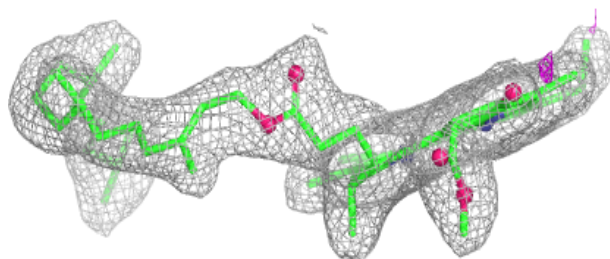
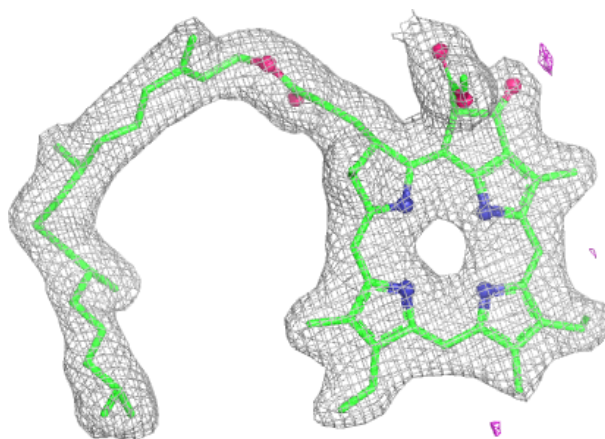
Electron density around PHO D 401:

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



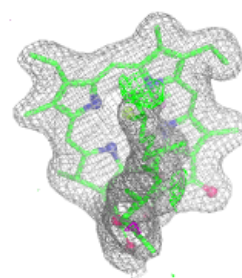
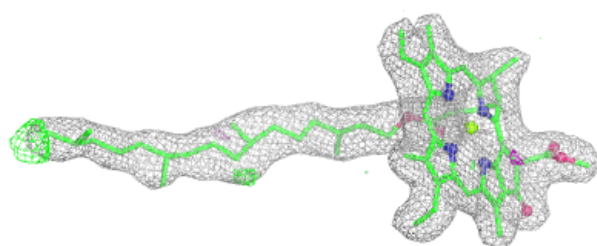
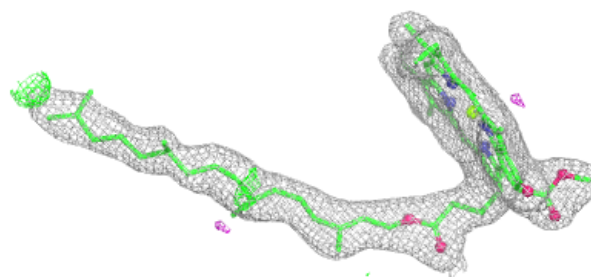
Electron density around PHO a 608:

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

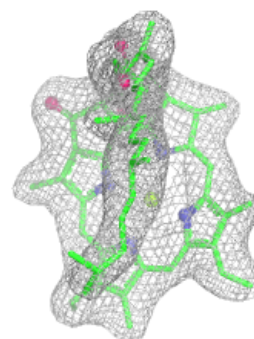
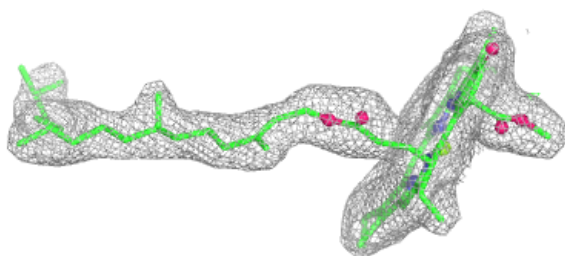
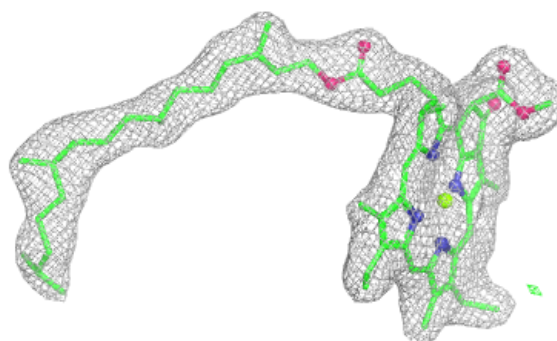


Electron density around CLA b 606:

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

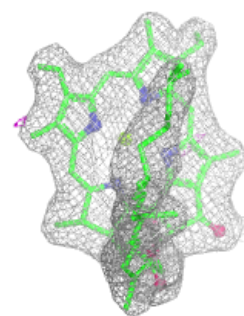
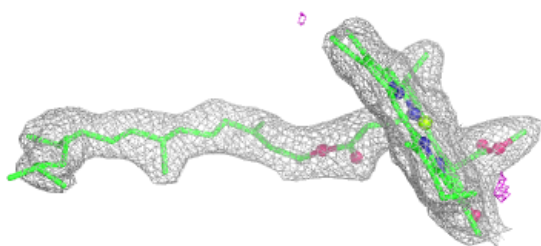
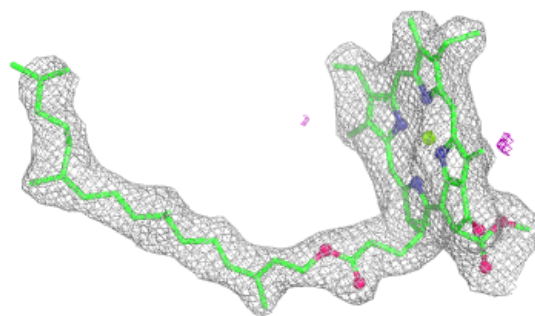
**Electron density around CLA B 609:**

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



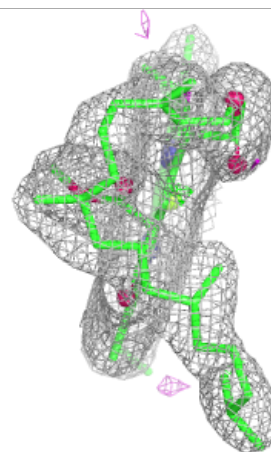
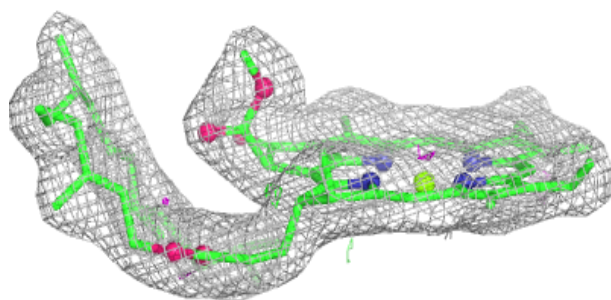
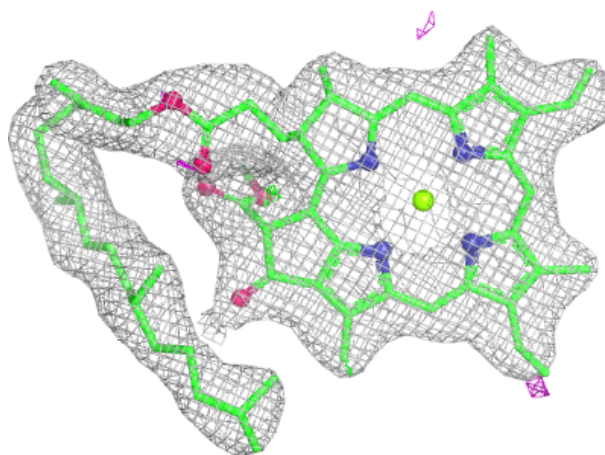
Electron density around CLA b 608:

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



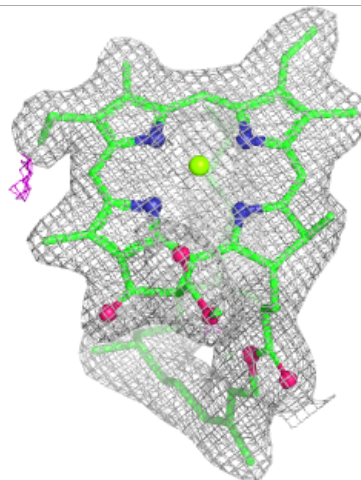
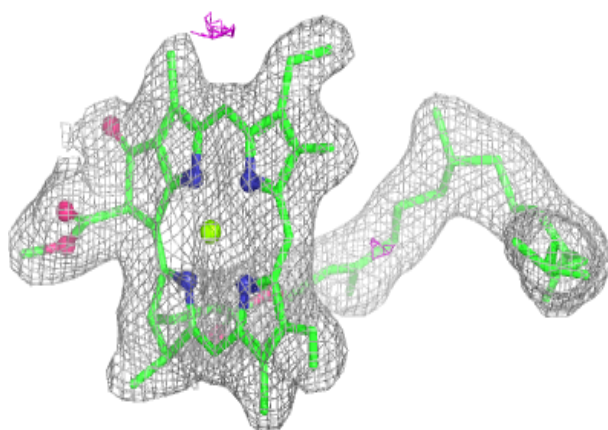
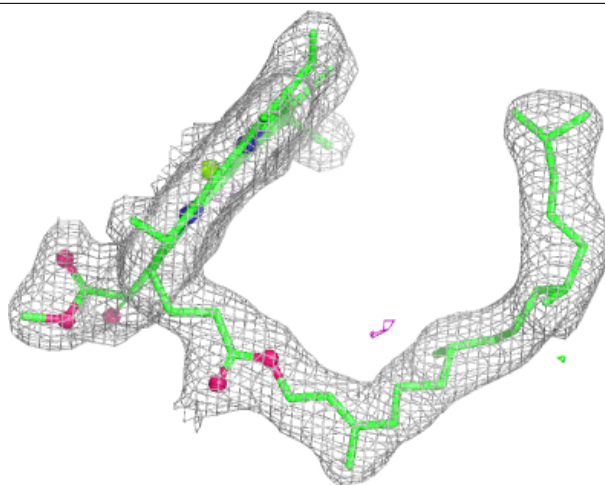
Electron density around CLA b 609:

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



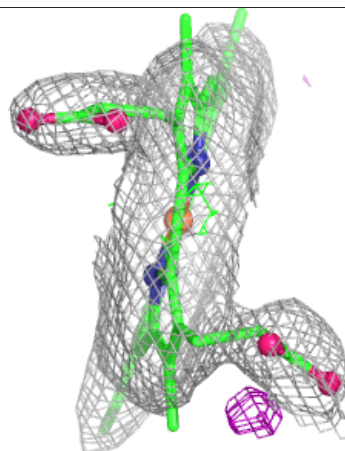
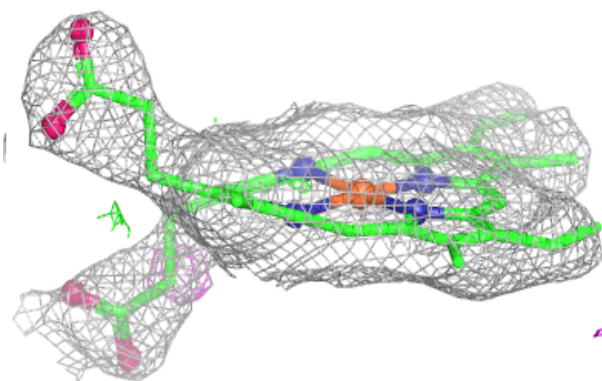
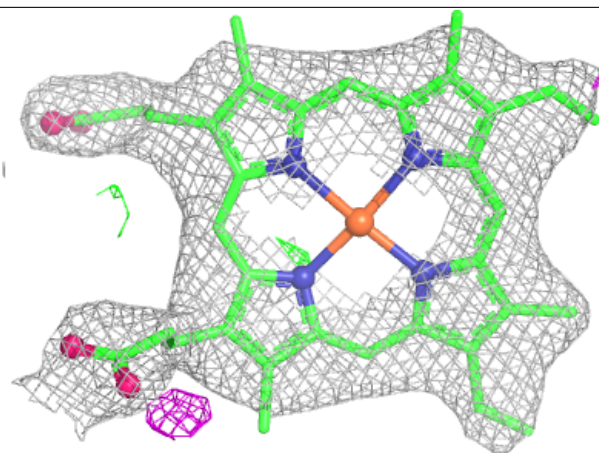
Electron density around CLA b 610:

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



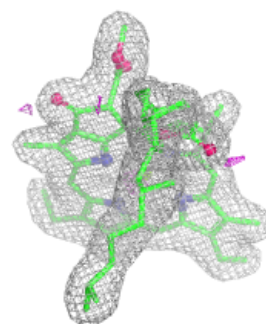
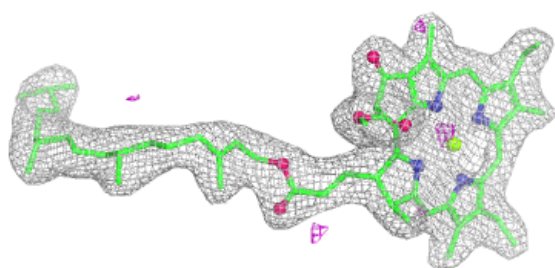
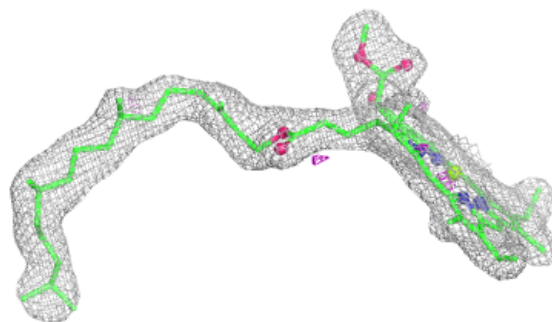
Electron density around HEM e 101:

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

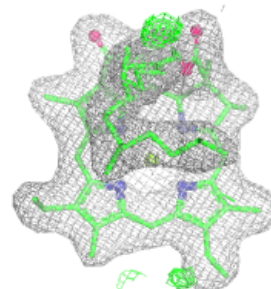
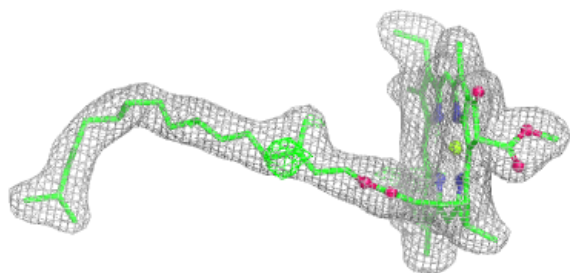
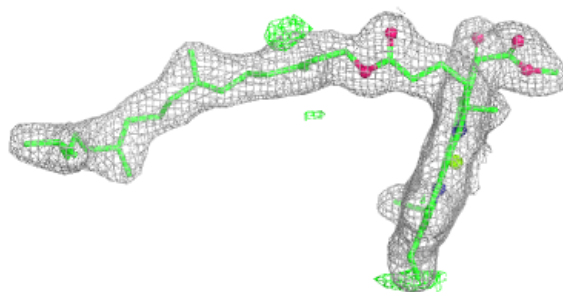


Electron density around CLA D 402:

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

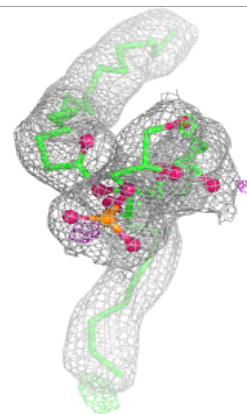
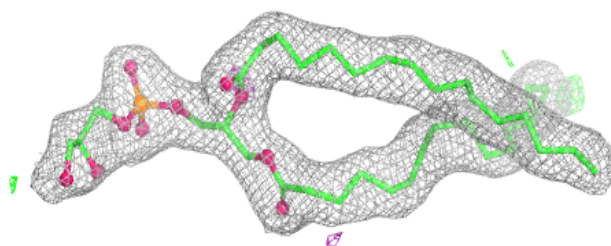
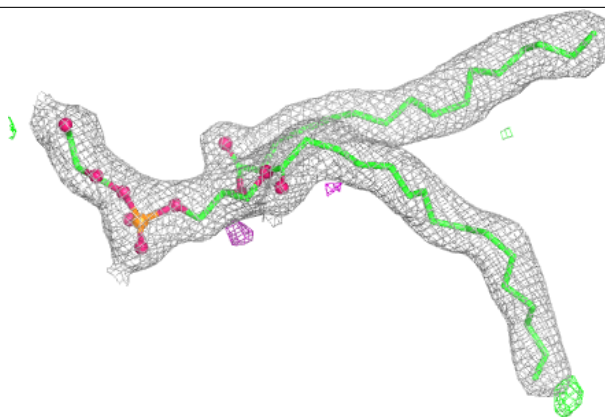
**Electron density around CLA B 605:**

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

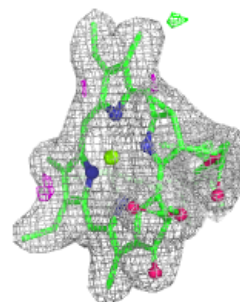
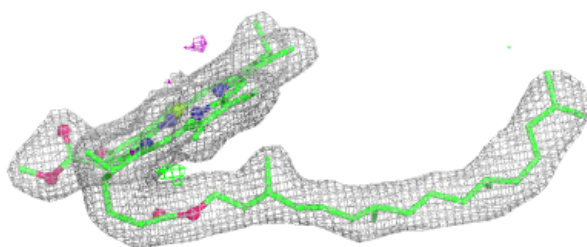
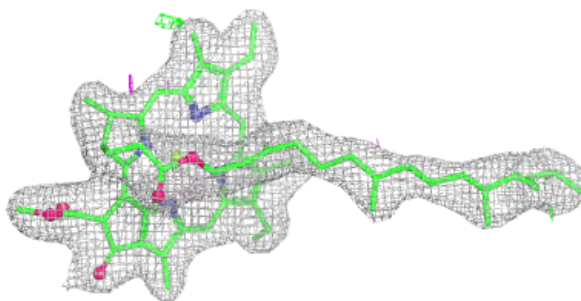


Electron density around LHG D 407:

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

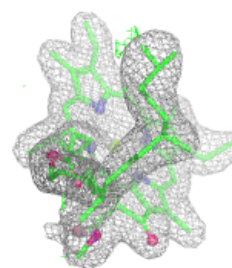
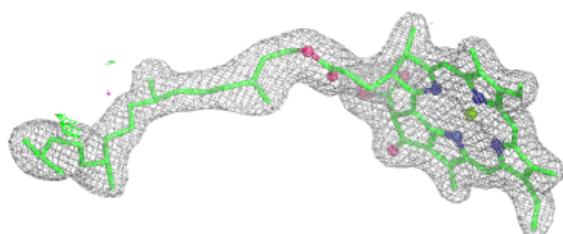
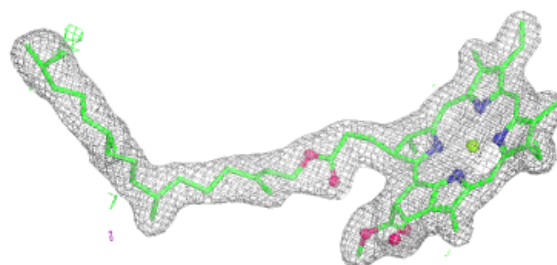
**Electron density around CLA B 608:**

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



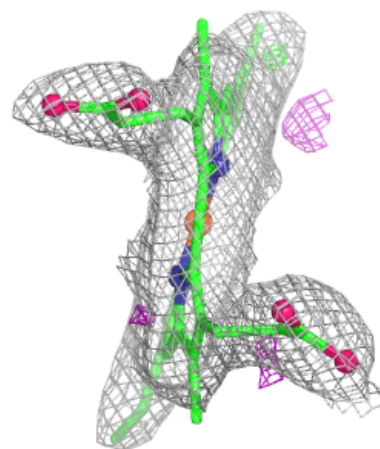
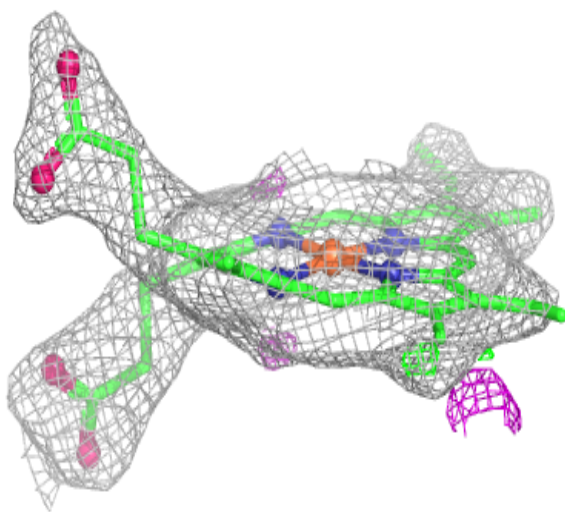
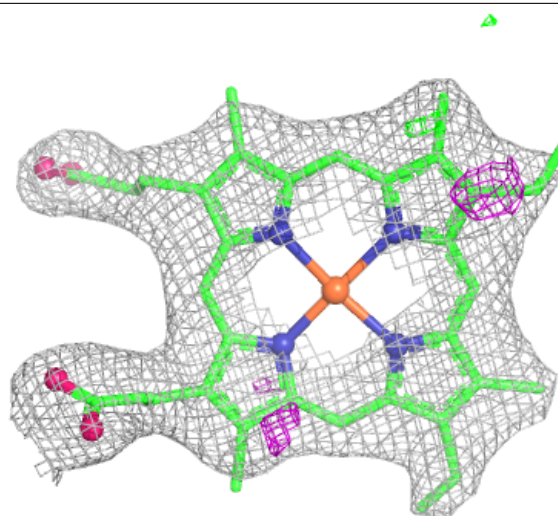
Electron density around CLA A 607:

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



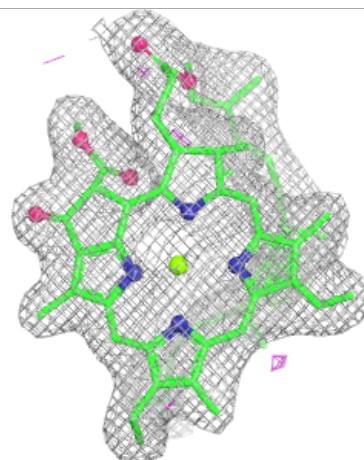
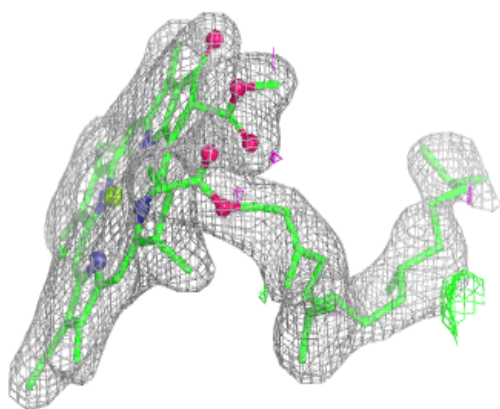
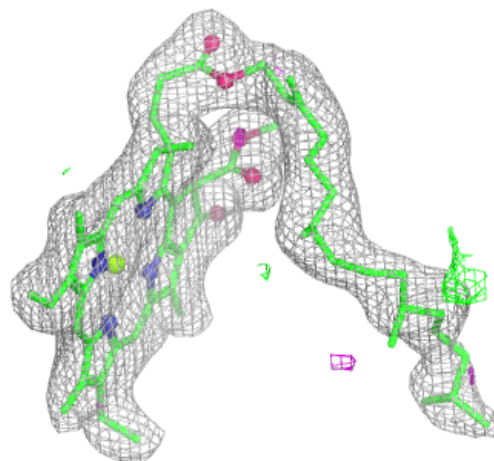
Electron density around HEM F 101:

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



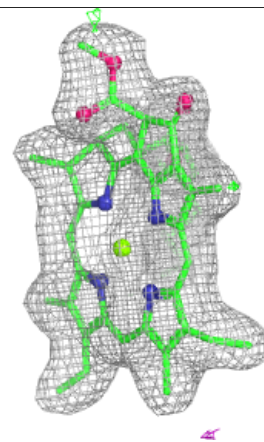
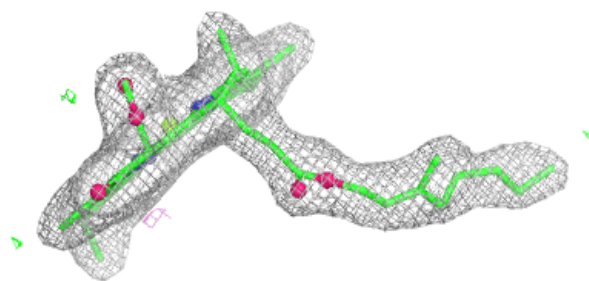
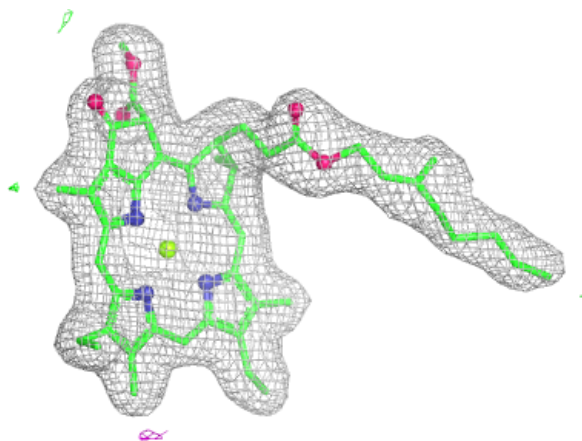
Electron density around CLA B 613:

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



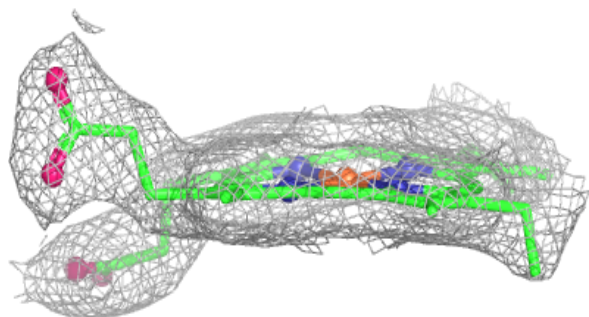
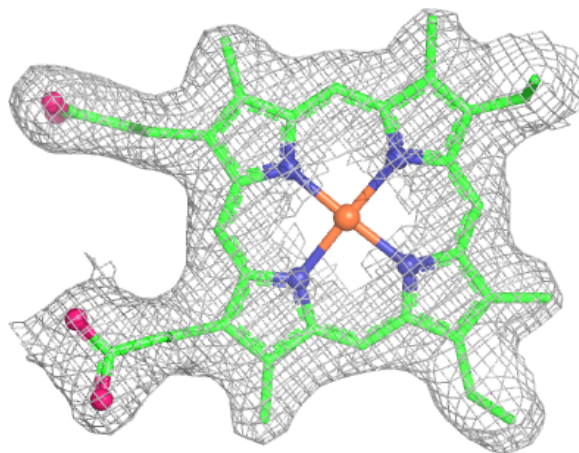
Electron density around CLA A 610:

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



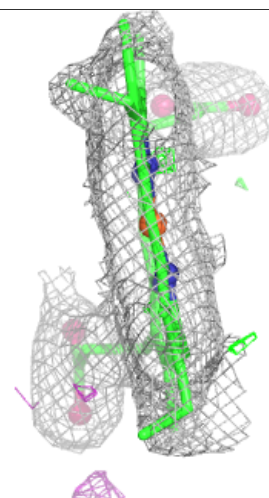
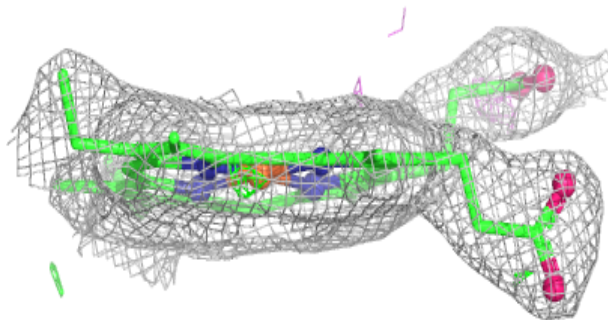
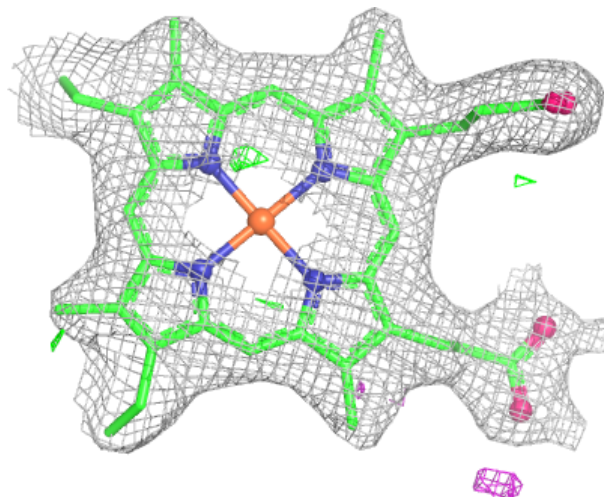
Electron density around HEC V 201:

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



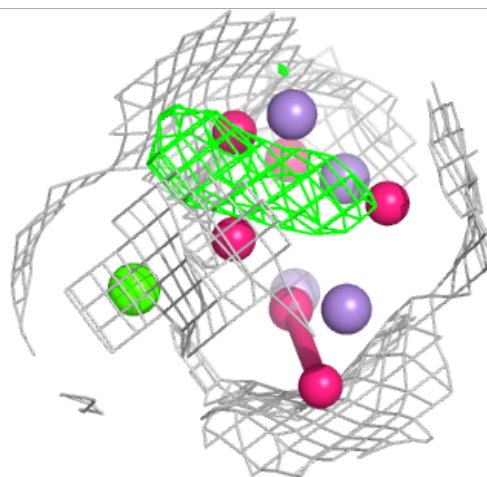
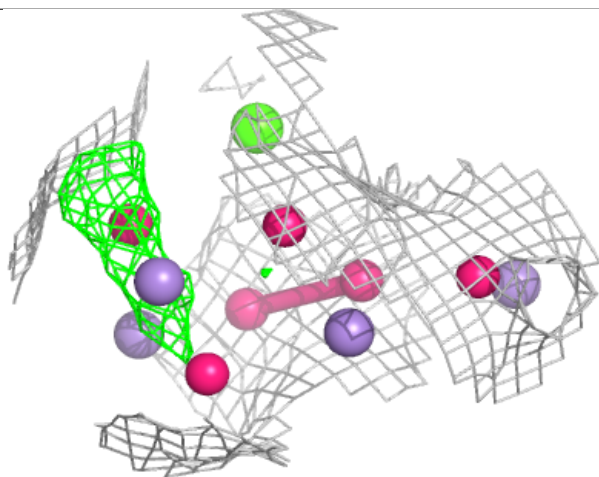
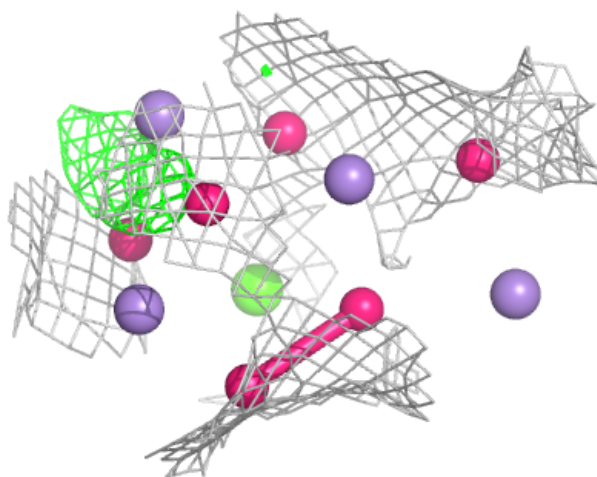
Electron density around HEC v 201:

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



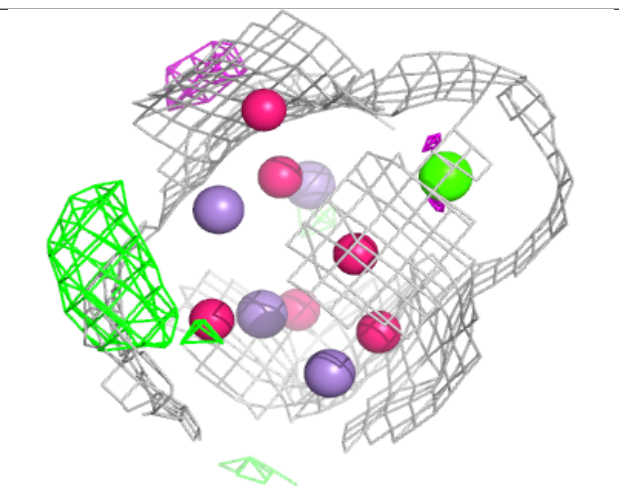
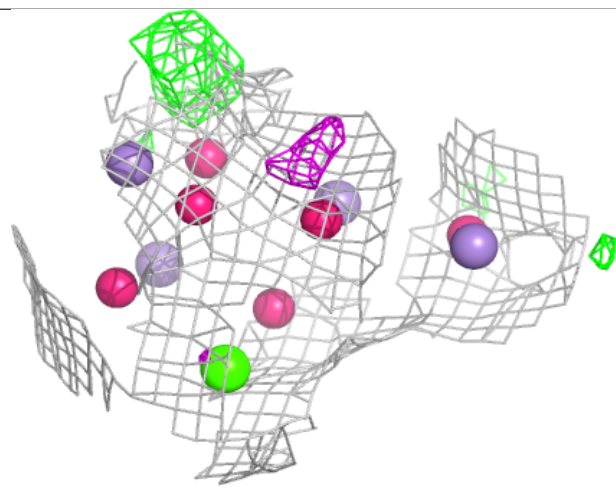
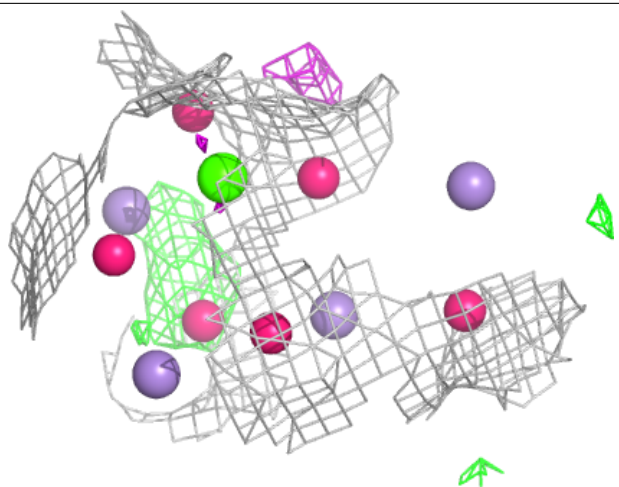
Electron density around OEY A 601 (C):

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



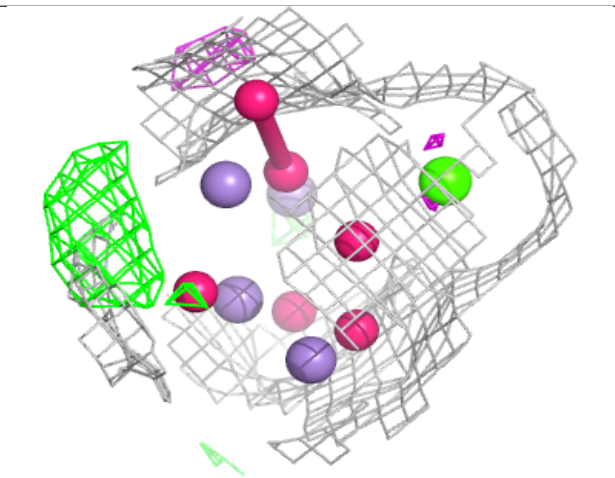
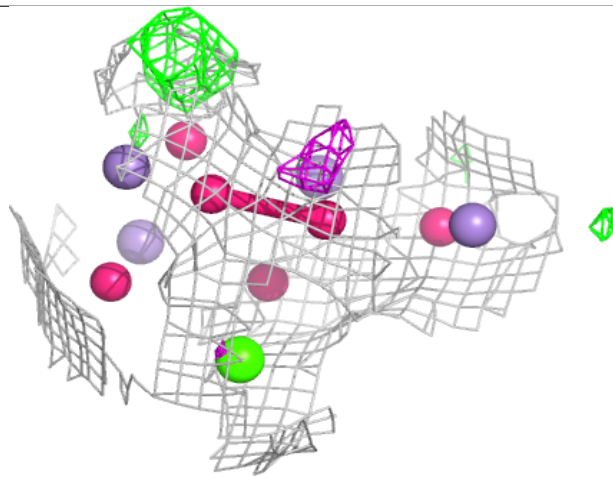
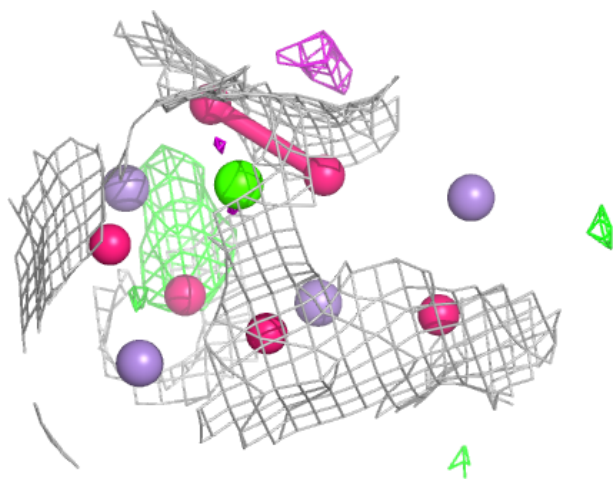
Electron density around OEY a 601 (A):

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



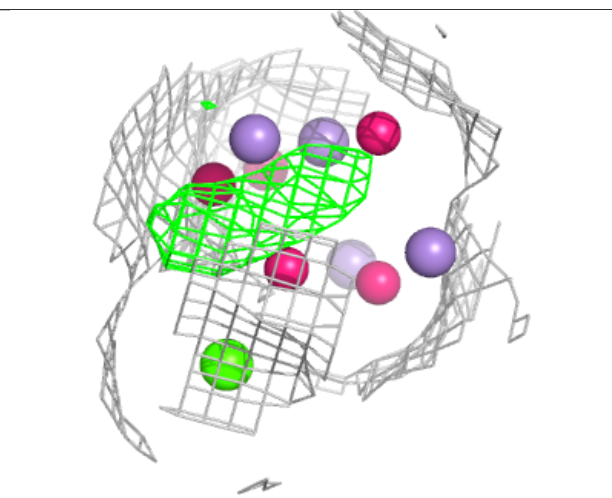
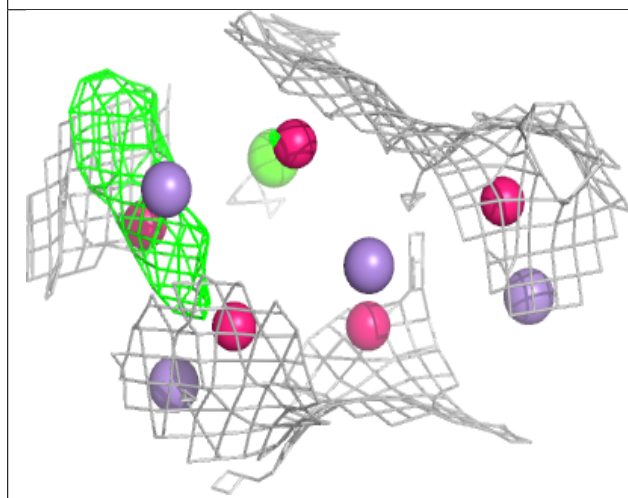
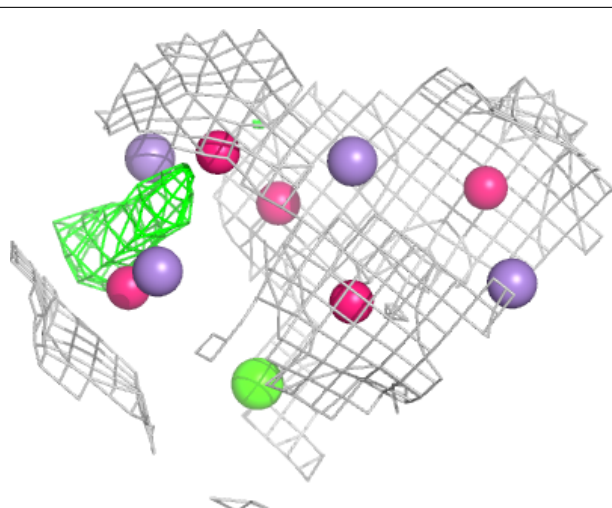
Electron density around OEY a 601 (C):

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



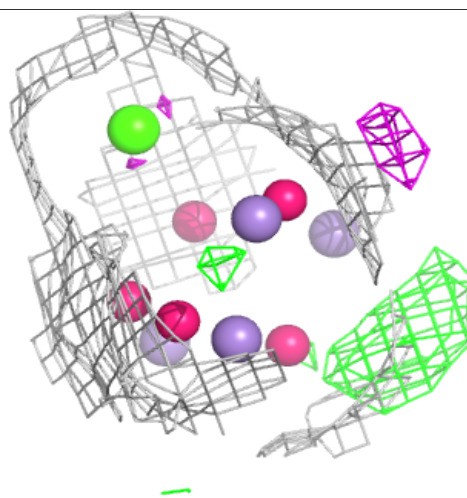
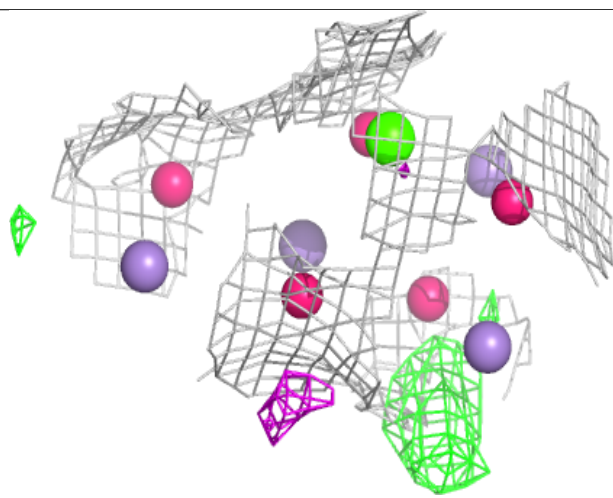
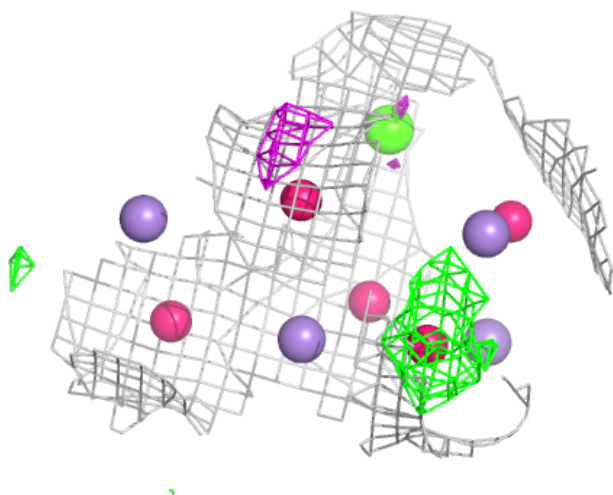
Electron density around OEX A 602 (B):

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



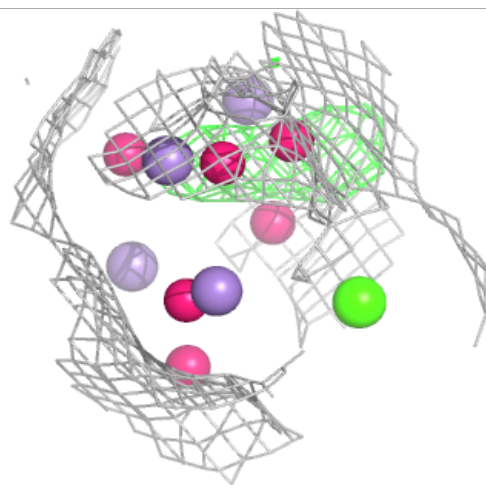
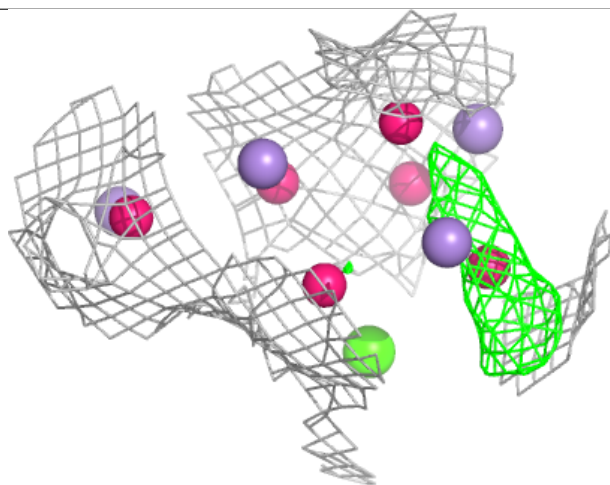
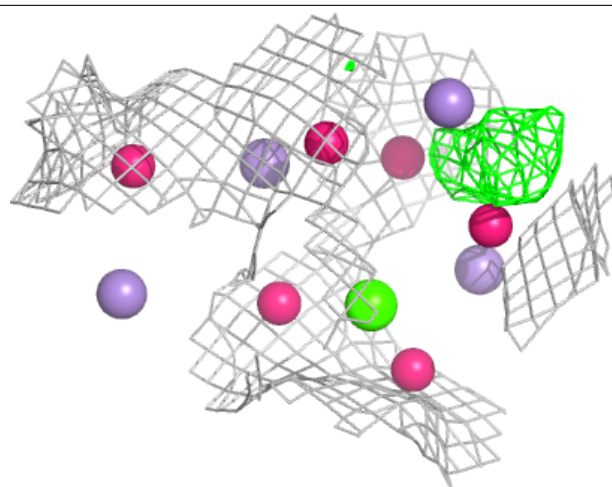
Electron density around OEX a 602 (B):

$2mF_o-DF_c$ (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 (A):

$2mF_o-DF_c$ (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.