



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 08:10 AM EDT

PDB ID : 8F4I / pdb_00008f4i
Title : RT XFEL structure of Photosystem II 2000 microseconds after the third illumination at 2.00 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 : 2.00 Å(reported)

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

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

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

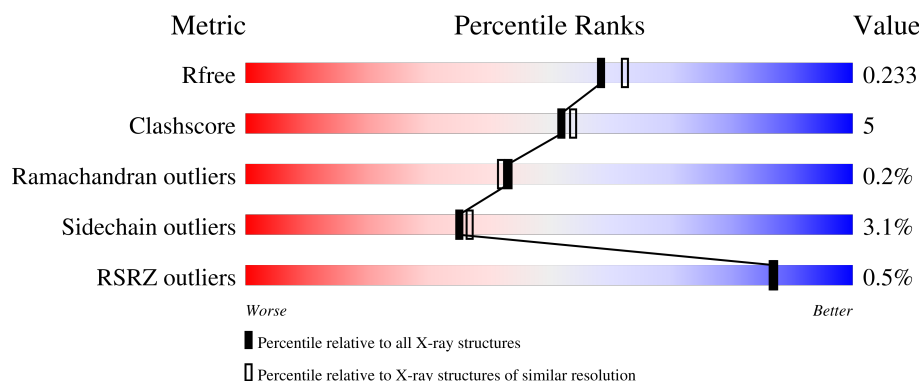
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
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 54640 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				

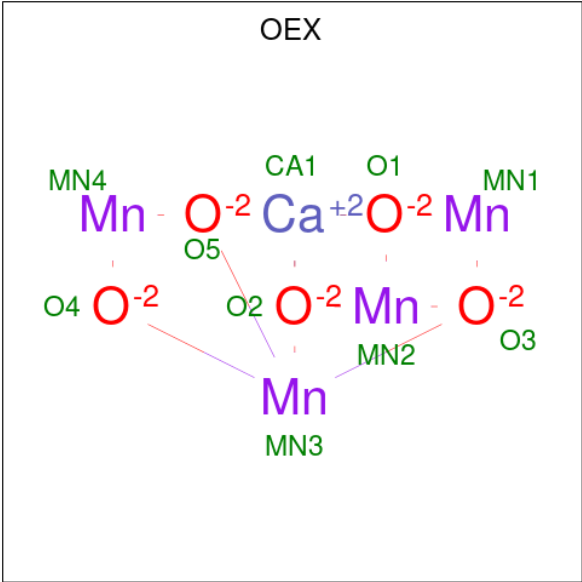
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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.

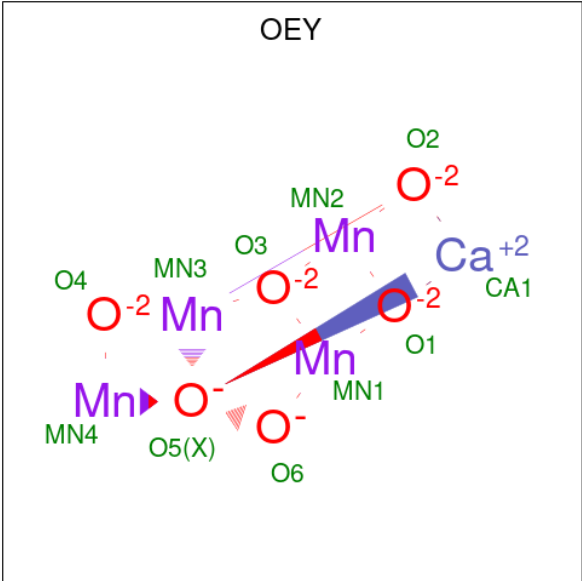
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O		0	0	0
			271	184	47	40				
20	r	31	Total	C	N	O		0	0	0
			246	166	43	37				

- Molecule 21 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	O	0	1
			20	2	8	10		
21	a	1	Total	Ca	Mn	O	0	1
			20	2	8	10		

- Molecule 22 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
22	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

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

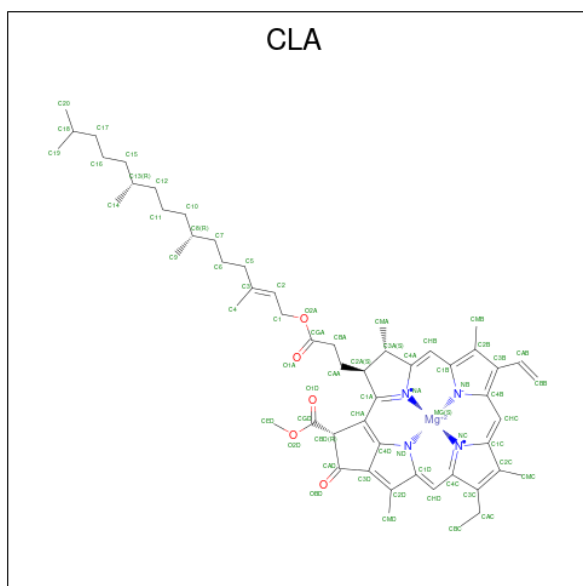
- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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

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

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



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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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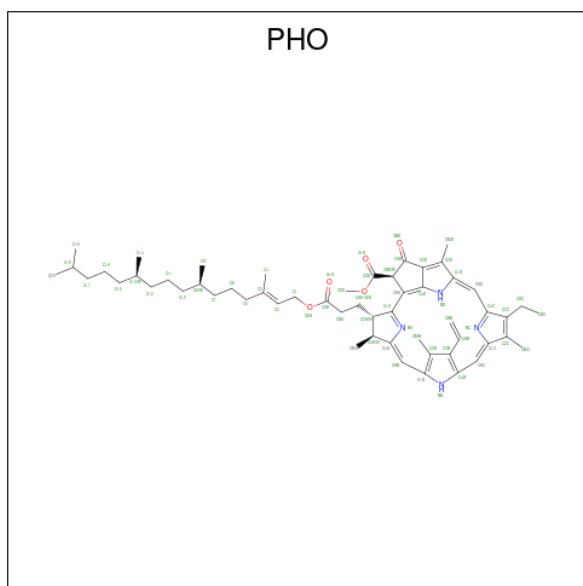
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N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

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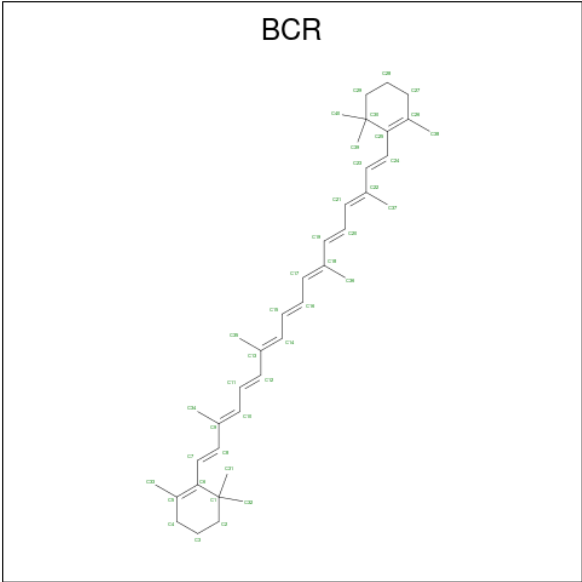
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

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



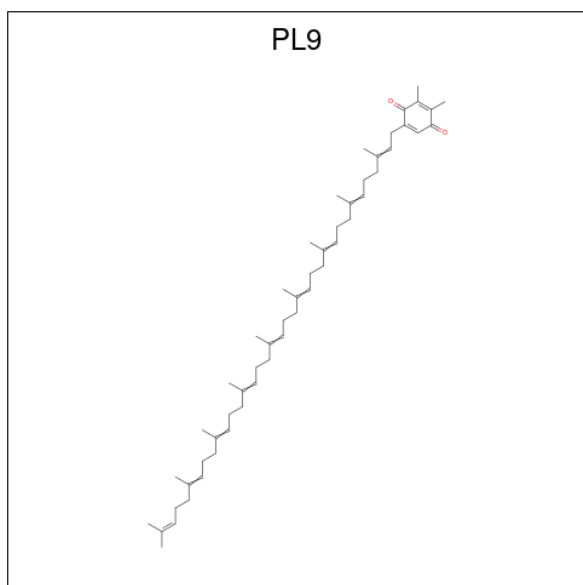
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total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

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

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



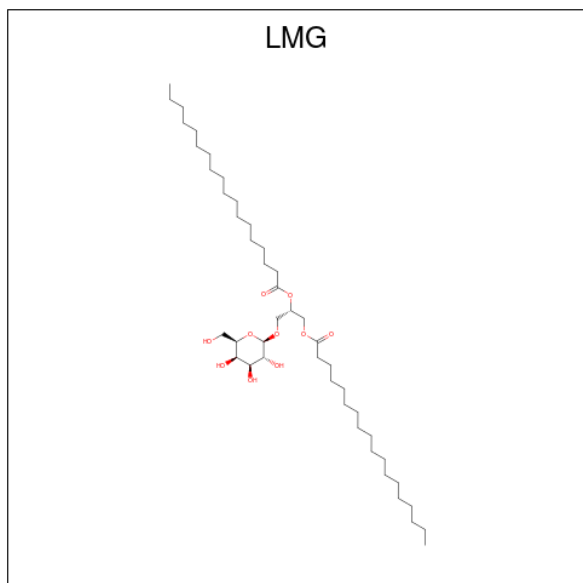
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 55 53 2	0	0
28	D	1	Total C O 55 53 2	0	0

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

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



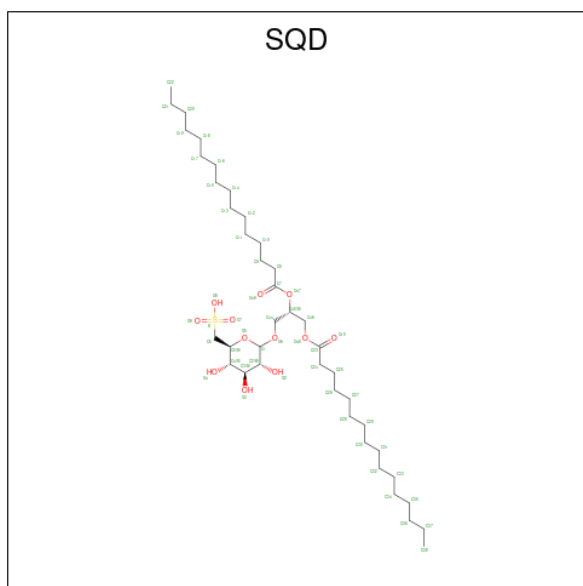
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			48	38	10		
29	B	1	Total	C	O	0	0
			51	41	10		
29	B	1	Total	C	O	0	0
			28	24	4		
29	C	1	Total	C	O	0	0
			48	38	10		
29	D	1	Total	C	O	0	0
			51	41	10		
29	D	1	Total	C	O	0	0
			33	27	6		
29	b	1	Total	C	O	0	0
			55	45	10		
29	c	1	Total	C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

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

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



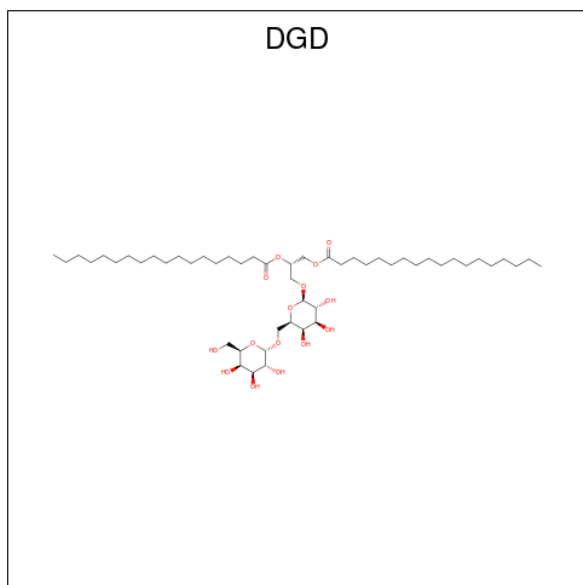
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			52	39	12	1		
30	A	1	Total	C	O		0	0
			39	35	4			
30	B	1	Total	C	O	S	0	0
			54	41	12	1		
30	D	1	Total	C	O	S	0	0
			36	25	10	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O		0	0
			36	31	5			
30	b	1	Total	C	O	S	0	0
			49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

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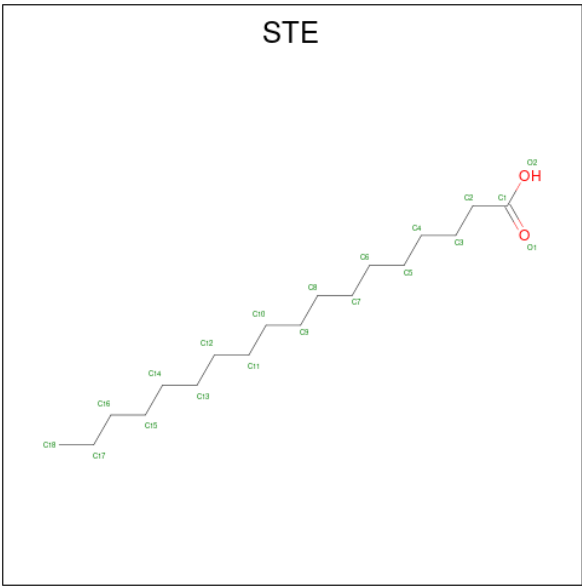
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	f	1	Total	C	O	S	0	0
			41	28	12	1		

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 32 is STEARIC ACID (CCD ID: STE) (formula: C₁₈H₃₆O₂).



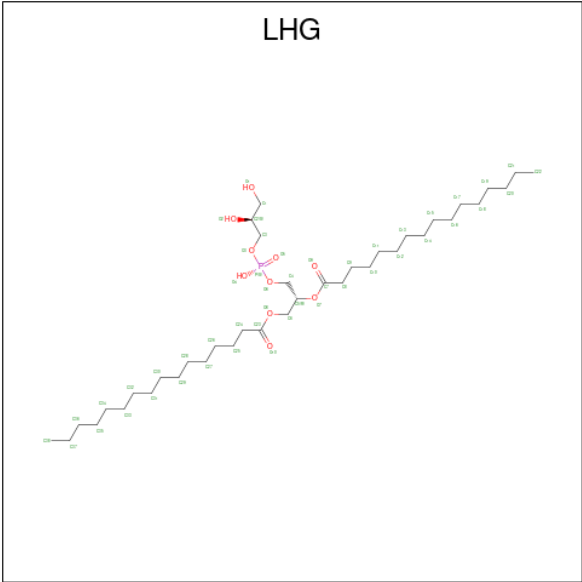
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B	1	Total	C	O	0	0
			17	15	2		
32	B	1	Total	C	O	0	0
			14	12	2		
32	B	1	Total	C	O	0	0
			12	10	2		
32	B	1	Total	C	O	0	0
			18	16	2		
32	B	1	Total	C	O	0	0
			12	10	2		
32	B	1	Total	C		0	0
			16	16			
32	C	1	Total	C	O	0	0
			12	10	2		
32	C	1	Total	C	O	0	0
			12	10	2		
32	C	1	Total	C		0	0
			16	16			
32	E	1	Total	C	O	0	0
			12	10	2		
32	H	1	Total	C		0	0
			18	18			
32	I	1	Total	C		0	0
			15	15			
32	J	1	Total	C	O	0	0
			12	10	2		

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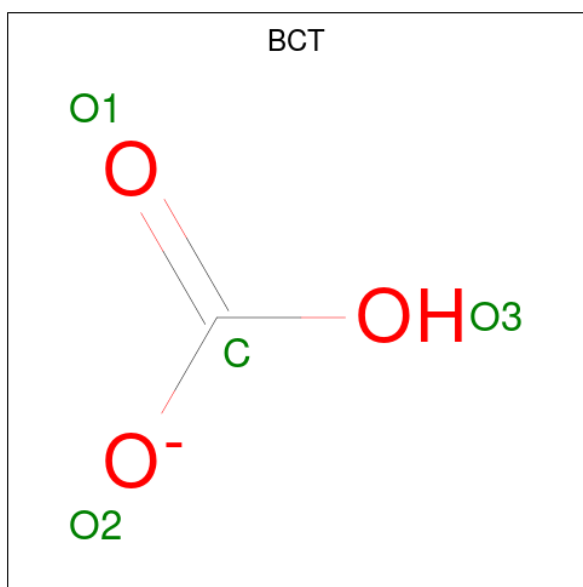
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	M	1	Total C O 15 13 2	0	0
32	M	1	Total C 10 10	0	0
32	T	1	Total C 16 16	0	0
32	T	1	Total C 15 15	0	0
32	X	1	Total C O 20 18 2	0	0
32	a	1	Total C O 12 10 2	0	0
32	b	1	Total C O 20 18 2	0	0
32	b	1	Total C O 16 14 2	0	0
32	b	1	Total C O 20 18 2	0	0
32	b	1	Total C 10 10	0	0
32	c	1	Total C O 20 18 2	0	0
32	c	1	Total C O 12 10 2	0	0
32	d	1	Total C O 17 15 2	0	0
32	d	1	Total C O 20 18 2	0	0
32	j	1	Total C O 12 10 2	0	0
32	l	1	Total C 18 18	0	0
32	m	1	Total C O 12 10 2	0	0
32	t	1	Total C 10 10	0	0

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



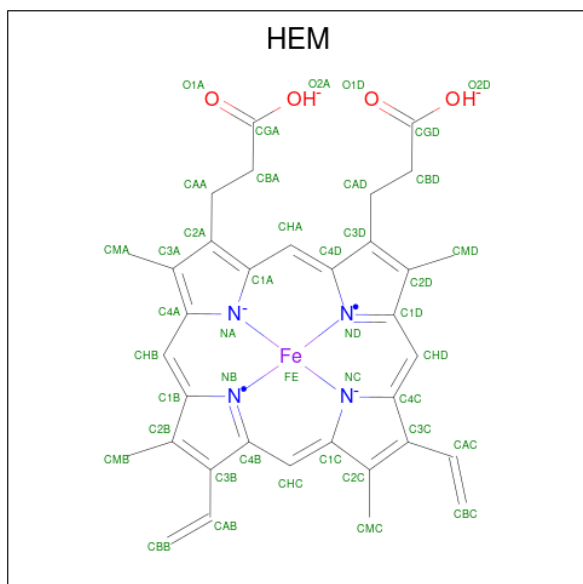
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total	C	O	P	0	0
			49	38	10	1		
33	D	1	Total	C	O	P	0	0
			49	38	10	1		
33	D	1	Total	C	O	P	0	0
			47	36	10	1		
33	D	1	Total	C	O	P	0	0
			49	38	10	1		
33	E	1	Total	C	O	P	0	0
			49	38	10	1		
33	a	1	Total	C	O	P	0	0
			49	38	10	1		
33	d	1	Total	C	O	P	0	0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

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



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

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



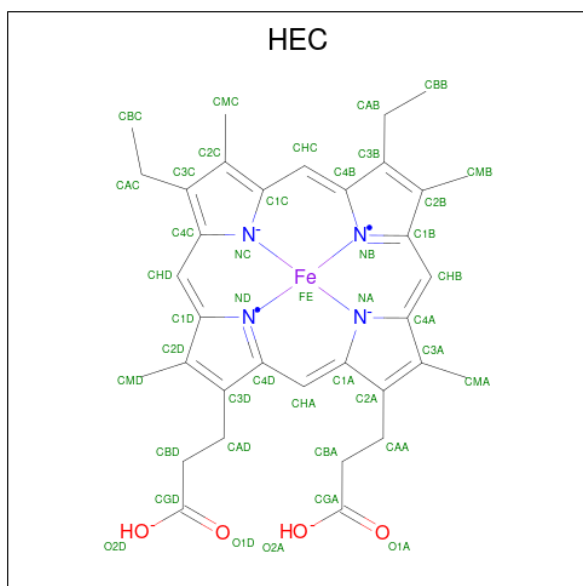
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
35	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	144	Total	O	0	4
			152	152		
37	B	218	Total	O	0	0
			218	218		
37	C	183	Total	O	0	0
			183	183		
37	D	124	Total	O	0	0
			124	124		
37	E	37	Total	O	0	0
			37	37		
37	F	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	H	30	Total 30	O 30	0	0
37	I	8	Total 8	O 8	0	0
37	J	8	Total 8	O 8	0	0
37	K	6	Total 6	O 6	0	0
37	L	10	Total 10	O 10	0	0
37	M	6	Total 6	O 6	0	0
37	O	97	Total 97	O 97	0	0
37	T	15	Total 15	O 15	0	0
37	U	47	Total 47	O 47	0	0
37	V	67	Total 67	O 67	0	0
37	Y	2	Total 2	O 2	0	0
37	X	8	Total 8	O 8	0	0
37	Z	9	Total 9	O 9	0	0
37	R	5	Total 5	O 5	0	0
37	a	133	Total 141	O 141	0	4
37	b	221	Total 221	O 221	0	0
37	c	182	Total 182	O 182	0	0
37	d	123	Total 123	O 123	0	0
37	e	24	Total 24	O 24	0	0
37	f	10	Total 10	O 10	0	0
37	h	19	Total 19	O 19	0	0

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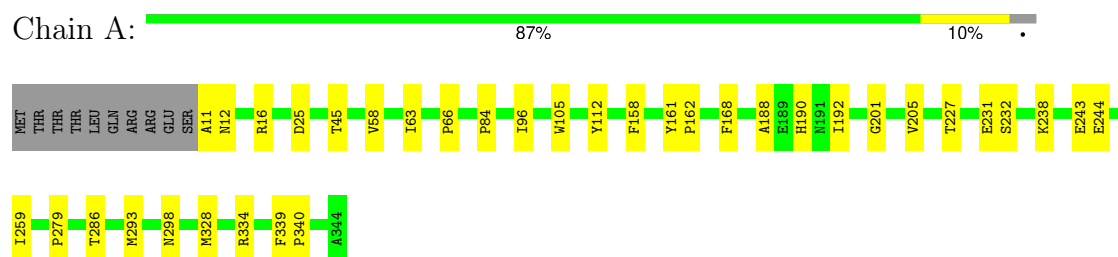
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	i	9	Total 9	O 9	0	0
37	j	10	Total 10	O 10	0	0
37	k	3	Total 3	O 3	0	0
37	l	7	Total 7	O 7	0	0
37	m	9	Total 9	O 9	0	0
37	o	88	Total 88	O 88	0	0
37	t	9	Total 9	O 9	0	0
37	u	61	Total 61	O 61	0	0
37	v	68	Total 68	O 68	0	0
37	y	3	Total 3	O 3	0	0
37	x	5	Total 5	O 5	0	0
37	z	7	Total 7	O 7	0	0

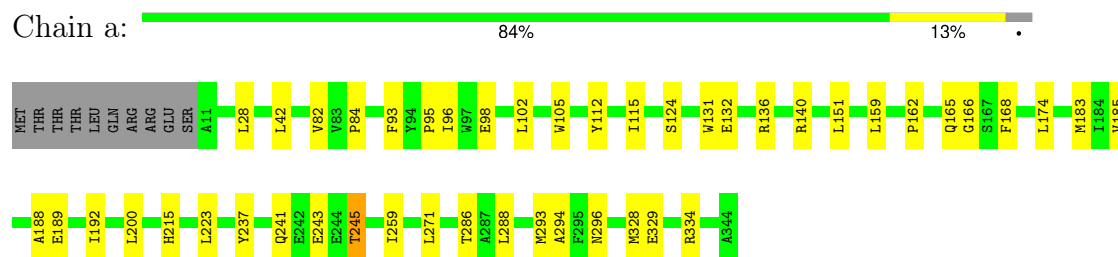
3 Residue-property plots [i](#)

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

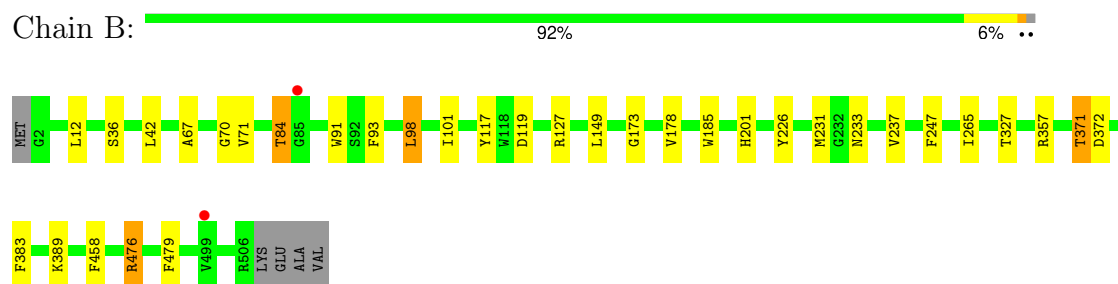
- Molecule 1: Photosystem II protein D1 1



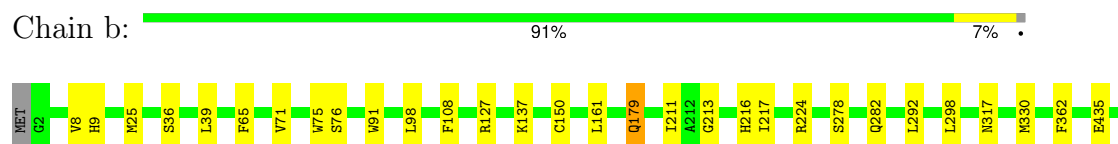
- Molecule 1: Photosystem II protein D1 1

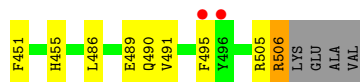


- Molecule 2: Photosystem II CP47 reaction center protein



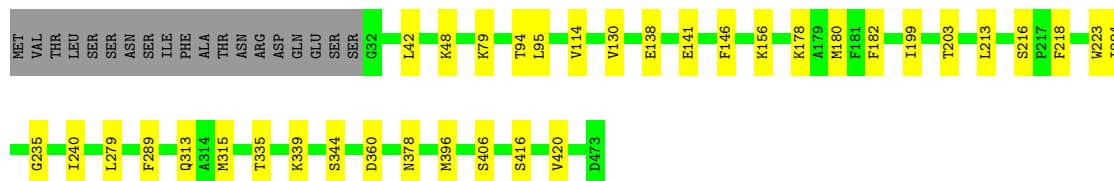
- Molecule 2: Photosystem II CP47 reaction center protein





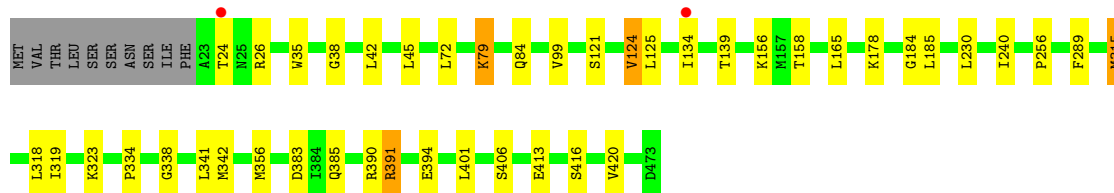
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 88% 8% .



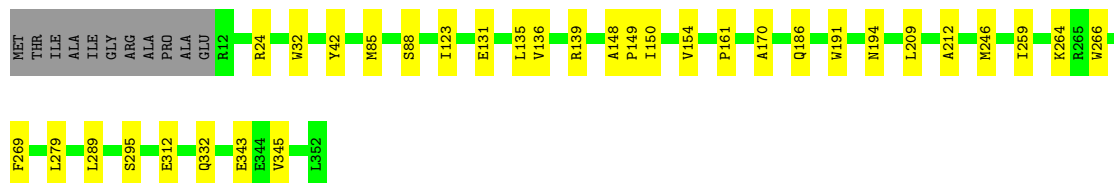
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 88% 9% ..



- Molecule 4: Photosystem II D2 protein

Chain D: 88% 9% .



- Molecule 4: Photosystem II D2 protein

Chain d: 89% 7% ..

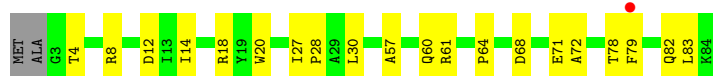
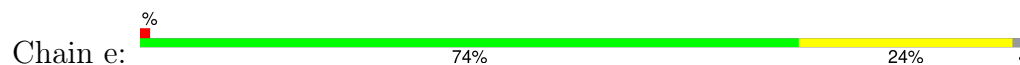


- Molecule 5: Cytochrome b559 subunit alpha

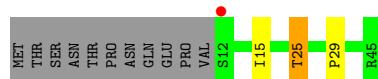
Chain E: 86% 12% .



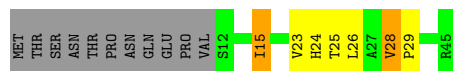
- Molecule 5: Cytochrome b559 subunit alpha



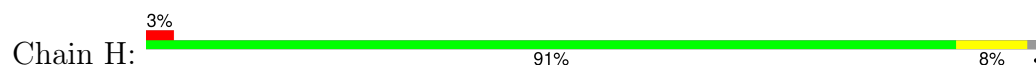
- Molecule 6: Cytochrome b559 subunit beta



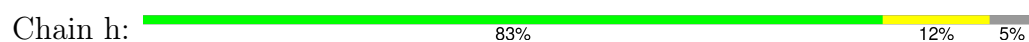
- Molecule 6: Cytochrome b559 subunit beta



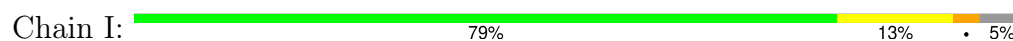
- Molecule 7: Photosystem II reaction center protein H



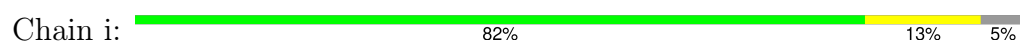
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I

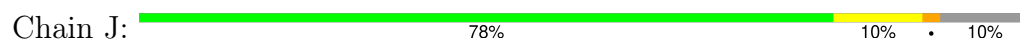


- Molecule 8: Photosystem II reaction center protein I





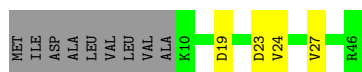
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



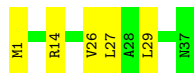
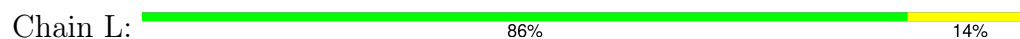
- Molecule 10: Photosystem II reaction center protein K



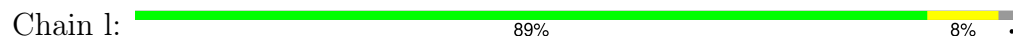
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L

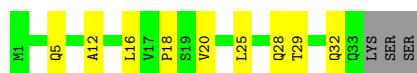


- Molecule 11: Photosystem II reaction center protein L



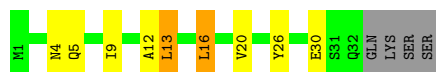
- Molecule 12: Photosystem II reaction center protein M





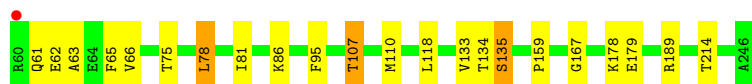
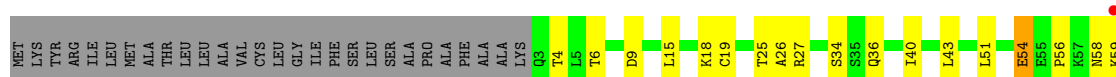
- Molecule 12: Photosystem II reaction center protein M

Chain m: 64% 19% 6% 11%



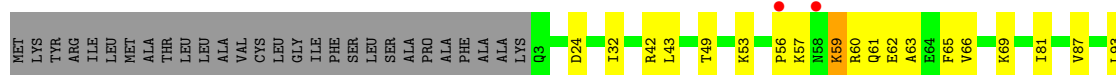
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 75% 13% 10%



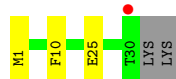
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 79% 10% 10%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 3% 84% 9% 6%



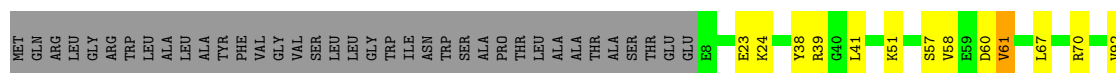
- Molecule 14: Photosystem II reaction center protein T

Chain t: 84% 9% 6%

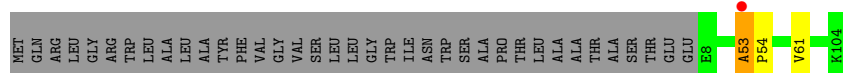


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 62% 10% 28%



- Molecule 15: Photosystem II 12 kDa extrinsic protein



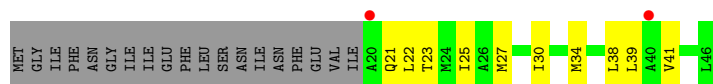
- Molecule 16: Cytochrome c-550



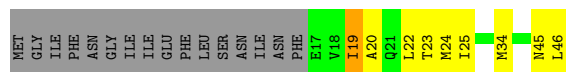
- Molecule 16: Cytochrome c-550



- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein

Chain X:  78% 12% 7%



- Molecule 18: Photosystem II reaction center X protein

Chain x:  5% 85% 10% 5%



- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  5% 76% 23% 1%



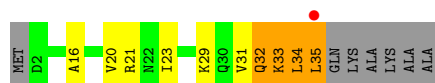
- Molecule 19: Photosystem II reaction center protein Z

Chain z:  2% 84% 16%



- Molecule 20: Photosystem II protein Y

Chain R:  2% 59% 15% 10% 17%



- Molecule 20: Photosystem II protein Y

Chain r:  59% 17% 24%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.31Å 222.59Å 308.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.72 – 2.00 19.72 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.72-2.00) 87.7 (19.72-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.47 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.186 , 0.232 0.186 , 0.233	Depositor DCC
R_{free} test set	4797 reflections (0.76%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	54640	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: OEY, HEM, LHG, FE2, DGD, BCT, PL9, CLA, BCR, CL, LMG, HEC, SQD, PHO, STE, OEX, FME

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	0.28	0/3717	0.45	0/5060
1	a	0.27	0/3714	0.44	0/5056
2	B	0.31	0/4155	0.47	0/5661
2	b	0.31	0/4118	0.49	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	0.32	0/2847	0.49	0/3874
5	E	0.24	0/688	0.44	0/940
5	e	0.22	0/683	0.42	0/932
6	F	0.27	0/284	0.42	0/387
6	f	0.25	0/284	0.46	0/387
7	H	0.31	0/523	0.45	0/713
7	h	0.28	0/511	0.44	0/697
8	I	0.29	0/293	0.48	0/396
8	i	0.31	0/293	0.42	0/396
9	J	0.25	0/263	0.43	0/356
9	j	0.22	0/263	0.42	0/356
10	K	0.24	0/303	0.39	0/416
10	k	0.24	0/303	0.39	0/416
11	L	0.34	0/311	0.45	0/422
11	l	0.37	0/303	0.50	0/412
12	M	0.29	0/249	0.50	0/341
12	m	0.30	0/244	0.51	0/334
13	O	0.30	0/1904	0.50	0/2585
13	o	0.30	0/1905	0.49	0/2583
14	T	0.34	0/257	0.50	0/349
14	t	0.30	0/255	0.41	0/346
15	U	0.28	0/785	0.47	0/1064
15	u	0.31	0/785	0.49	0/1064
16	V	0.29	0/1085	0.46	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.27	0/1085	0.42	0/1473
17	Y	0.20	0/197	0.34	0/264
17	y	0.19	0/219	0.40	0/294
18	X	0.22	0/284	0.35	0/384
18	x	0.19	0/289	0.27	0/391
19	Z	0.19	0/490	0.41	0/669
19	z	0.15	0/488	0.30	0/666
20	R	0.25	0/277	0.43	0/380
20	r	0.22	0/252	0.35	0/347
All	All	0.29	0/45246	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

There are no bond length outliers.

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

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	24	0
1	a	3601	0	3436	27	0
2	B	4005	0	3871	29	0
2	b	3978	0	3836	30	0
3	C	3592	0	3501	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3666	0	3574	26	0
4	D	2745	0	2653	25	0
4	d	2751	0	2659	22	0
5	E	666	0	651	6	0
5	e	664	0	648	16	0
6	F	275	0	282	4	0
6	f	275	0	282	6	0
7	H	510	0	532	4	0
7	h	498	0	518	5	0
8	I	296	0	311	3	0
8	i	296	0	311	4	0
9	J	257	0	268	3	0
9	j	257	0	268	6	0
10	K	293	0	305	3	0
10	k	293	0	305	5	0
11	L	304	0	316	7	0
11	l	296	0	304	1	0
12	M	256	0	269	7	0
12	m	251	0	267	7	0
13	O	1870	0	1830	27	0
13	o	1874	0	1846	17	0
14	T	258	0	261	2	0
14	t	256	0	256	1	0
15	U	774	0	773	6	0
15	u	774	0	773	1	0
16	V	1064	0	1073	12	0
16	v	1064	0	1073	16	0
17	Y	196	0	217	5	0
17	y	218	0	241	4	0
18	X	281	0	312	8	0
18	x	286	0	314	3	0
19	Z	479	0	516	9	0
19	z	477	0	509	4	0
20	R	271	0	298	7	0
20	r	246	0	263	1	0
21	A	20	0	0	0	0
21	a	20	0	0	0	0
22	A	11	0	0	1	0
22	a	11	0	0	1	0
23	A	1	0	0	0	0
23	a	1	0	0	0	0
24	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	2	0	0	0	0
25	A	249	0	264	6	0
25	B	1035	0	1139	37	0
25	C	839	0	922	18	0
25	D	130	0	144	7	0
25	a	260	0	288	11	0
25	b	1035	0	1139	32	0
25	c	839	0	919	24	0
25	d	130	0	144	2	0
26	A	64	0	74	1	0
26	D	64	0	74	2	0
26	a	64	0	74	0	0
26	d	64	0	74	2	0
27	A	40	0	56	3	0
27	B	120	0	168	7	0
27	C	120	0	168	7	0
27	D	40	0	56	2	0
27	H	40	0	56	2	0
27	K	40	0	56	0	0
27	T	40	0	56	2	0
27	a	40	0	56	1	0
27	b	120	0	168	5	0
27	c	40	0	56	3	0
27	d	40	0	56	1	0
27	k	120	0	168	3	0
27	t	40	0	56	2	0
27	x	40	0	56	2	0
28	A	55	0	80	5	0
28	D	55	0	80	1	0
28	a	55	0	80	7	0
28	d	55	0	80	2	0
29	A	48	0	66	4	0
29	B	79	0	112	2	0
29	C	48	0	66	2	0
29	D	84	0	117	3	0
29	b	55	0	86	1	0
29	c	134	0	181	3	0
29	d	67	0	92	2	0
29	m	51	0	72	3	0
30	A	91	0	136	2	0
30	B	54	0	78	0	0
30	D	36	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	90	0	134	3	0
30	b	49	0	65	1	0
30	f	41	0	49	1	0
31	A	66	0	96	5	0
31	C	186	0	246	4	0
31	H	62	0	82	2	0
31	a	44	0	75	6	0
31	c	186	0	246	6	0
31	h	62	0	82	1	0
32	B	89	0	137	4	0
32	C	40	0	63	1	0
32	E	12	0	16	0	0
32	H	18	0	35	1	0
32	I	15	0	26	2	0
32	J	12	0	16	1	0
32	M	25	0	38	1	0
32	T	31	0	60	0	0
32	X	20	0	35	2	0
32	a	12	0	16	0	0
32	b	66	0	110	10	0
32	c	32	0	51	1	0
32	d	37	0	61	2	0
32	j	12	0	16	0	0
32	l	18	0	35	1	0
32	m	12	0	16	0	0
32	t	10	0	16	0	0
33	B	49	0	74	2	0
33	D	145	0	215	5	0
33	E	49	0	74	3	0
33	a	49	0	74	1	0
33	d	88	0	125	5	0
33	e	42	0	57	1	0
33	l	49	0	74	1	0
34	D	4	0	1	1	0
34	d	4	0	1	0	0
35	F	43	0	30	2	0
35	e	43	0	30	4	0
36	V	43	0	30	0	0
36	v	43	0	30	2	0
37	A	152	0	0	3	0
37	B	218	0	0	2	0
37	C	183	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	D	124	0	0	1	0
37	E	37	0	0	1	0
37	F	6	0	0	0	0
37	H	30	0	0	1	0
37	I	8	0	0	0	0
37	J	8	0	0	0	0
37	K	6	0	0	1	0
37	L	10	0	0	0	0
37	M	6	0	0	1	0
37	O	97	0	0	5	0
37	R	5	0	0	0	0
37	T	15	0	0	0	0
37	U	47	0	0	0	0
37	V	67	0	0	2	0
37	X	8	0	0	1	0
37	Y	2	0	0	0	0
37	Z	9	0	0	2	0
37	a	141	0	0	2	0
37	b	221	0	0	0	0
37	c	182	0	0	4	0
37	d	123	0	0	1	0
37	e	24	0	0	0	0
37	f	10	0	0	0	0
37	h	19	0	0	2	0
37	i	9	0	0	1	0
37	j	10	0	0	1	0
37	k	3	0	0	1	0
37	l	7	0	0	0	0
37	m	9	0	0	0	0
37	o	88	0	0	0	0
37	t	9	0	0	0	0
37	u	61	0	0	0	0
37	v	68	0	0	1	0
37	x	5	0	0	0	0
37	y	3	0	0	0	0
37	z	7	0	0	0	0
All	All	54640	0	53863	547	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 (547) 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)
25:c:501:CLA:H192	25:c:507:CLA:HBB1	1.54	0.90
1:a:102:LEU:HD12	31:a:616:DGD:HB22	1.59	0.81
22:a:602[A]:OEY:O6	22:a:602[A]:OEY:O5	1.97	0.81
13:O:178:LYS:NZ	37:O:301:HOH:O	2.16	0.77
31:A:616:DGD:HE4	2:b:76:SER:HB3	1.67	0.76
22:A:602[A]:OEY:O6	22:A:602[A]:OEY:O5	2.03	0.75
4:D:279:LEU:HD22	26:D:402:PHO:HBC3	1.67	0.74
32:d:412:STE:H41	18:x:17:GLY:HA2	1.68	0.74
2:b:91:TRP:HE1	32:b:621:STE:H141	1.54	0.73
31:a:616:DGD:O3G	37:a:701:HOH:O	2.06	0.73
19:z:32:ASP:HA	19:z:35:ARG:HG3	1.72	0.71
9:J:15:THR:HG22	9:J:19:MET:HE2	1.71	0.71
5:e:57:ALA:H	5:e:60:GLN:HE21	1.38	0.70
3:C:378:ASN:OD1	37:C:601:HOH:O	2.08	0.70
10:k:21:LEU:HD13	17:y:24:MET:HE2	1.71	0.70
30:a:615:SQD:H222	31:a:616:DGD:HBV1	1.74	0.70
25:b:615:CLA:H2	25:b:616:CLA:HBB2	1.74	0.68
35:F:101:HEM:HBC2	35:F:101:HEM:HHD	1.75	0.68
3:C:146:PHE:O	3:C:156:LYS:NZ	2.27	0.68
4:D:332:GLN:NE2	37:D:501:HOH:O	2.19	0.68
4:d:12:ARG:N	37:d:501:HOH:O	2.26	0.68
15:U:23:GLU:HG3	15:U:24:LYS:HG2	1.74	0.68
25:B:601:CLA:H2	25:B:601:CLA:HAA2	1.74	0.68
7:h:64:ALA:O	37:h:201:HOH:O	2.10	0.68
13:o:56:PRO:HD3	13:o:63:ALA:HB2	1.75	0.67
28:d:406:PL9:H201	33:l:101:LHG:H202	1.77	0.67
12:m:4:ASN:ND2	29:m:101:LMG:O10	2.27	0.66
12:M:5:GLN:O	37:M:201:HOH:O	2.12	0.66
13:O:86:LYS:NZ	37:O:304:HOH:O	2.27	0.66
35:e:101:HEM:HBC2	35:e:101:HEM:HMC2	1.77	0.66
33:a:613:LHG:H211	25:b:613:CLA:H192	1.78	0.66
7:H:56:ASP:OD2	18:X:2:THR:N	2.30	0.65
2:B:91:TRP:HE1	32:B:621:STE:H32	1.60	0.65
33:B:623:LHG:H202	11:L:26:VAL:HG11	1.79	0.65
1:A:25:ASP:OD1	37:A:701:HOH:O	2.15	0.64
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	1.78	0.64
28:A:611:PL9:H253	25:D:403:CLA:H141	1.78	0.64
19:Z:11:ALA:N	37:Z:101:HOH:O	2.28	0.64
33:D:412:LHG:H222	12:M:18:PRO:HG3	1.78	0.64
25:B:606:CLA:H72	27:B:619:BCR:H311	1.79	0.64
20:R:32:GLN:HE21	20:R:33:LYS:N	1.96	0.64
5:e:14:ILE:O	5:e:20:TRP:NE1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:j:15:THR:HG22	9:j:19:MET:HE2	1.80	0.63
1:A:188[A]:ALA:HB2	1:A:328[A]:MET:HB2	1.80	0.63
2:b:211:ILE:HG23	32:b:625:STE:H22	1.80	0.63
28:A:611:PL9:H361	6:F:25:THR:HG21	1.80	0.63
25:b:614:CLA:H43	30:b:620:SQD:H102	1.81	0.62
13:o:24:ASP:OD1	13:o:203:LYS:NZ	2.25	0.62
1:a:188[C]:ALA:HB2	1:a:328[C]:MET:HB2	1.80	0.62
4:d:259:ILE:HD12	33:d:407:LHG:H291	1.81	0.62
25:c:503:CLA:H203	25:c:510:CLA:HAB	1.81	0.62
35:e:101:HEM:HHC	35:e:101:HEM:HBB2	1.82	0.62
4:d:246:MET:HE3	4:d:264:LYS:HG2	1.79	0.62
3:c:42:LEU:HD21	25:c:511:CLA:H2A	1.82	0.61
1:A:188[C]:ALA:HB2	1:A:328[C]:MET:HB2	1.82	0.61
4:d:42:TYR:CZ	6:f:25:THR:HG22	2.35	0.61
25:B:615:CLA:H2	25:B:616:CLA:HBB2	1.83	0.61
29:C:520:LMG:H191	10:K:27:VAL:HG11	1.83	0.61
4:d:126:MET:HE3	4:d:143:ALA:O	2.00	0.61
16:v:76:MET:HE3	36:v:201:HEC:HBB3	1.83	0.61
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.64	0.60
15:u:53:ALA:HB1	15:u:54:PRO:HD2	1.83	0.60
30:f:101:SQD:H312	18:x:27:VAL:HG11	1.84	0.60
25:B:610:CLA:HHC	25:B:610:CLA:HBB1	1.84	0.60
25:C:502:CLA:H61	25:C:512:CLA:H42	1.83	0.60
1:A:334[C]:ARG:NH1	37:A:702:HOH:O	2.29	0.59
25:A:609:CLA:H43	25:C:505:CLA:H191	1.84	0.59
4:D:24:ARG:NH2	18:X:35:ASP:OD2	2.35	0.59
32:B:627:STE:H152	12:m:12:ALA:HA	1.85	0.59
20:R:32:GLN:HE21	20:R:33:LYS:H	1.50	0.59
1:A:227:THR:HB	1:A:231:GLU:HG3	1.83	0.59
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.85	0.59
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.85	0.58
4:D:123:ILE:HD11	31:H:102:DGD:HAH1	1.84	0.58
29:b:622:LMG:H191	29:b:622:LMG:H332	1.85	0.58
2:b:489:GLU:HA	2:b:495:PHE:HD2	1.69	0.58
5:e:30:LEU:HD11	35:e:101:HEM:HBB2	1.85	0.58
12:M:29:THR:HA	12:M:32:GLN:HE21	1.68	0.58
1:A:334[C]:ARG:NH2	4:D:312:GLU:OE2	2.29	0.58
13:O:56:PRO:O	13:O:58:ASN:N	2.35	0.57
17:Y:39:LEU:HD21	19:Z:25:VAL:HA	1.84	0.57
19:Z:29:SER:HB3	19:Z:31:GLN:HG3	1.86	0.57
30:A:615:SQD:H312	27:b:619:BCR:H363	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:241:GLU:CD	4:d:241:GLU:H	2.12	0.57
15:U:57:SER:OG	15:U:60:ASP:OD1	2.23	0.57
5:e:57:ALA:HB3	5:e:60:GLN:HG2	1.86	0.56
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.87	0.56
2:B:371:THR:HG23	2:B:372:ASP:O	2.05	0.56
25:a:609:CLA:H52	25:a:609:CLA:H111	1.87	0.56
31:a:616:DGD:HG11	13:o:69:LYS:NZ	2.20	0.56
3:c:315:MET:HE3	3:c:319:ILE:HD11	1.86	0.56
17:Y:23:THR:HG22	17:Y:27:MET:HE3	1.87	0.56
4:D:343:GLU:HG2	16:V:135:VAL:HG11	1.88	0.56
27:T:101:BCR:H321	27:T:101:BCR:HC8	1.87	0.56
16:v:10:VAL:HG23	16:v:69:ILE:HD11	1.87	0.56
27:t:101:BCR:H321	27:t:101:BCR:HC8	1.87	0.56
4:D:264:LYS:NZ	34:D:401:BCT:O3	2.39	0.56
1:a:237:TYR:HB2	1:a:245:THR:HG21	1.88	0.55
15:U:38:TYR:HB2	15:U:41:LEU:HD12	1.88	0.55
13:O:58:ASN:ND2	13:O:61:GLN:OE1	2.35	0.55
16:v:76:MET:HE2	16:v:112:LEU:HD22	1.88	0.55
2:B:479[A]:PHE:O	4:D:139:ARG:NH2	2.32	0.55
20:R:29:LYS:HA	20:R:32:GLN:HE22	1.70	0.55
28:D:406:PL9:H412	11:L:29:LEU:HD23	1.87	0.55
2:B:327:THR:HG21	29:B:620:LMG:H291	1.89	0.55
1:a:271:LEU:HD21	28:a:611:PL9:HC71	1.89	0.55
25:b:601:CLA:HAB	25:b:601:CLA:H172	1.88	0.54
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.43	0.54
5:e:20:TRP:HD1	9:j:8:ILE:HD13	1.72	0.54
13:O:133:VAL:O	13:O:135:SER:N	2.40	0.54
29:A:613:LMG:H131	3:C:218:PHE:HE2	1.73	0.54
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.90	0.54
2:b:489:GLU:OE1	2:b:505:ARG:NH1	2.41	0.54
2:B:84:THR:HG21	13:o:66:VAL:HB	1.90	0.53
25:b:605:CLA:HHC	25:b:605:CLA:HBB1	1.90	0.53
28:A:611:PL9:H261	33:E:101:LHG:H211	1.90	0.53
1:a:165[C]:GLN:NE2	1:a:294:ALA:O	2.41	0.53
25:A:607:CLA:H101	25:D:403:CLA:H172	1.89	0.53
3:c:134:ILE:HD12	25:c:511:CLA:H43	1.89	0.53
10:k:18:PHE:HE2	19:z:13:VAL:HG21	1.73	0.53
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.09	0.53
31:A:616:DGD:HD5	2:b:75:TRP:HB3	1.89	0.53
3:c:79:LYS:HD3	3:c:84:GLN:HG2	1.90	0.53
3:C:48:LYS:HD2	3:C:138:GLU:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:133:VAL:C	13:O:135:SER:H	2.16	0.53
31:a:616:DGD:HG11	13:o:69:LYS:HZ1	1.74	0.53
3:c:406:SER:HA	3:c:420:VAL:HG23	1.90	0.53
13:o:62:GLU:OE1	13:o:63:ALA:N	2.42	0.53
4:D:32:TRP:CG	29:D:411:LMG:H161	2.45	0.52
13:o:216:GLU:OE2	13:o:234:LYS:HD2	2.09	0.52
1:A:63[B]:ILE:HB	3:C:335:THR:HG21	1.91	0.52
20:r:2:ASP:HB3	20:r:5:VAL:HG23	1.90	0.52
25:B:614:CLA:H202	25:B:614:CLA:H13	1.91	0.52
35:F:101:HEM:HBB2	35:F:101:HEM:HMB1	1.91	0.52
13:O:56:PRO:C	13:O:58:ASN:H	2.17	0.52
33:d:407:LHG:H281	14:t:17:PHE:CD1	2.43	0.52
3:C:406:SER:HA	3:C:420:VAL:HG23	1.91	0.52
2:b:91:TRP:CD1	32:b:621:STE:H162	2.44	0.52
16:v:76:MET:HE1	16:v:115:ILE:HD12	1.92	0.52
25:B:607:CLA:H111	25:B:613:CLA:H202	1.91	0.51
13:O:51:LEU:HB3	13:O:65:PHE:HB3	1.91	0.51
1:a:84:PRO:HA	1:a:112:TYR:CG	2.46	0.51
6:f:24:HIS:O	6:f:28:VAL:HG13	2.11	0.51
13:o:53:LYS:HB2	13:o:65:PHE:CE1	2.46	0.51
25:D:404:CLA:H192	18:X:15:LEU:HD21	1.92	0.51
13:O:179:GLU:OE1	37:O:302:HOH:O	2.19	0.51
3:C:203:THR:O	3:C:235:GLY:HA3	2.11	0.51
25:a:609:CLA:H2	8:i:12:VAL:HG11	1.93	0.51
25:B:601:CLA:HBA1	25:B:601:CLA:HBD	1.91	0.51
19:z:32:ASP:OD1	19:z:32:ASP:N	2.44	0.51
29:A:613:LMG:H141	25:C:505:CLA:H203	1.92	0.51
31:c:516:DGD:HA92	31:c:517:DGD:HB91	1.93	0.51
1:A:84:PRO:HA	1:A:112:TYR:CG	2.46	0.51
4:D:24:ARG:HD3	18:X:37:VAL:HG12	1.91	0.51
25:B:602:CLA:H191	31:H:102:DGD:HBT2	1.92	0.50
27:B:619:BCR:H382	30:a:615:SQD:H82	1.93	0.50
25:c:505:CLA:H43	27:c:514:BCR:HC7	1.93	0.50
5:e:30:LEU:HD11	35:e:101:HEM:CBB	2.41	0.50
4:D:85:MET:HE1	5:E:72:ALA:HB2	1.94	0.50
25:B:609:CLA:HBC1	32:H:103:STE:H51	1.94	0.50
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.47	0.50
2:b:39:LEU:HD22	32:b:624:STE:H51	1.93	0.50
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.42	0.50
10:K:23:ASP:OD2	17:Y:21:GLN:NE2	2.45	0.50
13:O:15:LEU:HA	13:O:18:LYS:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:158:THR:HG21	3:c:256:PRO:HD3	1.94	0.50
3:C:180:MET:HG2	3:C:199:ILE:O	2.11	0.50
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.94	0.50
25:b:602:CLA:H43	7:h:45:ILE:HG22	1.94	0.49
1:a:334[C]:ARG:NH2	37:a:715:HOH:O	2.45	0.49
25:b:610:CLA:HBB1	27:x:101:BCR:HC21	1.94	0.49
13:O:19:CYS:O	37:O:303:HOH:O	2.20	0.49
2:B:149[B]:LEU:HD11	25:B:604:CLA:H112	1.94	0.49
2:B:357:ARG:NE	37:B:705:HOH:O	2.29	0.49
13:O:56:PRO:O	13:O:58:ASN:ND2	2.46	0.49
25:a:607:CLA:H202	28:a:611:PL9:H222	1.94	0.49
3:C:114:VAL:HG22	32:C:523:STE:H102	1.95	0.49
8:I:2:GLU:O	8:I:6:ILE:HG12	2.13	0.49
13:O:78:LEU:HB3	13:O:81:ILE:HD11	1.94	0.49
1:a:329[C]:GLU:OE2	16:v:134:LYS:NZ	2.38	0.49
5:e:68:ASP:O	5:e:72:ALA:HB2	2.13	0.49
2:B:98:LEU:HD11	31:a:616:DGD:HBW2	1.95	0.49
16:V:41:HIS:HA	16:V:45:ILE:O	2.12	0.49
19:Z:23:VAL:HG22	19:Z:40:ILE:HD12	1.93	0.49
2:b:179:GLN:HE21	2:b:179:GLN:HA	1.78	0.49
8:i:34:ARG:NH2	37:i:101:HOH:O	2.46	0.49
16:v:26:TYR:OH	16:v:122:GLU:OE1	2.26	0.49
3:C:95:LEU:HD21	25:C:501:CLA:OBD	2.13	0.49
33:e:102:LHG:H262	33:e:102:LHG:H291	1.67	0.49
4:d:279:LEU:HD22	26:d:402:PHO:HBC3	1.94	0.48
31:A:616:DGD:HBF2	8:I:7:THR:HG21	1.95	0.48
13:O:27:ARG:NH1	37:O:306:HOH:O	2.31	0.48
28:A:611:PL9:H371	28:A:611:PL9:H351	1.56	0.48
20:R:16:ALA:O	20:R:20:VAL:HG23	2.13	0.48
25:c:504:CLA:H91	25:c:508:CLA:H172	1.95	0.48
4:D:266:TRP:CD1	33:D:409:LHG:HC31	2.49	0.48
16:V:28:GLU:HG2	37:V:353:HOH:O	2.12	0.48
25:c:501:CLA:C3D	25:c:503:CLA:H2	2.43	0.48
4:d:343:GLU:HG2	16:v:135:VAL:HG11	1.96	0.48
3:C:313:GLN:HB2	3:C:396:MET:HG3	1.96	0.48
18:X:2:THR:N	37:X:201:HOH:O	2.47	0.48
19:Z:7:LEU:O	37:Z:101:HOH:O	2.19	0.48
1:a:241:GLN:NE2	1:a:245:THR:HG23	2.28	0.48
1:A:45:THR:HG23	25:A:612:CLA:H191	1.96	0.48
2:B:119:ASP:H	11:L:1:MET:HE3	1.79	0.48
16:v:11:PRO:O	16:v:69:ILE:HD12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:607:CLA:H193	11:L:27:LEU:HD11	1.96	0.48
16:V:99:ASP:N	16:V:99:ASP:OD1	2.45	0.48
13:O:43:LEU:HB3	13:O:81:ILE:HB	1.96	0.48
4:D:269:PHE:CD2	33:D:412:LHG:HC12	2.48	0.47
16:V:87:GLU:OE1	16:V:96:ARG:NH1	2.46	0.47
16:v:2:GLU:OE2	37:v:301:HOH:O	2.20	0.47
3:c:121:SER:O	3:c:124:VAL:HG13	2.14	0.47
9:j:36:LEU:O	37:j:201:HOH:O	2.20	0.47
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.96	0.47
7:H:17:GLU:OE2	7:H:20:LYS:NZ	2.45	0.47
20:R:33:LYS:C	20:R:35:LEU:H	2.23	0.47
4:D:246:MET:HE3	4:D:264:LYS:HE2	1.97	0.47
2:B:247:PHE:CE1	25:B:602:CLA:H102	2.48	0.47
25:B:606:CLA:H91	25:B:606:CLA:H112	1.60	0.47
9:J:20:GLY:O	9:J:24:ILE:HG13	2.15	0.47
14:T:10:PHE:HE2	32:b:624:STE:H162	1.80	0.47
3:c:342:MET:SD	3:c:356[B]:MET:HE2	2.55	0.47
25:c:513:CLA:H61	25:c:513:CLA:H41	1.68	0.47
28:a:611:PL9:H371	28:a:611:PL9:H351	1.65	0.47
4:d:79:SER:HA	4:d:172:SER:HB3	1.96	0.47
25:B:613:CLA:H192	33:D:412:LHG:H211	1.97	0.47
3:C:213:LEU:HD21	27:C:515:BCR:C20	2.45	0.47
30:D:408:SQD:H341	18:X:23:LEU:HD22	1.97	0.47
2:B:36:SER:OG	27:B:618:BCR:H362	2.15	0.47
26:D:402:PHO:HBB1	26:D:402:PHO:HMB1	1.97	0.47
12:m:9:ILE:HG13	12:m:13:LEU:HD22	1.97	0.47
25:B:603:CLA:H2	25:B:605:CLA:H91	1.97	0.46
16:V:31:ARG:HH11	16:V:31:ARG:HB3	1.79	0.46
1:a:95:PRO:HD2	1:a:98:GLU:HG3	1.96	0.46
25:b:608:CLA:HBC2	25:b:609:CLA:H102	1.96	0.46
16:V:26:TYR:OH	16:V:122:GLU:OE1	2.32	0.46
3:c:26:ARG:HA	25:c:511:CLA:OBD	2.15	0.46
16:v:19:ILE:HG12	16:v:20:THR:N	2.30	0.46
25:D:404:CLA:H141	18:X:15:LEU:HD22	1.96	0.46
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.51	0.46
2:b:65:PHE:HE2	25:b:604:CLA:HED2	1.81	0.46
2:b:71:VAL:HG23	25:b:606:CLA:HMA2	1.96	0.46
25:B:615:CLA:H162	7:H:7:LEU:HD21	1.98	0.46
12:m:16:LEU:HD13	12:m:16:LEU:HA	1.67	0.46
31:C:518:DGD:HAN2	31:C:518:DGD:HAW1	1.73	0.46
4:d:246:MET:HE3	4:d:264:LYS:CG	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:57:LYS:HB3	13:o:59:LYS:HE3	1.98	0.46
29:D:407:LMG:H152	29:D:407:LMG:H121	1.40	0.46
12:M:20:VAL:HG11	12:m:20:VAL:HG22	1.98	0.46
4:d:42:TYR:CE1	6:f:25:THR:HG22	2.51	0.46
31:A:616:DGD:HB62	32:I:101:STE:H51	1.98	0.46
25:B:613:CLA:HBB1	25:B:613:CLA:HMB1	1.98	0.46
3:C:94:THR:HG22	25:C:501:CLA:HED1	1.97	0.46
25:b:606:CLA:C1C	32:b:621:STE:H61	2.45	0.46
5:e:18:ARG:HH22	6:f:15:ILE:HD11	1.80	0.46
25:B:614:CLA:HMD2	32:M:101:STE:H41	1.98	0.46
31:C:518:DGD:HA82	31:C:518:DGD:HAE2	1.69	0.46
3:c:38:GLY:HA3	25:c:511:CLA:HMD2	1.98	0.46
13:o:42:ARG:O	13:o:241:ALA:HA	2.16	0.46
5:e:57:ALA:H	5:e:60:GLN:NE2	2.10	0.45
7:h:12:ARG:NH2	7:h:15:ASN:O	2.47	0.45
33:D:412:LHG:H112	33:D:412:LHG:H352	1.99	0.45
1:a:140:ARG:HB2	4:d:220:ASN:HA	1.98	0.45
5:e:78:THR:O	5:e:82:GLN:HG3	2.16	0.45
27:k:102:BCR:H20C	27:k:102:BCR:H361	1.80	0.45
1:a:124:SER:HA	1:a:151:LEU:HD21	1.99	0.45
2:b:224:ARG:HG2	7:h:24:GLY:O	2.16	0.45
25:c:507:CLA:H61	25:c:507:CLA:H92	1.65	0.45
4:d:186:GLN:HB2	25:d:403:CLA:HBC1	1.99	0.45
5:e:8:ARG:NH1	5:e:12:ASP:OD1	2.49	0.45
2:B:149[A]:LEU:HD21	25:B:606:CLA:HBB2	1.98	0.45
28:a:611:PL9:H38	28:a:611:PL9:H422	1.62	0.45
2:b:224:ARG:HG3	7:h:25:TRP:CD2	2.52	0.45
1:A:201:GLY:HA3	1:A:286:THR:HB	1.98	0.45
26:A:608:PHO:HBB1	26:A:608:PHO:HMB3	1.99	0.45
25:B:607:CLA:H122	29:B:620:LMG:H241	1.99	0.45
25:B:612:CLA:H162	25:B:612:CLA:H122	1.79	0.45
4:D:42:TYR:CE1	6:F:25:THR:HG23	2.51	0.45
13:O:25:THR:O	13:O:27:ARG:N	2.49	0.45
13:O:54:GLU:O	13:O:63:ALA:HB3	2.16	0.45
19:Z:6:GLN:HE21	19:Z:6:GLN:HB3	1.54	0.45
3:c:338:GLY:HA3	3:c:341:LEU:O	2.16	0.45
3:c:383:ASP:O	3:c:385:GLN:NE2	2.44	0.45
27:C:515:BCR:H20C	27:C:515:BCR:H361	1.79	0.45
33:E:101:LHG:HC42	33:E:101:LHG:HC2	1.97	0.45
9:J:26:GLY:HA2	32:J:101:STE:H71	1.99	0.45
2:b:127:ARG:NH1	37:h:202:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:391[B]:ARG:HG2	37:c:607:HOH:O	2.16	0.45
10:k:27:VAL:O	10:k:30:VAL:HG22	2.16	0.45
32:l:102:STE:H182	32:l:102:STE:H151	1.76	0.45
3:C:279:LEU:HD12	25:C:509:CLA:HED2	1.98	0.45
5:E:68:ASP:O	5:E:72:ALA:HB2	2.16	0.45
2:b:150:CYS:HB2	25:b:603:CLA:CMC	2.46	0.45
25:b:607:CLA:H42	29:m:101:LMG:H311	1.99	0.45
27:B:618:BCR:H15C	27:B:618:BCR:H351	1.84	0.45
25:C:512:CLA:H91	25:C:512:CLA:H111	1.59	0.45
5:E:7:GLU:OE2	37:E:201:HOH:O	2.21	0.45
5:E:60:GLN:HG2	5:E:62:SER:H	1.81	0.45
16:V:87:GLU:CD	16:V:96:ARG:HH12	2.25	0.45
1:a:93:PHE:HZ	25:a:609:CLA:HAA1	1.82	0.45
3:c:323:LYS:HG3	37:c:635:HOH:O	2.16	0.45
2:B:117:TYR:HA	11:L:1:MET:HE1	1.98	0.45
25:C:506:CLA:H111	25:C:506:CLA:H172	1.99	0.45
25:A:607:CLA:H143	25:A:607:CLA:H161	1.79	0.44
16:V:90:GLU:HG3	16:V:91:VAL:HG13	1.98	0.44
12:m:26:TYR:OH	12:m:30:GLU:OE2	2.34	0.44
1:A:279:PRO:HG2	4:D:212:ALA:HB2	1.99	0.44
27:D:405:BCR:H361	27:D:405:BCR:H20C	1.75	0.44
13:O:54:GLU:HG3	13:O:110:MET:HE1	2.00	0.44
25:b:614:CLA:H93	25:b:614:CLA:H61	1.70	0.44
2:B:173:GLY:HA3	2:B:265:ILE:HD11	1.99	0.44
2:B:458:PHE:HB3	25:B:604:CLA:HBC2	1.99	0.44
8:I:29:ALA:O	8:I:35:LYS:HB3	2.17	0.44
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.51	0.44
25:b:614:CLA:H192	25:b:614:CLA:H162	1.87	0.44
25:c:509:CLA:H111	25:c:509:CLA:H142	1.65	0.44
25:c:510:CLA:H61	25:c:510:CLA:H2	1.58	0.44
4:d:172:SER:HB2	4:d:177:ALA:HB1	2.00	0.44
5:e:20:TRP:CD1	9:j:8:ILE:HD13	2.50	0.44
2:B:119:ASP:HB3	11:L:1:MET:HE3	1.99	0.44
28:a:611:PL9:H252	26:d:402:PHO:HBA2	1.99	0.44
28:A:611:PL9:H401	28:A:611:PL9:H422	1.63	0.44
37:A:781:HOH:O	13:O:107:THR:HG21	2.16	0.44
25:C:506:CLA:H8	27:C:515:BCR:H12C	1.99	0.44
27:D:405:BCR:H352	6:F:29:PRO:HG2	1.99	0.44
1:a:162[C]:PRO:O	1:a:166[C]:GLY:N	2.51	0.44
2:b:486:LEU:HD11	2:b:490:GLN:NE2	2.33	0.44
29:m:101:LMG:H361	29:m:101:LMG:H392	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:43:LEU:HB3	13:o:81:ILE:HB	2.00	0.44
25:C:506:CLA:H91	25:C:506:CLA:H203	1.99	0.44
4:D:148:ALA:HB3	4:D:149:PRO:HD3	2.00	0.44
1:a:185[C]:VAL:O	1:a:189[C]:GLU:HG3	2.18	0.44
25:a:607:CLA:HAB	25:d:403:CLA:H72	2.00	0.44
25:b:608:CLA:H203	31:h:101:DGD:HA71	1.99	0.44
3:c:413[A]:GLU:OE2	16:v:47:LYS:NZ	2.35	0.44
4:d:32:TRP:CD1	29:d:409:LMG:H112	2.53	0.44
29:D:407:LMG:H142	29:D:407:LMG:H171	1.77	0.44
19:Z:36:SER:O	19:Z:40:ILE:HG12	2.18	0.44
1:A:190[B]:HIS:ND1	1:A:298:ASN:OD1	2.51	0.44
25:B:607:CLA:H141	25:B:607:CLA:H161	1.73	0.44
25:b:611:CLA:H72	25:b:611:CLA:H112	1.73	0.44
10:K:19:ASP:OD1	37:K:201:HOH:O	2.21	0.43
2:b:278:SER:O	2:b:282:GLN:HG3	2.18	0.43
25:b:611:CLA:H143	25:b:611:CLA:H162	1.84	0.43
10:k:26:PRO:O	10:k:29:PRO:HD2	2.17	0.43
16:v:104:MET:HA	16:v:107:LEU:HD22	2.00	0.43
31:C:519:DGD:HA91	31:C:519:DGD:HAW1	1.80	0.43
33:d:408:LHG:H242	33:d:408:LHG:H272	1.59	0.43
11:L:14:ARG:HB3	14:T:25:GLU:HG2	1.99	0.43
25:a:609:CLA:H102	8:i:13:THR:HG23	1.99	0.43
31:c:517:DGD:HB92	31:c:517:DGD:HA91	2.00	0.43
31:C:519:DGD:HA51	31:C:519:DGD:HA22	1.67	0.43
16:V:63:THR:HG22	16:V:64:PRO:CD	2.49	0.43
25:a:606:CLA:CBD	25:a:612:CLA:HAC2	2.49	0.43
25:c:503:CLA:H102	25:c:503:CLA:H62	1.64	0.43
25:c:506:CLA:H62	25:c:506:CLA:H41	1.75	0.43
25:c:510:CLA:HMB1	25:c:510:CLA:HBB1	2.00	0.43
25:c:512:CLA:H142	25:c:512:CLA:H112	1.73	0.43
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.99	0.43
13:o:59:LYS:H	13:o:59:LYS:HG3	1.35	0.43
29:A:613:LMG:HC72	3:C:216:SER:HB2	2.01	0.43
29:A:613:LMG:H341	3:C:223:TRP:CE2	2.54	0.43
2:B:12:LEU:HB2	25:B:612:CLA:HMC2	2.00	0.43
25:C:506:CLA:H2	25:C:506:CLA:H62	1.85	0.43
25:a:609:CLA:H202	8:i:6:ILE:HG23	2.00	0.43
27:a:610:BCR:H20C	27:a:610:BCR:H361	1.87	0.43
2:b:36:SER:OG	27:b:618:BCR:H362	2.18	0.43
25:B:606:CLA:H122	25:B:606:CLA:H161	1.41	0.43
25:C:505:CLA:H193	25:C:505:CLA:H162	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:c:515:DGD:HA72	31:c:515:DGD:HA42	1.58	0.43
9:j:18:GLY:O	9:j:22:ILE:HD13	2.18	0.43
25:C:512:CLA:H111	25:C:513:CLA:H141	1.99	0.43
15:U:92:VAL:HG12	15:U:97:ARG:HD2	2.00	0.43
32:d:412:STE:H71	18:x:16:SER:HB3	2.00	0.43
25:b:614:CLA:H41	25:b:614:CLA:H62	1.37	0.43
13:o:180:GLU:CD	13:o:180:GLU:H	2.26	0.43
27:T:101:BCR:H331	27:T:101:BCR:HC7	1.70	0.43
1:a:215:HIS:ND1	28:a:611:PL9:O1	2.42	0.43
25:a:606:CLA:H192	33:d:407:LHG:H332	2.01	0.43
30:a:614:SQD:H111	30:a:614:SQD:H142	1.55	0.43
25:c:504:CLA:H62	25:c:504:CLA:H92	1.80	0.43
17:y:20:ALA:O	17:y:24:MET:HG2	2.19	0.43
27:C:515:BCR:H15C	27:C:515:BCR:H351	1.82	0.43
16:v:41:HIS:CD2	36:v:201:HEC:NB	2.86	0.43
29:C:520:LMG:H111	29:C:520:LMG:H142	1.86	0.42
25:c:513:CLA:H161	25:c:513:CLA:H141	1.80	0.42
27:C:514:BCR:H371	27:C:514:BCR:H24C	1.76	0.42
13:O:66:VAL:HG21	13:O:110:MET:HE3	2.01	0.42
1:a:296:ASN:HB3	3:c:401:LEU:HA	2.01	0.42
25:b:601:CLA:CHA	25:b:601:CLA:HBA2	2.49	0.42
3:c:35:TRP:CZ2	32:c:521:STE:H22	2.54	0.42
33:E:101:LHG:H352	33:E:101:LHG:H321	1.56	0.42
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	2.01	0.42
3:c:178:LYS:NZ	3:c:184:GLY:O	2.49	0.42
3:c:391[B]:ARG:NH1	37:c:607:HOH:O	2.41	0.42
25:c:505:CLA:H193	29:c:522:LMG:H131	2.00	0.42
5:e:57:ALA:N	5:e:60:GLN:HE21	2.12	0.42
2:B:185:TRP:HB3	25:B:601:CLA:HMA3	2.01	0.42
25:B:603:CLA:H91	25:B:603:CLA:H111	1.80	0.42
12:M:28:GLN:O	12:M:32:GLN:HG3	2.19	0.42
13:O:56:PRO:HG3	13:O:63:ALA:H	1.83	0.42
25:b:616:CLA:H62	25:b:616:CLA:H41	1.85	0.42
25:A:612:CLA:H162	25:A:612:CLA:H202	1.83	0.42
3:C:223:TRP:CG	3:C:224:ILE:H	2.36	0.42
19:Z:29:SER:HB3	19:Z:31:GLN:HE21	1.83	0.42
2:b:91:TRP:NE1	32:b:621:STE:H141	2.30	0.42
32:b:621:STE:H52	32:b:621:STE:H22	1.63	0.42
32:b:623:STE:H131	29:d:409:LMG:H401	2.01	0.42
25:c:509:CLA:H3A	25:c:509:CLA:HBA1	1.84	0.42
27:x:101:BCR:H24C	27:x:101:BCR:H371	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162[A]:PRO:HB3	1:A:168[A]:PHE:HA	2.02	0.42
2:B:233:ASN:HD21	2:B:476:ARG:NH1	2.18	0.42
3:C:42:LEU:HD21	25:C:511:CLA:H2A	2.02	0.42
27:C:515:BCR:H24C	27:C:515:BCR:H371	1.88	0.42
4:D:194:ASN:HA	4:D:295:SER:OG	2.20	0.42
6:F:15:ILE:HD13	20:R:23:ILE:HD11	2.02	0.42
1:a:131:TRP:CH2	25:c:505:CLA:HAA2	2.55	0.42
25:b:613:CLA:HBB1	25:b:613:CLA:HMB1	2.01	0.42
31:c:515:DGD:HB61	29:c:522:LMG:H402	2.00	0.42
27:A:610:BCR:H15C	27:A:610:BCR:H351	1.89	0.42
5:E:77:GLU:O	5:E:81:GLU:HG2	2.19	0.42
16:V:77:LYS:NZ	37:V:303:HOH:O	2.52	0.42
25:b:601:CLA:H91	25:b:601:CLA:H111	1.65	0.42
25:b:606:CLA:H193	25:b:606:CLA:H162	1.73	0.42
25:b:615:CLA:H152	25:b:615:CLA:H112	1.76	0.42
3:c:45:LEU:HA	3:c:139:THR:HG22	2.00	0.42
17:y:19:ILE:O	17:y:23:THR:HG22	2.20	0.42
1:A:339[A]:PHE:HB3	1:A:340[A]:PRO:HD2	2.02	0.42
25:B:611:CLA:H72	25:B:611:CLA:H112	1.52	0.42
25:C:513:CLA:H92	25:C:513:CLA:H61	1.75	0.42
20:R:31:VAL:O	20:R:34:LEU:HD22	2.20	0.42
2:b:505:ARG:HG3	2:b:506:ARG:N	2.34	0.42
25:b:607:CLA:HMB1	25:b:607:CLA:HBB1	2.02	0.42
2:B:149[B]:LEU:HD11	25:B:604:CLA:H162	2.01	0.42
2:B:247:PHE:HE1	25:B:602:CLA:H102	1.83	0.42
28:a:611:PL9:H251	28:a:611:PL9:H272	1.76	0.42
27:k:103:BCR:H24C	27:k:103:BCR:H371	1.80	0.42
3:C:360:ASP:OD1	37:C:602:HOH:O	2.22	0.42
7:H:2:ALA:N	37:H:202:HOH:O	2.53	0.42
18:X:21:LEU:HD11	32:X:101:STE:H182	2.02	0.42
25:b:609:CLA:H42	32:b:623:STE:H71	2.02	0.42
27:b:618:BCR:H15C	27:b:618:BCR:H351	1.90	0.42
28:d:406:PL9:H421	28:d:406:PL9:H401	1.87	0.42
5:e:64:PRO:HB2	5:e:79:PHE:CD2	2.55	0.42
19:z:57:LEU:HD23	19:z:57:LEU:HA	1.92	0.42
25:B:603:CLA:C2D	25:B:605:CLA:H2	2.50	0.41
27:B:619:BCR:H15C	27:B:619:BCR:H351	1.92	0.41
4:D:161:PRO:HG3	4:D:170:ALA:HB2	2.02	0.41
3:c:334:PRO:HA	13:o:153:THR:OG1	2.20	0.41
3:c:390:ARG:HD3	16:v:100:ILE:HD12	2.02	0.41
4:d:171:PRO:HG3	4:d:181:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:26:LEU:O	6:f:29:PRO:HD2	2.19	0.41
27:k:103:BCR:H20C	27:k:103:BCR:H361	1.90	0.41
1:A:158:PHE:O	1:A:162[C]:PRO:HG2	2.20	0.41
2:B:67:ALA:HA	2:B:71:VAL:O	2.20	0.41
32:B:625:STE:O2	37:B:701:HOH:O	2.22	0.41
25:b:605:CLA:H61	25:b:605:CLA:H41	1.88	0.41
31:c:515:DGD:HA61	31:c:515:DGD:HB51	2.03	0.41
4:d:272:LEU:C	4:d:272:LEU:HD23	2.46	0.41
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.55	0.41
30:A:614:SQD:H362	25:C:508:CLA:H191	2.02	0.41
2:B:237:VAL:HG22	25:B:610:CLA:HBC2	2.02	0.41
25:B:601:CLA:H92	27:H:101:BCR:H21C	2.02	0.41
19:Z:5:PHE:HB2	19:Z:57:LEU:HB3	2.01	0.41
27:c:514:BCR:H20C	27:c:514:BCR:H361	1.91	0.41
13:o:32:ILE:HG21	13:o:93:LEU:HD21	2.03	0.41
3:C:339:LYS:HB2	3:C:339:LYS:HE3	1.90	0.41
2:b:216:HIS:HE1	25:b:609:CLA:C1A	2.33	0.41
2:b:317:ASN:HA	2:b:330:MET:HE1	2.01	0.41
25:b:613:CLA:H143	25:b:613:CLA:H111	1.91	0.41
3:c:391[B]:ARG:NE	37:c:613:HOH:O	2.52	0.41
25:c:505:CLA:H2	25:c:505:CLA:H61	1.83	0.41
27:c:514:BCR:H24C	27:c:514:BCR:H371	1.90	0.41
31:c:516:DGD:HB32	31:c:516:DGD:HB61	1.85	0.41
17:y:22:LEU:HA	17:y:25:ILE:HG22	2.02	0.41
3:C:178:LYS:HA	3:C:182:PHE:HB2	2.01	0.41
25:C:507:CLA:H93	25:C:507:CLA:H112	1.93	0.41
25:C:512:CLA:H92	25:C:512:CLA:H61	1.76	0.41
15:U:58:VAL:O	15:U:61:VAL:HG22	2.21	0.41
25:a:612:CLA:HED2	4:d:198:MET:SD	2.61	0.41
27:d:405:BCR:H402	9:j:21:VAL:HG21	2.01	0.41
1:A:58[C]:VAL:O	1:A:66[C]:PRO:HA	2.20	0.41
25:B:602:CLA:H141	25:B:602:CLA:H161	1.81	0.41
12:M:20:VAL:HG11	12:m:20:VAL:CG2	2.51	0.41
13:O:34:SER:C	13:O:36:GLN:H	2.28	0.41
2:b:137:LYS:HE3	2:b:137:LYS:HB2	1.95	0.41
5:e:61:ARG:NH1	16:v:125:ILE:O	2.50	0.41
13:o:160:LYS:HD2	13:o:160:LYS:HA	1.84	0.41
1:A:232:SER:OG	33:B:623:LHG:O5	2.37	0.41
2:B:201:HIS:HB2	25:B:602:CLA:CHB	2.51	0.41
25:D:404:CLA:C1D	32:X:101:STE:H102	2.50	0.41
1:a:132:GLU:O	1:a:136:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:162[C]:PRO:HB3	1:a:168[C]:PHE:HA	2.02	0.41
2:b:451:PHE:CE2	2:b:455:HIS:CE1	3.09	0.41
3:c:391[B]:ARG:HH21	3:c:394:GLU:HG2	1.86	0.41
4:d:179:PHE:HA	4:d:182:LEU:HD22	2.01	0.41
16:v:72:LEU:HD23	16:v:72:LEU:HA	1.83	0.41
1:A:334[C]:ARG:HH21	13:O:159:PRO:HA	1.86	0.41
27:A:610:BCR:H371	27:A:610:BCR:H24C	1.87	0.41
27:C:514:BCR:H11C	27:C:514:BCR:H341	1.94	0.41
1:a:82:VAL:HG11	1:a:115:ILE:HD12	2.02	0.41
2:b:161:LEU:HD23	2:b:161:LEU:HA	1.90	0.41
25:b:614:CLA:H112	25:b:614:CLA:H152	1.81	0.41
3:c:185:LEU:HB2	3:c:230:LEU:HD13	2.03	0.41
4:d:194:ASN:HA	4:d:295:SER:OG	2.21	0.41
1:A:339[B]:PHE:HB3	1:A:340[B]:PRO:HD2	2.03	0.41
31:A:616:DGD:HB41	32:I:101:STE:H62	2.01	0.41
2:B:389:LYS:HA	2:B:389:LYS:HD3	1.78	0.41
25:B:602:CLA:H111	25:B:602:CLA:H91	1.77	0.41
3:C:79:LYS:NZ	37:C:614:HOH:O	2.53	0.41
4:D:186:GLN:HB2	25:D:403:CLA:HBC1	2.02	0.41
4:D:209:LEU:C	4:D:209:LEU:HD23	2.46	0.41
25:D:404:CLA:H112	25:D:404:CLA:H72	1.79	0.41
17:Y:34:MET:O	17:Y:38:LEU:HG	2.21	0.41
25:b:610:CLA:H51	25:b:610:CLA:H8	1.82	0.41
27:b:617:BCR:H351	27:b:617:BCR:H15C	1.81	0.41
10:k:10:LYS:N	37:k:202:HOH:O	2.53	0.41
25:B:605:CLA:HMB3	32:B:621:STE:H92	2.02	0.41
27:H:101:BCR:H11C	27:H:101:BCR:H341	1.90	0.41
1:a:183[B]:MET:HA	25:a:606:CLA:HMD2	2.03	0.41
2:b:292:LEU:HD21	2:b:298:LEU:HD23	2.02	0.41
1:A:161[A]:TYR:HB3	1:A:162[A]:PRO:HD3	2.02	0.40
2:B:42:LEU:HD21	2:B:93:PHE:HB3	2.03	0.40
27:B:617:BCR:H20C	27:B:617:BCR:H361	1.83	0.40
29:c:520:LMG:H292	29:c:520:LMG:HC91	1.81	0.40
1:A:11:ALA:O	1:A:16:ARG:NH2	2.54	0.40
2:B:226:TYR:CD2	2:B:231:MET:HB2	2.57	0.40
2:b:8:VAL:HG23	2:b:9:HIS:CD2	2.56	0.40
27:b:619:BCR:H20C	27:b:619:BCR:H361	1.92	0.40
13:o:53:LYS:HE3	13:o:65:PHE:CE2	2.56	0.40
27:A:610:BCR:H20C	27:A:610:BCR:H361	1.85	0.40
3:C:344:SER:O	13:O:75:THR:HG22	2.21	0.40
1:a:82:VAL:HB	1:a:174[B]:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:25:MET:HE1	2:b:108:PHE:CD1	2.57	0.40
25:c:502:CLA:H102	25:c:503:CLA:CHB	2.52	0.40
33:d:407:LHG:H152	11:l:22:LEU:HD21	2.03	0.40
27:B:619:BCR:H20C	27:B:619:BCR:H361	1.88	0.40
4:D:150:ILE:O	4:D:154:VAL:HG13	2.22	0.40
12:M:12:ALA:O	12:M:16:LEU:HB2	2.21	0.40
4:d:12:ARG:HA	4:d:12:ARG:HD3	1.94	0.40
25:A:606:CLA:HBD	25:A:612:CLA:HAC2	2.03	0.40
4:D:131:GLU:O	4:D:135:LEU:HG	2.21	0.40
15:U:70:ARG:NH2	16:V:85:GLU:OE1	2.55	0.40
2:b:213:GLY:O	2:b:217:ILE:HG13	2.22	0.40
3:c:318:LEU:C	3:c:318:LEU:HD23	2.47	0.40
27:t:101:BCR:H20C	27:t:101:BCR:H361	1.94	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%)	455 (99%)	2 (0%)	1 (0%)	43	42
1	a	458/344 (133%)	452 (99%)	5 (1%)	1 (0%)	43	42
2	B	507/510 (99%)	500 (99%)	7 (1%)	0	100	100
2	b	503/510 (99%)	492 (98%)	11 (2%)	0	100	100
3	C	461/461 (100%)	453 (98%)	7 (2%)	1 (0%)	43	42
3	c	471/461 (102%)	462 (98%)	8 (2%)	1 (0%)	43	42
4	D	341/352 (97%)	329 (96%)	12 (4%)	0	100	100
4	d	342/352 (97%)	332 (97%)	10 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	60 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	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%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	232 (96%)	7 (3%)	4 (2%)	7	3
13	o	242/272 (89%)	230 (95%)	11 (4%)	1 (0%)	30	27
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	26 (93%)	2 (7%)	0	100	100
15	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
15	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	11	7
16	V	135/163 (83%)	131 (97%)	3 (2%)	1 (1%)	18	14
16	v	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
17	Y	25/46 (54%)	25 (100%)	0	0	100	100
17	y	28/46 (61%)	27 (96%)	1 (4%)	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
20	R	32/41 (78%)	30 (94%)	2 (6%)	0	100	100
20	r	29/41 (71%)	28 (97%)	0	1 (3%)	3	1
All	All	5534/5700 (97%)	5398 (98%)	124 (2%)	12 (0%)	43	42

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	V	64	PRO
3	C	416	SER
3	c	416	SER
15	u	53	ALA
13	O	59	LYS
13	O	62	GLU
13	O	134	THR
13	O	26	ALA
13	o	61	GLN
20	r	30	GLN
1	A	259	ILE
1	a	259	ILE

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%)	369 (99%)	5 (1%)	61	68
1	a	373/280 (133%)	362 (97%)	11 (3%)	37	40
2	B	407/407 (100%)	401 (98%)	6 (2%)	57	64
2	b	402/407 (99%)	397 (99%)	5 (1%)	63	70
3	C	361/362 (100%)	356 (99%)	5 (1%)	59	66
3	c	370/362 (102%)	357 (96%)	13 (4%)	32	32
4	D	278/283 (98%)	275 (99%)	3 (1%)	65	73
4	d	279/283 (99%)	272 (98%)	7 (2%)	42	45
5	E	72/73 (99%)	69 (96%)	3 (4%)	26	25
5	e	71/73 (97%)	68 (96%)	3 (4%)	26	25
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	31
6	f	28/39 (72%)	25 (89%)	3 (11%)	6	4
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	53/55 (96%)	51 (96%)	2 (4%)	29	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	32/34 (94%)	30 (94%)	2 (6%)	16	13
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	25
9	j	24/28 (86%)	23 (96%)	1 (4%)	26	25
10	K	30/37 (81%)	29 (97%)	1 (3%)	33	34
10	k	30/37 (81%)	24 (80%)	6 (20%)	1	0
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	32 (94%)	2 (6%)	18	14
12	M	28/32 (88%)	27 (96%)	1 (4%)	31	31
12	m	28/32 (88%)	25 (89%)	3 (11%)	6	4
13	O	206/228 (90%)	198 (96%)	8 (4%)	28	28
13	o	207/228 (91%)	201 (97%)	6 (3%)	37	40
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	25/28 (89%)	24 (96%)	1 (4%)	28	27
15	U	84/112 (75%)	80 (95%)	4 (5%)	23	21
15	u	84/112 (75%)	83 (99%)	1 (1%)	63	70
16	V	117/138 (85%)	115 (98%)	2 (2%)	53	60
16	v	117/138 (85%)	113 (97%)	4 (3%)	32	33
17	Y	19/37 (51%)	17 (90%)	2 (10%)	6	4
17	y	22/37 (60%)	18 (82%)	4 (18%)	2	1
18	X	31/34 (91%)	30 (97%)	1 (3%)	34	35
18	x	31/34 (91%)	30 (97%)	1 (3%)	34	35
19	Z	52/52 (100%)	47 (90%)	5 (10%)	8	5
19	z	51/52 (98%)	45 (88%)	6 (12%)	5	3
20	R	28/33 (85%)	23 (82%)	5 (18%)	2	1
20	r	25/33 (76%)	21 (84%)	4 (16%)	2	1
All	All	4572/4654 (98%)	4434 (97%)	138 (3%)	35	38

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	205	VAL

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Mol	Chain	Res	Type
1	A	238	LYS
1	A	243	GLU
1	A	244	GLU
2	B	84	THR
2	B	98	LEU
2	B	101	ILE
2	B	127	ARG
2	B	371	THR
2	B	476	ARG
3	C	130	VAL
3	C	141	GLU
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
4	D	136	VAL
4	D	259	ILE
4	D	345	VAL
5	E	4	THR
5	E	22[A]	ILE
5	E	22[B]	ILE
6	F	25	THR
8	I	4	LEU
8	I	35	LYS
9	J	24	ILE
10	K	24	VAL
12	M	25	LEU
13	O	4	THR
13	O	54	GLU
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	135	SER
13	O	189	ARG
13	O	214	THR
15	U	39	ARG
15	U	51	LYS
15	U	61	VAL
15	U	67	LEU
16	V	7	VAL
16	V	86	GLN
17	Y	30	ILE
17	Y	41	VAL

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Mol	Chain	Res	Type
18	X	15	LEU
19	Z	6	GLN
19	Z	15	LEU
19	Z	35	ARG
19	Z	46	LEU
19	Z	50	LEU
20	R	21	ARG
20	R	32	GLN
20	R	33	LYS
20	R	34	LEU
20	R	35	LEU
1	a	28	LEU
1	a	42	LEU
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	243	GLU
1	a	245	THR
1	a	286	THR
1	a	288	LEU
2	b	98	LEU
2	b	179	GLN
2	b	362	PHE
2	b	435	GLU
2	b	506	ARG
3	c	24	THR
3	c	72	LEU
3	c	79	LYS
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	156	LYS
3	c	165	LEU
3	c	240	ILE
3	c	289	PHE
3	c	315	MET
3	c	391[A]	ARG
3	c	391[B]	ARG
4	d	90	LEU
4	d	182	LEU

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Mol	Chain	Res	Type
4	d	241	GLU
4	d	259	ILE
4	d	291	LEU
4	d	293	LEU
4	d	321	LEU
5	e	4	THR
5	e	71	GLU
5	e	83	LEU
6	f	15	ILE
6	f	23	VAL
6	f	28	VAL
7	h	7	LEU
7	h	56	ASP
9	j	21	VAL
10	k	10	LYS
10	k	13	GLU
10	k	25	LEU
10	k	27	VAL
10	k	30	VAL
10	k	35	LEU
11	l	21	LEU
11	l	30	LEU
12	m	5	GLN
12	m	13	LEU
12	m	16	LEU
13	o	49	THR
13	o	59	LYS
13	o	60	ARG
13	o	87	VAL
13	o	118	LEU
13	o	130	GLN
14	t	25	GLU
15	u	61	VAL
16	v	19	ILE
16	v	22	THR
16	v	69	ILE
16	v	107	LEU
17	y	19	ILE
17	y	34	MET
17	y	45	ASN
17	y	46	LEU
18	x	15	LEU

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Mol	Chain	Res	Type
19	z	2	THR
19	z	7	LEU
19	z	20	VAL
19	z	27	TYR
19	z	31	GLN
19	z	46	LEU
20	r	6	LEU
20	r	9	LEU
20	r	10	LEU
20	r	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	311	GLN
3	C	385	GLN
12	M	32	GLN
13	O	36	GLN
13	O	82	GLN
13	O	88	ASN
13	O	124	ASN
13	O	155	ASN
13	O	231	HIS
15	U	37	GLN
15	U	78	ASN
16	V	86	GLN
18	X	38	GLN
19	Z	38	GLN
20	R	22	ASN
20	R	32	GLN
1	a	19	ASN
1	a	234	ASN
2	b	14	ASN
2	b	179	GLN
2	b	331	ASN
2	b	338	GLN
2	b	409	GLN
3	c	311	GLN
3	c	382	ASN
5	e	60	GLN
5	e	82	GLN
7	h	59	ASN

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Mol	Chain	Res	Type
12	m	5	GLN
13	o	231	HIS
18	x	33	GLN
19	z	31	GLN
20	r	30	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	i	1	8	8,9,10	1.05	0	8,9,11	1.16	1 (12%)
12	FME	M	1	12	8,9,10	1.05	0	8,9,11	1.03	0
8	FME	I	1	8	8,9,10	1.01	0	8,9,11	1.13	0
12	FME	m	1	12	8,9,10	0.99	0	8,9,11	0.69	0
14	FME	t	1	14	8,9,10	0.97	0	8,9,11	1.27	1 (12%)
14	FME	T	1	14	8,9,10	1.16	1 (12%)	8,9,11	1.06	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
8	FME	i	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	5/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	t	1	14	-	2/7/9/11	-
14	FME	T	1	14	-	2/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	1	FME	CA-N	-2.24	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	CA-N-CN	-2.39	119.14	122.82
14	t	1	FME	CB-CA-N	2.22	114.56	110.52

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
27	BCR	D	405	-	41,41,41	1.07	3 (7%)	56,56,56	1.19	4 (7%)
32	STE	m	102	-	11,11,19	0.71	0	11,11,19	1.41	2 (18%)
25	CLA	B	613	2	69,73,73	1.31	8 (11%)	82,113,113	1.35	7 (8%)
25	CLA	D	404	4	69,73,73	1.24	7 (10%)	82,113,113	1.29	7 (8%)
22	OEY	a	602[A]	3,37,1	0,16,16	-	-	-		
25	CLA	B	601	37	69,73,73	1.37	8 (11%)	82,113,113	1.39	7 (8%)
32	STE	C	521	-	11,11,19	0.67	0	11,11,19	1.59	2 (18%)
29	LMG	A	613	-	48,48,55	0.75	0	56,56,63	1.37	6 (10%)
27	BCR	k	102	-	41,41,41	1.09	3 (7%)	56,56,56	1.07	3 (5%)
21	OEX	a	601[C]	3,37,1	0,14,14	-	-	-		
25	CLA	c	513	3	69,73,73	1.22	8 (11%)	82,113,113	1.25	8 (9%)
31	DGD	h	101	-	63,63,67	0.93	5 (7%)	77,77,81	1.42	13 (16%)
25	CLA	b	613	2	69,73,73	1.26	6 (8%)	82,113,113	1.44	11 (13%)
32	STE	B	621	-	16,16,19	0.70	0	16,16,19	1.06	0
25	CLA	c	508	3	68,72,73	1.30	8 (11%)	80,111,113	1.25	6 (7%)
36	HEC	V	201	16	50,50,50	1.66	6 (12%)	68,82,82	1.36	9 (13%)
33	LHG	d	407	-	48,48,48	0.70	2 (4%)	51,54,54	1.24	6 (11%)
25	CLA	B	616	2	64,68,73	1.40	6 (9%)	76,107,113	1.40	6 (7%)
25	CLA	b	601	37	69,73,73	1.29	7 (10%)	82,113,113	1.39	7 (8%)
25	CLA	B	611	2	69,73,73	1.22	6 (8%)	82,113,113	1.31	5 (6%)
21	OEX	a	601[B]	3,37,1	0,14,14	-	-	-		
22	OEY	A	602[A]	3,37,1	0,16,16	-	-	-		
27	BCR	A	610	-	41,41,41	0.96	3 (7%)	56,56,56	1.20	3 (5%)
27	BCR	B	618	-	41,41,41	1.04	2 (4%)	56,56,56	1.19	4 (7%)
33	LHG	l	101	-	48,48,48	0.60	0	51,54,54	1.18	6 (11%)
27	BCR	C	516	-	41,41,41	1.05	2 (4%)	56,56,56	1.10	3 (5%)
29	LMG	d	410	-	44,44,55	0.82	1 (2%)	52,52,63	1.30	6 (11%)
29	LMG	c	522	-	49,49,55	0.88	4 (8%)	57,57,63	1.28	6 (10%)
25	CLA	c	506	3	69,73,73	1.18	7 (10%)	82,113,113	1.27	4 (4%)
25	CLA	B	609	2	69,73,73	1.29	10 (14%)	82,113,113	1.37	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	611	2	69,73,73	1.30	6 (8%)	82,113,113	1.37	9 (10%)
28	PL9	d	406	-	55,55,55	1.05	3 (5%)	68,69,69	1.64	13 (19%)
32	STE	M	102	-	9,9,19	0.34	0	8,8,19	0.86	0
25	CLA	C	513	3	69,73,73	1.31	7 (10%)	82,113,113	1.40	6 (7%)
34	BCT	d	401	23	3,3,3	1.14	0	2,3,3	3.17	1 (50%)
25	CLA	C	502	3	69,73,73	1.21	7 (10%)	82,113,113	1.20	7 (8%)
25	CLA	b	605	2	69,73,73	1.22	6 (8%)	82,113,113	1.32	6 (7%)
29	LMG	B	622	-	26,26,55	0.69	2 (7%)	26,26,63	1.27	1 (3%)
30	SQD	A	614	-	50,52,54	1.59	7 (14%)	60,63,65	1.91	12 (20%)
32	STE	X	101	-	19,19,19	0.57	0	19,19,19	1.16	0
25	CLA	b	606	2	69,73,73	1.40	7 (10%)	82,113,113	1.48	6 (7%)
25	CLA	b	610	37	69,73,73	1.23	7 (10%)	82,113,113	1.41	7 (8%)
32	STE	a	617	-	11,11,19	0.81	0	11,11,19	0.99	0
30	SQD	A	615	-	38,38,54	1.76	5 (13%)	40,40,65	1.22	2 (5%)
31	DGD	C	517	-	63,63,67	1.00	5 (7%)	77,77,81	1.36	9 (11%)
31	DGD	c	515	-	63,63,67	0.95	3 (4%)	77,77,81	1.42	11 (14%)
32	STE	d	411	-	16,16,19	0.54	0	16,16,19	1.34	2 (12%)
21	OEX	A	601[C]	3,37,1	0,14,14	-	-	-	-	-
29	LMG	D	407	-	51,51,55	0.80	3 (5%)	59,59,63	1.38	6 (10%)
25	CLA	c	504	37	64,68,73	1.25	7 (10%)	76,107,113	1.25	8 (10%)
25	CLA	b	615	2	69,73,73	1.40	7 (10%)	82,113,113	1.28	8 (9%)
27	BCR	B	617	-	41,41,41	1.01	3 (7%)	56,56,56	1.18	6 (10%)
30	SQD	f	101	-	39,41,54	1.67	7 (17%)	49,52,65	1.66	10 (20%)
31	DGD	c	517	-	63,63,67	0.86	2 (3%)	77,77,81	1.30	6 (7%)
25	CLA	b	609	2	69,73,73	1.28	9 (13%)	82,113,113	1.32	7 (8%)
32	STE	c	519	-	19,19,19	0.61	0	19,19,19	1.00	0
35	HEM	e	101	5,6	50,50,50	1.47	8 (16%)	67,82,82	1.30	8 (11%)
30	SQD	b	620	-	47,49,54	1.60	8 (17%)	57,60,65	1.71	10 (17%)
32	STE	T	103	-	14,14,19	0.36	0	13,13,19	0.82	0
25	CLA	a	606	1	69,73,73	1.38	9 (13%)	82,113,113	1.20	9 (10%)
25	CLA	C	503	3	69,73,73	1.53	9 (13%)	82,113,113	1.44	5 (6%)
26	PHO	D	402	-	58,69,69	2.03	10 (17%)	55,99,99	1.46	9 (16%)
25	CLA	c	507	37	69,73,73	1.28	9 (13%)	82,113,113	1.35	9 (10%)
25	CLA	a	609	1	69,73,73	1.18	6 (8%)	82,113,113	1.26	6 (7%)
28	PL9	D	406	-	55,55,55	0.98	1 (1%)	68,69,69	1.55	13 (19%)
27	BCR	x	101	-	41,41,41	0.97	2 (4%)	56,56,56	1.25	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LHG	d	408	-	38,38,48	0.81	1 (2%)	41,44,54	1.19	4 (9%)
25	CLA	C	507	37	69,73,73	1.15	7 (10%)	82,113,113	1.42	7 (8%)
28	PL9	a	611	-	55,55,55	0.78	2 (3%)	68,69,69	1.60	11 (16%)
21	OEX	A	601[B]	3,37,1	0,14,14	-	-	-		
32	STE	b	621	-	19,19,19	0.59	0	19,19,19	1.06	0
25	CLA	B	606	2	69,73,73	1.38	6 (8%)	82,113,113	1.43	6 (7%)
25	CLA	C	506	3	69,73,73	1.43	9 (13%)	82,113,113	1.24	7 (8%)
32	STE	B	626	-	11,11,19	0.79	0	11,11,19	1.11	0
32	STE	B	627	-	17,17,19	0.64	0	17,17,19	1.21	1 (5%)
36	HEC	v	201	16	50,50,50	1.68	7 (14%)	68,82,82	1.17	7 (10%)
25	CLA	B	615	2	69,73,73	1.45	8 (11%)	82,113,113	1.30	6 (7%)
27	BCR	t	101	-	41,41,41	1.01	2 (4%)	56,56,56	1.37	7 (12%)
32	STE	b	624	-	19,19,19	0.64	0	19,19,19	1.09	1 (5%)
31	DGD	C	518	-	63,63,67	1.06	4 (6%)	77,77,81	1.35	10 (12%)
32	STE	B	629	-	15,15,19	0.34	0	14,14,19	0.80	0
25	CLA	C	509	3	69,73,73	1.22	8 (11%)	82,113,113	1.31	7 (8%)
25	CLA	b	608	2	69,73,73	1.36	8 (11%)	82,113,113	1.41	11 (13%)
25	CLA	A	607	37	69,73,73	1.12	8 (11%)	82,113,113	1.28	8 (9%)
25	CLA	B	602	2	69,73,73	1.25	6 (8%)	82,113,113	1.36	10 (12%)
27	BCR	k	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.31	10 (17%)
27	BCR	C	514	-	41,41,41	1.02	2 (4%)	56,56,56	1.22	6 (10%)
32	STE	M	101	-	14,14,19	0.72	0	14,14,19	1.02	0
25	CLA	b	602	2	69,73,73	1.13	7 (10%)	82,113,113	1.29	6 (7%)
27	BCR	C	515	-	41,41,41	1.07	2 (4%)	56,56,56	1.17	4 (7%)
31	DGD	C	519	-	63,63,67	0.81	2 (3%)	77,77,81	1.36	7 (9%)
25	CLA	d	404	4	69,73,73	1.15	6 (8%)	82,113,113	1.15	4 (4%)
25	CLA	b	616	2	64,68,73	1.19	6 (9%)	76,107,113	1.31	8 (10%)
32	STE	H	103	-	17,17,19	0.36	0	16,16,19	0.76	0
25	CLA	b	603	2	69,73,73	1.13	7 (10%)	82,113,113	1.39	10 (12%)
32	STE	J	101	-	11,11,19	0.74	0	11,11,19	1.13	0
25	CLA	c	512	3	69,73,73	1.25	7 (10%)	82,113,113	1.34	7 (8%)
25	CLA	d	403	4	69,73,73	1.19	7 (10%)	82,113,113	1.30	9 (10%)
25	CLA	c	505	3	69,73,73	1.08	7 (10%)	82,113,113	1.19	6 (7%)
32	STE	j	101	-	11,11,19	0.73	0	11,11,19	1.23	2 (18%)
25	CLA	B	610	37	69,73,73	1.13	7 (10%)	82,113,113	1.28	7 (8%)
25	CLA	A	606	1	69,73,73	1.22	8 (11%)	82,113,113	1.27	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LHG	D	410	-	46,46,48	0.95	2 (4%)	49,52,54	1.31	5 (10%)
31	DGD	c	516	-	63,63,67	1.01	5 (7%)	77,77,81	1.31	9 (11%)
25	CLA	D	403	4	69,73,73	1.07	5 (7%)	82,113,113	1.20	11 (13%)
25	CLA	b	612	2	69,73,73	1.13	9 (13%)	82,113,113	1.31	11 (13%)
28	PL9	A	611	-	55,55,55	0.64	0	68,69,69	1.53	10 (14%)
29	LMG	B	620	-	51,51,55	0.81	1 (1%)	59,59,63	1.38	7 (11%)
32	STE	E	102	-	11,11,19	0.76	0	11,11,19	1.13	1 (9%)
35	HEM	F	101	5,6	50,50,50	1.42	8 (16%)	67,82,82	1.09	2 (2%)
31	DGD	a	616	-	43,43,67	0.71	2 (4%)	45,45,81	1.37	7 (15%)
27	BCR	c	514	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
25	CLA	A	609	1	58,62,73	1.23	5 (8%)	68,99,113	1.40	6 (8%)
29	LMG	d	409	-	21,21,55	0.53	1 (4%)	20,20,63	1.26	2 (10%)
25	CLA	c	511	3	69,73,73	1.44	6 (8%)	82,113,113	1.46	4 (4%)
29	LMG	C	520	-	48,48,55	0.74	2 (4%)	56,56,63	1.38	8 (14%)
32	STE	C	523	-	15,15,19	0.34	0	14,14,19	0.87	0
32	STE	t	102	-	9,9,19	0.37	0	8,8,19	0.74	0
26	PHO	d	402	-	58,69,69	2.14	11 (18%)	55,99,99	1.48	8 (14%)
30	SQD	a	615	-	35,35,54	1.73	5 (14%)	37,37,65	1.46	5 (13%)
25	CLA	c	502	3	69,73,73	1.20	8 (11%)	82,113,113	1.28	8 (9%)
32	STE	c	521	-	11,11,19	0.77	0	11,11,19	1.08	0
25	CLA	C	508	3	69,73,73	1.17	8 (11%)	82,113,113	1.42	9 (10%)
29	LMG	c	520	-	48,48,55	0.91	3 (6%)	56,56,63	1.29	8 (14%)
25	CLA	B	603	2	69,73,73	1.10	7 (10%)	82,113,113	1.31	9 (10%)
25	CLA	c	510	3	69,73,73	1.33	7 (10%)	82,113,113	1.25	5 (6%)
25	CLA	a	612	37	69,73,73	1.28	6 (8%)	82,113,113	1.32	9 (10%)
25	CLA	C	511	3	69,73,73	1.29	6 (8%)	82,113,113	1.44	7 (8%)
25	CLA	c	503	3	69,73,73	1.24	10 (14%)	82,113,113	1.38	7 (8%)
33	LHG	E	101	-	48,48,48	0.75	2 (4%)	51,54,54	1.23	6 (11%)
31	DGD	H	102	-	63,63,67	1.05	4 (6%)	77,77,81	1.39	10 (12%)
33	LHG	a	613	-	48,48,48	0.75	3 (6%)	51,54,54	1.31	7 (13%)
32	STE	d	412	-	19,19,19	0.56	0	19,19,19	1.21	1 (5%)
27	BCR	B	619	-	41,41,41	1.00	2 (4%)	56,56,56	1.26	4 (7%)
25	CLA	B	608	2	69,73,73	1.13	6 (8%)	82,113,113	1.31	9 (10%)
32	STE	b	623	-	15,15,19	0.72	0	15,15,19	0.99	0
25	CLA	B	607	37	69,73,73	1.32	8 (11%)	82,113,113	1.16	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	605	2	69,73,73	1.21	6 (8%)	82,113,113	1.29	7 (8%)
30	SQD	D	408	-	34,36,54	1.49	5 (14%)	42,45,65	1.58	9 (21%)
25	CLA	B	614	2	69,73,73	1.24	5 (7%)	82,113,113	1.32	6 (7%)
27	BCR	b	617	-	41,41,41	0.95	2 (4%)	56,56,56	1.29	6 (10%)
25	CLA	B	604	2	69,73,73	1.31	7 (10%)	82,113,113	1.51	10 (12%)
32	STE	B	625	-	13,13,19	0.69	0	13,13,19	1.26	2 (15%)
27	BCR	k	103	-	41,41,41	1.05	2 (4%)	56,56,56	1.14	5 (8%)
25	CLA	B	612	2	69,73,73	1.09	5 (7%)	82,113,113	1.35	11 (13%)
34	BCT	D	401	23	3,3,3	1.13	0	2,3,3	3.21	1 (50%)
25	CLA	c	509	3	69,73,73	1.12	4 (5%)	82,113,113	1.41	7 (8%)
30	SQD	a	614	-	52,54,54	1.59	7 (13%)	62,65,65	1.78	11 (17%)
27	BCR	T	101	-	41,41,41	0.97	2 (4%)	56,56,56	1.26	8 (14%)
25	CLA	c	501	3	69,73,73	1.20	8 (11%)	82,113,113	1.35	9 (10%)
27	BCR	a	610	-	41,41,41	0.98	2 (4%)	56,56,56	1.15	2 (3%)
29	LMG	b	622	-	55,55,55	0.71	2 (3%)	63,63,63	1.36	9 (14%)
32	STE	B	628	-	11,11,19	0.77	0	11,11,19	1.17	1 (9%)
25	CLA	C	510	3	69,73,73	1.16	7 (10%)	82,113,113	1.35	8 (9%)
25	CLA	b	614	2	69,73,73	1.21	6 (8%)	82,113,113	1.25	7 (8%)
31	DGD	A	616	-	67,67,67	0.97	4 (5%)	81,81,81	1.32	12 (14%)
32	STE	l	102	-	17,17,19	0.29	0	16,16,19	0.96	0
26	PHO	A	608	-	58,69,69	1.94	8 (13%)	55,99,99	1.47	8 (14%)
32	STE	I	101	-	14,14,19	0.36	0	13,13,19	0.83	0
27	BCR	d	405	-	41,41,41	1.06	2 (4%)	56,56,56	1.22	6 (10%)
32	STE	C	522	-	11,11,19	0.69	0	11,11,19	1.22	1 (9%)
33	LHG	D	409	-	48,48,48	0.75	2 (4%)	51,54,54	1.25	7 (13%)
27	BCR	b	619	-	41,41,41	0.97	2 (4%)	56,56,56	1.16	3 (5%)
29	LMG	c	518	-	37,37,55	0.93	2 (5%)	45,45,63	1.35	6 (13%)
25	CLA	C	504	37	63,67,73	1.22	7 (11%)	74,105,113	1.29	7 (9%)
25	CLA	b	607	37	69,73,73	1.19	5 (7%)	82,113,113	1.19	7 (8%)
27	BCR	H	101	-	41,41,41	0.97	1 (2%)	56,56,56	1.23	6 (10%)
25	CLA	C	501	3	69,73,73	1.29	7 (10%)	82,113,113	1.32	6 (7%)
29	LMG	m	101	-	51,51,55	0.73	0	59,59,63	1.41	9 (15%)
32	STE	T	102	-	15,15,19	0.33	0	14,14,19	0.91	0
33	LHG	e	102	-	41,41,48	0.72	1 (2%)	44,47,54	1.30	6 (13%)
25	CLA	A	612	37	69,73,73	1.38	7 (10%)	82,113,113	1.24	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	C	512	3	69,73,73	1.29	9 (13%)	82,113,113	1.30	9 (10%)
26	PHO	a	608	-	58,69,69	2.12	10 (17%)	55,99,99	1.43	9 (16%)
25	CLA	C	505	3	69,73,73	1.37	8 (11%)	82,113,113	1.42	9 (10%)
30	SQD	B	624	-	52,54,54	1.58	10 (19%)	62,65,65	1.70	10 (16%)
32	STE	b	625	-	9,9,19	0.31	0	8,8,19	0.80	0
27	BCR	b	618	-	41,41,41	1.11	3 (7%)	56,56,56	1.17	5 (8%)
33	LHG	B	623	-	48,48,48	0.75	1 (2%)	51,54,54	1.17	3 (5%)
25	CLA	a	607	37	69,73,73	1.24	8 (11%)	82,113,113	1.24	6 (7%)
27	BCR	K	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.11	4 (7%)
29	LMG	D	411	-	31,31,55	0.63	1 (3%)	33,33,63	1.26	2 (6%)
25	CLA	b	604	2	69,73,73	1.08	6 (8%)	82,113,113	1.43	11 (13%)
33	LHG	D	412	-	48,48,48	0.80	1 (2%)	51,54,54	1.32	6 (11%)

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
27	BCR	D	405	-	-	5/29/63/63	0/2/2/2
32	STE	m	102	-	-	3/9/9/17	-
25	CLA	B	613	2	-	5/39/115/115	-
25	CLA	D	404	4	-	7/39/115/115	-
25	CLA	B	601	37	-	17/39/115/115	-
32	STE	C	521	-	-	3/9/9/17	-
29	LMG	A	613	-	-	18/43/63/70	0/1/1/1
27	BCR	k	102	-	-	6/29/63/63	0/2/2/2
25	CLA	c	513	3	-	10/39/115/115	-
31	DGD	h	101	-	-	17/51/91/95	0/2/2/2
25	CLA	b	613	2	-	7/39/115/115	-
32	STE	B	621	-	-	6/14/14/17	-
36	HEC	V	201	16	1/1/3/7	6/14/54/54	-
25	CLA	c	508	3	-	4/38/114/115	-
33	LHG	d	407	-	-	17/53/53/53	-
25	CLA	B	616	2	-	10/33/109/115	-
25	CLA	b	601	37	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	611	2	-	2/39/115/115	-
27	BCR	A	610	-	-	3/29/63/63	0/2/2/2
27	BCR	B	618	-	-	3/29/63/63	0/2/2/2
33	LHG	l	101	-	-	19/53/53/53	-
27	BCR	C	516	-	-	7/29/63/63	0/2/2/2
29	LMG	d	410	-	-	9/39/59/70	0/1/1/1
29	LMG	c	522	-	-	26/44/64/70	0/1/1/1
25	CLA	c	506	3	-	14/39/115/115	-
25	CLA	B	609	2	-	2/39/115/115	-
25	CLA	b	611	2	-	10/39/115/115	-
28	PL9	d	406	-	-	8/53/73/73	0/1/1/1
32	STE	M	102	-	-	2/7/7/17	-
25	CLA	C	513	3	-	12/39/115/115	-
25	CLA	C	502	3	-	9/39/115/115	-
25	CLA	b	605	2	-	9/39/115/115	-
29	LMG	B	622	-	-	10/22/22/70	-
30	SQD	A	614	-	-	20/47/67/69	0/1/1/1
32	STE	X	101	-	-	10/17/17/17	-
25	CLA	b	606	2	-	10/39/115/115	-
25	CLA	b	610	37	-	5/39/115/115	-
32	STE	a	617	-	-	4/9/9/17	-
30	SQD	A	615	-	-	16/39/39/69	-
31	DGD	C	517	-	-	22/51/91/95	0/2/2/2
31	DGD	c	515	-	-	28/51/91/95	0/2/2/2
32	STE	d	411	-	-	8/14/14/17	-
29	LMG	D	407	-	-	14/46/66/70	0/1/1/1
25	CLA	c	504	37	-	7/33/109/115	-
25	CLA	b	615	2	-	11/39/115/115	-
27	BCR	B	617	-	-	2/29/63/63	0/2/2/2
30	SQD	f	101	-	-	17/36/56/69	0/1/1/1
31	DGD	c	517	-	-	17/51/91/95	0/2/2/2
25	CLA	b	609	2	-	6/39/115/115	-
32	STE	c	519	-	-	9/17/17/17	-
35	HEM	e	101	5,6	-	5/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SQD	b	620	-	-	22/44/64/69	0/1/1/1
32	STE	T	103	-	-	9/12/12/17	-
25	CLA	a	606	1	-	4/39/115/115	-
25	CLA	C	503	3	-	3/39/115/115	-
26	PHO	D	402	-	-	2/37/103/103	0/5/6/6
25	CLA	c	507	37	-	7/39/115/115	-
25	CLA	a	609	1	-	8/39/115/115	-
28	PL9	D	406	-	-	6/53/73/73	0/1/1/1
27	BCR	x	101	-	-	7/29/63/63	0/2/2/2
33	LHG	d	408	-	-	13/43/43/53	-
25	CLA	C	507	37	-	9/39/115/115	-
28	PL9	a	611	-	-	22/53/73/73	0/1/1/1
32	STE	b	621	-	-	13/17/17/17	-
25	CLA	B	606	2	-	15/39/115/115	-
25	CLA	C	506	3	-	11/39/115/115	-
32	STE	B	626	-	-	6/9/9/17	-
32	STE	B	627	-	-	8/15/15/17	-
36	HEC	v	201	16	1/1/3/7	5/14/54/54	-
25	CLA	B	615	2	-	9/39/115/115	-
27	BCR	t	101	-	-	5/29/63/63	0/2/2/2
32	STE	b	624	-	-	8/17/17/17	-
31	DGD	C	518	-	-	19/51/91/95	0/2/2/2
32	STE	B	629	-	-	7/13/13/17	-
25	CLA	C	509	3	-	13/39/115/115	-
25	CLA	b	608	2	-	4/39/115/115	-
25	CLA	A	607	37	-	13/39/115/115	-
25	CLA	B	602	2	-	6/39/115/115	-
27	BCR	k	101	-	-	10/29/63/63	0/2/2/2
27	BCR	C	514	-	-	0/29/63/63	0/2/2/2
32	STE	M	101	-	-	7/12/12/17	-
25	CLA	b	602	2	-	4/39/115/115	-
27	BCR	C	515	-	-	4/29/63/63	0/2/2/2
31	DGD	C	519	-	-	16/51/91/95	0/2/2/2
25	CLA	d	404	4	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	616	2	-	7/33/109/115	-
32	STE	H	103	-	-	10/15/15/17	-
25	CLA	b	603	2	-	10/39/115/115	-
32	STE	J	101	-	-	5/9/9/17	-
25	CLA	c	512	3	-	19/39/115/115	-
25	CLA	d	403	4	-	4/39/115/115	-
25	CLA	c	505	3	-	8/39/115/115	-
32	STE	j	101	-	-	5/9/9/17	-
25	CLA	B	610	37	-	6/39/115/115	-
25	CLA	A	606	1	-	5/39/115/115	-
33	LHG	D	410	-	-	23/51/51/53	-
31	DGD	c	516	-	-	17/51/91/95	0/2/2/2
25	CLA	D	403	4	-	8/39/115/115	-
25	CLA	b	612	2	-	5/39/115/115	-
28	PL9	A	611	-	-	28/53/73/73	0/1/1/1
29	LMG	B	620	-	-	25/46/66/70	0/1/1/1
32	STE	E	102	-	-	3/9/9/17	-
35	HEM	F	101	5,6	-	3/14/54/54	-
31	DGD	a	616	-	-	31/45/45/95	-
27	BCR	c	514	-	-	3/29/63/63	0/2/2/2
25	CLA	A	609	1	-	4/26/102/115	-
29	LMG	d	409	-	-	7/17/17/70	-
25	CLA	c	511	3	-	4/39/115/115	-
29	LMG	C	520	-	-	19/43/63/70	0/1/1/1
32	STE	C	523	-	-	2/13/13/17	-
32	STE	t	102	-	-	3/7/7/17	-
26	PHO	d	402	-	-	4/37/103/103	0/5/6/6
30	SQD	a	615	-	-	16/37/37/69	-
25	CLA	c	502	3	-	3/39/115/115	-
32	STE	c	521	-	-	4/9/9/17	-
25	CLA	C	508	3	-	6/39/115/115	-
29	LMG	c	520	-	-	23/43/63/70	0/1/1/1
25	CLA	B	603	2	-	10/39/115/115	-
25	CLA	c	510	3	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	a	612	37	-	0/39/115/115	-
25	CLA	C	511	3	-	4/39/115/115	-
25	CLA	c	503	3	-	9/39/115/115	-
33	LHG	E	101	-	-	18/53/53/53	-
31	DGD	H	102	-	-	20/51/91/95	0/2/2/2
33	LHG	a	613	-	-	21/53/53/53	-
32	STE	d	412	-	-	9/17/17/17	-
27	BCR	B	619	-	-	6/29/63/63	0/2/2/2
25	CLA	B	608	2	-	3/39/115/115	-
32	STE	b	623	-	-	6/13/13/17	-
25	CLA	B	607	37	-	7/39/115/115	-
25	CLA	B	605	2	-	6/39/115/115	-
30	SQD	D	408	-	-	13/28/48/69	0/1/1/1
25	CLA	B	614	2	-	11/39/115/115	-
27	BCR	b	617	-	-	3/29/63/63	0/2/2/2
25	CLA	B	604	2	-	8/39/115/115	-
32	STE	B	625	-	-	3/11/11/17	-
27	BCR	k	103	-	-	4/29/63/63	0/2/2/2
25	CLA	B	612	2	-	7/39/115/115	-
25	CLA	c	509	3	-	13/39/115/115	-
30	SQD	a	614	-	-	21/49/69/69	0/1/1/1
27	BCR	T	101	-	-	7/29/63/63	0/2/2/2
25	CLA	c	501	3	-	4/39/115/115	-
27	BCR	a	610	-	-	0/29/63/63	0/2/2/2
29	LMG	b	622	-	-	28/50/70/70	0/1/1/1
32	STE	B	628	-	-	5/9/9/17	-
25	CLA	C	510	3	-	5/39/115/115	-
25	CLA	b	614	2	-	10/39/115/115	-
31	DGD	A	616	-	-	27/55/95/95	0/2/2/2
32	STE	l	102	-	-	6/15/15/17	-
26	PHO	A	608	-	-	2/37/103/103	0/5/6/6
32	STE	I	101	-	-	4/12/12/17	-
27	BCR	d	405	-	-	4/29/63/63	0/2/2/2
32	STE	C	522	-	-	4/9/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LHG	D	409	-	-	18/53/53/53	-
27	BCR	b	619	-	-	2/29/63/63	0/2/2/2
29	LMG	c	518	-	-	10/31/51/70	0/1/1/1
25	CLA	C	504	37	-	9/32/108/115	-
25	CLA	b	607	37	-	13/39/115/115	-
27	BCR	H	101	-	-	2/29/63/63	0/2/2/2
25	CLA	C	501	3	-	4/39/115/115	-
29	LMG	m	101	-	-	18/46/66/70	0/1/1/1
32	STE	T	102	-	-	8/13/13/17	-
33	LHG	e	102	-	-	27/46/46/53	-
25	CLA	A	612	37	-	4/39/115/115	-
25	CLA	C	512	3	-	13/39/115/115	-
26	PHO	a	608	-	-	2/37/103/103	0/5/6/6
25	CLA	C	505	3	-	13/39/115/115	-
30	SQD	B	624	-	-	23/49/69/69	0/1/1/1
32	STE	b	625	-	-	3/7/7/17	-
27	BCR	b	618	-	-	2/29/63/63	0/2/2/2
33	LHG	B	623	-	-	25/53/53/53	-
25	CLA	a	607	37	-	9/39/115/115	-
27	BCR	K	101	-	-	4/29/63/63	0/2/2/2
29	LMG	D	411	-	-	16/33/33/70	-
25	CLA	b	604	2	-	9/39/115/115	-
33	LHG	D	412	-	-	13/53/53/53	-

All (744) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	608	PHO	C1B-C2B	10.09	1.50	1.39
26	d	402	PHO	C1B-C2B	9.43	1.49	1.39
26	D	402	PHO	C1B-C2B	9.09	1.49	1.39
26	d	402	PHO	C3B-C4B	9.06	1.50	1.41
26	A	608	PHO	C1B-C2B	8.74	1.49	1.39
26	D	402	PHO	C3B-C4B	8.37	1.50	1.41
26	a	608	PHO	C3B-C4B	7.86	1.49	1.41
36	v	201	HEC	C3D-C2D	7.71	1.53	1.36
36	V	201	HEC	C3D-C2D	7.34	1.52	1.36
25	B	606	CLA	MG-NA	7.19	2.23	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	511	CLA	MG-NA	7.17	2.23	2.06
26	A	608	PHO	C3B-C4B	6.87	1.48	1.41
25	b	615	CLA	MG-NA	6.33	2.21	2.06
25	b	606	CLA	MG-NA	6.22	2.21	2.06
25	B	616	CLA	MG-NA	6.15	2.20	2.06
25	b	611	CLA	MG-NA	6.09	2.20	2.06
25	C	503	CLA	MG-NC	5.94	2.20	2.06
25	b	608	CLA	MG-NA	5.71	2.19	2.06
25	B	615	CLA	MG-NA	5.57	2.19	2.06
30	A	615	SQD	O47-C45	-5.41	1.37	1.47
30	a	614	SQD	O48-C23	5.25	1.48	1.33
25	c	510	CLA	MG-NA	5.12	2.18	2.06
25	a	612	CLA	MG-NA	5.08	2.18	2.06
25	C	511	CLA	MG-NA	5.07	2.18	2.06
30	a	615	SQD	O48-C23	4.97	1.47	1.33
25	b	613	CLA	MG-NA	4.97	2.18	2.06
25	B	604	CLA	MG-NA	4.94	2.18	2.06
25	b	601	CLA	MG-NA	4.93	2.18	2.06
30	A	615	SQD	O48-C23	4.84	1.47	1.33
25	B	613	CLA	MG-ND	-4.80	1.96	2.05
25	B	607	CLA	MG-NC	4.72	2.17	2.06
25	C	506	CLA	MG-NA	4.72	2.17	2.06
30	B	624	SQD	O48-C23	4.72	1.47	1.33
30	D	408	SQD	O48-C23	4.69	1.47	1.33
30	b	620	SQD	O48-C23	4.65	1.46	1.33
30	f	101	SQD	O48-C23	4.63	1.46	1.33
25	B	611	CLA	MG-NA	4.59	2.17	2.06
30	A	614	SQD	O48-C23	4.56	1.46	1.33
25	A	612	CLA	MG-NB	4.51	2.14	2.05
26	a	608	PHO	C1D-C2D	4.46	1.44	1.39
25	C	501	CLA	MG-NA	4.46	2.16	2.06
25	a	606	CLA	MG-NB	4.41	2.14	2.05
25	c	508	CLA	MG-NB	4.36	2.14	2.05
25	A	612	CLA	MG-NA	4.33	2.16	2.06
25	D	404	CLA	C1D-ND	4.32	1.43	1.37
25	B	601	CLA	C1D-ND	4.29	1.43	1.37
26	A	608	PHO	C1D-C2D	4.29	1.44	1.39
25	c	507	CLA	MG-NA	4.28	2.16	2.06
25	B	602	CLA	MG-NA	4.28	2.16	2.06
25	A	609	CLA	C1D-ND	4.26	1.43	1.37
25	C	513	CLA	MG-ND	4.23	2.14	2.05
25	B	609	CLA	MG-NA	4.21	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	505	CLA	MG-NA	4.18	2.16	2.06
25	B	607	CLA	C1D-ND	4.14	1.43	1.37
25	B	614	CLA	MG-NA	4.10	2.16	2.06
35	e	101	HEM	FE-NA	4.08	2.08	1.95
25	C	505	CLA	MG-NB	4.07	2.13	2.05
25	a	612	CLA	C1D-ND	4.05	1.43	1.37
25	A	612	CLA	C1D-ND	4.01	1.43	1.37
35	F	101	HEM	FE-NC	4.00	2.08	1.95
25	b	609	CLA	MG-NA	3.99	2.15	2.06
27	c	514	BCR	C1-C6	-3.98	1.48	1.53
25	B	616	CLA	C1D-ND	3.96	1.43	1.37
25	C	503	CLA	MG-NA	3.96	2.15	2.06
25	C	509	CLA	MG-NA	3.96	2.15	2.06
27	C	515	BCR	C1-C6	-3.95	1.48	1.53
33	D	410	LHG	P-O6	3.92	1.74	1.59
25	B	602	CLA	C1D-ND	3.92	1.43	1.37
25	C	512	CLA	MG-NB	3.92	2.13	2.05
25	C	501	CLA	C1D-ND	3.91	1.43	1.37
25	a	606	CLA	MG-NA	3.90	2.15	2.06
25	C	506	CLA	MG-NB	3.90	2.13	2.05
25	c	504	CLA	C4B-NB	3.89	1.43	1.37
25	C	503	CLA	C1D-ND	3.87	1.42	1.37
30	A	614	SQD	O47-C45	-3.86	1.37	1.46
25	c	510	CLA	C1D-ND	3.85	1.42	1.37
25	B	614	CLA	C1D-ND	3.84	1.42	1.37
25	C	502	CLA	MG-NA	3.83	2.15	2.06
25	B	615	CLA	MG-NB	3.82	2.13	2.05
26	d	402	PHO	C1D-C2D	3.81	1.43	1.39
30	a	615	SQD	O47-C7	3.79	1.45	1.34
35	e	101	HEM	FE-NB	3.79	2.06	1.94
25	B	604	CLA	MG-NC	3.78	2.15	2.06
25	b	610	CLA	C1D-ND	3.77	1.42	1.37
25	c	501	CLA	MG-ND	-3.75	1.98	2.05
25	C	506	CLA	C1D-ND	3.75	1.42	1.37
27	b	618	BCR	C30-C25	-3.71	1.49	1.53
26	D	402	PHO	C1D-C2D	3.70	1.43	1.39
35	e	101	HEM	FE-ND	3.69	2.06	1.94
25	b	614	CLA	C1D-ND	3.69	1.42	1.37
25	c	509	CLA	C1D-ND	3.68	1.42	1.37
25	b	610	CLA	MG-NB	-3.67	1.98	2.05
25	B	601	CLA	MG-NC	3.66	2.15	2.06
25	b	606	CLA	C1D-ND	3.64	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	609	CLA	C1D-ND	3.62	1.42	1.37
25	B	605	CLA	MG-NC	3.60	2.14	2.06
31	C	517	DGD	O2G-C2G	-3.60	1.38	1.46
25	d	404	CLA	MG-NC	3.59	2.14	2.06
25	b	609	CLA	C1D-ND	3.57	1.42	1.37
25	B	611	CLA	C1D-ND	3.57	1.42	1.37
25	B	604	CLA	C1D-ND	3.57	1.42	1.37
25	B	601	CLA	MG-NB	-3.57	1.98	2.05
30	a	614	SQD	O47-C7	3.56	1.44	1.34
27	B	618	BCR	C30-C25	-3.56	1.49	1.53
28	d	406	PL9	C6-C1	-3.56	1.42	1.48
25	B	614	CLA	C4B-NB	3.55	1.42	1.37
25	b	614	CLA	C4B-NB	3.55	1.42	1.37
36	V	201	HEC	FE-ND	3.55	2.05	1.94
25	A	612	CLA	MG-ND	-3.54	1.98	2.05
30	f	101	SQD	O47-C7	3.54	1.44	1.34
25	B	605	CLA	C1D-ND	3.53	1.42	1.37
30	B	624	SQD	O47-C7	3.53	1.44	1.34
25	C	513	CLA	C1D-ND	3.52	1.42	1.37
25	b	605	CLA	C4B-NB	3.52	1.42	1.37
25	c	508	CLA	MG-NC	3.51	2.14	2.06
25	B	615	CLA	C4B-NB	3.51	1.42	1.37
25	b	616	CLA	C1D-ND	3.50	1.42	1.37
25	b	605	CLA	MG-NA	3.50	2.14	2.06
27	k	102	BCR	C1-C6	-3.49	1.49	1.53
25	c	512	CLA	C1D-ND	3.49	1.42	1.37
27	D	405	BCR	C1-C6	-3.48	1.49	1.53
25	d	403	CLA	C1D-ND	3.48	1.42	1.37
26	d	402	PHO	C4D-CHA	3.47	1.44	1.39
25	C	505	CLA	MG-ND	-3.46	1.98	2.05
36	V	201	HEC	FE-NC	3.46	2.06	1.95
25	c	503	CLA	MG-NA	3.46	2.14	2.06
25	B	613	CLA	C1D-ND	3.45	1.42	1.37
25	B	609	CLA	C1D-ND	3.45	1.42	1.37
25	B	613	CLA	MG-NA	3.44	2.14	2.06
25	a	606	CLA	C1D-ND	3.44	1.42	1.37
25	c	508	CLA	C1D-ND	3.43	1.42	1.37
25	C	512	CLA	MG-NA	3.43	2.14	2.06
25	A	606	CLA	C1D-ND	3.43	1.42	1.37
30	f	101	SQD	O47-C45	-3.43	1.38	1.46
30	a	614	SQD	O47-C45	-3.42	1.38	1.46
27	c	514	BCR	C30-C25	-3.42	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	607	CLA	MG-NA	3.42	2.14	2.06
27	K	101	BCR	C30-C25	-3.42	1.49	1.53
27	H	101	BCR	C30-C25	-3.41	1.49	1.53
25	a	607	CLA	C1D-ND	3.40	1.42	1.37
26	a	608	PHO	C4D-CHA	3.40	1.44	1.39
25	b	612	CLA	C1D-ND	3.39	1.42	1.37
27	C	516	BCR	C1-C6	-3.38	1.49	1.53
25	C	511	CLA	C1D-ND	3.37	1.42	1.37
30	B	624	SQD	O47-C45	-3.37	1.38	1.46
36	v	201	HEC	FE-NA	3.37	2.06	1.95
25	c	509	CLA	C1B-C2B	3.36	1.51	1.43
25	C	507	CLA	C1D-ND	3.36	1.42	1.37
25	b	611	CLA	C1D-ND	3.36	1.42	1.37
30	b	620	SQD	O47-C7	3.35	1.43	1.34
25	C	509	CLA	C1D-ND	3.35	1.42	1.37
25	B	615	CLA	C1D-ND	3.34	1.42	1.37
25	C	506	CLA	MG-ND	-3.33	1.99	2.05
30	A	615	SQD	O47-C7	3.33	1.43	1.34
25	C	502	CLA	C4B-NB	3.33	1.42	1.37
25	B	606	CLA	C1D-ND	3.32	1.42	1.37
25	b	615	CLA	C1D-ND	3.32	1.42	1.37
25	B	609	CLA	C4B-NB	3.32	1.42	1.37
25	c	511	CLA	C4B-NB	3.31	1.42	1.37
25	C	503	CLA	MG-ND	3.31	2.12	2.05
25	C	507	CLA	C1B-C2B	3.30	1.50	1.43
30	b	620	SQD	O5-C1	3.29	1.50	1.41
25	b	608	CLA	C1D-ND	3.28	1.42	1.37
25	c	501	CLA	C1D-ND	3.28	1.42	1.37
25	c	503	CLA	C1D-ND	3.28	1.42	1.37
27	k	101	BCR	C30-C25	-3.28	1.49	1.53
25	c	513	CLA	C1D-ND	3.28	1.42	1.37
25	c	502	CLA	MG-ND	3.28	2.12	2.05
25	B	605	CLA	C1B-C2B	3.28	1.50	1.43
27	b	618	BCR	C1-C6	-3.27	1.49	1.53
25	B	601	CLA	C4B-NB	3.27	1.42	1.37
25	d	403	CLA	MG-NC	3.26	2.14	2.06
30	a	615	SQD	C24-C23	3.26	1.60	1.50
25	c	504	CLA	MG-NB	-3.24	1.99	2.05
27	k	102	BCR	C30-C25	-3.22	1.49	1.53
25	C	505	CLA	C4B-NB	3.22	1.42	1.37
27	k	103	BCR	C1-C6	-3.22	1.49	1.53
26	A	608	PHO	C4D-CHA	3.21	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	k	101	BCR	C1-C6	-3.21	1.49	1.53
25	C	505	CLA	C1D-ND	3.21	1.42	1.37
33	D	412	LHG	O7-C5	-3.21	1.39	1.46
25	c	502	CLA	C1D-ND	3.21	1.42	1.37
25	B	610	CLA	C1D-ND	3.21	1.42	1.37
30	A	614	SQD	C24-C23	3.21	1.60	1.50
25	B	612	CLA	C1D-ND	3.20	1.42	1.37
25	C	502	CLA	C1D-ND	3.20	1.42	1.37
25	b	607	CLA	C4B-NB	3.19	1.42	1.37
25	c	511	CLA	C1B-C2B	3.18	1.50	1.43
27	b	619	BCR	C1-C6	-3.18	1.49	1.53
25	b	601	CLA	C4B-NB	3.18	1.42	1.37
25	b	607	CLA	C1D-ND	3.17	1.42	1.37
30	a	614	SQD	C24-C23	3.17	1.59	1.50
30	A	615	SQD	C24-C23	3.17	1.59	1.50
30	A	614	SQD	O5-C1	3.17	1.50	1.41
25	c	511	CLA	C1D-ND	3.17	1.42	1.37
25	D	404	CLA	MG-NB	-3.17	1.99	2.05
25	B	615	CLA	C1B-C2B	3.16	1.50	1.43
25	b	601	CLA	C1D-ND	3.16	1.42	1.37
25	b	605	CLA	C1D-ND	3.16	1.42	1.37
31	H	102	DGD	O5D-C1E	3.16	1.45	1.40
31	C	517	DGD	C4E-C3E	3.16	1.60	1.52
25	c	513	CLA	MG-ND	-3.15	1.99	2.05
25	c	507	CLA	C4B-NB	3.15	1.42	1.37
27	d	405	BCR	C30-C25	-3.15	1.49	1.53
25	C	504	CLA	C1D-ND	3.14	1.42	1.37
30	D	408	SQD	C24-C23	3.14	1.59	1.50
25	C	513	CLA	MG-NC	3.14	2.13	2.06
25	C	505	CLA	C1B-C2B	3.13	1.50	1.43
25	b	606	CLA	C4B-NB	3.13	1.42	1.37
25	b	605	CLA	C1B-C2B	3.13	1.50	1.43
25	C	511	CLA	C4B-NB	3.13	1.42	1.37
27	a	610	BCR	C1-C6	-3.12	1.49	1.53
25	B	613	CLA	C4B-NB	3.12	1.42	1.37
30	B	624	SQD	O5-C1	3.11	1.49	1.41
30	f	101	SQD	C24-C23	3.11	1.59	1.50
25	c	507	CLA	C1B-C2B	3.10	1.50	1.43
25	a	607	CLA	C4B-NB	3.10	1.41	1.37
25	A	606	CLA	C1B-C2B	3.09	1.50	1.43
30	b	620	SQD	O47-C45	-3.08	1.39	1.46
25	B	616	CLA	C1B-C2B	3.08	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	E	101	LHG	P-O6	3.08	1.71	1.59
36	V	201	HEC	FE-NB	3.08	2.04	1.94
25	C	504	CLA	MG-NB	3.08	2.11	2.05
25	C	510	CLA	C1D-ND	3.07	1.41	1.37
25	C	513	CLA	C1B-C2B	3.07	1.50	1.43
27	B	619	BCR	C1-C6	-3.07	1.49	1.53
25	b	602	CLA	C1B-C2B	3.07	1.50	1.43
31	c	515	DGD	C4D-C3D	3.07	1.60	1.52
27	C	514	BCR	C1-C6	-3.07	1.49	1.53
27	d	405	BCR	C1-C6	-3.06	1.49	1.53
25	C	503	CLA	C4B-NB	3.06	1.41	1.37
25	C	503	CLA	C1B-C2B	3.05	1.50	1.43
25	B	607	CLA	C4B-NB	3.05	1.41	1.37
30	a	615	SQD	O47-C45	-3.04	1.39	1.46
25	C	501	CLA	C4B-NB	3.04	1.41	1.37
25	b	613	CLA	C4B-NB	3.03	1.41	1.37
25	d	403	CLA	C4B-NB	3.03	1.41	1.37
25	A	606	CLA	MG-NB	3.03	2.11	2.05
30	A	614	SQD	O47-C7	3.03	1.42	1.34
25	a	607	CLA	MG-ND	-3.02	1.99	2.05
25	c	507	CLA	MG-NB	-3.02	1.99	2.05
25	C	511	CLA	C1B-C2B	3.02	1.50	1.43
25	C	503	CLA	MG-NB	-3.02	1.99	2.05
25	b	610	CLA	C1B-C2B	3.02	1.50	1.43
25	B	608	CLA	C4B-NB	3.01	1.41	1.37
25	c	510	CLA	C1B-C2B	3.01	1.50	1.43
25	c	513	CLA	MG-NA	3.00	2.13	2.06
25	b	615	CLA	MG-NB	2.99	2.11	2.05
25	B	612	CLA	C4B-NB	2.99	1.41	1.37
25	C	505	CLA	CHC-C1C	2.99	1.44	1.38
25	B	606	CLA	C1B-C2B	2.99	1.50	1.43
25	b	601	CLA	C1B-C2B	2.99	1.50	1.43
25	b	602	CLA	C1D-ND	2.98	1.41	1.37
25	a	609	CLA	C4B-NB	2.98	1.41	1.37
35	e	101	HEM	CAC-C3C	2.98	1.55	1.47
25	b	608	CLA	C4B-NB	2.98	1.41	1.37
25	B	606	CLA	C4B-NB	2.97	1.41	1.37
25	B	608	CLA	C1D-ND	2.97	1.41	1.37
25	C	506	CLA	C4B-NB	2.97	1.41	1.37
25	a	606	CLA	C1B-C2B	2.96	1.50	1.43
25	C	507	CLA	C4B-NB	2.96	1.41	1.37
25	C	508	CLA	C1D-ND	2.95	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	617	BCR	C1-C6	-2.95	1.50	1.53
25	C	512	CLA	C4B-NB	2.95	1.41	1.37
25	B	602	CLA	C1B-C2B	2.94	1.50	1.43
25	b	611	CLA	C1B-C2B	2.94	1.50	1.43
25	c	512	CLA	MG-NB	2.94	2.11	2.05
25	c	507	CLA	C1D-ND	2.94	1.41	1.37
25	b	613	CLA	MG-NB	-2.94	2.00	2.05
25	d	404	CLA	C4B-NB	2.94	1.41	1.37
25	c	508	CLA	C1B-C2B	2.93	1.50	1.43
27	K	101	BCR	C1-C6	-2.93	1.50	1.53
35	F	101	HEM	CAB-C3B	2.93	1.55	1.47
25	C	509	CLA	C4B-NB	2.93	1.41	1.37
25	d	403	CLA	C1B-C2B	2.93	1.50	1.43
25	C	508	CLA	MG-NA	2.92	2.13	2.06
25	a	609	CLA	C1B-C2B	2.92	1.50	1.43
33	d	408	LHG	O7-C5	-2.92	1.39	1.46
30	f	101	SQD	O5-C1	2.92	1.49	1.41
25	C	512	CLA	C1D-ND	2.92	1.41	1.37
25	c	505	CLA	C4B-NB	2.92	1.41	1.37
25	B	611	CLA	C1B-C2B	2.91	1.50	1.43
25	B	602	CLA	C4B-NB	2.91	1.41	1.37
25	c	503	CLA	C1B-C2B	2.91	1.50	1.43
25	C	506	CLA	CHC-C1C	2.91	1.44	1.38
33	D	409	LHG	O7-C5	-2.91	1.39	1.46
25	C	504	CLA	C4B-NB	2.90	1.41	1.37
30	b	620	SQD	C24-C23	2.89	1.59	1.50
25	c	506	CLA	C1D-ND	2.89	1.41	1.37
27	C	514	BCR	C30-C25	-2.88	1.50	1.53
25	c	505	CLA	C1B-C2B	2.88	1.49	1.43
30	D	408	SQD	O5-C1	2.88	1.49	1.41
25	b	604	CLA	C1D-ND	2.88	1.41	1.37
25	b	609	CLA	C4B-NB	2.88	1.41	1.37
25	b	606	CLA	C1B-C2B	2.87	1.49	1.43
25	b	615	CLA	C4B-NB	2.87	1.41	1.37
25	c	504	CLA	C1D-ND	2.87	1.41	1.37
25	D	403	CLA	C1D-ND	2.86	1.41	1.37
25	C	508	CLA	C3B-C4B	2.86	1.51	1.42
25	b	603	CLA	C4B-NB	2.86	1.41	1.37
25	b	603	CLA	C1D-ND	2.86	1.41	1.37
25	a	607	CLA	MG-NC	2.86	2.13	2.06
25	B	601	CLA	C1B-C2B	2.85	1.49	1.43
26	D	402	PHO	C4D-CHA	2.85	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	617	BCR	C30-C25	-2.85	1.50	1.53
27	D	405	BCR	C30-C25	-2.85	1.50	1.53
25	b	615	CLA	C1B-C2B	2.85	1.49	1.43
25	B	611	CLA	C4B-NB	2.85	1.41	1.37
25	c	502	CLA	MG-NB	-2.85	2.00	2.05
27	b	617	BCR	C1-C6	-2.85	1.50	1.53
25	b	612	CLA	C4B-NB	2.85	1.41	1.37
25	b	616	CLA	C4B-NB	2.84	1.41	1.37
27	C	516	BCR	C30-C25	-2.84	1.50	1.53
25	c	512	CLA	C4B-NB	2.83	1.41	1.37
25	a	612	CLA	C1B-C2B	2.83	1.49	1.43
29	D	407	LMG	C4-C5	2.83	1.59	1.53
25	B	615	CLA	CHC-C1C	2.83	1.44	1.38
25	a	607	CLA	CHC-C1C	2.83	1.44	1.38
27	k	103	BCR	C30-C25	-2.83	1.50	1.53
25	B	601	CLA	MG-NA	2.83	2.13	2.06
30	a	614	SQD	O5-C1	2.83	1.49	1.41
25	C	512	CLA	C1B-C2B	2.82	1.49	1.43
25	d	404	CLA	C1D-ND	2.82	1.41	1.37
25	b	613	CLA	C1D-ND	2.82	1.41	1.37
25	C	513	CLA	C4B-NB	2.82	1.41	1.37
25	A	607	CLA	C1D-ND	2.82	1.41	1.37
25	c	501	CLA	C4B-NB	2.82	1.41	1.37
25	b	604	CLA	C4B-NB	2.81	1.41	1.37
25	A	612	CLA	C1B-C2B	2.81	1.49	1.43
25	B	603	CLA	C1D-ND	2.81	1.41	1.37
25	c	501	CLA	C1B-C2B	2.80	1.49	1.43
35	F	101	HEM	FE-NA	2.78	2.04	1.95
25	C	510	CLA	C1B-C2B	2.78	1.49	1.43
33	B	623	LHG	O7-C5	-2.78	1.40	1.46
27	T	101	BCR	C30-C25	-2.78	1.50	1.53
25	B	616	CLA	C4B-NB	2.77	1.41	1.37
25	c	510	CLA	CHC-C1C	2.77	1.44	1.38
25	A	607	CLA	C4B-NB	2.76	1.41	1.37
27	t	101	BCR	C1-C6	-2.76	1.50	1.53
25	B	609	CLA	MG-ND	2.74	2.11	2.05
25	b	610	CLA	C4B-NB	2.74	1.41	1.37
25	B	612	CLA	C1B-C2B	2.74	1.49	1.43
25	B	610	CLA	C3B-C4B	2.74	1.50	1.42
25	C	508	CLA	C4B-NB	2.74	1.41	1.37
25	b	606	CLA	MG-NB	-2.73	2.00	2.05
27	a	610	BCR	C30-C25	-2.73	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	507	CLA	MG-NA	2.73	2.12	2.06
36	v	201	HEC	FE-ND	2.73	2.03	1.94
25	a	606	CLA	MG-NC	2.73	2.12	2.06
25	A	606	CLA	MG-NC	2.72	2.12	2.06
25	c	512	CLA	CHC-C1C	2.72	1.43	1.38
25	c	506	CLA	C4B-NB	2.72	1.41	1.37
35	F	101	HEM	CAC-C3C	2.72	1.54	1.47
25	A	607	CLA	MG-NA	2.72	2.12	2.06
25	c	510	CLA	C4B-NB	2.72	1.41	1.37
25	b	614	CLA	CHC-C1C	2.72	1.43	1.38
25	D	404	CLA	C1B-C2B	2.72	1.49	1.43
25	c	512	CLA	C1B-C2B	2.72	1.49	1.43
25	B	607	CLA	C1B-C2B	2.72	1.49	1.43
25	C	508	CLA	C1B-C2B	2.71	1.49	1.43
26	A	608	PHO	C3D-C4D	2.71	1.44	1.41
25	A	607	CLA	C1B-C2B	2.71	1.49	1.43
25	C	506	CLA	C1B-C2B	2.71	1.49	1.43
25	C	501	CLA	C1B-C2B	2.71	1.49	1.43
25	C	506	CLA	C3B-C4B	2.71	1.50	1.42
27	A	610	BCR	C1-C6	-2.70	1.50	1.53
25	B	603	CLA	MG-NA	2.69	2.12	2.06
25	B	609	CLA	C1B-C2B	2.69	1.49	1.43
25	a	606	CLA	C4B-NB	2.69	1.41	1.37
26	D	402	PHO	CMD-C2D	-2.69	1.46	1.51
35	e	101	HEM	CAB-C3B	2.68	1.54	1.47
27	t	101	BCR	C30-C25	-2.68	1.50	1.53
25	B	607	CLA	MG-NB	-2.68	2.00	2.05
27	x	101	BCR	C30-C25	-2.68	1.50	1.53
25	c	509	CLA	C4B-NB	2.68	1.41	1.37
25	C	510	CLA	C4B-NB	2.67	1.41	1.37
25	c	513	CLA	C1B-C2B	2.67	1.49	1.43
25	b	616	CLA	C1B-C2B	2.66	1.49	1.43
25	c	501	CLA	MG-NC	2.66	2.12	2.06
25	c	506	CLA	C1B-C2B	2.66	1.49	1.43
25	d	404	CLA	C1B-C2B	2.66	1.49	1.43
25	C	512	CLA	C3B-C4B	2.65	1.50	1.42
26	D	402	PHO	C4D-ND	-2.65	1.34	1.38
27	B	618	BCR	C1-C6	-2.65	1.50	1.53
25	b	609	CLA	MG-ND	2.65	2.11	2.05
25	B	612	CLA	CHC-C1C	2.65	1.43	1.38
25	D	403	CLA	C1B-C2B	2.65	1.49	1.43
30	A	615	SQD	C46-C45	2.65	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	410	LHG	O3-C3	-2.65	1.34	1.44
25	B	610	CLA	C1B-C2B	2.64	1.49	1.43
25	b	608	CLA	CHC-C1C	2.63	1.43	1.38
25	B	604	CLA	C1B-C2B	2.63	1.49	1.43
25	b	615	CLA	C3B-C4B	2.63	1.50	1.42
33	a	613	LHG	C24-C23	2.63	1.58	1.50
25	b	611	CLA	C4B-NB	2.63	1.41	1.37
30	B	624	SQD	C24-C23	2.63	1.58	1.50
25	c	513	CLA	C3B-C4B	2.63	1.50	1.42
25	B	613	CLA	C1B-C2B	2.62	1.49	1.43
25	C	504	CLA	C3B-C4B	2.62	1.50	1.42
25	a	612	CLA	C4B-NB	2.62	1.41	1.37
26	A	608	PHO	C4D-ND	-2.62	1.34	1.38
25	a	609	CLA	MG-ND	-2.61	2.00	2.05
26	D	402	PHO	CMB-C2B	-2.61	1.46	1.51
25	C	502	CLA	C1B-C2B	2.61	1.49	1.43
31	C	518	DGD	C1G-C2G	2.61	1.59	1.50
25	b	607	CLA	C1B-C2B	2.60	1.49	1.43
25	b	614	CLA	MG-NA	2.60	2.12	2.06
25	C	503	CLA	C3B-C4B	2.60	1.50	1.42
25	b	605	CLA	C3B-C4B	2.60	1.50	1.42
25	C	509	CLA	CHC-C1C	2.60	1.43	1.38
28	a	611	PL9	C53-C6	-2.59	1.45	1.50
25	c	512	CLA	C3B-C4B	2.59	1.50	1.42
25	c	510	CLA	C3B-C4B	2.59	1.50	1.42
36	v	201	HEC	FE-NC	2.59	2.03	1.95
25	b	605	CLA	CHC-C1C	2.58	1.43	1.38
25	C	502	CLA	C3B-C4B	2.58	1.50	1.42
25	c	506	CLA	MG-NA	2.58	2.12	2.06
25	B	615	CLA	C3B-C4B	2.58	1.50	1.42
25	B	607	CLA	C3B-C4B	2.58	1.50	1.42
25	c	508	CLA	CHC-C1C	2.57	1.43	1.38
25	c	503	CLA	C4B-NB	2.57	1.41	1.37
25	B	604	CLA	C4B-NB	2.57	1.41	1.37
31	C	518	DGD	C4D-C3D	2.57	1.59	1.52
25	b	603	CLA	CMC-C2C	-2.56	1.45	1.50
25	B	605	CLA	MG-ND	-2.56	2.00	2.05
26	a	608	PHO	C3D-C4D	2.56	1.44	1.41
25	c	502	CLA	C1B-C2B	2.56	1.49	1.43
25	c	505	CLA	C1D-ND	2.56	1.41	1.37
25	b	603	CLA	C1B-C2B	2.56	1.49	1.43
31	H	102	DGD	C4D-C5D	2.55	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	604	CLA	C1B-C2B	2.55	1.49	1.43
25	a	607	CLA	C1B-C2B	2.55	1.49	1.43
31	c	517	DGD	O2G-C2G	-2.53	1.40	1.46
25	A	609	CLA	C1B-C2B	2.53	1.49	1.43
25	a	606	CLA	MG-ND	-2.52	2.00	2.05
25	b	608	CLA	C1B-C2B	2.52	1.49	1.43
25	C	502	CLA	CHC-C1C	2.52	1.43	1.38
25	C	505	CLA	C3B-C4B	2.52	1.50	1.42
25	A	612	CLA	CHC-C1C	2.52	1.43	1.38
25	C	511	CLA	C3B-C4B	2.52	1.50	1.42
25	C	510	CLA	MG-NA	2.51	2.12	2.06
25	b	613	CLA	C1B-C2B	2.51	1.49	1.43
25	c	508	CLA	C3B-C4B	2.51	1.50	1.42
25	b	601	CLA	CHC-C1C	2.50	1.43	1.38
27	C	515	BCR	C30-C25	-2.50	1.50	1.53
31	h	101	DGD	C4D-C3D	2.50	1.58	1.52
25	c	503	CLA	MG-NB	2.49	2.10	2.05
25	c	504	CLA	C1B-C2B	2.49	1.49	1.43
25	b	614	CLA	C3B-C4B	2.48	1.50	1.42
25	D	403	CLA	CHC-C1C	2.48	1.43	1.38
25	b	612	CLA	C1B-C2B	2.48	1.48	1.43
25	C	504	CLA	MG-NA	2.48	2.12	2.06
25	A	609	CLA	C4B-NB	2.48	1.41	1.37
25	C	512	CLA	CHC-C1C	2.47	1.43	1.38
25	D	403	CLA	C3B-C4B	2.47	1.49	1.42
25	c	503	CLA	MG-NC	2.46	2.12	2.06
29	c	520	LMG	C4-C3	2.46	1.58	1.52
25	b	615	CLA	CHC-C1C	2.46	1.43	1.38
25	c	506	CLA	CHC-C1C	2.46	1.43	1.38
25	b	602	CLA	C4B-NB	2.46	1.41	1.37
31	A	616	DGD	C4D-C3D	2.45	1.58	1.52
25	B	613	CLA	CHC-C1C	2.45	1.43	1.38
25	b	611	CLA	CHC-C1C	2.45	1.43	1.38
25	b	614	CLA	C1B-C2B	2.45	1.48	1.43
33	a	613	LHG	P-O6	2.45	1.69	1.59
31	A	616	DGD	C4D-C5D	2.45	1.58	1.53
30	f	101	SQD	O7-S	2.44	1.52	1.45
26	A	608	PHO	CMD-C2D	-2.44	1.46	1.51
31	H	102	DGD	O2G-C2G	-2.44	1.40	1.46
25	A	606	CLA	MG-NA	2.43	2.12	2.06
25	b	612	CLA	CHC-C1C	2.43	1.43	1.38
25	C	508	CLA	CHC-C1C	2.43	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	513	CLA	C4B-NB	2.43	1.41	1.37
25	B	602	CLA	CMB-C2B	-2.43	1.45	1.50
25	c	505	CLA	C3B-C4B	2.43	1.49	1.42
25	b	603	CLA	CMB-C2B	-2.43	1.45	1.50
25	c	508	CLA	C4B-NB	2.43	1.41	1.37
25	C	511	CLA	CHC-C1C	2.43	1.43	1.38
25	D	404	CLA	C4B-NB	2.42	1.41	1.37
29	B	622	LMG	O8-C28	2.42	1.38	1.30
25	b	608	CLA	C3B-C4B	2.42	1.49	1.42
25	B	608	CLA	MG-NB	-2.42	2.01	2.05
25	b	610	CLA	MG-NC	2.41	2.12	2.06
30	b	620	SQD	O9-S	2.41	1.51	1.45
27	T	101	BCR	C1-C6	-2.41	1.50	1.53
29	c	520	LMG	C3-C2	2.41	1.58	1.52
27	B	619	BCR	C30-C25	-2.41	1.50	1.53
26	A	608	PHO	CMC-C2C	-2.41	1.46	1.50
25	C	509	CLA	C1B-C2B	2.41	1.48	1.43
28	d	406	PL9	C53-C6	-2.41	1.45	1.50
25	D	404	CLA	MG-NC	2.41	2.12	2.06
30	a	614	SQD	O7-S	2.40	1.51	1.45
25	B	612	CLA	C3B-C4B	2.40	1.49	1.42
25	C	509	CLA	C3B-C4B	2.40	1.49	1.42
26	d	402	PHO	CMC-C2C	-2.39	1.46	1.50
28	d	406	PL9	C3-C4	-2.39	1.45	1.49
29	d	410	LMG	O7-C8	-2.38	1.41	1.46
25	b	612	CLA	C3B-C4B	2.38	1.49	1.42
25	c	502	CLA	C4B-NB	2.37	1.41	1.37
25	b	610	CLA	CMD-C2D	-2.37	1.45	1.50
25	B	610	CLA	CHC-C1C	2.37	1.43	1.38
29	C	520	LMG	O7-C8	-2.37	1.41	1.46
25	C	504	CLA	C1B-C2B	2.37	1.48	1.43
25	C	501	CLA	C3B-C4B	2.36	1.49	1.42
25	A	606	CLA	C3B-C4B	2.36	1.49	1.42
25	C	504	CLA	CHC-C1C	2.36	1.43	1.38
25	A	612	CLA	C3B-C4B	2.36	1.49	1.42
25	a	606	CLA	C3B-C4B	2.35	1.49	1.42
29	c	522	LMG	C4-C5	2.35	1.58	1.53
25	B	614	CLA	C1B-C2B	2.35	1.48	1.43
26	d	402	PHO	C1D-ND	2.35	1.42	1.38
25	b	609	CLA	CHC-C1C	2.35	1.43	1.38
31	C	518	DGD	O5D-C6D	-2.34	1.39	1.43
25	c	501	CLA	CHC-C1C	2.34	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	608	CLA	C1B-C2B	2.34	1.48	1.43
25	c	506	CLA	MG-ND	-2.33	2.01	2.05
30	B	624	SQD	O9-S	2.33	1.51	1.45
26	d	402	PHO	CAC-C3C	-2.33	1.47	1.51
25	c	503	CLA	CHC-C1C	2.33	1.43	1.38
36	V	201	HEC	CMB-C2B	2.33	1.55	1.50
25	b	603	CLA	CMD-C2D	-2.32	1.46	1.50
25	B	603	CLA	C1B-C2B	2.32	1.48	1.43
25	b	607	CLA	MG-NC	2.31	2.11	2.06
25	b	601	CLA	C3B-C4B	2.30	1.49	1.42
25	b	616	CLA	MG-NC	2.30	2.11	2.06
25	c	511	CLA	CHC-C1C	2.30	1.43	1.38
25	C	513	CLA	MG-NB	-2.30	2.01	2.05
25	c	512	CLA	C1D-C2D	2.30	1.49	1.45
31	c	516	DGD	O5D-C1E	2.30	1.44	1.40
31	H	102	DGD	C4E-C5E	2.30	1.57	1.53
35	F	101	HEM	CMD-C2D	2.30	1.55	1.50
31	c	516	DGD	C1G-C2G	2.29	1.58	1.50
25	b	606	CLA	MG-ND	2.29	2.10	2.05
33	e	102	LHG	P-O6	2.29	1.68	1.59
25	B	605	CLA	C3B-C4B	2.29	1.49	1.42
26	a	608	PHO	C4D-ND	-2.29	1.35	1.38
25	B	601	CLA	C3B-C4B	2.29	1.49	1.42
25	B	610	CLA	MG-NA	2.28	2.11	2.06
25	A	607	CLA	C3B-C4B	2.28	1.49	1.42
25	C	507	CLA	C3B-C4B	2.28	1.49	1.42
31	c	516	DGD	C3E-C2E	2.28	1.58	1.52
31	C	517	DGD	C6D-C5D	2.28	1.58	1.51
25	C	513	CLA	C3B-C4B	2.28	1.49	1.42
25	D	404	CLA	CMD-C2D	-2.28	1.46	1.50
29	b	622	LMG	C3-C2	2.27	1.58	1.52
25	A	609	CLA	C3D-C4D	2.27	1.49	1.44
25	d	403	CLA	CMD-C2D	-2.27	1.46	1.50
31	c	517	DGD	C4D-C5D	2.27	1.57	1.53
25	B	604	CLA	C3B-C4B	2.27	1.49	1.42
25	c	503	CLA	CMD-C2D	-2.27	1.46	1.50
25	c	505	CLA	CHC-C1C	2.26	1.43	1.38
31	A	616	DGD	C1E-C2E	2.26	1.59	1.52
25	a	606	CLA	CHC-C1C	2.26	1.43	1.38
28	D	406	PL9	C3-C4	-2.26	1.46	1.49
30	b	620	SQD	O5-C5	2.26	1.49	1.44
25	c	513	CLA	CHC-C1C	2.25	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	515	DGD	O1G-C1G	-2.25	1.40	1.45
25	B	611	CLA	CHC-C1C	2.25	1.43	1.38
25	A	607	CLA	CHC-C1C	2.25	1.43	1.38
25	B	605	CLA	C4B-NB	2.25	1.40	1.37
25	b	608	CLA	CMD-C2D	-2.25	1.46	1.50
25	c	505	CLA	MG-NA	2.25	2.11	2.06
25	d	404	CLA	C3B-C4B	2.25	1.49	1.42
27	b	617	BCR	C30-C25	-2.25	1.50	1.53
25	a	607	CLA	C3B-C4B	2.24	1.49	1.42
25	A	606	CLA	C4B-NB	2.24	1.40	1.37
25	B	610	CLA	C4B-NB	2.24	1.40	1.37
30	B	624	SQD	O7-S	2.24	1.51	1.45
27	b	619	BCR	C30-C25	-2.24	1.50	1.53
25	C	510	CLA	C3B-C4B	2.24	1.49	1.42
29	D	407	LMG	C7-C8	2.24	1.57	1.50
25	b	602	CLA	C3B-C4B	2.24	1.49	1.42
31	a	616	DGD	O1G-C1A	2.24	1.39	1.33
35	e	101	HEM	CMA-C3A	2.24	1.55	1.50
25	b	603	CLA	C3B-C4B	2.23	1.49	1.42
25	B	613	CLA	C3B-C4B	2.23	1.49	1.42
25	c	502	CLA	C3B-C4B	2.23	1.49	1.42
25	B	603	CLA	C4B-NB	2.23	1.40	1.37
25	C	501	CLA	CHC-C1C	2.23	1.43	1.38
25	C	510	CLA	CMD-C2D	-2.22	1.46	1.50
25	C	510	CLA	CHC-C1C	2.22	1.42	1.38
25	b	602	CLA	CMD-C2D	-2.22	1.46	1.50
31	C	518	DGD	O3D-C3D	-2.22	1.37	1.43
25	B	608	CLA	MG-NA	2.22	2.11	2.06
25	A	606	CLA	MG-ND	-2.22	2.01	2.05
25	C	507	CLA	CHC-C1C	2.22	1.42	1.38
31	A	616	DGD	O1G-C1G	-2.21	1.40	1.45
35	F	101	HEM	CMB-C2B	2.21	1.55	1.50
25	B	602	CLA	C3B-C4B	2.21	1.49	1.42
31	h	101	DGD	C4D-C5D	2.20	1.57	1.53
26	d	402	PHO	CMD-C2D	-2.20	1.47	1.51
26	a	608	PHO	CAC-C3C	-2.20	1.47	1.51
25	d	404	CLA	CHC-C1C	2.20	1.42	1.38
31	h	101	DGD	C1E-C2E	2.20	1.59	1.52
25	b	602	CLA	CHC-C1C	2.20	1.42	1.38
29	c	522	LMG	C3-C2	2.19	1.58	1.52
25	A	609	CLA	CMB-C2B	-2.19	1.46	1.50
26	d	402	PHO	C3D-C4D	2.19	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	603	CLA	C3B-C4B	2.19	1.49	1.42
25	a	609	CLA	C3B-C4B	2.18	1.49	1.42
25	b	604	CLA	MG-NA	2.18	2.11	2.06
25	C	501	CLA	C1D-C2D	2.18	1.49	1.45
36	v	201	HEC	CMD-C2D	2.18	1.55	1.50
25	C	509	CLA	CMD-C2D	-2.18	1.46	1.50
26	d	402	PHO	CMB-C2B	-2.18	1.47	1.51
29	c	522	LMG	O7-C8	-2.18	1.41	1.46
25	b	616	CLA	CHC-C1C	2.18	1.42	1.38
25	c	502	CLA	CHC-C1C	2.18	1.42	1.38
25	B	609	CLA	MG-NB	-2.17	2.01	2.05
25	b	612	CLA	CMC-C2C	-2.17	1.46	1.50
25	d	403	CLA	C3B-C4B	2.17	1.49	1.42
27	A	610	BCR	C33-C5	-2.17	1.47	1.50
36	V	201	HEC	CMC-C2C	2.17	1.55	1.50
25	b	604	CLA	C3B-C4B	2.17	1.49	1.42
33	d	407	LHG	O8-C6	-2.17	1.40	1.45
25	a	609	CLA	CMC-C2C	-2.16	1.46	1.50
25	b	606	CLA	CMB-C2B	-2.16	1.46	1.50
29	B	620	LMG	C4-C5	2.16	1.57	1.53
25	C	507	CLA	CMD-C2D	-2.16	1.46	1.50
25	C	508	CLA	C1D-C2D	2.16	1.49	1.45
25	B	609	CLA	CHC-C1C	2.16	1.42	1.38
29	D	407	LMG	O7-C8	-2.16	1.41	1.46
25	B	607	CLA	CMD-C2D	-2.16	1.46	1.50
25	B	609	CLA	C1D-C2D	2.16	1.49	1.45
33	E	101	LHG	O7-C5	-2.15	1.41	1.46
25	B	606	CLA	CHC-C1C	2.15	1.42	1.38
25	B	616	CLA	CHC-C1C	2.15	1.42	1.38
25	b	616	CLA	C3B-C4B	2.14	1.49	1.42
25	b	609	CLA	C1B-C2B	2.14	1.48	1.43
25	B	614	CLA	CHC-C1C	2.14	1.42	1.38
25	c	503	CLA	CMC-C2C	-2.14	1.46	1.50
25	b	612	CLA	CMB-C2B	-2.14	1.46	1.50
36	v	201	HEC	CMB-C2B	2.14	1.55	1.50
25	B	603	CLA	CHC-C1C	2.13	1.42	1.38
25	C	503	CLA	CHC-C1C	2.13	1.42	1.38
25	c	504	CLA	CHC-C1C	2.13	1.42	1.38
29	c	518	LMG	C4-C5	2.13	1.57	1.53
30	f	101	SQD	O9-S	2.13	1.51	1.45
25	b	609	CLA	C1D-C2D	2.13	1.49	1.45
25	c	509	CLA	C3B-C4B	2.13	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	F	101	HEM	FE-NB	2.13	2.01	1.94
30	D	408	SQD	O9-S	2.12	1.51	1.45
31	C	519	DGD	O1G-C1G	-2.12	1.40	1.45
30	a	615	SQD	C44-C45	2.12	1.56	1.51
25	b	602	CLA	MG-NA	2.12	2.11	2.06
29	C	520	LMG	C4-C5	2.12	1.57	1.53
30	b	620	SQD	O7-S	2.12	1.51	1.45
25	C	509	CLA	O2D-CGD	2.12	1.38	1.33
25	B	616	CLA	C3B-C4B	2.12	1.48	1.42
25	b	609	CLA	C3B-C4B	2.12	1.48	1.42
25	b	611	CLA	C1D-C2D	2.12	1.49	1.45
33	D	409	LHG	P-O6	2.11	1.67	1.59
25	B	613	CLA	CMD-C2D	-2.11	1.46	1.50
25	c	511	CLA	C3B-C4B	2.11	1.48	1.42
29	B	622	LMG	O7-C10	2.11	1.37	1.30
25	B	607	CLA	CMB-C2B	-2.11	1.46	1.50
29	c	522	LMG	C1-C2	2.11	1.58	1.52
25	b	601	CLA	CMC-C2C	-2.11	1.46	1.50
25	B	611	CLA	C3B-C4B	2.11	1.48	1.42
26	D	402	PHO	CMC-C2C	-2.10	1.47	1.50
25	B	615	CLA	C1D-C2D	2.10	1.49	1.45
25	b	612	CLA	MG-ND	-2.10	2.01	2.05
30	B	624	SQD	C8-C7	2.10	1.56	1.50
25	B	609	CLA	C3B-C4B	2.10	1.48	1.42
26	a	608	PHO	CMB-C2B	-2.10	1.47	1.51
36	v	201	HEC	CMC-C2C	2.10	1.55	1.50
27	D	405	BCR	C38-C26	-2.09	1.47	1.50
25	b	613	CLA	CMD-C2D	-2.09	1.46	1.50
30	A	614	SQD	C8-C7	2.09	1.56	1.50
31	h	101	DGD	C4E-C5E	2.09	1.57	1.53
31	C	517	DGD	C3D-C2D	2.09	1.57	1.52
25	D	404	CLA	C3B-C4B	2.09	1.48	1.42
30	A	614	SQD	O9-S	2.09	1.51	1.45
29	c	520	LMG	C1-C2	2.08	1.58	1.52
25	B	603	CLA	CMD-C2D	-2.08	1.46	1.50
25	c	503	CLA	C3B-C4B	2.07	1.48	1.42
25	C	512	CLA	CMB-C2B	-2.07	1.46	1.50
25	c	507	CLA	CMB-C2B	-2.07	1.46	1.50
25	b	610	CLA	C3B-C4B	2.07	1.48	1.42
25	B	610	CLA	CMB-C2B	-2.07	1.46	1.50
31	c	516	DGD	C6E-C5E	2.07	1.58	1.51
27	b	618	BCR	C38-C26	-2.06	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d	409	LMG	O7-C10	2.06	1.37	1.30
25	C	512	CLA	CMD-C2D	-2.06	1.46	1.50
26	a	608	PHO	O2D-CGD	2.06	1.38	1.33
30	a	614	SQD	C46-C45	2.06	1.57	1.50
33	d	407	LHG	O7-C5	-2.06	1.41	1.46
29	b	622	LMG	C4-C3	2.06	1.57	1.52
25	d	403	CLA	MG-NB	-2.06	2.01	2.05
29	c	518	LMG	C4-C3	2.06	1.57	1.52
25	c	502	CLA	MG-NA	2.06	2.11	2.06
25	B	608	CLA	C3B-C4B	2.05	1.48	1.42
25	b	604	CLA	CHC-C1C	2.05	1.42	1.38
31	c	516	DGD	C4D-C3D	2.05	1.57	1.52
33	a	613	LHG	O7-C5	-2.05	1.41	1.46
35	e	101	HEM	C3B-C2B	-2.05	1.33	1.37
25	c	504	CLA	CMC-C2C	-2.05	1.46	1.50
25	B	604	CLA	CHC-C1C	2.04	1.42	1.38
25	c	507	CLA	C3D-C4D	2.04	1.48	1.44
25	c	507	CLA	C3B-C4B	2.04	1.48	1.42
25	c	505	CLA	C3C-C2C	2.04	1.41	1.36
25	A	607	CLA	MG-NB	-2.04	2.01	2.05
31	a	616	DGD	C3G-C2G	2.04	1.56	1.51
25	c	506	CLA	CMC-C2C	-2.04	1.46	1.50
25	D	403	CLA	CMD-C2D	-2.04	1.46	1.50
26	D	402	PHO	CAC-C3C	-2.04	1.48	1.51
25	A	607	CLA	CMB-C2B	-2.03	1.46	1.50
27	x	101	BCR	C1-C6	-2.03	1.51	1.53
25	B	609	CLA	C3D-C4D	2.03	1.48	1.44
30	D	408	SQD	O7-S	2.03	1.50	1.45
26	d	402	PHO	C4D-ND	-2.03	1.35	1.38
29	D	411	LMG	C7-C8	2.03	1.56	1.51
26	a	608	PHO	CBD-CGD	-2.03	1.49	1.52
35	e	101	HEM	CMC-C2C	2.03	1.54	1.50
31	C	519	DGD	O3G-C3G	-2.03	1.40	1.43
25	C	502	CLA	CMB-C2B	-2.03	1.46	1.50
25	c	504	CLA	O2D-CGD	2.03	1.38	1.33
25	c	507	CLA	CHC-C1C	2.03	1.42	1.38
30	B	624	SQD	C44-C45	2.03	1.57	1.50
35	F	101	HEM	CMA-C3A	2.03	1.54	1.50
25	b	612	CLA	MG-NA	2.02	2.11	2.06
25	B	606	CLA	C3B-C4B	2.02	1.48	1.42
25	B	601	CLA	CMB-C2B	-2.02	1.46	1.50
25	c	508	CLA	C3C-C2C	2.02	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	612	CLA	C3B-C4B	2.02	1.48	1.42
25	c	501	CLA	CMC-C2C	-2.02	1.46	1.50
25	c	513	CLA	MG-NB	2.02	2.09	2.05
30	B	624	SQD	O5-C5	2.02	1.49	1.44
27	A	610	BCR	C30-C25	-2.02	1.51	1.53
27	B	617	BCR	C33-C5	-2.01	1.47	1.50
25	a	607	CLA	CMC-C2C	-2.01	1.46	1.50
25	c	501	CLA	C3B-C4B	2.01	1.48	1.42
31	C	517	DGD	C3G-C2G	2.01	1.57	1.50
25	C	508	CLA	CMD-C2D	-2.01	1.46	1.50
25	C	506	CLA	CMD-C2D	-2.01	1.46	1.50
25	b	609	CLA	CMC-C2C	-2.01	1.46	1.50
28	a	611	PL9	C7-C3	-2.01	1.48	1.51
25	c	510	CLA	CMD-C2D	-2.01	1.46	1.50
26	D	402	PHO	O2D-CGD	2.01	1.38	1.33
27	k	102	BCR	C33-C5	-2.00	1.47	1.50
31	h	101	DGD	O2G-C2G	-2.00	1.41	1.46
25	a	612	CLA	C3D-C4D	2.00	1.48	1.44
25	b	608	CLA	CMB-C2B	-2.00	1.46	1.50
31	c	515	DGD	C4E-C3E	2.00	1.57	1.52

All (1053) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	511	CLA	C4A-NA-C1A	8.79	110.69	106.68
25	b	606	CLA	C4A-NA-C1A	8.71	110.66	106.68
25	B	604	CLA	C4A-NA-C1A	8.48	110.55	106.68
25	B	606	CLA	C4A-NA-C1A	8.23	110.43	106.68
25	C	511	CLA	C4A-NA-C1A	8.22	110.43	106.68
25	C	513	CLA	C4A-NA-C1A	8.09	110.37	106.68
25	C	507	CLA	C4A-NA-C1A	7.98	110.32	106.68
25	C	503	CLA	C4A-NA-C1A	7.66	110.17	106.68
25	C	505	CLA	C4A-NA-C1A	7.34	110.03	106.68
25	b	601	CLA	C4A-NA-C1A	7.30	110.01	106.68
25	C	510	CLA	C4A-NA-C1A	7.24	109.98	106.68
25	c	507	CLA	C4A-NA-C1A	7.20	109.96	106.68
25	c	509	CLA	C4A-NA-C1A	7.08	109.91	106.68
25	B	601	CLA	C4A-NA-C1A	7.03	109.89	106.68
25	B	609	CLA	C4A-NA-C1A	6.96	109.85	106.68
25	B	605	CLA	C4A-NA-C1A	6.89	109.82	106.68
25	c	503	CLA	C4A-NA-C1A	6.79	109.78	106.68
25	C	501	CLA	C4A-NA-C1A	6.78	109.77	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	508	CLA	C4A-NA-C1A	6.78	109.77	106.68
25	b	604	CLA	C4A-NA-C1A	6.75	109.76	106.68
30	a	614	SQD	O6-C1-C2	6.74	118.51	108.27
25	B	611	CLA	C4A-NA-C1A	6.68	109.73	106.68
25	c	510	CLA	C4A-NA-C1A	6.65	109.71	106.68
25	c	501	CLA	C4A-NA-C1A	6.53	109.66	106.68
25	B	616	CLA	C4A-NA-C1A	6.52	109.65	106.68
25	c	506	CLA	C4A-NA-C1A	6.51	109.65	106.68
28	a	611	PL9	C7-C3-C4	6.50	122.26	116.91
25	C	509	CLA	C4A-NA-C1A	6.35	109.57	106.68
25	b	613	CLA	C4A-NA-C1A	6.17	109.50	106.68
25	A	606	CLA	C4A-NA-C1A	6.15	109.48	106.68
25	B	608	CLA	C4A-NA-C1A	6.10	109.46	106.68
25	b	602	CLA	C4A-NA-C1A	6.03	109.43	106.68
25	b	611	CLA	C4A-NA-C1A	6.01	109.42	106.68
25	D	404	CLA	C4A-NA-C1A	6.01	109.42	106.68
25	b	615	CLA	C4A-NA-C1A	6.00	109.42	106.68
26	A	608	PHO	C4D-CHA-CBD	-5.98	105.58	108.45
30	A	614	SQD	O6-C1-C2	5.98	117.35	108.27
28	d	406	PL9	C7-C3-C4	5.92	121.79	116.91
28	A	611	PL9	C7-C3-C4	5.91	121.78	116.91
25	B	615	CLA	C4A-NA-C1A	5.90	109.37	106.68
25	A	609	CLA	C4A-NA-C1A	5.85	109.35	106.68
25	A	612	CLA	C4A-NA-C1A	5.77	109.31	106.68
30	a	614	SQD	C1-O5-C5	-5.73	102.52	113.72
25	b	610	CLA	C4A-NA-C1A	5.71	109.28	106.68
25	d	403	CLA	C4A-NA-C1A	5.68	109.27	106.68
25	B	614	CLA	C4A-NA-C1A	5.60	109.24	106.68
26	a	608	PHO	C4D-CHA-CBD	-5.56	105.79	108.45
30	A	614	SQD	C1-O5-C5	-5.51	102.96	113.72
25	B	613	CLA	C1-C2-C3	-5.47	117.24	126.20
25	b	616	CLA	C4A-NA-C1A	5.43	109.16	106.68
25	C	504	CLA	C4A-NA-C1A	5.39	109.14	106.68
25	C	506	CLA	C4A-NA-C1A	5.35	109.12	106.68
25	b	608	CLA	C4A-NA-C1A	5.23	109.06	106.68
25	b	605	CLA	C4A-NA-C1A	5.21	109.06	106.68
28	a	611	PL9	C7-C3-C2	-5.17	117.30	123.39
25	B	607	CLA	C4A-NA-C1A	5.13	109.02	106.68
25	b	607	CLA	C4A-NA-C1A	5.12	109.02	106.68
25	c	513	CLA	C4A-NA-C1A	5.09	109.00	106.68
25	a	612	CLA	C4A-NA-C1A	5.06	108.99	106.68
25	b	609	CLA	C4A-NA-C1A	5.05	108.98	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	607	CLA	C4A-NA-C1A	5.04	108.98	106.68
25	c	502	CLA	C4A-NA-C1A	5.03	108.97	106.68
25	c	504	CLA	C4A-NA-C1A	5.03	108.97	106.68
25	B	612	CLA	C4A-NA-C1A	5.00	108.96	106.68
36	V	201	HEC	C1D-ND-C4D	4.99	111.11	105.21
30	a	615	SQD	O47-C7-C8	4.98	122.26	111.48
30	b	620	SQD	O6-C1-C2	4.94	115.78	108.27
25	B	602	CLA	C4A-NA-C1A	4.93	108.93	106.68
25	A	607	CLA	C4A-NA-C1A	4.92	108.92	106.68
25	c	505	CLA	C4A-NA-C1A	4.87	108.90	106.68
25	c	512	CLA	C4A-NA-C1A	4.87	108.90	106.68
25	B	613	CLA	C4A-NA-C1A	4.82	108.88	106.68
25	b	614	CLA	C4A-NA-C1A	4.77	108.85	106.68
25	b	603	CLA	C4A-NA-C1A	4.73	108.84	106.68
25	C	502	CLA	C4A-NA-C1A	4.67	108.81	106.68
25	C	512	CLA	C4A-NA-C1A	4.62	108.79	106.68
25	c	512	CLA	C1-C2-C3	-4.58	118.70	126.20
25	B	603	CLA	C4A-NA-C1A	4.57	108.76	106.68
28	D	406	PL9	C7-C3-C4	4.53	120.64	116.91
33	D	410	LHG	O4-P-O5	4.48	133.28	112.44
30	A	614	SQD	C1-C2-C3	-4.48	100.59	110.01
30	f	101	SQD	O6-C1-C2	4.48	115.07	108.27
26	D	402	PHO	C1-C2-C3	-4.45	118.91	126.20
28	d	406	PL9	C7-C3-C2	-4.43	118.16	123.39
25	a	606	CLA	C4A-NA-C1A	4.42	108.70	106.68
25	c	508	CLA	C4A-NA-C1A	4.41	108.69	106.68
33	e	102	LHG	O4-P-O5	4.40	132.91	112.44
30	B	624	SQD	O47-C7-C8	4.40	121.00	111.48
30	B	624	SQD	O6-C1-C2	4.40	114.95	108.27
30	b	620	SQD	O5-C5-C4	4.34	117.52	109.70
25	a	609	CLA	O2D-CGD-O1D	-4.32	115.43	123.85
33	B	623	LHG	O4-P-O5	4.30	132.46	112.44
30	B	624	SQD	C3-C4-C5	4.29	118.00	110.23
31	H	102	DGD	O3G-C3G-C2G	-4.28	100.41	110.82
33	l	101	LHG	O4-P-O5	4.27	132.31	112.44
25	d	404	CLA	C4A-NA-C1A	4.27	108.63	106.68
33	d	407	LHG	O4-P-O5	4.26	132.26	112.44
34	D	401	BCT	O2-C-O1	4.25	130.53	119.68
26	d	402	PHO	C4D-CHA-CBD	-4.23	106.42	108.45
25	b	606	CLA	O2D-CGD-O1D	-4.23	115.61	123.85
33	E	101	LHG	O4-P-O5	4.22	132.10	112.44
33	a	613	LHG	O4-P-O5	4.22	132.06	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	603	CLA	O2D-CGD-O1D	-4.20	115.68	123.85
33	d	408	LHG	O4-P-O5	4.15	131.73	112.44
30	f	101	SQD	O9-S-O7	-4.12	100.42	113.82
30	A	614	SQD	O47-C7-C8	4.11	120.38	111.48
33	D	412	LHG	O4-P-O5	4.10	131.51	112.44
36	v	201	HEC	C1D-ND-C4D	4.09	110.05	105.21
34	d	401	BCT	O2-C-O1	4.06	130.05	119.68
31	C	519	DGD	O3G-C3G-C2G	-4.05	100.96	110.82
33	D	409	LHG	O4-P-O5	4.04	131.26	112.44
28	A	611	PL9	C7-C3-C2	-4.02	118.66	123.39
25	b	613	CLA	C1-C2-C3	-4.00	119.64	126.20
31	C	518	DGD	O3G-C3G-C2G	-3.96	101.18	110.82
27	b	617	BCR	C2-C1-C6	3.94	116.16	110.44
26	D	402	PHO	C2B-C1B-NB	-3.93	106.59	109.43
25	B	601	CLA	O2D-CGD-O1D	-3.92	116.22	123.85
25	B	610	CLA	O2D-CGD-O1D	-3.91	116.23	123.85
25	B	615	CLA	C3B-C4B-NB	-3.90	107.05	110.53
28	d	406	PL9	C7-C8-C9	-3.87	120.17	126.83
30	b	620	SQD	O7-S-C6	3.86	112.51	106.76
25	a	606	CLA	C3B-C4B-NB	-3.82	107.12	110.53
25	a	609	CLA	O2D-CGD-CBD	3.82	117.90	111.23
25	A	607	CLA	C3B-C4B-NB	-3.81	107.13	110.53
25	A	607	CLA	C1-C2-C3	-3.80	119.97	126.20
25	c	509	CLA	O2A-CGA-O1A	-3.78	114.17	123.63
25	c	501	CLA	O2D-CGD-O1D	-3.77	116.50	123.85
30	B	624	SQD	C1-O5-C5	-3.76	106.38	113.72
25	B	614	CLA	O2D-CGD-O1D	-3.75	116.55	123.85
35	e	101	HEM	CBD-CAD-C3D	-3.74	102.20	112.53
25	c	512	CLA	C3B-C4B-NB	-3.73	107.20	110.53
30	A	614	SQD	O7-S-C6	3.71	112.30	106.76
26	d	402	PHO	C1-C2-C3	-3.71	120.12	126.20
31	C	517	DGD	O3G-C3G-C2G	-3.71	101.81	110.82
30	A	614	SQD	O9-S-O7	-3.70	101.78	113.82
27	B	619	BCR	C2-C1-C6	3.69	115.81	110.44
31	c	515	DGD	O3G-C3G-C2G	-3.69	101.84	110.82
30	f	101	SQD	O7-S-C6	3.69	112.26	106.76
25	b	605	CLA	C3B-C4B-NB	-3.68	107.25	110.53
25	b	608	CLA	C3B-C4B-NB	-3.67	107.25	110.53
32	C	521	STE	C3-C2-C1	-3.67	104.94	114.51
30	D	408	SQD	C1-O5-C5	-3.65	106.59	113.72
25	B	612	CLA	O2D-CGD-O1D	-3.64	116.76	123.85
25	A	609	CLA	O2D-CGD-O1D	-3.63	116.79	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	d	412	STE	C3-C2-C1	-3.62	105.07	114.51
33	a	613	LHG	O8-C23-C24	3.62	122.86	111.83
30	a	614	SQD	O47-C7-C8	3.61	119.30	111.48
28	D	406	PL9	C7-C3-C2	-3.61	119.14	123.39
25	B	613	CLA	C3B-C4B-NB	-3.61	107.31	110.53
27	D	405	BCR	C7-C8-C9	-3.60	120.91	126.23
25	b	612	CLA	O2D-CGD-O1D	-3.59	116.85	123.85
25	c	502	CLA	O2D-CGD-O1D	-3.59	116.86	123.85
25	B	614	CLA	C1-C2-C3	-3.59	120.32	126.20
25	B	603	CLA	C3B-C4B-NB	-3.58	107.33	110.53
31	a	616	DGD	O3G-C3G-C2G	-3.58	102.57	111.77
25	B	602	CLA	O2D-CGD-CBD	3.58	117.48	111.23
25	a	607	CLA	C3B-C4B-NB	-3.57	107.35	110.53
28	d	406	PL9	C22-C23-C24	-3.56	119.48	127.62
25	a	609	CLA	C4A-NA-C1A	3.55	108.30	106.68
25	C	506	CLA	C3B-C4B-NB	-3.55	107.36	110.53
25	B	610	CLA	C4A-NA-C1A	3.55	108.30	106.68
27	x	101	BCR	C2-C1-C6	3.54	115.58	110.44
25	b	615	CLA	C3B-C4B-NB	-3.53	107.38	110.53
25	C	504	CLA	C3B-C4B-NB	-3.53	107.38	110.53
31	C	519	DGD	O6D-C1D-O3G	-3.53	101.71	110.04
25	C	513	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
25	d	403	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
29	b	622	LMG	C1-O6-C5	-3.50	106.89	113.72
25	B	602	CLA	O2D-CGD-O1D	-3.50	117.04	123.85
25	C	507	CLA	CHB-C4A-NA	3.48	129.42	124.40
29	m	101	LMG	O1-C1-C2	-3.48	103.00	108.27
25	b	610	CLA	O2D-CGD-O1D	-3.47	117.09	123.85
25	b	611	CLA	O2D-CGD-O1D	-3.46	117.12	123.85
25	B	614	CLA	C3B-C4B-NB	-3.45	107.45	110.53
25	C	508	CLA	C3B-C4B-NB	-3.44	107.45	110.53
25	C	508	CLA	O2D-CGD-O1D	-3.42	117.18	123.85
30	a	615	SQD	O48-C23-C24	3.41	122.23	111.83
30	D	408	SQD	O9-S-C6	3.41	111.85	106.76
25	b	601	CLA	O2D-CGD-O1D	-3.41	117.21	123.85
25	B	606	CLA	O2D-CGD-O1D	-3.41	117.21	123.85
25	b	605	CLA	O2D-CGD-O1D	-3.40	117.23	123.85
30	B	624	SQD	O5-C5-C4	3.40	115.83	109.70
31	A	616	DGD	C3G-C2G-C1G	-3.38	103.91	111.78
25	C	505	CLA	C3B-C4B-NB	-3.37	107.52	110.53
25	b	606	CLA	O2D-CGD-CBD	3.36	117.11	111.23
30	A	615	SQD	O47-C7-C8	3.34	118.71	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	609	CLA	C3B-C4B-NB	-3.34	107.55	110.53
25	b	611	CLA	O2D-CGD-CBD	3.33	117.05	111.23
36	V	201	HEC	CBD-CAD-C3D	-3.33	103.33	112.53
25	A	612	CLA	C3B-C4B-NB	-3.32	107.57	110.53
25	b	601	CLA	C3B-C4B-NB	-3.32	107.57	110.53
27	b	617	BCR	C15-C14-C13	-3.32	122.63	127.28
25	b	616	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
29	C	520	LMG	O1-C7-C8	-3.30	102.80	110.82
28	a	611	PL9	C22-C23-C24	-3.29	120.09	127.62
25	B	604	CLA	C3B-C4B-NB	-3.29	107.59	110.53
30	A	614	SQD	O5-C1-C2	-3.29	103.62	110.37
25	b	608	CLA	CMB-C2B-C1B	-3.28	120.42	125.42
25	C	506	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
25	b	602	CLA	CHB-C4A-NA	3.27	129.12	124.40
25	C	503	CLA	C3B-C4B-NB	-3.27	107.61	110.53
30	B	624	SQD	O9-S-O7	-3.27	103.20	113.82
26	D	402	PHO	O2D-CGD-O1D	-3.26	117.49	123.85
25	C	512	CLA	CHB-C4A-NA	3.26	129.11	124.40
25	C	509	CLA	C3B-C4B-NB	-3.25	107.63	110.53
25	D	403	CLA	C3B-C4B-NB	-3.24	107.64	110.53
26	A	608	PHO	CMB-C2B-C3B	3.24	131.15	124.68
25	C	501	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
25	b	609	CLA	CMB-C2B-C1B	-3.23	120.51	125.42
26	d	402	PHO	C2B-C1B-NB	-3.22	107.10	109.43
27	B	617	BCR	C2-C1-C6	3.22	115.11	110.44
30	B	624	SQD	O48-C23-C24	3.22	121.64	111.83
29	D	407	LMG	O1-C1-C2	-3.22	103.39	108.27
25	A	609	CLA	O2D-CGD-CBD	3.21	116.85	111.23
25	C	510	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
25	B	610	CLA	C3B-C4B-NB	-3.21	107.67	110.53
31	C	517	DGD	CDB-CCB-CBB	-3.21	98.15	114.37
25	B	610	CLA	CHB-C4A-NA	3.21	129.03	124.40
28	D	406	PL9	C7-C8-C9	-3.20	121.31	126.83
25	b	604	CLA	C1-C2-C3	-3.20	120.95	126.20
25	C	505	CLA	O2D-CGD-O1D	-3.18	117.65	123.85
26	d	402	PHO	O1D-CGD-CBD	3.18	129.55	124.72
30	A	615	SQD	O48-C23-C24	3.18	121.53	111.83
25	b	601	CLA	CHB-C4A-NA	3.17	128.98	124.40
28	D	406	PL9	C37-C38-C39	-3.17	120.36	127.62
31	h	101	DGD	O3G-C3G-C2G	-3.16	103.13	110.82
27	t	101	BCR	C15-C16-C17	-3.16	117.05	123.52
25	c	509	CLA	O2D-CGD-O1D	-3.15	117.71	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	503	CLA	C7-C6-C5	-3.15	104.86	113.26
25	c	512	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
30	b	620	SQD	C1-C2-C3	-3.12	103.44	110.01
25	B	606	CLA	C3B-C4B-NB	-3.12	107.74	110.53
25	C	512	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
31	c	517	DGD	O3G-C3G-C2G	-3.12	103.24	110.82
30	b	620	SQD	O9-S-O7	-3.11	103.70	113.82
30	f	101	SQD	O9-S-C6	3.11	111.40	106.76
25	B	608	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
28	A	611	PL9	C40-C39-C41	3.11	120.62	115.23
25	b	612	CLA	CMB-C2B-C1B	-3.10	120.69	125.42
30	a	614	SQD	O48-C23-C24	3.10	121.30	111.83
25	C	512	CLA	C1-C2-C3	-3.10	121.12	126.20
30	D	408	SQD	O9-S-O7	-3.10	103.75	113.82
27	a	610	BCR	C27-C26-C25	3.09	126.89	122.70
25	b	610	CLA	C1-C2-C3	-3.08	121.14	126.20
26	D	402	PHO	C4D-CHA-CBD	-3.08	106.98	108.45
31	c	515	DGD	C3G-C2G-C1G	-3.08	104.60	111.78
25	c	508	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
25	b	614	CLA	C3B-C4B-NB	-3.08	107.78	110.53
25	C	501	CLA	C3B-C4B-NB	-3.07	107.79	110.53
25	c	507	CLA	C3B-C4B-NB	-3.07	107.79	110.53
27	c	514	BCR	C27-C26-C25	3.06	126.84	122.70
25	C	507	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
25	B	610	CLA	O2A-CGA-O1A	-3.06	115.99	123.63
25	a	612	CLA	O2D-CGD-O1D	-3.05	117.90	123.85
30	a	614	SQD	O9-S-O7	-3.04	103.92	113.82
25	B	612	CLA	CHB-C4A-NA	3.04	128.79	124.40
25	C	512	CLA	C3B-C4B-NB	-3.04	107.81	110.53
29	d	410	LMG	O6-C1-O1	-3.04	102.86	110.04
25	D	403	CLA	O2A-CGA-O1A	-3.03	116.04	123.63
27	T	101	BCR	C27-C26-C25	3.03	126.80	122.70
25	c	503	CLA	C3B-C4B-NB	-3.03	107.82	110.53
25	b	602	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
25	c	504	CLA	O2A-CGA-O1A	-3.02	116.08	123.63
35	F	101	HEM	CBD-CAD-C3D	-3.02	104.19	112.53
33	D	412	LHG	O8-C23-C24	3.02	121.03	111.83
25	c	502	CLA	C3B-C4B-NB	-3.01	107.84	110.53
28	d	406	PL9	C40-C39-C41	3.01	120.45	115.23
25	c	502	CLA	C1-C2-C3	-3.01	121.27	126.20
25	c	508	CLA	CHB-C4A-NA	3.00	128.74	124.40
25	C	511	CLA	C3B-C4B-NB	-3.00	107.85	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	519	DGD	O3E-C3E-C2E	-3.00	103.30	110.38
28	D	406	PL9	C40-C39-C41	3.00	120.44	115.23
25	A	609	CLA	CHB-C4A-NA	3.00	128.73	124.40
30	b	620	SQD	O48-C23-C24	2.99	120.94	111.83
25	B	612	CLA	C3B-C4B-NB	-2.99	107.86	110.53
25	A	606	CLA	CHB-C4A-NA	2.98	128.71	124.40
28	A	611	PL9	C22-C23-C24	-2.98	120.80	127.62
26	d	402	PHO	CMB-C2B-C3B	2.98	130.64	124.68
25	c	509	CLA	CHB-C4A-NA	2.98	128.69	124.40
25	d	404	CLA	C3B-C4B-NB	-2.97	107.88	110.53
26	A	608	PHO	O2D-CGD-O1D	-2.96	118.09	123.85
30	b	620	SQD	C3-C4-C5	2.95	115.58	110.23
28	D	406	PL9	C42-C43-C44	-2.94	120.88	127.62
27	t	101	BCR	C7-C8-C9	-2.94	121.88	126.23
31	c	516	DGD	O6D-C1D-O3G	-2.94	103.09	110.04
25	b	604	CLA	C3B-C4B-NB	-2.94	107.91	110.53
25	C	501	CLA	O2D-CGD-CBD	2.94	116.37	111.23
30	a	614	SQD	C1-C2-C3	-2.94	103.83	110.01
31	c	516	DGD	O3G-C3G-C2G	-2.93	103.68	110.82
25	B	603	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
25	C	502	CLA	C3B-C4B-NB	-2.93	107.91	110.53
27	k	101	BCR	C27-C26-C25	2.93	126.67	122.70
27	k	102	BCR	C33-C5-C6	-2.93	121.29	124.48
26	a	608	PHO	CMB-C2B-C3B	2.93	130.53	124.68
27	d	405	BCR	C27-C26-C25	2.92	126.66	122.70
25	b	603	CLA	C3B-C4B-NB	-2.92	107.92	110.53
30	D	408	SQD	O8-S-C6	2.91	111.60	105.97
25	B	611	CLA	C3B-C4B-NB	-2.91	107.93	110.53
25	B	609	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
31	c	517	DGD	CDB-CCB-CBB	-2.91	99.67	114.37
31	h	101	DGD	CDB-CCB-CBB	-2.90	99.71	114.37
25	b	614	CLA	C1-C2-C3	-2.89	121.45	126.20
25	d	403	CLA	CHB-C4A-NA	2.89	128.57	124.40
26	A	608	PHO	C2B-C1B-NB	-2.89	107.34	109.43
30	B	624	SQD	O7-S-C6	2.89	111.07	106.76
30	f	101	SQD	O5-C5-C4	2.88	114.89	109.70
33	e	102	LHG	O8-C23-C24	2.88	120.61	111.83
25	c	508	CLA	C3B-C4B-NB	-2.88	107.96	110.53
31	C	517	DGD	O6D-C1D-O3G	-2.88	103.25	110.04
25	B	602	CLA	CHB-C4A-NA	2.88	128.55	124.40
25	b	612	CLA	C11-C12-C13	-2.87	106.41	115.97
25	B	608	CLA	CMB-C2B-C1B	-2.87	121.05	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	503	CLA	C1-C2-C3	-2.87	121.50	126.20
27	B	619	BCR	C3-C4-C5	-2.87	108.94	114.06
25	C	509	CLA	CED-O2D-CGD	2.87	122.42	115.92
27	H	101	BCR	C27-C26-C25	2.87	126.58	122.70
33	d	407	LHG	O8-C23-C24	2.86	120.56	111.83
25	B	612	CLA	C1-C2-C3	-2.86	121.51	126.20
25	b	610	CLA	O2A-CGA-O1A	-2.86	116.47	123.63
27	B	617	BCR	C27-C26-C25	2.86	126.57	122.70
25	b	612	CLA	C3B-C4B-NB	-2.86	107.98	110.53
25	b	612	CLA	C1-C2-C3	-2.86	121.52	126.20
25	d	403	CLA	O2A-CGA-O1A	-2.86	116.48	123.63
27	T	101	BCR	C33-C5-C6	-2.85	121.37	124.48
25	b	605	CLA	C1-C2-C3	-2.85	121.52	126.20
30	b	620	SQD	O47-C7-C8	2.85	117.65	111.48
25	b	604	CLA	CHB-C4A-NA	2.85	128.51	124.40
25	A	606	CLA	C3B-C4B-NB	-2.85	107.99	110.53
25	b	607	CLA	C3B-C4B-NB	-2.85	107.99	110.53
25	B	604	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
25	c	505	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
27	b	618	BCR	C15-C14-C13	-2.84	123.30	127.28
25	C	513	CLA	C3B-C4B-NB	-2.84	108.00	110.53
31	C	519	DGD	CDB-CCB-CBB	-2.84	100.02	114.37
33	D	409	LHG	O8-C23-C24	2.84	120.49	111.83
25	b	604	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
29	c	520	LMG	O6-C1-O1	-2.84	103.34	110.04
27	k	101	BCR	C2-C1-C6	2.83	114.55	110.44
27	t	101	BCR	C11-C10-C9	-2.83	123.31	127.28
29	A	613	LMG	O6-C1-O1	-2.82	103.37	110.04
25	B	615	CLA	CHB-C4A-NA	2.82	128.47	124.40
27	k	103	BCR	C11-C10-C9	-2.82	123.32	127.28
25	b	616	CLA	C3B-C4B-NB	-2.82	108.01	110.53
30	a	614	SQD	O9-S-C6	2.82	110.97	106.76
25	C	503	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
27	C	514	BCR	C2-C1-C6	2.82	114.53	110.44
25	c	508	CLA	O2D-CGD-CBD	2.82	116.16	111.23
25	C	508	CLA	CHD-C1D-ND	-2.82	120.84	124.80
25	C	502	CLA	O2A-CGA-O1A	-2.81	116.59	123.63
36	v	201	HEC	CHA-C4D-ND	2.81	127.45	124.42
25	d	403	CLA	O2D-CGD-CBD	2.81	116.14	111.23
30	D	408	SQD	O48-C23-C24	2.81	120.39	111.83
25	c	505	CLA	C3B-C4B-NB	-2.80	108.03	110.53
25	c	513	CLA	CMB-C2B-C1B	-2.80	121.15	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	402	PHO	CMB-C2B-C3B	2.80	130.28	124.68
27	C	516	BCR	C27-C26-C25	2.80	126.48	122.70
30	A	614	SQD	O8-S-C6	2.80	111.37	105.97
28	D	406	PL9	C12-C13-C14	-2.79	121.25	127.62
27	t	101	BCR	C33-C5-C6	-2.78	121.45	124.48
31	a	616	DGD	CDB-CCB-CBB	-2.78	100.31	114.37
27	k	101	BCR	C7-C8-C9	-2.78	122.12	126.23
25	a	607	CLA	CHB-C4A-NA	2.78	128.41	124.40
25	B	605	CLA	C3B-C4B-NB	-2.77	108.06	110.53
25	c	506	CLA	C3B-C4B-NB	-2.77	108.06	110.53
25	B	602	CLA	C1-C2-C3	-2.77	121.67	126.20
25	c	511	CLA	C3B-C4B-NB	-2.76	108.06	110.53
31	h	101	DGD	C1D-C2D-C3D	-2.76	104.20	110.01
30	D	408	SQD	O6-C1-C2	2.76	112.47	108.27
25	B	616	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
25	B	601	CLA	C3B-C4B-NB	-2.76	108.07	110.53
25	b	610	CLA	CHB-C4A-NA	2.76	128.38	124.40
25	C	511	CLA	O2A-CGA-O1A	-2.75	116.74	123.63
25	C	506	CLA	C1-C2-C3	-2.75	121.69	126.20
29	b	622	LMG	O2-C2-C1	-2.75	103.52	110.08
25	b	612	CLA	O2A-CGA-O1A	-2.75	116.75	123.63
31	c	515	DGD	O6D-C1D-O3G	-2.75	103.55	110.04
25	a	609	CLA	CHB-C4A-NA	2.74	128.35	124.40
25	c	512	CLA	CHB-C4A-NA	2.74	128.35	124.40
25	c	513	CLA	C3B-C4B-NB	-2.73	108.09	110.53
26	A	608	PHO	O2D-CGD-CBD	2.73	113.95	110.95
25	c	513	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
25	c	513	CLA	CHB-C4A-NA	2.72	128.32	124.40
25	b	612	CLA	C4A-NA-C1A	2.72	107.92	106.68
25	a	606	CLA	O2A-CGA-O1A	-2.72	116.83	123.63
27	B	619	BCR	C29-C30-C25	2.72	114.39	110.44
25	c	504	CLA	CMB-C2B-C1B	-2.72	121.28	125.42
31	C	517	DGD	O5D-C6D-C5D	-2.72	103.30	109.42
33	E	101	LHG	O8-C23-C24	2.71	120.11	111.83
25	c	506	CLA	CHB-C4A-NA	2.71	128.31	124.40
31	A	616	DGD	CDB-CCB-CBB	-2.71	100.66	114.37
27	A	610	BCR	C15-C16-C17	-2.71	117.97	123.52
33	a	613	LHG	O8-C23-O10	-2.71	116.86	123.63
35	e	101	HEM	C3B-C2B-C1B	2.70	108.44	106.41
31	C	518	DGD	CDB-CCB-CBB	-2.70	100.72	114.37
28	d	406	PL9	C37-C38-C39	-2.70	121.45	127.62
25	C	510	CLA	O2D-CGD-CBD	2.70	115.95	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	101	SQD	O48-C23-C24	2.70	120.06	111.83
27	k	103	BCR	C27-C26-C25	2.70	126.35	122.70
27	B	618	BCR	C15-C14-C13	-2.70	123.50	127.28
25	A	612	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
27	A	610	BCR	C2-C1-C6	2.69	114.35	110.44
27	t	101	BCR	C27-C26-C25	2.69	126.34	122.70
27	C	514	BCR	C15-C14-C13	-2.69	123.50	127.28
25	C	501	CLA	O2A-CGA-O1A	-2.69	116.90	123.63
25	b	611	CLA	C1-C2-C3	-2.69	121.79	126.20
25	B	604	CLA	O2A-CGA-O1A	-2.69	116.91	123.63
28	d	406	PL9	C12-C13-C14	-2.69	121.48	127.62
35	e	101	HEM	CBA-CAA-C2A	-2.69	105.11	112.53
28	a	611	PL9	C40-C39-C41	2.69	119.89	115.23
30	B	624	SQD	C4-C3-C2	2.68	115.53	110.83
25	B	611	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
29	D	411	LMG	O1-C7-C8	-2.68	104.89	111.77
25	B	601	CLA	CAA-C2A-C3A	-2.68	105.77	113.00
25	B	609	CLA	C3B-C4B-NB	-2.68	108.14	110.53
25	C	512	CLA	C6-C5-C3	-2.67	106.96	113.47
25	D	403	CLA	C4A-NA-C1A	2.67	107.90	106.68
25	b	603	CLA	O2D-CGD-CBD	2.67	115.90	111.23
25	B	615	CLA	C6-C7-C8	-2.67	107.11	115.97
27	c	514	BCR	C15-C16-C17	-2.66	118.07	123.52
25	c	507	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
26	D	402	PHO	O1D-CGD-CBD	2.66	128.76	124.72
25	B	607	CLA	C3B-C4B-NB	-2.66	108.15	110.53
25	B	606	CLA	O2D-CGD-CBD	2.66	115.88	111.23
25	B	607	CLA	CMB-C2B-C1B	-2.66	121.37	125.42
25	a	612	CLA	O2D-CGD-CBD	2.65	115.87	111.23
27	D	405	BCR	C27-C26-C25	2.65	126.29	122.70
25	b	601	CLA	O2A-CGA-O1A	-2.65	117.00	123.63
33	D	412	LHG	C11-C10-C9	-2.65	100.97	114.37
25	c	508	CLA	C1-C2-C3	-2.65	121.85	126.20
25	C	511	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
27	C	514	BCR	C27-C26-C25	2.64	126.27	122.70
28	D	406	PL9	C27-C28-C29	-2.64	121.58	127.62
25	C	513	CLA	O2A-CGA-O1A	-2.64	117.02	123.63
31	H	102	DGD	O6D-C1D-O3G	-2.64	103.80	110.04
29	D	407	LMG	O6-C1-O1	-2.64	103.81	110.04
28	a	611	PL9	O2-C1-C6	2.64	124.68	120.48
31	A	616	DGD	O3G-C3G-C2G	-2.64	104.40	110.82
25	B	612	CLA	O2A-CGA-O1A	-2.63	117.04	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	H	101	BCR	C16-C15-C14	-2.63	118.13	123.52
26	d	402	PHO	CMA-C3A-C4A	-2.63	108.94	114.61
25	B	616	CLA	C1-C2-C3	-2.63	121.89	126.20
25	B	603	CLA	O2A-CGA-O1A	-2.63	117.06	123.63
27	C	515	BCR	C27-C26-C25	2.63	126.25	122.70
25	B	614	CLA	CHB-C4A-NA	2.62	128.19	124.40
25	b	614	CLA	CHB-C4A-NA	2.62	128.19	124.40
29	c	518	LMG	O2-C2-C1	-2.62	103.83	110.08
27	k	102	BCR	C27-C26-C25	2.62	126.25	122.70
25	b	609	CLA	CMB-C2B-C3B	2.62	132.71	126.55
25	c	505	CLA	C1-C2-C3	-2.62	121.91	126.20
27	C	514	BCR	C15-C16-C17	-2.62	118.16	123.52
27	d	405	BCR	C11-C10-C9	-2.62	123.61	127.28
36	V	201	HEC	CHB-C1B-NB	2.61	127.24	124.42
25	B	604	CLA	CHB-C4A-NA	2.61	128.17	124.40
27	k	101	BCR	C15-C16-C17	-2.61	118.17	123.52
25	b	602	CLA	C3B-C4B-NB	-2.61	108.20	110.53
25	b	603	CLA	CMB-C2B-C1B	-2.61	121.45	125.42
25	d	404	CLA	CHB-C4A-NA	2.60	128.16	124.40
25	D	403	CLA	O2D-CGD-CBD	2.60	115.78	111.23
30	A	614	SQD	O9-S-C6	2.60	110.63	106.76
25	C	509	CLA	CHB-C4A-NA	2.60	128.15	124.40
25	c	510	CLA	C3B-C4B-NB	-2.60	108.21	110.53
31	H	102	DGD	CDB-CCB-CBB	-2.60	101.24	114.37
25	C	510	CLA	C3B-C4B-NB	-2.59	108.22	110.53
25	b	608	CLA	CHB-C4A-NA	2.59	128.14	124.40
33	D	409	LHG	C20-C19-C18	-2.59	101.28	114.37
27	A	610	BCR	C27-C26-C25	2.58	126.20	122.70
30	D	408	SQD	O5-C5-C4	2.58	114.35	109.70
25	b	609	CLA	O2A-CGA-O1A	-2.58	117.17	123.63
30	f	101	SQD	O5-C1-C2	-2.58	105.07	110.37
27	x	101	BCR	C27-C26-C25	2.58	126.19	122.70
29	A	613	LMG	C40-C39-C38	-2.58	101.33	114.37
25	C	505	CLA	C1-C2-C3	-2.58	121.97	126.20
31	c	515	DGD	C3D-C4D-C5D	-2.58	105.56	110.23
25	D	404	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
27	c	514	BCR	C33-C5-C6	-2.58	121.67	124.48
25	C	504	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
27	d	405	BCR	C38-C26-C25	-2.57	121.67	124.48
25	C	508	CLA	CMB-C2B-C1B	-2.57	121.50	125.42
31	c	516	DGD	CDB-CCB-CBB	-2.57	101.36	114.37
28	D	406	PL9	C22-C23-C24	-2.57	121.74	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	503	CLA	C7-C6-C5	-2.57	106.41	113.26
27	b	618	BCR	C27-C26-C25	2.57	126.18	122.70
25	b	608	CLA	CMB-C2B-C3B	2.57	132.60	126.55
25	C	513	CLA	CHB-C4A-NA	2.57	128.11	124.40
25	c	510	CLA	CHB-C4A-NA	2.57	128.10	124.40
25	B	604	CLA	C2D-C1D-ND	-2.57	107.59	110.13
33	d	408	LHG	O8-C23-C24	2.56	119.65	111.83
25	b	616	CLA	CHB-C4A-NA	2.56	128.10	124.40
25	b	613	CLA	C2A-C1A-CHA	2.56	128.31	123.87
33	D	410	LHG	C11-C10-C9	-2.56	101.42	114.37
33	D	410	LHG	O8-C23-C24	2.56	119.64	111.83
31	C	518	DGD	C3E-C4E-C5E	-2.56	105.60	110.23
25	b	612	CLA	CMB-C2B-C3B	2.56	132.56	126.55
25	B	602	CLA	CMB-C2B-C1B	-2.56	121.53	125.42
25	A	607	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
25	b	603	CLA	C4-C3-C5	2.55	119.66	115.23
27	C	514	BCR	C24-C23-C22	-2.55	122.46	126.23
36	v	201	HEC	CHD-C1D-ND	2.55	127.53	124.37
30	f	101	SQD	O47-C7-C8	2.55	120.31	110.93
31	C	518	DGD	O6D-C1D-O3G	-2.55	104.02	110.04
25	A	612	CLA	O2D-CGD-CBD	2.55	115.69	111.23
33	l	101	LHG	O8-C23-C24	2.55	119.61	111.83
32	d	411	STE	C3-C2-C1	-2.55	107.85	114.51
27	H	101	BCR	C11-C10-C9	-2.55	123.70	127.28
27	b	619	BCR	C29-C30-C25	2.55	114.14	110.44
27	C	515	BCR	C15-C16-C17	-2.55	118.31	123.52
26	D	402	PHO	O2D-CGD-CBD	2.55	113.74	110.95
28	d	406	PL9	C35-C34-C36	2.55	119.65	115.23
36	v	201	HEC	CBD-CAD-C3D	-2.54	105.50	112.53
31	c	517	DGD	O6D-C1D-O3G	-2.54	104.03	110.04
33	D	412	LHG	C20-C19-C18	-2.54	101.51	114.37
25	c	507	CLA	CHB-C4A-NA	2.54	128.07	124.40
25	B	611	CLA	O2D-CGD-CBD	2.54	115.67	111.23
26	a	608	PHO	C1-C2-C3	-2.53	122.04	126.20
29	m	101	LMG	O3-C3-C2	-2.53	104.40	110.38
25	C	506	CLA	CHB-C4A-NA	2.53	128.05	124.40
29	c	518	LMG	O6-C1-O1	-2.53	104.06	110.04
30	a	615	SQD	C46-C45-C44	-2.53	105.96	111.80
31	C	518	DGD	O2D-C2D-C1D	-2.53	104.05	110.08
25	a	607	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
25	A	612	CLA	O2A-CGA-O1A	-2.53	117.31	123.63
25	b	607	CLA	C1-O2A-CGA	2.52	122.76	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	F	101	HEM	CHC-C4B-NB	2.52	127.14	124.42
27	k	101	BCR	C3-C4-C5	-2.52	109.56	114.06
29	C	520	LMG	O6-C1-O1	-2.52	104.09	110.04
27	B	618	BCR	C2-C1-C6	2.52	114.10	110.44
28	a	611	PL9	C37-C38-C39	-2.52	121.86	127.62
25	B	612	CLA	CMB-C2B-C3B	2.52	132.47	126.55
25	C	510	CLA	CHB-C4A-NA	2.52	128.03	124.40
27	b	619	BCR	C27-C26-C25	2.51	126.10	122.70
25	b	613	CLA	CHB-C4A-NA	2.51	128.03	124.40
27	C	515	BCR	C15-C14-C13	-2.51	123.75	127.28
29	A	613	LMG	C38-C37-C36	-2.51	101.69	114.37
29	B	620	LMG	C40-C39-C38	-2.51	101.69	114.37
29	m	101	LMG	C6-C5-C4	-2.51	106.87	113.02
25	a	612	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
25	b	616	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
28	D	406	PL9	C32-C33-C34	-2.50	121.90	127.62
25	B	602	CLA	O2A-CGA-O1A	-2.50	117.37	123.63
27	k	103	BCR	C16-C15-C14	-2.50	118.41	123.52
31	c	515	DGD	O3G-C1D-C2D	-2.50	104.48	108.27
28	A	611	PL9	O2-C1-C6	2.50	124.45	120.48
25	A	612	CLA	CHB-C4A-NA	2.49	128.00	124.40
25	C	510	CLA	CMB-C2B-C1B	-2.49	121.62	125.42
27	b	617	BCR	C27-C26-C25	2.49	126.07	122.70
25	c	501	CLA	C1-C2-C3	-2.49	122.12	126.20
31	c	515	DGD	CDB-CCB-CBB	-2.49	101.80	114.37
33	a	613	LHG	C11-C10-C9	-2.49	101.80	114.37
32	m	102	STE	O2-C1-C2	2.49	121.86	114.00
25	b	601	CLA	O2D-CGD-CBD	2.49	115.58	111.23
25	b	615	CLA	CHB-C4A-NA	2.48	127.98	124.40
30	D	408	SQD	C1-C2-C3	-2.48	104.79	110.01
25	B	601	CLA	CAA-CBA-CGA	-2.48	106.17	113.21
25	c	504	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
29	c	522	LMG	C38-C37-C36	-2.48	101.83	114.37
25	c	511	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
25	b	609	CLA	CHB-C4A-NA	2.48	127.98	124.40
25	C	505	CLA	CHB-C4A-NA	2.48	127.98	124.40
25	c	513	CLA	O2A-CGA-O1A	-2.48	117.44	123.63
25	C	512	CLA	O2D-CGD-CBD	2.47	115.56	111.23
25	a	612	CLA	C3B-C4B-NB	-2.47	108.32	110.53
25	b	614	CLA	O2A-CGA-O1A	-2.47	117.45	123.63
31	c	515	DGD	O3E-C3E-C2E	-2.47	104.55	110.38
25	B	612	CLA	C11-C12-C13	-2.47	107.76	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	513	CLA	CMB-C2B-C3B	2.47	132.35	126.55
25	B	605	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
28	a	611	PL9	O2-C1-C2	-2.47	116.22	121.83
29	A	613	LMG	O8-C28-O10	-2.47	117.46	123.63
27	B	618	BCR	C27-C26-C25	2.47	126.03	122.70
25	B	612	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
25	c	512	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
25	C	511	CLA	CHB-C4A-NA	2.46	127.95	124.40
25	b	610	CLA	O1D-CGD-CBD	2.46	129.38	124.52
27	b	617	BCR	C29-C30-C25	2.46	114.01	110.44
25	B	603	CLA	CHD-C4C-NC	2.46	128.04	124.23
25	a	607	CLA	O2A-CGA-O1A	-2.46	117.48	123.63
27	c	514	BCR	C7-C8-C9	-2.45	122.60	126.23
30	A	614	SQD	O48-C23-C24	2.45	119.32	111.83
30	a	614	SQD	O8-S-C6	2.45	110.71	105.97
25	B	616	CLA	O2A-CGA-O1A	-2.45	117.49	123.63
25	B	605	CLA	CHC-C4B-NB	2.45	127.73	124.05
26	a	608	PHO	O2A-CGA-O1A	-2.45	117.49	123.63
29	b	622	LMG	O1-C1-C2	-2.45	104.55	108.27
25	C	508	CLA	CHD-C1D-C2D	2.45	130.58	125.49
25	b	607	CLA	CHC-C4B-NB	2.45	127.72	124.05
31	c	516	DGD	C1D-C2D-C3D	-2.45	104.87	110.01
25	C	507	CLA	C3B-C4B-NB	-2.44	108.35	110.53
25	D	403	CLA	CMB-C2B-C1B	-2.44	121.70	125.42
27	k	101	BCR	C15-C14-C13	-2.44	123.85	127.28
28	A	611	PL9	O2-C1-C2	-2.44	116.28	121.83
25	B	602	CLA	CAC-C3C-C4C	2.44	127.96	124.79
33	D	412	LHG	C18-C17-C16	-2.44	102.04	114.37
30	f	101	SQD	C1-O5-C5	-2.44	108.96	113.72
25	b	612	CLA	CHB-C4A-NA	2.44	127.92	124.40
25	b	603	CLA	O2A-CGA-O1A	-2.43	117.54	123.63
27	x	101	BCR	C11-C10-C9	-2.43	123.86	127.28
31	A	616	DGD	C1D-C2D-C3D	-2.43	104.89	110.01
25	b	606	CLA	CHC-C4B-NB	2.43	127.70	124.05
29	d	409	LMG	C38-C37-C36	-2.43	102.07	114.37
25	B	609	CLA	C7-C6-C5	-2.43	106.78	113.26
25	b	607	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
25	b	615	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
25	b	613	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
30	a	614	SQD	O7-S-C6	2.43	110.38	106.76
29	C	520	LMG	C40-C39-C38	-2.43	102.10	114.37
27	a	610	BCR	C33-C5-C6	-2.43	121.84	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	516	BCR	C33-C5-C6	-2.42	121.84	124.48
29	b	622	LMG	O1-C7-C8	-2.42	104.93	110.82
25	b	614	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
30	A	614	SQD	O47-C7-O49	-2.42	118.05	123.70
29	d	410	LMG	O2-C2-C1	-2.42	104.31	110.08
27	H	101	BCR	C2-C1-C6	2.42	113.95	110.44
29	d	409	LMG	C40-C39-C38	-2.42	102.15	114.37
31	h	101	DGD	O6E-C5E-C4E	2.42	114.05	109.70
29	d	410	LMG	C40-C39-C38	-2.42	102.16	114.37
32	d	411	STE	O2-C1-C2	2.41	121.63	114.00
29	c	518	LMG	C40-C39-C38	-2.41	102.18	114.37
29	B	620	LMG	C38-C37-C36	-2.41	102.19	114.37
25	B	606	CLA	O2A-CGA-O1A	-2.41	117.60	123.63
25	D	404	CLA	CHB-C4A-NA	2.41	127.87	124.40
29	c	522	LMG	C40-C39-C38	-2.41	102.21	114.37
25	b	608	CLA	CHB-C1B-NB	2.40	127.65	124.05
35	e	101	HEM	CHD-C4C-NC	2.40	127.07	124.45
31	A	616	DGD	C4E-C3E-C2E	-2.40	106.61	110.83
25	B	615	CLA	CHD-C1D-ND	-2.40	121.42	124.80
26	a	608	PHO	OBD-CAD-CBD	-2.40	122.30	125.82
25	C	512	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
25	b	613	CLA	CHA-C1A-NA	-2.40	120.96	126.39
25	C	509	CLA	CMB-C2B-C1B	-2.40	121.77	125.42
33	d	407	LHG	C11-C10-C9	-2.39	102.26	114.37
25	B	609	CLA	C1-C2-C3	-2.39	122.28	126.20
29	B	620	LMG	C1-O6-C5	-2.39	109.05	113.72
33	E	101	LHG	C11-C10-C9	-2.39	102.29	114.37
25	b	613	CLA	CHC-C4B-NB	2.39	127.63	124.05
29	C	520	LMG	C1-O6-C5	-2.39	109.06	113.72
25	c	509	CLA	O1D-CGD-CBD	2.39	129.22	124.52
25	B	603	CLA	CHB-C1B-NB	2.38	127.63	124.05
25	c	507	CLA	O2A-CGA-O1A	-2.38	117.66	123.63
32	B	627	STE	C3-C2-C1	-2.38	108.29	114.51
27	b	618	BCR	C11-C10-C9	-2.38	123.94	127.28
25	b	613	CLA	CHB-C1B-NB	2.38	127.62	124.05
33	d	407	LHG	C18-C17-C16	-2.38	102.33	114.37
25	b	611	CLA	CHB-C4A-NA	2.38	127.83	124.40
25	A	609	CLA	O2A-CGA-O1A	-2.37	117.69	123.63
25	B	601	CLA	O1D-CGD-CBD	2.37	129.20	124.52
29	c	520	LMG	C40-C39-C38	-2.37	102.37	114.37
25	C	501	CLA	CHB-C4A-NA	2.37	127.82	124.40
35	e	101	HEM	CAB-C3B-C2B	-2.37	120.72	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	608	CLA	C3B-C4B-NB	-2.37	108.41	110.53
25	C	502	CLA	CHB-C1B-NB	2.37	127.60	124.05
25	B	610	CLA	O2D-CGD-CBD	2.37	115.37	111.23
31	h	101	DGD	CBB-CAB-C9B	-2.37	102.40	114.37
25	c	501	CLA	O2A-CGA-O1A	-2.37	117.71	123.63
25	b	616	CLA	CMB-C2B-C3B	2.37	132.11	126.55
28	A	611	PL9	C27-C28-C29	-2.36	122.21	127.62
25	c	502	CLA	CHD-C1D-ND	-2.36	121.48	124.80
25	b	608	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
33	D	409	LHG	C27-C26-C25	-2.36	102.45	114.37
25	B	610	CLA	CHD-C1D-ND	-2.36	121.49	124.80
25	a	606	CLA	CHB-C4A-NA	2.36	127.80	124.40
31	H	102	DGD	O1G-C1A-O1A	-2.36	117.74	123.63
25	D	404	CLA	O2D-CGD-CBD	2.36	115.35	111.23
35	e	101	HEM	C3B-C4B-NB	-2.35	107.78	109.47
30	a	615	SQD	C9-C8-C7	-2.35	105.07	113.69
26	a	608	PHO	C2B-C1B-NB	-2.35	107.73	109.43
32	m	102	STE	C3-C2-C1	-2.35	108.37	114.51
25	b	616	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
29	B	620	LMG	O2-C2-C1	-2.35	104.48	110.08
31	a	616	DGD	C8B-C7B-C6B	-2.35	102.50	114.37
25	b	611	CLA	C3B-C4B-NB	-2.35	108.44	110.53
26	A	608	PHO	C1-C2-C3	-2.34	122.36	126.20
25	A	607	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
27	C	514	BCR	C33-C5-C6	-2.34	121.93	124.48
25	C	510	CLA	C11-C12-C13	-2.34	108.20	115.97
27	B	617	BCR	C3-C4-C5	-2.33	109.90	114.06
25	B	608	CLA	CMB-C2B-C3B	2.33	132.03	126.55
27	k	102	BCR	C24-C23-C22	-2.33	122.79	126.23
28	A	611	PL9	C36-C34-C33	-2.33	115.94	121.17
33	e	102	LHG	C11-C10-C9	-2.33	102.61	114.37
25	D	403	CLA	CED-O2D-CGD	2.33	121.19	115.92
25	b	604	CLA	O2A-CGA-O1A	-2.32	117.81	123.63
25	c	503	CLA	CHB-C4A-NA	2.32	127.75	124.40
25	c	507	CLA	C2A-C1A-CHA	2.32	127.90	123.87
25	a	607	CLA	O2D-CGD-CBD	2.32	115.29	111.23
25	d	403	CLA	C3B-C4B-NB	-2.32	108.46	110.53
33	E	101	LHG	C20-C19-C18	-2.32	102.63	114.37
33	e	102	LHG	C20-C19-C18	-2.32	102.63	114.37
29	m	101	LMG	C38-C37-C36	-2.32	102.64	114.37
25	b	605	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
25	B	613	CLA	O2D-CGD-O1D	-2.32	119.33	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	404	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
25	A	609	CLA	CHD-C4C-NC	2.32	127.82	124.23
31	C	517	DGD	CBB-CAB-C9B	-2.32	102.66	114.37
31	C	518	DGD	O5D-C6D-C5D	-2.31	104.20	109.42
25	c	503	CLA	O2D-CGD-O1D	-2.31	119.34	123.85
32	j	101	STE	O2-C1-C2	2.31	121.31	114.00
28	A	611	PL9	C20-C19-C21	2.31	119.24	115.23
25	C	508	CLA	CMB-C2B-C3B	2.31	131.99	126.55
29	m	101	LMG	C40-C39-C38	-2.31	102.68	114.37
25	B	615	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
29	D	411	LMG	O7-C10-O9	-2.31	118.31	123.70
25	B	614	CLA	O2D-CGD-CBD	2.31	115.27	111.23
25	D	403	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
27	k	103	BCR	C33-C5-C6	-2.31	121.97	124.48
29	m	101	LMG	O1-C7-C8	-2.31	105.21	110.82
33	D	409	LHG	O8-C23-O10	-2.31	117.86	123.63
29	D	407	LMG	O2-C2-C1	-2.31	104.58	110.08
25	C	502	CLA	CHA-C1A-NA	-2.30	121.17	126.39
31	A	616	DGD	O2D-C2D-C1D	-2.30	104.58	110.08
33	l	101	LHG	C11-C10-C9	-2.30	102.73	114.37
25	b	606	CLA	C3B-C4B-NB	-2.30	108.47	110.53
30	b	620	SQD	O8-S-C6	2.30	110.41	105.97
29	c	522	LMG	O6-C1-O1	-2.30	104.61	110.04
31	c	515	DGD	O5D-C6D-C5D	-2.30	104.24	109.42
31	A	616	DGD	O6D-C1D-O3G	-2.29	104.62	110.04
29	m	101	LMG	O7-C10-O9	-2.29	118.35	123.70
25	C	509	CLA	CMB-C2B-C3B	2.29	131.94	126.55
25	B	607	CLA	CMB-C2B-C3B	2.29	131.94	126.55
25	C	511	CLA	C1-C2-C3	-2.29	122.45	126.20
27	B	617	BCR	C11-C10-C9	-2.29	124.07	127.28
26	d	402	PHO	O2D-CGD-O1D	-2.28	119.40	123.85
25	b	602	CLA	C1-C2-C3	-2.28	122.46	126.20
25	b	603	CLA	CMB-C2B-C3B	2.28	131.92	126.55
33	B	623	LHG	C20-C19-C18	-2.28	102.84	114.37
25	B	605	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
32	B	628	STE	O2-C1-C2	2.28	121.19	114.00
33	E	101	LHG	C27-C26-C25	-2.28	102.86	114.37
25	B	601	CLA	C2A-C1A-CHA	2.28	127.82	123.87
26	a	608	PHO	CMA-C3A-C4A	-2.27	109.71	114.61
31	c	515	DGD	CBB-CAB-C9B	-2.27	102.88	114.37
32	E	102	STE	O2-C1-C2	2.27	121.17	114.00
31	a	616	DGD	CFB-CEB-CDB	-2.27	102.92	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	606	CLA	CMB-C2B-C1B	-2.26	121.97	125.42
25	b	610	CLA	CAA-C2A-C3A	-2.26	106.89	113.00
29	b	622	LMG	C8-O7-C10	2.26	123.20	117.80
27	b	617	BCR	C35-C13-C14	-2.26	119.16	122.82
31	h	101	DGD	O6E-C5E-C6E	-2.25	100.86	106.44
28	a	611	PL9	C20-C19-C21	2.25	119.14	115.23
25	d	403	CLA	C4-C3-C5	2.25	119.14	115.23
25	b	611	CLA	C7-C6-C5	-2.25	107.27	113.26
26	a	608	PHO	O2D-CGD-O1D	-2.25	119.47	123.85
31	a	616	DGD	C5B-C4B-C3B	-2.25	103.00	114.37
25	b	603	CLA	CHD-C1D-ND	-2.25	121.64	124.80
25	B	607	CLA	O2D-CGD-O1D	-2.24	119.48	123.85
29	B	622	LMG	C38-C37-C36	-2.24	103.02	114.37
33	D	410	LHG	C27-C26-C25	-2.24	103.04	114.37
25	a	606	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
25	B	612	CLA	CHD-C1D-ND	-2.24	121.65	124.80
25	b	607	CLA	CHB-C4A-NA	2.24	127.63	124.40
27	k	101	BCR	C11-C10-C9	-2.24	124.14	127.28
31	C	519	DGD	CBB-CAB-C9B	-2.24	103.06	114.37
29	m	101	LMG	O6-C1-O1	-2.24	104.76	110.04
31	c	517	DGD	C8B-C7B-C6B	-2.24	103.07	114.37
29	b	622	LMG	C40-C39-C38	-2.24	103.07	114.37
25	a	612	CLA	CHC-C4B-NB	2.23	127.40	124.05
27	d	405	BCR	C1-C6-C5	-2.23	119.58	122.64
25	B	608	CLA	CHB-C1B-NB	2.23	127.39	124.05
25	C	506	CLA	O1D-CGD-CBD	2.23	128.91	124.52
27	k	101	BCR	C24-C23-C22	-2.23	122.94	126.23
25	c	501	CLA	CMB-C2B-C1B	-2.22	122.03	125.42
25	b	613	CLA	O2D-CGD-CBD	2.22	115.12	111.23
27	t	101	BCR	C15-C14-C13	-2.22	124.16	127.28
31	h	101	DGD	O6D-C1D-O3G	-2.22	104.79	110.04
29	c	520	LMG	O3-C3-C2	-2.22	105.14	110.38
36	v	201	HEC	CHB-C1B-NB	2.22	126.81	124.42
25	b	615	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
27	T	101	BCR	C2-C1-C6	2.22	113.66	110.44
25	b	614	CLA	CHD-C1D-ND	-2.22	121.68	124.80
25	c	503	CLA	C11-C12-C13	-2.22	108.60	115.97
25	B	608	CLA	O2D-CGD-CBD	2.22	115.10	111.23
29	B	620	LMG	O7-C10-O9	-2.22	118.53	123.70
25	c	504	CLA	C3B-C4B-NB	-2.21	108.55	110.53
25	B	613	CLA	CHB-C4A-NA	2.21	127.59	124.40
25	B	605	CLA	CHB-C4A-NA	2.21	127.59	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	616	DGD	C3E-C4E-C5E	-2.21	106.22	110.23
31	h	101	DGD	C7B-C6B-C5B	-2.21	103.20	114.37
27	d	405	BCR	C30-C25-C26	-2.21	119.62	122.64
25	c	510	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
27	c	514	BCR	C2-C1-C6	2.21	113.65	110.44
25	A	607	CLA	O2D-CGD-CBD	2.21	115.09	111.23
36	V	201	HEC	C1D-C2D-C3D	-2.21	104.66	106.98
30	a	614	SQD	C44-O6-C1	-2.21	109.07	113.80
29	C	520	LMG	C38-C37-C36	-2.21	103.22	114.37
25	D	403	CLA	C1-C2-C3	-2.21	122.58	126.20
25	C	503	CLA	CHC-C4B-NB	2.20	127.36	124.05
25	C	504	CLA	CHD-C1D-ND	-2.20	121.70	124.80
29	C	520	LMG	O8-C28-O10	-2.20	118.12	123.63
25	C	502	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
25	B	604	CLA	O2D-CGD-CBD	2.20	115.08	111.23
25	A	606	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
33	d	407	LHG	C20-C19-C18	-2.20	103.24	114.37
25	c	504	CLA	O2D-CGD-CBD	2.20	115.08	111.23
33	D	410	LHG	C18-C17-C16	-2.20	103.25	114.37
29	c	522	LMG	O7-C10-O9	-2.20	118.56	123.70
25	A	607	CLA	C1D-ND-C4D	2.20	107.86	106.31
25	C	506	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
25	D	403	CLA	CMB-C2B-C3B	2.20	131.72	126.55
28	a	611	PL9	C7-C8-C9	-2.20	123.04	126.83
27	B	617	BCR	C33-C5-C6	-2.20	122.09	124.48
25	C	505	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
25	C	504	CLA	CHB-C4A-NA	2.19	127.57	124.40
25	C	504	CLA	CHD-C4C-NC	2.19	127.63	124.23
25	b	604	CLA	O2D-CGD-CBD	2.19	115.06	111.23
27	K	101	BCR	C27-C26-C25	2.19	125.66	122.70
29	c	518	LMG	O1-C7-C8	-2.19	105.50	110.82
36	V	201	HEC	CMC-C2C-C1C	-2.19	122.09	125.42
25	C	502	CLA	CHD-C1D-ND	-2.19	121.73	124.80
25	a	609	CLA	CAA-CBA-CGA	-2.19	107.00	113.21
31	c	515	DGD	O1G-C1A-C2A	-2.18	105.18	111.83
31	c	516	DGD	C5B-C4B-C3B	-2.18	103.36	114.37
25	b	611	CLA	CMB-C2B-C3B	2.18	131.67	126.55
30	a	614	SQD	O5-C1-C2	-2.18	105.89	110.37
26	a	608	PHO	O1D-CGD-CBD	2.18	128.03	124.72
29	c	518	LMG	C38-C37-C36	-2.17	103.38	114.37
25	b	612	CLA	O2D-CGD-CBD	2.17	115.03	111.23
25	D	403	CLA	C4-C3-C5	2.17	119.00	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	406	PL9	O2-C1-C2	-2.17	116.89	121.83
25	b	602	CLA	O2D-CGD-CBD	2.17	115.02	111.23
33	D	409	LHG	C18-C17-C16	-2.17	103.41	114.37
25	C	504	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
25	C	505	CLA	O1D-CGD-CBD	2.17	128.79	124.52
31	C	517	DGD	CAB-C9B-C8B	-2.17	103.41	114.37
31	c	517	DGD	CBB-CAB-C9B	-2.16	103.43	114.37
31	C	517	DGD	C6B-C5B-C4B	-2.16	103.44	114.37
25	A	612	CLA	CMB-C2B-C3B	2.16	131.63	126.55
32	b	624	STE	C3-C2-C1	-2.16	108.87	114.51
29	c	522	LMG	C1-O6-C5	-2.16	109.50	113.72
29	d	410	LMG	C38-C37-C36	-2.16	103.46	114.37
31	C	518	DGD	C1D-C2D-C3D	-2.16	105.47	110.01
25	c	510	CLA	O2D-CGD-O1D	-2.16	119.65	123.85
25	b	613	CLA	C7-C6-C5	-2.16	107.51	113.26
32	C	521	STE	O2-C1-C2	2.16	120.81	114.00
29	b	622	LMG	C42-C41-C40	-2.16	103.47	114.37
25	A	606	CLA	CAA-CBA-CGA	-2.16	107.09	113.21
27	k	101	BCR	C38-C26-C25	-2.16	122.13	124.48
25	d	403	CLA	C1-C2-C3	-2.16	122.67	126.20
27	H	101	BCR	C16-C17-C18	-2.15	124.26	127.28
27	b	618	BCR	C30-C25-C26	-2.15	119.69	122.64
31	A	616	DGD	CBB-CAB-C9B	-2.15	103.48	114.37
25	b	604	CLA	C6-C7-C8	-2.15	108.81	115.97
33	E	101	LHG	C18-C17-C16	-2.15	103.48	114.37
25	a	612	CLA	CBC-CAC-C3C	-2.15	106.58	112.42
27	b	618	BCR	C8-C7-C6	-2.15	121.25	127.00
29	C	520	LMG	O3-C3-C2	-2.15	105.30	110.38
28	d	406	PL9	C8-C7-C3	2.15	117.59	112.03
25	c	501	CLA	CMB-C2B-C3B	2.15	131.60	126.55
33	e	102	LHG	C18-C17-C16	-2.15	103.50	114.37
25	c	501	CLA	C3B-C4B-NB	-2.15	108.61	110.53
31	C	518	DGD	CAB-C9B-C8B	-2.15	103.52	114.37
25	B	602	CLA	CMB-C2B-C3B	2.15	131.60	126.55
25	B	604	CLA	CHC-C4B-NB	2.15	127.27	124.05
27	C	515	BCR	C2-C1-C6	2.15	113.56	110.44
31	c	517	DGD	CAB-C9B-C8B	-2.15	103.52	114.37
25	b	601	CLA	CHD-C1D-ND	-2.14	121.78	124.80
27	c	514	BCR	C35-C13-C14	-2.14	119.34	122.82
25	b	611	CLA	CHD-C1D-ND	-2.14	121.79	124.80
27	b	617	BCR	C33-C5-C6	-2.14	122.15	124.48
27	K	101	BCR	C2-C1-C6	2.14	113.55	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	509	CLA	C1-O2A-CGA	-2.14	111.47	116.65
27	k	101	BCR	C33-C5-C6	-2.14	122.15	124.48
27	B	618	BCR	C3-C4-C5	-2.14	110.24	114.06
25	D	403	CLA	CHB-C4A-NA	2.14	127.48	124.40
28	d	406	PL9	C36-C34-C33	-2.14	116.37	121.17
27	K	101	BCR	C24-C23-C22	-2.14	123.07	126.23
29	m	101	LMG	C9-C8-C7	-2.14	106.80	111.78
25	a	609	CLA	CMD-C2D-C3D	2.14	132.59	127.69
25	c	504	CLA	CMB-C2B-C3B	2.13	131.57	126.55
25	C	505	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
31	H	102	DGD	O6E-C5E-C4E	2.13	113.54	109.70
25	D	404	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
26	A	608	PHO	O1D-CGD-CBD	2.13	127.95	124.72
28	d	406	PL9	C42-C43-C44	-2.13	122.75	127.62
31	h	101	DGD	O5D-C1E-C2E	2.13	111.50	108.27
33	D	409	LHG	C11-C10-C9	-2.13	103.62	114.37
30	B	624	SQD	O8-S-C6	2.13	110.08	105.97
33	d	407	LHG	O8-C23-O10	-2.13	118.31	123.63
25	C	508	CLA	O2D-CGD-CBD	2.13	114.94	111.23
31	c	516	DGD	O2D-C2D-C1D	-2.12	105.01	110.08
25	C	508	CLA	C1-C2-C3	-2.12	122.72	126.20
28	D	406	PL9	O2-C1-C2	-2.12	117.00	121.83
27	T	101	BCR	C31-C1-C6	2.12	113.57	110.24
25	b	608	CLA	O2D-CGD-CBD	2.12	114.94	111.23
32	B	625	STE	O2-C1-C2	2.12	120.70	114.00
36	V	201	HEC	CAD-CBD-CGD	-2.12	108.04	113.67
25	c	501	CLA	O2D-CGD-CBD	2.12	114.94	111.23
28	D	406	PL9	C8-C7-C3	2.12	117.51	112.03
25	c	502	CLA	CHB-C4A-NA	2.12	127.46	124.40
27	x	101	BCR	C35-C13-C14	-2.12	119.38	122.82
31	A	616	DGD	CAB-C9B-C8B	-2.12	103.67	114.37
31	H	102	DGD	CBB-CAB-C9B	-2.12	103.67	114.37
29	D	407	LMG	C40-C39-C38	-2.12	103.67	114.37
29	d	410	LMG	O1-C7-C8	-2.12	105.67	110.82
25	c	506	CLA	C1-C2-C3	-2.12	122.73	126.20
36	v	201	HEC	CBA-CAA-C2A	-2.12	106.68	112.53
25	c	507	CLA	CHC-C4B-NB	2.12	127.22	124.05
30	b	620	SQD	O9-S-C6	2.11	109.91	106.76
29	D	407	LMG	C38-C37-C36	-2.11	103.68	114.37
27	D	405	BCR	C38-C26-C25	-2.11	122.18	124.48
25	C	507	CLA	C2A-C1A-CHA	2.11	127.53	123.87
25	D	404	CLA	CMB-C2B-C3B	2.11	131.52	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	603	CLA	CMB-C2B-C3B	2.11	131.52	126.55
31	c	516	DGD	C8B-C7B-C6B	-2.11	103.69	114.37
32	B	625	STE	C3-C2-C1	-2.11	109.00	114.51
27	d	405	BCR	C33-C5-C6	-2.11	122.18	124.48
29	d	410	LMG	O3-C3-C2	-2.11	105.40	110.38
25	b	615	CLA	CHD-C4C-NC	2.11	127.50	124.23
31	C	518	DGD	CBB-CAB-C9B	-2.11	103.71	114.37
25	c	511	CLA	C1-C2-C3	-2.11	122.74	126.20
30	f	101	SQD	C1-C2-C3	-2.11	105.58	110.01
29	D	407	LMG	O3-C3-C2	-2.11	105.41	110.38
25	b	608	CLA	CHD-C4C-NC	2.11	127.50	124.23
31	H	102	DGD	C8B-C7B-C6B	-2.11	103.72	114.37
25	c	504	CLA	CHB-C4A-NA	2.11	127.44	124.40
29	c	520	LMG	C38-C37-C36	-2.10	103.74	114.37
25	C	510	CLA	CMB-C2B-C3B	2.10	131.49	126.55
31	C	517	DGD	C3D-C4D-C5D	-2.10	106.42	110.23
31	A	616	DGD	O5D-C6D-C5D	-2.10	104.69	109.42
31	a	616	DGD	C1G-C2G-C3G	-2.10	106.95	111.80
33	l	101	LHG	C18-C17-C16	-2.10	103.76	114.37
31	h	101	DGD	C6D-C5D-C4D	2.10	116.47	112.07
25	c	505	CLA	CHB-C4A-NA	2.10	127.43	124.40
25	B	609	CLA	CHC-C4B-NB	2.10	127.19	124.05
25	a	606	CLA	C7-C6-C5	-2.10	107.68	113.26
32	C	522	STE	O2-C1-C2	2.09	120.62	114.00
25	B	603	CLA	O2D-CGD-CBD	2.09	114.89	111.23
33	l	101	LHG	C20-C19-C18	-2.09	103.79	114.37
25	b	604	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
30	A	614	SQD	O6-C44-C45	-2.09	105.73	110.82
25	B	604	CLA	CHA-C4D-ND	2.09	136.86	132.55
27	T	101	BCR	C1-C6-C5	-2.09	119.78	122.64
25	c	505	CLA	O2D-CGD-CBD	2.09	114.88	111.23
25	B	604	CLA	C1-O2A-CGA	-2.09	111.60	116.65
36	V	201	HEC	CMC-C2C-C3C	2.08	130.04	125.62
25	b	607	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
25	B	608	CLA	CHB-C4A-NA	2.08	127.41	124.40
28	a	611	PL9	C35-C34-C36	2.08	118.84	115.23
27	H	101	BCR	C35-C13-C12	2.08	121.27	118.09
25	B	603	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
29	c	520	LMG	C9-C8-C7	-2.08	106.93	111.78
29	c	518	LMG	O8-C28-O10	-2.08	118.42	123.63
25	C	507	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
25	c	502	CLA	O1D-CGD-CBD	2.08	128.61	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	613	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
25	C	513	CLA	O1D-CGD-CBD	2.08	128.61	124.52
25	B	602	CLA	CHA-C4D-ND	2.08	136.83	132.55
28	d	406	PL9	C32-C33-C34	-2.07	122.88	127.62
25	c	509	CLA	O2A-CGA-CBA	2.07	118.16	111.83
25	b	615	CLA	CHA-C4D-ND	2.07	136.83	132.55
31	C	518	DGD	C5B-C4B-C3B	-2.07	103.89	114.37
25	A	607	CLA	CHB-C4A-NA	2.07	127.39	124.40
25	c	512	CLA	CHD-C1D-ND	-2.07	121.89	124.80
31	H	102	DGD	C1E-O6E-C5E	2.07	117.76	113.72
27	b	619	BCR	C2-C1-C6	2.07	113.44	110.44
33	D	412	LHG	C15-C14-C13	-2.07	103.93	114.37
25	B	612	CLA	O2D-CGD-CBD	2.06	114.84	111.23
27	T	101	BCR	C1-C6-C7	2.06	121.25	115.65
36	V	201	HEC	CHA-C4D-ND	2.06	126.64	124.42
25	b	609	CLA	CED-O2D-CGD	2.06	120.59	115.92
25	a	612	CLA	CHB-C4A-NA	2.06	127.38	124.40
27	T	101	BCR	C30-C25-C26	-2.06	119.82	122.64
25	c	513	CLA	C1-C2-C3	-2.06	122.82	126.20
33	e	102	LHG	C27-C26-C25	-2.06	103.97	114.37
33	d	408	LHG	C27-C26-C25	-2.06	103.97	114.37
25	C	512	CLA	CHD-C1D-ND	-2.06	121.91	124.80
29	c	522	LMG	O8-C28-O10	-2.06	118.48	123.63
25	B	616	CLA	O2D-CGD-CBD	2.06	114.82	111.23
25	b	603	CLA	CHC-C4B-NB	2.05	127.13	124.05
25	C	505	CLA	CMB-C2B-C3B	2.05	131.38	126.55
25	d	404	CLA	CHA-C1A-NA	-2.05	121.74	126.39
29	A	613	LMG	O1-C7-C8	-2.05	105.82	110.82
29	c	520	LMG	C42-C41-C40	-2.05	104.00	114.37
25	b	612	CLA	CHB-C1B-NB	2.05	127.13	124.05
27	D	405	BCR	C33-C5-C6	-2.05	122.25	124.48
27	t	101	BCR	C30-C25-C26	-2.05	119.83	122.64
25	C	509	CLA	C1-C2-C3	-2.05	122.84	126.20
30	D	408	SQD	C3-C4-C5	2.05	113.95	110.23
31	h	101	DGD	C1E-O6E-C5E	2.05	117.72	113.72
27	T	101	BCR	C4-C5-C6	2.05	125.47	122.70
25	B	609	CLA	C16-C15-C13	-2.05	109.16	115.97
33	a	613	LHG	O8-C6-C5	-2.05	102.50	108.40
25	c	502	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
31	c	515	DGD	C1D-C2D-C3D	-2.05	105.70	110.01
31	c	516	DGD	CBB-CAB-C9B	-2.05	104.03	114.37
31	A	616	DGD	C7A-C6A-C5A	-2.05	104.03	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	608	CLA	C1D-ND-C4D	2.05	107.75	106.31
27	x	101	BCR	C3-C4-C5	-2.04	110.41	114.06
25	a	606	CLA	O1D-CGD-CBD	2.04	128.55	124.52
33	a	613	LHG	C20-C19-C18	-2.04	104.04	114.37
27	B	617	BCR	C15-C16-C17	-2.04	119.34	123.52
25	C	507	CLA	CHC-C4B-NB	2.04	127.11	124.05
31	h	101	DGD	O3E-C3E-C2E	-2.04	105.56	110.38
31	c	516	DGD	C3E-C4E-C5E	-2.04	106.53	110.23
33	B	623	LHG	C27-C26-C25	-2.04	104.05	114.37
26	d	402	PHO	C1A-C2A-C3A	-2.04	100.90	102.84
29	B	620	LMG	C22-C21-C20	-2.04	104.06	114.37
25	c	507	CLA	CHA-C1A-NA	-2.04	121.78	126.39
25	b	604	CLA	CMB-C2B-C3B	2.04	131.34	126.55
25	b	616	CLA	CHD-C1D-ND	-2.04	121.94	124.80
28	A	611	PL9	C12-C13-C14	-2.03	122.97	127.62
25	B	613	CLA	CMB-C2B-C3B	2.03	131.34	126.55
25	a	606	CLA	CMB-C2B-C1B	-2.03	122.32	125.42
25	b	604	CLA	C11-C12-C13	-2.03	109.21	115.97
25	C	511	CLA	CHD-C4C-NC	2.03	127.38	124.23
29	b	622	LMG	O5-C6-C5	-2.03	104.41	111.33
33	a	613	LHG	C18-C17-C16	-2.03	104.10	114.37
31	C	519	DGD	CAB-C9B-C8B	-2.03	104.10	114.37
32	j	101	STE	C3-C2-C1	-2.03	109.21	114.51
25	B	611	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
27	x	101	BCR	C16-C15-C14	-2.03	119.37	123.52
29	B	620	LMG	O1-C7-C8	-2.03	105.88	110.82
27	C	516	BCR	C8-C7-C6	-2.03	121.58	127.00
28	D	406	PL9	C36-C34-C33	-2.03	116.61	121.17
29	C	520	LMG	O2-C2-C1	-2.03	105.24	110.08
27	K	101	BCR	C15-C14-C13	-2.03	124.44	127.28
31	H	102	DGD	C1D-C2D-C3D	-2.03	105.75	110.01
25	a	612	CLA	CMB-C2B-C3B	2.03	131.31	126.55
26	D	402	PHO	C3B-C4B-NB	-2.03	106.14	107.46
25	b	608	CLA	CHD-C1D-C2D	2.02	129.70	125.49
29	c	520	LMG	O2-C2-C1	-2.02	105.25	110.08
25	B	608	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
25	c	501	CLA	O1D-CGD-CBD	2.02	128.51	124.52
26	D	402	PHO	CBA-CAA-C2A	-2.02	107.82	113.78
25	b	615	CLA	CHD-C1D-ND	-2.02	121.96	124.80
25	B	607	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
25	B	613	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
36	v	201	HEC	CMC-C2C-C1C	-2.02	122.34	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	517	DGD	O2D-C2D-C1D	-2.02	105.26	110.08
25	b	605	CLA	CHA-C1A-NA	-2.02	121.82	126.39
27	k	103	BCR	C24-C23-C22	-2.02	123.25	126.23
31	C	519	DGD	C3G-C2G-C1G	-2.02	107.08	111.78
30	a	615	SQD	O49-C7-C8	-2.02	115.89	123.78
25	B	609	CLA	CHB-C4A-NA	2.02	127.31	124.40
25	B	616	CLA	CMB-C2B-C3B	2.02	131.29	126.55
27	B	619	BCR	C15-C14-C13	-2.01	124.46	127.28
25	B	605	CLA	C16-C15-C13	-2.01	109.28	115.97
26	A	608	PHO	O2A-CGA-O1A	-2.01	118.60	123.63
25	B	606	CLA	C1-C2-C3	-2.01	122.91	126.20
35	e	101	HEM	CHB-C1B-NB	2.01	126.85	124.37
33	d	408	LHG	O8-C23-O10	-2.01	118.61	123.63
29	b	622	LMG	C24-C23-C22	-2.01	104.23	114.37
31	H	102	DGD	CAB-C9B-C8B	-2.01	104.23	114.37
31	a	616	DGD	CBB-CAB-C9B	-2.01	104.23	114.37
25	d	403	CLA	CMA-C3A-C4A	-2.00	106.39	111.77
25	B	609	CLA	CHD-C1D-ND	-2.00	121.98	124.80
33	l	101	LHG	C27-C26-C25	-2.00	104.24	114.37
25	c	507	CLA	O2D-CGD-CBD	2.00	114.73	111.23
28	a	611	PL9	C27-C28-C29	-2.00	123.04	127.62
29	A	613	LMG	O7-C10-O9	-2.00	119.02	123.70
29	c	520	LMG	O8-C28-O10	-2.00	118.62	123.63
25	a	606	CLA	CHC-C4B-NB	2.00	127.05	124.05
31	h	101	DGD	CAB-C9B-C8B	-2.00	104.25	114.37
35	e	101	HEM	C1B-NB-C4B	2.00	107.58	105.21
36	V	201	HEC	CMD-C2D-C1D	2.00	128.16	125.03

All (2) chirality outliers are listed below:

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

All (1700) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	607	CLA	C2B-C3B-CAB-CBB
25	A	607	CLA	C4B-C3B-CAB-CBB
25	A	612	CLA	C14-C13-C15-C16
25	B	601	CLA	C1A-C2A-CAA-CBA
25	B	614	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	B	614	CLA	CAD-CBD-CGD-O2D
25	C	502	CLA	C14-C13-C15-C16
25	C	507	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O2D
25	C	507	CLA	C11-C10-C8-C9
25	C	509	CLA	CHA-CBD-CGD-O2D
25	C	512	CLA	C2B-C3B-CAB-CBB
25	C	512	CLA	C4B-C3B-CAB-CBB
25	C	512	CLA	C6-C7-C8-C9
25	a	607	CLA	C2B-C3B-CAB-CBB
25	a	607	CLA	C4B-C3B-CAB-CBB
25	b	601	CLA	C1A-C2A-CAA-CBA
25	b	606	CLA	C14-C13-C15-C16
25	b	614	CLA	CAD-CBD-CGD-O1D
25	b	614	CLA	CAD-CBD-CGD-O2D
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	502	CLA	CAD-CBD-CGD-O2D
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O2D
25	c	512	CLA	C6-C7-C8-C9
27	C	515	BCR	C11-C12-C13-C14
27	C	516	BCR	C5-C6-C7-C8
27	C	516	BCR	C20-C21-C22-C37
27	C	516	BCR	C37-C22-C23-C24
27	D	405	BCR	C37-C22-C23-C24
27	d	405	BCR	C20-C21-C22-C37
27	d	405	BCR	C37-C22-C23-C24
27	d	405	BCR	C22-C23-C24-C25
27	k	102	BCR	C5-C6-C7-C8
27	t	101	BCR	C7-C8-C9-C34
28	A	611	PL9	C22-C23-C24-C25
28	A	611	PL9	C22-C23-C24-C26
28	A	611	PL9	C37-C38-C39-C40
28	A	611	PL9	C37-C38-C39-C41
28	D	406	PL9	C32-C33-C34-C36
28	D	406	PL9	C47-C48-C49-C51
28	a	611	PL9	C22-C23-C24-C25
28	a	611	PL9	C32-C33-C34-C35
28	a	611	PL9	C32-C33-C34-C36
28	d	406	PL9	C32-C33-C34-C35
28	d	406	PL9	C32-C33-C34-C36
28	d	406	PL9	C42-C43-C44-C46

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Mol	Chain	Res	Type	Atoms
29	A	613	LMG	O6-C1-O1-C7
29	A	613	LMG	O9-C10-O7-C8
29	D	411	LMG	C11-C10-O7-C8
29	c	522	LMG	O6-C1-O1-C7
30	B	624	SQD	O6-C44-C45-O47
30	B	624	SQD	O49-C7-O47-C45
30	B	624	SQD	C8-C7-O47-C45
30	D	408	SQD	C45-C44-O6-C1
30	a	614	SQD	O6-C44-C45-O47
30	a	615	SQD	O47-C45-C46-O48
30	a	615	SQD	O49-C7-O47-C45
30	f	101	SQD	C2-C1-O6-C44
30	f	101	SQD	O5-C1-O6-C44
30	f	101	SQD	C8-C7-O47-C45
31	A	616	DGD	C2B-C1B-O2G-C2G
31	A	616	DGD	O1B-C1B-O2G-C2G
31	A	616	DGD	O2G-C2G-C3G-O3G
31	a	616	DGD	C2B-C1B-O2G-C2G
33	B	623	LHG	C4-O6-P-O3
33	B	623	LHG	C4-O6-P-O4
33	B	623	LHG	C4-O6-P-O5
33	D	409	LHG	C3-O3-P-O5
33	D	409	LHG	C3-O3-P-O6
33	D	409	LHG	C4-O6-P-O3
33	D	409	LHG	C4-O6-P-O4
33	D	410	LHG	C3-O3-P-O5
33	D	410	LHG	C3-O3-P-O6
33	D	412	LHG	C3-O3-P-O4
33	a	613	LHG	O1-C1-C2-C3
33	a	613	LHG	C3-O3-P-O4
33	a	613	LHG	C3-O3-P-O5
33	a	613	LHG	C3-O3-P-O6
33	d	407	LHG	C4-O6-P-O3
33	d	407	LHG	C4-O6-P-O4
33	d	408	LHG	C4-O6-P-O4
33	e	102	LHG	O1-C1-C2-C3
33	e	102	LHG	C1-C2-C3-O3
33	e	102	LHG	C3-O3-P-O4
33	e	102	LHG	O10-C23-O8-C6
33	e	102	LHG	C24-C23-O8-C6
33	l	101	LHG	C4-O6-P-O3
33	l	101	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
33	l	101	LHG	C4-O6-P-O5
25	b	601	CLA	O1D-CGD-O2D-CED
25	B	601	CLA	CBD-CGD-O2D-CED
25	b	601	CLA	CBD-CGD-O2D-CED
29	c	522	LMG	O10-C28-O8-C9
30	b	620	SQD	O10-C23-O48-C46
30	f	101	SQD	O10-C23-O48-C46
28	D	406	PL9	C47-C48-C49-C50
28	a	611	PL9	C47-C48-C49-C51
29	c	520	LMG	C29-C28-O8-C9
30	b	620	SQD	C24-C23-O48-C46
29	B	620	LMG	O10-C28-O8-C9
29	c	520	LMG	O10-C28-O8-C9
33	E	101	LHG	O10-C23-O8-C6
25	B	601	CLA	O1D-CGD-O2D-CED
29	D	411	LMG	O9-C10-O7-C8
29	c	520	LMG	O9-C10-O7-C8
30	f	101	SQD	O49-C7-O47-C45
31	a	616	DGD	O1B-C1B-O2G-C2G
25	A	609	CLA	C3-C5-C6-C7
25	b	614	CLA	C3-C5-C6-C7
25	C	513	CLA	CBA-CGA-O2A-C1
29	c	522	LMG	C29-C28-O8-C9
30	f	101	SQD	C24-C23-O48-C46
33	E	101	LHG	C24-C23-O8-C6
25	c	513	CLA	CBD-CGD-O2D-CED
29	A	613	LMG	C11-C10-O7-C8
29	c	520	LMG	C11-C10-O7-C8
30	a	615	SQD	C8-C7-O47-C45
25	B	614	CLA	C4-C3-C5-C6
25	C	504	CLA	C4-C3-C5-C6
25	C	513	CLA	C4-C3-C5-C6
25	b	603	CLA	C4-C3-C5-C6
25	b	604	CLA	C4-C3-C5-C6
25	b	614	CLA	C4-C3-C5-C6
25	c	507	CLA	C4-C3-C5-C6
25	c	513	CLA	C4-C3-C5-C6
28	A	611	PL9	C35-C34-C36-C37
28	A	611	PL9	C40-C39-C41-C42
28	a	611	PL9	C35-C34-C36-C37
25	C	513	CLA	C2-C3-C5-C6
25	b	603	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	b	604	CLA	C2-C3-C5-C6
25	b	614	CLA	C2-C3-C5-C6
25	c	507	CLA	C2-C3-C5-C6
28	A	611	PL9	C38-C39-C41-C42
28	a	611	PL9	C23-C24-C26-C27
28	a	611	PL9	C33-C34-C36-C37
28	d	406	PL9	C38-C39-C41-C42
25	C	513	CLA	C3-C5-C6-C7
25	b	602	CLA	C3-C5-C6-C7
25	B	616	CLA	CBA-CGA-O2A-C1
29	c	520	LMG	C4-C5-C6-O5
28	a	611	PL9	C42-C43-C44-C45
28	a	611	PL9	C22-C23-C24-C26
28	a	611	PL9	C42-C43-C44-C46
25	B	616	CLA	O1A-CGA-O2A-C1
30	a	615	SQD	O10-C23-O48-C46
28	a	611	PL9	C47-C48-C49-C50
25	C	511	CLA	CBD-CGD-O2D-CED
25	c	501	CLA	CBD-CGD-O2D-CED
33	D	409	LHG	O2-C2-C3-O3
33	d	407	LHG	O2-C2-C3-O3
29	B	620	LMG	C29-C28-O8-C9
25	C	513	CLA	O1A-CGA-O2A-C1
29	C	520	LMG	C11-C10-O7-C8
30	b	620	SQD	C8-C7-O47-C45
29	c	518	LMG	C11-C10-O7-C8
25	C	512	CLA	C3-C5-C6-C7
25	b	604	CLA	C3-C5-C6-C7
25	C	509	CLA	CBD-CGD-O2D-CED
30	a	615	SQD	C24-C23-O48-C46
36	V	201	HEC	C2C-C3C-CAC-CBC
25	b	605	CLA	C4-C3-C5-C6
25	B	614	CLA	C2-C3-C5-C6
25	C	504	CLA	C2-C3-C5-C6
28	A	611	PL9	C23-C24-C26-C27
28	A	611	PL9	C33-C34-C36-C37
31	c	517	DGD	O1A-C1A-O1G-C1G
28	A	611	PL9	C34-C36-C37-C38
28	D	406	PL9	C44-C46-C47-C48
28	a	611	PL9	C24-C26-C27-C28
28	a	611	PL9	C34-C36-C37-C38
29	b	622	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
29	b	622	LMG	O6-C1-O1-C7
30	B	624	SQD	O5-C1-O6-C44
29	c	520	LMG	O6-C5-C6-O5
25	C	501	CLA	CBD-CGD-O2D-CED
25	C	512	CLA	CBD-CGD-O2D-CED
25	c	512	CLA	CBD-CGD-O2D-CED
31	h	101	DGD	O6E-C5E-C6E-O5E
26	d	402	PHO	CBD-CGD-O2D-CED
30	b	620	SQD	O49-C7-O47-C45
33	D	409	LHG	C1-C2-C3-O3
25	B	601	CLA	CBA-CGA-O2A-C1
25	c	506	CLA	CBA-CGA-O2A-C1
30	D	408	SQD	C24-C23-O48-C46
32	H	103	STE	C14-C15-C16-C17
32	b	621	STE	C2-C3-C4-C5
33	d	408	LHG	C24-C25-C26-C27
30	A	614	SQD	C30-C31-C32-C33
33	E	101	LHG	C32-C33-C34-C35
31	A	616	DGD	O6E-C5E-C6E-O5E
28	A	611	PL9	C45-C44-C46-C47
25	b	605	CLA	C2-C3-C5-C6
25	c	513	CLA	C2-C3-C5-C6
28	A	611	PL9	C43-C44-C46-C47
25	B	606	CLA	C11-C10-C8-C9
25	B	607	CLA	C14-C13-C15-C16
25	B	610	CLA	C14-C13-C15-C16
25	B	616	CLA	C11-C10-C8-C9
25	C	503	CLA	C11-C10-C8-C9
25	C	509	CLA	C11-C10-C8-C9
25	C	512	CLA	C11-C10-C8-C9
25	C	513	CLA	C6-C7-C8-C9
25	b	602	CLA	C11-C10-C8-C9
25	b	605	CLA	C11-C10-C8-C9
25	b	606	CLA	C11-C10-C8-C9
25	c	509	CLA	C6-C7-C8-C9
25	c	509	CLA	C11-C12-C13-C14
25	c	511	CLA	C14-C13-C15-C16
32	C	521	STE	C4-C5-C6-C7
29	b	622	LMG	C2-C1-O1-C7
29	c	522	LMG	C2-C1-O1-C7
30	B	624	SQD	C2-C1-O6-C44
33	D	410	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
33	e	102	LHG	O2-C2-C3-O3
25	c	506	CLA	O1A-CGA-O2A-C1
31	a	616	DGD	O1A-C1A-O1G-C1G
31	A	616	DGD	C4E-C5E-C6E-O5E
25	c	513	CLA	O1D-CGD-O2D-CED
27	B	619	BCR	C11-C12-C13-C35
27	B	619	BCR	C37-C22-C23-C24
27	C	515	BCR	C7-C8-C9-C34
27	C	515	BCR	C11-C12-C13-C35
27	C	516	BCR	C7-C8-C9-C34
27	K	101	BCR	C37-C22-C23-C24
27	b	619	BCR	C37-C22-C23-C24
27	k	102	BCR	C7-C8-C9-C34
27	x	101	BCR	C7-C8-C9-C34
27	D	405	BCR	C21-C22-C23-C24
31	h	101	DGD	C4E-C5E-C6E-O5E
25	b	601	CLA	C2A-CAA-CBA-CGA
30	B	624	SQD	C34-C35-C36-C37
30	D	408	SQD	O10-C23-O48-C46
36	V	201	HEC	C2B-C3B-CAB-CBB
25	C	513	CLA	C15-C16-C17-C18
30	A	614	SQD	C23-C24-C25-C26
32	B	629	STE	C11-C12-C13-C14
25	B	610	CLA	C15-C16-C17-C18
25	a	607	CLA	C13-C15-C16-C17
25	b	603	CLA	C13-C15-C16-C17
25	b	607	CLA	C5-C6-C7-C8
33	e	102	LHG	O1-C1-C2-O2
29	D	411	LMG	C10-C11-C12-C13
25	B	606	CLA	C12-C13-C15-C16
25	D	403	CLA	C12-C13-C15-C16
25	b	606	CLA	C6-C7-C8-C10
25	b	614	CLA	C11-C12-C13-C15
25	b	615	CLA	C11-C12-C13-C15
31	a	616	DGD	C2A-C1A-O1G-C1G
30	a	614	SQD	C11-C12-C13-C14
29	B	620	LMG	O6-C5-C6-O5
31	a	616	DGD	C1A-C2A-C3A-C4A
32	d	412	STE	C1-C2-C3-C4
28	A	611	PL9	C29-C31-C32-C33
25	D	404	CLA	C13-C15-C16-C17
33	d	407	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
36	v	201	HEC	C2C-C3C-CAC-CBC
29	B	620	LMG	C10-C11-C12-C13
30	f	101	SQD	C23-C24-C25-C26
31	a	616	DGD	C1B-C2B-C3B-C4B
32	B	626	STE	C1-C2-C3-C4
32	b	621	STE	C1-C2-C3-C4
32	b	623	STE	C1-C2-C3-C4
33	E	101	LHG	C23-C24-C25-C26
33	l	101	LHG	C23-C24-C25-C26
25	B	601	CLA	O1A-CGA-O2A-C1
25	c	512	CLA	CBA-CGA-O2A-C1
25	B	601	CLA	C5-C6-C7-C8
25	B	601	CLA	C13-C15-C16-C17
25	B	606	CLA	C8-C10-C11-C12
25	B	606	CLA	C13-C15-C16-C17
25	C	506	CLA	C8-C10-C11-C12
25	C	509	CLA	C10-C11-C12-C13
25	c	509	CLA	C10-C11-C12-C13
25	b	606	CLA	C2A-CAA-CBA-CGA
25	C	505	CLA	C15-C16-C17-C18
25	b	601	CLA	C13-C15-C16-C17
25	c	509	CLA	C5-C6-C7-C8
31	c	515	DGD	O6E-C5E-C6E-O5E
29	D	407	LMG	C10-C11-C12-C13
30	A	614	SQD	C7-C8-C9-C10
33	e	102	LHG	C7-C8-C9-C10
36	V	201	HEC	C4C-C3C-CAC-CBC
30	b	620	SQD	O5-C1-O6-C44
25	A	607	CLA	C10-C11-C12-C13
25	B	603	CLA	C8-C10-C11-C12
25	B	613	CLA	C8-C10-C11-C12
25	B	615	CLA	C5-C6-C7-C8
25	C	502	CLA	C15-C16-C17-C18
25	C	503	CLA	C5-C6-C7-C8
25	b	605	CLA	C5-C6-C7-C8
25	b	614	CLA	C13-C15-C16-C17
25	b	615	CLA	C5-C6-C7-C8
25	c	510	CLA	C10-C11-C12-C13
33	a	613	LHG	O2-C2-C3-O3
31	c	517	DGD	C2A-C1A-O1G-C1G
25	B	601	CLA	C15-C16-C17-C18
25	a	606	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	b	615	CLA	C10-C11-C12-C13
25	C	505	CLA	C5-C6-C7-C8
25	b	607	CLA	C10-C11-C12-C13
25	c	509	CLA	C13-C15-C16-C17
25	c	510	CLA	C5-C6-C7-C8
25	c	512	CLA	C13-C15-C16-C17
29	d	410	LMG	C28-C29-C30-C31
31	c	516	DGD	C1A-C2A-C3A-C4A
33	D	412	LHG	C23-C24-C25-C26
25	B	606	CLA	C15-C16-C17-C18
25	B	607	CLA	C5-C6-C7-C8
25	C	512	CLA	C13-C15-C16-C17
25	b	611	CLA	C13-C15-C16-C17
25	c	510	CLA	C15-C16-C17-C18
32	b	624	STE	C2-C3-C4-C5
25	b	601	CLA	C3-C5-C6-C7
29	C	520	LMG	O9-C10-O7-C8
33	e	102	LHG	O9-C7-O7-C5
33	a	613	LHG	C1-C2-C3-O3
25	B	606	CLA	C2A-CAA-CBA-CGA
30	b	620	SQD	C12-C13-C14-C15
33	e	102	LHG	C26-C27-C28-C29
25	B	604	CLA	C10-C11-C12-C13
25	a	607	CLA	C8-C10-C11-C12
25	a	609	CLA	C5-C6-C7-C8
25	b	602	CLA	C13-C15-C16-C17
25	b	607	CLA	C8-C10-C11-C12
25	b	616	CLA	C5-C6-C7-C8
25	c	506	CLA	C13-C15-C16-C17
25	B	611	CLA	C8-C10-C11-C12
25	C	510	CLA	C8-C10-C11-C12
25	c	503	CLA	C5-C6-C7-C8
25	c	510	CLA	C8-C10-C11-C12
25	c	513	CLA	C13-C15-C16-C17
25	B	614	CLA	C13-C15-C16-C17
25	C	509	CLA	C13-C15-C16-C17
25	C	512	CLA	C10-C11-C12-C13
25	b	601	CLA	C8-C10-C11-C12
25	b	601	CLA	C10-C11-C12-C13
25	b	609	CLA	C15-C16-C17-C18
25	b	614	CLA	C8-C10-C11-C12
25	c	507	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	c	506	CLA	C4-C3-C5-C6
28	A	611	PL9	C25-C24-C26-C27
28	d	406	PL9	C40-C39-C41-C42
28	A	611	PL9	C47-C48-C49-C51
25	C	511	CLA	O1D-CGD-O2D-CED
31	C	518	DGD	C2E-C1E-O5D-C6D
25	C	509	CLA	O1D-CGD-O2D-CED
25	b	601	CLA	C16-C17-C18-C19
25	c	512	CLA	O1A-CGA-O2A-C1
27	C	516	BCR	C16-C17-C18-C36
27	D	405	BCR	C20-C21-C22-C37
27	T	101	BCR	C35-C13-C14-C15
27	T	101	BCR	C16-C17-C18-C36
27	c	514	BCR	C35-C13-C14-C15
27	k	101	BCR	C11-C10-C9-C34
27	k	101	BCR	C35-C13-C14-C15
29	m	101	LMG	C10-C11-C12-C13
25	b	614	CLA	C5-C6-C7-C8
27	B	618	BCR	C7-C8-C9-C34
27	b	618	BCR	C7-C8-C9-C34
30	b	620	SQD	C10-C11-C12-C13
25	c	511	CLA	C15-C16-C17-C18
33	d	408	LHG	O1-C1-C2-C3
33	B	623	LHG	C23-C24-C25-C26
29	D	411	LMG	C9-C8-O7-C10
30	b	620	SQD	C46-C45-O47-C7
25	b	607	CLA	C16-C17-C18-C20
25	c	504	CLA	C11-C12-C13-C14
27	B	619	BCR	C12-C13-C14-C15
27	C	515	BCR	C11-C10-C9-C8
27	K	101	BCR	C11-C10-C9-C8
27	T	101	BCR	C12-C13-C14-C15
27	T	101	BCR	C16-C17-C18-C19
27	k	102	BCR	C20-C21-C22-C23
27	x	101	BCR	C11-C10-C9-C8
27	x	101	BCR	C16-C17-C18-C19
31	C	518	DGD	O6E-C1E-O5D-C6D
25	c	503	CLA	C8-C10-C11-C12
25	c	501	CLA	O1D-CGD-O2D-CED
25	c	512	CLA	O1D-CGD-O2D-CED
33	E	101	LHG	C27-C28-C29-C30
25	B	603	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
25	B	609	CLA	C16-C17-C18-C20
25	b	607	CLA	C16-C17-C18-C19
25	c	503	CLA	C16-C17-C18-C20
25	c	512	CLA	C16-C17-C18-C19
29	b	622	LMG	C35-C36-C37-C38
29	c	522	LMG	C13-C14-C15-C16
31	A	616	DGD	C6B-C7B-C8B-C9B
32	B	625	STE	C6-C7-C8-C9
32	H	103	STE	C7-C8-C9-C10
32	b	621	STE	C7-C8-C9-C10
32	b	623	STE	C5-C6-C7-C8
29	A	613	LMG	C16-C17-C18-C19
30	B	624	SQD	C17-C18-C19-C20
31	a	616	DGD	CBA-CCA-CDA-CEA
31	h	101	DGD	C3B-C4B-C5B-C6B
32	B	628	STE	C2-C3-C4-C5
33	D	410	LHG	C11-C12-C13-C14
33	D	410	LHG	C29-C30-C31-C32
33	a	613	LHG	C32-C33-C34-C35
25	B	603	CLA	C13-C15-C16-C17
25	C	506	CLA	C13-C15-C16-C17
25	b	606	CLA	C15-C16-C17-C18
29	c	520	LMG	C33-C34-C35-C36
31	H	102	DGD	C5B-C6B-C7B-C8B
31	c	515	DGD	C3B-C4B-C5B-C6B
32	H	103	STE	C5-C6-C7-C8
32	H	103	STE	C12-C13-C14-C15
32	I	101	STE	C11-C10-C9-C8
32	T	103	STE	C11-C12-C13-C14
33	B	623	LHG	C17-C18-C19-C20
33	D	409	LHG	C11-C10-C9-C8
29	C	520	LMG	C17-C18-C19-C20
29	D	407	LMG	C39-C40-C41-C42
30	A	615	SQD	C28-C29-C30-C31
31	a	616	DGD	C8B-C9B-CAB-CBB
31	c	515	DGD	C4B-C5B-C6B-C7B
31	c	517	DGD	CBA-CCA-CDA-CEA
32	C	522	STE	C3-C4-C5-C6
32	X	101	STE	C14-C15-C16-C17
32	d	411	STE	C11-C10-C9-C8
33	D	409	LHG	C12-C13-C14-C15
33	D	410	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
33	E	101	LHG	C24-C25-C26-C27
33	e	102	LHG	C14-C15-C16-C17
33	a	613	LHG	O1-C1-C2-O2
29	d	409	LMG	C33-C34-C35-C36
30	A	614	SQD	C11-C12-C13-C14
30	a	614	SQD	C24-C25-C26-C27
32	T	102	STE	C5-C6-C7-C8
32	c	519	STE	C9-C10-C11-C12
32	d	412	STE	C4-C5-C6-C7
33	E	101	LHG	C16-C17-C18-C19
33	a	613	LHG	C10-C11-C12-C13
25	C	513	CLA	C10-C11-C12-C13
25	C	502	CLA	C4B-C3B-CAB-CBB
25	c	512	CLA	C4B-C3B-CAB-CBB
29	b	622	LMG	C41-C42-C43-C44
31	h	101	DGD	CBA-CCA-CDA-CEA
32	B	629	STE	C11-C10-C9-C8
33	a	613	LHG	C15-C16-C17-C18
25	B	601	CLA	C16-C17-C18-C19
25	B	601	CLA	C16-C17-C18-C20
25	B	603	CLA	C16-C17-C18-C19
25	B	606	CLA	C16-C17-C18-C19
25	B	616	CLA	C11-C12-C13-C15
25	a	606	CLA	C16-C17-C18-C19
25	c	512	CLA	C16-C17-C18-C20
25	d	403	CLA	C16-C17-C18-C19
25	d	403	CLA	C16-C17-C18-C20
30	D	408	SQD	C25-C26-C27-C28
25	B	615	CLA	C15-C16-C17-C18
25	C	504	CLA	C8-C10-C11-C12
25	b	608	CLA	C13-C15-C16-C17
29	c	522	LMG	C12-C13-C14-C15
31	c	515	DGD	C8B-C9B-CAB-CBB
25	B	611	CLA	C11-C10-C8-C7
29	b	622	LMG	C31-C32-C33-C34
31	A	616	DGD	C4B-C5B-C6B-C7B
31	A	616	DGD	C5B-C6B-C7B-C8B
31	c	517	DGD	C5A-C6A-C7A-C8A
32	B	628	STE	C3-C4-C5-C6
32	H	103	STE	C11-C10-C9-C8
29	D	407	LMG	O6-C5-C6-O5
31	C	519	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
31	a	616	DGD	C8A-C9A-CAA-CBA
31	c	515	DGD	C6A-C7A-C8A-C9A
31	c	517	DGD	C4A-C5A-C6A-C7A
32	T	102	STE	C4-C5-C6-C7
32	c	519	STE	C2-C3-C4-C5
32	c	521	STE	C2-C3-C4-C5
32	d	411	STE	C9-C10-C11-C12
29	b	622	LMG	C4-C5-C6-O5
25	b	601	CLA	C3A-C2A-CAA-CBA
25	C	512	CLA	O1D-CGD-O2D-CED
31	c	516	DGD	C6A-C7A-C8A-C9A
32	b	624	STE	C12-C13-C14-C15
25	b	615	CLA	C15-C16-C17-C18
29	d	410	LMG	C38-C39-C40-C41
27	k	101	BCR	C13-C14-C15-C16
25	B	606	CLA	C16-C17-C18-C20
25	B	616	CLA	C11-C12-C13-C14
25	a	606	CLA	C16-C17-C18-C20
29	A	613	LMG	O6-C5-C6-O5
29	c	520	LMG	C30-C31-C32-C33
29	m	101	LMG	C17-C18-C19-C20
32	b	624	STE	C3-C4-C5-C6
32	d	412	STE	C3-C4-C5-C6
33	B	623	LHG	C27-C28-C29-C30
25	C	513	CLA	C8-C10-C11-C12
29	b	622	LMG	C16-C17-C18-C19
29	c	522	LMG	C38-C39-C40-C41
29	d	409	LMG	C35-C36-C37-C38
30	D	408	SQD	C30-C31-C32-C33
30	b	620	SQD	C26-C27-C28-C29
33	B	623	LHG	C13-C14-C15-C16
25	C	501	CLA	O1D-CGD-O2D-CED
30	B	624	SQD	C24-C23-O48-C46
32	B	625	STE	C11-C10-C9-C8
33	B	623	LHG	C30-C31-C32-C33
33	D	410	LHG	C25-C26-C27-C28
33	D	410	LHG	C33-C34-C35-C36
25	B	605	CLA	C3-C5-C6-C7
33	a	613	LHG	C7-C8-C9-C10
29	A	613	LMG	C35-C36-C37-C38
29	d	409	LMG	C32-C33-C34-C35
30	a	614	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
31	H	102	DGD	CBB-CCB-CDB-CEB
31	a	616	DGD	C4A-C5A-C6A-C7A
31	c	515	DGD	C3A-C4A-C5A-C6A
31	c	516	DGD	CCA-CDA-CEA-CFA
32	B	625	STE	C3-C4-C5-C6
32	C	522	STE	C5-C6-C7-C8
32	H	103	STE	C6-C7-C8-C9
32	T	102	STE	C6-C7-C8-C9
33	l	101	LHG	C9-C10-C11-C12
29	D	411	LMG	C14-C15-C16-C17
30	a	614	SQD	C30-C31-C32-C33
31	c	517	DGD	C6A-C7A-C8A-C9A
32	d	412	STE	C12-C13-C14-C15
32	l	102	STE	C4-C5-C6-C7
31	H	102	DGD	C9A-CAA-CBA-CCA
32	c	521	STE	C4-C5-C6-C7
32	l	102	STE	C13-C14-C15-C16
33	D	409	LHG	C30-C31-C32-C33
29	D	407	LMG	C37-C38-C39-C40
30	A	614	SQD	C34-C35-C36-C37
31	A	616	DGD	CBA-CCA-CDA-CEA
32	j	101	STE	C2-C3-C4-C5
33	D	409	LHG	C33-C34-C35-C36
33	a	613	LHG	C28-C29-C30-C31
28	d	406	PL9	C42-C43-C44-C45
25	B	615	CLA	C16-C17-C18-C20
25	c	503	CLA	C16-C17-C18-C19
31	A	616	DGD	C1B-C2B-C3B-C4B
33	e	102	LHG	C23-C24-C25-C26
25	c	512	CLA	C2B-C3B-CAB-CBB
27	C	516	BCR	C1-C6-C7-C8
27	D	405	BCR	C23-C24-C25-C30
27	k	102	BCR	C1-C6-C7-C8
27	t	101	BCR	C1-C6-C7-C8
27	t	101	BCR	C5-C6-C7-C8
29	A	613	LMG	C34-C35-C36-C37
31	A	616	DGD	CCB-CDB-CEB-CFB
33	D	409	LHG	C32-C33-C34-C35
30	A	614	SQD	C11-C10-C9-C8
30	a	614	SQD	C32-C33-C34-C35
30	a	615	SQD	C30-C31-C32-C33
30	f	101	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
30	f	101	SQD	C31-C32-C33-C34
32	H	103	STE	C13-C14-C15-C16
29	C	520	LMG	C31-C32-C33-C34
30	f	101	SQD	C25-C26-C27-C28
33	E	101	LHG	C18-C19-C20-C21
33	a	613	LHG	C29-C30-C31-C32
33	e	102	LHG	C18-C19-C20-C21
31	c	517	DGD	C7B-C8B-C9B-CAB
32	T	102	STE	C7-C8-C9-C10
32	d	411	STE	C6-C7-C8-C9
32	d	412	STE	C7-C8-C9-C10
32	l	102	STE	C9-C10-C11-C12
29	b	622	LMG	O9-C10-O7-C8
29	C	520	LMG	C14-C15-C16-C17
29	c	520	LMG	C31-C32-C33-C34
31	c	515	DGD	C5B-C6B-C7B-C8B
31	h	101	DGD	C6B-C7B-C8B-C9B
32	C	521	STE	C5-C6-C7-C8
28	A	611	PL9	C12-C13-C14-C16
27	B	619	BCR	C10-C11-C12-C13
27	k	101	BCR	C18-C19-C20-C21
25	c	504	CLA	C8-C10-C11-C12
25	c	504	CLA	C11-C12-C13-C15
30	A	614	SQD	C27-C28-C29-C30
30	b	620	SQD	C24-C25-C26-C27
32	B	627	STE	C5-C6-C7-C8
32	T	103	STE	C12-C13-C14-C15
33	B	623	LHG	C16-C17-C18-C19
33	D	410	LHG	C32-C33-C34-C35
29	c	520	LMG	C10-C11-C12-C13
25	b	611	CLA	C14-C13-C15-C16
30	A	614	SQD	C28-C29-C30-C31
30	B	624	SQD	C32-C33-C34-C35
31	h	101	DGD	C5A-C6A-C7A-C8A
32	X	101	STE	C12-C13-C14-C15
33	d	408	LHG	C32-C33-C34-C35
33	e	102	LHG	C27-C28-C29-C30
33	l	101	LHG	C14-C15-C16-C17
33	l	101	LHG	C17-C18-C19-C20
30	b	620	SQD	C9-C10-C11-C12
33	l	101	LHG	C27-C28-C29-C30
29	B	620	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
30	B	624	SQD	C11-C12-C13-C14
31	c	516	DGD	C7B-C8B-C9B-CAB
32	B	629	STE	C6-C7-C8-C9
32	j	101	STE	C5-C6-C7-C8
25	B	607	CLA	C13-C15-C16-C17
29	m	101	LMG	C32-C33-C34-C35
31	a	616	DGD	CDA-CEA-CFA-CGA
33	D	409	LHG	C15-C16-C17-C18
33	D	410	LHG	C24-C25-C26-C27
30	b	620	SQD	C23-C24-C25-C26
31	c	515	DGD	C1A-C2A-C3A-C4A
30	A	614	SQD	C16-C17-C18-C19
31	C	519	DGD	C5A-C6A-C7A-C8A
32	X	101	STE	C7-C8-C9-C10
32	X	101	STE	C11-C12-C13-C14
33	D	412	LHG	C28-C29-C30-C31
29	C	520	LMG	C13-C14-C15-C16
31	C	518	DGD	C8B-C9B-CAB-CBB
32	C	521	STE	C6-C7-C8-C9
32	J	101	STE	C4-C5-C6-C7
32	J	101	STE	C6-C7-C8-C9
32	b	625	STE	C3-C4-C5-C6
33	d	408	LHG	C27-C28-C29-C30
33	e	102	LHG	C8-C7-O7-C5
29	b	622	LMG	C10-C11-C12-C13
29	B	620	LMG	C37-C38-C39-C40
29	m	101	LMG	C14-C15-C16-C17
31	c	515	DGD	CAB-CBB-CCB-CDB
31	h	101	DGD	C5B-C6B-C7B-C8B
33	B	623	LHG	C9-C10-C11-C12
33	E	101	LHG	C9-C10-C11-C12
25	B	602	CLA	C13-C15-C16-C17
27	c	514	BCR	C7-C8-C9-C34
31	a	616	DGD	CEB-CFB-CGB-CHB
27	k	102	BCR	C21-C22-C23-C24
31	H	102	DGD	CBA-CCA-CDA-CEA
25	B	610	CLA	C16-C17-C18-C20
25	B	615	CLA	C16-C17-C18-C19
25	C	502	CLA	C16-C17-C18-C19
29	A	613	LMG	C38-C39-C40-C41
32	b	621	STE	C14-C15-C16-C17
32	b	625	STE	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
25	C	506	CLA	C4-C3-C5-C6
29	c	520	LMG	C14-C15-C16-C17
33	D	412	LHG	C29-C30-C31-C32
30	a	614	SQD	C27-C28-C29-C30
31	a	616	DGD	C3B-C4B-C5B-C6B
32	B	629	STE	C5-C6-C7-C8
30	B	624	SQD	O10-C23-O48-C46
25	B	616	CLA	C8-C10-C11-C12
25	C	506	CLA	C15-C16-C17-C18
29	c	520	LMG	C39-C40-C41-C42
29	c	522	LMG	C18-C19-C20-C21
29	d	410	LMG	C14-C15-C16-C17
30	D	408	SQD	C23-C24-C25-C26
32	B	621	STE	C1-C2-C3-C4
29	B	620	LMG	C16-C17-C18-C19
29	B	620	LMG	C32-C33-C34-C35
29	c	520	LMG	C11-C12-C13-C14
31	C	518	DGD	C4A-C5A-C6A-C7A
31	C	519	DGD	CBA-CCA-CDA-CEA
31	c	515	DGD	CCB-CDB-CEB-CFB
32	H	103	STE	C4-C5-C6-C7
28	a	611	PL9	C39-C41-C42-C43
25	B	613	CLA	C5-C6-C7-C8
29	b	622	LMG	C34-C35-C36-C37
31	a	616	DGD	C3A-C4A-C5A-C6A
31	H	102	DGD	C3A-C4A-C5A-C6A
32	b	621	STE	C13-C14-C15-C16
29	c	522	LMG	C28-C29-C30-C31
29	c	518	LMG	C36-C37-C38-C39
29	c	522	LMG	C37-C38-C39-C40
33	d	407	LHG	C29-C30-C31-C32
30	A	614	SQD	C14-C15-C16-C17
32	X	101	STE	C10-C11-C12-C13
33	d	407	LHG	C34-C35-C36-C37
29	d	410	LMG	O6-C5-C6-O5
29	D	411	LMG	C28-C29-C30-C31
29	B	622	LMG	C13-C14-C15-C16
36	V	201	HEC	C4B-C3B-CAB-CBB
29	D	407	LMG	C17-C18-C19-C20
30	a	615	SQD	C11-C10-C9-C8
32	T	103	STE	C11-C10-C9-C8
32	d	412	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
33	D	412	LHG	C25-C26-C27-C28
26	d	402	PHO	O1D-CGD-O2D-CED
29	A	613	LMG	C17-C18-C19-C20
29	d	409	LMG	C37-C38-C39-C40
30	a	614	SQD	C14-C15-C16-C17
31	c	515	DGD	C9B-CAB-CBB-CCB
25	C	506	CLA	C2-C3-C5-C6
33	d	407	LHG	C1-C2-C3-O3
31	C	519	DGD	C3A-C4A-C5A-C6A
32	T	103	STE	C14-C15-C16-C17
32	c	519	STE	C4-C5-C6-C7
33	E	101	LHG	C33-C34-C35-C36
30	a	614	SQD	C10-C11-C12-C13
31	C	517	DGD	C5B-C6B-C7B-C8B
32	b	624	STE	C14-C15-C16-C17
32	c	519	STE	C11-C12-C13-C14
29	B	620	LMG	C12-C13-C14-C15
32	X	101	STE	C6-C7-C8-C9
29	b	622	LMG	C15-C16-C17-C18
33	E	101	LHG	C34-C35-C36-C37
30	b	620	SQD	C11-C10-C9-C8
31	c	515	DGD	C2A-C3A-C4A-C5A
31	h	101	DGD	C6A-C7A-C8A-C9A
32	B	628	STE	C5-C6-C7-C8
33	D	410	LHG	C10-C11-C12-C13
29	d	410	LMG	C36-C37-C38-C39
30	D	408	SQD	C34-C35-C36-C37
25	a	609	CLA	C1A-C2A-CAA-CBA
25	c	508	CLA	C1A-C2A-CAA-CBA
25	c	513	CLA	C1A-C2A-CAA-CBA
25	C	513	CLA	C5-C6-C7-C8
30	A	614	SQD	C24-C25-C26-C27
30	A	615	SQD	C10-C11-C12-C13
32	M	101	STE	C11-C10-C9-C8
33	D	410	LHG	C30-C31-C32-C33
29	B	622	LMG	C14-C15-C16-C17
25	B	602	CLA	C8-C10-C11-C12
25	c	511	CLA	C13-C15-C16-C17
29	c	522	LMG	O9-C10-O7-C8
29	D	407	LMG	C30-C31-C32-C33
29	c	522	LMG	C29-C30-C31-C32
25	A	607	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	B	604	CLA	C11-C10-C8-C7
25	B	604	CLA	C12-C13-C15-C16
25	B	605	CLA	C11-C10-C8-C7
25	B	616	CLA	C6-C7-C8-C10
25	C	506	CLA	C12-C13-C15-C16
25	C	510	CLA	C11-C10-C8-C7
25	C	512	CLA	C6-C7-C8-C10
25	a	607	CLA	C11-C10-C8-C7
25	b	604	CLA	C12-C13-C15-C16
25	b	607	CLA	C6-C7-C8-C10
25	b	611	CLA	C11-C10-C8-C7
25	c	504	CLA	C11-C10-C8-C7
25	c	506	CLA	C6-C7-C8-C10
25	c	506	CLA	C11-C10-C8-C7
25	d	403	CLA	C11-C12-C13-C15
25	d	404	CLA	C12-C13-C15-C16
30	a	614	SQD	C28-C29-C30-C31
32	E	102	STE	C4-C5-C6-C7
29	b	622	LMG	C19-C20-C21-C22
32	X	101	STE	C9-C10-C11-C12
33	d	408	LHG	C26-C27-C28-C29
33	l	101	LHG	C13-C14-C15-C16
29	c	518	LMG	O6-C5-C6-O5
25	B	601	CLA	C8-C10-C11-C12
25	d	404	CLA	C10-C11-C12-C13
29	b	622	LMG	C11-C10-O7-C8
25	A	607	CLA	C11-C12-C13-C14
25	B	606	CLA	C14-C13-C15-C16
25	C	505	CLA	C6-C7-C8-C9
25	C	506	CLA	C14-C13-C15-C16
25	D	403	CLA	C14-C13-C15-C16
25	b	615	CLA	C11-C10-C8-C9
25	b	615	CLA	C11-C12-C13-C14
25	c	505	CLA	C11-C10-C8-C9
25	c	506	CLA	C6-C7-C8-C9
25	c	506	CLA	C11-C10-C8-C9
25	c	513	CLA	C11-C12-C13-C14
31	h	101	DGD	CBB-CCB-CDB-CEB
32	b	625	STE	C4-C5-C6-C7
29	m	101	LMG	C28-C29-C30-C31
30	A	615	SQD	C9-C10-C11-C12
32	H	103	STE	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
29	A	613	LMG	C29-C28-O8-C9
28	A	611	PL9	C17-C18-C19-C20
33	E	101	LHG	C30-C31-C32-C33
29	B	622	LMG	C29-C30-C31-C32
31	H	102	DGD	CCA-CDA-CEA-CFA
29	b	622	LMG	O1-C7-C8-C9
29	c	520	LMG	O1-C7-C8-C9
30	a	614	SQD	O6-C44-C45-C46
30	a	615	SQD	C44-C45-C46-O48
25	A	609	CLA	C5-C6-C7-C8
29	C	520	LMG	C32-C33-C34-C35
29	c	520	LMG	C41-C42-C43-C44
31	a	616	DGD	C2B-C3B-C4B-C5B
29	D	407	LMG	C36-C37-C38-C39
29	d	409	LMG	C31-C32-C33-C34
30	a	614	SQD	C19-C20-C21-C22
29	c	520	LMG	C28-C29-C30-C31
25	C	502	CLA	C16-C17-C18-C20
29	B	620	LMG	C33-C34-C35-C36
30	D	408	SQD	C29-C30-C31-C32
30	a	614	SQD	C9-C10-C11-C12
27	b	618	BCR	C35-C13-C14-C15
27	b	619	BCR	C20-C21-C22-C37
25	b	603	CLA	C8-C10-C11-C12
29	D	411	LMG	C31-C32-C33-C34
29	b	622	LMG	C29-C30-C31-C32
31	C	517	DGD	O6E-C5E-C6E-O5E
32	B	627	STE	C13-C14-C15-C16
30	a	614	SQD	C17-C18-C19-C20
25	B	614	CLA	C8-C10-C11-C12
29	B	620	LMG	C29-C30-C31-C32
29	C	520	LMG	C37-C38-C39-C40
29	D	407	LMG	C15-C16-C17-C18
32	M	101	STE	C7-C8-C9-C10
32	T	103	STE	C10-C11-C12-C13
33	B	623	LHG	C32-C33-C34-C35
33	a	613	LHG	C16-C17-C18-C19
25	b	606	CLA	C10-C11-C12-C13
25	c	505	CLA	C15-C16-C17-C18
33	d	407	LHG	C11-C12-C13-C14
29	c	518	LMG	C39-C40-C41-C42
30	A	614	SQD	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
31	A	616	DGD	C2B-C3B-C4B-C5B
32	c	519	STE	C1-C2-C3-C4
31	C	517	DGD	C9B-CAB-CBB-CCB
31	c	517	DGD	C8B-C9B-CAB-CBB
33	D	409	LHG	C25-C26-C27-C28
32	m	102	STE	C6-C7-C8-C9
33	a	613	LHG	C30-C31-C32-C33
31	c	515	DGD	O6D-C5D-C6D-O5D
25	D	403	CLA	C15-C16-C17-C18
32	B	627	STE	C6-C7-C8-C9
32	B	628	STE	C6-C7-C8-C9
33	D	409	LHG	C16-C17-C18-C19
29	m	101	LMG	C11-C12-C13-C14
30	B	624	SQD	C9-C10-C11-C12
30	D	408	SQD	C31-C32-C33-C34
32	T	102	STE	C13-C14-C15-C16
33	D	410	LHG	C11-C10-C9-C8
33	d	408	LHG	C23-C24-C25-C26
31	c	516	DGD	C3A-C4A-C5A-C6A
27	B	619	BCR	C11-C10-C9-C8
31	C	519	DGD	CBB-CCB-CDB-CEB
32	T	103	STE	C6-C7-C8-C9
32	l	102	STE	C14-C15-C16-C17
31	c	516	DGD	CDA-CEA-CFA-CGA
30	A	614	SQD	C26-C27-C28-C29
32	d	412	STE	C15-C16-C17-C18
29	C	520	LMG	C38-C39-C40-C41
29	c	518	LMG	C35-C36-C37-C38
25	A	609	CLA	C4-C3-C5-C6
28	A	611	PL9	C20-C19-C21-C22
25	C	505	CLA	C2-C3-C5-C6
25	c	506	CLA	C2-C3-C5-C6
31	C	517	DGD	C2B-C3B-C4B-C5B
32	a	617	STE	C4-C5-C6-C7
33	D	409	LHG	C13-C14-C15-C16
29	D	407	LMG	C38-C39-C40-C41
29	c	520	LMG	C34-C35-C36-C37
31	C	519	DGD	C4B-C5B-C6B-C7B
32	B	627	STE	C4-C5-C6-C7
33	d	407	LHG	C12-C13-C14-C15
32	l	102	STE	C1-C2-C3-C4
31	c	517	DGD	C1A-C2A-C3A-C4A

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Mol	Chain	Res	Type	Atoms
29	B	620	LMG	C19-C20-C21-C22
31	c	515	DGD	CBB-CCB-CDB-CEB
32	b	623	STE	C10-C11-C12-C13
32	l	102	STE	C10-C11-C12-C13
33	d	408	LHG	C33-C34-C35-C36
29	c	520	LMG	O7-C8-C9-O8
32	J	101	STE	C7-C8-C9-C10
31	A	616	DGD	C2A-C3A-C4A-C5A
29	C	520	LMG	C30-C31-C32-C33
29	b	622	LMG	C17-C18-C19-C20
29	c	522	LMG	C39-C40-C41-C42
33	e	102	LHG	C13-C14-C15-C16
30	A	614	SQD	C17-C18-C19-C20
25	D	403	CLA	C16-C17-C18-C19
25	C	513	CLA	C13-C15-C16-C17
30	A	615	SQD	C11-C12-C13-C14
30	B	624	SQD	C19-C20-C21-C22
33	D	410	LHG	C31-C32-C33-C34
31	H	102	DGD	CDB-CEB-CFB-CGB
28	D	406	PL9	C32-C33-C34-C35
29	B	620	LMG	C17-C18-C19-C20
29	c	522	LMG	C34-C35-C36-C37
25	a	609	CLA	C10-C11-C12-C13
32	B	627	STE	C2-C3-C4-C5
30	b	620	SQD	C19-C20-C21-C22
31	A	616	DGD	CEB-CFB-CGB-CHB
25	D	403	CLA	C16-C17-C18-C20
28	A	611	PL9	C15-C14-C16-C17
28	d	406	PL9	C45-C44-C46-C47
31	C	518	DGD	C6A-C7A-C8A-C9A
25	C	505	CLA	C10-C11-C12-C13
29	m	101	LMG	C38-C39-C40-C41
33	a	613	LHG	C17-C18-C19-C20
32	B	629	STE	C3-C4-C5-C6
33	e	102	LHG	C11-C10-C9-C8
33	l	101	LHG	C30-C31-C32-C33
25	A	607	CLA	C11-C10-C8-C9
25	B	603	CLA	C11-C10-C8-C9
25	B	604	CLA	C11-C10-C8-C9
25	B	604	CLA	C14-C13-C15-C16
25	B	605	CLA	C11-C10-C8-C9
25	B	616	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	C	505	CLA	C11-C10-C8-C9
25	a	607	CLA	C11-C10-C8-C9
25	a	609	CLA	C14-C13-C15-C16
25	b	604	CLA	C14-C13-C15-C16
25	b	607	CLA	C6-C7-C8-C9
25	d	403	CLA	C11-C12-C13-C14
25	d	404	CLA	C6-C7-C8-C9
25	d	404	CLA	C14-C13-C15-C16
25	B	606	CLA	C4B-C3B-CAB-CBB
25	b	601	CLA	C4B-C3B-CAB-CBB
25	b	610	CLA	C4B-C3B-CAB-CBB
25	c	503	CLA	C4B-C3B-CAB-CBB
29	D	411	LMG	C36-C37-C38-C39
32	d	411	STE	C2-C3-C4-C5
25	B	612	CLA	C16-C17-C18-C20
29	B	620	LMG	C20-C21-C22-C23
28	A	611	PL9	C32-C33-C34-C36
29	B	622	LMG	C33-C34-C35-C36
30	A	614	SQD	C13-C14-C15-C16
31	C	518	DGD	C6B-C7B-C8B-C9B
32	a	617	STE	C2-C3-C4-C5
32	m	102	STE	C5-C6-C7-C8
31	c	516	DGD	C2E-C1E-O5D-C6D
30	A	614	SQD	C35-C36-C37-C38
33	e	102	LHG	O6-C4-C5-C6
31	h	101	DGD	C2B-C3B-C4B-C5B
33	D	412	LHG	C19-C20-C21-C22
31	a	616	DGD	C5A-C6A-C7A-C8A
25	A	607	CLA	C11-C12-C13-C15
25	A	612	CLA	C12-C13-C15-C16
25	B	616	CLA	C11-C10-C8-C7
25	C	502	CLA	C12-C13-C15-C16
25	C	505	CLA	C6-C7-C8-C10
25	C	505	CLA	C11-C10-C8-C7
25	C	507	CLA	C11-C10-C8-C7
25	b	604	CLA	C11-C12-C13-C15
25	b	606	CLA	C12-C13-C15-C16
25	b	611	CLA	C11-C12-C13-C15
25	b	615	CLA	C11-C10-C8-C7
25	c	505	CLA	C6-C7-C8-C10
25	c	505	CLA	C11-C10-C8-C7
25	c	512	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	c	513	CLA	C11-C12-C13-C15
25	c	503	CLA	C15-C16-C17-C18
25	c	506	CLA	C8-C10-C11-C12
31	C	518	DGD	CDB-CEB-CFB-CGB
32	B	621	STE	C12-C13-C14-C15
32	t	102	STE	C5-C6-C7-C8
29	B	622	LMG	C37-C38-C39-C40
29	c	522	LMG	C40-C41-C42-C43
29	d	410	LMG	C32-C33-C34-C35
25	C	507	CLA	C5-C6-C7-C8
25	C	512	CLA	C8-C10-C11-C12
32	M	101	STE	C10-C11-C12-C13
31	a	616	DGD	CBB-CCB-CDB-CEB
25	c	503	CLA	C10-C11-C12-C13
29	D	407	LMG	C20-C21-C22-C23
32	b	624	STE	C9-C10-C11-C12
27	B	619	BCR	C7-C8-C9-C34
27	k	101	BCR	C7-C8-C9-C10
30	A	615	SQD	C14-C15-C16-C17
32	T	103	STE	C9-C10-C11-C12
29	c	520	LMG	C7-C8-C9-O8
31	A	616	DGD	O1G-C1G-C2G-C3G
31	A	616	DGD	C1G-C2G-C3G-O3G
33	E	101	LHG	C4-C5-C6-O8
31	a	616	DGD	CEA-CFA-CGA-CHA
31	h	101	DGD	C4A-C5A-C6A-C7A
25	c	510	CLA	C3-C5-C6-C7
33	B	623	LHG	C19-C20-C21-C22
25	b	601	CLA	C16-C17-C18-C20
25	B	608	CLA	C15-C16-C17-C18
26	d	402	PHO	C5-C6-C7-C8
29	B	620	LMG	C4-C5-C6-O5
32	B	629	STE	C4-C5-C6-C7
29	D	411	LMG	C15-C16-C17-C18
25	B	612	CLA	C10-C11-C12-C13
29	D	407	LMG	C12-C13-C14-C15
25	C	505	CLA	C4-C3-C5-C6
25	b	616	CLA	C4-C3-C5-C6
28	a	611	PL9	C40-C39-C41-C42
30	b	620	SQD	C18-C19-C20-C21
31	C	517	DGD	CCB-CDB-CEB-CFB
33	D	410	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	B	616	CLA	C3-C5-C6-C7
25	b	615	CLA	C13-C15-C16-C17
25	A	607	CLA	C16-C17-C18-C20
31	C	517	DGD	C1B-C2B-C3B-C4B
33	e	102	LHG	O6-C4-C5-O7
32	m	102	STE	C3-C4-C5-C6
33	D	412	LHG	C27-C28-C29-C30
27	B	617	BCR	C1-C6-C7-C8
27	b	617	BCR	C1-C6-C7-C8
27	k	101	BCR	C23-C24-C25-C30
25	c	509	CLA	CAA-CBA-CGA-O2A
25	c	512	CLA	C15-C16-C17-C18
29	c	518	LMG	C38-C39-C40-C41
29	d	409	LMG	C34-C35-C36-C37
33	E	101	LHG	C25-C26-C27-C28
25	B	609	CLA	C16-C17-C18-C19
25	D	404	CLA	C16-C17-C18-C19
25	A	606	CLA	C2C-C3C-CAC-CBC
29	A	613	LMG	O1-C7-C8-O7
29	B	620	LMG	O7-C8-C9-O8
29	b	622	LMG	O1-C7-C8-O7
29	c	520	LMG	O1-C7-C8-O7
30	f	101	SQD	O6-C44-C45-O47
33	E	101	LHG	O7-C5-C6-O8
31	C	517	DGD	C4A-C5A-C6A-C7A
32	X	101	STE	C4-C5-C6-C7
28	A	611	PL9	C4-C3-C7-C8
28	D	406	PL9	C4-C3-C7-C8
28	a	611	PL9	C4-C3-C7-C8
29	B	620	LMG	C31-C32-C33-C34
29	d	409	LMG	C39-C40-C41-C42
31	H	102	DGD	C4A-C5A-C6A-C7A
25	c	510	CLA	C4-C3-C5-C6
31	C	519	DGD	CCB-CDB-CEB-CFB
27	T	101	BCR	C18-C19-C20-C21
27	d	405	BCR	C18-C19-C20-C21
29	b	622	LMG	C13-C14-C15-C16
31	c	517	DGD	C3B-C4B-C5B-C6B
32	b	624	STE	C4-C5-C6-C7
33	d	407	LHG	C14-C15-C16-C17
25	B	610	CLA	C16-C17-C18-C19
29	d	410	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
30	b	620	SQD	C28-C29-C30-C31
29	m	101	LMG	O10-C28-O8-C9
25	B	603	CLA	C14-C13-C15-C16
25	B	615	CLA	C11-C12-C13-C14
25	C	504	CLA	C11-C10-C8-C9
25	C	508	CLA	C11-C12-C13-C14
25	C	510	CLA	C11-C10-C8-C9
25	b	601	CLA	C11-C12-C13-C14
25	b	609	CLA	C14-C13-C15-C16
25	b	611	CLA	C11-C12-C13-C14
25	c	504	CLA	C11-C10-C8-C9
31	A	616	DGD	C7B-C8B-C9B-CAB
31	c	517	DGD	C3A-C4A-C5A-C6A
31	c	516	DGD	O6E-C1E-O5D-C6D
29	m	101	LMG	C31-C32-C33-C34
36	v	201	HEC	C4C-C3C-CAC-CBC
28	A	611	PL9	C44-C46-C47-C48
28	a	611	PL9	C19-C21-C22-C23
28	a	611	PL9	C44-C46-C47-C48
29	A	613	LMG	C29-C30-C31-C32
33	B	623	LHG	C18-C19-C20-C21
25	c	512	CLA	C2A-CAA-CBA-CGA
29	c	522	LMG	C15-C16-C17-C18
30	B	624	SQD	C13-C14-C15-C16
32	T	102	STE	C11-C10-C9-C8
25	B	615	CLA	C13-C15-C16-C17
33	D	409	LHG	O1-C1-C2-O2
25	C	506	CLA	C3-C5-C6-C7
25	B	614	CLA	C16-C17-C18-C20
25	D	404	CLA	C16-C17-C18-C20
31	H	102	DGD	C3B-C4B-C5B-C6B
30	A	615	SQD	C12-C13-C14-C15
31	C	517	DGD	C6A-C7A-C8A-C9A
31	C	519	DGD	C6A-C7A-C8A-C9A
32	T	102	STE	C10-C11-C12-C13
32	t	102	STE	C6-C7-C8-C9
27	A	610	BCR	C11-C10-C9-C34
27	K	101	BCR	C11-C10-C9-C34
27	T	101	BCR	C11-C10-C9-C34
27	b	617	BCR	C16-C17-C18-C36
27	x	101	BCR	C16-C17-C18-C36
31	H	102	DGD	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
25	a	609	CLA	C13-C15-C16-C17
25	c	505	CLA	C16-C17-C18-C20
25	C	507	CLA	C10-C11-C12-C13
25	B	603	CLA	C12-C13-C15-C16
25	B	606	CLA	C6-C7-C8-C10
25	B	606	CLA	C11-C12-C13-C15
25	B	610	CLA	C12-C13-C15-C16
25	C	508	CLA	C11-C12-C13-C15
25	C	509	CLA	C12-C13-C15-C16
25	C	513	CLA	C6-C7-C8-C10
25	D	404	CLA	C11-C12-C13-C15
25	a	607	CLA	C12-C13-C15-C16
25	a	609	CLA	C12-C13-C15-C16
25	b	607	CLA	C11-C12-C13-C15
25	b	609	CLA	C12-C13-C15-C16
25	c	511	CLA	C12-C13-C15-C16
25	d	404	CLA	C11-C12-C13-C15
30	A	614	SQD	C10-C11-C12-C13
31	C	518	DGD	C2A-C3A-C4A-C5A
31	C	518	DGD	CDA-CEA-CFA-CGA
25	c	509	CLA	C8-C10-C11-C12
27	C	516	BCR	C21-C22-C23-C24
27	c	514	BCR	C7-C8-C9-C10
27	t	101	BCR	C7-C8-C9-C10
33	D	410	LHG	C26-C27-C28-C29
33	B	623	LHG	O10-C23-O8-C6
30	B	624	SQD	C45-C44-O6-C1
31	C	518	DGD	C5D-C6D-O5D-C1E
31	c	516	DGD	C5D-C6D-O5D-C1E
25	B	612	CLA	C16-C17-C18-C19
30	a	615	SQD	C12-C13-C14-C15
32	T	103	STE	C15-C16-C17-C18
29	C	520	LMG	C12-C13-C14-C15
32	B	621	STE	C11-C12-C13-C14
33	e	102	LHG	C28-C29-C30-C31
29	b	622	LMG	C9-C8-O7-C10
30	A	615	SQD	C18-C19-C20-C21
31	C	518	DGD	C8A-C9A-CAA-CBA
31	C	517	DGD	C4B-C5B-C6B-C7B
32	M	102	STE	C5-C6-C7-C8
32	j	101	STE	C3-C4-C5-C6
25	A	607	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	m	101	LMG	C37-C38-C39-C40
33	E	101	LHG	C12-C13-C14-C15
32	T	103	STE	C4-C5-C6-C7
33	B	623	LHG	O6-C4-C5-O7
33	l	101	LHG	O6-C4-C5-O7
31	C	519	DGD	CAB-CBB-CCB-CDB
31	C	518	DGD	O6D-C1D-O3G-C3G
31	C	517	DGD	C5A-C6A-C7A-C8A
28	A	611	PL9	C19-C21-C22-C23
29	B	620	LMG	C7-C8-C9-O8
29	D	411	LMG	C7-C8-C9-O8
30	B	624	SQD	O6-C44-C45-C46
31	c	515	DGD	O1G-C1G-C2G-C3G
25	b	611	CLA	C10-C11-C12-C13
35	e	101	HEM	C4B-C3B-CAB-CBB
31	H	102	DGD	C6B-C7B-C8B-C9B
32	t	102	STE	C3-C4-C5-C6
25	c	509	CLA	C15-C16-C17-C18
30	f	101	SQD	C27-C28-C29-C30
31	C	519	DGD	C4A-C5A-C6A-C7A
31	c	515	DGD	C8A-C9A-CAA-CBA
29	D	411	LMG	O7-C8-C9-O8
31	A	616	DGD	O1G-C1G-C2G-O2G
25	B	603	CLA	C11-C12-C13-C14
25	B	613	CLA	C11-C12-C13-C14
25	C	507	CLA	C11-C12-C13-C14
25	D	404	CLA	C11-C12-C13-C14
25	a	607	CLA	C14-C13-C15-C16
25	b	604	CLA	C11-C12-C13-C14
25	b	607	CLA	C11-C12-C13-C14
31	C	517	DGD	CAB-CBB-CCB-CDB
33	d	407	LHG	C33-C34-C35-C36
31	H	102	DGD	C6A-C7A-C8A-C9A
29	c	518	LMG	C28-C29-C30-C31
30	A	615	SQD	C30-C31-C32-C33
31	C	517	DGD	CCA-CDA-CEA-CFA
31	c	515	DGD	C7A-C8A-C9A-CAA
31	c	515	DGD	C4D-C5D-C6D-O5D
30	b	620	SQD	C17-C18-C19-C20
25	c	506	CLA	C2-C1-O2A-CGA
25	b	613	CLA	C16-C17-C18-C19
25	B	614	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	c	513	CLA	C5-C6-C7-C8
32	b	623	STE	C11-C12-C13-C14
32	C	522	STE	C4-C5-C6-C7
25	c	505	CLA	C16-C17-C18-C19
25	A	607	CLA	C13-C15-C16-C17
27	x	101	BCR	C14-C15-C16-C17
29	c	518	LMG	C31-C32-C33-C34
30	B	624	SQD	C30-C31-C32-C33
30	f	101	SQD	C33-C34-C35-C36
31	C	518	DGD	C5B-C6B-C7B-C8B
31	a	616	DGD	C6A-C7A-C8A-C9A
32	X	101	STE	C11-C10-C9-C8
32	c	519	STE	C3-C4-C5-C6
29	B	620	LMG	C14-C15-C16-C17
29	B	620	LMG	C39-C40-C41-C42
29	c	522	LMG	C32-C33-C34-C35
31	a	616	DGD	CCA-CDA-CEA-CFA
25	b	609	CLA	C13-C15-C16-C17
33	d	408	LHG	O1-C1-C2-O2
33	B	623	LHG	C12-C13-C14-C15
25	B	601	CLA	C4B-C3B-CAB-CBB
25	c	512	CLA	C1A-C2A-CAA-CBA
29	m	101	LMG	C29-C28-O8-C9
29	A	613	LMG	C14-C15-C16-C17
29	B	620	LMG	C13-C14-C15-C16
31	C	517	DGD	C2A-C3A-C4A-C5A
33	D	410	LHG	C7-C8-C9-C10
32	B	626	STE	C4-C5-C6-C7
25	c	510	CLA	C2-C3-C5-C6
32	I	101	STE	C5-C6-C7-C8
29	c	522	LMG	C11-C12-C13-C14
33	D	412	LHG	C11-C10-C9-C8
32	T	102	STE	C11-C12-C13-C14
33	B	623	LHG	O6-C4-C5-C6
33	l	101	LHG	O6-C4-C5-C6
25	b	602	CLA	C8-C10-C11-C12
30	B	624	SQD	C25-C26-C27-C28
33	D	412	LHG	C32-C33-C34-C35
25	B	606	CLA	C11-C10-C8-C7
25	B	615	CLA	C6-C7-C8-C10
25	B	615	CLA	C11-C12-C13-C15
25	C	504	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	C	512	CLA	C11-C10-C8-C7
25	b	601	CLA	C11-C12-C13-C15
25	b	603	CLA	C11-C12-C13-C15
25	b	606	CLA	C11-C10-C8-C7
29	c	522	LMG	C31-C32-C33-C34
30	D	408	SQD	C27-C28-C29-C30
33	a	613	LHG	C27-C28-C29-C30
25	B	603	CLA	C10-C11-C12-C13
29	b	622	LMG	C18-C19-C20-C21
31	H	102	DGD	C7A-C8A-C9A-CAA
33	d	408	LHG	C30-C31-C32-C33
25	b	607	CLA	CBA-CGA-O2A-C1
31	H	102	DGD	C2B-C3B-C4B-C5B
25	C	505	CLA	C13-C15-C16-C17
31	H	102	DGD	C7B-C8B-C9B-CAB
33	D	409	LHG	C28-C29-C30-C31
25	b	603	CLA	C16-C17-C18-C20
33	l	101	LHG	C29-C30-C31-C32
28	d	406	PL9	C43-C44-C46-C47
25	B	605	CLA	C15-C16-C17-C18
33	d	407	LHG	C28-C29-C30-C31
31	C	518	DGD	C1A-C2A-C3A-C4A
25	c	505	CLA	C6-C7-C8-C9
25	d	404	CLA	C11-C12-C13-C14
25	b	607	CLA	O1A-CGA-O2A-C1
29	A	613	LMG	C28-C29-C30-C31
25	b	612	CLA	C13-C15-C16-C17
31	c	516	DGD	C9B-CAB-CBB-CCB
31	C	518	DGD	CAA-CBA-CCA-CDA
31	c	515	DGD	O1G-C1G-C2G-O2G
32	E	102	STE	C3-C4-C5-C6
29	c	520	LMG	C36-C37-C38-C39
29	c	522	LMG	O1-C7-C8-C9
31	a	616	DGD	O1G-C1G-C2G-C3G
25	b	611	CLA	C4-C3-C5-C6
31	H	102	DGD	CDA-CEA-CFA-CGA
31	c	517	DGD	CCB-CDB-CEB-CFB
25	B	601	CLA	CAD-CBD-CGD-O2D
25	C	502	CLA	CAD-CBD-CGD-O2D
25	c	504	CLA	CAD-CBD-CGD-O2D
30	A	614	SQD	O10-C23-O48-C46
29	c	522	LMG	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
30	A	614	SQD	C24-C23-O48-C46
25	b	615	CLA	C8-C10-C11-C12
30	a	615	SQD	C15-C16-C17-C18
25	B	614	CLA	C16-C17-C18-C19
25	C	509	CLA	C3-C5-C6-C7
31	c	517	DGD	C4B-C5B-C6B-C7B
32	M	101	STE	C3-C4-C5-C6
25	B	608	CLA	C13-C15-C16-C17
30	A	615	SQD	C32-C33-C34-C35
32	c	521	STE	C6-C7-C8-C9
32	M	101	STE	C6-C7-C8-C9
25	B	601	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	504	CLA	CAD-CBD-CGD-O1D
25	C	509	CLA	CHA-CBD-CGD-O1D
25	b	616	CLA	CHA-CBD-CGD-O1D
25	b	616	CLA	CHA-CBD-CGD-O2D
25	c	504	CLA	CAD-CBD-CGD-O1D
33	D	409	LHG	C3-O3-P-O4
33	d	407	LHG	C3-O3-P-O5
33	d	407	LHG	C4-O6-P-O5
33	B	623	LHG	C31-C32-C33-C34
31	C	517	DGD	C8B-C9B-CAB-CBB
28	A	611	PL9	C47-C48-C49-C50
32	J	101	STE	C3-C4-C5-C6
33	B	623	LHG	C15-C16-C17-C18
25	B	601	CLA	C2B-C3B-CAB-CBB
25	C	502	CLA	C2B-C3B-CAB-CBB
25	b	601	CLA	C2B-C3B-CAB-CBB
31	c	516	DGD	C9A-CAA-CBA-CCA
32	b	624	STE	C11-C12-C13-C14
25	A	609	CLA	C2-C3-C5-C6
28	a	611	PL9	C38-C39-C41-C42
30	b	620	SQD	C11-C12-C13-C14
29	D	407	LMG	C35-C36-C37-C38
32	M	102	STE	C1-C2-C3-C4
25	b	605	CLA	C10-C11-C12-C13
25	C	504	CLA	C11-C12-C13-C14
30	a	614	SQD	C26-C27-C28-C29
31	A	616	DGD	CFB-CGB-CHB-CIB
29	b	622	LMG	C38-C39-C40-C41
32	b	623	STE	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
32	c	519	STE	C11-C10-C9-C8
25	C	508	CLA	C5-C6-C7-C8
26	a	608	PHO	C8-C10-C11-C12
32	I	101	STE	C1-C2-C3-C4
29	A	613	LMG	C32-C33-C34-C35
32	E	102	STE	C5-C6-C7-C8
33	d	407	LHG	C25-C26-C27-C28
33	d	408	LHG	C25-C26-C27-C28
31	c	516	DGD	C8B-C9B-CAB-CBB
33	l	101	LHG	C15-C16-C17-C18
33	l	101	LHG	C33-C34-C35-C36
25	A	607	CLA	C6-C7-C8-C9
25	B	605	CLA	C6-C7-C8-C9
25	B	606	CLA	C11-C12-C13-C14
25	C	509	CLA	C14-C13-C15-C16
25	b	601	CLA	C11-C10-C8-C9
25	b	612	CLA	C14-C13-C15-C16
31	C	519	DGD	C2B-C3B-C4B-C5B
25	C	505	CLA	C12-C13-C15-C16
25	b	613	CLA	C11-C10-C8-C7
27	K	101	BCR	C20-C21-C22-C23
30	a	615	SQD	C11-C12-C13-C14
33	D	410	LHG	C1-C2-C3-O3
32	B	626	STE	C2-C3-C4-C5
32	J	101	STE	C2-C3-C4-C5
25	b	605	CLA	C16-C17-C18-C20
33	B	623	LHG	C10-C11-C12-C13
31	C	517	DGD	O1A-C1A-O1G-C1G
30	a	615	SQD	C10-C11-C12-C13
31	c	517	DGD	C1B-C2B-C3B-C4B
25	b	603	CLA	C16-C17-C18-C19
31	c	515	DGD	C9A-CAA-CBA-CCA
33	D	412	LHG	C18-C19-C20-C21
31	H	102	DGD	C4B-C5B-C6B-C7B
33	B	623	LHG	C26-C27-C28-C29
28	a	611	PL9	C37-C38-C39-C40
29	D	411	LMG	C11-C12-C13-C14
31	C	517	DGD	O1G-C1G-C2G-O2G
31	a	616	DGD	O1G-C1G-C2G-O2G
33	B	623	LHG	C33-C34-C35-C36
33	B	623	LHG	C24-C25-C26-C27
29	c	518	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
25	A	606	CLA	C16-C17-C18-C20
31	H	102	DGD	CAB-CBB-CCB-CDB
25	C	501	CLA	C2A-CAA-CBA-CGA
31	A	616	DGD	O6D-C5D-C6D-O5D
25	C	509	CLA	C2-C1-O2A-CGA
30	A	615	SQD	C24-C25-C26-C27
31	a	616	DGD	CAA-CBA-CCA-CDA
25	a	607	CLA	C15-C16-C17-C18
29	C	520	LMG	O1-C7-C8-C9
31	a	616	DGD	C5B-C6B-C7B-C8B
29	b	622	LMG	C28-C29-C30-C31
30	a	614	SQD	C23-C24-C25-C26
33	a	613	LHG	C25-C26-C27-C28
30	D	408	SQD	O48-C23-C24-C25
25	D	403	CLA	C2C-C3C-CAC-CBC
33	d	407	LHG	C15-C16-C17-C18
33	D	410	LHG	C27-C28-C29-C30
25	c	513	CLA	C2A-CAA-CBA-CGA
25	C	511	CLA	C16-C17-C18-C20
25	B	604	CLA	CBD-CGD-O2D-CED
31	c	516	DGD	C8A-C9A-CAA-CBA
29	D	411	LMG	C37-C38-C39-C40
31	c	515	DGD	O1G-C1A-C2A-C3A
31	h	101	DGD	O2G-C1B-C2B-C3B
25	B	602	CLA	C11-C12-C13-C14
25	B	604	CLA	C11-C12-C13-C14
31	C	519	DGD	C3B-C4B-C5B-C6B
25	c	510	CLA	CBA-CGA-O2A-C1
29	C	520	LMG	C29-C28-O8-C9
31	C	519	DGD	C7A-C8A-C9A-CAA
30	B	624	SQD	C23-C24-C25-C26
32	B	621	STE	C2-C3-C4-C5
25	A	606	CLA	C4C-C3C-CAC-CBC
25	b	610	CLA	C16-C17-C18-C20
31	A	616	DGD	C4D-C5D-C6D-O5D
33	D	412	LHG	C24-C23-O8-C6
25	b	611	CLA	C8-C10-C11-C12
33	E	101	LHG	C19-C20-C21-C22
31	a	616	DGD	CFB-CGB-CHB-CIB
29	m	101	LMG	C30-C31-C32-C33
25	b	611	CLA	C2-C3-C5-C6
31	C	518	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
31	c	515	DGD	O1A-C1A-O1G-C1G
29	D	411	LMG	C29-C30-C31-C32
25	B	602	CLA	C11-C12-C13-C15
25	c	509	CLA	C11-C12-C13-C15
25	b	604	CLA	C5-C6-C7-C8
29	D	407	LMG	C11-C12-C13-C14
33	l	101	LHG	C34-C35-C36-C37
25	c	510	CLA	O1A-CGA-O2A-C1
29	c	520	LMG	C38-C39-C40-C41
30	A	615	SQD	O49-C7-O47-C45
33	a	613	LHG	C26-C27-C28-C29
25	C	511	CLA	C16-C17-C18-C19
29	D	411	LMG	C16-C17-C18-C19
25	B	601	CLA	C3A-C2A-CAA-CBA
31	c	515	DGD	C4A-C5A-C6A-C7A
33	e	102	LHG	C24-C25-C26-C27
33	a	613	LHG	C19-C20-C21-C22
33	E	101	LHG	C2-C3-O3-P
33	d	408	LHG	C2-C3-O3-P
32	b	621	STE	C11-C12-C13-C14
25	b	610	CLA	C8-C10-C11-C12
30	f	101	SQD	C24-C25-C26-C27
36	v	201	HEC	CAD-CBD-CGD-O1D
25	c	506	CLA	C15-C16-C17-C18
31	h	101	DGD	CAB-CBB-CCB-CDB
25	c	508	CLA	C4-C3-C5-C6
25	c	512	CLA	C4-C3-C5-C6
29	B	622	LMG	C31-C32-C33-C34
32	b	621	STE	O1-C1-C2-C3
28	A	611	PL9	C39-C41-C42-C43
31	C	517	DGD	O6D-C5D-C6D-O5D
31	C	519	DGD	O6D-C5D-C6D-O5D
31	a	616	DGD	CFA-CGA-CHA-CIA
31	C	517	DGD	C3A-C4A-C5A-C6A
25	a	609	CLA	C6-C7-C8-C9
25	b	603	CLA	C6-C7-C8-C9
25	b	616	CLA	C11-C10-C8-C9
25	c	506	CLA	C11-C12-C13-C14
25	c	512	CLA	C11-C12-C13-C14
31	C	519	DGD	C2A-C3A-C4A-C5A
33	e	102	LHG	C19-C20-C21-C22
25	c	509	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
32	b	621	STE	C11-C10-C9-C8
33	D	410	LHG	C14-C15-C16-C17
29	A	613	LMG	C9-C8-O7-C10
31	a	616	DGD	C1G-C2G-O2G-C1B
29	B	622	LMG	O7-C10-C11-C12
36	v	201	HEC	CAD-CBD-CGD-O2D
29	c	522	LMG	C36-C37-C38-C39
31	a	616	DGD	C7B-C8B-C9B-CAB
28	A	611	PL9	C13-C14-C16-C17
32	M	101	STE	O1-C1-C2-C3
32	M	101	STE	O2-C1-C2-C3
32	c	519	STE	O1-C1-C2-C3
25	c	501	CLA	C2A-CAA-CBA-CGA
25	c	503	CLA	C1A-C2A-CAA-CBA
29	C	520	LMG	C18-C19-C20-C21
25	B	606	CLA	C2B-C3B-CAB-CBB
25	c	503	CLA	C2B-C3B-CAB-CBB
27	A	610	BCR	C23-C24-C25-C30
27	D	405	BCR	C23-C24-C25-C26
27	H	101	BCR	C23-C24-C25-C30
27	b	617	BCR	C5-C6-C7-C8
27	k	101	BCR	C1-C6-C7-C8
27	k	101	BCR	C23-C24-C25-C26
27	x	101	BCR	C23-C24-C25-C30
35	F	101	HEM	CAD-CBD-CGD-O2D
25	b	616	CLA	C10-C11-C12-C13
29	m	101	LMG	C13-C14-C15-C16
32	b	621	STE	C9-C10-C11-C12
32	B	628	STE	C4-C5-C6-C7
25	b	616	CLA	C2-C3-C5-C6
32	b	621	STE	O2-C1-C2-C3
36	V	201	HEC	CAD-CBD-CGD-O2D
25	A	607	CLA	C6-C7-C8-C10
25	B	604	CLA	C11-C12-C13-C15
25	C	503	CLA	C11-C10-C8-C7
25	C	509	CLA	C11-C10-C8-C7
25	b	603	CLA	C6-C7-C8-C10
25	b	605	CLA	C11-C10-C8-C7
25	b	612	CLA	C12-C13-C15-C16
30	a	614	SQD	O47-C45-C46-O48
30	b	620	SQD	O6-C44-C45-O47
31	c	516	DGD	O1G-C1G-C2G-O2G

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Mol	Chain	Res	Type	Atoms
32	c	519	STE	O2-C1-C2-C3
32	B	626	STE	C5-C6-C7-C8
31	A	616	DGD	CDB-CEB-CFB-CGB
33	l	101	LHG	C31-C32-C33-C34
25	b	606	CLA	C16-C17-C18-C19
29	D	407	LMG	C14-C15-C16-C17
32	a	617	STE	C6-C7-C8-C9
32	H	103	STE	C1-C2-C3-C4
25	C	509	CLA	C8-C10-C11-C12
29	B	622	LMG	O9-C10-C11-C12
25	c	505	CLA	C5-C6-C7-C8
25	c	508	CLA	C2-C3-C5-C6
25	c	512	CLA	C2-C3-C5-C6
32	B	621	STE	C6-C7-C8-C9
32	a	617	STE	C7-C8-C9-C10
29	b	622	LMG	C32-C33-C34-C35
25	A	606	CLA	C15-C16-C17-C18
32	B	626	STE	O2-C1-C2-C3
25	b	615	CLA	C16-C17-C18-C20
25	D	403	CLA	C3-C5-C6-C7
29	c	522	LMG	C17-C18-C19-C20
32	d	411	STE	O2-C1-C2-C3
36	V	201	HEC	CAD-CBD-CGD-O1D
31	h	101	DGD	O1B-C1B-C2B-C3B
29	B	622	LMG	C32-C33-C34-C35
29	C	520	LMG	C15-C16-C17-C18
25	B	605	CLA	C8-C10-C11-C12
33	D	412	LHG	C24-C25-C26-C27
30	A	615	SQD	C19-C20-C21-C22
30	a	614	SQD	O10-C23-O48-C46
25	C	507	CLA	C4-C3-C5-C6
28	A	611	PL9	C30-C29-C31-C32
35	F	101	HEM	CAD-CBD-CGD-O1D
31	c	516	DGD	CBB-CCB-CDB-CEB
31	h	101	DGD	CDA-CEA-CFA-CGA
25	b	615	CLA	C16-C17-C18-C19
25	b	608	CLA	CBA-CGA-O2A-C1
29	B	620	LMG	O9-C10-O7-C8
32	d	411	STE	C3-C4-C5-C6
32	b	621	STE	C12-C13-C14-C15
25	b	613	CLA	C13-C15-C16-C17
25	C	506	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	v	201	HEC	C2B-C3B-CAB-CBB
31	C	518	DGD	C3B-C4B-C5B-C6B
32	B	627	STE	O2-C1-C2-C3
31	C	517	DGD	O1G-C1A-C2A-C3A
31	H	102	DGD	O2G-C1B-C2B-C3B
30	b	620	SQD	C29-C30-C31-C32
29	d	410	LMG	C34-C35-C36-C37
25	b	608	CLA	O1A-CGA-O2A-C1
25	C	501	CLA	C16-C17-C18-C20
26	D	402	PHO	CHA-CBD-CGD-O1D
26	D	402	PHO	CHA-CBD-CGD-O2D
27	B	618	BCR	C20-C21-C22-C37
27	k	103	BCR	C20-C21-C22-C37
27	t	101	BCR	C20-C21-C22-C37
25	B	612	CLA	C13-C15-C16-C17
25	c	509	CLA	C3-C5-C6-C7
29	m	101	LMG	C40-C41-C42-C43
31	h	101	DGD	CDB-CEB-CFB-CGB
25	C	506	CLA	CBD-CGD-O2D-CED
30	a	614	SQD	C29-C30-C31-C32
33	D	412	LHG	C10-C11-C12-C13
25	c	506	CLA	C11-C12-C13-C15
32	d	412	STE	C14-C15-C16-C17
32	c	521	STE	C1-C2-C3-C4
31	C	519	DGD	C5B-C6B-C7B-C8B
32	C	522	STE	C1-C2-C3-C4
32	b	624	STE	C5-C6-C7-C8
32	d	411	STE	O1-C1-C2-C3
25	C	508	CLA	C11-C10-C8-C9
25	C	510	CLA	C6-C7-C8-C9
25	b	603	CLA	C11-C12-C13-C14
25	c	507	CLA	C6-C7-C8-C9
31	A	616	DGD	C6A-C7A-C8A-C9A
32	B	626	STE	O1-C1-C2-C3
25	B	614	CLA	C2A-CAA-CBA-CGA
25	B	613	CLA	C2-C1-O2A-CGA
25	C	506	CLA	C2-C1-O2A-CGA
25	D	403	CLA	C2-C1-O2A-CGA
30	a	614	SQD	C24-C23-O48-C46
29	D	411	LMG	C33-C34-C35-C36
25	B	601	CLA	C4-C3-C5-C6
25	c	512	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	c	515	DGD	CAA-CBA-CCA-CDA
25	a	606	CLA	C2C-C3C-CAC-CBC
32	j	101	STE	C1-C2-C3-C4
30	B	624	SQD	C29-C30-C31-C32
30	B	624	SQD	C33-C34-C35-C36
29	c	522	LMG	C9-C8-O7-C10
27	k	101	BCR	C10-C11-C12-C13
29	d	410	LMG	C30-C31-C32-C33
30	D	408	SQD	C24-C25-C26-C27
32	b	623	STE	C2-C3-C4-C5
27	k	102	BCR	C14-C15-C16-C17
25	b	608	CLA	C16-C17-C18-C19
33	B	623	LHG	C14-C15-C16-C17
32	I	101	STE	C2-C3-C4-C5
25	b	609	CLA	C4-C3-C5-C6
30	a	615	SQD	C17-C18-C19-C20
31	c	517	DGD	CCA-CDA-CEA-CFA
32	B	627	STE	O1-C1-C2-C3
29	C	520	LMG	C36-C37-C38-C39
31	C	517	DGD	C4D-C5D-C6D-O5D
32	b	621	STE	C5-C6-C7-C8
29	A	613	LMG	O1-C7-C8-C9
29	A	613	LMG	C7-C8-C9-O8
29	B	620	LMG	O1-C7-C8-C9
30	f	101	SQD	O6-C44-C45-C46
33	e	102	LHG	C4-C5-C6-O8
25	B	607	CLA	C8-C10-C11-C12
35	F	101	HEM	C4C-C3C-CAC-CBC
29	c	518	LMG	C34-C35-C36-C37
33	D	410	LHG	C15-C16-C17-C18
25	C	505	CLA	C8-C10-C11-C12
33	l	101	LHG	C18-C19-C20-C21
30	a	615	SQD	O48-C23-C24-C25
29	c	522	LMG	O1-C7-C8-O7
25	b	610	CLA	C15-C16-C17-C18
27	T	101	BCR	C14-C15-C16-C17
25	B	607	CLA	C11-C10-C8-C9
25	B	614	CLA	C11-C12-C13-C14
25	B	615	CLA	C6-C7-C8-C9
25	D	404	CLA	C6-C7-C8-C9
25	b	605	CLA	C11-C12-C13-C14
25	b	607	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	C	512	CLA	C16-C17-C18-C20
25	B	612	CLA	CAA-CBA-CGA-O2A
32	C	523	STE	C3-C4-C5-C6
30	f	101	SQD	O48-C23-C24-C25
25	B	607	CLA	C12-C13-C15-C16
25	C	508	CLA	C11-C10-C8-C7
25	C	510	CLA	C6-C7-C8-C10
25	a	609	CLA	C6-C7-C8-C10
25	b	610	CLA	C2B-C3B-CAB-CBB
25	c	501	CLA	C2B-C3B-CAB-CBB
27	A	610	BCR	C23-C24-C25-C26
27	B	617	BCR	C5-C6-C7-C8
27	B	618	BCR	C23-C24-C25-C30
27	H	101	BCR	C23-C24-C25-C26
27	k	101	BCR	C5-C6-C7-C8
27	k	103	BCR	C1-C6-C7-C8
27	k	103	BCR	C5-C6-C7-C8
27	x	101	BCR	C23-C24-C25-C26
25	d	404	CLA	C5-C6-C7-C8
30	A	615	SQD	C8-C7-O47-C45
29	C	520	LMG	C39-C40-C41-C42
31	c	516	DGD	C5B-C6B-C7B-C8B
30	B	624	SQD	C12-C13-C14-C15
30	a	614	SQD	C15-C16-C17-C18
25	b	613	CLA	C16-C17-C18-C20
31	c	517	DGD	CDB-CEB-CFB-CGB
32	B	629	STE	C7-C8-C9-C10
25	B	612	CLA	CBA-CGA-O2A-C1
25	B	613	CLA	C4-C3-C5-C6
25	b	609	CLA	C2-C3-C5-C6
25	b	614	CLA	C2A-CAA-CBA-CGA
29	m	101	LMG	C20-C21-C22-C23
31	C	518	DGD	C9B-CAB-CBB-CCB
33	e	102	LHG	O8-C23-C24-C25
33	a	613	LHG	C11-C12-C13-C14
32	d	412	STE	C2-C3-C4-C5
33	l	101	LHG	C32-C33-C34-C35
31	c	515	DGD	C4E-C5E-C6E-O5E
32	d	411	STE	C12-C13-C14-C15
27	k	103	BCR	C19-C20-C21-C22
33	d	408	LHG	C29-C30-C31-C32
31	c	517	DGD	C7A-C8A-C9A-CAA

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Mol	Chain	Res	Type	Atoms
28	A	611	PL9	C18-C19-C21-C22
35	e	101	HEM	CAD-CBD-CGD-O2D
31	c	515	DGD	O1B-C1B-O2G-C2G
35	e	101	HEM	CAD-CBD-CGD-O1D
25	b	607	CLA	C11-C10-C8-C9
33	e	102	LHG	C16-C17-C18-C19
31	c	515	DGD	C1G-C2G-C3G-O3G
25	B	602	CLA	C1A-C2A-CAA-CBA
25	C	504	CLA	C4B-C3B-CAB-CBB
25	C	508	CLA	C1A-C2A-CAA-CBA
29	b	622	LMG	C36-C37-C38-C39
25	b	613	CLA	C4-C3-C5-C6
28	a	611	PL9	C25-C24-C26-C27
25	b	613	CLA	CAA-CBA-CGA-O2A
29	B	620	LMG	C15-C16-C17-C18
33	d	407	LHG	C11-C10-C9-C8
25	C	507	CLA	C2-C3-C5-C6
32	B	627	STE	C12-C13-C14-C15
32	C	523	STE	C12-C13-C14-C15
35	e	101	HEM	CAA-CBA-CGA-O2A
29	c	522	LMG	C4-C5-C6-O5
25	A	607	CLA	C2C-C3C-CAC-CBC
25	B	607	CLA	C11-C10-C8-C7
25	b	605	CLA	C11-C12-C13-C15
25	b	611	CLA	C12-C13-C15-C16
25	c	509	CLA	C6-C7-C8-C10
30	D	408	SQD	C32-C33-C34-C35
26	a	608	PHO	O2A-C1-C2-C3
25	c	508	CLA	C10-C11-C12-C13
32	B	621	STE	C10-C11-C12-C13
29	b	622	LMG	C39-C40-C41-C42
29	m	101	LMG	C12-C13-C14-C15
25	c	507	CLA	C8-C10-C11-C12
32	b	621	STE	C4-C5-C6-C7
25	B	610	CLA	C2A-CAA-CBA-CGA
25	d	404	CLA	C16-C17-C18-C19
29	B	620	LMG	C28-C29-C30-C31
25	B	602	CLA	C3A-C2A-CAA-CBA
25	B	603	CLA	C4-C3-C5-C6
26	d	402	PHO	C3A-C2A-CAA-CBA
25	b	604	CLA	C16-C17-C18-C19
25	c	502	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
31	a	616	DGD	O1G-C1A-C2A-C3A
26	A	608	PHO	C8-C10-C11-C12
29	c	520	LMG	C29-C30-C31-C32
31	c	515	DGD	O1B-C1B-C2B-C3B
25	C	505	CLA	C14-C13-C15-C16
25	b	606	CLA	C6-C7-C8-C9
25	c	512	CLA	C14-C13-C15-C16
32	j	101	STE	C4-C5-C6-C7
29	b	622	LMG	O9-C10-C11-C12
31	A	616	DGD	C8B-C9B-CAB-CBB
25	B	608	CLA	C4-C3-C5-C6
30	b	620	SQD	C13-C14-C15-C16
28	a	611	PL9	C28-C29-C31-C32
30	f	101	SQD	O10-C23-C24-C25
32	X	101	STE	C3-C4-C5-C6
25	A	612	CLA	C4C-C3C-CAC-CBC
31	a	616	DGD	O2G-C1B-C2B-C3B
25	b	612	CLA	C10-C11-C12-C13
29	b	622	LMG	C8-C7-O1-C1
29	m	101	LMG	C8-C7-O1-C1
31	C	517	DGD	C5D-C6D-O5D-C1E
29	C	520	LMG	O1-C7-C8-O7
33	e	102	LHG	O7-C5-C6-O8
31	C	518	DGD	C2D-C1D-O3G-C3G
25	B	612	CLA	CAA-CBA-CGA-O1A
31	c	516	DGD	O1B-C1B-C2B-C3B
25	b	612	CLA	CAA-CBA-CGA-O2A
29	C	520	LMG	O7-C10-C11-C12
30	B	624	SQD	C14-C15-C16-C17
25	A	606	CLA	C16-C17-C18-C19
31	h	101	DGD	C1G-C2G-C3G-O3G
29	m	101	LMG	O9-C10-C11-C12
30	a	615	SQD	O10-C23-C24-C25
33	D	410	LHG	O10-C23-C24-C25
25	A	612	CLA	C13-C15-C16-C17
35	e	101	HEM	CAA-CBA-CGA-O1A
31	C	517	DGD	O1B-C1B-C2B-C3B
33	B	623	LHG	O9-C7-C8-C9
25	C	504	CLA	CAD-CBD-CGD-O2D
25	D	404	CLA	CAD-CBD-CGD-O2D
26	A	608	PHO	CAD-CBD-CGD-O2D
30	A	615	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
33	e	102	LHG	O10-C23-C24-C25
30	A	615	SQD	O48-C23-C24-C25
33	D	410	LHG	O8-C23-C24-C25
30	a	615	SQD	O6-C44-C45-C46
30	A	615	SQD	C16-C17-C18-C19
25	c	509	CLA	C2A-CAA-CBA-CGA
31	H	102	DGD	C8B-C9B-CAB-CBB
25	b	613	CLA	CAA-CBA-CGA-O1A
30	b	620	SQD	O47-C7-C8-C9
29	B	622	LMG	C28-C29-C30-C31
31	A	616	DGD	CCA-CDA-CEA-CFA
31	a	616	DGD	O1B-C1B-C2B-C3B
30	A	614	SQD	C15-C16-C17-C18
31	A	616	DGD	C5A-C6A-C7A-C8A
31	A	616	DGD	CBB-CCB-CDB-CEB

There are no ring outliers.

147 monomers are involved in 267 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	D	405	BCR	2	0
25	B	613	CLA	3	0
25	D	404	CLA	4	0
22	a	602[A]	OEY	1	0
25	B	601	CLA	4	0
29	A	613	LMG	4	0
27	k	102	BCR	1	0
25	c	513	CLA	2	0
31	h	101	DGD	1	0
25	b	613	CLA	3	0
32	B	621	STE	2	0
25	c	508	CLA	1	0
33	d	407	LHG	4	0
25	B	616	CLA	1	0
25	b	601	CLA	3	0
25	B	611	CLA	1	0
22	A	602[A]	OEY	1	0
27	A	610	BCR	3	0
27	B	618	BCR	2	0
33	l	101	LHG	1	0
29	c	522	LMG	2	0
25	c	506	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	609	CLA	1	0
25	b	611	CLA	2	0
28	d	406	PL9	2	0
25	C	513	CLA	2	0
25	C	502	CLA	1	0
25	b	605	CLA	2	0
30	A	614	SQD	1	0
32	X	101	STE	2	0
25	b	606	CLA	3	0
25	b	610	CLA	2	0
30	A	615	SQD	1	0
31	c	515	DGD	3	0
29	D	407	LMG	2	0
25	c	504	CLA	2	0
25	b	615	CLA	2	0
27	B	617	BCR	1	0
30	f	101	SQD	1	0
31	c	517	DGD	2	0
25	b	609	CLA	3	0
35	e	101	HEM	4	0
30	b	620	SQD	1	0
25	a	606	CLA	3	0
26	D	402	PHO	2	0
25	c	507	CLA	2	0
25	a	609	CLA	5	0
28	D	406	PL9	1	0
27	x	101	BCR	2	0
33	d	408	LHG	1	0
25	C	507	CLA	1	0
28	a	611	PL9	7	0
32	b	621	STE	5	0
25	B	606	CLA	4	0
25	C	506	CLA	4	0
32	B	627	STE	1	0
36	v	201	HEC	2	0
25	B	615	CLA	2	0
27	t	101	BCR	2	0
32	b	624	STE	2	0
31	C	518	DGD	2	0
25	C	509	CLA	1	0
25	b	608	CLA	2	0
25	A	607	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	602	CLA	6	0
27	C	514	BCR	2	0
32	M	101	STE	1	0
25	b	602	CLA	1	0
27	C	515	BCR	5	0
31	C	519	DGD	2	0
25	b	616	CLA	2	0
32	H	103	STE	1	0
25	b	603	CLA	1	0
32	J	101	STE	1	0
25	c	512	CLA	1	0
25	d	403	CLA	2	0
25	c	505	CLA	4	0
25	B	610	CLA	2	0
25	A	606	CLA	1	0
31	c	516	DGD	2	0
25	D	403	CLA	3	0
28	A	611	PL9	5	0
29	B	620	LMG	2	0
35	F	101	HEM	2	0
31	a	616	DGD	6	0
27	c	514	BCR	3	0
25	A	609	CLA	1	0
29	d	409	LMG	2	0
25	c	511	CLA	4	0
29	C	520	LMG	2	0
32	C	523	STE	1	0
26	d	402	PHO	2	0
30	a	615	SQD	2	0
25	c	502	CLA	1	0
32	c	521	STE	1	0
25	C	508	CLA	1	0
29	c	520	LMG	1	0
25	B	603	CLA	3	0
25	c	510	CLA	3	0
25	a	612	CLA	2	0
25	C	511	CLA	1	0
25	c	503	CLA	4	0
33	E	101	LHG	3	0
31	H	102	DGD	2	0
33	a	613	LHG	1	0
32	d	412	STE	2	0

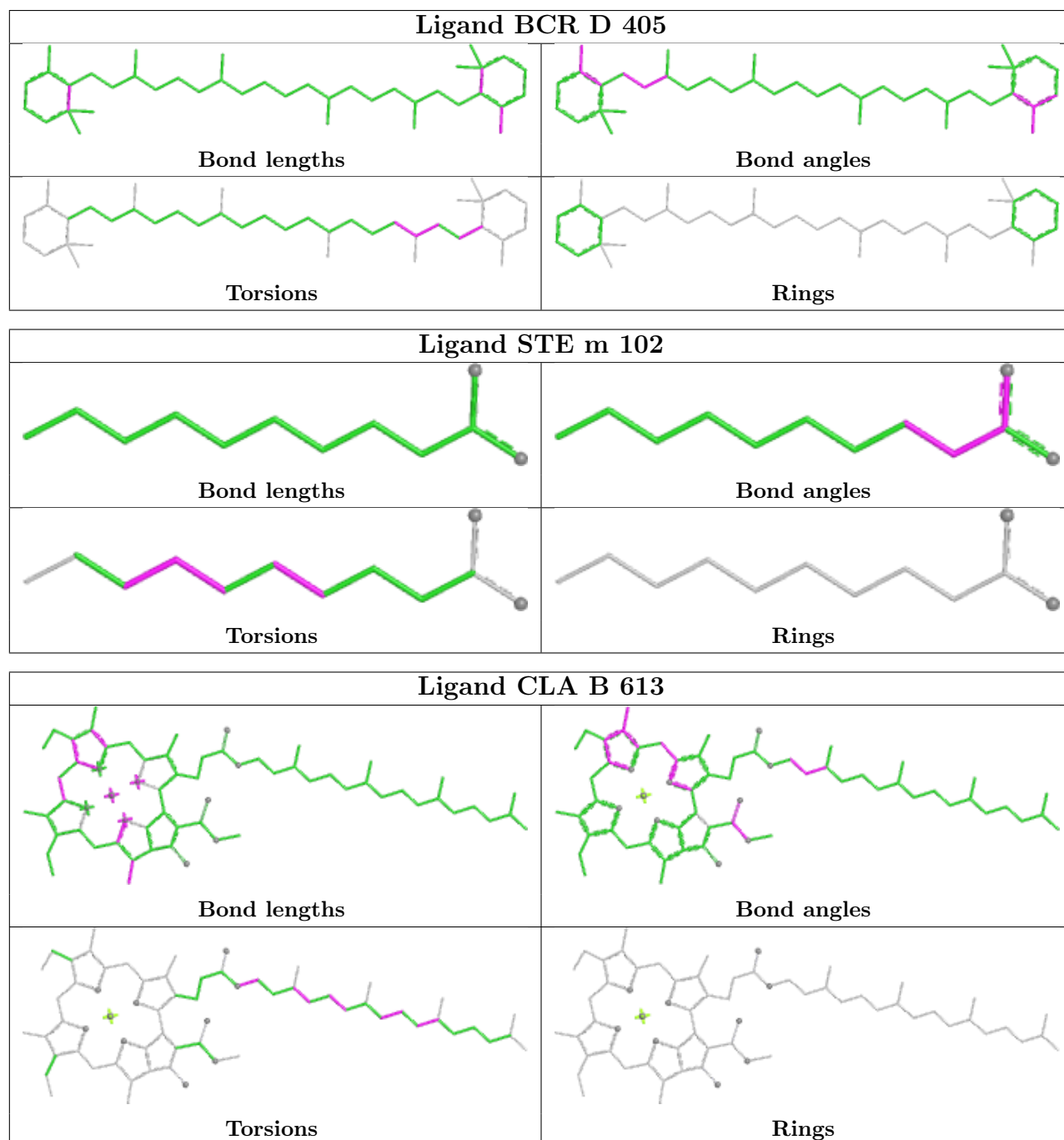
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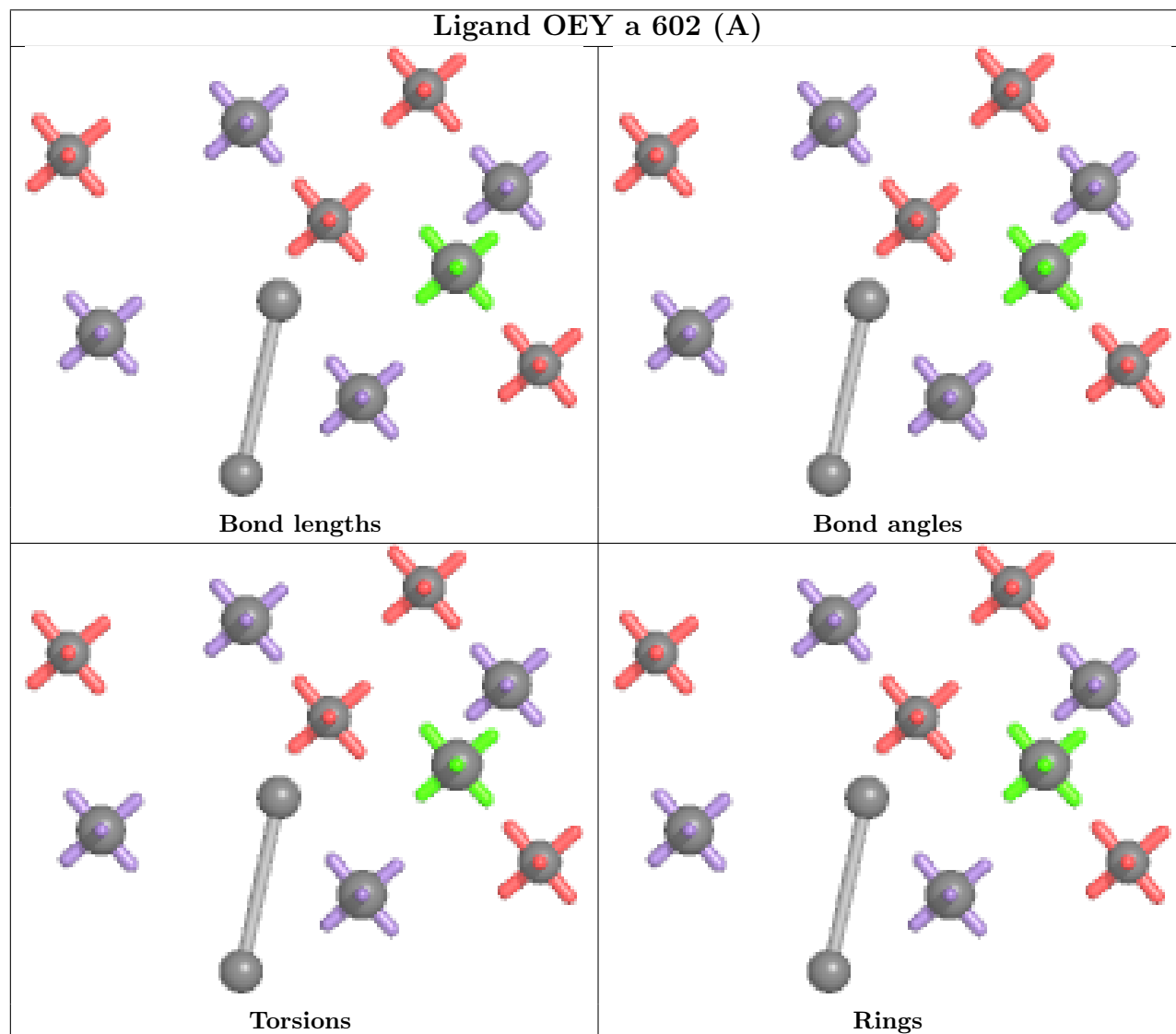
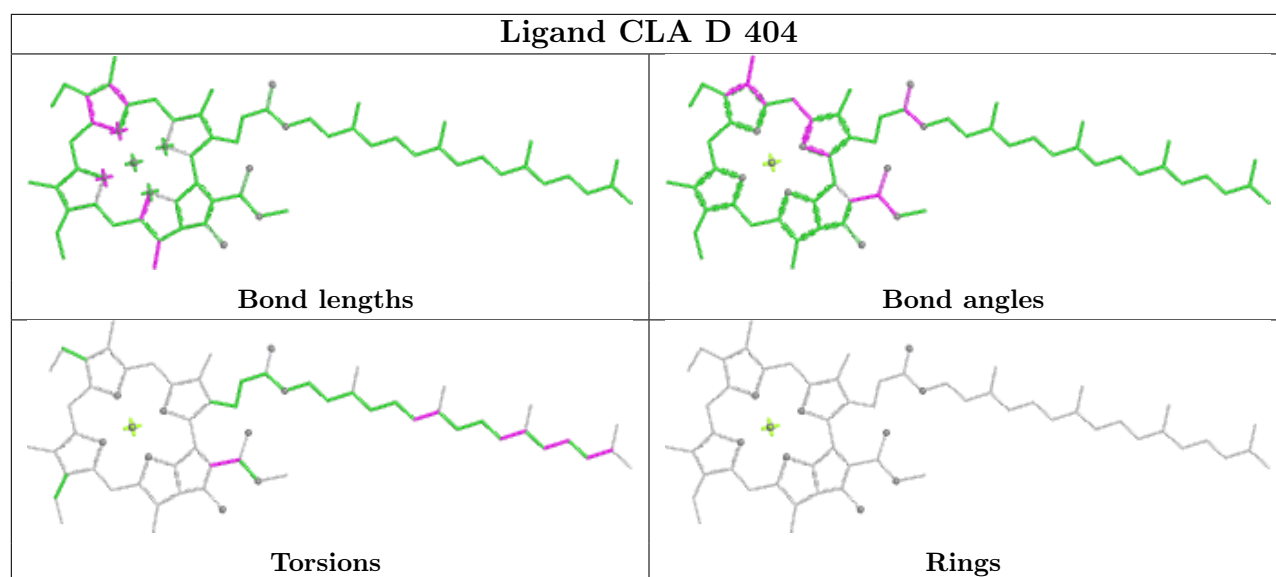
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	619	BCR	4	0
32	b	623	STE	2	0
25	B	607	CLA	4	0
25	B	605	CLA	3	0
30	D	408	SQD	1	0
25	B	614	CLA	2	0
27	b	617	BCR	1	0
25	B	604	CLA	3	0
32	B	625	STE	1	0
27	k	103	BCR	2	0
25	B	612	CLA	2	0
34	D	401	BCT	1	0
25	c	509	CLA	2	0
30	a	614	SQD	1	0
27	T	101	BCR	2	0
25	c	501	CLA	2	0
27	a	610	BCR	1	0
29	b	622	LMG	1	0
25	b	614	CLA	5	0
31	A	616	DGD	5	0
32	l	102	STE	1	0
26	A	608	PHO	1	0
32	I	101	STE	2	0
27	d	405	BCR	1	0
33	D	409	LHG	1	0
27	b	619	BCR	2	0
25	b	607	CLA	2	0
27	H	101	BCR	2	0
25	C	501	CLA	2	0
29	m	101	LMG	3	0
33	e	102	LHG	1	0
25	A	612	CLA	3	0
25	C	512	CLA	4	0
25	C	505	CLA	3	0
32	b	625	STE	1	0
27	b	618	BCR	2	0
33	B	623	LHG	2	0
25	a	607	CLA	2	0
29	D	411	LMG	1	0
25	b	604	CLA	1	0
33	D	412	LHG	4	0

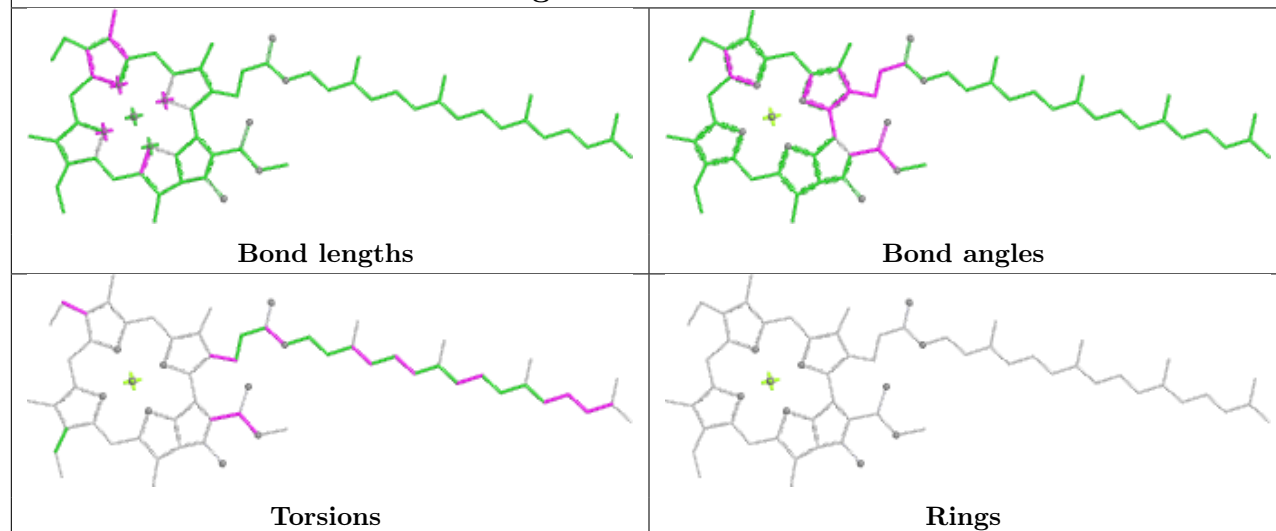
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

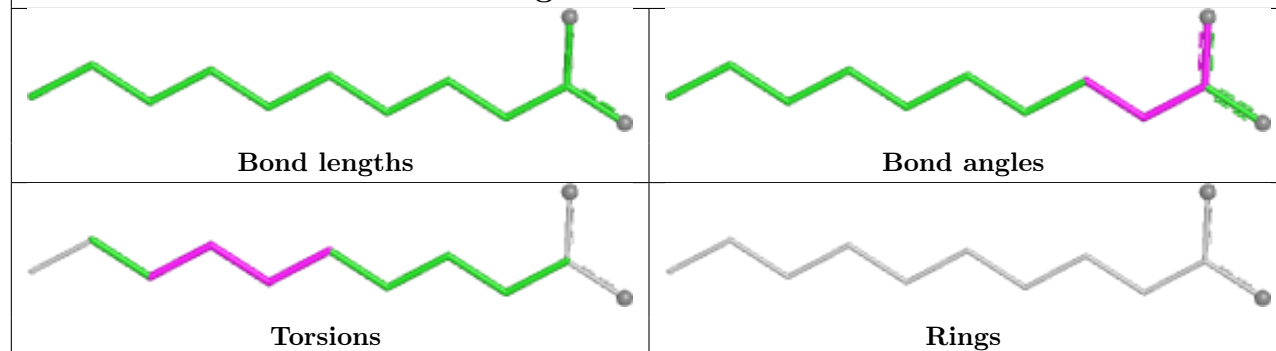




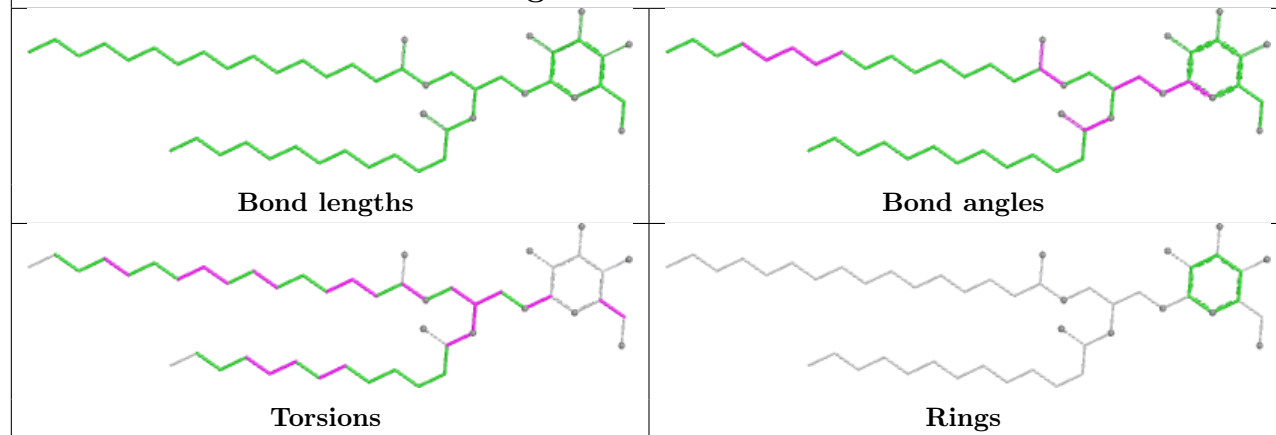
Ligand CLA B 601

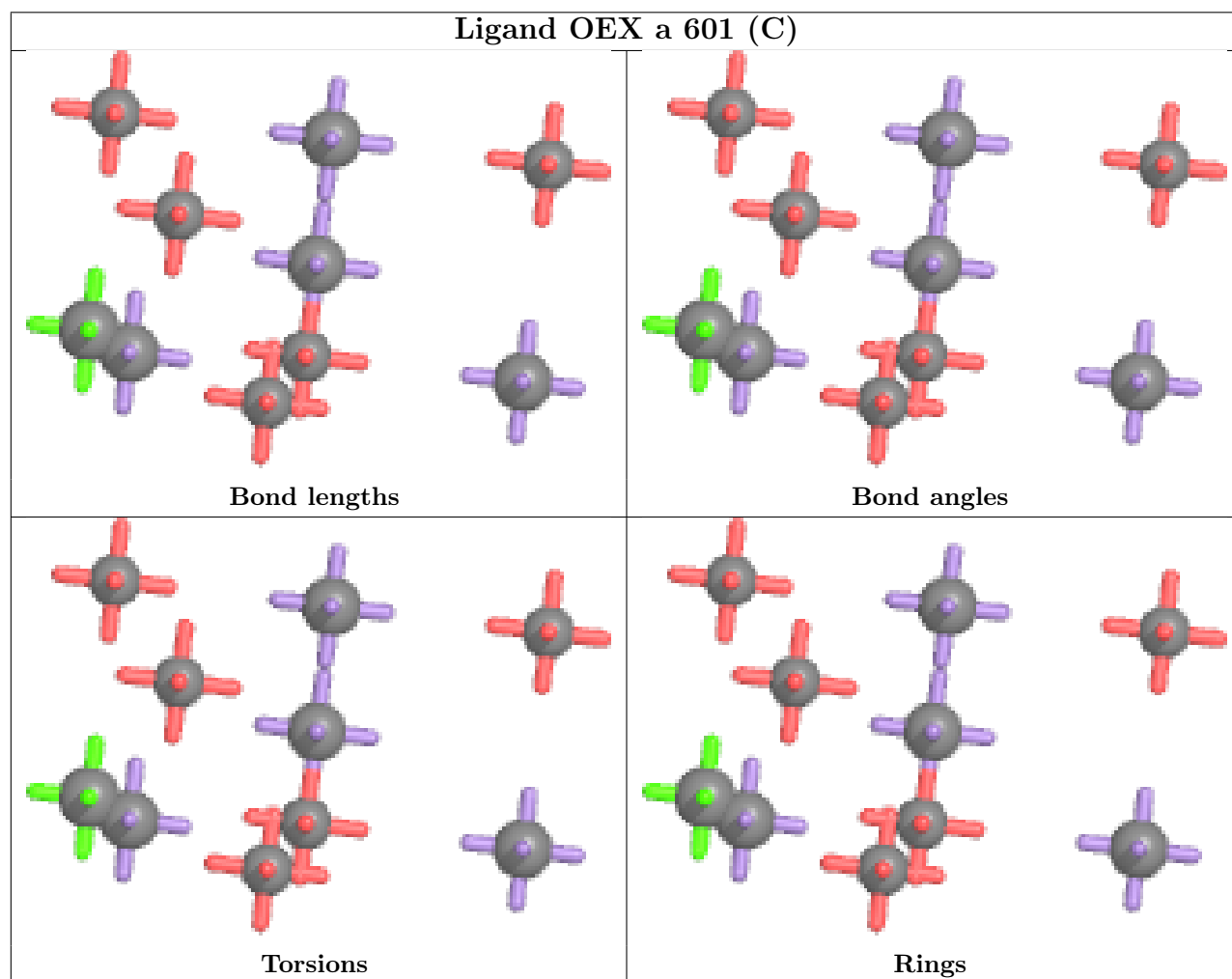
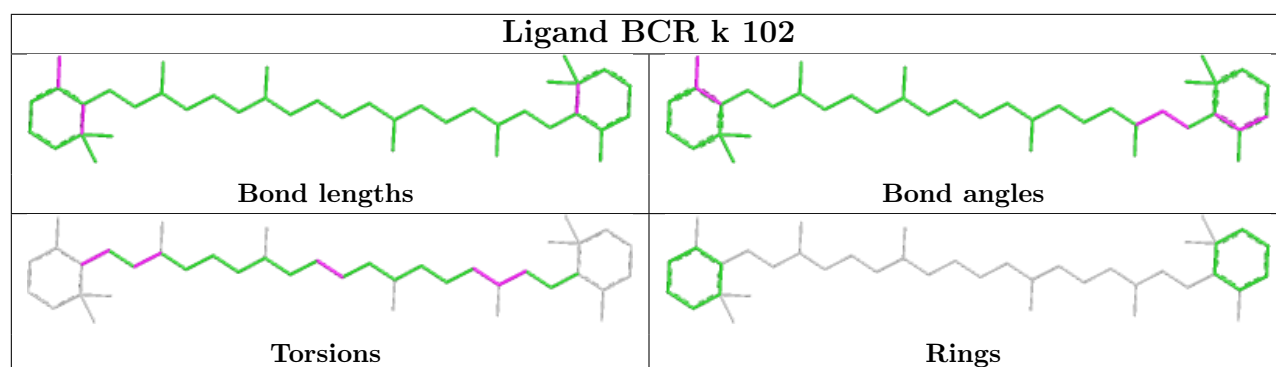


Ligand STE C 521

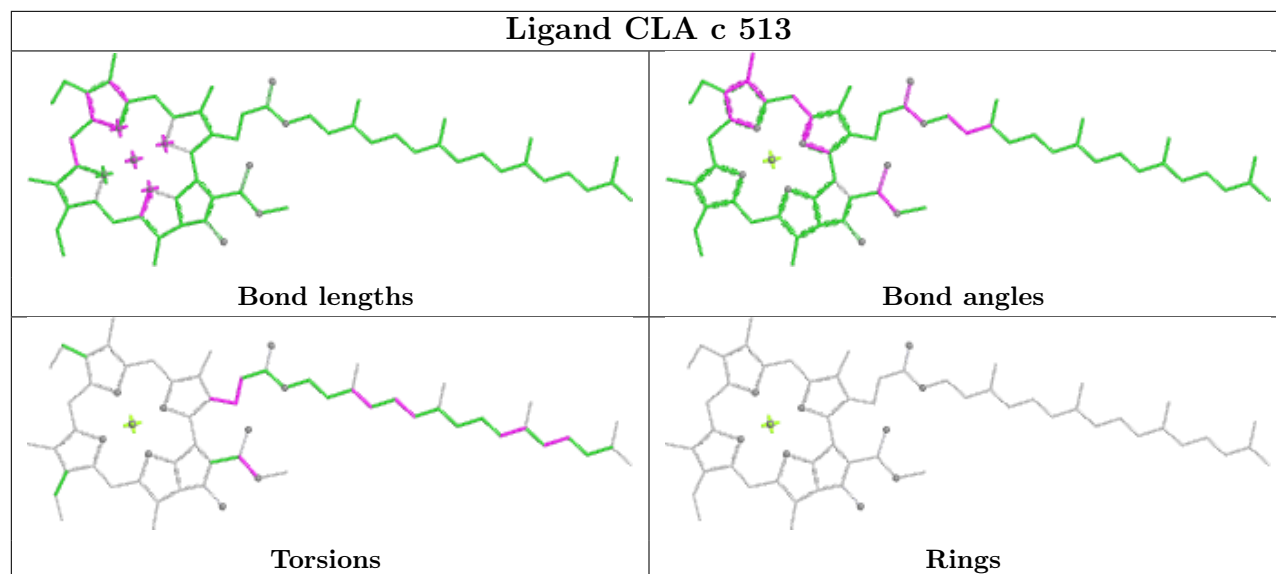


Ligand LMG A 613

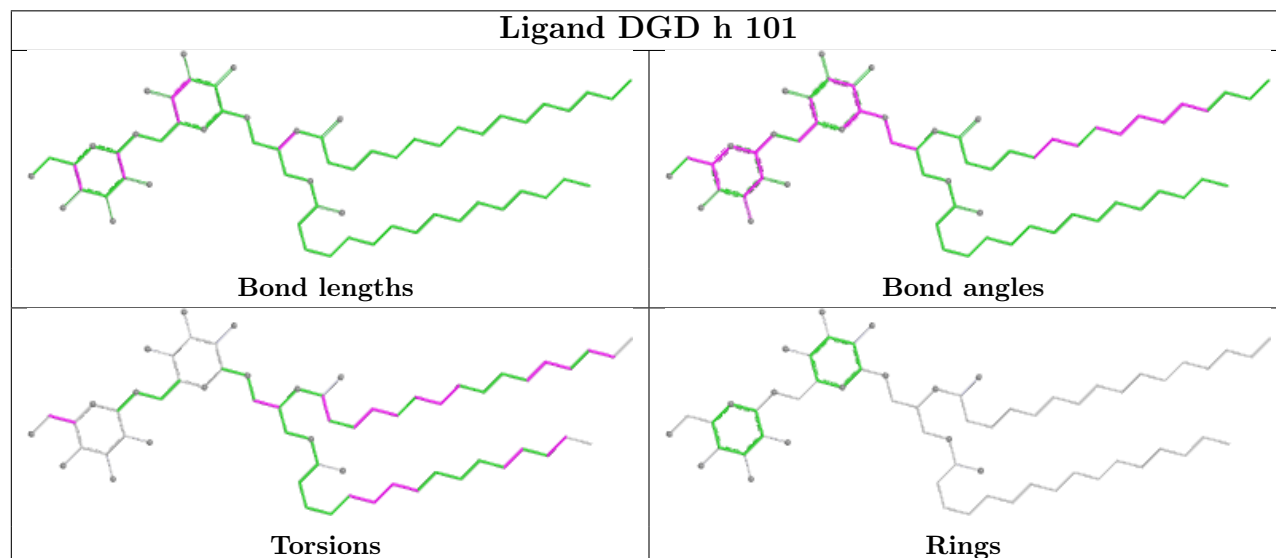




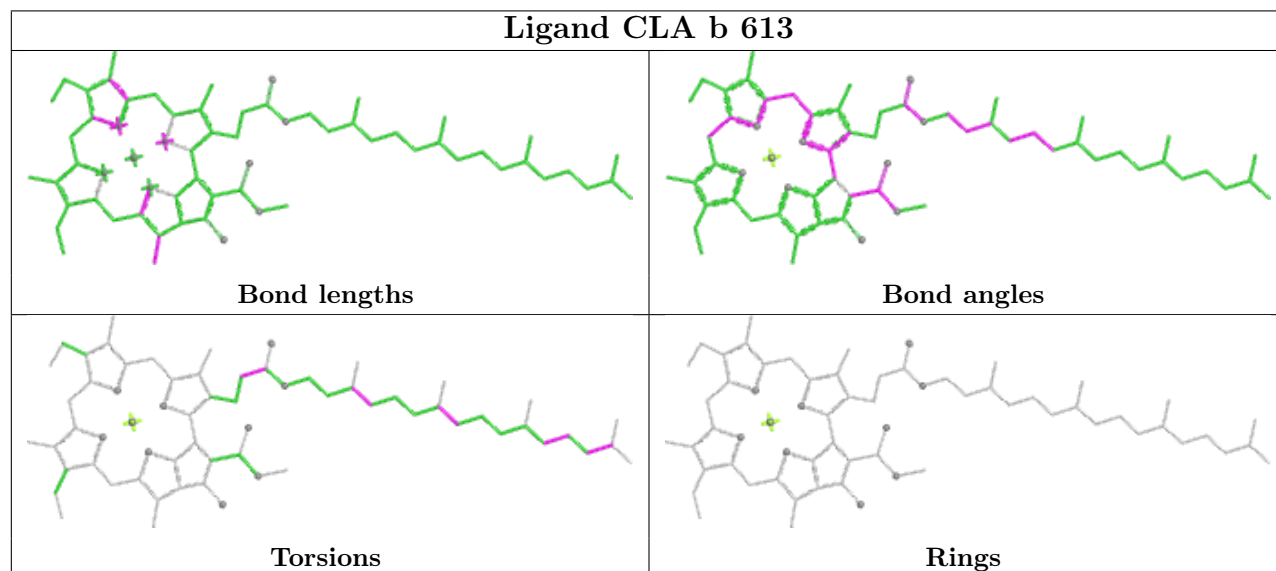
Ligand CLA c 513

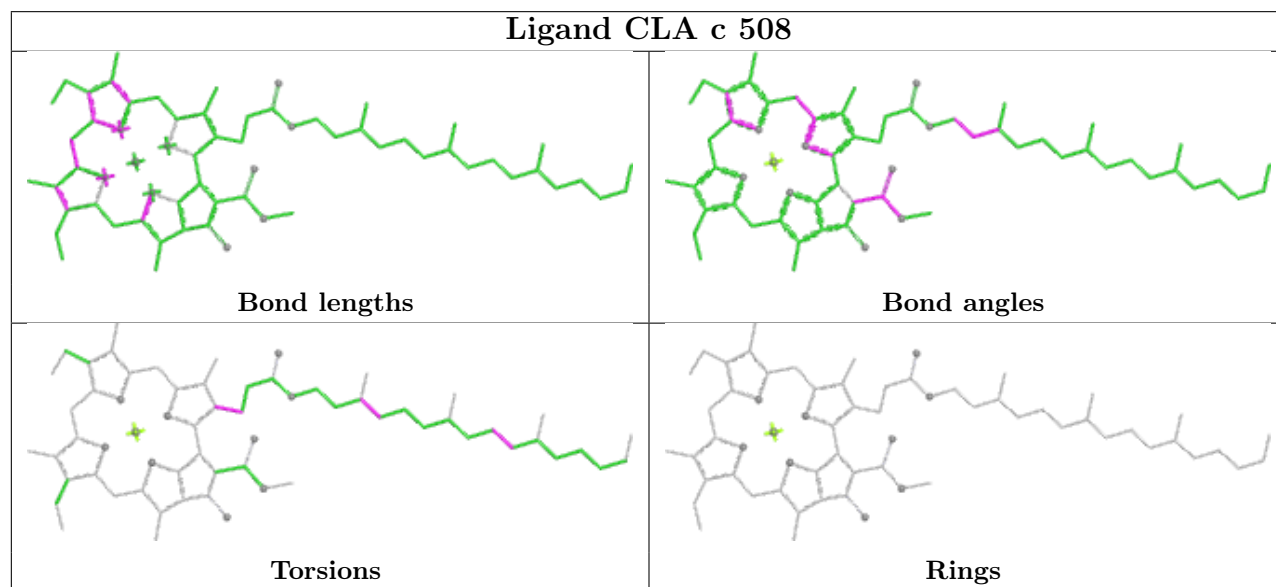
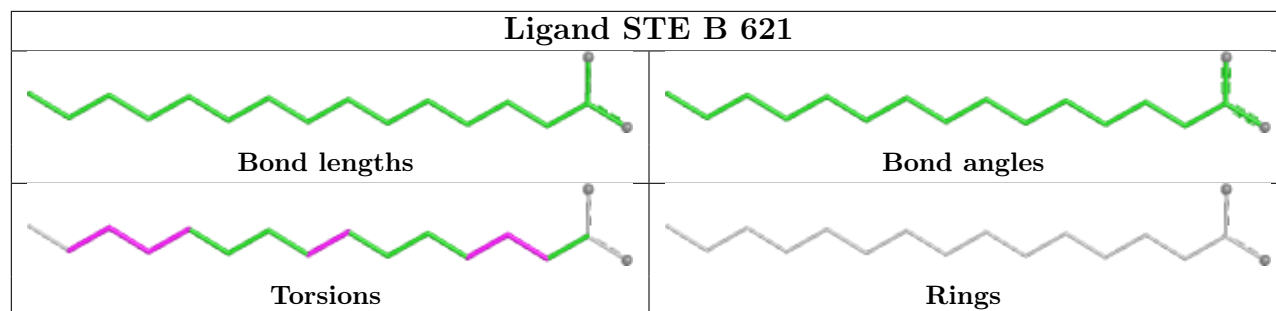


Ligand DGD h 101

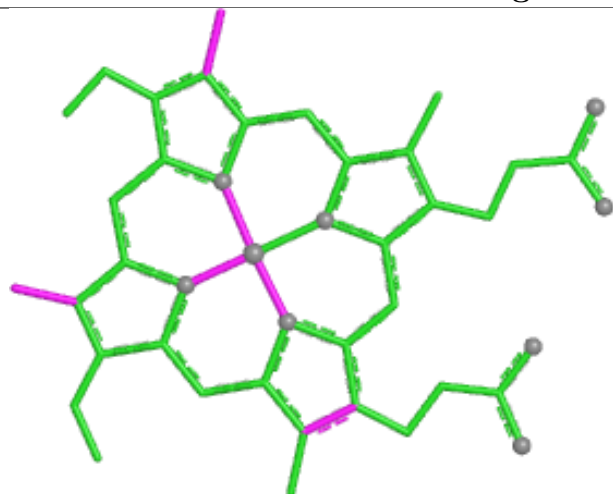


Ligand CLA b 613

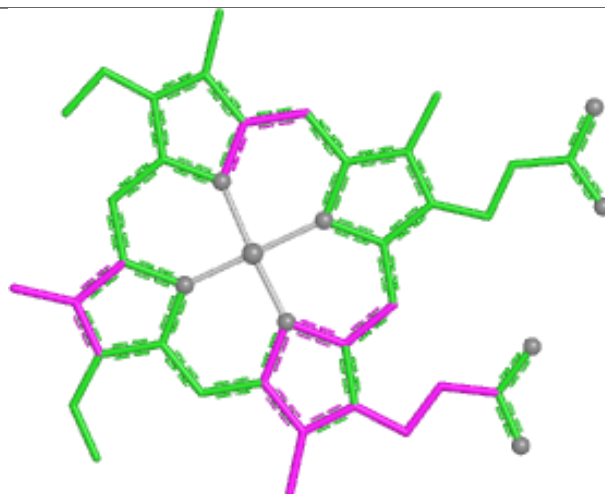




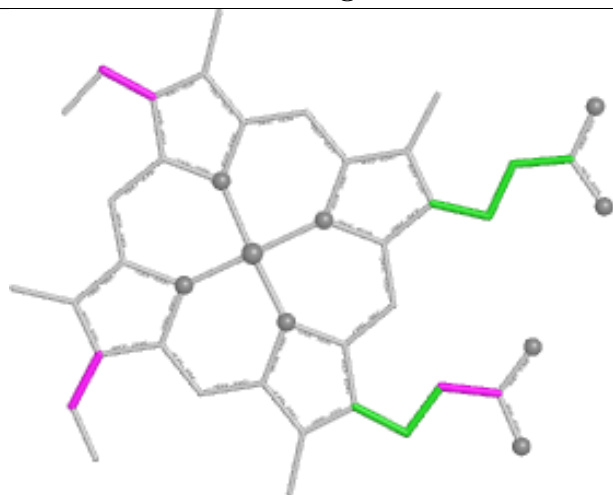
Ligand HEC V 201



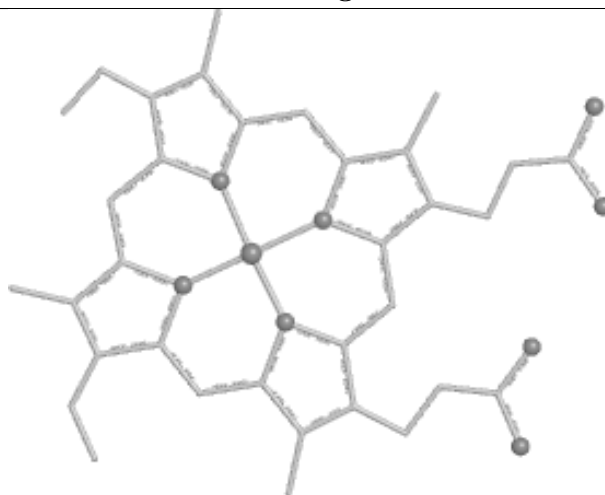
Bond lengths



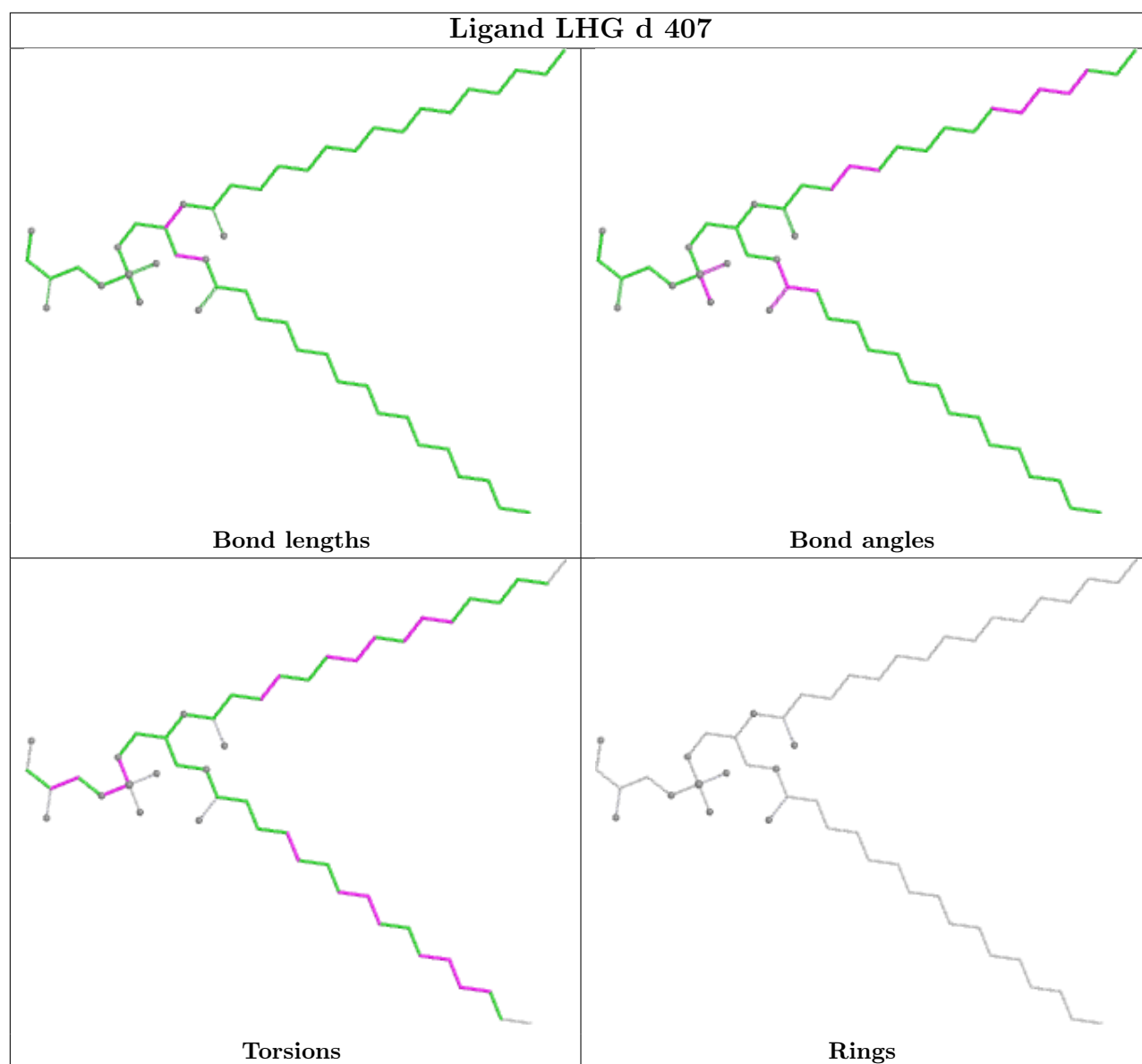
Bond angles

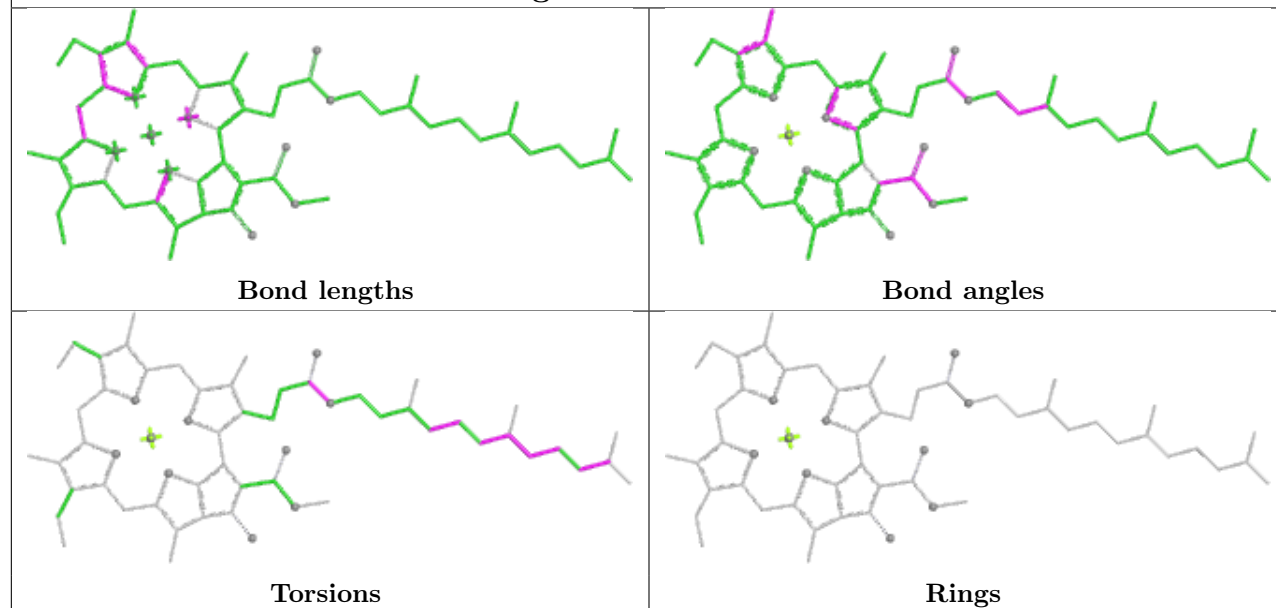
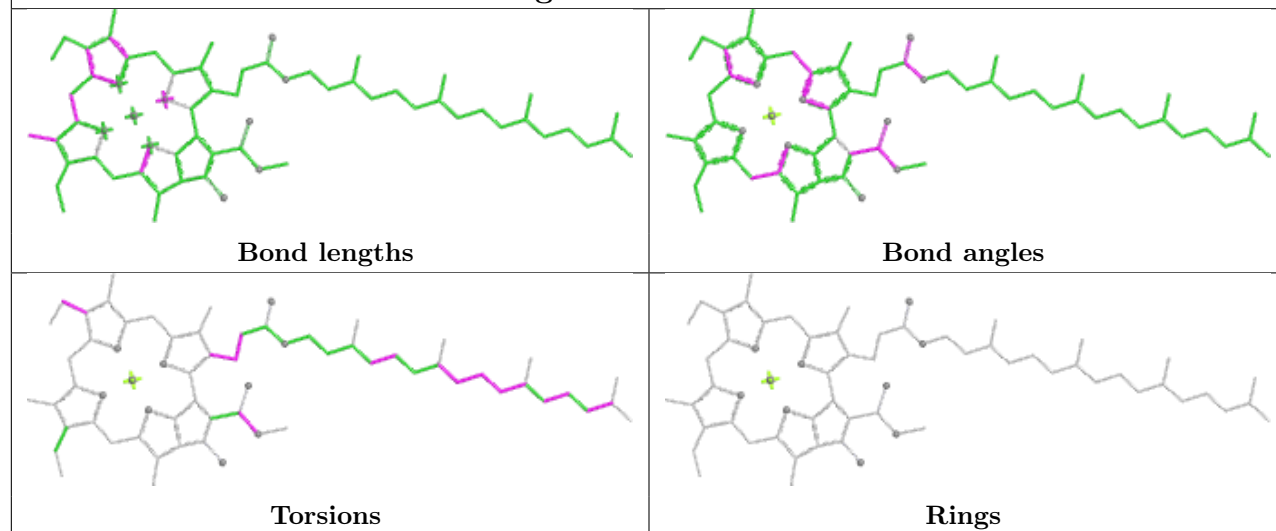


Torsions

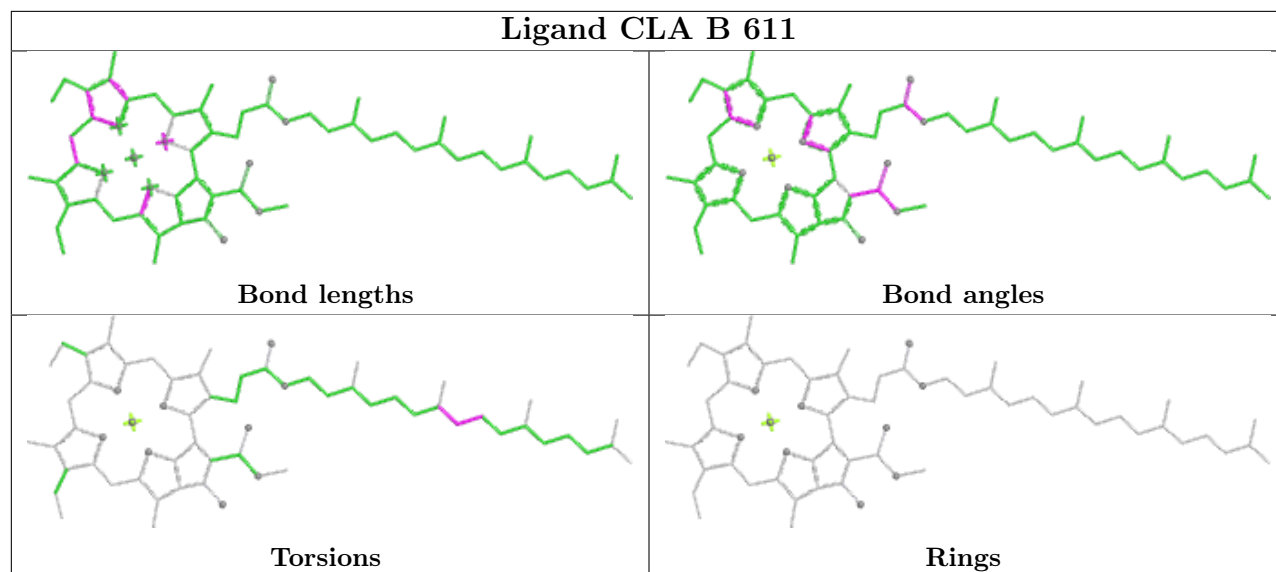


Rings

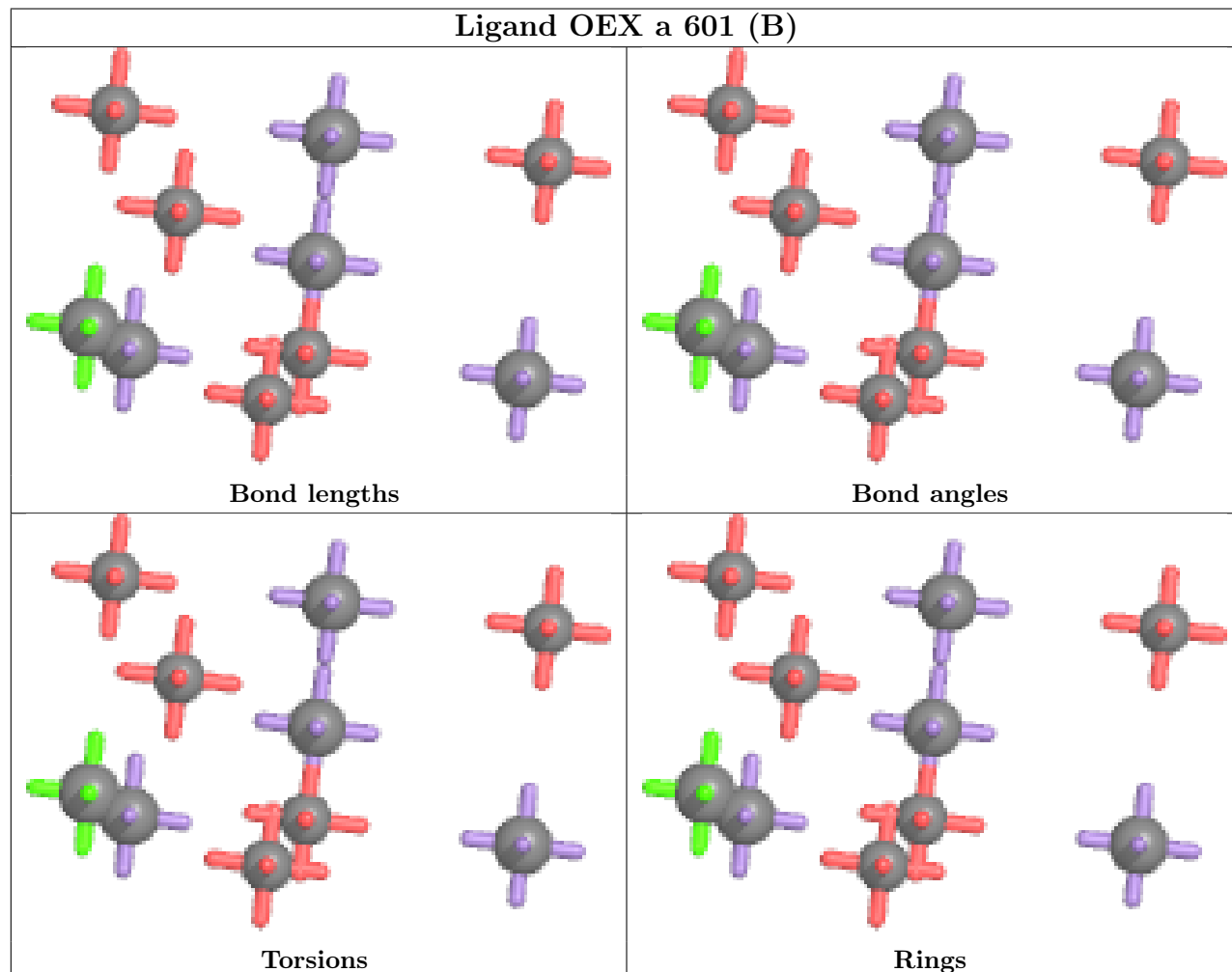


Ligand CLA B 616**Ligand CLA b 601**

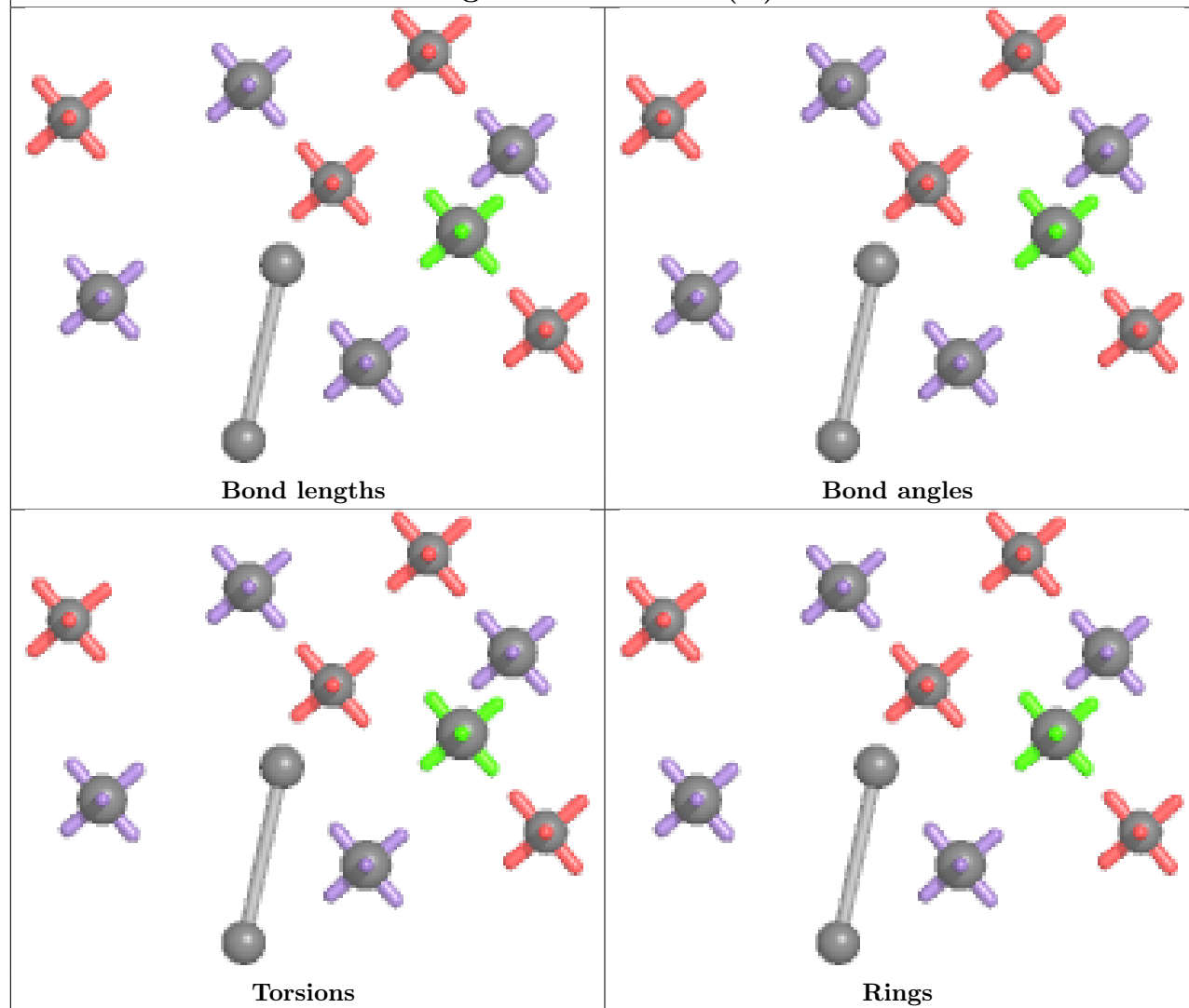
Ligand CLA B 611



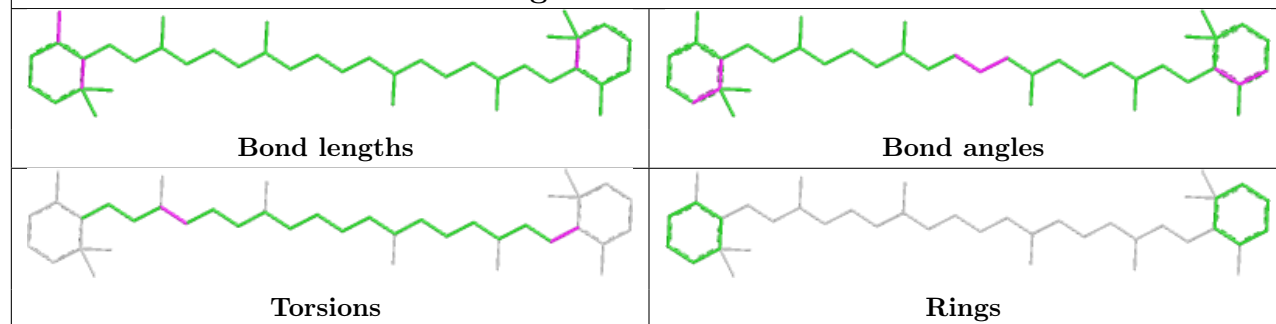
Ligand OEX a 601 (B)

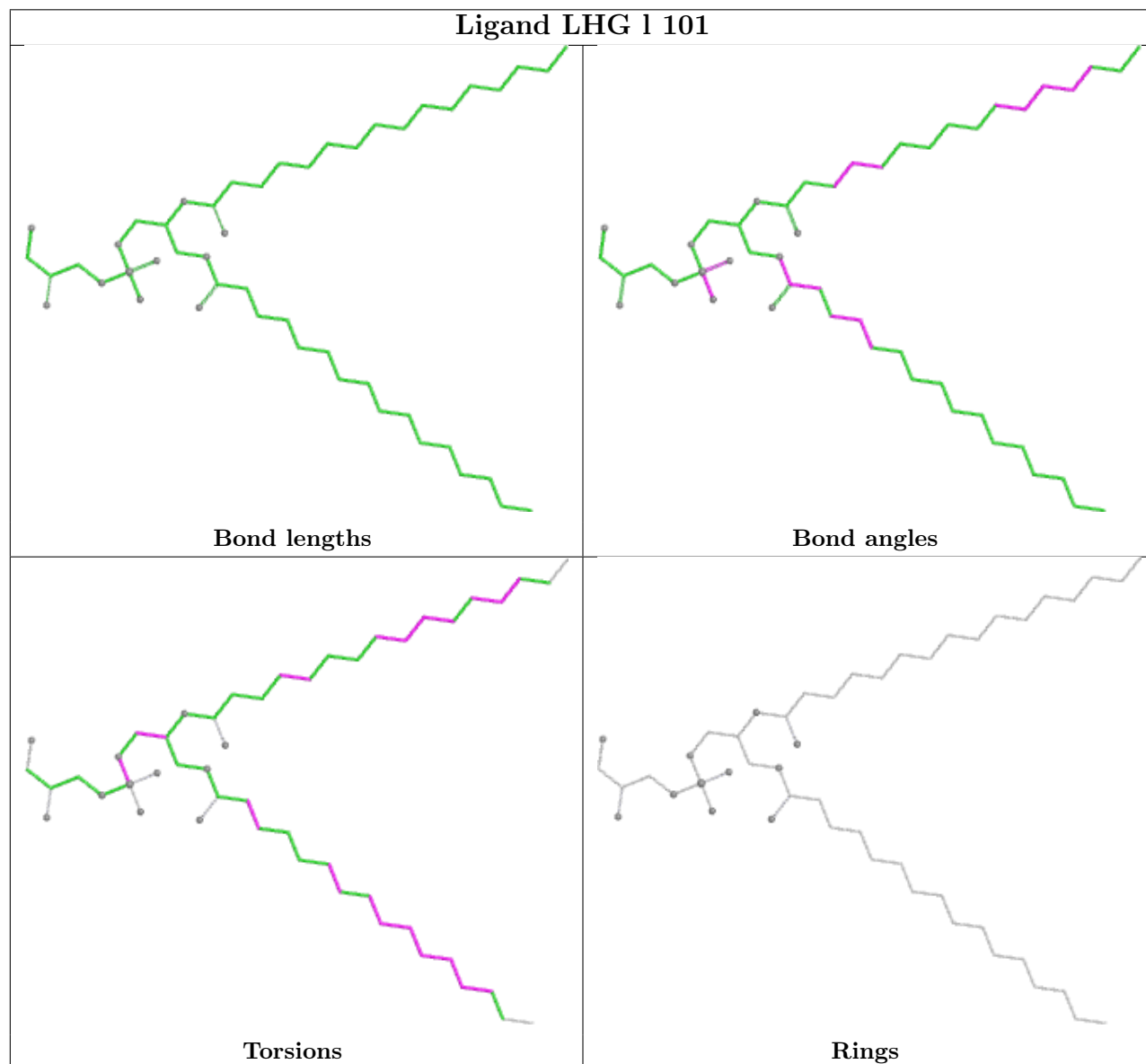
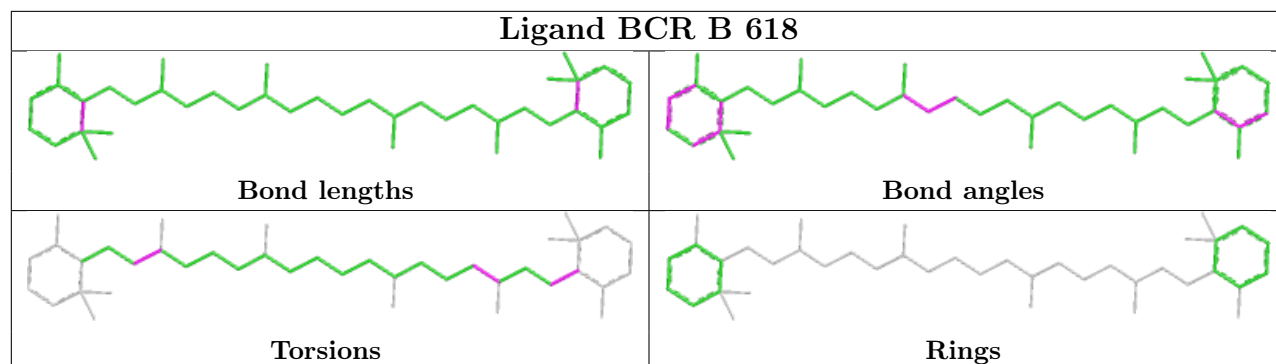


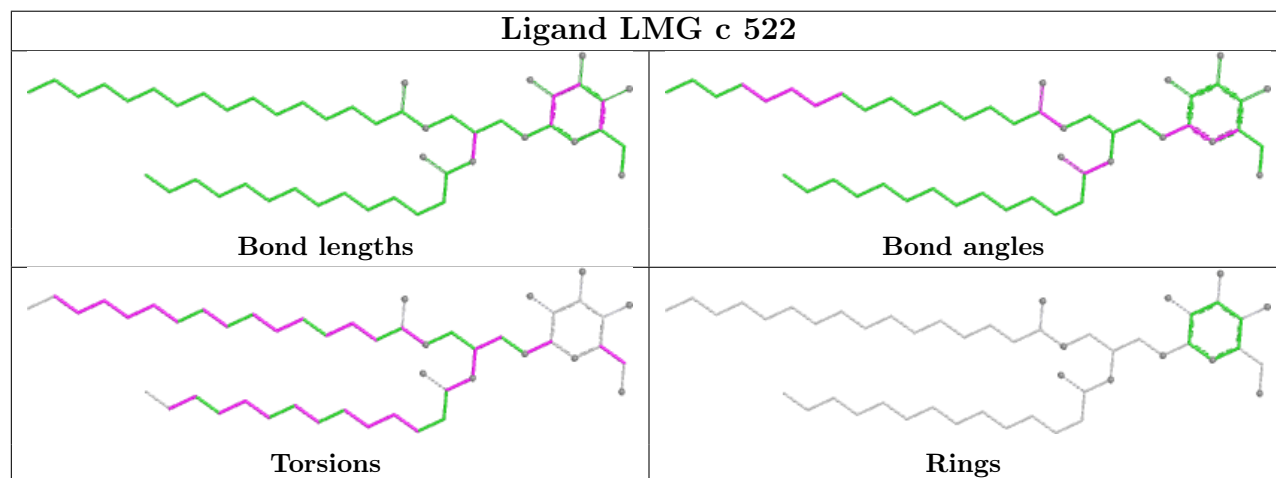
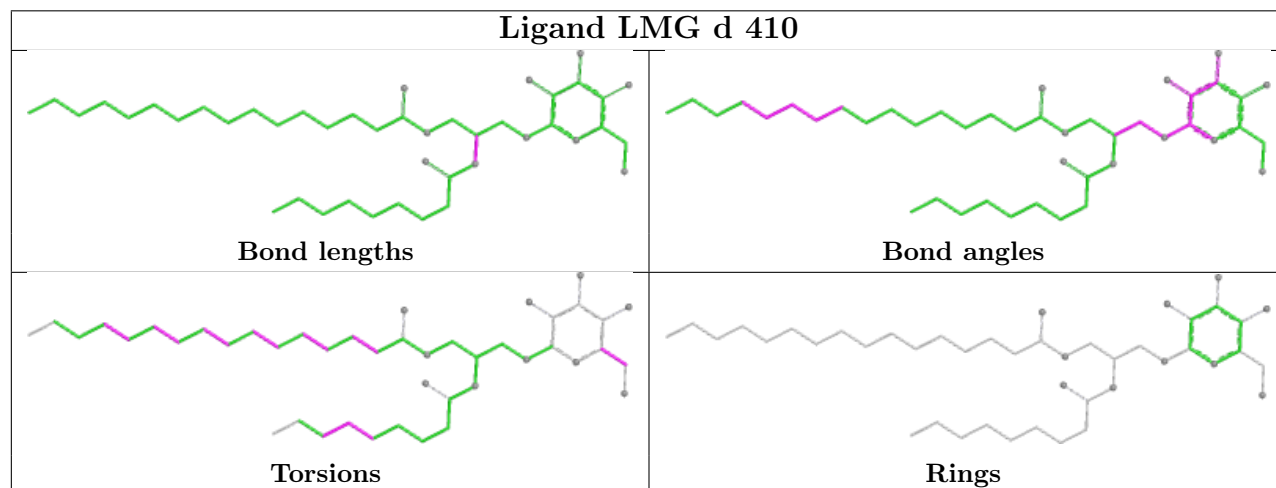
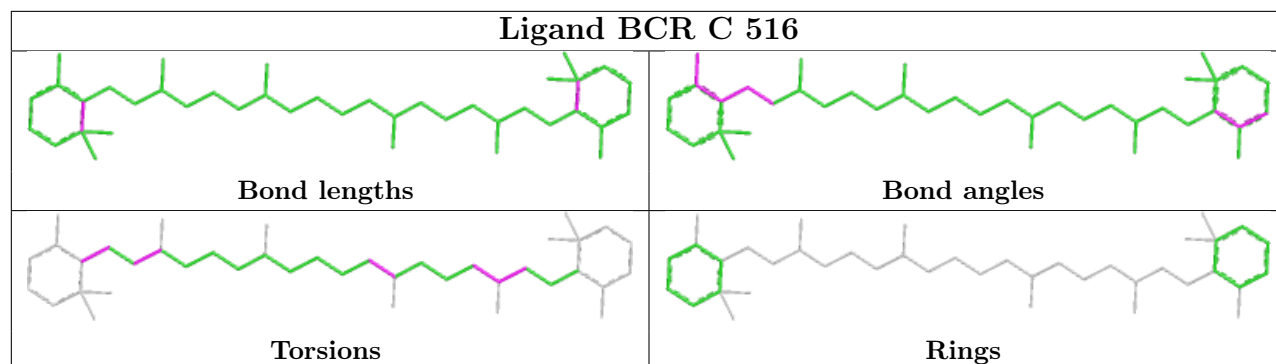
Ligand OEY A 602 (A)



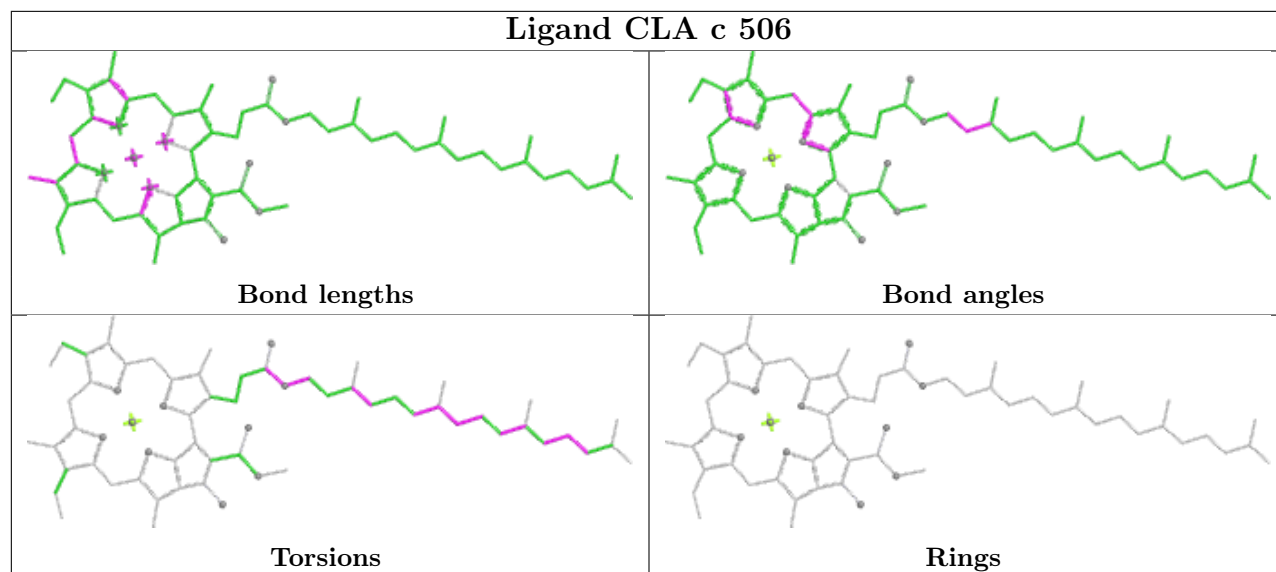
Ligand BCR A 610



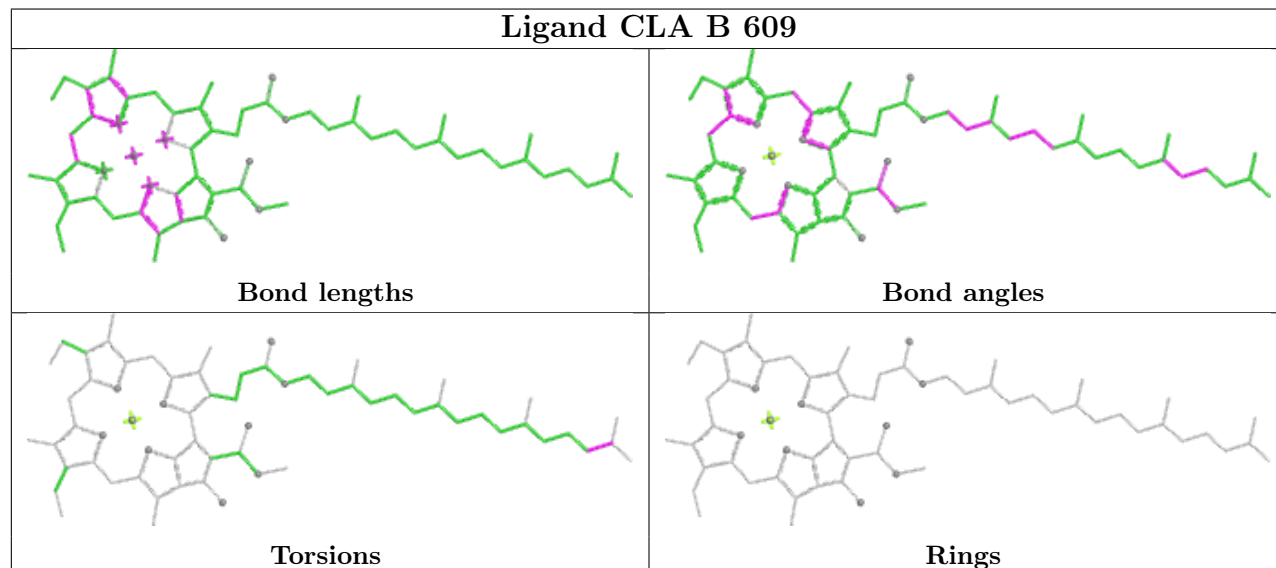




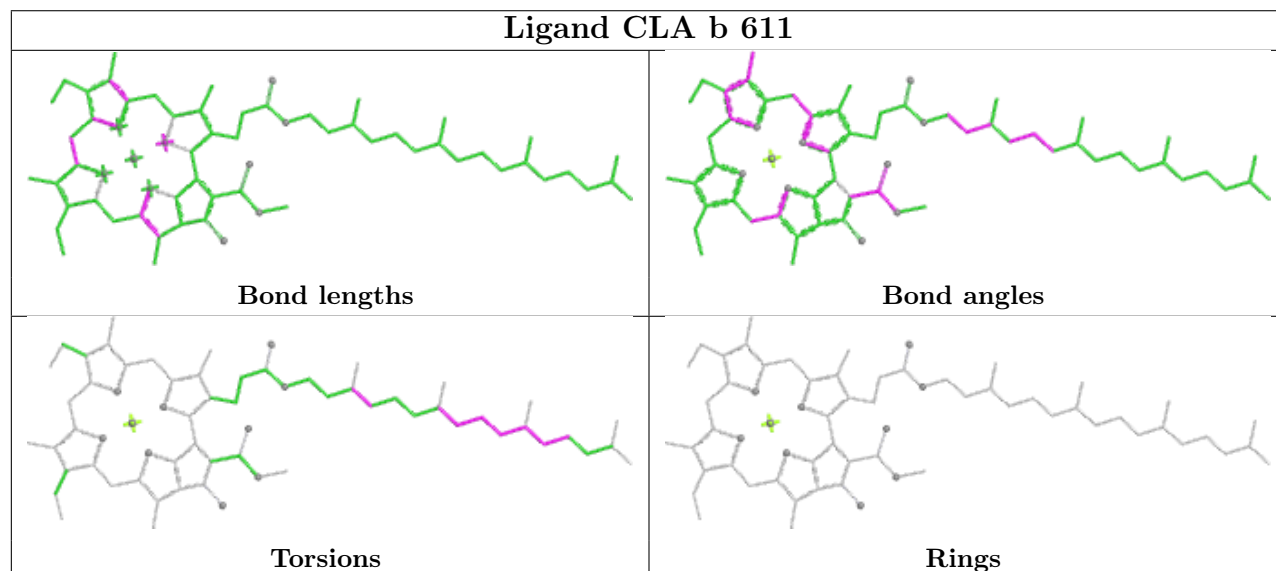
Ligand CLA c 506

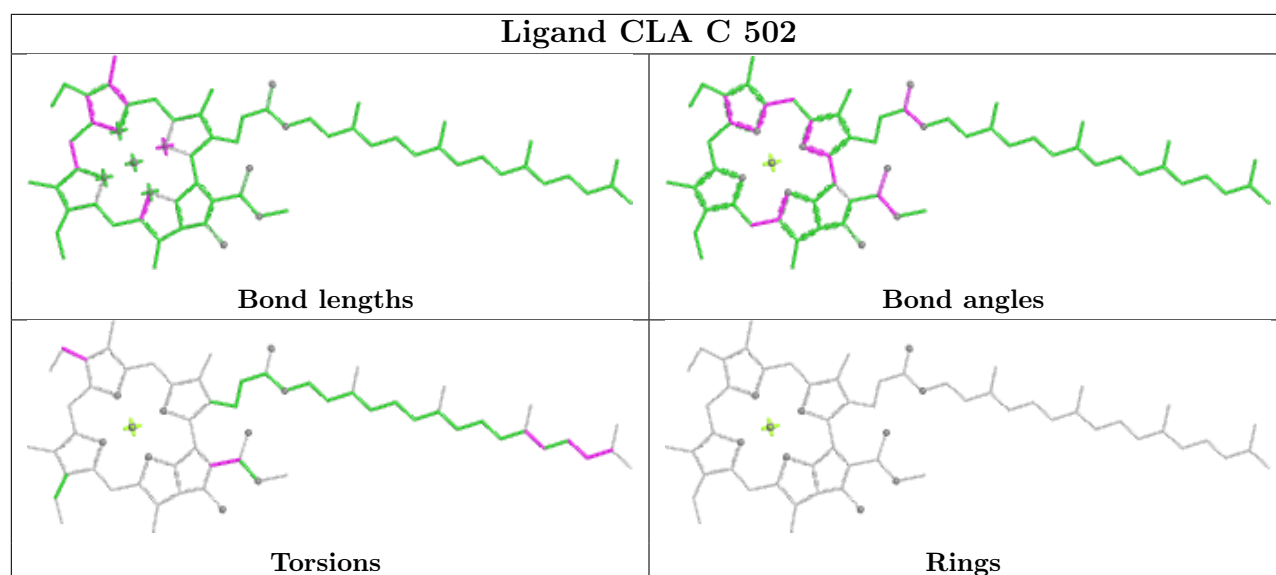
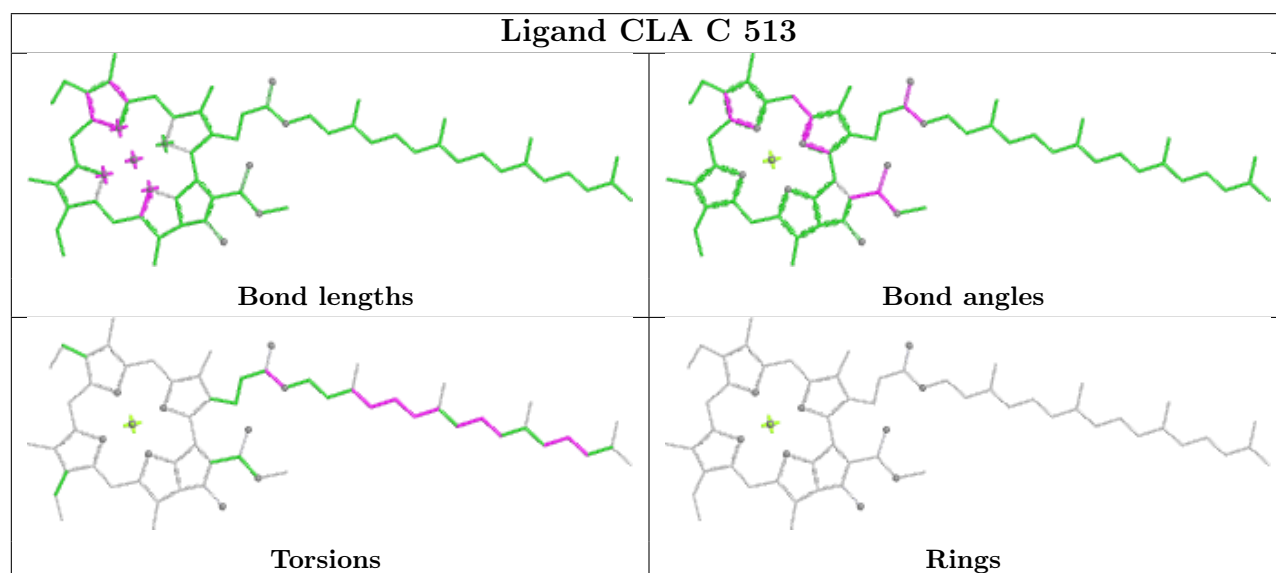
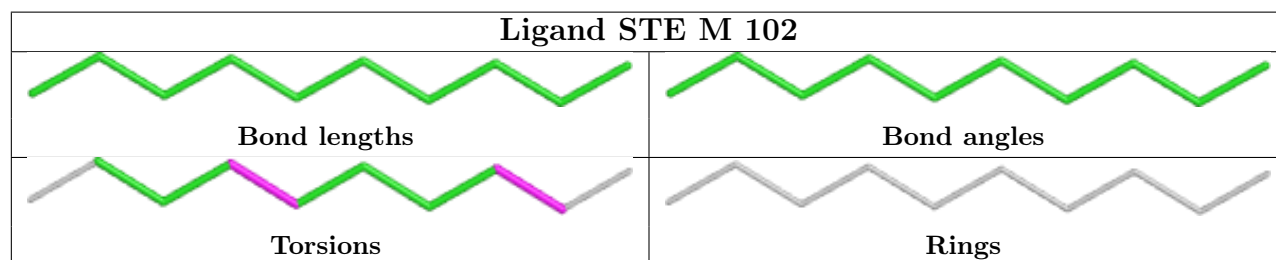
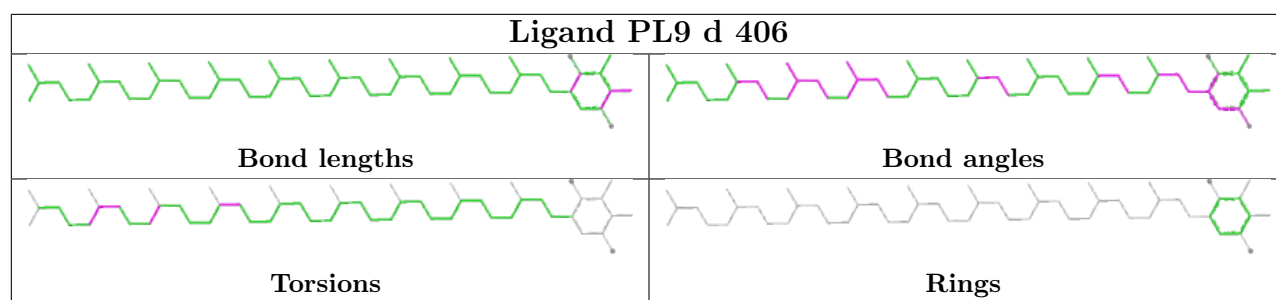


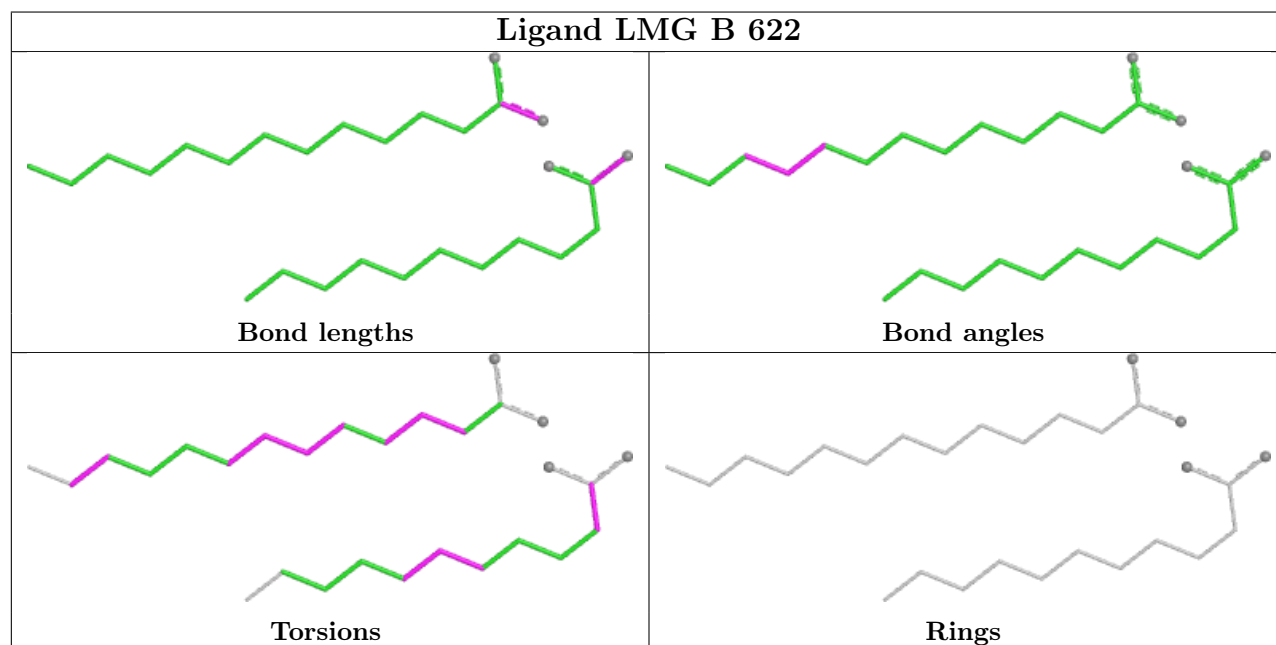
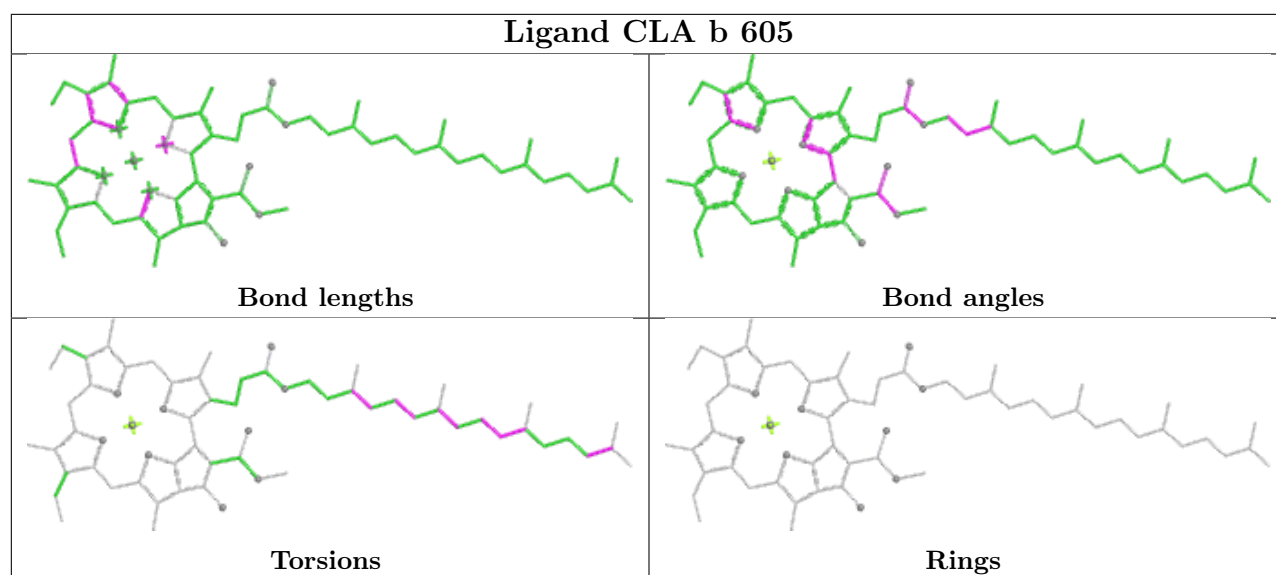
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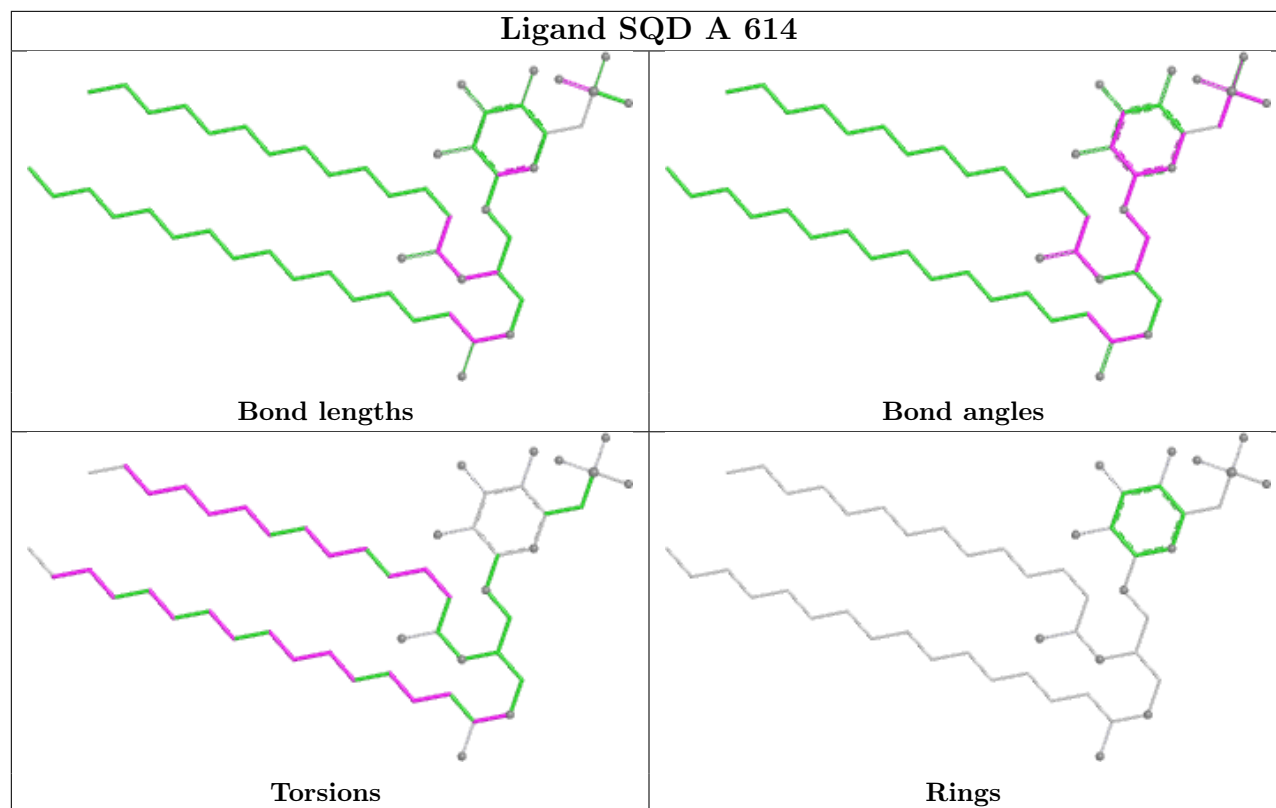
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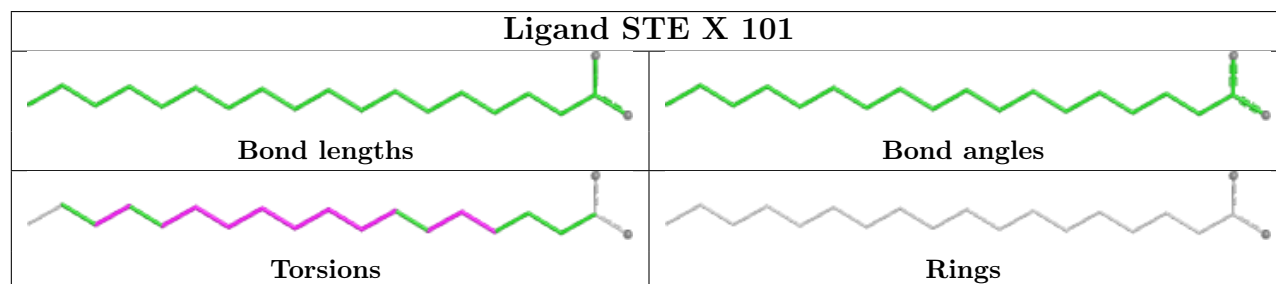




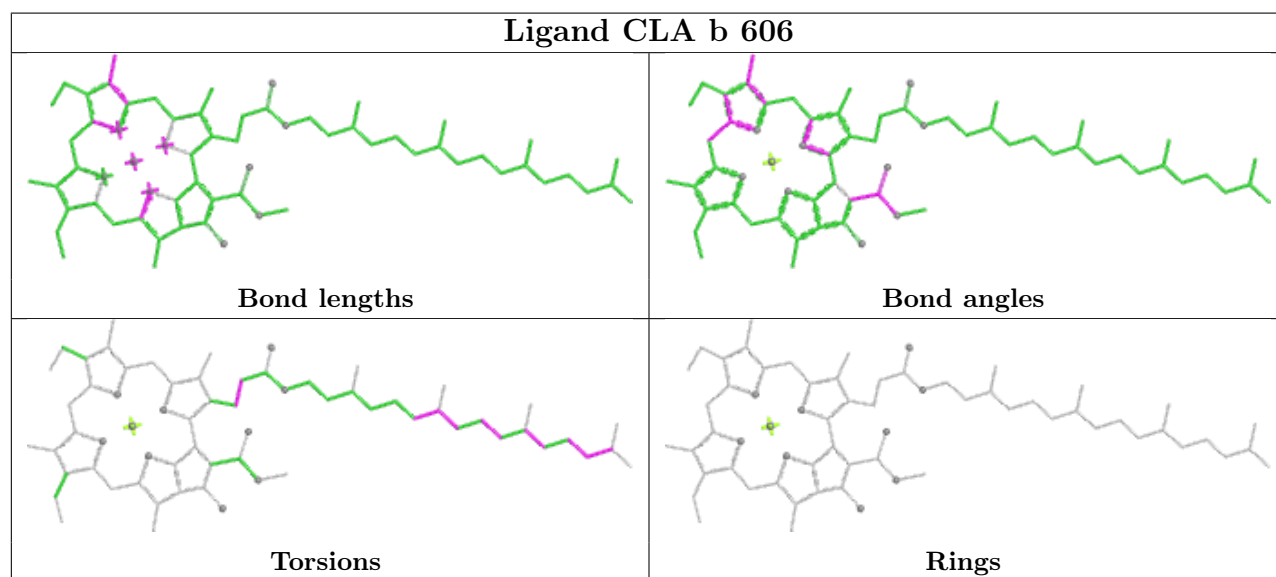
Ligand SQD A 614



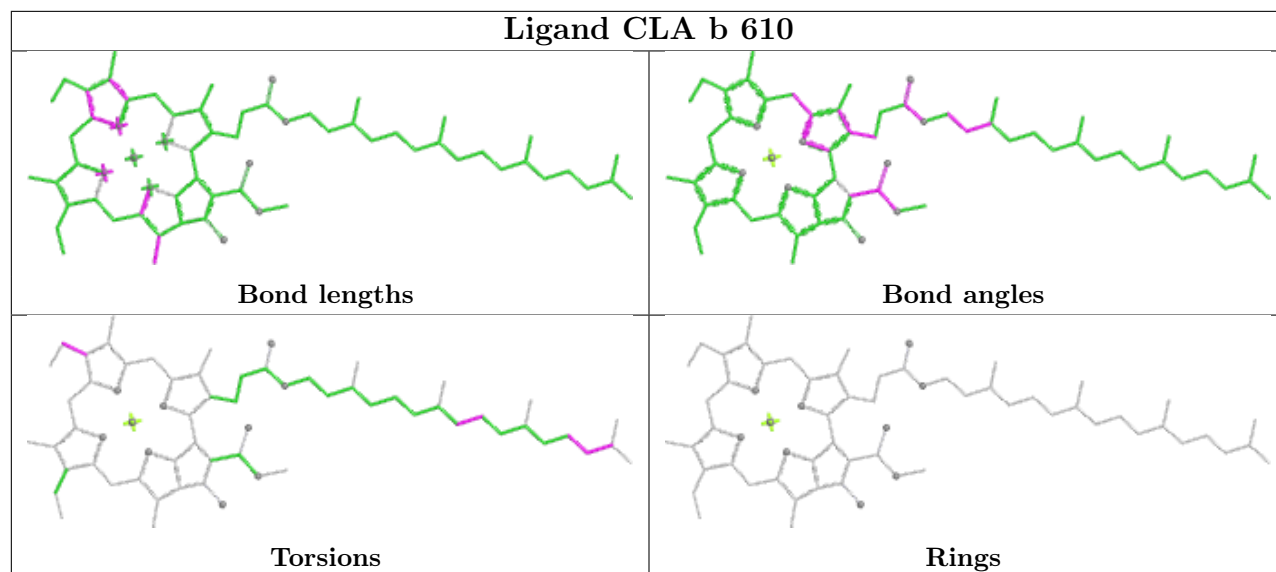
Ligand STE X 101



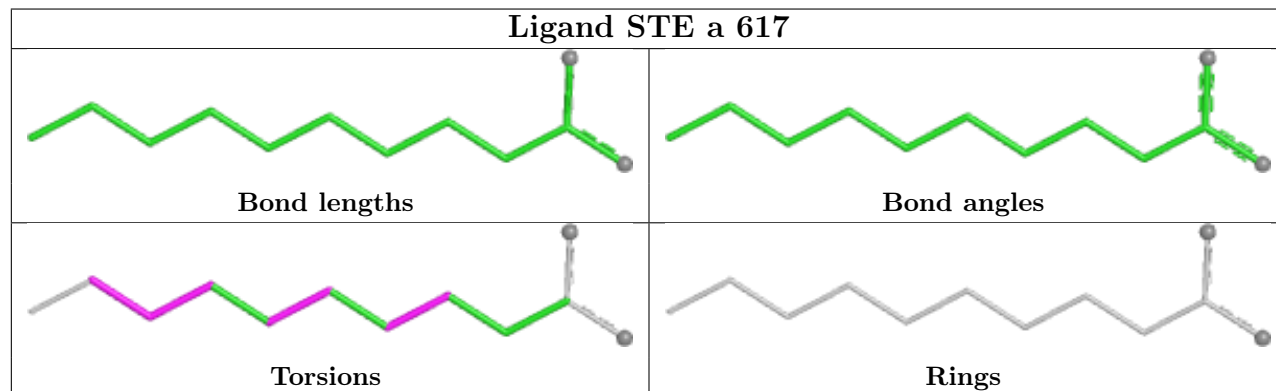
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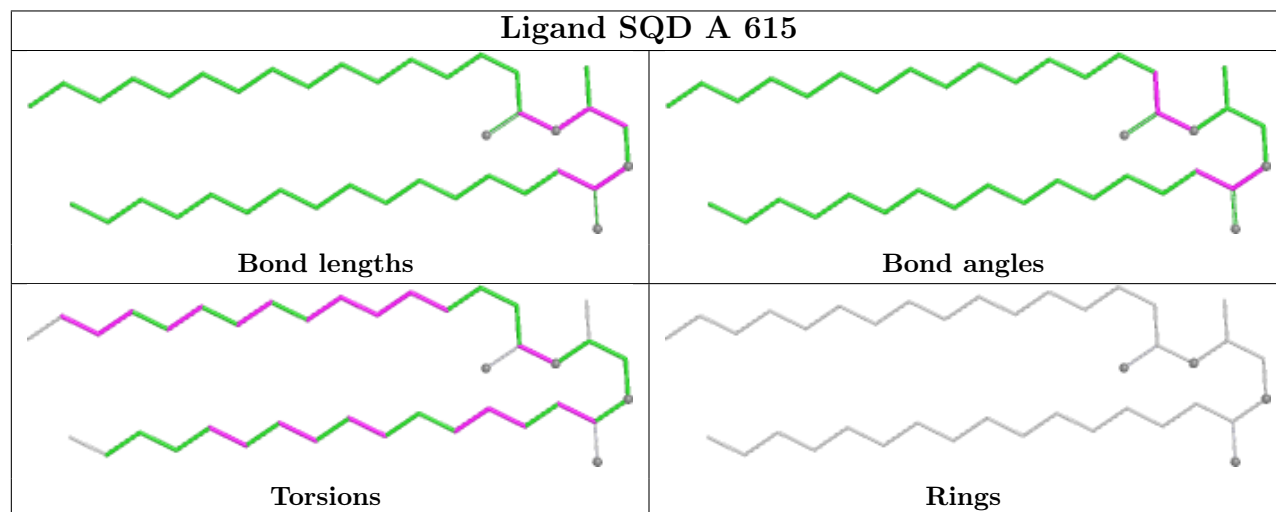
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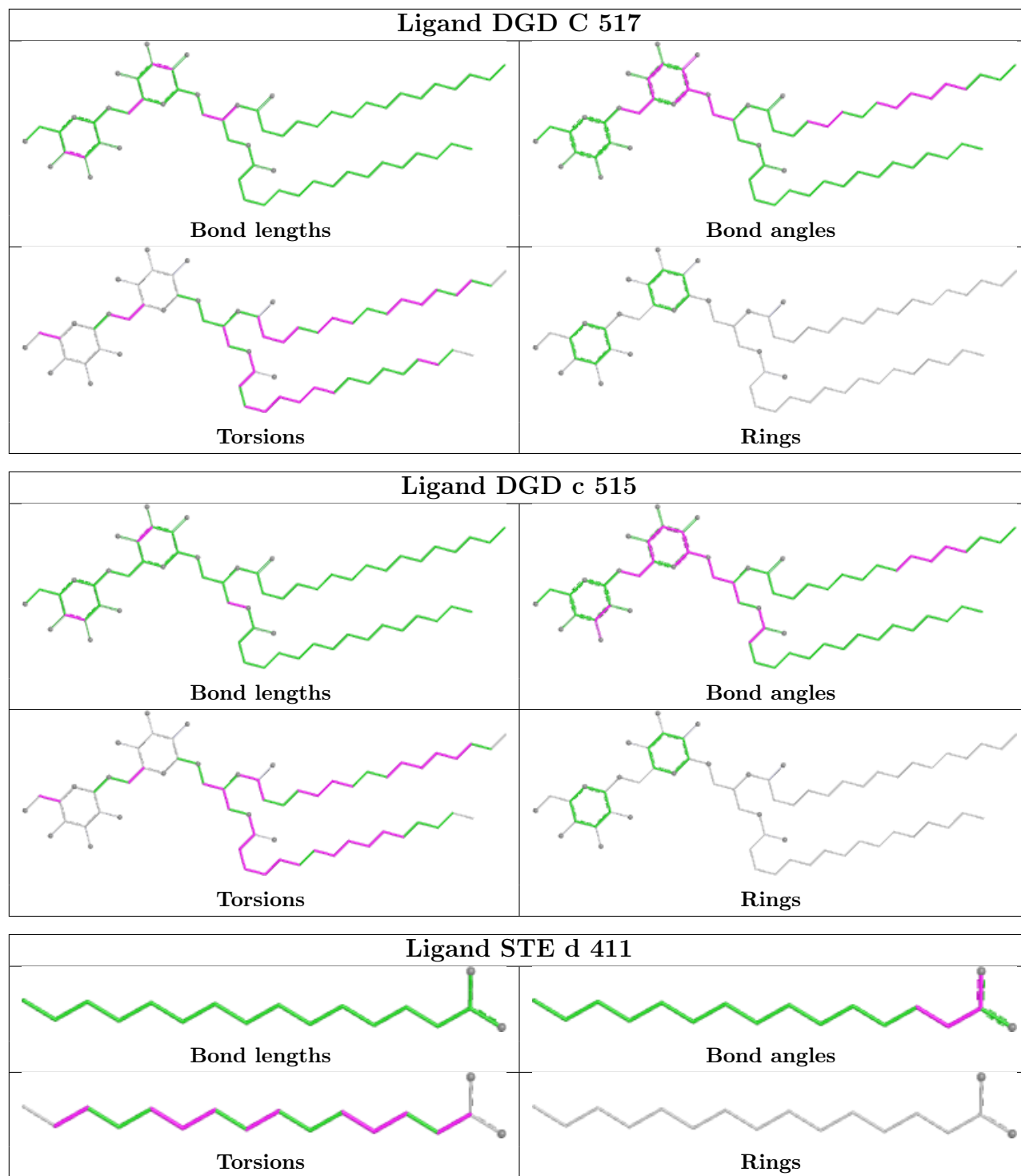


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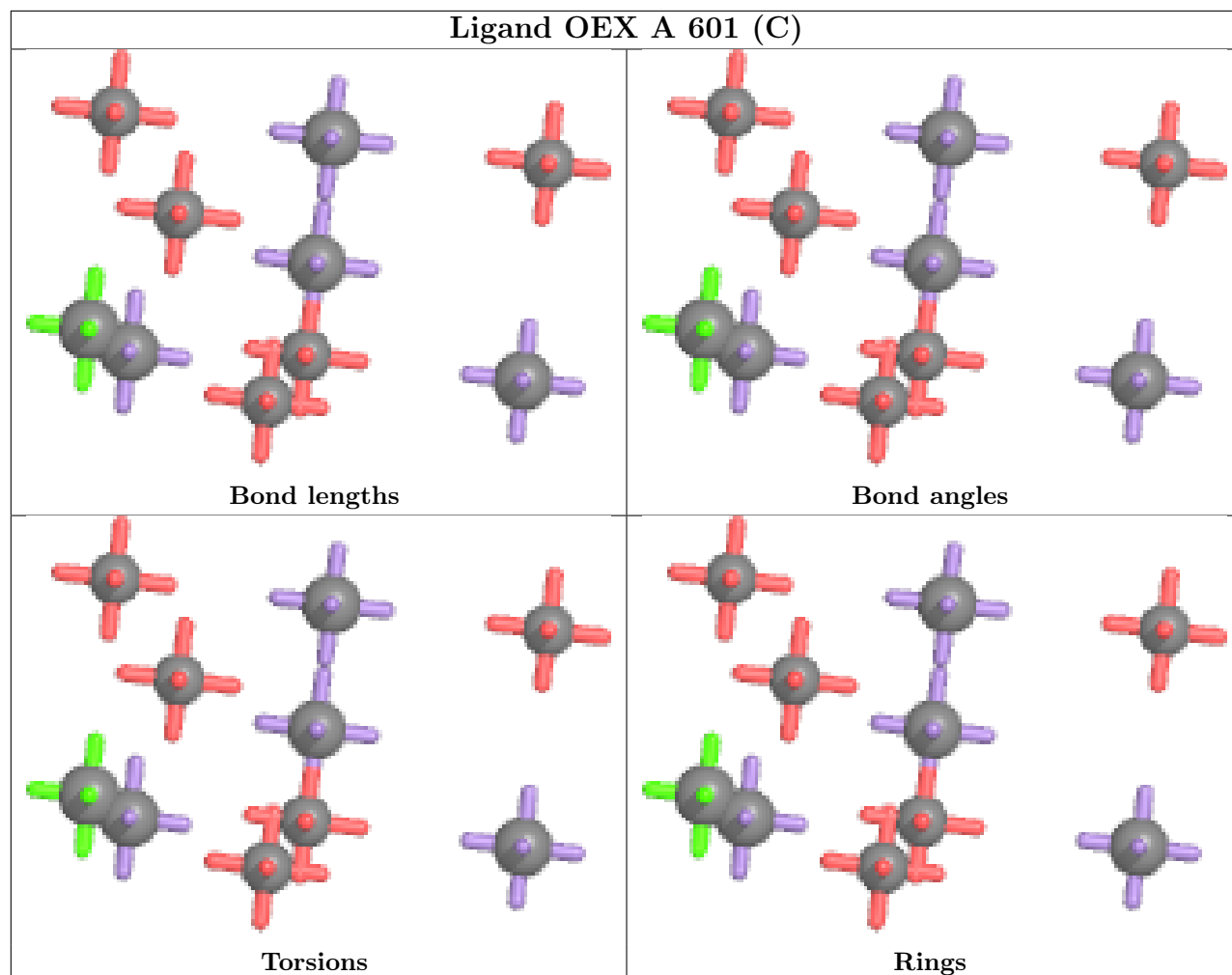


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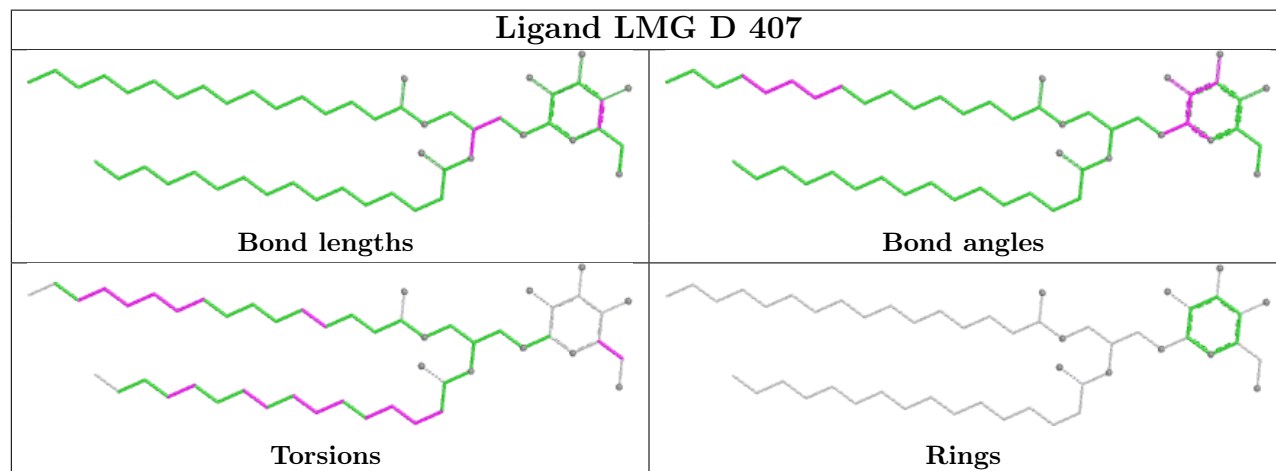


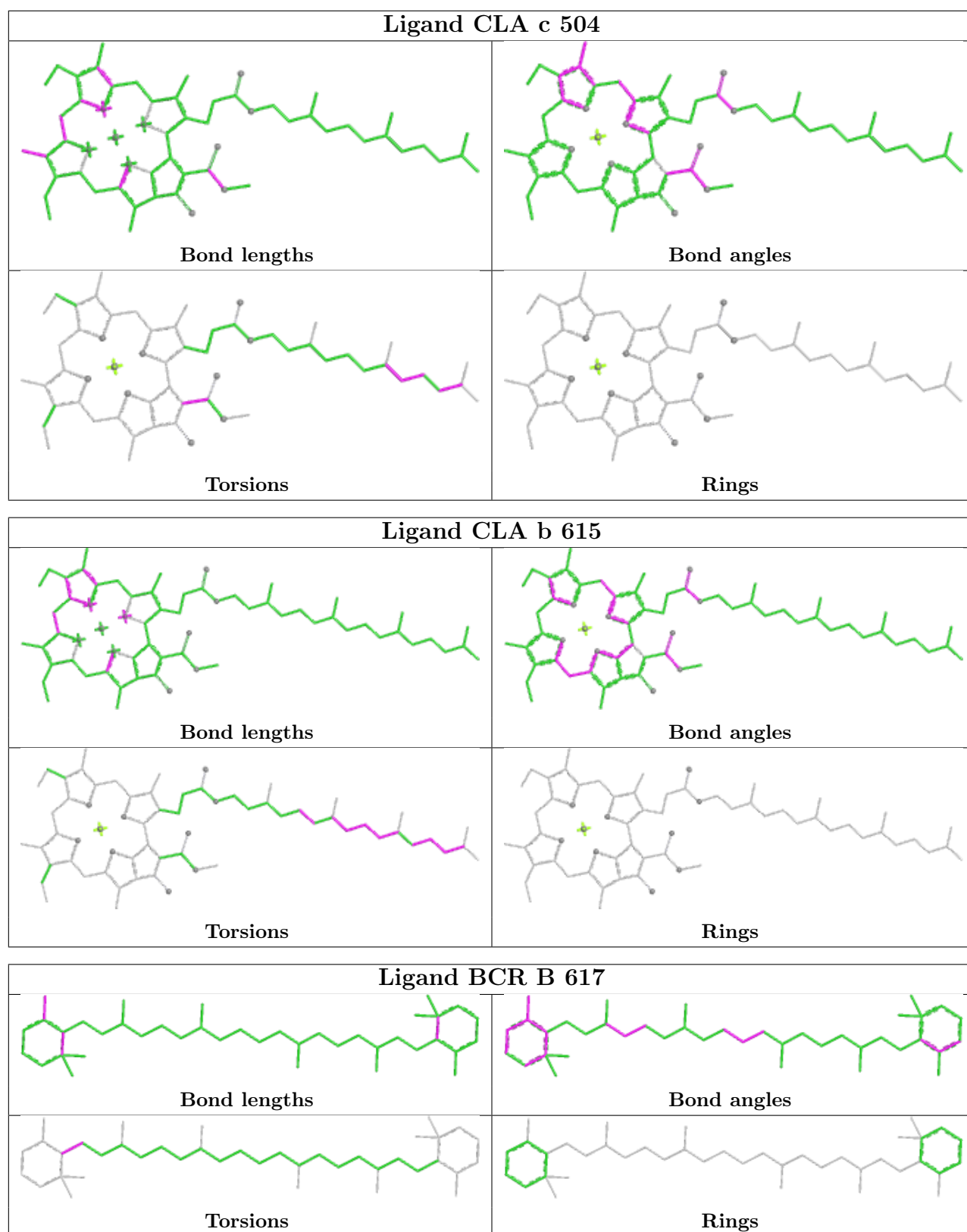


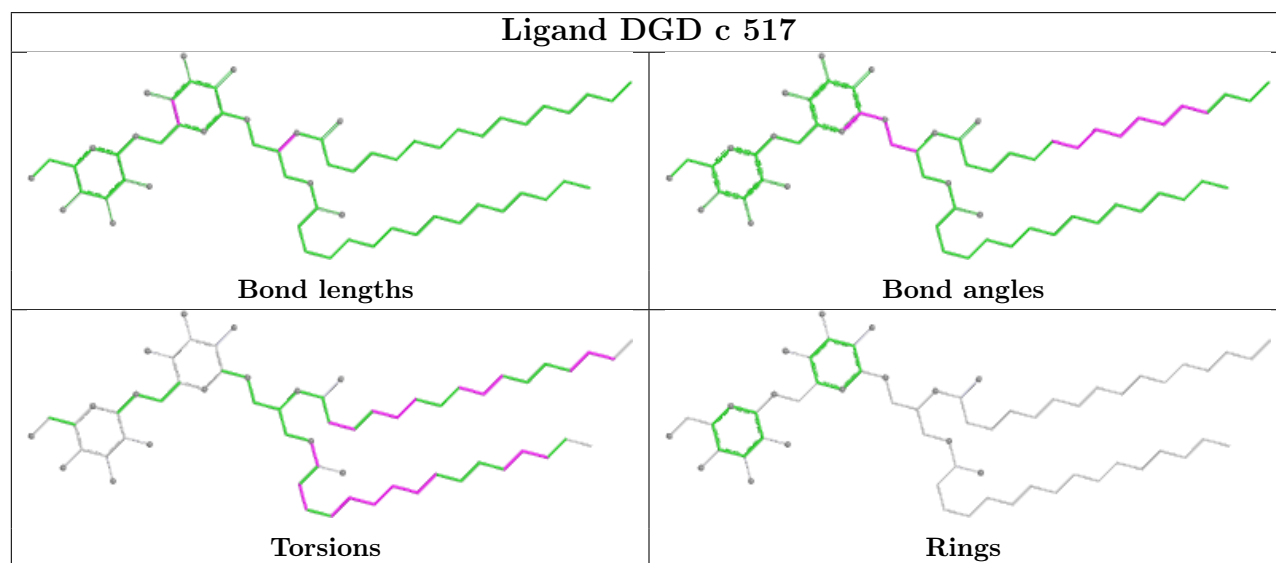
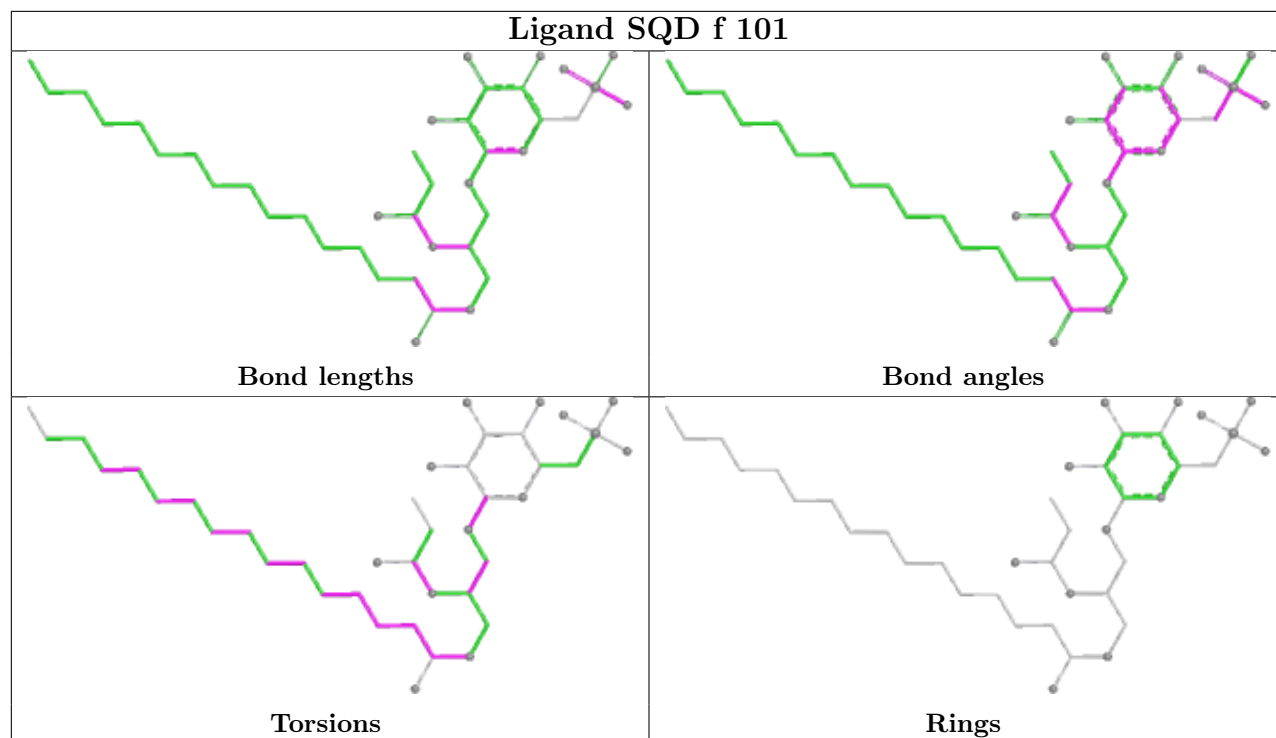
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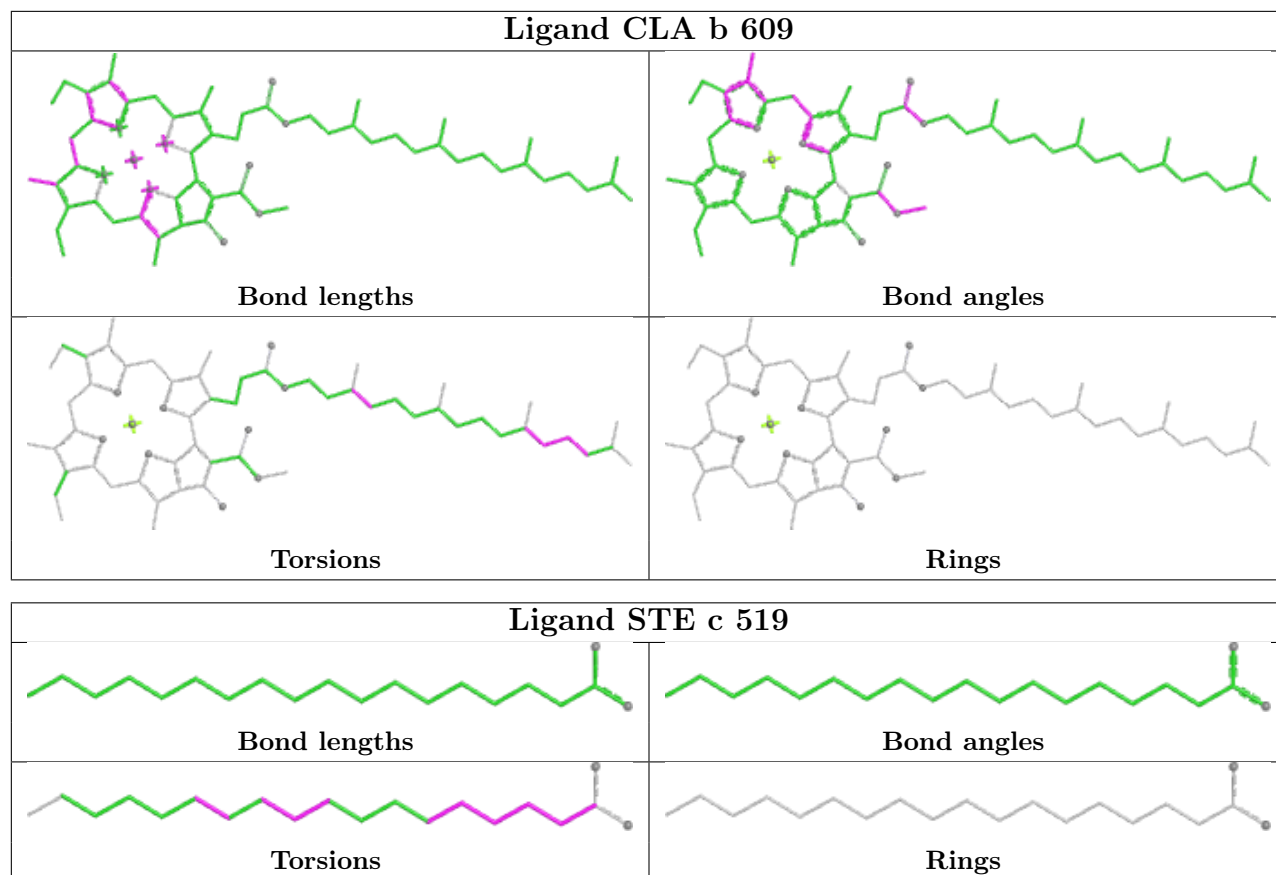


Ligand LMG D 407

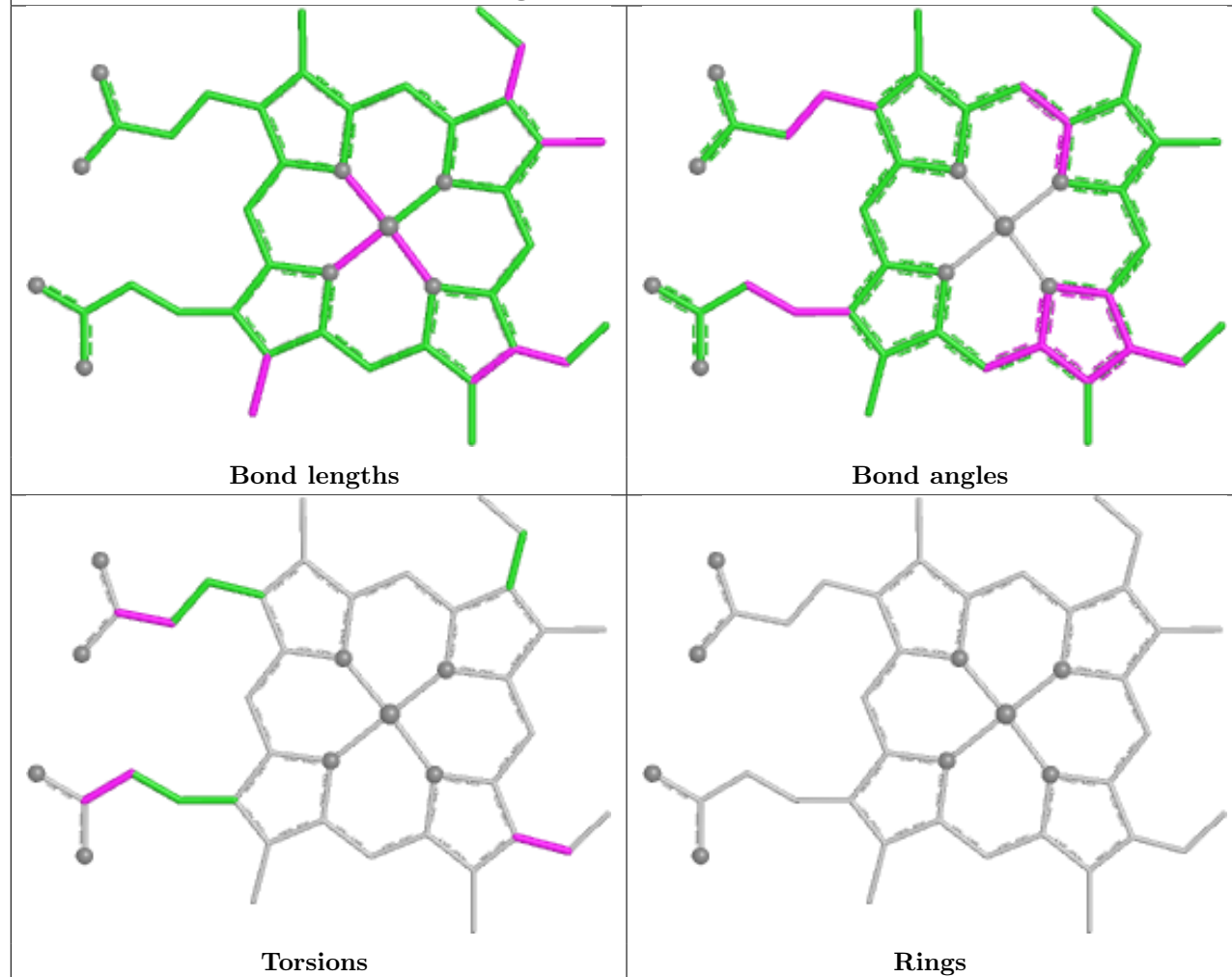


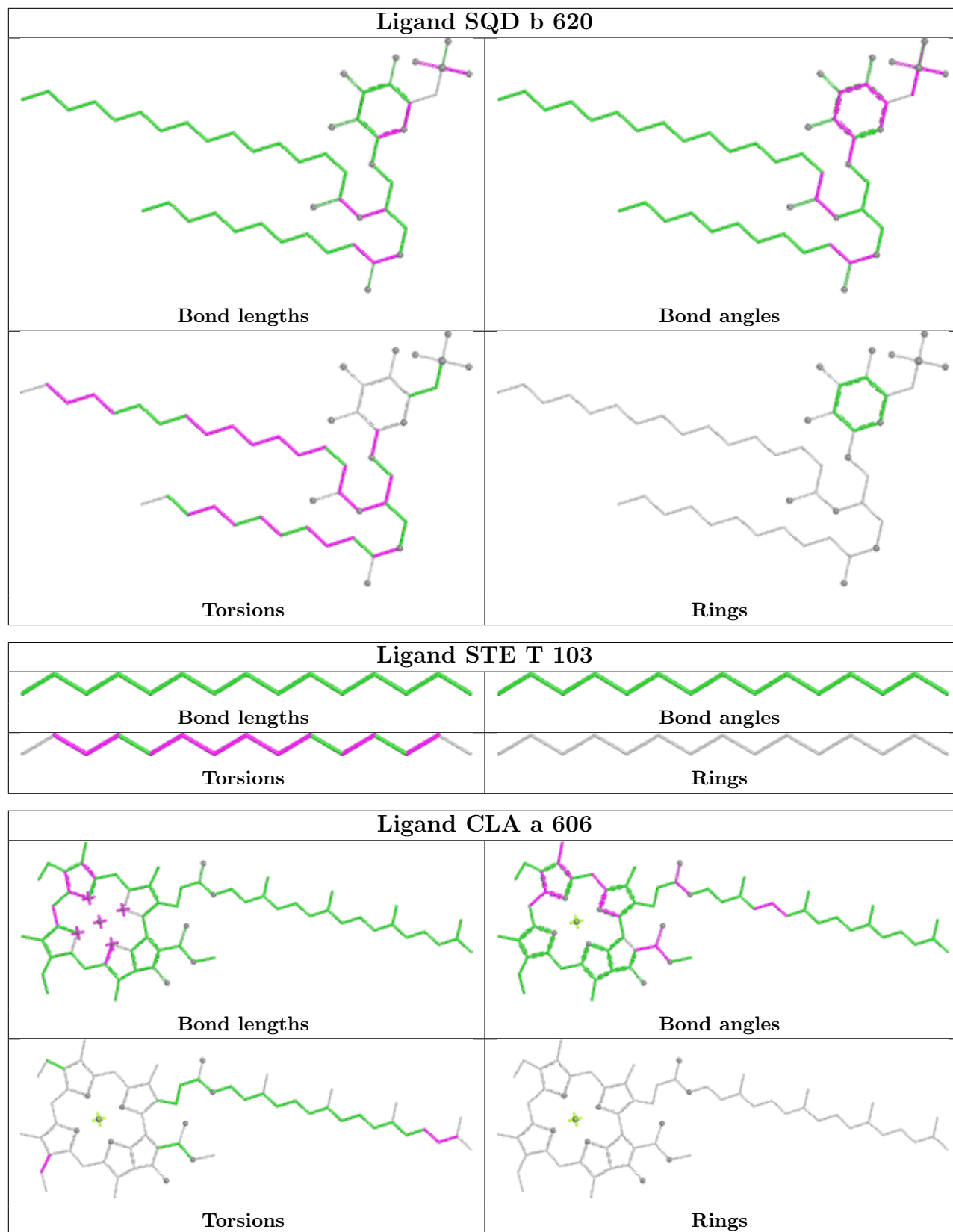


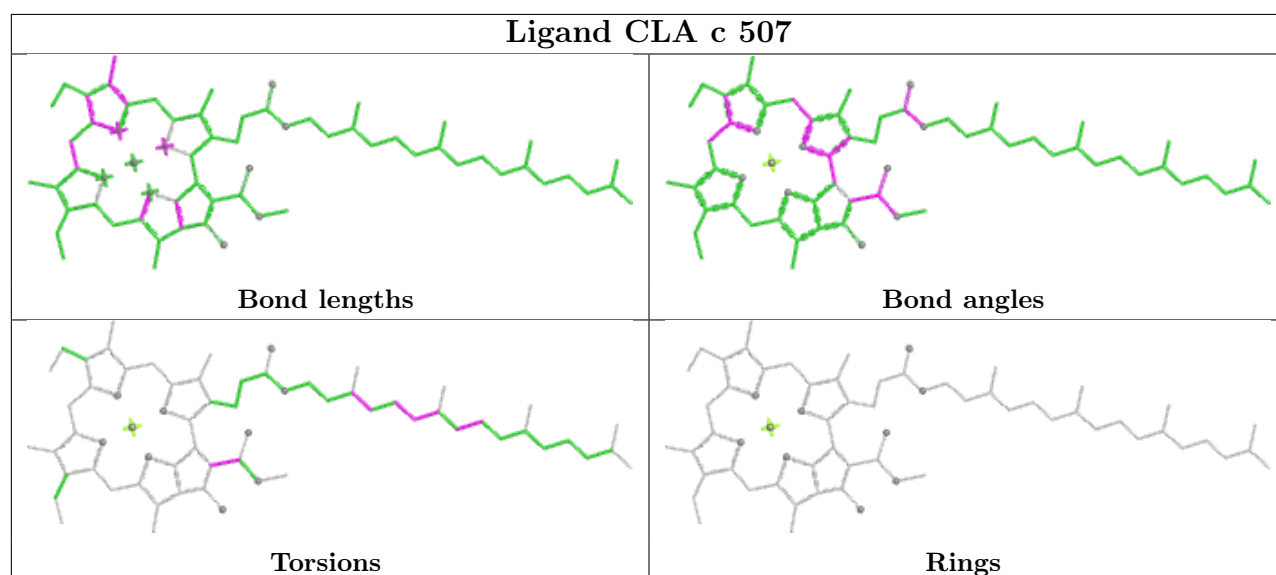
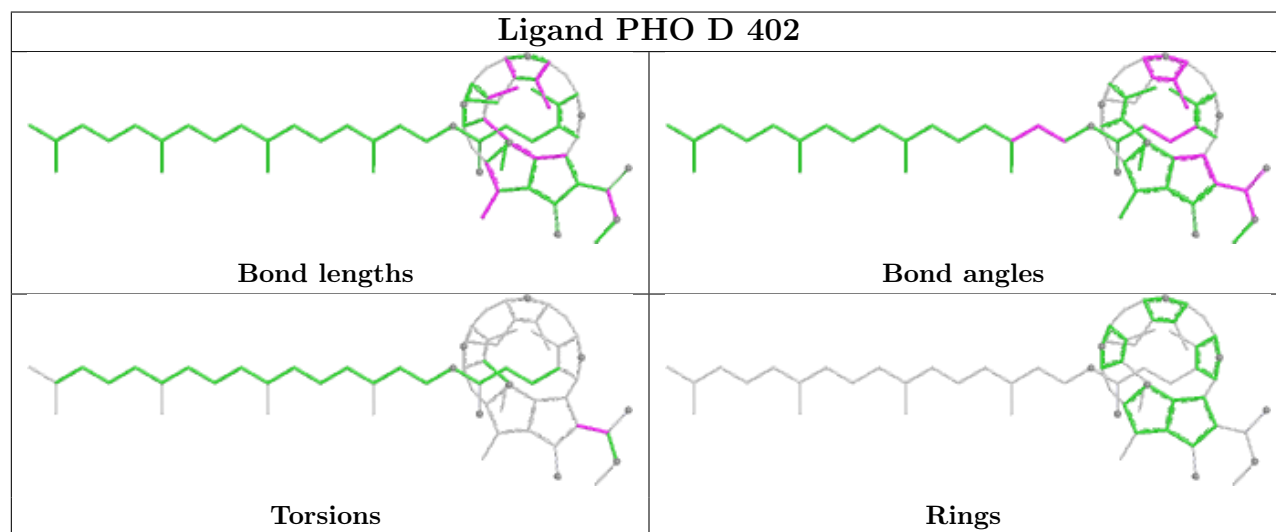
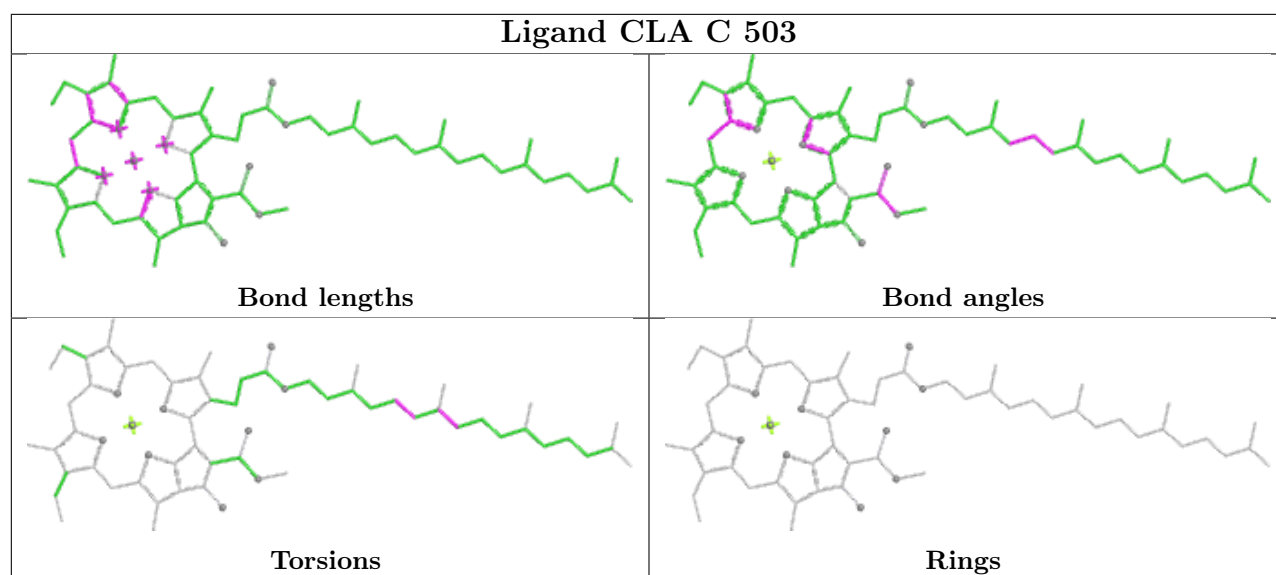


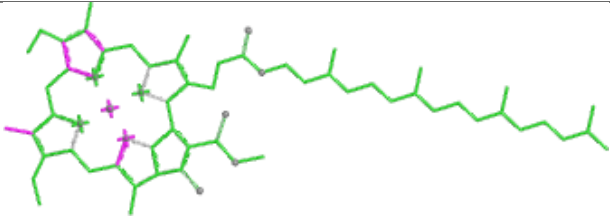
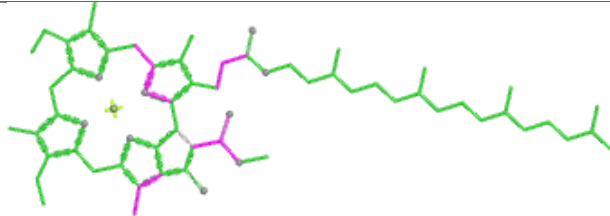
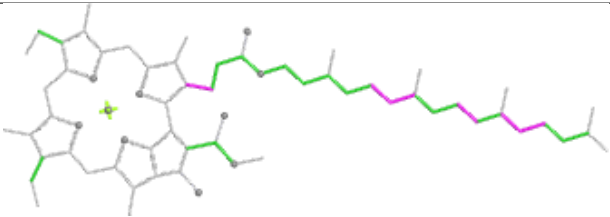
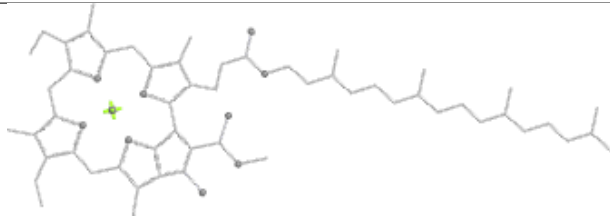
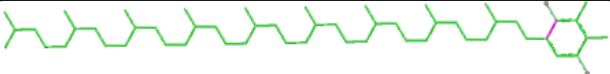
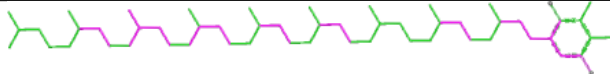
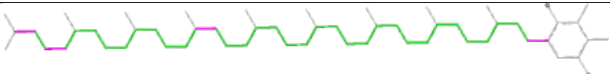
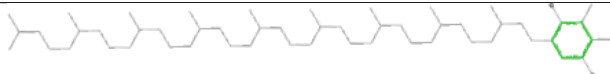
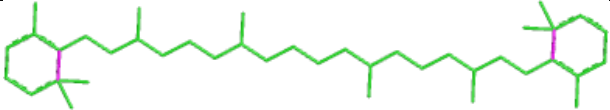
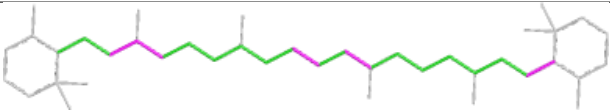
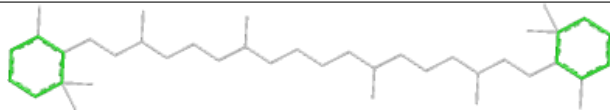


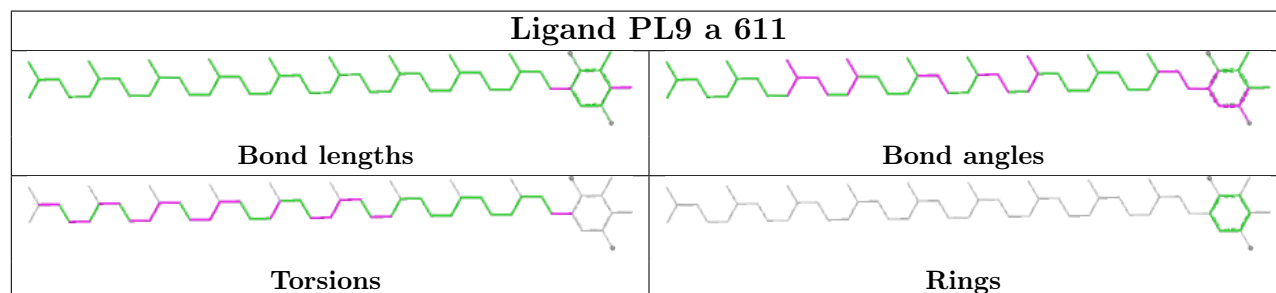
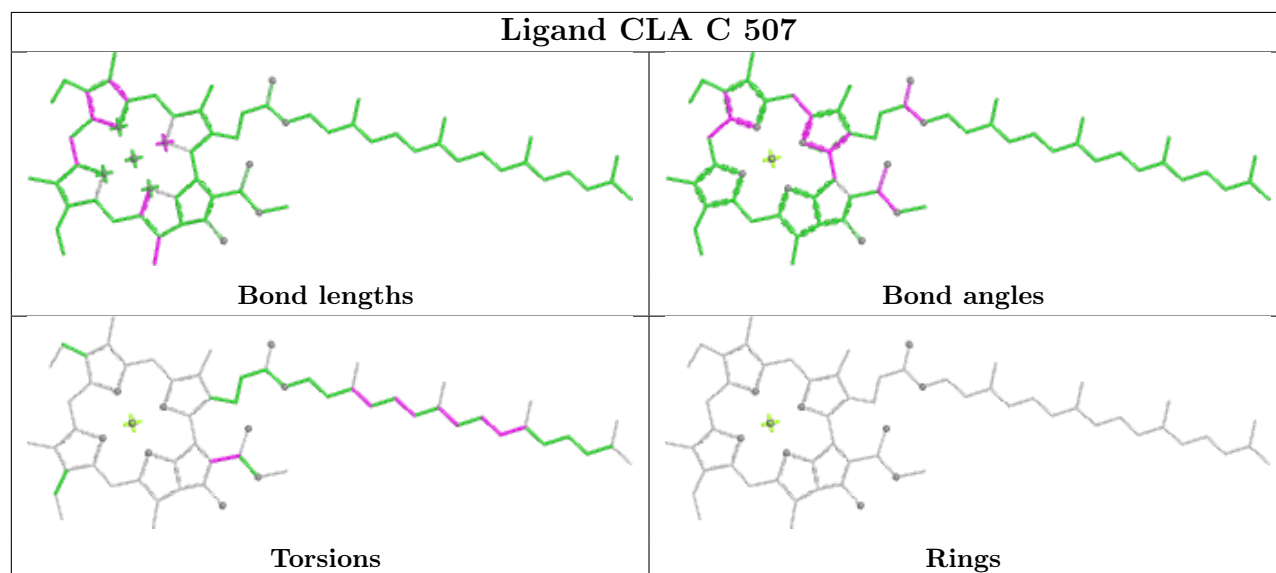
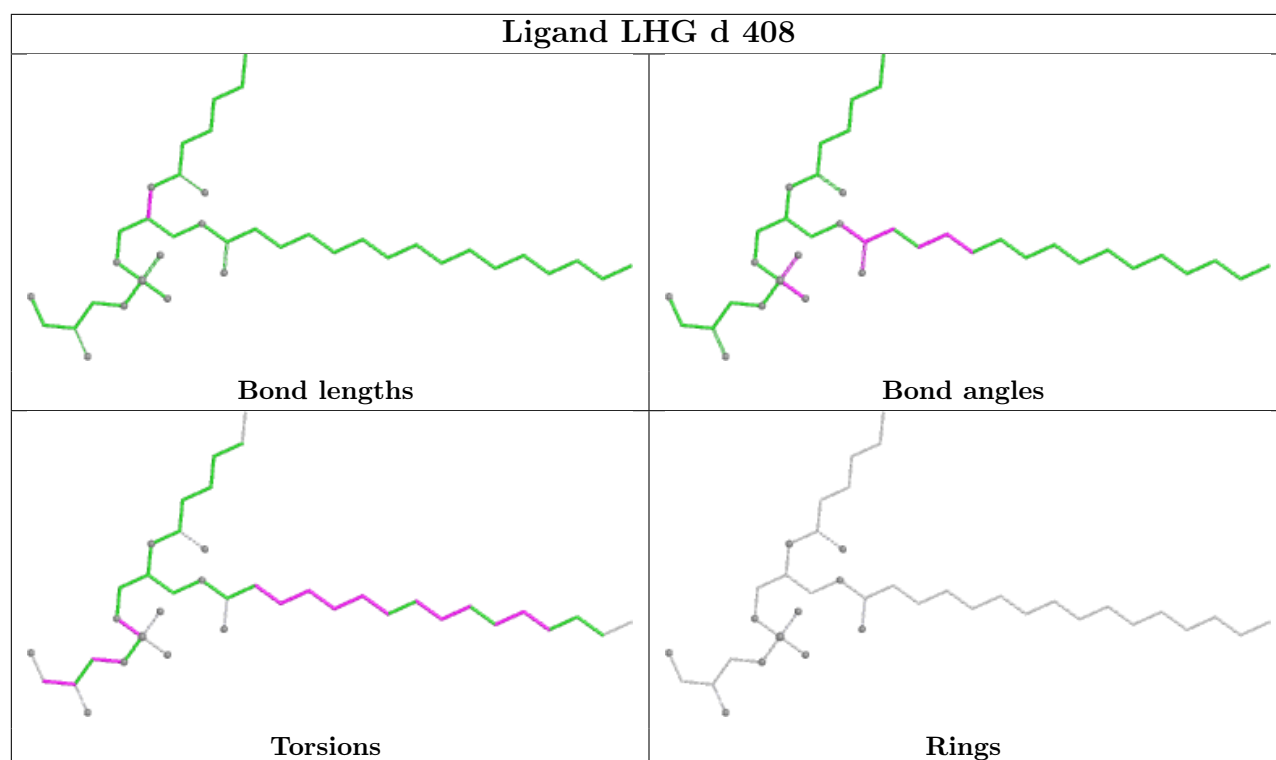
Ligand HEM e 101

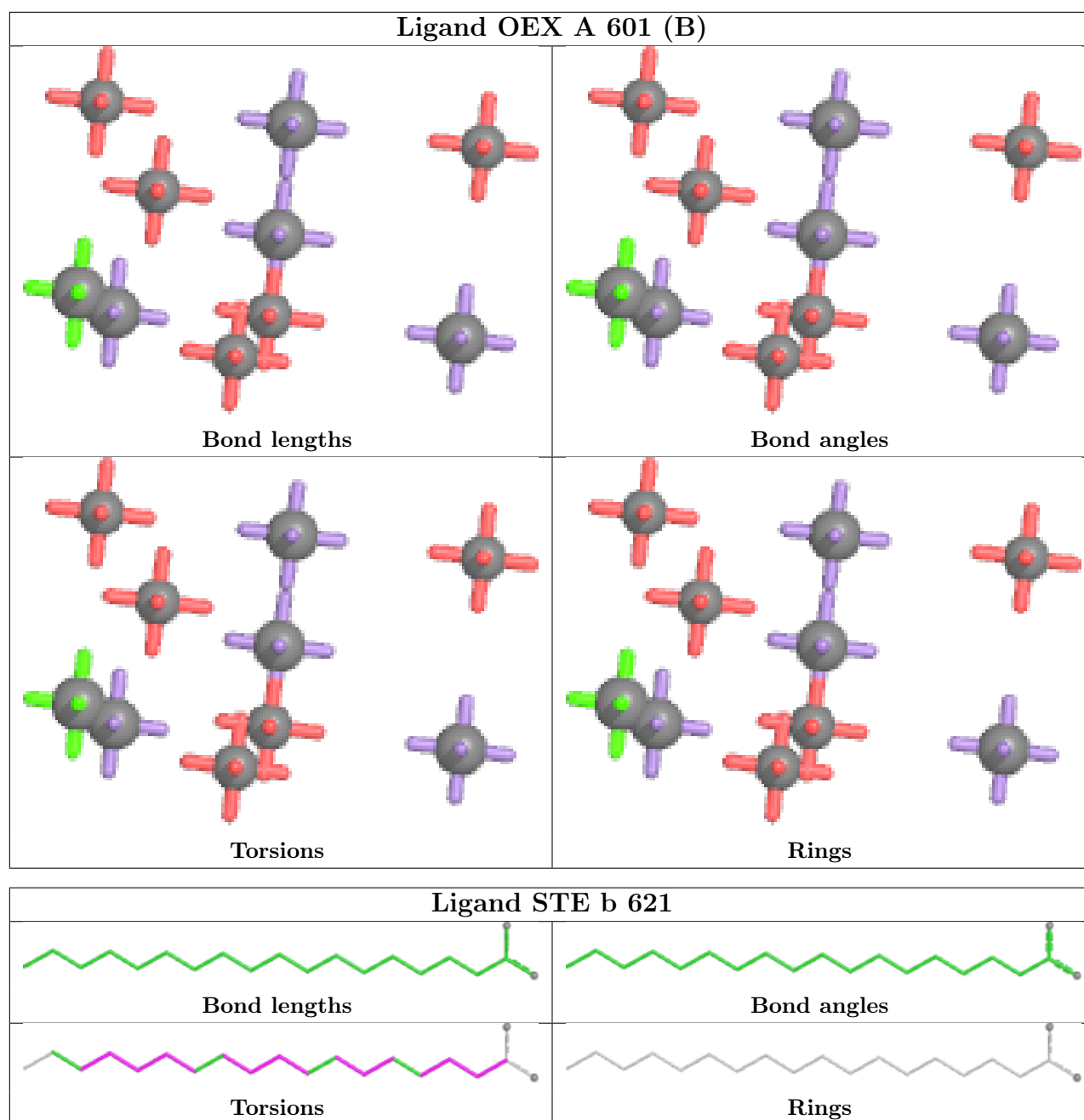




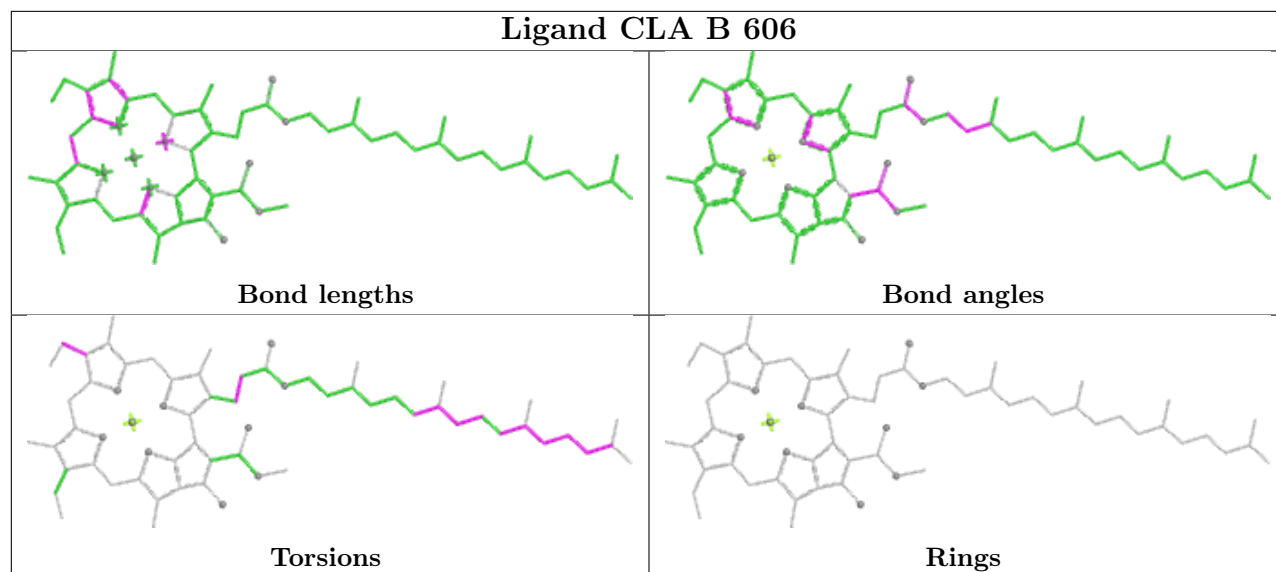


Ligand CLA a 609	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 D 406	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR x 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

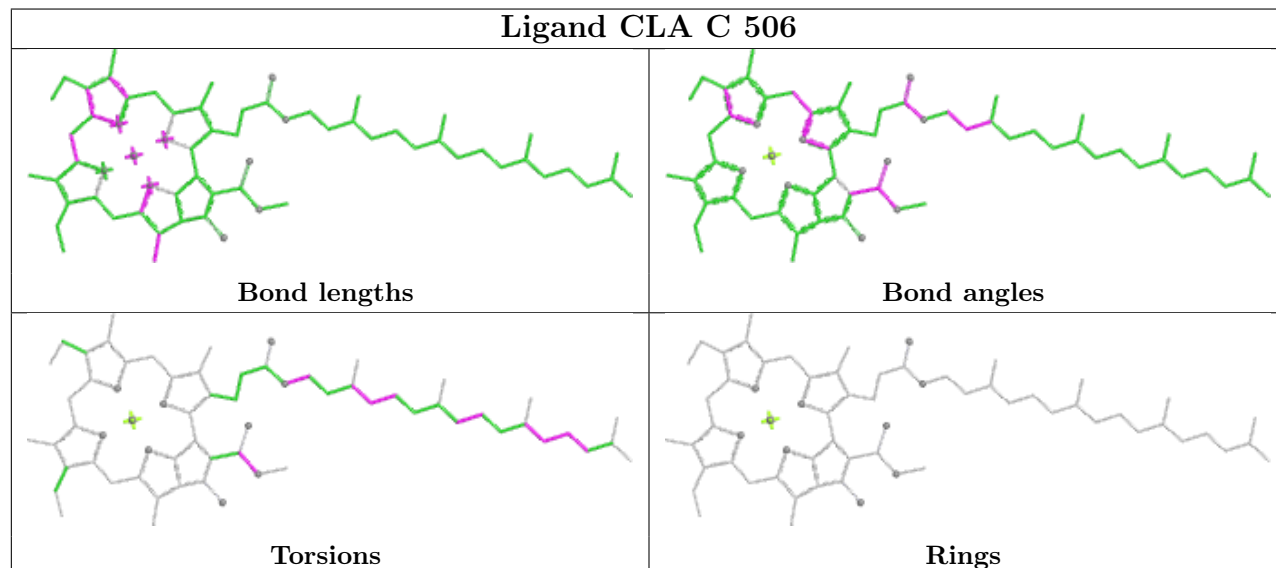




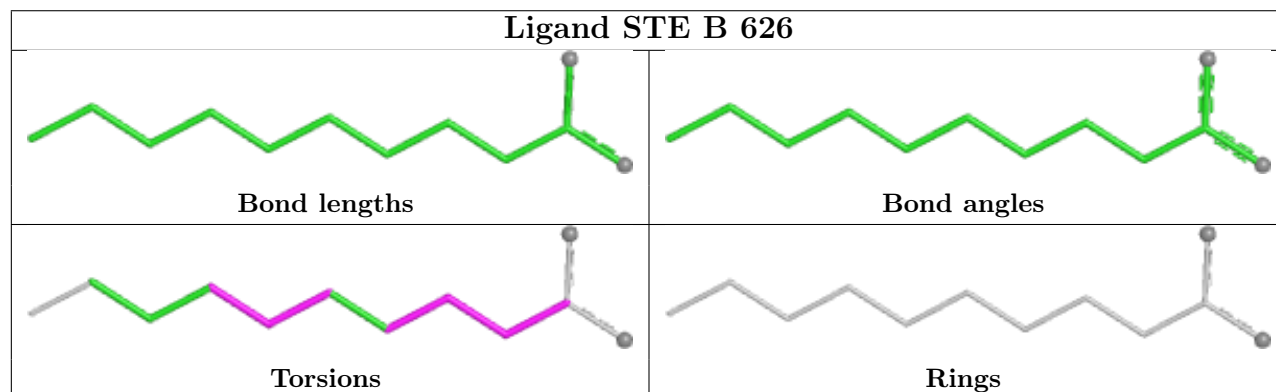
Ligand CLA B 606

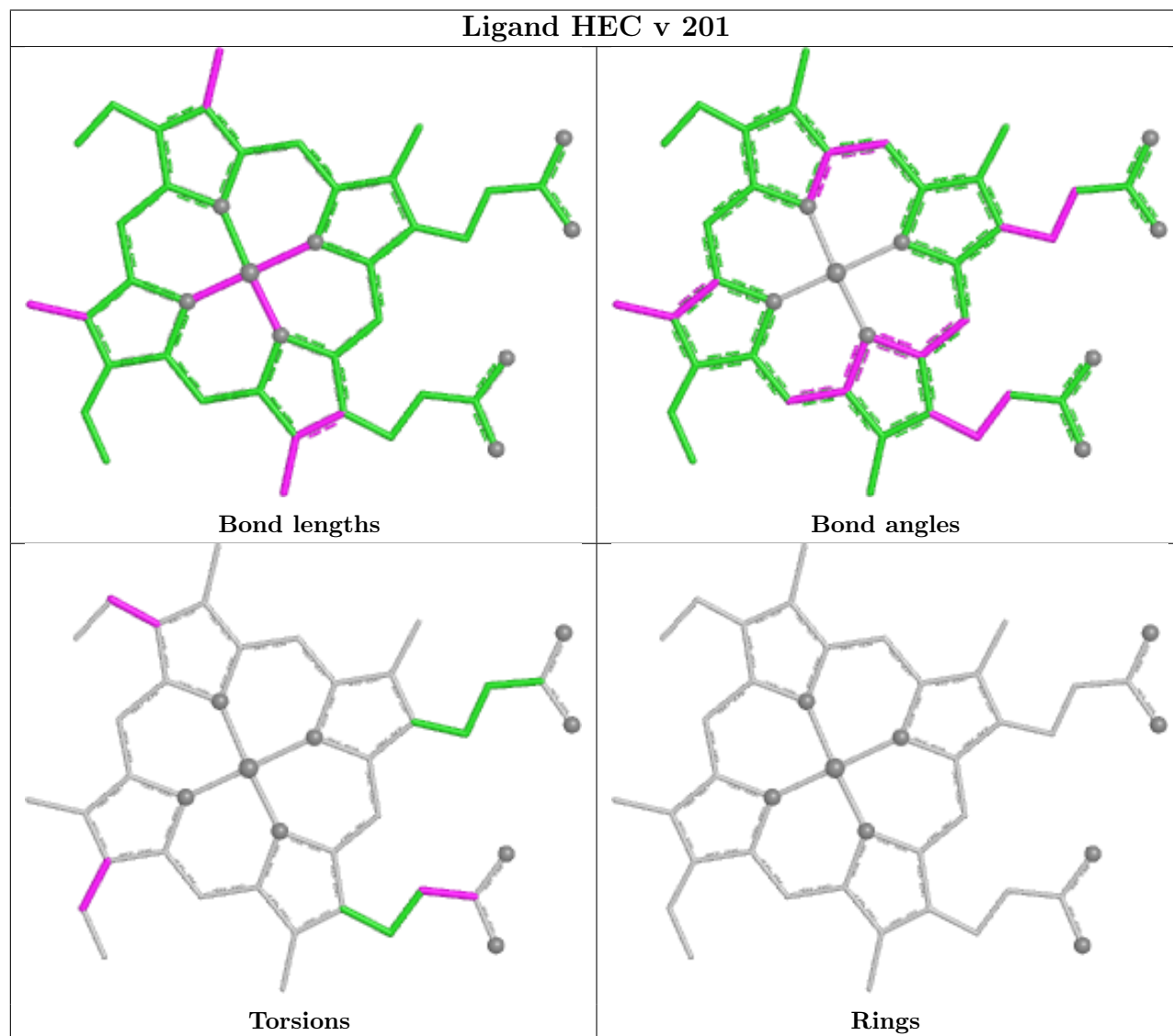
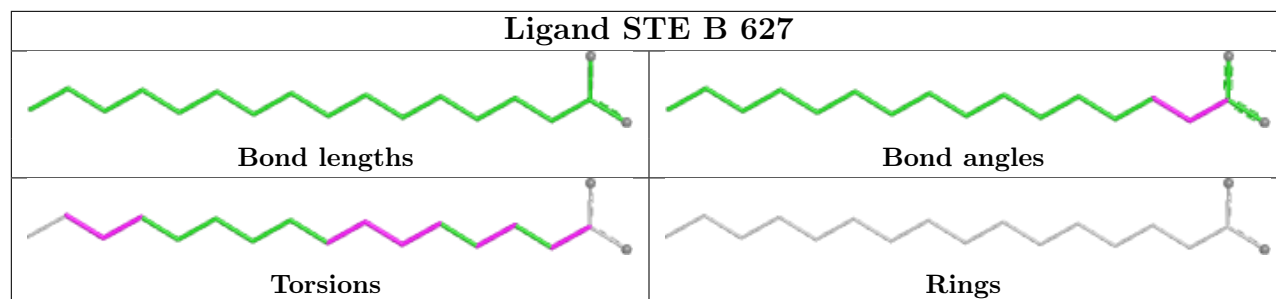


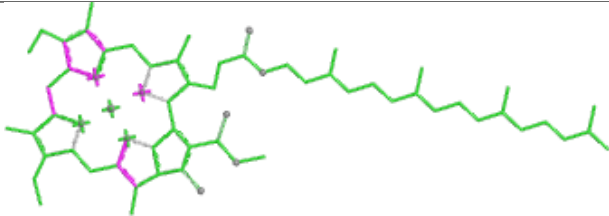
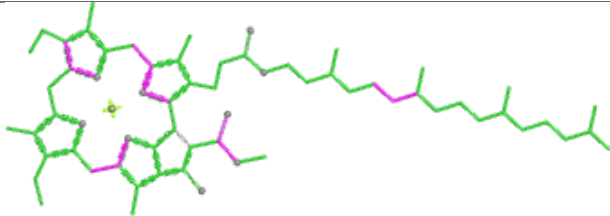
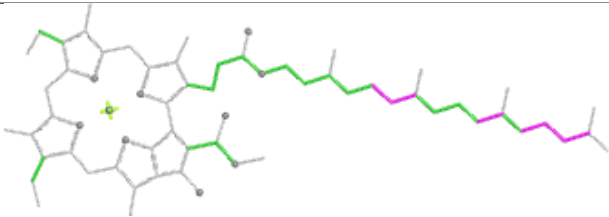
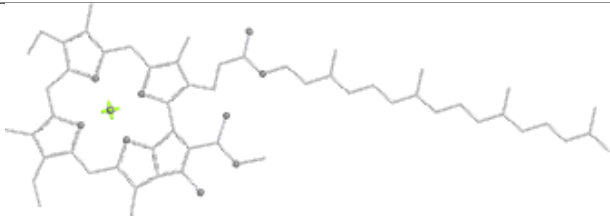
Ligand CLA C 506

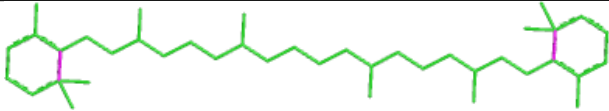
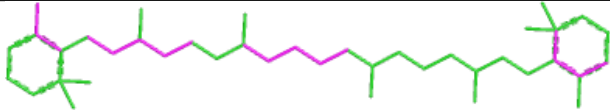
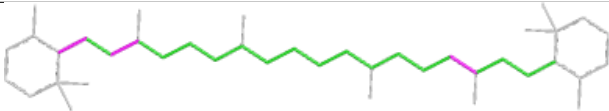
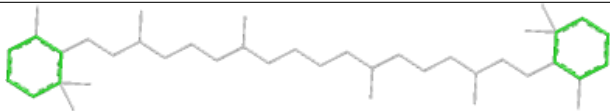


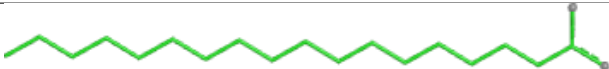
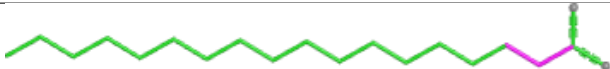
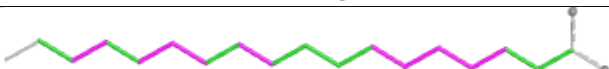
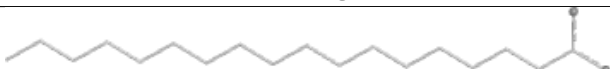
Ligand STE B 626

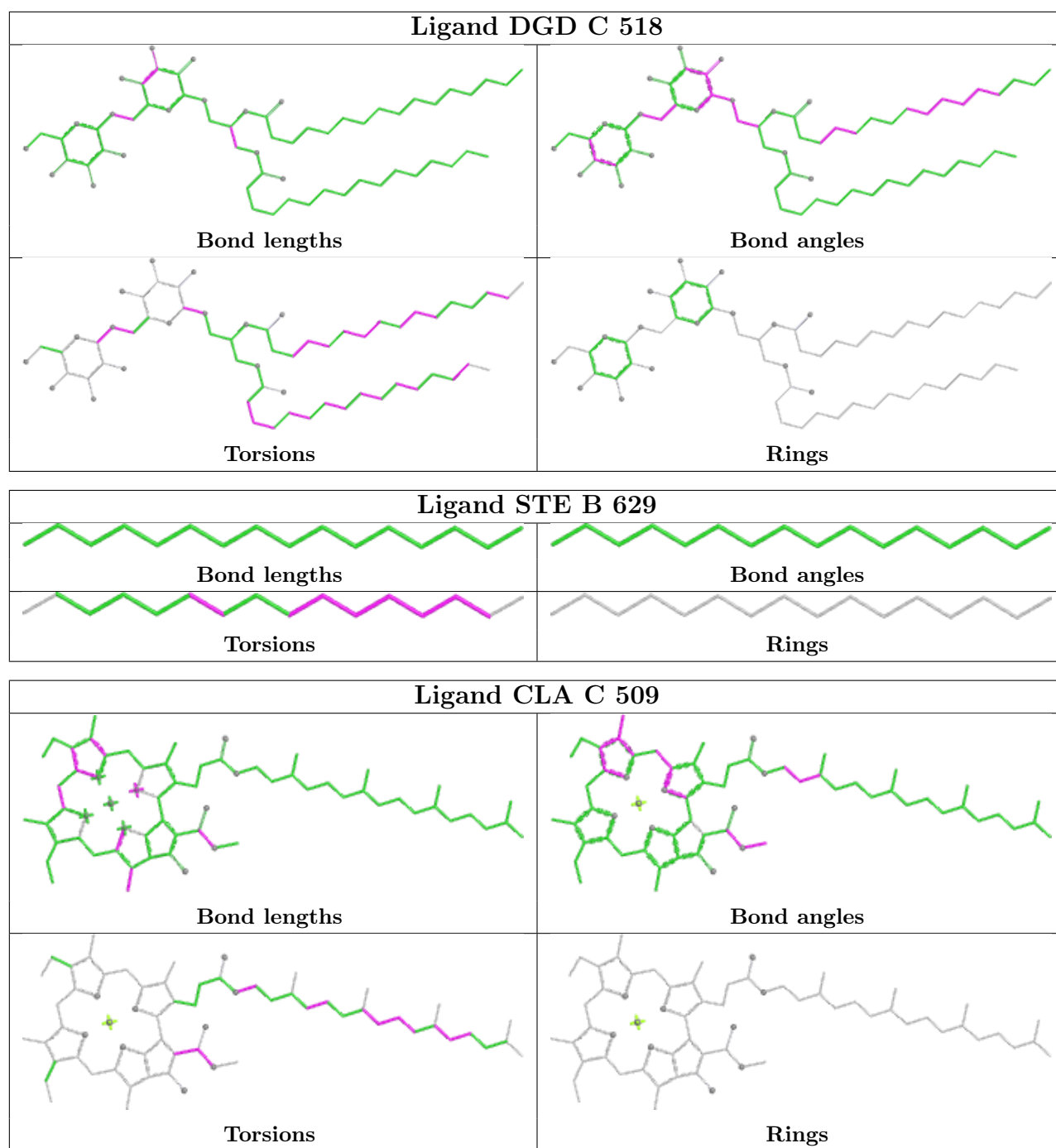


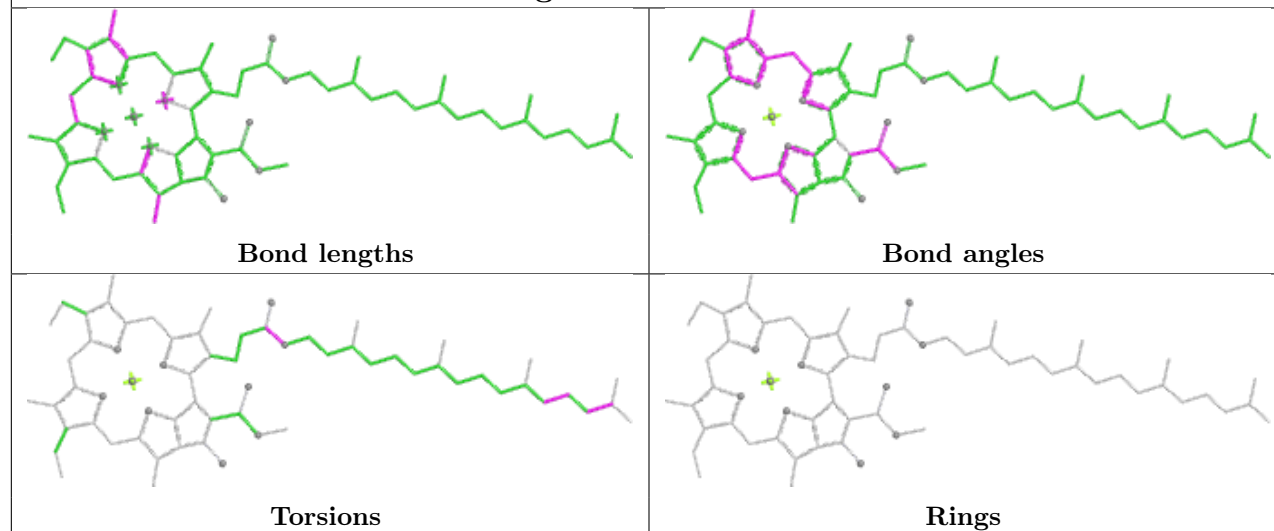
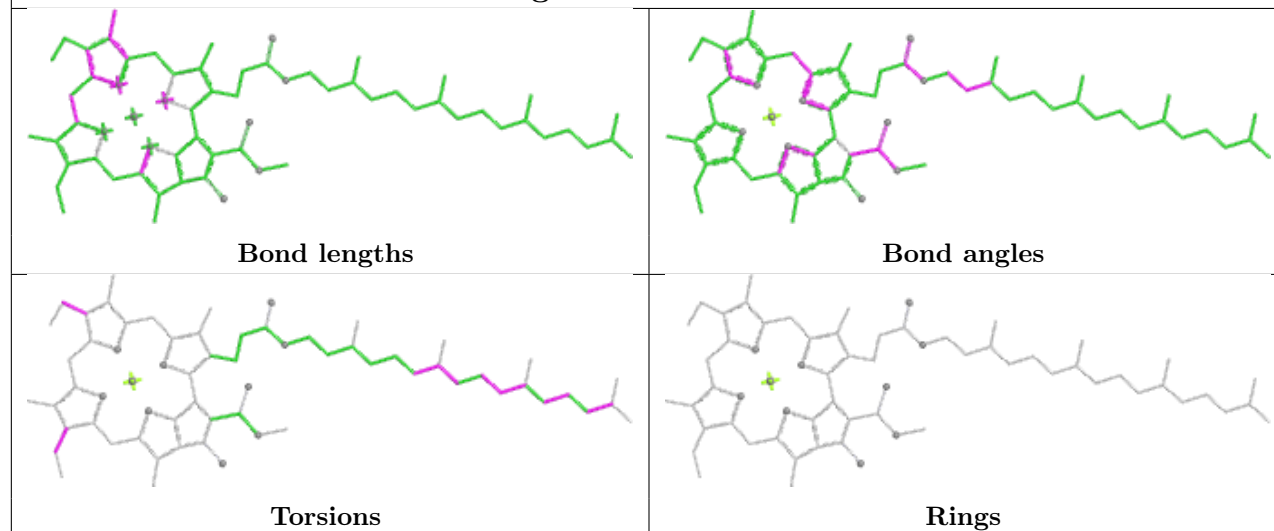
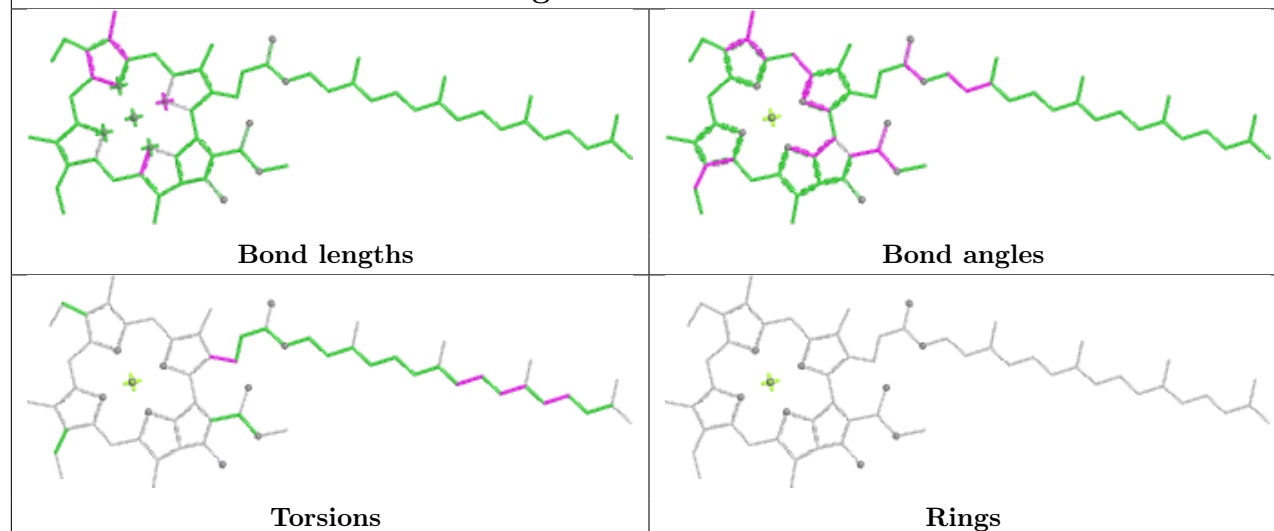


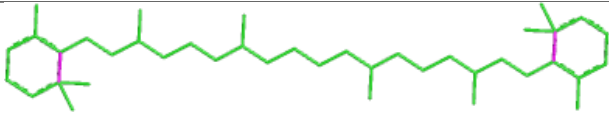
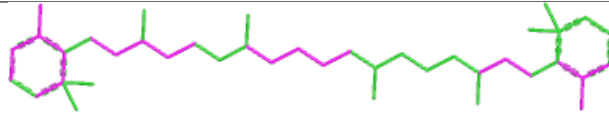
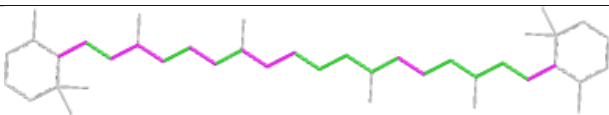
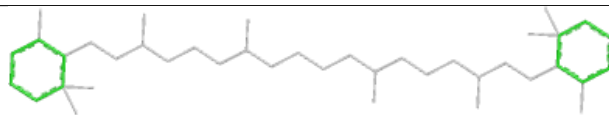
Ligand CLA B 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

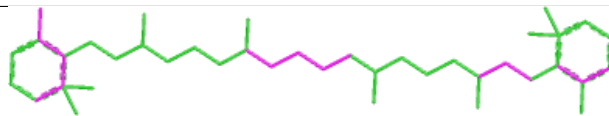
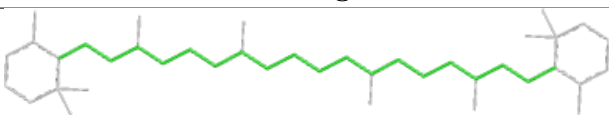
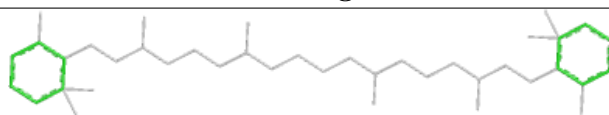
Ligand BCR t 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

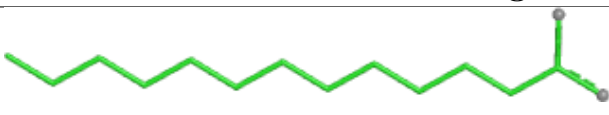
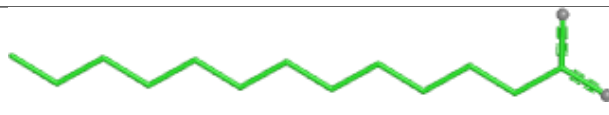
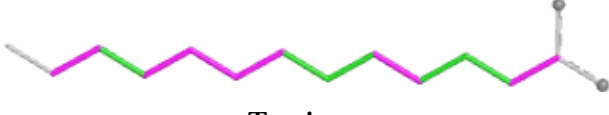
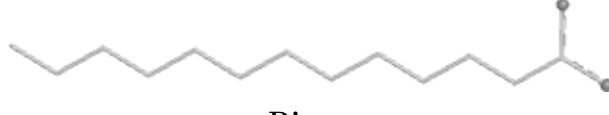
Ligand STE b 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

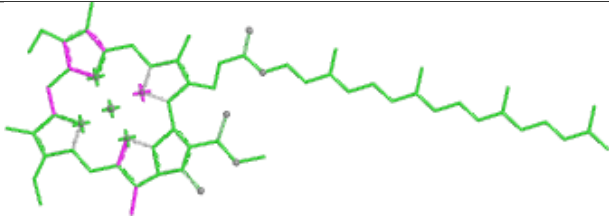
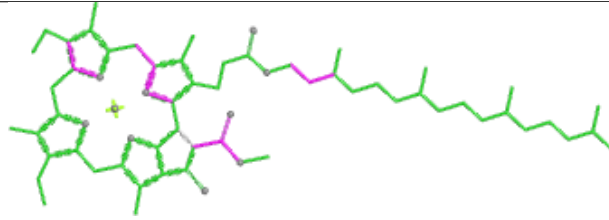
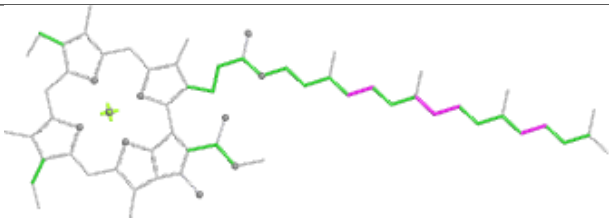
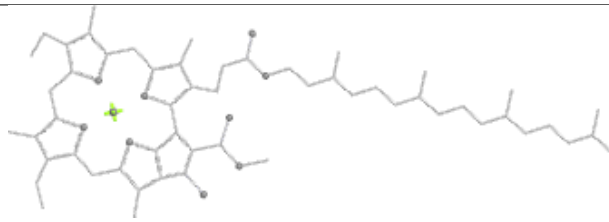


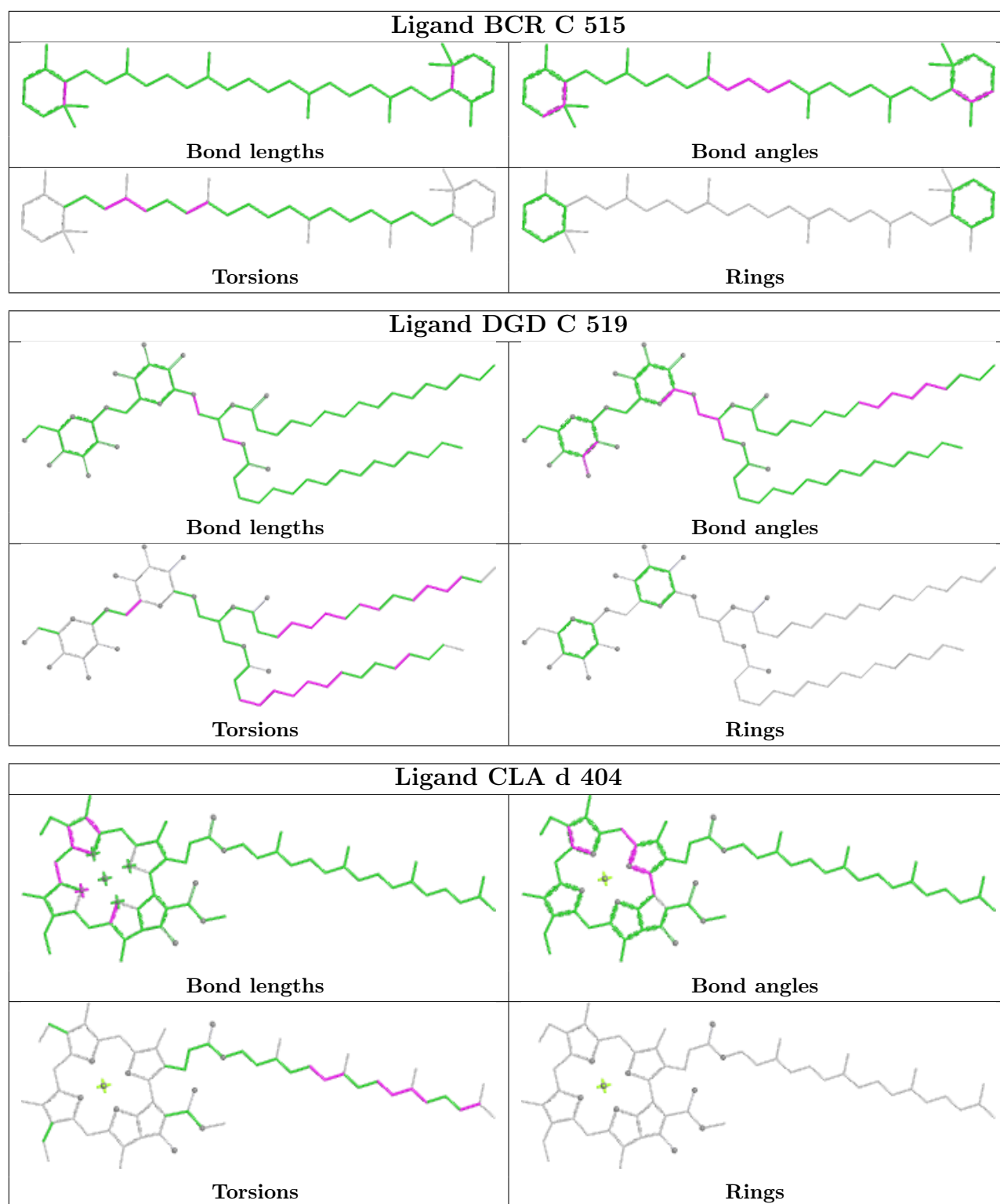
Ligand CLA b 608**Ligand CLA A 607****Ligand CLA B 602**

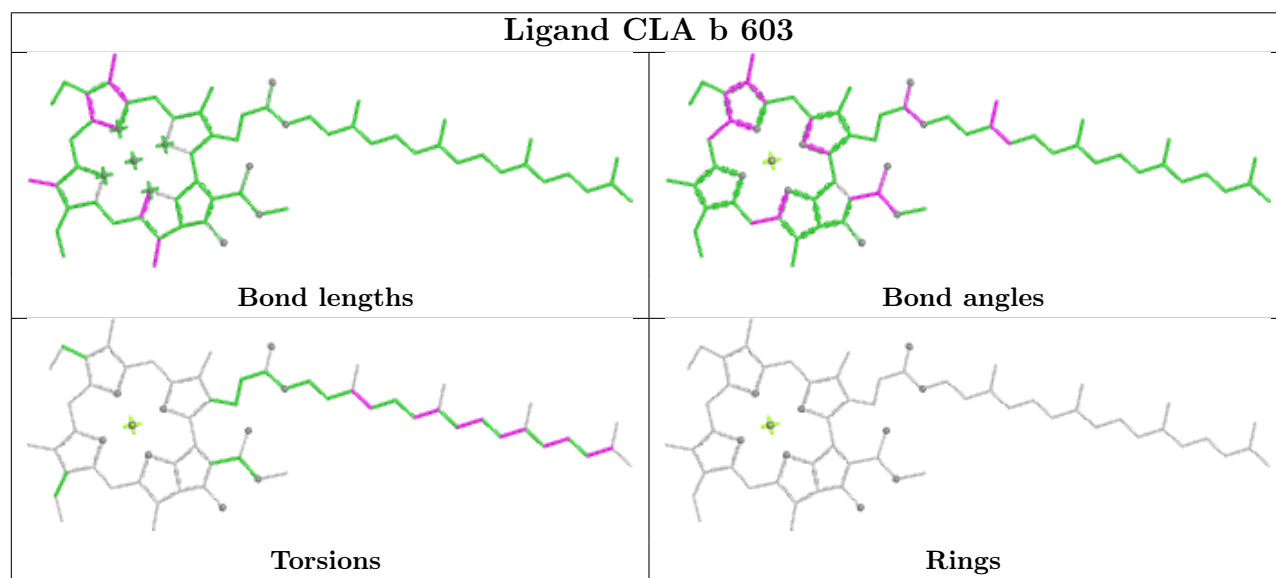
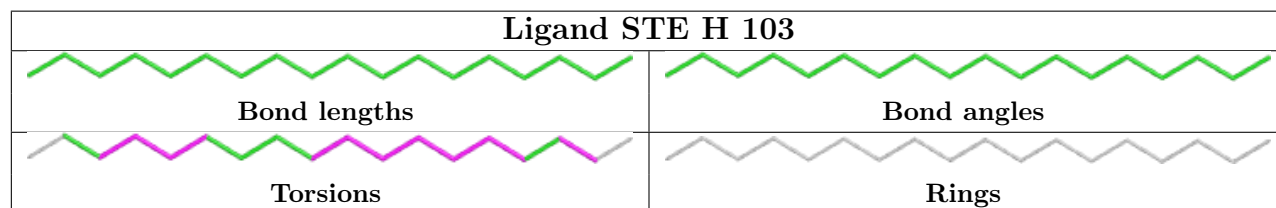
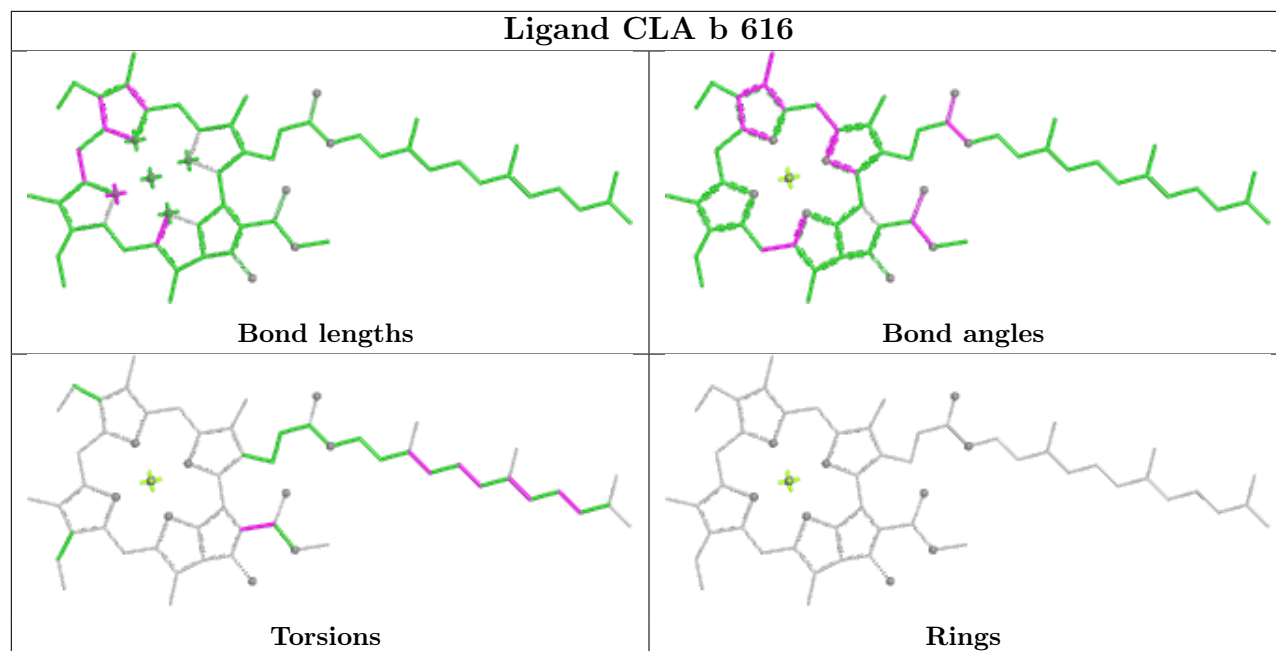
Ligand BCR k 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

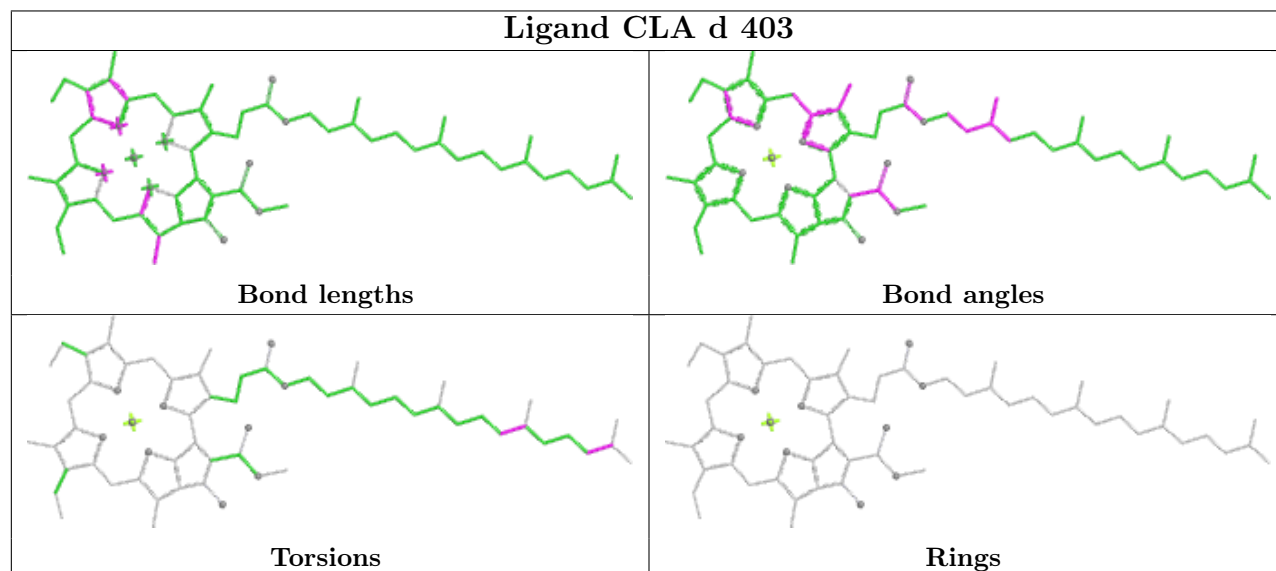
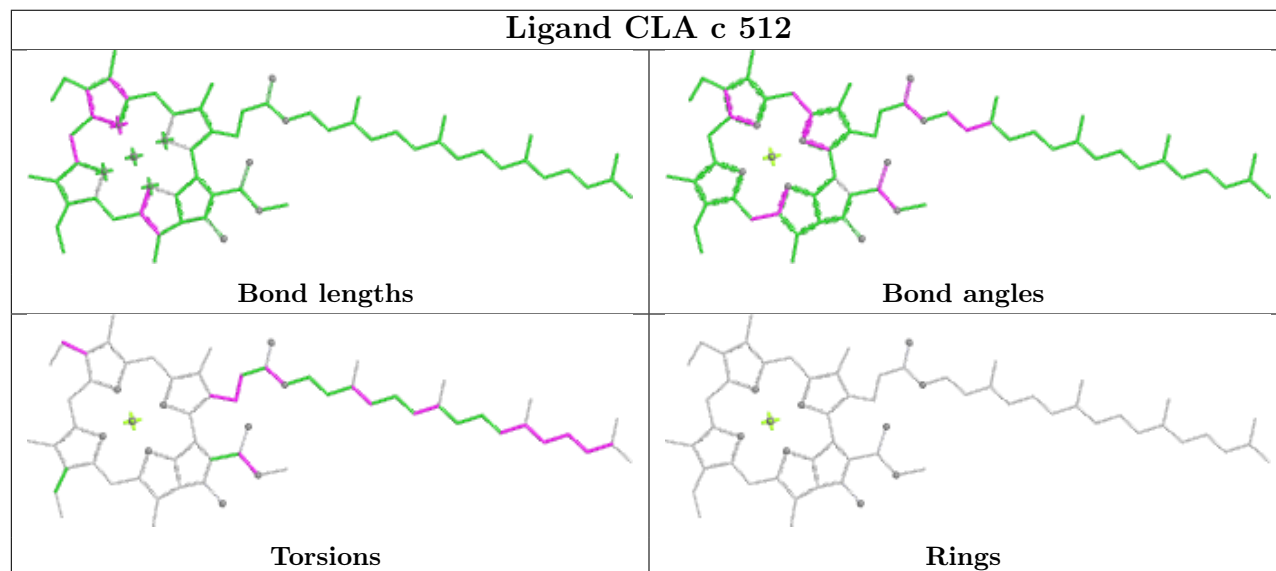
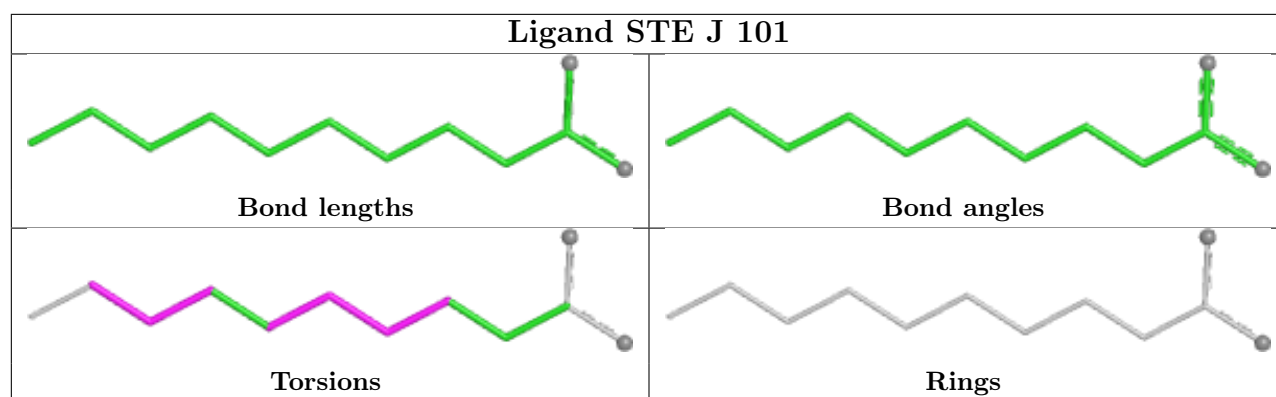
Ligand BCR C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE M 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

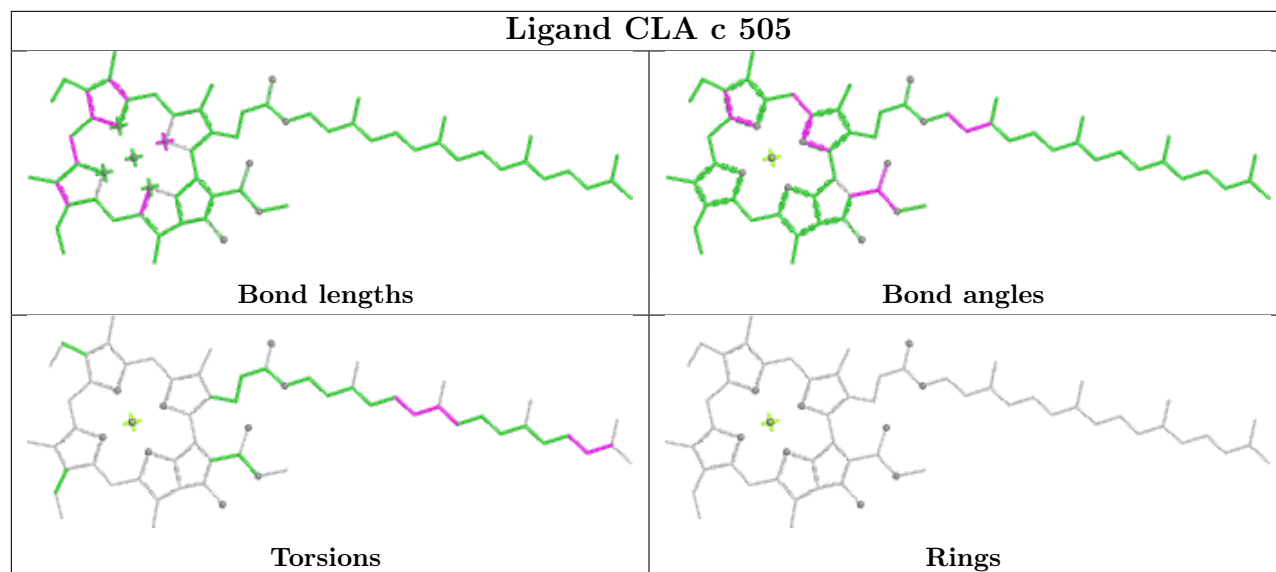
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Bond lengths	Bond angles
	
Torsions	Rings



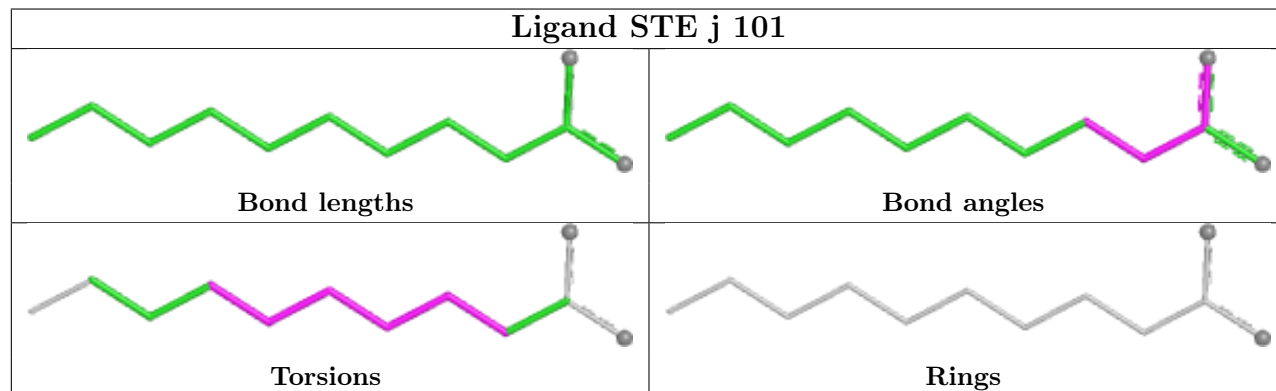




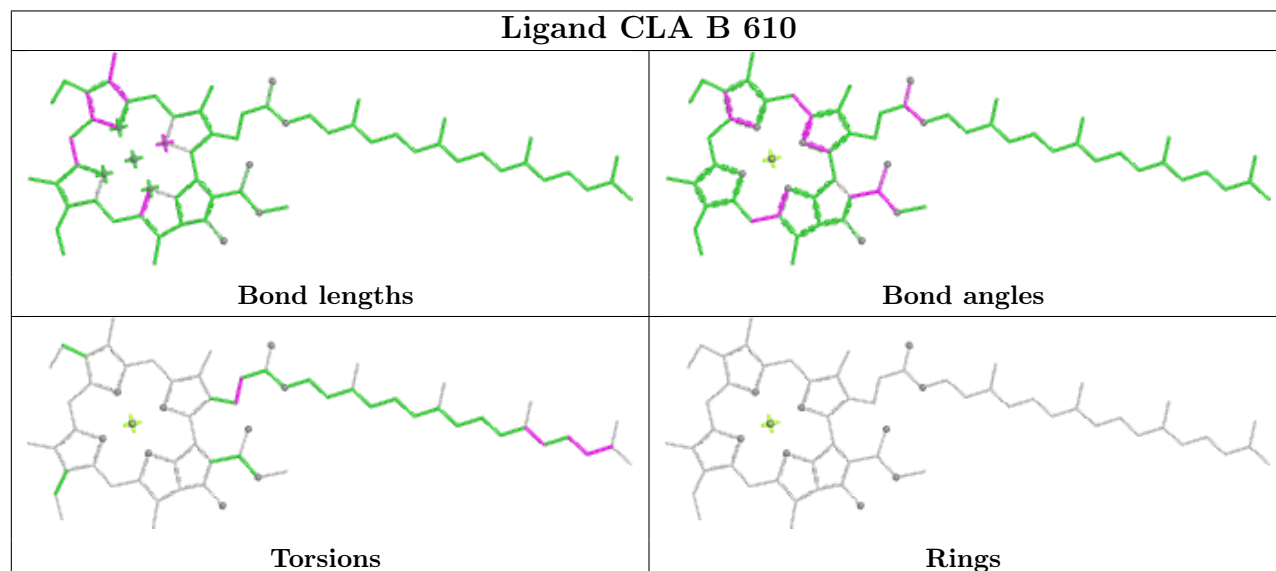
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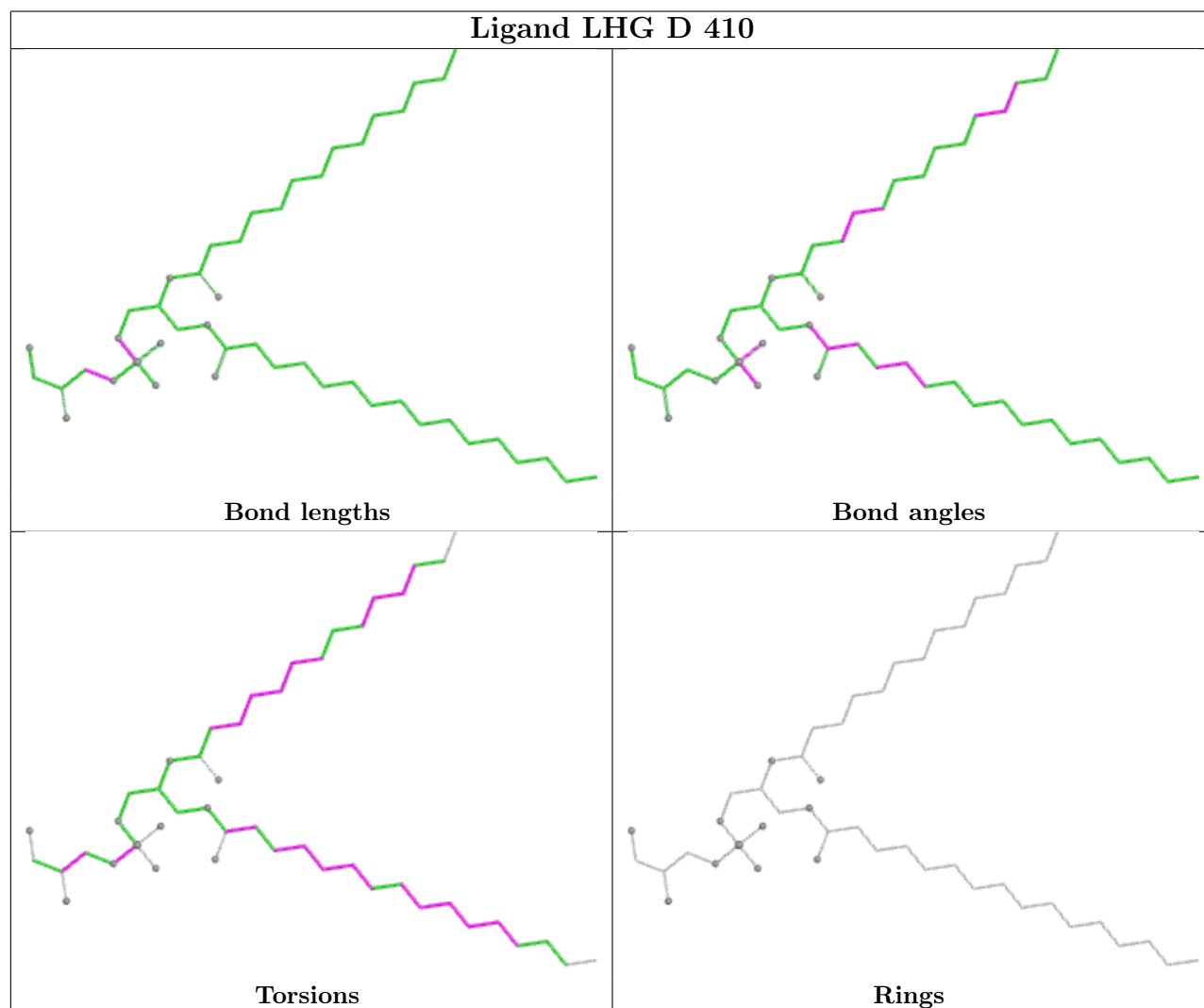
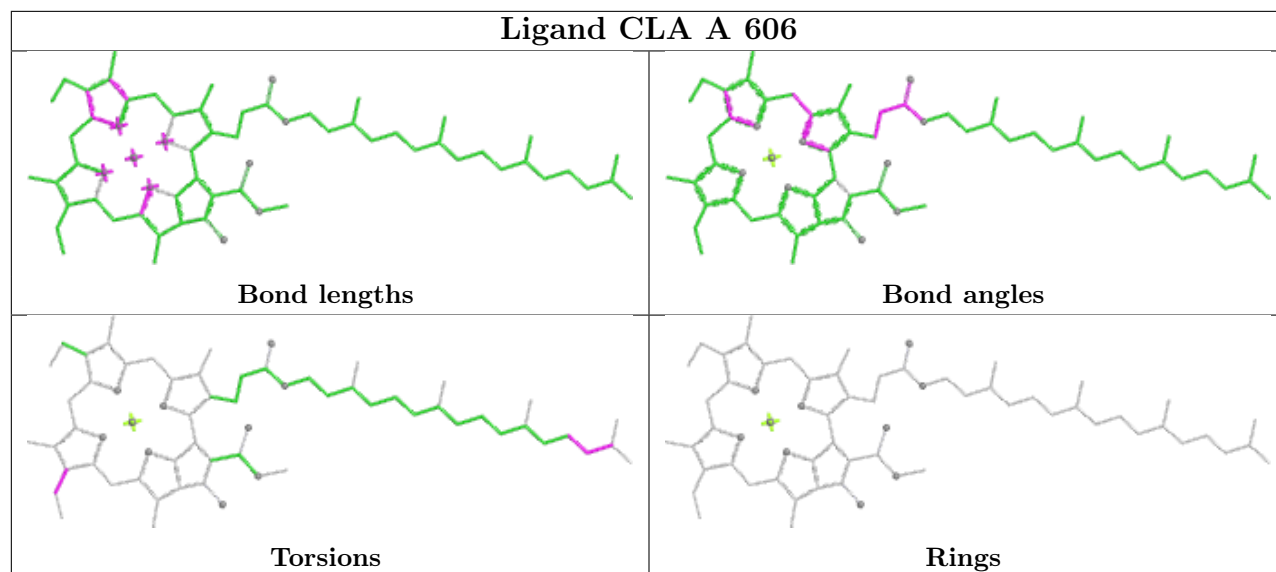


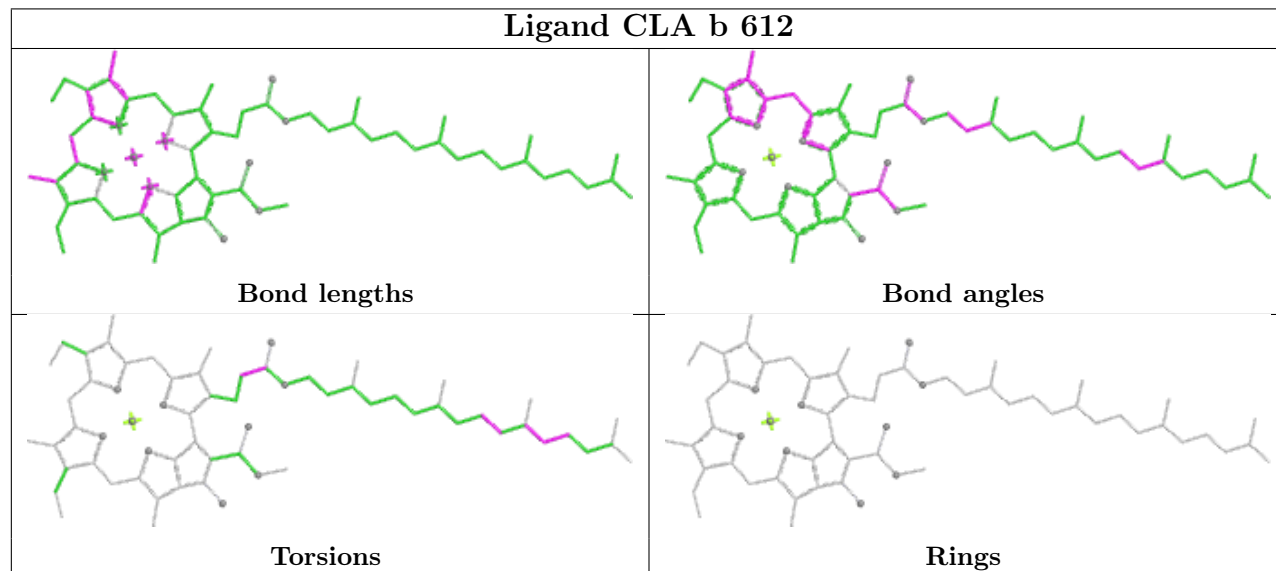
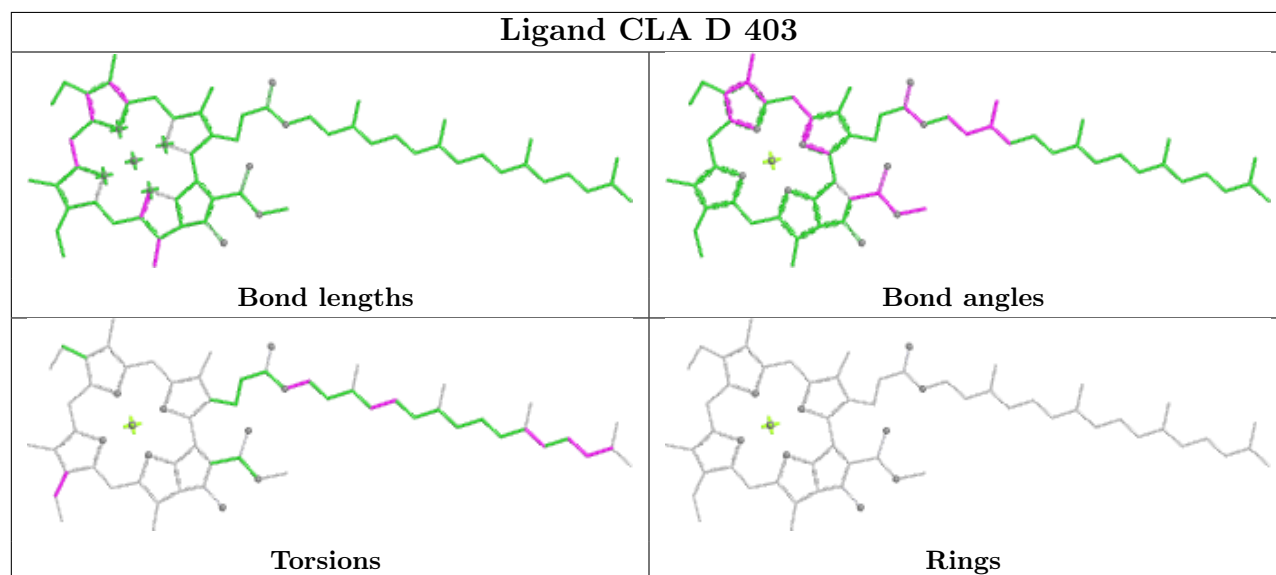
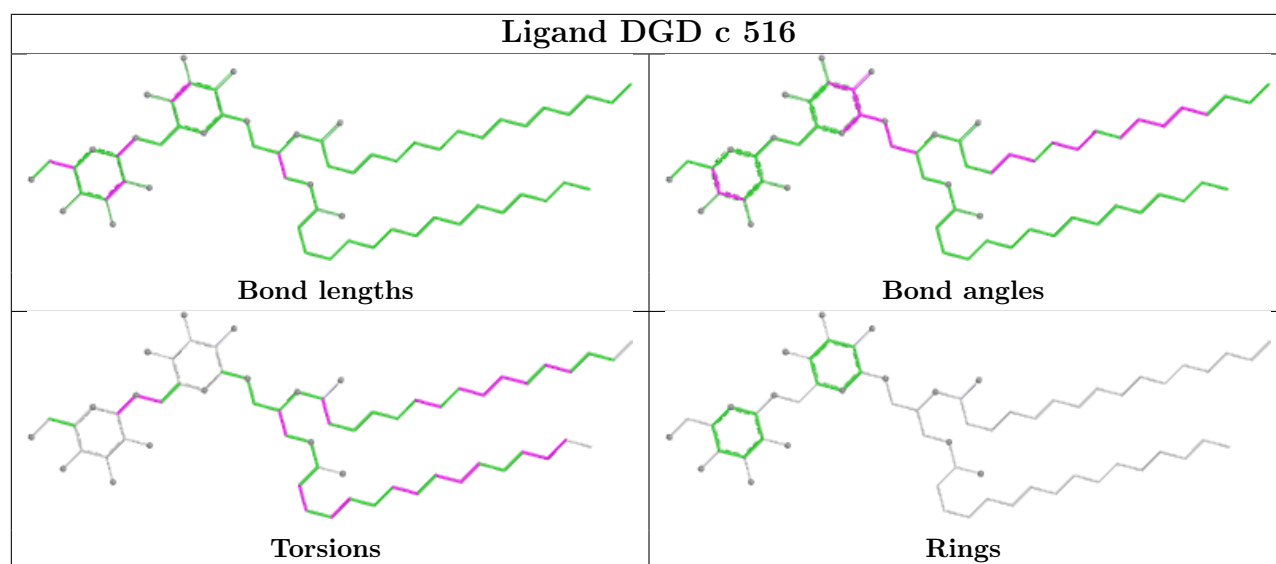
Ligand STE j 101

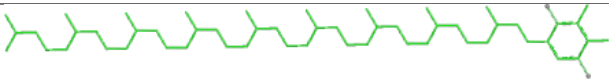
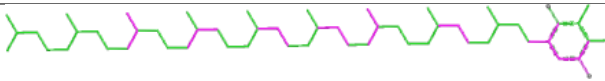
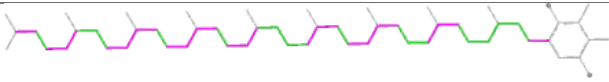
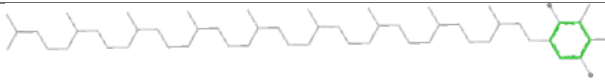


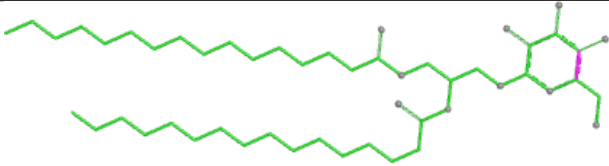
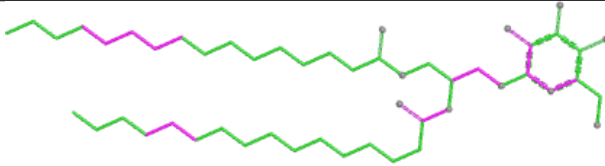
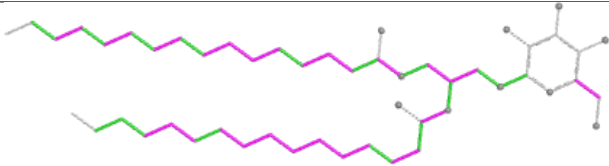
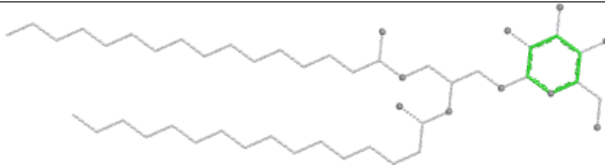
Ligand CLA B 610

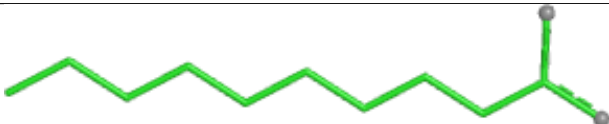
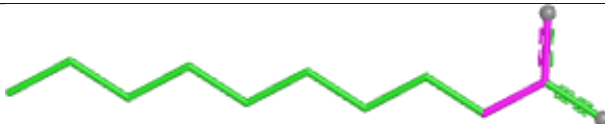
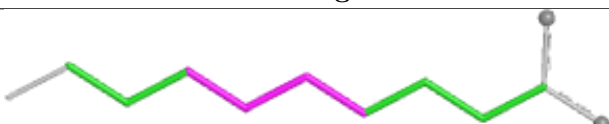
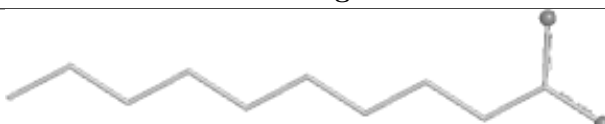


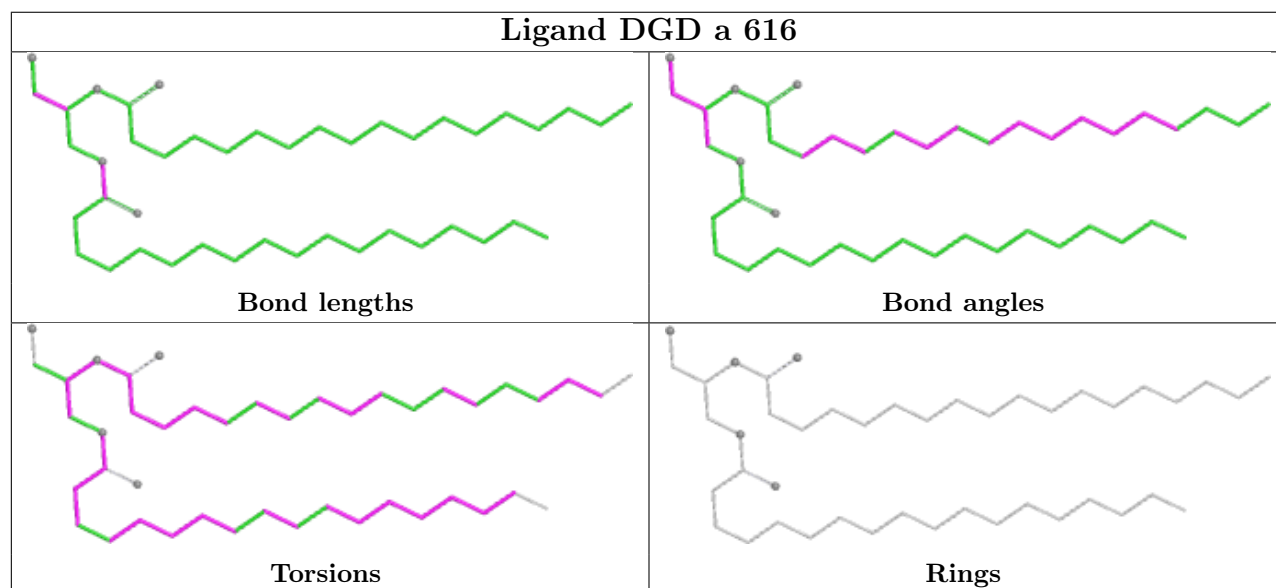
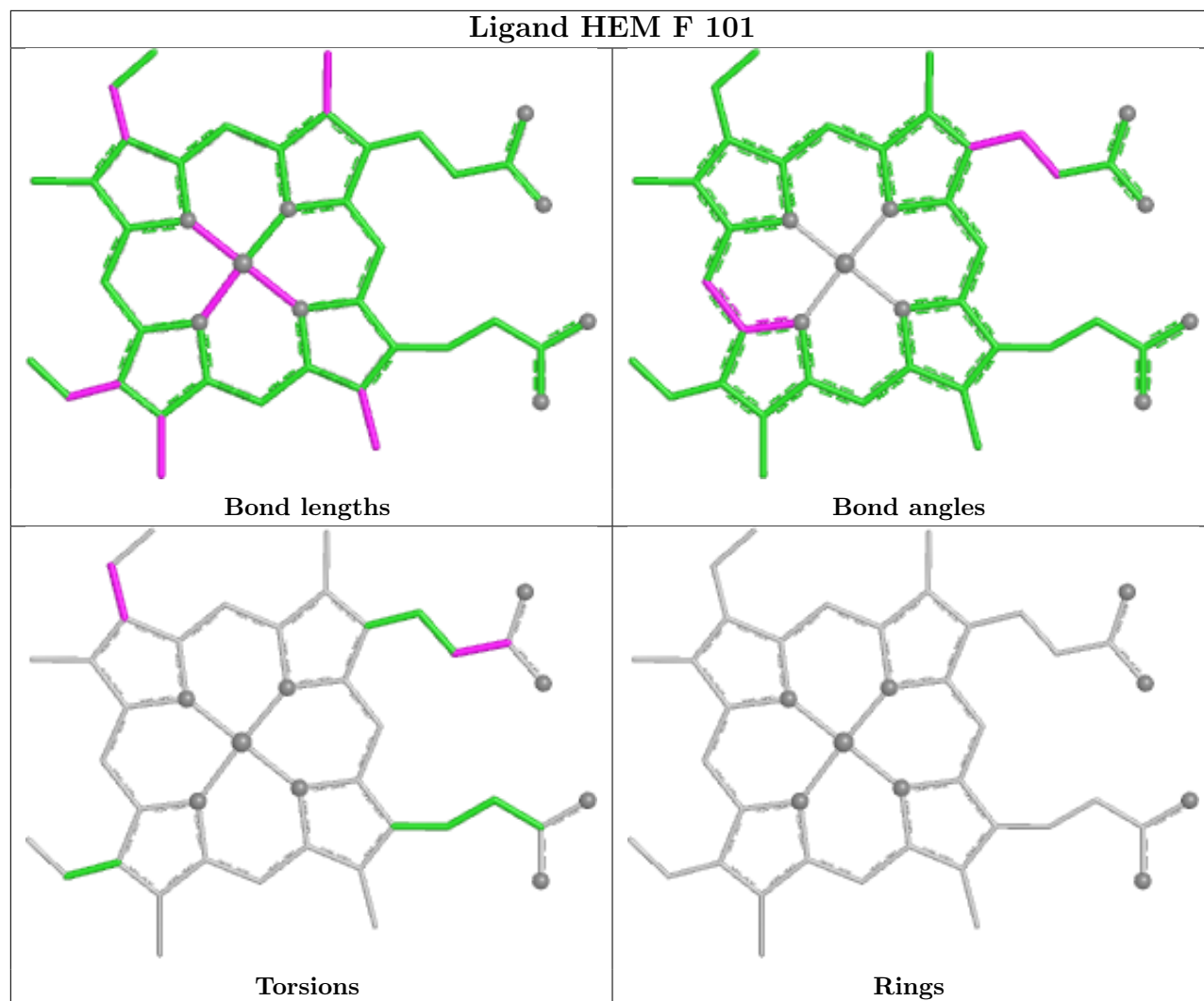


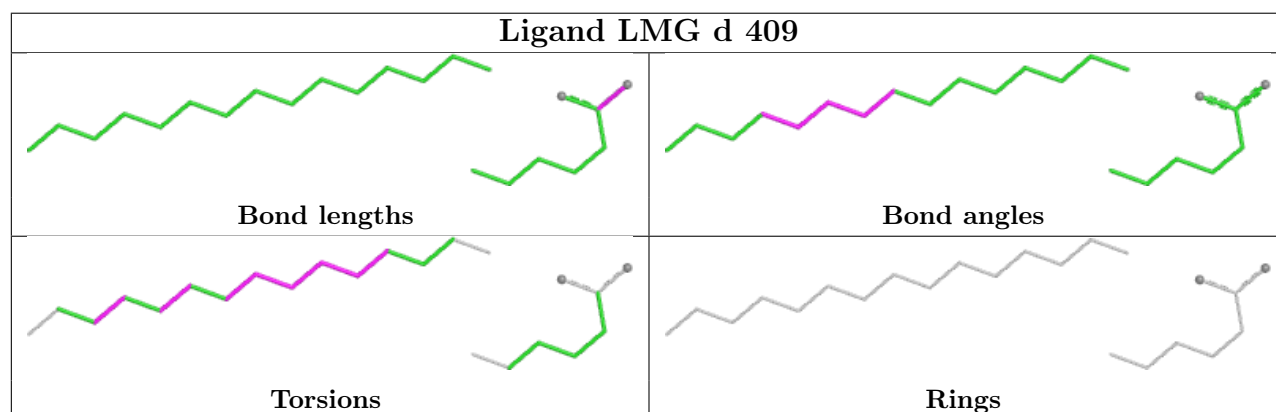
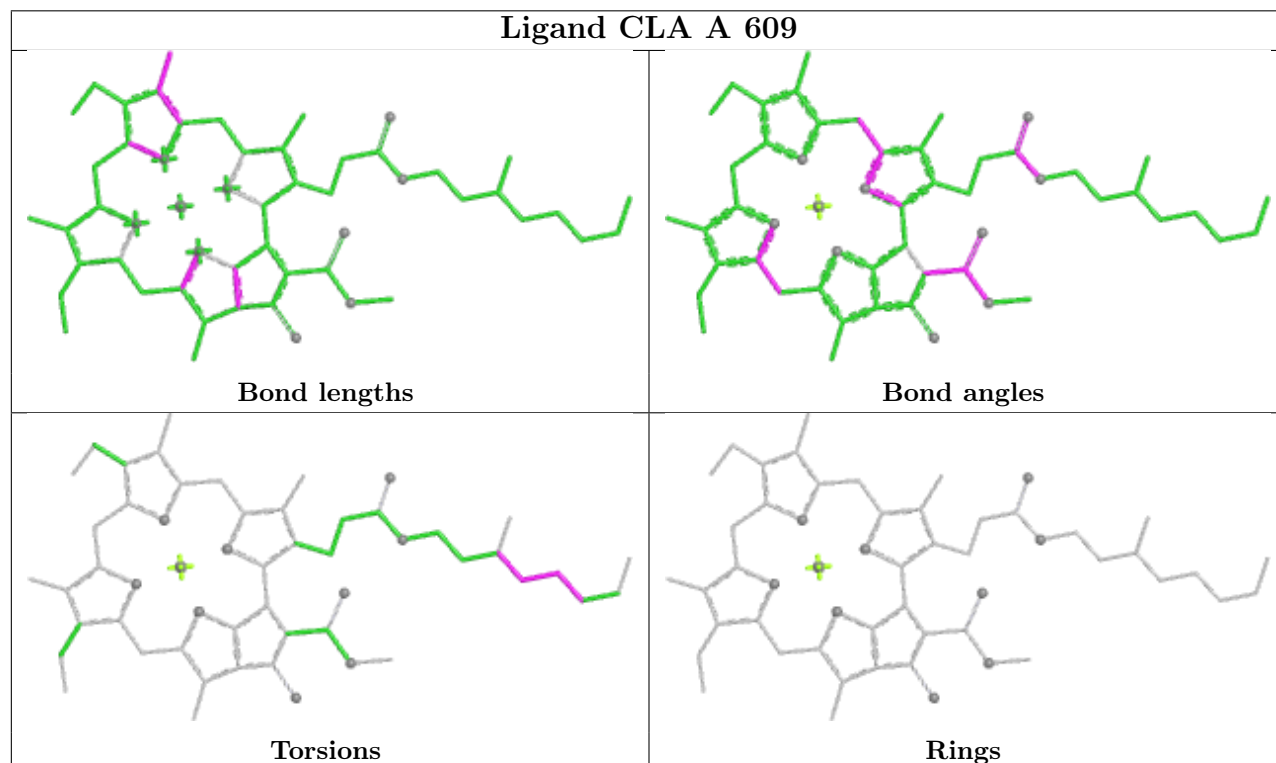
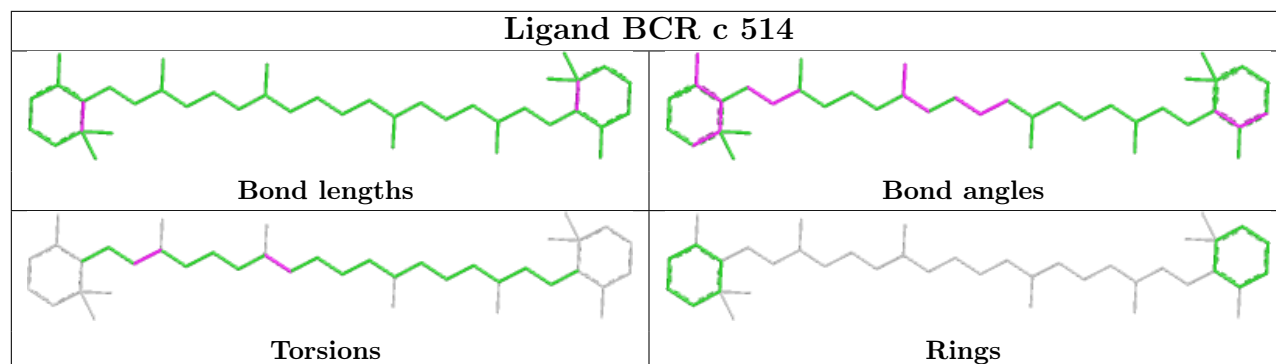


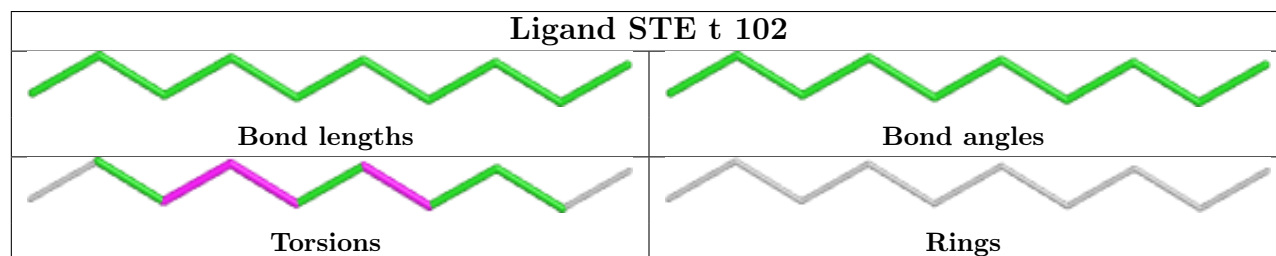
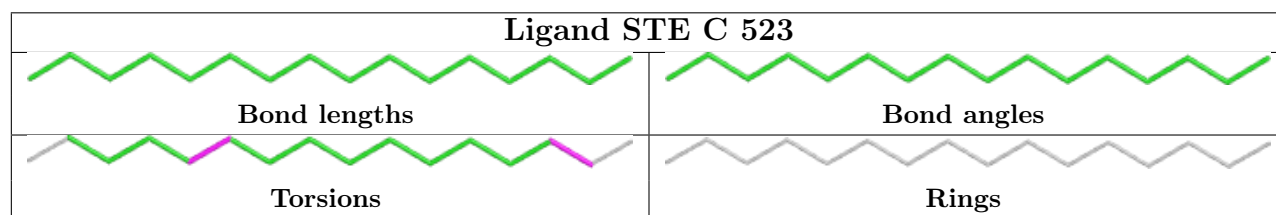
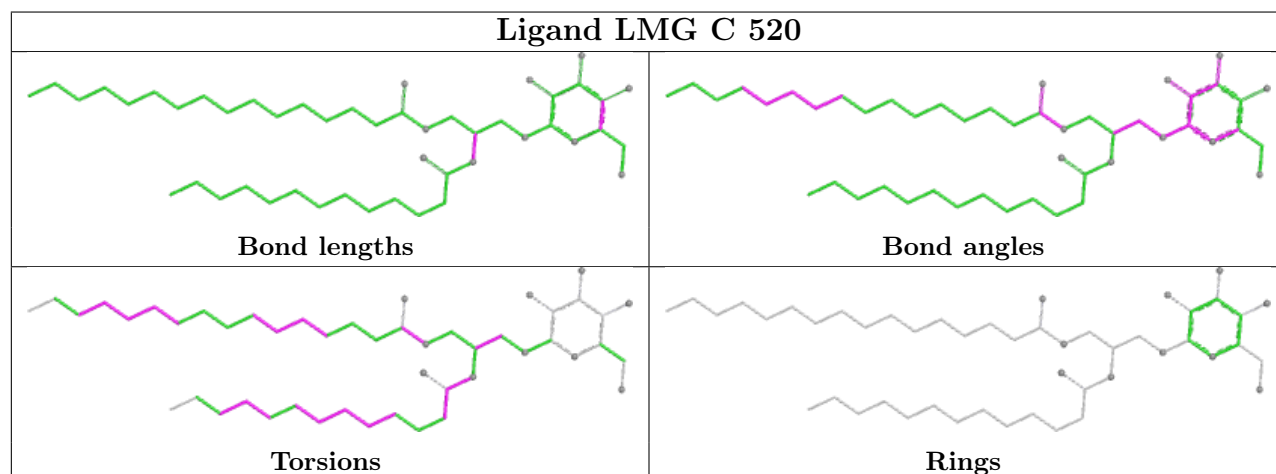
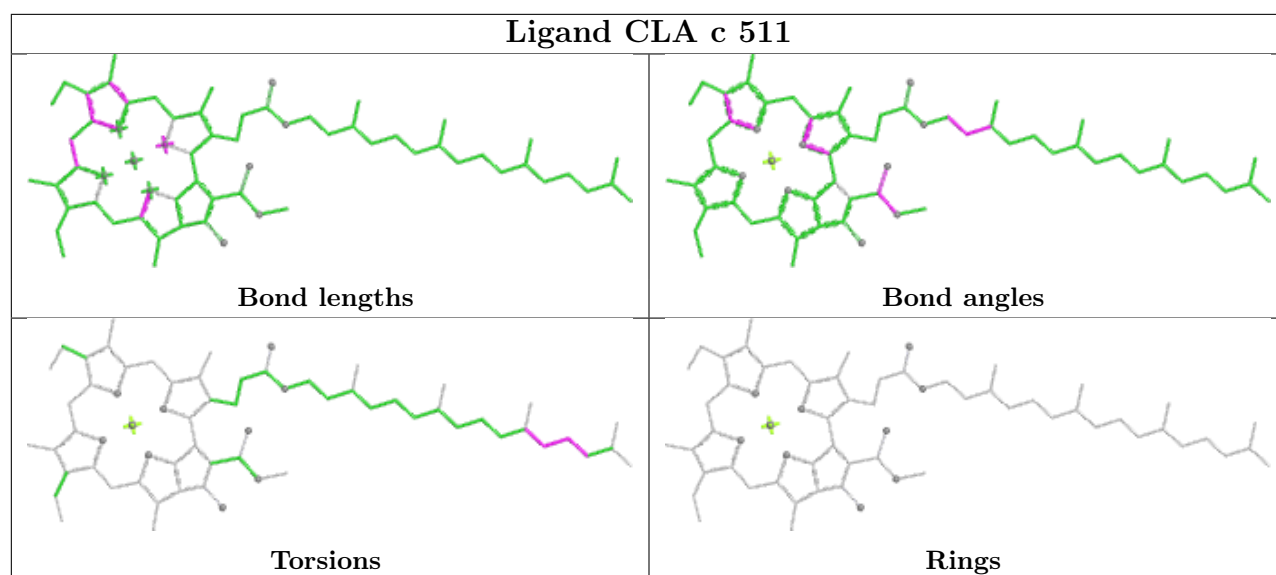
Ligand PL9 A 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

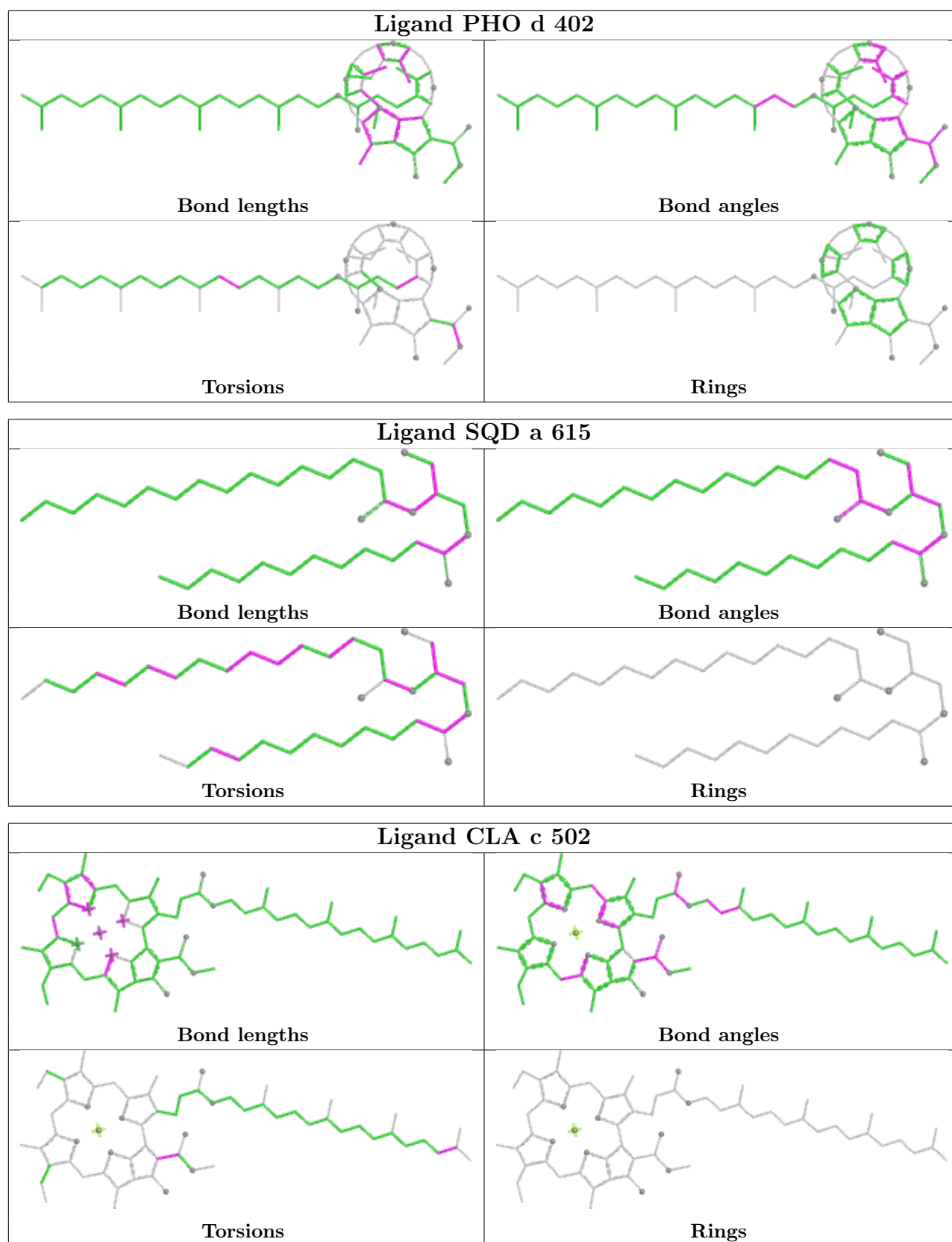
Ligand LMG B 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

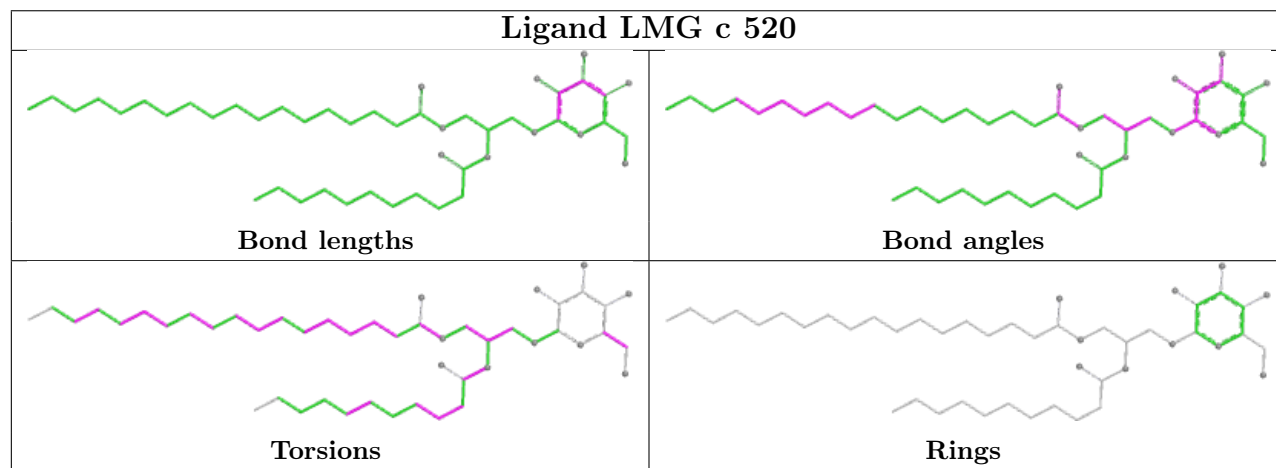
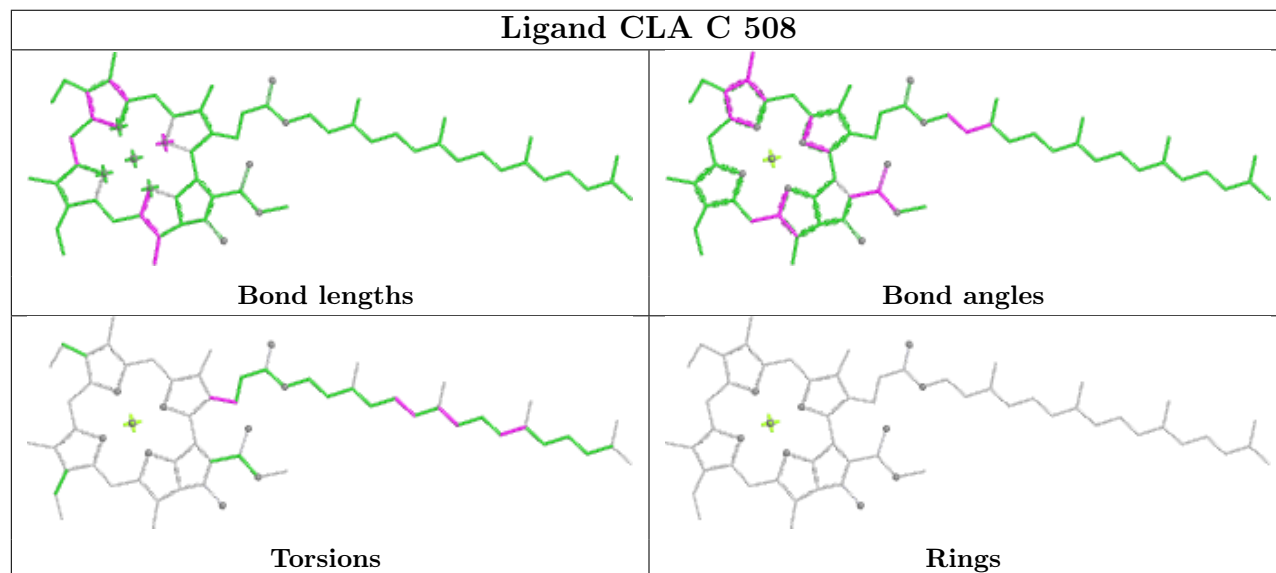
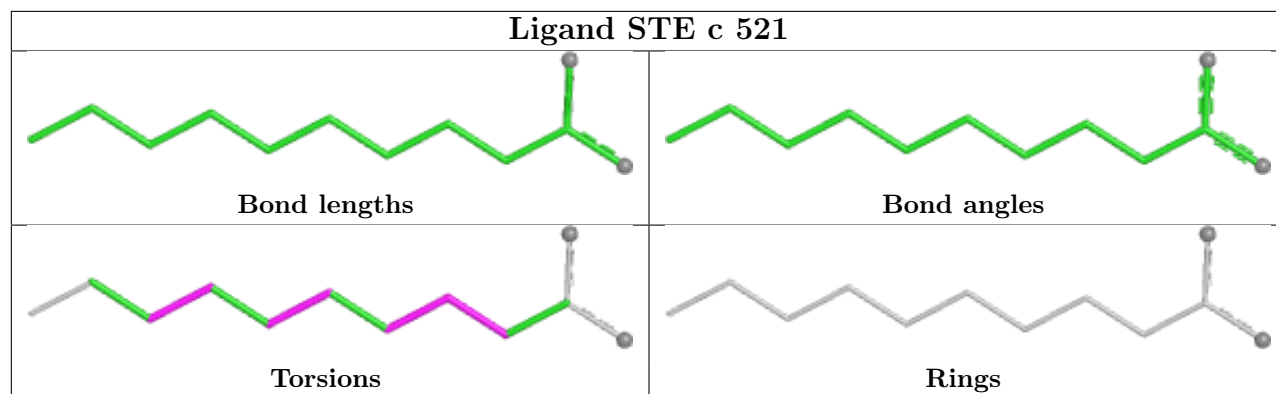
Ligand STE E 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

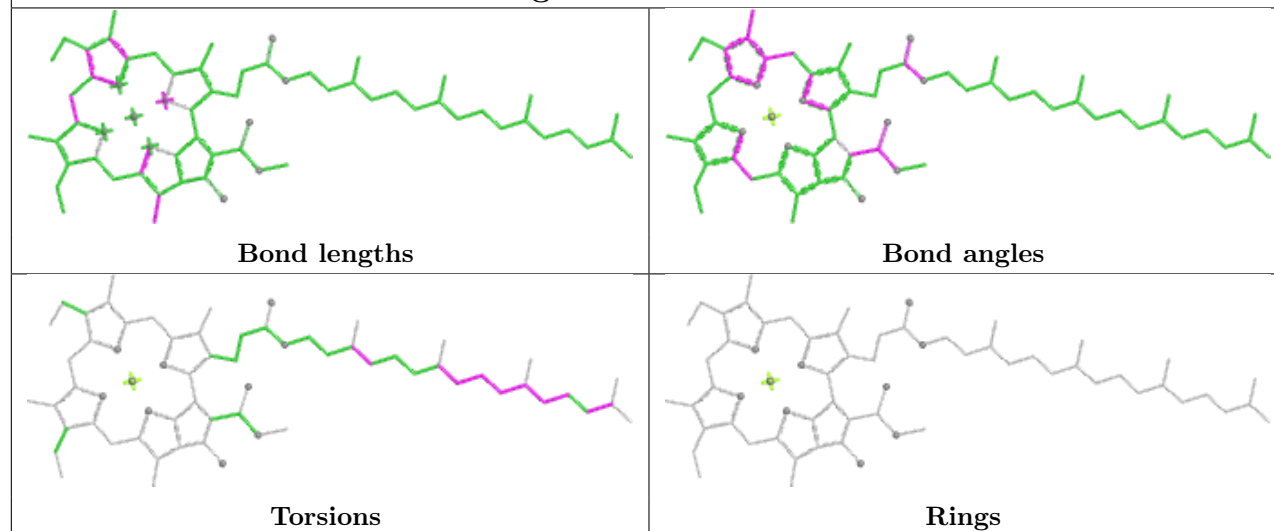
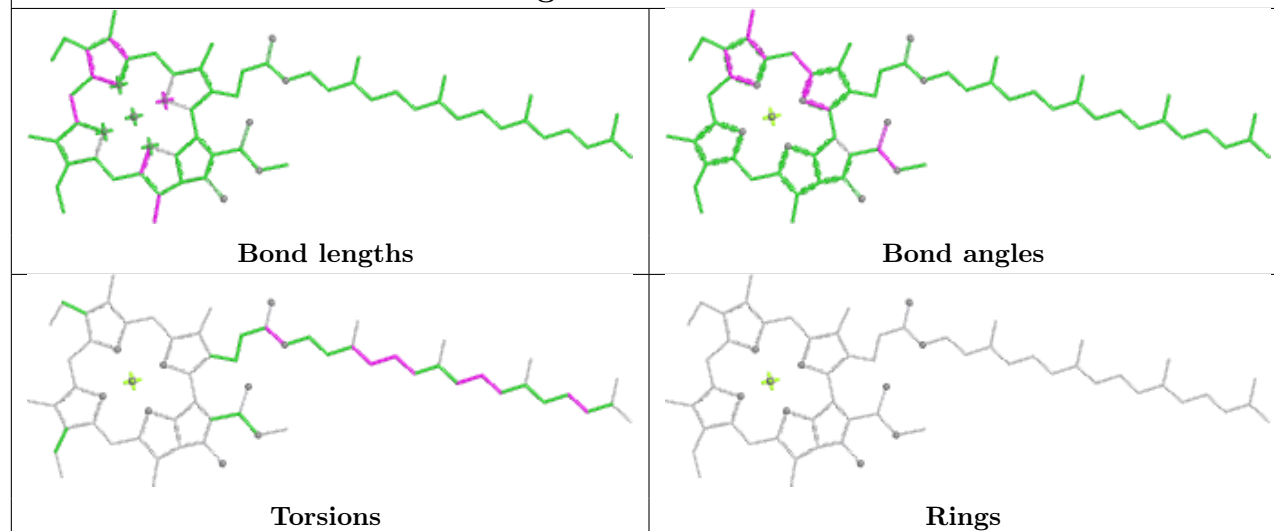
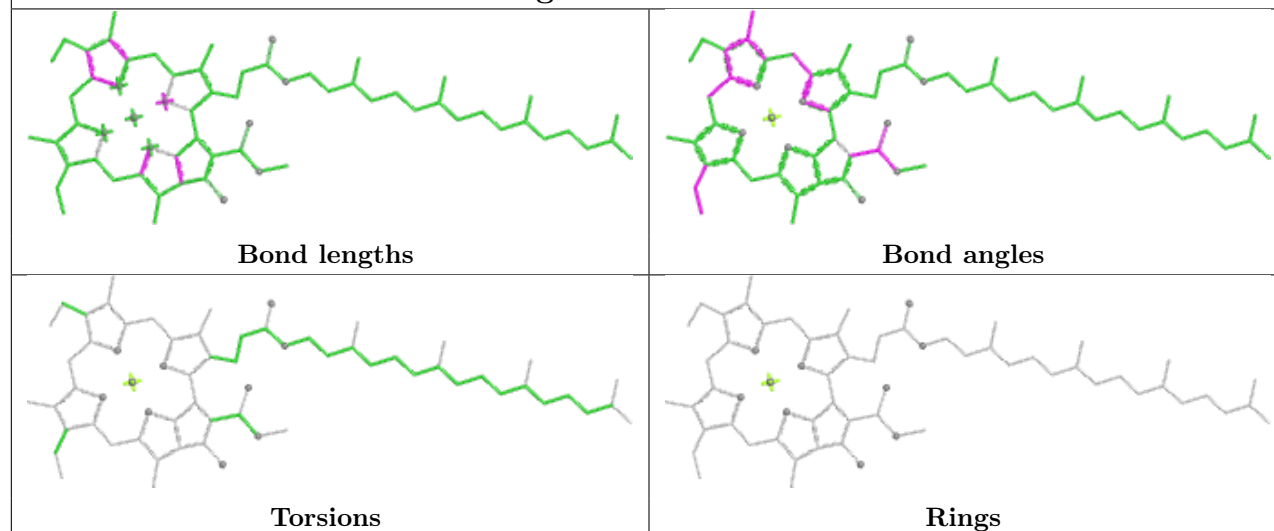




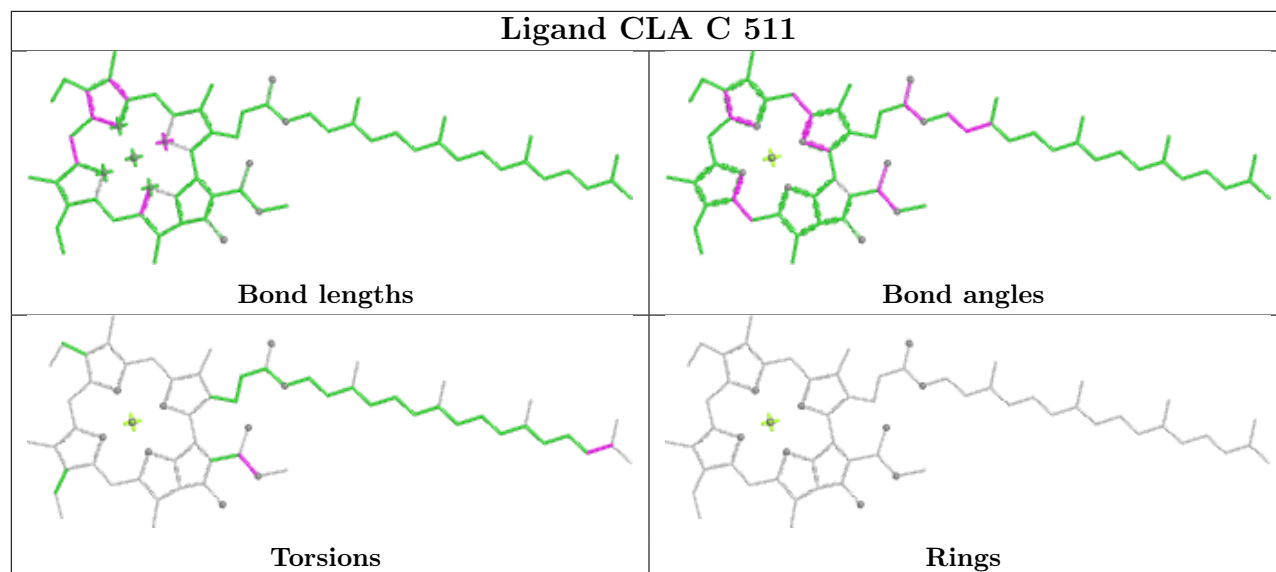




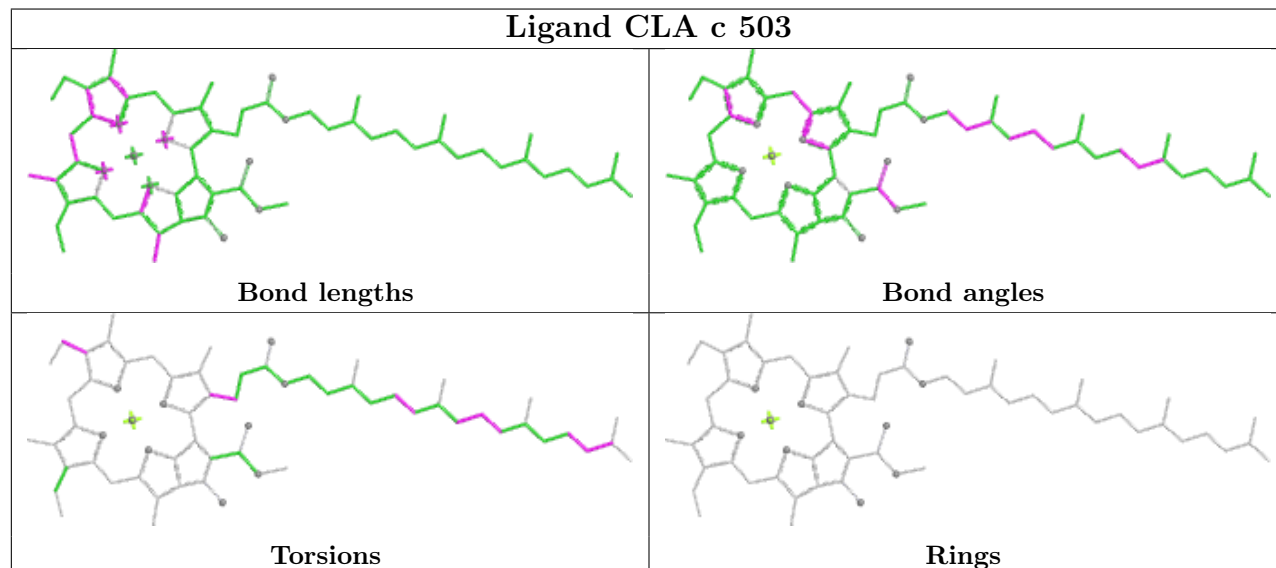


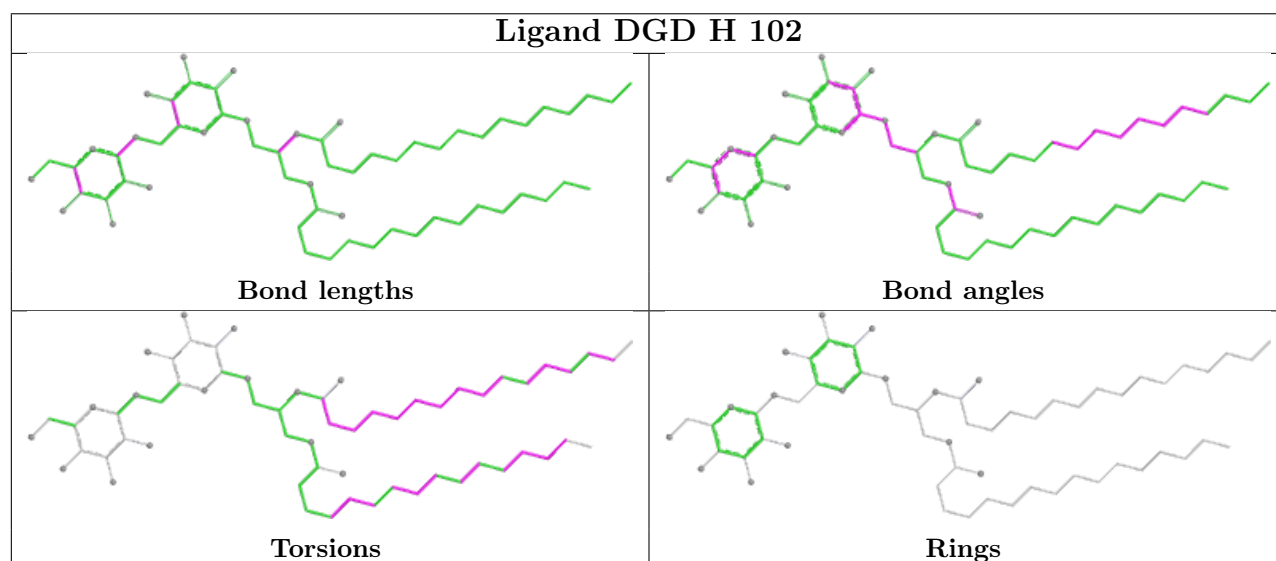
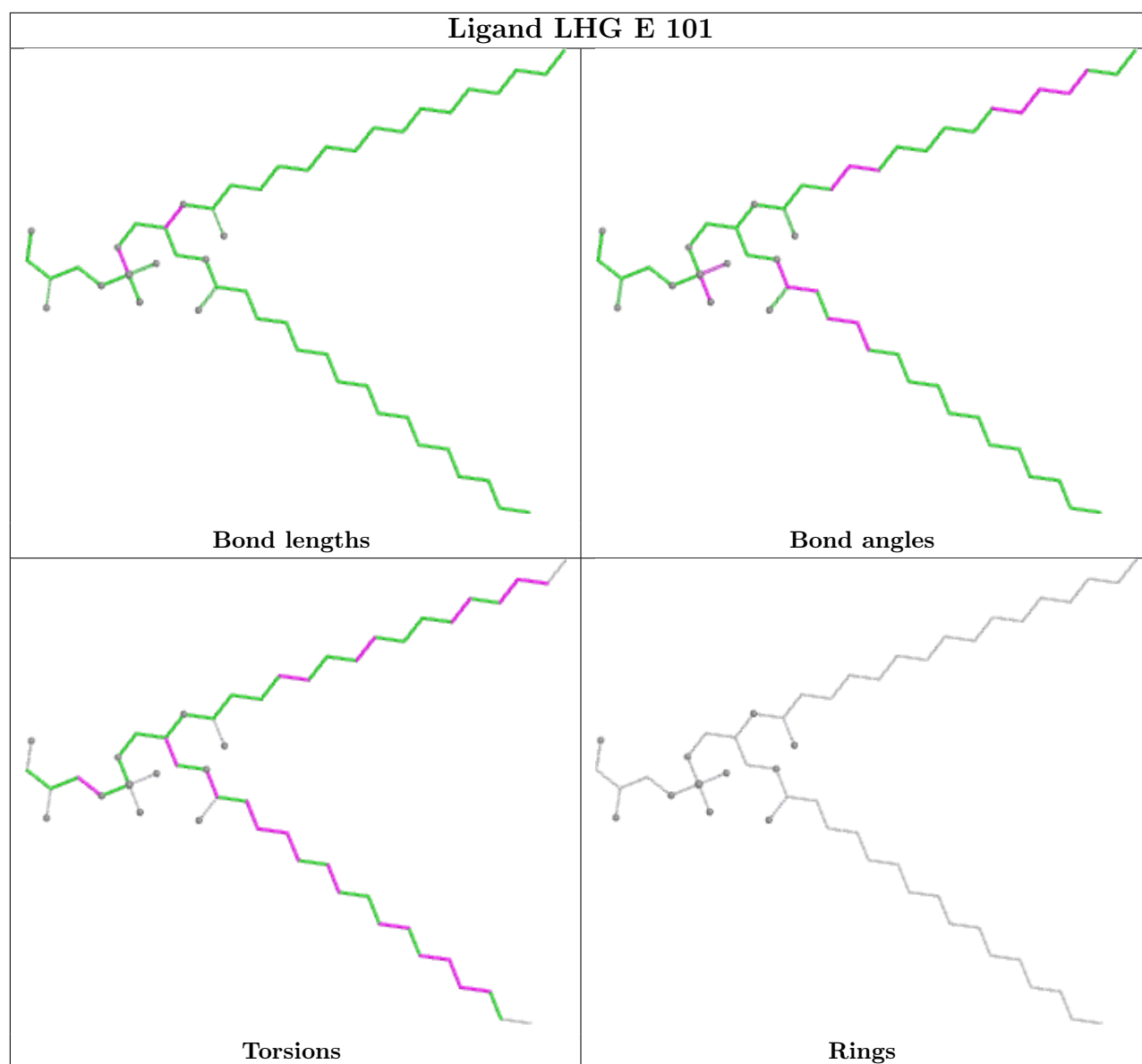
Ligand CLA B 603**Ligand CLA c 510****Ligand CLA a 612**

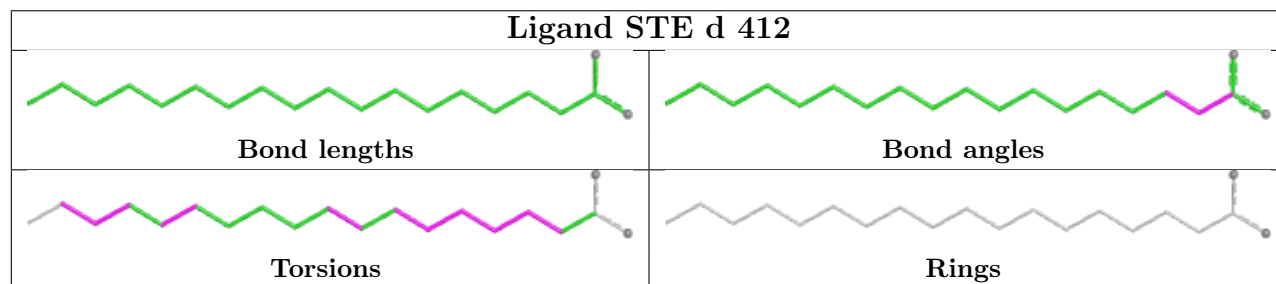
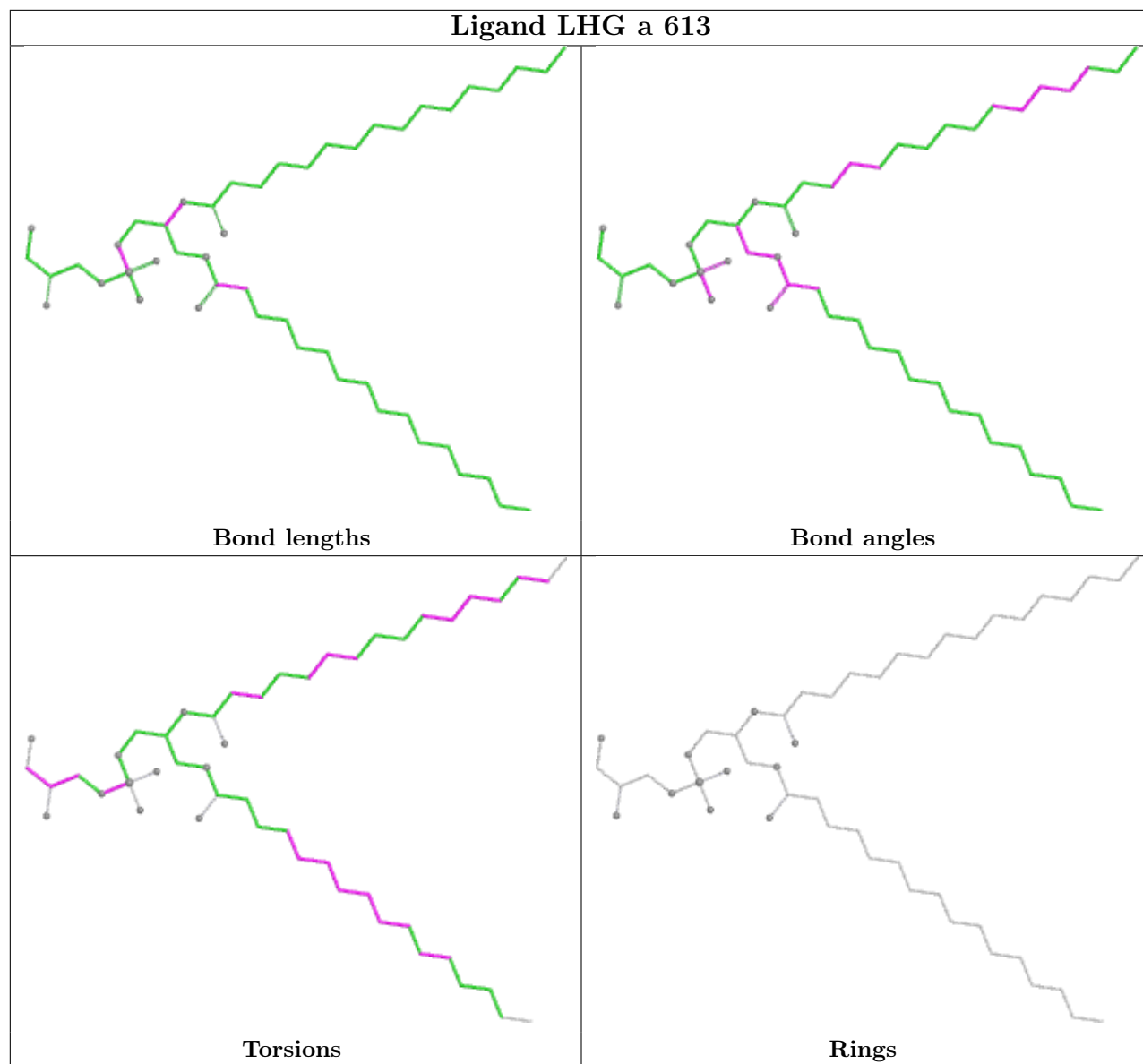
Ligand CLA C 511

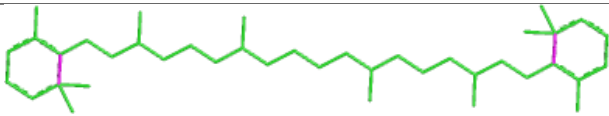
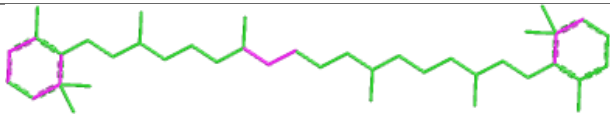
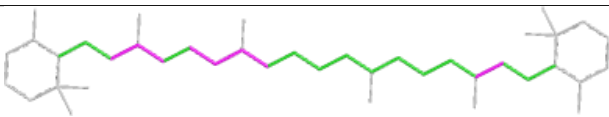
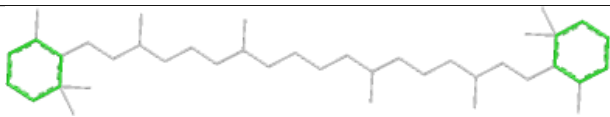


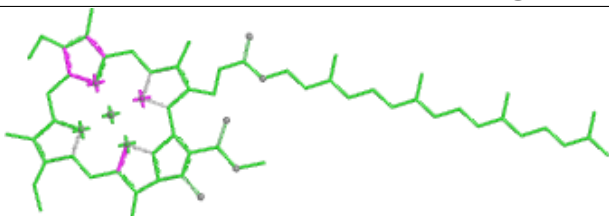
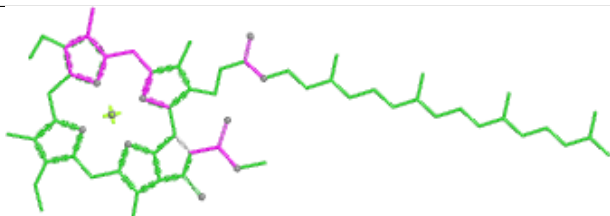
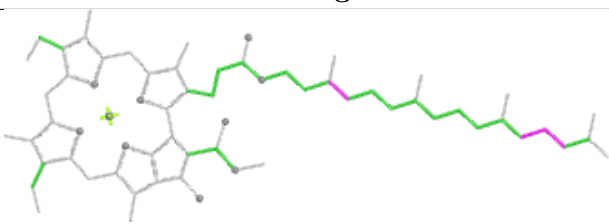
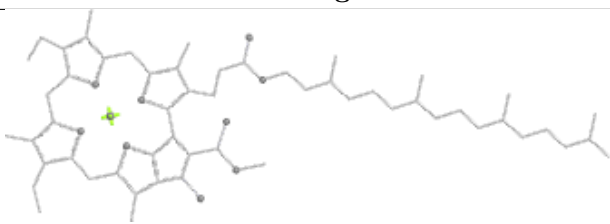
Ligand CLA c 503

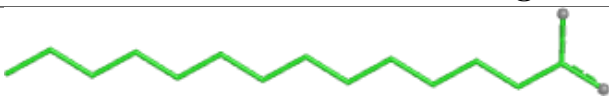
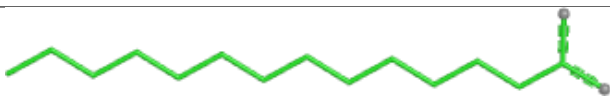
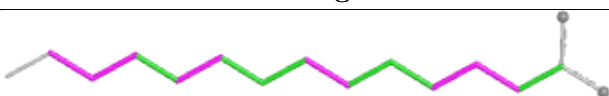
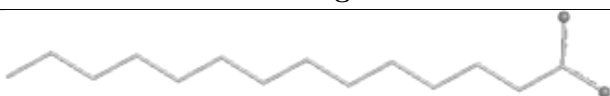


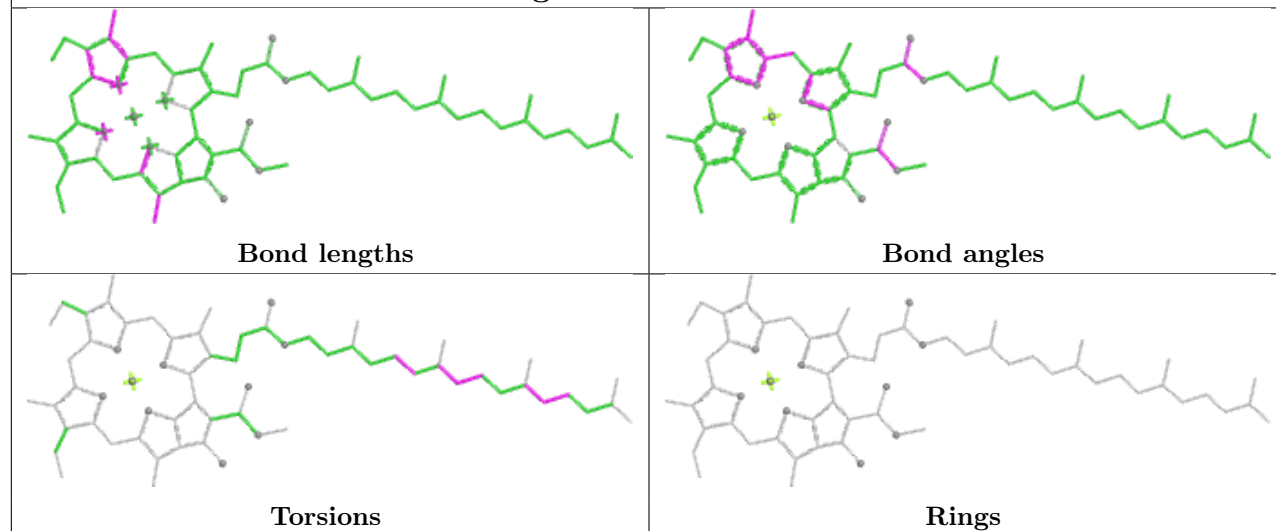
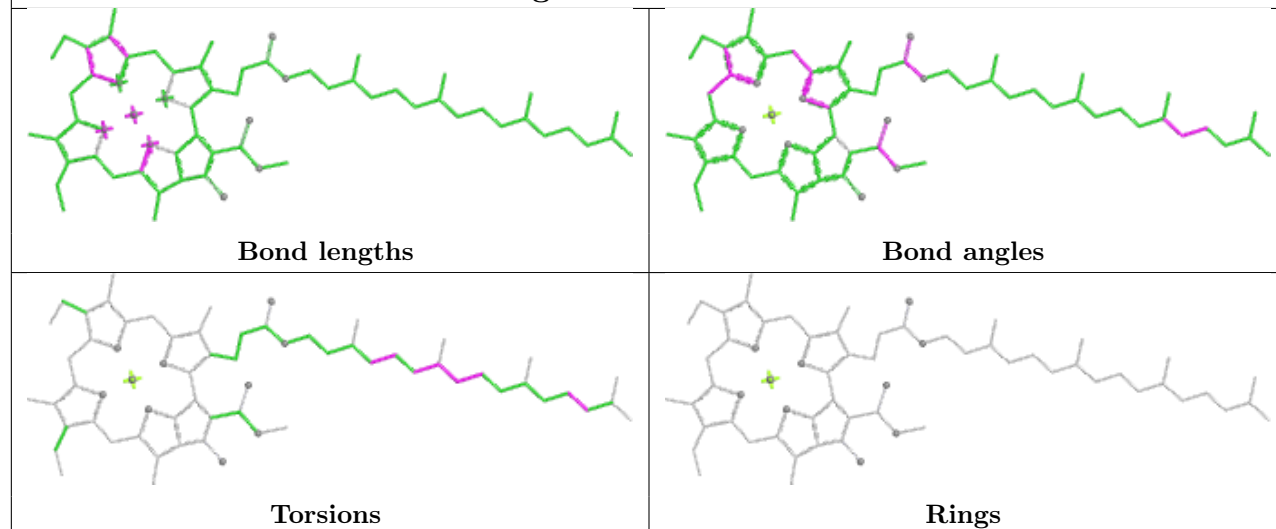


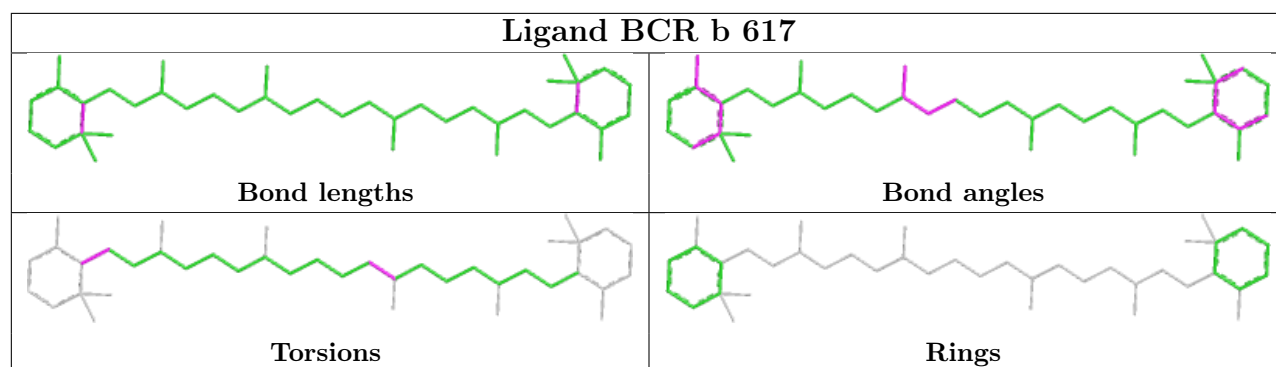
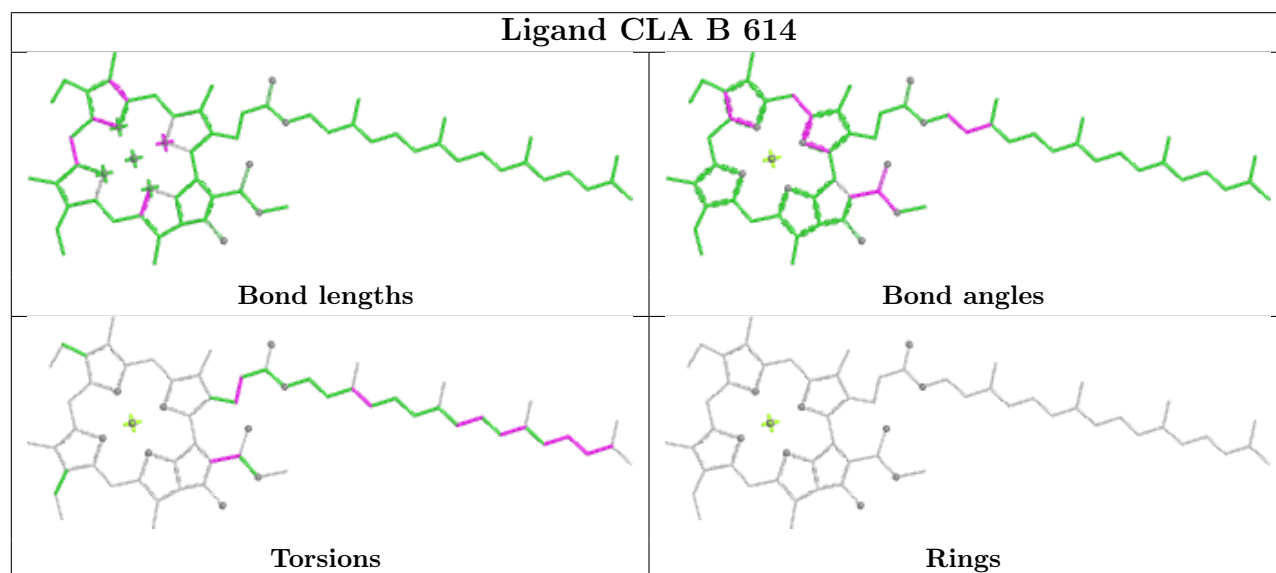
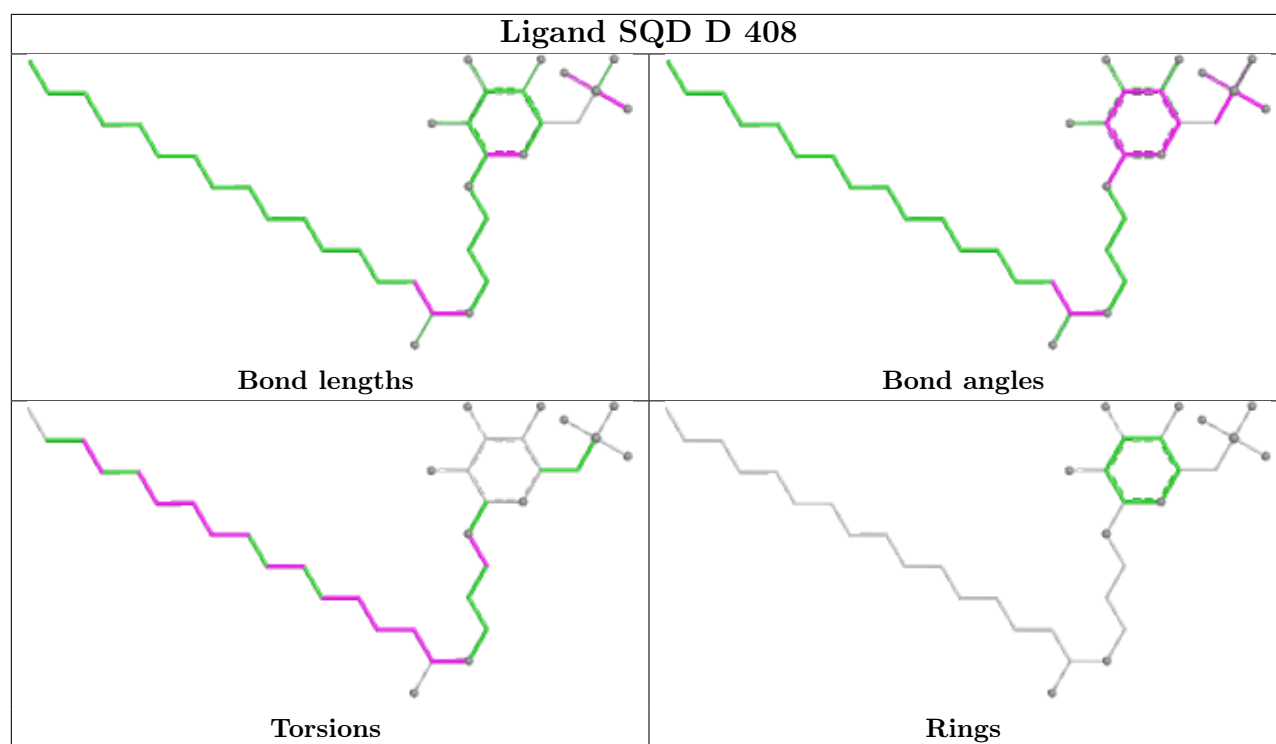


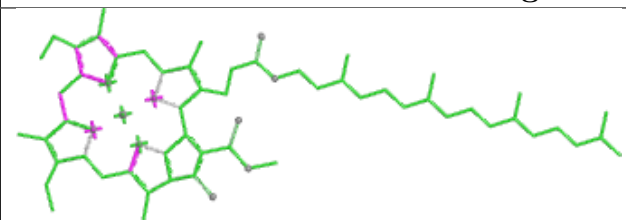
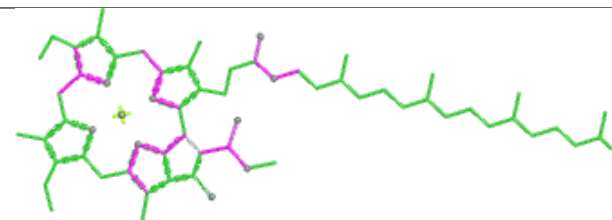
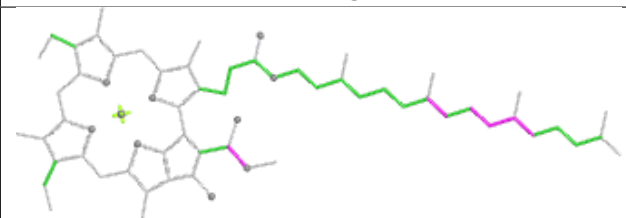
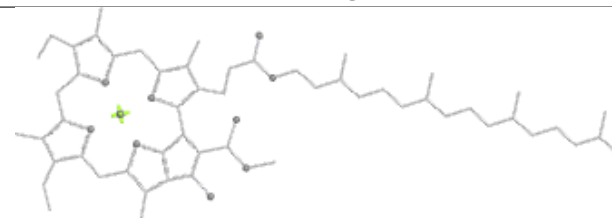
Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

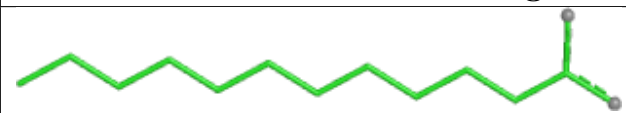
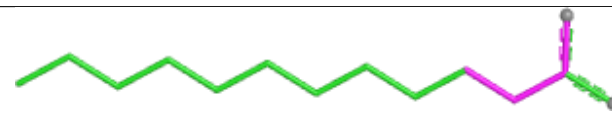
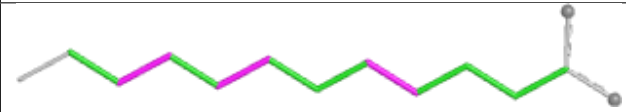
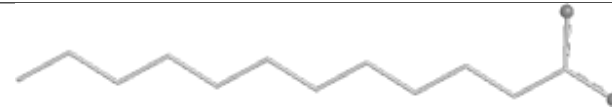
Ligand CLA B 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

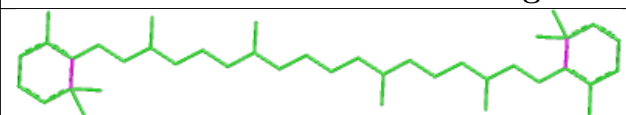
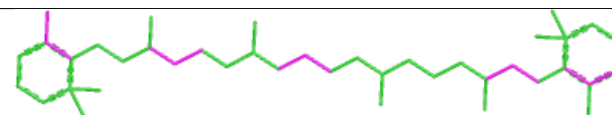
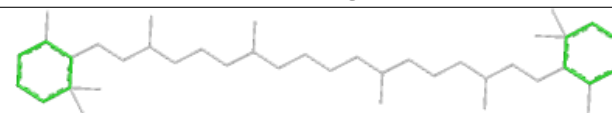
Ligand STE b 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

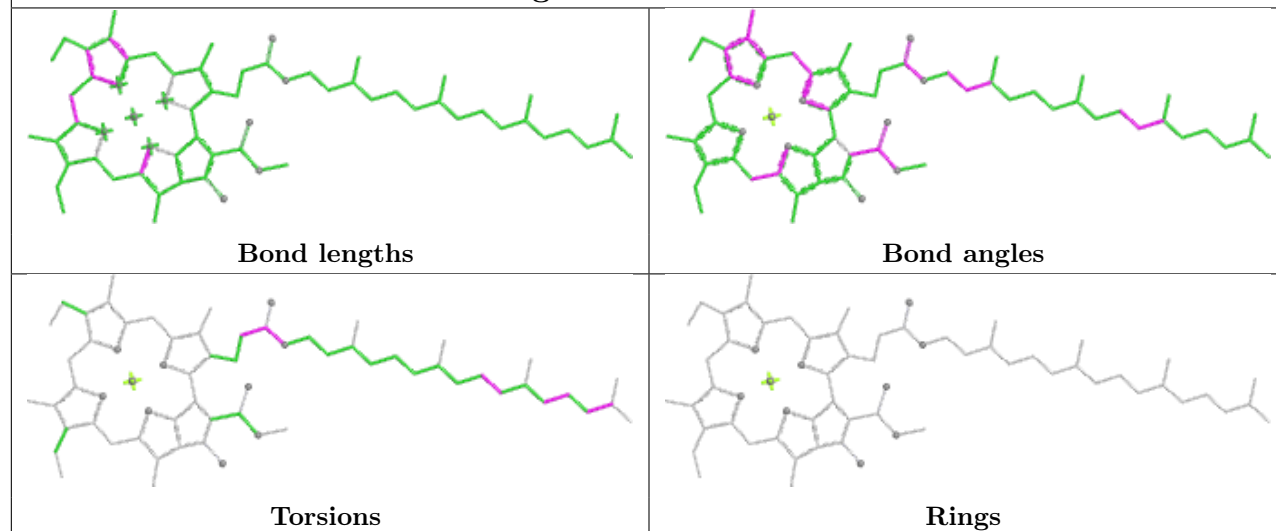
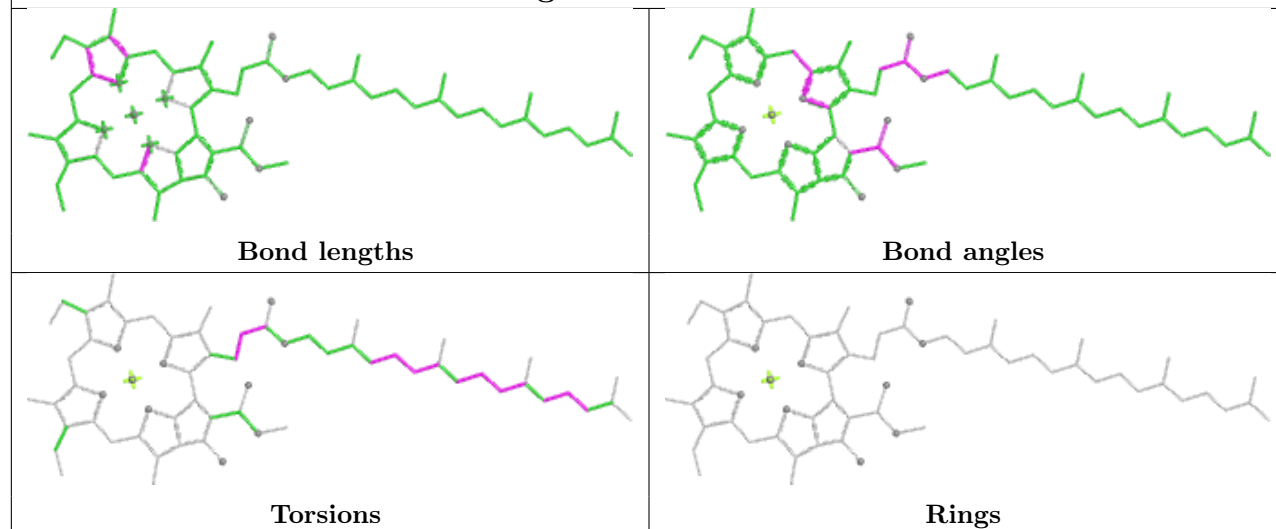
Ligand CLA B 607**Ligand CLA B 605**

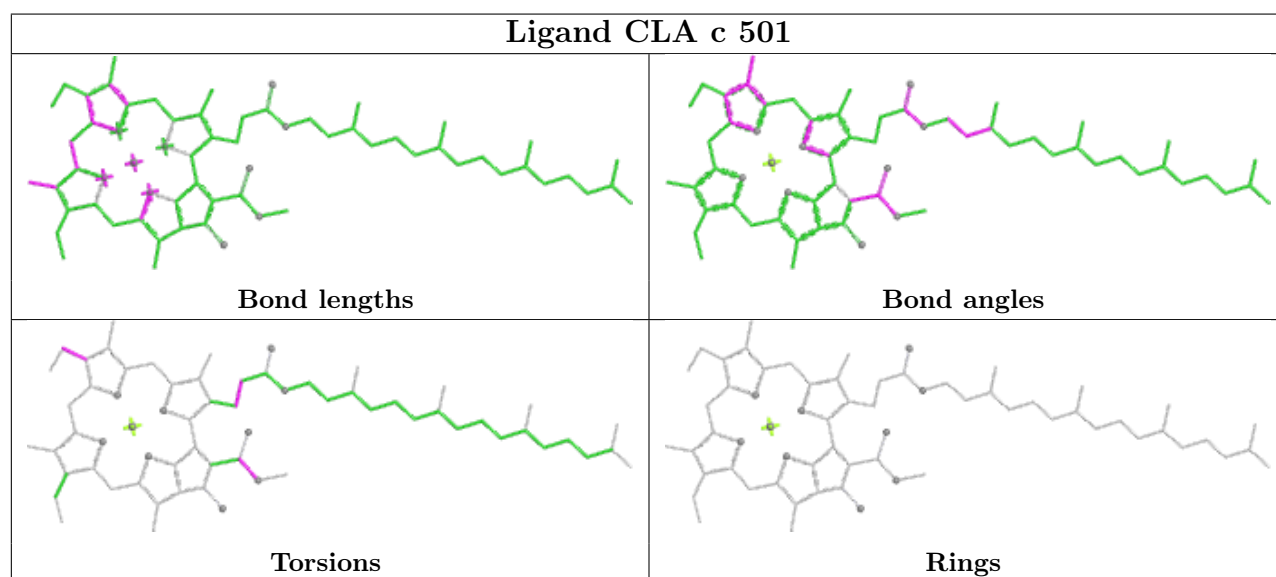
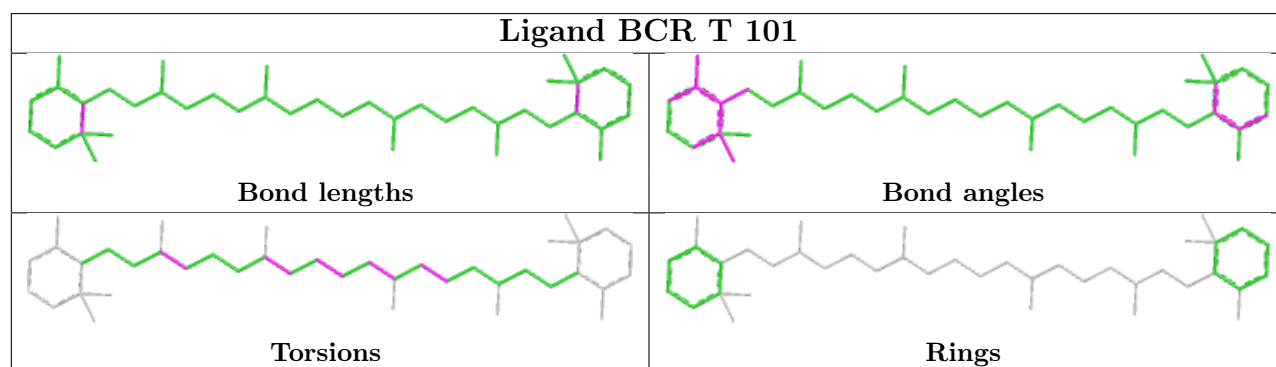
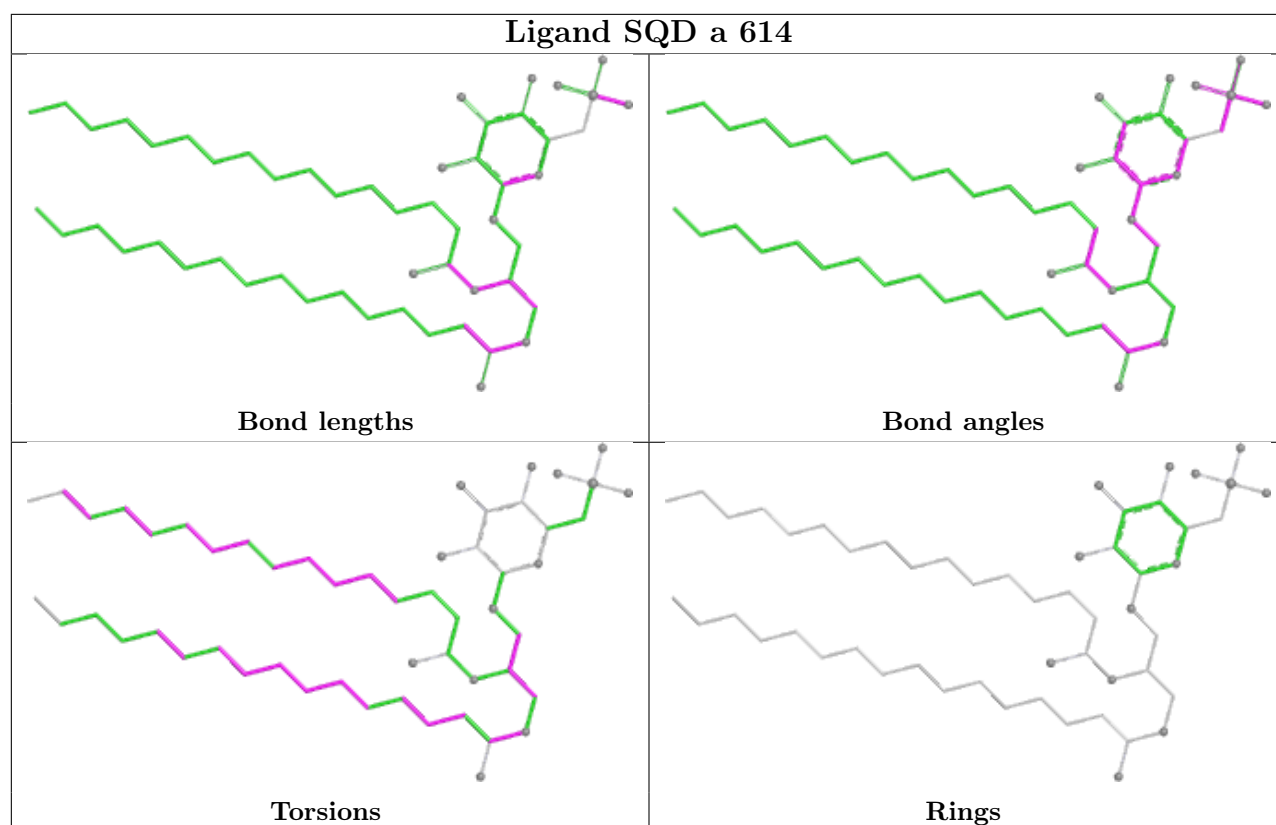


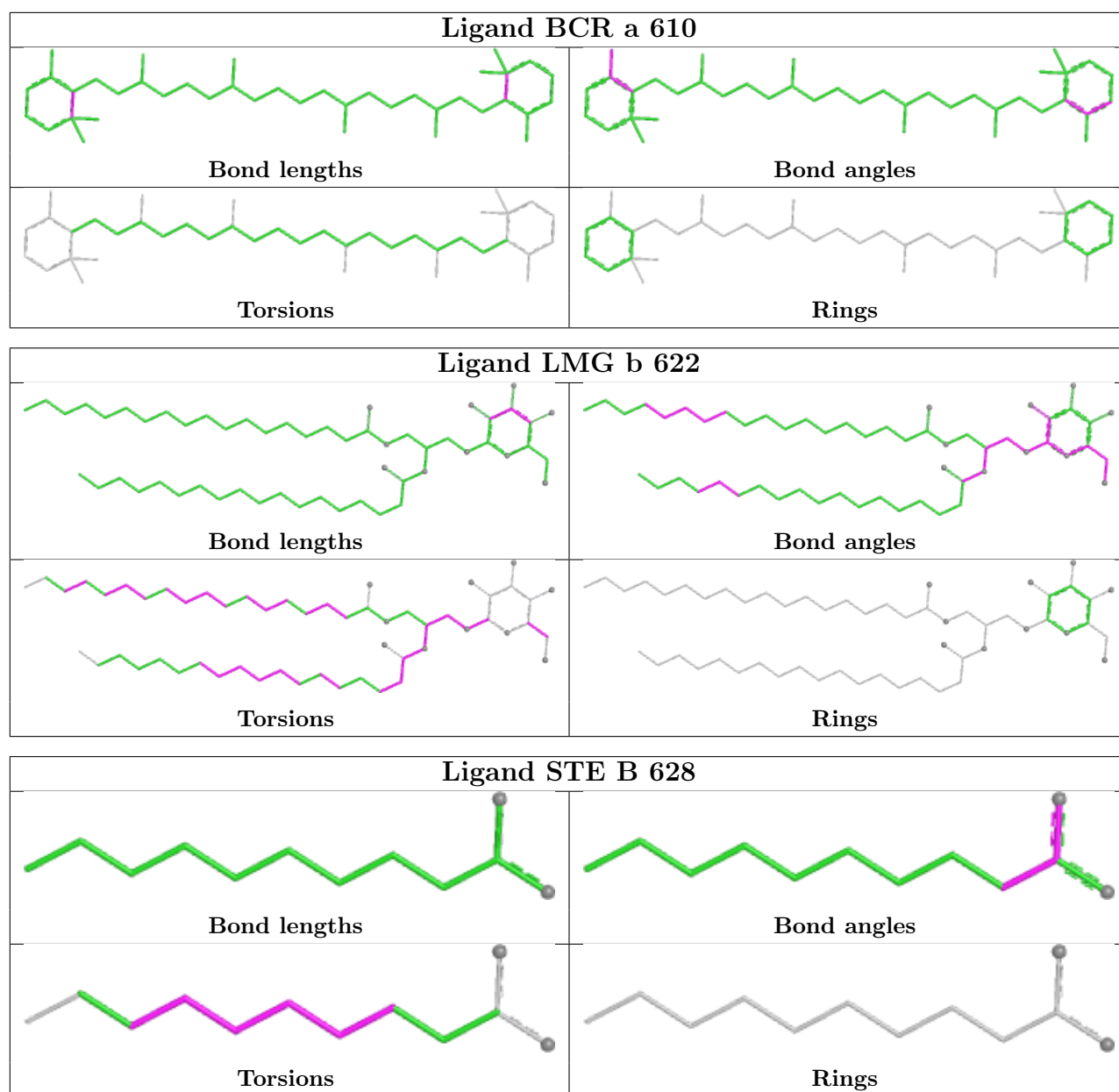
Ligand CLA B 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

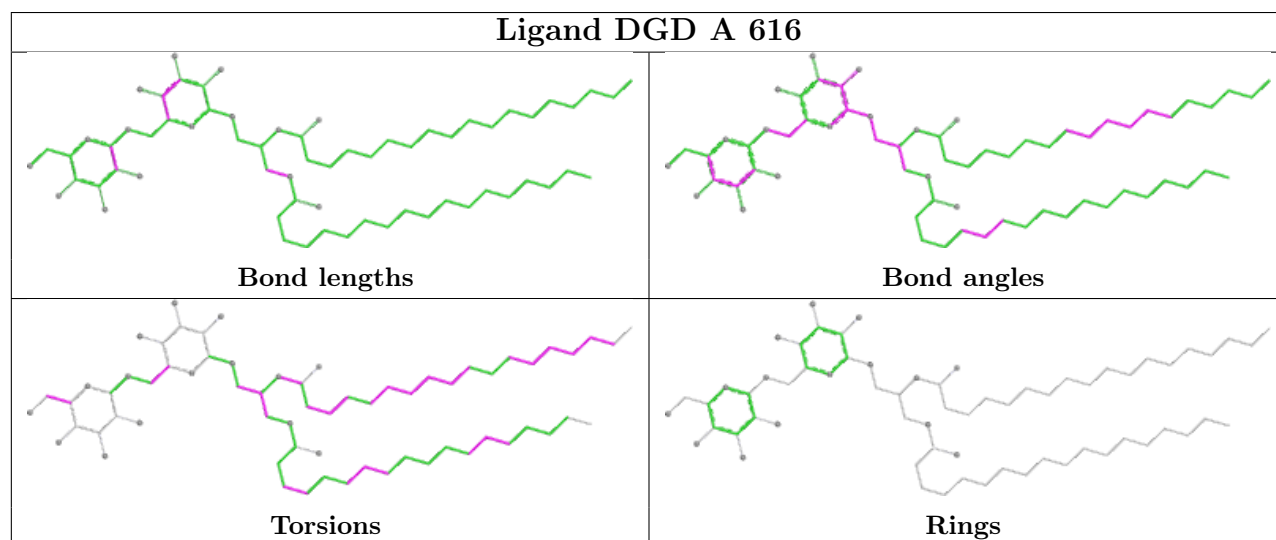
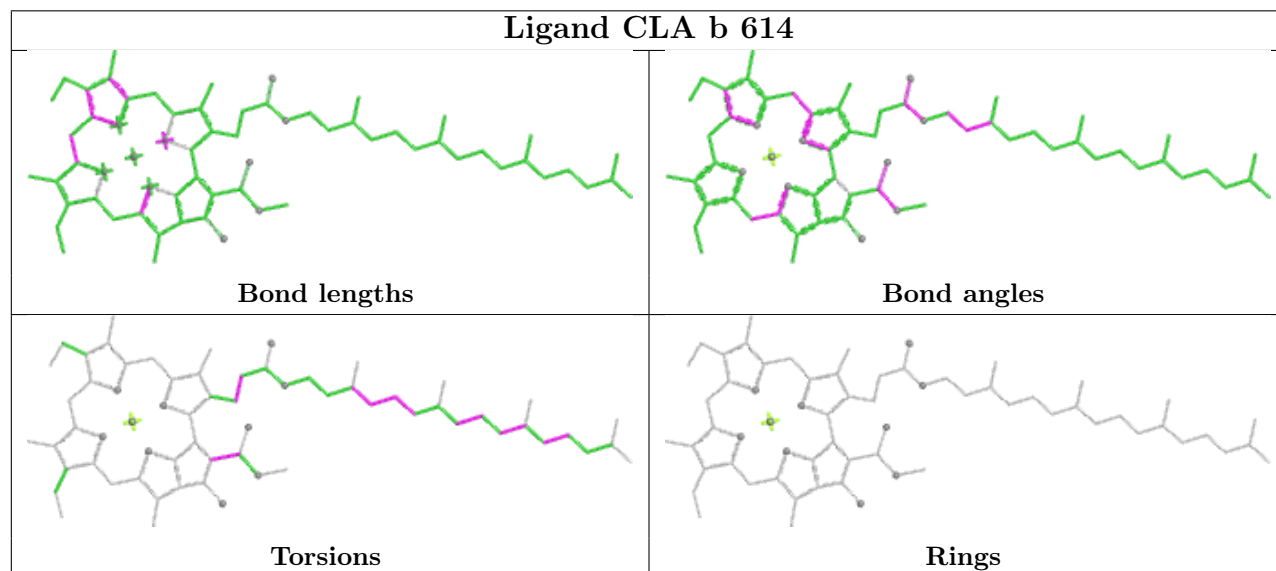
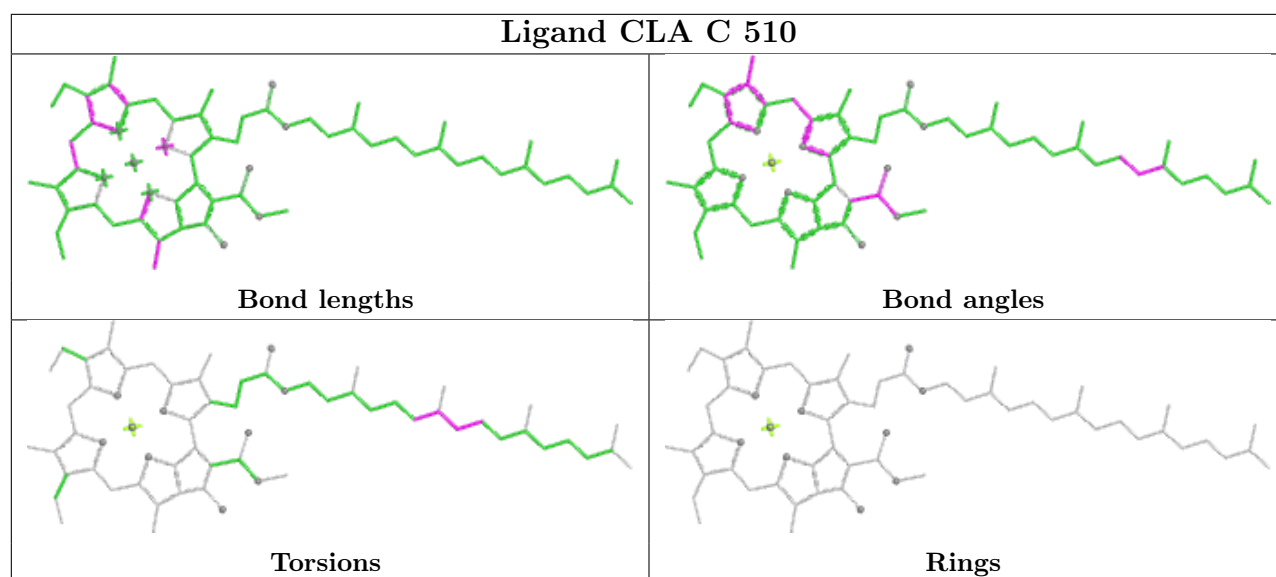
Ligand STE B 625	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR k 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

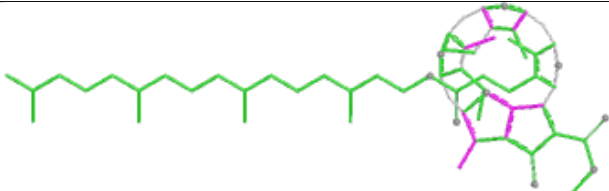
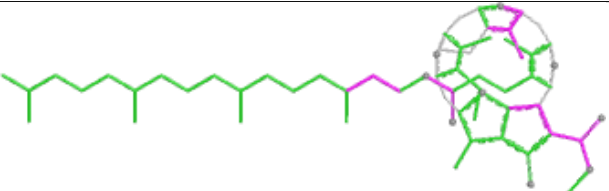
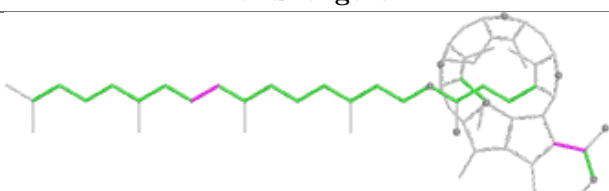
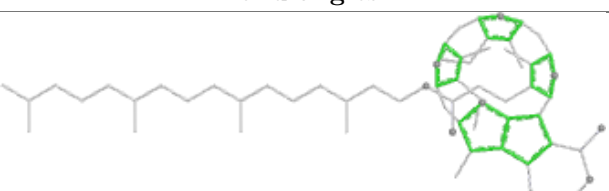
Ligand CLA B 612**Ligand CLA c 509**



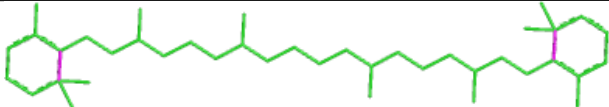
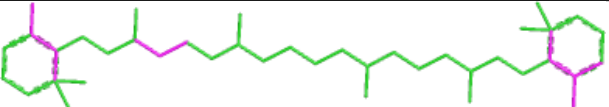
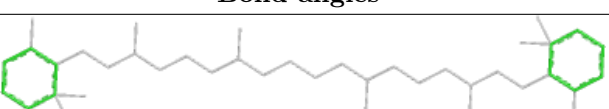


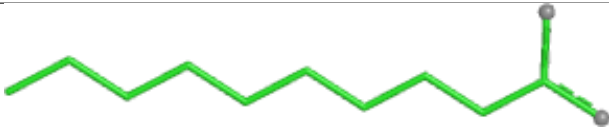
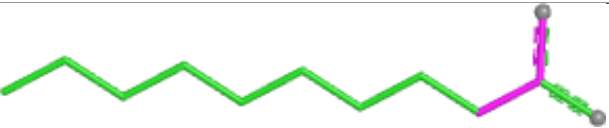
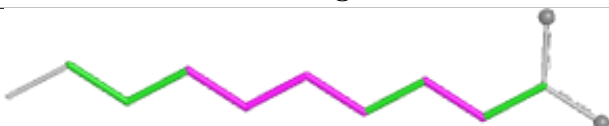
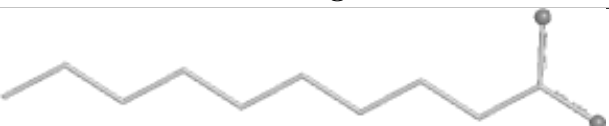


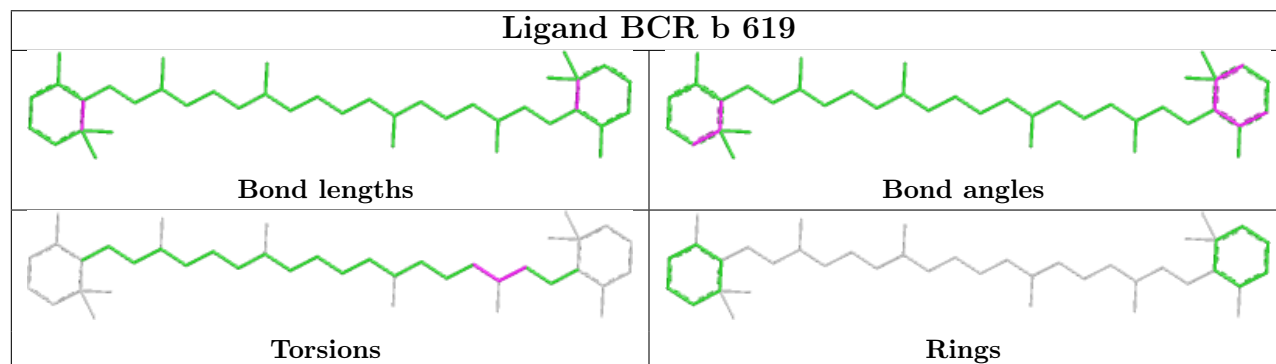
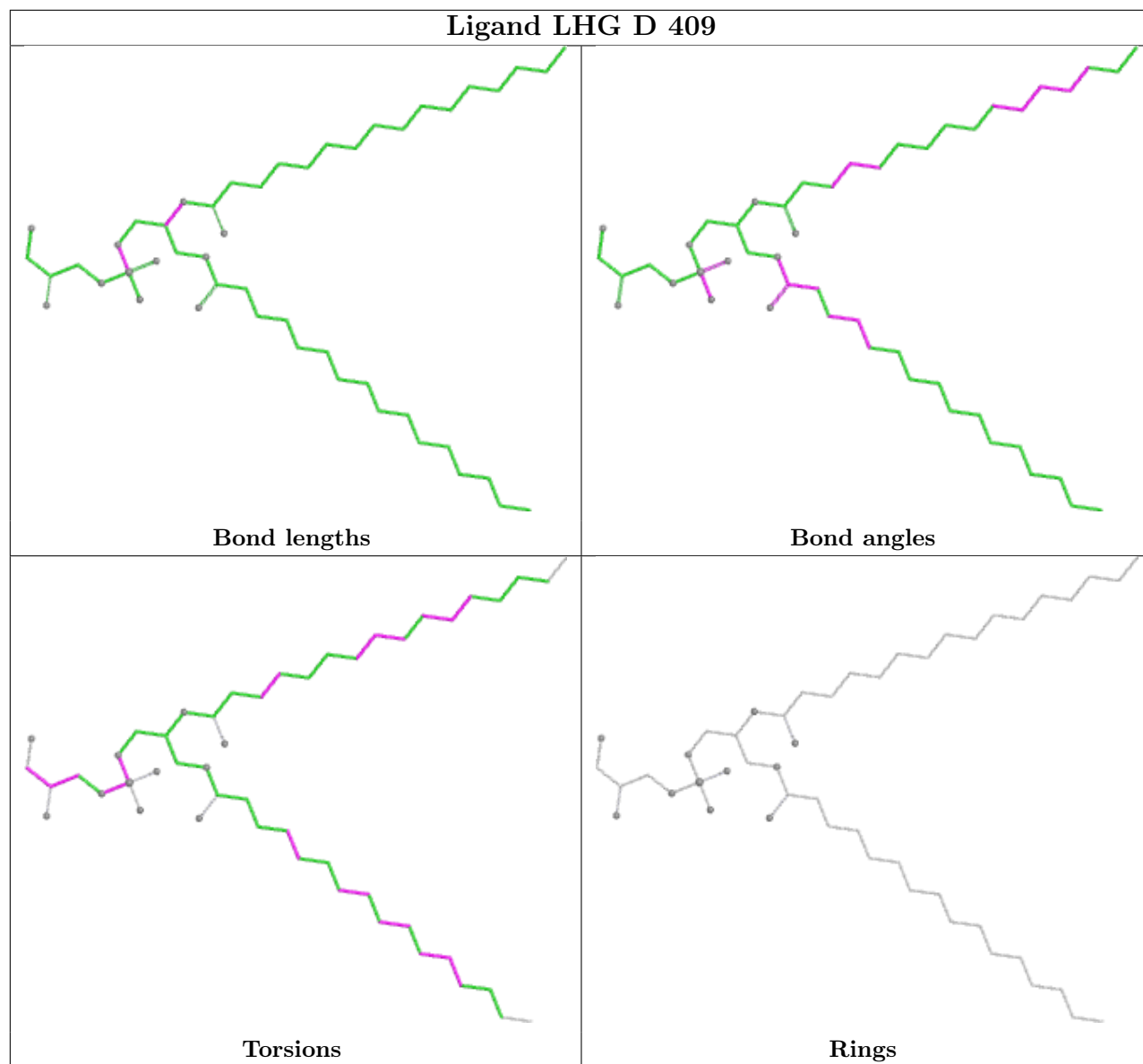
Ligand STE I 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

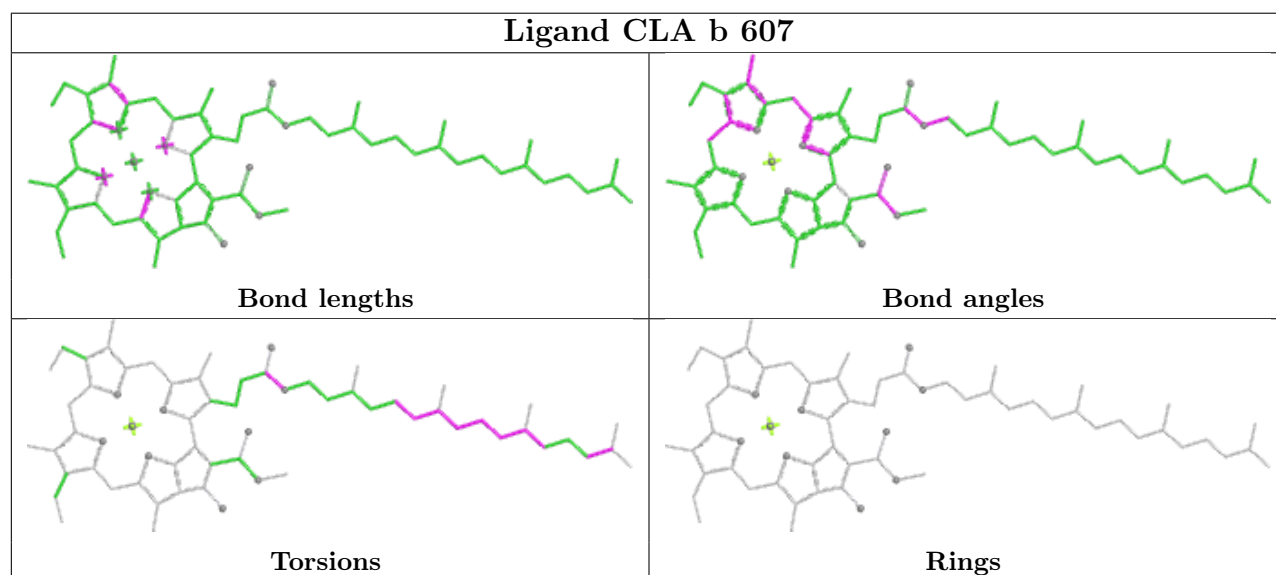
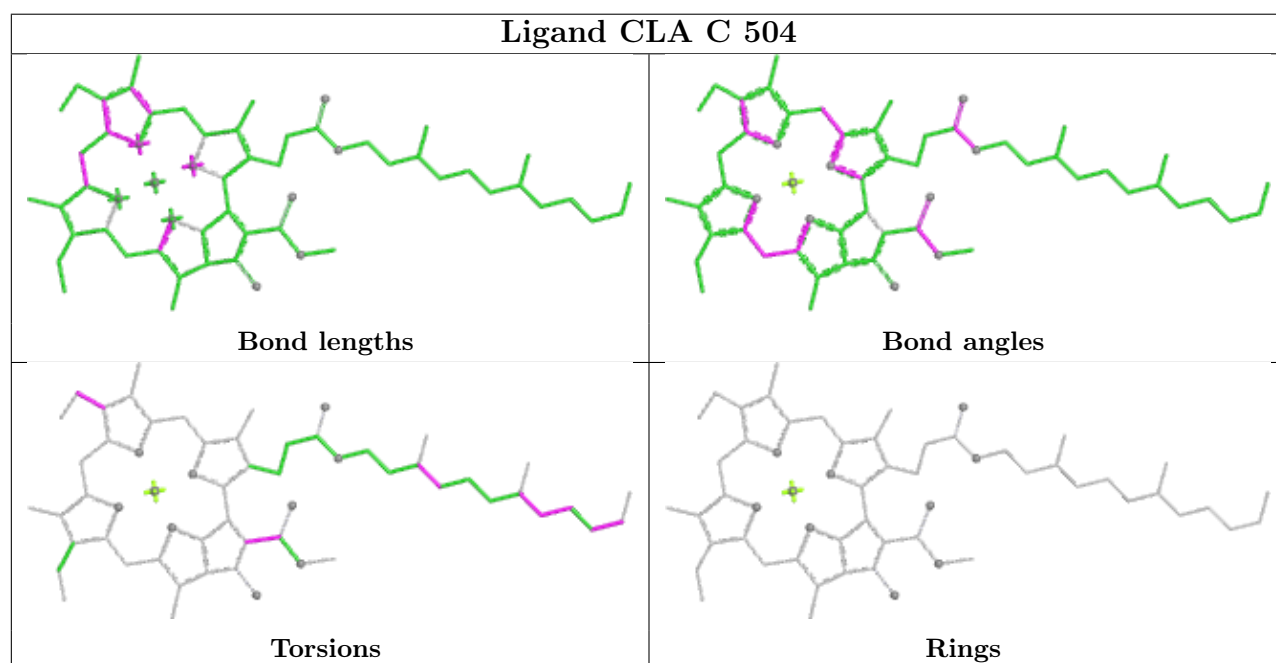
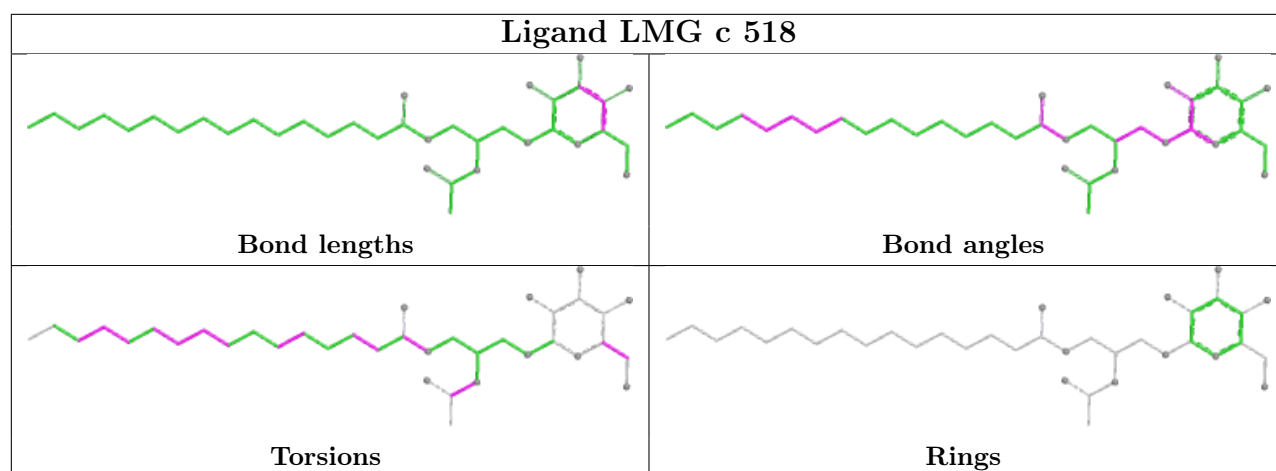
Ligand PHO A 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

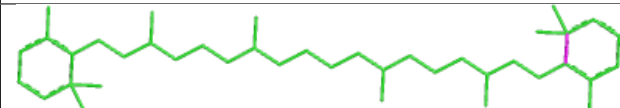
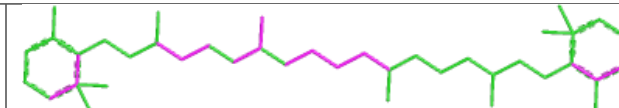
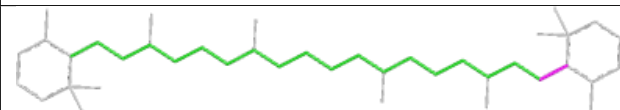
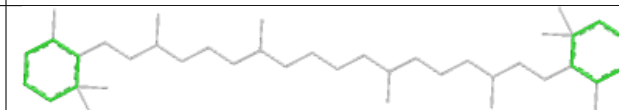
Ligand STE I 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

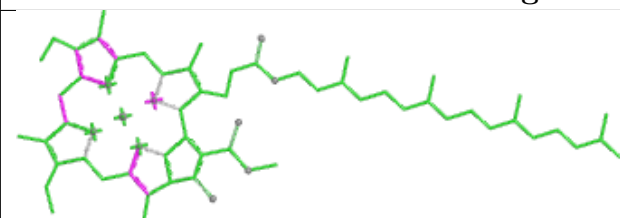
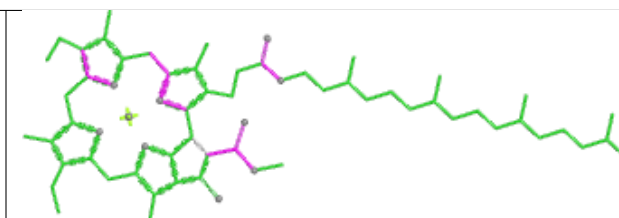
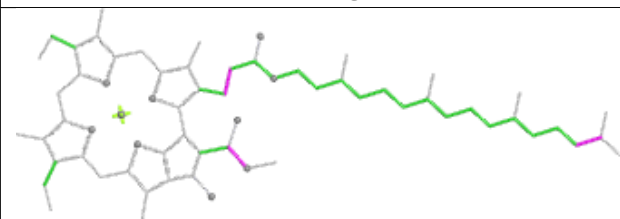
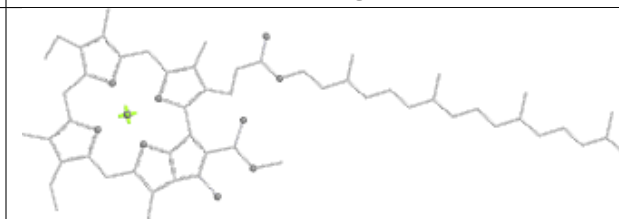
Ligand BCR d 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

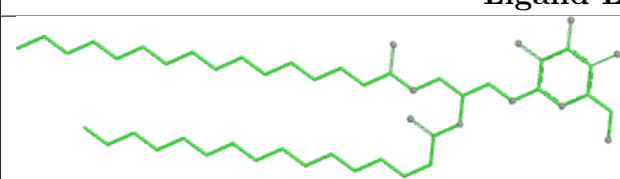
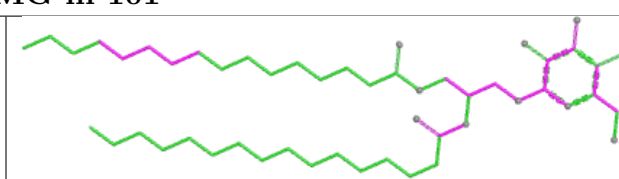
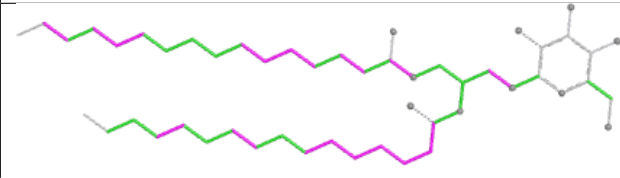
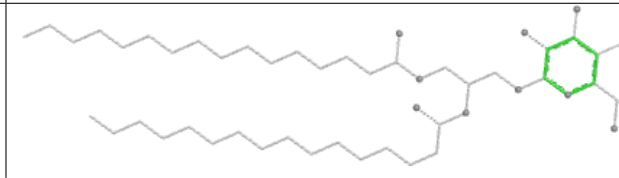
Ligand STE C 522	
 Bond lengths	 Bond angles
 Torsions	 Rings

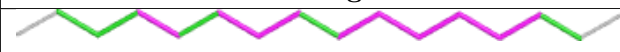
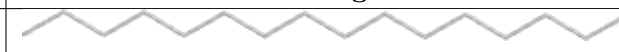


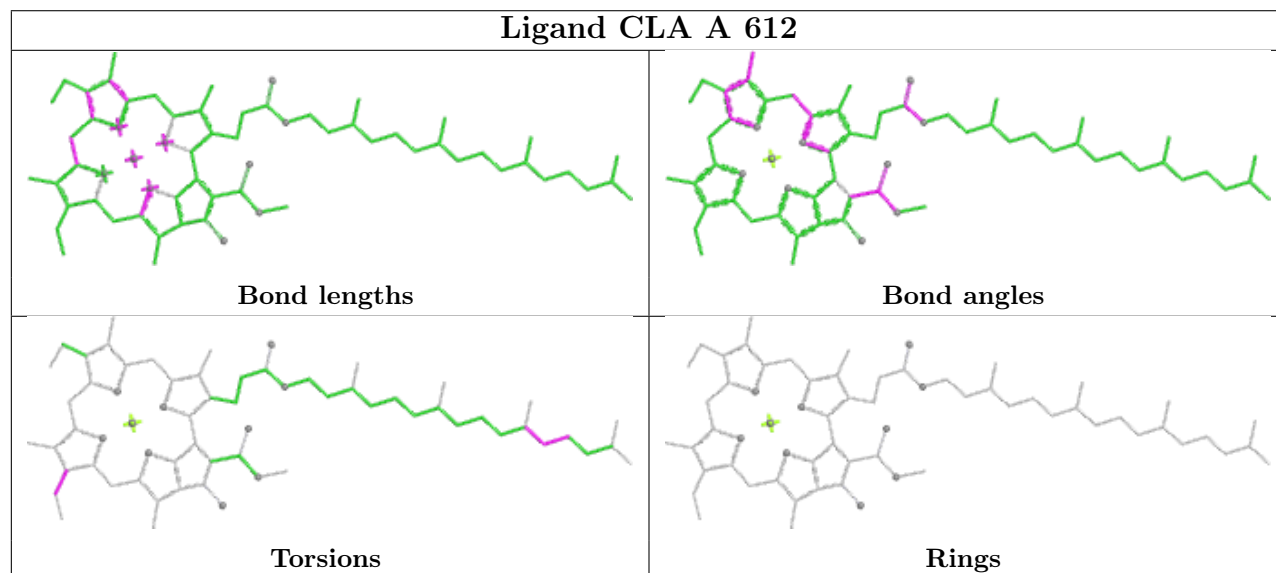
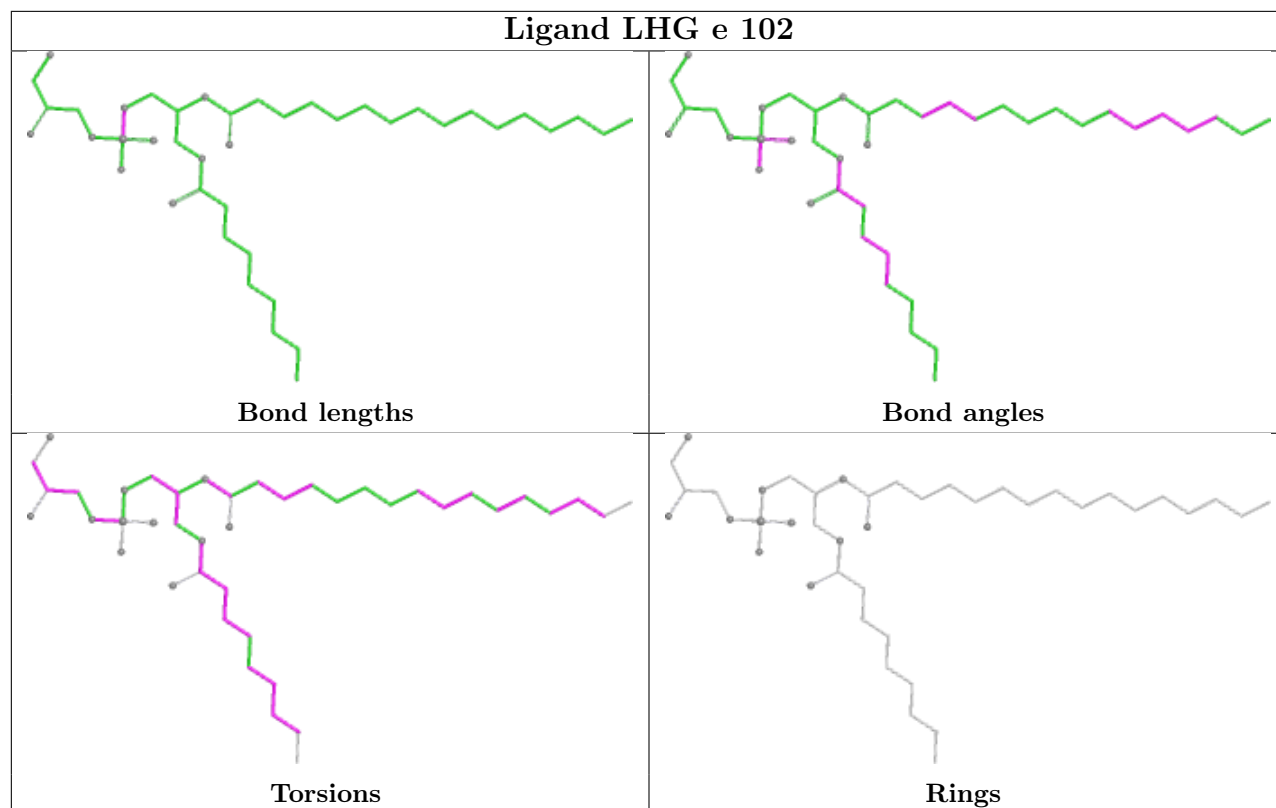


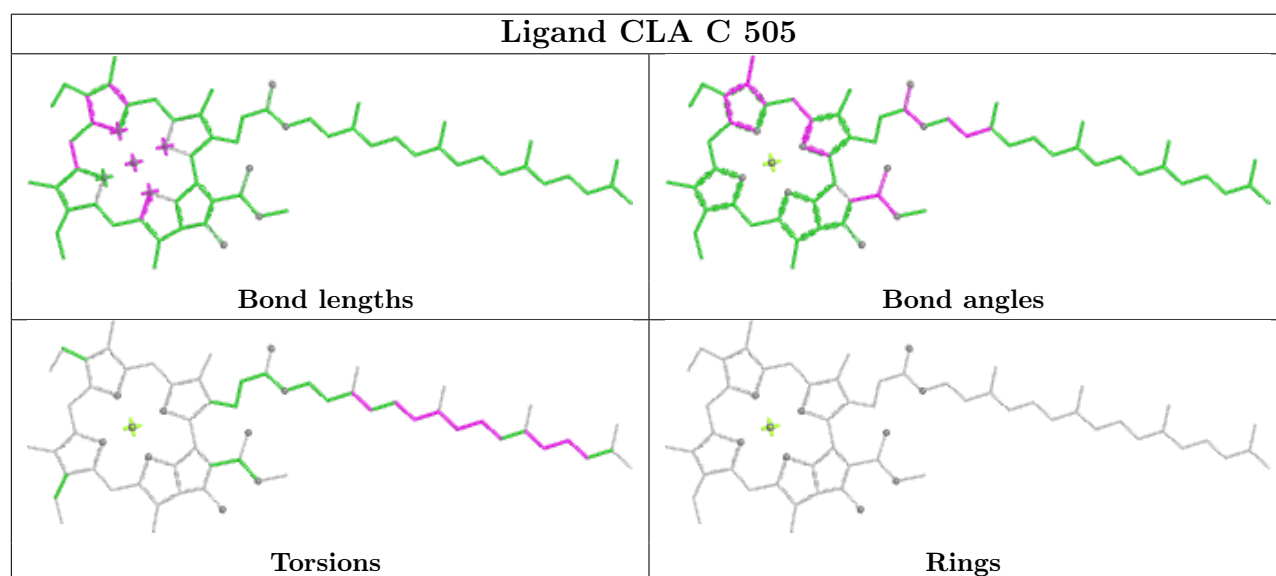
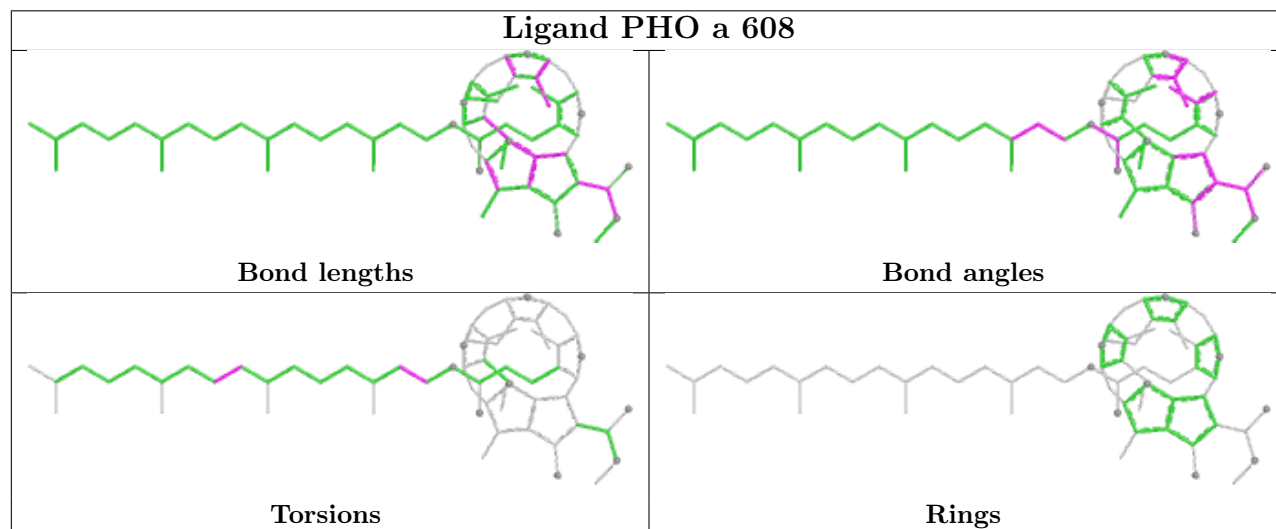
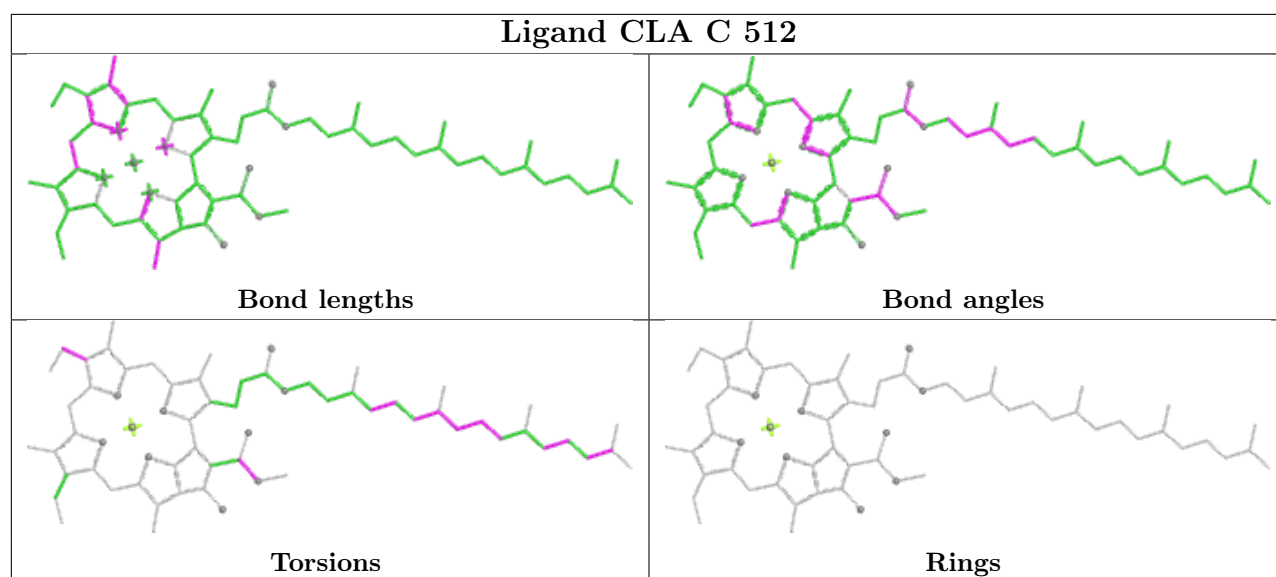
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

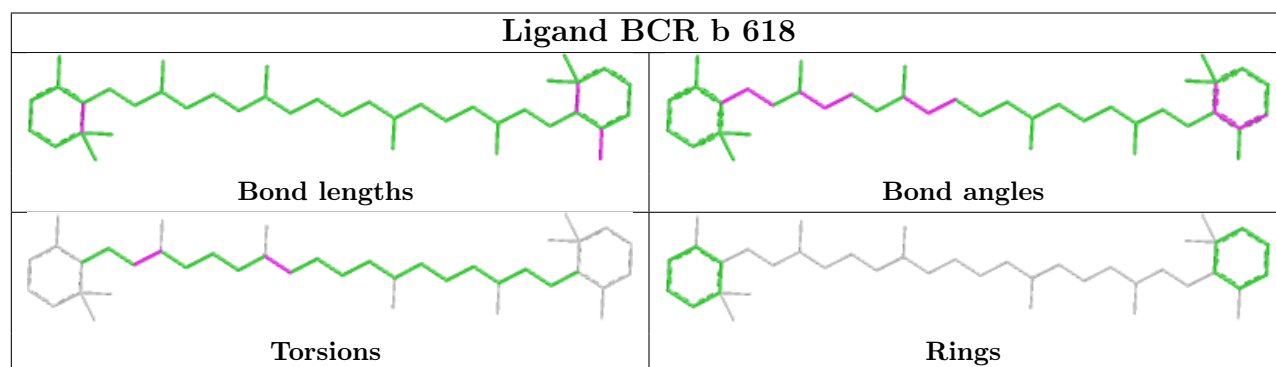
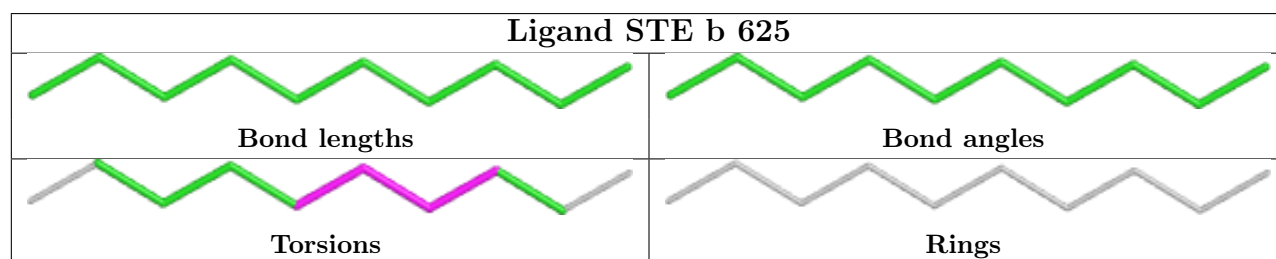
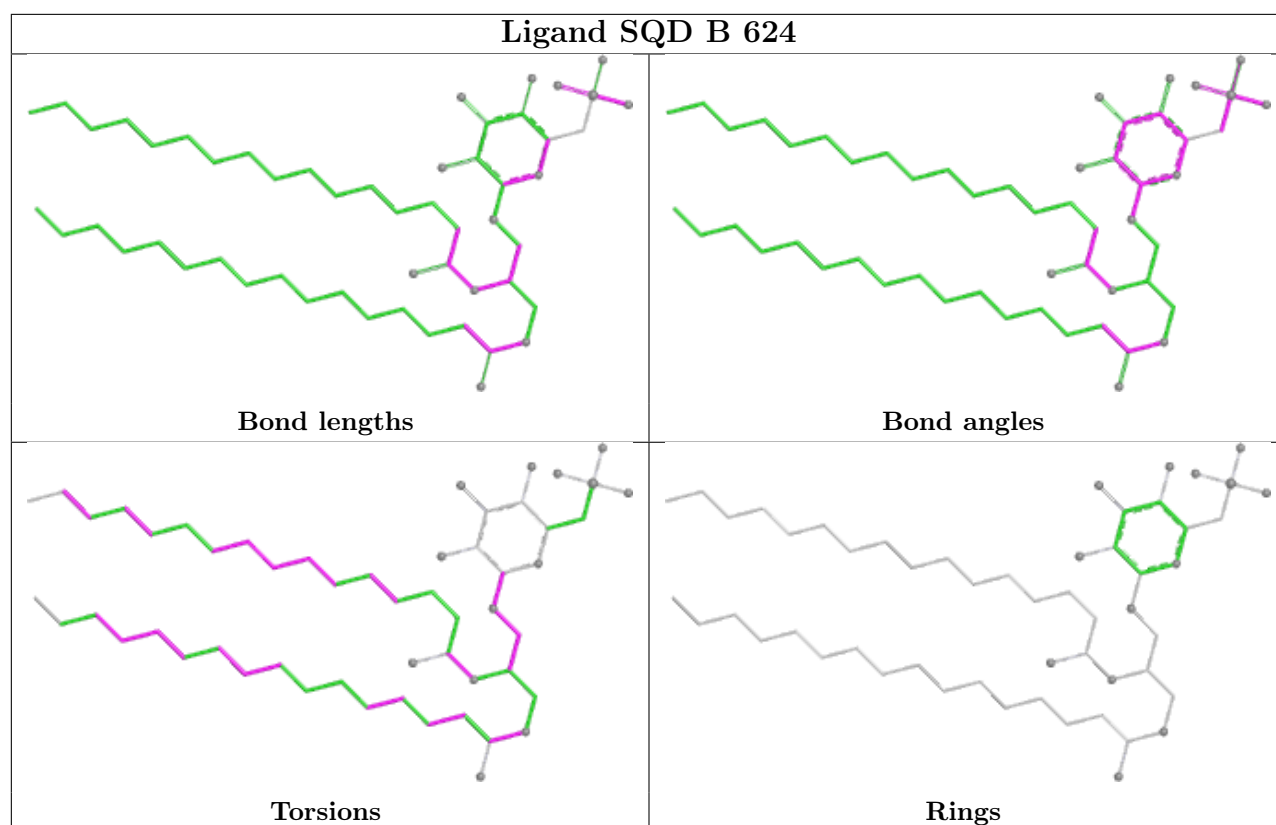
Ligand CLA C 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

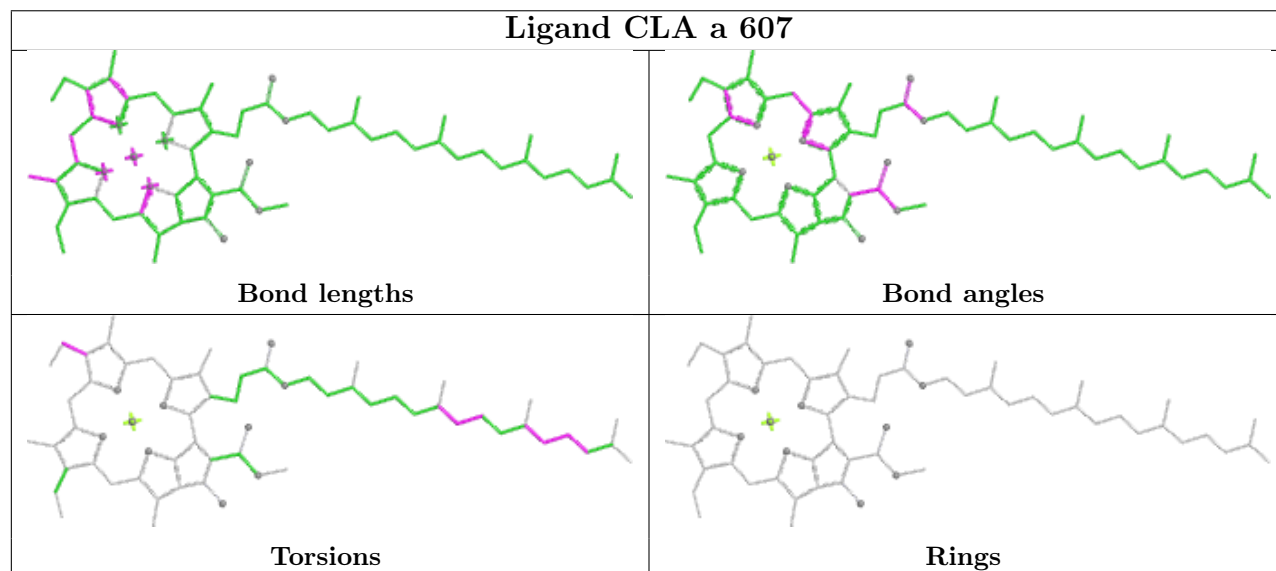
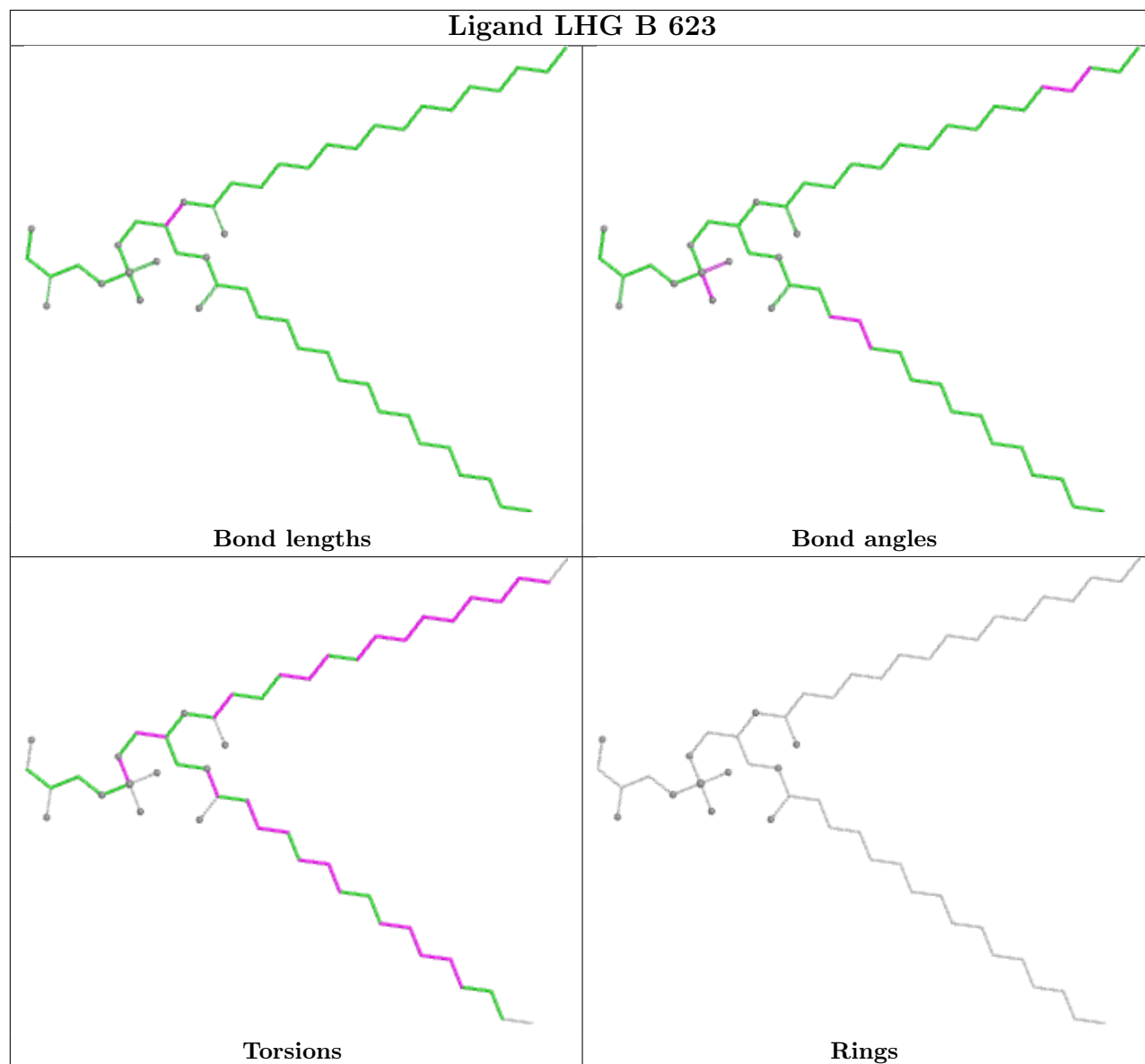
Ligand LMG m 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

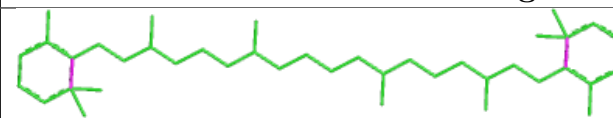
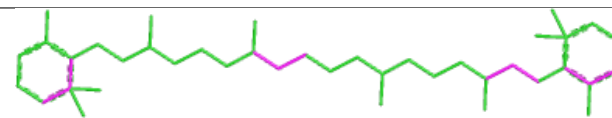
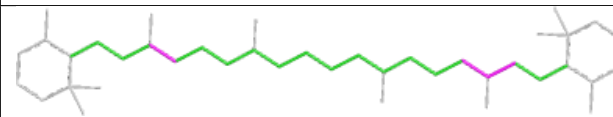
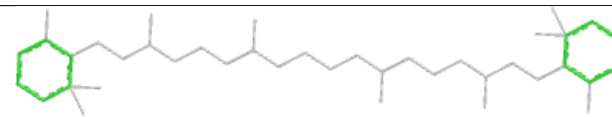
Ligand STE T 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

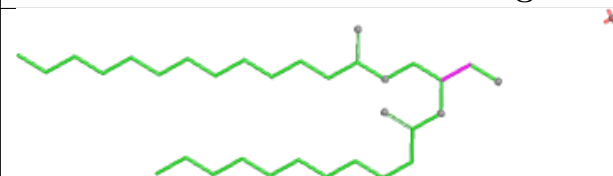
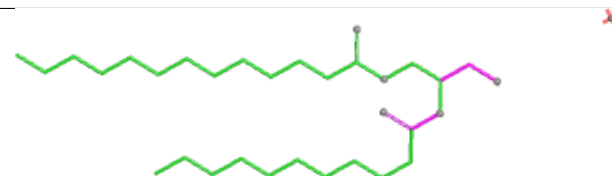
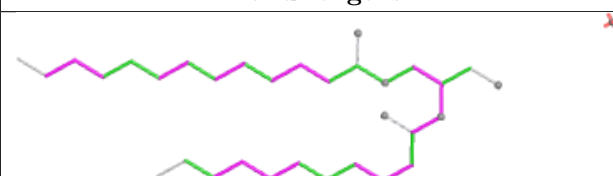
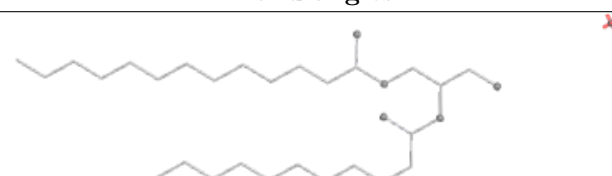


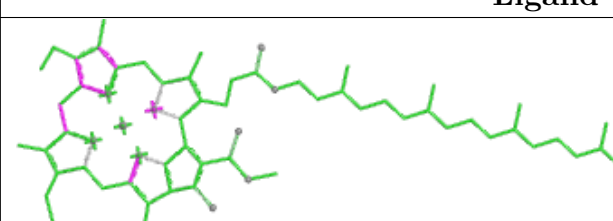
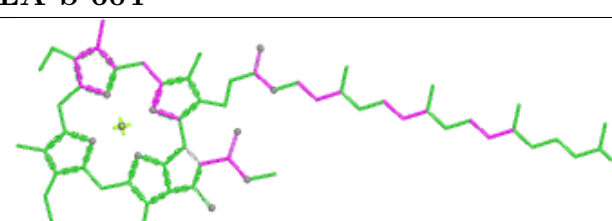
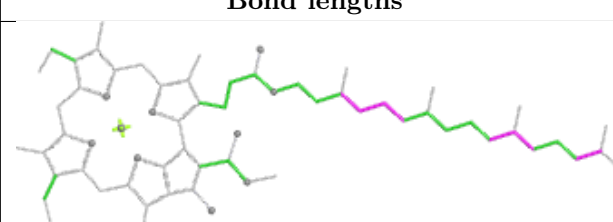
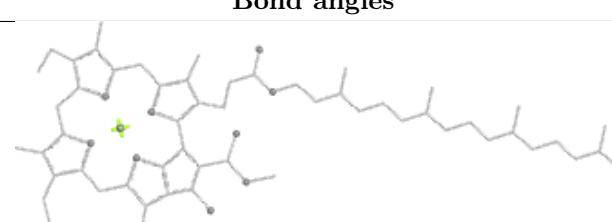


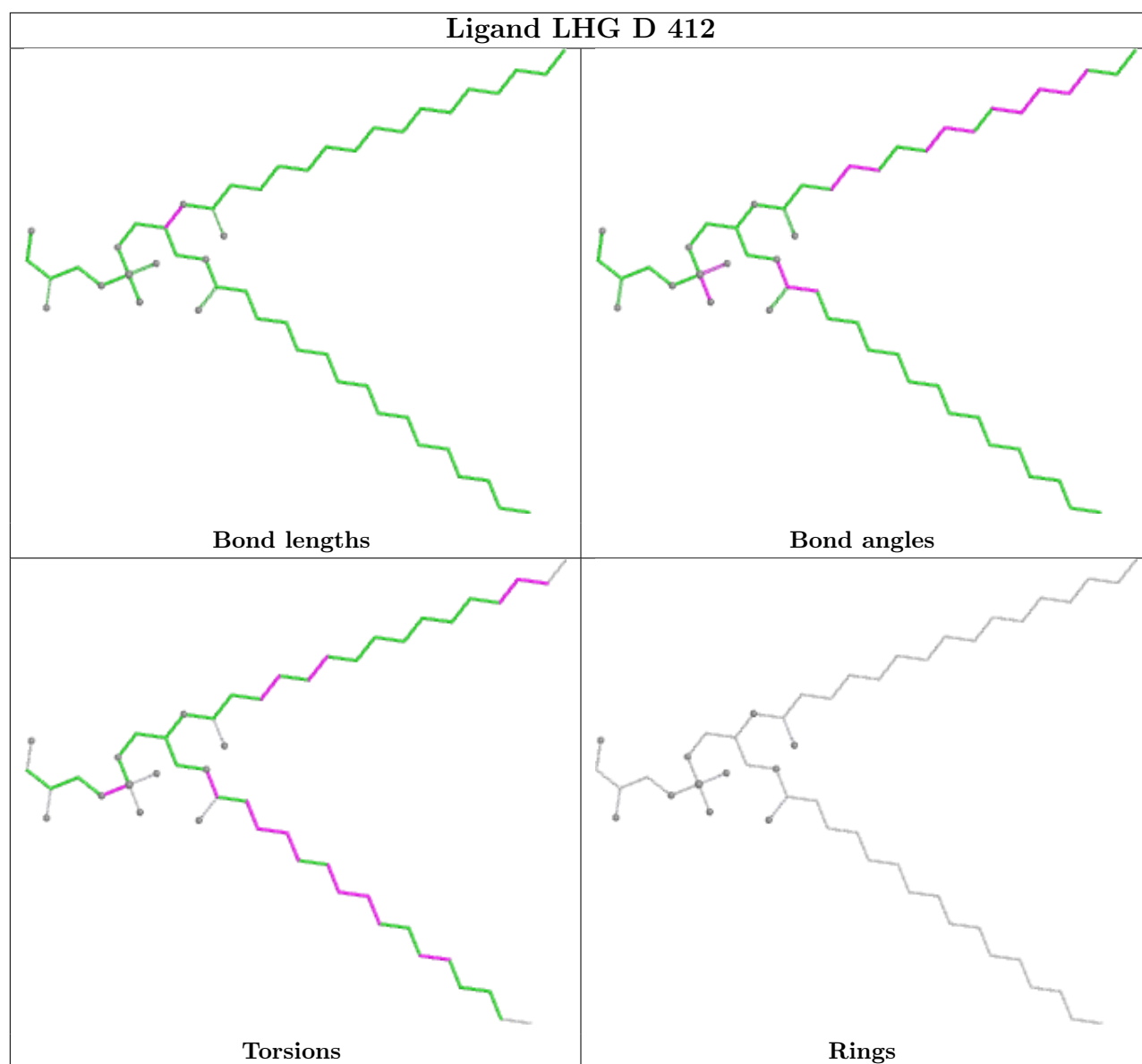




Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG D 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 604	
	
Bond lengths	Bond angles
	
Torsions	Rings



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%)	-0.57	0 100 100	7, 26, 45, 71	64 (19%)
1	a	334/344 (97%)	-0.48	0 100 100	8, 28, 52, 74	64 (19%)
2	B	505/510 (99%)	-0.46	2 (0%) 88 88	17, 31, 58, 85	4 (0%)
2	b	505/510 (99%)	-0.35	2 (0%) 88 88	24, 35, 64, 100	0
3	C	442/461 (95%)	-0.47	0 100 100	9, 34, 49, 66	11 (2%)
3	c	451/461 (97%)	-0.33	2 (0%) 88 88	9, 37, 57, 93	12 (2%)
4	D	341/352 (96%)	-0.62	0 100 100	10, 28, 44, 74	2 (0%)
4	d	341/352 (96%)	-0.46	0 100 100	9, 32, 53, 76	3 (0%)
5	E	82/84 (97%)	0.11	1 (1%) 76 76	30, 48, 70, 85	1 (1%)
5	e	82/84 (97%)	0.22	1 (1%) 76 76	38, 55, 72, 85	0
6	F	34/45 (75%)	-0.18	1 (2%) 53 52	34, 41, 58, 81	0
6	f	34/45 (75%)	0.03	0 100 100	38, 48, 72, 79	0
7	H	65/66 (98%)	-0.23	2 (3%) 51 50	33, 40, 54, 64	0
7	h	63/66 (95%)	-0.03	0 100 100	37, 48, 59, 63	0
8	I	35/38 (92%)	-0.36	0 100 100	31, 38, 62, 78	0
8	i	35/38 (92%)	-0.33	0 100 100	31, 38, 66, 76	0
9	J	36/40 (90%)	-0.08	0 100 100	33, 47, 68, 84	0
9	j	36/40 (90%)	-0.02	0 100 100	37, 50, 82, 86	0
10	K	37/46 (80%)	-0.18	0 100 100	40, 47, 62, 69	0
10	k	37/46 (80%)	0.02	0 100 100	43, 51, 64, 76	0
11	L	37/37 (100%)	-0.44	0 100 100	23, 28, 60, 62	0
11	l	36/37 (97%)	-0.45	0 100 100	25, 29, 61, 78	0
12	M	32/36 (88%)	-0.46	0 100 100	26, 32, 55, 63	0
12	m	31/36 (86%)	-0.45	0 100 100	27, 32, 51, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.27	2 (0%) 82 82	23, 40, 78, 122	1 (0%)
13	o	244/272 (89%)	-0.22	2 (0%) 82 82	25, 39, 73, 108	0
14	T	29/32 (90%)	-0.60	1 (3%) 48 47	25, 30, 52, 64	0
14	t	29/32 (90%)	-0.56	0 100 100	26, 30, 62, 79	0
15	U	97/134 (72%)	-0.22	0 100 100	30, 40, 66, 83	0
15	u	97/134 (72%)	-0.28	1 (1%) 79 79	28, 38, 52, 78	0
16	V	137/163 (84%)	-0.36	0 100 100	28, 38, 53, 68	0
16	v	137/163 (84%)	-0.22	0 100 100	32, 44, 63, 78	0
17	Y	27/46 (58%)	0.59	2 (7%) 20 19	47, 63, 77, 83	0
17	y	30/46 (65%)	0.32	0 100 100	55, 64, 75, 92	0
18	X	38/41 (92%)	-0.10	0 100 100	41, 48, 66, 71	0
18	x	39/41 (95%)	0.30	2 (5%) 33 32	46, 56, 79, 93	0
19	Z	62/62 (100%)	0.68	3 (4%) 35 34	52, 63, 100, 109	0
19	z	62/62 (100%)	0.43	1 (1%) 70 70	54, 65, 106, 112	0
20	R	34/41 (82%)	0.55	1 (2%) 53 52	56, 63, 72, 78	0
20	r	31/41 (75%)	0.83	0 100 100	66, 77, 93, 94	0
All	All	5302/5700 (93%)	-0.32	26 (0%) 87 87	7, 36, 67, 122	162 (3%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Z	33	TRP	3.4
19	Z	62	VAL	3.4
18	x	37	VAL	3.0
19	Z	4	LEU	2.9
13	o	58	ASN	2.8
19	z	33	TRP	2.8
13	O	60	ARG	2.8
2	b	495	PHE	2.7
20	R	35	LEU	2.7
7	H	65	LEU	2.6
7	H	41	PHE	2.5
6	F	12	SER	2.5
15	u	53	ALA	2.5
17	Y	20	ALA	2.5
2	B	499	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
13	O	59	LYS	2.4
18	x	40	SER	2.3
2	B	85	GLY	2.3
13	o	56	PRO	2.2
5	E	3	GLY	2.2
3	c	24	THR	2.2
14	T	30	THR	2.2
2	b	496	TYR	2.2
3	c	134	ILE	2.0
5	e	79	PHE	2.0
17	Y	40	ALA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	T	1	10/11	0.91	0.10	30,35,53,62	0
12	FME	M	1	10/11	0.92	0.10	36,47,61,62	0
14	FME	t	1	10/11	0.93	0.07	30,33,53,58	0
8	FME	I	1	10/11	0.95	0.07	38,44,53,54	0
12	FME	m	1	10/11	0.96	0.07	31,46,60,64	0
8	FME	i	1	10/11	0.96	0.06	41,46,49,50	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	STE	H	103	18/20	0.67	0.14	55,61,68,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	STE	b	624	20/20	0.71	0.14	42,54,64,65	0
29	LMG	d	409	23/55	0.75	0.14	44,59,65,67	0
32	STE	c	521	12/20	0.75	0.13	51,62,67,72	0
32	STE	B	628	12/20	0.77	0.12	50,58,67,68	0
29	LMG	b	622	55/55	0.77	0.13	47,60,69,72	0
32	STE	a	617	12/20	0.77	0.11	55,60,65,66	0
28	PL9	a	611	55/55	0.77	0.14	40,60,76,79	0
31	DGD	a	616	44/66	0.77	0.12	39,50,65,71	0
32	STE	b	623	16/20	0.78	0.11	53,56,72,73	0
33	LHG	E	101	49/49	0.78	0.13	42,70,88,94	0
32	STE	B	627	18/20	0.79	0.12	40,49,70,74	0
28	PL9	A	611	55/55	0.79	0.12	37,57,70,73	0
32	STE	B	621	17/20	0.80	0.13	33,44,61,62	0
29	LMG	D	411	33/55	0.80	0.11	38,52,70,74	0
29	LMG	c	520	48/55	0.80	0.12	50,63,77,80	0
33	LHG	e	102	42/49	0.80	0.11	55,75,89,97	0
32	STE	b	621	20/20	0.81	0.11	36,46,66,70	0
31	DGD	A	616	66/66	0.81	0.10	46,55,64,69	0
25	CLA	b	601	65/65	0.82	0.11	43,60,76,81	0
32	STE	m	102	12/20	0.82	0.12	48,54,60,63	0
32	STE	T	103	15/20	0.82	0.12	44,50,65,66	0
32	STE	E	102	12/20	0.82	0.11	58,65,68,69	0
29	LMG	A	613	48/55	0.83	0.10	38,53,64,69	0
32	STE	I	101	15/20	0.83	0.12	41,50,61,61	0
32	STE	J	101	12/20	0.83	0.12	45,52,57,59	0
32	STE	d	412	20/20	0.83	0.13	41,53,59,60	0
32	STE	B	629	16/20	0.83	0.11	42,55,68,70	0
32	STE	t	102	10/20	0.83	0.11	44,55,62,65	0
32	STE	C	522	12/20	0.83	0.10	45,52,60,61	0
30	SQD	a	615	36/54	0.83	0.10	38,53,64,68	0
32	STE	j	101	12/20	0.84	0.10	45,53,57,60	0
32	STE	C	521	12/20	0.85	0.11	38,42,54,55	0
30	SQD	B	624	54/54	0.85	0.10	37,54,77,83	0
32	STE	B	625	14/20	0.85	0.09	39,43,52,55	0
29	LMG	c	522	49/55	0.85	0.09	38,50,69,76	0
29	LMG	c	518	37/55	0.85	0.09	40,55,66,66	0
30	SQD	A	615	39/54	0.85	0.10	42,51,72,78	0
30	SQD	f	101	41/54	0.86	0.11	57,70,83,85	0
29	LMG	B	622	28/55	0.86	0.10	39,49,57,63	0
32	STE	T	102	16/20	0.86	0.10	37,44,53,55	0
30	SQD	b	620	49/54	0.86	0.09	35,51,73,77	0
32	STE	b	625	10/20	0.86	0.10	46,52,56,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	STE	X	101	20/20	0.86	0.12	35,47,61,70	0
32	STE	c	519	20/20	0.87	0.10	39,48,73,74	0
27	BCR	d	405	40/40	0.87	0.10	38,46,72,72	0
25	CLA	B	601	65/65	0.88	0.10	37,53,73,86	0
32	STE	B	626	12/20	0.88	0.12	43,50,55,57	0
29	LMG	m	101	51/55	0.88	0.08	37,48,58,60	0
27	BCR	k	102	40/40	0.89	0.09	41,51,56,62	0
32	STE	l	102	18/20	0.89	0.10	33,43,60,63	0
31	DGD	H	102	62/66	0.89	0.09	29,40,49,53	0
29	LMG	B	620	51/55	0.89	0.08	31,47,57,60	0
32	STE	M	102	10/20	0.89	0.09	42,45,48,49	0
27	BCR	x	101	40/40	0.89	0.09	38,48,62,64	0
29	LMG	C	520	48/55	0.90	0.09	39,57,65,70	0
31	DGD	h	101	62/66	0.90	0.09	31,43,49,55	0
32	STE	M	101	15/20	0.90	0.09	34,43,54,57	0
27	BCR	C	514	40/40	0.90	0.09	41,49,54,55	0
32	STE	d	411	17/20	0.90	0.09	45,50,60,61	0
27	BCR	C	516	40/40	0.90	0.09	39,48,55,57	0
25	CLA	c	512	65/65	0.91	0.09	42,51,72,74	0
27	BCR	k	103	40/40	0.91	0.10	41,47,54,57	0
27	BCR	D	405	40/40	0.91	0.09	31,39,67,71	0
27	BCR	H	101	40/40	0.91	0.08	33,43,55,57	0
31	DGD	C	518	62/66	0.91	0.08	30,41,77,86	0
30	SQD	A	614	52/54	0.91	0.10	31,46,68,75	0
25	CLA	C	513	65/65	0.91	0.08	41,49,71,74	0
27	BCR	k	101	40/40	0.91	0.09	41,51,55,57	0
30	SQD	D	408	36/54	0.91	0.10	43,61,66,70	0
30	SQD	a	614	54/54	0.91	0.09	38,54,66,69	0
31	DGD	c	516	62/66	0.92	0.08	32,44,69,73	0
29	LMG	D	407	51/55	0.92	0.08	28,44,67,69	0
32	STE	C	523	16/20	0.92	0.08	37,47,54,55	0
31	DGD	c	515	62/66	0.93	0.07	23,35,57,67	0
27	BCR	B	619	40/40	0.93	0.07	28,37,49,52	0
25	CLA	C	506	65/65	0.93	0.07	29,37,61,65	0
25	CLA	c	508	64/65	0.93	0.07	30,38,71,85	0
25	CLA	B	606	65/65	0.93	0.07	25,32,55,63	0
25	CLA	c	513	65/65	0.93	0.08	42,52,83,86	0
27	BCR	b	617	40/40	0.93	0.07	28,36,44,47	0
27	BCR	b	618	40/40	0.93	0.07	25,36,46,47	0
31	DGD	C	517	62/66	0.93	0.08	23,34,67,72	0
27	BCR	b	619	40/40	0.93	0.07	30,41,55,58	0
33	LHG	D	412	49/49	0.93	0.07	30,38,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	BCR	c	514	40/40	0.93	0.07	26,40,50,52	0
33	LHG	a	613	49/49	0.93	0.07	34,44,57,62	0
27	BCR	A	610	40/40	0.93	0.06	23,31,39,40	0
34	BCT	d	401	4/4	0.93	0.08	32,38,41,47	0
25	CLA	C	503	65/65	0.94	0.07	30,37,41,49	0
27	BCR	t	101	40/40	0.94	0.06	26,33,44,47	0
25	CLA	d	404	65/65	0.94	0.08	30,40,72,76	0
25	CLA	a	606	65/65	0.94	0.07	18,26,37,46	0
28	PL9	D	406	55/55	0.94	0.06	22,28,37,38	0
27	BCR	B	617	40/40	0.94	0.06	27,34,42,44	0
28	PL9	d	406	55/55	0.94	0.06	24,30,35,39	0
31	DGD	C	519	62/66	0.94	0.07	29,37,65,68	0
27	BCR	B	618	40/40	0.94	0.06	24,35,42,45	0
25	CLA	C	508	65/65	0.94	0.07	27,33,74,81	0
25	CLA	b	606	65/65	0.94	0.07	28,34,61,68	0
27	BCR	C	515	40/40	0.94	0.07	28,37,45,50	0
31	DGD	c	517	62/66	0.94	0.08	27,42,64,68	0
25	CLA	b	608	65/65	0.94	0.07	30,36,49,55	0
25	CLA	b	610	65/65	0.94	0.07	24,33,40,42	0
25	CLA	b	614	65/65	0.94	0.07	22,33,56,66	0
27	BCR	K	101	40/40	0.94	0.08	35,42,55,57	0
27	BCR	T	101	40/40	0.94	0.06	28,33,43,46	0
25	CLA	b	616	60/65	0.94	0.08	26,37,78,82	0
25	CLA	c	503	65/65	0.94	0.07	34,38,44,50	0
33	LHG	D	410	47/49	0.94	0.08	27,39,70,76	0
25	CLA	c	506	65/65	0.94	0.08	32,40,77,79	0
25	CLA	C	510	65/65	0.94	0.07	30,38,48,51	0
25	CLA	c	509	65/65	0.94	0.08	32,38,51,56	0
25	CLA	c	511	65/65	0.94	0.08	37,46,56,62	0
25	CLA	C	512	65/65	0.94	0.08	38,45,70,82	0
29	LMG	d	410	44/55	0.95	0.07	36,44,65,71	0
25	CLA	c	501	65/65	0.95	0.06	28,35,42,47	0
25	CLA	c	502	65/65	0.95	0.06	28,34,45,49	0
25	CLA	a	607	65/65	0.95	0.07	27,33,71,74	0
25	CLA	c	504	60/65	0.95	0.06	28,38,64,66	0
25	CLA	c	505	65/65	0.95	0.07	31,35,55,65	0
25	CLA	B	609	65/65	0.95	0.06	24,33,44,49	0
25	CLA	c	507	65/65	0.95	0.07	26,36,48,51	0
25	CLA	B	610	65/65	0.95	0.06	21,27,35,37	0
25	CLA	C	511	65/65	0.95	0.07	33,42,51,54	0
25	CLA	c	510	65/65	0.95	0.07	29,39,50,54	0
27	BCR	a	610	40/40	0.95	0.06	23,31,40,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	b	609	65/65	0.95	0.07	28,40,55,65	0
33	LHG	B	623	49/49	0.95	0.07	27,35,44,51	0
25	CLA	C	502	65/65	0.95	0.06	27,32,44,48	0
25	CLA	b	612	65/65	0.95	0.07	23,29,41,48	0
25	CLA	d	403	65/65	0.95	0.06	22,28,49,54	0
25	CLA	A	606	65/65	0.95	0.06	18,24,39,43	0
33	LHG	d	408	39/49	0.95	0.07	31,39,57,58	0
26	PHO	d	402	64/64	0.95	0.06	27,35,40,43	0
33	LHG	l	101	49/49	0.95	0.07	29,39,46,54	0
25	CLA	A	607	65/65	0.95	0.07	22,29,78,81	0
25	CLA	C	501	65/65	0.96	0.06	26,32,41,47	0
25	CLA	b	602	65/65	0.96	0.06	29,36,50,53	0
25	CLA	b	604	65/65	0.96	0.06	22,28,59,72	0
25	CLA	b	605	65/65	0.96	0.06	22,29,39,45	0
26	PHO	D	402	64/64	0.96	0.05	22,29,34,39	0
26	PHO	a	608	64/64	0.96	0.05	19,27,32,40	0
25	CLA	A	612	65/65	0.96	0.06	18,24,38,48	0
25	CLA	B	607	65/65	0.96	0.06	19,27,52,54	0
25	CLA	C	504	59/65	0.96	0.06	28,34,60,63	0
25	CLA	C	505	65/65	0.96	0.06	25,34,51,60	0
25	CLA	B	608	65/65	0.96	0.06	22,29,47,54	0
25	CLA	b	613	65/65	0.96	0.06	21,28,59,61	0
25	CLA	C	507	65/65	0.96	0.06	25,33,46,48	0
25	CLA	b	615	65/65	0.96	0.06	26,35,47,53	0
25	CLA	B	602	65/65	0.96	0.06	24,32,46,50	0
25	CLA	C	509	65/65	0.96	0.07	26,35,50,54	0
25	CLA	B	604	65/65	0.96	0.07	21,26,56,61	0
25	CLA	B	611	65/65	0.96	0.05	19,26,40,44	0
33	LHG	D	409	49/49	0.96	0.06	26,34,42,46	0
25	CLA	B	613	65/65	0.96	0.06	19,25,55,64	0
25	CLA	B	614	65/65	0.96	0.06	22,32,55,63	0
25	CLA	D	403	65/65	0.96	0.06	18,24,44,52	0
25	CLA	D	404	65/65	0.96	0.07	26,32,76,85	0
33	LHG	d	407	49/49	0.96	0.06	29,37,46,53	0
25	CLA	B	615	65/65	0.96	0.06	23,30,48,58	0
25	CLA	B	616	60/65	0.96	0.07	24,32,71,76	0
25	CLA	a	609	65/65	0.96	0.09	21,28,62,66	0
34	BCT	D	401	4/4	0.96	0.06	29,29,31,34	0
25	CLA	a	612	65/65	0.96	0.05	21,27,39,44	0
26	PHO	A	608	64/64	0.97	0.05	20,25,30,35	0
25	CLA	b	611	65/65	0.97	0.05	23,29,44,50	0
25	CLA	B	605	65/65	0.97	0.05	20,27,37,41	0

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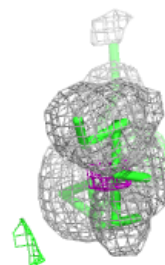
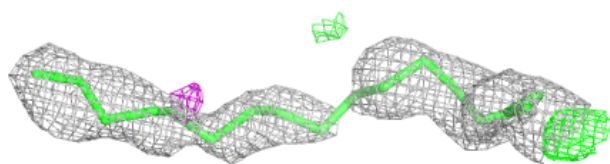
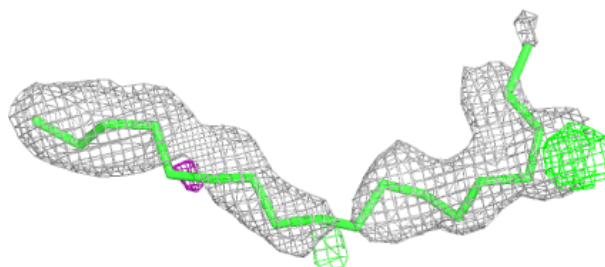
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	B	612	65/65	0.97	0.06	20,27,36,41	0
25	CLA	b	607	65/65	0.97	0.06	23,30,56,61	0
25	CLA	B	603	65/65	0.97	0.06	20,28,50,52	0
25	CLA	b	603	65/65	0.97	0.06	23,30,55,63	0
25	CLA	A	609	54/65	0.97	0.06	20,25,57,61	0
35	HEM	F	101	43/43	0.97	0.08	39,44,53,58	0
35	HEM	e	101	43/43	0.97	0.09	45,53,66,78	0
36	HEC	V	201	43/43	0.98	0.06	24,29,37,44	0
36	HEC	v	201	43/43	0.98	0.06	27,33,36,41	0
24	CL	A	605	1/1	0.99	0.04	27,27,27,27	0
24	CL	a	604	1/1	0.99	0.06	26,26,26,26	0
21	OEX	A	601[B]	10/10	0.99	0.03	24,28,32,32	10
21	OEX	A	601[C]	10/10	0.99	0.03	18,22,26,27	10
21	OEX	a	601[B]	10/10	0.99	0.02	25,29,31,31	10
21	OEX	a	601[C]	10/10	0.99	0.02	17,24,26,28	10
22	OXY	A	602[A]	11/11	0.99	0.04	25,28,31,31	11
22	OXY	a	602[A]	11/11	0.99	0.03	27,29,33,33	11
23	FE2	a	603	1/1	0.99	0.02	33,33,33,33	0
24	CL	A	604	1/1	0.99	0.03	27,27,27,27	0
23	FE2	A	603	1/1	1.00	0.02	26,26,26,26	0
24	CL	a	605	1/1	1.00	0.07	28,28,28,28	0

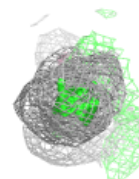
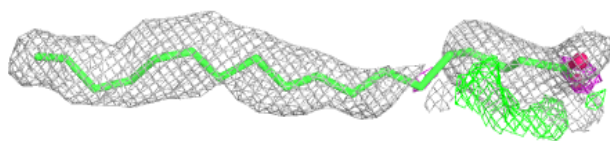
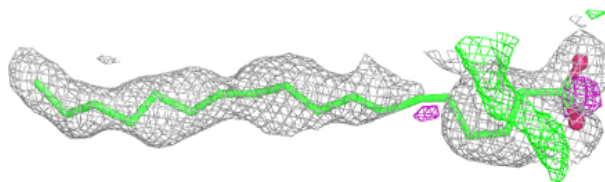
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE 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)

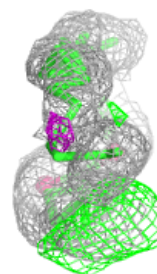
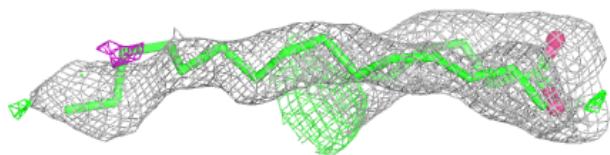
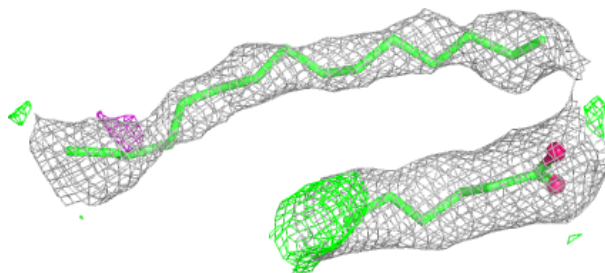
**Electron density around STE b 624:**

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

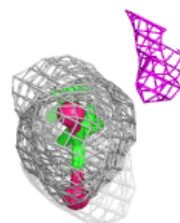
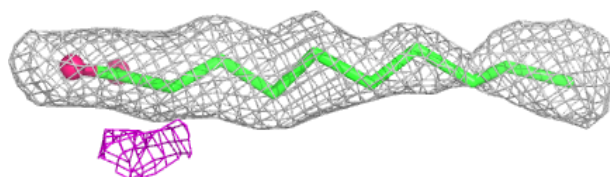
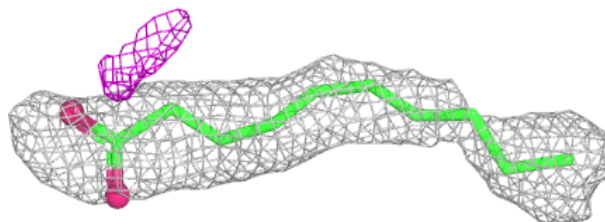


Electron density around LMG d 409:

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

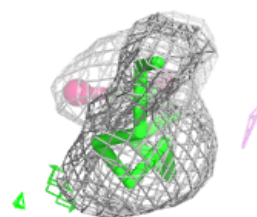
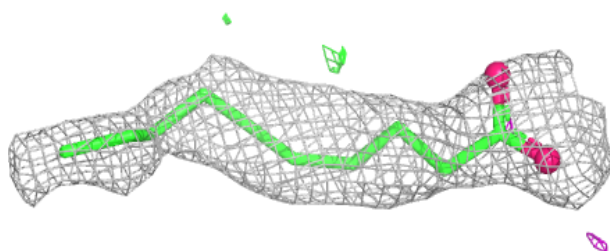
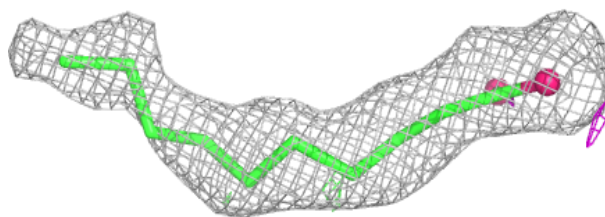
**Electron density around STE c 521:**

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

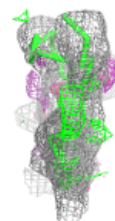
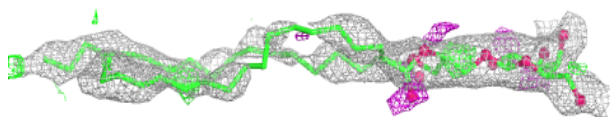
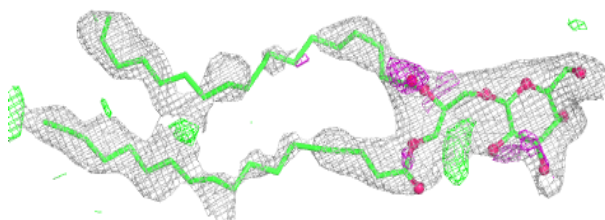


Electron density around STE B 628:

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

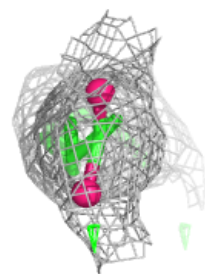
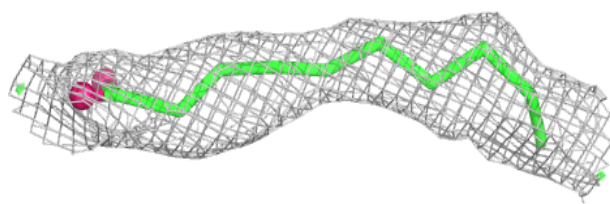
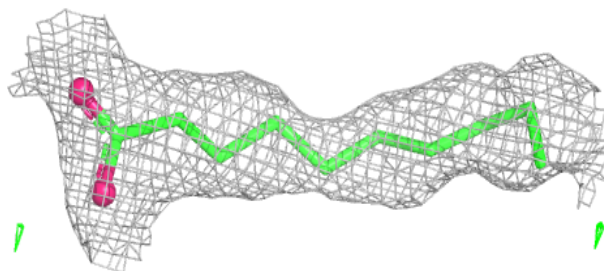
**Electron density around LMG b 622:**

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

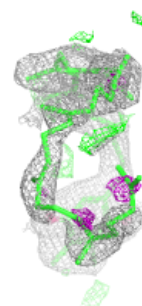
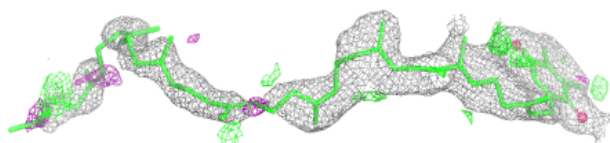
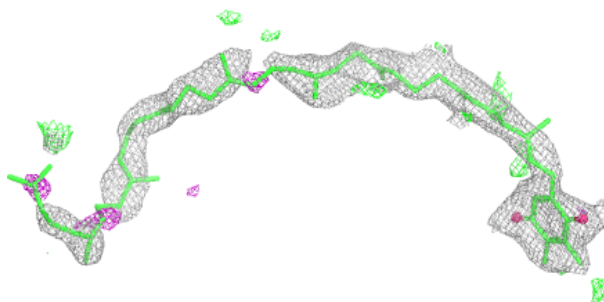


Electron density around STE a 617:

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

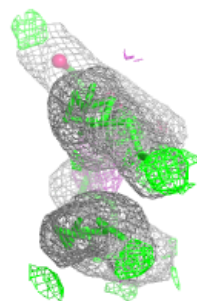
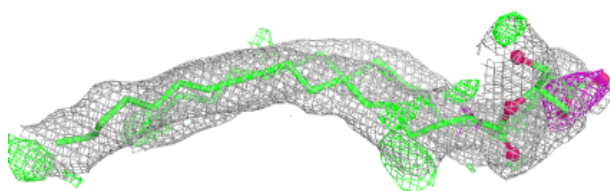
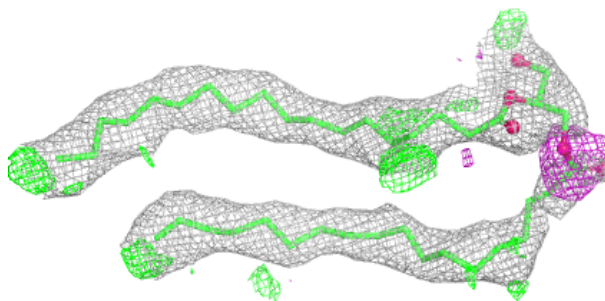
**Electron density around PL9 a 611:**

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

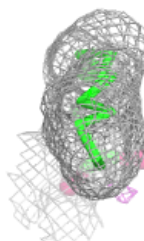
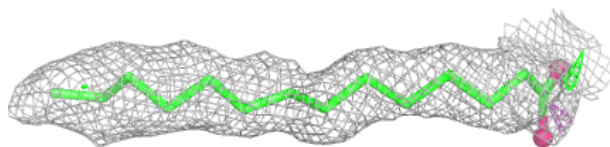
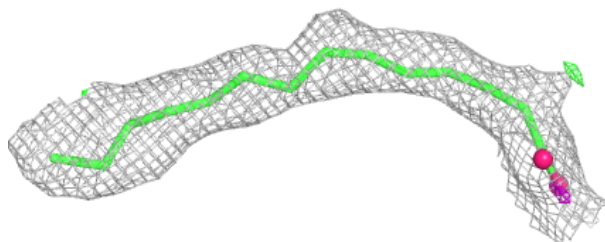


Electron density around DGD a 616:

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

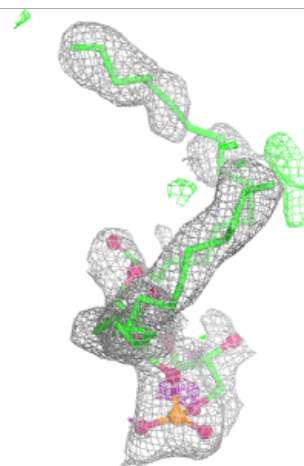
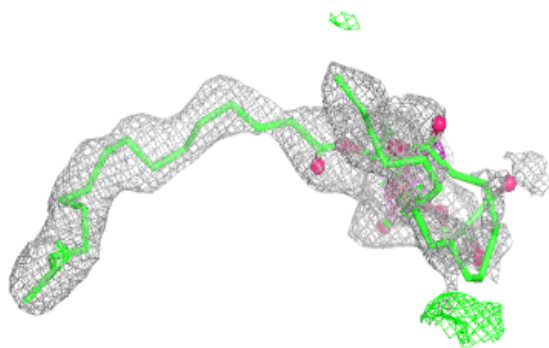
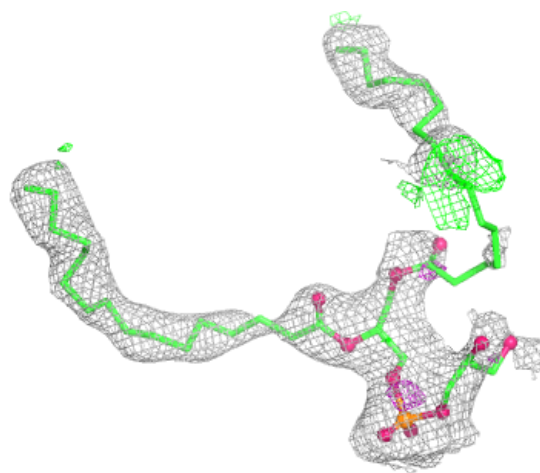
**Electron density around STE b 623:**

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



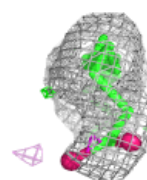
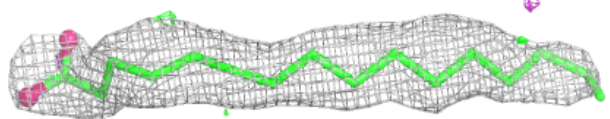
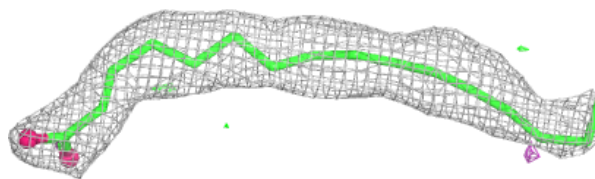
Electron density around LHG E 101:

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

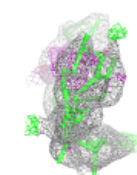
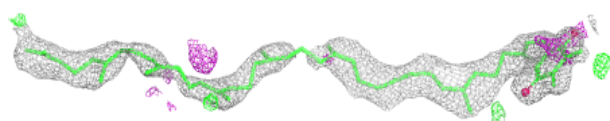
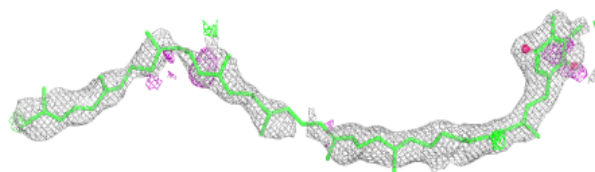


Electron density around STE B 627:

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

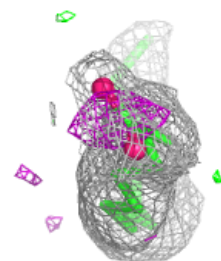
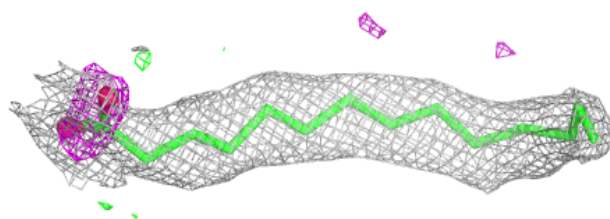
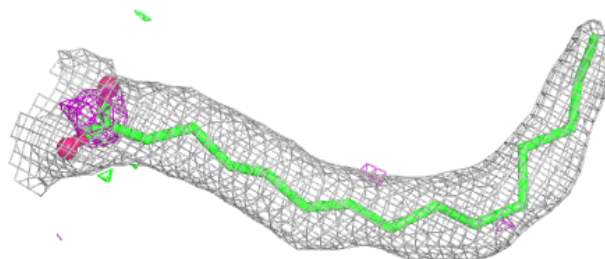
**Electron density around PL9 A 611:**

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

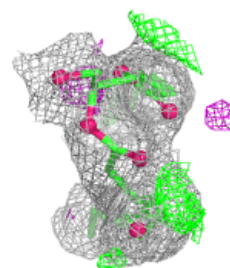
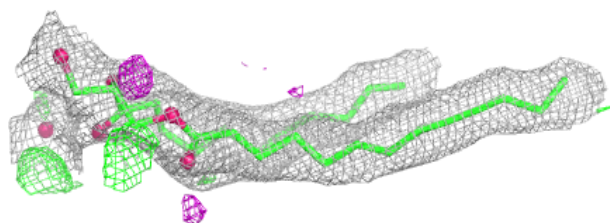
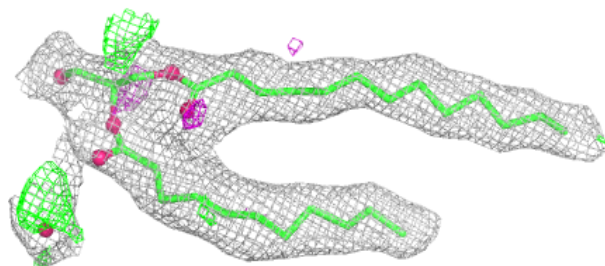


Electron density around STE B 621:

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

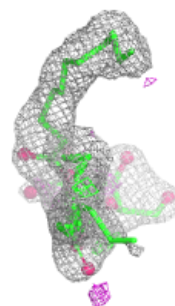
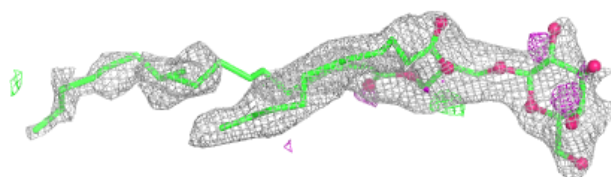
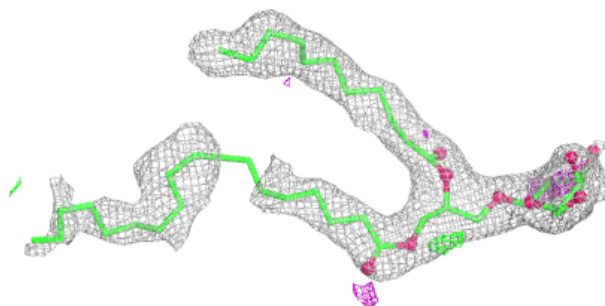
**Electron density around LMG D 411:**

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

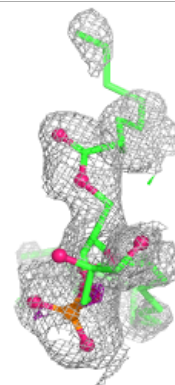
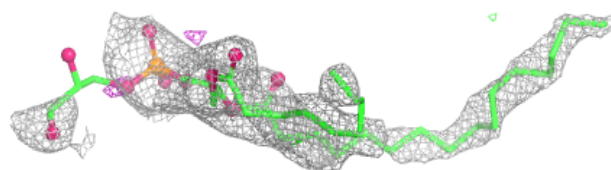
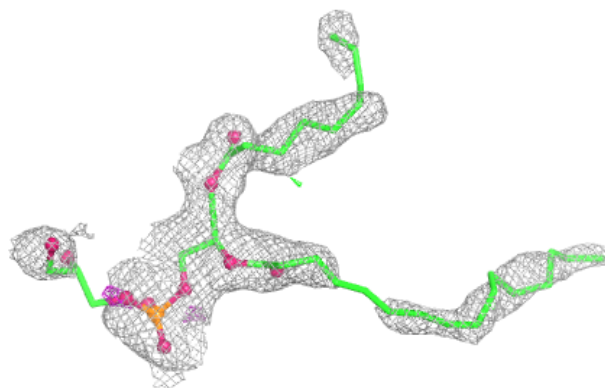


Electron density around LMG c 520:

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

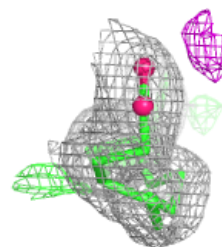
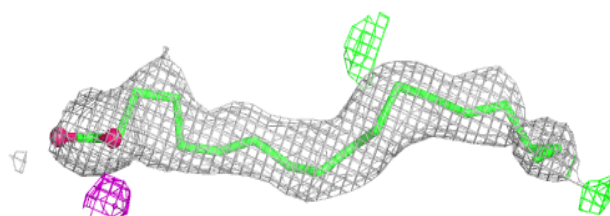
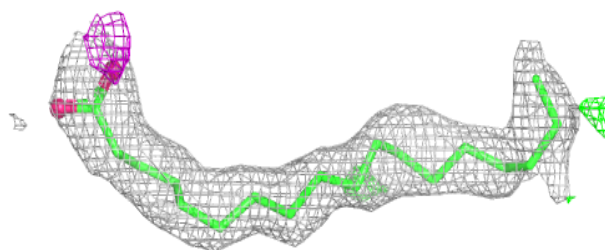
**Electron density around LHG e 102:**

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

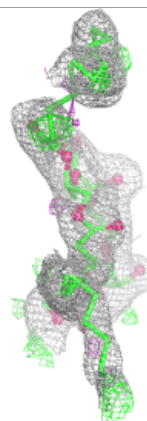
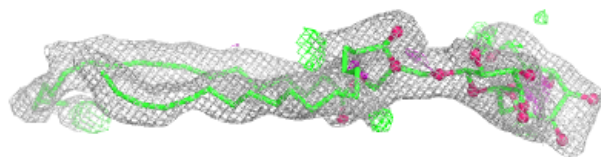
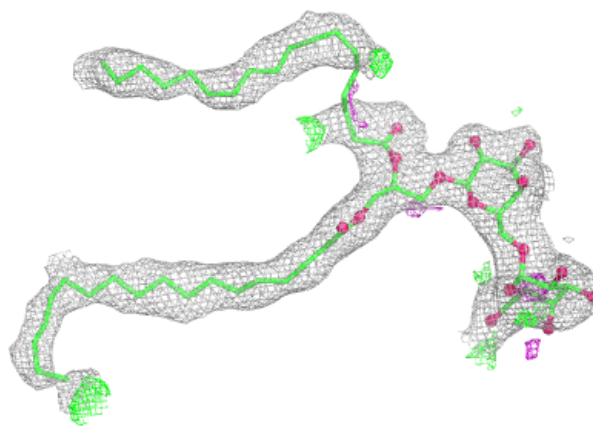


Electron density around STE b 621:

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

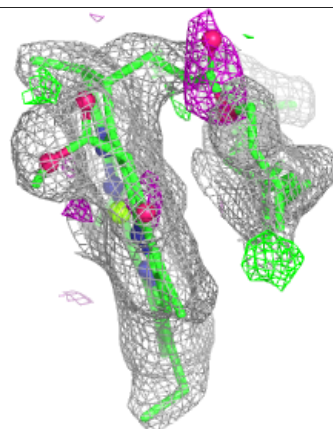
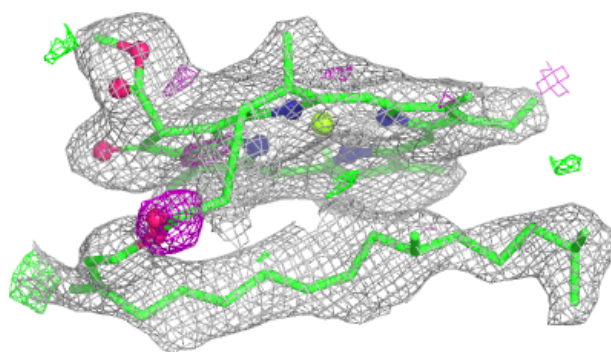
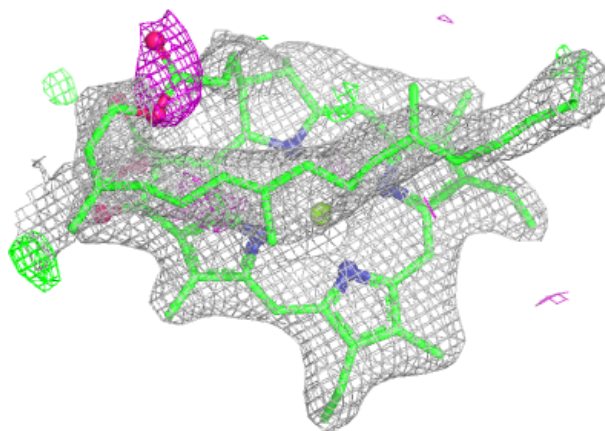
**Electron density around DGD A 616:**

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

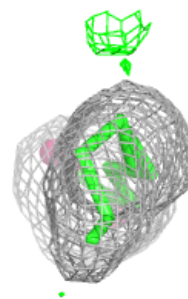
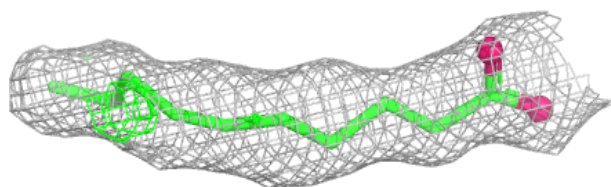
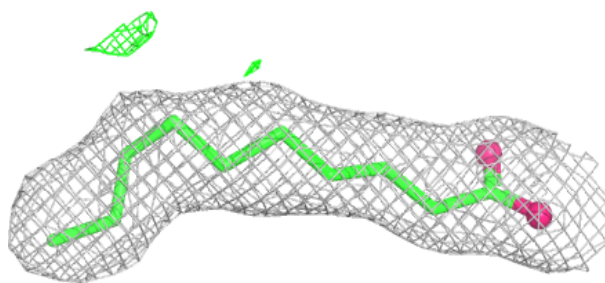


Electron density around CLA b 601:

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

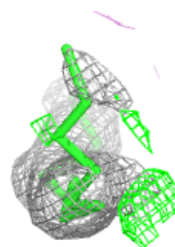
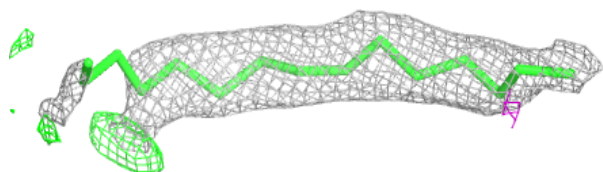
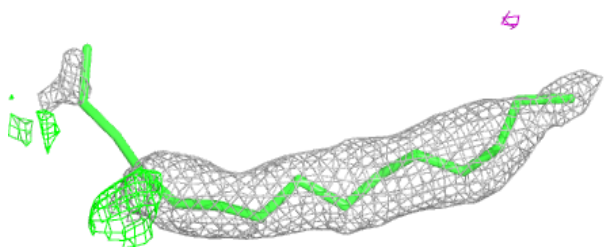
**Electron density around STE m 102:**

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

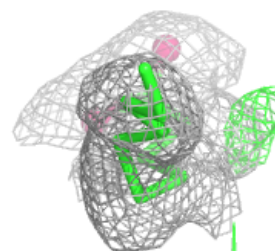
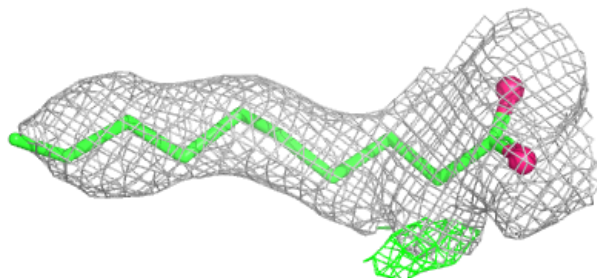
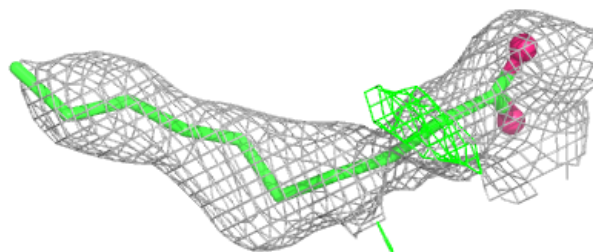


Electron density around STE T 103:

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

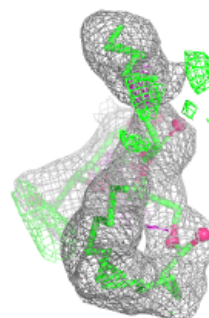
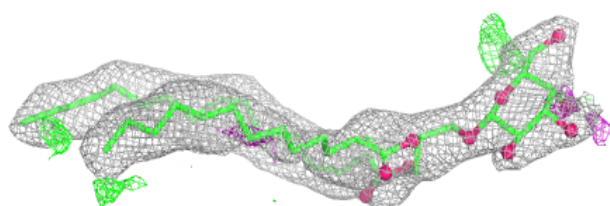
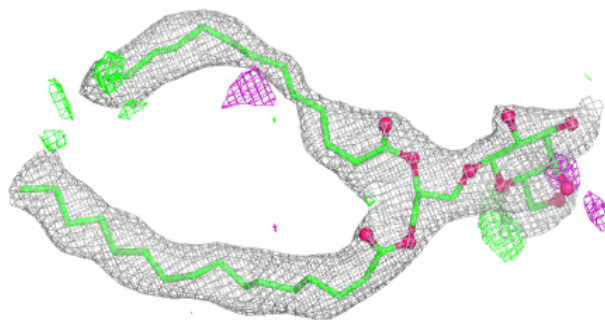
**Electron density around STE E 102:**

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

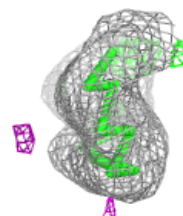
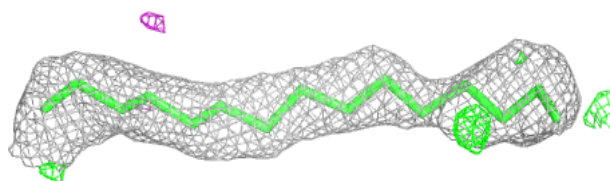
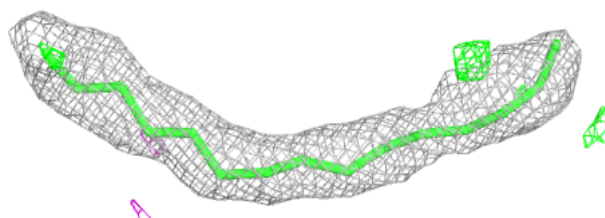


Electron density around LMG A 613:

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

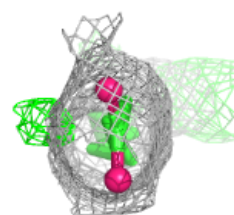
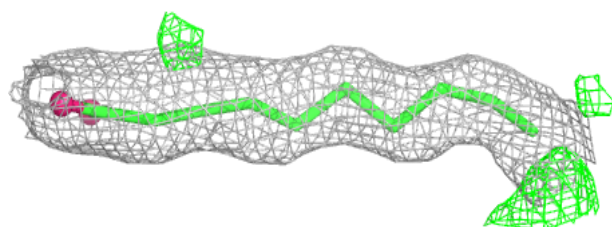
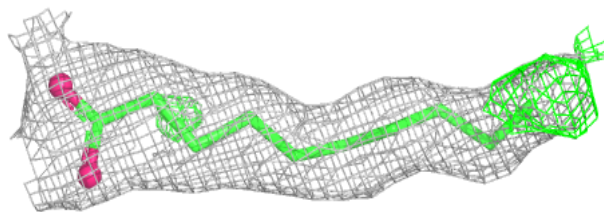
**Electron density around STE I 101:**

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

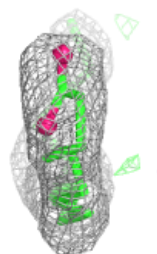
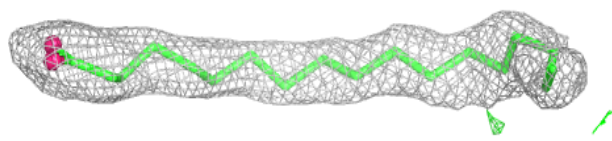
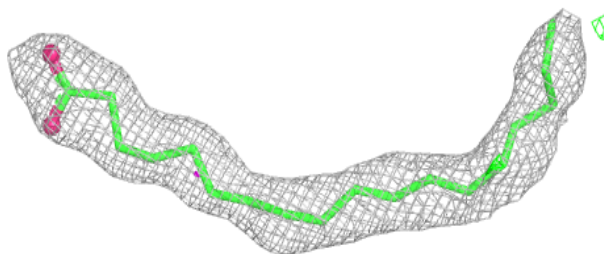


Electron density around STE J 101:

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

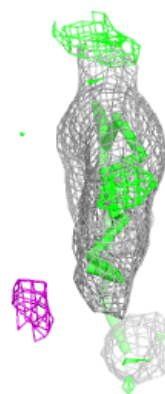
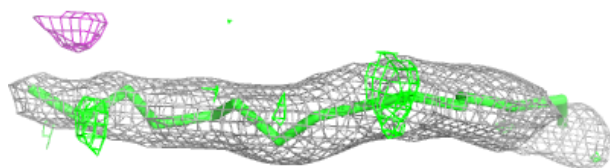
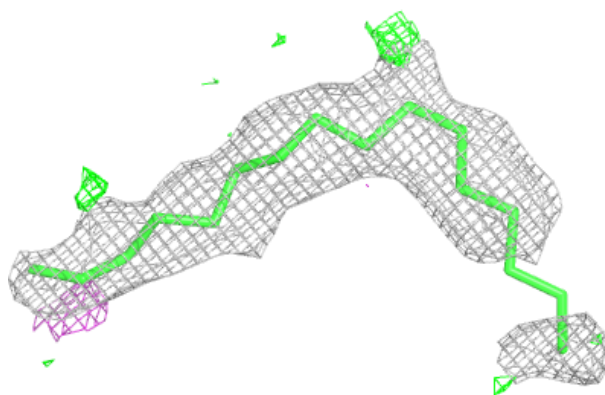
**Electron density around STE d 412:**

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

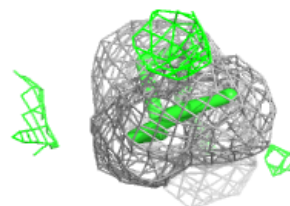
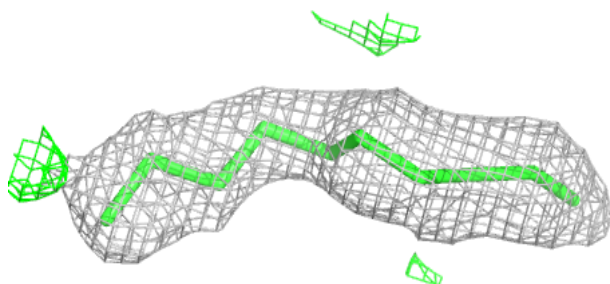
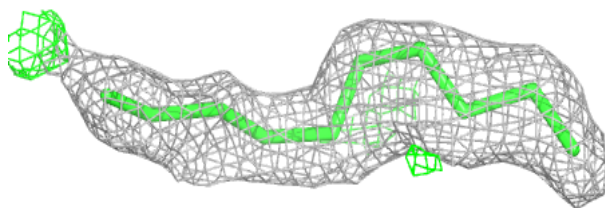


Electron density around STE B 629:

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

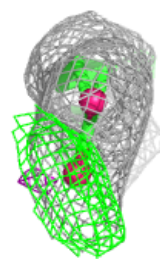
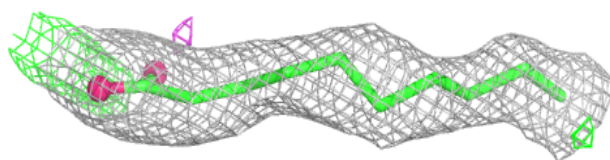
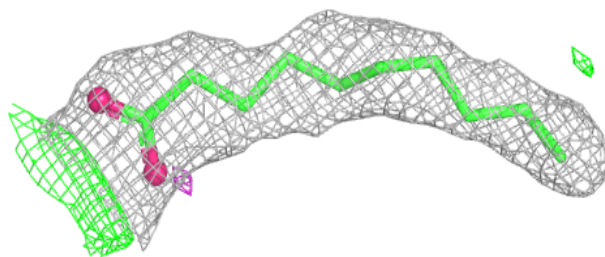
**Electron density around STE t 102:**

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



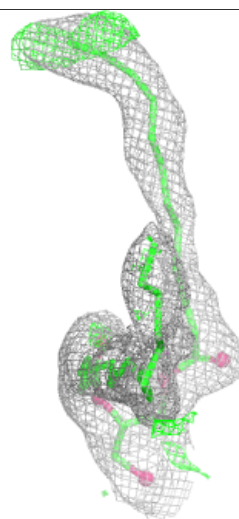
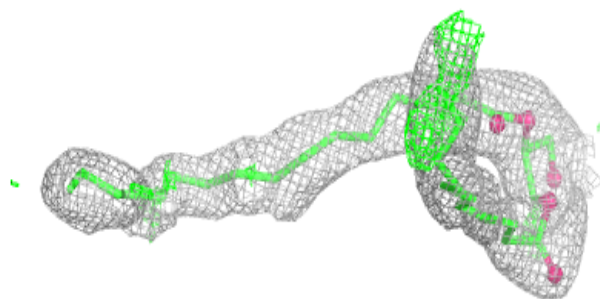
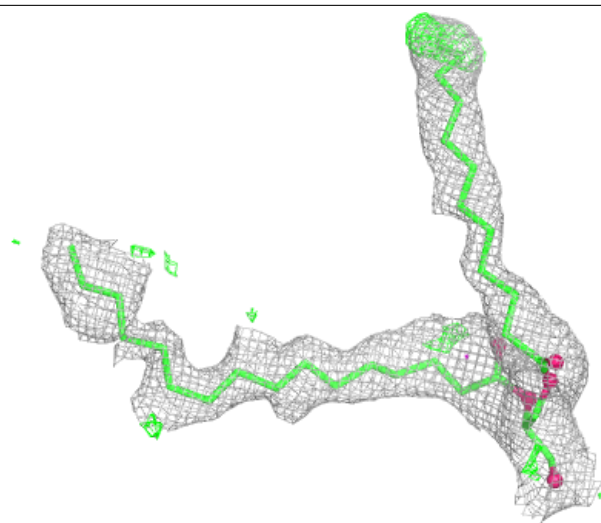
Electron density around STE C 522:

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



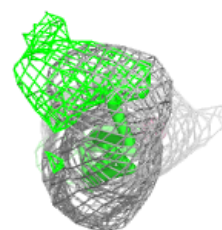
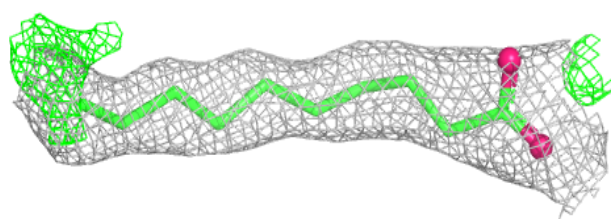
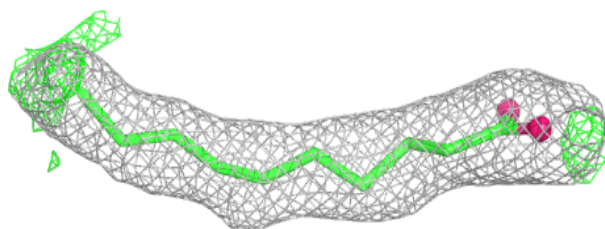
Electron density around SQD a 615:

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

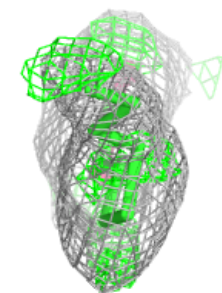
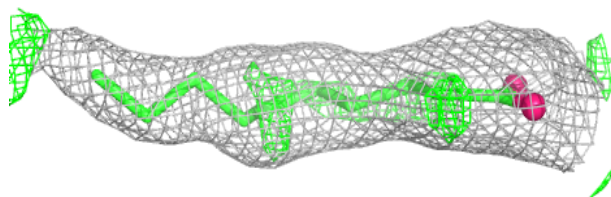
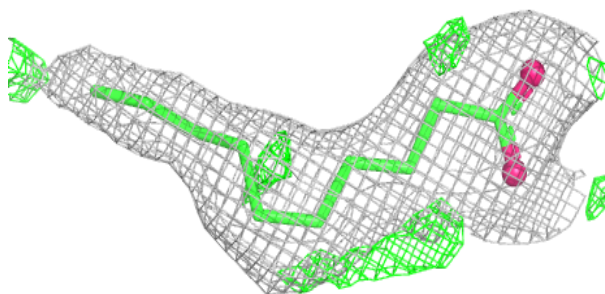


Electron density around STE j 101:

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

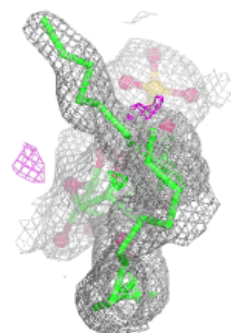
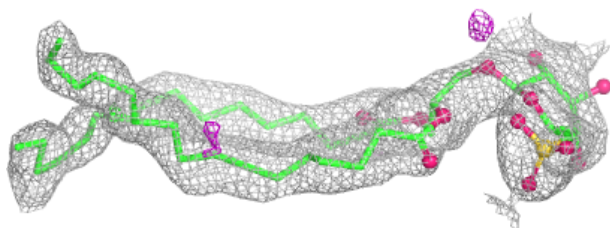
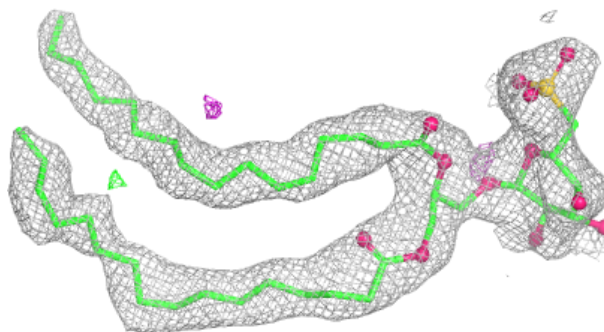
**Electron density around STE C 521:**

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

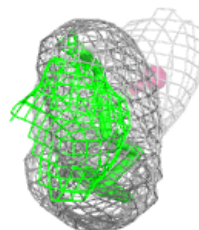
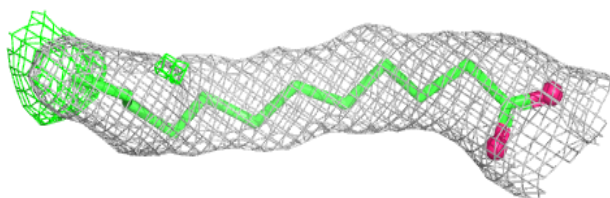
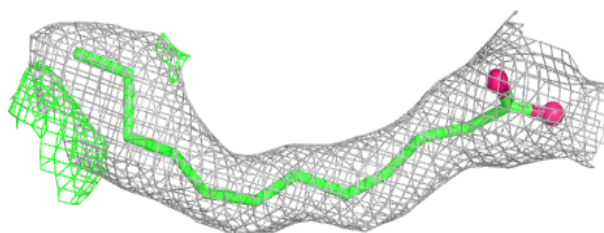


Electron density around SQD B 624:

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

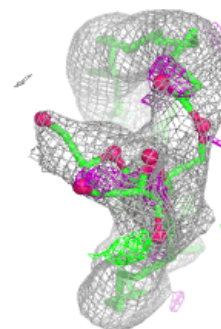
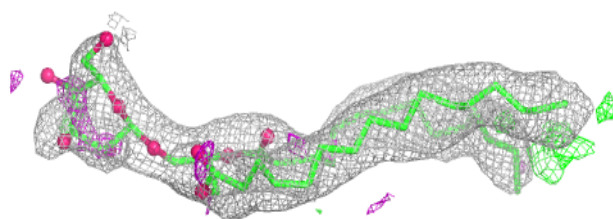
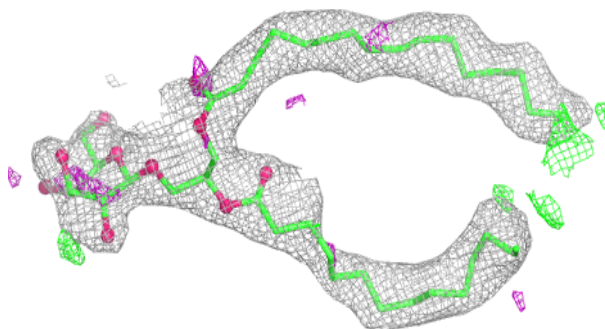
**Electron density around STE B 625:**

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

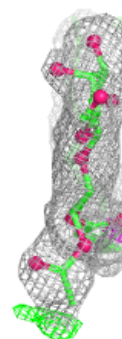
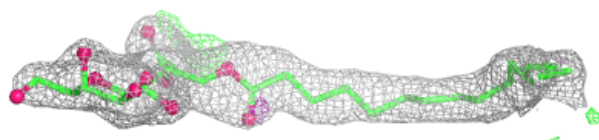
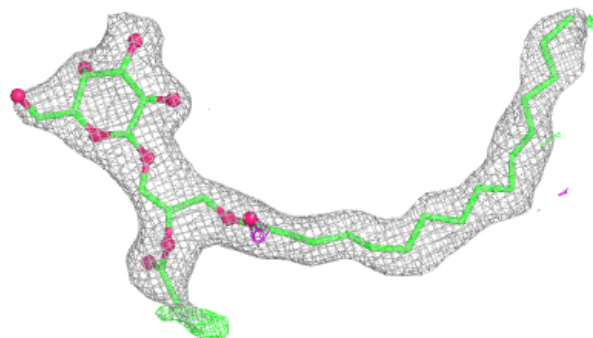


Electron density around LMG c 522:

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

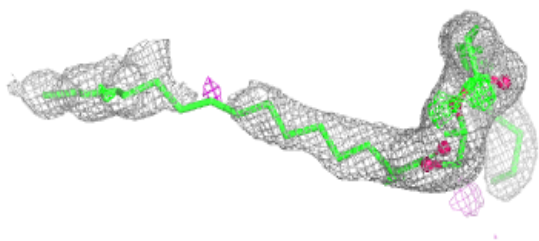
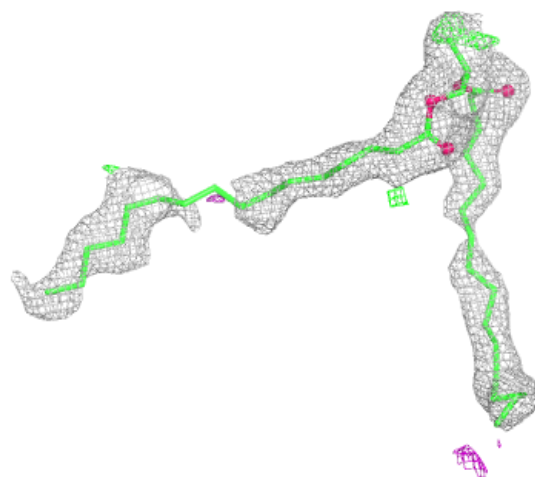
**Electron density around LMG c 518:**

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



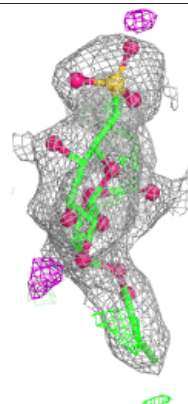
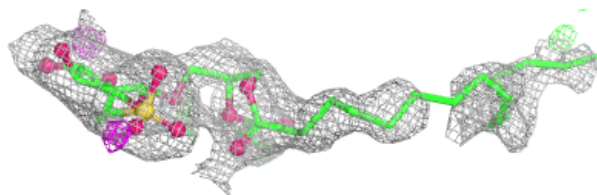
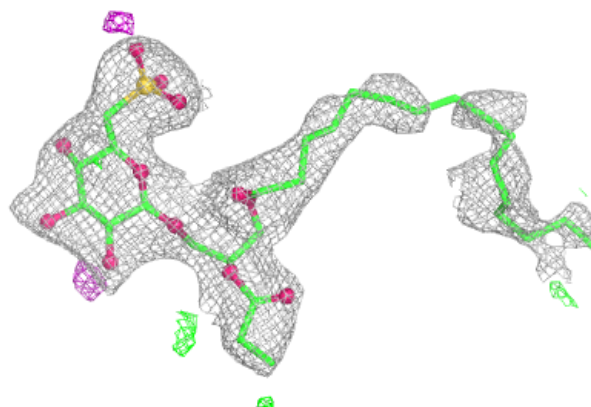
Electron density around SQD A 615:

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

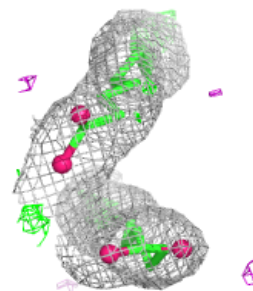
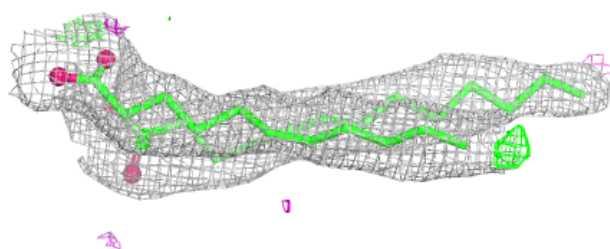
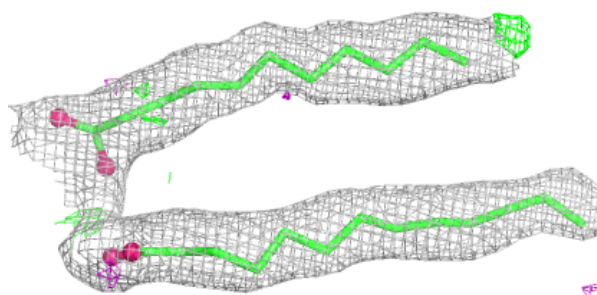


Electron density around SQD f 101:

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

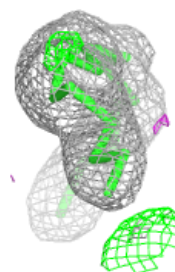
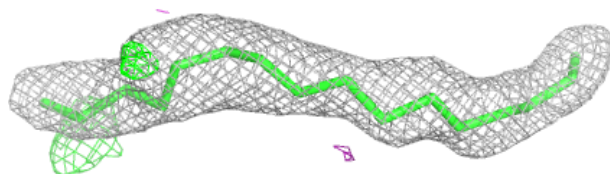
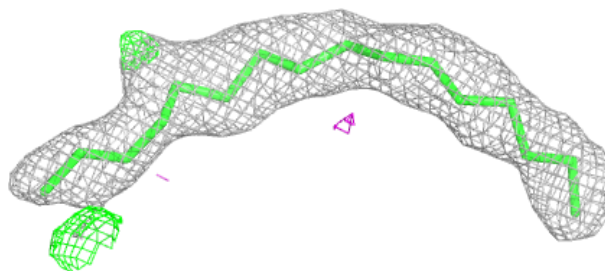
**Electron density around LMG B 622:**

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

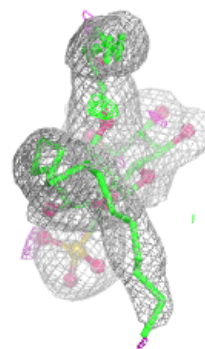
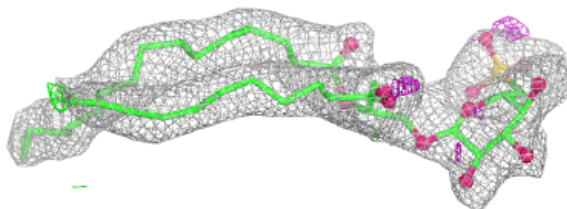
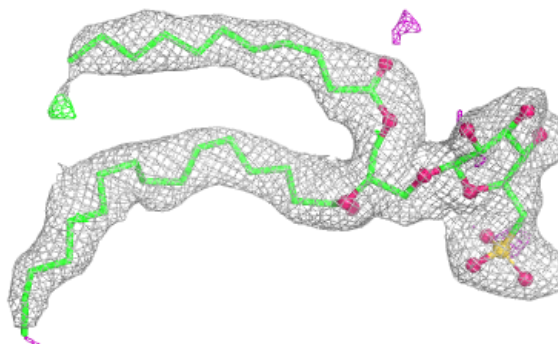


Electron density around STE T 102:

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

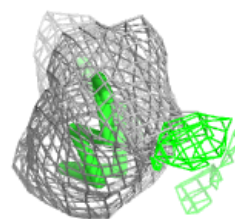
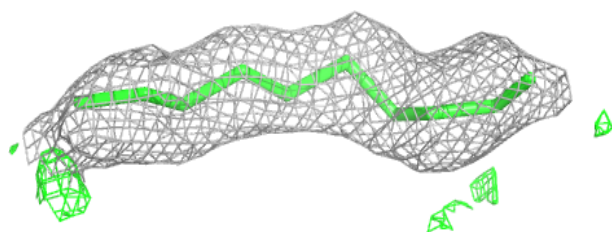
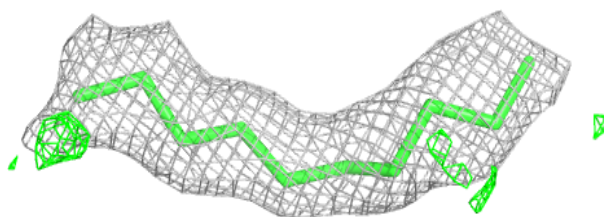
**Electron density around SQD b 620:**

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

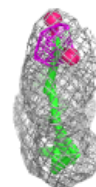
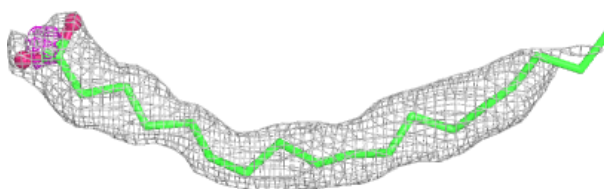


Electron density around STE b 625:

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

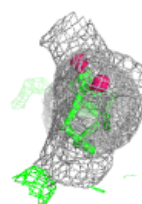
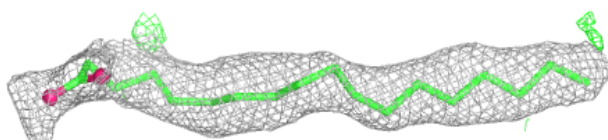
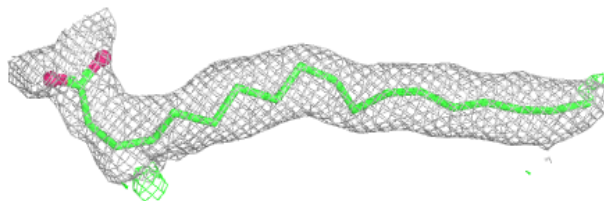
**Electron density around STE X 101:**

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

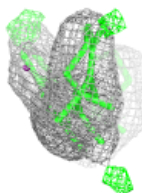
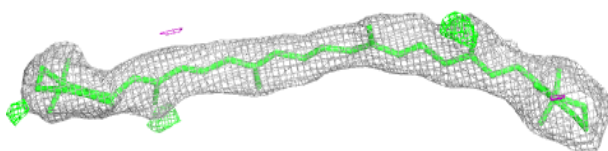
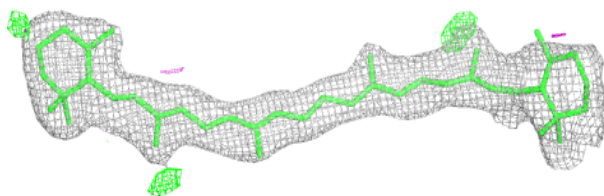


Electron density around STE c 519:

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

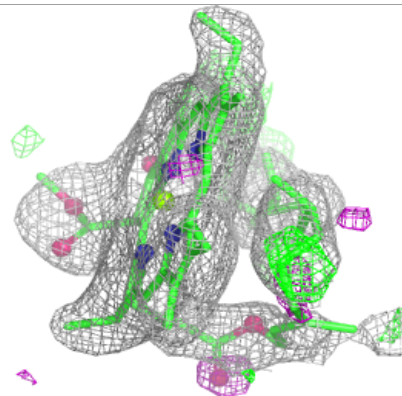
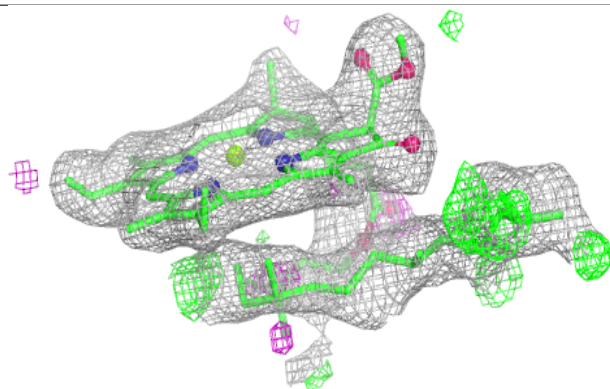
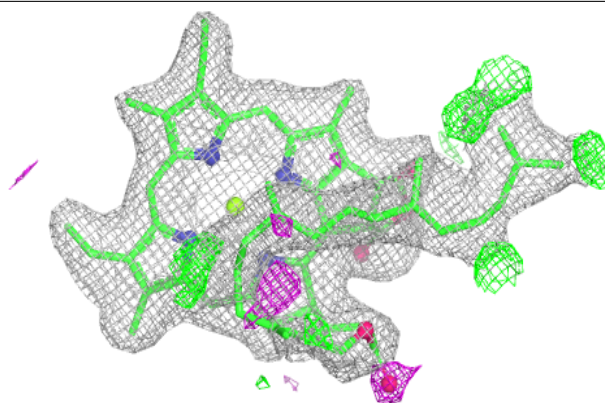
**Electron density around BCR d 405:**

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

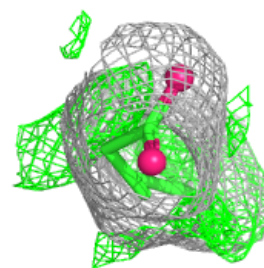
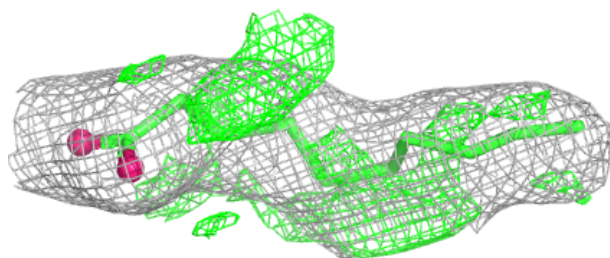
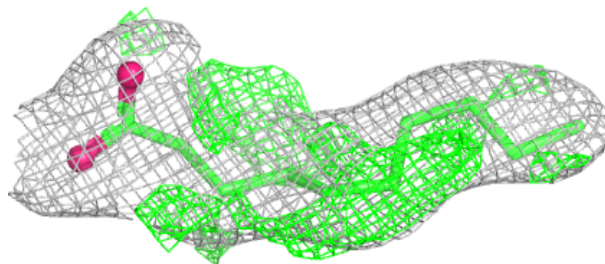


Electron density around CLA B 601:

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

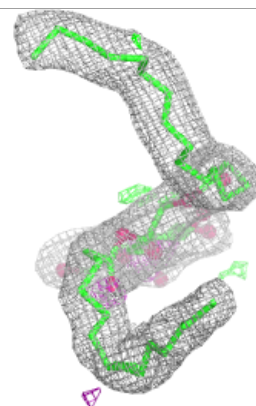
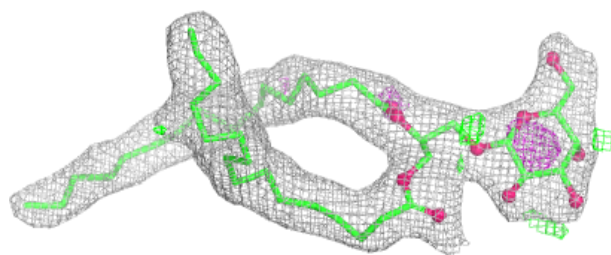
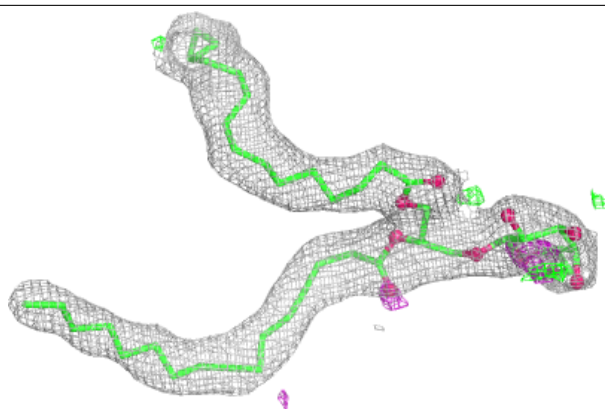
**Electron density around STE B 626:**

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

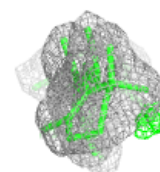
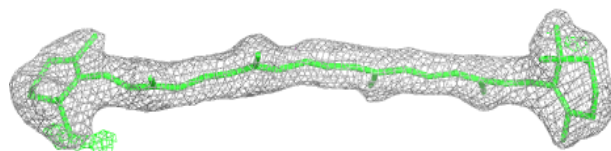
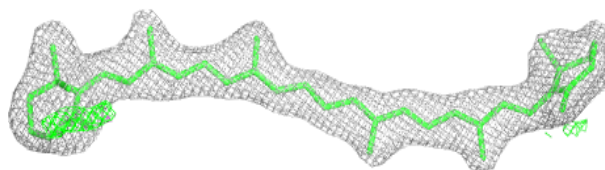


Electron density around LMG m 101:

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

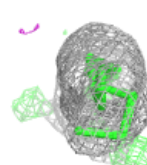
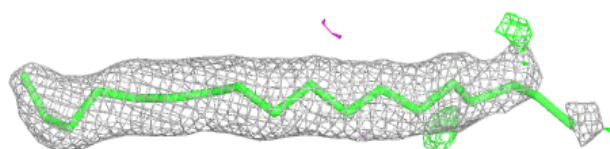
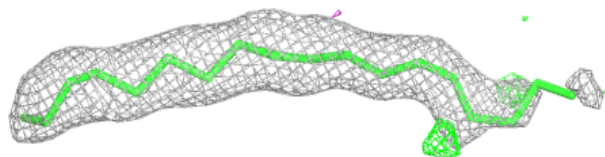
**Electron density around BCR k 102:**

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

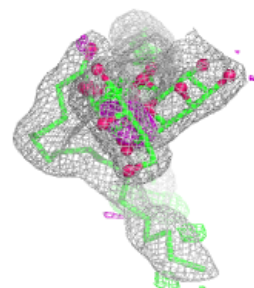
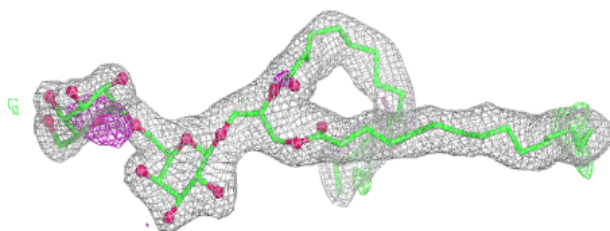
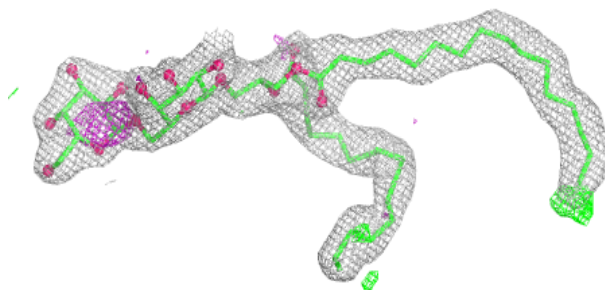


Electron density around STE I 102:

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

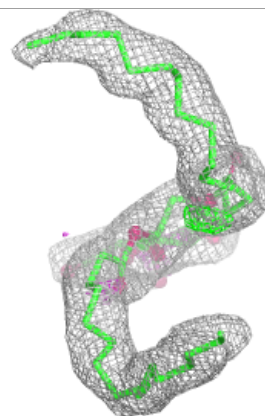
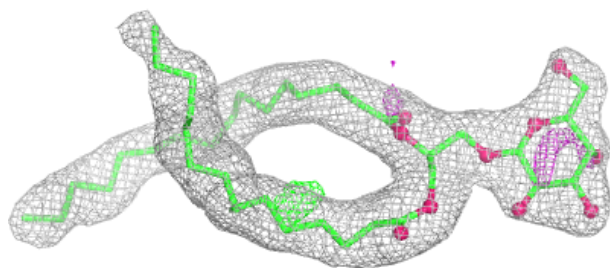
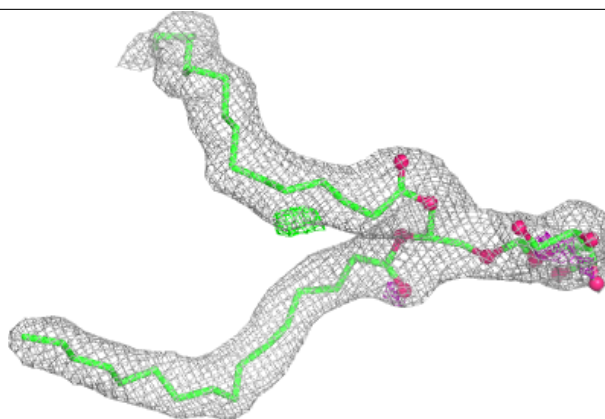
**Electron density around DGD H 102:**

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

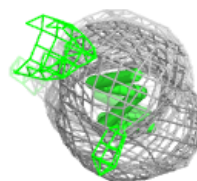
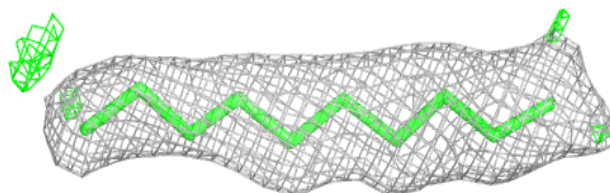
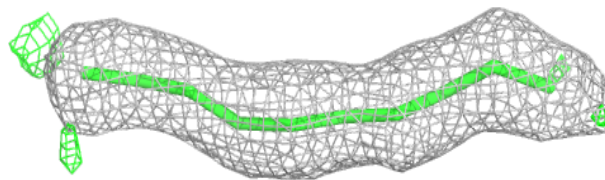


Electron density around LMG B 620:

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

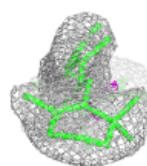
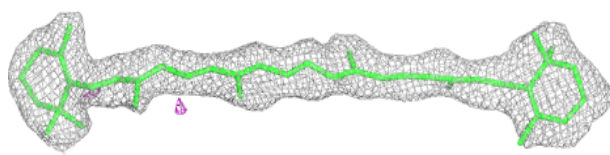
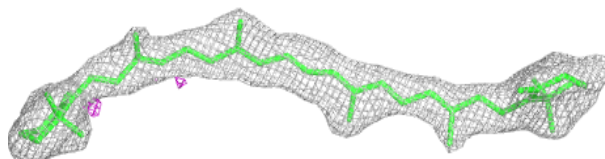
**Electron density around STE M 102:**

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

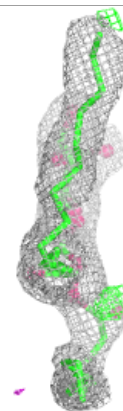
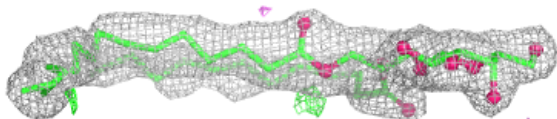
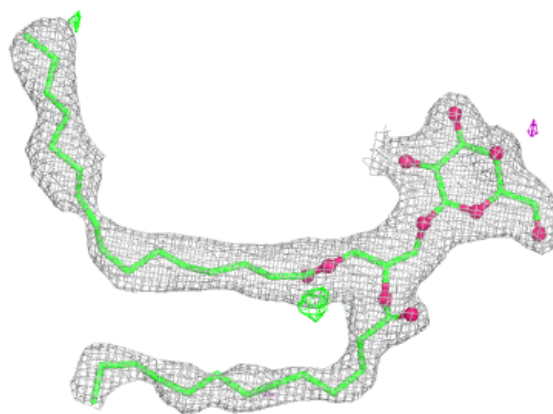


Electron density around BCR x 101:

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

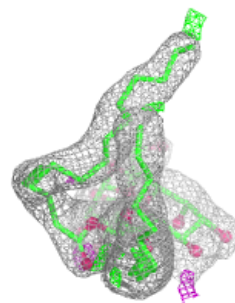
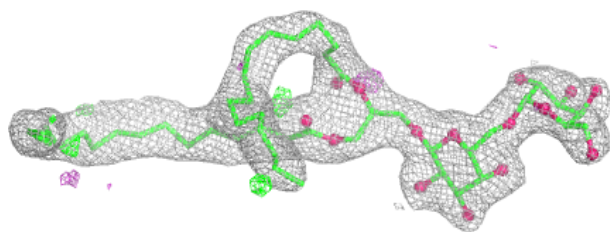
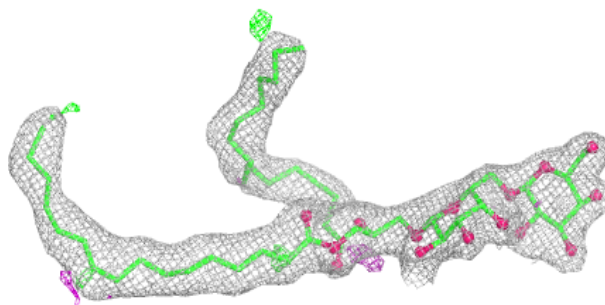
**Electron density around LMG C 520:**

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

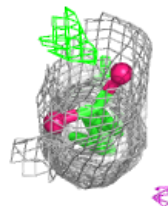
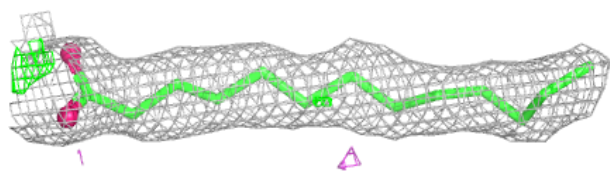
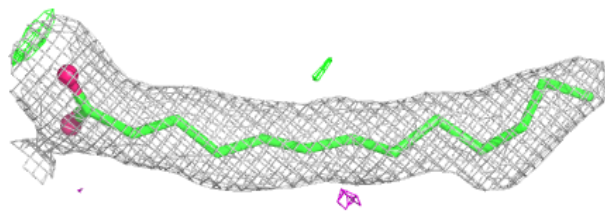


Electron density around DGD h 101:

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

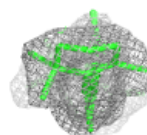
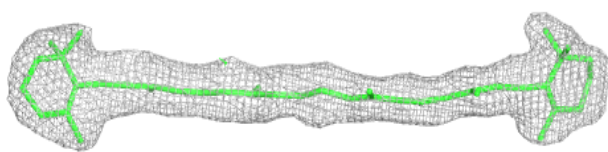
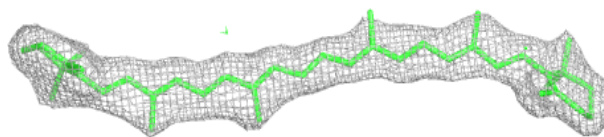
**Electron density around STE M 101:**

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

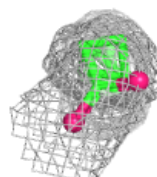
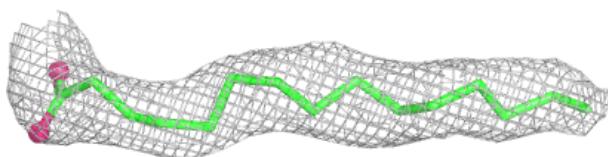
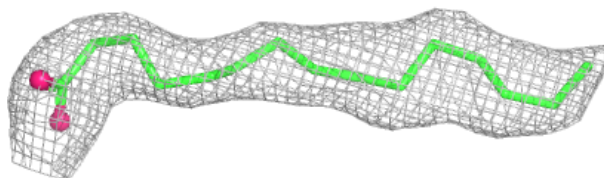


Electron density around BCR C 514:

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

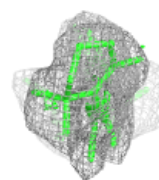
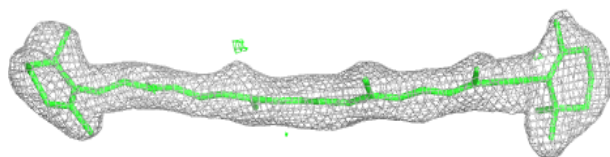
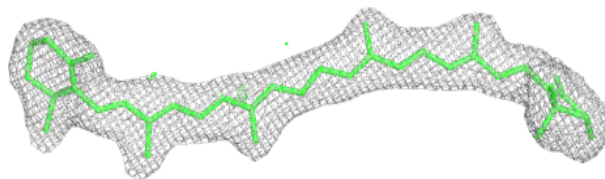
**Electron density around STE d 411:**

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



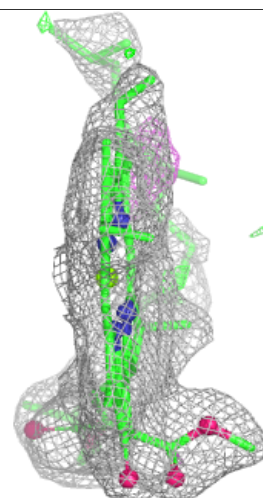
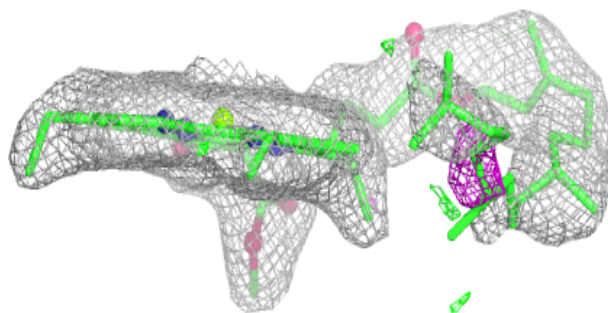
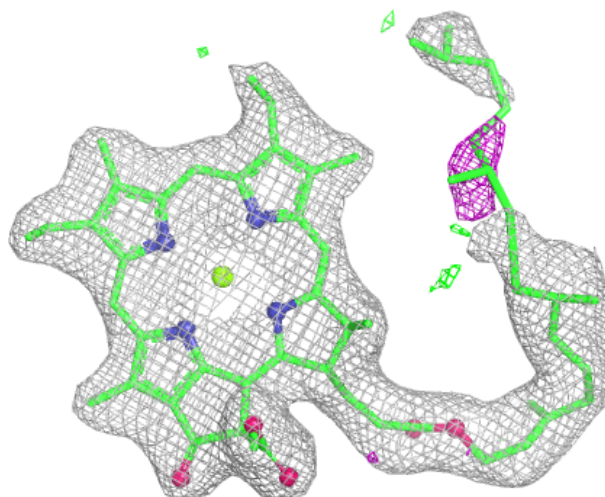
Electron density around BCR C 516:

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



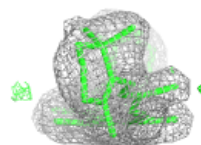
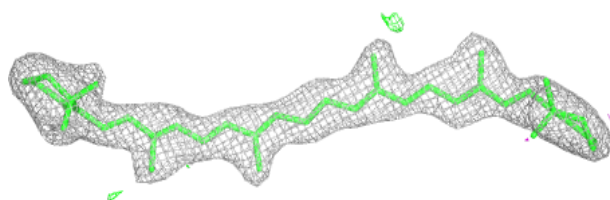
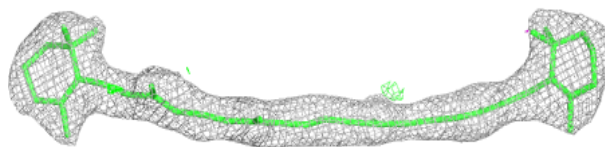
Electron density around CLA c 512:

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

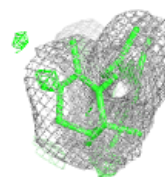
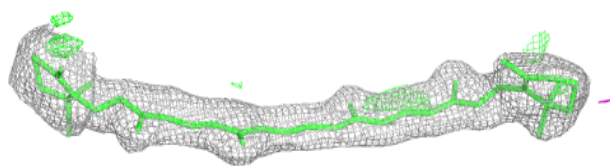
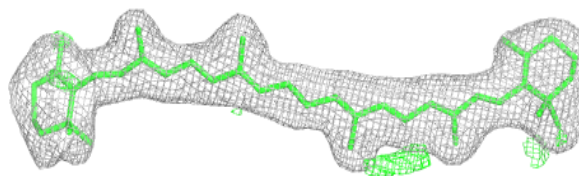


Electron density around BCR k 103:

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

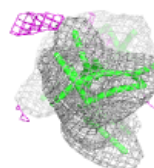
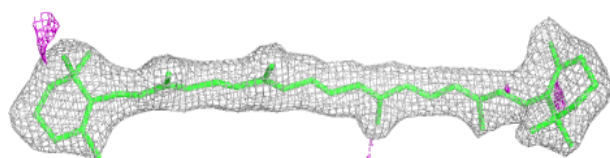
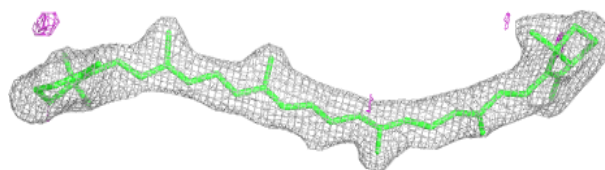
**Electron density around BCR D 405:**

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

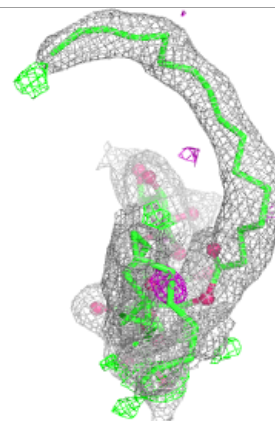
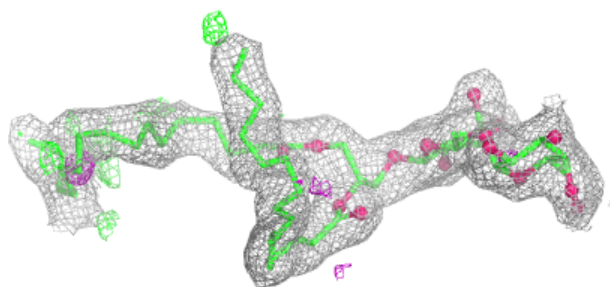
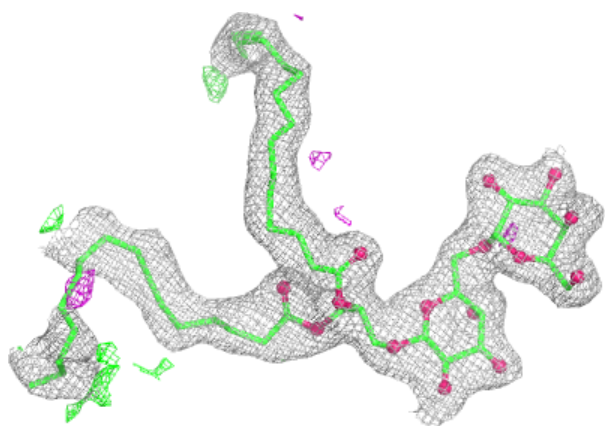


Electron density around BCR H 101:

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

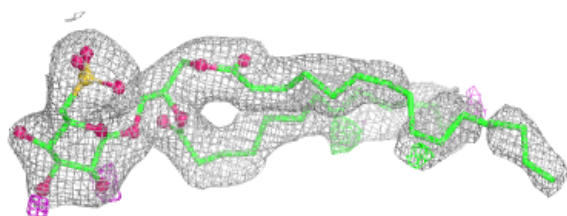
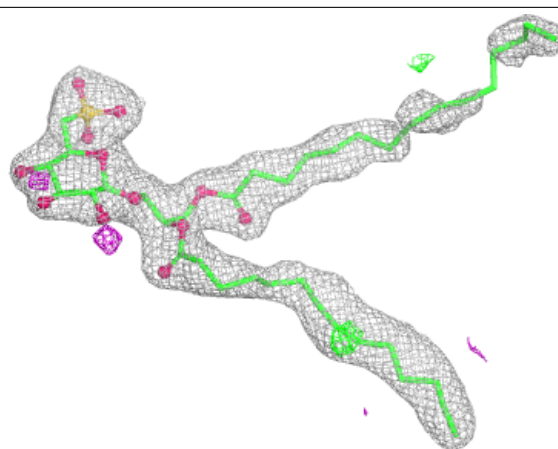
**Electron density around DGD C 518:**

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

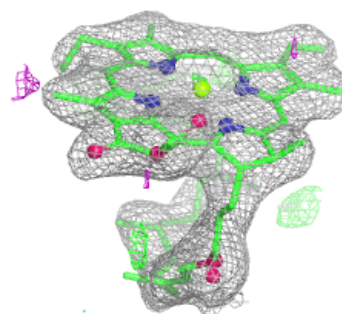
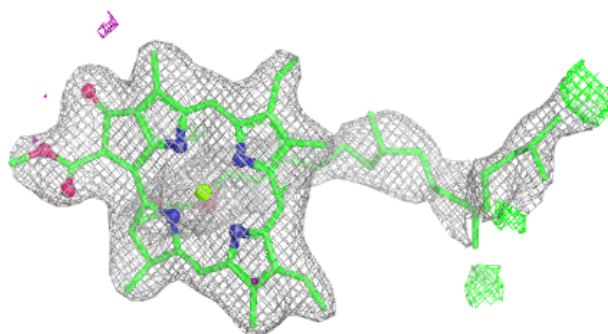
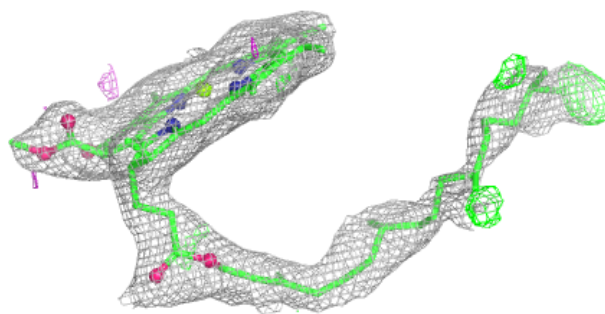


Electron density around SQD A 614:

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

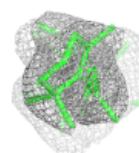
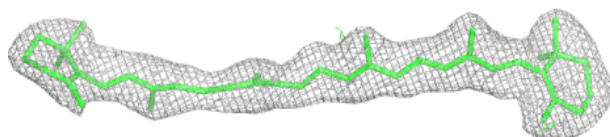
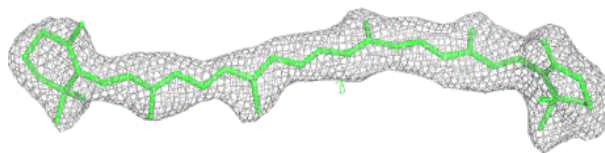
**Electron density around CLA C 513:**

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

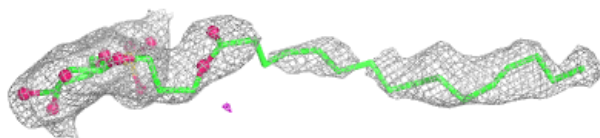
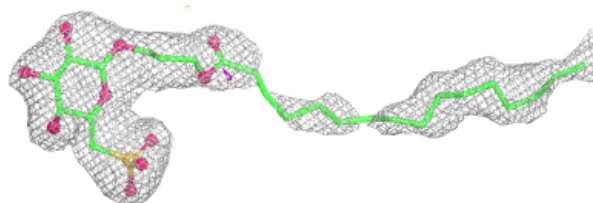


Electron density around BCR k 101:

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

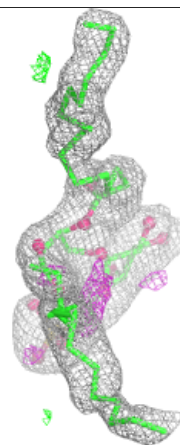
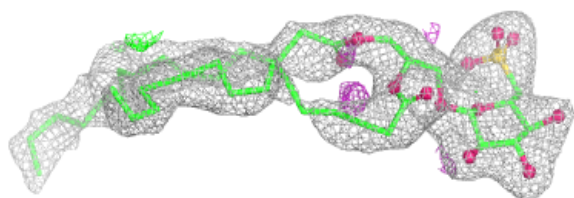
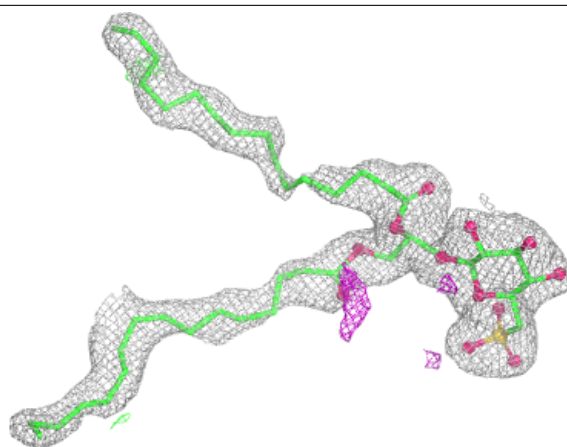
**Electron density around SQD D 408:**

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

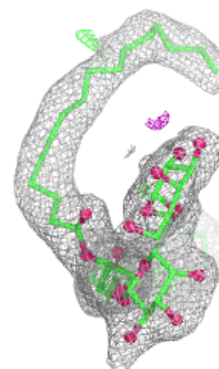
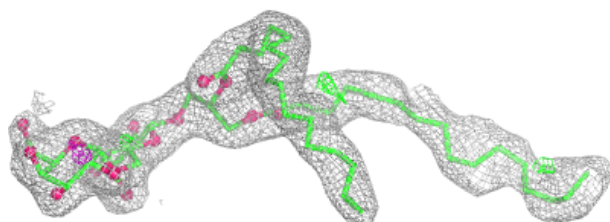
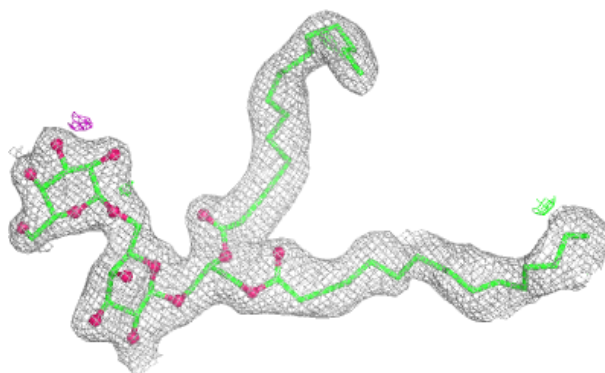


Electron density around SQD a 614:

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

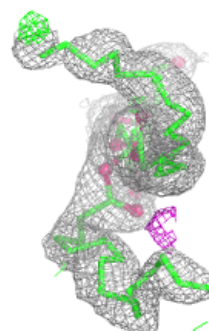
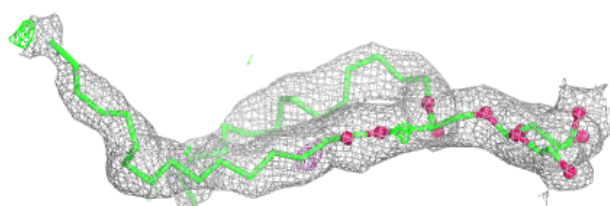
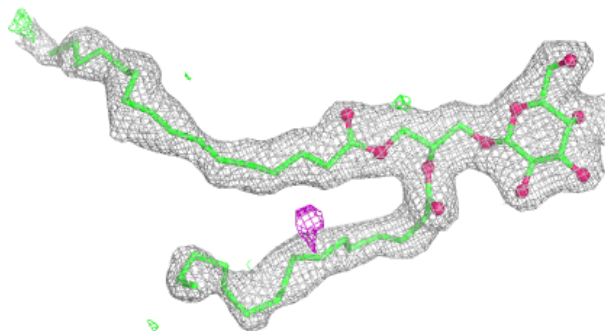
**Electron density around DGD c 516:**

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

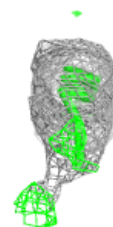
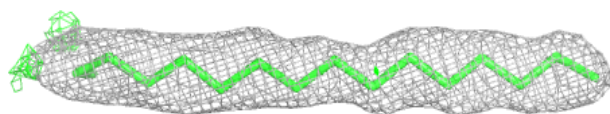
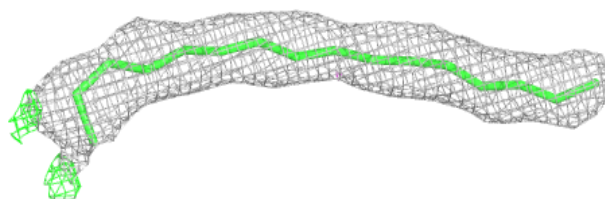


Electron density around LMG D 407:

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

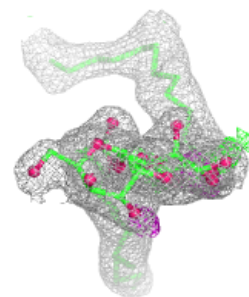
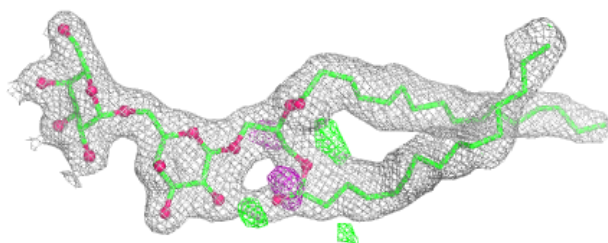
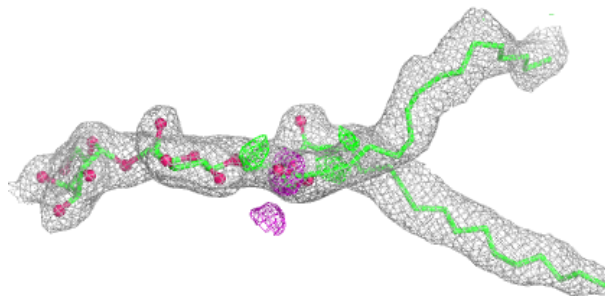
**Electron density around STE C 523:**

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

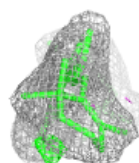
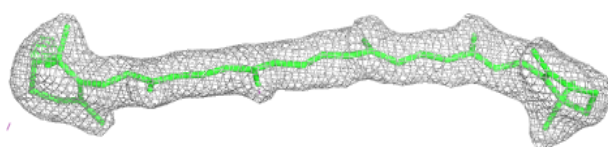
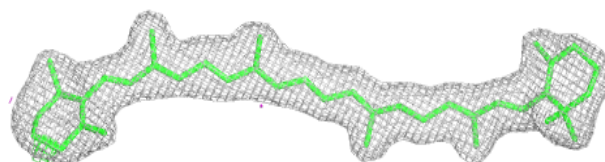


Electron density around DGD c 515:

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

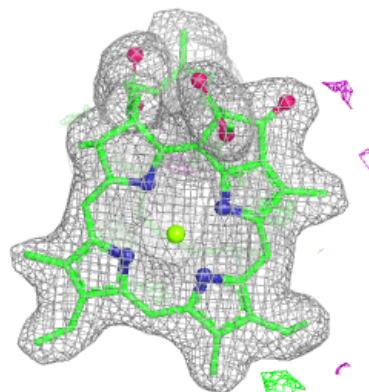
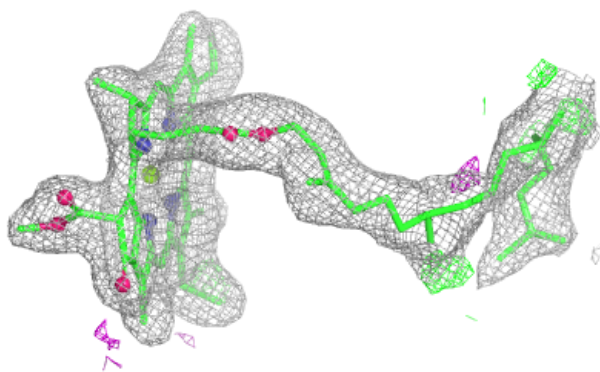
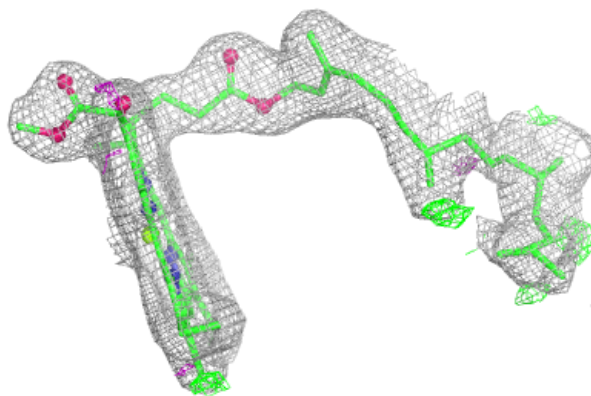
**Electron density around BCR B 619:**

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

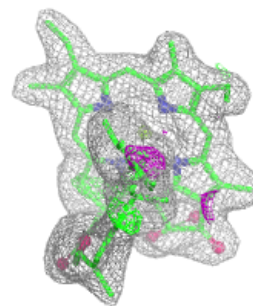
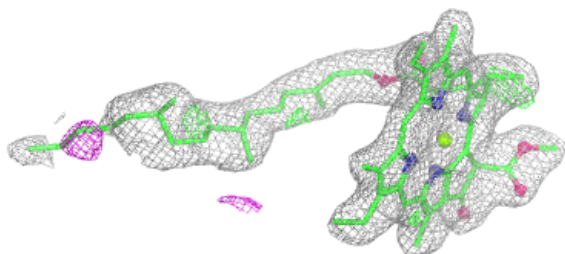
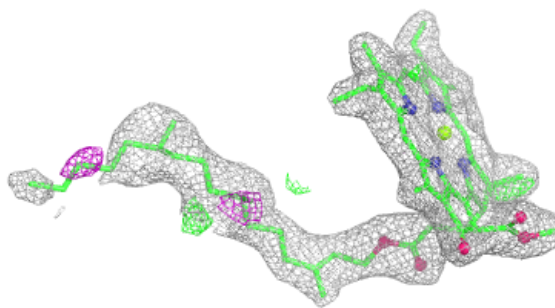


Electron density around CLA C 506:

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

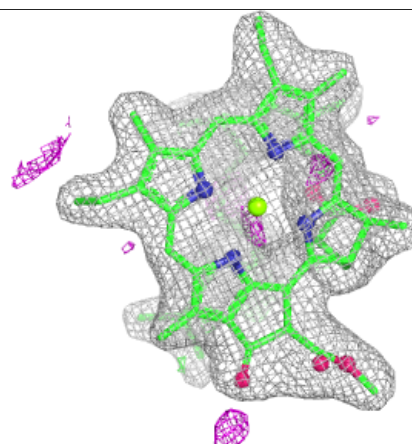
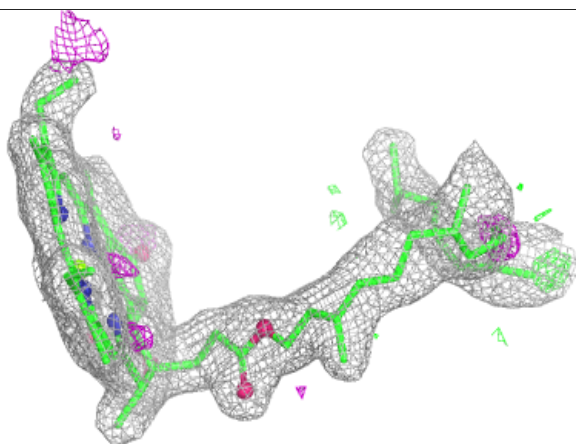
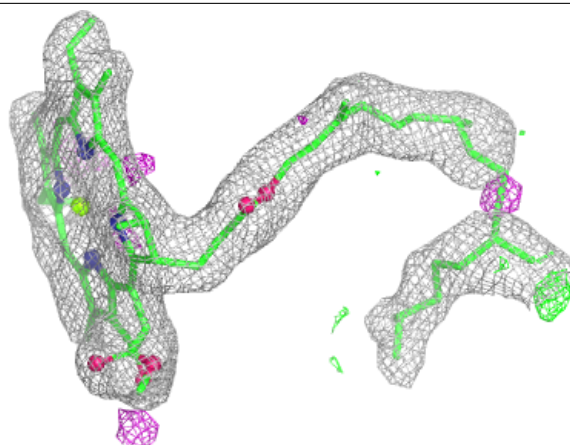
**Electron density around CLA c 508:**

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

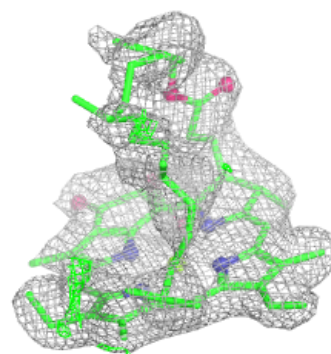
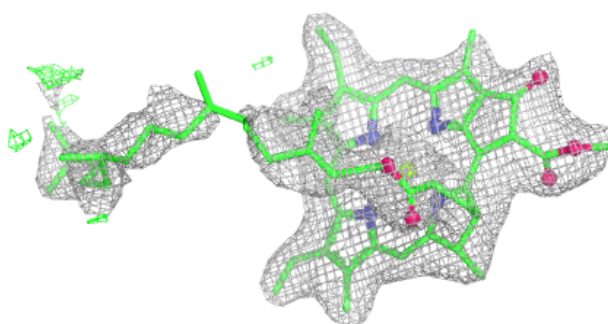
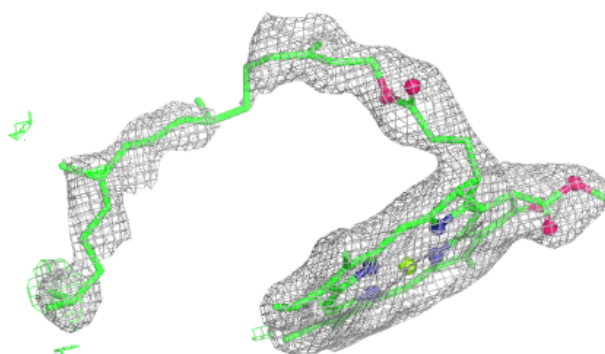


Electron density around CLA B 606:

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

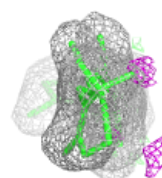
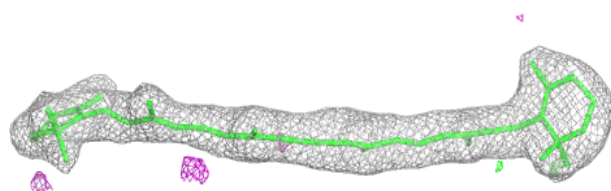
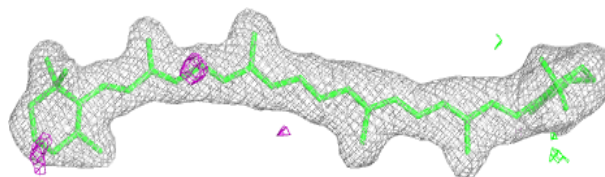
**Electron density around CLA c 513:**

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

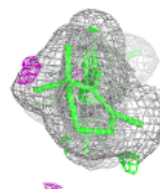
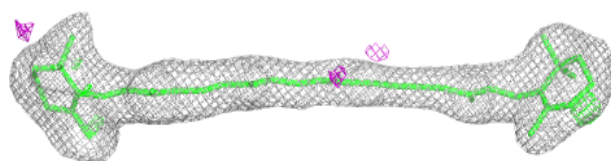
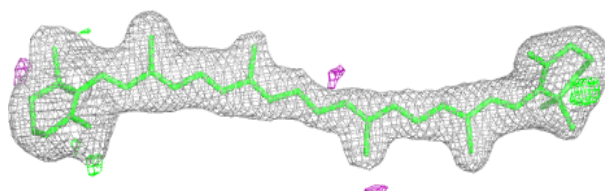


Electron density around BCR b 617:

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

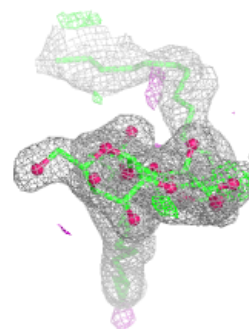
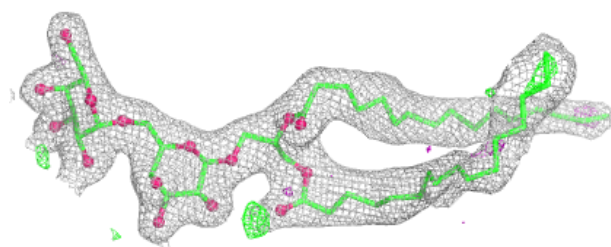
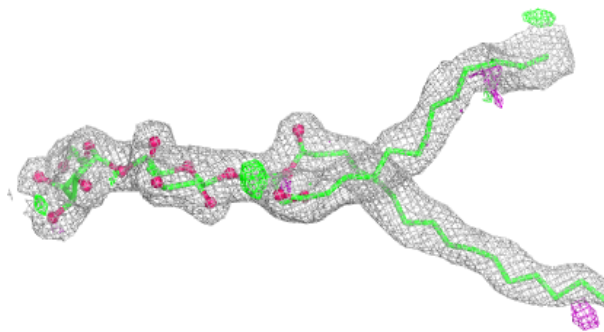
**Electron density around BCR b 618:**

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

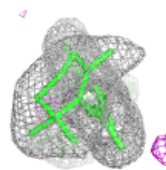
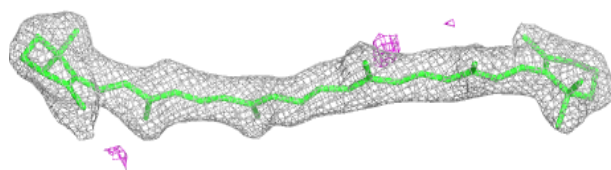
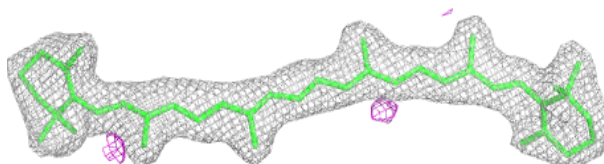


Electron density around DGD C 517:

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

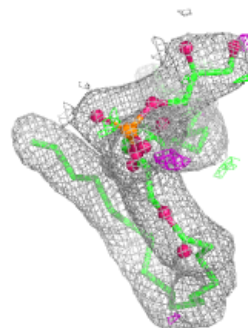
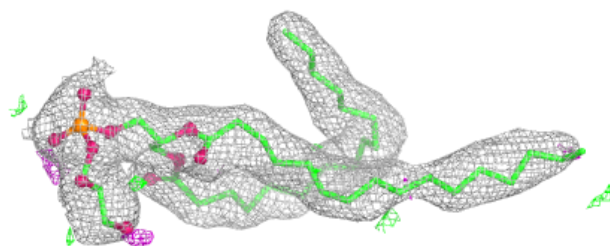
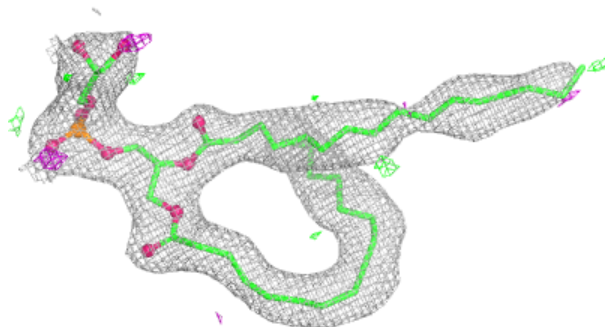
**Electron density around BCR b 619:**

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

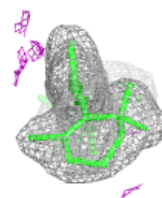
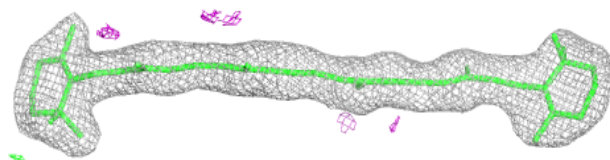
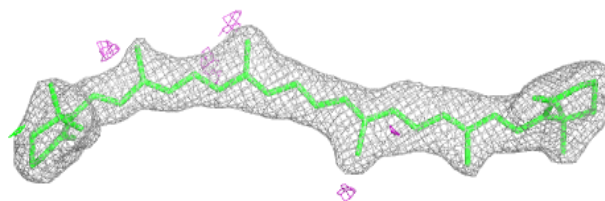


Electron density around LHG D 412:

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

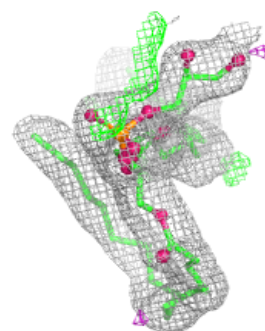
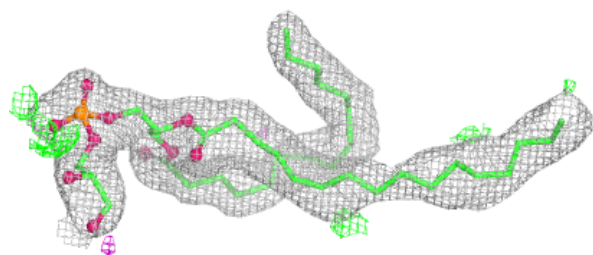
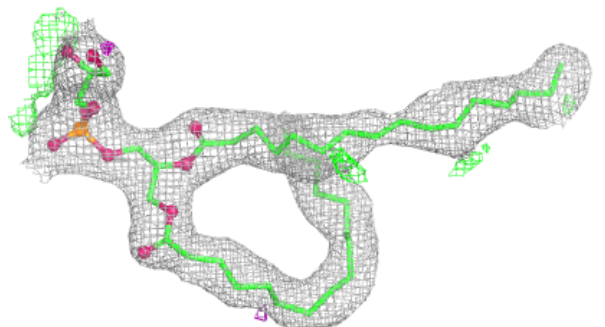
**Electron density around BCR c 514:**

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

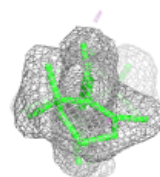
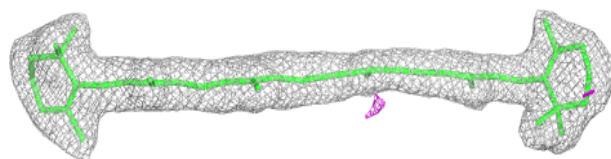
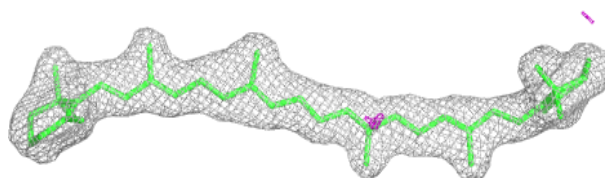


Electron density around LHG a 613:

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

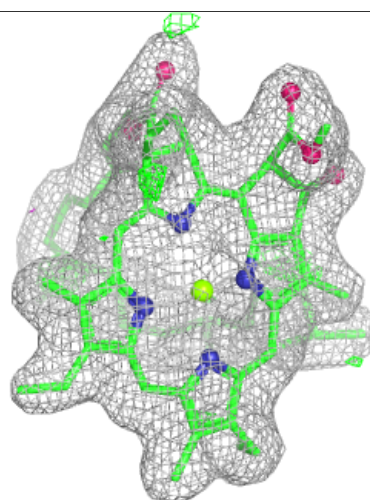
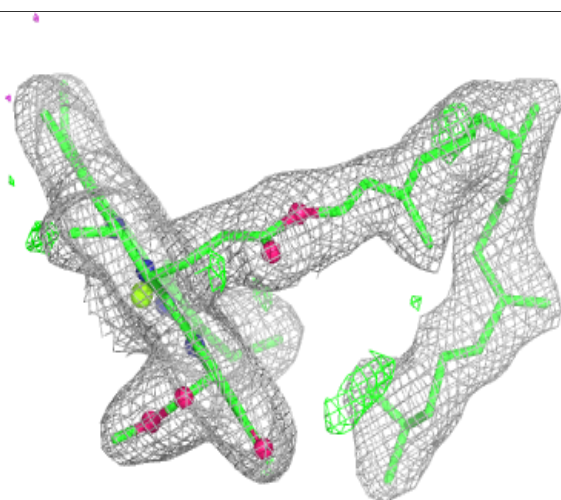
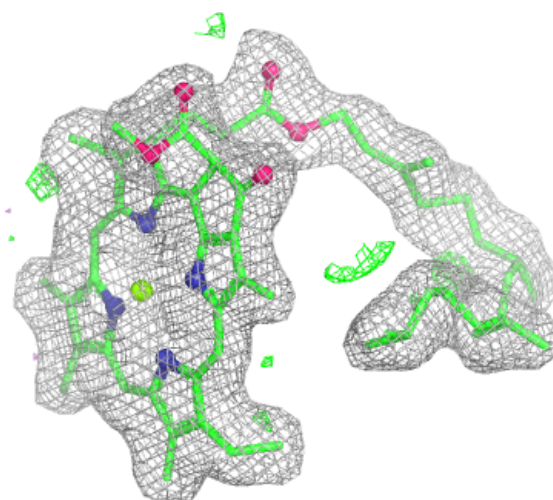
**Electron density around BCR A 610:**

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



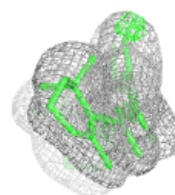
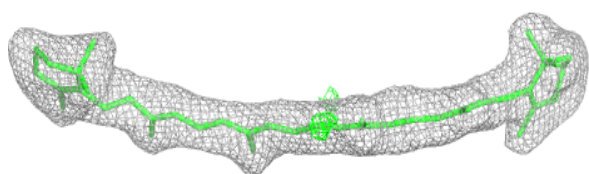
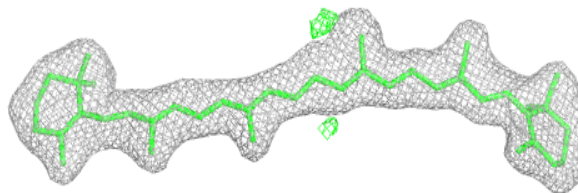
Electron density around CLA C 503:

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

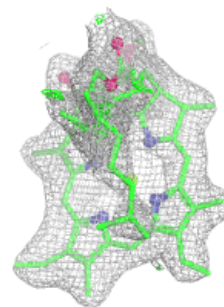
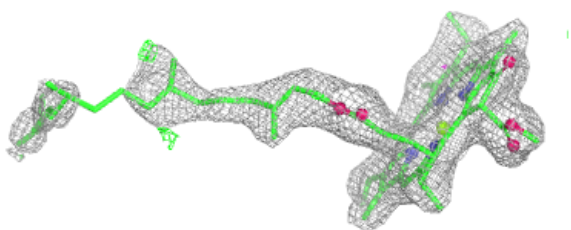
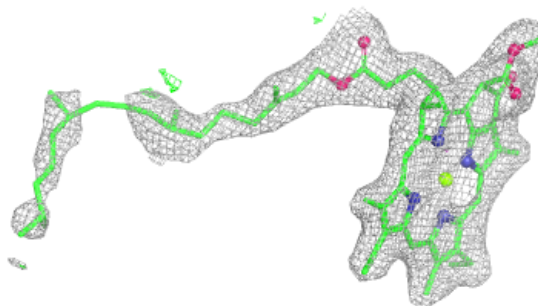


Electron density around BCR t 101:

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

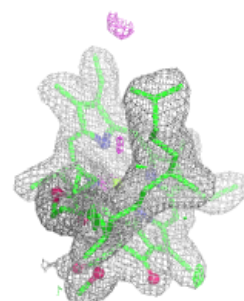
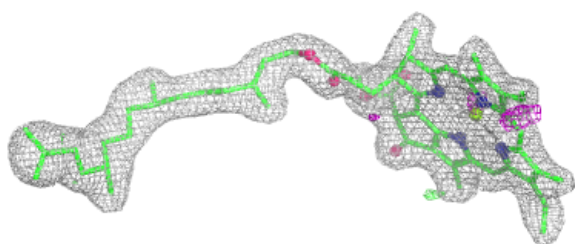
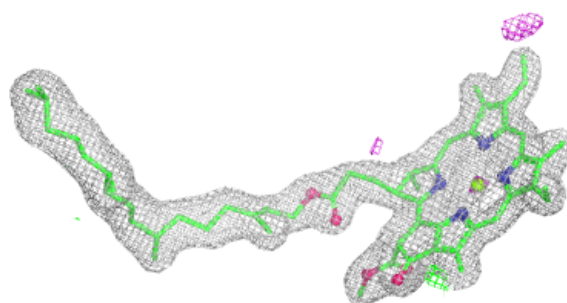
**Electron density around CLA d 404:**

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

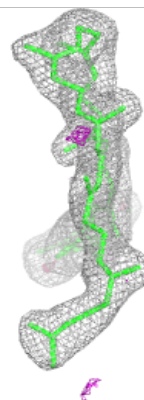
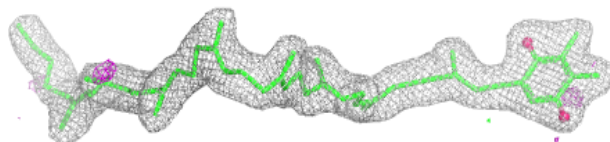
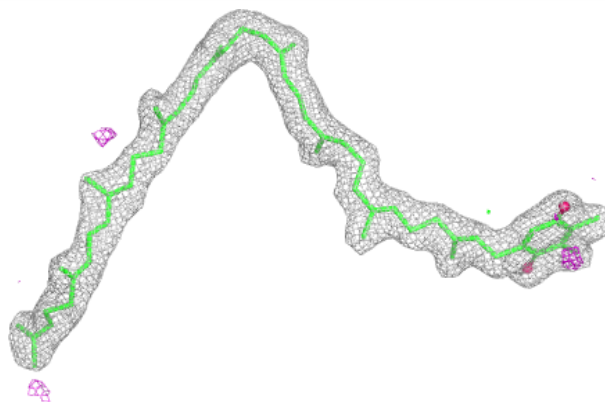


Electron density around CLA a 606:

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

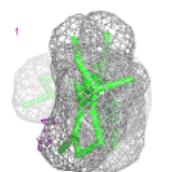
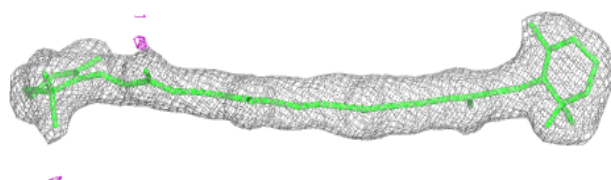
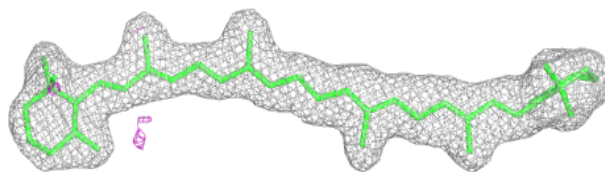
**Electron density around PL9 D 406:**

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

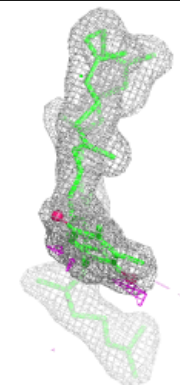
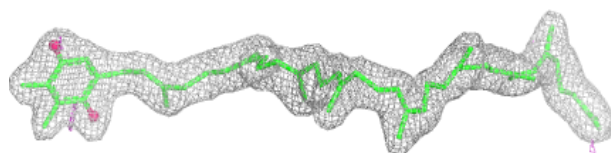
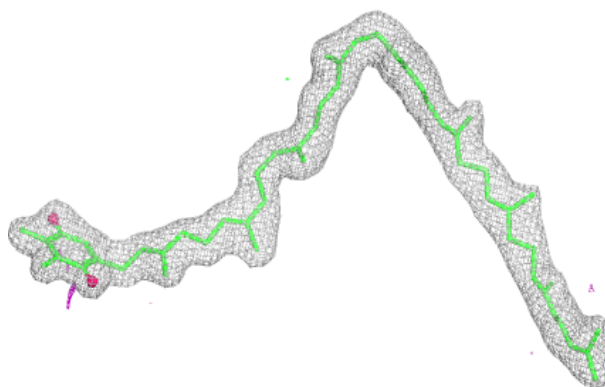


Electron density around BCR B 617:

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

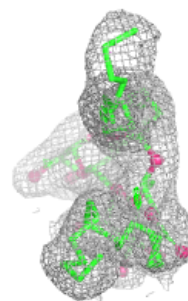
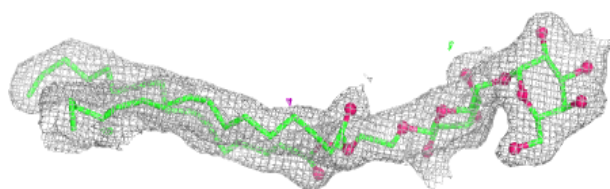
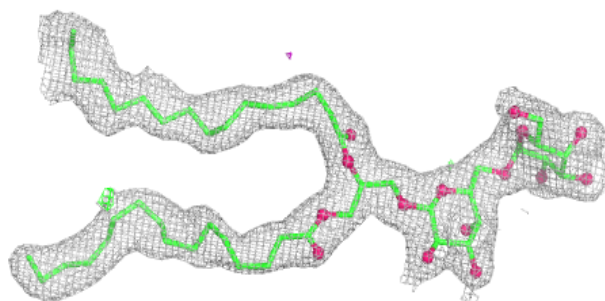
**Electron density around PL9 d 406:**

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

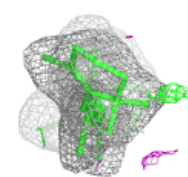
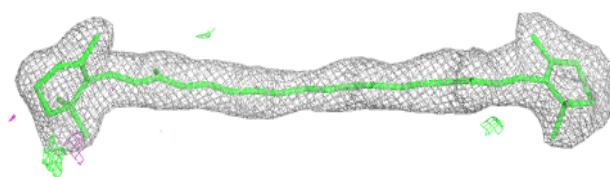
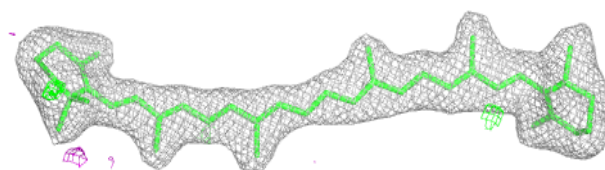


Electron density around DGD C 519:

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

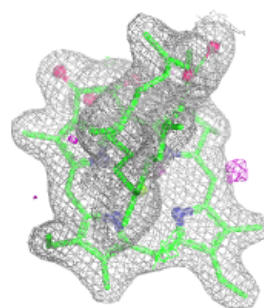
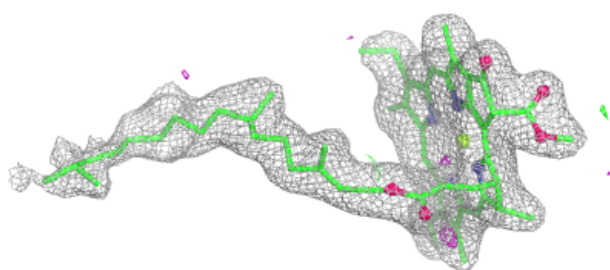
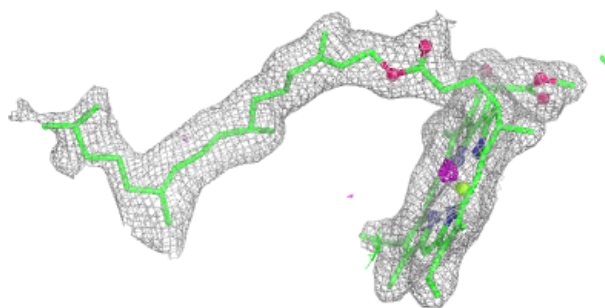
**Electron density around BCR B 618:**

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

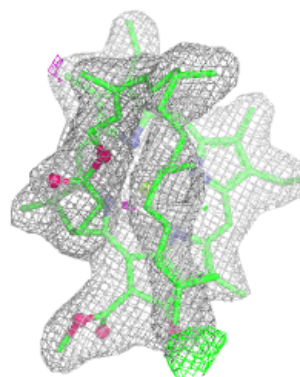
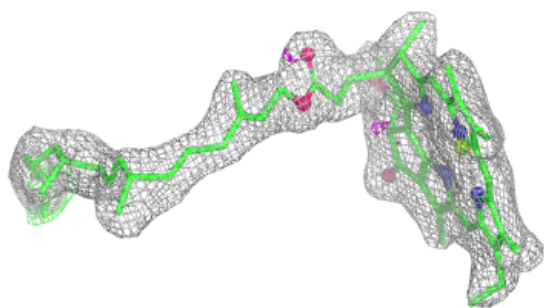
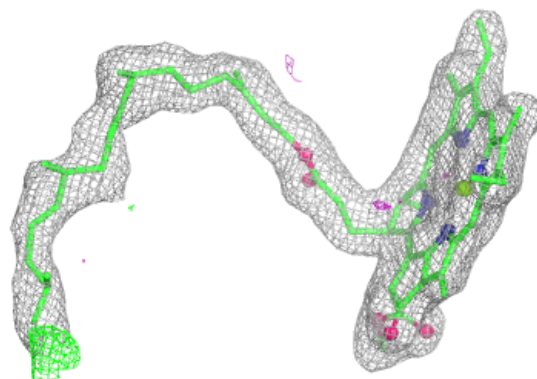


Electron density around CLA C 508:

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

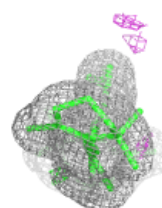
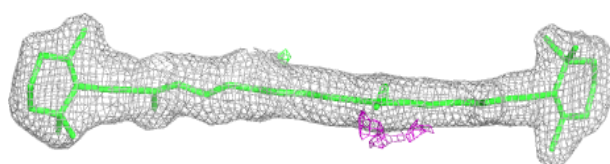
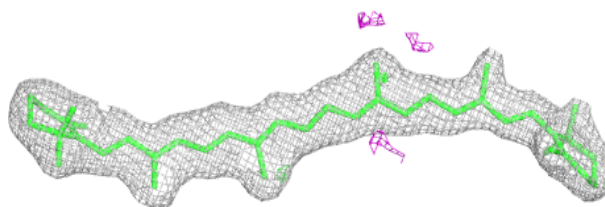
**Electron density around CLA b 606:**

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

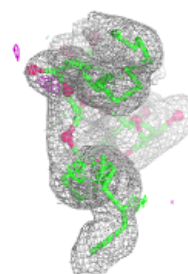
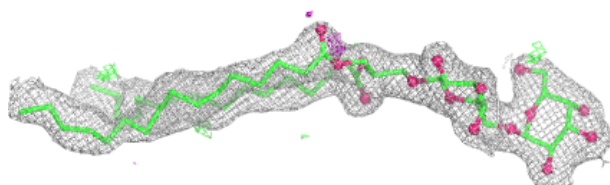
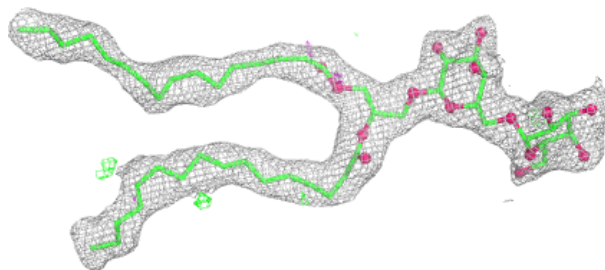


Electron density around BCR C 515:

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

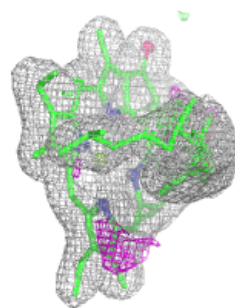
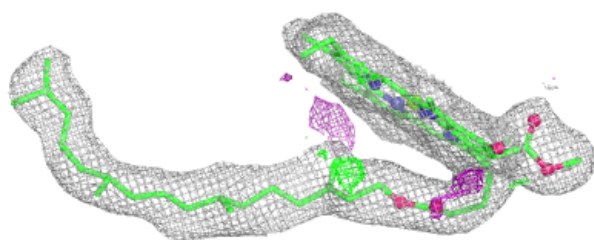
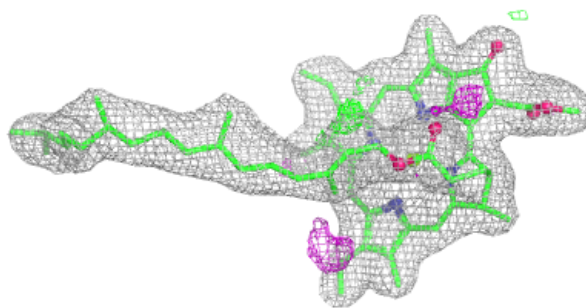
**Electron density around DGD c 517:**

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



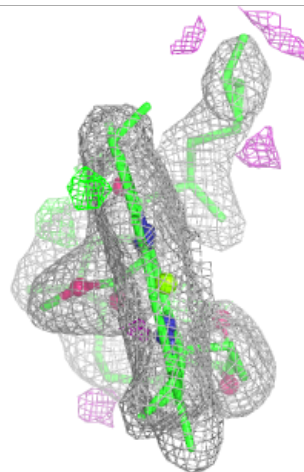
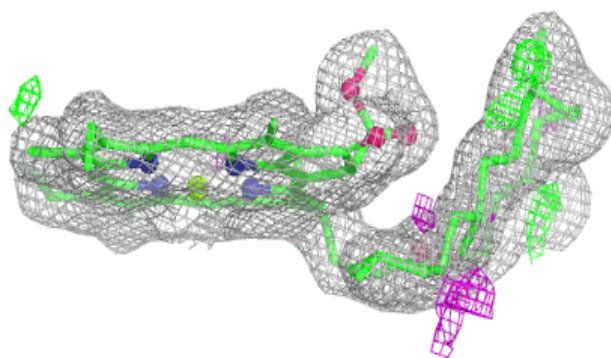
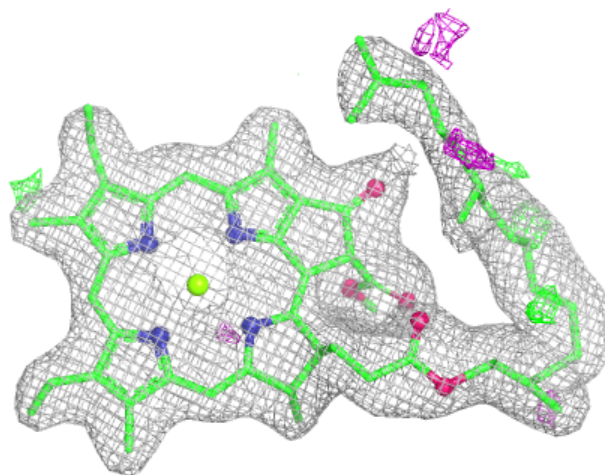
Electron density around CLA b 608:

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



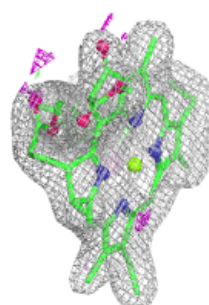
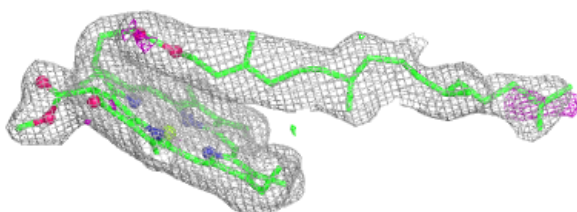
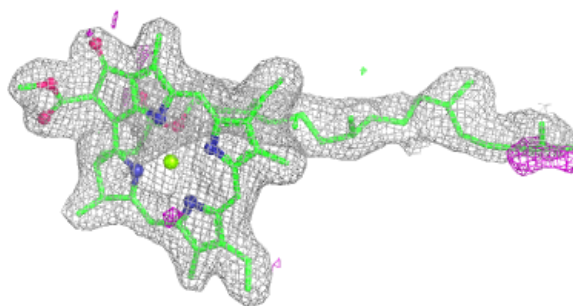
Electron density around CLA b 610:

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

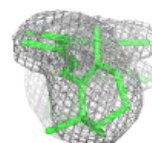
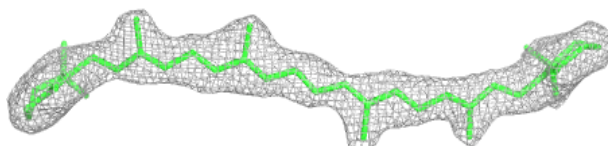
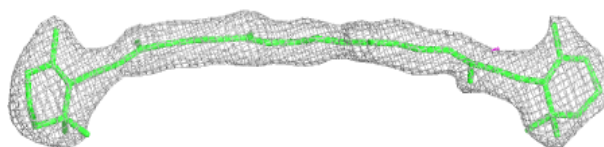


Electron density around CLA b 614:

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

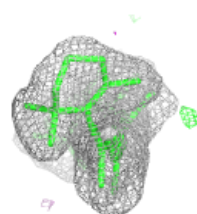
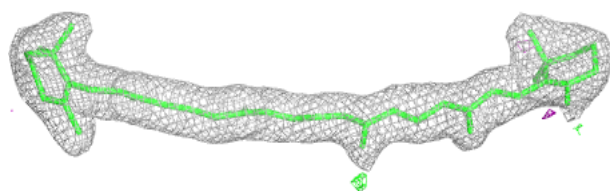
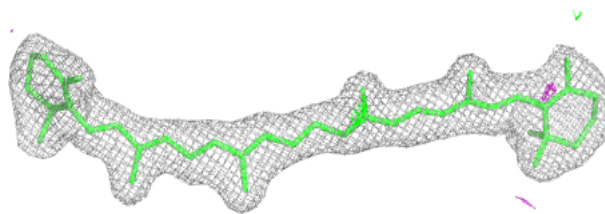
**Electron density around BCR K 101:**

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



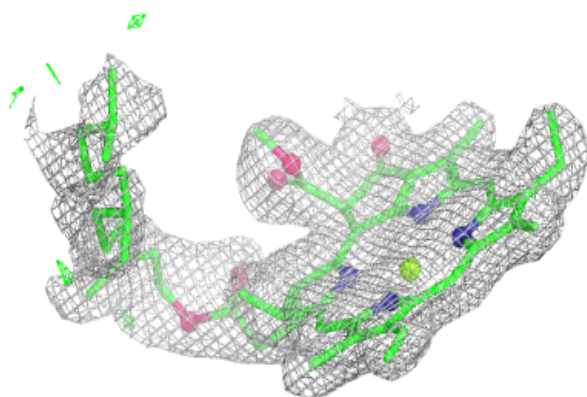
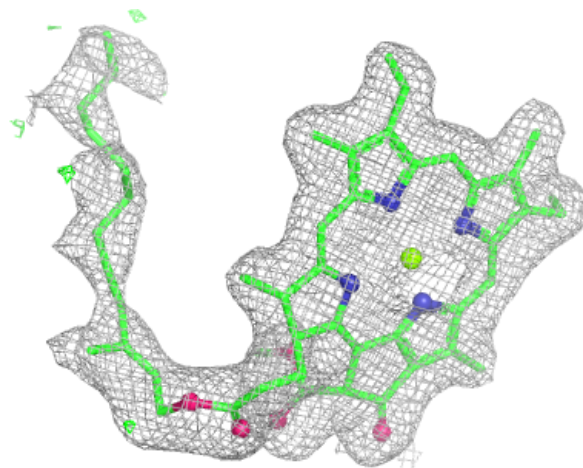
Electron density around BCR T 101:

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



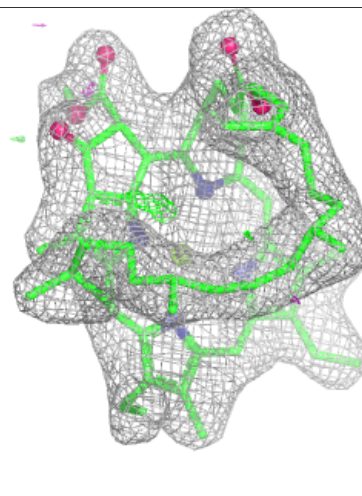
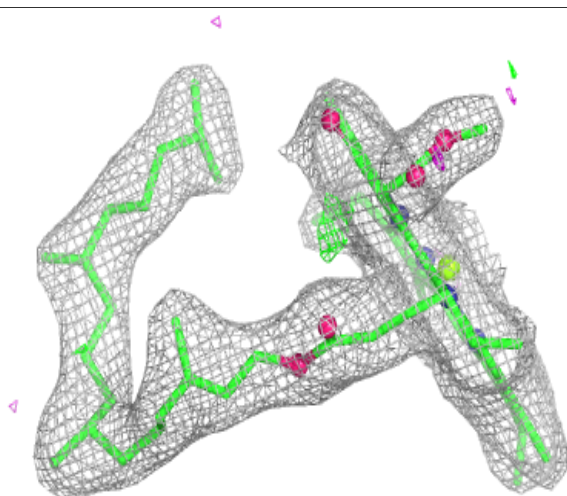
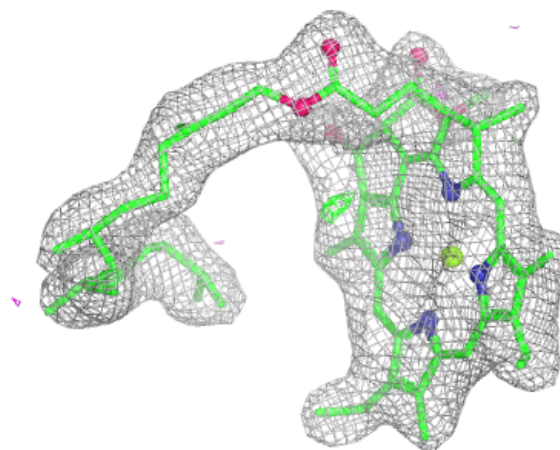
Electron density around CLA b 616:

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



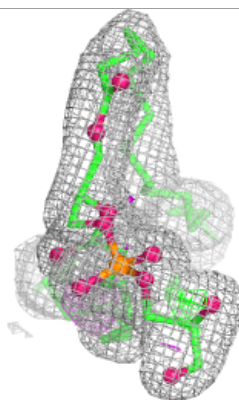
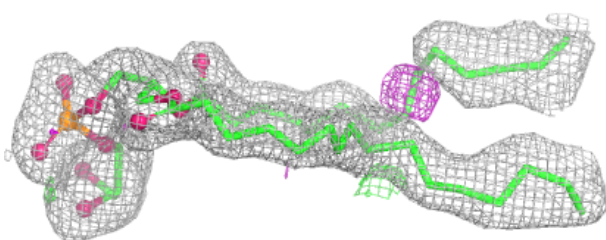
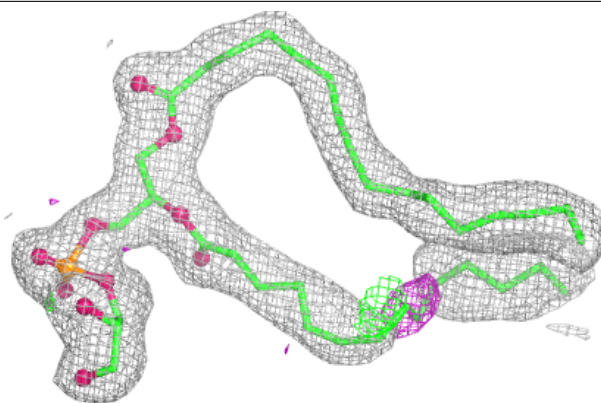
Electron density around CLA c 503:

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

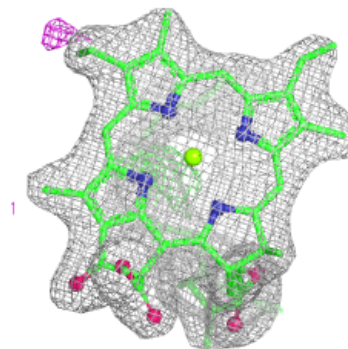
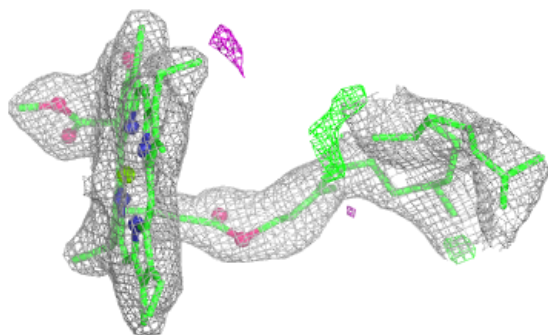
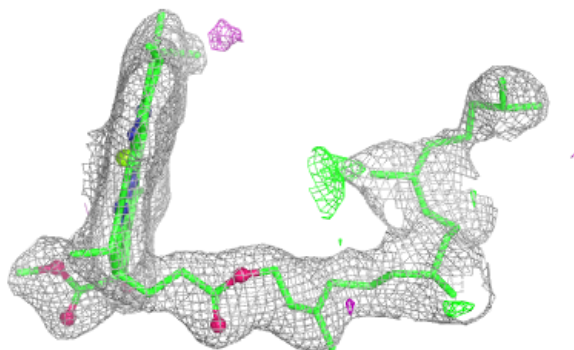


Electron density around LHG D 410:

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

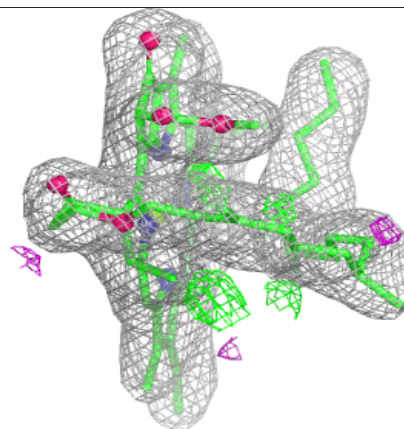
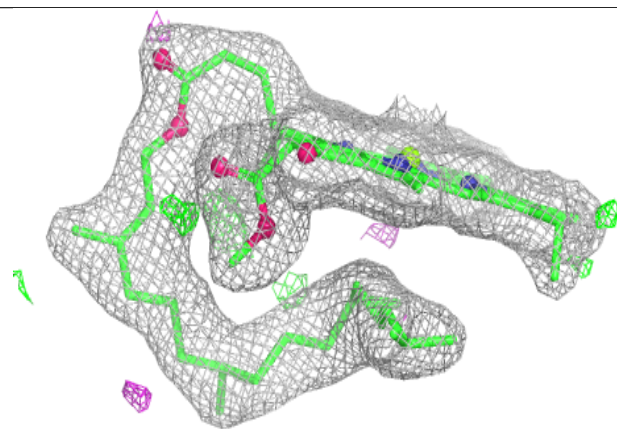
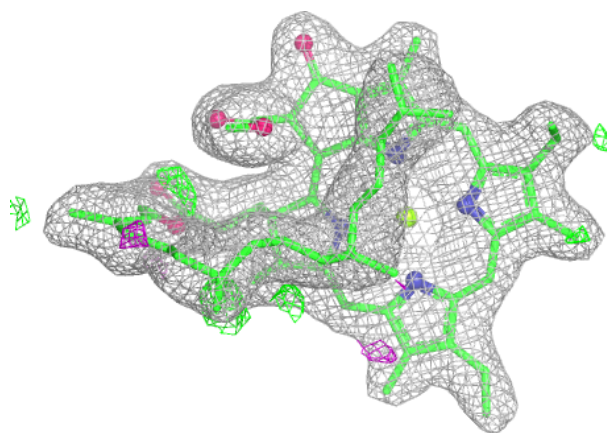
**Electron density around CLA c 506:**

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



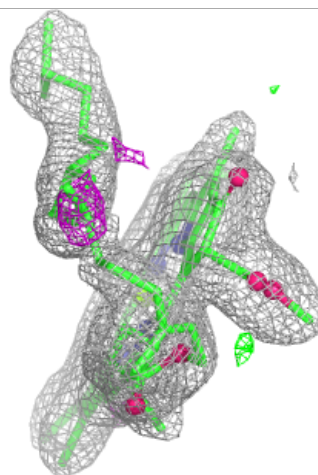
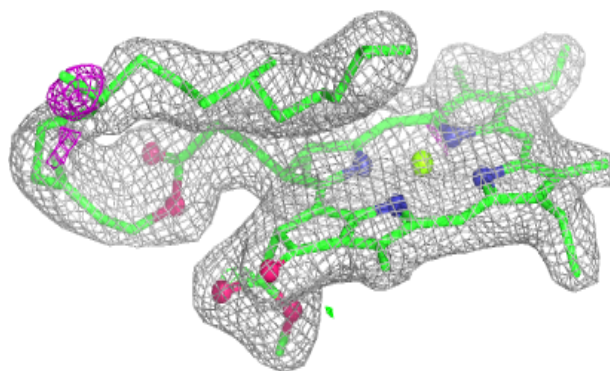
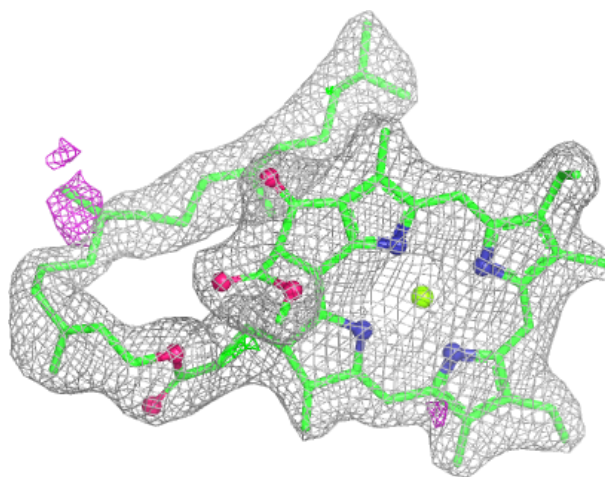
Electron density around CLA C 510:

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



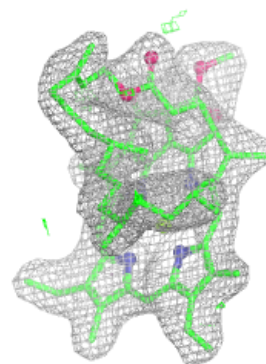
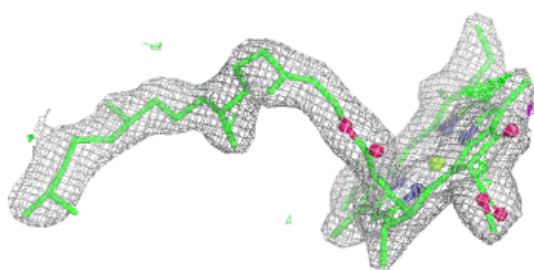
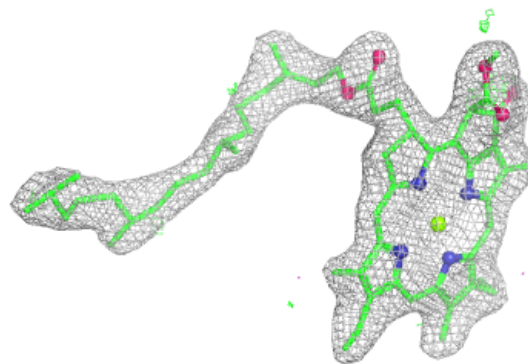
Electron density around CLA c 509:

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



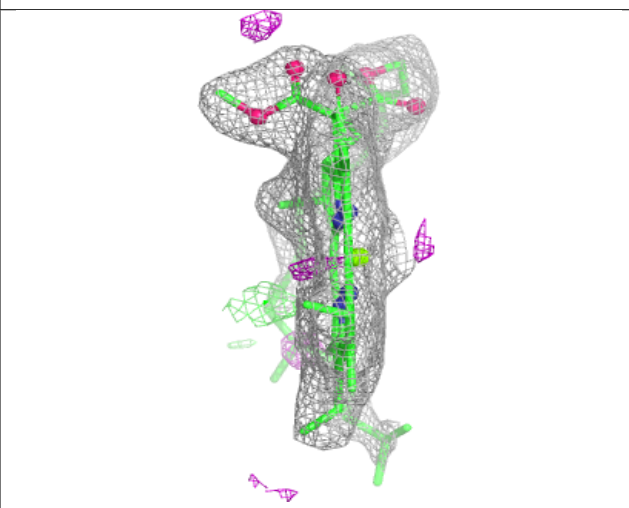
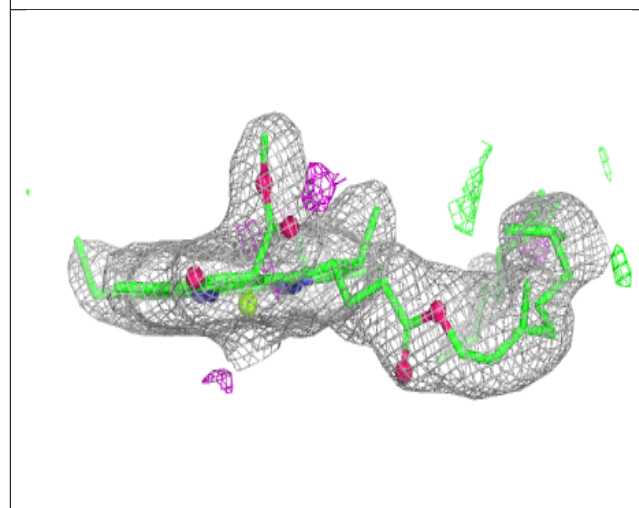
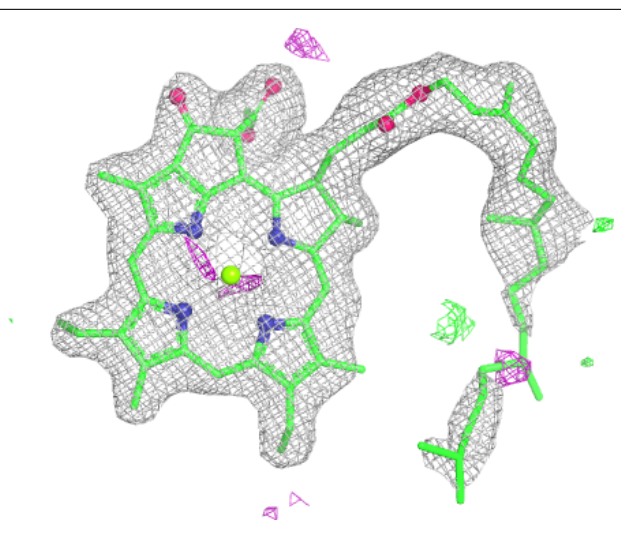
Electron density around CLA c 511:

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



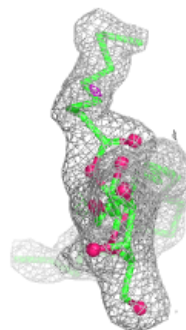
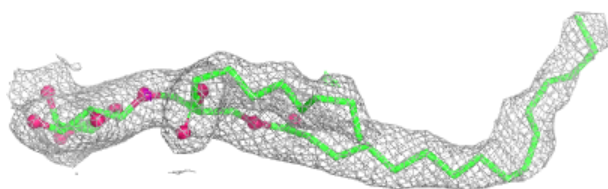
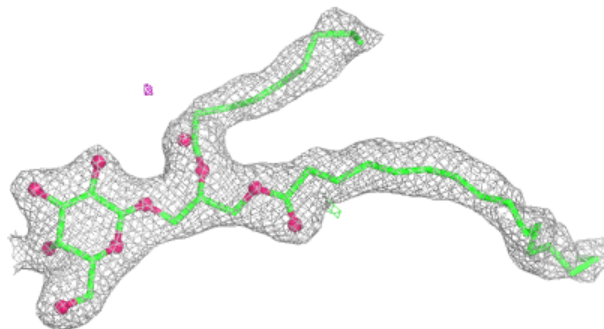
Electron density around CLA C 512:

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

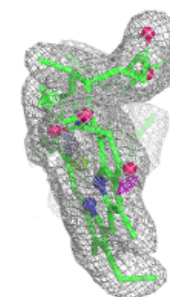
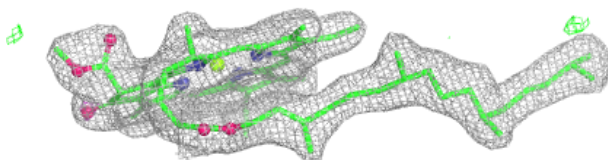
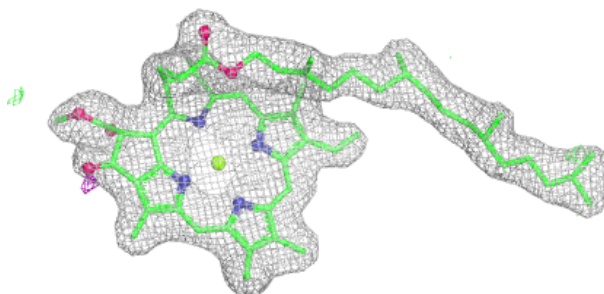


Electron density around LMG d 410:

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

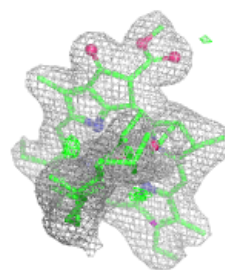
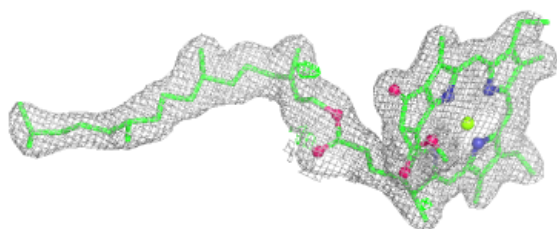
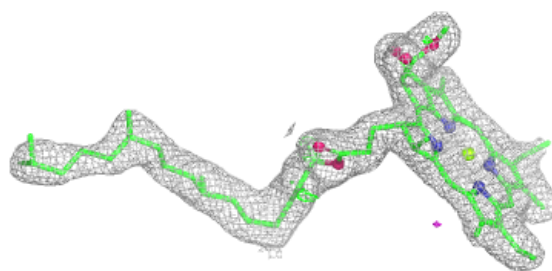
**Electron density around CLA c 501:**

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

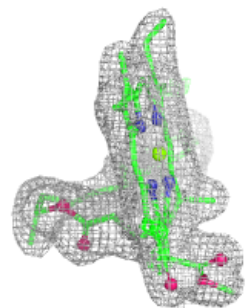
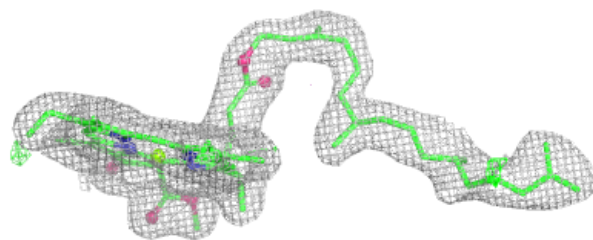
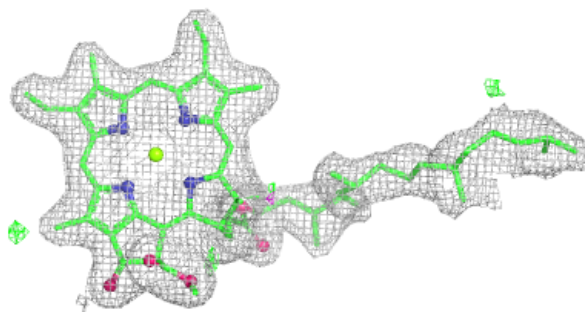


Electron density around CLA c 502:

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

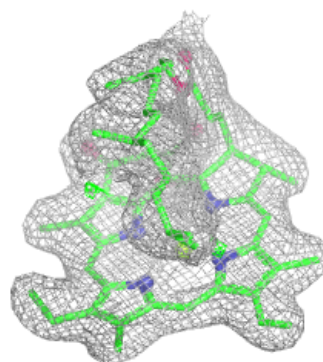
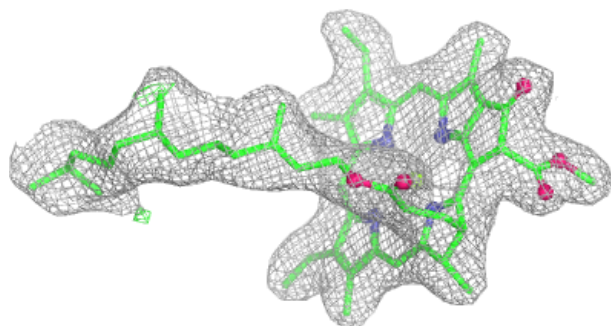
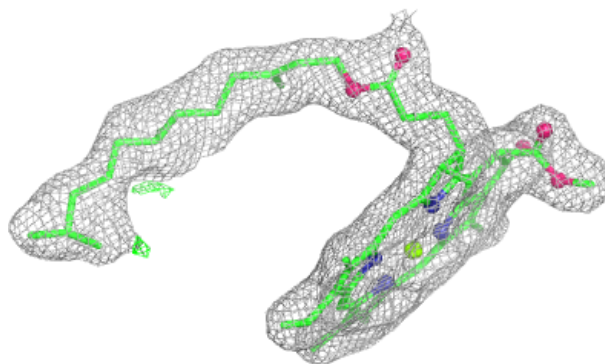
**Electron density around CLA a 607:**

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

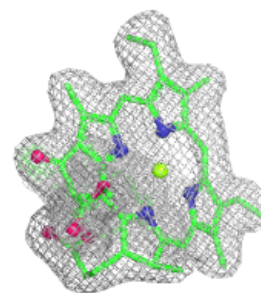
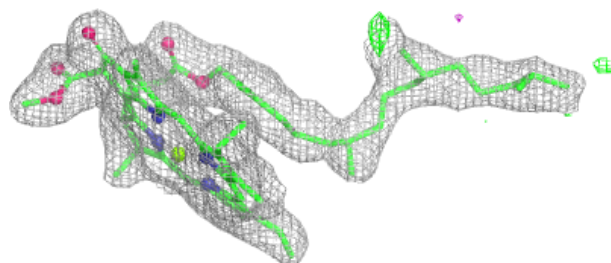
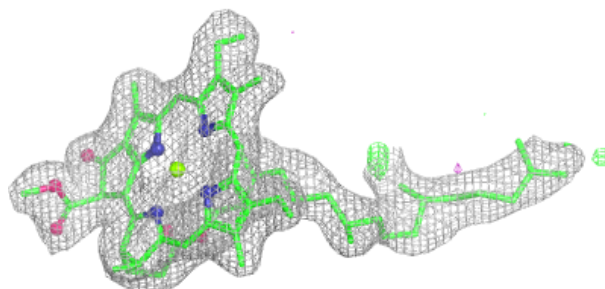


Electron density around CLA c 504:

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

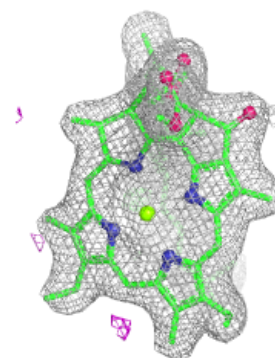
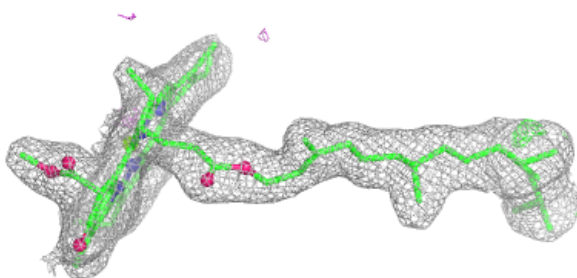
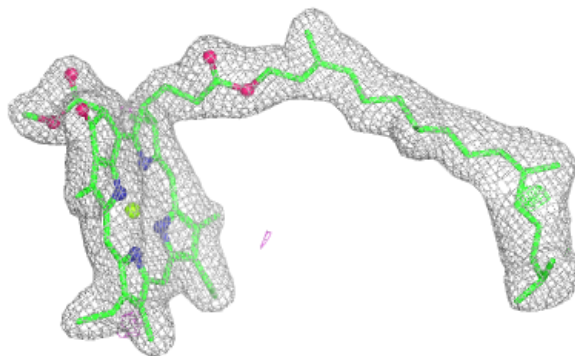
**Electron density around CLA c 505:**

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



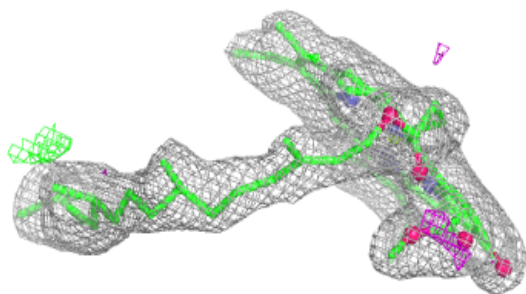
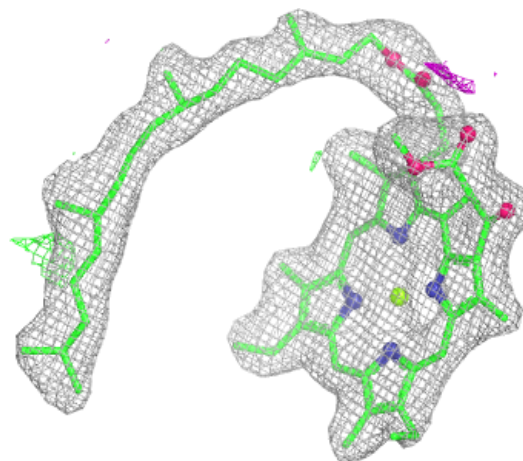
Electron density around CLA B 609:

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



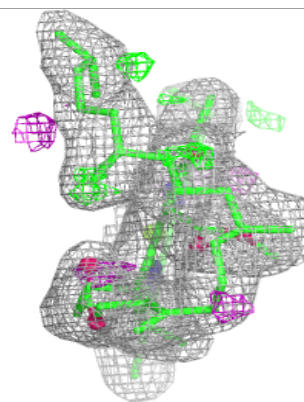
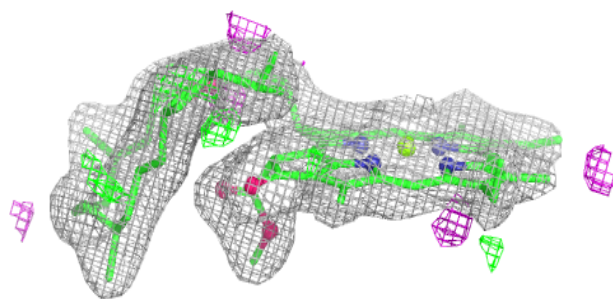
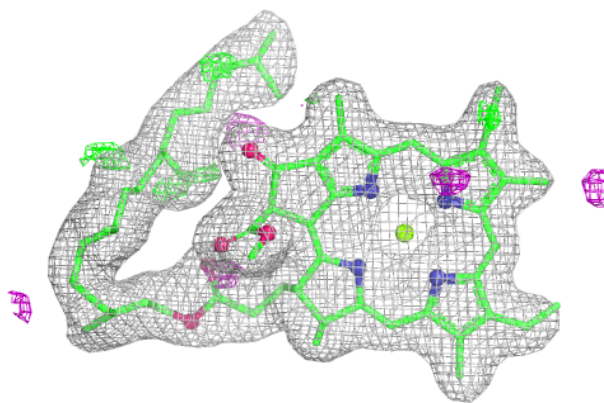
Electron density around CLA c 507:

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

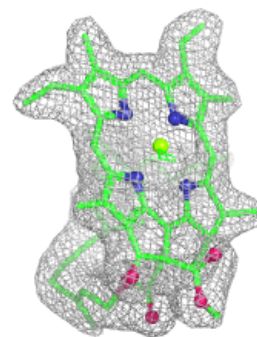
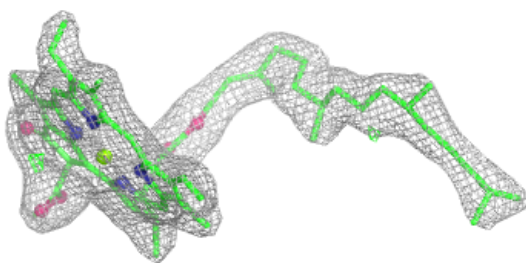
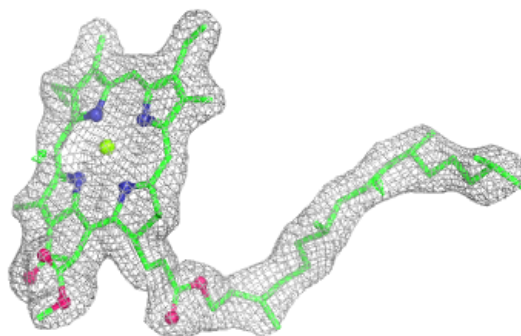


Electron density around CLA B 610:

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

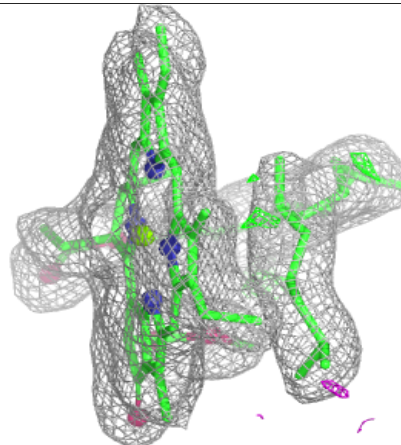
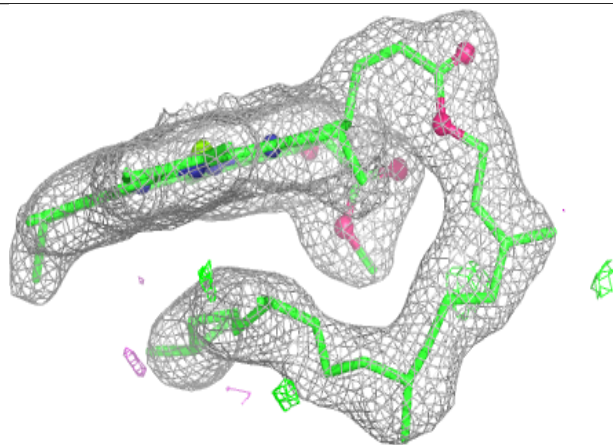
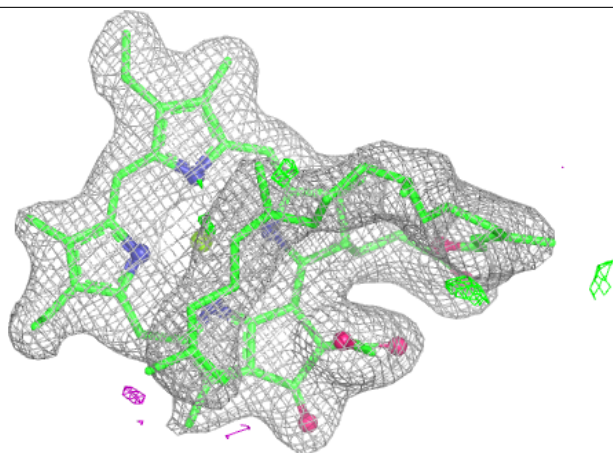
**Electron density around CLA C 511:**

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

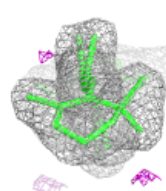
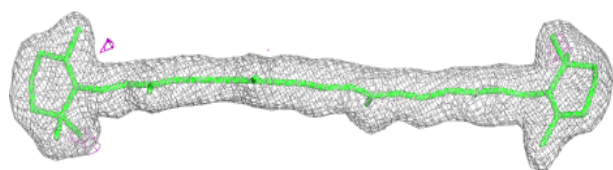
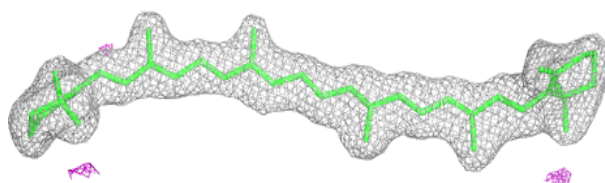


Electron density around CLA c 510:

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

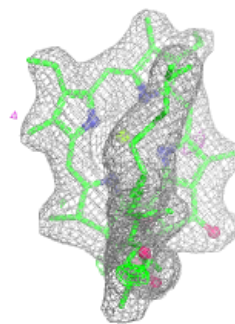
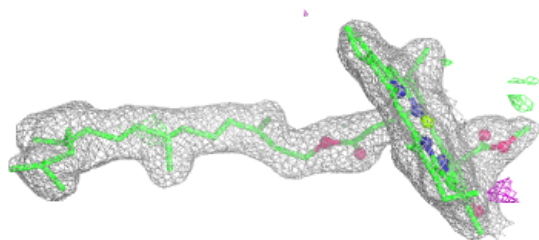
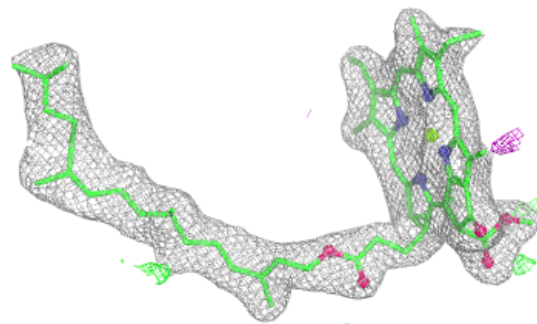
**Electron density around BCR a 610:**

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



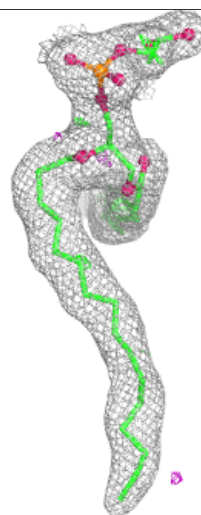
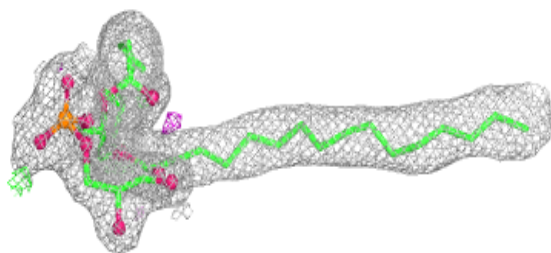
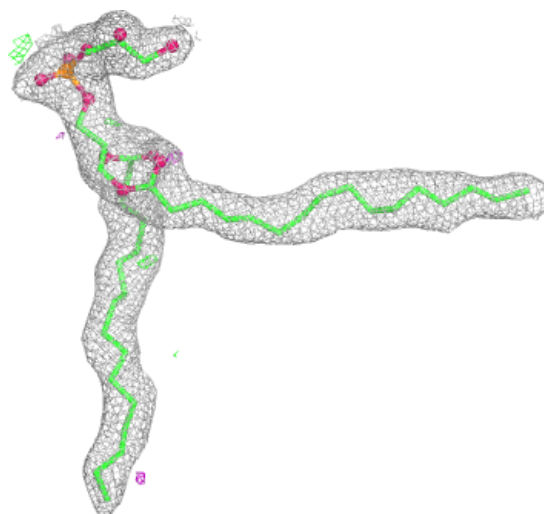
Electron density around CLA b 609:

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



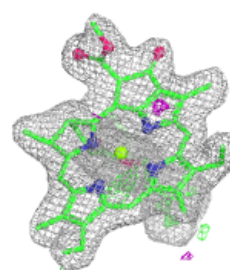
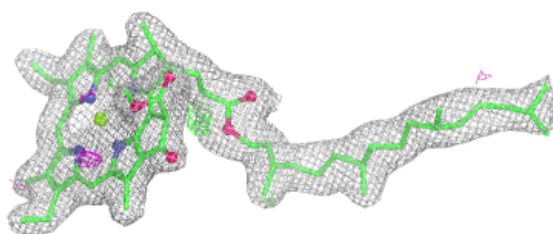
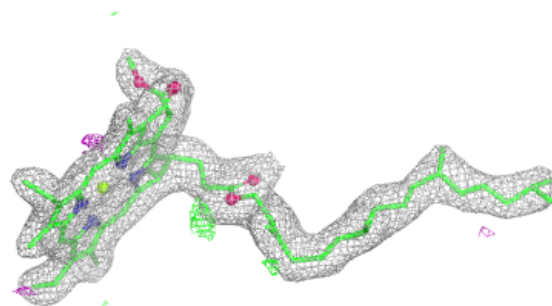
Electron density around LHG B 623:

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



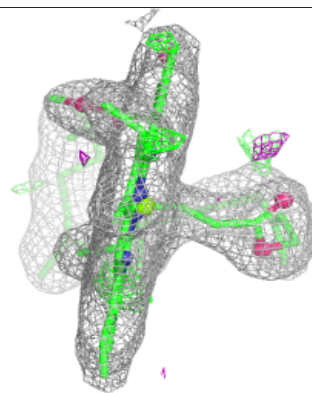
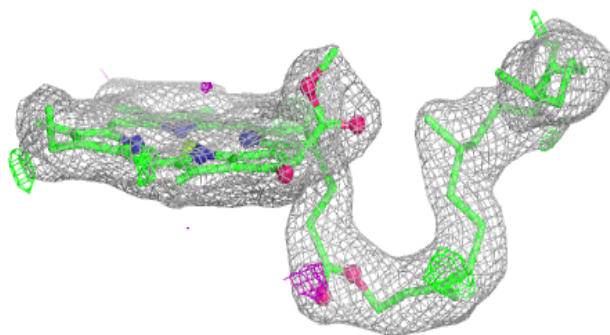
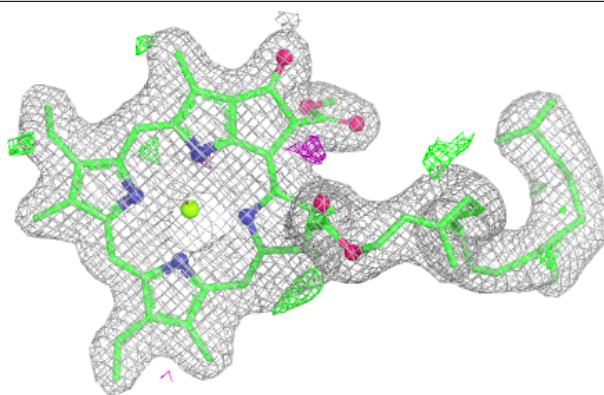
Electron density around CLA C 502:

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



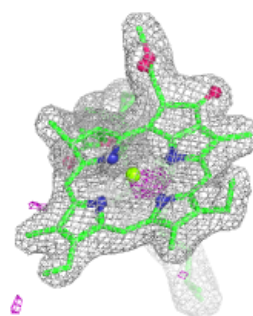
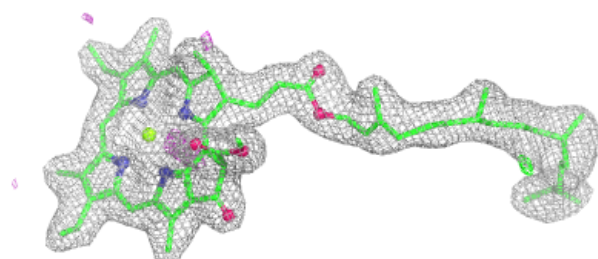
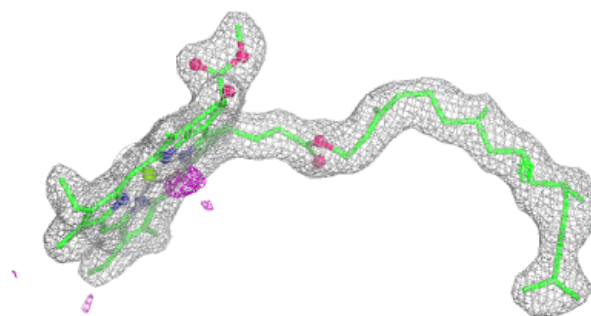
Electron density around CLA b 612:

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

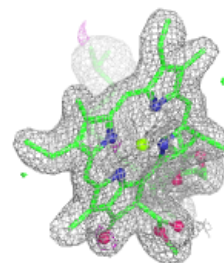
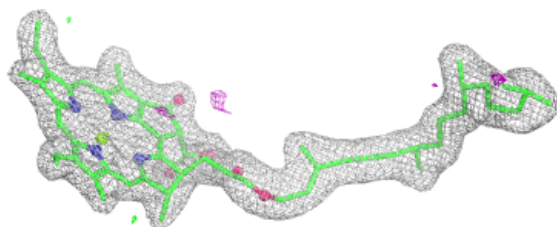
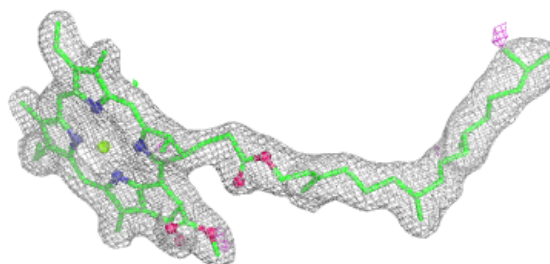


Electron density around CLA d 403:

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

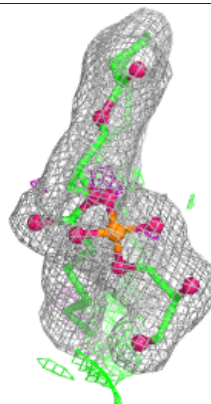
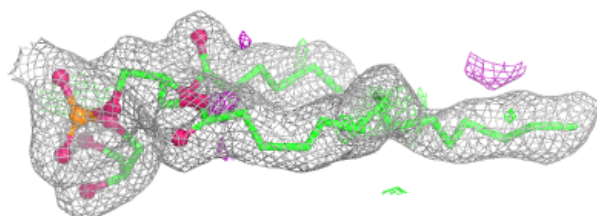
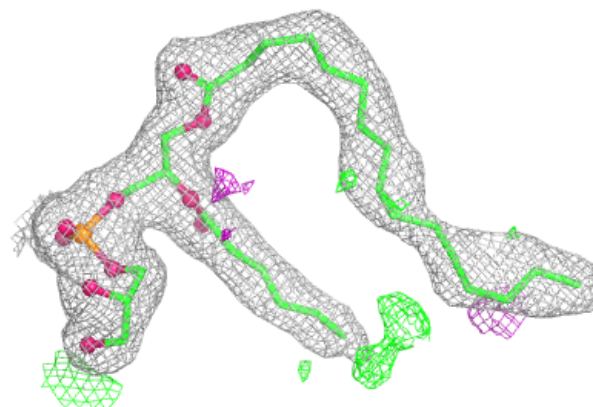
**Electron density around CLA A 606:**

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

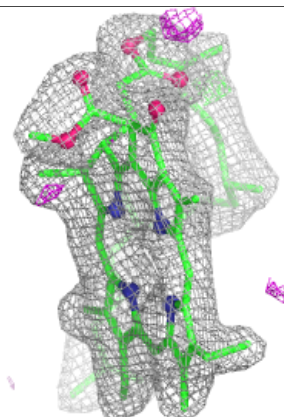
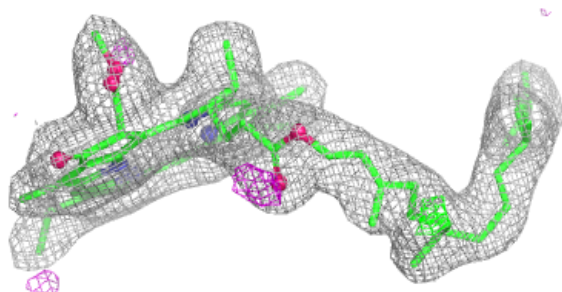
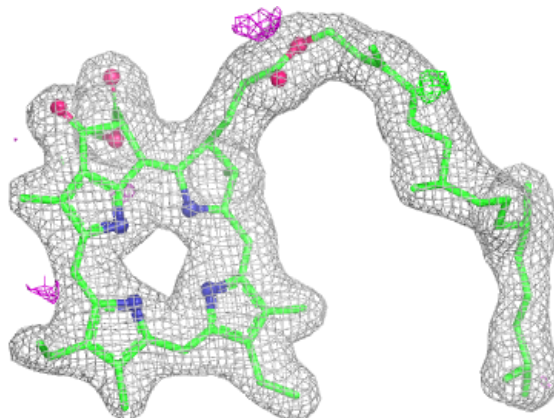


Electron density around LHG d 408:

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

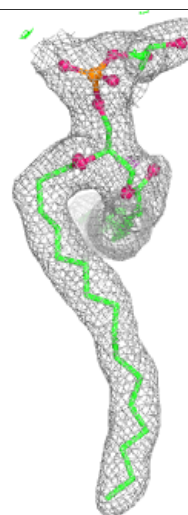
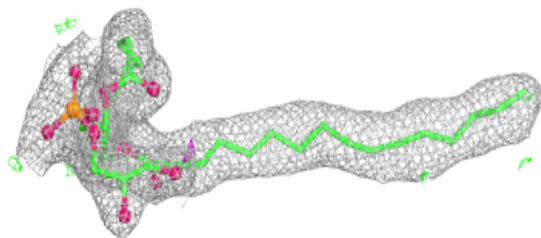
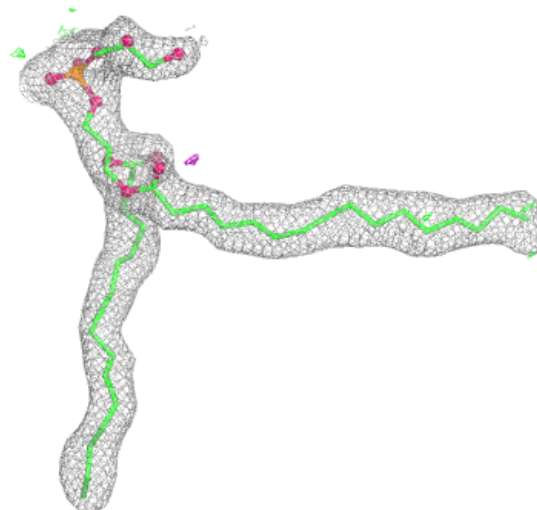
**Electron density around PHO d 402:**

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



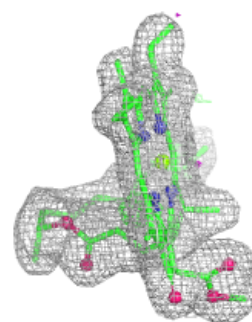
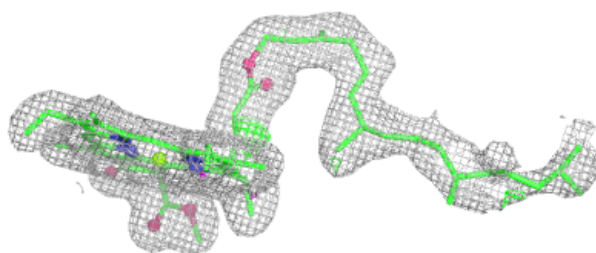
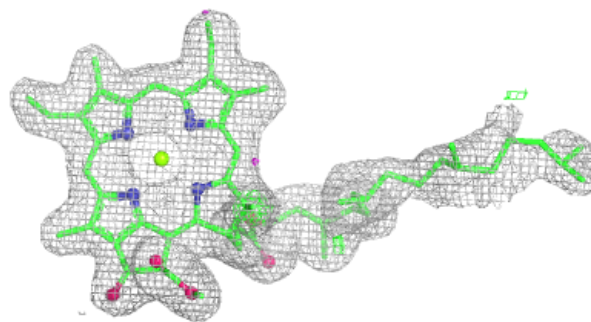
Electron density around LHG 1 101:

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

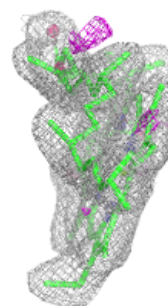
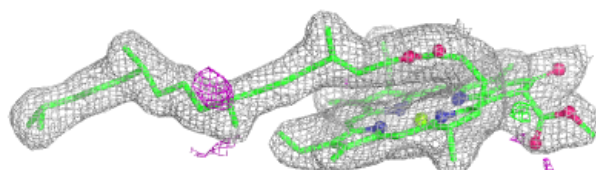
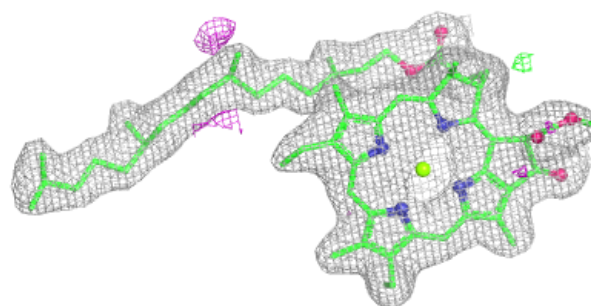


Electron density around CLA A 607:

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

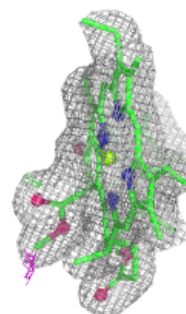
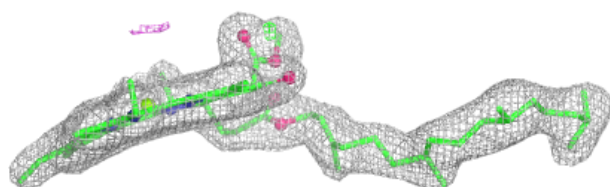
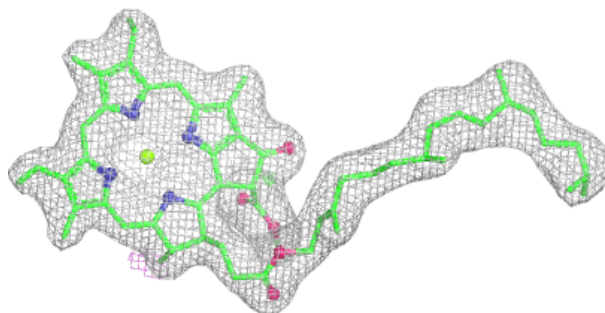
**Electron density around CLA C 501:**

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

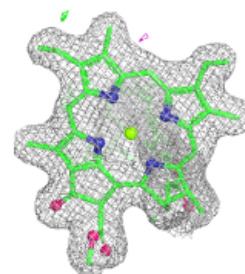
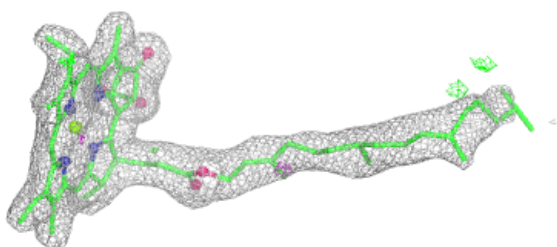
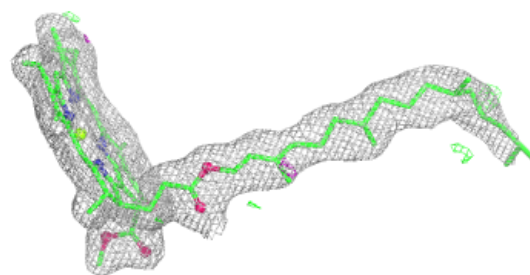


Electron density around CLA b 602:

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

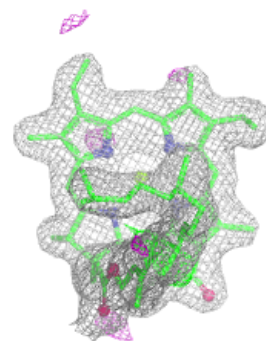
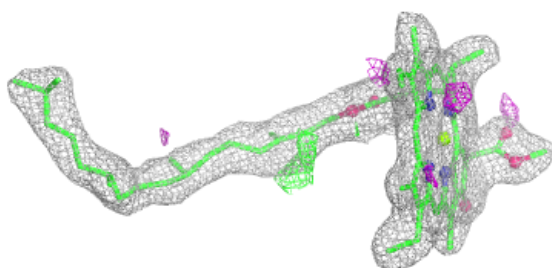
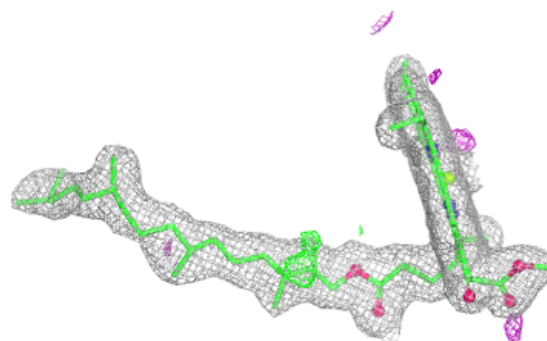
**Electron density around CLA b 604:**

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

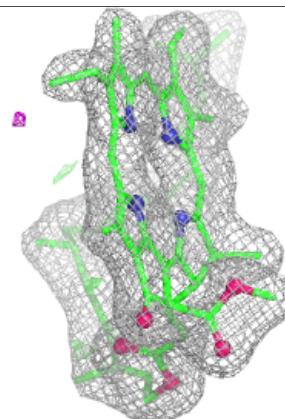
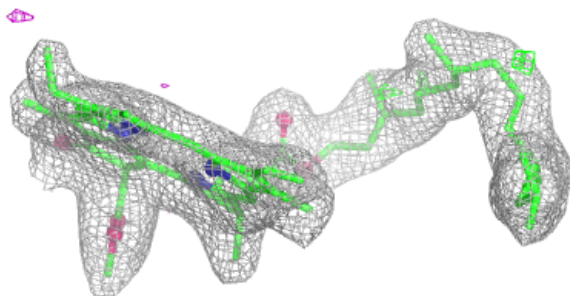
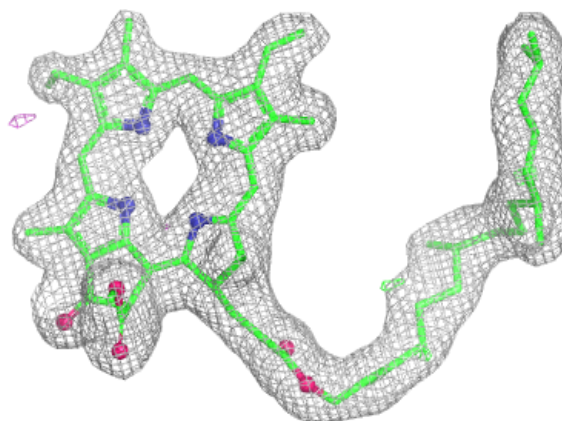


Electron density around CLA b 605:

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

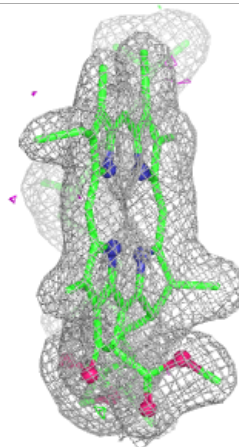
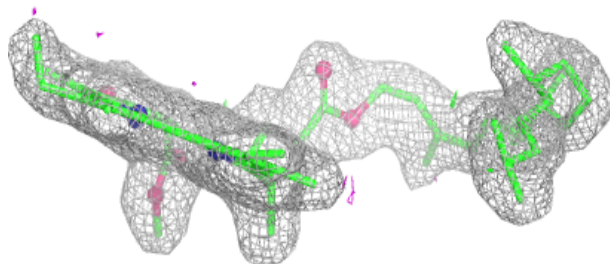
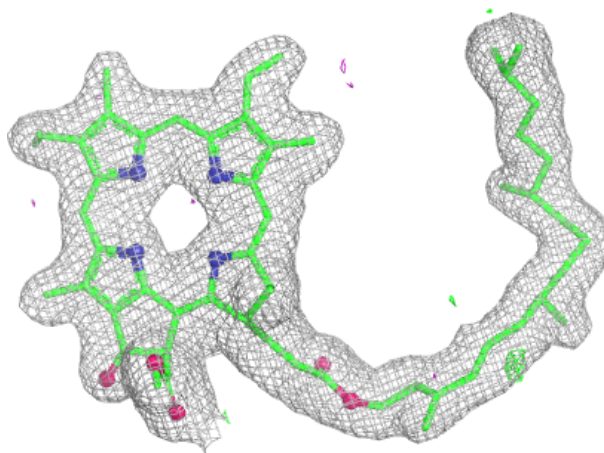
**Electron density around PHO D 402:**

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



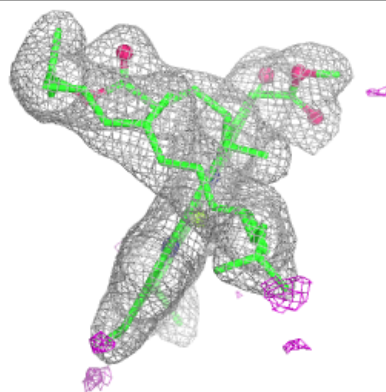
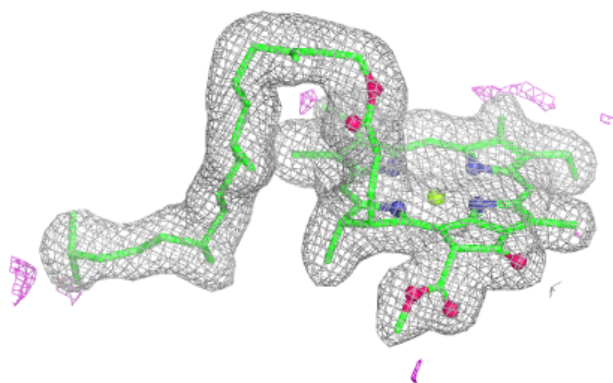
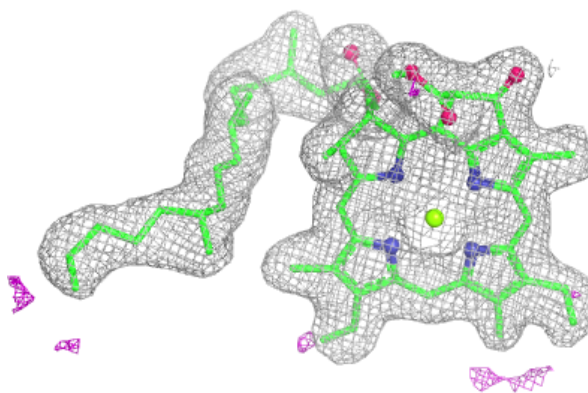
Electron density around PHO a 608:

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

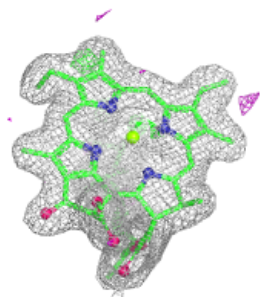
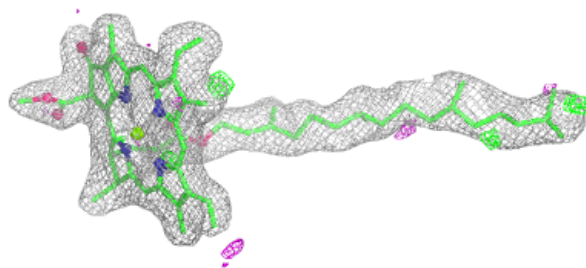
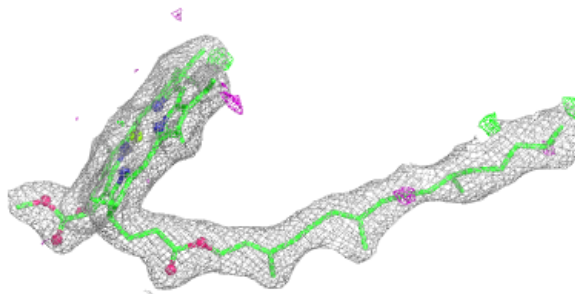


Electron density around CLA A 612:

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

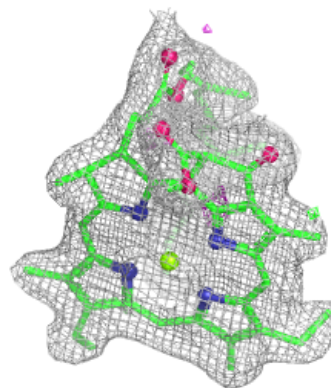
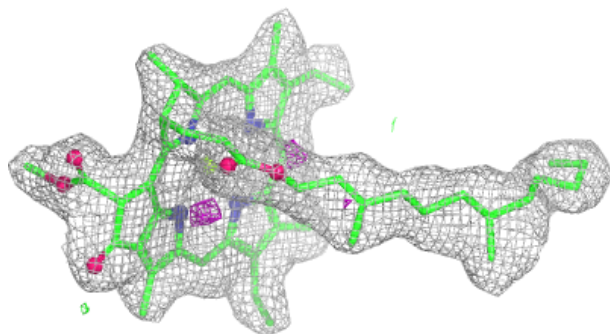
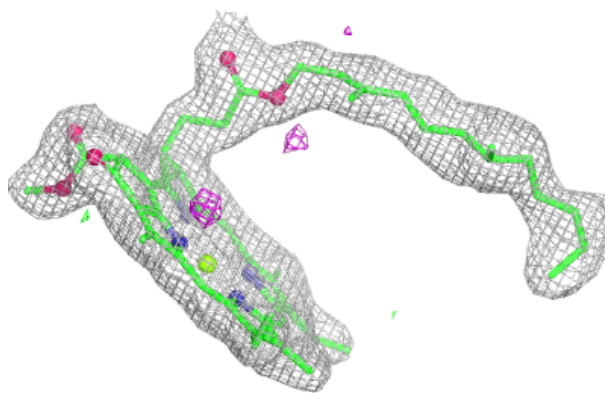
**Electron density around CLA B 607:**

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

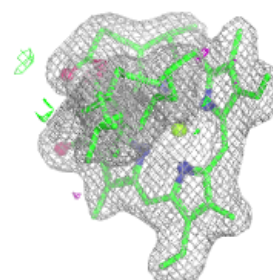
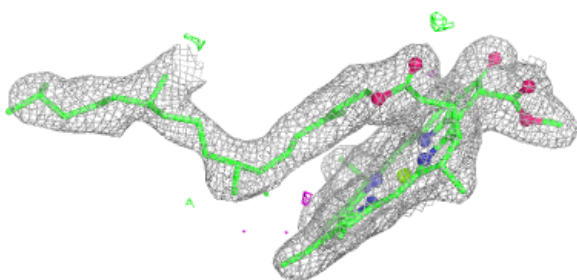
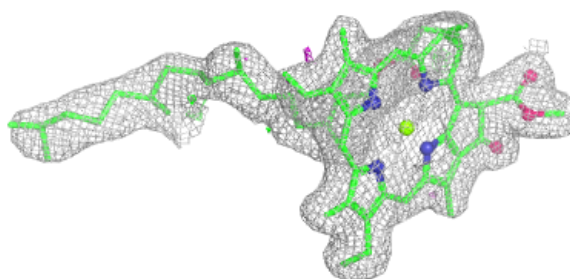


Electron density around CLA C 504:

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

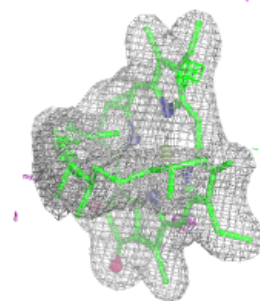
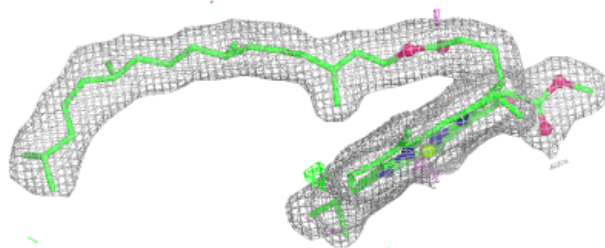
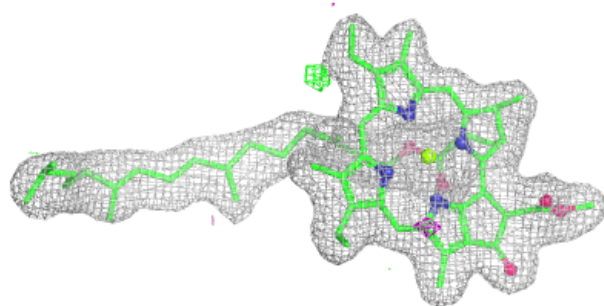
**Electron density around CLA C 505:**

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



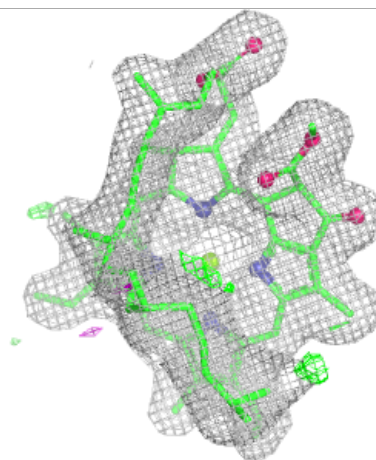
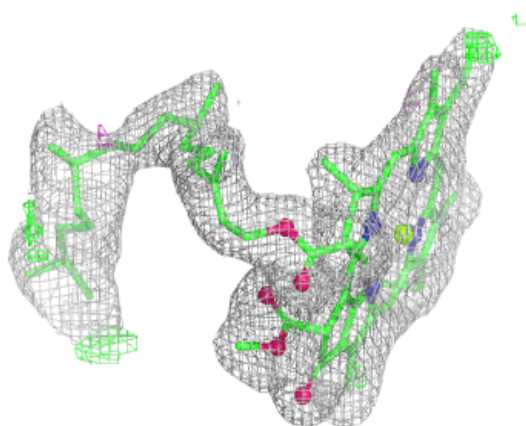
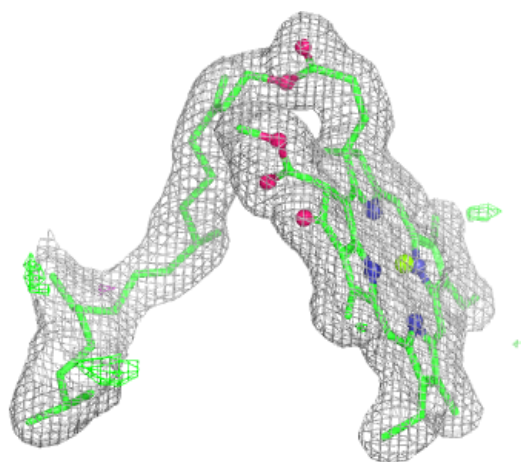
Electron density around CLA B 608:

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



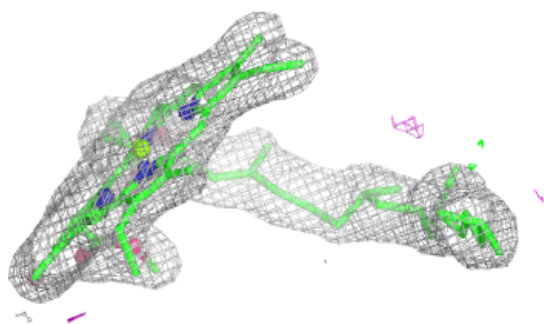
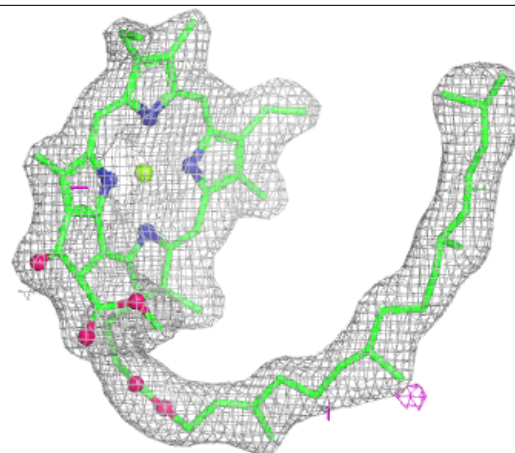
Electron density around CLA b 613:

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



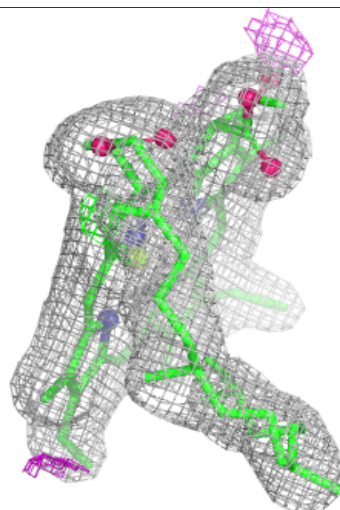
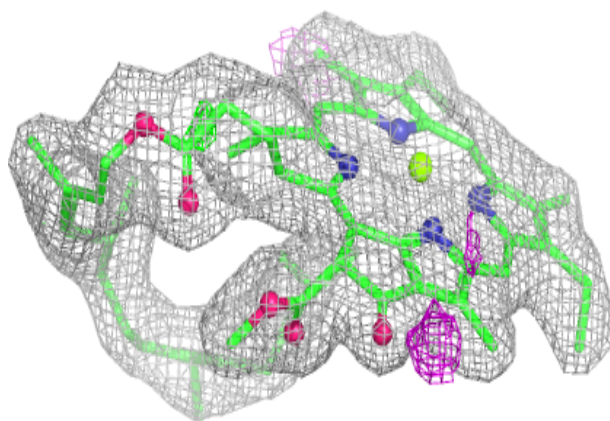
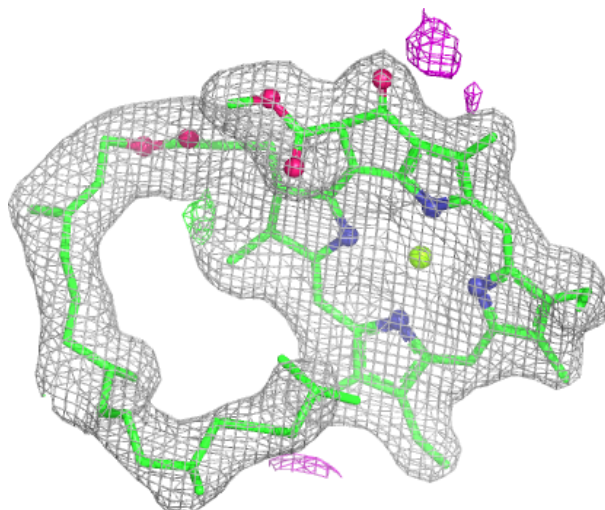
Electron density around CLA C 507:

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



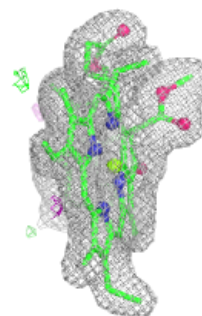
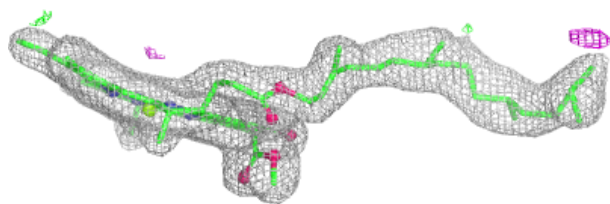
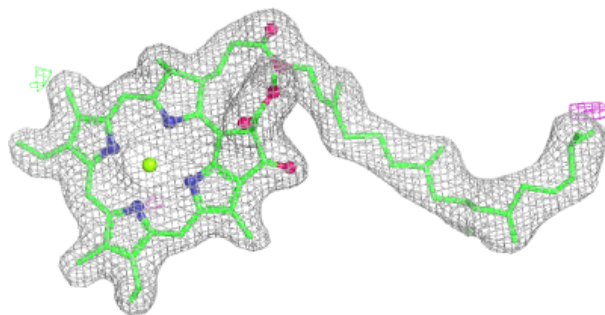
Electron density around CLA b 615:

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



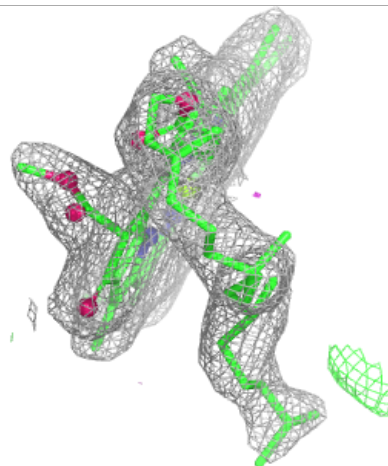
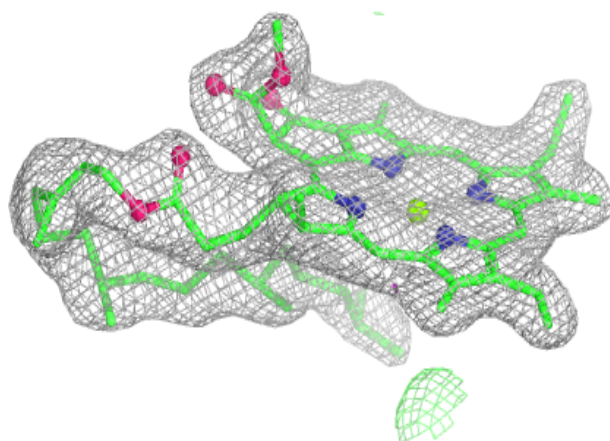
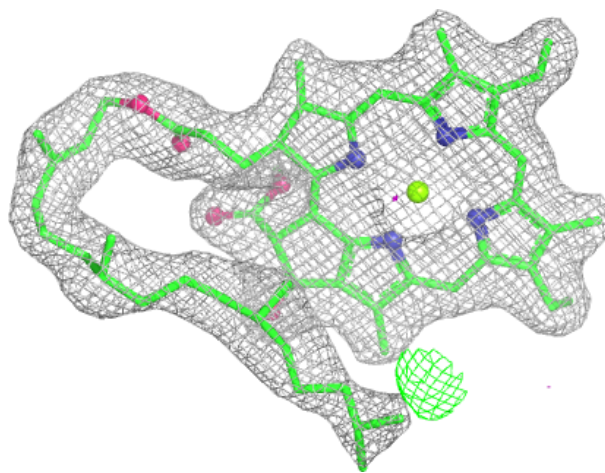
Electron density around CLA B 602:

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



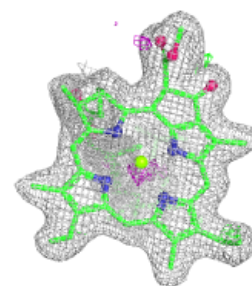
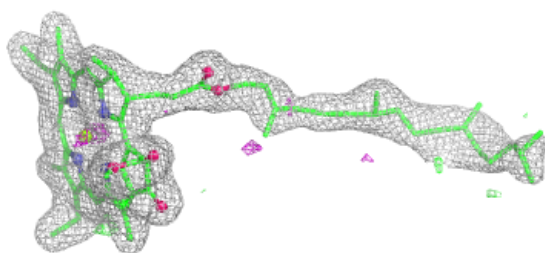
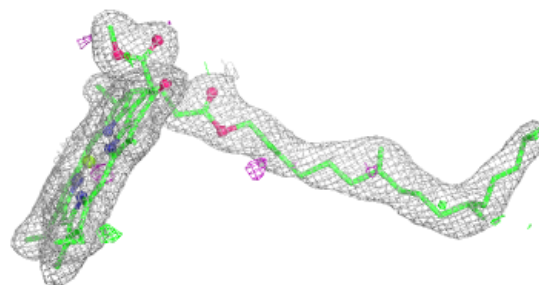
Electron density around CLA C 509:

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



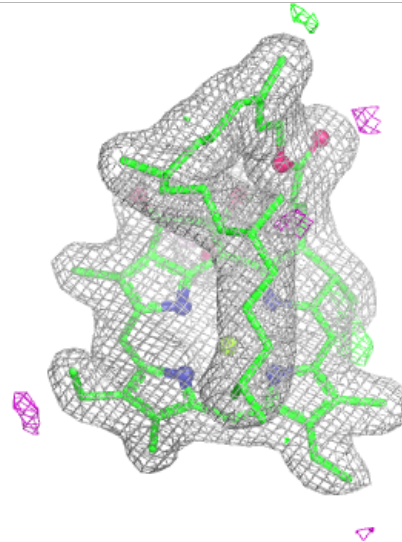
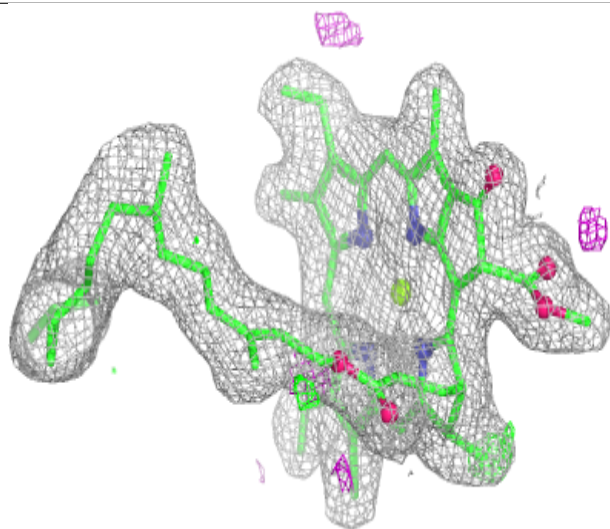
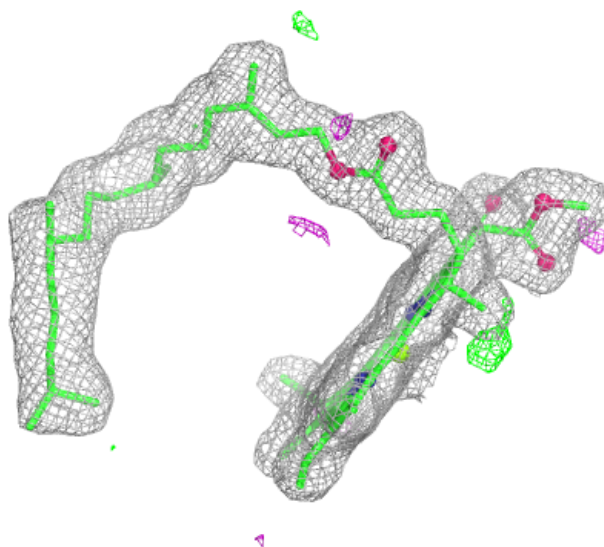
Electron density around CLA B 604:

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



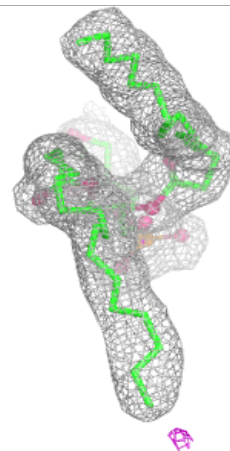
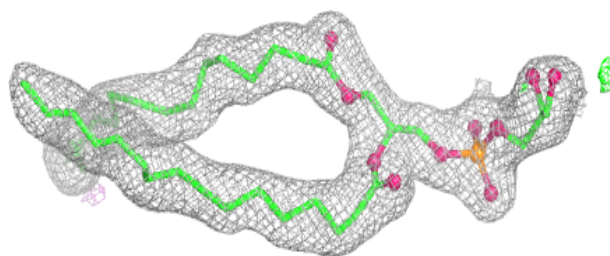
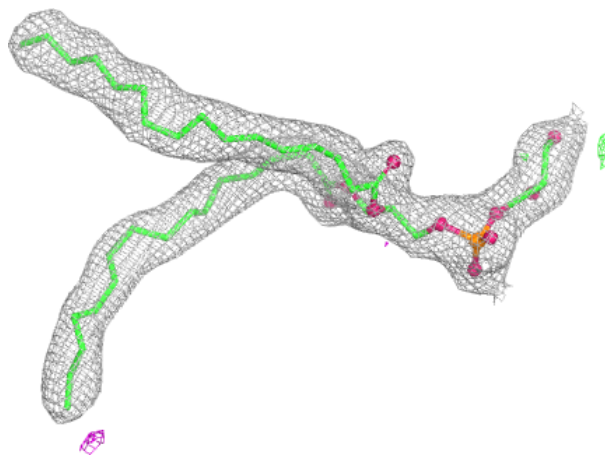
Electron density around CLA B 611:

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



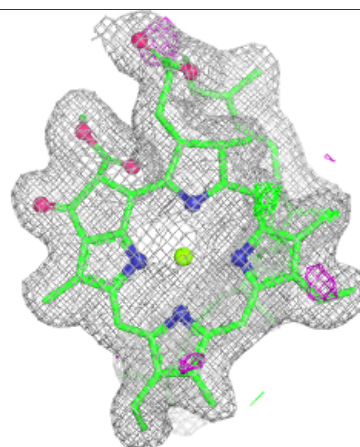
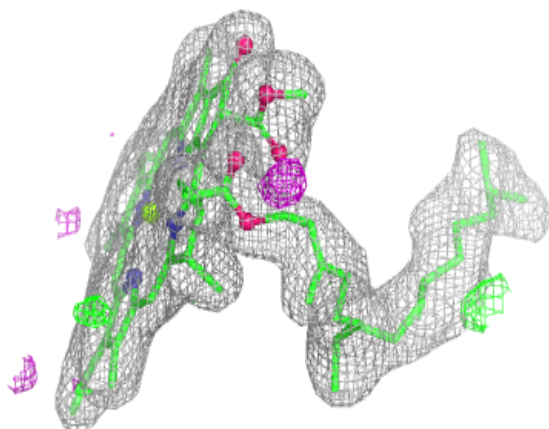
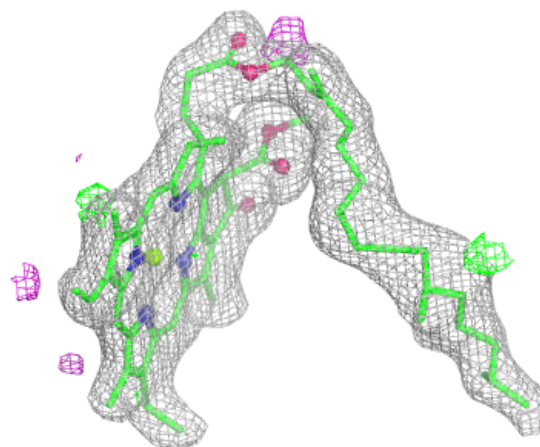
Electron density around LHG D 409:

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



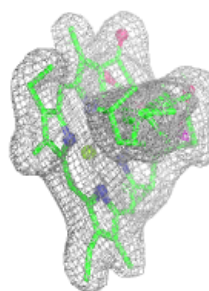
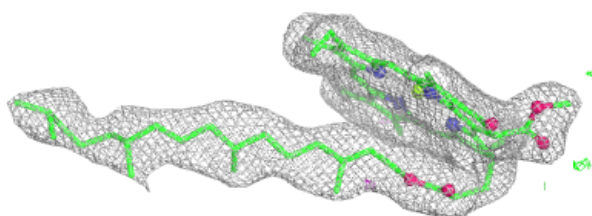
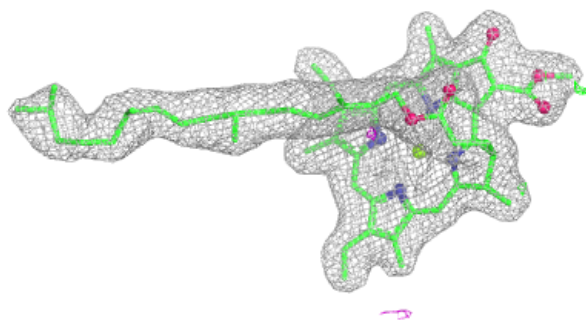
Electron density around CLA B 613:

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

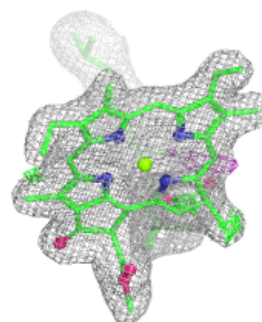
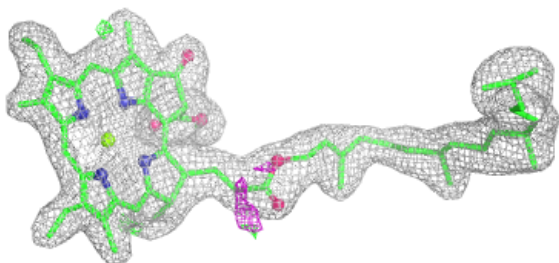
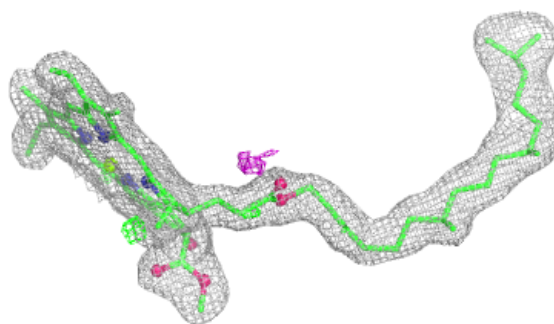


Electron density around CLA B 614:

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

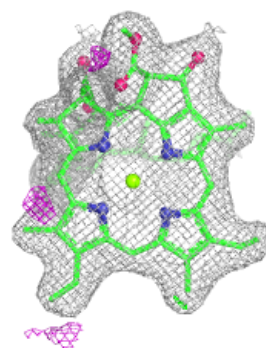
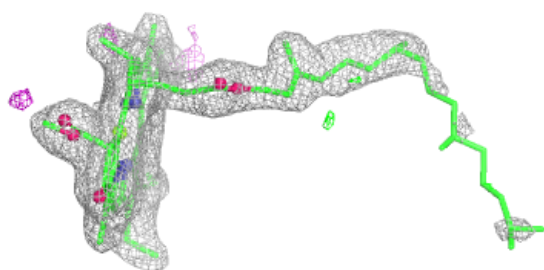
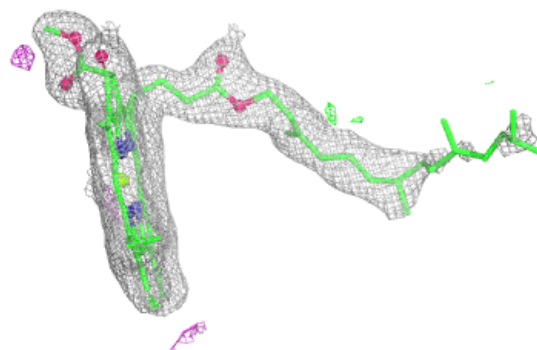
**Electron density around CLA D 403:**

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

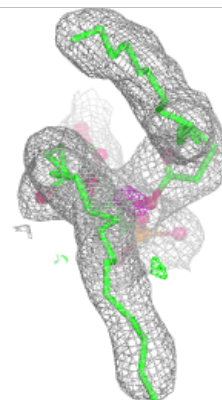
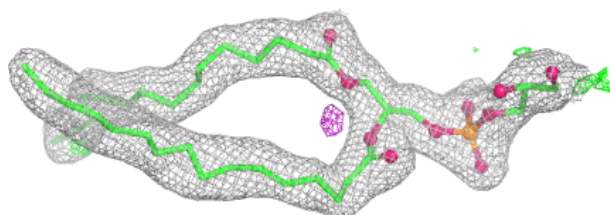
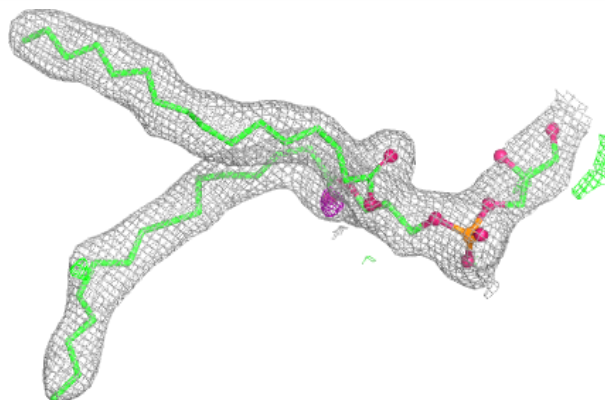


Electron density around CLA D 404:

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

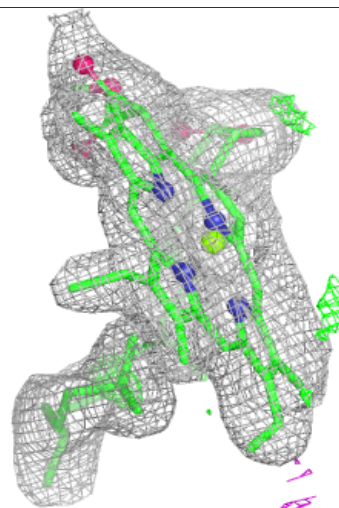
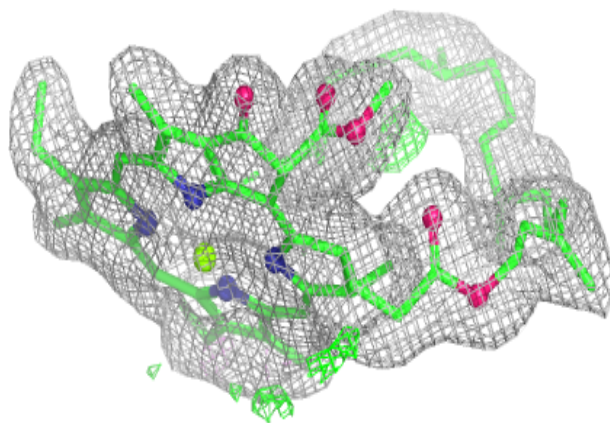
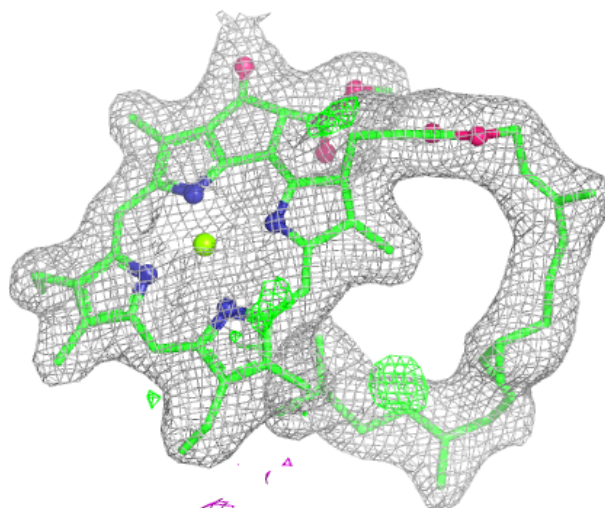
**Electron density around LHG d 407:**

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



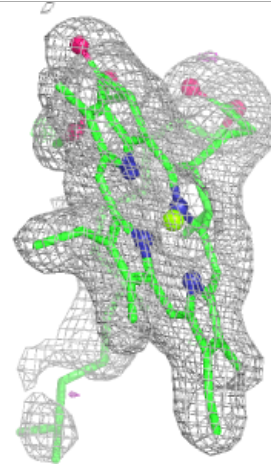
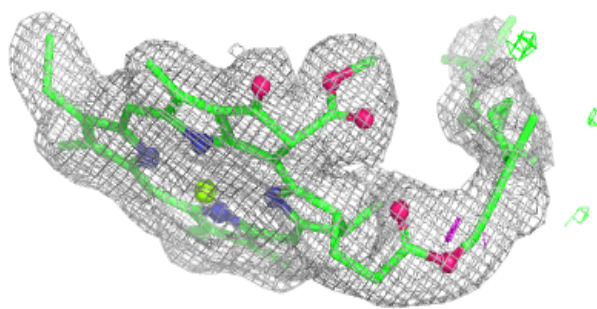
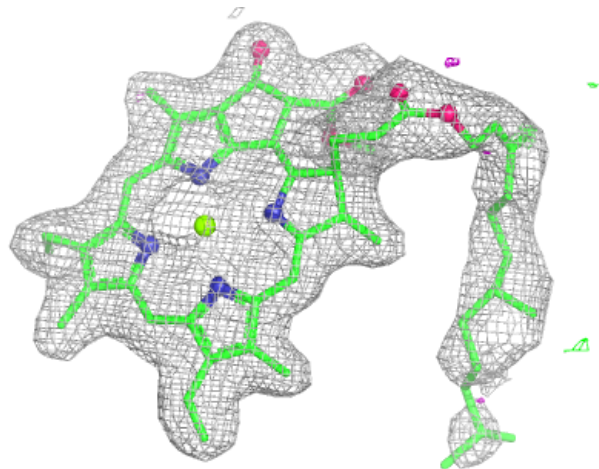
Electron density around CLA B 615:

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



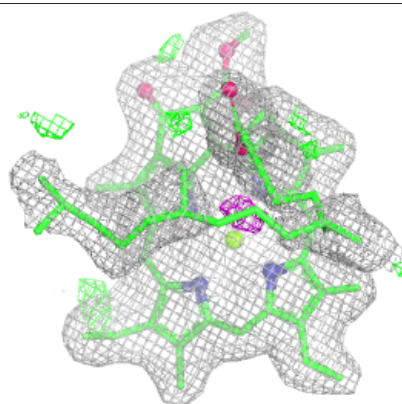
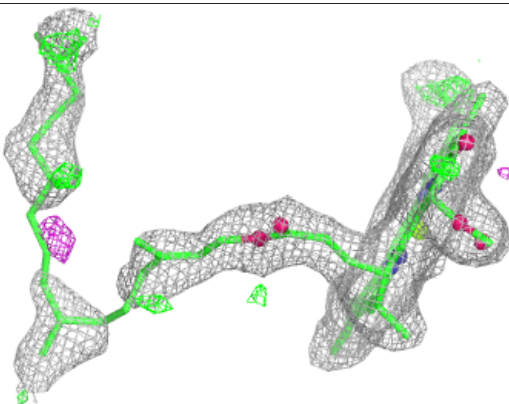
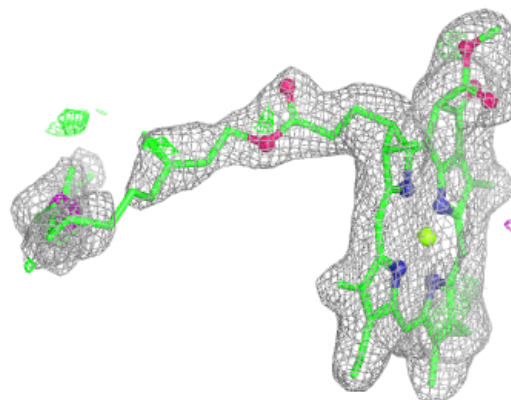
Electron density around CLA B 616:

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

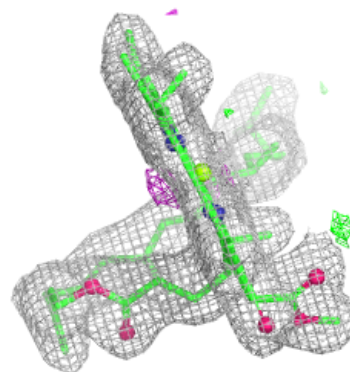
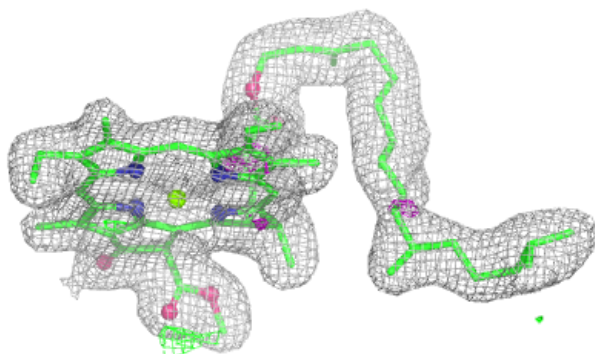
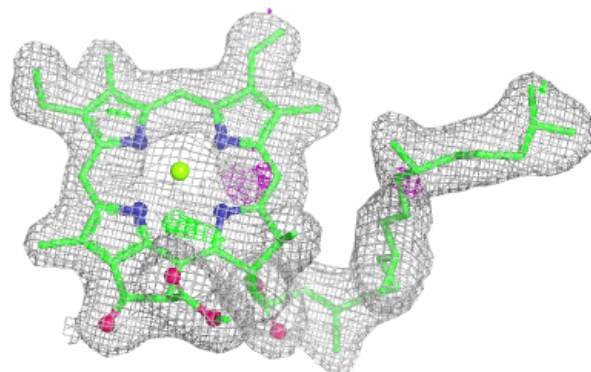


Electron density around CLA a 609:

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

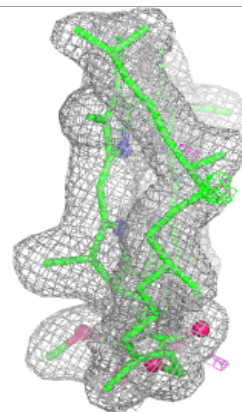
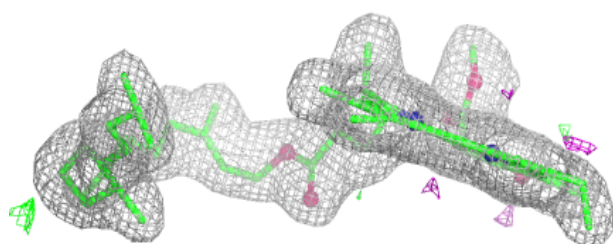
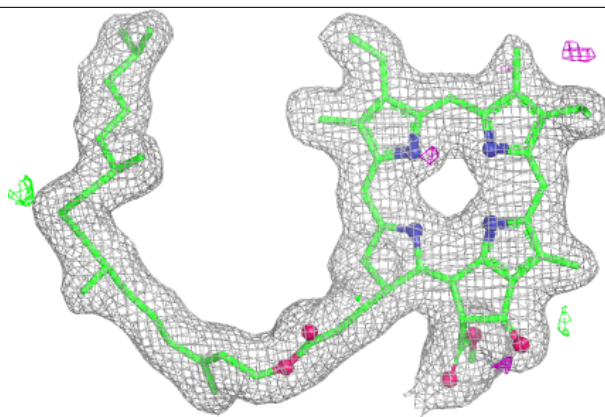
**Electron density around CLA a 612:**

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



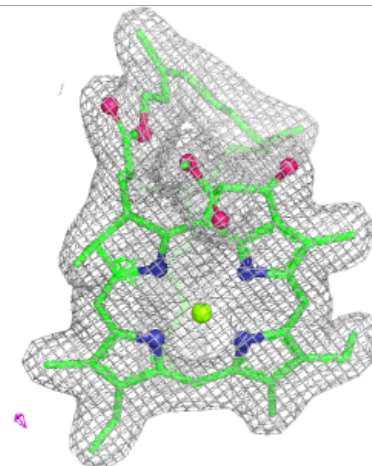
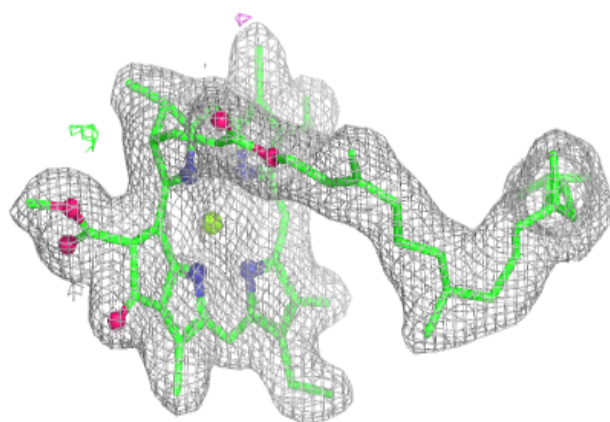
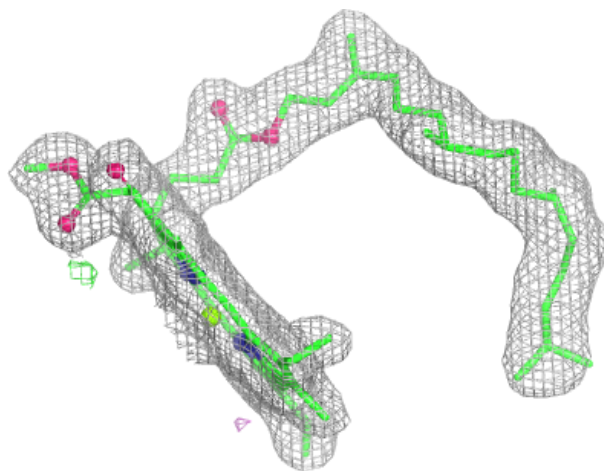
Electron density around PHO A 608:

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



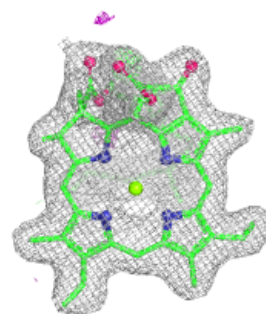
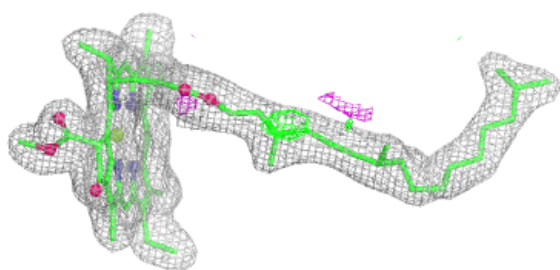
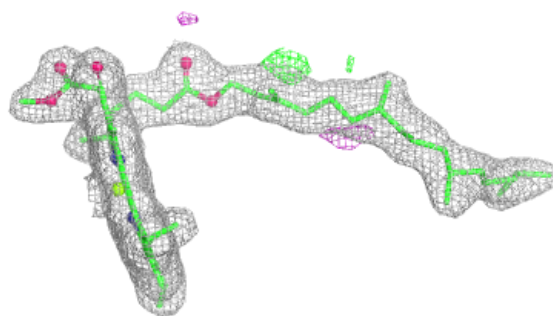
Electron density around CLA b 611:

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

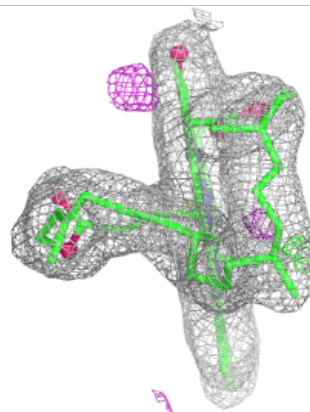
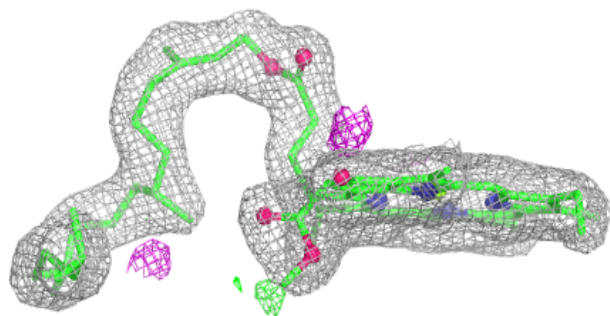
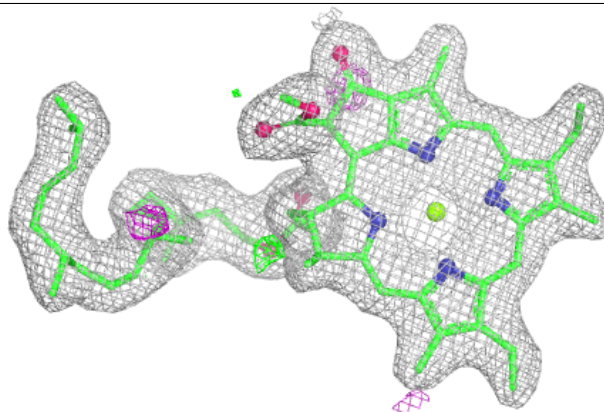


Electron density around CLA B 605:

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

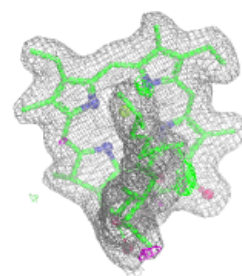
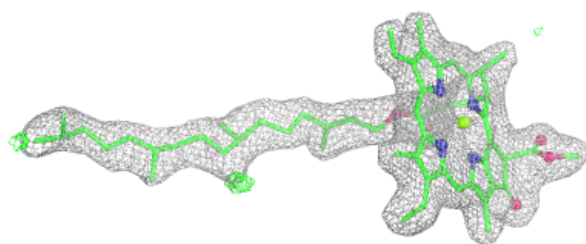
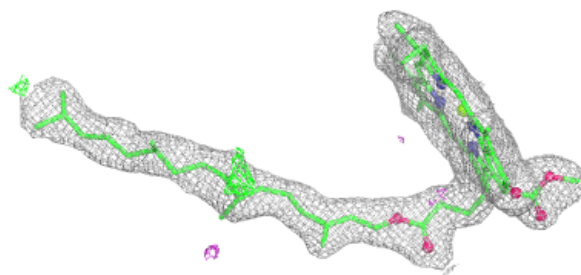
**Electron density around CLA B 612:**

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

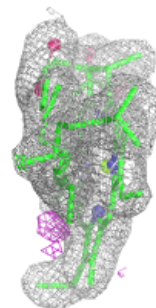
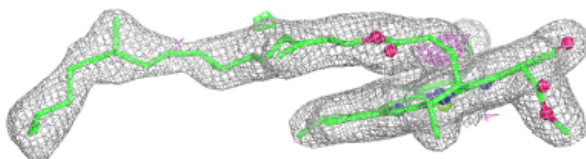
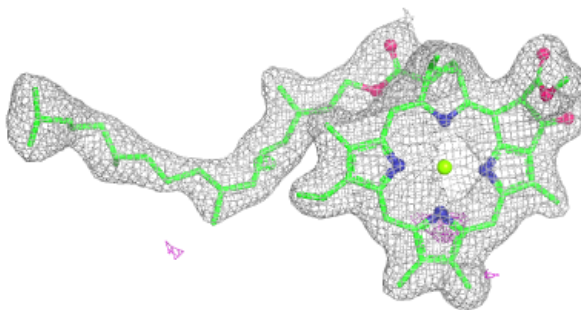


Electron density around CLA b 607:

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

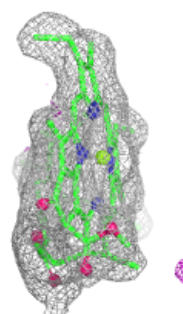
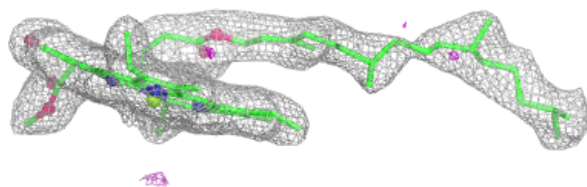
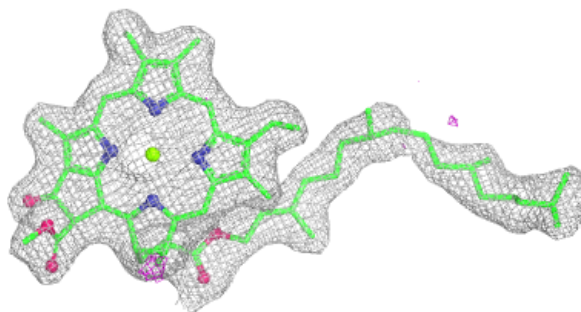
**Electron density around CLA B 603:**

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

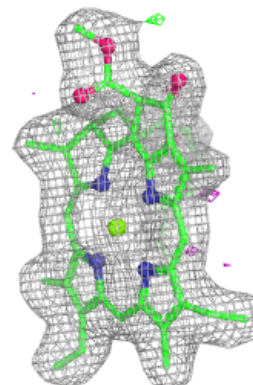
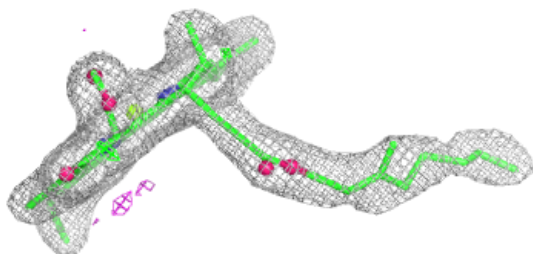
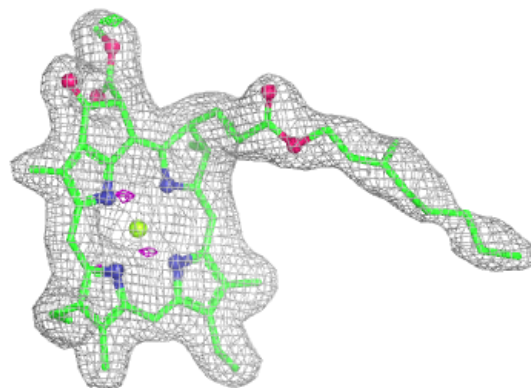


Electron density around CLA b 603:

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

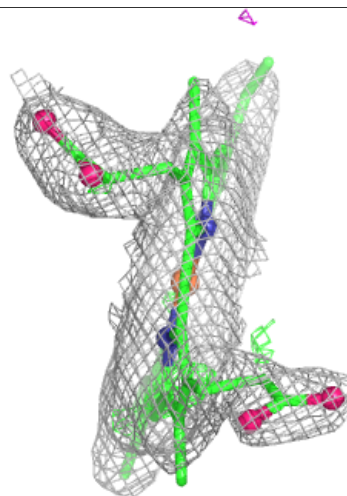
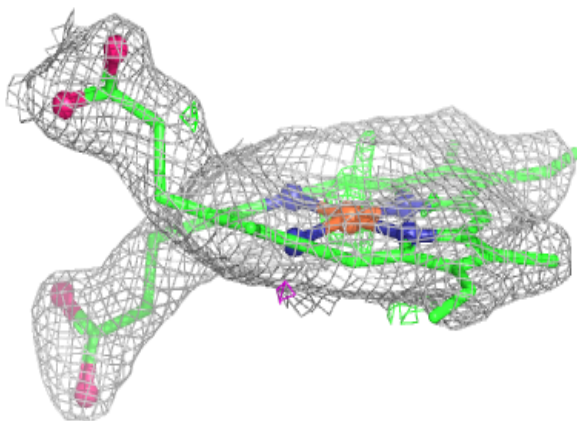
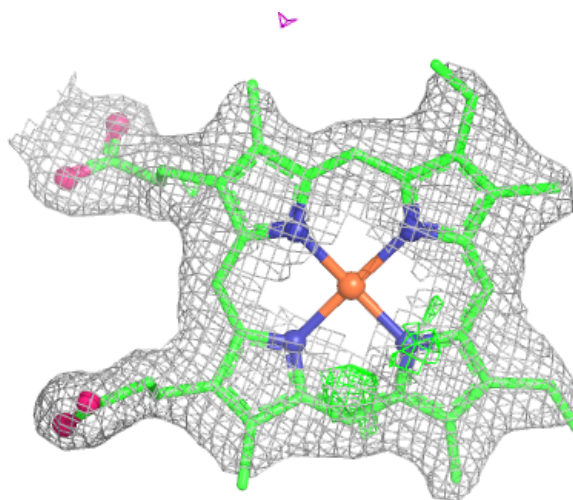
**Electron density around CLA A 609:**

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



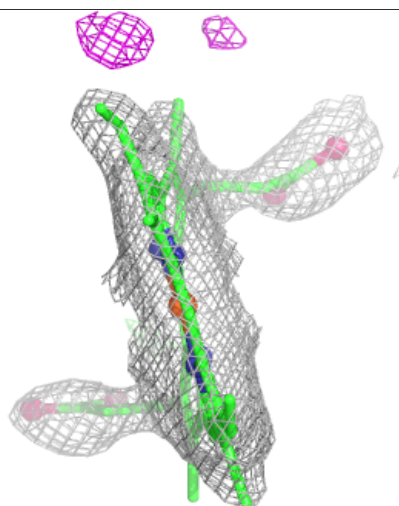
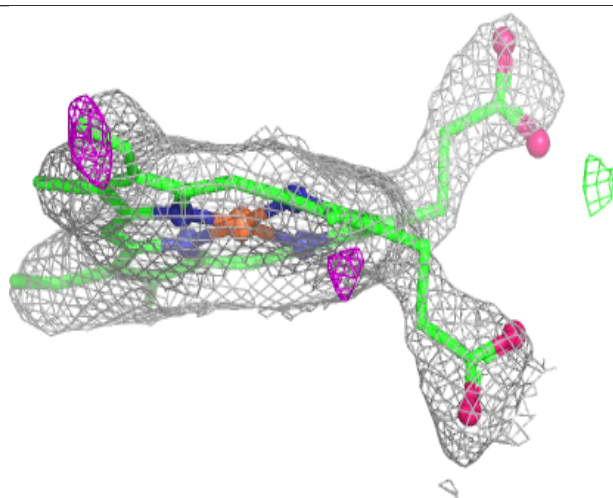
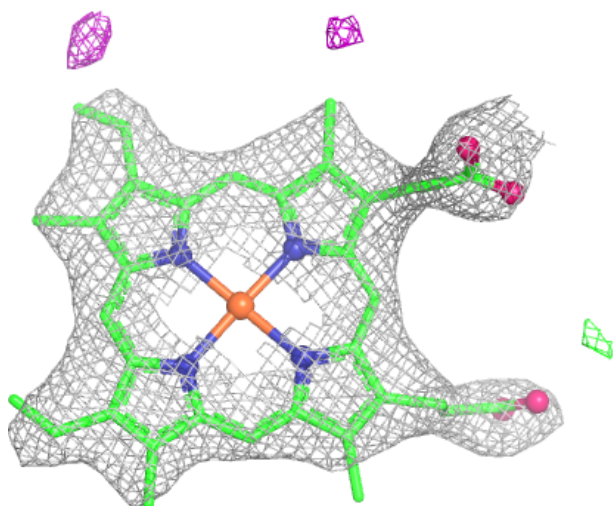
Electron density around HEM F 101:

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



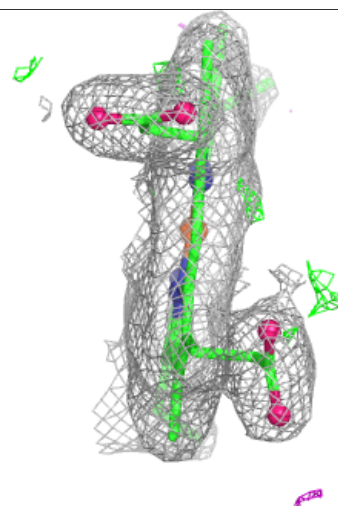
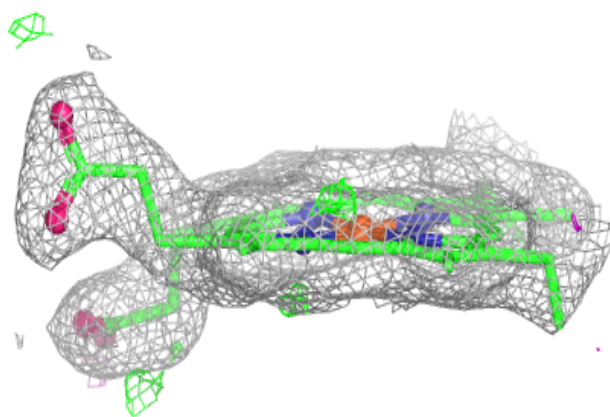
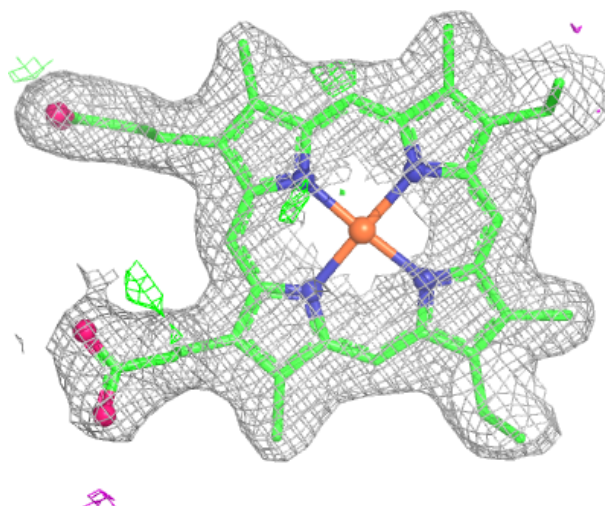
Electron density around HEM e 101:

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



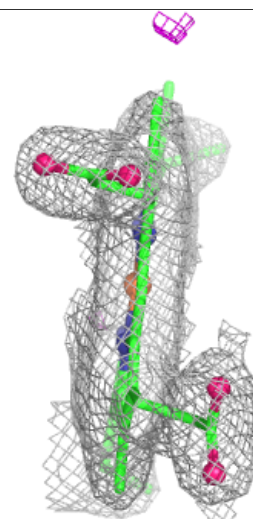
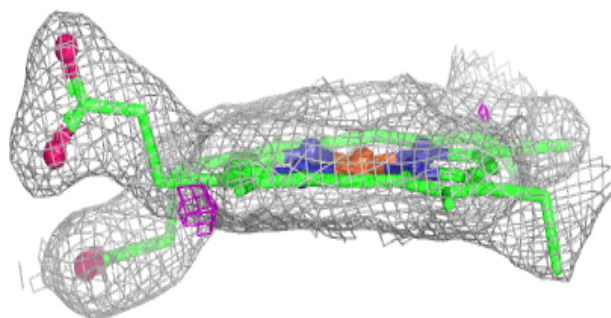
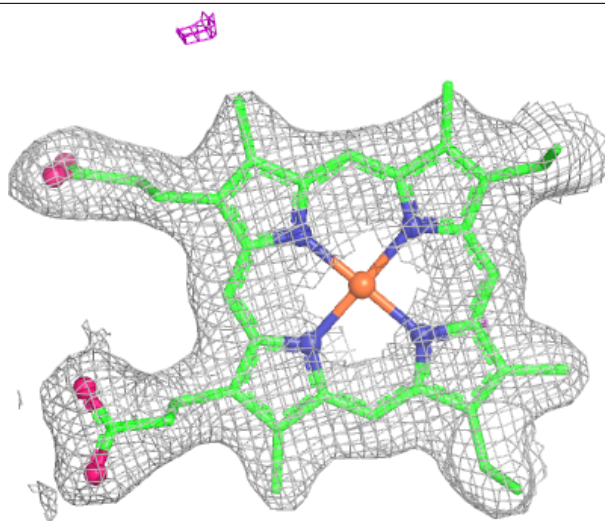
Electron density around HEC V 201:

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



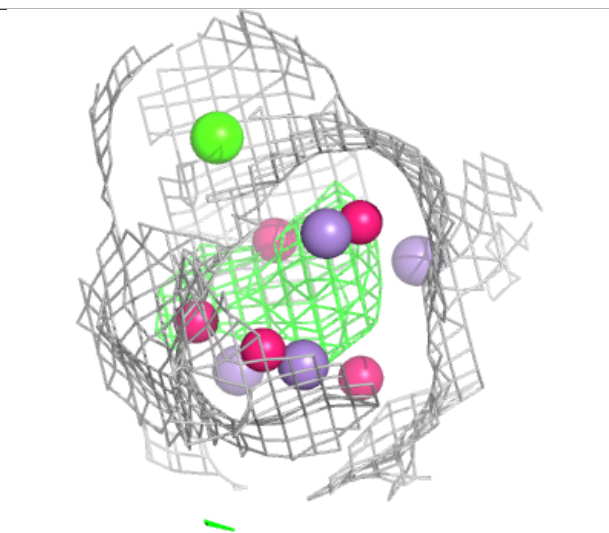
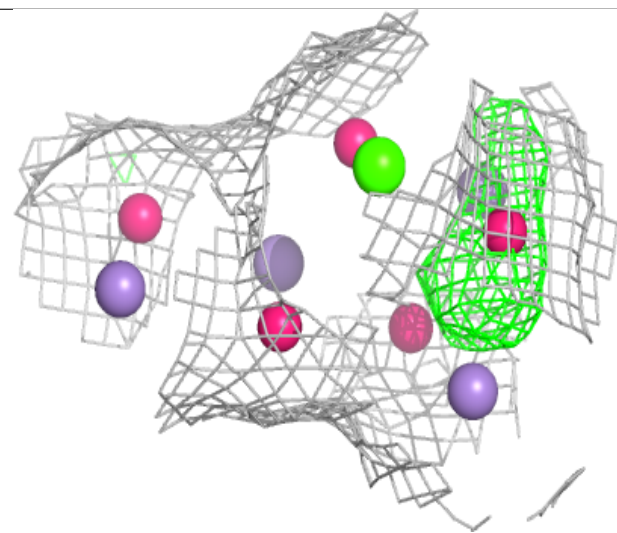
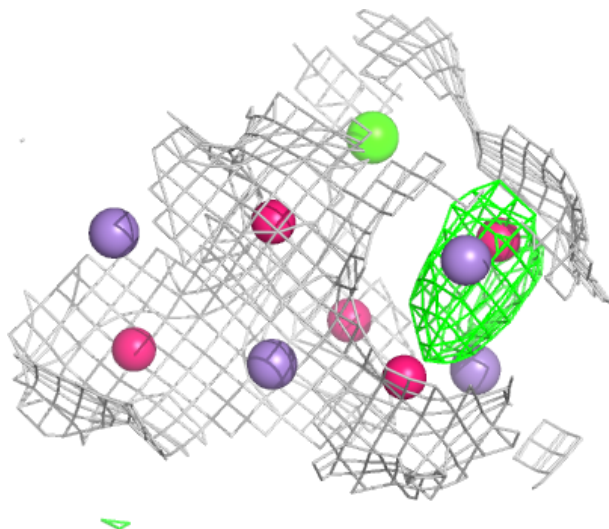
Electron density around HEC v 201:

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



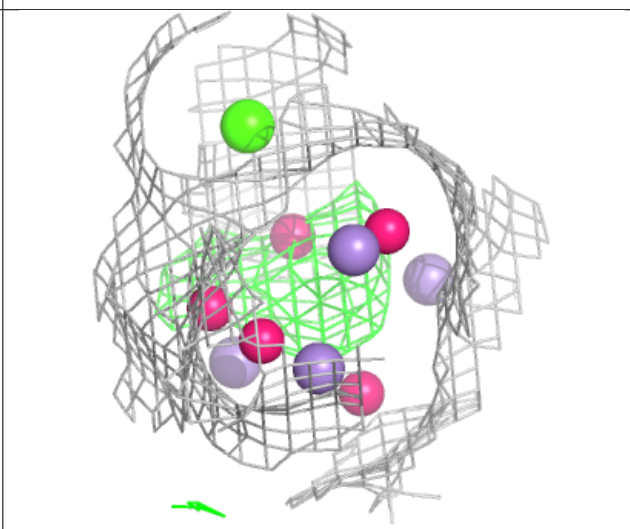
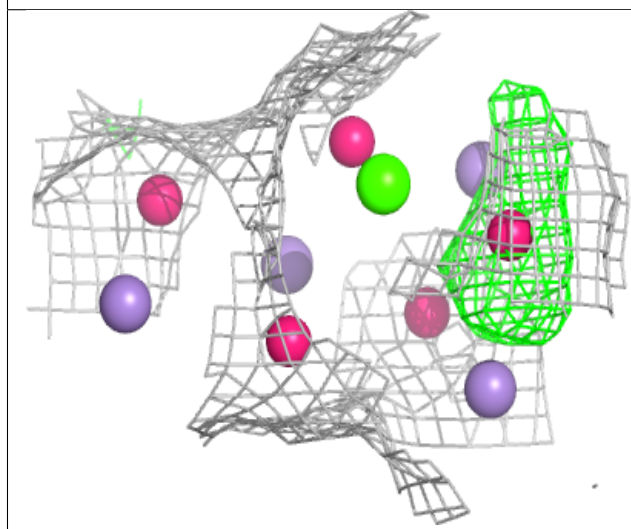
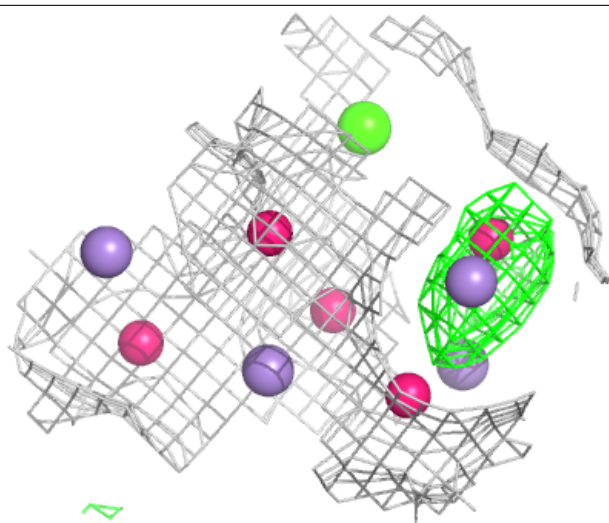
Electron density around OEX A 601 (B):

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



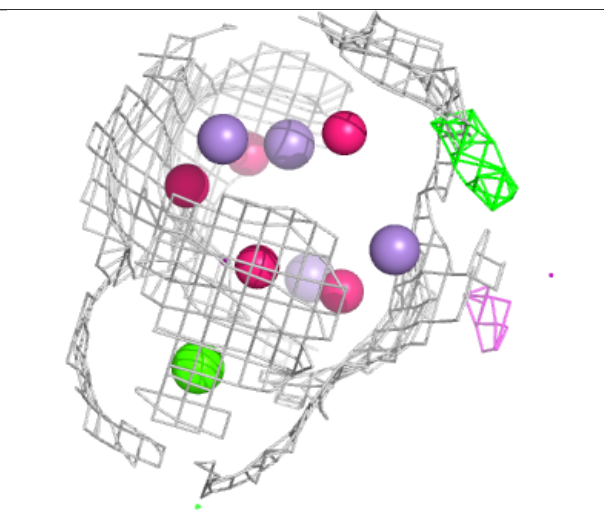
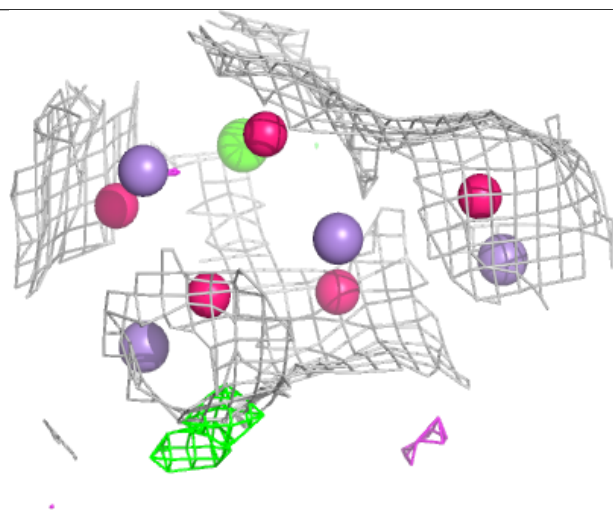
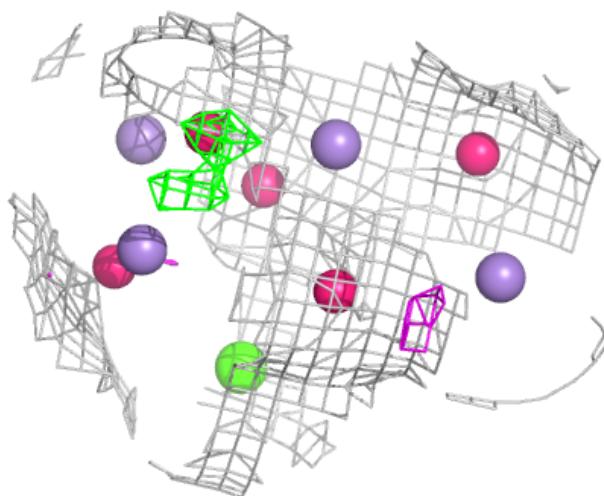
Electron density around OEX A 601 (C):

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



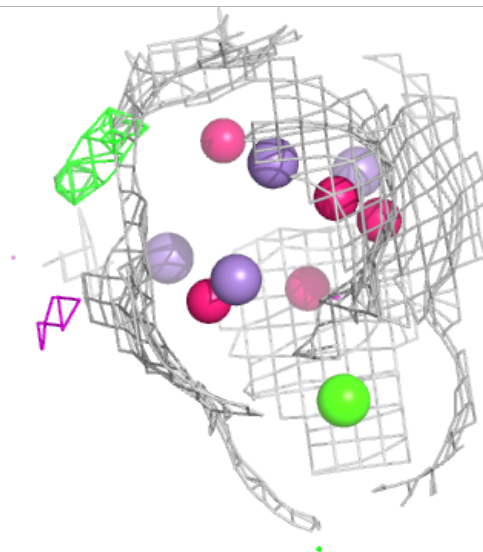
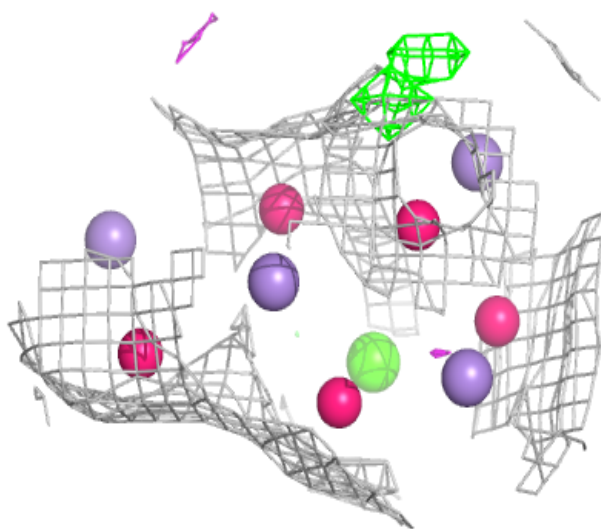
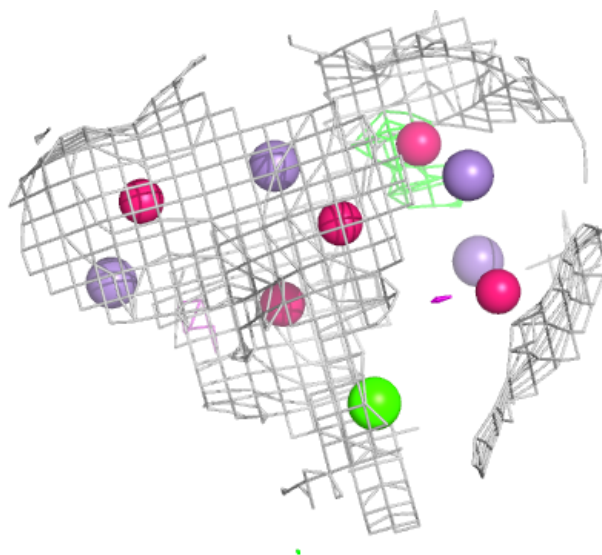
Electron density around OEX a 601 (B):

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



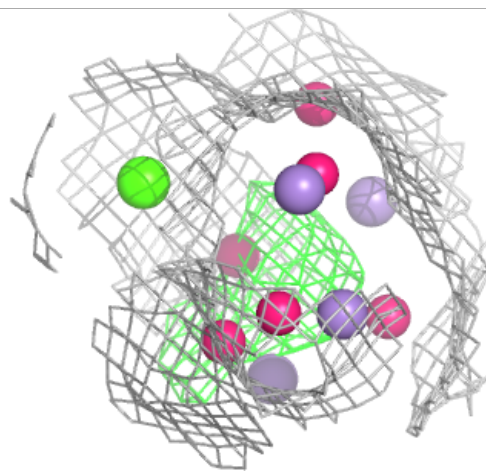
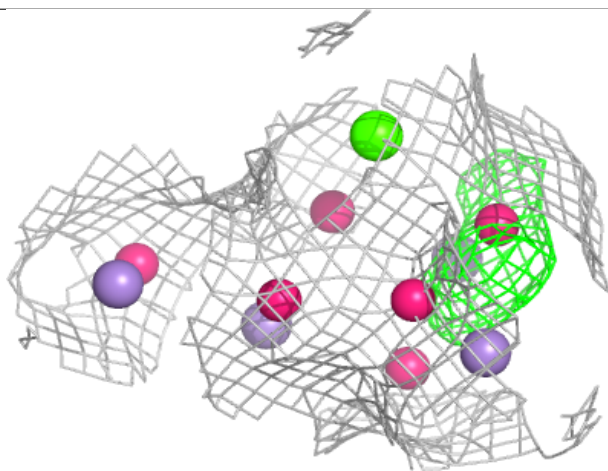
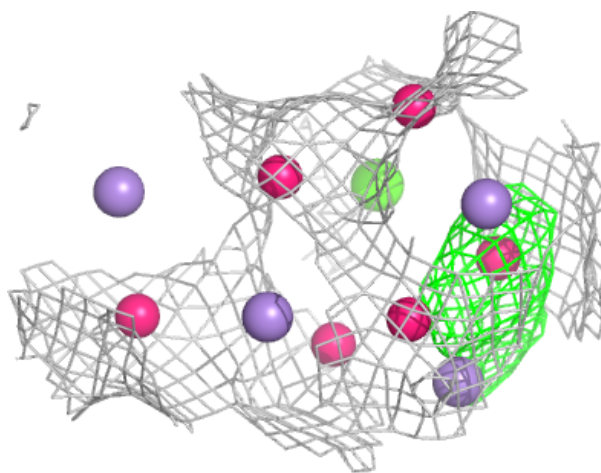
Electron density around OEX a 601 (C):

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



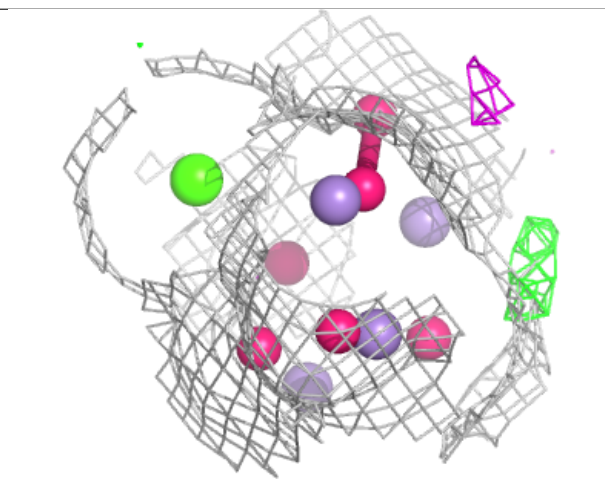
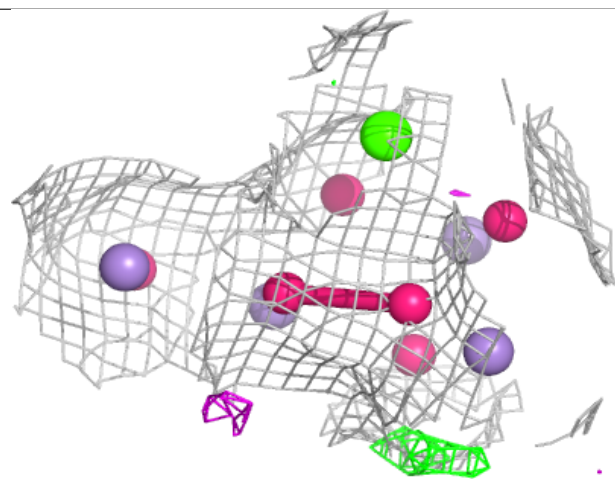
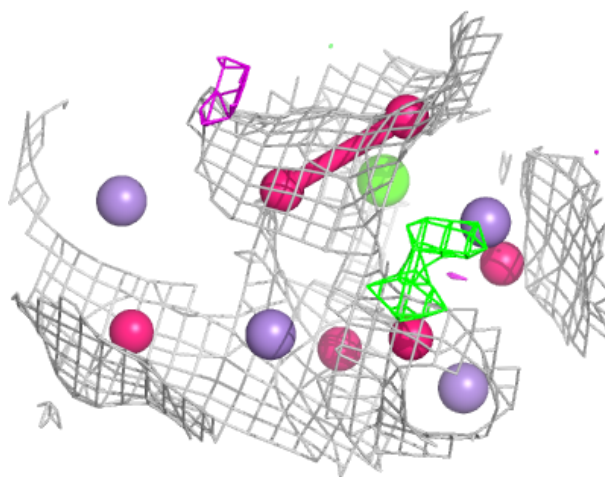
Electron density around OEY A 602 (A):

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



Electron density around OEY a 602 (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.