



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2026 – 02:09 PM EDT

PDB ID : 9Z37 / pdb_00009z37
Title : RT XFEL structure of two-flash state of Photosystem II (2F, S3 rich) at 2.11 Angstrom obtained from anomalous data at 7 keV
Authors : Bhowmick, A.; Kern, J.; Yano, J.; Yachandra, V.K.; Minnetian, N.M.; Zhang, M.
Deposited on : 2025-11-05
Resolution : 2.11 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
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

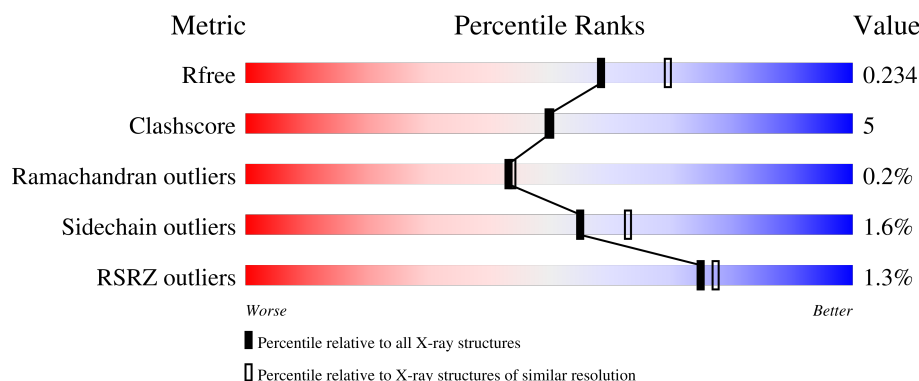
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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.



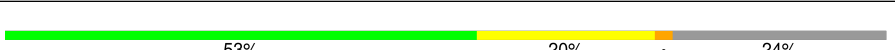
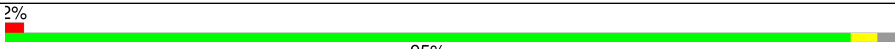
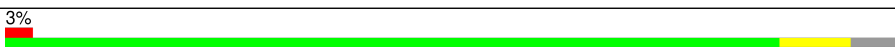
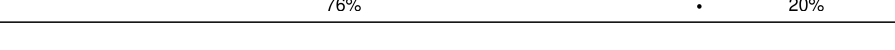
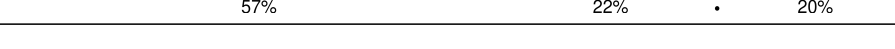
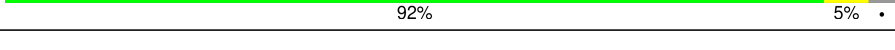
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	
2	B	510	
2	b	510	

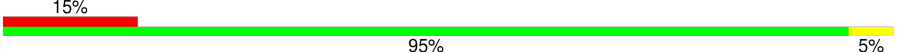
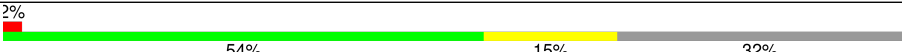
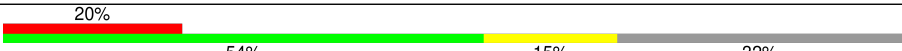
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
14	T	32	
14	t	32	
15	U	134	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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 54355 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	69	0
			3152	2055	520	558	19			
1	a	334	Total	C	N	O	S	0	69	0
			3149	2052	520	558	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	5	0
			4016	2637	670	696	13			
2	b	505	Total	C	N	O	S	0	1	0
			3984	2614	665	692	13			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	10	0
			2805	1859	456	478	12			
4	d	341	Total	C	N	O	S	0	11	0
			2811	1863	456	480	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
			505	335	82	85	3			
7	h	63	Total	C	N	O	S	0	0	0
			493	327	80	83	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	41	CYS	PHE	conflict	UNP Q8DJ43
h	41	CYS	PHE	conflict	UNP Q8DJ43

- 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			
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.

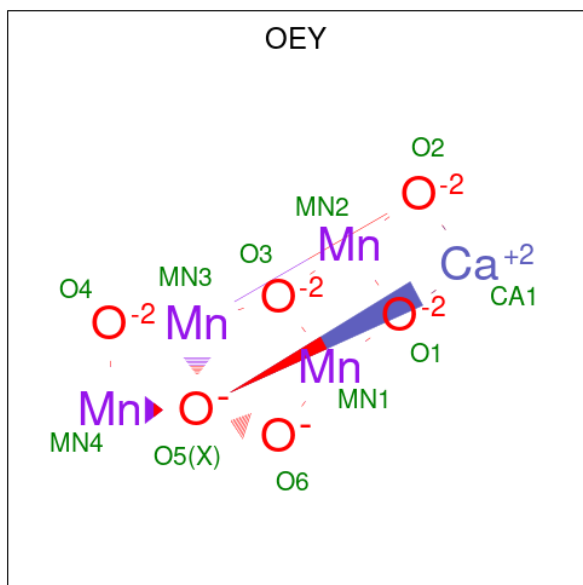
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	28	Total	C	N	O	0	0	0
			221	151	38	32			

Continued on next page...

Continued from previous page...

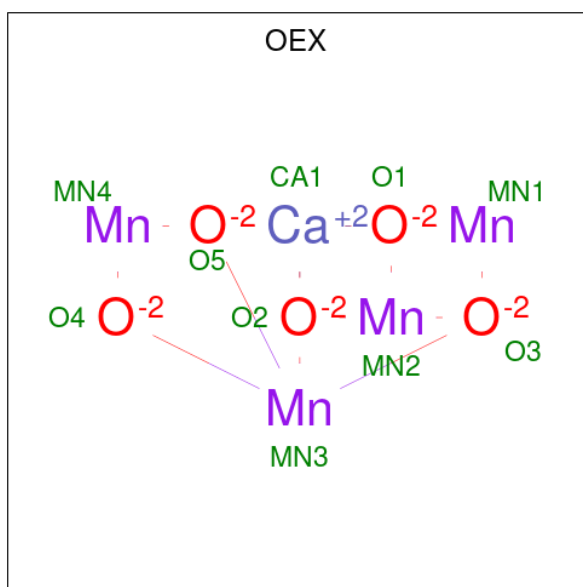
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	r	28	Total	C	N	O	0	0	0
			221	151	38	32			

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



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

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



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

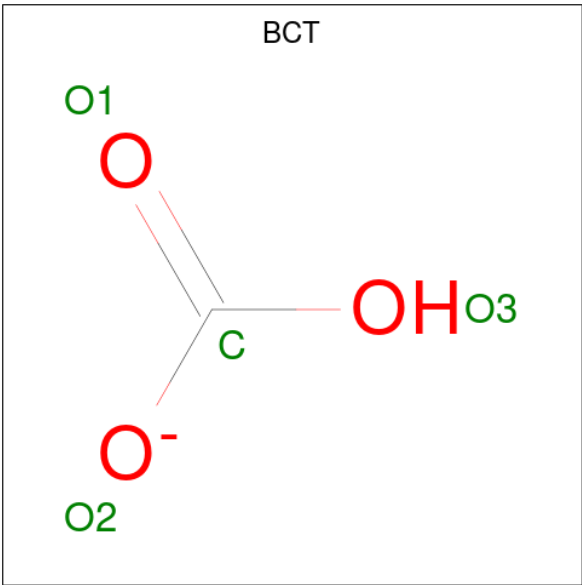
- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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

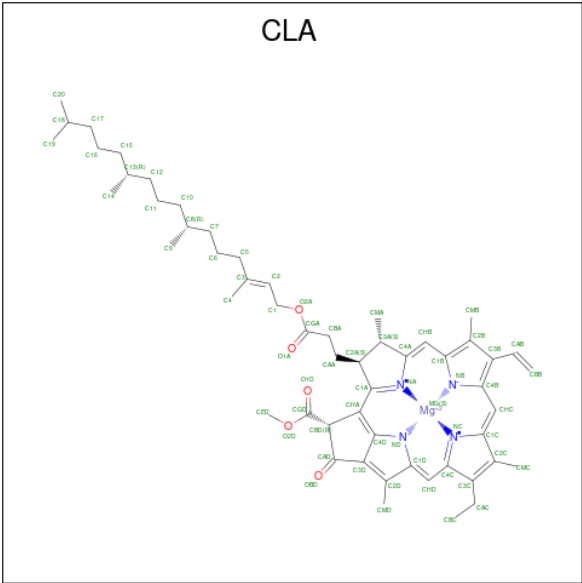
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	2	Total	Cl	0	0
			2	2		
24	a	2	Total	Cl	0	0
			2	2		

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



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

- Molecule 26 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

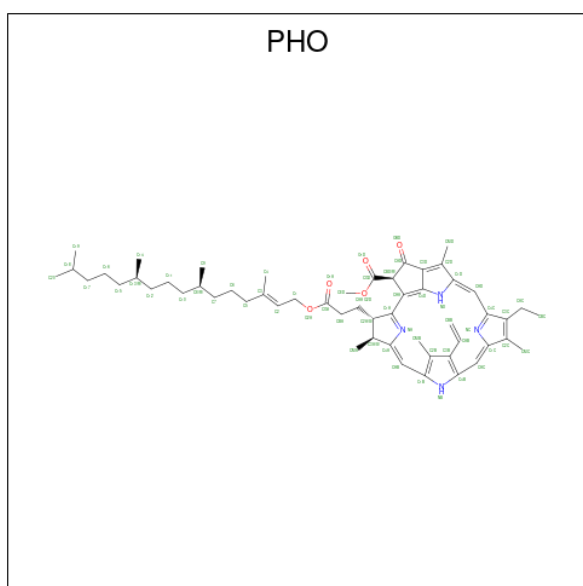
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N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

Continued on next page...

Continued from previous page...

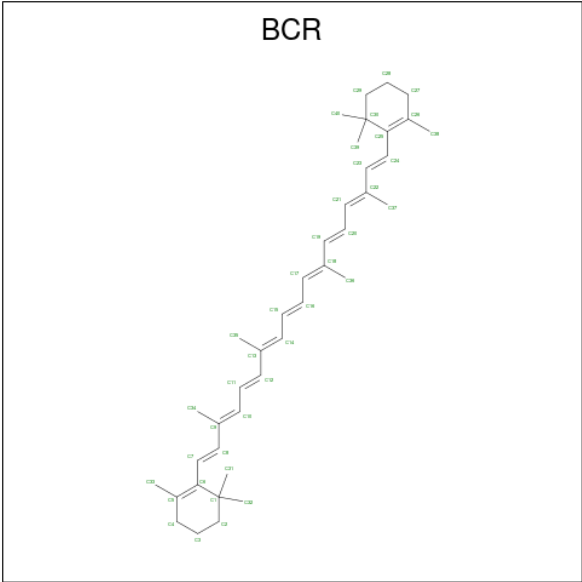
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

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



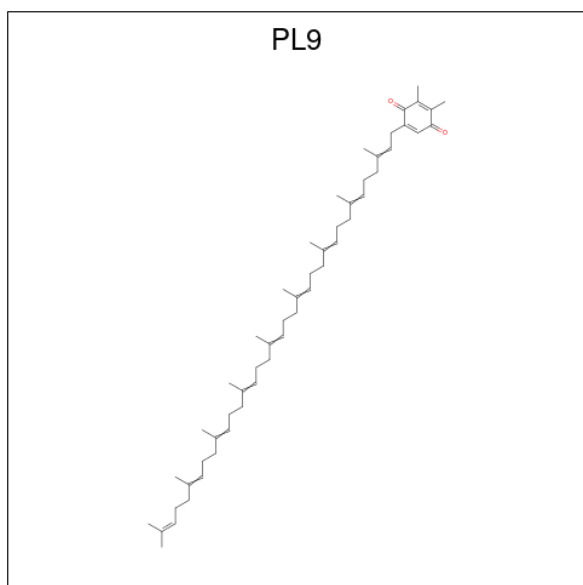
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C 40 40	0	0
28	B	1	Total C 40 40	0	0
28	B	1	Total C 40 40	0	0
28	B	1	Total C 40 40	0	0
28	C	1	Total C 40 40	0	0
28	D	1	Total C 40 40	0	0
28	K	1	Total C 40 40	0	0
28	K	1	Total C 40 40	0	0
28	K	1	Total C 40 40	0	0
28	T	1	Total C 40 40	0	0
28	X	1	Total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

Continued on next page...

Continued from previous page...

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

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



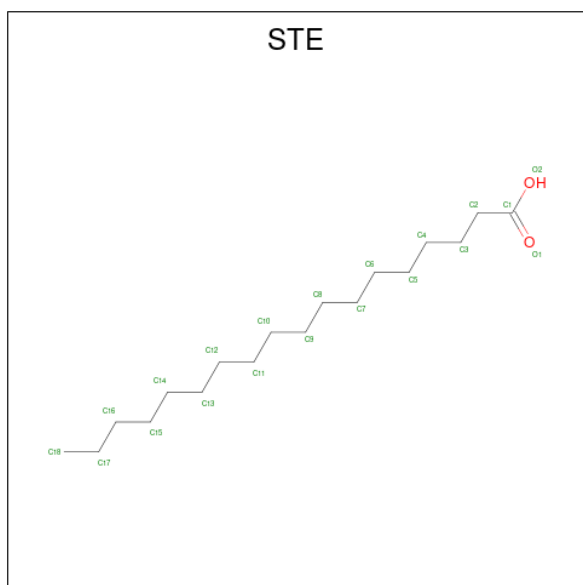
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 55 53 2	0	0
29	D	1	Total C O 55 53 2	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 30 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C		0	0
			9	9			
30	A	1	Total	C		0	0
			8	8			
30	A	1	Total	C		0	0
			17	17			
30	A	1	Total	C		0	0
			11	11			
30	B	1	Total	C	O	0	0
			17	15	2		
30	B	1	Total	C	O	0	0
			18	16	2		
30	B	1	Total	C	O	0	0
			12	10	2		
30	B	1	Total	C		0	0
			15	15			
30	C	1	Total	C	O	0	0
			14	12	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	C	1	Total C 5 5	0	0
30	C	1	Total C 7 7	0	0
30	C	1	Total C 10 10	0	0
30	C	1	Total C O 12 10 2	0	0
30	C	1	Total C 16 16	0	0
30	C	1	Total C 14 14	0	0
30	D	1	Total C O 20 18 2	0	0
30	E	1	Total C O 12 10 2	0	0
30	E	1	Total C 12 12	0	0
30	E	1	Total C O 20 18 2	0	0
30	H	1	Total C 18 18	0	0
30	H	1	Total C 9 9	0	0
30	I	1	Total C O 17 15 2	0	0
30	I	1	Total C O 15 13 2	0	0
30	J	1	Total C O 12 10 2	0	0
30	K	1	Total C 14 14	0	0
30	M	1	Total C O 15 13 2	0	0
30	M	1	Total C 10 10	0	0
30	M	1	Total C 15 15	0	0
30	T	1	Total C 16 16	0	0
30	Z	1	Total C 17 17	0	0

Continued on next page...

Continued from previous page...

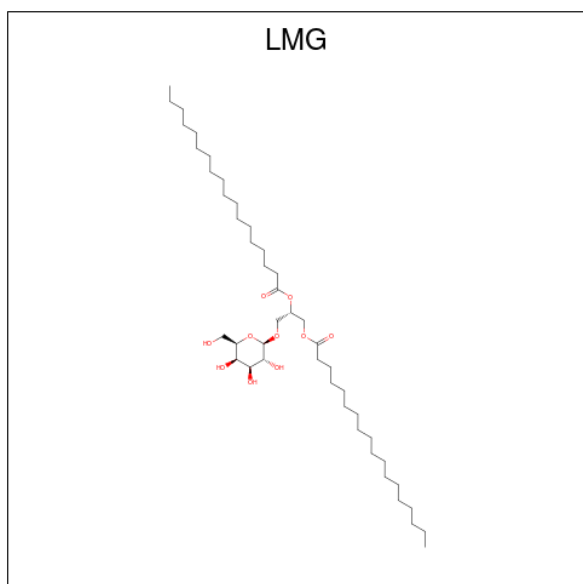
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	a	1	Total C 10 10	0	0
30	a	1	Total C O 12 10 2	0	0
30	b	1	Total C O 20 18 2	0	0
30	b	1	Total C O 16 14 2	0	0
30	b	1	Total C 10 10	0	0
30	c	1	Total C 13 13	0	0
30	c	1	Total C 18 18	0	0
30	d	1	Total C O 20 18 2	0	0
30	d	1	Total C O 20 18 2	0	0
30	d	1	Total C O 20 18 2	0	0
30	e	1	Total C 9 9	0	0
30	e	1	Total C 8 8	0	0
30	e	1	Total C 9 9	0	0
30	e	1	Total C O 13 11 2	0	0
30	h	1	Total C 10 10	0	0
30	h	1	Total C 11 11	0	0
30	i	1	Total C O 12 10 2	0	0
30	i	1	Total C 6 6	0	0
30	j	1	Total C O 12 10 2	0	0
30	j	1	Total C 16 16	0	0
30	k	1	Total C O 14 12 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	m	1	Total C O 12 10 2	0	0
30	m	1	Total C 18 18	0	0
30	t	1	Total C O 14 12 2	0	0
30	z	1	Total C 9 9	0	0

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



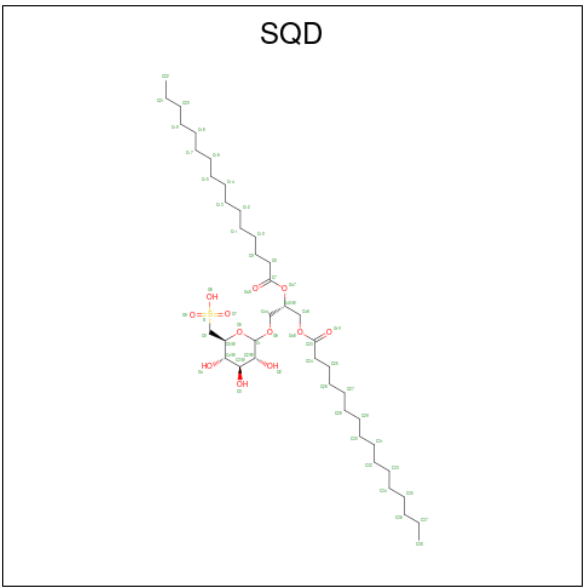
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 48 38 10	0	0
31	B	1	Total C O 45 35 10	0	0
31	C	1	Total C O 36 26 10	0	0
31	C	1	Total C O 48 38 10	0	0
31	D	1	Total C O 50 40 10	0	0
31	D	1	Total C O 51 41 10	0	0
31	M	1	Total C O 51 41 10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	a	1	Total	C	O	0	0
			55	45	10		
31	b	1	Total	C	O	0	0
			55	45	10		
31	c	1	Total	C	O	0	0
			30	25	5		
31	c	1	Total	C	O	0	0
			46	36	10		
31	c	1	Total	C	O	0	0
			48	38	10		
31	c	1	Total	C	O	0	0
			49	39	10		
31	d	1	Total	C	O	0	0
			44	34	10		
31	m	1	Total	C	O	0	0
			51	41	10		

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



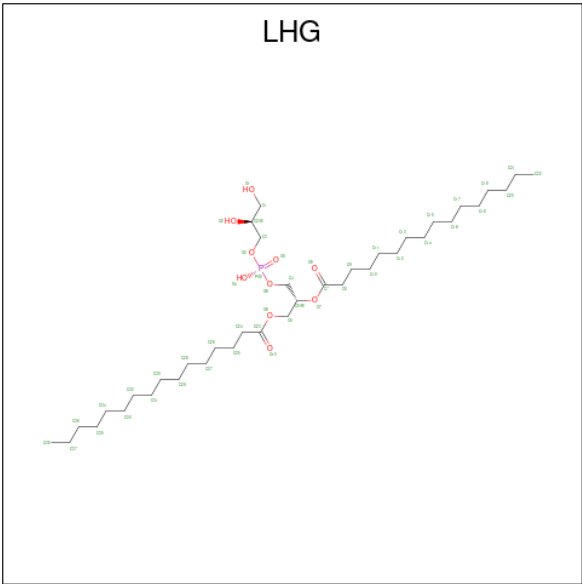
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	O	S	0	0
			52	39	12	1		
32	A	1	Total	C	O	S	0	0
			43	30	12	1		
32	B	1	Total	C	O	S	0	0
			54	41	12	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	F	1	Total	C	O	S	0	0
			36	25	10	1		
32	a	1	Total	C	O	S	0	0
			54	41	12	1		
32	a	1	Total	C	O	S	0	0
			54	41	12	1		
32	b	1	Total	C	O	S	0	0
			49	36	12	1		
32	f	1	Total	C	O	S	0	0
			41	28	12	1		

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



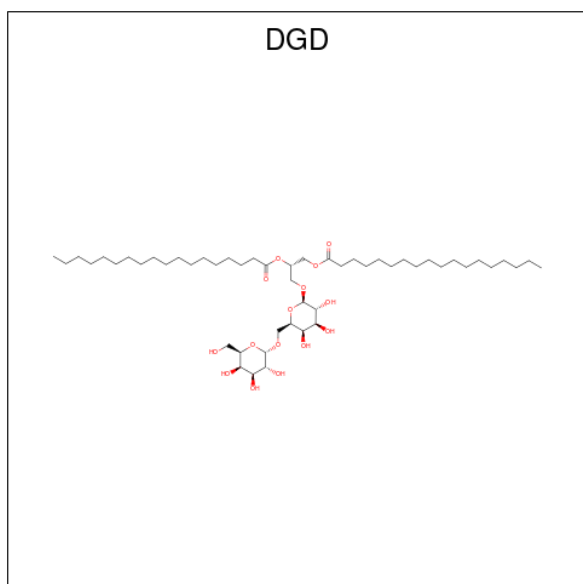
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	A	1	Total	C	O	P	0	0
			49	38	10	1		
33	D	1	Total	C	O	P	0	0
			49	38	10	1		
33	D	1	Total	C	O	P	0	0
			47	36	10	1		
33	D	1	Total	C	O	P	0	0
			49	38	10	1		
33	L	1	Total	C	O	P	0	0
			49	38	10	1		
33	a	1	Total	C	O	P	0	0
			39	28	10	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	a	1	Total	C	O	P	0	0
			42	31	10	1		
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	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



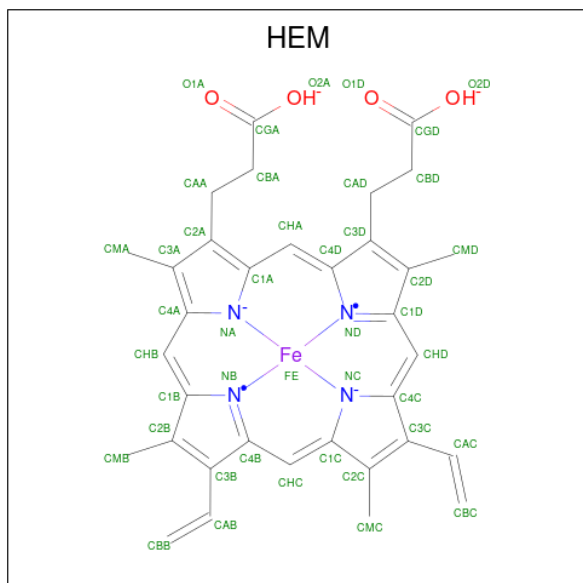
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	A	1	Total	C	O	0	0
			66	51	15		
34	C	1	Total	C	O	0	0
			62	47	15		
34	C	1	Total	C	O	0	0
			62	47	15		
34	C	1	Total	C	O	0	0
			62	47	15		
34	H	1	Total	C	O	0	0
			62	47	15		
34	c	1	Total	C	O	0	0
			62	47	15		
34	c	1	Total	C	O	0	0
			62	47	15		

Continued on next page...

Continued from previous page...

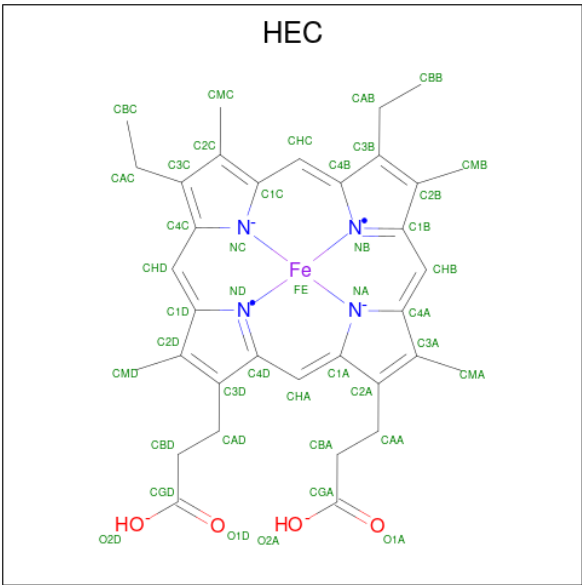
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	c	1	Total 62	C 47	O 15	0	0
34	h	1	Total 62	C 47	O 15	0	0

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



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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
36	V	1	Total	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	154	Total	O	0	4
			158	158		
37	B	268	Total	O	0	0
			268	268		
37	C	194	Total	O	0	0
			194	194		
37	D	137	Total	O	0	0
			137	137		
37	E	42	Total	O	0	0
			42	42		
37	F	6	Total	O	0	0
			6	6		
37	H	38	Total	O	0	0
			38	38		
37	I	13	Total	O	0	0
			13	13		
37	J	13	Total	O	0	0
			13	13		
37	K	6	Total	O	0	0
			6	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	L	9	Total O 9 9	0	0
37	M	13	Total O 13 13	0	0
37	O	139	Total O 139 139	0	0
37	T	12	Total O 12 12	0	0
37	U	53	Total O 53 53	0	0
37	V	87	Total O 87 87	0	0
37	X	12	Total O 12 12	0	0
37	Z	4	Total O 4 4	0	0
37	R	4	Total O 4 4	0	0
37	a	140	Total O 144 144	0	4
37	b	255	Total O 255 255	0	0
37	c	202	Total O 202 202	0	0
37	d	138	Total O 138 138	0	0
37	e	25	Total O 25 25	0	0
37	f	8	Total O 8 8	0	0
37	h	22	Total O 22 22	0	0
37	i	11	Total O 11 11	0	0
37	j	14	Total O 14 14	0	0
37	k	7	Total O 7 7	0	0
37	l	16	Total O 16 16	0	0
37	m	22	Total O 22 22	0	0

Continued on next page...

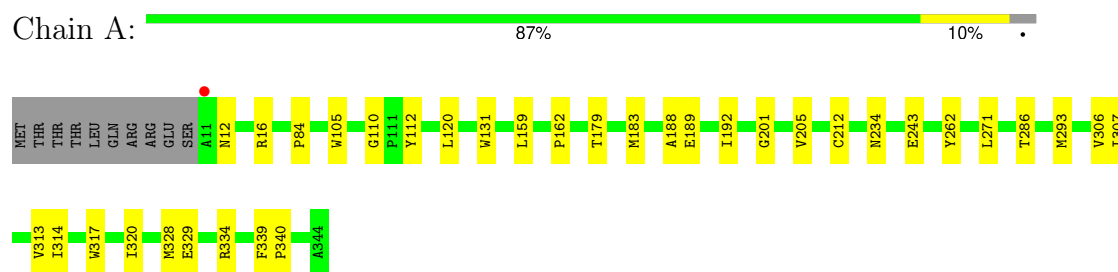
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	o	128	Total 128	O 128	0	0
37	t	12	Total 12	O 12	0	0
37	u	72	Total 72	O 72	0	0
37	v	76	Total 76	O 76	0	0
37	y	8	Total 8	O 8	0	0
37	x	15	Total 15	O 15	0	0
37	z	8	Total 8	O 8	0	0
37	r	2	Total 2	O 2	0	0

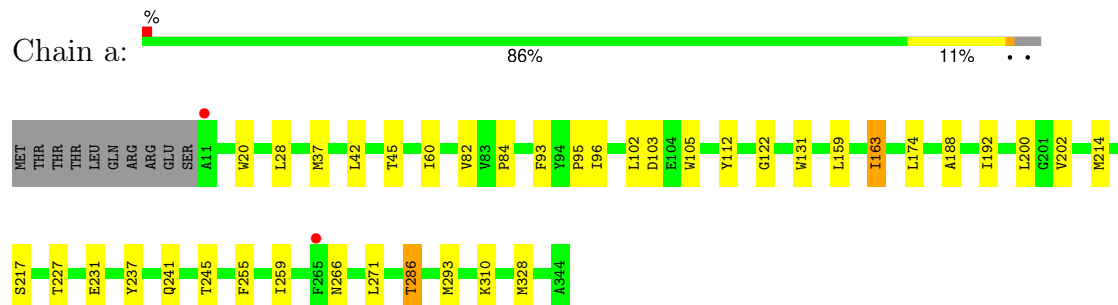
3 Residue-property plots [i](#)

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.

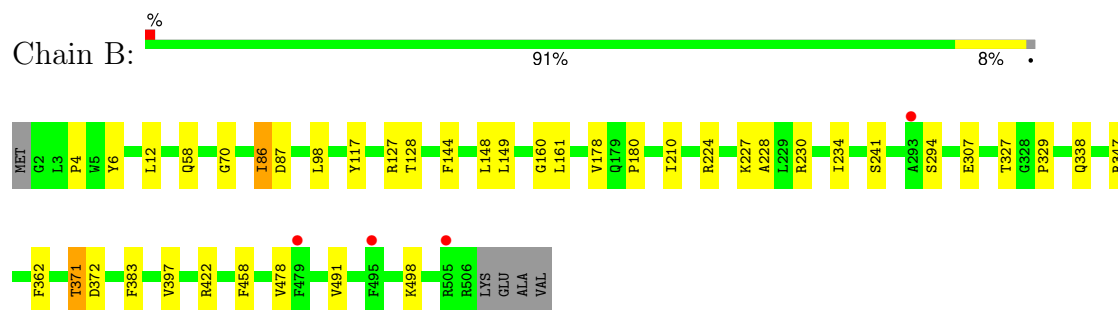
- Molecule 1: Photosystem II protein D1 1



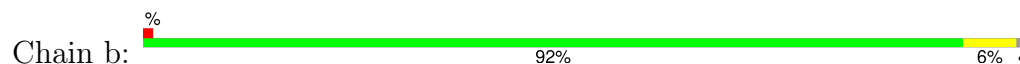
- Molecule 1: Photosystem II protein D1 1

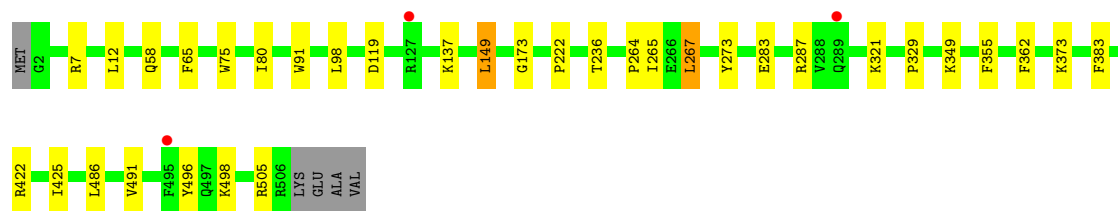


- Molecule 2: Photosystem II CP47 reaction center protein



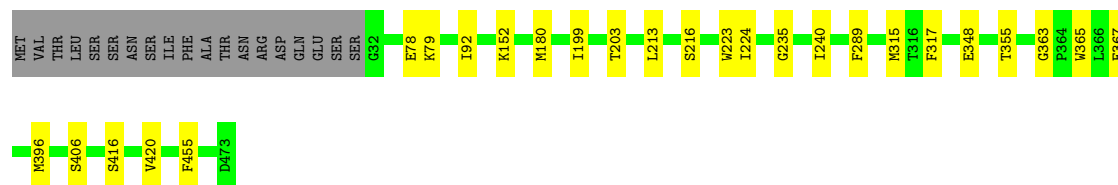
- Molecule 2: Photosystem II CP47 reaction center protein





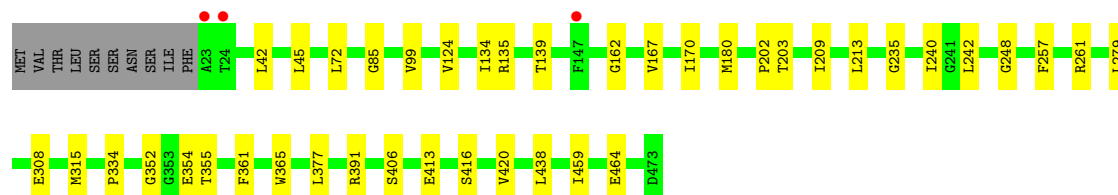
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 90% 6% .



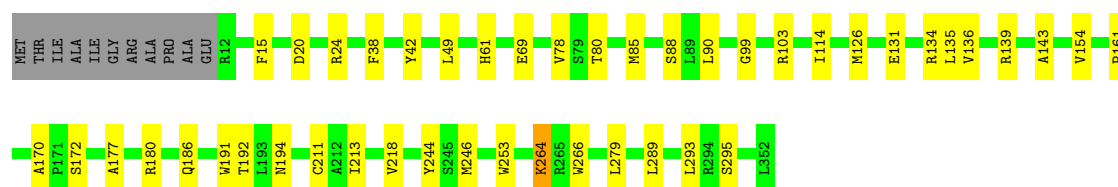
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 89% 9% .



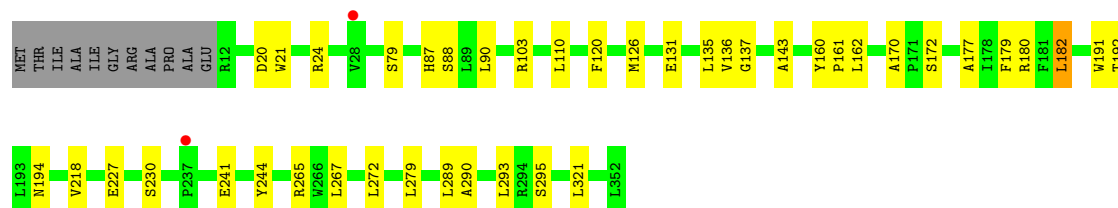
- Molecule 4: Photosystem II D2 protein

Chain D: 84% 13% .

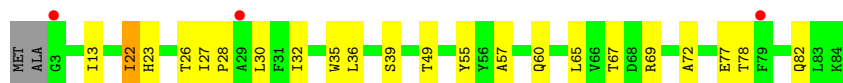


- Molecule 4: Photosystem II D2 protein

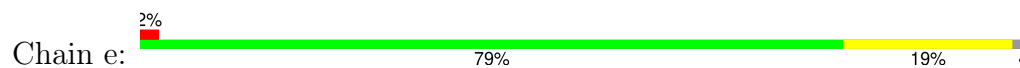
Chain d: 85% 12% .



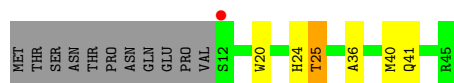
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta



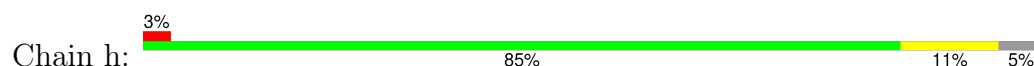
- Molecule 6: Cytochrome b559 subunit beta



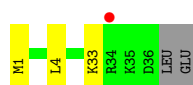
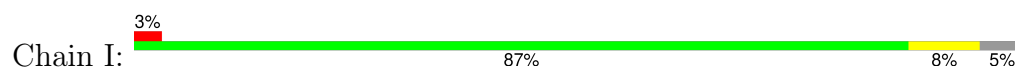
- Molecule 7: Photosystem II reaction center protein H



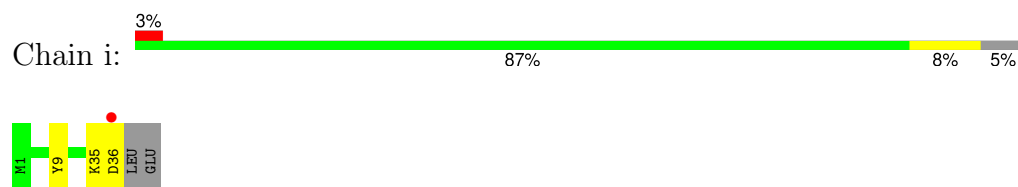
- Molecule 7: Photosystem II reaction center protein H



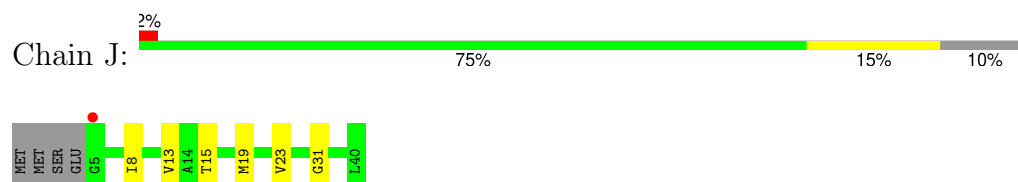
- Molecule 8: Photosystem II reaction center protein I



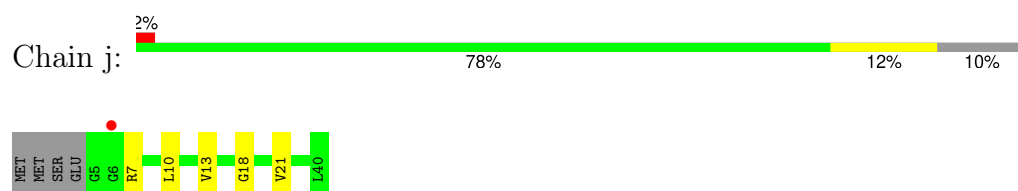
- Molecule 8: Photosystem II reaction center protein I



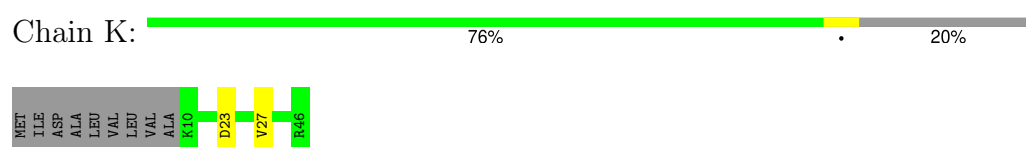
- Molecule 9: Photosystem II reaction center protein J



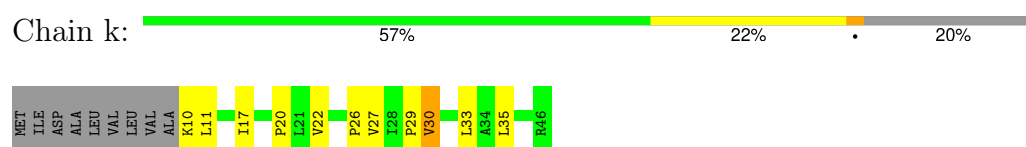
- Molecule 9: Photosystem II reaction center protein J



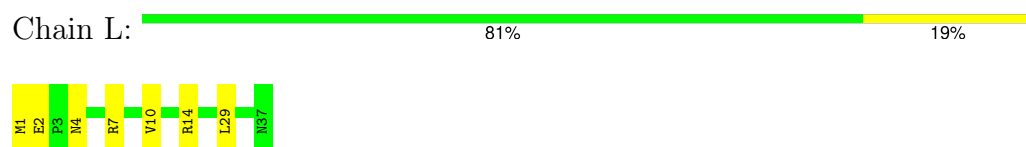
- Molecule 10: Photosystem II reaction center protein K



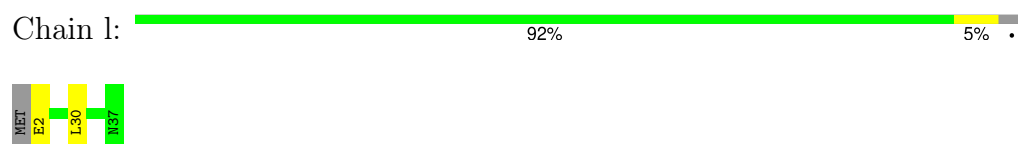
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M

Chain M:  69% 19% 8%



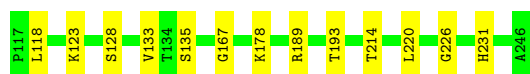
- Molecule 12: Photosystem II reaction center protein M

Chain m:  69% 19% 11%



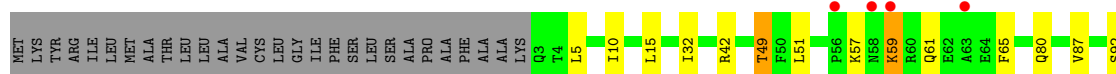
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  79% 11% 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  81% 8% 10%



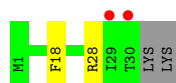
- Molecule 14: Photosystem II reaction center protein T

Chain T:  81% 12% 6%



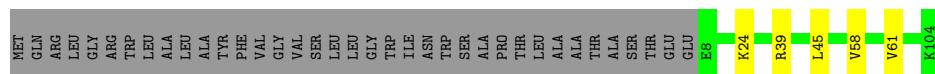
- Molecule 14: Photosystem II reaction center protein T

Chain t:  88% 6% 6%



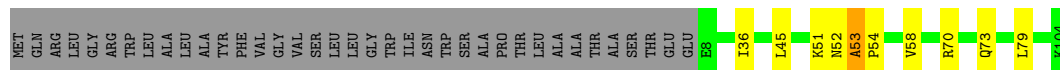
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  69% 28%



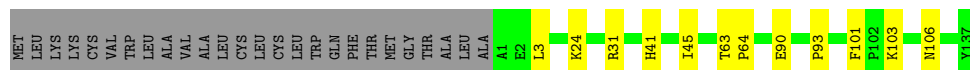
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  65% 7% 28%



- Molecule 16: Cytochrome c-550

Chain V:  77% 7% 16%



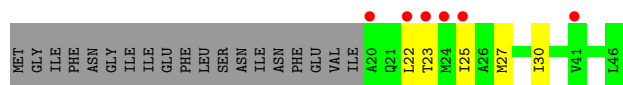
- Molecule 16: Cytochrome c-550

Chain v:  71% 12% 16%



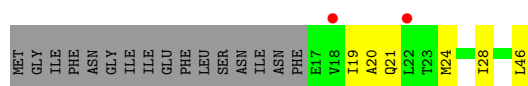
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:  13% 48% 11% 41%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  4% 52% 13% 35%



- Molecule 18: Photosystem II reaction center X protein

Chain X:  5% 80% 12% 7%



- Molecule 18: Photosystem II reaction center X protein

Chain x: 85% 10% 5%



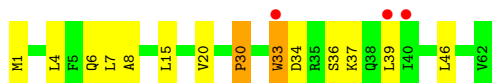
- Molecule 19: Photosystem II reaction center protein Z

Chain Z: 15% 95% 5%



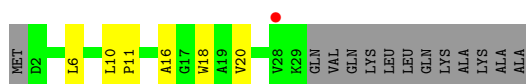
- Molecule 19: Photosystem II reaction center protein Z

Chain z: 5% 77% 19%



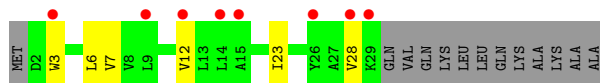
- Molecule 20: Photosystem II protein Y

Chain R: 2% 54% 15% 32%



- Molecule 20: Photosystem II protein Y

Chain r: 20% 54% 15% 32%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.58Å 222.82Å 309.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.85 – 2.11 37.85 – 2.11	Depositor EDS
% Data completeness (in resolution range)	98.0 (37.85-2.11) 82.4 (37.85-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.37 (at 2.12Å)	Xtriage
Refinement program	PHENIX 2.0_5848	Depositor
R, R_{free}	0.194 , 0.234 0.194 , 0.234	Depositor DCC
R_{free} test set	4113 reflections (0.65%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 62.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	54355	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: STE, DGD, LMG, PL9, FME, BCT, CLA, SQD, CL, BCR, LHG, OEX, HEM, OEY, HEC, FE2, PHO

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	0.32	0/3252	0.48	0/4430
1	a	0.31	0/3249	0.46	0/4426
2	B	0.33	0/4166	0.47	0/5675
2	b	0.32	0/4127	0.46	0/5623
3	C	0.32	0/3625	0.46	0/4935
3	c	0.31	0/3705	0.45	0/5042
4	D	0.34	0/2902	0.49	0/3951
4	d	0.33	0/2911	0.48	0/3963
5	E	0.27	0/688	0.43	0/940
5	e	0.24	0/683	0.43	0/932
6	F	0.26	0/284	0.39	0/387
6	f	0.26	0/284	0.49	0/387
7	H	0.32	0/517	0.48	0/705
7	h	0.28	0/505	0.45	0/689
8	I	0.33	0/293	0.49	0/396
8	i	0.33	0/293	0.41	0/396
9	J	0.27	0/263	0.43	0/356
9	j	0.25	0/263	0.42	0/356
10	K	0.26	0/303	0.46	0/416
10	k	0.26	0/303	0.46	0/416
11	L	0.36	0/311	0.48	0/422
11	l	0.35	0/303	0.44	0/412
12	M	0.31	0/249	0.47	0/341
12	m	0.32	0/244	0.53	0/334
13	O	0.31	0/1904	0.52	0/2585
13	o	0.32	0/1905	0.50	0/2583
14	T	0.36	0/257	0.53	0/349
14	t	0.33	0/255	0.40	0/346
15	U	0.28	0/785	0.44	0/1064
15	u	0.29	0/785	0.51	0/1064
16	V	0.32	0/1085	0.51	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.28	0/1085	0.45	0/1473
17	Y	0.21	0/197	0.35	0/264
17	y	0.21	0/219	0.38	0/294
18	X	0.26	0/284	0.40	0/384
18	x	0.22	0/289	0.37	0/391
19	Z	0.22	0/490	0.43	0/669
19	z	0.21	0/488	0.40	0/666
20	R	0.20	0/227	0.36	0/313
20	r	0.23	0/227	0.35	0/313
All	All	0.31	0/44205	0.47	0/60161

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3152	0	3015	27	0
1	a	3149	0	3006	32	0
2	B	4016	0	3883	29	0
2	b	3984	0	3842	26	0
3	C	3509	0	3426	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3583	0	3499	25	0
4	D	2805	0	2702	37	0
4	d	2811	0	2708	29	0
5	E	666	0	651	18	0
5	e	664	0	648	15	0
6	F	275	0	282	5	0
6	f	275	0	282	8	0
7	H	505	0	528	2	0
7	h	493	0	514	4	0
8	I	296	0	311	1	0
8	i	296	0	311	2	0
9	J	257	0	268	5	0
9	j	257	0	268	5	0
10	K	293	0	305	2	0
10	k	293	0	305	7	0
11	L	304	0	316	5	0
11	l	296	0	304	1	0
12	M	256	0	269	7	0
12	m	251	0	267	6	0
13	O	1870	0	1830	18	0
13	o	1874	0	1846	19	0
14	T	258	0	261	5	0
14	t	256	0	256	2	0
15	U	774	0	773	1	0
15	u	774	0	773	9	0
16	V	1064	0	1073	8	0
16	v	1064	0	1073	16	0
17	Y	196	0	217	3	0
17	y	218	0	241	6	0
18	X	281	0	312	5	0
18	x	286	0	314	2	0
19	Z	479	0	516	2	0
19	z	477	0	509	10	0
20	R	221	0	238	5	0
20	r	221	0	238	4	0
21	A	11	0	0	2	0
21	a	11	0	0	1	0
22	A	10	0	0	0	0
22	a	10	0	0	0	0
23	A	1	0	0	0	0
23	a	1	0	0	0	0
24	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	2	0	0	0	0
25	A	4	0	1	0	0
25	a	4	0	1	0	0
26	A	249	0	264	10	0
26	B	1035	0	1139	24	0
26	C	839	0	922	14	0
26	D	130	0	144	2	0
26	a	260	0	288	9	0
26	b	1035	0	1139	27	0
26	c	839	0	919	24	0
26	d	130	0	144	1	0
27	A	64	0	74	2	0
27	D	64	0	74	0	0
27	a	64	0	74	1	0
27	d	64	0	74	3	0
28	A	40	0	56	0	0
28	B	120	0	168	2	0
28	C	40	0	56	2	0
28	D	40	0	56	3	0
28	K	120	0	168	3	0
28	T	40	0	56	5	0
28	X	40	0	56	3	0
28	a	40	0	56	0	0
28	b	120	0	168	5	0
28	c	80	0	112	2	0
28	d	40	0	56	1	0
28	h	40	0	56	3	0
28	k	80	0	112	3	0
28	t	40	0	56	3	0
29	A	55	0	80	7	0
29	D	55	0	80	1	0
29	a	55	0	80	5	0
29	d	55	0	80	1	0
30	A	45	0	83	5	0
30	B	62	0	96	4	0
30	C	78	0	126	0	0
30	D	20	0	35	3	0
30	E	44	0	74	3	0
30	H	27	0	52	1	0
30	I	32	0	48	1	0
30	J	12	0	16	0	0
30	K	14	0	27	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	M	40	0	67	1	0
30	T	16	0	31	2	0
30	Z	17	0	33	1	0
30	a	22	0	32	2	0
30	b	46	0	75	2	0
30	c	31	0	57	1	0
30	d	60	0	105	6	0
30	e	39	0	67	1	0
30	h	21	0	40	2	0
30	i	18	0	24	1	0
30	j	28	0	47	0	0
30	k	14	0	20	0	0
30	m	30	0	51	3	0
30	t	14	0	20	0	0
30	z	9	0	14	1	0
31	A	48	0	66	3	0
31	B	45	0	60	5	0
31	C	84	0	106	4	0
31	D	101	0	142	13	0
31	M	51	0	72	3	0
31	a	55	0	86	5	0
31	b	55	0	86	0	0
31	c	173	0	240	5	0
31	d	44	0	58	0	0
31	m	51	0	72	2	0
32	A	95	0	124	0	0
32	B	54	0	78	2	0
32	F	36	0	46	1	0
32	a	108	0	156	4	0
32	b	49	0	65	1	0
32	f	41	0	49	0	0
33	A	49	0	74	5	0
33	D	145	0	215	8	0
33	L	49	0	74	1	0
33	a	81	0	108	3	0
33	b	49	0	74	0	0
33	d	49	0	74	0	0
33	l	49	0	74	1	0
34	A	66	0	96	4	0
34	C	186	0	246	7	0
34	H	62	0	82	0	0
34	c	186	0	246	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	h	62	0	82	2	0
35	F	43	0	30	3	0
35	e	43	0	30	2	0
36	V	43	0	30	0	0
36	v	43	0	30	0	0
37	A	158	0	0	7	0
37	B	268	0	0	3	0
37	C	194	0	0	2	0
37	D	137	0	0	5	0
37	E	42	0	0	1	0
37	F	6	0	0	0	0
37	H	38	0	0	1	0
37	I	13	0	0	0	0
37	J	13	0	0	2	0
37	K	6	0	0	0	0
37	L	9	0	0	1	0
37	M	13	0	0	1	0
37	O	139	0	0	5	0
37	R	4	0	0	2	0
37	T	12	0	0	0	0
37	U	53	0	0	0	0
37	V	87	0	0	1	0
37	X	12	0	0	0	0
37	Z	4	0	0	0	0
37	a	144	0	0	7	0
37	b	255	0	0	9	0
37	c	202	0	0	3	0
37	d	138	0	0	2	0
37	e	25	0	0	3	0
37	f	8	0	0	1	0
37	h	22	0	0	2	0
37	i	11	0	0	0	0
37	j	14	0	0	0	0
37	k	7	0	0	0	0
37	l	16	0	0	2	0
37	m	22	0	0	3	0
37	o	128	0	0	5	0
37	r	2	0	0	0	0
37	t	12	0	0	0	0
37	u	72	0	0	2	0
37	v	76	0	0	1	0
37	x	15	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	y	8	0	0	1	0
37	z	8	0	0	3	0
All	All	54355	0	53500	557	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 (557) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:102:LEU:H	31:a:618:LMG:H121	1.43	0.83
7:H:7:LEU:HB3	37:H:201:HOH:O	1.81	0.81
33:D:410:LHG:H152	33:L:101:LHG:H281	1.62	0.79
35:F:101:HEM:HBC2	35:F:101:HEM:HHD	1.67	0.77
3:c:180:MET:HE1	31:c:523:LMG:HC72	1.67	0.76
28:t:101:BCR:HC8	28:t:101:BCR:H311	1.67	0.75
26:A:608:CLA:H172	29:A:612:PL9:H23	1.69	0.75
26:b:615:CLA:H2	26:b:616:CLA:HBB2	1.69	0.74
21:A:601[B]:OEY:O5	21:A:601[B]:OEY:O6	2.08	0.72
2:B:491:VAL:HG12	4:D:136:VAL:HG13	1.72	0.72
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.55	0.72
9:J:15:THR:HG22	9:J:19:MET:HE2	1.71	0.71
26:b:615:CLA:HHC	26:b:615:CLA:HBB1	1.72	0.70
31:B:620:LMG:HC92	31:D:406:LMG:H152	1.74	0.69
21:a:601[B]:OEY:O5	21:a:601[B]:OEY:O6	2.11	0.68
35:e:102:HEM:HHD	35:e:102:HEM:HBC2	1.76	0.68
28:T:101:BCR:H311	28:T:101:BCR:HC8	1.74	0.68
17:Y:23:THR:HG22	17:Y:27:MET:HE3	1.75	0.68
26:C:502:CLA:H61	26:C:512:CLA:H42	1.77	0.67
31:B:620:LMG:HC71	4:D:134:ARG:HG2	1.77	0.66
19:z:36:SER:HA	19:z:39:LEU:HD23	1.78	0.66
13:o:10:ILE:HG23	37:o:301:HOH:O	1.96	0.66
13:o:15:LEU:HB2	37:o:301:HOH:O	1.96	0.66
4:D:15:PHE:HE2	31:D:406:LMG:H121	1.61	0.65
3:C:78:GLU:HG2	16:V:106:ASN:HD22	1.63	0.64
19:z:4:LEU:HA	19:z:7:LEU:HB2	1.80	0.64
15:u:70:ARG:NH1	15:u:73:GLN:HE21	1.96	0.64
37:A:719:HOH:O	13:O:69:LYS:HB3	1.98	0.64
35:e:102:HEM:HHC	35:e:102:HEM:HBB2	1.80	0.63
19:z:34:ASP:HA	19:z:37:LYS:HD3	1.81	0.63
37:A:702:HOH:O	4:D:264:LYS:HD3	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.79	0.63
5:e:17:VAL:H	9:j:7:ARG:HD2	1.64	0.63
3:C:213:LEU:HG	26:C:506:CLA:H193	1.79	0.63
2:b:498:LYS:HE3	4:d:20:ASP:HA	1.81	0.62
26:c:501:CLA:H192	26:c:507:CLA:HBB1	1.80	0.62
2:B:241:SER:HB3	26:B:612:CLA:HED3	1.82	0.62
2:b:91:TRP:HE1	30:b:621:STE:H41	1.64	0.62
3:c:42:LEU:HD21	26:c:511:CLA:H2A	1.81	0.62
30:A:621:STE:H162	30:A:622:STE:H122	1.82	0.62
12:M:31:SER:HB3	37:m:204:HOH:O	1.98	0.62
13:O:5:LEU:HD13	13:O:10:ILE:HD11	1.81	0.62
1:a:20:TRP:HB2	30:a:620:STE:H22	1.82	0.62
2:b:264:PRO:HG2	2:b:267:LEU:HD22	1.81	0.61
1:a:237:TYR:HB2	1:a:245:THR:HG21	1.81	0.61
26:a:610:CLA:H111	26:a:610:CLA:H52	1.82	0.61
31:D:406:LMG:H341	31:D:406:LMG:H132	1.81	0.61
26:a:610:CLA:H171	8:i:9:TYR:HB3	1.83	0.61
34:A:619:DGD:HD5	2:b:75:TRP:HB3	1.81	0.61
29:A:612:PL9:H361	6:F:25:THR:HG21	1.84	0.60
28:X:101:BCR:H331	28:X:101:BCR:HC8	1.83	0.60
5:e:30:LEU:HD23	20:r:12:VAL:HG12	1.83	0.60
1:a:103:ASP:OD2	31:a:618:LMG:H112	2.01	0.60
27:A:609:PHO:HBC3	4:D:279:LEU:HD22	1.82	0.59
1:a:84:PRO:HA	1:a:112:TYR:CG	2.37	0.59
4:D:69:GLU:HG3	37:D:502:HOH:O	2.02	0.59
37:f:207:HOH:O	16:v:30:LYS:HE3	2.02	0.59
34:C:522:DGD:HAH1	31:D:407:LMG:H212	1.83	0.59
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.83	0.59
30:d:410:STE:H32	18:x:12:ILE:HG21	1.85	0.58
15:u:53:ALA:HB1	15:u:54:PRO:HD2	1.83	0.58
1:A:271:LEU:HD11	29:A:612:PL9:HC71	1.85	0.58
30:d:408:STE:H101	30:h:104:STE:H162	1.84	0.58
6:f:26:LEU:O	6:f:29:PRO:HD2	2.03	0.58
2:B:227:LYS:HD3	31:B:620:LMG:O3	2.04	0.58
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.04	0.58
28:h:101:BCR:HC8	28:h:101:BCR:H331	1.85	0.58
26:c:501:CLA:C3D	26:c:503:CLA:H2	2.34	0.58
16:v:60:ALA:HA	37:v:302:HOH:O	2.03	0.58
29:a:612:PL9:HC2	37:a:831:HOH:O	2.04	0.57
26:B:615:CLA:H2	26:B:616:CLA:HBB2	1.85	0.57
3:c:438:LEU:HD11	26:c:505:CLA:HBB1	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:1:FME:HCN	30:T:102:STE:H102	1.86	0.57
32:B:622:SQD:H172	32:B:622:SQD:H352	1.87	0.57
4:D:246:MET:HE3	4:D:264:LYS:HE2	1.87	0.57
13:O:189:ARG:NH1	13:O:226:GLY:HA3	2.20	0.57
3:c:377:LEU:H	13:o:80:GLN:HE22	1.53	0.57
30:D:411:STE:H102	18:X:16:SER:HB3	1.87	0.57
15:U:58:VAL:O	15:U:61:VAL:HG22	2.04	0.57
1:a:28:LEU:HD22	37:d:541:HOH:O	2.05	0.57
4:D:69:GLU:HG2	5:E:55:TYR:OH	2.05	0.56
31:B:620:LMG:HC2	31:D:406:LMG:O2	2.04	0.56
4:d:103:ARG:HG3	5:e:73:LYS:HE2	1.88	0.56
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.40	0.56
1:a:102:LEU:N	31:a:618:LMG:H121	2.18	0.56
29:a:612:PL9:H38	29:a:612:PL9:H472	1.88	0.56
13:o:92:SER:HB3	13:o:131:PRO:HA	1.86	0.56
37:a:779:HOH:O	4:d:230:SER:HB2	2.06	0.56
1:a:227:THR:HB	1:a:231:GLU:HG3	1.88	0.55
2:B:498:LYS:HE2	31:D:406:LMG:HC62	1.88	0.55
31:D:406:LMG:H111	37:D:526:HOH:O	2.06	0.55
31:a:618:LMG:H142	31:a:618:LMG:H291	1.88	0.55
28:B:618:BCR:H363	28:t:101:BCR:H19C	1.89	0.55
30:B:623:STE:H21	12:M:6:LEU:HD11	1.89	0.54
3:C:152:LYS:HE3	37:C:684:HOH:O	2.07	0.54
37:B:810:HOH:O	31:D:406:LMG:HC3	2.06	0.54
5:E:57:ALA:HB3	5:E:60:GLN:HB3	1.90	0.54
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.88	0.54
1:a:122:GLY:HA2	37:a:761:HOH:O	2.08	0.54
3:c:391[B]:ARG:HH11	3:c:391[B]:ARG:HB2	1.72	0.54
16:v:104:MET:HA	16:v:107:LEU:HD22	1.90	0.54
19:z:8:ALA:HB3	37:z:205:HOH:O	2.07	0.54
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	1.89	0.54
1:a:245:THR:HB	4:d:265:ARG:HE	1.73	0.54
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.42	0.54
16:v:110:LYS:HE3	16:v:111:ASP:OD1	2.07	0.54
33:D:409:LHG:H141	33:D:409:LHG:H341	1.90	0.54
2:B:327:THR:HG21	31:M:101:LMG:H291	1.90	0.53
30:d:406:STE:H31	30:d:408:STE:H81	1.89	0.53
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.90	0.53
2:B:307:GLU:OE1	13:o:59:LYS:HD3	2.07	0.53
4:D:99:GLY:HA3	30:D:411:STE:H21	1.90	0.53
1:a:214:MET:HE2	27:d:401:PHO:HED3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:615:CLA:H2	26:b:616:CLA:CBB	2.38	0.53
16:v:28:GLU:HG2	16:v:110:LYS:NZ	2.23	0.53
16:v:76:MET:HE2	16:v:112:LEU:HD22	1.89	0.53
3:c:134:ILE:HD12	26:c:511:CLA:H43	1.89	0.53
10:k:11:LEU:HD11	10:k:22:VAL:HG21	1.91	0.53
31:A:615:LMG:H142	34:C:520:DGD:HA91	1.91	0.53
1:a:245:THR:HG22	37:a:733:HOH:O	2.08	0.53
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.90	0.53
5:e:68:ASP:O	5:e:72:ALA:HB2	2.08	0.53
26:B:604:CLA:H43	26:B:605:CLA:H2	1.90	0.53
30:d:408:STE:H82	30:h:104:STE:H172	1.90	0.53
2:b:12:LEU:HB2	26:b:612:CLA:HMC2	1.91	0.53
1:A:234:ASN:HD21	33:D:410:LHG:HC11	1.74	0.53
2:B:12:LEU:HB2	26:B:612:CLA:HMC2	1.91	0.52
3:C:406:SER:HA	3:C:420:VAL:HG23	1.92	0.52
13:O:107:THR:HG22	37:O:334:HOH:O	2.09	0.52
4:d:192:THR:HG23	26:d:402:CLA:HBC2	1.91	0.52
30:D:411:STE:H31	18:X:12:ILE:HG21	1.91	0.52
16:v:41:HIS:HA	16:v:45:ILE:O	2.10	0.52
30:B:625:STE:H112	37:B:954:HOH:O	2.10	0.52
3:c:213:LEU:HD11	28:c:515:BCR:C20	2.40	0.52
15:u:53:ALA:HB3	37:u:226:HOH:O	2.10	0.52
2:B:230:ARG:NH2	31:B:620:LMG:HC5	2.25	0.52
4:d:21:TRP:O	4:d:24:ARG:HG3	2.10	0.52
1:A:189[B]:GLU:CD	21:A:601[B]:OEY:O6	2.48	0.51
14:t:18:PHE:HB2	28:t:101:BCR:HC8	1.92	0.51
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	1.91	0.51
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.46	0.51
28:T:101:BCR:H352	28:b:618:BCR:H382	1.93	0.51
28:d:404:BCR:H403	28:d:404:BCR:H23C	1.92	0.51
6:f:36:ALA:O	6:f:40:MET:HG3	2.10	0.51
2:b:283:GLU:O	2:b:287:ARG:HG3	2.11	0.51
26:b:608:CLA:H172	26:b:609:CLA:H192	1.91	0.51
5:E:22[A]:ILE:HA	20:R:18:TRP:HE1	1.76	0.51
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.45	0.51
13:O:27:ARG:HG3	37:O:302:HOH:O	2.10	0.51
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.93	0.51
2:b:222:PRO:HB3	7:h:26:GLY:HA3	1.93	0.51
3:C:180:MET:HG2	3:C:199:ILE:O	2.12	0.50
1:a:271:LEU:HD21	29:a:612:PL9:HC71	1.93	0.50
3:c:45:LEU:HA	3:c:139:THR:HG22	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:8:ARG:HD2	5:e:12:ASP:OD1	2.12	0.50
17:y:20:ALA:O	17:y:24:MET:HG2	2.11	0.50
31:C:523:LMG:H191	10:K:27:VAL:HG11	1.93	0.50
20:R:18:TRP:HD1	37:R:103:HOH:O	1.95	0.50
5:e:61:ARG:HA	37:e:211:HOH:O	2.10	0.50
33:D:408:LHG:H321	14:T:21:ILE:HD11	1.94	0.50
9:J:8:ILE:HG22	37:J:202:HOH:O	2.12	0.50
1:a:217:SER:HA	4:d:272:LEU:HD12	1.93	0.50
31:A:615:LMG:HC72	3:C:216:SER:HB2	1.94	0.49
3:c:315:MET:HE2	3:c:365:TRP:HZ3	1.77	0.49
10:k:27:VAL:O	10:k:30:VAL:HG13	2.12	0.49
12:M:20:VAL:HG11	12:m:20:VAL:HG22	1.93	0.49
16:v:13:ASN:HD21	16:v:17:LYS:HB3	1.77	0.49
4:D:186:GLN:HB2	26:D:402:CLA:HBC1	1.94	0.49
2:b:273:TYR:HD2	37:b:721:HOH:O	1.94	0.49
3:c:170:ILE:HD11	31:c:523:LMG:H381	1.93	0.49
1:a:214:MET:HE1	1:a:255:PHE:CE1	2.48	0.49
26:b:602:CLA:H172	34:h:102:DGD:HAE1	1.95	0.49
20:r:3:TRP:O	20:r:7:VAL:HG13	2.13	0.49
1:a:45:THR:HG23	26:a:613:CLA:H201	1.94	0.49
26:c:501:CLA:C2D	26:c:503:CLA:H2	2.43	0.49
19:z:15:LEU:HD22	19:z:46:LEU:HD23	1.94	0.49
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.47	0.49
26:C:506:CLA:H91	26:C:506:CLA:H203	1.94	0.49
4:d:126:MET:HE3	4:d:143:ALA:O	2.12	0.49
13:o:5:LEU:HD13	13:o:10:ILE:HD11	1.95	0.49
1:A:306:VAL:HG12	1:A:314:ILE:HB	1.94	0.48
30:e:103:STE:H162	6:f:43:ILE:HG12	1.95	0.48
1:A:262:TYR:HD1	33:A:617:LHG:H262	1.77	0.48
34:C:521:DGD:HG32	31:C:523:LMG:HC92	1.94	0.48
4:D:61:HIS:HD2	37:D:624:HOH:O	1.97	0.48
1:a:37:MET:HA	37:a:761:HOH:O	2.12	0.48
31:a:618:LMG:H362	31:a:618:LMG:H331	1.56	0.48
1:a:163[A]:ILE:HG13	37:c:780:HOH:O	2.12	0.48
7:h:8:GLY:HA3	37:h:201:HOH:O	2.14	0.48
26:c:503:CLA:H203	26:c:510:CLA:HAB	1.95	0.48
5:E:13:ILE:HA	37:E:202:HOH:O	2.13	0.48
28:T:101:BCR:H341	28:b:618:BCR:H381	1.95	0.48
26:b:612:CLA:H162	26:b:612:CLA:H122	1.66	0.48
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.49	0.48
1:a:286:THR:HG23	26:a:607:CLA:HED3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:79:SER:HA	4:d:172:SER:HB3	1.95	0.48
30:i:101:STE:H61	30:i:101:STE:H32	1.68	0.48
2:b:65:PHE:HE1	26:b:604:CLA:HED2	1.79	0.48
26:b:609:CLA:H141	26:b:609:CLA:H161	1.64	0.48
26:c:504:CLA:H93	26:c:508:CLA:H192	1.95	0.48
3:c:315:MET:HE2	3:c:365:TRP:CZ3	2.49	0.48
26:A:607:CLA:HBD	26:A:614:CLA:HAC2	1.94	0.48
13:o:87:VAL:HG23	37:o:386:HOH:O	2.13	0.48
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.44	0.47
4:D:192:THR:HG23	26:D:402:CLA:HBC2	1.96	0.47
26:c:513:CLA:HBA2	30:c:516:STE:H121	1.96	0.47
31:c:522:LMG:H142	31:c:522:LMG:H292	1.96	0.47
4:d:241:GLU:CD	4:d:241:GLU:H	2.22	0.47
13:o:49:THR:HG23	13:o:236:GLN:HB2	1.96	0.47
2:B:371:THR:HG23	2:B:372:ASP:O	2.14	0.47
5:E:26:THR:HG23	37:R:103:HOH:O	2.13	0.47
33:a:614:LHG:H242	33:a:614:LHG:H272	1.69	0.47
11:l:2:GLU:HB2	37:l:212:HOH:O	2.13	0.47
3:C:363:GLY:O	3:C:367:GLU:HG2	2.15	0.47
31:D:406:LMG:H141	31:D:406:LMG:H172	1.66	0.47
11:L:14:ARG:HB3	14:T:25:GLU:HG2	1.97	0.47
9:j:18:GLY:O	9:j:21:VAL:HG22	2.14	0.47
3:C:455:PHE:HD2	8:I:33:LYS:HG3	1.79	0.47
26:A:607:CLA:CBF	26:A:614:CLA:HAC2	2.45	0.47
5:e:25:ILE:HG12	37:e:201:HOH:O	2.13	0.47
4:D:49:LEU:HD13	28:D:404:BCR:C15	2.45	0.47
26:c:512:CLA:H142	26:c:513:CLA:H111	1.97	0.47
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.44	0.47
5:e:57:ALA:H	5:e:60:GLN:HG2	1.79	0.47
1:A:179[B]:THR:O	1:A:183[B]:MET:HG3	2.15	0.47
30:A:620:STE:H171	37:b:954:HOH:O	2.15	0.47
4:D:15:PHE:CE2	31:D:406:LMG:H121	2.47	0.47
16:V:93:PRO:HA	16:V:101:PHE:CD2	2.49	0.47
2:b:486:LEU:HD11	37:b:765:HOH:O	2.14	0.47
3:c:334:PRO:HA	13:o:153:THR:OG1	2.15	0.47
4:d:180:ARG:NH1	37:d:501:HOH:O	2.47	0.47
31:A:615:LMG:H141	26:C:505:CLA:H203	1.96	0.47
1:A:183[B]:MET:HA	26:A:607:CLA:HMD1	1.97	0.47
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.50	0.47
26:B:611:CLA:H112	26:B:611:CLA:H72	1.62	0.47
26:C:509:CLA:H91	26:C:509:CLA:H112	1.69	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:617:SQD:H302	32:a:617:SQD:H331	1.61	0.47
3:c:459:ILE:HG21	3:c:464:GLU:HG3	1.96	0.47
2:b:98:LEU:HD11	26:b:606:CLA:H152	1.97	0.46
26:b:602:CLA:H112	26:b:602:CLA:H152	1.57	0.46
12:m:23:ILE:HD13	30:m:102:STE:H82	1.97	0.46
29:A:612:PL9:H422	29:A:612:PL9:H401	1.66	0.46
2:B:86:ILE:HG12	2:B:87:ASP:N	2.29	0.46
2:B:228:ALA:HB2	31:D:406:LMG:H322	1.96	0.46
4:D:42:TYR:CE1	6:F:25:THR:HG23	2.50	0.46
26:c:507:CLA:H61	26:c:507:CLA:H41	1.78	0.46
10:k:10:LYS:N	10:k:10:LYS:HE2	2.30	0.46
2:b:329:PRO:HD3	31:m:101:LMG:HC61	1.97	0.46
26:B:608:CLA:H152	26:B:609:CLA:H192	1.97	0.46
5:E:22[A]:ILE:HG23	5:E:23:HIS:HD1	1.81	0.46
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.97	0.46
3:c:406:SER:HA	3:c:420:VAL:HG23	1.95	0.46
13:o:59:LYS:HB2	13:o:61:GLN:OE1	2.16	0.46
3:C:315:MET:HE2	3:C:365:TRP:CZ3	2.50	0.46
2:b:422:ARG:O	2:b:425:ILE:HG12	2.16	0.46
10:k:20:PRO:HB3	17:y:21:GLN:HG3	1.98	0.46
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.97	0.46
26:B:614:CLA:H191	30:B:623:STE:H111	1.98	0.46
20:R:10:LEU:HB3	20:R:11:PRO:HD3	1.97	0.46
29:a:612:PL9:H38	29:a:612:PL9:H503	1.97	0.46
31:m:101:LMG:H371	31:m:101:LMG:H342	1.81	0.46
15:u:70:ARG:HH11	15:u:73:GLN:HB3	1.81	0.46
16:v:110:LYS:HD2	16:v:110:LYS:C	2.41	0.46
37:D:502:HOH:O	5:E:49:THR:HG21	2.15	0.46
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.98	0.46
13:o:178:LYS:HA	13:o:178:LYS:HD3	1.79	0.46
16:v:95:LEU:HD11	16:v:112:LEU:HD11	1.98	0.46
1:A:307:ILE:HG22	1:A:313:VAL:HA	1.98	0.46
1:A:329[A]:GLU:HG3	37:A:792:HOH:O	2.16	0.46
2:B:4:PRO:HB2	2:B:6:TYR:CE1	2.51	0.46
3:c:167:VAL:HG13	26:c:512:CLA:H102	1.98	0.46
4:d:179:PHE:HA	4:d:182:LEU:HD22	1.97	0.46
2:B:58:GLN:C	2:B:329:PRO:HB3	2.41	0.46
26:C:507:CLA:H141	26:C:507:CLA:H161	1.72	0.46
4:D:24:ARG:HH11	18:X:37:VAL:HG12	1.81	0.46
5:E:32:ILE:HD13	30:E:103:STE:H62	1.98	0.46
13:O:40:ILE:HD13	13:O:95:PHE:CD1	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:496:TYR:CE1	2:b:505:ARG:HG2	2.51	0.46
4:D:126:MET:HE3	4:D:143:ALA:O	2.16	0.45
13:O:93:LEU:O	13:O:128:SER:HA	2.16	0.45
19:Z:48:ILE:HD11	30:Z:101:STE:H131	1.99	0.45
26:a:613:CLA:H43	26:a:613:CLA:O1A	2.16	0.45
4:d:218:VAL:HG13	4:d:244:TYR:CD1	2.52	0.45
28:k:102:BCR:H311	28:k:102:BCR:HC7	1.72	0.45
13:o:181:GLU:HB2	37:o:303:HOH:O	2.16	0.45
2:B:498:LYS:HE3	4:D:20:ASP:HA	1.98	0.45
31:D:406:LMG:HC71	37:D:526:HOH:O	2.16	0.45
30:T:102:STE:H122	30:T:102:STE:H91	1.53	0.45
2:B:224:ARG:HD3	31:D:406:LMG:H292	1.99	0.45
26:C:511:CLA:H141	26:C:511:CLA:H162	1.70	0.45
26:a:608:CLA:H121	29:a:612:PL9:H212	1.98	0.45
32:a:615:SQD:H332	32:a:615:SQD:H301	1.51	0.45
1:A:159[A]:LEU:C	1:A:162[A]:PRO:HD2	2.42	0.45
3:C:92:ILE:HD11	26:C:503:CLA:HED2	1.98	0.45
3:C:203:THR:O	3:C:235:GLY:HA3	2.16	0.45
4:d:160:TYR:HA	4:d:290:ALA:HB2	1.99	0.45
26:B:606:CLA:H112	26:B:606:CLA:H93	1.65	0.45
5:E:65:LEU:O	5:E:67:THR:HG23	2.16	0.45
16:V:90:GLU:HG2	37:V:350:HOH:O	2.17	0.45
26:A:608:CLA:H111	29:A:612:PL9:H221	1.99	0.45
26:b:614:CLA:H62	26:b:614:CLA:H41	1.52	0.45
28:b:617:BCR:H383	32:b:620:SQD:H82	1.99	0.45
26:c:510:CLA:H191	10:k:33:LEU:HD22	1.99	0.45
4:d:279:LEU:HD21	27:d:401:PHO:HMC2	1.97	0.45
32:F:102:SQD:H382	18:X:20:VAL:HG22	1.99	0.45
5:e:8:ARG:HG2	5:e:13:ILE:HG13	1.98	0.45
2:B:422:ARG:HD2	37:O:332:HOH:O	2.16	0.45
26:a:607:CLA:H122	27:a:609:PHO:H3A	1.99	0.45
3:C:317:PHE:HE2	3:C:396:MET:HE1	1.82	0.45
12:M:33:GLN:HA	37:M:210:HOH:O	2.16	0.45
26:b:602:CLA:H43	7:h:45:ILE:HG22	1.99	0.45
26:b:608:CLA:H141	26:b:608:CLA:H161	1.65	0.45
2:B:149[B]:LEU:HD11	26:B:604:CLA:H162	1.98	0.44
3:C:78:GLU:HG2	16:V:106:ASN:ND2	2.30	0.44
37:C:677:HOH:O	13:O:10:ILE:HB	2.18	0.44
5:e:18:ARG:HH11	20:r:23:ILE:HD11	1.80	0.44
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	1.99	0.44
2:b:355:PHE:HZ	2:b:373:LYS:HE3	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:509:CLA:H142	26:c:509:CLA:H111	1.70	0.44
16:V:41:HIS:HA	16:V:45:ILE:O	2.17	0.44
13:o:32:ILE:HD13	13:o:32:ILE:HA	1.84	0.44
2:B:144:PHE:CE2	2:B:148:LEU:HD11	2.52	0.44
2:B:161:LEU:HD12	2:B:161:LEU:HA	1.81	0.44
5:E:22[A]:ILE:HG23	5:E:23:HIS:ND1	2.32	0.44
2:b:119:ASP:HB3	37:h:204:HOH:O	2.17	0.44
26:b:608:CLA:H111	4:d:120:PHE:CE1	2.51	0.44
30:m:103:STE:H52	30:m:103:STE:H22	1.68	0.44
2:B:127:ARG:HG2	2:B:128:THR:HG23	2.00	0.44
4:D:266:TRP:CD1	33:D:408:LHG:HC31	2.53	0.44
16:V:24:LYS:HB2	16:V:24:LYS:HE2	1.47	0.44
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.99	0.44
26:c:511:CLA:H171	19:z:20:VAL:HA	2.00	0.44
16:v:76:MET:HE1	16:v:115:ILE:HB	2.00	0.44
31:C:523:LMG:H112	10:K:23:ASP:HB3	2.00	0.44
1:A:84:PRO:HA	1:A:112:TYR:CG	2.53	0.44
2:B:458:PHE:HB3	26:B:604:CLA:HBC2	1.99	0.44
26:B:603:CLA:H141	26:B:603:CLA:H161	1.60	0.44
34:C:521:DGD:HB71	31:C:523:LMG:H401	2.00	0.44
13:O:133:VAL:C	13:O:135:SER:H	2.26	0.44
2:B:160:GLY:HA3	2:B:180:PRO:HB3	2.00	0.44
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.99	0.44
13:O:178:LYS:HE3	13:O:178:LYS:HB2	1.75	0.44
3:c:257:PHE:O	3:c:261:ARG:HG3	2.17	0.44
4:d:172:SER:HB2	4:d:177:ALA:HB1	2.00	0.44
29:d:405:PL9:H201	33:l:101:LHG:H202	1.99	0.44
33:D:409:LHG:H152	33:D:409:LHG:H182	1.74	0.44
26:b:615:CLA:H92	26:b:615:CLA:H61	1.78	0.44
26:C:512:CLA:H193	26:C:512:CLA:H161	1.82	0.43
30:K:104:STE:H112	30:K:104:STE:H81	1.56	0.43
17:Y:30:ILE:HD12	17:Y:30:ILE:HA	1.88	0.43
3:c:162:GLY:HA2	3:c:248:GLY:HA2	2.00	0.43
3:c:202:PRO:HB2	37:c:768:HOH:O	2.17	0.43
12:m:16:LEU:HB3	37:m:218:HOH:O	2.18	0.43
26:B:616:CLA:HMB1	26:B:616:CLA:HBB1	1.99	0.43
2:b:349:LYS:HD3	37:b:850:HOH:O	2.17	0.43
28:k:101:BCR:H10C	17:y:28:ILE:HG23	2.00	0.43
1:A:243:GLU:N	1:A:243:GLU:CD	2.76	0.43
26:A:607:CLA:HMB1	26:A:607:CLA:HBB1	2.00	0.43
30:A:622:STE:H132	30:A:622:STE:H162	1.78	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:605:CLA:H61	26:B:605:CLA:H41	1.79	0.43
9:J:13:VAL:HG23	37:J:202:HOH:O	2.18	0.43
9:J:19:MET:O	9:J:23:VAL:HG23	2.18	0.43
31:M:101:LMG:H361	31:M:101:LMG:H332	1.69	0.43
34:c:521:DGD:HB72	34:c:521:DGD:HBT2	1.79	0.43
4:d:267:LEU:C	4:d:267:LEU:HD23	2.42	0.43
14:t:28:ARG:HA	14:t:28:ARG:HD3	1.78	0.43
15:u:51:LYS:HB2	15:u:51:LYS:HE2	1.84	0.43
7:H:56:ASP:OD2	18:X:2:THR:HA	2.18	0.43
26:c:511:CLA:H191	30:z:101:STE:H81	2.00	0.43
29:A:612:PL9:H351	29:A:612:PL9:H371	1.63	0.43
26:B:613:CLA:HBB1	26:B:613:CLA:HMB1	1.99	0.43
20:R:16:ALA:O	20:R:20:VAL:HG23	2.18	0.43
4:d:90:LEU:HD23	4:d:90:LEU:HA	1.90	0.43
6:F:20:TRP:CE2	6:F:24:HIS:CE1	3.07	0.43
16:V:31:ARG:HH11	16:V:31:ARG:HB3	1.84	0.43
1:a:163[B]:ILE:HG13	37:c:780:HOH:O	2.19	0.43
37:a:727:HOH:O	2:b:7:ARG:HD2	2.18	0.43
26:c:502:CLA:H203	26:c:502:CLA:H161	1.84	0.43
1:A:320:ILE:HB	37:A:842:HOH:O	2.19	0.43
26:B:601:CLA:H102	28:X:101:BCR:H402	2.00	0.43
26:B:608:CLA:H143	26:B:608:CLA:H161	1.80	0.43
26:C:508:CLA:H192	34:C:521:DGD:HA92	1.99	0.43
33:D:409:LHG:H142	33:D:409:LHG:H322	2.00	0.43
13:O:103:PHE:HB3	13:O:123:LYS:HE2	1.99	0.43
6:f:19:ARG:O	6:f:23:VAL:HG13	2.19	0.43
10:k:17:ILE:HD11	19:z:6:GLN:HG2	1.99	0.43
1:A:212:CYS:HB2	4:D:211:CYS:HB2	2.01	0.43
33:A:617:LHG:H301	33:A:617:LHG:H271	1.85	0.43
28:D:404:BCR:H392	28:D:404:BCR:H23C	2.00	0.43
1:a:60[B]:ILE:HD12	1:a:84:PRO:HD2	2.00	0.43
1:a:310:LYS:HD2	16:v:1:ALA:HB1	1.99	0.43
26:b:612:CLA:H161	37:b:780:HOH:O	2.18	0.43
27:d:401:PHO:HBC2	27:d:401:PHO:HHD	2.01	0.43
19:z:1:MET:HA	37:z:208:HOH:O	2.17	0.43
2:B:117:TYR:HA	11:L:1:MET:HE1	2.01	0.43
26:B:602:CLA:H193	26:B:602:CLA:H162	1.78	0.43
26:B:614:CLA:H112	32:B:622:SQD:H371	2.01	0.43
28:C:514:BCR:H20C	28:C:514:BCR:H361	1.85	0.43
8:i:35:LYS:HB3	8:i:35:LYS:HE3	1.88	0.43
26:B:608:CLA:H91	26:B:608:CLA:H112	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:616:LHG:H122	33:a:616:LHG:HC92	1.73	0.43
12:m:17:VAL:HB	12:m:18:PRO:HD3	2.01	0.43
15:u:36:ILE:HD13	16:v:52:LEU:HD13	2.01	0.43
26:b:604:CLA:H192	26:b:604:CLA:H161	1.88	0.42
4:d:87:HIS:CD2	4:d:162:LEU:HD23	2.54	0.42
12:m:5:GLN:HB2	37:m:209:HOH:O	2.18	0.42
13:O:231:HIS:HE1	37:O:394:HOH:O	2.02	0.42
3:c:242:LEU:HD21	31:c:523:LMG:H311	1.99	0.42
13:o:42:ARG:O	13:o:241:ALA:HA	2.19	0.42
26:A:608:CLA:HMB2	27:A:609:PHO:H172	2.01	0.42
26:B:610:CLA:HHC	26:B:610:CLA:HBB1	2.02	0.42
26:C:511:CLA:H193	26:C:511:CLA:H161	1.79	0.42
28:C:514:BCR:H371	28:C:514:BCR:H24C	1.83	0.42
34:C:520:DGD:HAE1	34:C:520:DGD:HA82	1.62	0.42
26:b:603:CLA:H142	26:b:603:CLA:H111	1.71	0.42
26:c:507:CLA:H142	26:c:507:CLA:H112	1.77	0.42
9:j:10:LEU:O	9:j:13:VAL:HG22	2.19	0.42
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.20	0.42
30:M:104:STE:H183	26:b:614:CLA:H202	2.01	0.42
26:b:604:CLA:H13	30:b:621:STE:H162	2.01	0.42
3:c:203:THR:O	3:c:235:GLY:HA3	2.20	0.42
4:d:293:LEU:HD12	4:d:293:LEU:HA	1.92	0.42
1:A:16:ARG:HG2	30:A:622:STE:H183	2.01	0.42
1:A:201:GLY:HA3	1:A:286:THR:HB	2.00	0.42
4:D:293:LEU:HD12	4:D:293:LEU:HA	1.94	0.42
13:O:193:THR:HG21	13:O:220:LEU:HD12	2.01	0.42
34:A:619:DGD:HG12	30:I:102:STE:H71	2.02	0.42
30:H:103:STE:H152	30:H:103:STE:H121	1.81	0.42
10:k:26:PRO:O	10:k:29:PRO:HD2	2.20	0.42
6:F:36:ALA:O	6:F:40:MET:HG3	2.18	0.42
28:K:103:BCR:H371	28:K:103:BCR:H24C	1.82	0.42
1:a:82:VAL:HB	1:a:174[B]:LEU:HB2	2.02	0.42
26:b:614:CLA:H141	26:b:614:CLA:H162	1.58	0.42
16:v:17:LYS:HE3	16:v:18:THR:O	2.19	0.42
1:A:105:TRP:CE2	1:A:110:GLY:HA3	2.55	0.42
30:A:622:STE:H152	37:A:771:HOH:O	2.19	0.42
4:D:78:VAL:HG11	4:D:114:ILE:HD12	2.02	0.42
12:M:20:VAL:HG11	12:m:20:VAL:CG2	2.50	0.42
3:c:135:ARG:HH22	19:z:33:TRP:NE1	2.17	0.42
26:c:510:CLA:H161	26:c:510:CLA:H121	1.79	0.42
26:c:511:CLA:H91	26:c:511:CLA:H111	1.80	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:h:101:BCR:H331	28:h:101:BCR:C8	2.50	0.42
17:y:20:ALA:HB3	37:y:101:HOH:O	2.19	0.42
29:D:405:PL9:H412	11:L:29:LEU:HD23	2.01	0.42
5:E:78:THR:O	5:E:82:GLN:HG3	2.20	0.42
26:b:604:CLA:H62	26:b:604:CLA:H41	1.73	0.42
31:c:523:LMG:H382	31:c:523:LMG:H352	1.73	0.42
26:B:616:CLA:H112	26:B:616:CLA:H91	1.77	0.42
12:M:4:ASN:HD22	12:M:5:GLN:N	2.17	0.42
5:e:17:VAL:H	9:j:7:ARG:CD	2.30	0.42
1:A:320:ILE:HD13	37:A:842:HOH:O	2.20	0.41
34:A:619:DGD:HBE1	34:A:619:DGD:HB82	1.91	0.41
26:C:511:CLA:H143	19:Z:20:VAL:HG13	2.02	0.41
1:a:241:GLN:NE2	1:a:245:THR:HG23	2.34	0.41
3:c:352:GLY:O	3:c:355[B]:THR:HG22	2.19	0.41
2:B:338:GLN:O	13:o:59:LYS:HG2	2.20	0.41
20:R:6:LEU:HD23	20:R:6:LEU:HA	1.87	0.41
33:a:616:LHG:H251	33:a:616:LHG:H282	1.68	0.41
30:a:620:STE:H51	30:a:620:STE:H21	1.71	0.41
34:c:519:DGD:HA22	34:c:519:DGD:HA51	1.84	0.41
7:h:4:ARG:HE	7:h:4:ARG:HB3	1.62	0.41
30:B:625:STE:H112	30:B:625:STE:H141	1.46	0.41
1:a:131:TRP:CH2	26:c:505:CLA:HAA2	2.55	0.41
2:b:149:LEU:HD23	2:b:149:LEU:HA	1.92	0.41
26:c:509:CLA:H3A	26:c:509:CLA:HBA1	1.69	0.41
4:d:110:LEU:HD23	4:d:110:LEU:HA	1.95	0.41
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.56	0.41
30:d:408:STE:H32	30:d:408:STE:H61	1.72	0.41
1:A:131:TRP:CH2	26:C:505:CLA:HAA2	2.55	0.41
26:B:614:CLA:H62	26:B:614:CLA:H41	1.72	0.41
28:B:618:BCR:H20C	28:B:618:BCR:H361	1.83	0.41
4:D:90:LEU:HD23	4:D:90:LEU:HA	1.93	0.41
28:T:101:BCR:H382	28:T:101:BCR:H23C	2.02	0.41
28:X:101:BCR:H371	28:X:101:BCR:H24C	1.85	0.41
5:e:35:TRP:CD2	6:f:39:ALA:HB2	2.55	0.41
28:h:101:BCR:H361	28:h:101:BCR:H20C	1.78	0.41
33:A:617:LHG:H222	4:D:38:PHE:CE1	2.56	0.41
26:B:613:CLA:C14	31:M:101:LMG:H241	2.51	0.41
4:D:85:MET:HE1	5:E:72:ALA:HB2	2.01	0.41
4:D:218:VAL:HG22	4:D:244:TYR:CE1	2.55	0.41
5:E:35:TRP:HE1	30:E:103:STE:H141	1.84	0.41
26:b:602:CLA:H203	26:b:602:CLA:H162	1.75	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:c:514:BCR:H24C	28:c:514:BCR:H371	1.85	0.41
17:y:46:LEU:HD23	17:y:46:LEU:HA	1.92	0.41
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.03	0.41
28:D:404:BCR:H20C	28:D:404:BCR:H361	1.76	0.41
32:a:617:SQD:H1	37:a:760:HOH:O	2.20	0.41
26:b:602:CLA:H3A	37:b:827:HOH:O	2.21	0.41
3:c:209:ILE:HD13	3:c:209:ILE:HA	1.87	0.41
5:e:17:VAL:HB	9:j:7:ARG:HH11	1.86	0.41
37:e:219:HOH:O	6:f:15:ILE:HG13	2.20	0.41
13:o:57:LYS:O	13:o:59:LYS:HG3	2.21	0.41
33:A:617:LHG:HC41	30:E:102:STE:H141	2.02	0.41
26:C:507:CLA:H92	26:C:507:CLA:H61	1.74	0.41
4:D:194:ASN:HA	4:D:295:SER:OG	2.20	0.41
35:F:101:HEM:HBB2	35:F:101:HEM:HMB1	2.02	0.41
1:a:202:VAL:HG11	26:a:608:CLA:C3D	2.50	0.41
13:o:228:HIS:HD2	37:o:312:HOH:O	2.02	0.41
26:A:608:CLA:H141	26:A:608:CLA:H161	1.62	0.41
4:D:131:GLU:O	4:D:135:LEU:HG	2.21	0.41
2:b:137:LYS:HE2	37:b:773:HOH:O	2.20	0.41
37:b:765:HOH:O	4:d:137:GLY:HA3	2.19	0.41
34:A:619:DGD:HG31	2:b:75:TRP:CD2	2.56	0.41
3:C:79:LYS:HG2	16:V:103:LYS:HD3	2.03	0.41
11:L:4:ASN:HB3	11:L:7:ARG:HD3	2.03	0.41
37:L:204:HOH:O	14:T:25:GLU:HG3	2.21	0.41
26:b:615:CLA:HBA1	26:b:615:CLA:H3A	1.87	0.41
28:b:618:BCR:H361	28:b:618:BCR:H20C	1.85	0.41
34:h:102:DGD:HBH1	34:h:102:DGD:HBT1	1.80	0.41
37:l:214:HOH:O	30:m:103:STE:H21	2.20	0.41
16:v:77:LYS:HG2	16:v:95:LEU:HD12	2.02	0.41
17:y:21:GLN:HE21	17:y:21:GLN:HB2	1.57	0.41
19:z:30:PRO:HA	37:z:201:HOH:O	2.21	0.41
37:B:706:HOH:O	11:L:2:GLU:HG2	2.20	0.41
34:C:522:DGD:HBH1	34:C:522:DGD:HBT2	1.80	0.41
26:b:614:CLA:H93	26:b:614:CLA:H61	1.75	0.41
28:b:617:BCR:H24C	28:b:617:BCR:H371	1.82	0.41
4:d:194:ASN:HA	4:d:295:SER:OG	2.21	0.41
1:A:183[A]:MET:HA	26:A:607:CLA:HMD1	2.03	0.40
1:A:243:GLU:CD	1:A:243:GLU:H	2.28	0.40
1:A:334[B]:ARG:HD3	37:A:822:HOH:O	2.20	0.40
1:A:339[B]:PHE:HB3	1:A:340[B]:PRO:HD2	2.02	0.40
2:B:144:PHE:CE1	2:B:210:ILE:HG23	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:58:GLN:C	2:b:329:PRO:HB3	2.46	0.40
15:u:52:ASN:C	37:u:201:HOH:O	2.63	0.40
2:B:347:ARG:O	2:B:397:VAL:HA	2.22	0.40
3:C:223:TRP:CG	3:C:224:ILE:H	2.39	0.40
28:K:101:BCR:H20C	28:K:101:BCR:H361	1.83	0.40
4:d:131:GLU:O	4:d:135:LEU:HG	2.21	0.40
5:e:18:ARG:NH1	20:r:23:ILE:HD11	2.35	0.40
15:u:45:LEU:HD23	15:u:45:LEU:HA	1.95	0.40
26:A:608:CLA:H161	26:A:608:CLA:H202	1.79	0.40
29:A:612:PL9:H271	33:A:617:LHG:H223	2.03	0.40
33:D:410:LHG:H211	12:M:14:PHE:CE2	2.56	0.40
5:E:36:LEU:HA	5:E:39:SER:OG	2.21	0.40
13:O:116:ILE:HD12	13:O:231:HIS:CD2	2.56	0.40
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.55	0.40
1:a:266:ASN:ND2	1:a:266:ASN:H	2.19	0.40
37:b:885:HOH:O	30:d:408:STE:H112	2.22	0.40
26:c:505:CLA:H72	26:c:505:CLA:H112	1.77	0.40
1:A:120:LEU:HD23	1:A:120:LEU:HA	1.86	0.40
28:K:102:BCR:H312	28:K:103:BCR:H353	2.02	0.40
2:b:321:LYS:HD2	2:b:321:LYS:HA	1.96	0.40
6:f:26:LEU:C	6:f:29:PRO:HD2	2.46	0.40
28:k:101:BCR:H321	28:k:101:BCR:HC8	2.03	0.40
18:x:14:LEU:HD23	18:x:14:LEU:HA	1.92	0.40
2:B:478:VAL:O	4:D:139:ARG:HG2	2.21	0.40
26:B:606:CLA:H143	26:B:606:CLA:H111	1.66	0.40
3:C:348:GLU:OE2	13:O:11:VAL:HA	2.21	0.40
4:D:61:HIS:HE1	4:D:80:THR:O	2.04	0.40
5:E:30:LEU:HD11	35:F:101:HEM:HAB	2.03	0.40
13:O:115:ARG:HD3	37:O:398:HOH:O	2.21	0.40
14:T:18:PHE:HB2	28:T:101:BCR:HC8	2.03	0.40
26:a:613:CLA:H191	32:a:617:SQD:H212	2.04	0.40
3:c:85:GLY:O	26:c:504:CLA:HED2	2.22	0.40
13:o:51:LEU:HB3	13:o:65:PHE:HB3	2.01	0.40
16:v:93:PRO:HA	16:v:101:PHE:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	400/344 (116%)	394 (98%)	6 (2%)	0	100	100
1	a	400/344 (116%)	394 (98%)	5 (1%)	1 (0%)	36	36
2	B	508/510 (100%)	501 (99%)	6 (1%)	1 (0%)	43	44
2	b	504/510 (99%)	496 (98%)	8 (2%)	0	100	100
3	C	451/461 (98%)	438 (97%)	12 (3%)	1 (0%)	43	44
3	c	461/461 (100%)	448 (97%)	12 (3%)	1 (0%)	43	44
4	D	348/352 (99%)	340 (98%)	8 (2%)	0	100	100
4	d	349/352 (99%)	341 (98%)	8 (2%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	61 (97%)	2 (3%)	0	100	100
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	231 (95%)	11 (4%)	1 (0%)	30	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	232 (96%)	10 (4%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
15	u	95/134 (71%)	90 (95%)	4 (4%)	1 (1%)	11	7
16	V	135/163 (83%)	131 (97%)	3 (2%)	1 (1%)	18	15
16	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
17	Y	25/46 (54%)	24 (96%)	1 (4%)	0	100	100
17	y	28/46 (61%)	28 (100%)	0	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	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%)	55 (92%)	3 (5%)	2 (3%)	3	1
20	R	26/41 (63%)	26 (100%)	0	0	100	100
20	r	26/41 (63%)	25 (96%)	1 (4%)	0	100	100
All	All	5405/5700 (95%)	5274 (98%)	122 (2%)	9 (0%)	43	44

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	294	SER
3	C	416	SER
16	V	64	PRO
3	c	416	SER
15	u	53	ALA
19	z	33	TRP
13	O	57	LYS
19	z	30	PRO
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	326/280 (116%)	324 (99%)	2 (1%)	78	85
1	a	325/280 (116%)	318 (98%)	7 (2%)	45	52
2	B	408/407 (100%)	403 (99%)	5 (1%)	63	71
2	b	403/407 (99%)	398 (99%)	5 (1%)	63	71
3	C	353/362 (98%)	349 (99%)	4 (1%)	65	74
3	c	362/362 (100%)	353 (98%)	9 (2%)	42	47
4	D	285/283 (101%)	283 (99%)	2 (1%)	76	83
4	d	286/283 (101%)	282 (99%)	4 (1%)	59	67
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	42
5	e	71/73 (97%)	70 (99%)	1 (1%)	59	67
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	33
6	f	28/39 (72%)	27 (96%)	1 (4%)	31	33
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	53/55 (96%)	50 (94%)	3 (6%)	18	16
8	I	32/34 (94%)	31 (97%)	1 (3%)	35	38
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	38
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	28 (93%)	2 (7%)	15	12
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	41
11	l	34/35 (97%)	33 (97%)	1 (3%)	37	41
12	M	28/32 (88%)	26 (93%)	2 (7%)	13	10
12	m	28/32 (88%)	27 (96%)	1 (4%)	31	33
13	O	206/228 (90%)	201 (98%)	5 (2%)	43	48
13	o	207/228 (91%)	202 (98%)	5 (2%)	43	48
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	25/28 (89%)	25 (100%)	0	100	100
15	U	84/112 (75%)	81 (96%)	3 (4%)	31	33
15	u	84/112 (75%)	84 (100%)	0	100	100
16	V	117/138 (85%)	116 (99%)	1 (1%)	70	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	v	117/138 (85%)	115 (98%)	2 (2%)	53	61
17	Y	19/37 (51%)	19 (100%)	0	100	100
17	y	22/37 (60%)	21 (96%)	1 (4%)	24	24
18	X	31/34 (91%)	31 (100%)	0	100	100
18	x	31/34 (91%)	29 (94%)	2 (6%)	15	13
19	Z	52/52 (100%)	51 (98%)	1 (2%)	50	57
19	z	51/52 (98%)	51 (100%)	0	100	100
20	R	22/33 (67%)	22 (100%)	0	100	100
20	r	22/33 (67%)	20 (91%)	2 (9%)	9	6
All	All	4467/4654 (96%)	4390 (98%)	77 (2%)	55	61

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	205	VAL
2	B	86	ILE
2	B	98	LEU
2	B	234	ILE
2	B	362	PHE
2	B	371	THR
3	C	240	ILE
3	C	289	PHE
3	C	355[A]	THR
3	C	355[B]	THR
4	D	154	VAL
4	D	264	LYS
5	E	22[A]	ILE
5	E	22[B]	ILE
6	F	25	THR
8	I	4	LEU
11	L	10	VAL
12	M	20	VAL
12	M	25	LEU
13	O	49	THR
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	214	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	U	24	LYS
15	U	39	ARG
15	U	45	LEU
16	V	3	LEU
19	Z	7	LEU
1	a	42	LEU
1	a	159[A]	LEU
1	a	159[B]	LEU
1	a	163[A]	ILE
1	a	163[B]	ILE
1	a	200	LEU
1	a	286	THR
2	b	80	ILE
2	b	149	LEU
2	b	236	THR
2	b	267	LEU
2	b	362	PHE
3	c	72	LEU
3	c	99	VAL
3	c	124	VAL
3	c	240	ILE
3	c	279	LEU
3	c	354[A]	GLU
3	c	354[B]	GLU
3	c	413[A]	GLU
3	c	413[B]	GLU
4	d	182	LEU
4	d	227[A]	GLU
4	d	227[B]	GLU
4	d	321	LEU
5	e	54	SER
6	f	23	VAL
7	h	5	THR
7	h	43	LEU
7	h	56	ASP
8	i	36	ASP
10	k	30	VAL
10	k	35	LEU
11	l	30	LEU
12	m	13	LEU
13	o	49	THR
13	o	59	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	o	118	LEU
13	o	134	THR
13	o	135	SER
16	v	52	LEU
16	v	107	LEU
17	y	19	ILE
18	x	2	THR
18	x	7	LEU
20	r	6	LEU
20	r	28	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	GLN
1	A	234	ASN
2	B	282	GLN
2	B	374	ASN
2	B	490	GLN
3	C	155	ASN
3	C	201	ASN
3	C	415	ASN
4	D	98	GLN
4	D	250	ASN
5	E	82	GLN
12	M	4	ASN
12	M	5	GLN
12	M	32	GLN
13	O	231	HIS
15	U	73	GLN
15	U	78	ASN
16	V	106	ASN
17	Y	21	GLN
19	Z	6	GLN
20	R	22	ASN
1	a	234	ASN
1	a	266	ASN
2	b	282	GLN
2	b	289	GLN
2	b	338	GLN
2	b	409	GLN
2	b	490	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	c	322	GLN
3	c	378	ASN
4	d	61	HIS
5	e	82	GLN
6	f	44	GLN
12	m	5	GLN
13	o	36	GLN
13	o	80	GLN
13	o	82	GLN
13	o	88	ASN
13	o	132	ASN
13	o	155	ASN
13	o	200	ASN
15	u	37	GLN
15	u	73	GLN
17	y	21	GLN
18	x	33	GLN
19	z	6	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	FME	m	1	12	8,9,10	0.49	0	8,9,11	0.75	0
14	FME	t	1	14	8,9,10	0.53	0	8,9,11	0.91	0
8	FME	I	1	8	8,9,10	0.51	0	8,9,11	1.30	1 (12%)
14	FME	T	1	14	8,9,10	0.40	0	8,9,11	0.81	0
8	FME	i	1	8	8,9,10	0.45	0	8,9,11	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	FME	M	1	12	8,9,10	0.52	0	8,9,11	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	m	1	12	-	0/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	2/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	0/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1	FME	CA-N-CN	-2.99	118.22	122.82

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 213 ligands modelled in this entry, 6 are monoatomic - leaving 207 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	$\# Z > 2$
28	BCR	d	404	-	41,41,41	0.43	0	56,56,56	1.19	5 (8%)
29	PL9	D	405	-	55,55,55	1.01	3 (5%)	68,69,69	1.55	15 (22%)
34	DGD	c	520	-	63,63,67	0.58	0	77,77,81	0.92	6 (7%)
30	STE	B	621	-	16,16,19	0.66	0	16,16,19	1.09	0
28	BCR	B	618	-	41,41,41	0.47	0	56,56,56	0.91	1 (1%)
26	CLA	C	501	3	69,73,73	1.49	6 (8%)	82,113,113	1.45	5 (6%)
30	STE	M	103	-	9,9,19	0.40	0	8,8,19	0.64	0
30	STE	h	103	-	9,9,19	0.37	0	8,8,19	0.69	0
26	CLA	B	616	2	64,68,73	1.27	7 (10%)	76,107,113	1.43	11 (14%)
35	HEM	F	101	6,5	50,50,50	1.48	9 (18%)	67,82,82	1.14	2 (2%)
26	CLA	b	603	2	69,73,73	1.20	9 (13%)	82,113,113	1.34	7 (8%)
28	BCR	k	102	-	41,41,41	0.39	0	56,56,56	0.91	1 (1%)
26	CLA	A	608	37	69,73,73	1.30	8 (11%)	82,113,113	1.33	6 (7%)
26	CLA	c	501	3	69,73,73	1.16	9 (13%)	82,113,113	1.28	7 (8%)
26	CLA	B	603	2	69,73,73	1.29	6 (8%)	82,113,113	1.28	8 (9%)
30	STE	I	101	-	16,16,19	0.73	0	16,16,19	0.98	1 (6%)
30	STE	B	625	-	14,14,19	0.40	0	13,13,19	0.62	0
26	CLA	c	507	37	69,73,73	1.21	6 (8%)	82,113,113	1.34	6 (7%)
26	CLA	a	610	1	69,73,73	1.30	6 (8%)	82,113,113	1.25	7 (8%)
26	CLA	c	511	3	69,73,73	1.38	7 (10%)	82,113,113	1.49	5 (6%)
26	CLA	c	504	37	64,68,73	1.23	7 (10%)	76,107,113	1.44	9 (11%)
32	SQD	A	616	-	50,52,54	1.59	6 (12%)	60,63,65	1.98	12 (20%)
28	BCR	c	514	-	41,41,41	0.38	0	56,56,56	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	STE	z	101	-	8,8,19	0.40	0	7,7,19	0.62	0
26	CLA	B	604	2	69,73,73	1.27	5 (7%)	82,113,113	1.51	7 (8%)
28	BCR	K	101	-	41,41,41	0.36	0	56,56,56	0.65	0
26	CLA	C	503	3	69,73,73	1.46	8 (11%)	82,113,113	1.65	9 (10%)
26	CLA	c	508	3	68,72,73	1.32	8 (11%)	80,111,113	1.36	9 (11%)
26	CLA	b	605	2	69,73,73	1.22	7 (10%)	82,113,113	1.27	9 (10%)
28	BCR	K	103	-	41,41,41	0.41	0	56,56,56	1.04	3 (5%)
30	STE	e	101	-	8,8,19	0.40	0	7,7,19	0.59	0
27	PHO	a	609	-	58,69,69	2.00	8 (13%)	55,99,99	1.59	9 (16%)
26	CLA	B	608	2	69,73,73	1.23	6 (8%)	82,113,113	1.32	9 (10%)
26	CLA	b	601	37	69,73,73	1.31	6 (8%)	82,113,113	1.38	5 (6%)
31	LMG	M	101	-	51,51,55	0.52	0	59,59,63	0.86	3 (5%)
33	LHG	D	408	-	48,48,48	0.56	0	51,54,54	0.63	1 (1%)
26	CLA	D	402	4	69,73,73	1.12	7 (10%)	82,113,113	1.33	9 (10%)
30	STE	H	103	-	8,8,19	0.38	0	7,7,19	0.63	0
30	STE	t	102	-	13,13,19	0.69	0	13,13,19	1.27	2 (15%)
30	STE	e	105	-	12,12,19	0.69	0	12,12,19	1.18	1 (8%)
28	BCR	T	101	-	41,41,41	0.47	0	56,56,56	0.93	1 (1%)
26	CLA	C	513	3	69,73,73	1.34	8 (11%)	82,113,113	1.35	11 (13%)
28	BCR	K	102	-	41,41,41	0.35	0	56,56,56	0.85	0
31	LMG	a	618	-	55,55,55	0.50	0	63,63,63	1.12	5 (7%)
26	CLA	C	512	3	69,73,73	1.48	11 (15%)	82,113,113	1.36	8 (9%)
32	SQD	a	615	-	52,54,54	1.54	7 (13%)	62,65,65	1.90	11 (17%)
30	STE	m	102	-	11,11,19	0.72	0	11,11,19	1.24	0
30	STE	E	101	-	11,11,19	0.76	0	11,11,19	1.10	0
34	DGD	C	522	-	63,63,67	0.58	1 (1%)	77,77,81	0.88	1 (1%)
27	PHO	d	401	-	58,69,69	2.17	12 (20%)	55,99,99	1.64	10 (18%)
26	CLA	B	614	2	69,73,73	1.23	7 (10%)	82,113,113	1.32	10 (12%)
30	STE	E	102	-	11,11,19	0.38	0	10,10,19	0.69	0
30	STE	b	621	-	19,19,19	0.61	0	19,19,19	1.22	1 (5%)
26	CLA	A	614	37	69,73,73	1.24	6 (8%)	82,113,113	1.33	6 (7%)
28	BCR	D	404	-	41,41,41	0.41	0	56,56,56	0.97	2 (3%)
28	BCR	b	618	-	41,41,41	0.41	0	56,56,56	1.04	3 (5%)
32	SQD	F	102	-	34,36,54	1.49	5 (14%)	42,45,65	1.65	9 (21%)
33	LHG	D	410	-	48,48,48	0.56	0	51,54,54	0.77	0
26	CLA	c	509	3	69,73,73	1.17	6 (8%)	82,113,113	1.34	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	d	402	4	69,73,73	1.32	9 (13%)	82,113,113	1.30	7 (8%)
28	BCR	t	101	-	41,41,41	0.48	0	56,56,56	1.14	4 (7%)
26	CLA	C	507	37	69,73,73	1.31	5 (7%)	82,113,113	1.54	6 (7%)
28	BCR	B	619	-	41,41,41	0.38	0	56,56,56	0.78	0
28	BCR	b	619	-	41,41,41	0.40	0	56,56,56	0.85	1 (1%)
26	CLA	C	511	3	69,73,73	1.43	8 (11%)	82,113,113	1.44	6 (7%)
28	BCR	X	101	-	41,41,41	0.50	0	56,56,56	1.15	5 (8%)
31	LMG	c	523	-	48,48,55	0.47	0	56,56,63	0.84	1 (1%)
28	BCR	C	514	-	41,41,41	0.32	0	56,56,56	0.84	1 (1%)
26	CLA	b	606	2	69,73,73	1.29	7 (10%)	82,113,113	1.50	10 (12%)
26	CLA	C	509	3	69,73,73	1.19	8 (11%)	82,113,113	1.32	8 (9%)
32	SQD	B	622	-	52,54,54	1.56	6 (11%)	62,65,65	1.86	13 (20%)
30	STE	I	102	-	14,14,19	0.70	0	14,14,19	1.16	1 (7%)
31	LMG	D	407	-	51,51,55	0.52	0	59,59,63	0.64	0
26	CLA	c	513	3	69,73,73	1.25	8 (11%)	82,113,113	1.17	7 (8%)
30	STE	A	613	-	8,8,19	0.41	0	7,7,19	0.60	0
26	CLA	B	611	2	69,73,73	1.25	8 (11%)	82,113,113	1.39	8 (9%)
30	STE	d	406	-	19,19,19	0.69	0	19,19,19	0.93	1 (5%)
26	CLA	C	502	3	69,73,73	1.28	8 (11%)	82,113,113	1.27	9 (10%)
26	CLA	b	604	2	69,73,73	1.18	6 (8%)	82,113,113	1.53	11 (13%)
21	OEY	A	601[B]	37,1,3	0,16,16	-	-	-	-	-
26	CLA	a	613	37	69,73,73	1.22	4 (5%)	82,113,113	1.31	8 (9%)
26	CLA	b	614	2	69,73,73	1.29	8 (11%)	82,113,113	1.30	9 (10%)
29	PL9	a	612	-	55,55,55	0.82	1 (1%)	68,69,69	1.54	13 (19%)
32	SQD	f	101	-	39,41,54	1.66	7 (17%)	49,52,65	1.93	12 (24%)
26	CLA	B	601	37	69,73,73	1.33	7 (10%)	82,113,113	1.33	7 (8%)
30	STE	C	515	-	13,13,19	0.76	0	13,13,19	0.95	0
30	STE	K	104	-	13,13,19	0.35	0	12,12,19	0.80	0
26	CLA	b	615	2	69,73,73	1.42	10 (14%)	82,113,113	1.30	7 (8%)
33	LHG	a	614	-	38,38,48	0.58	0	41,44,54	0.67	0
28	BCR	h	101	-	41,41,41	0.42	0	56,56,56	1.04	2 (3%)
26	CLA	B	607	37	69,73,73	1.22	7 (10%)	82,113,113	1.26	9 (10%)
30	STE	A	622	-	10,10,19	0.30	0	9,9,19	0.96	0
30	STE	C	524	-	11,11,19	0.89	0	11,11,19	1.14	1 (9%)
26	CLA	b	610	37	69,73,73	1.28	5 (7%)	82,113,113	1.29	8 (9%)
33	LHG	d	407	-	48,48,48	0.48	0	51,54,54	0.75	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	c	502	3	69,73,73	1.20	5 (7%)	82,113,113	1.35	6 (7%)
30	STE	C	517	-	4,4,19	0.39	0	3,3,19	0.46	0
26	CLA	a	607	1	69,73,73	1.41	9 (13%)	82,113,113	1.32	6 (7%)
30	STE	e	104	-	8,8,19	0.41	0	7,7,19	0.62	0
30	STE	m	103	-	17,17,19	0.34	0	16,16,19	0.83	0
30	STE	d	408	-	19,19,19	0.55	0	19,19,19	1.08	1 (5%)
32	SQD	a	617	-	52,54,54	1.68	8 (15%)	62,65,65	1.46	10 (16%)
31	LMG	B	620	-	45,45,55	0.53	0	53,53,63	0.96	3 (5%)
30	STE	c	516	-	12,12,19	0.35	0	11,11,19	0.78	0
31	LMG	b	622	-	55,55,55	0.46	0	63,63,63	1.06	4 (6%)
26	CLA	C	510	3	69,73,73	1.30	9 (13%)	82,113,113	1.39	5 (6%)
26	CLA	c	505	3	69,73,73	1.15	7 (10%)	82,113,113	1.42	8 (9%)
28	BCR	A	611	-	41,41,41	0.47	0	56,56,56	0.67	0
26	CLA	B	606	2	69,73,73	1.43	8 (11%)	82,113,113	1.52	9 (10%)
30	STE	H	102	-	17,17,19	0.41	0	16,16,19	0.75	0
30	STE	T	102	-	15,15,19	0.38	0	14,14,19	0.73	0
35	HEM	e	102	6,5	50,50,50	1.60	11 (22%)	67,82,82	1.48	9 (13%)
26	CLA	B	613	2	69,73,73	1.32	7 (10%)	82,113,113	1.31	7 (8%)
26	CLA	b	616	2	64,68,73	1.23	6 (9%)	76,107,113	1.41	9 (11%)
31	LMG	C	523	-	48,48,55	0.50	0	56,56,63	0.66	0
31	LMG	d	409	-	44,44,55	0.52	0	52,52,63	0.70	0
34	DGD	h	102	-	63,63,67	0.59	0	77,77,81	0.93	6 (7%)
30	STE	b	625	-	9,9,19	0.39	0	8,8,19	0.65	0
30	STE	c	517	-	17,17,19	0.38	0	16,16,19	0.74	0
30	STE	a	619	-	9,9,19	0.44	0	8,8,19	0.59	0
30	STE	Z	101	-	16,16,19	0.37	0	15,15,19	0.71	0
34	DGD	C	520	-	63,63,67	0.59	0	77,77,81	0.83	2 (2%)
33	LHG	A	617	-	48,48,48	0.54	0	51,54,54	0.54	0
26	CLA	c	512	3	69,73,73	1.28	11 (15%)	82,113,113	1.41	8 (9%)
30	STE	A	621	-	16,16,19	0.44	0	15,15,19	0.60	0
21	OEY	a	601[B]	37,1,3	0,16,16	-	-	-	-	-
30	STE	i	101	-	11,11,19	0.75	0	11,11,19	1.11	1 (9%)
33	LHG	a	616	-	41,41,48	0.60	0	44,47,54	0.60	0
26	CLA	B	612	2	69,73,73	1.15	6 (8%)	82,113,113	1.46	10 (12%)
28	BCR	k	101	-	41,41,41	0.41	0	56,56,56	0.95	2 (3%)
30	STE	D	411	-	19,19,19	0.59	0	19,19,19	1.12	1 (5%)
30	STE	b	624	-	15,15,19	0.76	0	15,15,19	1.06	2 (13%)
31	LMG	c	518	-	29,29,55	0.43	0	31,31,63	0.61	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	b	611	2	69,73,73	1.29	6 (8%)	82,113,113	1.35	9 (10%)
26	CLA	a	608	37	69,73,73	1.21	6 (8%)	82,113,113	1.24	6 (7%)
26	CLA	d	403	4	69,73,73	1.34	8 (11%)	82,113,113	1.24	10 (12%)
31	LMG	c	522	-	46,46,55	0.54	0	54,54,63	0.66	1 (1%)
32	SQD	A	618	-	41,43,54	1.84	10 (24%)	51,54,65	1.49	7 (13%)
30	STE	J	101	-	11,11,19	0.73	0	11,11,19	1.22	0
29	PL9	d	405	-	55,55,55	1.09	4 (7%)	68,69,69	1.60	15 (22%)
30	STE	j	101	-	11,11,19	0.68	0	11,11,19	1.22	1 (9%)
34	DGD	c	519	-	63,63,67	0.62	0	77,77,81	0.89	3 (3%)
33	LHG	D	409	-	46,46,48	0.59	0	49,52,54	0.61	0
33	LHG	b	623	-	48,48,48	0.57	1 (2%)	51,54,54	0.64	1 (1%)
26	CLA	B	615	2	69,73,73	1.44	8 (11%)	82,113,113	1.38	4 (4%)
26	CLA	b	608	2	69,73,73	1.32	10 (14%)	82,113,113	1.35	11 (13%)
29	PL9	A	612	-	55,55,55	0.89	3 (5%)	68,69,69	1.52	12 (17%)
26	CLA	C	504	37	63,67,73	1.29	9 (14%)	74,105,113	1.21	7 (9%)
30	STE	A	620	-	7,7,19	0.34	0	6,6,19	0.79	0
30	STE	B	623	-	17,17,19	0.58	0	17,17,19	1.29	2 (11%)
31	LMG	C	516	-	35,35,55	0.53	0	43,43,63	1.46	5 (11%)
25	BCT	A	606	23	3,3,3	0.75	0	2,3,3	2.43	1 (50%)
26	CLA	C	508	3	69,73,73	1.29	9 (13%)	82,113,113	1.45	9 (10%)
32	SQD	b	620	-	47,49,54	1.60	11 (23%)	57,60,65	1.92	15 (26%)
26	CLA	b	607	37	69,73,73	1.18	8 (11%)	82,113,113	1.27	9 (10%)
28	BCR	a	611	-	41,41,41	0.39	0	56,56,56	0.67	0
26	CLA	b	609	2	69,73,73	1.28	6 (8%)	82,113,113	1.43	13 (15%)
26	CLA	b	602	2	69,73,73	1.19	6 (8%)	82,113,113	1.30	8 (9%)
30	STE	j	102	-	15,15,19	0.38	0	14,14,19	0.77	0
30	STE	C	519	-	9,9,19	0.39	0	8,8,19	0.70	0
30	STE	i	102	-	5,5,19	0.41	0	4,4,19	0.43	0
30	STE	M	102	-	14,14,19	0.69	0	14,14,19	1.14	1 (7%)
30	STE	a	620	-	11,11,19	0.77	0	11,11,19	0.96	0
30	STE	M	104	-	14,14,19	0.29	0	13,13,19	0.95	0
30	STE	E	103	-	19,19,19	0.68	0	19,19,19	0.97	0
34	DGD	H	101	-	63,63,67	0.59	0	77,77,81	0.93	3 (3%)
25	BCT	a	606	23	3,3,3	0.77	0	2,3,3	2.20	1 (50%)
30	STE	h	104	-	10,10,19	0.35	0	9,9,19	0.77	0
30	STE	d	410	-	19,19,19	0.62	0	19,19,19	1.02	1 (5%)
22	OEX	A	602[A]	37,1,3	0,14,14	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMG	c	524	-	49,49,55	0.49	0	57,57,63	0.79	3 (5%)
34	DGD	C	521	-	63,63,67	0.59	0	77,77,81	0.79	1 (1%)
31	LMG	m	101	-	51,51,55	0.46	0	59,59,63	0.92	2 (3%)
22	OEX	a	602[A]	37,1,3	0,14,14	-	-	-		
27	PHO	D	401	-	58,69,69	2.03	10 (17%)	55,99,99	1.64	11 (20%)
26	CLA	B	605	2	69,73,73	1.40	9 (13%)	82,113,113	1.35	6 (7%)
28	BCR	b	617	-	41,41,41	0.36	0	56,56,56	0.73	1 (1%)
30	STE	C	518	-	6,6,19	0.42	0	5,5,19	0.55	0
26	CLA	b	613	2	69,73,73	1.20	8 (11%)	82,113,113	1.38	11 (13%)
26	CLA	c	506	3	69,73,73	1.16	6 (8%)	82,113,113	1.24	9 (10%)
28	BCR	c	515	-	41,41,41	0.40	0	56,56,56	0.80	0
36	HEC	v	201	16	50,50,50	1.73	6 (12%)	68,82,82	1.47	9 (13%)
34	DGD	c	521	-	63,63,67	0.58	0	77,77,81	0.79	2 (2%)
31	LMG	A	615	-	48,48,55	0.47	0	56,56,63	0.67	1 (1%)
31	LMG	D	406	-	50,50,55	0.43	0	58,58,63	1.13	7 (12%)
26	CLA	A	607	1	69,73,73	1.20	6 (8%)	82,113,113	1.30	6 (7%)
26	CLA	c	503	3	69,73,73	1.35	9 (13%)	82,113,113	1.48	6 (7%)
28	BCR	B	617	-	41,41,41	0.48	0	56,56,56	0.73	1 (1%)
26	CLA	A	610	1	58,62,73	1.22	5 (8%)	68,99,113	1.27	9 (13%)
33	LHG	L	101	-	48,48,48	0.50	0	51,54,54	0.62	0
36	HEC	V	201	16	50,50,50	1.90	7 (14%)	68,82,82	1.58	11 (16%)
27	PHO	A	609	-	58,69,69	2.01	8 (13%)	55,99,99	1.81	10 (18%)
30	STE	B	624	-	11,11,19	0.81	0	11,11,19	1.14	0
30	STE	k	103	-	13,13,19	0.72	0	13,13,19	1.15	1 (7%)
26	CLA	B	610	37	69,73,73	1.34	9 (13%)	82,113,113	1.41	9 (10%)
30	STE	C	525	-	15,15,19	0.37	0	14,14,19	0.76	0
26	CLA	b	612	2	69,73,73	1.38	9 (13%)	82,113,113	1.39	10 (12%)
30	STE	C	526	-	13,13,19	0.34	0	12,12,19	0.84	0
34	DGD	A	619	-	67,67,67	0.53	0	81,81,81	0.92	3 (3%)
30	STE	e	103	-	7,7,19	0.38	0	6,6,19	0.71	0
26	CLA	c	510	3	69,73,73	1.24	6 (8%)	82,113,113	1.19	6 (7%)
33	LHG	l	101	-	48,48,48	0.46	0	51,54,54	0.59	0
26	CLA	C	505	3	69,73,73	1.29	8 (11%)	82,113,113	1.40	9 (10%)
26	CLA	B	609	2	69,73,73	1.22	5 (7%)	82,113,113	1.39	8 (9%)
26	CLA	B	602	2	69,73,73	1.32	7 (10%)	82,113,113	1.34	11 (13%)
26	CLA	D	403	4	69,73,73	1.33	6 (8%)	82,113,113	1.26	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	C	506	3	69,73,73	1.17	6 (8%)	82,113,113	1.33	7 (8%)

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
28	BCR	d	404	-	-	4/29/63/63	0/2/2/2
29	PL9	D	405	-	-	13/53/73/73	0/1/1/1
34	DGD	c	520	-	-	17/51/91/95	0/2/2/2
30	STE	B	621	-	-	7/14/14/17	-
28	BCR	B	618	-	-	1/29/63/63	0/2/2/2
26	CLA	C	501	3	-	5/39/115/115	-
30	STE	M	103	-	-	4/7/7/17	-
30	STE	h	103	-	-	4/7/7/17	-
26	CLA	B	616	2	-	10/33/109/115	-
35	HEM	F	101	6,5	-	3/14/54/54	-
26	CLA	b	603	2	-	10/39/115/115	-
28	BCR	k	102	-	-	2/29/63/63	0/2/2/2
26	CLA	A	608	37	-	11/39/115/115	-
26	CLA	c	501	3	-	5/39/115/115	-
26	CLA	B	603	2	-	7/39/115/115	-
30	STE	I	101	-	-	10/14/14/17	-
30	STE	B	625	-	-	12/12/12/17	-
26	CLA	c	507	37	-	13/39/115/115	-
26	CLA	a	610	1	-	8/39/115/115	-
26	CLA	c	511	3	-	7/39/115/115	-
26	CLA	c	504	37	-	7/33/109/115	-
32	SQD	A	616	-	-	15/47/67/69	0/1/1/1
28	BCR	c	514	-	-	0/29/63/63	0/2/2/2
30	STE	z	101	-	-	3/6/6/17	-
26	CLA	B	604	2	-	10/39/115/115	-
28	BCR	K	101	-	-	2/29/63/63	0/2/2/2
26	CLA	C	503	3	-	6/39/115/115	-
26	CLA	c	508	3	-	7/38/114/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	b	605	2	-	10/39/115/115	-
28	BCR	K	103	-	-	2/29/63/63	0/2/2/2
30	STE	e	101	-	-	3/6/6/17	-
27	PHO	a	609	-	-	0/37/103/103	0/5/6/6
26	CLA	B	608	2	-	8/39/115/115	-
26	CLA	b	601	37	-	14/39/115/115	-
31	LMG	M	101	-	-	26/46/66/70	0/1/1/1
33	LHG	D	408	-	-	19/53/53/53	-
26	CLA	D	402	4	-	5/39/115/115	-
30	STE	H	103	-	-	4/6/6/17	-
30	STE	t	102	-	-	4/11/11/17	-
30	STE	e	105	-	-	6/10/10/17	-
28	BCR	T	101	-	-	5/29/63/63	0/2/2/2
26	CLA	C	513	3	-	9/39/115/115	-
28	BCR	K	102	-	-	4/29/63/63	0/2/2/2
31	LMG	a	618	-	-	24/50/70/70	0/1/1/1
26	CLA	C	512	3	-	10/39/115/115	-
32	SQD	a	615	-	-	20/49/69/69	0/1/1/1
30	STE	m	102	-	-	4/9/9/17	-
30	STE	E	101	-	-	3/9/9/17	-
34	DGD	C	522	-	-	8/51/91/95	0/2/2/2
27	PHO	d	401	-	-	2/37/103/103	0/5/6/6
26	CLA	B	614	2	-	15/39/115/115	-
30	STE	E	102	-	-	3/9/9/17	-
30	STE	b	621	-	-	9/17/17/17	-
26	CLA	A	614	37	-	5/39/115/115	-
28	BCR	D	404	-	-	2/29/63/63	0/2/2/2
28	BCR	b	618	-	-	0/29/63/63	0/2/2/2
32	SQD	F	102	-	-	14/28/48/69	0/1/1/1
33	LHG	D	410	-	-	19/53/53/53	-
26	CLA	c	509	3	-	17/39/115/115	-
26	CLA	d	402	4	-	10/39/115/115	-
28	BCR	t	101	-	-	4/29/63/63	0/2/2/2
26	CLA	C	507	37	-	11/39/115/115	-
28	BCR	B	619	-	-	0/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	BCR	b	619	-	-	0/29/63/63	0/2/2/2
26	CLA	C	511	3	-	6/39/115/115	-
28	BCR	X	101	-	-	5/29/63/63	0/2/2/2
31	LMG	c	523	-	-	17/43/63/70	0/1/1/1
28	BCR	C	514	-	-	0/29/63/63	0/2/2/2
26	CLA	b	606	2	-	5/39/115/115	-
26	CLA	C	509	3	-	9/39/115/115	-
32	SQD	B	622	-	-	24/49/69/69	0/1/1/1
30	STE	I	102	-	-	8/12/12/17	-
31	LMG	D	407	-	-	11/46/66/70	0/1/1/1
26	CLA	c	513	3	-	12/39/115/115	-
30	STE	A	613	-	-	4/6/6/17	-
26	CLA	B	611	2	-	4/39/115/115	-
30	STE	d	406	-	-	8/17/17/17	-
26	CLA	C	502	3	-	11/39/115/115	-
26	CLA	b	604	2	-	13/39/115/115	-
26	CLA	a	613	37	-	5/39/115/115	-
26	CLA	b	614	2	-	24/39/115/115	-
29	PL9	a	612	-	-	17/53/73/73	0/1/1/1
32	SQD	f	101	-	-	16/36/56/69	0/1/1/1
26	CLA	B	601	37	-	22/39/115/115	-
30	STE	C	515	-	-	7/11/11/17	-
30	STE	K	104	-	-	7/11/11/17	-
26	CLA	b	615	2	-	7/39/115/115	-
33	LHG	a	614	-	-	9/43/43/53	-
28	BCR	h	101	-	-	3/29/63/63	0/2/2/2
26	CLA	B	607	37	-	8/39/115/115	-
30	STE	A	622	-	-	3/8/8/17	-
30	STE	C	524	-	-	2/9/9/17	-
26	CLA	b	610	37	-	5/39/115/115	-
33	LHG	d	407	-	-	18/53/53/53	-
26	CLA	c	502	3	-	13/39/115/115	-
30	STE	C	517	-	-	0/2/2/17	-
26	CLA	a	607	1	-	3/39/115/115	-
30	STE	e	104	-	-	3/6/6/17	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	STE	m	103	-	-	12/15/15/17	-
30	STE	d	408	-	-	11/17/17/17	-
32	SQD	a	617	-	-	19/49/69/69	0/1/1/1
31	LMG	B	620	-	-	19/40/60/70	0/1/1/1
30	STE	c	516	-	-	5/10/10/17	-
31	LMG	b	622	-	-	27/50/70/70	0/1/1/1
26	CLA	C	510	3	-	5/39/115/115	-
26	CLA	c	505	3	-	6/39/115/115	-
28	BCR	A	611	-	-	0/29/63/63	0/2/2/2
26	CLA	B	606	2	-	12/39/115/115	-
30	STE	H	102	-	-	6/15/15/17	-
30	STE	T	102	-	-	7/13/13/17	-
35	HEM	e	102	6,5	-	6/14/54/54	-
26	CLA	B	613	2	-	13/39/115/115	-
26	CLA	b	616	2	-	9/33/109/115	-
31	LMG	C	523	-	-	19/43/63/70	0/1/1/1
31	LMG	d	409	-	-	4/39/59/70	0/1/1/1
34	DGD	h	102	-	-	17/51/91/95	0/2/2/2
30	STE	b	625	-	-	4/7/7/17	-
30	STE	c	517	-	-	9/15/15/17	-
30	STE	a	619	-	-	3/7/7/17	-
30	STE	Z	101	-	-	7/14/14/17	-
34	DGD	C	520	-	-	22/51/91/95	0/2/2/2
33	LHG	A	617	-	-	19/53/53/53	-
26	CLA	c	512	3	-	17/39/115/115	-
30	STE	A	621	-	-	8/14/14/17	-
30	STE	i	101	-	-	5/9/9/17	-
33	LHG	a	616	-	-	17/46/46/53	-
26	CLA	B	612	2	-	9/39/115/115	-
28	BCR	k	101	-	-	5/29/63/63	0/2/2/2
30	STE	D	411	-	-	7/17/17/17	-
30	STE	b	624	-	-	6/13/13/17	-
31	LMG	c	518	-	-	10/31/31/70	-
26	CLA	b	611	2	-	4/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	a	608	37	-	8/39/115/115	-
26	CLA	d	403	4	-	13/39/115/115	-
31	LMG	c	522	-	-	15/41/61/70	0/1/1/1
32	SQD	A	618	-	-	15/38/58/69	0/1/1/1
30	STE	J	101	-	-	7/9/9/17	-
29	PL9	d	405	-	-	10/53/73/73	0/1/1/1
30	STE	j	101	-	-	4/9/9/17	-
34	DGD	c	519	-	-	17/51/91/95	0/2/2/2
33	LHG	D	409	-	-	15/51/51/53	-
33	LHG	b	623	-	-	13/53/53/53	-
26	CLA	B	615	2	-	9/39/115/115	-
26	CLA	b	608	2	-	7/39/115/115	-
29	PL9	A	612	-	-	21/53/73/73	0/1/1/1
26	CLA	C	504	37	-	5/32/108/115	-
30	STE	A	620	-	-	3/5/5/17	-
30	STE	B	623	-	-	11/15/15/17	-
31	LMG	C	516	-	-	13/30/50/70	0/1/1/1
26	CLA	C	508	3	-	4/39/115/115	-
32	SQD	b	620	-	-	20/44/64/69	0/1/1/1
26	CLA	b	607	37	-	15/39/115/115	-
28	BCR	a	611	-	-	2/29/63/63	0/2/2/2
26	CLA	b	609	2	-	7/39/115/115	-
26	CLA	b	602	2	-	13/39/115/115	-
30	STE	j	102	-	-	6/13/13/17	-
30	STE	C	519	-	-	7/7/7/17	-
30	STE	i	102	-	-	2/3/3/17	-
30	STE	M	102	-	-	8/12/12/17	-
30	STE	a	620	-	-	6/9/9/17	-
30	STE	M	104	-	-	4/12/12/17	-
30	STE	E	103	-	-	11/17/17/17	-
34	DGD	H	101	-	-	14/51/91/95	0/2/2/2
30	STE	h	104	-	-	3/8/8/17	-
30	STE	d	410	-	-	10/17/17/17	-
31	LMG	c	524	-	-	18/44/64/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	DGD	C	521	-	-	17/51/91/95	0/2/2/2
31	LMG	m	101	-	-	25/46/66/70	0/1/1/1
27	PHO	D	401	-	-	3/37/103/103	0/5/6/6
26	CLA	B	605	2	-	10/39/115/115	-
28	BCR	b	617	-	-	4/29/63/63	0/2/2/2
30	STE	C	518	-	-	2/4/4/17	-
26	CLA	b	613	2	-	7/39/115/115	-
26	CLA	c	506	3	-	16/39/115/115	-
28	BCR	c	515	-	-	0/29/63/63	0/2/2/2
36	HEC	v	201	16	1/1/3/7	5/14/54/54	-
34	DGD	c	521	-	-	15/51/91/95	0/2/2/2
31	LMG	A	615	-	-	18/43/63/70	0/1/1/1
31	LMG	D	406	-	-	17/45/65/70	0/1/1/1
26	CLA	A	607	1	-	5/39/115/115	-
26	CLA	c	503	3	-	11/39/115/115	-
28	BCR	B	617	-	-	2/29/63/63	0/2/2/2
26	CLA	A	610	1	-	4/26/102/115	-
33	LHG	L	101	-	-	22/53/53/53	-
36	HEC	V	201	16	1/1/3/7	4/14/54/54	-
27	PHO	A	609	-	-	3/37/103/103	0/5/6/6
30	STE	B	624	-	-	2/9/9/17	-
30	STE	k	103	-	-	5/11/11/17	-
26	CLA	B	610	37	-	5/39/115/115	-
30	STE	C	525	-	-	10/13/13/17	-
26	CLA	b	612	2	-	6/39/115/115	-
30	STE	C	526	-	-	8/11/11/17	-
34	DGD	A	619	-	-	21/55/95/95	0/2/2/2
30	STE	e	103	-	-	4/5/5/17	-
26	CLA	c	510	3	-	19/39/115/115	-
33	LHG	l	101	-	-	19/53/53/53	-
26	CLA	C	505	3	-	10/39/115/115	-
26	CLA	B	609	2	-	8/39/115/115	-
26	CLA	B	602	2	-	6/39/115/115	-
26	CLA	D	403	4	-	7/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	C	506	3	-	12/39/115/115	-

All (651) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	401	PHO	C3B-C4B	9.41	1.51	1.41
27	d	401	PHO	C1B-C2B	9.15	1.49	1.39
27	A	609	PHO	C1B-C2B	8.45	1.48	1.39
27	D	401	PHO	C1B-C2B	8.07	1.48	1.39
27	a	609	PHO	C3B-C4B	7.93	1.49	1.41
27	a	609	PHO	C1B-C2B	7.93	1.48	1.39
27	A	609	PHO	C3B-C4B	7.86	1.49	1.41
27	D	401	PHO	C3B-C4B	7.85	1.49	1.41
26	B	606	CLA	MG-NA	7.73	2.24	2.06
36	V	201	HEC	C3D-C2D	7.69	1.53	1.36
36	v	201	HEC	C3D-C2D	7.24	1.52	1.36
36	V	201	HEC	FE-ND	7.22	2.17	1.94
26	C	501	CLA	MG-NA	6.96	2.22	2.06
26	C	507	CLA	MG-NA	6.30	2.21	2.06
26	C	511	CLA	MG-NA	6.27	2.21	2.06
26	c	511	CLA	MG-NA	6.13	2.20	2.06
26	C	512	CLA	MG-NB	5.90	2.17	2.05
26	B	603	CLA	MG-NA	5.82	2.20	2.06
26	b	615	CLA	MG-NB	5.70	2.17	2.05
26	b	610	CLA	MG-NB	-5.63	1.94	2.05
35	e	102	HEM	FE-NB	5.57	2.12	1.94
26	B	615	CLA	MG-NA	5.53	2.19	2.06
26	b	609	CLA	MG-NA	5.36	2.19	2.06
26	b	611	CLA	MG-NA	5.31	2.18	2.06
26	b	606	CLA	MG-NA	5.28	2.18	2.06
26	B	604	CLA	MG-NA	5.18	2.18	2.06
26	a	607	CLA	MG-NB	5.07	2.15	2.05
26	a	613	CLA	MG-NA	5.05	2.18	2.06
32	a	617	SQD	O48-C23	5.01	1.48	1.33
26	d	403	CLA	MG-NA	5.01	2.18	2.06
26	b	612	CLA	MG-ND	-4.92	1.96	2.05
32	F	102	SQD	O48-C23	4.90	1.47	1.33
32	A	618	SQD	O48-C23	4.88	1.47	1.33
27	a	609	PHO	C1D-C2D	4.86	1.44	1.39
32	A	616	SQD	O48-C23	4.72	1.47	1.33
26	B	609	CLA	MG-NA	4.72	2.17	2.06
27	D	401	PHO	C1D-C2D	4.71	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	615	SQD	O48-C23	4.69	1.47	1.33
32	B	622	SQD	O48-C23	4.69	1.47	1.33
32	f	101	SQD	O48-C23	4.66	1.46	1.33
26	C	503	CLA	MG-ND	4.65	2.15	2.05
36	v	201	HEC	FE-NA	4.64	2.10	1.95
27	A	609	PHO	C1D-C2D	4.64	1.44	1.39
26	a	610	CLA	C1D-ND	4.53	1.43	1.37
26	B	601	CLA	MG-NA	4.47	2.16	2.06
26	D	403	CLA	MG-NA	4.40	2.16	2.06
26	B	610	CLA	MG-NA	4.39	2.16	2.06
26	B	615	CLA	MG-NB	4.38	2.14	2.05
26	B	613	CLA	MG-NC	4.38	2.16	2.06
26	B	605	CLA	C1D-ND	4.37	1.43	1.37
36	v	201	HEC	FE-ND	4.35	2.08	1.94
26	A	608	CLA	MG-NA	4.35	2.16	2.06
26	C	513	CLA	MG-ND	4.33	2.14	2.05
35	e	102	HEM	FE-NA	4.32	2.09	1.95
26	C	503	CLA	MG-NC	4.32	2.16	2.06
26	c	510	CLA	MG-NA	4.21	2.16	2.06
26	c	503	CLA	MG-NA	4.21	2.16	2.06
26	b	612	CLA	C1D-ND	4.18	1.43	1.37
35	F	101	HEM	FE-NB	4.18	2.07	1.94
26	C	513	CLA	MG-NA	4.18	2.16	2.06
26	B	610	CLA	C1D-ND	4.18	1.43	1.37
26	b	608	CLA	MG-NB	4.16	2.14	2.05
27	d	401	PHO	C1D-C2D	4.09	1.44	1.39
26	a	607	CLA	C1D-ND	4.07	1.43	1.37
32	b	620	SQD	O48-C23	4.04	1.45	1.33
32	a	617	SQD	O5-C1	4.04	1.52	1.41
26	D	403	CLA	C1D-ND	4.03	1.43	1.37
26	c	503	CLA	MG-NC	4.03	2.15	2.06
26	C	512	CLA	MG-ND	-4.03	1.97	2.05
26	b	601	CLA	MG-NA	4.02	2.15	2.06
26	a	610	CLA	MG-ND	-4.00	1.97	2.05
26	a	610	CLA	C4B-NB	4.00	1.43	1.37
26	C	501	CLA	C1D-ND	3.99	1.43	1.37
26	c	502	CLA	C1D-ND	3.99	1.43	1.37
26	B	608	CLA	MG-NA	3.97	2.15	2.06
26	B	608	CLA	C1D-ND	3.97	1.43	1.37
26	B	616	CLA	MG-NC	3.95	2.15	2.06
32	b	620	SQD	O47-C7	3.93	1.45	1.34
26	b	616	CLA	C1D-ND	3.93	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	610	CLA	C1D-ND	3.91	1.43	1.37
26	B	602	CLA	C1D-ND	3.90	1.43	1.37
26	b	604	CLA	MG-NA	3.89	2.15	2.06
26	A	607	CLA	MG-NA	3.89	2.15	2.06
26	C	503	CLA	C1D-ND	3.88	1.43	1.37
26	c	509	CLA	C1D-ND	3.88	1.43	1.37
26	b	614	CLA	C4B-NB	3.88	1.43	1.37
26	C	503	CLA	MG-NA	3.87	2.15	2.06
26	a	607	CLA	MG-NA	3.87	2.15	2.06
26	B	604	CLA	C1D-ND	3.86	1.42	1.37
26	A	607	CLA	C1D-ND	3.86	1.42	1.37
26	B	614	CLA	MG-NA	3.86	2.15	2.06
26	B	602	CLA	MG-ND	-3.86	1.98	2.05
32	A	618	SQD	O5-C1	3.86	1.51	1.41
26	b	614	CLA	C1D-ND	3.81	1.42	1.37
26	b	606	CLA	C1D-ND	3.80	1.42	1.37
26	B	602	CLA	MG-NC	3.79	2.15	2.06
26	c	508	CLA	MG-NC	3.76	2.15	2.06
26	d	403	CLA	C1D-ND	3.75	1.42	1.37
26	d	402	CLA	C1D-ND	3.74	1.42	1.37
26	c	511	CLA	C1D-ND	3.74	1.42	1.37
26	C	505	CLA	C1D-ND	3.73	1.42	1.37
32	a	615	SQD	O47-C45	-3.73	1.37	1.46
26	C	505	CLA	MG-NC	3.72	2.15	2.06
26	A	614	CLA	C1D-ND	3.70	1.42	1.37
26	b	601	CLA	C1D-ND	3.70	1.42	1.37
26	B	613	CLA	C1D-ND	3.69	1.42	1.37
26	B	605	CLA	C4B-NB	3.69	1.42	1.37
26	B	605	CLA	MG-NB	3.69	2.13	2.05
26	B	615	CLA	C1D-ND	3.68	1.42	1.37
26	c	504	CLA	C4B-NB	3.68	1.42	1.37
26	b	613	CLA	MG-NC	3.67	2.15	2.06
26	d	402	CLA	MG-ND	-3.67	1.98	2.05
26	B	613	CLA	MG-NB	-3.67	1.98	2.05
35	F	101	HEM	FE-NC	3.67	2.07	1.95
26	d	403	CLA	C4B-NB	3.66	1.42	1.37
26	b	605	CLA	MG-NB	3.66	2.13	2.05
26	B	616	CLA	C1D-ND	3.65	1.42	1.37
26	C	501	CLA	C4B-NB	3.63	1.42	1.37
32	A	616	SQD	O47-C45	-3.63	1.38	1.46
32	f	101	SQD	O47-C7	3.62	1.44	1.34
26	B	610	CLA	C4B-NB	3.61	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	608	CLA	MG-NA	3.60	2.14	2.06
26	b	612	CLA	MG-NA	3.59	2.14	2.06
26	b	608	CLA	C1D-ND	3.59	1.42	1.37
26	c	508	CLA	C4B-NB	3.59	1.42	1.37
27	D	401	PHO	C4D-CHA	3.58	1.44	1.39
26	b	607	CLA	MG-NA	3.57	2.14	2.06
26	C	502	CLA	C1D-ND	3.56	1.42	1.37
26	b	604	CLA	C1D-ND	3.56	1.42	1.37
26	c	510	CLA	C1D-ND	3.56	1.42	1.37
27	a	609	PHO	C4D-CHA	3.56	1.44	1.39
26	C	504	CLA	C4B-NB	3.55	1.42	1.37
26	B	607	CLA	C1D-ND	3.55	1.42	1.37
26	C	509	CLA	MG-NA	3.54	2.14	2.06
26	B	601	CLA	C1D-ND	3.53	1.42	1.37
26	C	509	CLA	C1D-ND	3.53	1.42	1.37
26	A	607	CLA	C1B-C2B	3.52	1.51	1.43
26	D	403	CLA	MG-ND	-3.51	1.98	2.05
26	B	602	CLA	C4B-NB	3.51	1.42	1.37
26	A	608	CLA	C1D-ND	3.51	1.42	1.37
26	c	512	CLA	C1D-ND	3.51	1.42	1.37
26	C	511	CLA	C1D-ND	3.50	1.42	1.37
26	c	513	CLA	C1D-ND	3.49	1.42	1.37
32	A	618	SQD	O47-C45	-3.49	1.38	1.46
26	b	602	CLA	C1D-ND	3.49	1.42	1.37
26	B	611	CLA	C1D-ND	3.49	1.42	1.37
36	V	201	HEC	FE-NA	3.48	2.06	1.95
26	C	513	CLA	C1D-ND	3.46	1.42	1.37
26	A	610	CLA	C4B-NB	3.46	1.42	1.37
26	B	609	CLA	C1D-ND	3.46	1.42	1.37
26	B	612	CLA	C1D-ND	3.45	1.42	1.37
26	b	602	CLA	MG-ND	-3.45	1.99	2.05
26	b	603	CLA	C1D-ND	3.43	1.42	1.37
26	C	502	CLA	MG-NA	3.42	2.14	2.06
26	B	601	CLA	C4B-NB	3.42	1.42	1.37
26	c	506	CLA	C1D-ND	3.42	1.42	1.37
32	a	617	SQD	O47-C7	3.42	1.43	1.34
26	d	402	CLA	MG-NA	3.41	2.14	2.06
26	c	503	CLA	C1D-ND	3.40	1.42	1.37
26	B	607	CLA	MG-NA	3.40	2.14	2.06
35	F	101	HEM	FE-NA	3.40	2.06	1.95
26	c	507	CLA	MG-NA	3.39	2.14	2.06
32	A	618	SQD	O47-C7	3.38	1.43	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	511	CLA	C1B-C2B	3.38	1.51	1.43
32	B	622	SQD	O47-C45	-3.38	1.38	1.46
26	B	614	CLA	C1D-ND	3.38	1.42	1.37
26	C	504	CLA	MG-NA	3.37	2.14	2.06
32	a	617	SQD	O47-C45	-3.35	1.38	1.46
27	D	401	PHO	C3D-C4D	3.34	1.45	1.41
26	C	506	CLA	C1D-ND	3.34	1.42	1.37
26	c	508	CLA	C1D-ND	3.34	1.42	1.37
32	B	622	SQD	O47-C7	3.33	1.43	1.34
26	A	614	CLA	MG-NA	3.31	2.14	2.06
26	C	508	CLA	C4B-NB	3.30	1.42	1.37
32	A	618	SQD	C24-C23	3.30	1.60	1.50
26	B	615	CLA	C1B-C2B	3.30	1.50	1.43
26	C	503	CLA	C1B-C2B	3.30	1.50	1.43
26	B	605	CLA	C1B-C2B	3.29	1.50	1.43
26	B	606	CLA	C4B-NB	3.28	1.42	1.37
26	c	513	CLA	MG-NA	3.28	2.14	2.06
32	f	101	SQD	O47-C45	-3.28	1.38	1.46
32	a	617	SQD	C24-C23	3.28	1.60	1.50
26	C	512	CLA	C1D-ND	3.28	1.42	1.37
27	A	609	PHO	C4D-CHA	3.27	1.44	1.39
26	c	513	CLA	C4B-NB	3.27	1.42	1.37
26	C	501	CLA	CHC-C1C	3.27	1.45	1.38
26	b	613	CLA	C1D-ND	3.26	1.42	1.37
26	b	615	CLA	C1D-ND	3.26	1.42	1.37
26	B	603	CLA	C1D-ND	3.26	1.42	1.37
26	C	508	CLA	C1D-ND	3.26	1.42	1.37
26	C	503	CLA	C4B-NB	3.26	1.42	1.37
26	b	612	CLA	C4B-NB	3.26	1.42	1.37
26	c	512	CLA	MG-NB	3.26	2.12	2.05
26	B	614	CLA	C4B-NB	3.25	1.42	1.37
26	b	613	CLA	C4B-NB	3.25	1.42	1.37
32	A	616	SQD	C24-C23	3.25	1.60	1.50
26	c	507	CLA	C4B-NB	3.25	1.42	1.37
32	B	622	SQD	C24-C23	3.25	1.60	1.50
26	C	510	CLA	C1D-ND	3.25	1.42	1.37
26	B	612	CLA	MG-NA	3.24	2.14	2.06
29	d	405	PL9	C3-C4	-3.24	1.44	1.49
26	C	512	CLA	MG-NA	3.24	2.14	2.06
32	F	102	SQD	C24-C23	3.23	1.60	1.50
26	b	615	CLA	MG-ND	-3.22	1.99	2.05
36	V	201	HEC	FE-NC	3.21	2.05	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	620	SQD	O5-C1	3.21	1.50	1.41
26	C	510	CLA	C1B-C2B	3.20	1.50	1.43
29	a	612	PL9	C53-C6	-3.19	1.44	1.50
27	d	401	PHO	C4D-CHA	3.18	1.44	1.39
26	c	503	CLA	C1B-C2B	3.17	1.50	1.43
26	C	506	CLA	C4B-NB	3.17	1.42	1.37
26	C	502	CLA	C4B-NB	3.17	1.42	1.37
26	d	402	CLA	C4B-NB	3.16	1.42	1.37
26	a	607	CLA	C1B-C2B	3.16	1.50	1.43
26	c	507	CLA	C1B-C2B	3.16	1.50	1.43
26	a	613	CLA	C1D-ND	3.15	1.42	1.37
26	c	501	CLA	MG-NA	3.14	2.13	2.06
26	B	611	CLA	C1B-C2B	3.14	1.50	1.43
26	c	509	CLA	C1B-C2B	3.13	1.50	1.43
26	B	601	CLA	C1B-C2B	3.13	1.50	1.43
26	c	502	CLA	MG-NA	3.13	2.13	2.06
26	C	506	CLA	C1B-C2B	3.13	1.50	1.43
26	c	512	CLA	C4B-NB	3.12	1.42	1.37
26	B	611	CLA	MG-NC	3.12	2.13	2.06
26	a	613	CLA	C1B-C2B	3.12	1.50	1.43
26	b	601	CLA	C4B-NB	3.12	1.42	1.37
26	c	505	CLA	C4B-NB	3.12	1.42	1.37
26	B	605	CLA	MG-NC	3.12	2.13	2.06
32	f	101	SQD	C24-C23	3.11	1.59	1.50
26	C	510	CLA	C4B-NB	3.11	1.42	1.37
26	C	505	CLA	C1B-C2B	3.11	1.50	1.43
26	B	616	CLA	C4B-NB	3.11	1.41	1.37
26	b	605	CLA	C4B-NB	3.11	1.41	1.37
32	a	615	SQD	O47-C7	3.11	1.43	1.34
26	b	615	CLA	C4B-NB	3.09	1.41	1.37
26	C	511	CLA	C4B-NB	3.08	1.41	1.37
26	b	616	CLA	MG-NC	3.07	2.13	2.06
26	C	513	CLA	C4B-NB	3.07	1.41	1.37
32	b	620	SQD	O47-C45	-3.07	1.39	1.46
26	c	501	CLA	C1D-ND	3.06	1.41	1.37
26	A	608	CLA	C1B-C2B	3.06	1.50	1.43
26	C	507	CLA	C4B-NB	3.06	1.41	1.37
26	b	609	CLA	C1D-ND	3.06	1.41	1.37
26	B	609	CLA	C1B-C2B	3.05	1.50	1.43
26	A	610	CLA	C1D-ND	3.05	1.41	1.37
26	C	508	CLA	MG-NC	3.05	2.13	2.06
26	a	610	CLA	C1B-C2B	3.05	1.50	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	611	CLA	C4B-NB	3.04	1.41	1.37
32	A	616	SQD	O47-C7	3.04	1.42	1.34
26	c	508	CLA	CHC-C1C	3.04	1.44	1.38
26	c	503	CLA	C4B-NB	3.02	1.41	1.37
26	c	504	CLA	C1B-C2B	3.02	1.50	1.43
26	b	611	CLA	C4B-NB	3.02	1.41	1.37
26	c	507	CLA	C1D-ND	3.02	1.41	1.37
26	C	502	CLA	MG-NB	-3.01	1.99	2.05
26	b	607	CLA	C1D-ND	3.01	1.41	1.37
26	A	608	CLA	C4B-NB	3.00	1.41	1.37
26	D	403	CLA	C4B-NB	3.00	1.41	1.37
32	a	615	SQD	C24-C23	2.99	1.59	1.50
26	b	601	CLA	C1B-C2B	2.99	1.50	1.43
32	A	616	SQD	O5-C1	2.99	1.49	1.41
26	b	603	CLA	C4B-NB	2.98	1.41	1.37
26	C	502	CLA	C1B-C2B	2.98	1.50	1.43
26	c	511	CLA	C1B-C2B	2.98	1.50	1.43
26	b	615	CLA	C3B-C4B	2.97	1.51	1.42
26	b	611	CLA	C1D-ND	2.97	1.41	1.37
26	a	607	CLA	CHC-C1C	2.97	1.44	1.38
26	B	606	CLA	C1D-ND	2.97	1.41	1.37
26	b	605	CLA	C1B-C2B	2.96	1.50	1.43
26	C	508	CLA	C1B-C2B	2.95	1.50	1.43
26	C	507	CLA	C1D-ND	2.95	1.41	1.37
29	d	405	PL9	C7-C3	2.95	1.55	1.51
26	B	611	CLA	MG-NA	2.95	2.13	2.06
27	a	609	PHO	C3D-C4D	2.95	1.45	1.41
26	b	608	CLA	MG-NA	2.95	2.13	2.06
35	e	102	HEM	FE-NC	2.94	2.04	1.95
35	e	102	HEM	CAC-C3C	2.94	1.55	1.47
26	C	510	CLA	MG-NA	2.94	2.13	2.06
26	c	512	CLA	C1B-C2B	2.93	1.50	1.43
26	b	603	CLA	C1B-C2B	2.92	1.50	1.43
26	c	511	CLA	C4B-NB	2.92	1.41	1.37
26	b	612	CLA	CHC-C1C	2.92	1.44	1.38
26	c	512	CLA	CHC-C1C	2.92	1.44	1.38
26	C	505	CLA	MG-NA	2.91	2.13	2.06
27	A	609	PHO	CMD-C2D	-2.91	1.45	1.51
26	c	505	CLA	CHC-C1C	2.91	1.44	1.38
26	B	613	CLA	C4B-NB	2.91	1.41	1.37
26	A	614	CLA	C1B-C2B	2.91	1.50	1.43
26	a	608	CLA	C1D-ND	2.91	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	603	CLA	C1B-C2B	2.91	1.50	1.43
26	b	609	CLA	C4B-NB	2.91	1.41	1.37
26	b	608	CLA	C4B-NB	2.90	1.41	1.37
32	a	615	SQD	O5-C1	2.90	1.49	1.41
26	b	606	CLA	C4B-NB	2.90	1.41	1.37
26	C	509	CLA	C4B-NB	2.89	1.41	1.37
26	b	610	CLA	C1B-C2B	2.89	1.49	1.43
26	C	507	CLA	C1B-C2B	2.89	1.49	1.43
26	C	508	CLA	MG-NA	2.88	2.13	2.06
26	C	510	CLA	MG-NC	2.88	2.13	2.06
26	B	606	CLA	C1B-C2B	2.88	1.49	1.43
26	A	608	CLA	MG-NB	-2.87	2.00	2.05
26	A	614	CLA	C4B-NB	2.86	1.41	1.37
26	d	402	CLA	MG-NC	2.85	2.13	2.06
35	F	101	HEM	CAB-C3B	2.85	1.55	1.47
26	c	506	CLA	MG-ND	-2.85	2.00	2.05
26	c	508	CLA	C1B-C2B	2.84	1.49	1.43
26	C	504	CLA	C1D-ND	2.84	1.41	1.37
26	b	616	CLA	C4B-NB	2.84	1.41	1.37
26	d	402	CLA	C1B-C2B	2.83	1.49	1.43
26	b	613	CLA	C1B-C2B	2.83	1.49	1.43
26	a	608	CLA	C4B-NB	2.83	1.41	1.37
26	D	403	CLA	C1B-C2B	2.82	1.49	1.43
26	D	402	CLA	C1B-C2B	2.82	1.49	1.43
36	V	201	HEC	FE-NB	2.82	2.03	1.94
26	b	602	CLA	C4B-NB	2.82	1.41	1.37
26	B	607	CLA	MG-NB	-2.81	2.00	2.05
32	f	101	SQD	O5-C1	2.81	1.49	1.41
26	d	403	CLA	C1B-C2B	2.81	1.49	1.43
26	b	614	CLA	MG-NA	2.81	2.12	2.06
32	B	622	SQD	O5-C1	2.81	1.49	1.41
26	C	510	CLA	CHC-C1C	2.81	1.44	1.38
26	B	608	CLA	C4B-NB	2.81	1.41	1.37
26	c	510	CLA	C4B-NB	2.79	1.41	1.37
26	C	501	CLA	C3B-C4B	2.78	1.50	1.42
26	B	615	CLA	C4B-NB	2.78	1.41	1.37
26	B	602	CLA	C1B-C2B	2.78	1.49	1.43
26	c	505	CLA	C3B-C4B	2.77	1.50	1.42
26	B	613	CLA	C1B-C2B	2.77	1.49	1.43
26	b	603	CLA	MG-ND	-2.77	2.00	2.05
26	c	510	CLA	C1B-C2B	2.76	1.49	1.43
32	A	618	SQD	O9-S	2.76	1.52	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	614	CLA	MG-ND	-2.75	2.00	2.05
26	c	502	CLA	C1B-C2B	2.75	1.49	1.43
32	F	102	SQD	O5-C1	2.75	1.48	1.41
26	C	505	CLA	CHC-C1C	2.75	1.44	1.38
26	b	609	CLA	C1B-C2B	2.75	1.49	1.43
26	b	604	CLA	C1B-C2B	2.75	1.49	1.43
26	b	614	CLA	MG-NC	2.75	2.12	2.06
26	B	608	CLA	CHC-C1C	2.75	1.44	1.38
26	C	506	CLA	MG-NC	2.74	2.12	2.06
26	b	611	CLA	C1B-C2B	2.74	1.49	1.43
26	c	513	CLA	C3B-C4B	2.73	1.50	1.42
27	A	609	PHO	CMC-C2C	-2.73	1.46	1.50
26	b	602	CLA	C1B-C2B	2.72	1.49	1.43
29	A	612	PL9	C53-C6	-2.72	1.45	1.50
26	b	605	CLA	MG-NA	2.72	2.12	2.06
26	D	402	CLA	MG-NA	2.72	2.12	2.06
26	C	504	CLA	C1B-C2B	2.71	1.49	1.43
26	C	513	CLA	C1B-C2B	2.71	1.49	1.43
26	B	605	CLA	CHC-C1C	2.71	1.43	1.38
26	c	504	CLA	C1D-ND	2.71	1.41	1.37
26	b	608	CLA	CHC-C1C	2.70	1.43	1.38
26	B	610	CLA	C1B-C2B	2.70	1.49	1.43
26	c	508	CLA	C3B-C4B	2.70	1.50	1.42
26	b	605	CLA	C3B-C4B	2.69	1.50	1.42
26	c	512	CLA	MG-NA	2.69	2.12	2.06
26	b	608	CLA	C3B-C4B	2.69	1.50	1.42
26	B	616	CLA	C1B-C2B	2.69	1.49	1.43
26	b	614	CLA	CHC-C1C	2.69	1.43	1.38
32	b	620	SQD	C24-C23	2.69	1.58	1.50
26	b	603	CLA	MG-NA	2.68	2.12	2.06
26	c	504	CLA	MG-NA	2.68	2.12	2.06
26	c	502	CLA	C4B-NB	2.68	1.41	1.37
26	C	508	CLA	C3B-C4B	2.68	1.50	1.42
26	C	512	CLA	C4B-NB	2.67	1.41	1.37
26	c	501	CLA	C1B-C2B	2.67	1.49	1.43
27	d	401	PHO	CMC-C2C	-2.67	1.46	1.50
32	A	618	SQD	O7-S	2.66	1.52	1.45
26	b	605	CLA	C1D-ND	2.66	1.41	1.37
26	D	402	CLA	C4B-NB	2.65	1.41	1.37
26	b	614	CLA	C1B-C2B	2.65	1.49	1.43
26	A	614	CLA	MG-NC	2.65	2.12	2.06
26	C	501	CLA	C1B-C2B	2.64	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	605	CLA	CHC-C1C	2.64	1.43	1.38
26	B	614	CLA	CMB-C2B	-2.64	1.45	1.50
26	c	505	CLA	C1D-ND	2.64	1.41	1.37
35	F	101	HEM	CAC-C3C	2.64	1.54	1.47
26	c	505	CLA	C1B-C2B	2.64	1.49	1.43
35	e	102	HEM	CAB-C3B	2.64	1.54	1.47
26	C	507	CLA	CHC-C1C	2.63	1.43	1.38
26	c	509	CLA	C4B-NB	2.63	1.41	1.37
36	v	201	HEC	FE-NC	2.63	2.03	1.95
26	B	605	CLA	C3B-C4B	2.63	1.50	1.42
26	C	510	CLA	C3B-C4B	2.62	1.50	1.42
26	b	615	CLA	MG-NA	2.62	2.12	2.06
29	D	405	PL9	C52-C5	-2.62	1.45	1.50
26	b	607	CLA	C1B-C2B	2.61	1.49	1.43
27	D	401	PHO	CMC-C2C	-2.60	1.46	1.50
32	a	617	SQD	O5-C5	2.60	1.50	1.44
26	a	608	CLA	C1B-C2B	2.60	1.49	1.43
26	B	610	CLA	MG-ND	-2.59	2.00	2.05
27	d	401	PHO	CMD-C2D	-2.59	1.46	1.51
26	b	612	CLA	C3B-C4B	2.59	1.50	1.42
26	b	616	CLA	C1B-C2B	2.59	1.49	1.43
26	C	512	CLA	C1B-C2B	2.59	1.49	1.43
26	C	512	CLA	MG-NC	2.58	2.12	2.06
26	B	609	CLA	C4B-NB	2.58	1.41	1.37
26	B	608	CLA	C1B-C2B	2.58	1.49	1.43
26	c	513	CLA	CHC-C1C	2.57	1.43	1.38
26	C	509	CLA	C1B-C2B	2.57	1.49	1.43
26	b	615	CLA	C1B-C2B	2.57	1.49	1.43
26	A	610	CLA	CHC-C1C	2.55	1.43	1.38
26	b	602	CLA	CMD-C2D	-2.55	1.45	1.50
26	B	605	CLA	MG-ND	-2.55	2.00	2.05
26	C	502	CLA	C3B-C4B	2.55	1.50	1.42
26	d	402	CLA	C3B-C4B	2.54	1.50	1.42
32	a	617	SQD	O9-S	2.54	1.52	1.45
32	a	617	SQD	O7-S	2.54	1.52	1.45
26	d	403	CLA	CHC-C1C	2.54	1.43	1.38
26	C	511	CLA	C3B-C4B	2.53	1.50	1.42
26	C	504	CLA	C3B-C4B	2.53	1.50	1.42
26	B	601	CLA	C3B-C4B	2.53	1.50	1.42
26	C	513	CLA	CHC-C1C	2.52	1.43	1.38
26	B	612	CLA	C1B-C2B	2.52	1.49	1.43
26	B	601	CLA	CHC-C1C	2.52	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	508	CLA	MG-ND	2.52	2.10	2.05
26	c	506	CLA	C4B-NB	2.51	1.41	1.37
26	B	604	CLA	C1B-C2B	2.51	1.49	1.43
26	B	610	CLA	C3B-C4B	2.50	1.50	1.42
27	d	401	PHO	C3D-C4D	2.50	1.44	1.41
26	b	604	CLA	C4B-NB	2.50	1.41	1.37
27	a	609	PHO	CBD-CGD	-2.50	1.49	1.52
26	A	607	CLA	C3B-C4B	2.49	1.50	1.42
26	b	608	CLA	C1B-C2B	2.49	1.49	1.43
26	B	612	CLA	C4B-NB	2.49	1.41	1.37
27	A	609	PHO	CMB-C2B	-2.49	1.46	1.51
32	B	622	SQD	O9-S	2.48	1.52	1.45
26	C	505	CLA	C3B-C4B	2.47	1.49	1.42
27	a	609	PHO	CMB-C2B	-2.47	1.46	1.51
32	b	620	SQD	O9-S	2.46	1.52	1.45
26	c	512	CLA	C3B-C4B	2.46	1.49	1.42
26	c	510	CLA	MG-NB	-2.46	2.00	2.05
26	C	509	CLA	C3B-C4B	2.45	1.49	1.42
36	v	201	HEC	FE-NB	2.44	2.02	1.94
26	b	606	CLA	CHC-C1C	2.44	1.43	1.38
26	C	513	CLA	C3B-C4B	2.44	1.49	1.42
26	a	610	CLA	CMC-C2C	-2.43	1.45	1.50
26	b	611	CLA	CHC-C1C	2.43	1.43	1.38
26	c	501	CLA	MG-ND	-2.42	2.01	2.05
32	F	102	SQD	O9-S	2.42	1.51	1.45
26	b	607	CLA	C4B-NB	2.42	1.41	1.37
26	C	511	CLA	MG-NB	-2.41	2.01	2.05
26	B	603	CLA	CMD-C2D	-2.41	1.45	1.50
26	C	505	CLA	C4B-NB	2.41	1.41	1.37
26	A	614	CLA	CHC-C1C	2.41	1.43	1.38
26	B	610	CLA	CHC-C1C	2.41	1.43	1.38
26	c	504	CLA	CHC-C1C	2.41	1.43	1.38
26	B	611	CLA	CHC-C1C	2.40	1.43	1.38
32	f	101	SQD	O7-S	2.40	1.51	1.45
26	C	505	CLA	MG-NB	2.40	2.10	2.05
26	c	506	CLA	CHC-C1C	2.40	1.43	1.38
27	d	401	PHO	C4D-ND	-2.40	1.34	1.38
26	b	604	CLA	C3B-C4B	2.40	1.49	1.42
26	C	504	CLA	CHC-C1C	2.39	1.43	1.38
26	B	607	CLA	C4B-NB	2.39	1.41	1.37
26	d	403	CLA	C3B-C4B	2.39	1.49	1.42
26	b	612	CLA	C1B-C2B	2.39	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	607	CLA	C1B-C2B	2.38	1.48	1.43
26	A	610	CLA	C1B-C2B	2.38	1.48	1.43
26	b	615	CLA	CHC-C1C	2.38	1.43	1.38
26	b	606	CLA	C1B-C2B	2.38	1.48	1.43
26	B	615	CLA	C1D-C2D	2.38	1.50	1.45
26	b	606	CLA	MG-NC	2.38	2.11	2.06
26	b	601	CLA	C3B-C4B	2.38	1.49	1.42
26	b	613	CLA	CHC-C1C	2.38	1.43	1.38
26	B	603	CLA	C3B-C4B	2.38	1.49	1.42
26	a	610	CLA	C3B-C4B	2.38	1.49	1.42
27	D	401	PHO	CMD-C2D	-2.37	1.46	1.51
26	c	509	CLA	C3B-C4B	2.37	1.49	1.42
26	b	615	CLA	CMD-C2D	-2.36	1.45	1.50
32	f	101	SQD	O9-S	2.36	1.51	1.45
26	b	614	CLA	C3B-C4B	2.36	1.49	1.42
26	A	607	CLA	C4B-NB	2.35	1.41	1.37
26	c	501	CLA	C4B-NB	2.35	1.40	1.37
26	c	506	CLA	MG-NC	2.34	2.11	2.06
26	B	608	CLA	C3B-C4B	2.34	1.49	1.42
26	b	612	CLA	MG-NB	2.34	2.10	2.05
26	B	607	CLA	CMB-C2B	-2.34	1.46	1.50
26	C	512	CLA	C3B-C4B	2.34	1.49	1.42
26	A	608	CLA	CHC-C1C	2.33	1.43	1.38
26	C	509	CLA	CHC-C1C	2.33	1.43	1.38
26	B	613	CLA	C3B-C4B	2.33	1.49	1.42
26	b	611	CLA	C3B-C4B	2.33	1.49	1.42
26	b	604	CLA	MG-ND	-2.32	2.01	2.05
26	b	603	CLA	CMD-C2D	-2.32	1.46	1.50
26	B	606	CLA	CHC-C1C	2.32	1.43	1.38
26	c	511	CLA	CHC-C1C	2.32	1.43	1.38
26	C	508	CLA	CHC-C1C	2.32	1.43	1.38
32	A	616	SQD	O9-S	2.32	1.51	1.45
26	B	603	CLA	C4B-NB	2.32	1.40	1.37
26	c	513	CLA	MG-ND	-2.32	2.01	2.05
26	d	402	CLA	CHC-C1C	2.31	1.43	1.38
26	D	402	CLA	C1D-ND	2.31	1.40	1.37
26	b	610	CLA	CMD-C2D	-2.29	1.46	1.50
36	V	201	HEC	CMB-C2B	2.29	1.55	1.50
29	D	405	PL9	C31-C29	-2.29	1.46	1.51
26	A	608	CLA	MG-NC	2.29	2.11	2.06
26	C	512	CLA	CMD-C2D	-2.28	1.46	1.50
26	B	615	CLA	CMB-C2B	-2.28	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d	405	PL9	C31-C29	-2.28	1.46	1.51
26	c	501	CLA	CHC-C1C	2.28	1.43	1.38
26	D	403	CLA	CMD-C2D	-2.28	1.46	1.50
29	d	405	PL9	C6-C1	-2.28	1.44	1.48
26	b	603	CLA	CMC-C2C	-2.27	1.46	1.50
26	b	616	CLA	CMC-C2C	-2.27	1.46	1.50
26	B	604	CLA	CHC-C1C	2.27	1.43	1.38
27	D	401	PHO	C1D-ND	2.26	1.42	1.38
26	c	509	CLA	CHC-C1C	2.26	1.43	1.38
26	b	607	CLA	MG-NB	-2.25	2.01	2.05
26	b	603	CLA	C3B-C4B	2.25	1.49	1.42
26	a	608	CLA	CHC-C1C	2.25	1.43	1.38
26	B	604	CLA	C4B-NB	2.25	1.40	1.37
26	b	616	CLA	C3B-C4B	2.24	1.49	1.42
26	C	511	CLA	CHC-C1C	2.24	1.43	1.38
26	b	609	CLA	CHC-C1C	2.24	1.43	1.38
26	B	613	CLA	CHC-C1C	2.24	1.43	1.38
26	A	608	CLA	C3B-C4B	2.24	1.49	1.42
32	A	618	SQD	O5-C5	2.24	1.49	1.44
26	b	609	CLA	C3B-C4B	2.24	1.49	1.42
36	V	201	HEC	CMC-C2C	2.23	1.55	1.50
26	b	613	CLA	CMD-C2D	-2.23	1.46	1.50
26	C	503	CLA	C3B-C4B	2.23	1.49	1.42
26	c	501	CLA	CMC-C2C	-2.22	1.46	1.50
26	b	601	CLA	CHC-C1C	2.22	1.42	1.38
26	c	513	CLA	C1B-C2B	2.22	1.48	1.43
26	b	614	CLA	CMC-C2C	-2.22	1.46	1.50
26	c	510	CLA	CMB-C2B	-2.22	1.46	1.50
26	c	504	CLA	C3B-C4B	2.22	1.49	1.42
29	D	405	PL9	C3-C4	-2.21	1.46	1.49
26	B	605	CLA	MG-NA	2.21	2.11	2.06
35	e	102	HEM	CMB-C2B	2.21	1.55	1.50
26	c	503	CLA	C3B-C4B	2.21	1.49	1.42
26	c	509	CLA	MG-NB	-2.20	2.01	2.05
26	b	612	CLA	CMC-C2C	-2.20	1.46	1.50
26	c	505	CLA	CMB-C2B	-2.20	1.46	1.50
32	A	618	SQD	C46-C45	2.20	1.57	1.50
35	e	102	HEM	CMA-C3A	2.20	1.55	1.50
27	a	609	PHO	CMD-C2D	-2.19	1.47	1.51
26	b	608	CLA	MG-ND	-2.19	2.01	2.05
26	c	503	CLA	CMC-C2C	-2.19	1.46	1.50
26	c	503	CLA	CMD-C2D	-2.19	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	610	CLA	C3D-C4D	2.19	1.49	1.44
26	C	502	CLA	CHC-C1C	2.18	1.42	1.38
26	B	614	CLA	C1B-C2B	2.18	1.48	1.43
35	F	101	HEM	CMD-C2D	2.18	1.55	1.50
27	A	609	PHO	C4D-ND	-2.18	1.35	1.38
32	b	620	SQD	O7-S	2.18	1.51	1.45
26	B	614	CLA	CHC-C1C	2.17	1.42	1.38
26	B	602	CLA	CMB-C2B	-2.17	1.46	1.50
26	c	511	CLA	C3B-C4B	2.17	1.49	1.42
26	C	512	CLA	CHC-C1C	2.17	1.42	1.38
32	a	615	SQD	O7-S	2.16	1.51	1.45
26	C	508	CLA	C1D-C2D	2.16	1.49	1.45
26	b	607	CLA	CMC-C2C	-2.16	1.46	1.50
29	A	612	PL9	C7-C3	-2.16	1.48	1.51
26	B	606	CLA	CMB-C2B	-2.16	1.46	1.50
26	c	512	CLA	C3C-C2C	2.16	1.41	1.36
26	B	612	CLA	C3B-C4B	2.16	1.49	1.42
26	b	615	CLA	CMB-C2B	-2.16	1.46	1.50
26	B	616	CLA	C3B-C4B	2.15	1.49	1.42
26	a	607	CLA	C4B-NB	2.15	1.40	1.37
26	C	504	CLA	CMD-C2D	-2.15	1.46	1.50
27	D	401	PHO	CMB-C2B	-2.15	1.47	1.51
26	B	602	CLA	C3B-C4B	2.15	1.49	1.42
26	a	607	CLA	CMD-C2D	-2.15	1.46	1.50
26	b	610	CLA	C4B-NB	2.15	1.40	1.37
26	B	609	CLA	C3B-C4B	2.15	1.49	1.42
26	C	506	CLA	C3B-C4B	2.14	1.49	1.42
26	C	510	CLA	CMD-C2D	-2.14	1.46	1.50
26	c	512	CLA	CMB-C2B	-2.14	1.46	1.50
26	c	512	CLA	C1D-C2D	2.14	1.49	1.45
26	b	608	CLA	CMB-C2B	-2.14	1.46	1.50
36	v	201	HEC	CMB-C2B	2.13	1.55	1.50
26	C	504	CLA	CMB-C2B	-2.12	1.46	1.50
26	B	611	CLA	C3B-C4B	2.12	1.48	1.42
26	c	504	CLA	CMB-C2B	-2.12	1.46	1.50
26	D	402	CLA	MG-NB	2.12	2.10	2.05
26	C	510	CLA	C3C-C2C	2.12	1.41	1.36
26	C	502	CLA	CMB-C2B	-2.12	1.46	1.50
26	b	606	CLA	C3B-C4B	2.11	1.48	1.42
26	a	607	CLA	CMC-C2C	-2.11	1.46	1.50
35	e	102	HEM	C2A-C3A	-2.11	1.33	1.38
26	A	610	CLA	MG-NC	2.11	2.11	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	613	CLA	C3B-C4B	2.11	1.48	1.42
27	d	401	PHO	CMB-C2B	-2.11	1.47	1.51
26	C	509	CLA	O2D-CGD	2.10	1.38	1.33
26	d	402	CLA	CMB-C2B	-2.10	1.46	1.50
26	a	613	CLA	C4B-NB	2.10	1.40	1.37
26	d	403	CLA	MG-ND	-2.10	2.01	2.05
26	c	503	CLA	CHC-C1C	2.10	1.42	1.38
26	b	613	CLA	MG-NA	2.10	2.11	2.06
26	c	501	CLA	CMD-C2D	-2.09	1.46	1.50
35	e	102	HEM	CMC-C2C	2.09	1.55	1.50
26	B	611	CLA	CMD-C2D	-2.09	1.46	1.50
26	c	502	CLA	C3B-C4B	2.08	1.48	1.42
35	F	101	HEM	CMB-C2B	2.08	1.55	1.50
33	b	623	LHG	O7-C5	-2.08	1.41	1.46
32	F	102	SQD	O7-S	2.08	1.51	1.45
32	a	615	SQD	O9-S	2.08	1.51	1.45
26	C	509	CLA	CMD-C2D	-2.08	1.46	1.50
35	e	102	HEM	C3B-C2B	-2.08	1.32	1.37
26	B	601	CLA	C1D-C2D	2.08	1.49	1.45
26	c	507	CLA	C3D-C4D	2.08	1.48	1.44
26	a	608	CLA	C3B-C4B	2.08	1.48	1.42
26	C	512	CLA	CMB-C2B	-2.07	1.46	1.50
26	c	507	CLA	C3B-C4B	2.07	1.48	1.42
27	D	401	PHO	C4C-NC	2.07	1.44	1.37
26	D	402	CLA	C3B-C4B	2.07	1.48	1.42
26	B	606	CLA	CMD-C2D	-2.07	1.46	1.50
26	B	616	CLA	CHC-C1C	2.06	1.42	1.38
35	F	101	HEM	CMA-C3A	2.06	1.55	1.50
26	C	503	CLA	C1D-C2D	2.06	1.49	1.45
26	c	508	CLA	CMD-C2D	-2.06	1.46	1.50
26	c	506	CLA	C1B-C2B	2.06	1.48	1.43
32	b	620	SQD	O6-C44	2.06	1.47	1.43
26	B	612	CLA	CMC-C2C	-2.05	1.46	1.50
32	b	620	SQD	O5-C5	2.05	1.49	1.44
26	c	512	CLA	CMD-C2D	-2.05	1.46	1.50
35	F	101	HEM	FE-ND	2.05	2.01	1.94
26	b	608	CLA	MG-NC	2.05	2.11	2.06
26	c	511	CLA	C3C-C2C	2.05	1.41	1.36
35	e	102	HEM	CMD-C2D	2.05	1.55	1.50
26	b	607	CLA	C3B-C4B	2.04	1.48	1.42
26	B	606	CLA	C3B-C4B	2.04	1.48	1.42
26	C	506	CLA	CMC-C2C	-2.04	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	513	CLA	C1D-C2D	2.04	1.49	1.45
27	d	401	PHO	O2D-CGD	2.04	1.38	1.33
27	d	401	PHO	CAC-C3C	-2.04	1.48	1.51
32	b	620	SQD	C8-C7	2.03	1.56	1.50
32	b	620	SQD	C44-C45	2.03	1.57	1.50
29	A	612	PL9	C3-C4	-2.03	1.46	1.49
26	A	607	CLA	CMC-C2C	-2.03	1.46	1.50
26	D	402	CLA	CHC-C1C	2.03	1.42	1.38
26	c	508	CLA	MG-NA	2.03	2.11	2.06
26	b	602	CLA	C3B-C4B	2.03	1.48	1.42
26	c	513	CLA	MG-NC	2.03	2.11	2.06
26	b	603	CLA	CHC-C1C	2.03	1.42	1.38
26	C	504	CLA	O2D-CGD	2.03	1.38	1.33
34	C	522	DGD	O3G-C3G	-2.03	1.40	1.43
26	c	505	CLA	MG-NA	2.02	2.11	2.06
27	d	401	PHO	C4C-NC	2.02	1.43	1.37
26	B	615	CLA	CHC-C1C	2.02	1.42	1.38
32	A	618	SQD	C8-C7	2.02	1.56	1.50
26	c	501	CLA	C3B-C4B	2.02	1.48	1.42
26	C	511	CLA	CMD-C2D	-2.01	1.46	1.50
26	d	403	CLA	CMD-C2D	-2.01	1.46	1.50
26	B	616	CLA	CMC-C2C	-2.01	1.46	1.50
26	b	607	CLA	CMD-C2D	-2.00	1.46	1.50
26	B	607	CLA	C3B-C4B	2.00	1.48	1.42
26	B	610	CLA	C1D-C2D	2.00	1.49	1.45
26	a	607	CLA	C3B-C4B	2.00	1.48	1.42

All (892) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	503	CLA	C4A-NA-C1A	10.03	111.26	106.68
26	C	507	CLA	C4A-NA-C1A	9.44	110.98	106.68
26	c	511	CLA	C4A-NA-C1A	9.12	110.84	106.68
26	C	511	CLA	C4A-NA-C1A	8.93	110.75	106.68
26	c	503	CLA	C4A-NA-C1A	8.86	110.72	106.68
26	B	606	CLA	C4A-NA-C1A	8.57	110.59	106.68
26	B	615	CLA	C4A-NA-C1A	8.30	110.47	106.68
26	B	604	CLA	C4A-NA-C1A	8.03	110.34	106.68
26	b	606	CLA	C4A-NA-C1A	7.70	110.19	106.68
26	B	612	CLA	C4A-NA-C1A	7.69	110.19	106.68
26	C	510	CLA	C4A-NA-C1A	7.60	110.15	106.68
26	C	506	CLA	C4A-NA-C1A	7.47	110.09	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	509	CLA	C4A-NA-C1A	7.40	110.06	106.68
26	C	501	CLA	C4A-NA-C1A	7.35	110.03	106.68
26	c	505	CLA	C4A-NA-C1A	7.31	110.02	106.68
26	b	601	CLA	C4A-NA-C1A	7.16	109.94	106.68
26	b	604	CLA	C4A-NA-C1A	7.08	109.91	106.68
26	c	504	CLA	C4A-NA-C1A	7.04	109.89	106.68
26	B	601	CLA	C4A-NA-C1A	7.01	109.88	106.68
26	C	508	CLA	C4A-NA-C1A	6.91	109.83	106.68
26	B	609	CLA	C4A-NA-C1A	6.90	109.83	106.68
32	a	615	SQD	O6-C1-C2	6.87	118.70	108.27
32	A	616	SQD	O6-C1-C2	6.75	118.52	108.27
26	c	507	CLA	C4A-NA-C1A	6.69	109.73	106.68
26	B	605	CLA	C4A-NA-C1A	6.65	109.71	106.68
26	A	614	CLA	C4A-NA-C1A	6.64	109.71	106.68
26	A	608	CLA	C4A-NA-C1A	6.55	109.67	106.68
26	c	502	CLA	C4A-NA-C1A	6.49	109.64	106.68
32	b	620	SQD	O6-C1-C2	6.48	118.12	108.27
26	B	611	CLA	C4A-NA-C1A	6.37	109.58	106.68
26	C	509	CLA	C4A-NA-C1A	6.30	109.56	106.68
26	a	607	CLA	C4A-NA-C1A	6.19	109.50	106.68
26	b	613	CLA	C4A-NA-C1A	6.17	109.49	106.68
26	c	512	CLA	C4A-NA-C1A	6.16	109.49	106.68
26	b	611	CLA	C4A-NA-C1A	6.08	109.45	106.68
26	A	607	CLA	C4A-NA-C1A	5.97	109.40	106.68
36	V	201	HEC	C1D-ND-C4D	5.94	112.24	105.21
26	C	505	CLA	C4A-NA-C1A	5.90	109.37	106.68
26	B	610	CLA	C4A-NA-C1A	5.87	109.36	106.68
26	b	609	CLA	C4A-NA-C1A	5.86	109.35	106.68
29	A	612	PL9	C7-C3-C4	5.83	121.71	116.91
32	A	616	SQD	C1-O5-C5	-5.80	102.39	113.72
26	c	506	CLA	C4A-NA-C1A	5.75	109.30	106.68
26	c	501	CLA	C4A-NA-C1A	5.69	109.28	106.68
27	d	401	PHO	C4D-CHA-CBD	-5.64	105.75	108.45
26	C	512	CLA	C4A-NA-C1A	5.57	109.22	106.68
26	b	616	CLA	C4A-NA-C1A	5.54	109.21	106.68
26	B	608	CLA	C4A-NA-C1A	5.51	109.19	106.68
36	v	201	HEC	C1D-ND-C4D	5.49	111.70	105.21
32	a	615	SQD	C1-O5-C5	-5.48	103.01	113.72
27	a	609	PHO	C4D-CHA-CBD	-5.48	105.83	108.45
32	f	101	SQD	C1-O5-C5	-5.44	103.10	113.72
26	b	603	CLA	C4A-NA-C1A	5.41	109.15	106.68
26	C	513	CLA	C4A-NA-C1A	5.39	109.14	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	602	CLA	C4A-NA-C1A	5.37	109.13	106.68
26	B	607	CLA	C4A-NA-C1A	5.36	109.12	106.68
26	b	615	CLA	C4A-NA-C1A	5.36	109.12	106.68
26	b	612	CLA	C4A-NA-C1A	5.35	109.12	106.68
26	c	510	CLA	C4A-NA-C1A	5.32	109.11	106.68
26	D	402	CLA	C4A-NA-C1A	5.32	109.11	106.68
26	d	402	CLA	C4A-NA-C1A	5.29	109.09	106.68
26	a	608	CLA	C4A-NA-C1A	5.29	109.09	106.68
26	b	607	CLA	C4A-NA-C1A	5.25	109.07	106.68
26	B	613	CLA	C4A-NA-C1A	5.24	109.07	106.68
26	b	602	CLA	C4A-NA-C1A	5.23	109.06	106.68
32	B	622	SQD	O6-C1-C2	5.19	116.16	108.27
29	a	612	PL9	C7-C3-C4	5.18	121.18	116.91
27	D	401	PHO	C4D-CHA-CBD	-5.17	105.97	108.45
32	f	101	SQD	O6-C1-C2	5.14	116.08	108.27
29	D	405	PL9	C7-C3-C4	5.10	121.11	116.91
26	a	613	CLA	C4A-NA-C1A	5.06	108.99	106.68
26	B	613	CLA	C1-C2-C3	-5.06	117.90	126.20
26	c	508	CLA	C4A-NA-C1A	5.04	108.98	106.68
26	b	610	CLA	C4A-NA-C1A	5.02	108.97	106.68
31	C	516	LMG	C8-O7-C10	4.97	129.70	117.80
27	A	609	PHO	O1D-CGD-CBD	4.97	132.26	124.72
26	b	614	CLA	C4A-NA-C1A	4.92	108.92	106.68
26	D	403	CLA	C4A-NA-C1A	4.85	108.89	106.68
26	C	504	CLA	C4A-NA-C1A	4.82	108.88	106.68
26	B	616	CLA	C4A-NA-C1A	4.72	108.83	106.68
26	B	614	CLA	C4A-NA-C1A	4.72	108.83	106.68
26	d	403	CLA	C4A-NA-C1A	4.72	108.83	106.68
26	b	603	CLA	O2D-CGD-O1D	-4.71	114.68	123.85
27	A	609	PHO	CBC-CAC-C3C	4.63	119.51	112.87
32	B	622	SQD	C1-O5-C5	-4.61	104.72	113.72
29	d	405	PL9	C7-C3-C4	4.58	120.68	116.91
26	b	608	CLA	C4A-NA-C1A	4.58	108.77	106.68
32	B	622	SQD	O7-S-C6	4.57	113.58	106.76
31	b	622	LMG	C8-O7-C10	4.53	128.63	117.80
32	A	616	SQD	C1-C2-C3	-4.51	100.51	110.01
32	A	616	SQD	O7-S-C6	4.51	113.49	106.76
32	A	616	SQD	O47-C7-C8	4.49	121.19	111.48
27	A	609	PHO	C4D-CHA-CBD	-4.45	106.32	108.45
32	f	101	SQD	O9-S-O7	-4.44	99.38	113.82
26	C	502	CLA	C4A-NA-C1A	4.42	108.69	106.68
26	c	505	CLA	C3B-C4B-NB	-4.40	106.60	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	618	SQD	O47-C7-C8	4.39	120.98	111.48
29	A	612	PL9	C7-C3-C2	-4.38	118.22	123.39
27	a	609	PHO	CMA-C3A-C4A	-4.37	105.19	114.61
32	F	102	SQD	O6-C1-C2	4.37	114.91	108.27
31	a	618	LMG	O1-C1-C2	4.35	114.88	108.27
32	b	620	SQD	O47-C7-C8	4.35	120.89	111.48
26	C	501	CLA	C3B-C4B-NB	-4.33	106.66	110.53
32	b	620	SQD	O9-S-O7	-4.33	99.74	113.82
32	B	622	SQD	O47-C7-C8	4.33	120.84	111.48
26	c	513	CLA	C4A-NA-C1A	4.31	108.64	106.68
26	b	615	CLA	C3B-C4B-NB	-4.29	106.70	110.53
32	a	617	SQD	O5-C5-C4	4.28	117.41	109.70
31	C	516	LMG	C7-O1-C1	4.28	122.97	113.80
35	e	102	HEM	CBD-CAD-C3D	-4.24	100.82	112.53
31	D	406	LMG	C1-O6-C5	4.19	121.90	113.72
26	b	605	CLA	C4A-NA-C1A	4.19	108.59	106.68
32	A	616	SQD	O9-S-O7	-4.18	100.23	113.82
26	c	501	CLA	O2D-CGD-O1D	-4.14	115.78	123.85
32	a	615	SQD	C1-C2-C3	-4.14	101.30	110.01
26	B	614	CLA	O2D-CGD-O1D	-4.13	115.80	123.85
32	f	101	SQD	O7-S-C6	4.12	112.90	106.76
26	A	610	CLA	C4A-NA-C1A	4.11	108.55	106.68
26	D	403	CLA	O2D-CGD-O1D	-4.06	115.95	123.85
27	D	401	PHO	CMA-C3A-C4A	-4.03	105.93	114.61
32	a	617	SQD	O47-C7-C8	3.99	120.12	111.48
26	B	616	CLA	O2D-CGD-O1D	-3.99	116.09	123.85
32	a	615	SQD	O47-C7-C8	3.98	120.09	111.48
26	B	608	CLA	C3B-C4B-NB	-3.98	106.98	110.53
26	b	606	CLA	O2D-CGD-O1D	-3.95	116.15	123.85
26	c	512	CLA	C1-C2-C3	-3.95	119.73	126.20
26	B	611	CLA	O2D-CGD-O1D	-3.94	116.19	123.85
29	d	405	PL9	C37-C38-C39	-3.93	118.63	127.62
27	A	609	PHO	C1-C2-C3	-3.92	119.77	126.20
26	C	505	CLA	O2D-CGD-O1D	-3.88	116.30	123.85
26	b	614	CLA	C1-C2-C3	-3.87	119.85	126.20
26	B	608	CLA	O2D-CGD-O1D	-3.87	116.31	123.85
26	C	502	CLA	O2D-CGD-O1D	-3.83	116.40	123.85
26	c	513	CLA	C3B-C4B-NB	-3.81	107.13	110.53
26	C	513	CLA	O2D-CGD-O1D	-3.81	116.44	123.85
26	C	501	CLA	O2D-CGD-O1D	-3.80	116.45	123.85
26	b	604	CLA	O2D-CGD-O1D	-3.80	116.45	123.85
26	a	610	CLA	C4A-NA-C1A	3.79	108.41	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	603	CLA	O2D-CGD-O1D	-3.78	116.49	123.85
35	e	102	HEM	CBA-CAA-C2A	-3.77	102.10	112.53
27	A	609	PHO	C2B-C1B-NB	-3.77	106.70	109.43
26	b	612	CLA	O2D-CGD-O1D	-3.77	116.51	123.85
32	a	615	SQD	O9-S-O7	-3.77	101.58	113.82
26	C	508	CLA	O2D-CGD-O1D	-3.71	116.64	123.85
26	c	508	CLA	C1-C2-C3	-3.70	120.13	126.20
26	b	614	CLA	O2D-CGD-O1D	-3.66	116.72	123.85
28	B	618	BCR	C24-C23-C22	3.65	131.64	126.23
36	V	201	HEC	C4B-NB-C1B	3.65	109.53	105.21
26	d	402	CLA	O2D-CGD-O1D	-3.64	116.76	123.85
26	b	606	CLA	O2D-CGD-CBD	3.64	117.60	111.23
26	b	616	CLA	O2D-CGD-O1D	-3.63	116.78	123.85
26	B	610	CLA	C1-C2-C3	-3.63	120.25	126.20
26	B	602	CLA	O2D-CGD-O1D	-3.62	116.80	123.85
32	B	622	SQD	O48-C23-C24	3.61	122.85	111.83
26	c	508	CLA	C3B-C4B-NB	-3.61	107.31	110.53
34	A	619	DGD	C2G-O2G-C1B	3.60	126.42	117.80
26	b	603	CLA	O2D-CGD-CBD	3.60	117.53	111.23
36	v	201	HEC	CBD-CAD-C3D	-3.56	102.68	112.53
26	c	512	CLA	C3B-C4B-NB	-3.56	107.35	110.53
26	B	609	CLA	O2D-CGD-O1D	-3.56	116.92	123.85
26	b	613	CLA	O2D-CGD-O1D	-3.56	116.92	123.85
26	B	602	CLA	O2D-CGD-CBD	3.56	117.45	111.23
32	a	617	SQD	O9-S-O7	-3.55	102.27	113.82
26	C	510	CLA	C3B-C4B-NB	-3.53	107.38	110.53
32	F	102	SQD	O8-S-C6	3.51	112.75	105.97
26	C	507	CLA	O2D-CGD-O1D	-3.51	117.02	123.85
26	B	610	CLA	O2D-CGD-O1D	-3.51	117.02	123.85
26	b	611	CLA	O2D-CGD-O1D	-3.50	117.04	123.85
26	C	511	CLA	O2D-CGD-O1D	-3.49	117.05	123.85
29	a	612	PL9	C7-C3-C2	-3.49	119.28	123.39
32	b	620	SQD	O7-S-C6	3.48	111.95	106.76
26	a	610	CLA	O2D-CGD-O1D	-3.47	117.09	123.85
26	B	614	CLA	O2D-CGD-CBD	3.47	117.30	111.23
27	d	401	PHO	O1D-CGD-CBD	3.47	129.98	124.72
29	D	405	PL9	C7-C3-C2	-3.47	119.30	123.39
31	a	618	LMG	C1-C2-C3	-3.46	102.72	110.01
26	B	605	CLA	C7-C6-C5	-3.46	104.04	113.26
27	A	609	PHO	CMA-C3A-C4A	-3.46	107.16	114.61
31	C	516	LMG	O1-C1-C2	3.46	113.53	108.27
26	B	606	CLA	C3B-C4B-NB	-3.46	107.44	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	613	CLA	O2D-CGD-O1D	-3.45	117.13	123.85
26	B	604	CLA	C3B-C4B-NB	-3.43	107.47	110.53
32	B	622	SQD	C3-C4-C5	3.42	116.43	110.23
32	b	620	SQD	O5-C5-C4	3.41	115.85	109.70
26	c	505	CLA	O2D-CGD-O1D	-3.41	117.20	123.85
27	A	609	PHO	O2D-CGD-O1D	-3.40	117.23	123.85
26	B	616	CLA	C1-C2-C3	-3.40	120.63	126.20
26	C	512	CLA	CHB-C4A-NA	3.40	129.30	124.40
32	f	101	SQD	O9-S-C6	3.39	111.82	106.76
26	B	606	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
26	A	607	CLA	O2A-CGA-O1A	-3.37	115.19	123.63
26	b	608	CLA	C3B-C4B-NB	-3.37	107.52	110.53
26	C	510	CLA	O2D-CGD-O1D	-3.37	117.28	123.85
31	D	406	LMG	C7-O1-C1	3.37	121.02	113.80
29	a	612	PL9	C22-C23-C24	-3.37	119.91	127.62
26	d	403	CLA	C3B-C4B-NB	-3.37	107.53	110.53
26	B	603	CLA	C3B-C4B-NB	-3.37	107.53	110.53
26	b	616	CLA	O2D-CGD-CBD	3.36	117.11	111.23
26	A	608	CLA	O2D-CGD-O1D	-3.35	117.32	123.85
26	B	603	CLA	C4A-NA-C1A	3.35	108.21	106.68
26	c	511	CLA	C3B-C4B-NB	-3.35	107.54	110.53
26	b	606	CLA	C3B-C4B-NB	-3.35	107.54	110.53
26	b	601	CLA	O2D-CGD-O1D	-3.34	117.34	123.85
32	a	617	SQD	O7-S-C6	3.34	111.75	106.76
26	b	608	CLA	O2D-CGD-O1D	-3.34	117.34	123.85
26	B	601	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
26	A	610	CLA	C3B-C4B-NB	-3.32	107.56	110.53
26	b	605	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
26	b	608	CLA	CHB-C4A-NA	3.31	129.18	124.40
27	d	401	PHO	C1-C2-C3	-3.30	120.78	126.20
32	F	102	SQD	O9-S-O7	-3.30	103.09	113.82
26	B	610	CLA	C3B-C4B-NB	-3.30	107.59	110.53
26	c	504	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
26	c	506	CLA	C3B-C4B-NB	-3.29	107.59	110.53
31	C	516	LMG	C4-C3-C2	3.28	116.59	110.83
26	c	502	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
29	D	405	PL9	C7-C8-C9	-3.28	121.19	126.83
26	B	611	CLA	O2D-CGD-CBD	3.27	116.95	111.23
36	v	201	HEC	CHB-C1B-NB	3.26	127.94	124.42
31	c	523	LMG	C3-C4-C5	-3.26	104.31	110.23
32	A	618	SQD	O48-C23-C24	3.26	121.78	111.83
26	a	607	CLA	C3B-C4B-NB	-3.26	107.62	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	509	CLA	O2A-CGA-O1A	-3.25	115.49	123.63
32	A	618	SQD	O9-S-O7	-3.24	103.28	113.82
26	B	604	CLA	C1-O2A-CGA	-3.23	108.82	116.65
26	C	504	CLA	C3B-C4B-NB	-3.23	107.65	110.53
26	b	609	CLA	C1-C2-C3	-3.23	120.91	126.20
31	B	620	LMG	O3-C3-C2	-3.22	102.78	110.38
27	D	401	PHO	CMB-C2B-C3B	3.22	131.12	124.68
28	k	102	BCR	C7-C8-C9	-3.22	121.47	126.23
27	a	609	PHO	C1-C2-C3	-3.22	120.92	126.20
26	B	614	CLA	C3B-C4B-NB	-3.22	107.66	110.53
32	A	616	SQD	O9-S-C6	3.22	111.56	106.76
36	V	201	HEC	C3B-C4B-NB	-3.22	106.64	110.17
26	b	614	CLA	C3B-C4B-NB	-3.21	107.66	110.53
26	b	616	CLA	C3B-C4B-NB	-3.21	107.66	110.53
28	X	101	BCR	C16-C17-C18	-3.20	122.79	127.28
32	B	622	SQD	O9-S-O7	-3.19	103.45	113.82
26	c	507	CLA	CHB-C4A-NA	3.18	129.00	124.40
28	X	101	BCR	C29-C30-C25	3.18	115.06	110.44
26	b	607	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
26	C	503	CLA	O2D-CGD-O1D	-3.18	117.67	123.85
27	D	401	PHO	C2B-C1B-NB	-3.17	107.14	109.43
26	B	615	CLA	CHB-C4A-NA	3.17	128.97	124.40
26	D	402	CLA	C3B-C4B-NB	-3.17	107.70	110.53
27	A	609	PHO	CMB-C2B-C3B	3.16	131.00	124.68
26	D	402	CLA	O2A-CGA-O1A	-3.16	115.73	123.63
26	C	512	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
26	a	607	CLA	CHB-C4A-NA	3.14	128.94	124.40
28	X	101	BCR	C33-C5-C6	3.14	127.92	124.48
26	c	512	CLA	CHB-C4A-NA	3.14	128.94	124.40
26	b	604	CLA	O2D-CGD-CBD	3.14	116.72	111.23
29	D	405	PL9	C22-C23-C24	-3.14	120.44	127.62
34	c	520	DGD	C6E-C5E-C4E	-3.13	105.33	113.02
26	c	508	CLA	O2A-CGA-O1A	-3.13	115.80	123.63
26	B	610	CLA	CHB-C4A-NA	3.13	128.91	124.40
26	b	602	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
27	a	609	PHO	CMB-C2B-C3B	3.12	130.92	124.68
28	h	101	BCR	C2-C1-C6	3.12	114.97	110.44
26	b	615	CLA	CHB-C4A-NA	3.11	128.89	124.40
26	b	604	CLA	C1-C2-C3	-3.11	121.10	126.20
26	c	506	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
26	c	507	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
26	C	507	CLA	C3B-C4B-NB	-3.10	107.76	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	612	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
29	d	405	PL9	C40-C39-C41	3.10	120.61	115.23
27	d	401	PHO	CMB-C2B-C3B	3.10	130.87	124.68
26	a	608	CLA	C3B-C4B-NB	-3.09	107.77	110.53
32	a	615	SQD	C44-O6-C1	-3.09	107.17	113.80
26	B	611	CLA	C3B-C4B-NB	-3.09	107.78	110.53
26	C	501	CLA	O2D-CGD-CBD	3.09	116.62	111.23
26	b	610	CLA	C1-C2-C3	-3.09	121.14	126.20
26	A	614	CLA	C3B-C4B-NB	-3.09	107.78	110.53
26	b	604	CLA	C6-C7-C8	-3.08	105.72	115.97
26	b	603	CLA	O2A-CGA-O1A	-3.08	115.93	123.63
32	F	102	SQD	O9-S-C6	3.07	111.34	106.76
26	b	612	CLA	C3B-C4B-NB	-3.05	107.81	110.53
26	D	403	CLA	O2D-CGD-CBD	3.05	116.56	111.23
26	b	605	CLA	C3B-C4B-NB	-3.04	107.81	110.53
26	b	604	CLA	CHB-C4A-NA	3.03	128.77	124.40
26	A	607	CLA	CHB-C4A-NA	3.03	128.77	124.40
28	d	404	BCR	C30-C25-C26	-3.02	118.50	122.64
26	d	402	CLA	C3B-C4B-NB	-3.02	107.83	110.53
27	D	401	PHO	C3B-C4B-NB	-3.02	105.50	107.46
29	d	405	PL9	C27-C28-C29	-3.01	120.73	127.62
26	C	509	CLA	C3B-C4B-NB	-3.01	107.85	110.53
26	b	608	CLA	CMB-C2B-C1B	-3.00	120.85	125.42
26	B	605	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
26	b	608	CLA	O2D-CGD-CBD	3.00	116.47	111.23
26	b	601	CLA	C3B-C4B-NB	-2.99	107.86	110.53
36	v	201	HEC	C2A-C1A-NA	-2.99	107.44	110.32
26	A	608	CLA	C3B-C4B-NB	-2.99	107.86	110.53
32	a	615	SQD	O48-C23-C24	2.99	120.94	111.83
27	d	401	PHO	CMA-C3A-C4A	-2.98	108.19	114.61
26	b	616	CLA	CHB-C4A-NA	2.97	128.69	124.40
26	b	602	CLA	O2D-CGD-CBD	2.97	116.42	111.23
26	b	602	CLA	CHB-C4A-NA	2.97	128.68	124.40
26	B	601	CLA	C3B-C4B-NB	-2.96	107.89	110.53
32	b	620	SQD	C1-C2-C3	-2.96	103.78	110.01
32	f	101	SQD	C46-C45-C44	-2.94	104.93	111.78
27	a	609	PHO	C2B-C1B-NB	-2.93	107.31	109.43
30	B	623	STE	C3-C2-C1	-2.93	106.86	114.51
26	a	608	CLA	CHB-C4A-NA	2.93	128.62	124.40
26	a	610	CLA	C1-C2-C3	-2.92	121.41	126.20
26	b	610	CLA	CAA-CBA-CGA	-2.92	104.91	113.21
29	D	405	PL9	C27-C28-C29	-2.92	120.94	127.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	505	CLA	O2D-CGD-CBD	2.92	116.33	111.23
25	A	606	BCT	O2-C-O1	2.91	127.13	119.68
26	c	503	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
26	C	513	CLA	O2D-CGD-CBD	2.91	116.31	111.23
26	C	507	CLA	CHB-C4A-NA	2.90	128.59	124.40
26	c	512	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
26	C	502	CLA	O2A-CGA-O1A	-2.90	116.37	123.63
26	b	606	CLA	C1-C2-C3	-2.90	121.45	126.20
26	C	508	CLA	C3B-C4B-NB	-2.89	107.95	110.53
26	d	402	CLA	O2A-CGA-O1A	-2.89	116.40	123.63
26	a	610	CLA	O2D-CGD-CBD	2.89	116.28	111.23
26	c	501	CLA	O2D-CGD-CBD	2.89	116.27	111.23
26	c	509	CLA	CHB-C4A-NA	2.88	128.56	124.40
32	B	622	SQD	O5-C5-C4	2.88	114.89	109.70
32	f	101	SQD	O5-C5-C4	2.88	114.89	109.70
32	a	615	SQD	O8-S-C6	2.88	111.53	105.97
32	b	620	SQD	O9-S-C6	2.88	111.05	106.76
27	d	401	PHO	CAA-C2A-C3A	-2.88	105.22	113.00
26	B	605	CLA	C3B-C4B-NB	-2.88	107.96	110.53
26	C	505	CLA	CAC-C3C-C4C	2.88	128.53	124.79
26	C	509	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
26	C	506	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
26	c	508	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
26	b	604	CLA	O2A-CGA-O1A	-2.87	116.46	123.63
26	b	613	CLA	C3B-C4B-NB	-2.86	107.98	110.53
28	K	103	BCR	C20-C21-C22	-2.86	123.27	127.28
29	a	612	PL9	C27-C28-C29	-2.86	121.08	127.62
29	d	405	PL9	C7-C3-C2	-2.86	120.02	123.39
26	B	611	CLA	C1-C2-C3	-2.85	121.52	126.20
26	B	608	CLA	O2D-CGD-CBD	2.85	116.21	111.23
26	C	512	CLA	C1-C2-C3	-2.85	121.53	126.20
27	d	401	PHO	O2D-CGD-O1D	-2.85	118.31	123.85
34	c	519	DGD	C3G-O3G-C1D	2.84	119.89	113.80
28	b	618	BCR	C33-C5-C6	2.84	127.58	124.48
26	B	612	CLA	O2A-CGA-O1A	-2.84	116.53	123.63
26	a	613	CLA	O2D-CGD-CBD	2.84	116.19	111.23
26	b	614	CLA	CHB-C4A-NA	2.84	128.49	124.40
26	B	612	CLA	CHB-C4A-NA	2.83	128.49	124.40
26	b	611	CLA	O2D-CGD-CBD	2.83	116.17	111.23
26	c	504	CLA	C1-C2-C3	-2.82	121.58	126.20
26	B	616	CLA	C3B-C4B-NB	-2.82	108.02	110.53
26	c	505	CLA	O2D-CGD-CBD	2.82	116.15	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	513	CLA	CHD-C1D-ND	-2.81	120.84	124.80
26	b	612	CLA	CMB-C2B-C1B	-2.81	121.14	125.42
26	C	501	CLA	O2A-CGA-O1A	-2.81	116.60	123.63
26	D	402	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
29	A	612	PL9	O2-C1-C2	-2.80	115.47	121.83
35	F	101	HEM	CBD-CAD-C3D	-2.80	104.80	112.53
26	c	504	CLA	O2A-CGA-O1A	-2.79	116.65	123.63
26	b	613	CLA	CHB-C4A-NA	2.79	128.43	124.40
26	B	604	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
26	a	608	CLA	O2A-CGA-O1A	-2.77	116.69	123.63
29	d	405	PL9	C22-C23-C24	-2.77	121.28	127.62
26	A	607	CLA	C1-C2-C3	-2.77	121.65	126.20
32	f	101	SQD	O5-C1-C2	-2.77	104.68	110.37
26	b	604	CLA	C3B-C4B-NB	-2.77	108.06	110.53
28	B	617	BCR	C29-C30-C25	2.77	114.46	110.44
26	A	614	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
26	a	607	CLA	O2D-CGD-O1D	-2.77	118.47	123.85
26	c	513	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
34	h	102	DGD	C6D-C5D-C4D	2.75	117.83	112.07
26	B	615	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
26	b	612	CLA	CHB-C4A-NA	2.74	128.36	124.40
26	c	505	CLA	CHB-C4A-NA	2.74	128.36	124.40
26	C	512	CLA	C3B-C4B-NB	-2.74	108.08	110.53
26	b	610	CLA	O2A-CGA-O1A	-2.74	116.78	123.63
27	d	401	PHO	C2B-C1B-NB	-2.73	107.45	109.43
32	F	102	SQD	O5-C1-C2	-2.73	104.76	110.37
25	a	606	BCT	O2-C-O1	2.73	126.65	119.68
32	a	617	SQD	O48-C23-C24	2.72	120.14	111.83
32	b	620	SQD	O5-C1-C2	-2.72	104.79	110.37
26	c	507	CLA	C3B-C4B-NB	-2.72	108.10	110.53
26	b	602	CLA	C1-C2-C3	-2.72	121.75	126.20
26	B	603	CLA	O2A-CGA-O1A	-2.71	116.84	123.63
26	C	513	CLA	C3B-C4B-NB	-2.70	108.12	110.53
26	C	506	CLA	C1-C2-C3	-2.70	121.78	126.20
26	C	513	CLA	CMB-C2B-C1B	-2.70	121.31	125.42
26	D	402	CLA	CHB-C4A-NA	2.69	128.28	124.40
26	c	504	CLA	CMB-C2B-C1B	-2.69	121.33	125.42
26	c	511	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
26	D	402	CLA	C1-C2-C3	-2.68	121.81	126.20
26	B	606	CLA	CHB-C1B-NB	2.68	128.06	124.05
26	C	507	CLA	C2A-C1A-CHA	2.68	128.51	123.87
34	H	101	DGD	C3E-C4E-C5E	-2.68	105.38	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	f	101	SQD	O47-C7-C8	2.68	120.76	110.93
26	b	611	CLA	C3B-C4B-NB	-2.68	108.14	110.53
26	B	602	CLA	CMB-C2B-C1B	-2.67	121.35	125.42
26	B	605	CLA	O2A-CGA-O1A	-2.67	116.94	123.63
26	C	502	CLA	C3B-C4B-NB	-2.67	108.14	110.53
28	C	514	BCR	C2-C1-C6	2.67	114.32	110.44
32	B	622	SQD	O9-S-C6	2.67	110.75	106.76
31	m	101	LMG	O1-C7-C8	-2.67	104.33	110.82
29	d	405	PL9	C42-C43-C44	-2.67	121.52	127.62
27	a	609	PHO	OBD-CAD-CBD	-2.66	121.92	125.82
29	a	612	PL9	C37-C38-C39	-2.65	121.55	127.62
26	c	506	CLA	CMB-C2B-C1B	-2.65	121.39	125.42
32	A	618	SQD	O6-C1-C2	2.65	112.30	108.27
27	D	401	PHO	CMA-C3A-C2A	-2.65	103.90	114.13
28	d	404	BCR	C38-C26-C25	-2.65	121.59	124.48
26	B	610	CLA	O2D-CGD-CBD	2.65	115.86	111.23
29	a	612	PL9	C32-C33-C34	-2.65	121.56	127.62
26	C	503	CLA	CHB-C4A-NA	2.64	128.22	124.40
26	B	614	CLA	O2A-CGA-O1A	-2.64	117.02	123.63
35	e	102	HEM	C3B-C4B-NB	-2.64	107.57	109.47
29	A	612	PL9	C40-C39-C41	2.64	119.81	115.23
26	B	612	CLA	C1-C2-C3	-2.64	121.88	126.20
32	F	102	SQD	O48-C23-C24	2.64	119.88	111.83
26	b	605	CLA	O2A-CGA-O1A	-2.63	117.04	123.63
26	c	501	CLA	C3B-C4B-NB	-2.63	108.18	110.53
26	b	613	CLA	C7-C6-C5	-2.63	106.26	113.26
32	b	620	SQD	O8-S-C6	2.63	111.05	105.97
26	A	614	CLA	CHC-C4B-NB	2.63	127.99	124.05
36	V	201	HEC	CHA-C4D-ND	2.62	127.25	124.42
26	b	615	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
26	b	613	CLA	CED-O2D-CGD	2.62	121.85	115.92
26	c	501	CLA	CMB-C2B-C1B	-2.62	121.44	125.42
26	b	601	CLA	CHB-C4A-NA	2.61	128.17	124.40
32	b	620	SQD	C3-C4-C5	2.61	114.97	110.23
26	B	602	CLA	CHB-C4A-NA	2.61	128.17	124.40
26	a	610	CLA	CHB-C4A-NA	2.60	128.16	124.40
26	B	607	CLA	CHB-C1B-NB	2.60	127.95	124.05
30	M	102	STE	C3-C2-C1	-2.59	107.75	114.51
26	c	513	CLA	CMB-C2B-C1B	-2.59	121.48	125.42
26	C	506	CLA	CHB-C4A-NA	2.59	128.13	124.40
29	a	612	PL9	C40-C39-C41	2.58	119.71	115.23
35	e	102	HEM	C3B-C2B-C1B	2.58	108.35	106.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	609	CLA	CMB-C2B-C1B	-2.58	121.49	125.42
34	C	520	DGD	C3D-C4D-C5D	-2.58	105.56	110.23
36	V	201	HEC	CBD-CAD-C3D	-2.58	105.41	112.53
26	b	609	CLA	O2A-CGA-O1A	-2.58	117.19	123.63
26	C	503	CLA	C3B-C4B-NB	-2.58	108.23	110.53
26	C	509	CLA	CMB-C2B-C1B	-2.57	121.50	125.42
29	D	405	PL9	C37-C38-C39	-2.57	121.73	127.62
29	A	612	PL9	O2-C1-C6	2.57	124.57	120.48
29	d	405	PL9	C8-C7-C3	2.57	118.68	112.03
29	d	405	PL9	C32-C33-C34	-2.57	121.74	127.62
26	d	403	CLA	CHB-C4A-NA	2.57	128.11	124.40
26	d	403	CLA	O2D-CGD-O1D	-2.57	118.86	123.85
29	d	405	PL9	C20-C19-C21	2.56	119.68	115.23
26	b	609	CLA	C3B-C4B-NB	-2.56	108.24	110.53
26	c	504	CLA	CHB-C4A-NA	2.56	128.10	124.40
28	t	101	BCR	C2-C1-C6	2.55	114.15	110.44
26	C	512	CLA	O2A-CGA-O1A	-2.55	117.24	123.63
26	B	604	CLA	O2D-CGD-CBD	2.54	115.68	111.23
26	B	616	CLA	O2A-CGA-O1A	-2.54	117.28	123.63
32	B	622	SQD	O5-C1-C2	-2.53	105.16	110.37
32	b	620	SQD	O2-C2-C1	2.53	116.11	110.08
26	B	602	CLA	CHC-C4B-NB	2.53	127.84	124.05
26	b	605	CLA	CHB-C4A-NA	2.53	128.05	124.40
32	A	616	SQD	O5-C1-C2	-2.53	105.18	110.37
26	b	613	CLA	O1D-CGD-CBD	2.52	129.50	124.52
26	B	614	CLA	CHB-C4A-NA	2.52	128.04	124.40
26	b	601	CLA	O2D-CGD-CBD	2.52	115.63	111.23
26	C	508	CLA	CHD-C1D-ND	-2.52	121.26	124.80
26	B	606	CLA	O2A-CGA-O1A	-2.52	117.34	123.63
26	B	609	CLA	C3B-C4B-NB	-2.51	108.28	110.53
26	C	508	CLA	O2A-CGA-O1A	-2.51	117.34	123.63
26	b	606	CLA	CHB-C1B-NB	2.51	127.81	124.05
28	K	103	BCR	C16-C17-C18	2.51	130.79	127.28
26	C	507	CLA	O2D-CGD-CBD	2.51	115.61	111.23
26	A	608	CLA	CHC-C4B-NB	2.50	127.81	124.05
31	b	622	LMG	C1-O6-C5	-2.50	108.83	113.72
26	B	604	CLA	O2A-CGA-O1A	-2.50	117.37	123.63
32	a	617	SQD	C1-O5-C5	2.50	118.61	113.72
26	C	513	CLA	O2A-CGA-O1A	-2.50	117.38	123.63
26	a	613	CLA	C1-C2-C3	-2.50	122.11	126.20
26	C	511	CLA	CHB-C4A-NA	2.49	128.00	124.40
26	b	610	CLA	CHB-C4A-NA	2.49	128.00	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	610	CLA	O2A-CGA-O1A	-2.49	117.39	123.63
28	d	404	BCR	C33-C5-C6	-2.49	121.77	124.48
26	B	602	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
36	V	201	HEC	C2B-C1B-NB	-2.49	107.02	109.90
26	C	513	CLA	CHD-C1D-C2D	2.49	130.66	125.49
32	b	620	SQD	O48-C23-C24	2.48	119.41	111.83
27	D	401	PHO	CAA-C2A-C3A	-2.48	106.29	113.00
26	b	608	CLA	C1-C2-C3	-2.48	122.13	126.20
32	a	617	SQD	O8-S-C6	2.48	110.77	105.97
27	a	609	PHO	OBD-CAD-C3D	2.48	131.76	127.89
26	c	503	CLA	C3B-C4B-NB	-2.48	108.31	110.53
32	A	616	SQD	C45-O47-C7	-2.48	111.86	117.80
27	a	609	PHO	C3B-C4B-NB	-2.48	105.85	107.46
32	A	618	SQD	O9-S-C6	2.48	110.45	106.76
26	b	607	CLA	C1-O2A-CGA	2.48	122.64	116.65
26	C	504	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
26	b	609	CLA	C1-O2A-CGA	2.47	122.63	116.65
26	b	612	CLA	O1D-CGD-CBD	2.47	129.39	124.52
26	b	612	CLA	O2A-CGA-O1A	-2.47	117.46	123.63
26	A	614	CLA	CHB-C4A-NA	2.46	127.96	124.40
26	b	610	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
26	A	614	CLA	O2D-CGD-CBD	2.46	115.53	111.23
29	a	612	PL9	O1-C4-C3	-2.46	118.13	120.73
31	c	524	LMG	O3-C3-C4	2.46	116.18	110.38
26	B	609	CLA	CHB-C4A-NA	2.46	127.95	124.40
26	a	613	CLA	CHB-C4A-NA	2.46	127.95	124.40
26	D	403	CLA	O2A-CGA-O1A	-2.46	117.48	123.63
29	D	405	PL9	C40-C39-C41	2.46	119.50	115.23
32	A	618	SQD	O7-S-C6	2.46	110.43	106.76
26	c	510	CLA	C3B-C4B-NB	-2.46	108.34	110.53
26	B	610	CLA	CHD-C1D-ND	-2.45	121.35	124.80
26	A	610	CLA	CHB-C4A-NA	2.45	127.94	124.40
26	D	402	CLA	O2D-CGD-CBD	2.45	115.52	111.23
26	B	616	CLA	O2D-CGD-CBD	2.45	115.51	111.23
26	A	608	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
27	a	609	PHO	CMA-C3A-C2A	-2.45	104.67	114.13
26	C	502	CLA	O1D-CGD-CBD	2.45	129.34	124.52
29	a	612	PL9	O2-C1-C2	-2.45	116.27	121.83
26	A	610	CLA	O2D-CGD-O1D	-2.45	119.09	123.85
26	b	608	CLA	CMB-C2B-C3B	2.44	132.29	126.55
26	b	609	CLA	C7-C6-C5	-2.44	106.76	113.26
29	d	405	PL9	C7-C8-C9	-2.44	122.63	126.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	609	CLA	C7-C6-C5	-2.44	106.77	113.26
26	C	509	CLA	CHB-C4A-NA	2.43	127.91	124.40
26	a	608	CLA	O2D-CGD-CBD	2.43	115.48	111.23
32	a	615	SQD	O9-S-C6	2.43	110.39	106.76
26	B	604	CLA	CHB-C4A-NA	2.43	127.91	124.40
34	c	520	DGD	O4D-C4D-C5D	2.43	115.31	109.32
26	C	508	CLA	O2D-CGD-CBD	2.43	115.48	111.23
26	c	513	CLA	CHB-C4A-NA	2.43	127.90	124.40
26	b	603	CLA	C3B-C4B-NB	-2.43	108.36	110.53
32	A	616	SQD	O48-C23-C24	2.43	119.23	111.83
36	V	201	HEC	C3D-C4D-ND	-2.43	108.01	110.35
26	a	608	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
31	c	524	LMG	O1-C1-C2	2.42	111.95	108.27
26	b	612	CLA	CMB-C2B-C3B	2.42	132.24	126.55
26	C	511	CLA	O2A-CGA-O1A	-2.42	117.58	123.63
32	a	617	SQD	O5-C1-C2	2.42	115.34	110.37
26	c	502	CLA	CHB-C4A-NA	2.42	127.89	124.40
26	b	616	CLA	CMB-C2B-C1B	-2.42	121.74	125.42
28	T	101	BCR	C38-C26-C27	-2.42	108.44	113.60
26	a	610	CLA	O2A-CGA-O1A	-2.41	117.59	123.63
26	b	611	CLA	CMB-C2B-C1B	-2.41	121.75	125.42
26	d	403	CLA	CMB-C2B-C1B	-2.41	121.75	125.42
26	c	510	CLA	O2A-CGA-O1A	-2.41	117.60	123.63
36	v	201	HEC	C4B-NB-C1B	2.41	108.06	105.21
26	a	607	CLA	O2A-CGA-O1A	-2.41	117.60	123.63
26	c	507	CLA	CHC-C4B-NB	2.41	127.66	124.05
35	e	102	HEM	C4D-ND-C1D	2.40	108.05	105.21
29	D	405	PL9	C35-C34-C36	2.40	119.40	115.23
26	c	501	CLA	CMB-C2B-C3B	2.40	132.19	126.55
26	b	608	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
26	C	509	CLA	CMB-C2B-C3B	2.40	132.19	126.55
34	A	619	DGD	O3G-C3G-C2G	2.40	116.65	110.82
26	B	603	CLA	CHB-C1B-NB	2.39	127.64	124.05
26	c	508	CLA	O2D-CGD-CBD	2.39	115.42	111.23
26	b	605	CLA	CHD-C1D-ND	-2.39	121.44	124.80
32	b	620	SQD	C46-O48-C23	-2.39	108.37	117.12
35	e	102	HEM	CAB-C3B-C2B	-2.39	120.66	128.43
26	B	612	CLA	O1D-CGD-CBD	2.39	129.22	124.52
27	d	401	PHO	O2A-CGA-O1A	-2.38	117.66	123.63
26	C	502	CLA	C1-C2-C3	-2.38	122.29	126.20
26	B	611	CLA	C2D-C1D-ND	-2.38	107.77	110.13
26	b	606	CLA	CHC-C4B-NB	2.38	127.62	124.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	f	101	SQD	C1-C2-C3	-2.38	105.00	110.01
26	b	607	CLA	C3B-C4B-NB	-2.38	108.40	110.53
30	t	102	STE	O2-C1-C2	2.38	121.52	114.00
27	A	609	PHO	CMA-C3A-C2A	-2.38	104.94	114.13
34	h	102	DGD	C6D-O5D-C1E	2.38	118.90	113.80
29	A	612	PL9	C7-C8-C9	-2.38	122.73	126.83
31	a	618	LMG	O8-C9-C8	2.38	115.25	108.40
26	a	607	CLA	O1D-CGD-CBD	2.38	129.20	124.52
28	d	404	BCR	C32-C1-C6	2.37	113.97	110.24
34	h	102	DGD	O4E-C4E-C5E	2.37	115.16	109.32
26	a	610	CLA	CAA-CBA-CGA	-2.37	106.48	113.21
26	c	508	CLA	CHD-C4C-NC	2.37	127.90	124.23
26	c	505	CLA	CHD-C1D-ND	-2.37	121.47	124.80
31	b	622	LMG	C3-C4-C5	-2.37	105.94	110.23
26	B	612	CLA	C3B-C4B-NB	-2.36	108.42	110.53
26	C	506	CLA	C3B-C4B-NB	-2.36	108.42	110.53
26	b	616	CLA	CMB-C2B-C3B	2.36	132.10	126.55
26	B	614	CLA	C1-C2-C3	-2.36	122.34	126.20
26	B	601	CLA	O2D-CGD-CBD	2.36	115.35	111.23
29	d	405	PL9	C12-C13-C14	-2.36	122.23	127.62
26	B	608	CLA	C6-C7-C8	-2.36	108.14	115.97
26	c	512	CLA	CHD-C1D-ND	-2.35	121.49	124.80
29	A	612	PL9	O1-C4-C3	-2.35	118.25	120.73
26	C	503	CLA	C1D-ND-C4D	2.35	107.96	106.31
26	B	613	CLA	C3B-C4B-NB	-2.35	108.43	110.53
31	D	406	LMG	O4-C4-C5	2.35	115.11	109.32
29	d	405	PL9	O1-C4-C3	-2.35	118.25	120.73
26	C	505	CLA	C11-C10-C8	-2.35	108.17	115.97
28	d	404	BCR	C16-C15-C14	-2.35	118.72	123.52
26	B	607	CLA	CMB-C2B-C1B	-2.35	121.85	125.42
26	b	613	CLA	C16-C15-C13	-2.35	108.17	115.97
26	c	510	CLA	O2D-CGD-O1D	-2.34	119.28	123.85
26	d	403	CLA	O2D-CGD-CBD	2.34	115.33	111.23
31	D	406	LMG	C8-O7-C10	2.34	123.41	117.80
32	F	102	SQD	C46-C45-C44	-2.34	106.09	113.67
26	b	612	CLA	C11-C12-C13	-2.34	108.17	115.97
26	b	606	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
26	c	504	CLA	C3B-C4B-NB	-2.33	108.45	110.53
26	c	503	CLA	C7-C6-C5	-2.33	107.05	113.26
26	C	505	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
26	B	613	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
26	c	506	CLA	CHB-C4A-NA	2.32	127.75	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	v	201	HEC	CHA-C4D-ND	2.32	126.92	124.42
34	h	102	DGD	C3D-C4D-C5D	-2.32	106.02	110.23
26	B	613	CLA	O1D-CGD-CBD	2.32	129.09	124.52
28	t	101	BCR	C11-C10-C9	-2.32	124.03	127.28
27	D	401	PHO	O2D-CGD-CBD	2.32	113.49	110.95
30	j	101	STE	O2-C1-C2	2.32	121.33	114.00
31	c	524	LMG	C3-C4-C5	-2.32	106.03	110.23
26	b	611	CLA	CHD-C1D-ND	-2.32	121.54	124.80
26	c	511	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
26	A	610	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
32	A	616	SQD	O47-C7-O49	-2.31	118.30	123.70
26	b	612	CLA	C1-C2-C3	-2.31	122.41	126.20
26	C	513	CLA	CMB-C2B-C3B	2.31	131.99	126.55
26	B	616	CLA	CHC-C4B-NB	2.31	127.52	124.05
26	d	402	CLA	C4-C3-C5	2.31	119.23	115.23
28	X	101	BCR	C7-C6-C5	2.30	126.86	121.56
26	b	609	CLA	CHA-C1A-NA	-2.30	121.19	126.39
31	m	101	LMG	C4-C3-C2	2.30	114.86	110.83
31	M	101	LMG	C1-C2-C3	-2.30	105.18	110.01
32	a	617	SQD	C9-C8-C7	-2.30	105.28	113.69
26	c	505	CLA	C11-C12-C13	-2.30	108.33	115.97
34	H	101	DGD	O3E-C3E-C4E	2.30	115.79	110.38
26	c	512	CLA	O2A-CGA-O1A	-2.30	117.89	123.63
26	c	504	CLA	O2D-CGD-CBD	2.29	115.24	111.23
26	B	602	CLA	C3B-C4B-NB	-2.29	108.48	110.53
26	B	616	CLA	CAA-CBA-CGA	-2.29	106.70	113.21
26	A	608	CLA	O2D-CGD-CBD	2.29	115.23	111.23
31	M	101	LMG	O7-C8-C7	-2.29	100.14	108.34
29	A	612	PL9	C36-C34-C33	-2.29	116.04	121.17
26	B	608	CLA	CHB-C4A-NA	2.28	127.70	124.40
26	b	603	CLA	CHB-C4A-NA	2.28	127.70	124.40
34	c	520	DGD	C6D-O5D-C1E	2.28	118.69	113.80
26	A	610	CLA	O2D-CGD-CBD	2.28	115.22	111.23
27	d	401	PHO	OBD-CAD-CBD	-2.27	122.49	125.82
26	C	513	CLA	CHD-C4C-NC	2.27	127.76	124.23
26	C	505	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
34	c	520	DGD	O6E-C5E-C4E	2.27	113.78	109.70
26	B	614	CLA	CHB-C1B-NB	2.26	127.44	124.05
26	b	607	CLA	C6-C7-C8	-2.26	108.44	115.97
31	D	406	LMG	O6-C5-C4	2.26	113.77	109.70
27	D	401	PHO	C3D-C4D-ND	2.26	110.60	107.71
26	C	508	CLA	CHD-C1D-C2D	2.26	130.19	125.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	503	CLA	CHB-C4A-NA	2.26	127.66	124.40
26	D	402	CLA	C4-C3-C5	2.26	119.15	115.23
26	d	402	CLA	C6-C5-C3	2.26	118.97	113.47
34	C	522	DGD	C6D-O5D-C1E	2.26	118.63	113.80
26	C	503	CLA	O1D-CGD-CBD	2.26	128.97	124.52
26	b	605	CLA	CHD-C4C-NC	2.26	127.73	124.23
30	t	102	STE	C3-C2-C1	-2.25	108.62	114.51
26	b	608	CLA	CHB-C1B-NB	2.25	127.43	124.05
26	C	509	CLA	C1-C2-C3	-2.25	122.51	126.20
29	d	405	PL9	C36-C34-C33	-2.25	116.11	121.17
26	c	506	CLA	CMB-C2B-C3B	2.25	131.84	126.55
26	C	505	CLA	C3B-C4B-NB	-2.25	108.52	110.53
34	A	619	DGD	O4E-C4E-C5E	2.25	114.86	109.32
26	c	508	CLA	CHB-C4A-NA	2.25	127.64	124.40
26	b	613	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
26	B	609	CLA	C1-C2-C3	-2.25	122.51	126.20
26	B	602	CLA	C1-C2-C3	-2.25	122.52	126.20
26	C	505	CLA	CHB-C4A-NA	2.24	127.64	124.40
26	b	602	CLA	C11-C10-C8	-2.24	108.51	115.97
29	d	405	PL9	O2-C1-C6	2.24	124.05	120.48
26	C	504	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
27	D	401	PHO	O2D-CGD-O1D	-2.24	119.49	123.85
28	b	618	BCR	C1-C6-C5	-2.24	119.58	122.64
36	V	201	HEC	C2A-C1A-NA	-2.24	108.16	110.32
26	c	507	CLA	O2D-CGD-CBD	2.24	115.14	111.23
26	d	403	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
26	b	602	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
26	B	607	CLA	C3B-C4B-NB	-2.24	108.53	110.53
32	B	622	SQD	C45-O47-C7	-2.24	112.45	117.80
26	b	616	CLA	CHC-C4B-NB	2.24	127.40	124.05
26	b	611	CLA	CHB-C4A-NA	2.23	127.62	124.40
31	D	406	LMG	O6-C1-O1	-2.23	104.77	110.04
26	B	609	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
28	t	101	BCR	C35-C13-C12	2.23	121.49	118.09
30	I	102	STE	C3-C2-C1	-2.23	108.70	114.51
26	b	615	CLA	C1-C2-C3	-2.23	122.55	126.20
26	c	509	CLA	C3B-C4B-NB	-2.22	108.54	110.53
28	k	101	BCR	C23-C22-C21	-2.22	115.51	119.01
26	B	603	CLA	C4-C3-C5	2.22	119.09	115.23
32	b	620	SQD	O48-C23-O10	-2.22	118.07	123.63
26	b	607	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
34	h	102	DGD	O3E-C3E-C2E	-2.22	105.14	110.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	510	CLA	O2D-CGD-CBD	2.22	115.11	111.23
26	b	602	CLA	CMB-C2B-C3B	2.22	131.77	126.55
32	A	618	SQD	O48-C46-C45	2.22	114.79	108.40
36	V	201	HEC	CMD-C2D-C1D	2.22	128.50	125.03
29	D	405	PL9	C8-C7-C3	2.22	117.76	112.03
26	a	613	CLA	CHD-C1D-ND	-2.22	121.68	124.80
36	v	201	HEC	C3D-C4D-ND	-2.22	108.21	110.35
34	c	520	DGD	C3D-C4D-C5D	-2.22	106.22	110.23
26	D	403	CLA	CHC-C4B-NB	2.22	127.37	124.05
26	C	511	CLA	C3B-C4B-NB	-2.21	108.56	110.53
26	b	606	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
26	D	403	CLA	CHB-C4A-NA	2.21	127.59	124.40
26	C	513	CLA	CHB-C4A-NA	2.21	127.59	124.40
34	H	101	DGD	O5D-C1E-C2E	2.21	111.63	108.27
32	F	102	SQD	C1-O5-C5	-2.21	109.41	113.72
32	f	101	SQD	O48-C23-C24	2.21	118.56	111.83
29	a	612	PL9	O2-C1-C6	2.21	123.99	120.48
34	C	520	DGD	C6D-O5D-C1E	2.21	118.52	113.80
34	c	521	DGD	C3G-O3G-C1D	2.21	118.52	113.80
33	d	407	LHG	O4-P-O5	2.20	122.70	112.44
26	C	503	CLA	C2D-C1D-ND	-2.20	107.95	110.13
26	B	609	CLA	O1D-CGD-CBD	2.20	128.85	124.52
26	C	504	CLA	CHB-C4A-NA	2.20	127.57	124.40
26	B	603	CLA	CHC-C4B-NB	2.20	127.34	124.05
26	b	613	CLA	CHC-C4B-NB	2.20	127.34	124.05
26	a	613	CLA	CHC-C4B-NB	2.19	127.34	124.05
30	b	624	STE	O2-C1-C2	2.19	120.92	114.00
26	B	602	CLA	CMB-C2B-C3B	2.19	131.69	126.55
34	c	519	DGD	C3D-C4D-C5D	-2.19	106.27	110.23
30	D	411	STE	O2-C1-C2	2.19	120.91	114.00
26	b	609	CLA	CMB-C2B-C3B	2.19	131.69	126.55
26	c	506	CLA	C1-O2A-CGA	2.18	121.94	116.65
26	B	608	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
30	d	406	STE	O2-C1-C2	2.18	120.89	114.00
26	d	403	CLA	CHC-C4B-NB	2.18	127.32	124.05
26	d	403	CLA	C1-C2-C3	-2.18	122.63	126.20
26	C	506	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
26	B	607	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
33	b	623	LHG	O7-C5-C4	-2.18	100.54	108.34
26	B	603	CLA	O1D-CGD-CBD	2.17	128.80	124.52
26	b	605	CLA	O1D-CGD-CBD	2.17	128.80	124.52
31	B	620	LMG	O3-C3-C4	2.17	115.50	110.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	603	CLA	CHC-C4B-NB	2.17	127.31	124.05
26	b	616	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
30	B	623	STE	O2-C1-C2	2.17	120.86	114.00
29	D	405	PL9	C12-C13-C14	-2.17	122.66	127.62
26	b	614	CLA	O2D-CGD-CBD	2.17	115.02	111.23
26	b	607	CLA	CMB-C2B-C3B	2.17	131.65	126.55
36	v	201	HEC	CMD-C2D-C1D	2.17	128.42	125.03
26	B	608	CLA	CMB-C2B-C3B	2.17	131.65	126.55
35	e	102	HEM	O1A-CGA-CBA	-2.17	116.22	123.09
26	b	608	CLA	C6-C7-C8	-2.16	108.77	115.97
26	B	607	CLA	CHB-C4A-NA	2.16	127.52	124.40
35	e	102	HEM	CHC-C1C-NC	2.16	126.81	124.45
26	b	614	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
26	b	610	CLA	O1D-CGD-CBD	2.16	128.78	124.52
26	B	601	CLA	CAA-CBA-CGA	-2.16	107.08	113.21
36	V	201	HEC	CHB-C1B-NB	2.16	126.75	124.42
26	d	402	CLA	O2D-CGD-CBD	2.16	115.00	111.23
28	X	101	BCR	C2-C3-C4	-2.16	106.54	111.28
31	a	618	LMG	C1-O6-C5	-2.16	109.51	113.72
26	c	512	CLA	CHD-C1D-C2D	2.15	129.97	125.49
28	D	404	BCR	C38-C26-C25	-2.15	122.14	124.48
29	A	612	PL9	C22-C23-C24	-2.15	122.70	127.62
26	b	613	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
26	C	504	CLA	CHB-C1B-NB	2.15	127.27	124.05
31	B	620	LMG	C4-C3-C2	2.15	114.60	110.83
26	A	607	CLA	C3B-C4B-NB	-2.15	108.61	110.53
26	b	604	CLA	C2A-C1A-CHA	2.15	127.59	123.87
26	b	609	CLA	C2A-C1A-CHA	2.15	127.59	123.87
30	I	101	STE	O2-C1-C2	2.14	120.78	114.00
35	F	101	HEM	O2D-CGD-CBD	2.14	120.75	114.00
31	c	518	LMG	C8-O7-C10	2.13	122.90	117.80
26	C	504	CLA	C1-C2-C3	-2.13	122.70	126.20
26	B	615	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
28	b	619	BCR	C4-C5-C6	-2.13	119.83	122.70
26	A	610	CLA	CMB-C2B-C3B	2.13	131.56	126.55
30	C	524	STE	O2-C1-C2	2.13	120.72	114.00
30	b	621	STE	O2-C1-C2	2.13	120.72	114.00
26	c	513	CLA	CMB-C2B-C3B	2.13	131.55	126.55
29	a	612	PL9	C20-C19-C21	2.12	118.92	115.23
26	C	511	CLA	O2D-CGD-CBD	2.12	114.93	111.23
26	B	608	CLA	CHB-C1B-NB	2.12	127.22	124.05
26	c	508	CLA	CMB-C2B-C1B	-2.12	122.20	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	610	CLA	CMB-C2B-C3B	2.11	131.52	126.55
26	B	611	CLA	C1D-ND-C4D	2.11	107.79	106.31
31	D	406	LMG	O6-C1-C2	2.11	114.71	110.37
26	c	513	CLA	CHB-C1B-NB	2.11	127.21	124.05
31	b	622	LMG	O7-C8-C9	2.11	115.91	108.34
30	k	103	STE	O2-C1-C2	2.11	120.65	114.00
26	b	606	CLA	CMB-C2B-C3B	2.11	131.50	126.55
28	D	404	BCR	C23-C22-C21	-2.10	115.70	119.01
29	D	405	PL9	C20-C19-C21	2.10	118.88	115.23
26	B	616	CLA	C4D-C3D-CAD	-2.10	105.82	108.11
26	B	606	CLA	C2A-C1A-CHA	2.10	127.52	123.87
26	B	602	CLA	C16-C15-C13	-2.10	108.98	115.97
26	C	503	CLA	CHD-C1D-C2D	2.10	129.86	125.49
34	C	521	DGD	C3E-C4E-C5E	-2.10	106.42	110.23
32	B	622	SQD	O48-C23-O10	-2.10	118.37	123.63
26	C	502	CLA	CHD-C1D-ND	-2.10	121.85	124.80
26	C	508	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
26	D	403	CLA	C3B-C4B-NB	-2.10	108.66	110.53
26	B	606	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
26	B	614	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
26	A	607	CLA	O1D-CGD-CBD	2.09	128.65	124.52
36	V	201	HEC	C3C-C4C-NC	-2.09	107.83	110.15
29	D	405	PL9	O2-C1-C2	-2.09	117.07	121.83
26	d	403	CLA	CMB-C2B-C3B	2.09	131.47	126.55
35	e	102	HEM	C4C-NC-C1C	2.09	109.23	105.82
26	c	509	CLA	O2A-CGA-CBA	2.09	118.21	111.83
32	B	622	SQD	C25-C24-C23	-2.09	106.03	113.69
26	B	610	CLA	CHA-C1A-NA	-2.09	121.66	126.39
29	D	405	PL9	C32-C33-C34	-2.09	122.84	127.62
26	B	606	CLA	CHA-C4D-ND	2.09	136.85	132.55
26	b	609	CLA	CHB-C4A-NA	2.08	127.41	124.40
28	k	101	BCR	C20-C21-C22	2.08	130.20	127.28
26	C	510	CLA	C11-C10-C8	-2.08	109.05	115.97
29	D	405	PL9	O2-C1-C6	2.08	123.79	120.48
26	b	611	CLA	CMB-C2B-C3B	2.08	131.44	126.55
26	C	509	CLA	O2D-CGD-CBD	2.08	114.86	111.23
26	C	508	CLA	CHB-C1B-NB	2.08	127.17	124.05
26	B	605	CLA	O1D-CGD-CBD	2.08	128.61	124.52
26	B	607	CLA	CHC-C4B-NB	2.08	127.16	124.05
28	b	617	BCR	C33-C5-C6	-2.07	122.22	124.48
29	A	612	PL9	C42-C43-C44	-2.07	122.88	127.62
28	K	103	BCR	C7-C6-C5	2.07	126.32	121.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	616	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
30	i	101	STE	O2-C1-C2	2.07	120.54	114.00
26	A	610	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
34	c	519	DGD	O6D-C1D-O3G	-2.06	105.17	110.04
26	B	613	CLA	CHB-C4A-NA	2.06	127.38	124.40
26	c	503	CLA	C1-C2-C3	-2.06	122.82	126.20
26	B	612	CLA	C11-C12-C13	-2.06	109.11	115.97
31	a	618	LMG	O4-C4-C5	2.06	114.40	109.32
26	b	615	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
26	b	614	CLA	CHA-C4D-ND	2.06	136.80	132.55
26	b	607	CLA	CHC-C4B-NB	2.06	127.14	124.05
26	c	509	CLA	CMB-C2B-C3B	2.06	131.39	126.55
26	b	609	CLA	C4D-CHA-C1A	2.06	123.70	121.24
26	c	510	CLA	CHB-C4A-NA	2.06	127.37	124.40
26	B	601	CLA	CHB-C4A-NA	2.06	127.37	124.40
27	A	609	PHO	O2A-CGA-O1A	-2.06	118.48	123.63
32	F	102	SQD	O5-C5-C4	2.05	113.40	109.70
26	c	510	CLA	C1-C2-C3	-2.05	122.83	126.20
26	B	612	CLA	C16-C15-C13	-2.05	109.14	115.97
26	b	609	CLA	CHC-C4B-NB	2.05	127.13	124.05
32	a	615	SQD	O5-C1-C2	-2.05	106.16	110.37
27	D	401	PHO	C4D-ND-C1D	-2.05	106.42	108.87
26	c	502	CLA	C1-C2-C3	-2.05	122.84	126.20
26	B	616	CLA	CMB-C2B-C3B	2.05	131.36	126.55
32	b	620	SQD	C46-C45-C44	-2.05	107.02	111.78
26	C	503	CLA	CHC-C4B-NB	2.05	127.12	124.05
28	t	101	BCR	C23-C22-C21	-2.04	115.79	119.01
30	d	408	STE	C3-C2-C1	-2.04	109.17	114.51
26	c	506	CLA	O1D-CGD-CBD	2.04	128.55	124.52
26	B	614	CLA	CHD-C1D-ND	-2.04	121.93	124.80
32	A	616	SQD	C44-O6-C1	-2.04	109.41	113.80
31	M	101	LMG	O7-C10-C11	-2.04	107.06	111.48
26	C	502	CLA	CHB-C4A-NA	2.04	127.35	124.40
26	b	615	CLA	C11-C12-C13	-2.04	109.18	115.97
26	C	506	CLA	O1D-CGD-CBD	2.04	128.54	124.52
29	A	612	PL9	C50-C49-C48	-2.04	116.53	122.66
28	b	618	BCR	C3-C4-C5	2.04	117.69	114.06
31	A	615	LMG	O3-C3-C4	2.04	115.18	110.38
26	b	605	CLA	C1-C2-C3	-2.04	122.86	126.20
26	C	502	CLA	CHA-C1A-NA	-2.04	121.78	126.39
26	b	611	CLA	CHD-C1D-C2D	2.04	129.72	125.49
26	c	511	CLA	CHB-C4A-NA	2.03	127.34	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	505	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
34	c	521	DGD	C6D-C5D-C4D	2.03	116.33	112.07
30	b	624	STE	O2-C1-O1	-2.03	118.11	123.33
29	a	612	PL9	C7-C8-C9	-2.03	123.33	126.83
26	B	601	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
31	c	522	LMG	O1-C7-C8	-2.03	105.88	110.82
26	c	506	CLA	CHC-C4B-NB	2.03	127.09	124.05
26	a	613	CLA	C3B-C4B-NB	-2.03	108.72	110.53
30	e	105	STE	O2-C1-C2	2.03	120.41	114.00
26	B	607	CLA	CHA-C1A-NA	-2.03	121.80	126.39
26	C	512	CLA	C6-C7-C8	-2.03	109.23	115.97
29	D	405	PL9	C36-C34-C33	-2.03	116.62	121.17
26	B	613	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
32	a	615	SQD	O7-S-C6	2.02	109.78	106.76
26	c	502	CLA	O1D-CGD-CBD	2.02	128.51	124.52
31	C	516	LMG	O1-C7-C8	-2.02	105.90	110.82
29	A	612	PL9	C30-C29-C31	-2.02	111.72	115.23
34	c	520	DGD	C6D-C5D-C4D	2.02	116.31	112.07
26	C	512	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
36	v	201	HEC	CHD-C1D-ND	2.02	126.87	124.37
32	a	617	SQD	O9-S-C6	2.02	109.77	106.76
26	c	502	CLA	CHD-C1D-ND	-2.02	121.96	124.80
26	B	611	CLA	CHC-C4B-NB	2.02	127.08	124.05
32	f	101	SQD	C3-C4-C5	2.02	113.89	110.23
26	c	501	CLA	CHB-C4A-NA	2.02	127.31	124.40
26	b	614	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
28	h	101	BCR	C7-C6-C5	2.01	126.19	121.56
26	B	606	CLA	C2B-C1B-NB	-2.01	108.24	110.33
26	D	402	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
26	A	610	CLA	CHB-C1B-NB	2.01	127.06	124.05
26	b	607	CLA	CHB-C1B-NB	2.01	127.06	124.05
33	D	408	LHG	C5-O7-C7	2.01	122.60	117.80
30	d	410	STE	O2-C1-C2	2.01	120.34	114.00
26	b	604	CLA	C11-C10-C8	-2.01	109.30	115.97
26	B	607	CLA	C2A-C1A-CHA	2.00	127.35	123.87
26	b	604	CLA	CHA-C4D-ND	2.00	136.68	132.55
26	c	504	CLA	CHD-C1D-ND	-2.00	121.98	124.80
34	h	102	DGD	C3E-C4E-C5E	-2.00	106.60	110.23
26	B	612	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
29	a	612	PL9	C35-C34-C36	2.00	118.70	115.23

All (2) chirality outliers are listed below:

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

All (1828) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	B	601	CLA	C1A-C2A-CAA-CBA
26	B	611	CLA	C12-C13-C15-C16
26	B	615	CLA	C6-C7-C8-C9
26	C	504	CLA	C4B-C3B-CAB-CBB
26	C	507	CLA	CHA-CBD-CGD-O1D
26	C	507	CLA	CHA-CBD-CGD-O2D
26	a	608	CLA	C2B-C3B-CAB-CBB
26	a	608	CLA	C4B-C3B-CAB-CBB
26	b	604	CLA	C2-C3-C5-C6
26	b	604	CLA	C4-C3-C5-C6
26	b	614	CLA	CAD-CBD-CGD-O1D
26	b	614	CLA	CAD-CBD-CGD-O2D
26	c	507	CLA	CHA-CBD-CGD-O2D
26	d	403	CLA	C1A-C2A-CAA-CBA
26	d	403	CLA	C3A-C2A-CAA-CBA
28	D	404	BCR	C23-C24-C25-C26
28	D	404	BCR	C23-C24-C25-C30
28	K	102	BCR	C1-C6-C7-C8
28	K	102	BCR	C5-C6-C7-C8
28	K	102	BCR	C21-C22-C23-C24
28	T	101	BCR	C7-C8-C9-C10
28	X	101	BCR	C5-C6-C7-C8
28	d	404	BCR	C21-C22-C23-C24
28	k	101	BCR	C1-C6-C7-C8
28	k	101	BCR	C5-C6-C7-C8
28	k	101	BCR	C17-C18-C19-C20
28	k	101	BCR	C36-C18-C19-C20
28	k	102	BCR	C7-C8-C9-C10
28	k	102	BCR	C7-C8-C9-C34
28	t	101	BCR	C7-C8-C9-C10
29	A	612	PL9	C27-C28-C29-C30
29	A	612	PL9	C27-C28-C29-C31
29	D	405	PL9	C12-C13-C14-C15
29	D	405	PL9	C12-C13-C14-C16
29	D	405	PL9	C32-C33-C34-C36
29	a	612	PL9	C22-C23-C24-C25
29	a	612	PL9	C22-C23-C24-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	a	612	PL9	C37-C38-C39-C41
29	a	612	PL9	C42-C43-C44-C45
29	d	405	PL9	C32-C33-C34-C36
31	A	615	LMG	O6-C1-O1-C7
31	A	615	LMG	O9-C10-O7-C8
31	A	615	LMG	C11-C10-O7-C8
31	C	516	LMG	C2-C1-O1-C7
31	C	523	LMG	C11-C10-O7-C8
31	D	406	LMG	O6-C1-O1-C7
31	D	406	LMG	O9-C10-O7-C8
31	D	406	LMG	C11-C10-O7-C8
31	a	618	LMG	O6-C1-O1-C7
31	a	618	LMG	O7-C8-C9-O8
31	c	518	LMG	O1-C7-C8-O7
31	c	524	LMG	C2-C1-O1-C7
31	c	524	LMG	O6-C1-O1-C7
31	m	101	LMG	O6-C1-O1-C7
32	A	618	SQD	O5-C5-C6-S
32	B	622	SQD	C2-C1-O6-C44
32	B	622	SQD	O5-C1-O6-C44
32	B	622	SQD	O6-C44-C45-O47
32	B	622	SQD	O49-C7-O47-C45
32	F	102	SQD	C2-C1-O6-C44
32	F	102	SQD	O5-C1-O6-C44
32	a	617	SQD	O6-C44-C45-O47
32	a	617	SQD	O5-C5-C6-S
32	b	620	SQD	O5-C1-O6-C44
32	b	620	SQD	C8-C7-O47-C45
32	f	101	SQD	C2-C1-O6-C44
32	f	101	SQD	O5-C1-O6-C44
33	D	408	LHG	C3-O3-P-O4
33	D	408	LHG	C3-O3-P-O6
33	D	410	LHG	C1-C2-C3-O3
33	D	410	LHG	C3-O3-P-O4
33	L	101	LHG	C4-O6-P-O4
33	a	616	LHG	C3-O3-P-O5
33	a	616	LHG	C3-O3-P-O6
33	b	623	LHG	O1-C1-C2-C3
33	d	407	LHG	O1-C1-C2-C3
33	l	101	LHG	C4-O6-P-O3
33	l	101	LHG	C4-O6-P-O4
33	l	101	LHG	C4-O6-P-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	b	601	CLA	O1D-CGD-O2D-CED
26	b	601	CLA	CBD-CGD-O2D-CED
26	c	513	CLA	CBD-CGD-O2D-CED
26	B	601	CLA	O1A-CGA-O2A-C1
32	F	102	SQD	O10-C23-O48-C46
29	A	612	PL9	C47-C48-C49-C50
29	A	612	PL9	C47-C48-C49-C51
26	B	601	CLA	CBA-CGA-O2A-C1
31	B	620	LMG	O10-C28-O8-C9
31	M	101	LMG	O10-C28-O8-C9
31	b	622	LMG	O10-C28-O8-C9
32	f	101	SQD	O10-C23-O48-C46
26	B	614	CLA	C13-C15-C16-C17
31	C	523	LMG	O9-C10-O7-C8
32	b	620	SQD	O49-C7-O47-C45
32	f	101	SQD	O49-C7-O47-C45
34	A	619	DGD	O1B-C1B-O2G-C2G
26	b	602	CLA	C3-C5-C6-C7
26	b	604	CLA	C3-C5-C6-C7
26	b	614	CLA	C3-C5-C6-C7
26	d	403	CLA	C3-C5-C6-C7
31	B	620	LMG	C29-C28-O8-C9
31	M	101	LMG	C29-C28-O8-C9
32	F	102	SQD	C24-C23-O48-C46
32	f	101	SQD	C24-C23-O48-C46
26	B	614	CLA	CBD-CGD-O2D-CED
26	C	501	CLA	CBD-CGD-O2D-CED
26	c	503	CLA	CBD-CGD-O2D-CED
26	c	508	CLA	CBD-CGD-O2D-CED
32	B	622	SQD	C8-C7-O47-C45
32	f	101	SQD	C8-C7-O47-C45
26	A	610	CLA	C4-C3-C5-C6
26	B	603	CLA	C4-C3-C5-C6
26	B	605	CLA	C4-C3-C5-C6
26	B	614	CLA	C4-C3-C5-C6
26	C	504	CLA	C4-C3-C5-C6
26	D	403	CLA	C4-C3-C5-C6
26	b	602	CLA	C4-C3-C5-C6
26	b	603	CLA	C4-C3-C5-C6
26	b	605	CLA	C4-C3-C5-C6
26	b	614	CLA	C4-C3-C5-C6
26	c	507	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	B	603	CLA	C2-C3-C5-C6
26	B	605	CLA	C2-C3-C5-C6
26	B	614	CLA	C2-C3-C5-C6
26	C	504	CLA	C2-C3-C5-C6
26	b	602	CLA	C2-C3-C5-C6
26	b	603	CLA	C2-C3-C5-C6
26	b	605	CLA	C2-C3-C5-C6
26	b	614	CLA	C2-C3-C5-C6
29	A	612	PL9	C38-C39-C41-C42
26	b	601	CLA	C3-C5-C6-C7
26	B	616	CLA	CBA-CGA-O2A-C1
31	b	622	LMG	C29-C28-O8-C9
32	B	622	SQD	C24-C23-O48-C46
29	A	612	PL9	C37-C38-C39-C40
29	A	612	PL9	C37-C38-C39-C41
29	a	612	PL9	C32-C33-C34-C36
29	a	612	PL9	C42-C43-C44-C46
26	B	616	CLA	O1A-CGA-O2A-C1
33	D	408	LHG	O2-C2-C3-O3
33	D	410	LHG	O2-C2-C3-O3
31	m	101	LMG	C29-C28-O8-C9
34	A	619	DGD	C2B-C1B-O2G-C2G
31	D	406	LMG	C4-C5-C6-O5
26	B	615	CLA	C3-C5-C6-C7
26	C	512	CLA	C3-C5-C6-C7
26	C	512	CLA	CBD-CGD-O2D-CED
31	b	622	LMG	O6-C5-C6-O5
26	c	513	CLA	O1D-CGD-O2D-CED
29	A	612	PL9	C35-C34-C36-C37
26	A	610	CLA	C2-C3-C5-C6
26	c	507	CLA	C2-C3-C5-C6
29	A	612	PL9	C24-C26-C27-C28
29	A	612	PL9	C29-C31-C32-C33
29	A	612	PL9	C34-C36-C37-C38
29	A	612	PL9	C39-C41-C42-C43
29	A	612	PL9	C44-C46-C47-C48
29	a	612	PL9	C34-C36-C37-C38
30	d	408	STE	C5-C6-C7-C8
33	b	623	LHG	C10-C11-C12-C13
31	m	101	LMG	O10-C28-O8-C9
32	B	622	SQD	O10-C23-O48-C46
31	b	622	LMG	O6-C1-O1-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	C	520	DGD	C8A-C9A-CAA-CBA
26	c	506	CLA	CBA-CGA-O2A-C1
26	C	505	CLA	CBD-CGD-O2D-CED
26	C	511	CLA	CBD-CGD-O2D-CED
26	C	513	CLA	CBD-CGD-O2D-CED
33	l	101	LHG	C7-C8-C9-C10
34	c	521	DGD	C7B-C8B-C9B-CAB
29	A	612	PL9	C22-C23-C24-C25
29	D	405	PL9	C32-C33-C34-C35
30	C	524	STE	C2-C3-C4-C5
26	c	501	CLA	CBD-CGD-O2D-CED
26	c	512	CLA	C15-C16-C17-C18
31	C	516	LMG	C29-C28-O8-C9
30	B	625	STE	C11-C12-C13-C14
34	A	619	DGD	O6E-C5E-C6E-O5E
34	A	619	DGD	C4E-C5E-C6E-O5E
34	A	619	DGD	C8B-C9B-CAB-CBB
34	C	521	DGD	C3B-C4B-C5B-C6B
31	c	523	LMG	C35-C36-C37-C38
32	a	615	SQD	C12-C13-C14-C15
34	h	102	DGD	C6B-C7B-C8B-C9B
26	b	607	CLA	C4-C3-C5-C6
26	D	403	CLA	C2-C3-C5-C6
26	b	607	CLA	C2-C3-C5-C6
29	A	612	PL9	C33-C34-C36-C37
29	a	612	PL9	C33-C34-C36-C37
29	d	405	PL9	C38-C39-C41-C42
26	B	604	CLA	C11-C10-C8-C9
26	B	605	CLA	C6-C7-C8-C9
26	B	606	CLA	C11-C12-C13-C14
26	B	608	CLA	C14-C13-C15-C16
26	B	610	CLA	C14-C13-C15-C16
26	B	613	CLA	C11-C12-C13-C14
26	B	615	CLA	C14-C13-C15-C16
26	C	503	CLA	C11-C10-C8-C9
26	C	509	CLA	C11-C10-C8-C9
26	C	512	CLA	C11-C10-C8-C9
26	a	608	CLA	C11-C12-C13-C14
26	a	613	CLA	C14-C13-C15-C16
26	b	601	CLA	C11-C10-C8-C9
26	b	602	CLA	C6-C7-C8-C9
26	b	603	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	b	605	CLA	C11-C10-C8-C9
26	b	606	CLA	C14-C13-C15-C16
26	b	607	CLA	C11-C10-C8-C9
26	b	610	CLA	C14-C13-C15-C16
26	b	614	CLA	C6-C7-C8-C9
26	b	616	CLA	C6-C7-C8-C9
26	c	509	CLA	C11-C12-C13-C14
26	c	510	CLA	C11-C10-C8-C9
26	c	510	CLA	C11-C12-C13-C14
26	c	511	CLA	C14-C13-C15-C16
26	c	513	CLA	C11-C12-C13-C14
26	d	403	CLA	C6-C7-C8-C9
31	b	622	LMG	C2-C1-O1-C7
33	b	623	LHG	C7-C8-C9-C10
26	B	614	CLA	O1D-CGD-O2D-CED
31	D	406	LMG	O6-C5-C6-O5
33	a	616	LHG	C9-C10-C11-C12
31	C	516	LMG	O10-C28-O8-C9
34	c	521	DGD	C6A-C7A-C8A-C9A
28	K	102	BCR	C37-C22-C23-C24
28	T	101	BCR	C7-C8-C9-C34
28	b	617	BCR	C36-C18-C19-C20
28	d	404	BCR	C37-C22-C23-C24
28	h	101	BCR	C7-C8-C9-C34
28	t	101	BCR	C7-C8-C9-C34
30	C	515	STE	C1-C2-C3-C4
33	L	101	LHG	C7-C8-C9-C10
29	D	405	PL9	C47-C48-C49-C51
34	c	521	DGD	O6E-C5E-C6E-O5E
26	B	608	CLA	C15-C16-C17-C18
30	a	620	STE	C2-C3-C4-C5
32	a	615	SQD	C30-C31-C32-C33
29	a	612	PL9	C32-C33-C34-C35
31	D	407	LMG	C16-C17-C18-C19
31	m	101	LMG	C38-C39-C40-C41
33	a	614	LHG	C24-C25-C26-C27
26	B	608	CLA	C13-C15-C16-C17
26	D	403	CLA	C8-C10-C11-C12
26	B	607	CLA	C3-C5-C6-C7
26	b	611	CLA	C8-C10-C11-C12
26	B	606	CLA	C12-C13-C15-C16
26	C	503	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	C	508	CLA	C12-C13-C15-C16
26	b	606	CLA	C6-C7-C8-C10
26	c	506	CLA	C12-C13-C15-C16
26	c	510	CLA	C12-C13-C15-C16
30	e	105	STE	C1-C2-C3-C4
31	C	516	LMG	C28-C29-C30-C31
32	a	615	SQD	C7-C8-C9-C10
33	a	616	LHG	C25-C26-C27-C28
34	C	520	DGD	O6E-C5E-C6E-O5E
26	c	503	CLA	O1D-CGD-O2D-CED
34	c	521	DGD	C4A-C5A-C6A-C7A
26	B	601	CLA	C5-C6-C7-C8
26	C	503	CLA	C5-C6-C7-C8
30	a	620	STE	C1-C2-C3-C4
31	c	524	LMG	C10-C11-C12-C13
26	c	506	CLA	O1A-CGA-O2A-C1
26	C	512	CLA	C10-C11-C12-C13
26	b	607	CLA	C10-C11-C12-C13
31	B	620	LMG	C4-C5-C6-O5
26	B	601	CLA	C2A-CAA-CBA-CGA
26	B	606	CLA	C8-C10-C11-C12
26	B	613	CLA	C8-C10-C11-C12
26	C	502	CLA	C15-C16-C17-C18
26	C	505	CLA	C15-C16-C17-C18
26	C	507	CLA	C5-C6-C7-C8
26	a	613	CLA	C15-C16-C17-C18
26	b	615	CLA	C8-C10-C11-C12
26	c	509	CLA	C13-C15-C16-C17
26	c	513	CLA	C13-C15-C16-C17
31	a	618	LMG	C28-C29-C30-C31
31	c	522	LMG	C28-C29-C30-C31
32	F	102	SQD	C23-C24-C25-C26
33	A	617	LHG	C23-C24-C25-C26
31	C	516	LMG	O6-C1-O1-C7
31	M	101	LMG	C33-C34-C35-C36
26	B	603	CLA	C13-C15-C16-C17
26	B	607	CLA	C13-C15-C16-C17
26	B	609	CLA	C13-C15-C16-C17
26	B	616	CLA	C5-C6-C7-C8
26	C	507	CLA	C13-C15-C16-C17
26	C	508	CLA	C15-C16-C17-C18
26	C	509	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	C	512	CLA	C13-C15-C16-C17
26	a	608	CLA	C15-C16-C17-C18
26	b	613	CLA	C10-C11-C12-C13
26	c	504	CLA	C10-C11-C12-C13
26	c	510	CLA	C8-C10-C11-C12
34	C	521	DGD	C7A-C8A-C9A-CAA
33	d	407	LHG	O2-C2-C3-O3
30	H	103	STE	C12-C13-C14-C15
26	B	612	CLA	CBD-CGD-O2D-CED
31	a	618	LMG	C10-C11-C12-C13
31	d	409	LMG	C28-C29-C30-C31
26	A	608	CLA	C15-C16-C17-C18
26	B	606	CLA	C10-C11-C12-C13
26	b	601	CLA	C10-C11-C12-C13
26	b	614	CLA	C8-C10-C11-C12
26	b	614	CLA	C13-C15-C16-C17
26	c	507	CLA	C5-C6-C7-C8
26	c	508	CLA	O1D-CGD-O2D-CED
30	B	623	STE	C1-C2-C3-C4
30	d	410	STE	C1-C2-C3-C4
26	C	506	CLA	C15-C16-C17-C18
26	a	608	CLA	C8-C10-C11-C12
26	c	509	CLA	C10-C11-C12-C13
36	V	201	HEC	C2C-C3C-CAC-CBC
33	D	408	LHG	C1-C2-C3-O3
33	d	407	LHG	C1-C2-C3-O3
26	b	606	CLA	C2A-CAA-CBA-CGA
26	C	501	CLA	O1D-CGD-O2D-CED
33	L	101	LHG	C27-C28-C29-C30
26	a	607	CLA	C15-C16-C17-C18
26	b	604	CLA	C13-C15-C16-C17
26	b	607	CLA	C8-C10-C11-C12
26	c	506	CLA	C15-C16-C17-C18
26	C	512	CLA	O1D-CGD-O2D-CED
26	b	615	CLA	C5-C6-C7-C8
26	c	513	CLA	C8-C10-C11-C12
26	B	605	CLA	C13-C15-C16-C17
26	C	509	CLA	C13-C15-C16-C17
26	b	602	CLA	C15-C16-C17-C18
26	d	403	CLA	C10-C11-C12-C13
31	D	406	LMG	C10-C11-C12-C13
32	B	622	SQD	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	a	612	PL9	C35-C34-C36-C37
26	B	614	CLA	C8-C10-C11-C12
26	C	509	CLA	C3-C5-C6-C7
32	f	101	SQD	C25-C26-C27-C28
31	B	620	LMG	C2-C1-O1-C7
32	A	618	SQD	C2-C1-O6-C44
30	E	103	STE	C1-C2-C3-C4
33	b	623	LHG	C23-C24-C25-C26
31	C	523	LMG	C29-C28-O8-C9
26	B	616	CLA	C11-C12-C13-C14
26	b	604	CLA	C16-C17-C18-C20
33	A	617	LHG	C27-C28-C29-C30
34	c	520	DGD	C4E-C5E-C6E-O5E
28	X	101	BCR	C7-C8-C9-C34
31	B	620	LMG	O6-C5-C6-O5
28	b	617	BCR	C17-C18-C19-C20
28	h	101	BCR	C7-C8-C9-C10
26	c	512	CLA	C2A-CAA-CBA-CGA
26	b	603	CLA	C13-C15-C16-C17
33	D	410	LHG	O1-C1-C2-C3
33	a	614	LHG	O1-C1-C2-C3
30	m	102	STE	C1-C2-C3-C4
32	B	622	SQD	C23-C24-C25-C26
31	b	622	LMG	C9-C8-O7-C10
32	b	620	SQD	C46-C45-O47-C7
34	C	522	DGD	CAB-CBB-CCB-CDB
26	B	615	CLA	C16-C17-C18-C20
26	C	510	CLA	C16-C17-C18-C19
26	c	507	CLA	C16-C17-C18-C19
26	c	512	CLA	C16-C17-C18-C19
31	B	620	LMG	O6-C1-O1-C7
31	c	523	LMG	C11-C10-O7-C8
32	a	615	SQD	C26-C27-C28-C29
32	a	617	SQD	C27-C28-C29-C30
26	c	512	CLA	CBA-CGA-O2A-C1
26	b	616	CLA	C2-C1-O2A-CGA
26	c	506	CLA	C2-C1-O2A-CGA
26	B	606	CLA	C16-C17-C18-C19
26	B	607	CLA	C16-C17-C18-C20
26	C	501	CLA	C16-C17-C18-C19
26	b	602	CLA	C16-C17-C18-C19
26	c	503	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	c	512	CLA	C16-C17-C18-C20
30	B	623	STE	C10-C11-C12-C13
30	C	519	STE	C7-C8-C9-C10
31	B	620	LMG	C11-C12-C13-C14
32	B	622	SQD	C13-C14-C15-C16
33	l	101	LHG	C34-C35-C36-C37
34	C	522	DGD	C8A-C9A-CAA-CBA
34	H	101	DGD	C8B-C9B-CAB-CBB
34	c	520	DGD	C3B-C4B-C5B-C6B
30	C	519	STE	C5-C6-C7-C8
30	H	103	STE	C14-C15-C16-C17
30	M	102	STE	C9-C10-C11-C12
30	b	621	STE	C7-C8-C9-C10
30	b	624	STE	C7-C8-C9-C10
30	d	410	STE	C5-C6-C7-C8
30	m	103	STE	C9-C10-C11-C12
30	z	101	STE	C2-C3-C4-C5
31	A	615	LMG	C33-C34-C35-C36
31	a	618	LMG	C15-C16-C17-C18
31	b	622	LMG	C16-C17-C18-C19
31	c	524	LMG	C31-C32-C33-C34
31	m	101	LMG	C12-C13-C14-C15
32	F	102	SQD	C27-C28-C29-C30
32	b	620	SQD	C10-C11-C12-C13
33	A	617	LHG	C15-C16-C17-C18
33	A	617	LHG	C28-C29-C30-C31
33	b	623	LHG	C17-C18-C19-C20
33	l	101	LHG	C29-C30-C31-C32
34	c	521	DGD	C9A-CAA-CBA-CCA
34	h	102	DGD	C5B-C6B-C7B-C8B
30	c	516	STE	C5-C6-C7-C8
30	h	103	STE	C12-C13-C14-C15
30	k	103	STE	C7-C8-C9-C10
31	c	518	LMG	C32-C33-C34-C35
34	C	521	DGD	C6B-C7B-C8B-C9B
34	h	102	DGD	C2B-C3B-C4B-C5B
34	c	519	DGD	O6D-C5D-C6D-O5D
30	A	613	STE	C2-C3-C4-C5
30	B	623	STE	C6-C7-C8-C9
30	B	625	STE	C6-C7-C8-C9
30	K	104	STE	C7-C8-C9-C10
30	M	103	STE	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	a	620	STE	C6-C7-C8-C9
30	b	621	STE	C4-C5-C6-C7
30	e	104	STE	C12-C13-C14-C15
30	m	103	STE	C5-C6-C7-C8
31	C	523	LMG	C12-C13-C14-C15
31	M	101	LMG	C13-C14-C15-C16
31	b	622	LMG	C15-C16-C17-C18
32	A	618	SQD	C14-C15-C16-C17
32	f	101	SQD	C27-C28-C29-C30
33	D	409	LHG	C29-C30-C31-C32
34	C	522	DGD	C9A-CAA-CBA-CCA
34	c	520	DGD	CAA-CBA-CCA-CDA
33	D	408	LHG	O1-C1-C2-O2
33	D	410	LHG	O1-C1-C2-O2
33	b	623	LHG	O1-C1-C2-O2
30	b	621	STE	C11-C10-C9-C8
30	d	410	STE	C3-C4-C5-C6
31	B	620	LMG	C29-C30-C31-C32
34	h	102	DGD	CBB-CCB-CDB-CEB
26	b	605	CLA	C4B-C3B-CAB-CBB
26	c	505	CLA	C4B-C3B-CAB-CBB
26	c	512	CLA	C4B-C3B-CAB-CBB
30	E	101	STE	C1-C2-C3-C4
31	C	523	LMG	C28-C29-C30-C31
34	c	520	DGD	C1A-C2A-C3A-C4A
30	C	515	STE	C3-C4-C5-C6
30	D	411	STE	C3-C4-C5-C6
30	H	102	STE	C2-C3-C4-C5
31	M	101	LMG	C32-C33-C34-C35
32	b	620	SQD	C27-C28-C29-C30
26	B	615	CLA	C16-C17-C18-C19
26	c	507	CLA	C16-C17-C18-C20
26	c	510	CLA	C16-C17-C18-C20
26	B	606	CLA	C2A-CAA-CBA-CGA
30	c	516	STE	C7-C8-C9-C10
31	D	407	LMG	C39-C40-C41-C42
32	A	616	SQD	C9-C10-C11-C12
26	A	608	CLA	C13-C15-C16-C17
26	B	601	CLA	C8-C10-C11-C12
26	B	611	CLA	C8-C10-C11-C12
26	B	614	CLA	C15-C16-C17-C18
26	c	513	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	I	101	STE	C2-C3-C4-C5
34	h	102	DGD	C8A-C9A-CAA-CBA
26	B	608	CLA	C12-C13-C15-C16
26	B	614	CLA	C11-C12-C13-C15
26	b	602	CLA	C11-C12-C13-C15
26	b	614	CLA	C11-C10-C8-C7
26	c	503	CLA	C6-C7-C8-C10
26	d	403	CLA	C11-C12-C13-C15
31	A	615	LMG	C34-C35-C36-C37
31	c	524	LMG	C37-C38-C39-C40
30	B	621	STE	C1-C2-C3-C4
30	I	101	STE	C1-C2-C3-C4
30	t	102	STE	C11-C10-C9-C8
31	B	620	LMG	C33-C34-C35-C36
31	b	622	LMG	C12-C13-C14-C15
31	b	622	LMG	C36-C37-C38-C39
34	C	520	DGD	C6B-C7B-C8B-C9B
34	H	101	DGD	C4E-C5E-C6E-O5E
30	B	625	STE	C4-C5-C6-C7
32	a	617	SQD	C18-C19-C20-C21
30	A	621	STE	C6-C7-C8-C9
30	B	625	STE	C11-C10-C9-C8
30	Z	101	STE	C14-C15-C16-C17
26	B	613	CLA	C10-C11-C12-C13
26	a	610	CLA	C5-C6-C7-C8
26	c	510	CLA	C5-C6-C7-C8
36	V	201	HEC	C4C-C3C-CAC-CBC
26	C	513	CLA	O1D-CGD-O2D-CED
34	A	619	DGD	C7B-C8B-C9B-CAB
26	C	510	CLA	C16-C17-C18-C20
26	b	614	CLA	C16-C17-C18-C20
31	B	620	LMG	C34-C35-C36-C37
31	b	622	LMG	C34-C35-C36-C37
26	b	605	CLA	C5-C6-C7-C8
31	C	523	LMG	C11-C12-C13-C14
32	A	616	SQD	C32-C33-C34-C35
32	B	622	SQD	C33-C34-C35-C36
34	h	102	DGD	C9A-CAA-CBA-CCA
34	c	521	DGD	C4E-C5E-C6E-O5E
30	A	620	STE	C12-C13-C14-C15
30	C	526	STE	C7-C8-C9-C10
32	A	616	SQD	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	D	408	LHG	C11-C12-C13-C14
33	D	408	LHG	C18-C19-C20-C21
33	L	101	LHG	C34-C35-C36-C37
33	a	616	LHG	C26-C27-C28-C29
34	c	521	DGD	C2A-C3A-C4A-C5A
32	A	616	SQD	C7-C8-C9-C10
32	b	620	SQD	C23-C24-C25-C26
30	J	101	STE	C6-C7-C8-C9
31	a	618	LMG	C11-C12-C13-C14
31	c	524	LMG	C30-C31-C32-C33
31	m	101	LMG	C29-C30-C31-C32
33	D	408	LHG	C14-C15-C16-C17
34	C	521	DGD	C4A-C5A-C6A-C7A
26	c	512	CLA	O1A-CGA-O2A-C1
30	m	103	STE	C3-C4-C5-C6
30	C	526	STE	C9-C10-C11-C12
30	E	103	STE	C10-C11-C12-C13
30	H	102	STE	C14-C15-C16-C17
31	m	101	LMG	C36-C37-C38-C39
30	C	518	STE	C4-C5-C6-C7
30	E	103	STE	C13-C14-C15-C16
30	M	102	STE	C7-C8-C9-C10
30	d	408	STE	C10-C11-C12-C13
31	b	622	LMG	C29-C30-C31-C32
32	A	616	SQD	C15-C16-C17-C18
32	f	101	SQD	C26-C27-C28-C29
33	D	408	LHG	C13-C14-C15-C16
34	c	519	DGD	C3B-C4B-C5B-C6B
26	C	513	CLA	C16-C17-C18-C19
26	C	504	CLA	C2B-C3B-CAB-CBB
26	c	505	CLA	C2B-C3B-CAB-CBB
26	c	512	CLA	C2B-C3B-CAB-CBB
28	B	617	BCR	C1-C6-C7-C8
28	B	617	BCR	C5-C6-C7-C8
28	T	101	BCR	C1-C6-C7-C8
28	T	101	BCR	C5-C6-C7-C8
28	T	101	BCR	C23-C24-C25-C26
28	X	101	BCR	C23-C24-C25-C26
28	b	617	BCR	C1-C6-C7-C8
28	b	617	BCR	C5-C6-C7-C8
28	h	101	BCR	C5-C6-C7-C8
28	t	101	BCR	C1-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	C	525	STE	C5-C6-C7-C8
30	M	104	STE	C11-C12-C13-C14
32	A	618	SQD	C12-C13-C14-C15
34	c	519	DGD	C7B-C8B-C9B-CAB
31	c	522	LMG	C11-C10-O7-C8
26	C	509	CLA	C8-C10-C11-C12
30	i	102	STE	C7-C8-C9-C10
30	B	621	STE	C7-C8-C9-C10
32	a	615	SQD	C14-C15-C16-C17
34	A	619	DGD	C9A-CAA-CBA-CCA
31	C	523	LMG	C30-C31-C32-C33
30	J	101	STE	C1-C2-C3-C4
31	c	524	LMG	C28-C29-C30-C31
30	D	411	STE	C2-C3-C4-C5
30	H	102	STE	C11-C10-C9-C8
30	K	104	STE	C10-C11-C12-C13
30	K	104	STE	C12-C13-C14-C15
31	C	523	LMG	O10-C28-O8-C9
29	A	612	PL9	C4-C3-C7-C8
30	B	625	STE	C3-C4-C5-C6
30	M	104	STE	C9-C10-C11-C12
30	b	624	STE	C2-C3-C4-C5
31	c	522	LMG	C13-C14-C15-C16
31	c	524	LMG	C16-C17-C18-C19
32	b	620	SQD	C25-C26-C27-C28
32	f	101	SQD	C28-C29-C30-C31
33	L	101	LHG	C29-C30-C31-C32
31	c	523	LMG	O9-C10-O7-C8
30	A	621	STE	C13-C14-C15-C16
30	I	101	STE	C4-C5-C6-C7
30	c	517	STE	C6-C7-C8-C9
34	C	521	DGD	CBA-CCA-CDA-CEA
30	H	102	STE	C6-C7-C8-C9
30	T	102	STE	C9-C10-C11-C12
30	T	102	STE	C14-C15-C16-C17
30	c	516	STE	C3-C4-C5-C6
32	a	615	SQD	C11-C12-C13-C14
33	L	101	LHG	C17-C18-C19-C20
33	L	101	LHG	C26-C27-C28-C29
33	l	101	LHG	C13-C14-C15-C16
34	c	520	DGD	C9A-CAA-CBA-CCA
34	c	521	DGD	CCA-CDA-CEA-CFA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	a	615	SQD	C23-C24-C25-C26
26	c	502	CLA	C6-C7-C8-C9
30	B	621	STE	C11-C10-C9-C8
30	I	101	STE	C5-C6-C7-C8
30	A	613	STE	C5-C6-C7-C8
31	C	523	LMG	C39-C40-C41-C42
31	D	407	LMG	C30-C31-C32-C33
33	L	101	LHG	C14-C15-C16-C17
33	l	101	LHG	C25-C26-C27-C28
34	c	521	DGD	C9B-CAB-CBB-CCB
32	A	618	SQD	O5-C1-O6-C44
30	e	103	STE	C12-C13-C14-C15
30	m	103	STE	C6-C7-C8-C9
31	d	409	LMG	C36-C37-C38-C39
31	C	516	LMG	O6-C5-C6-O5
31	C	523	LMG	C2-C1-O1-C7
26	c	503	CLA	C10-C11-C12-C13
30	A	622	STE	C14-C15-C16-C17
30	C	525	STE	C4-C5-C6-C7
30	B	621	STE	C6-C7-C8-C9
30	E	101	STE	C4-C5-C6-C7
30	I	101	STE	C9-C10-C11-C12
30	M	102	STE	C6-C7-C8-C9
30	j	102	STE	C13-C14-C15-C16
30	A	621	STE	C10-C11-C12-C13
30	B	623	STE	C5-C6-C7-C8
30	E	103	STE	C14-C15-C16-C17
30	b	625	STE	C4-C5-C6-C7
30	k	103	STE	C2-C3-C4-C5
31	B	620	LMG	C12-C13-C14-C15
33	L	101	LHG	C32-C33-C34-C35
34	C	520	DGD	C4B-C5B-C6B-C7B
34	c	519	DGD	C3A-C4A-C5A-C6A
26	A	614	CLA	C16-C17-C18-C20
26	B	606	CLA	C16-C17-C18-C20
26	b	614	CLA	C16-C17-C18-C19
26	c	503	CLA	C16-C17-C18-C19
31	M	101	LMG	C11-C10-O7-C8
31	M	101	LMG	C10-C11-C12-C13
31	c	523	LMG	C10-C11-C12-C13
31	C	516	LMG	C11-C12-C13-C14
32	A	616	SQD	C30-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	c	522	LMG	O9-C10-O7-C8
30	C	525	STE	C7-C8-C9-C10
32	b	620	SQD	C26-C27-C28-C29
33	A	617	LHG	C16-C17-C18-C19
34	h	102	DGD	CCB-CDB-CEB-CFB
30	c	517	STE	C9-C10-C11-C12
31	a	618	LMG	C35-C36-C37-C38
31	d	409	LMG	O6-C5-C6-O5
27	A	609	PHO	C2C-C3C-CAC-CBC
32	a	617	SQD	C31-C32-C33-C34
33	a	616	LHG	C11-C12-C13-C14
31	D	406	LMG	C28-C29-C30-C31
31	m	101	LMG	C10-C11-C12-C13
26	C	511	CLA	CBA-CGA-O2A-C1
34	C	521	DGD	C2G-C3G-O3G-C1D
34	C	521	DGD	C5D-C6D-O5D-C1E
26	b	612	CLA	C13-C15-C16-C17
26	B	605	CLA	C16-C17-C18-C20
26	C	513	CLA	C16-C17-C18-C20
26	c	505	CLA	C16-C17-C18-C19
26	c	510	CLA	CBD-CGD-O2D-CED
30	c	517	STE	C11-C12-C13-C14
30	d	410	STE	C2-C3-C4-C5
33	D	410	LHG	C24-C25-C26-C27
26	C	506	CLA	C4-C3-C5-C6
29	A	612	PL9	C40-C39-C41-C42
29	d	405	PL9	C15-C14-C16-C17
29	d	405	PL9	C45-C44-C46-C47
31	b	622	LMG	C4-C5-C6-O5
31	M	101	LMG	C20-C21-C22-C23
26	C	508	CLA	C10-C11-C12-C13
30	E	103	STE	C6-C7-C8-C9
33	A	617	LHG	C30-C31-C32-C33
32	B	622	SQD	C35-C36-C37-C38
30	D	411	STE	C7-C8-C9-C10
30	d	406	STE	C7-C8-C9-C10
33	a	614	LHG	C25-C26-C27-C28
34	C	521	DGD	C7B-C8B-C9B-CAB
26	d	402	CLA	C3-C5-C6-C7
26	A	614	CLA	C15-C16-C17-C18
31	m	101	LMG	C11-C12-C13-C14
30	M	102	STE	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	I	101	STE	C7-C8-C9-C10
30	d	408	STE	C14-C15-C16-C17
33	D	410	LHG	C29-C30-C31-C32
27	d	401	PHO	C2C-C3C-CAC-CBC
34	c	519	DGD	O6E-C5E-C6E-O5E
30	J	101	STE	C4-C5-C6-C7
33	l	101	LHG	C17-C18-C19-C20
34	A	619	DGD	C4B-C5B-C6B-C7B
26	c	504	CLA	C8-C10-C11-C12
26	c	507	CLA	C8-C10-C11-C12
26	B	616	CLA	C11-C12-C13-C15
30	e	101	STE	C13-C14-C15-C16
33	D	409	LHG	C15-C16-C17-C18
26	B	607	CLA	C15-C16-C17-C18
26	b	606	CLA	C15-C16-C17-C18
26	b	609	CLA	C15-C16-C17-C18
26	C	505	CLA	O1D-CGD-O2D-CED
30	E	101	STE	C6-C7-C8-C9
30	d	410	STE	C6-C7-C8-C9
33	D	410	LHG	C17-C18-C19-C20
32	A	618	SQD	O6-C44-C45-O47
34	A	619	DGD	O2G-C2G-C3G-O3G
31	c	522	LMG	C12-C13-C14-C15
30	H	102	STE	C12-C13-C14-C15
26	B	612	CLA	C10-C11-C12-C13
30	B	621	STE	C9-C10-C11-C12
30	m	103	STE	C11-C10-C9-C8
33	L	101	LHG	C33-C34-C35-C36
33	l	101	LHG	C10-C11-C12-C13
34	c	520	DGD	C2A-C3A-C4A-C5A
30	C	526	STE	C10-C11-C12-C13
30	M	102	STE	C11-C10-C9-C8
32	a	617	SQD	C11-C12-C13-C14
26	B	601	CLA	C2-C1-O2A-CGA
30	A	621	STE	C11-C12-C13-C14
30	B	625	STE	C10-C11-C12-C13
30	I	102	STE	C6-C7-C8-C9
31	B	620	LMG	C35-C36-C37-C38
31	c	523	LMG	C16-C17-C18-C19
34	C	522	DGD	C9B-CAB-CBB-CCB
30	h	103	STE	C10-C11-C12-C13
31	M	101	LMG	O9-C10-O7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	C	515	STE	C5-C6-C7-C8
30	H	103	STE	C11-C12-C13-C14
31	D	407	LMG	C13-C14-C15-C16
32	F	102	SQD	C30-C31-C32-C33
32	f	101	SQD	C30-C31-C32-C33
33	a	614	LHG	C27-C28-C29-C30
26	b	610	CLA	C2A-CAA-CBA-CGA
26	C	511	CLA	O1D-CGD-O2D-CED
30	B	623	STE	C4-C5-C6-C7
30	e	104	STE	C13-C14-C15-C16
33	D	410	LHG	C27-C28-C29-C30
26	b	602	CLA	C10-C11-C12-C13
31	M	101	LMG	C31-C32-C33-C34
34	h	102	DGD	CDA-CEA-CFA-CGA
31	a	618	LMG	C31-C32-C33-C34
33	d	407	LHG	O1-C1-C2-O2
30	Z	101	STE	C11-C12-C13-C14
30	c	516	STE	C6-C7-C8-C9
30	m	103	STE	C2-C3-C4-C5
33	D	408	LHG	C34-C35-C36-C37
26	c	508	CLA	C1A-C2A-CAA-CBA
31	M	101	LMG	C28-C29-C30-C31
30	B	625	STE	C7-C8-C9-C10
30	d	406	STE	C4-C5-C6-C7
31	A	615	LMG	C14-C15-C16-C17
32	a	615	SQD	C31-C32-C33-C34
26	A	608	CLA	C8-C10-C11-C12
30	b	621	STE	C11-C12-C13-C14
31	M	101	LMG	C12-C13-C14-C15
26	B	604	CLA	C11-C10-C8-C7
26	B	606	CLA	C11-C12-C13-C15
26	B	613	CLA	C11-C10-C8-C7
26	B	613	CLA	C12-C13-C15-C16
26	B	615	CLA	C6-C7-C8-C10
26	C	506	CLA	C6-C7-C8-C10
26	C	506	CLA	C11-C12-C13-C15
26	C	506	CLA	C12-C13-C15-C16
26	a	610	CLA	C6-C7-C8-C10
26	b	601	CLA	C11-C10-C8-C7
26	b	602	CLA	C11-C10-C8-C7
26	b	608	CLA	C11-C12-C13-C15
26	b	615	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	c	510	CLA	C11-C10-C8-C7
26	c	513	CLA	C12-C13-C15-C16
26	d	403	CLA	C6-C7-C8-C10
30	A	621	STE	C9-C10-C11-C12
30	b	624	STE	C3-C4-C5-C6
26	c	506	CLA	C16-C17-C18-C20
26	A	607	CLA	C15-C16-C17-C18
34	H	101	DGD	O6E-C5E-C6E-O5E
26	B	615	CLA	C5-C6-C7-C8
26	C	505	CLA	C10-C11-C12-C13
34	C	521	DGD	C6A-C7A-C8A-C9A
31	m	101	LMG	C4-C5-C6-O5
29	d	405	PL9	C13-C14-C16-C17
30	i	101	STE	C2-C3-C4-C5
30	A	613	STE	C4-C5-C6-C7
26	B	605	CLA	C8-C10-C11-C12
26	c	503	CLA	C8-C10-C11-C12
26	A	608	CLA	C11-C10-C8-C9
26	B	601	CLA	C14-C13-C15-C16
26	B	604	CLA	C14-C13-C15-C16
26	B	606	CLA	C14-C13-C15-C16
26	C	506	CLA	C6-C7-C8-C9
26	C	506	CLA	C14-C13-C15-C16
26	C	513	CLA	C11-C10-C8-C9
26	a	610	CLA	C6-C7-C8-C9
26	b	614	CLA	C11-C12-C13-C14
30	e	105	STE	C5-C6-C7-C8
31	b	622	LMG	C33-C34-C35-C36
32	B	622	SQD	C10-C11-C12-C13
33	l	101	LHG	C14-C15-C16-C17
32	A	616	SQD	C11-C12-C13-C14
34	c	519	DGD	C4B-C5B-C6B-C7B
34	C	521	DGD	CDB-CEB-CFB-CGB
33	d	407	LHG	C26-C27-C28-C29
34	H	101	DGD	C3B-C4B-C5B-C6B
34	c	519	DGD	C2A-C3A-C4A-C5A
29	D	405	PL9	C47-C48-C49-C50
31	D	406	LMG	C2-C1-O1-C7
31	C	523	LMG	O1-C7-C8-C9
31	M	101	LMG	C7-C8-C9-O8
31	c	518	LMG	C7-C8-C9-O8
32	A	618	SQD	O6-C44-C45-C46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	B	622	SQD	O6-C44-C45-C46
32	a	615	SQD	O6-C44-C45-C46
32	a	615	SQD	C44-C45-C46-O48
34	A	619	DGD	O1G-C1G-C2G-C3G
31	C	523	LMG	C32-C33-C34-C35
33	D	410	LHG	C26-C27-C28-C29
30	m	102	STE	C3-C4-C5-C6
31	a	618	LMG	C21-C22-C23-C24
33	A	617	LHG	C24-C25-C26-C27
33	A	617	LHG	O2-C2-C3-O3
31	C	523	LMG	C17-C18-C19-C20
26	B	601	CLA	C16-C17-C18-C19
26	B	605	CLA	C16-C17-C18-C19
26	b	603	CLA	C16-C17-C18-C19
30	B	625	STE	C9-C10-C11-C12
30	D	411	STE	C5-C6-C7-C8
31	a	618	LMG	C20-C21-C22-C23
32	A	618	SQD	C18-C19-C20-C21
33	D	408	LHG	C15-C16-C17-C18
34	c	519	DGD	C4D-C5D-C6D-O5D
26	c	501	CLA	O1D-CGD-O2D-CED
30	C	525	STE	C11-C10-C9-C8
31	c	524	LMG	C38-C39-C40-C41
33	D	408	LHG	C26-C27-C28-C29
31	a	618	LMG	C13-C14-C15-C16
26	B	612	CLA	O1D-CGD-O2D-CED
26	c	512	CLA	C5-C6-C7-C8
30	T	102	STE	C11-C12-C13-C14
34	c	520	DGD	C8B-C9B-CAB-CBB
26	C	511	CLA	O1A-CGA-O2A-C1
30	Z	101	STE	C10-C11-C12-C13
33	D	410	LHG	C28-C29-C30-C31
26	C	507	CLA	C4-C3-C5-C6
26	C	506	CLA	C2-C3-C5-C6
26	B	616	CLA	C10-C11-C12-C13
30	K	104	STE	C9-C10-C11-C12
30	d	410	STE	C10-C11-C12-C13
31	C	523	LMG	C37-C38-C39-C40
31	c	522	LMG	O6-C5-C6-O5
31	c	523	LMG	O6-C5-C6-O5
34	c	521	DGD	O6D-C5D-C6D-O5D
26	a	610	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	b	624	STE	C6-C7-C8-C9
30	m	103	STE	C7-C8-C9-C10
31	c	523	LMG	C30-C31-C32-C33
31	D	407	LMG	O6-C5-C6-O5
30	B	623	STE	C7-C8-C9-C10
31	c	524	LMG	C33-C34-C35-C36
32	F	102	SQD	C33-C34-C35-C36
32	a	617	SQD	C9-C10-C11-C12
34	c	520	DGD	C8A-C9A-CAA-CBA
26	B	606	CLA	C5-C6-C7-C8
26	C	509	CLA	C10-C11-C12-C13
30	m	102	STE	C4-C5-C6-C7
31	D	407	LMG	C20-C21-C22-C23
31	c	524	LMG	C34-C35-C36-C37
30	C	525	STE	C12-C13-C14-C15
30	h	104	STE	C13-C14-C15-C16
31	C	523	LMG	C15-C16-C17-C18
32	A	616	SQD	C11-C10-C9-C8
31	a	618	LMG	C29-C28-O8-C9
30	I	101	STE	C11-C10-C9-C8
30	J	101	STE	C5-C6-C7-C8
32	B	622	SQD	C16-C17-C18-C19
32	a	617	SQD	C30-C31-C32-C33
26	c	511	CLA	C15-C16-C17-C18
30	e	103	STE	C14-C15-C16-C17
31	A	615	LMG	C36-C37-C38-C39
31	a	618	LMG	C36-C37-C38-C39
31	b	622	LMG	C31-C32-C33-C34
31	m	101	LMG	C17-C18-C19-C20
31	m	101	LMG	C20-C21-C22-C23
32	F	102	SQD	C34-C35-C36-C37
32	a	617	SQD	C24-C25-C26-C27
32	a	617	SQD	C33-C34-C35-C36
33	L	101	LHG	C28-C29-C30-C31
34	C	522	DGD	C3A-C4A-C5A-C6A
28	K	103	BCR	C9-C10-C11-C12
26	b	603	CLA	C16-C17-C18-C20
31	c	523	LMG	C14-C15-C16-C17
26	b	607	CLA	C3-C5-C6-C7
32	B	622	SQD	C11-C12-C13-C14
33	L	101	LHG	C31-C32-C33-C34
31	D	407	LMG	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	b	620	SQD	C17-C18-C19-C20
33	A	617	LHG	C9-C10-C11-C12
32	a	615	SQD	C25-C26-C27-C28
34	c	520	DGD	C7B-C8B-C9B-CAB
29	d	405	PL9	C47-C48-C49-C51
30	A	621	STE	C7-C8-C9-C10
30	b	625	STE	C2-C3-C4-C5
32	a	617	SQD	C34-C35-C36-C37
26	a	610	CLA	C4-C3-C5-C6
30	d	410	STE	C7-C8-C9-C10
32	a	615	SQD	C16-C17-C18-C19
33	D	408	LHG	C33-C34-C35-C36
33	d	407	LHG	C29-C30-C31-C32
34	C	521	DGD	CAB-CBB-CCB-CDB
34	c	519	DGD	CBA-CCA-CDA-CEA
26	b	607	CLA	C16-C17-C18-C20
31	M	101	LMG	C36-C37-C38-C39
31	b	622	LMG	C21-C22-C23-C24
31	b	622	LMG	C40-C41-C42-C43
32	F	102	SQD	C32-C33-C34-C35
33	d	407	LHG	C13-C14-C15-C16
34	A	619	DGD	C4A-C5A-C6A-C7A
34	C	522	DGD	C7A-C8A-C9A-CAA
32	a	615	SQD	O6-C44-C45-O47
32	a	615	SQD	O47-C45-C46-O48
32	f	101	SQD	O6-C44-C45-O47
33	D	409	LHG	C13-C14-C15-C16
30	C	519	STE	C9-C10-C11-C12
32	b	620	SQD	C30-C31-C32-C33
31	M	101	LMG	C37-C38-C39-C40
30	A	620	STE	C11-C12-C13-C14
30	C	525	STE	C3-C4-C5-C6
31	c	518	LMG	C12-C13-C14-C15
34	c	521	DGD	C4B-C5B-C6B-C7B
30	e	101	STE	C11-C12-C13-C14
33	L	101	LHG	C10-C11-C12-C13
30	a	619	STE	C1-C2-C3-C4
30	b	625	STE	C7-C8-C9-C10
34	c	521	DGD	CDA-CEA-CFA-CGA
30	b	621	STE	C5-C6-C7-C8
33	D	409	LHG	C33-C34-C35-C36
31	c	524	LMG	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	c	518	LMG	C33-C34-C35-C36
31	c	522	LMG	C17-C18-C19-C20
30	E	103	STE	C9-C10-C11-C12
31	m	101	LMG	C19-C20-C21-C22
31	A	615	LMG	C15-C16-C17-C18
31	c	522	LMG	C11-C12-C13-C14
31	c	522	LMG	C14-C15-C16-C17
30	M	103	STE	C7-C8-C9-C10
30	C	526	STE	C11-C10-C9-C8
30	c	517	STE	C1-C2-C3-C4
26	c	508	CLA	C8-C10-C11-C12
26	b	607	CLA	C16-C17-C18-C19
26	c	509	CLA	C4-C3-C5-C6
26	C	512	CLA	C8-C10-C11-C12
30	h	104	STE	C15-C16-C17-C18
32	a	615	SQD	C19-C20-C21-C22
30	A	620	STE	C13-C14-C15-C16
30	E	103	STE	C2-C3-C4-C5
32	F	102	SQD	C45-C44-O6-C1
26	B	601	CLA	C11-C10-C8-C9
26	B	612	CLA	C14-C13-C15-C16
26	B	613	CLA	C14-C13-C15-C16
26	B	614	CLA	C14-C13-C15-C16
26	C	506	CLA	C11-C12-C13-C14
26	a	610	CLA	C14-C13-C15-C16
26	b	602	CLA	C11-C10-C8-C9
26	b	604	CLA	C14-C13-C15-C16
26	b	607	CLA	C11-C12-C13-C14
26	b	608	CLA	C11-C12-C13-C14
26	b	614	CLA	C11-C10-C8-C9
26	b	615	CLA	C11-C12-C13-C14
26	c	512	CLA	C11-C12-C13-C14
26	c	513	CLA	C14-C13-C15-C16
26	d	403	CLA	C11-C12-C13-C14
33	A	617	LHG	C13-C14-C15-C16
34	A	619	DGD	C3B-C4B-C5B-C6B
33	a	614	LHG	C2-C3-O3-P
26	D	402	CLA	C4B-C3B-CAB-CBB
26	b	601	CLA	C4B-C3B-CAB-CBB
26	c	502	CLA	C4B-C3B-CAB-CBB
26	d	402	CLA	C4B-C3B-CAB-CBB
30	B	621	STE	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	B	623	STE	C11-C10-C9-C8
31	M	101	LMG	C29-C30-C31-C32
30	B	623	STE	C13-C14-C15-C16
26	c	510	CLA	O1D-CGD-O2D-CED
26	b	608	CLA	C13-C15-C16-C17
30	C	519	STE	C11-C10-C9-C8
34	c	520	DGD	C2E-C1E-O5D-C6D
26	B	612	CLA	C8-C10-C11-C12
30	C	515	STE	C6-C7-C8-C9
34	c	520	DGD	CAB-CBB-CCB-CDB
30	M	102	STE	C10-C11-C12-C13
31	C	516	LMG	C16-C17-C18-C19
31	D	406	LMG	C14-C15-C16-C17
33	a	614	LHG	C34-C35-C36-C37
26	A	608	CLA	C11-C10-C8-C7
26	A	608	CLA	C11-C12-C13-C15
26	B	601	CLA	C11-C10-C8-C7
26	B	601	CLA	C12-C13-C15-C16
26	B	604	CLA	C6-C7-C8-C10
26	B	608	CLA	C6-C7-C8-C10
26	B	612	CLA	C12-C13-C15-C16
26	B	614	CLA	C12-C13-C15-C16
26	C	502	CLA	C12-C13-C15-C16
26	C	513	CLA	C11-C10-C8-C7
26	D	403	CLA	C11-C12-C13-C15
26	a	610	CLA	C12-C13-C15-C16
26	b	602	CLA	C6-C7-C8-C10
26	b	604	CLA	C12-C13-C15-C16
26	b	606	CLA	C12-C13-C15-C16
26	b	614	CLA	C11-C12-C13-C15
26	c	507	CLA	C12-C13-C15-C16
26	c	509	CLA	C11-C12-C13-C15
26	c	512	CLA	C11-C12-C13-C15
26	d	402	CLA	C11-C12-C13-C15
26	d	403	CLA	C12-C13-C15-C16
26	b	614	CLA	C15-C16-C17-C18
31	b	622	LMG	C30-C31-C32-C33
32	A	616	SQD	C12-C13-C14-C15
33	b	623	LHG	C11-C10-C9-C8
33	l	101	LHG	C5-C6-O8-C23
30	I	102	STE	C10-C11-C12-C13
31	m	101	LMG	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	I	102	STE	C5-C6-C7-C8
33	D	410	LHG	C11-C12-C13-C14
26	B	601	CLA	C16-C17-C18-C20
26	b	604	CLA	C16-C17-C18-C19
30	b	624	STE	C11-C12-C13-C14
31	d	409	LMG	C35-C36-C37-C38
26	B	601	CLA	C3A-C2A-CAA-CBA
26	c	509	CLA	C3A-C2A-CAA-CBA
26	B	615	CLA	C10-C11-C12-C13
29	D	405	PL9	C43-C44-C46-C47
30	c	517	STE	C12-C13-C14-C15
33	L	101	LHG	C11-C10-C9-C8
26	b	601	CLA	C13-C15-C16-C17
30	M	103	STE	C6-C7-C8-C9
28	k	101	BCR	C19-C20-C21-C22
31	m	101	LMG	C14-C15-C16-C17
34	C	521	DGD	C5B-C6B-C7B-C8B
34	c	520	DGD	O6E-C5E-C6E-O5E
30	K	104	STE	C11-C10-C9-C8
31	M	101	LMG	C30-C31-C32-C33
32	A	618	SQD	C16-C17-C18-C19
33	D	410	LHG	C25-C26-C27-C28
34	C	520	DGD	C9A-CAA-CBA-CCA
26	C	513	CLA	C13-C15-C16-C17
30	i	101	STE	C3-C4-C5-C6
31	c	522	LMG	C16-C17-C18-C19
33	d	407	LHG	C18-C19-C20-C21
26	A	610	CLA	C6-C7-C8-C9
31	c	524	LMG	C15-C16-C17-C18
32	A	618	SQD	C13-C14-C15-C16
34	c	519	DGD	C6A-C7A-C8A-C9A
29	a	612	PL9	C24-C26-C27-C28
31	a	618	LMG	C7-C8-C9-O8
31	b	622	LMG	O1-C7-C8-C9
32	a	617	SQD	O6-C44-C45-C46
34	A	619	DGD	C1G-C2G-C3G-O3G
26	c	513	CLA	C3-C5-C6-C7
34	c	519	DGD	C9B-CAB-CBB-CCB
26	A	614	CLA	C16-C17-C18-C19
26	c	504	CLA	C11-C12-C13-C15
26	c	503	CLA	C15-C16-C17-C18
26	c	509	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	D	409	LHG	C35-C36-C37-C38
30	b	624	STE	C5-C6-C7-C8
30	d	406	STE	C10-C11-C12-C13
32	A	616	SQD	C27-C28-C29-C30
34	C	520	DGD	C7A-C8A-C9A-CAA
34	C	520	DGD	C5B-C6B-C7B-C8B
31	c	518	LMG	O1-C7-C8-C9
30	B	621	STE	C12-C13-C14-C15
30	I	102	STE	C9-C10-C11-C12
30	T	102	STE	C12-C13-C14-C15
30	e	103	STE	C13-C14-C15-C16
31	M	101	LMG	C19-C20-C21-C22
32	F	102	SQD	C29-C30-C31-C32
32	a	615	SQD	C17-C18-C19-C20
34	C	520	DGD	O6D-C5D-C6D-O5D
30	d	408	STE	C12-C13-C14-C15
29	d	405	PL9	C43-C44-C46-C47
31	D	407	LMG	C12-C13-C14-C15
26	c	511	CLA	CBD-CGD-O2D-CED
31	D	407	LMG	C22-C23-C24-C25
29	a	612	PL9	C37-C38-C39-C40
26	b	602	CLA	C16-C17-C18-C20
26	b	609	CLA	C16-C17-C18-C20
26	b	601	CLA	C2B-C3B-CAB-CBB
26	b	605	CLA	C2B-C3B-CAB-CBB
28	t	101	BCR	C5-C6-C7-C8
31	D	406	LMG	C32-C33-C34-C35
26	b	614	CLA	CBD-CGD-O2D-CED
30	m	103	STE	C4-C5-C6-C7
32	b	620	SQD	C13-C14-C15-C16
30	C	519	STE	C4-C5-C6-C7
30	z	101	STE	C4-C5-C6-C7
27	D	401	PHO	C16-C17-C18-C20
31	m	101	LMG	O7-C8-C9-O8
32	A	616	SQD	O6-C44-C45-O47
32	b	620	SQD	O47-C45-C46-O48
33	A	617	LHG	O7-C5-C6-O8
33	a	616	LHG	O7-C5-C6-O8
29	a	612	PL9	C4-C3-C7-C8
32	B	622	SQD	C9-C10-C11-C12
33	a	616	LHG	C11-C10-C9-C8
31	a	618	LMG	O10-C28-O8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	D	405	PL9	C15-C14-C16-C17
30	b	621	STE	C13-C14-C15-C16
26	c	509	CLA	C2-C3-C5-C6
29	D	405	PL9	C13-C14-C16-C17
29	D	405	PL9	C28-C29-C31-C32
29	a	612	PL9	C43-C44-C46-C47
31	M	101	LMG	C14-C15-C16-C17
26	c	505	CLA	C16-C17-C18-C20
32	a	617	SQD	C25-C26-C27-C28
32	A	618	SQD	C23-C24-C25-C26
31	m	101	LMG	C30-C31-C32-C33
26	B	604	CLA	C6-C7-C8-C9
26	B	605	CLA	C11-C10-C8-C9
26	B	614	CLA	C6-C7-C8-C9
26	C	505	CLA	C14-C13-C15-C16
26	C	507	CLA	C14-C13-C15-C16
26	D	403	CLA	C11-C12-C13-C14
26	c	504	CLA	C11-C10-C8-C9
26	d	403	CLA	C14-C13-C15-C16
30	C	525	STE	C6-C7-C8-C9
26	C	505	CLA	C8-C10-C11-C12
30	C	525	STE	C11-C12-C13-C14
33	D	408	LHG	C11-C10-C9-C8
33	d	407	LHG	C12-C13-C14-C15
26	A	608	CLA	C16-C17-C18-C20
26	c	504	CLA	C11-C12-C13-C14
26	c	506	CLA	C16-C17-C18-C19
26	c	510	CLA	C16-C17-C18-C19
30	B	623	STE	C9-C10-C11-C12
30	M	102	STE	C5-C6-C7-C8
30	H	102	STE	C1-C2-C3-C4
30	B	624	STE	C6-C7-C8-C9
29	A	612	PL9	C19-C21-C22-C23
30	C	515	STE	C7-C8-C9-C10
31	B	620	LMG	C18-C19-C20-C21
32	a	617	SQD	C14-C15-C16-C17
31	b	622	LMG	C37-C38-C39-C40
34	h	102	DGD	CAB-CBB-CCB-CDB
26	d	403	CLA	C13-C15-C16-C17
34	h	102	DGD	C7B-C8B-C9B-CAB
26	c	509	CLA	CAA-CBA-CGA-O2A
30	H	103	STE	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	C	521	DGD	CDA-CEA-CFA-CGA
34	c	520	DGD	CDB-CEB-CFB-CGB
26	B	607	CLA	C16-C17-C18-C19
26	C	501	CLA	C16-C17-C18-C20
31	b	622	LMG	C22-C23-C24-C25
30	h	103	STE	C11-C12-C13-C14
30	j	101	STE	C5-C6-C7-C8
34	c	519	DGD	CBB-CCB-CDB-CEB
26	C	513	CLA	C8-C10-C11-C12
26	b	603	CLA	C10-C11-C12-C13
26	c	505	CLA	C15-C16-C17-C18
30	A	621	STE	C14-C15-C16-C17
30	d	410	STE	C11-C12-C13-C14
31	A	615	LMG	C16-C17-C18-C19
32	a	617	SQD	C10-C11-C12-C13
33	l	101	LHG	C28-C29-C30-C31
30	E	103	STE	C4-C5-C6-C7
33	D	408	LHG	C9-C10-C11-C12
33	D	409	LHG	C25-C26-C27-C28
26	a	607	CLA	C2C-C3C-CAC-CBC
26	c	511	CLA	C8-C10-C11-C12
34	H	101	DGD	CAB-CBB-CCB-CDB
26	B	601	CLA	C6-C7-C8-C10
26	B	602	CLA	C11-C12-C13-C15
26	B	604	CLA	C12-C13-C15-C16
26	B	605	CLA	C11-C10-C8-C7
26	B	613	CLA	C11-C12-C13-C15
26	B	615	CLA	C12-C13-C15-C16
26	C	505	CLA	C6-C7-C8-C10
26	C	505	CLA	C12-C13-C15-C16
26	C	509	CLA	C12-C13-C15-C16
26	C	512	CLA	C11-C10-C8-C7
26	b	601	CLA	C6-C7-C8-C10
26	b	603	CLA	C11-C12-C13-C15
26	b	607	CLA	C11-C12-C13-C15
26	b	608	CLA	C11-C10-C8-C7
30	B	623	STE	C12-C13-C14-C15
30	d	410	STE	C4-C5-C6-C7
34	c	521	DGD	CBB-CCB-CDB-CEB
28	X	101	BCR	C7-C8-C9-C10
31	a	618	LMG	C8-C7-O1-C1
34	c	520	DGD	C2G-C3G-O3G-C1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	B	625	STE	C2-C3-C4-C5
26	c	502	CLA	C13-C15-C16-C17
26	B	610	CLA	C2A-CAA-CBA-CGA
30	j	102	STE	C7-C8-C9-C10
31	M	101	LMG	C18-C19-C20-C21
33	D	408	LHG	O1-C1-C2-C3
30	T	102	STE	C13-C14-C15-C16
33	L	101	LHG	C30-C31-C32-C33
26	B	604	CLA	O2A-C1-C2-C3
31	A	615	LMG	C9-C8-O7-C10
31	a	618	LMG	C33-C34-C35-C36
32	a	617	SQD	C11-C10-C9-C8
26	B	610	CLA	C16-C17-C18-C19
34	h	102	DGD	O2G-C1B-C2B-C3B
33	b	623	LHG	C26-C27-C28-C29
30	C	515	STE	C9-C10-C11-C12
31	C	523	LMG	O6-C1-O1-C7
31	C	516	LMG	C7-C8-C9-O8
31	m	101	LMG	C7-C8-C9-O8
33	A	617	LHG	C4-C5-C6-O8
33	a	616	LHG	C4-C5-C6-O8
31	m	101	LMG	C11-C10-O7-C8
35	F	101	HEM	C4C-C3C-CAC-CBC
35	e	102	HEM	C4B-C3B-CAB-CBB
35	e	102	HEM	C4C-C3C-CAC-CBC
26	b	608	CLA	C16-C17-C18-C19
31	D	406	LMG	C33-C34-C35-C36
31	c	518	LMG	C11-C12-C13-C14
26	b	605	CLA	C10-C11-C12-C13
34	C	520	DGD	C4D-C5D-C6D-O5D
26	B	610	CLA	C15-C16-C17-C18
26	C	506	CLA	C13-C15-C16-C17
34	A	619	DGD	CAB-CBB-CCB-CDB
31	c	522	LMG	C29-C30-C31-C32
26	b	614	CLA	O1D-CGD-O2D-CED
31	C	523	LMG	O1-C7-C8-O7
31	M	101	LMG	O7-C8-C9-O8
31	c	523	LMG	O7-C8-C9-O8
26	A	614	CLA	C13-C15-C16-C17
26	B	601	CLA	C6-C7-C8-C9
26	b	608	CLA	C11-C10-C8-C9
26	c	504	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	c	511	CLA	C11-C10-C8-C9
30	A	621	STE	C12-C13-C14-C15
33	b	623	LHG	C25-C26-C27-C28
30	B	624	STE	C4-C5-C6-C7
30	M	103	STE	C5-C6-C7-C8
31	b	622	LMG	C11-C12-C13-C14
32	f	101	SQD	C33-C34-C35-C36
34	C	520	DGD	C5A-C6A-C7A-C8A
30	E	102	STE	C14-C15-C16-C17
31	B	620	LMG	C17-C18-C19-C20
31	D	406	LMG	C18-C19-C20-C21
33	A	617	LHG	C31-C32-C33-C34
33	L	101	LHG	C15-C16-C17-C18
33	D	408	LHG	C16-C17-C18-C19
34	C	521	DGD	C1B-C2B-C3B-C4B
30	M	104	STE	C14-C15-C16-C17
33	D	410	LHG	C11-C10-C9-C8
26	B	613	CLA	C5-C6-C7-C8
30	C	525	STE	C15-C16-C17-C18
26	C	510	CLA	C10-C11-C12-C13
29	a	612	PL9	C20-C19-C21-C22
30	K	104	STE	C14-C15-C16-C17
30	c	517	STE	C10-C11-C12-C13
31	C	523	LMG	C38-C39-C40-C41
33	A	617	LHG	C19-C20-C21-C22
30	j	102	STE	C5-C6-C7-C8
26	B	610	CLA	C16-C17-C18-C20
26	d	402	CLA	C16-C17-C18-C20
27	D	401	PHO	C16-C17-C18-C19
33	D	410	LHG	C13-C14-C15-C16
30	K	104	STE	C13-C14-C15-C16
30	a	619	STE	C4-C5-C6-C7
26	b	607	CLA	CBD-CGD-O2D-CED
31	B	620	LMG	C11-C10-O7-C8
34	c	520	DGD	C4A-C5A-C6A-C7A
31	A	615	LMG	C12-C13-C14-C15
26	b	610	CLA	C15-C16-C17-C18
26	c	510	CLA	C10-C11-C12-C13
26	B	601	CLA	C4B-C3B-CAB-CBB
26	b	601	CLA	C1A-C2A-CAA-CBA
26	c	512	CLA	C1A-C2A-CAA-CBA
26	c	513	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	a	619	STE	C7-C8-C9-C10
26	b	609	CLA	C4-C3-C5-C6
29	D	405	PL9	C30-C29-C31-C32
30	M	104	STE	C12-C13-C14-C15
30	d	408	STE	C11-C10-C9-C8
33	A	617	LHG	C25-C26-C27-C28
29	a	612	PL9	C18-C19-C21-C22
31	c	524	LMG	O6-C5-C6-O5
31	m	101	LMG	C31-C32-C33-C34
33	d	407	LHG	C14-C15-C16-C17
30	k	103	STE	C9-C10-C11-C12
33	D	408	LHG	C19-C20-C21-C22
26	c	502	CLA	C3-C5-C6-C7
31	c	523	LMG	C11-C12-C13-C14
31	c	524	LMG	C12-C13-C14-C15
31	m	101	LMG	O9-C10-O7-C8
32	a	615	SQD	C10-C11-C12-C13
32	b	620	SQD	C5-C6-S-O7
31	c	524	LMG	C20-C21-C22-C23
26	B	602	CLA	C13-C15-C16-C17
30	M	102	STE	C4-C5-C6-C7
26	B	605	CLA	C6-C7-C8-C10
26	C	507	CLA	C11-C12-C13-C15
26	C	510	CLA	C11-C10-C8-C7
26	a	608	CLA	C11-C12-C13-C15
26	b	605	CLA	C11-C10-C8-C7
26	b	616	CLA	C6-C7-C8-C10
26	b	616	CLA	C11-C10-C8-C7
26	c	501	CLA	C11-C12-C13-C15
26	c	504	CLA	C11-C10-C8-C7
26	c	513	CLA	C11-C12-C13-C15
33	a	614	LHG	C29-C30-C31-C32
26	c	502	CLA	C16-C17-C18-C20
26	c	509	CLA	C16-C17-C18-C19
31	C	516	LMG	C15-C16-C17-C18
31	D	406	LMG	C37-C38-C39-C40
30	C	526	STE	C6-C7-C8-C9
33	l	101	LHG	C18-C19-C20-C21
33	D	410	LHG	C23-C24-C25-C26
33	D	409	LHG	C2-C3-O3-P
26	C	507	CLA	C2-C3-C5-C6
31	B	620	LMG	O9-C10-O7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	B	608	CLA	C6-C7-C8-C9
26	C	509	CLA	C14-C13-C15-C16
26	b	613	CLA	C6-C7-C8-C9
26	c	506	CLA	C14-C13-C15-C16
31	a	618	LMG	C29-C30-C31-C32
30	J	101	STE	C7-C8-C9-C10
26	c	511	CLA	O1D-CGD-O2D-CED
31	A	615	LMG	O1-C7-C8-O7
31	C	516	LMG	O7-C8-C9-O8
31	M	101	LMG	O1-C7-C8-O7
31	b	622	LMG	O1-C7-C8-O7
31	c	518	LMG	O7-C8-C9-O8
31	m	101	LMG	O1-C7-C8-O7
33	A	617	LHG	C1-C2-C3-O3
26	B	604	CLA	C10-C11-C12-C13
31	M	101	LMG	O1-C7-C8-C9
31	c	523	LMG	C7-C8-C9-O8
32	b	620	SQD	C44-C45-C46-O48
33	d	407	LHG	C19-C20-C21-C22
26	A	610	CLA	C3-C5-C6-C7
26	B	601	CLA	CAD-CBD-CGD-O2D
26	B	607	CLA	CAD-CBD-CGD-O2D
26	B	614	CLA	CAD-CBD-CGD-O2D
26	C	502	CLA	CAD-CBD-CGD-O2D
26	c	502	CLA	CAD-CBD-CGD-O2D
30	c	517	STE	C14-C15-C16-C17
30	j	101	STE	C2-C3-C4-C5
30	e	104	STE	C11-C12-C13-C14
32	A	616	SQD	C24-C25-C26-C27
26	a	608	CLA	C13-C15-C16-C17
30	z	101	STE	C3-C4-C5-C6
26	a	613	CLA	C16-C17-C18-C20
26	d	402	CLA	C16-C17-C18-C19
26	c	509	CLA	C2A-CAA-CBA-CGA
30	d	406	STE	C5-C6-C7-C8
30	e	105	STE	C6-C7-C8-C9
34	C	520	DGD	CAB-CBB-CCB-CDB
30	C	524	STE	C3-C4-C5-C6
34	h	102	DGD	C6A-C7A-C8A-C9A
30	t	102	STE	C6-C7-C8-C9
26	B	601	CLA	CAD-CBD-CGD-O1D
26	B	614	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	C	502	CLA	CAD-CBD-CGD-O1D
26	C	506	CLA	CAD-CBD-CGD-O1D
26	c	502	CLA	CAD-CBD-CGD-O1D
26	c	507	CLA	CHA-CBD-CGD-O1D
26	c	509	CLA	CHA-CBD-CGD-O2D
33	L	101	LHG	C4-O6-P-O3
33	a	616	LHG	C3-O3-P-O4
33	b	623	LHG	C18-C19-C20-C21
31	c	523	LMG	C37-C38-C39-C40
26	B	601	CLA	C4-C3-C5-C6
26	a	610	CLA	C2-C3-C5-C6
34	H	101	DGD	C4B-C5B-C6B-C7B
31	c	523	LMG	C28-C29-C30-C31
28	d	404	BCR	C36-C18-C19-C20
31	c	524	LMG	C40-C41-C42-C43
30	d	406	STE	C2-C3-C4-C5
26	B	613	CLA	C16-C17-C18-C19
26	b	612	CLA	C16-C17-C18-C20
30	C	518	STE	C2-C3-C4-C5
34	C	520	DGD	CCB-CDB-CEB-CFB
33	b	623	LHG	C28-C29-C30-C31
32	F	102	SQD	C25-C26-C27-C28
30	m	103	STE	C12-C13-C14-C15
34	C	520	DGD	C2B-C3B-C4B-C5B
30	E	103	STE	C15-C16-C17-C18
33	a	614	LHG	C33-C34-C35-C36
31	D	406	LMG	C7-C8-O7-C10
30	I	101	STE	C11-C12-C13-C14
31	D	406	LMG	O8-C28-C29-C30
34	c	519	DGD	C1B-C2B-C3B-C4B
32	a	615	SQD	C28-C29-C30-C31
30	B	625	STE	C12-C13-C14-C15
26	A	608	CLA	C16-C17-C18-C19
26	a	613	CLA	C16-C17-C18-C19
26	d	403	CLA	C8-C10-C11-C12
26	b	614	CLA	CBA-CGA-O2A-C1
26	b	614	CLA	O1A-CGA-O2A-C1
30	c	517	STE	C5-C6-C7-C8
26	A	608	CLA	C11-C12-C13-C14
26	B	602	CLA	C11-C12-C13-C14
26	C	502	CLA	C14-C13-C15-C16
26	C	505	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	C	510	CLA	C11-C10-C8-C9
26	b	604	CLA	C11-C12-C13-C14
26	b	614	CLA	C14-C13-C15-C16
26	c	507	CLA	C14-C13-C15-C16
26	c	512	CLA	C6-C7-C8-C9
26	d	402	CLA	C11-C12-C13-C14
26	B	609	CLA	C11-C12-C13-C15
26	b	604	CLA	C11-C12-C13-C15
32	b	620	SQD	C11-C12-C13-C14
31	c	523	LMG	O6-C1-O1-C7
26	b	609	CLA	C16-C17-C18-C19
32	b	620	SQD	C29-C30-C31-C32
34	A	619	DGD	C7A-C8A-C9A-CAA
34	H	101	DGD	C9A-CAA-CBA-CCA
34	C	521	DGD	CCA-CDA-CEA-CFA
31	m	101	LMG	C2-C1-O1-C7
26	c	512	CLA	C4-C3-C5-C6
33	D	409	LHG	C17-C18-C19-C20
26	A	607	CLA	C2C-C3C-CAC-CBC
26	B	613	CLA	C16-C17-C18-C20
31	D	406	LMG	C15-C16-C17-C18
31	c	524	LMG	C11-C12-C13-C14
34	A	619	DGD	O1G-C1G-C2G-O2G
26	B	602	CLA	C15-C16-C17-C18
33	l	101	LHG	C30-C31-C32-C33
28	B	618	BCR	C15-C16-C17-C18
33	l	101	LHG	C19-C20-C21-C22
26	b	611	CLA	C16-C17-C18-C20
26	c	502	CLA	C16-C17-C18-C19
26	c	506	CLA	C8-C10-C11-C12
31	c	523	LMG	C34-C35-C36-C37
32	a	615	SQD	C35-C36-C37-C38
34	h	102	DGD	C4A-C5A-C6A-C7A
26	c	507	CLA	C2-C1-O2A-CGA
29	D	405	PL9	C45-C44-C46-C47
26	B	604	CLA	C16-C17-C18-C20
32	F	102	SQD	O48-C23-C24-C25
31	m	101	LMG	O1-C7-C8-C9
32	f	101	SQD	O6-C44-C45-C46
31	M	101	LMG	C15-C16-C17-C18
34	c	519	DGD	C2B-C3B-C4B-C5B
26	b	609	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	K	103	BCR	C19-C20-C21-C22
28	X	101	BCR	C9-C10-C11-C12
26	b	612	CLA	C16-C17-C18-C19
34	c	520	DGD	O6E-C1E-O5D-C6D
26	b	604	CLA	C10-C11-C12-C13
26	b	609	CLA	C2-C3-C5-C6
30	j	101	STE	C4-C5-C6-C7
30	E	102	STE	C9-C10-C11-C12
26	B	609	CLA	C11-C12-C13-C14
26	c	501	CLA	C11-C12-C13-C14
26	c	508	CLA	C11-C10-C8-C9
26	C	502	CLA	C4B-C3B-CAB-CBB
32	a	615	SQD	C34-C35-C36-C37
26	b	608	CLA	C16-C17-C18-C20
26	b	613	CLA	C16-C17-C18-C19
33	L	101	LHG	C24-C25-C26-C27
34	C	520	DGD	C4E-C5E-C6E-O5E
26	c	501	CLA	C2A-CAA-CBA-CGA
26	c	506	CLA	C4-C3-C5-C6
34	h	102	DGD	CDB-CEB-CFB-CGB
30	i	102	STE	C11-C10-C9-C8
26	b	601	CLA	C8-C10-C11-C12
31	M	101	LMG	C17-C18-C19-C20
30	A	613	STE	C6-C7-C8-C9
30	B	623	STE	C2-C3-C4-C5
34	C	522	DGD	C5A-C6A-C7A-C8A
31	A	615	LMG	C18-C19-C20-C21
26	C	507	CLA	C11-C10-C8-C7
26	b	614	CLA	C5-C6-C7-C8
33	a	616	LHG	C17-C18-C19-C20
33	L	101	LHG	C5-C6-O8-C23
30	d	406	STE	C6-C7-C8-C9
33	a	616	LHG	C14-C15-C16-C17
29	d	405	PL9	C42-C43-C44-C45
26	c	512	CLA	C3A-C2A-CAA-CBA
26	A	607	CLA	C4C-C3C-CAC-CBC
30	E	103	STE	C3-C4-C5-C6
32	b	620	SQD	C18-C19-C20-C21
30	b	621	STE	C12-C13-C14-C15
34	H	101	DGD	C7A-C8A-C9A-CAA
26	C	503	CLA	C15-C16-C17-C18
30	b	621	STE	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	D	411	STE	O2-C1-C2-C3
33	D	409	LHG	C9-C10-C11-C12
30	b	621	STE	C9-C10-C11-C12
33	D	409	LHG	C12-C13-C14-C15
35	e	102	HEM	CAD-CBD-CGD-O2D
26	b	611	CLA	C13-C15-C16-C17
28	d	404	BCR	C17-C18-C19-C20
30	D	411	STE	C11-C12-C13-C14
26	B	601	CLA	C2-C3-C5-C6
31	c	523	LMG	C36-C37-C38-C39
35	e	102	HEM	CAD-CBD-CGD-O1D
36	V	201	HEC	CAD-CBD-CGD-O2D
26	a	607	CLA	C4C-C3C-CAC-CBC
32	A	616	SQD	O6-C44-C45-C46
30	Z	101	STE	C5-C6-C7-C8
30	Z	101	STE	C6-C7-C8-C9
30	t	102	STE	C5-C6-C7-C8
30	b	625	STE	C5-C6-C7-C8
26	B	608	CLA	C11-C12-C13-C14
26	B	614	CLA	C11-C12-C13-C14
26	C	502	CLA	C6-C7-C8-C9
26	C	507	CLA	C11-C10-C8-C9
26	b	607	CLA	C14-C13-C15-C16
26	b	609	CLA	C6-C7-C8-C9
30	c	517	STE	C2-C3-C4-C5
32	B	622	SQD	C31-C32-C33-C34
32	B	622	SQD	C46-C45-O47-C7
26	C	506	CLA	C8-C10-C11-C12
30	C	525	STE	C10-C11-C12-C13
26	A	614	CLA	C3-C5-C6-C7
26	B	616	CLA	C3-C5-C6-C7
26	B	603	CLA	C16-C17-C18-C20
34	H	101	DGD	O2G-C1B-C2B-C3B
26	c	512	CLA	C2-C3-C5-C6
33	l	101	LHG	C9-C10-C11-C12
30	I	101	STE	O2-C1-C2-C3
30	a	620	STE	O1-C1-C2-C3
30	h	103	STE	C13-C14-C15-C16
32	A	618	SQD	C19-C20-C21-C22
36	v	201	HEC	C2B-C3B-CAB-CBB
34	C	520	DGD	C3B-C4B-C5B-C6B
26	B	601	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	B	609	CLA	C2B-C3B-CAB-CBB
26	C	502	CLA	C2B-C3B-CAB-CBB
26	c	502	CLA	C2B-C3B-CAB-CBB
26	d	402	CLA	C2B-C3B-CAB-CBB
33	D	409	LHG	C24-C25-C26-C27
33	D	409	LHG	C27-C28-C29-C30
30	J	101	STE	O2-C1-C2-C3
30	k	103	STE	O1-C1-C2-C3
30	C	519	STE	C6-C7-C8-C9
30	e	101	STE	C15-C16-C17-C18
34	H	101	DGD	CBB-CCB-CDB-CEB
30	I	101	STE	O1-C1-C2-C3
30	d	408	STE	O1-C1-C2-C3
26	B	603	CLA	C11-C10-C8-C7
26	B	616	CLA	C6-C7-C8-C10
26	c	503	CLA	C11-C10-C8-C7
26	c	509	CLA	C11-C10-C8-C7
26	d	402	CLA	C6-C7-C8-C10
26	b	613	CLA	C15-C16-C17-C18
31	C	516	LMG	O1-C7-C8-O7
30	J	101	STE	O1-C1-C2-C3
30	d	408	STE	O2-C1-C2-C3
30	i	101	STE	O1-C1-C2-C3
32	f	101	SQD	C24-C25-C26-C27
33	b	623	LHG	C16-C17-C18-C19
26	c	508	CLA	C16-C17-C18-C19
32	a	617	SQD	C26-C27-C28-C29
26	B	612	CLA	C13-C15-C16-C17
26	b	602	CLA	C13-C15-C16-C17
26	b	615	CLA	O1D-CGD-O2D-CED
29	A	612	PL9	C15-C14-C16-C17
26	c	506	CLA	C5-C6-C7-C8
34	A	619	DGD	CFB-CGB-CHB-CIB
34	h	102	DGD	CCA-CDA-CEA-CFA
26	B	613	CLA	C2-C1-O2A-CGA
26	C	504	CLA	C11-C12-C13-C14
33	d	407	LHG	C28-C29-C30-C31
34	C	520	DGD	CAA-CBA-CCA-CDA
31	b	622	LMG	C24-C25-C26-C27
30	D	411	STE	O1-C1-C2-C3
26	B	611	CLA	C14-C13-C15-C16
26	c	509	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	c	510	CLA	C14-C13-C15-C16
26	D	403	CLA	C5-C6-C7-C8
26	b	616	CLA	C10-C11-C12-C13
30	a	620	STE	C3-C4-C5-C6
33	A	617	LHG	C34-C35-C36-C37
26	B	604	CLA	C16-C17-C18-C19
30	a	620	STE	O2-C1-C2-C3
30	i	101	STE	O2-C1-C2-C3
31	B	620	LMG	C32-C33-C34-C35
34	c	520	DGD	C5B-C6B-C7B-C8B
26	D	402	CLA	C15-C16-C17-C18
31	a	618	LMG	C42-C43-C44-C45
26	B	603	CLA	C16-C17-C18-C19
36	V	201	HEC	CAD-CBD-CGD-O1D
33	a	616	LHG	C23-C24-C25-C26
30	j	102	STE	C11-C10-C9-C8
29	A	612	PL9	C9-C11-C12-C13
31	b	622	LMG	C7-C8-C9-O8
30	k	103	STE	O2-C1-C2-C3
35	e	102	HEM	CAA-CBA-CGA-O2A
26	B	607	CLA	O1A-CGA-O2A-C1
30	C	515	STE	C11-C10-C9-C8
33	D	410	LHG	C9-C10-C11-C12
33	a	616	LHG	O6-C4-C5-O7
30	C	526	STE	C5-C6-C7-C8
26	C	505	CLA	C2C-C3C-CAC-CBC
30	A	622	STE	C10-C11-C12-C13
32	B	622	SQD	C45-C46-O48-C23
31	D	407	LMG	C11-C12-C13-C14
26	B	609	CLA	C4B-C3B-CAB-CBB
26	b	604	CLA	C4B-C3B-CAB-CBB
26	c	502	CLA	O1A-CGA-O2A-C1
34	C	522	DGD	CCB-CDB-CEB-CFB
33	D	409	LHG	C32-C33-C34-C35
30	c	516	STE	C9-C10-C11-C12
27	A	609	PHO	CHA-CBD-CGD-O1D
30	C	519	STE	C3-C4-C5-C6
26	C	502	CLA	O1A-CGA-O2A-C1
26	b	616	CLA	O1A-CGA-O2A-C1
31	m	101	LMG	O6-C5-C6-O5
34	c	519	DGD	O6E-C1E-O5D-C6D
26	b	612	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	a	616	LHG	C2-C3-O3-P
26	B	608	CLA	C11-C12-C13-C15
26	b	603	CLA	C11-C10-C8-C7
26	c	506	CLA	C6-C7-C8-C10
26	c	507	CLA	C11-C10-C8-C7
31	D	407	LMG	C40-C41-C42-C43
30	d	408	STE	C6-C7-C8-C9
30	m	103	STE	C10-C11-C12-C13
32	f	101	SQD	C32-C33-C34-C35
34	c	521	DGD	CBA-CCA-CDA-CEA
31	A	615	LMG	C11-C12-C13-C14
33	d	407	LHG	C9-C10-C11-C12
31	a	618	LMG	C32-C33-C34-C35
35	e	102	HEM	CAA-CBA-CGA-O1A
26	A	608	CLA	C14-C13-C15-C16
26	C	508	CLA	C11-C10-C8-C9
26	b	603	CLA	C11-C10-C8-C9
26	c	505	CLA	C11-C12-C13-C14
26	c	506	CLA	C6-C7-C8-C9
30	j	102	STE	C9-C10-C11-C12
30	h	104	STE	C9-C10-C11-C12
32	a	617	SQD	C5-C6-S-O8
33	D	409	LHG	C11-C12-C13-C14
26	C	501	CLA	C2A-CAA-CBA-CGA
26	D	402	CLA	C2-C1-O2A-CGA
26	B	609	CLA	C16-C17-C18-C19
26	b	610	CLA	C16-C17-C18-C20
31	C	523	LMG	C19-C20-C21-C22
31	c	522	LMG	C29-C28-O8-C9
29	d	405	PL9	C33-C34-C36-C37
30	Z	101	STE	C2-C3-C4-C5
31	a	618	LMG	C30-C31-C32-C33
31	b	622	LMG	C35-C36-C37-C38
32	b	620	SQD	O48-C23-C24-C25
34	c	519	DGD	C2E-C1E-O5D-C6D
31	a	618	LMG	C9-C8-O7-C10
32	B	622	SQD	C44-C45-O47-C7
34	A	619	DGD	C3G-C2G-O2G-C1B
26	b	611	CLA	C16-C17-C18-C19
26	c	509	CLA	C16-C17-C18-C20
27	d	401	PHO	C8-C10-C11-C12
34	c	519	DGD	C4A-C5A-C6A-C7A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	A	617	LHG	C17-C18-C19-C20
31	c	522	LMG	O10-C28-O8-C9
31	A	615	LMG	C31-C32-C33-C34
26	c	502	CLA	C15-C16-C17-C18
26	B	607	CLA	CBA-CGA-O2A-C1
26	C	502	CLA	CBA-CGA-O2A-C1
34	C	520	DGD	C2A-C1A-O1G-C1G
31	A	615	LMG	O1-C7-C8-C9
34	C	520	DGD	C4A-C5A-C6A-C7A
31	c	523	LMG	C32-C33-C34-C35
26	c	502	CLA	CBA-CGA-O2A-C1
26	b	612	CLA	CAA-CBA-CGA-O2A
30	I	102	STE	C4-C5-C6-C7
30	j	101	STE	C7-C8-C9-C10
34	A	619	DGD	CDA-CEA-CFA-CGA
30	e	105	STE	O2-C1-C2-C3
31	A	615	LMG	O7-C8-C9-O8
30	d	406	STE	O1-C1-C2-C3
36	v	201	HEC	CAD-CBD-CGD-O1D
26	D	403	CLA	C10-C11-C12-C13
26	C	507	CLA	C11-C12-C13-C14
26	C	512	CLA	C11-C12-C13-C14
26	b	605	CLA	C11-C12-C13-C14
26	c	503	CLA	C11-C10-C8-C9
27	A	609	PHO	C6-C7-C8-C9
33	d	407	LHG	O9-C7-O7-C5
33	a	616	LHG	C28-C29-C30-C31
34	C	520	DGD	C8B-C9B-CAB-CBB
33	b	623	LHG	C15-C16-C17-C18
30	d	408	STE	C3-C4-C5-C6
30	m	103	STE	C14-C15-C16-C17
30	d	406	STE	O2-C1-C2-C3
36	v	201	HEC	CAD-CBD-CGD-O2D
32	B	622	SQD	C29-C30-C31-C32
26	B	611	CLA	C11-C10-C8-C7
26	C	503	CLA	C11-C10-C8-C7
26	b	607	CLA	C11-C10-C8-C7
26	b	614	CLA	C6-C7-C8-C10
26	c	502	CLA	C11-C10-C8-C7
26	c	506	CLA	C11-C10-C8-C7
26	c	511	CLA	C12-C13-C15-C16
26	D	402	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	b	604	CLA	C2B-C3B-CAB-CBB
26	b	610	CLA	C2B-C3B-CAB-CBB
28	K	101	BCR	C23-C24-C25-C26
28	a	611	BCR	C5-C6-C7-C8
28	a	611	BCR	C23-C24-C25-C26
31	c	518	LMG	O8-C28-C29-C30
30	T	102	STE	C3-C4-C5-C6
34	H	101	DGD	C6B-C7B-C8B-C9B
26	c	509	CLA	CAA-CBA-CGA-O1A
29	d	405	PL9	C34-C36-C37-C38
26	b	607	CLA	O1D-CGD-O2D-CED
34	c	521	DGD	C8B-C9B-CAB-CBB
33	d	407	LHG	C8-C7-O7-C5
26	c	510	CLA	C15-C16-C17-C18
26	c	510	CLA	CAA-CBA-CGA-O2A
33	D	408	LHG	C28-C29-C30-C31
33	D	409	LHG	C30-C31-C32-C33
30	d	408	STE	C4-C5-C6-C7
26	c	513	CLA	C4-C3-C5-C6
32	A	618	SQD	C7-C8-C9-C10
30	j	102	STE	C3-C4-C5-C6
26	c	510	CLA	C2-C3-C5-C6
29	D	405	PL9	C38-C39-C41-C42
30	e	105	STE	C2-C3-C4-C5
30	C	526	STE	C12-C13-C14-C15
33	d	407	LHG	C11-C12-C13-C14
30	I	102	STE	O2-C1-C2-C3
35	F	101	HEM	CAD-CBD-CGD-O1D
34	C	521	DGD	CBB-CCB-CDB-CEB
31	a	618	LMG	C37-C38-C39-C40
26	b	601	CLA	C6-C7-C8-C9
26	d	402	CLA	C6-C7-C8-C9
30	Z	101	STE	C7-C8-C9-C10
34	h	102	DGD	C4B-C5B-C6B-C7B
33	l	101	LHG	O7-C7-C8-C9
31	A	615	LMG	C7-C8-C9-O8
26	B	602	CLA	C1A-C2A-CAA-CBA
26	C	502	CLA	C1A-C2A-CAA-CBA
26	C	511	CLA	C1A-C2A-CAA-CBA
26	c	509	CLA	C1A-C2A-CAA-CBA
29	a	612	PL9	C45-C44-C46-C47
26	B	613	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	F	101	HEM	CAD-CBD-CGD-O2D
33	d	407	LHG	C30-C31-C32-C33
26	b	616	CLA	CBA-CGA-O2A-C1
33	D	410	LHG	C10-C11-C12-C13
34	h	102	DGD	C2A-C3A-C4A-C5A
32	A	616	SQD	O47-C7-C8-C9
32	A	618	SQD	O48-C23-C24-C25
33	l	101	LHG	C24-C25-C26-C27
26	b	614	CLA	C2A-CAA-CBA-CGA
26	c	503	CLA	C5-C6-C7-C8
26	d	403	CLA	C15-C16-C17-C18
34	H	101	DGD	CDA-CEA-CFA-CGA
30	m	102	STE	C5-C6-C7-C8
33	a	614	LHG	C28-C29-C30-C31
33	d	407	LHG	C11-C10-C9-C8
34	H	101	DGD	C5B-C6B-C7B-C8B
29	A	612	PL9	C42-C43-C44-C45
26	B	612	CLA	CAA-CBA-CGA-O2A
33	L	101	LHG	O7-C7-C8-C9
34	C	520	DGD	O1A-C1A-O1G-C1G
32	a	617	SQD	C5-C6-S-O9
26	B	609	CLA	C4-C3-C5-C6
26	c	510	CLA	C4-C3-C5-C6
26	C	509	CLA	C11-C10-C8-C7
26	C	512	CLA	C12-C13-C15-C16
26	a	608	CLA	C12-C13-C15-C16
26	a	613	CLA	C12-C13-C15-C16
26	b	605	CLA	C11-C12-C13-C15
26	c	510	CLA	C11-C12-C13-C15
30	e	105	STE	O1-C1-C2-C3
31	C	516	LMG	C7-C8-O7-C10
34	A	619	DGD	C1G-C2G-O2G-C1B
30	d	408	STE	C15-C16-C17-C18
33	D	410	LHG	C31-C32-C33-C34
33	A	617	LHG	C10-C11-C12-C13
28	K	101	BCR	C15-C16-C17-C18
26	B	614	CLA	C2A-CAA-CBA-CGA
26	B	616	CLA	C2A-CAA-CBA-CGA
30	E	102	STE	C11-C10-C9-C8
26	B	606	CLA	O1D-CGD-O2D-CED
30	t	102	STE	C3-C4-C5-C6
31	c	522	LMG	C40-C41-C42-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	B	602	CLA	C3A-C2A-CAA-CBA
26	c	508	CLA	C3A-C2A-CAA-CBA
31	c	518	LMG	O10-C28-C29-C30
26	B	606	CLA	C15-C16-C17-C18
26	b	614	CLA	C10-C11-C12-C13
30	A	622	STE	C13-C14-C15-C16
36	v	201	HEC	C4B-C3B-CAB-CBB
33	L	101	LHG	C18-C19-C20-C21
31	a	618	LMG	O6-C5-C6-O5
30	E	103	STE	C11-C12-C13-C14
26	B	603	CLA	C11-C10-C8-C9
26	B	616	CLA	C6-C7-C8-C9
26	b	616	CLA	C11-C10-C8-C9
26	c	506	CLA	C11-C10-C8-C9
26	c	507	CLA	C11-C10-C8-C9
31	D	406	LMG	C36-C37-C38-C39
34	C	520	DGD	C2A-C3A-C4A-C5A
32	B	622	SQD	C25-C26-C27-C28
26	B	612	CLA	CAA-CBA-CGA-O1A
32	A	618	SQD	O10-C23-C24-C25
26	B	609	CLA	C2-C3-C5-C6
26	c	506	CLA	C2-C3-C5-C6
26	b	613	CLA	C13-C15-C16-C17
30	e	103	STE	C11-C12-C13-C14
26	b	615	CLA	CBD-CGD-O2D-CED
33	L	101	LHG	O9-C7-C8-C9
30	d	410	STE	C9-C10-C11-C12
31	B	620	LMG	C36-C37-C38-C39
30	i	101	STE	C6-C7-C8-C9
31	B	620	LMG	C8-C7-O1-C1
32	b	620	SQD	C45-C44-O6-C1
34	C	520	DGD	C5D-C6D-O5D-C1E
33	a	616	LHG	O10-C23-O8-C6
31	b	622	LMG	C20-C21-C22-C23
30	I	102	STE	O1-C1-C2-C3
26	D	402	CLA	C3-C5-C6-C7
32	B	622	SQD	C14-C15-C16-C17
26	b	612	CLA	CAA-CBA-CGA-O1A
26	c	510	CLA	CAA-CBA-CGA-O1A
26	b	613	CLA	CAA-CBA-CGA-O2A
30	T	102	STE	C10-C11-C12-C13
34	A	619	DGD	C6B-C7B-C8B-C9B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	c	512	CLA	C13-C15-C16-C17
26	b	601	CLA	CAA-CBA-CGA-O2A
32	A	616	SQD	O49-C7-C8-C9
36	v	201	HEC	C4C-C3C-CAC-CBC
31	M	101	LMG	C38-C39-C40-C41
31	c	522	LMG	C33-C34-C35-C36
26	C	503	CLA	CAD-CBD-CGD-O2D
26	C	513	CLA	CAD-CBD-CGD-O2D
26	b	607	CLA	CAD-CBD-CGD-O2D
26	b	616	CLA	CAD-CBD-CGD-O2D
26	c	510	CLA	CAD-CBD-CGD-O2D
27	D	401	PHO	CAD-CBD-CGD-O2D
26	b	615	CLA	C15-C16-C17-C18
26	A	608	CLA	C4C-C3C-CAC-CBC
34	H	101	DGD	C9B-CAB-CBB-CCB
34	C	521	DGD	O6E-C1E-O5D-C6D
26	A	607	CLA	C2-C1-O2A-CGA
26	d	402	CLA	C2-C1-O2A-CGA
26	B	613	CLA	CAA-CBA-CGA-O1A
30	I	102	STE	C3-C4-C5-C6
30	m	103	STE	C13-C14-C15-C16
26	b	613	CLA	CAA-CBA-CGA-O1A
30	B	625	STE	C1-C2-C3-C4
26	A	607	CLA	C16-C17-C18-C19
26	C	511	CLA	C16-C17-C18-C19
30	B	625	STE	C5-C6-C7-C8
30	C	526	STE	C15-C16-C17-C18

There are no ring outliers.

139 monomers are involved in 262 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	d	404	BCR	1	0
29	D	405	PL9	1	0
28	B	618	BCR	2	0
26	B	616	CLA	3	0
35	F	101	HEM	3	0
26	b	603	CLA	1	0
28	k	102	BCR	1	0
26	A	608	CLA	5	0
26	c	501	CLA	3	0
26	B	603	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	B	625	STE	2	0
26	c	507	CLA	3	0
26	a	610	CLA	2	0
26	c	511	CLA	5	0
26	c	504	CLA	2	0
28	c	514	BCR	1	0
30	z	101	STE	1	0
26	B	604	CLA	3	0
28	K	101	BCR	1	0
26	C	503	CLA	1	0
26	c	508	CLA	1	0
28	K	103	BCR	2	0
27	a	609	PHO	1	0
26	B	608	CLA	3	0
31	M	101	LMG	3	0
33	D	408	LHG	2	0
26	D	402	CLA	2	0
30	H	103	STE	1	0
28	T	101	BCR	5	0
28	K	102	BCR	1	0
31	a	618	LMG	5	0
26	C	512	CLA	2	0
32	a	615	SQD	1	0
30	m	102	STE	1	0
34	C	522	DGD	2	0
27	d	401	PHO	3	0
26	B	614	CLA	3	0
30	E	102	STE	1	0
30	b	621	STE	2	0
26	A	614	CLA	2	0
28	D	404	BCR	3	0
28	b	618	BCR	3	0
32	F	102	SQD	1	0
33	D	410	LHG	3	0
26	c	509	CLA	2	0
26	d	402	CLA	1	0
28	t	101	BCR	3	0
26	C	507	CLA	2	0
26	C	511	CLA	3	0
28	X	101	BCR	3	0
31	c	523	LMG	4	0
28	C	514	BCR	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	b	606	CLA	1	0
26	C	509	CLA	1	0
32	B	622	SQD	2	0
30	I	102	STE	1	0
31	D	407	LMG	1	0
26	c	513	CLA	2	0
26	B	611	CLA	1	0
30	d	406	STE	1	0
26	C	502	CLA	1	0
26	b	604	CLA	4	0
21	A	601[B]	OEY	2	0
26	a	613	CLA	3	0
26	b	614	CLA	4	0
29	a	612	PL9	5	0
26	B	601	CLA	1	0
30	K	104	STE	1	0
26	b	615	CLA	5	0
33	a	614	LHG	1	0
28	h	101	BCR	3	0
30	A	622	STE	4	0
26	c	502	CLA	1	0
26	a	607	CLA	2	0
30	m	103	STE	2	0
30	d	408	STE	5	0
32	a	617	SQD	3	0
31	B	620	LMG	5	0
30	c	516	STE	1	0
26	c	505	CLA	3	0
26	B	606	CLA	2	0
30	T	102	STE	2	0
35	e	102	HEM	2	0
26	B	613	CLA	2	0
26	b	616	CLA	2	0
31	C	523	LMG	4	0
34	h	102	DGD	2	0
30	Z	101	STE	1	0
34	C	520	DGD	2	0
33	A	617	LHG	5	0
26	c	512	CLA	2	0
30	A	621	STE	1	0
21	a	601[B]	OEY	1	0
30	i	101	STE	1	0

Continued on next page...

Continued from previous page...

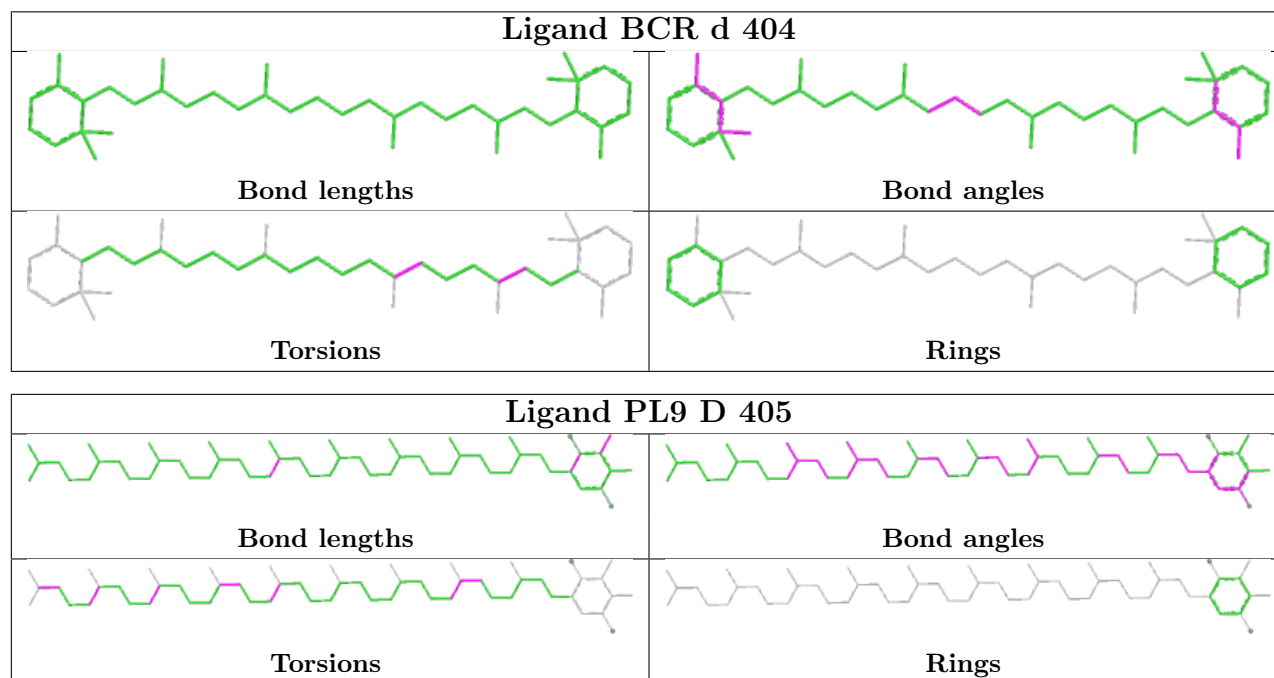
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	a	616	LHG	2	0
26	B	612	CLA	2	0
28	k	101	BCR	2	0
30	D	411	STE	3	0
26	a	608	CLA	2	0
31	c	522	LMG	1	0
29	d	405	PL9	1	0
34	c	519	DGD	1	0
33	D	409	LHG	3	0
26	B	615	CLA	1	0
26	b	608	CLA	3	0
29	A	612	PL9	7	0
30	A	620	STE	1	0
30	B	623	STE	2	0
26	C	508	CLA	1	0
32	b	620	SQD	1	0
26	b	609	CLA	2	0
26	b	602	CLA	5	0
30	a	620	STE	2	0
30	M	104	STE	1	0
30	E	103	STE	2	0
30	h	104	STE	2	0
30	d	410	STE	1	0
34	C	521	DGD	3	0
31	m	101	LMG	2	0
26	B	605	CLA	2	0
28	b	617	BCR	2	0
28	c	515	BCR	1	0
34	c	521	DGD	1	0
31	A	615	LMG	3	0
31	D	406	LMG	12	0
26	A	607	CLA	5	0
26	c	503	CLA	3	0
33	L	101	LHG	1	0
27	A	609	PHO	2	0
26	B	610	CLA	1	0
26	b	612	CLA	3	0
34	A	619	DGD	4	0
30	e	103	STE	1	0
26	c	510	CLA	3	0
33	l	101	LHG	1	0
26	C	505	CLA	2	0

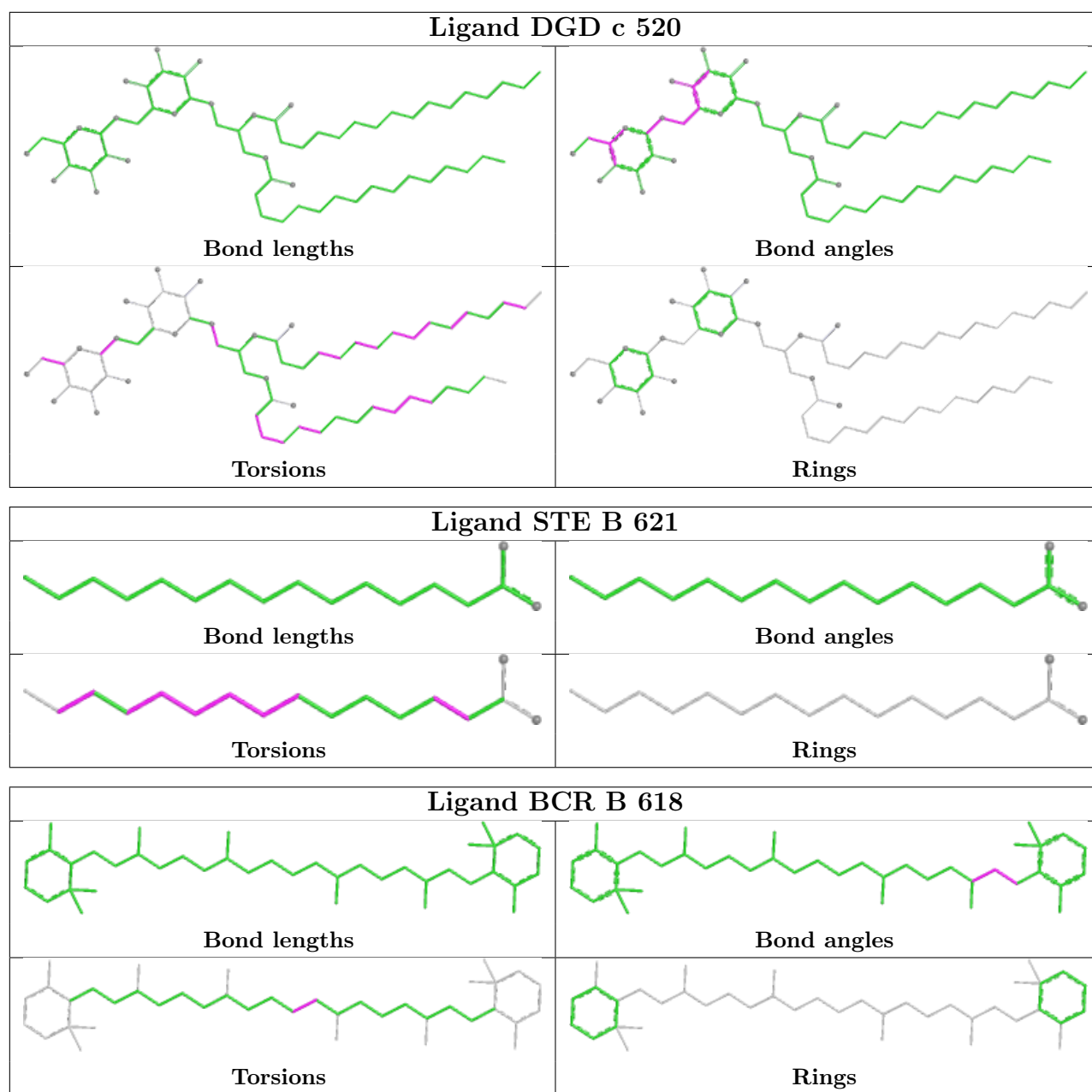
Continued on next page...

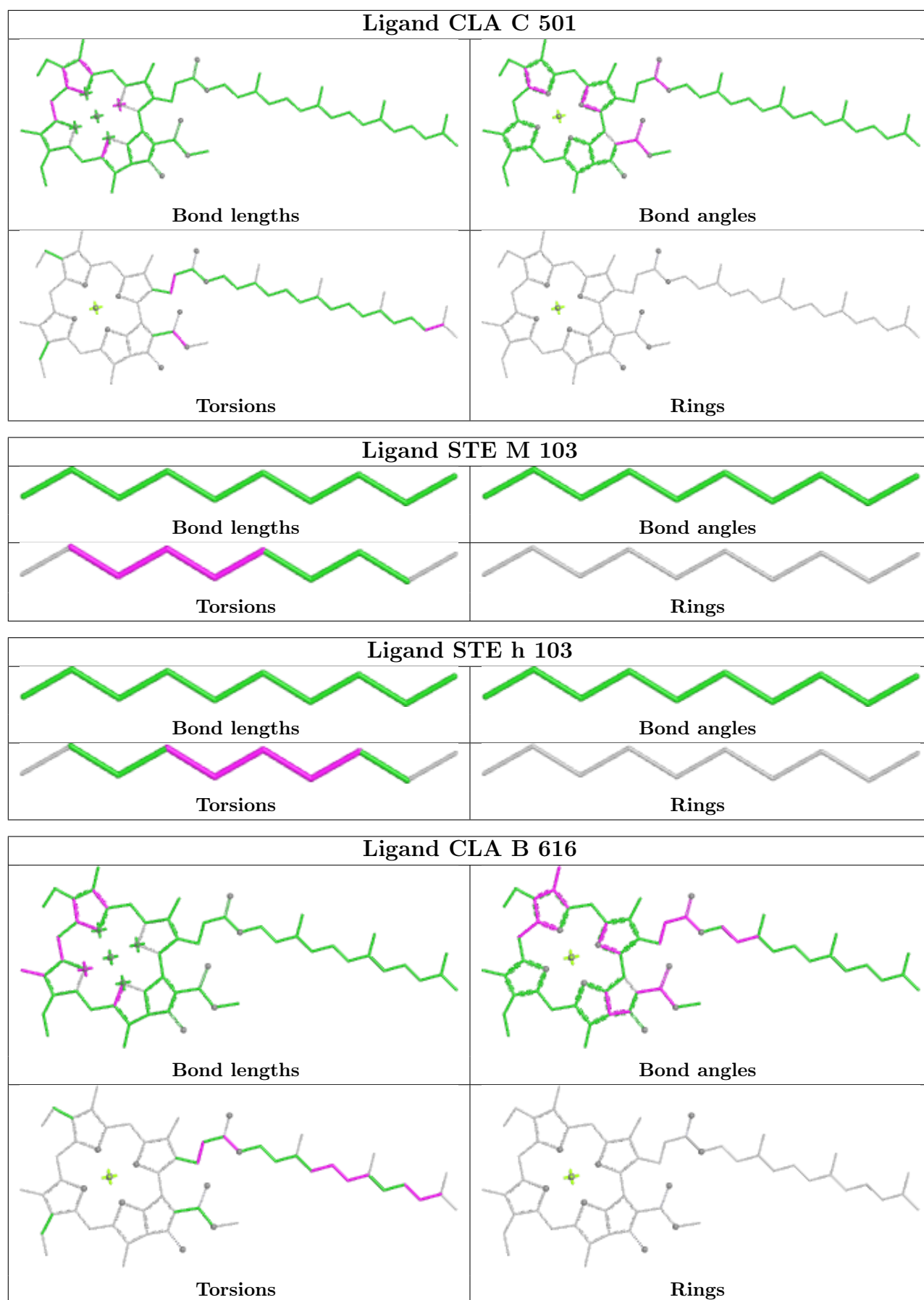
Continued from previous page...

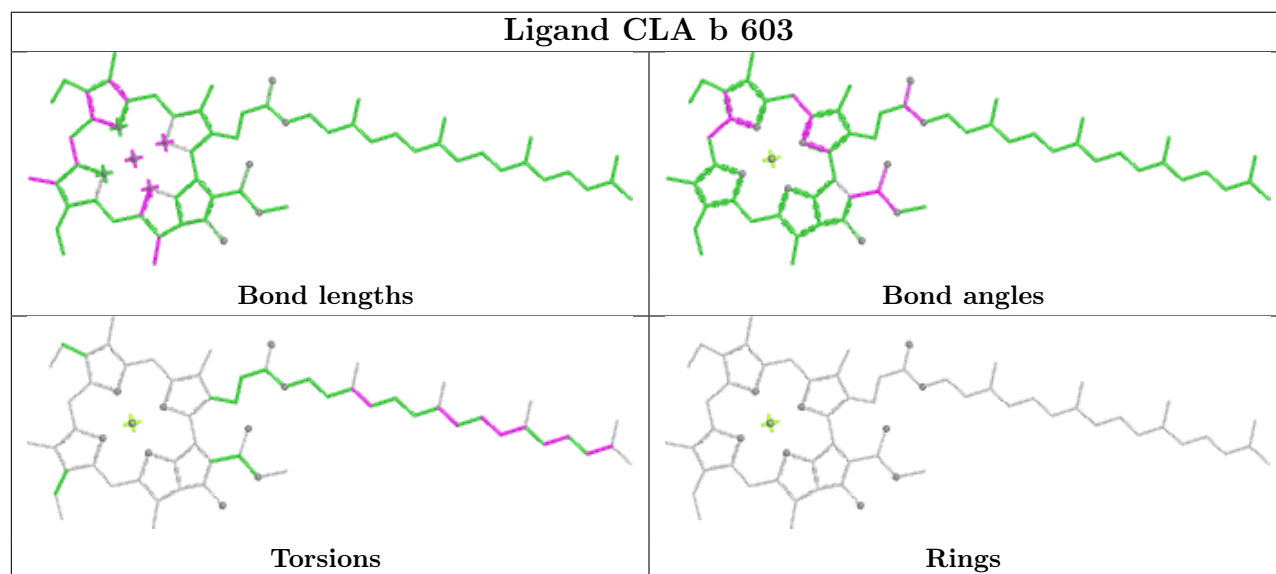
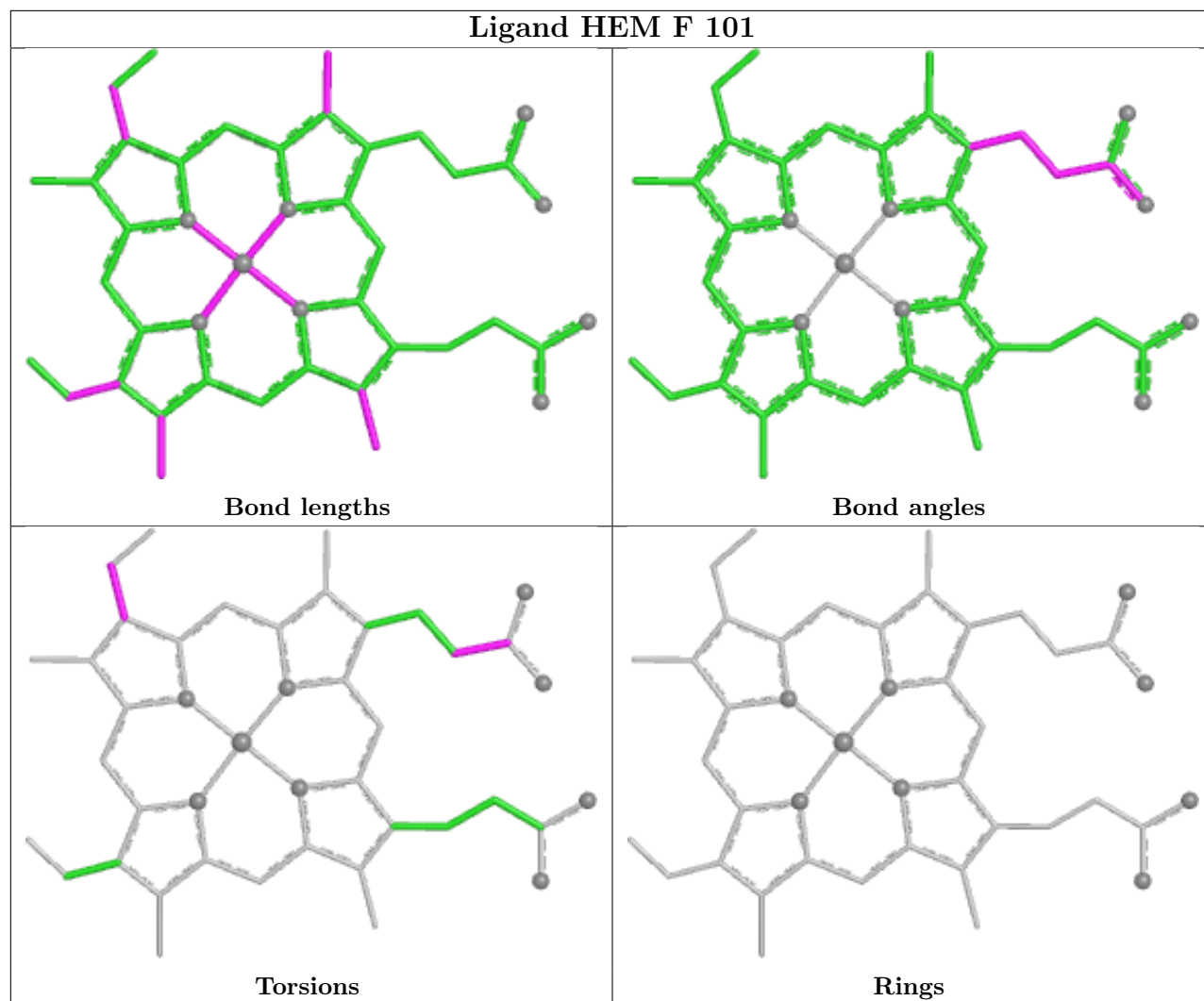
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	609	CLA	1	0
26	B	602	CLA	1	0
26	C	506	CLA	2	0

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

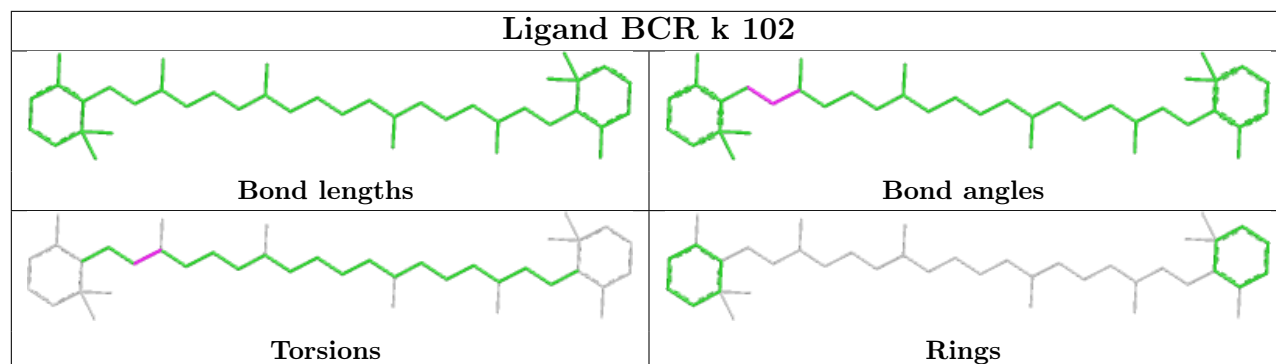




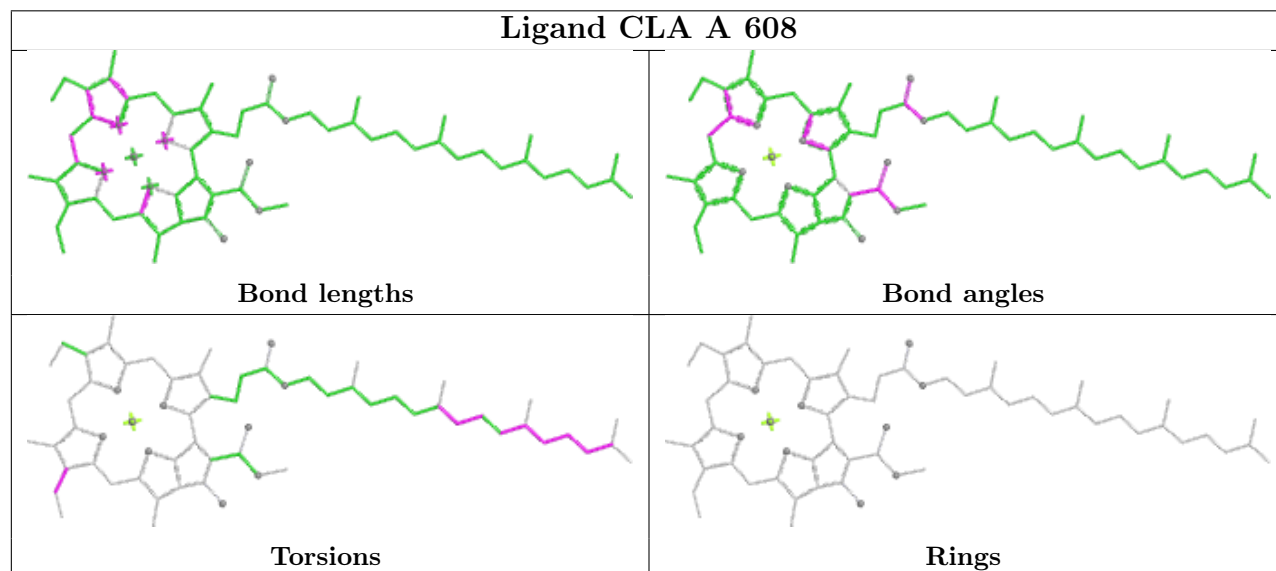




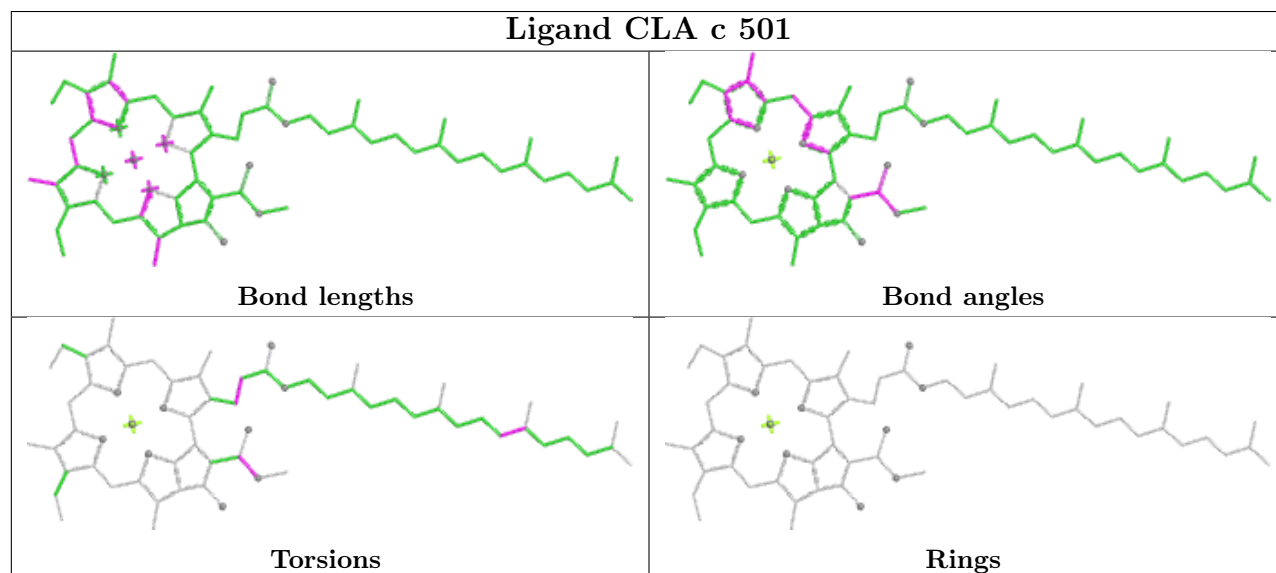
Ligand BCR k 102

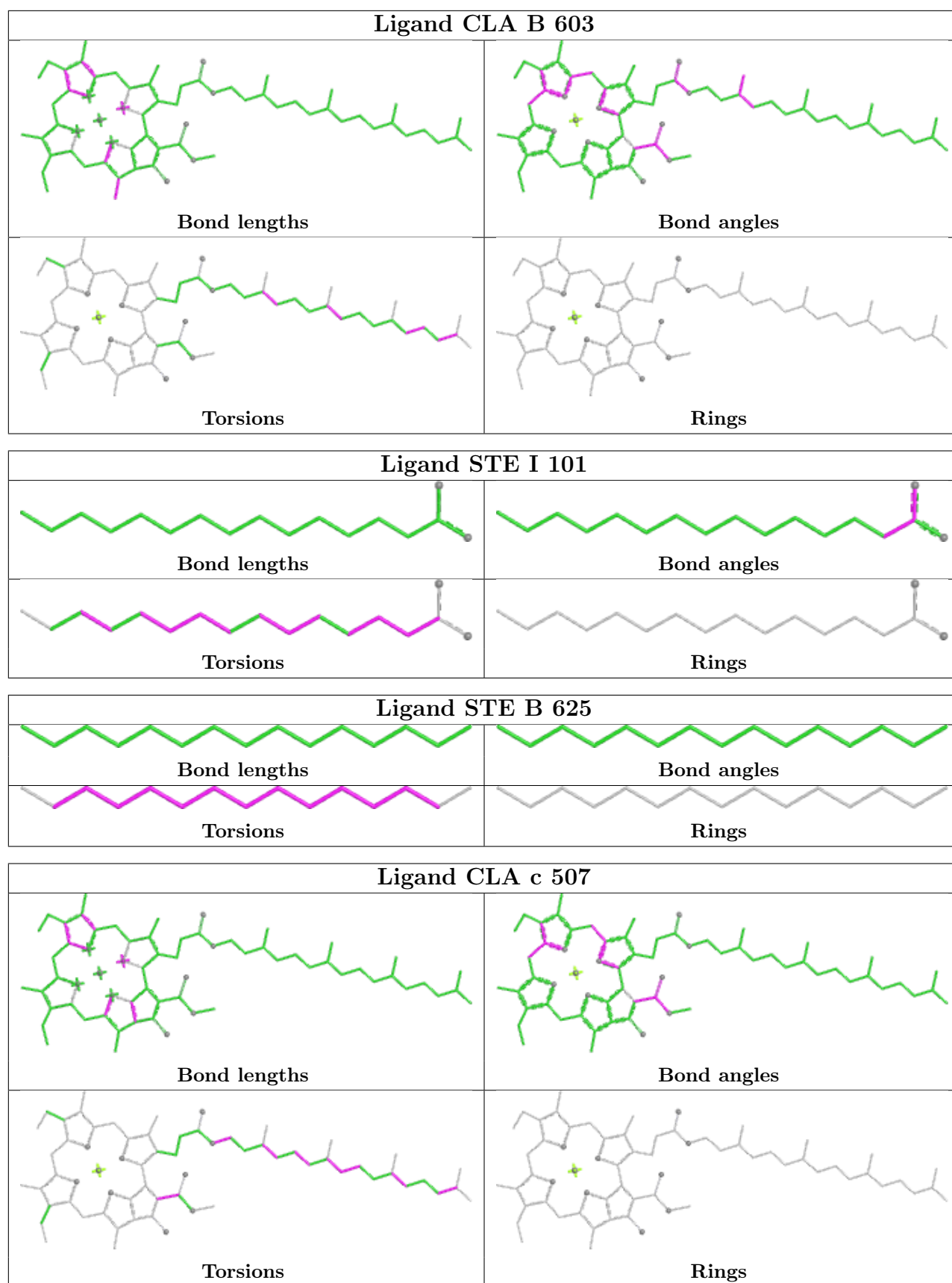


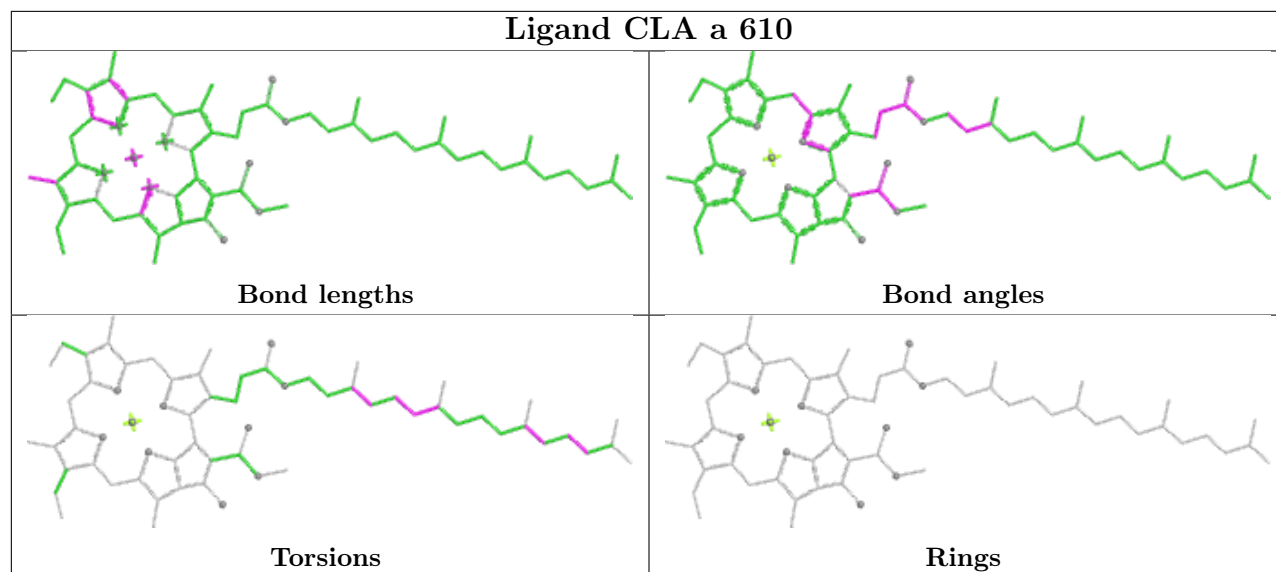
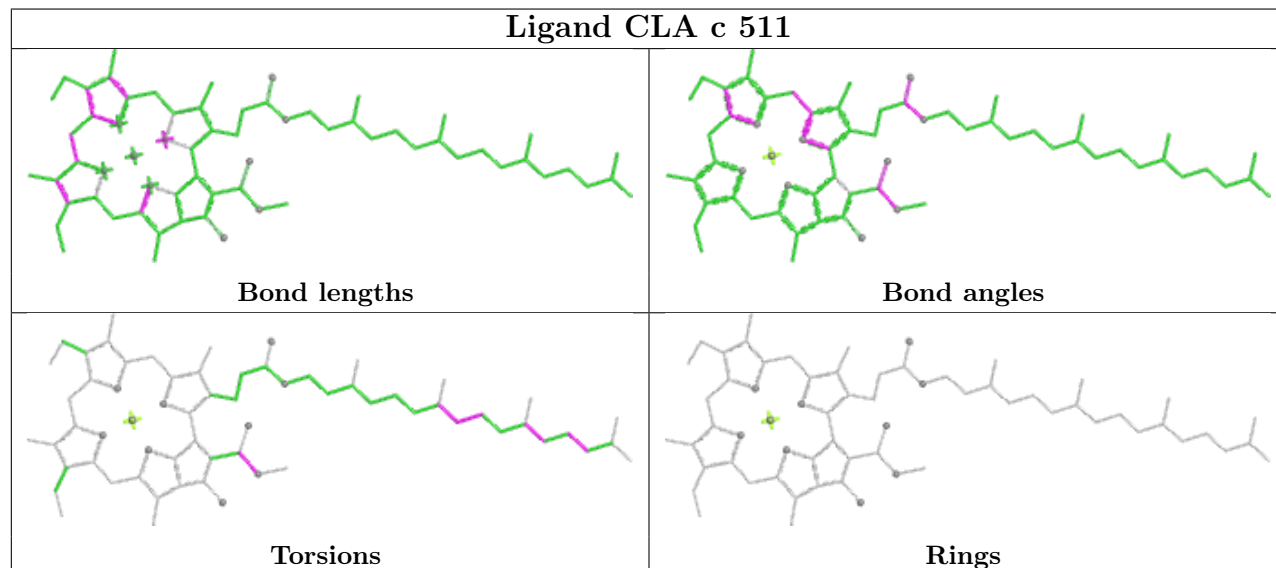
Ligand CLA A 608



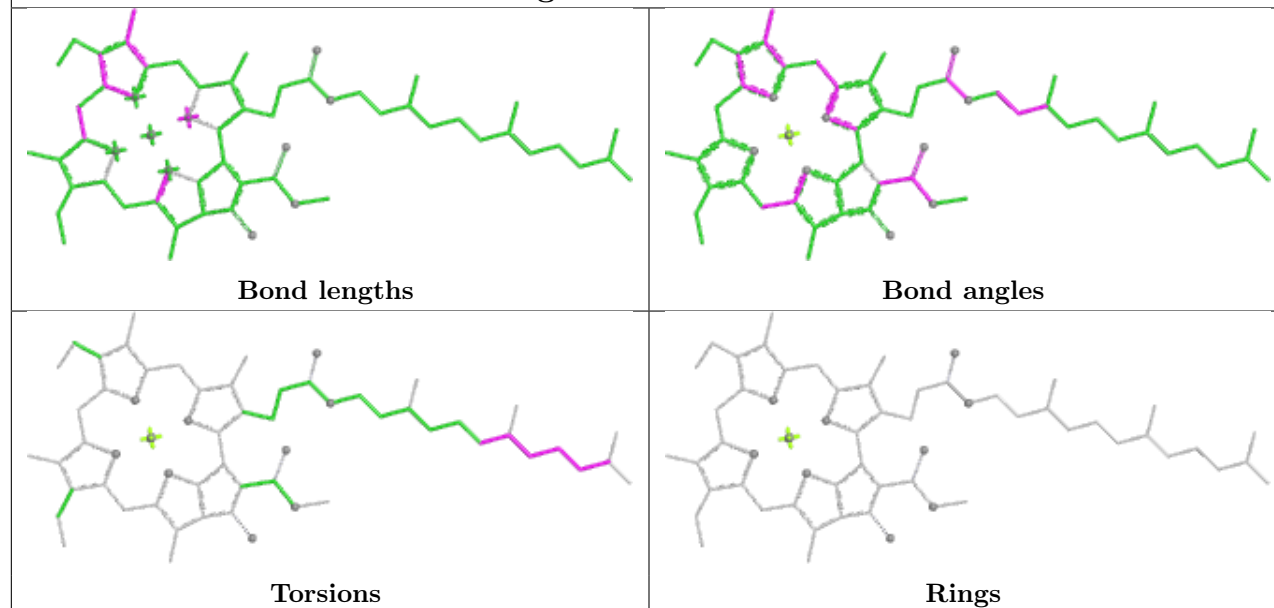
Ligand CLA c 501



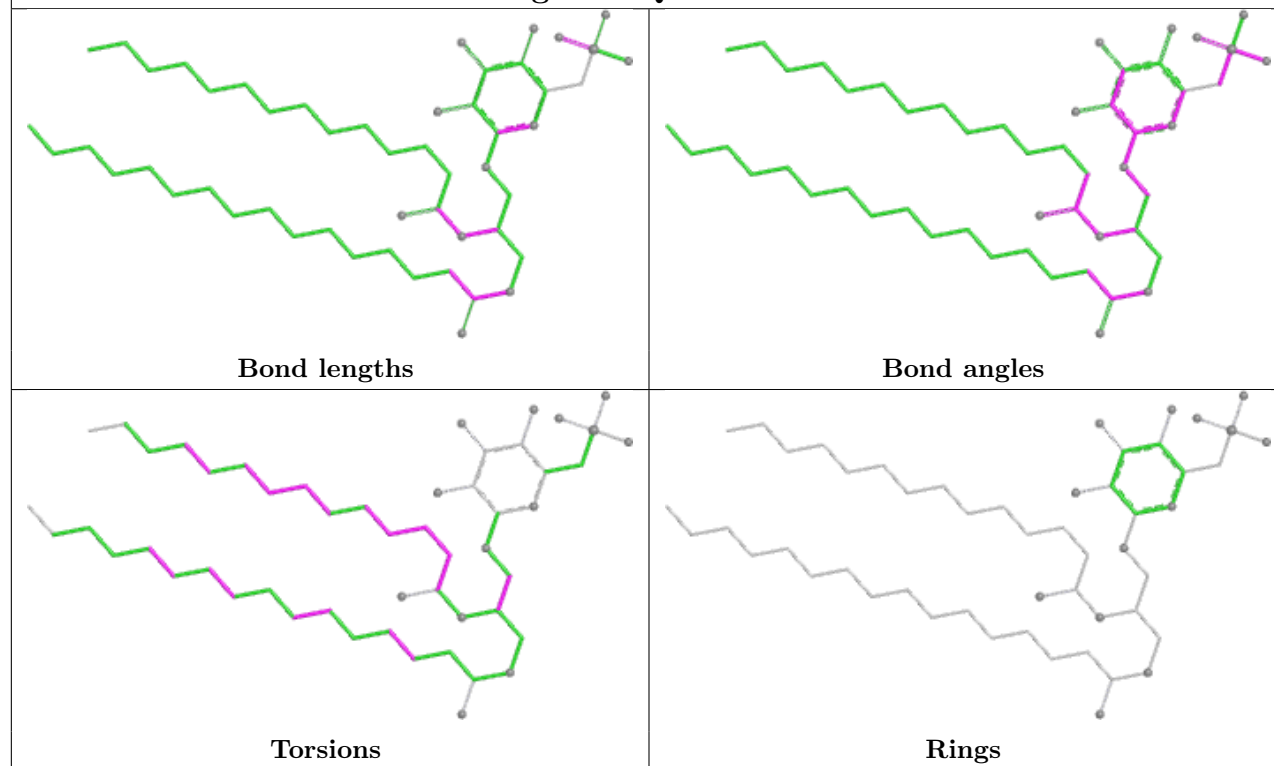


Ligand CLA a 610**Ligand CLA c 511**

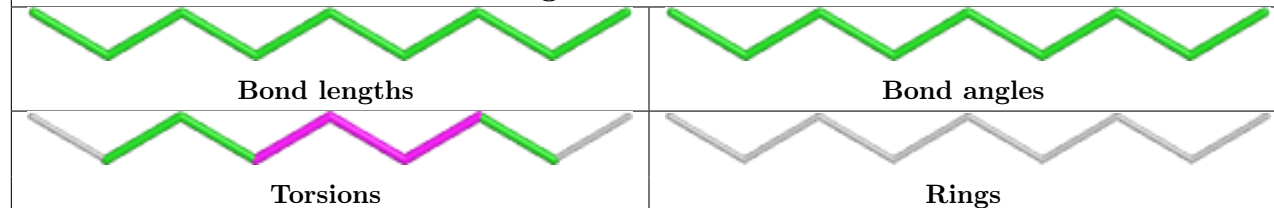
Ligand CLA c 504

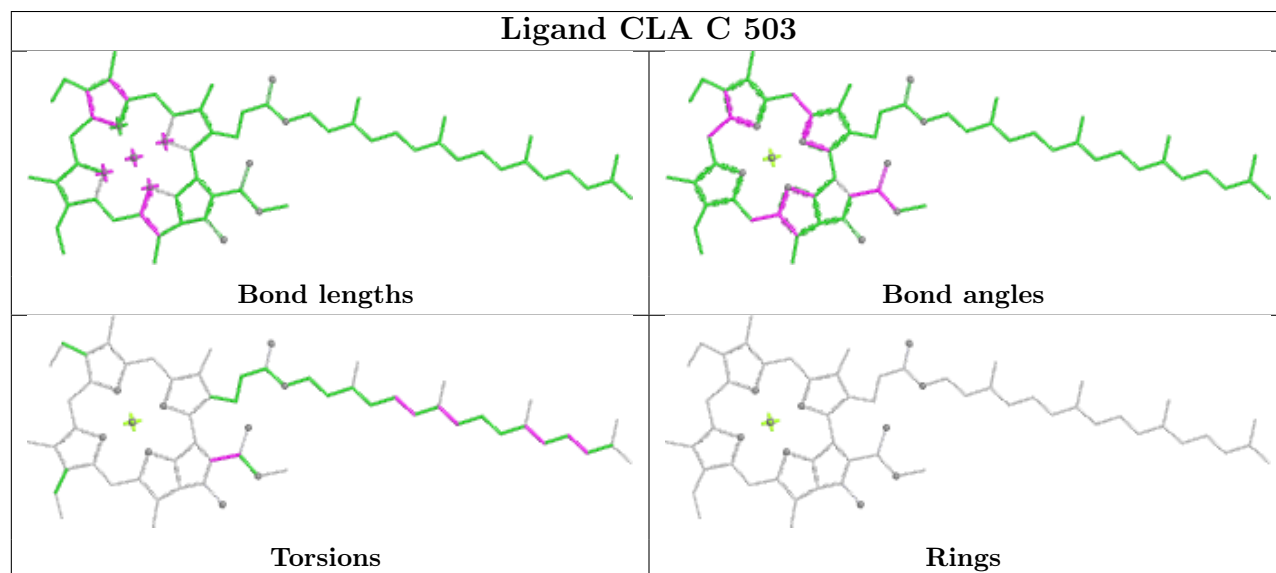
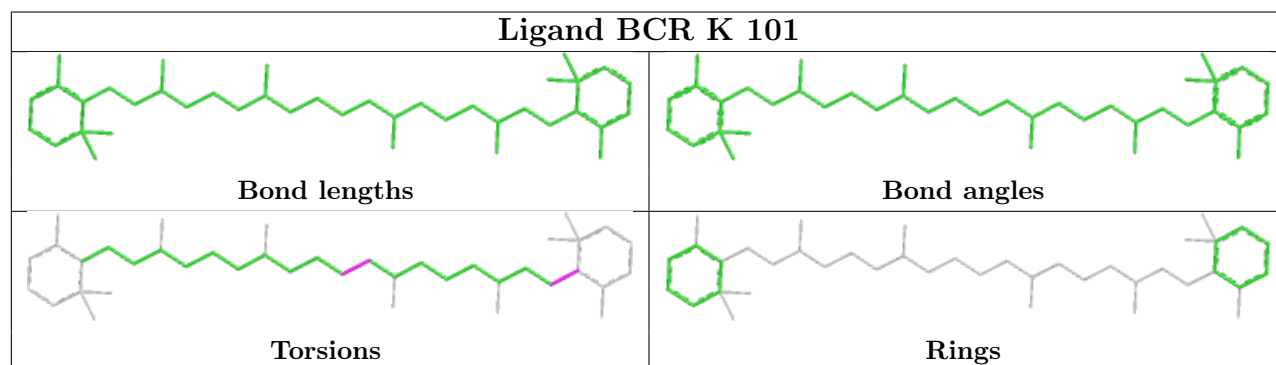
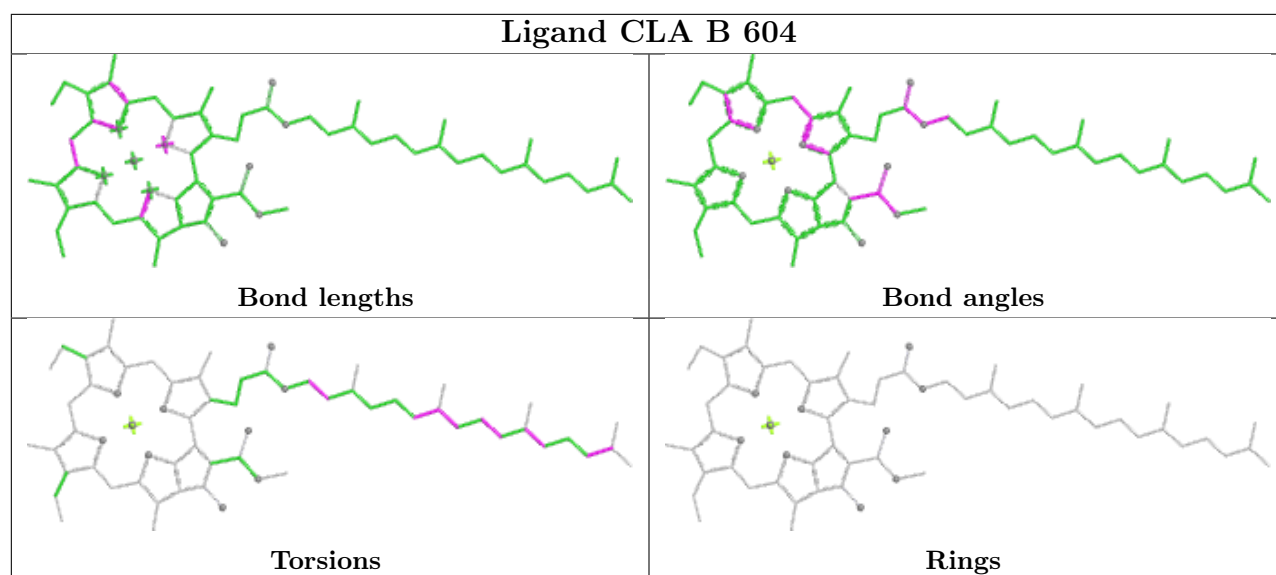


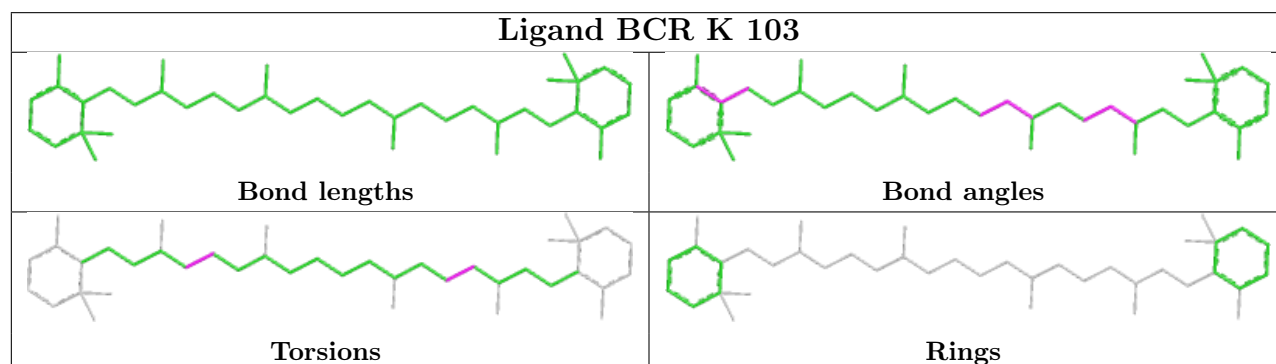
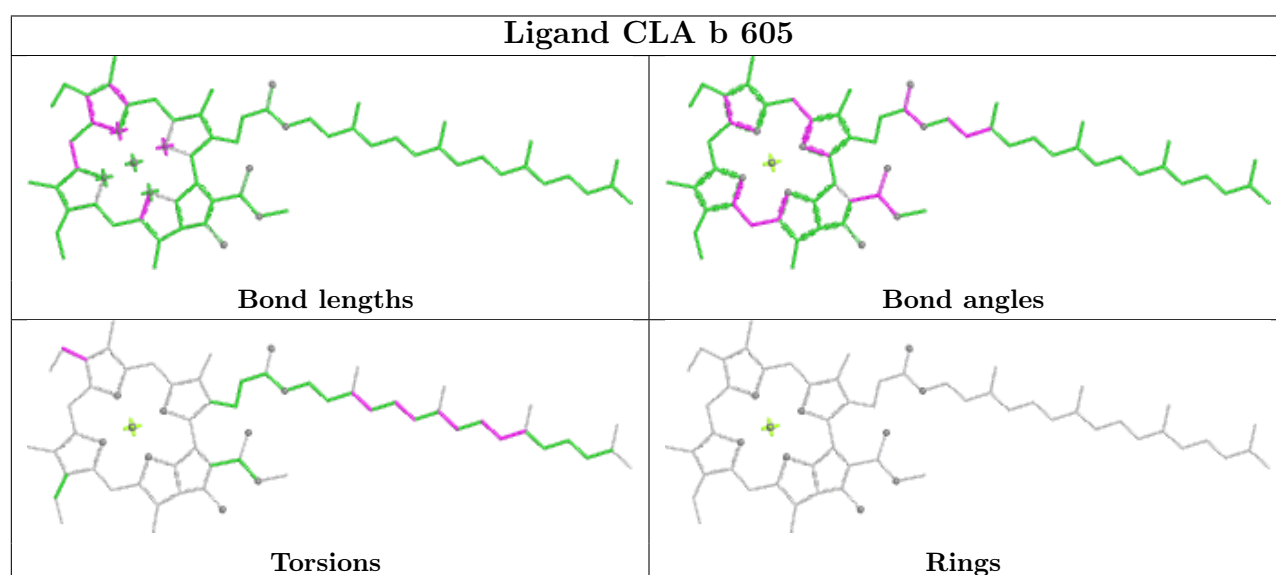
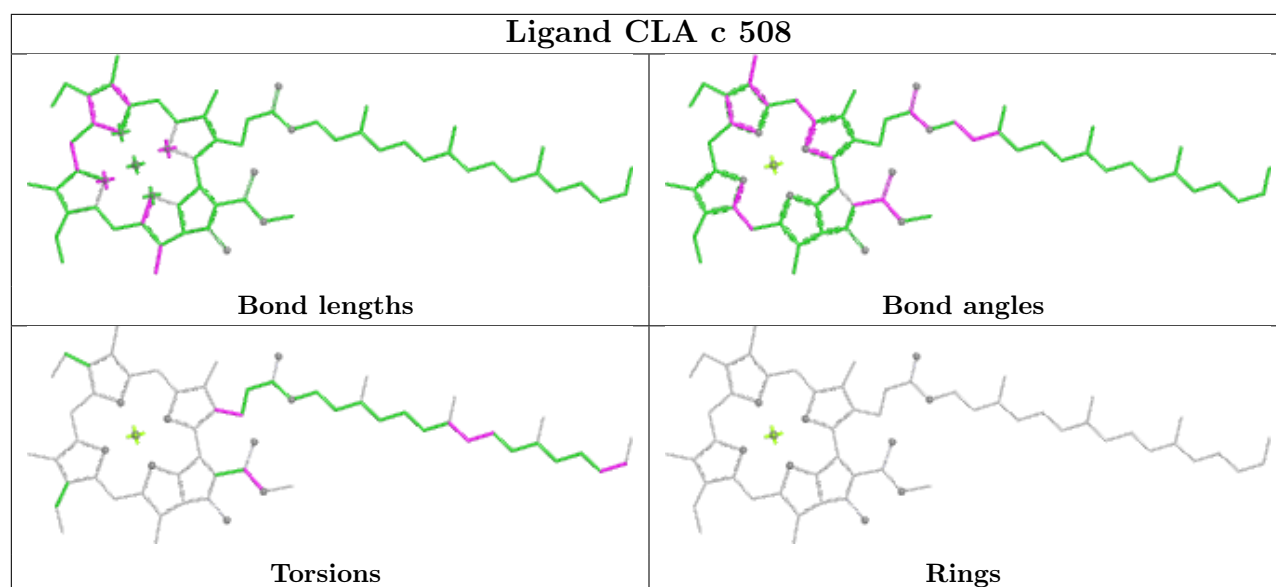
Ligand SQD A 616

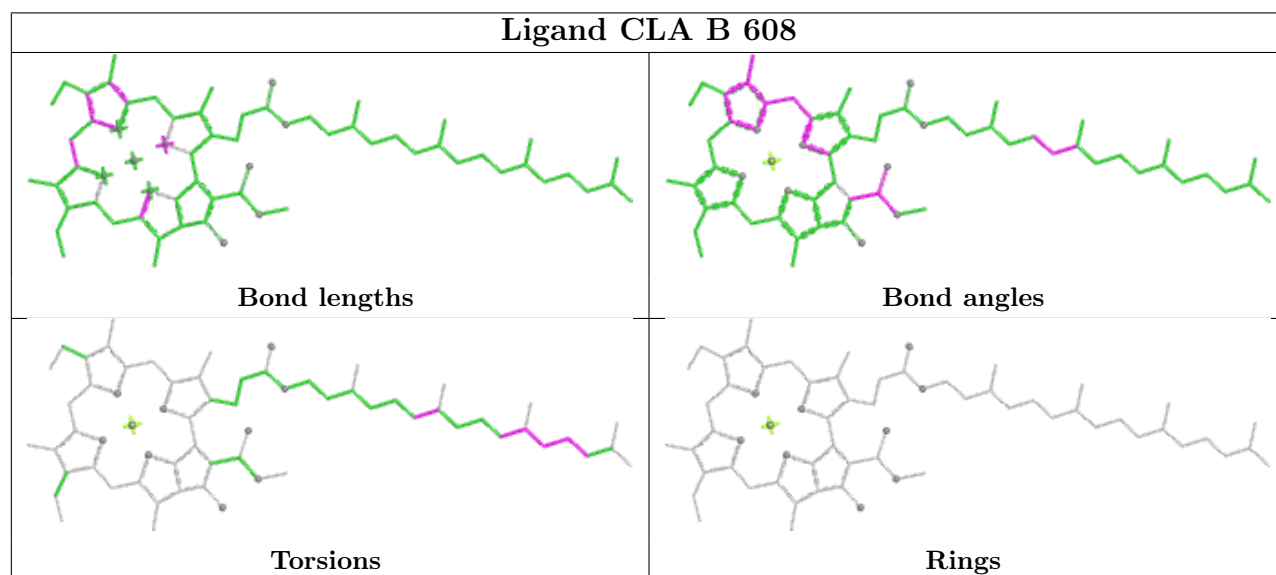
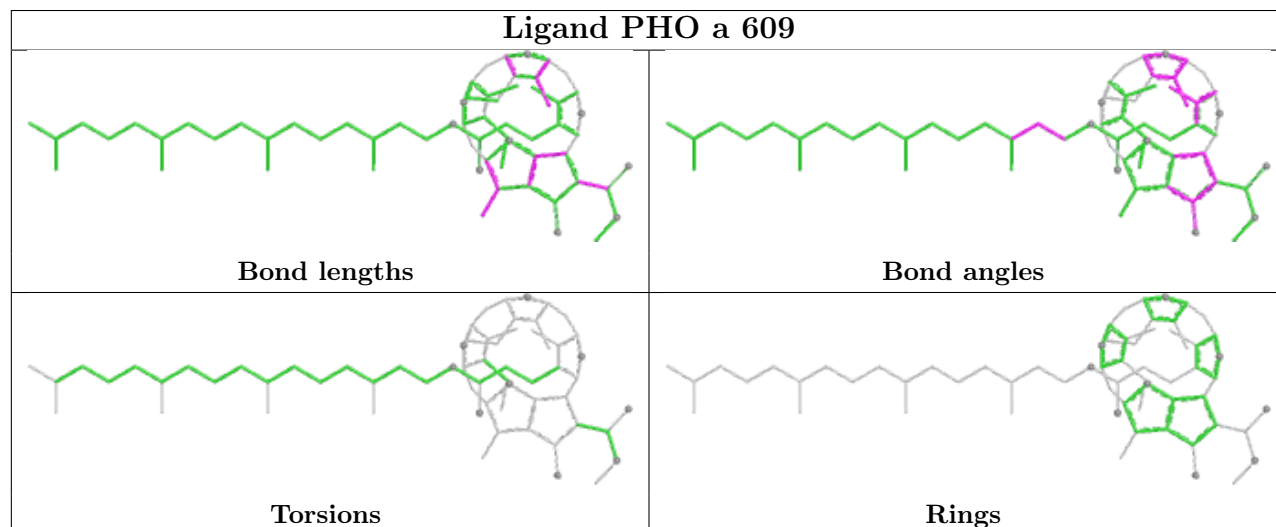
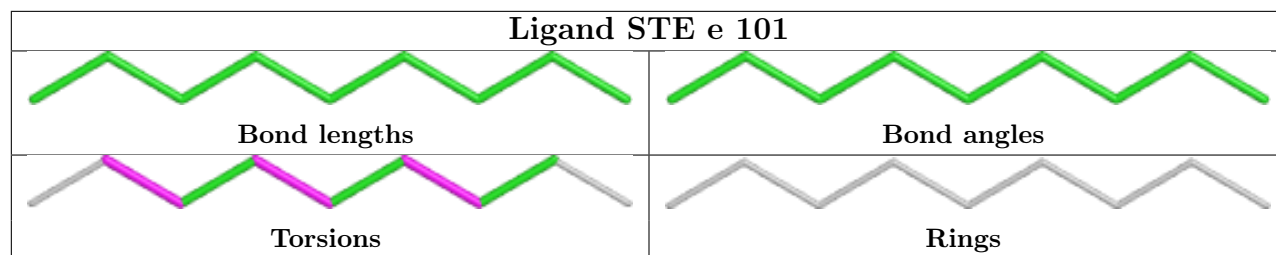


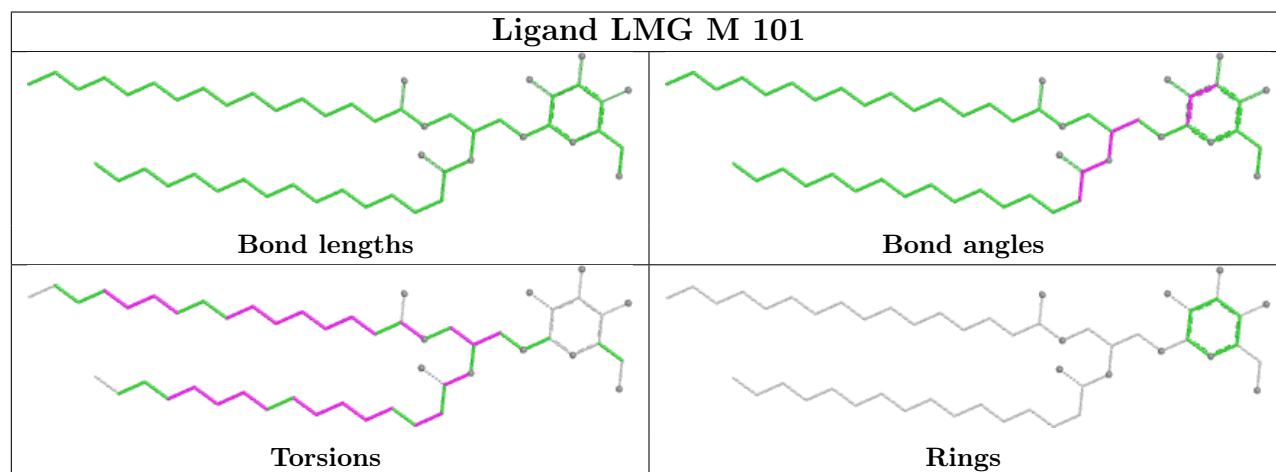
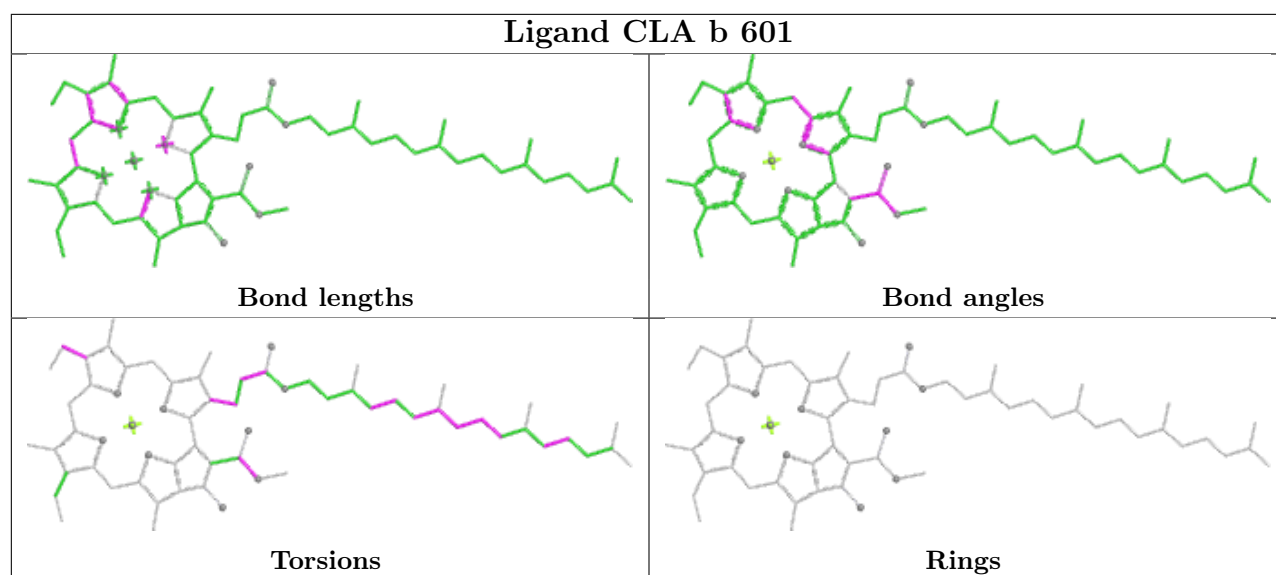
Ligand STE z 101

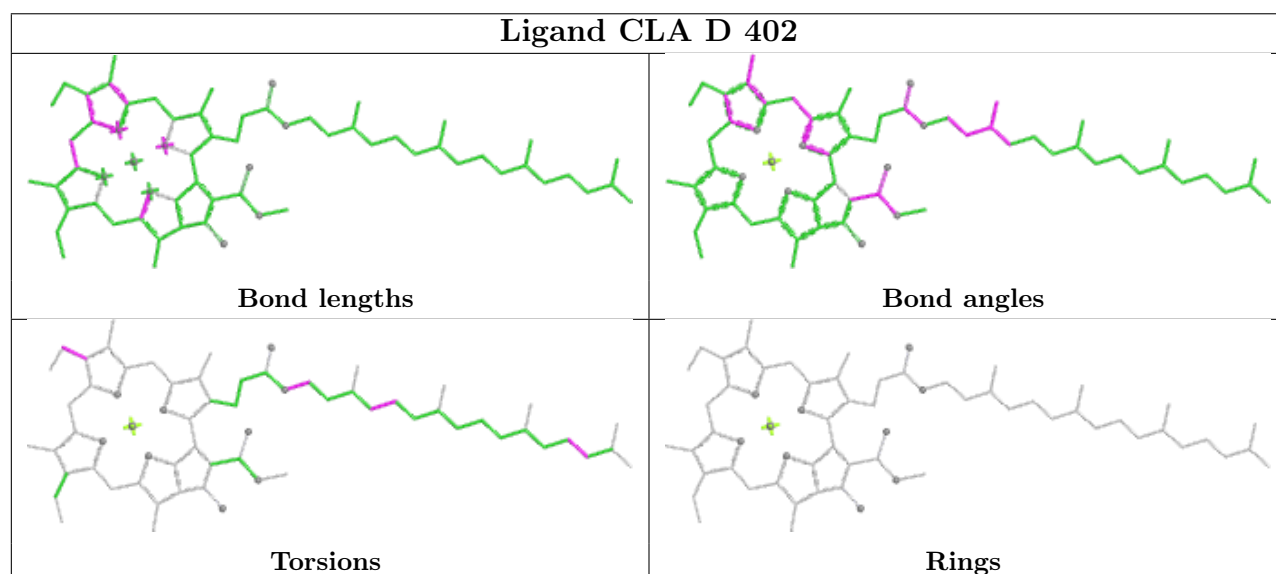
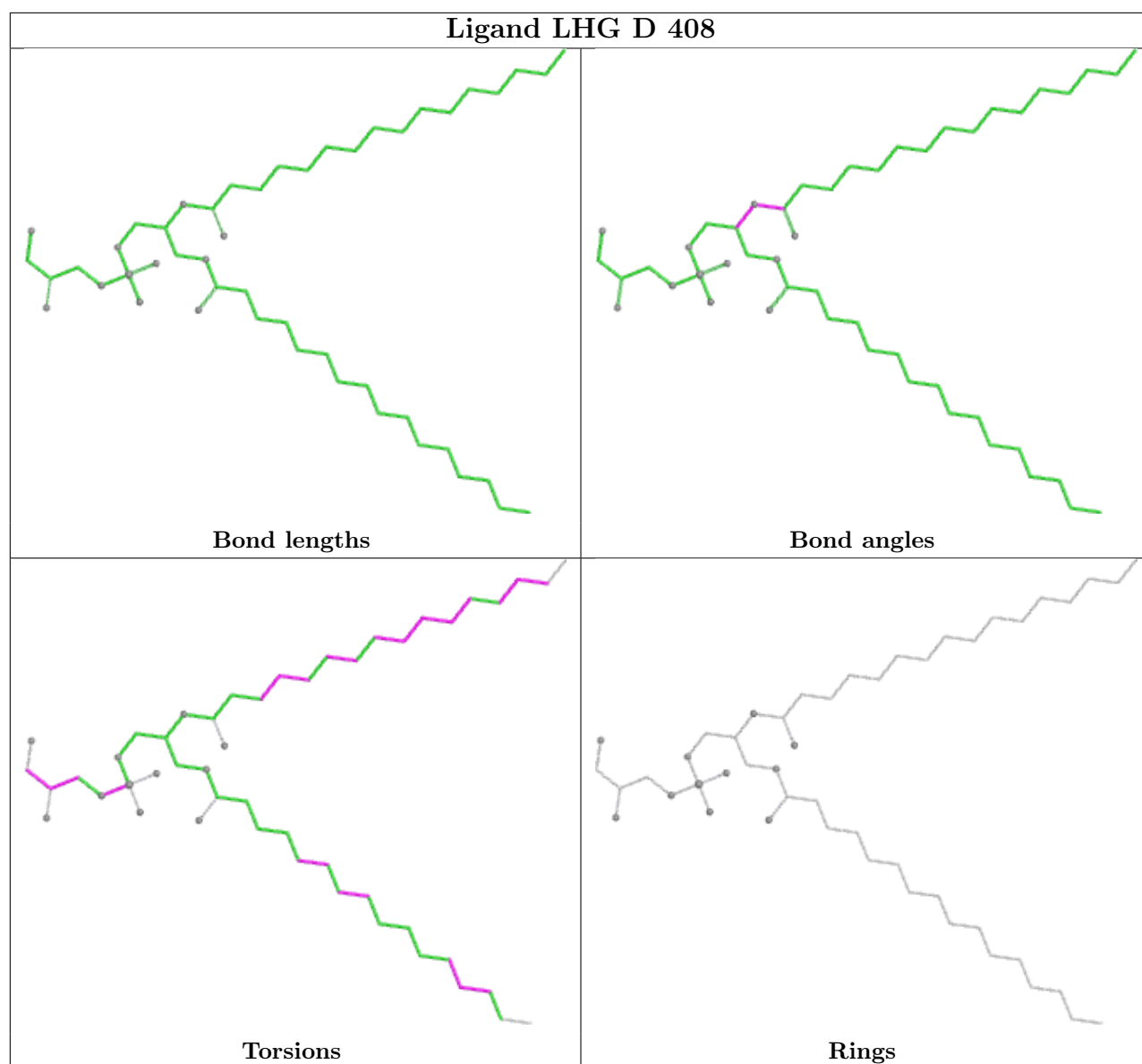


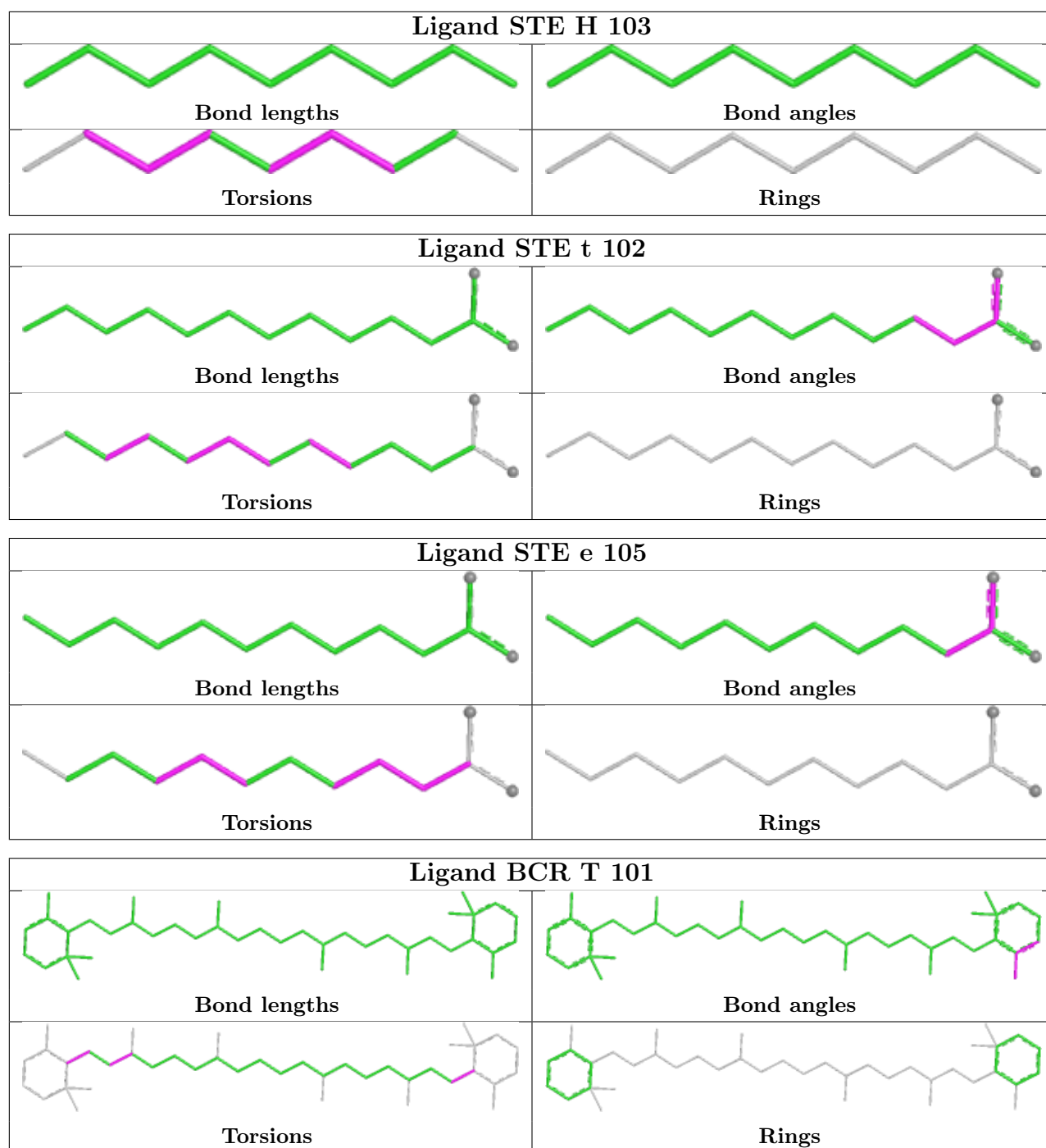


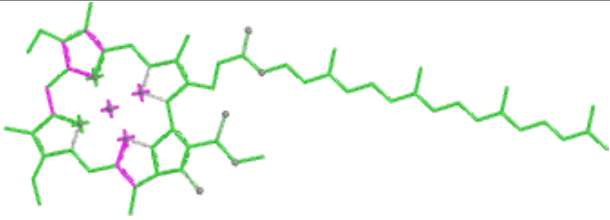
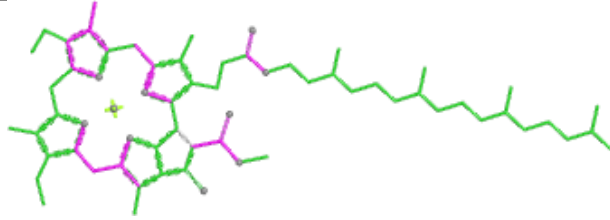
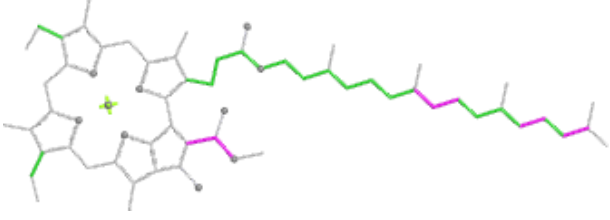
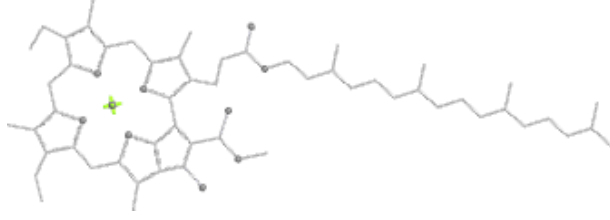
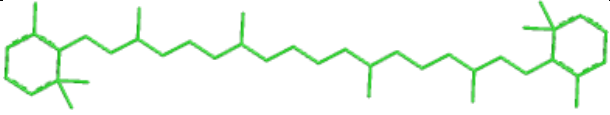
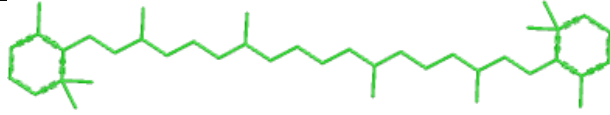
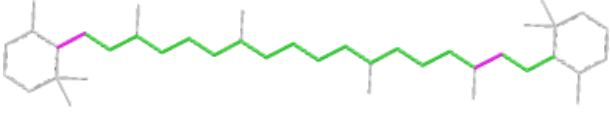
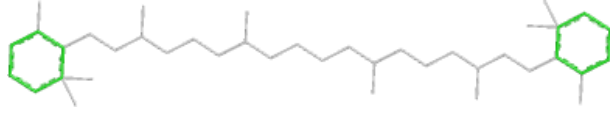
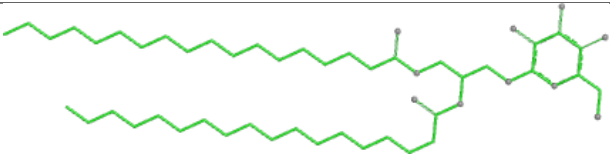
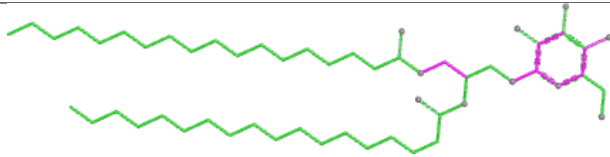
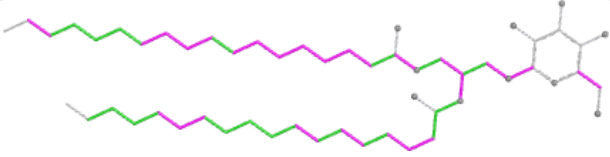
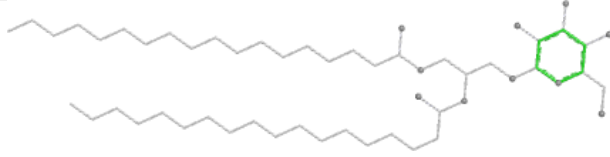




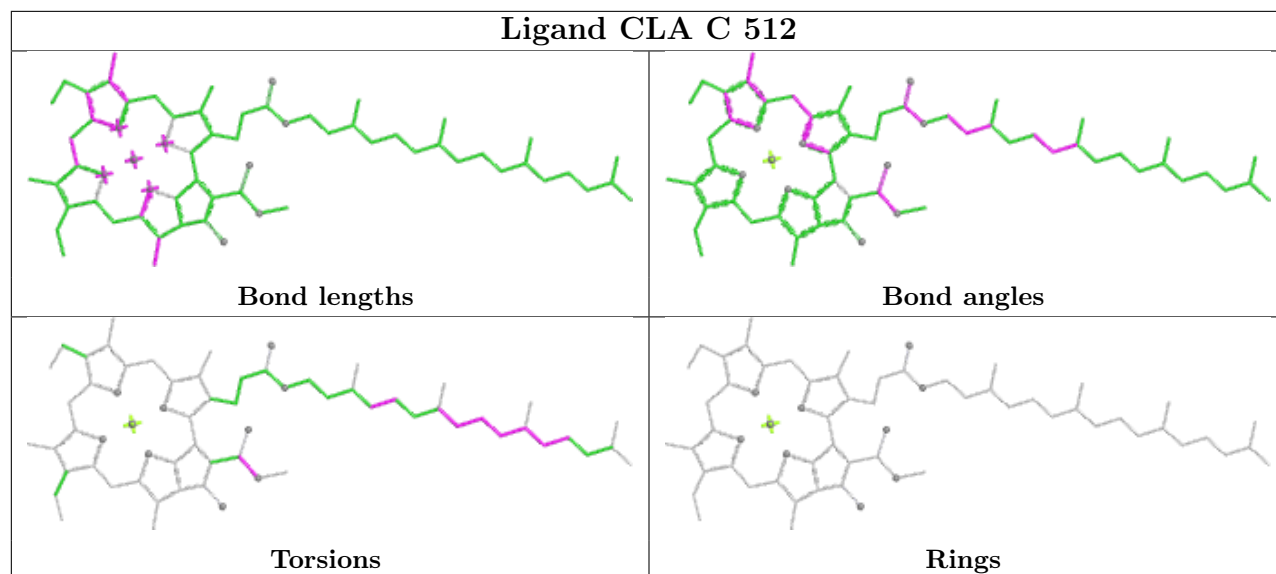




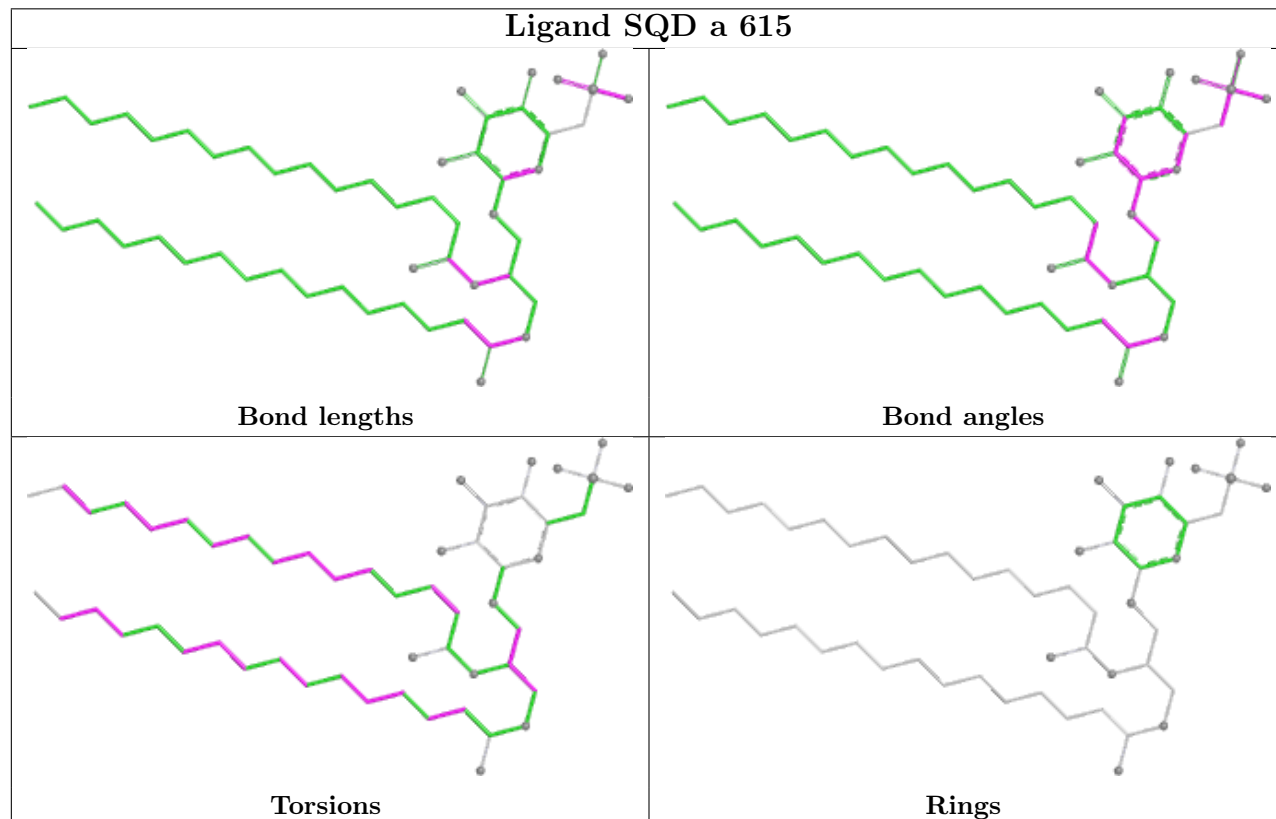


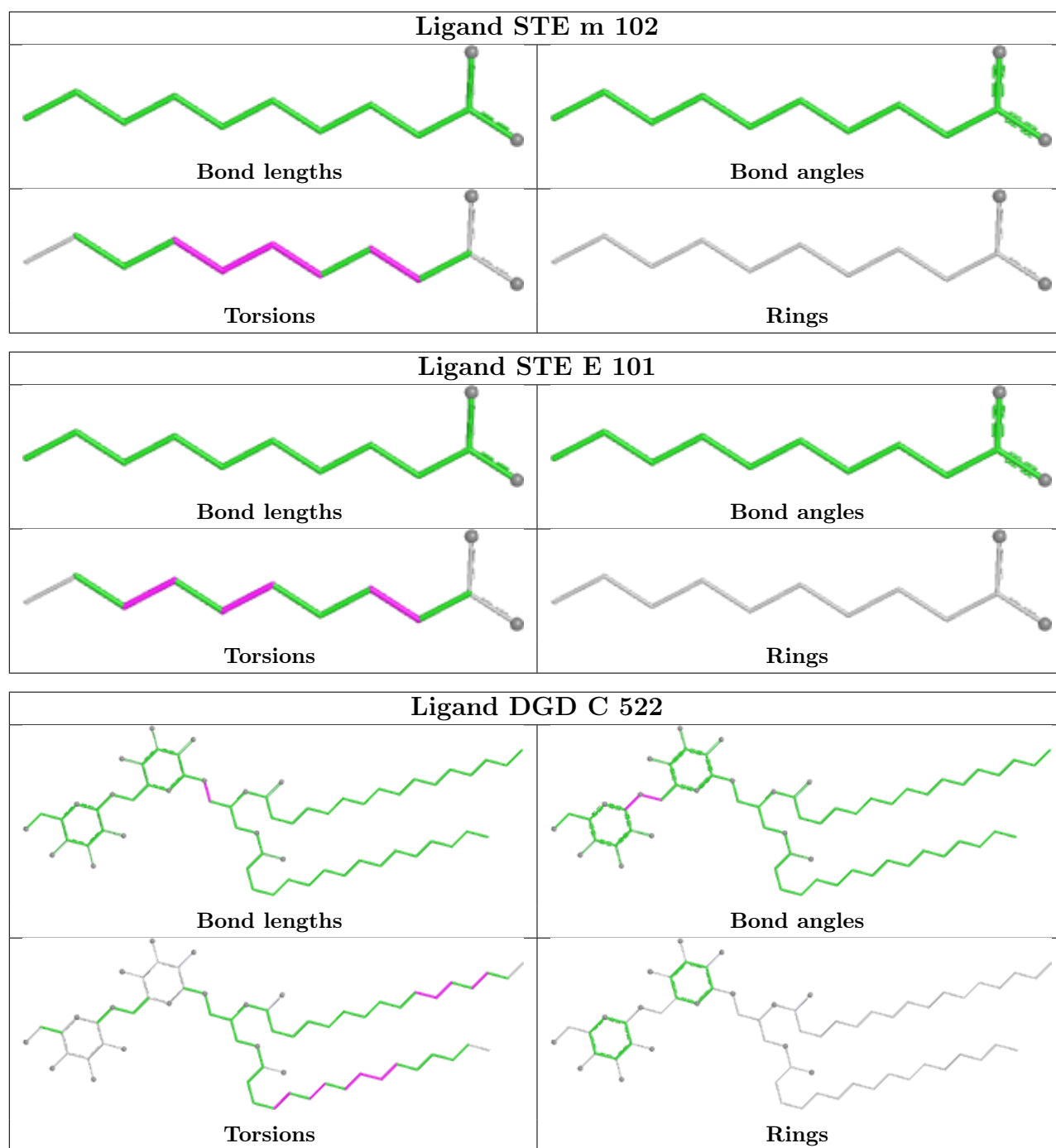
Ligand CLA C 513	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR K 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG a 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

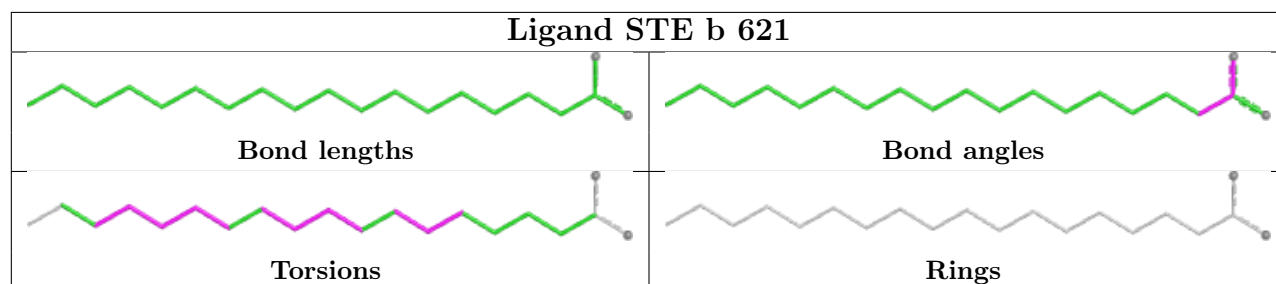
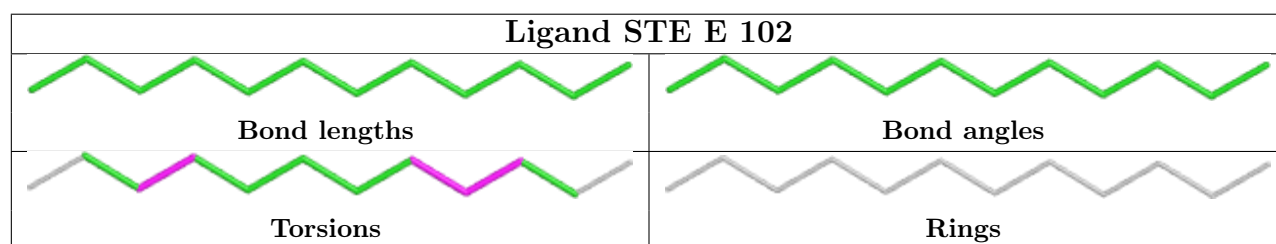
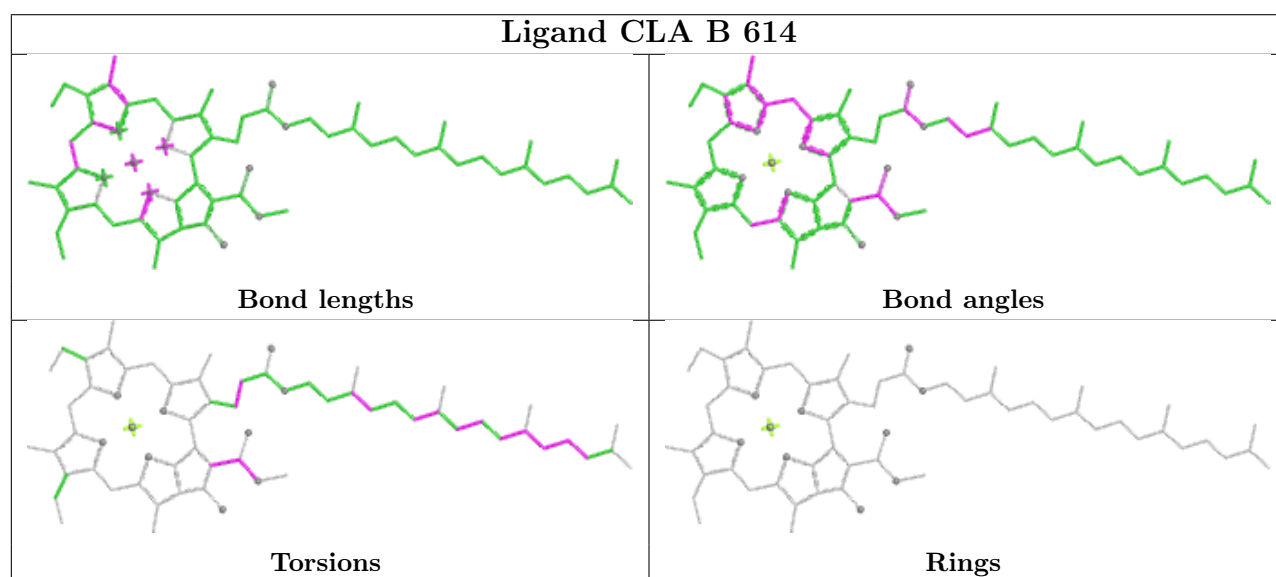
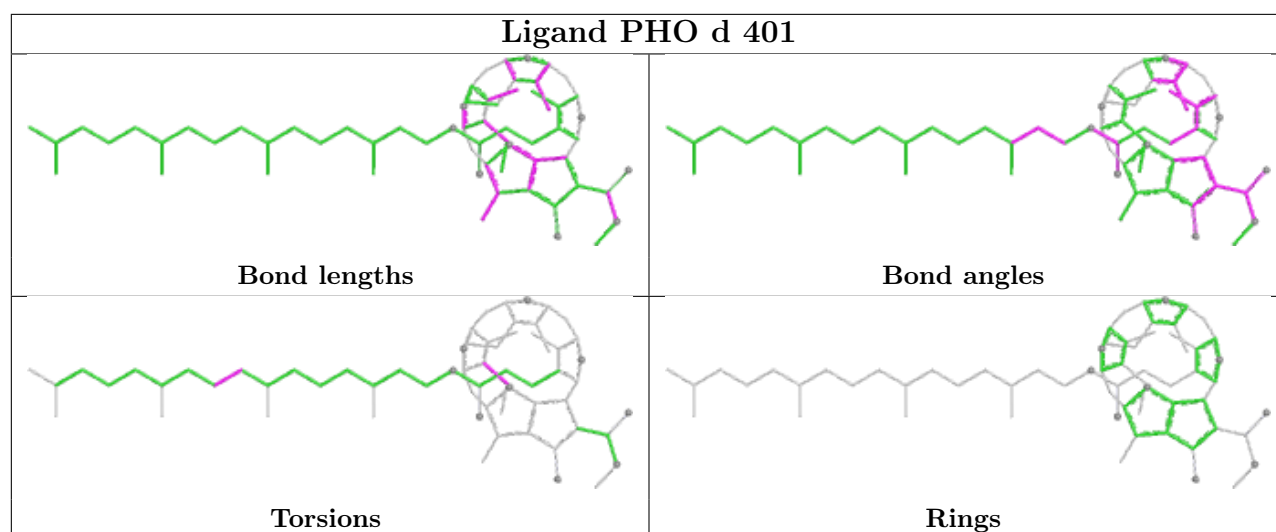
Ligand CLA C 512

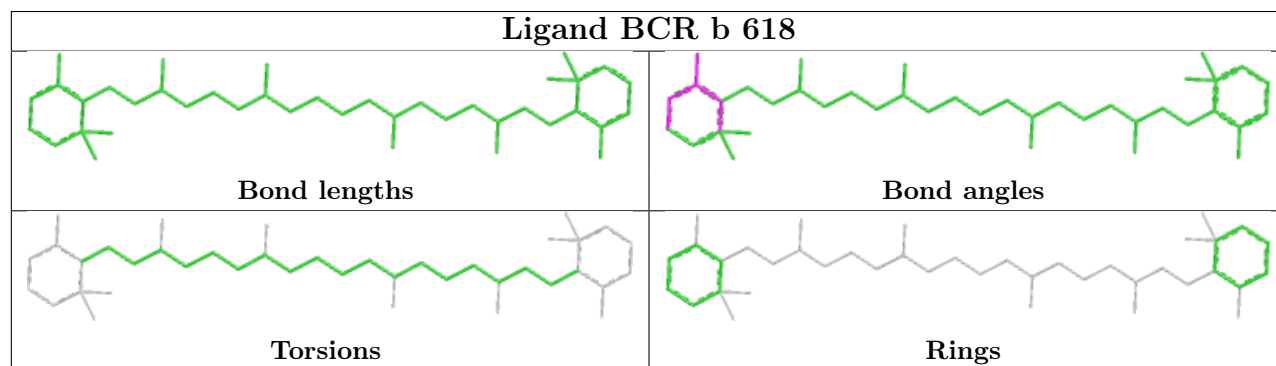
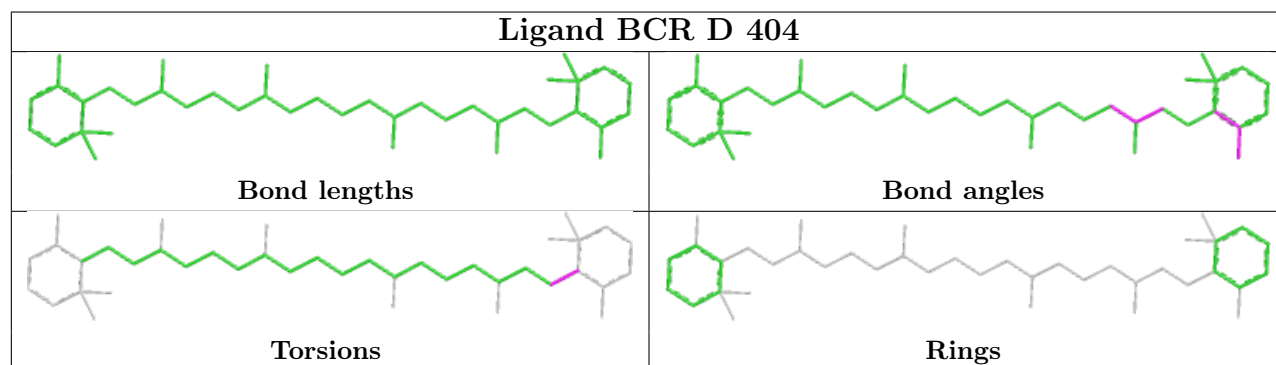
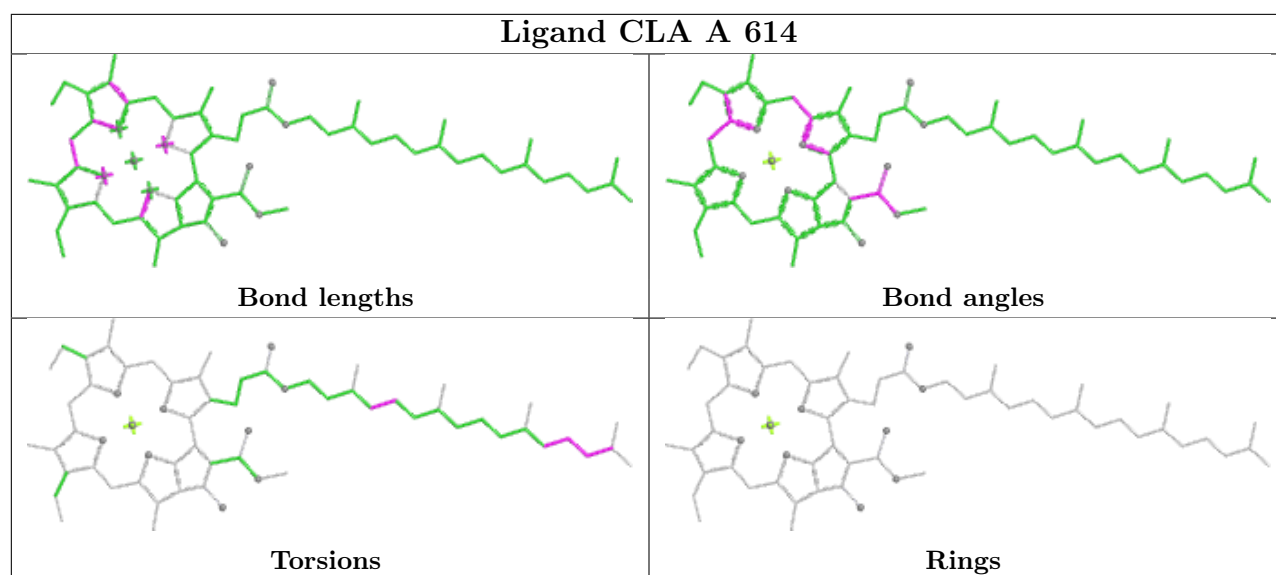


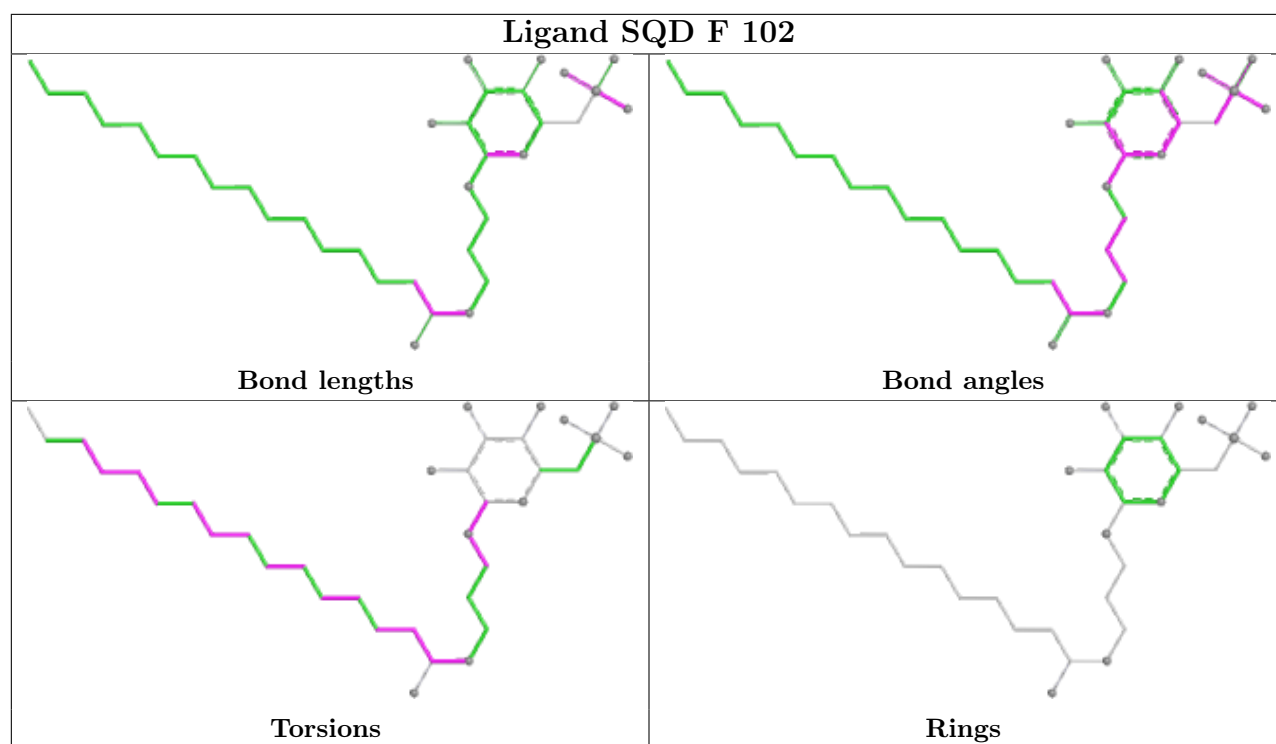
Ligand SQD a 615

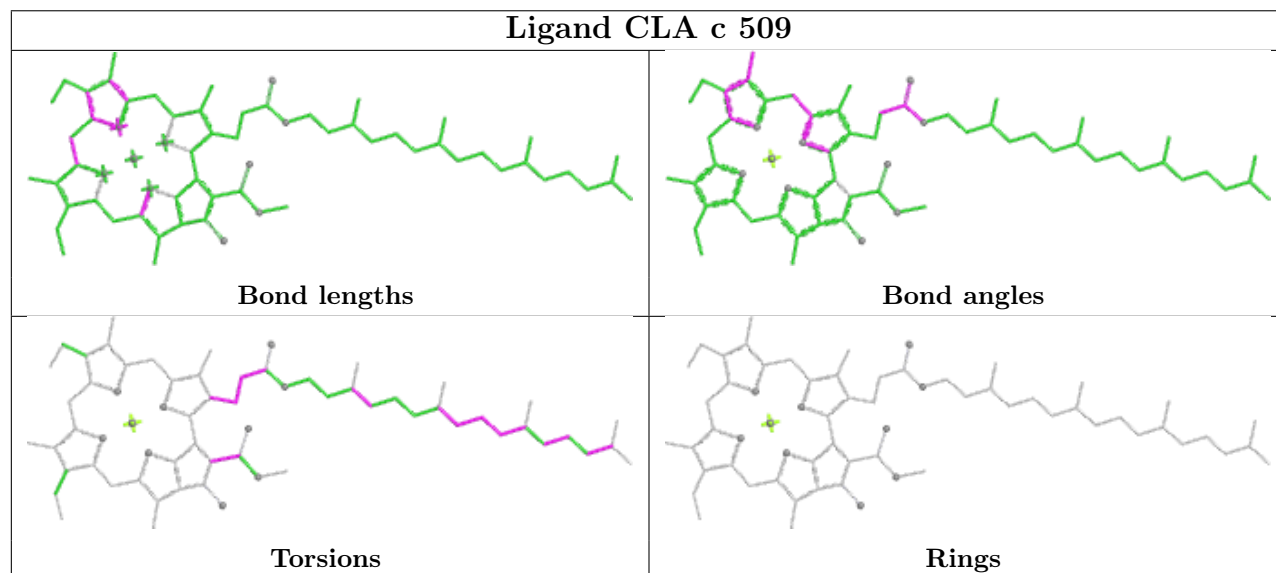
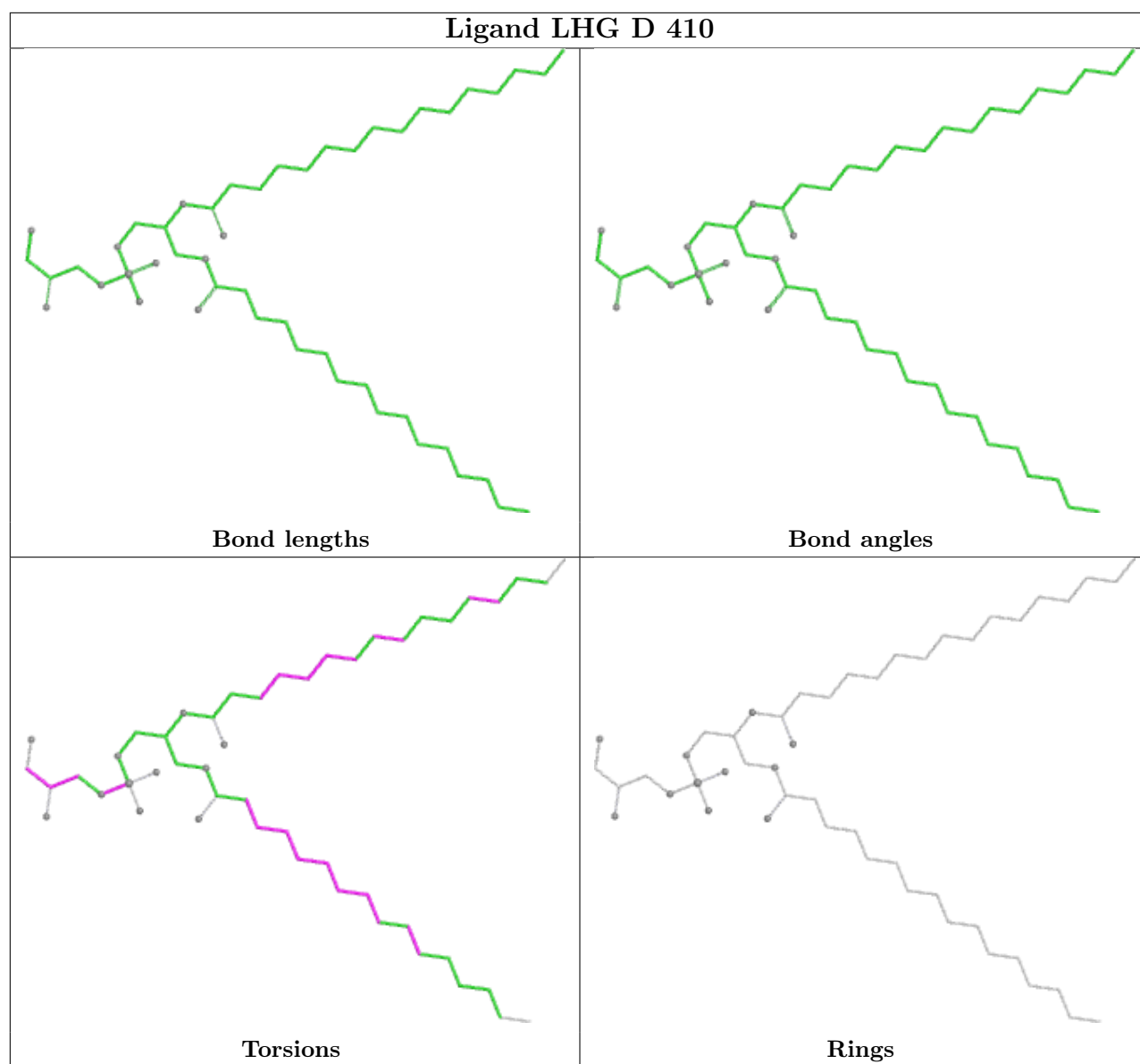


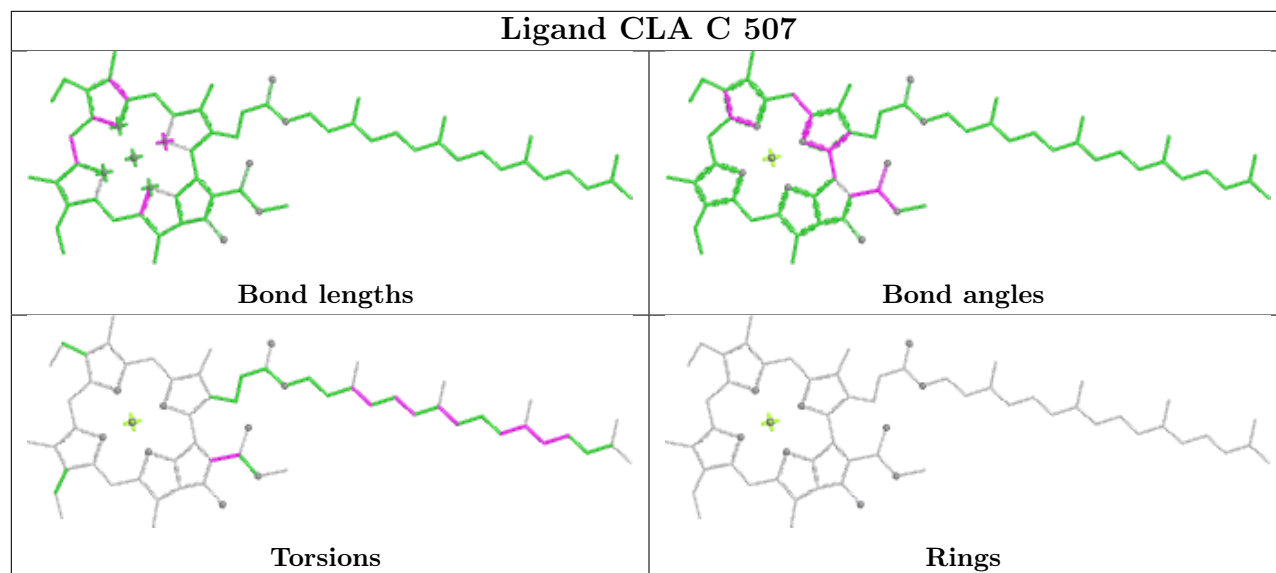
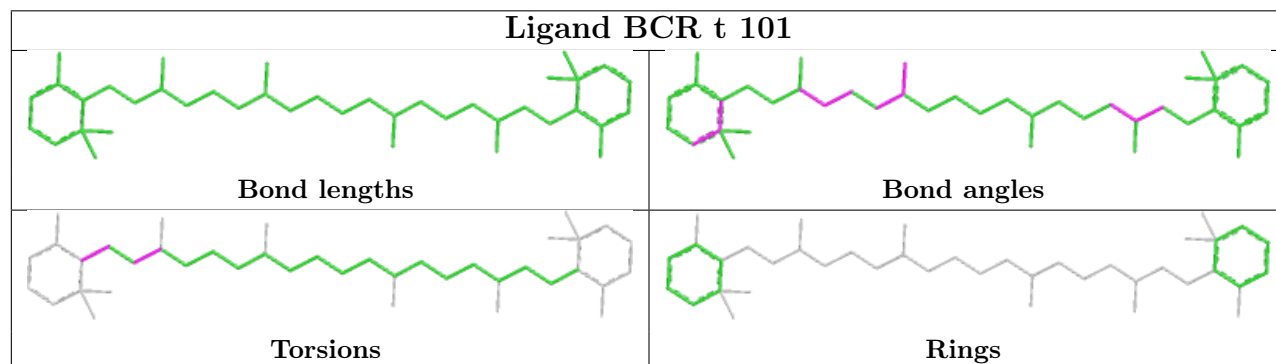
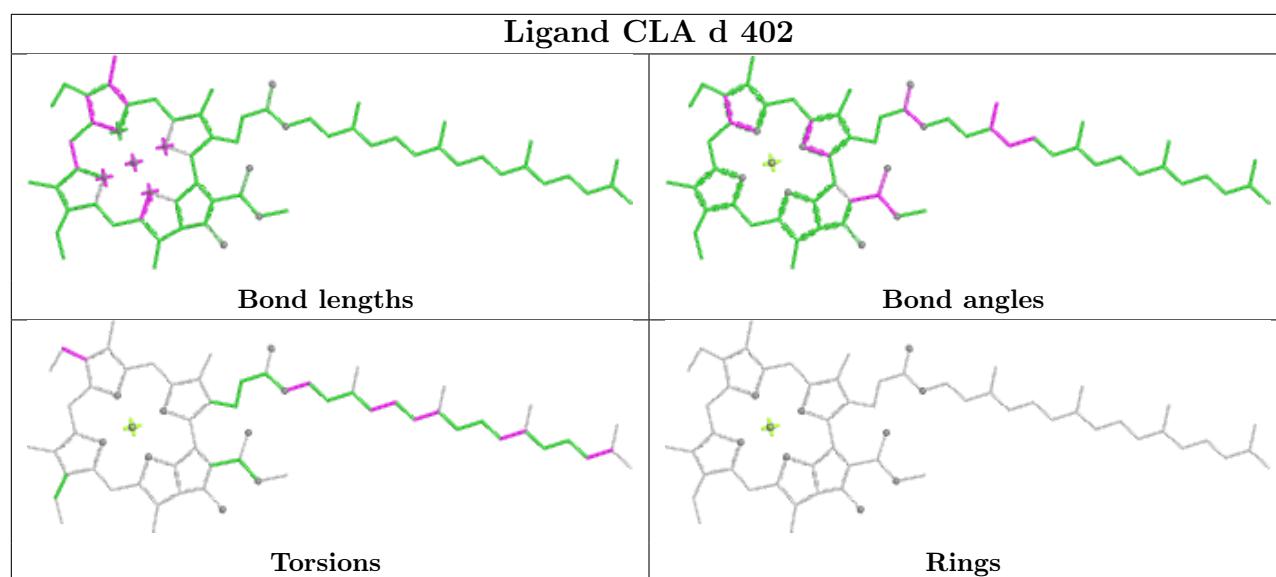


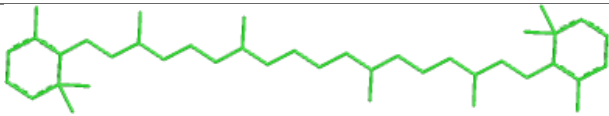
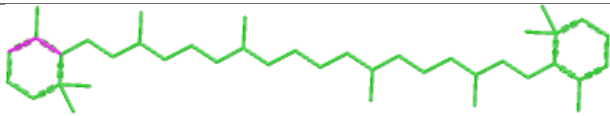
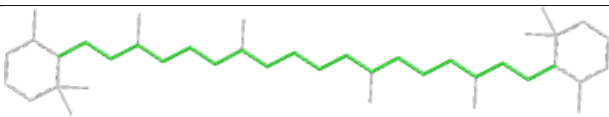
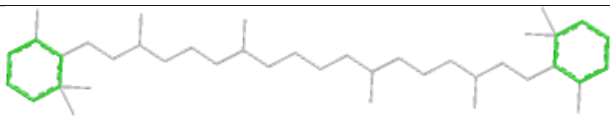


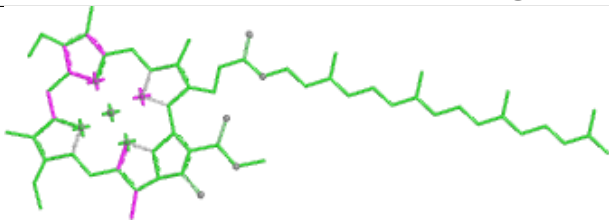
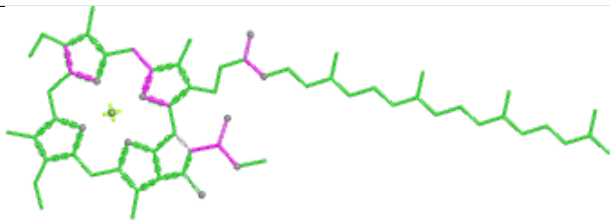
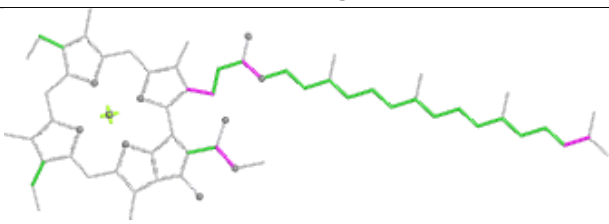
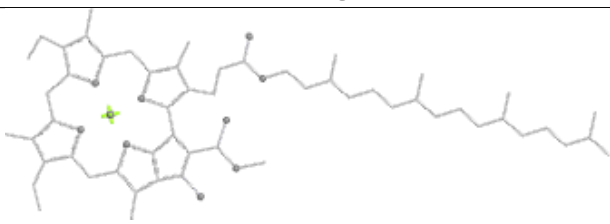


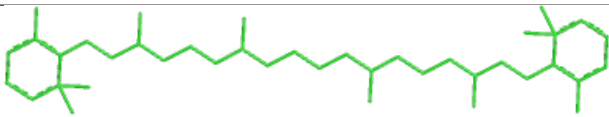
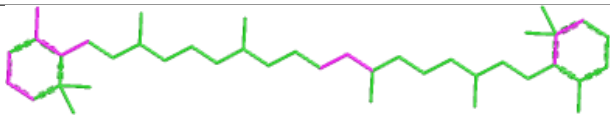
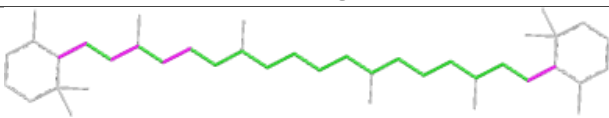
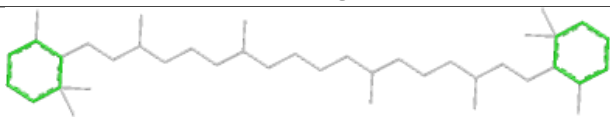


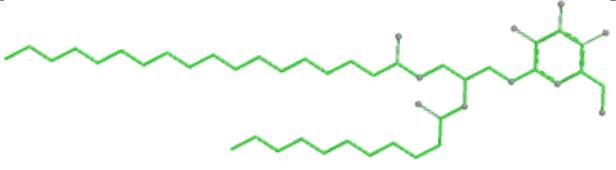
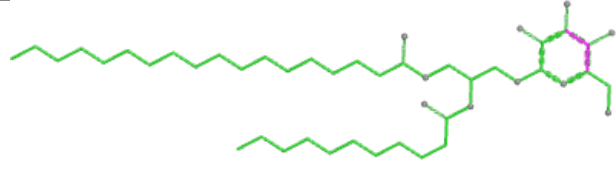
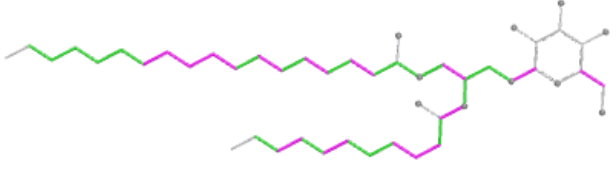
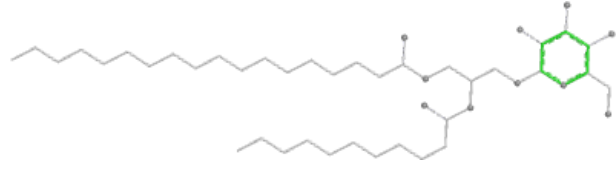


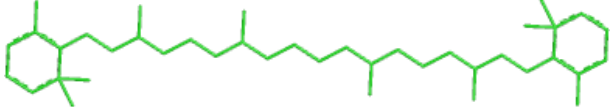
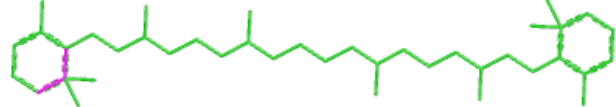
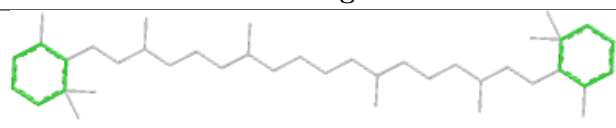


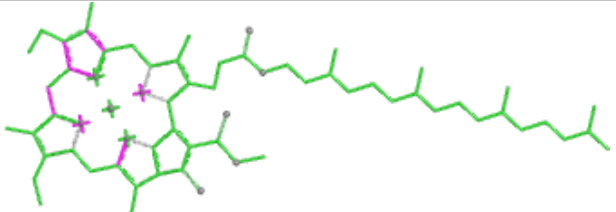
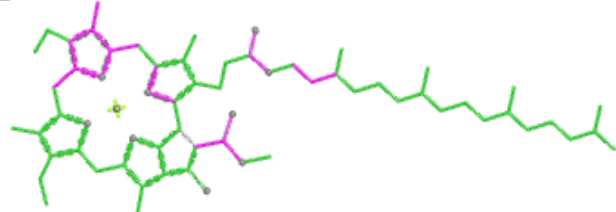
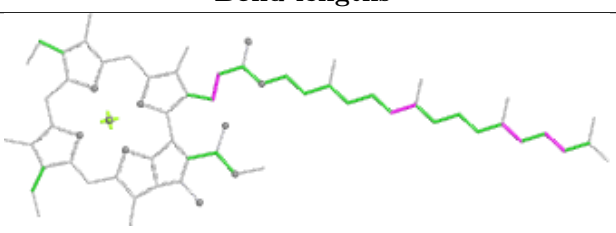
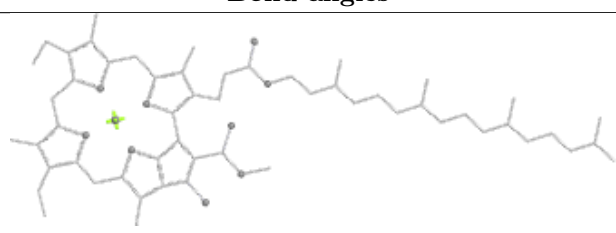
Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

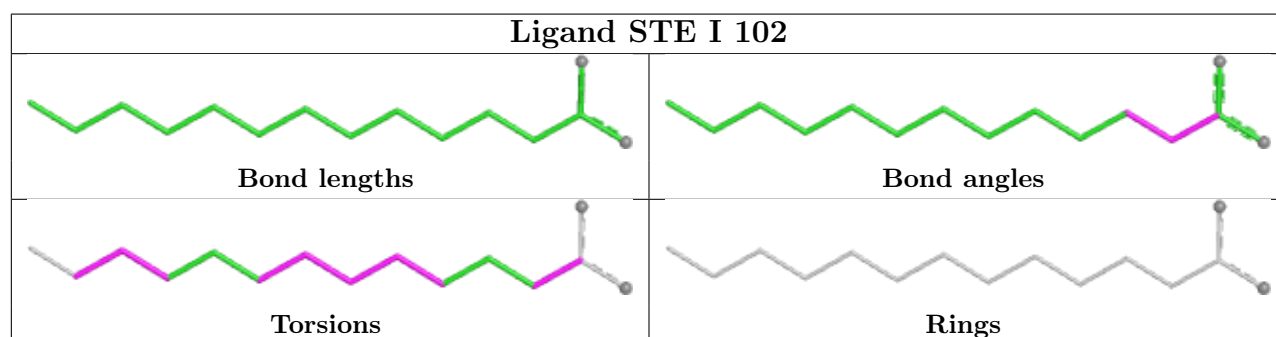
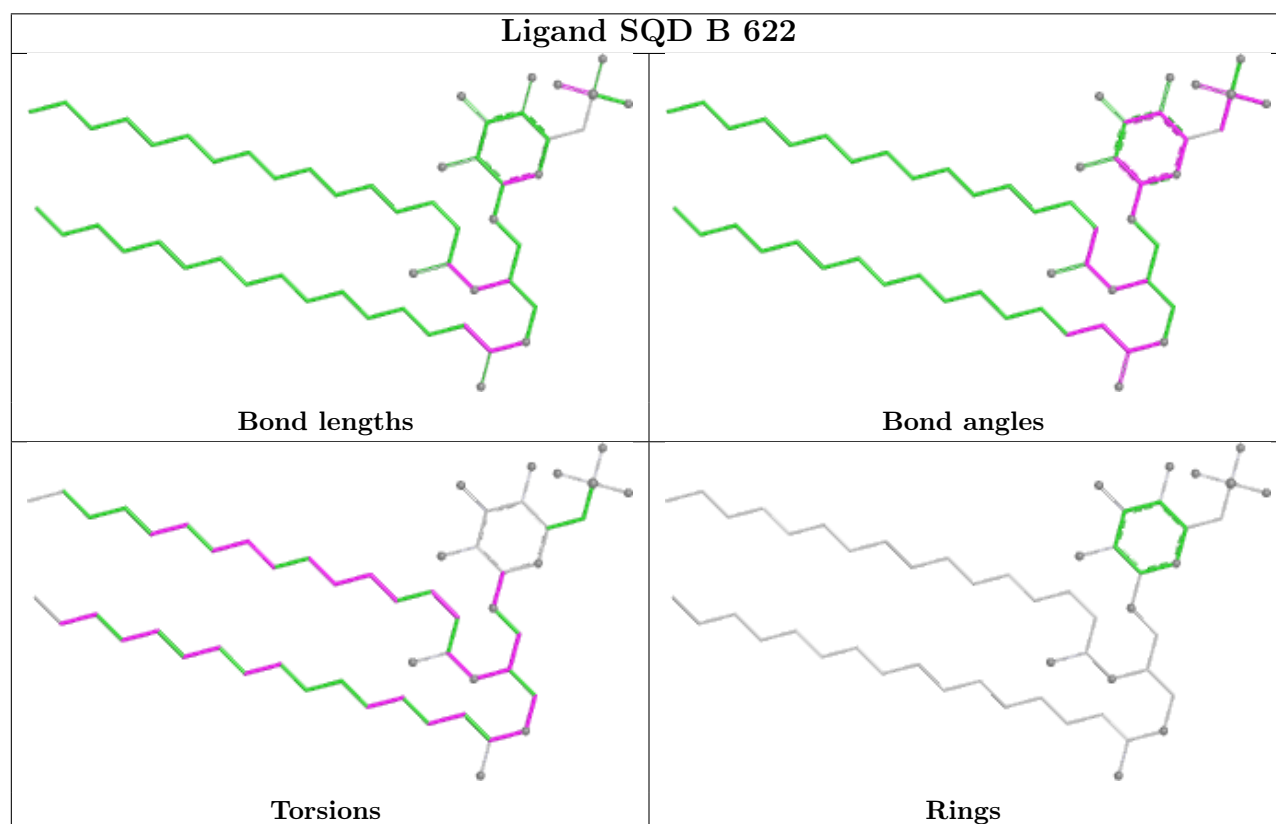
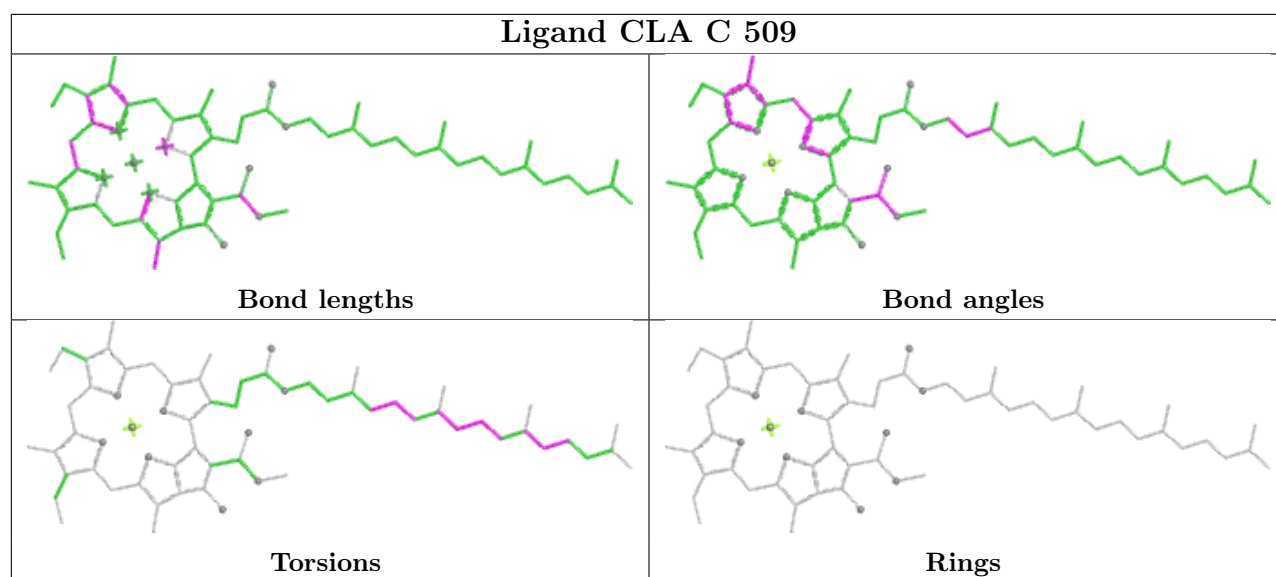
Ligand CLA C 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

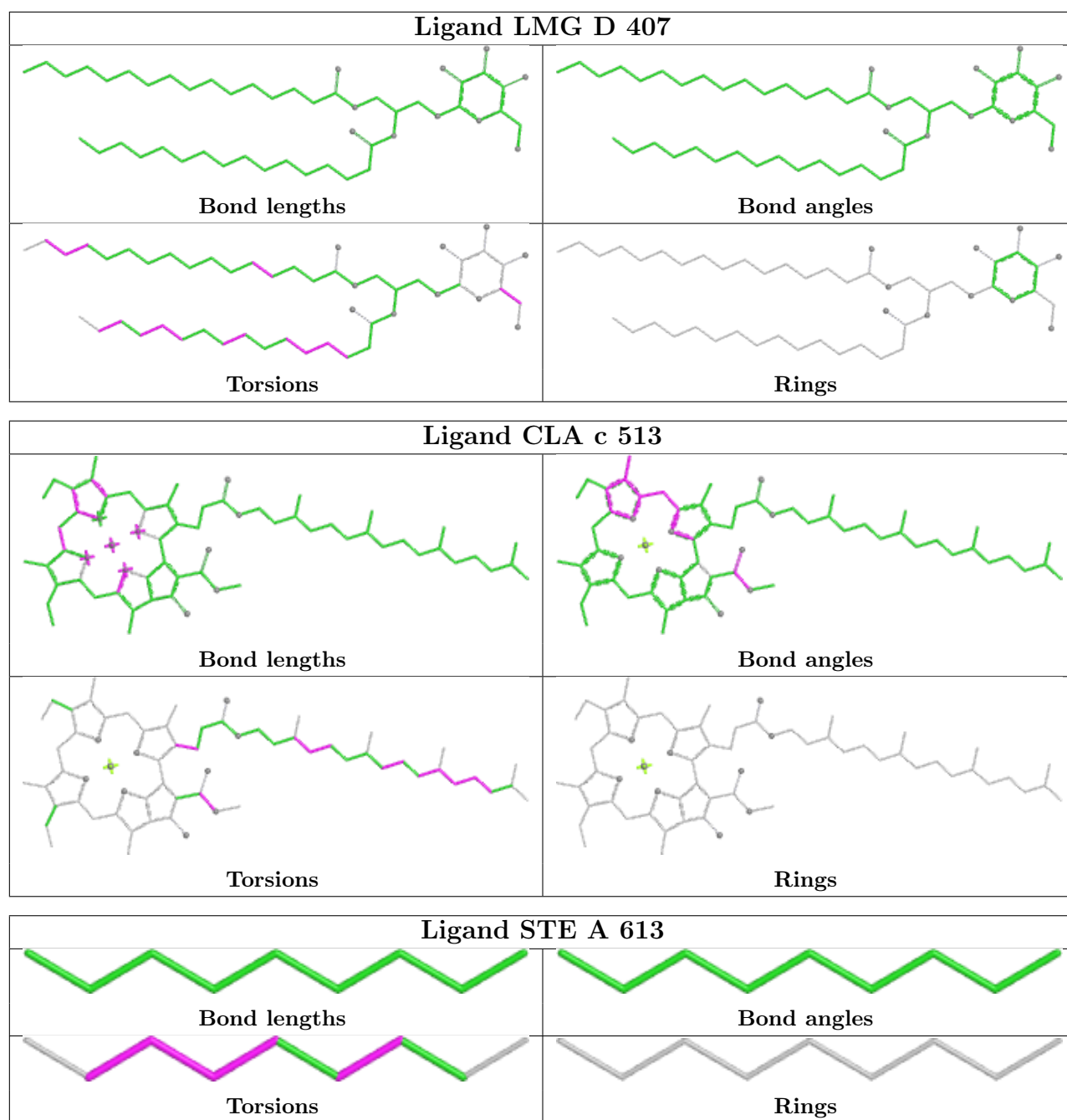
Ligand BCR X 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

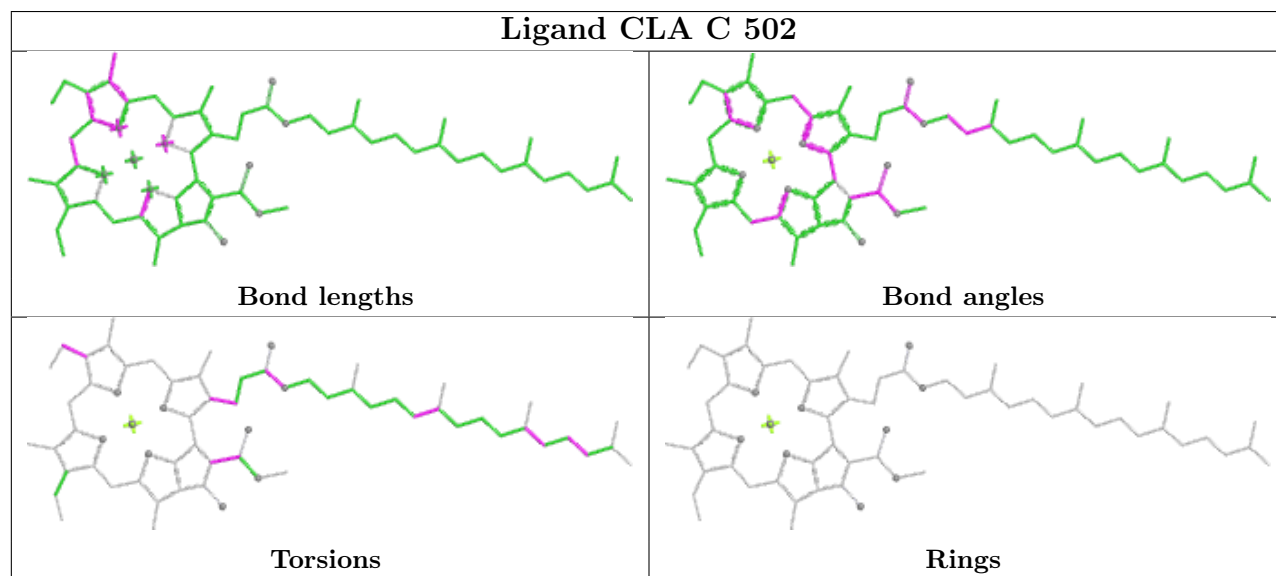
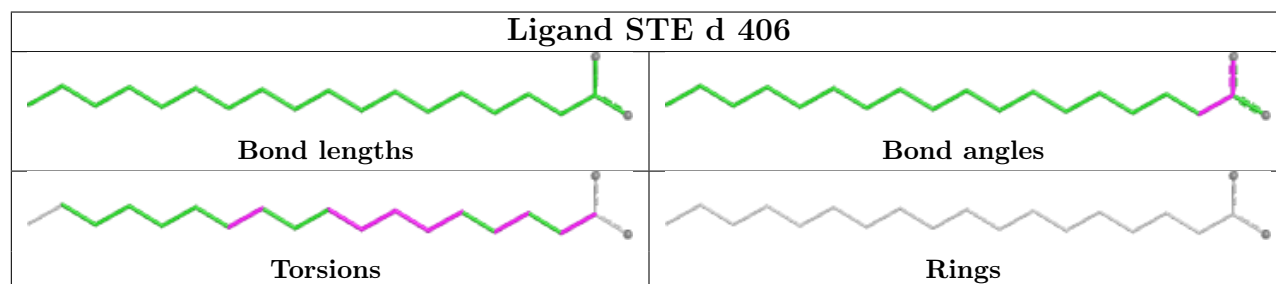
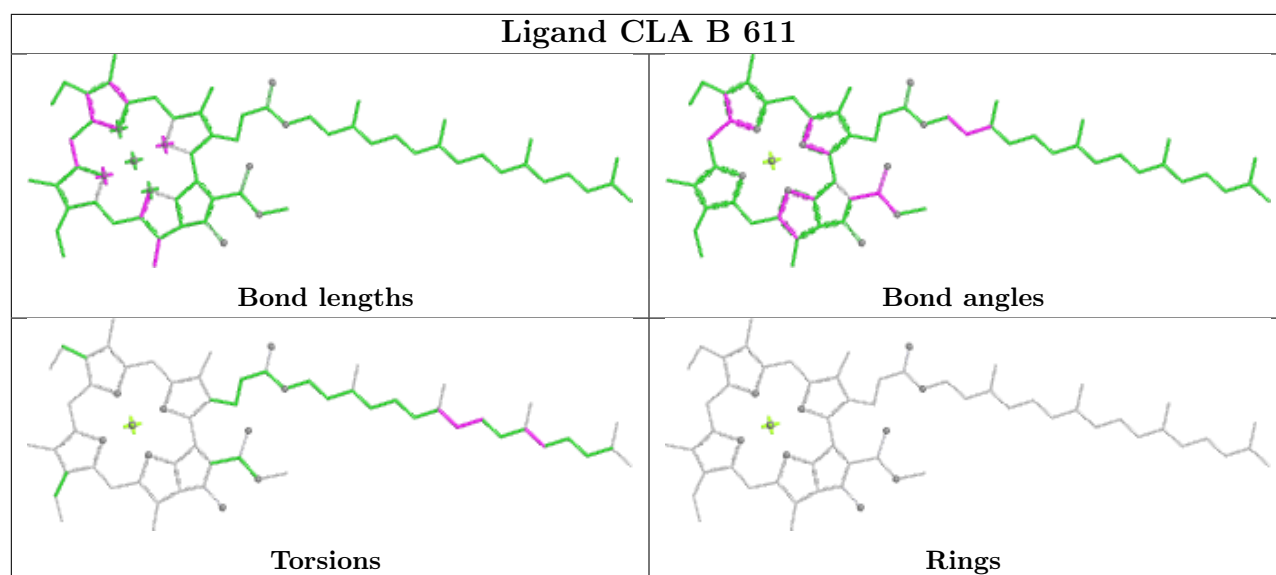
Ligand LMG c 523	
	
Bond lengths	Bond angles
	
Torsions	Rings

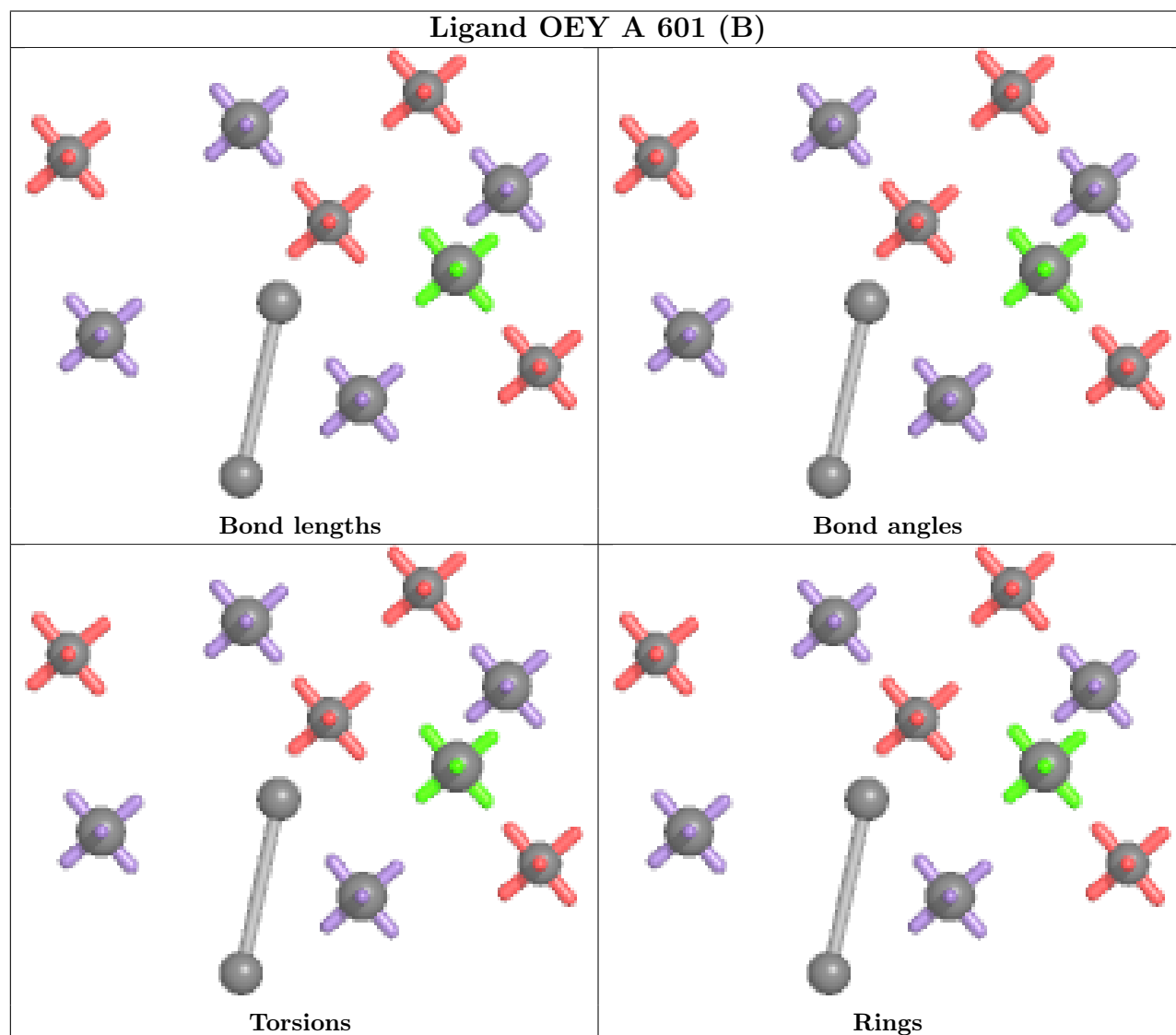
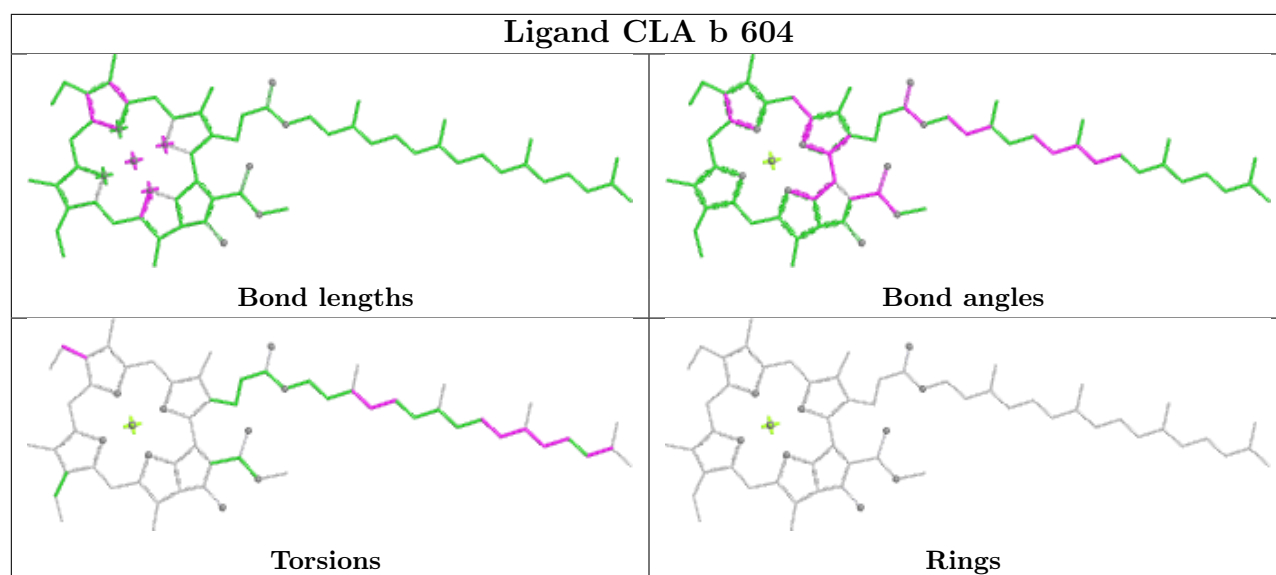
Ligand BCR C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

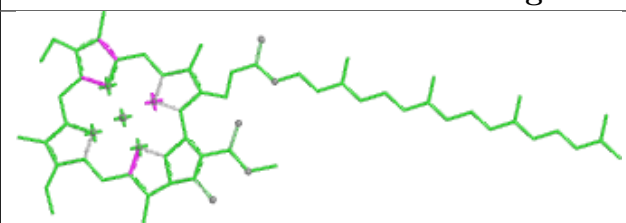
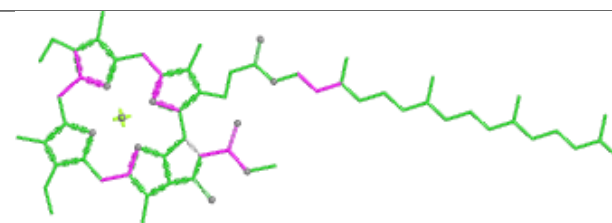
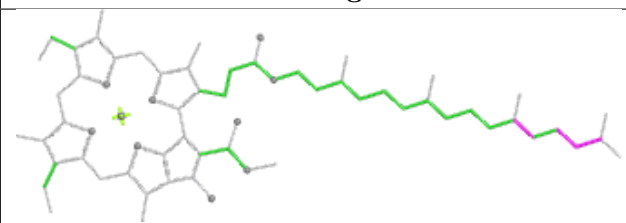
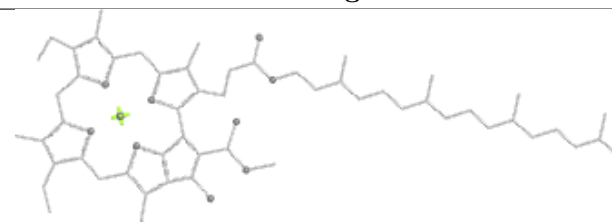
Ligand CLA b 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

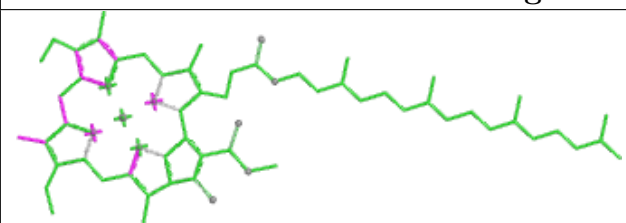
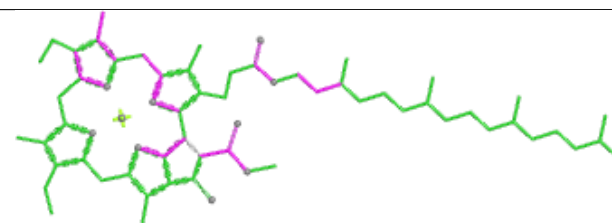
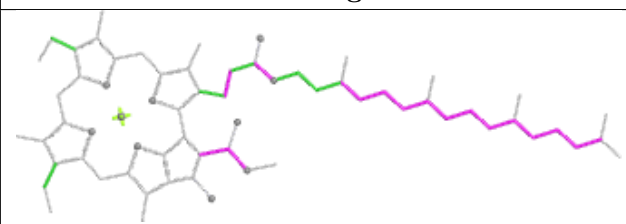
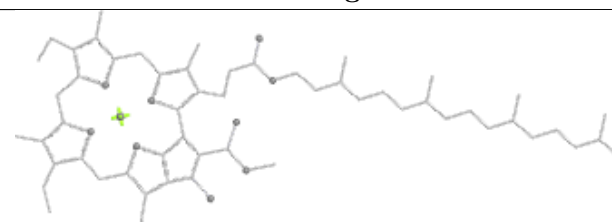




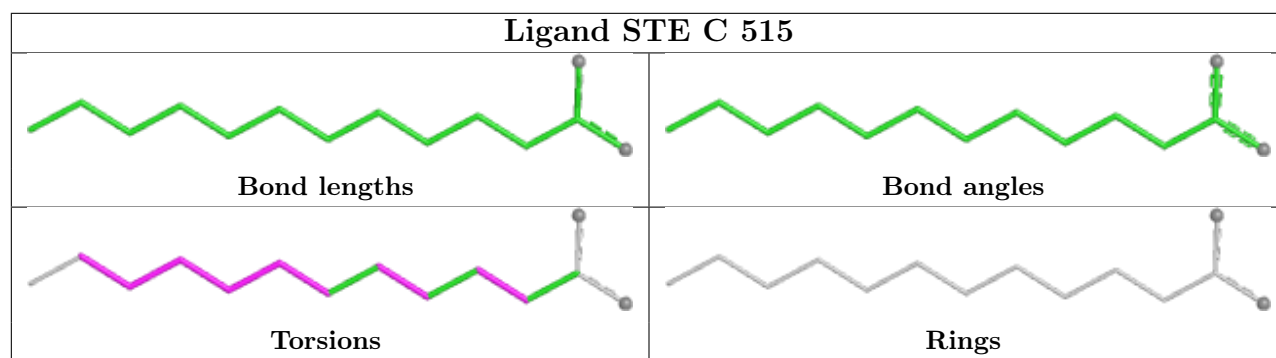
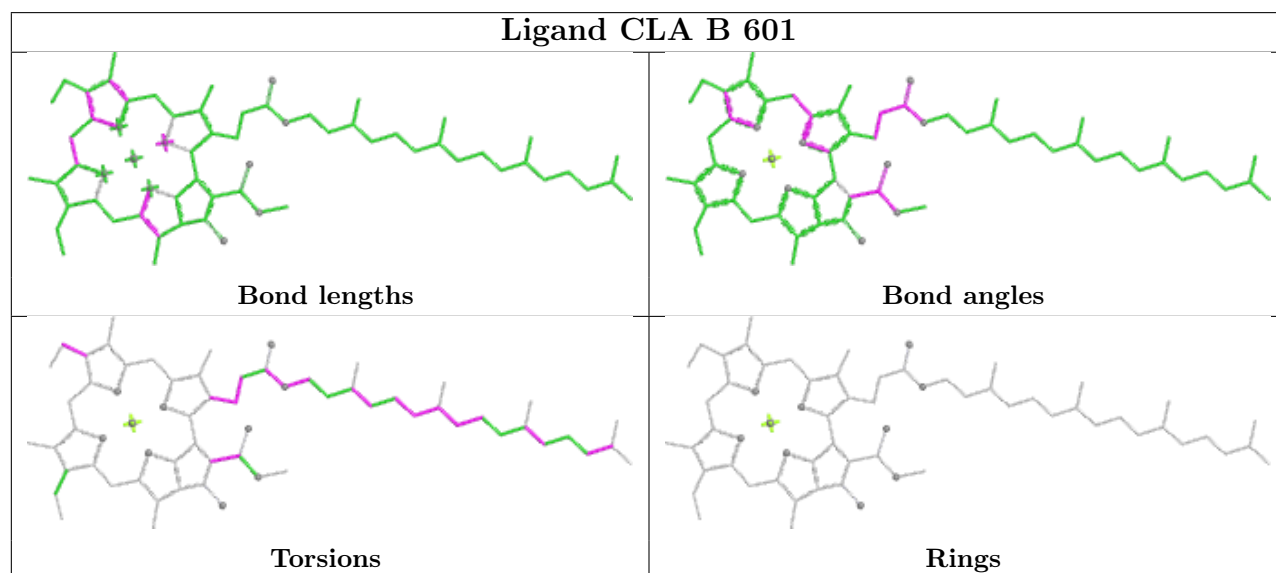
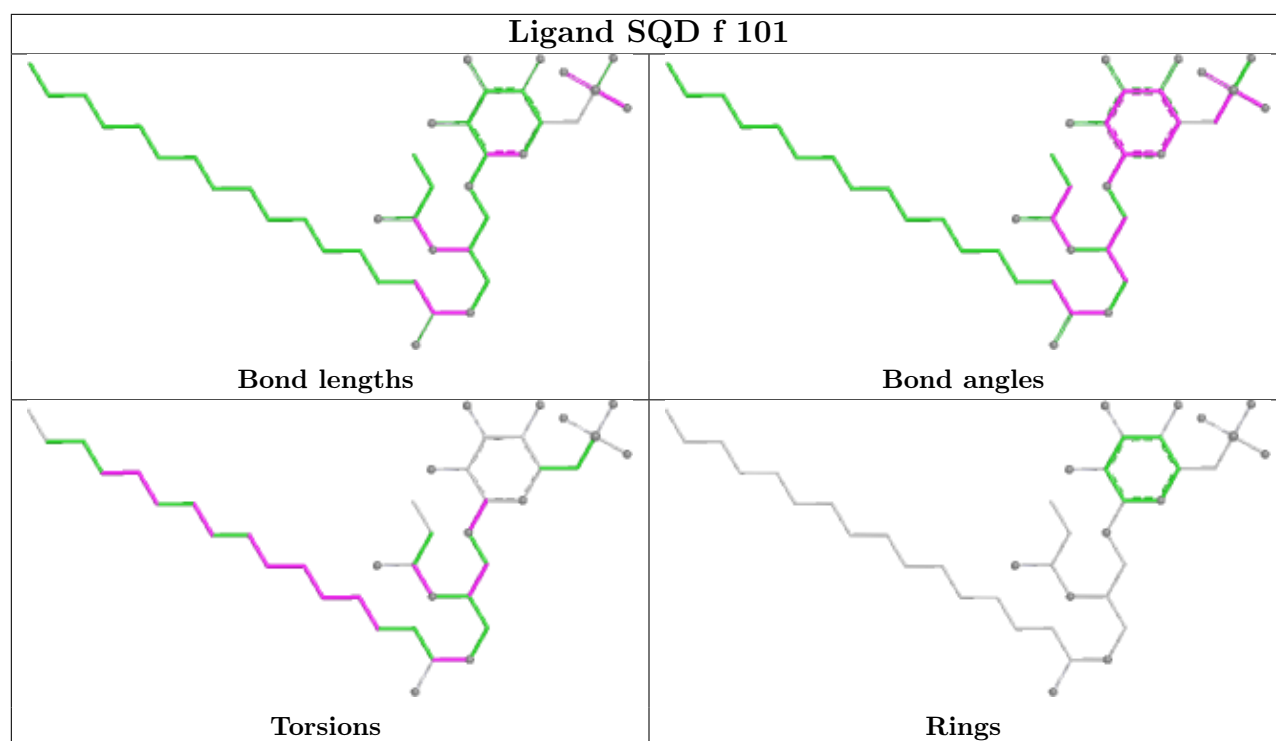


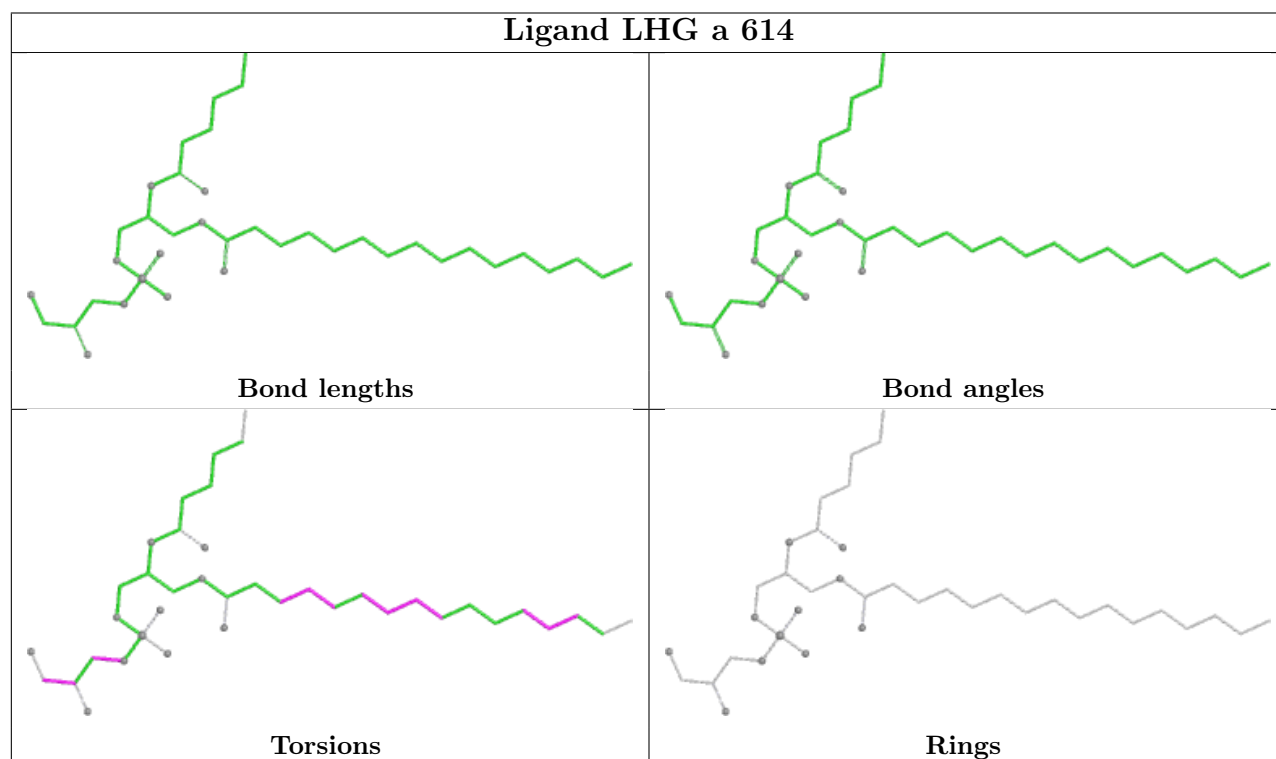
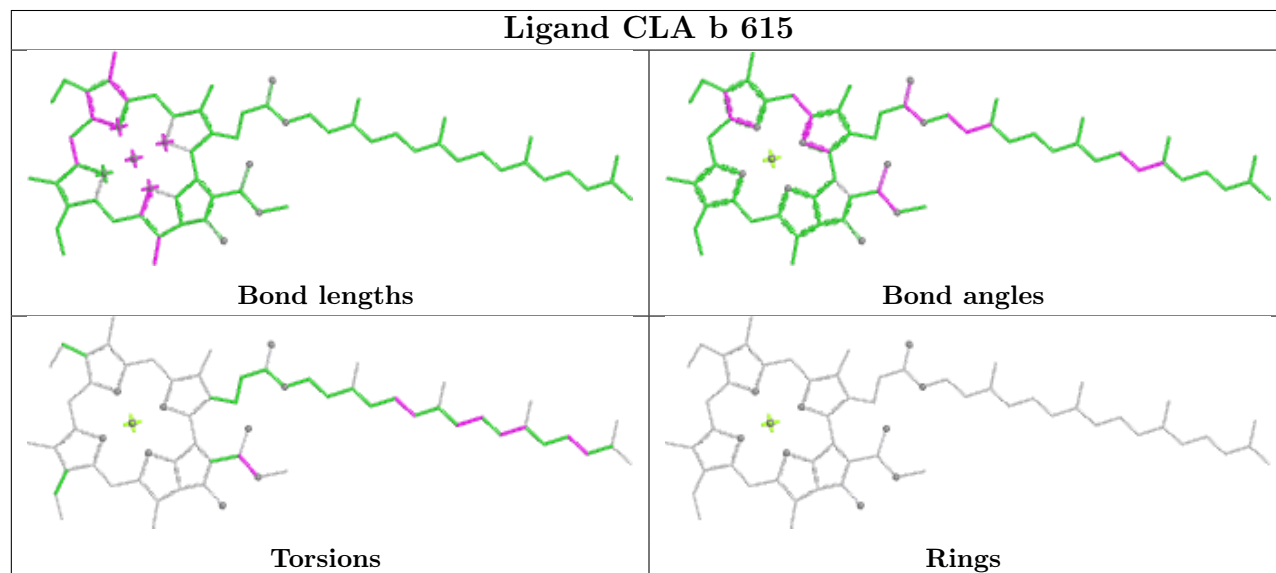
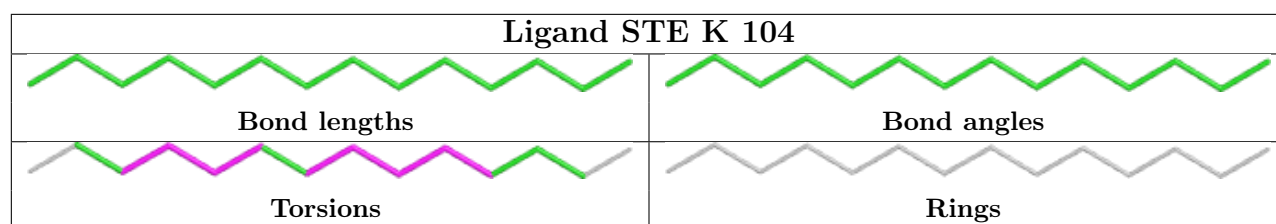


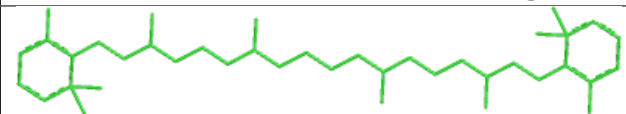
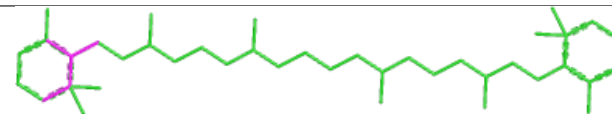
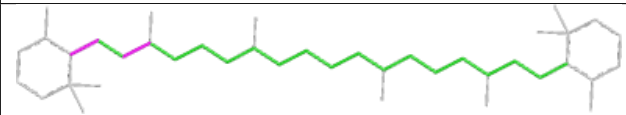
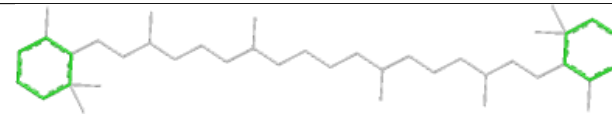
Ligand CLA a 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

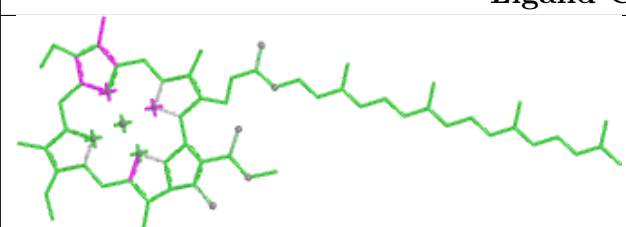
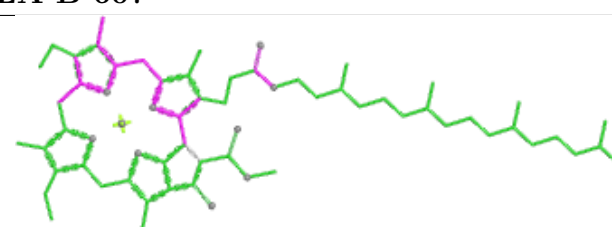
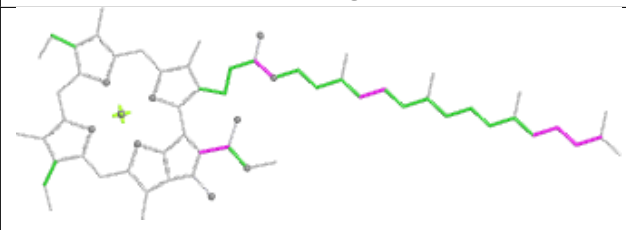
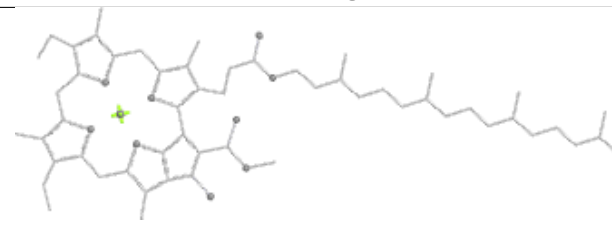
Ligand CLA b 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

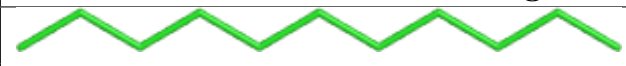
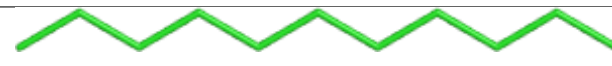
Ligand PL9 a 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

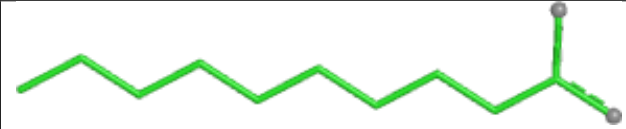
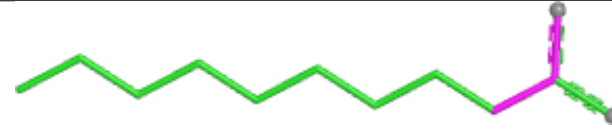
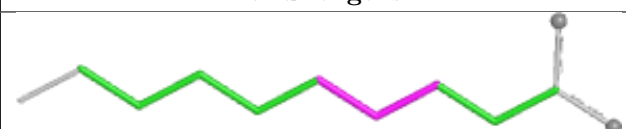
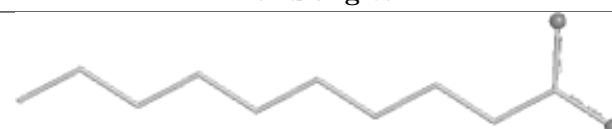


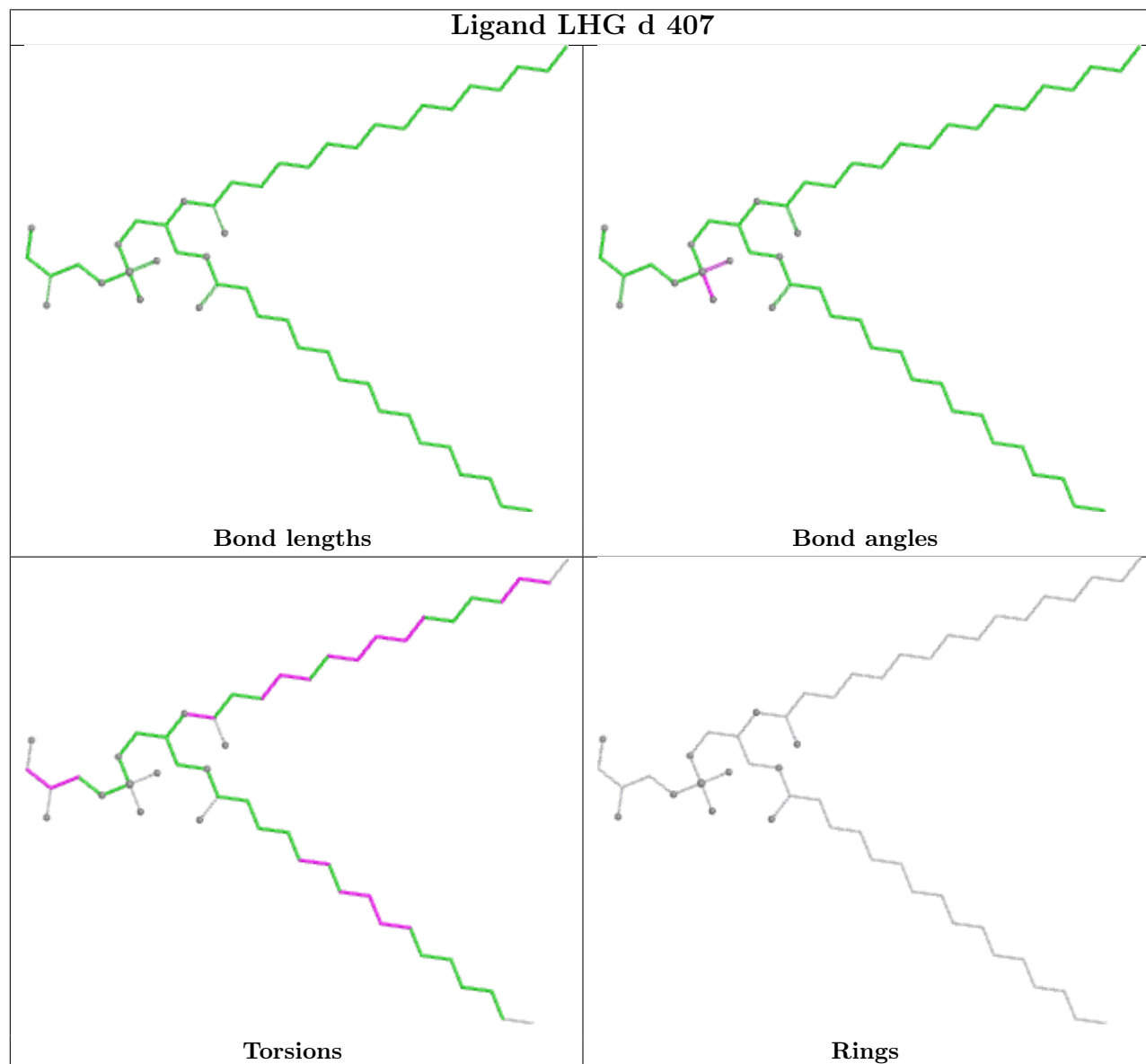
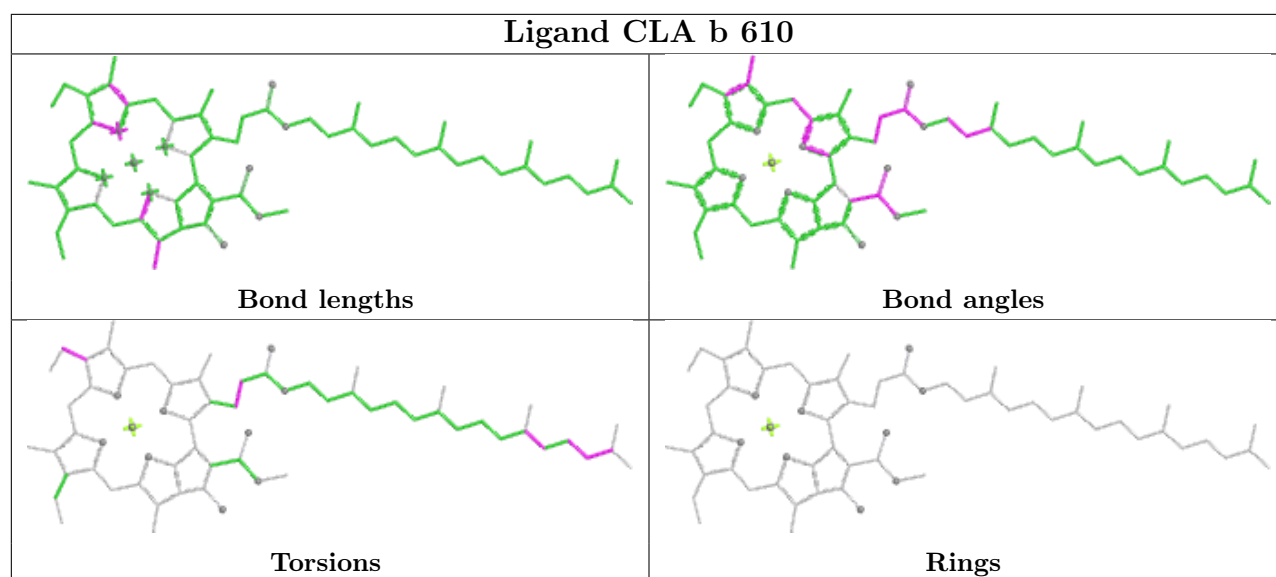


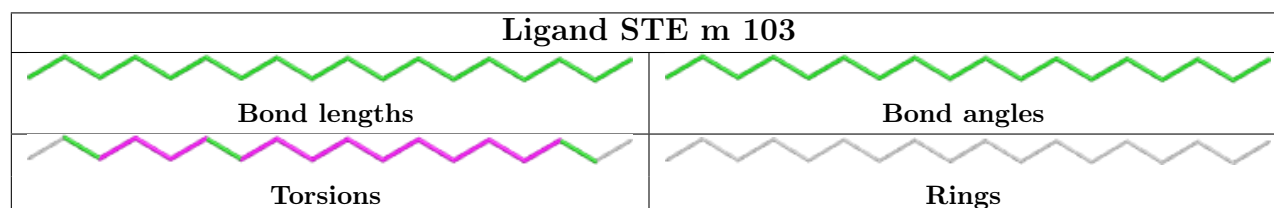
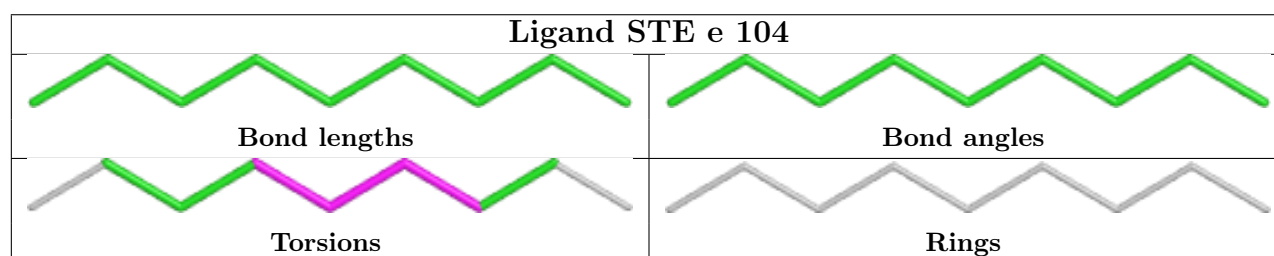
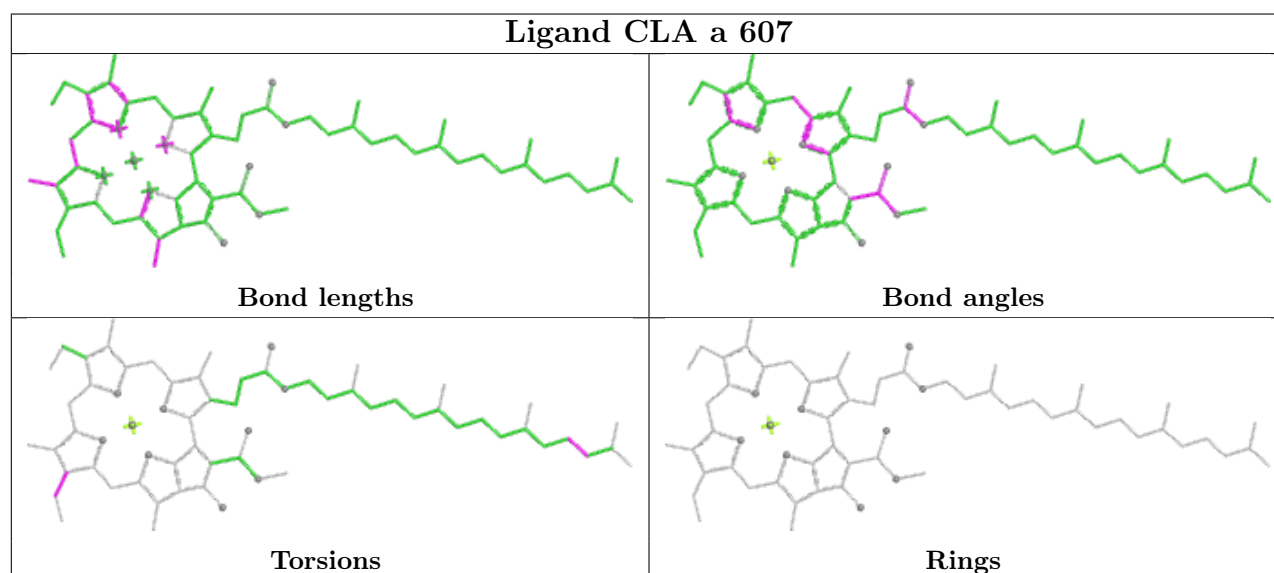
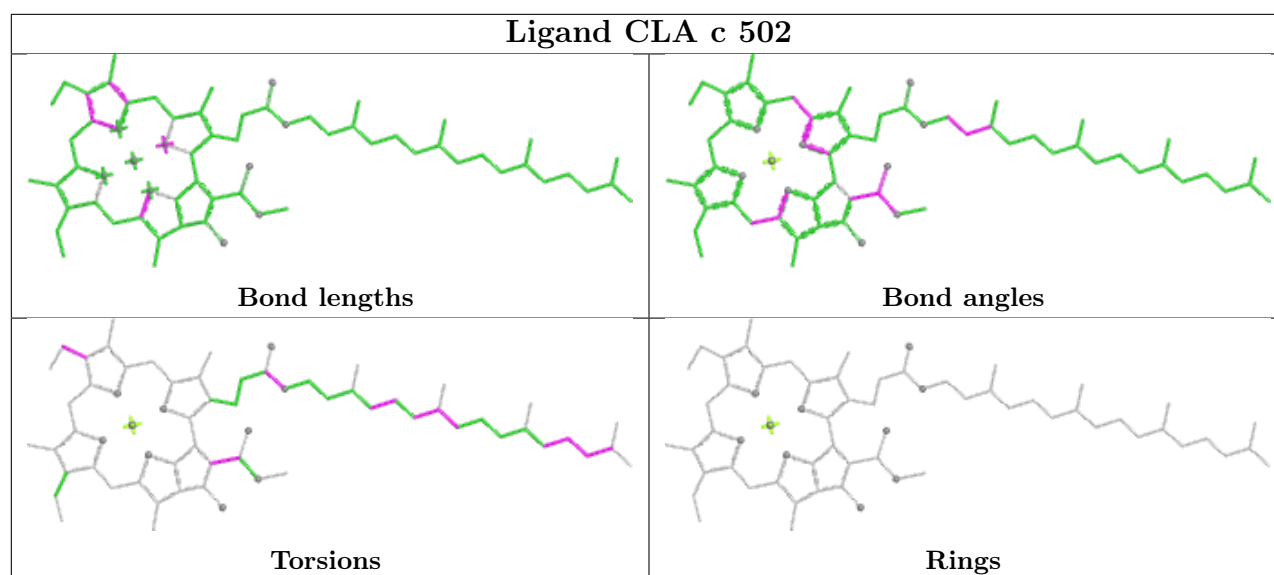
Ligand BCR h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

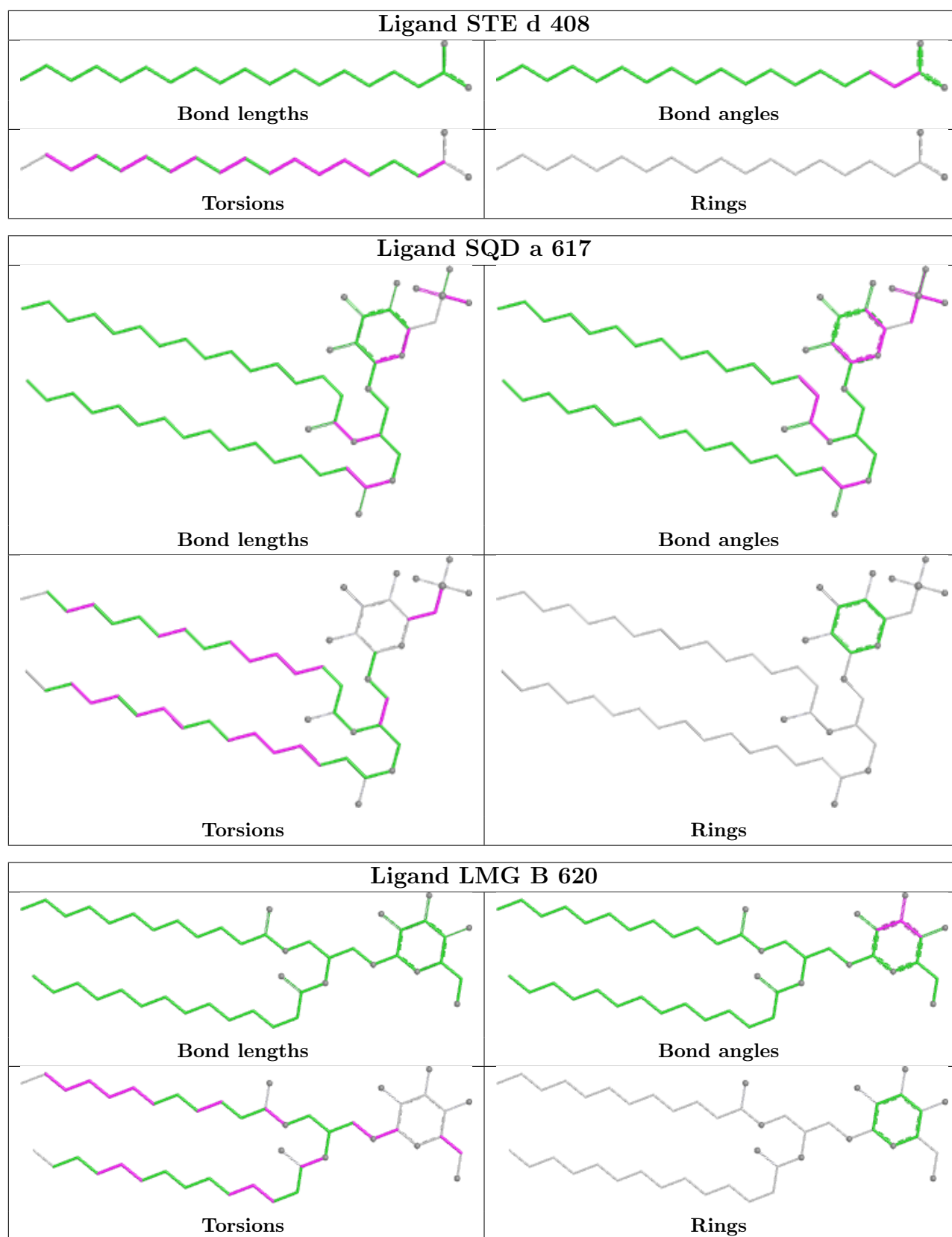
Ligand CLA B 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

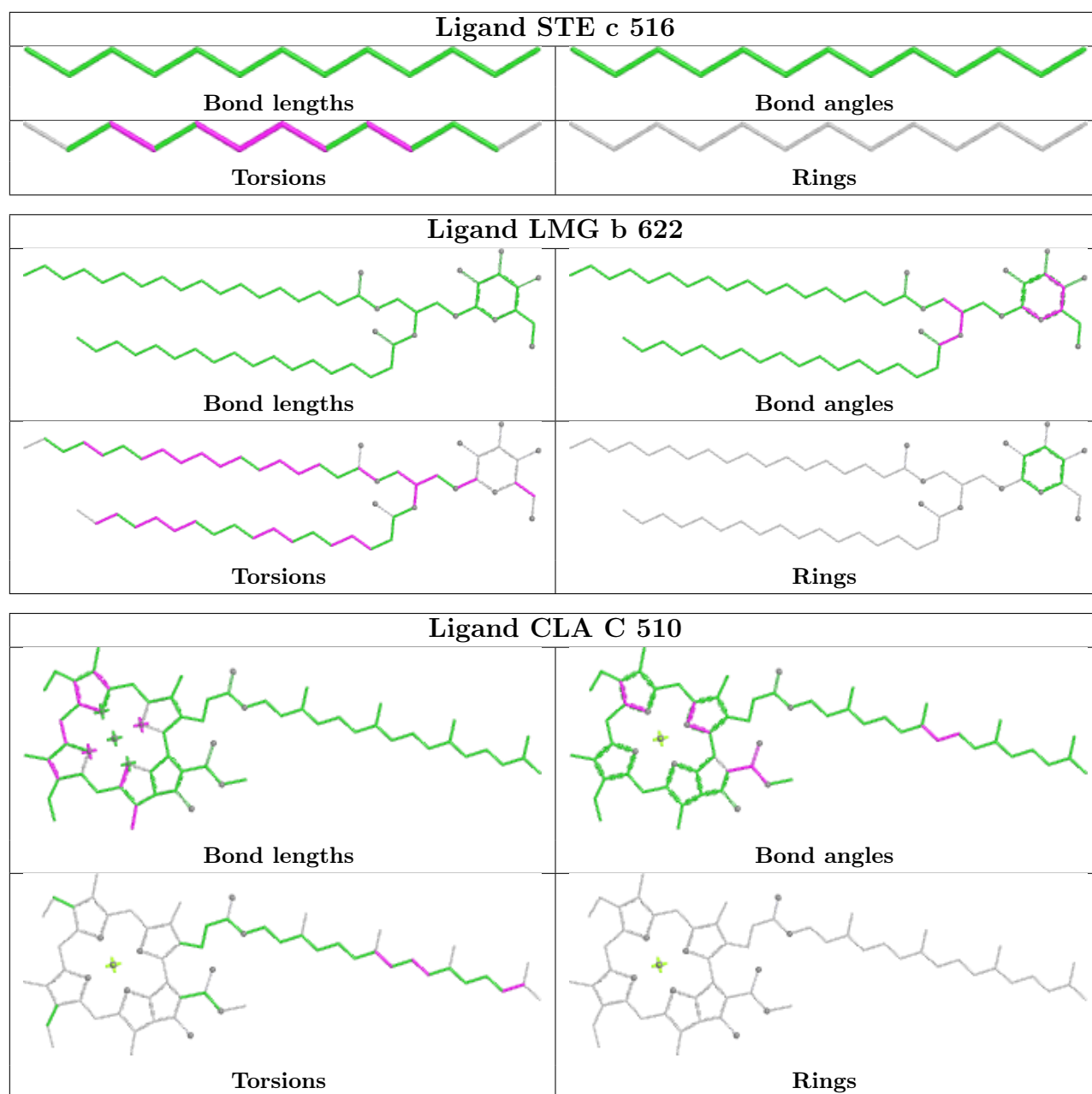
Ligand STE A 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

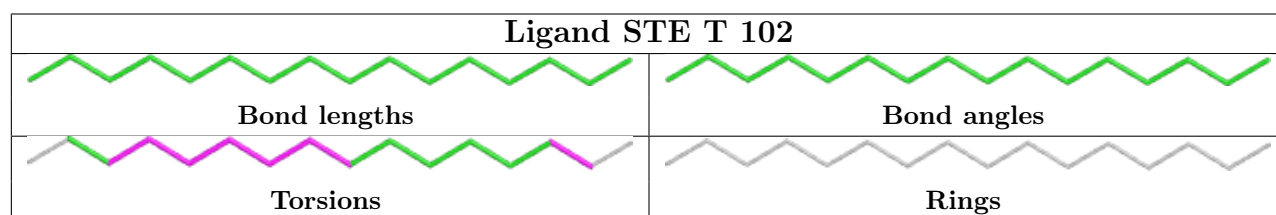
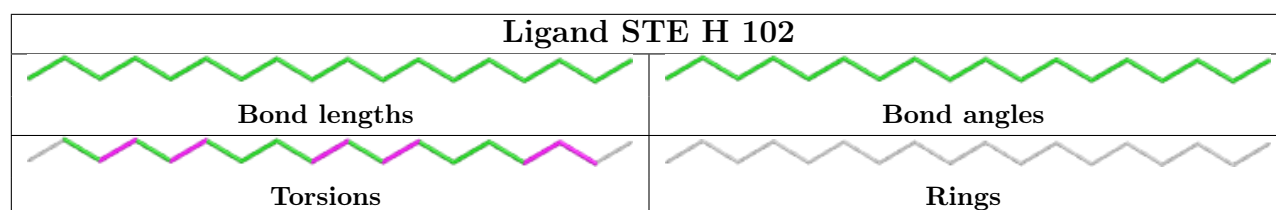
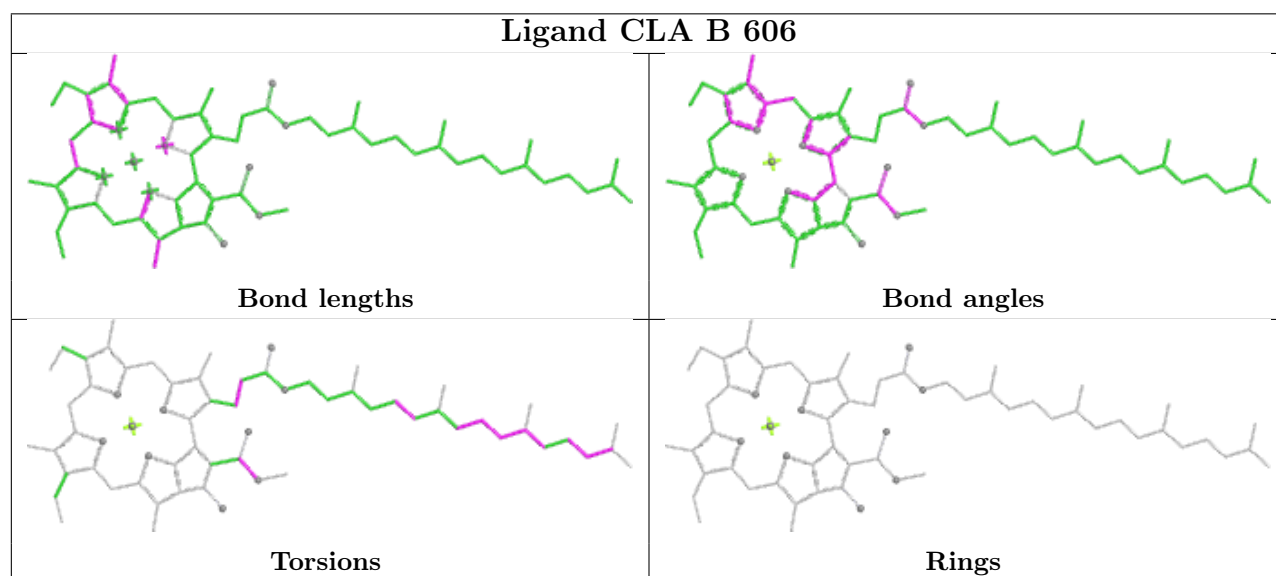
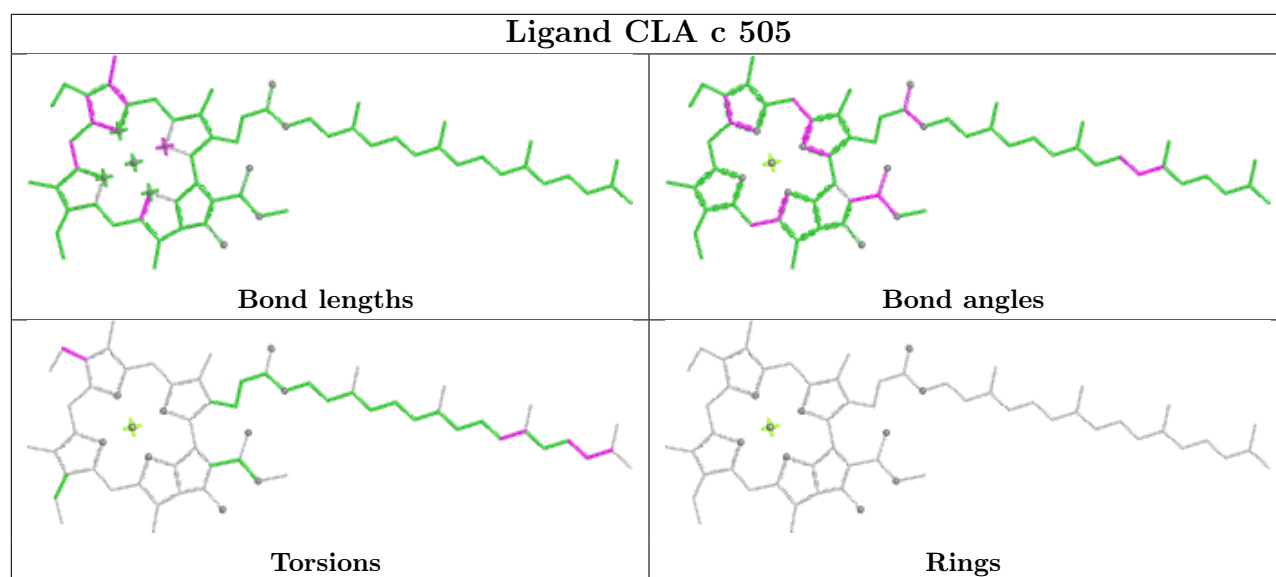
Ligand STE C 524	
	
Bond lengths	Bond angles
	
Torsions	Rings



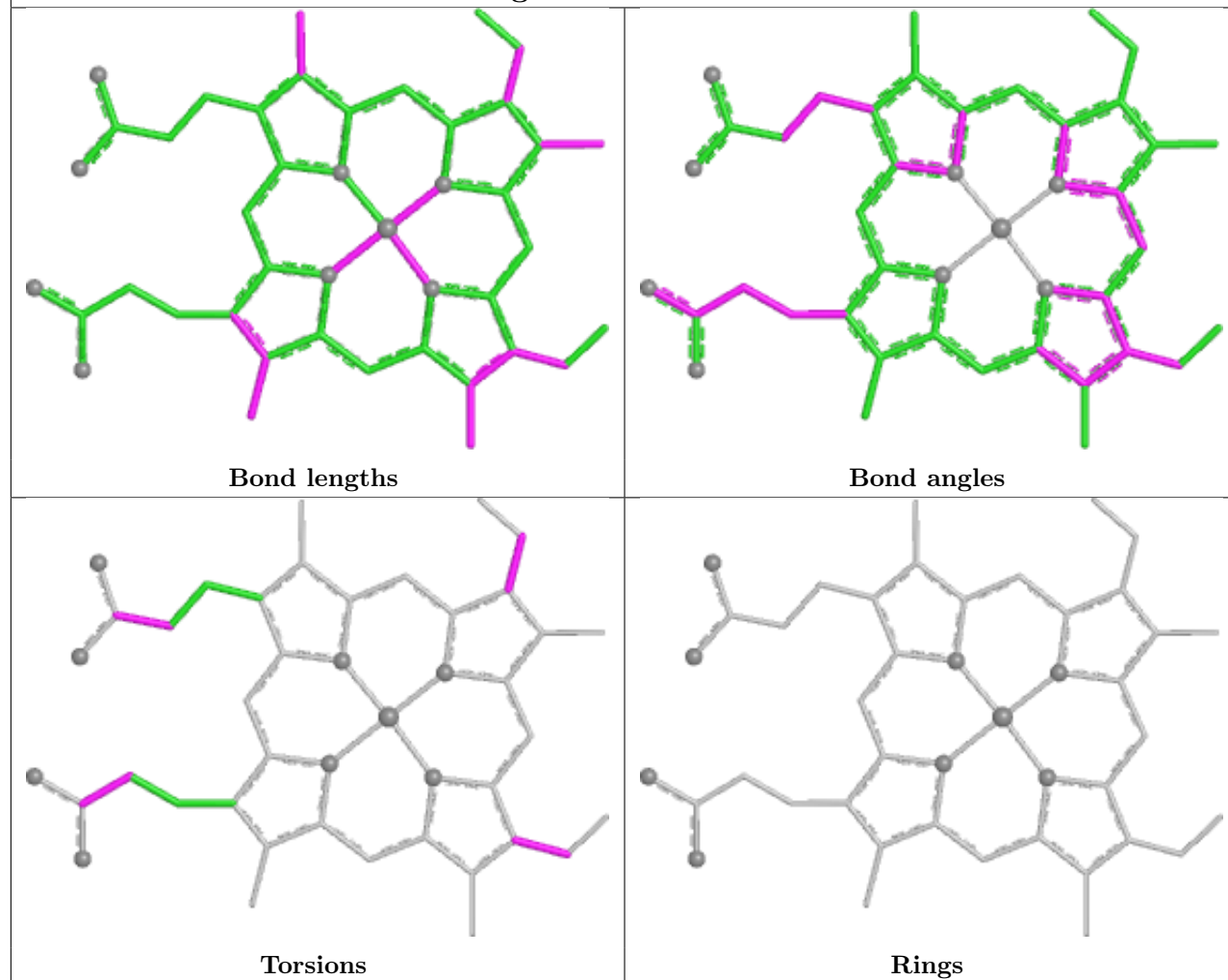




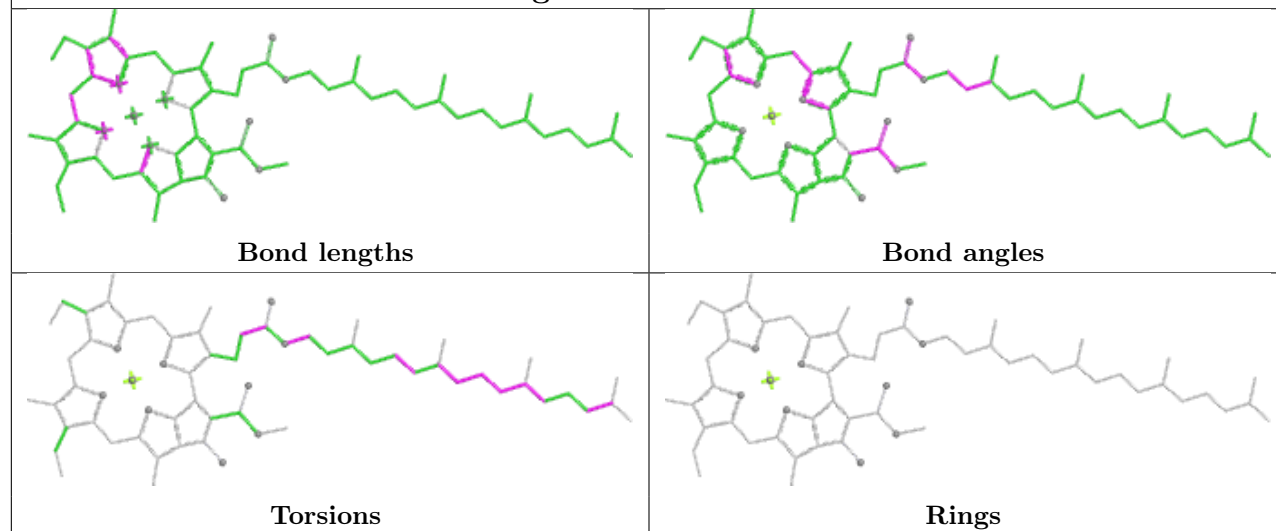


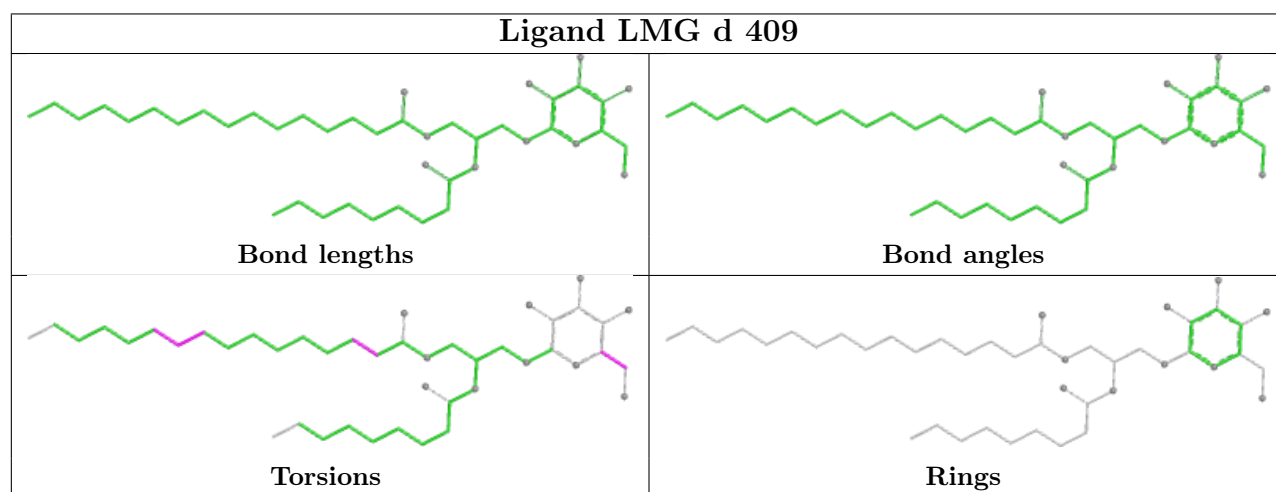
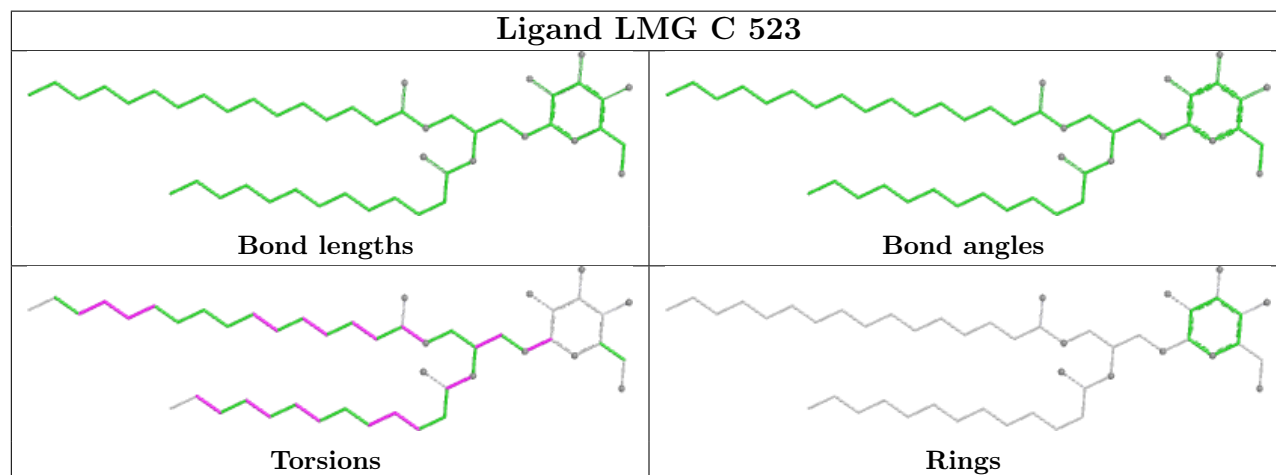
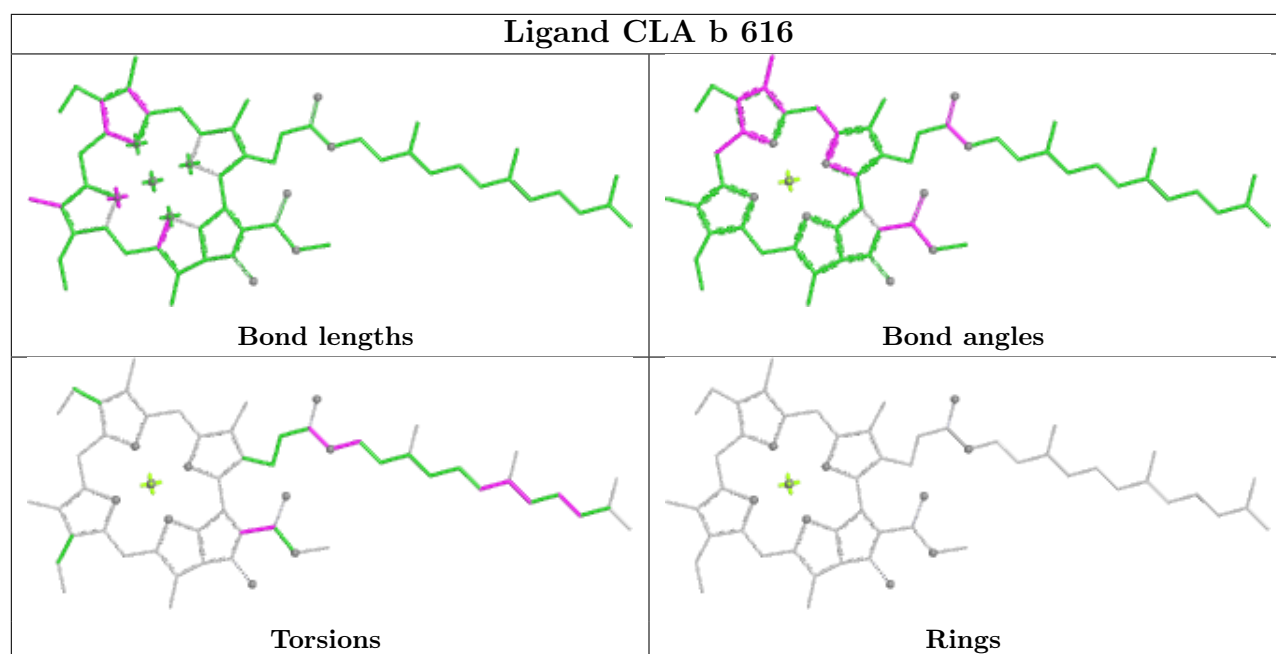


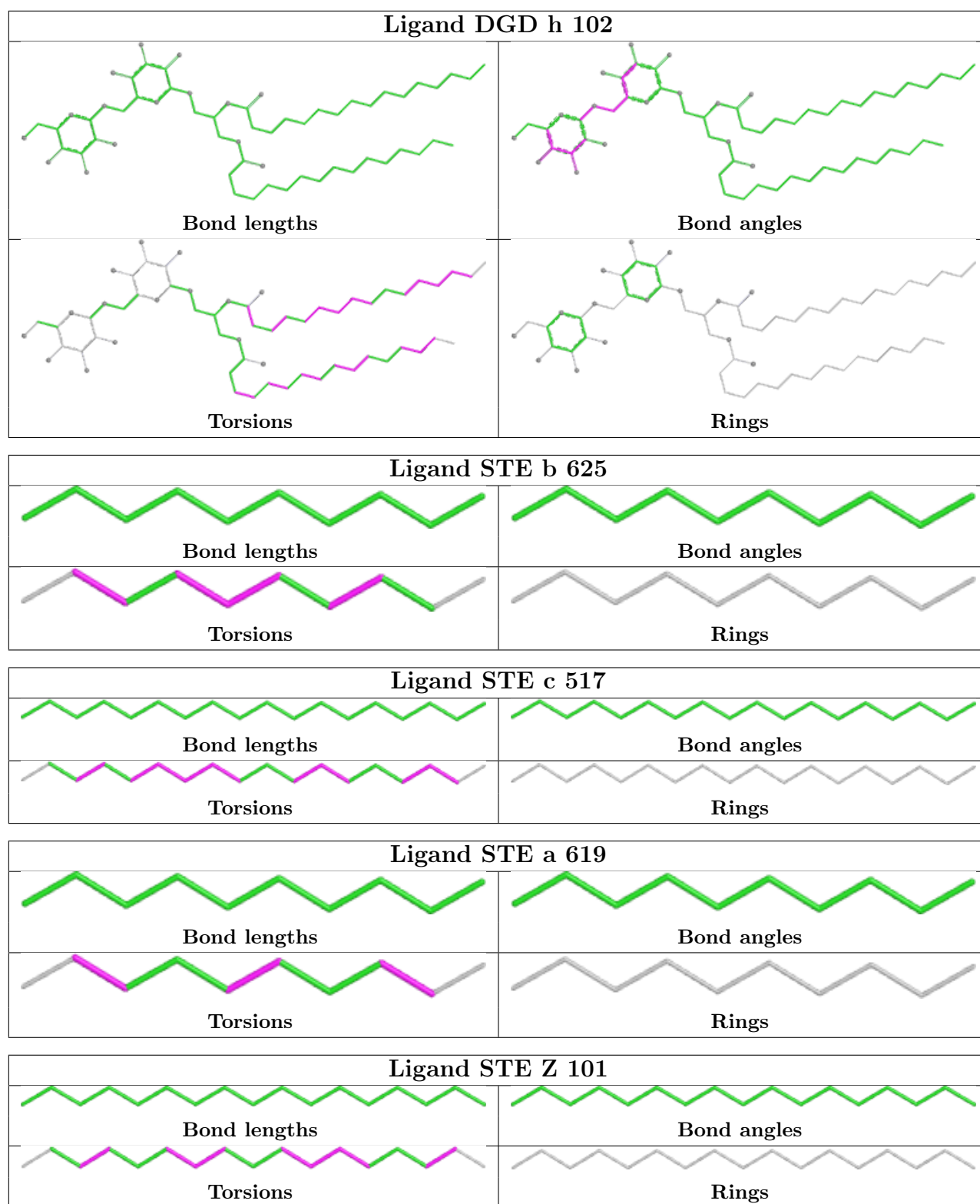
Ligand HEM e 102

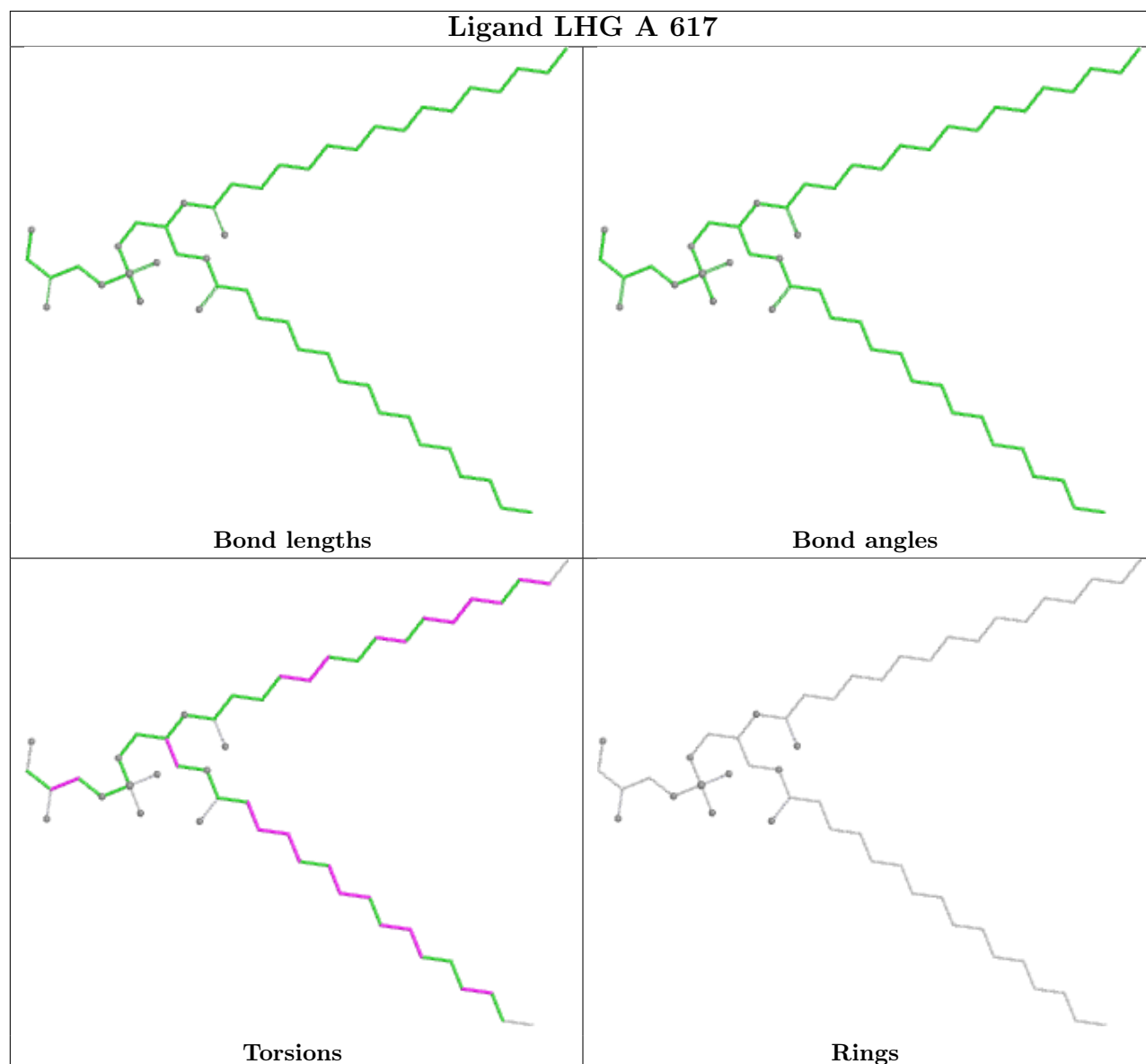
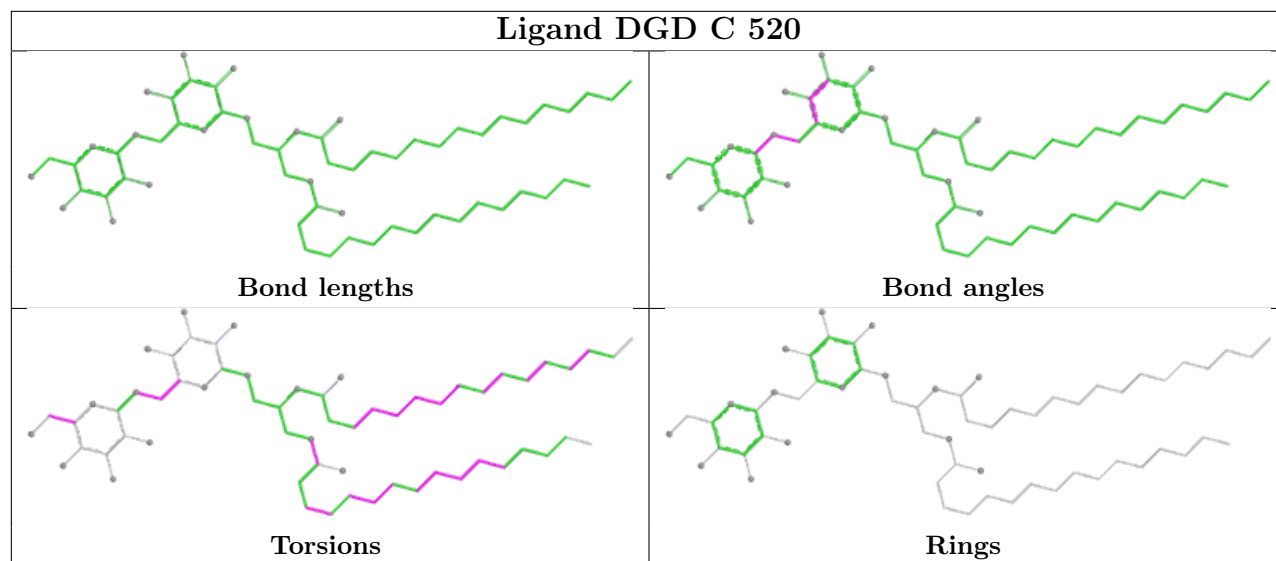


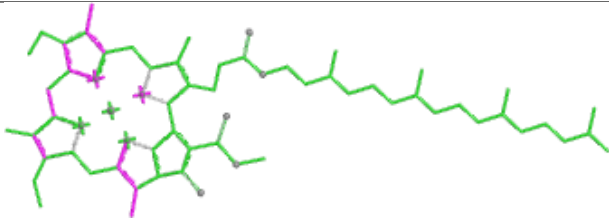
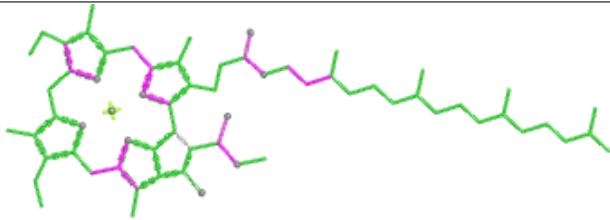
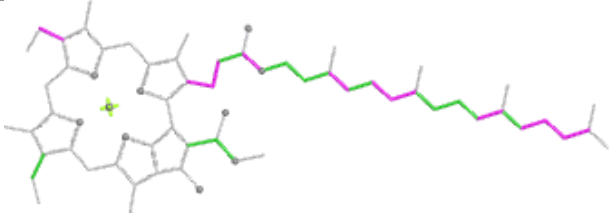
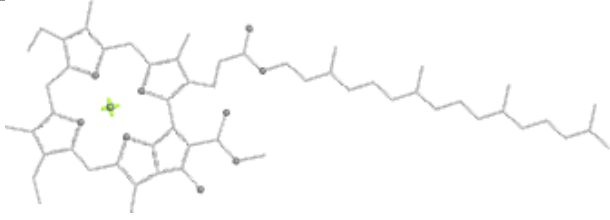
Ligand CLA B 613





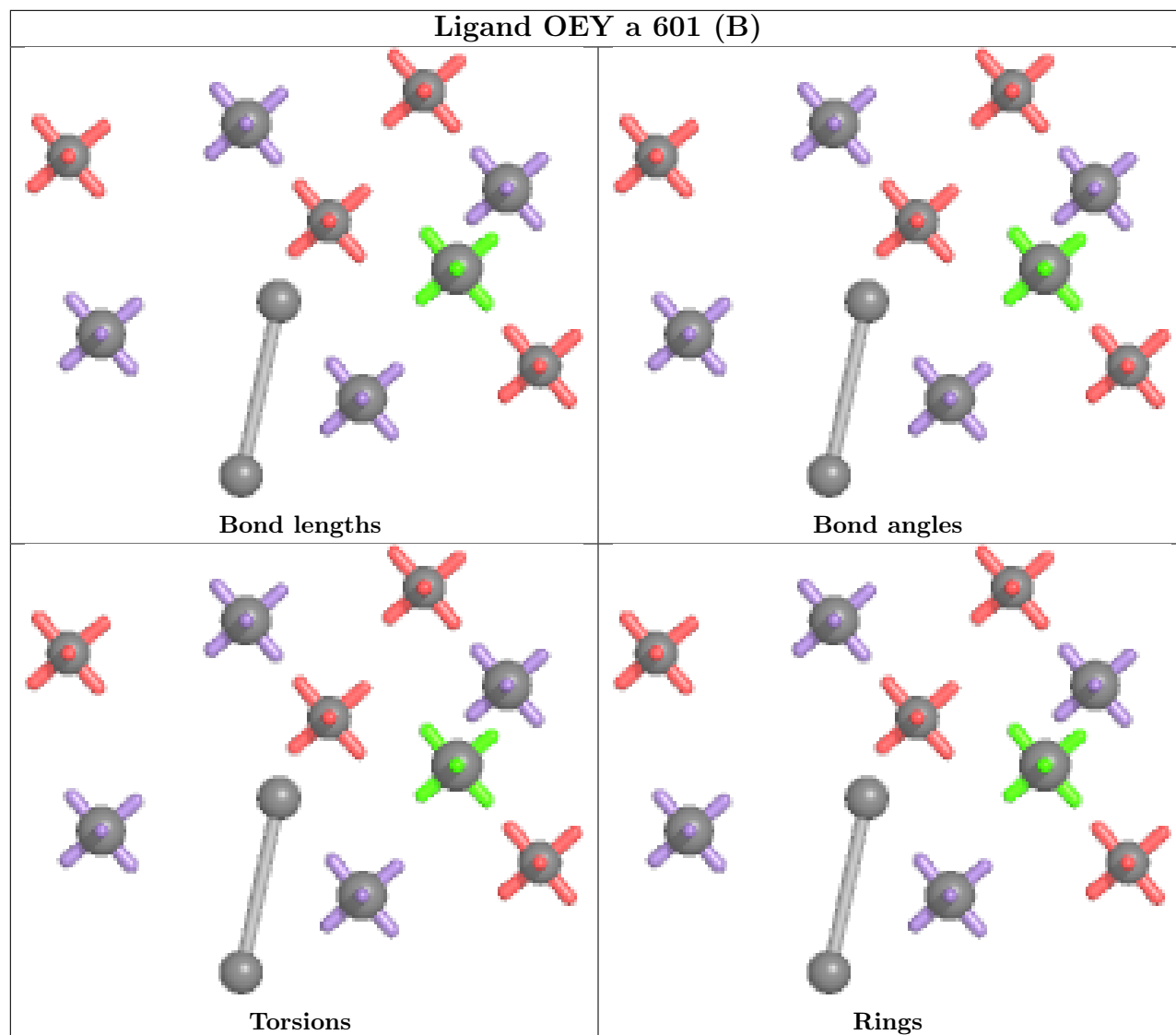




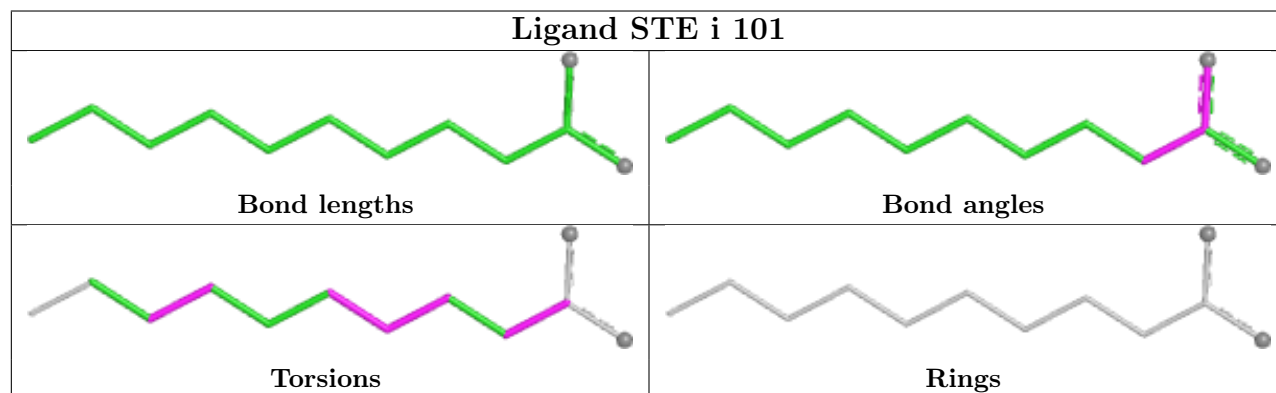
Ligand CLA c 512	
	Bond lengths
	Bond angles
	Torsions
	Rings

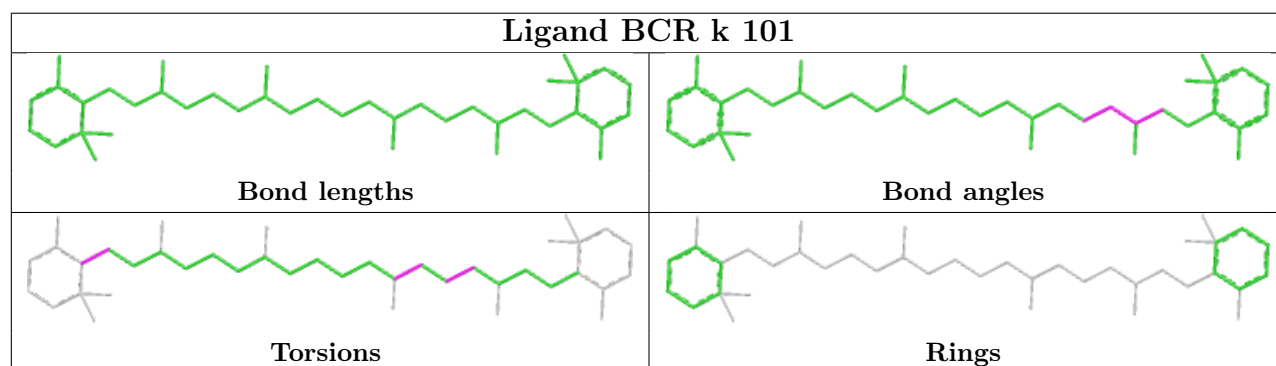
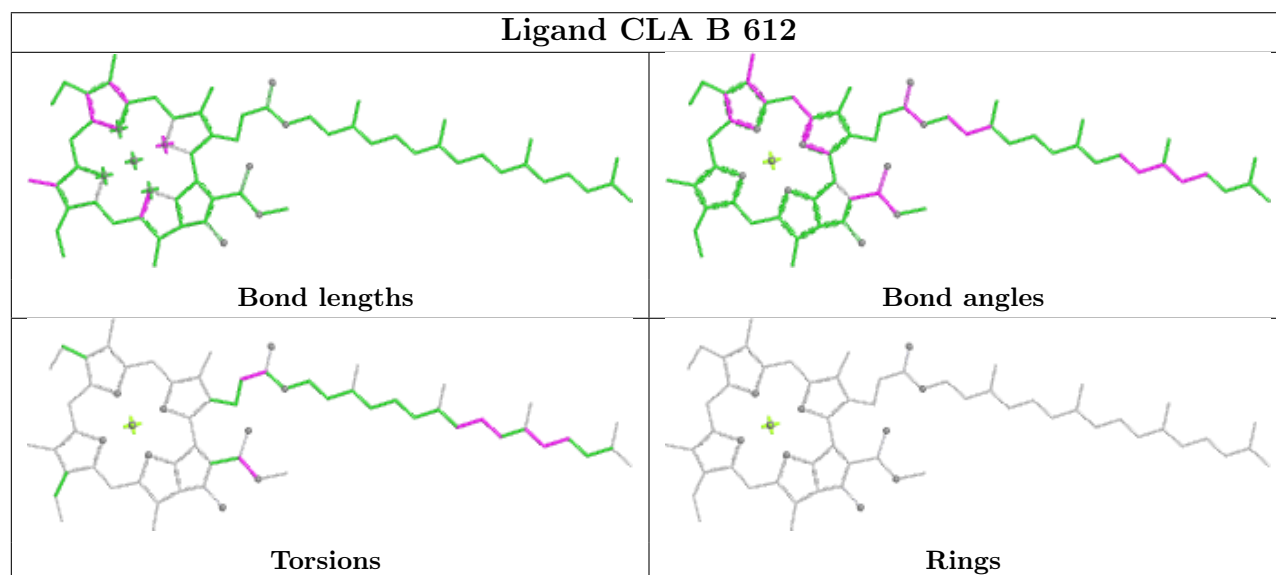
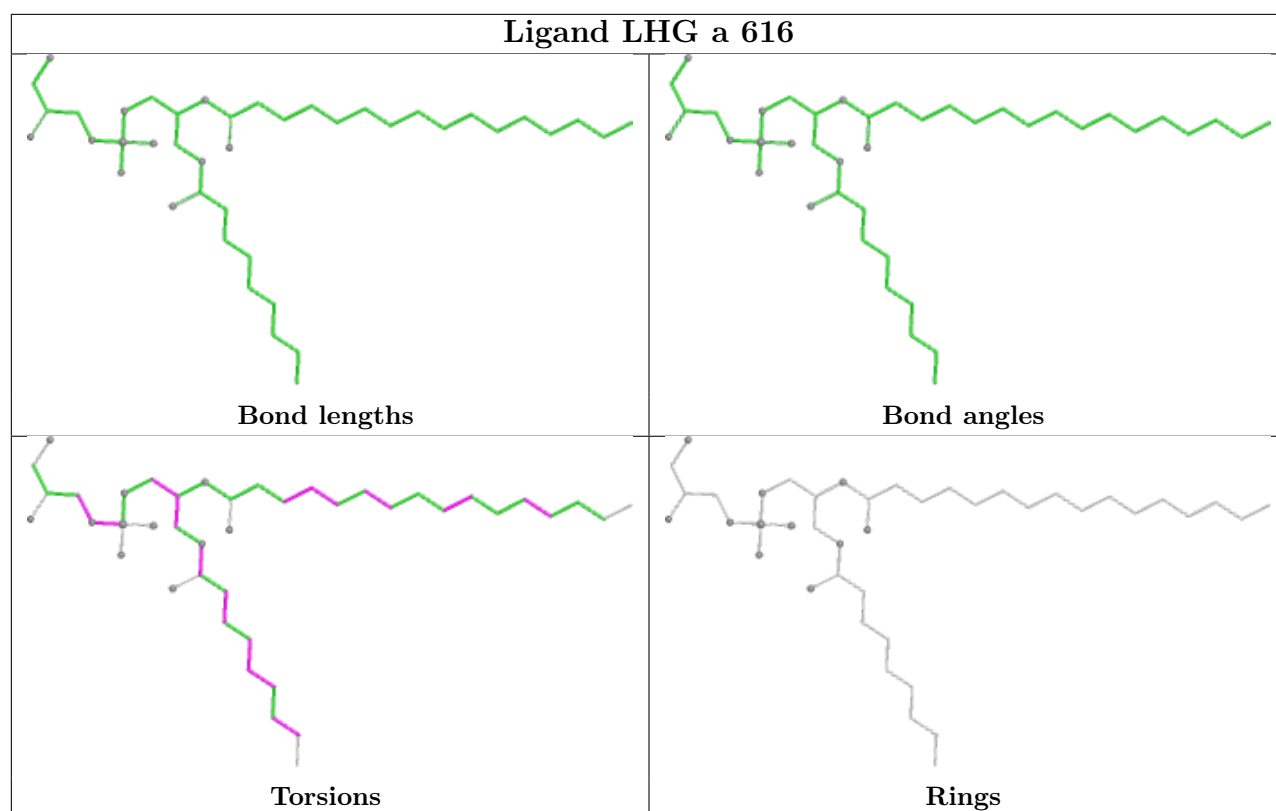
Ligand STE A 621	
	Bond lengths
	Bond angles
	Torsions
	Rings

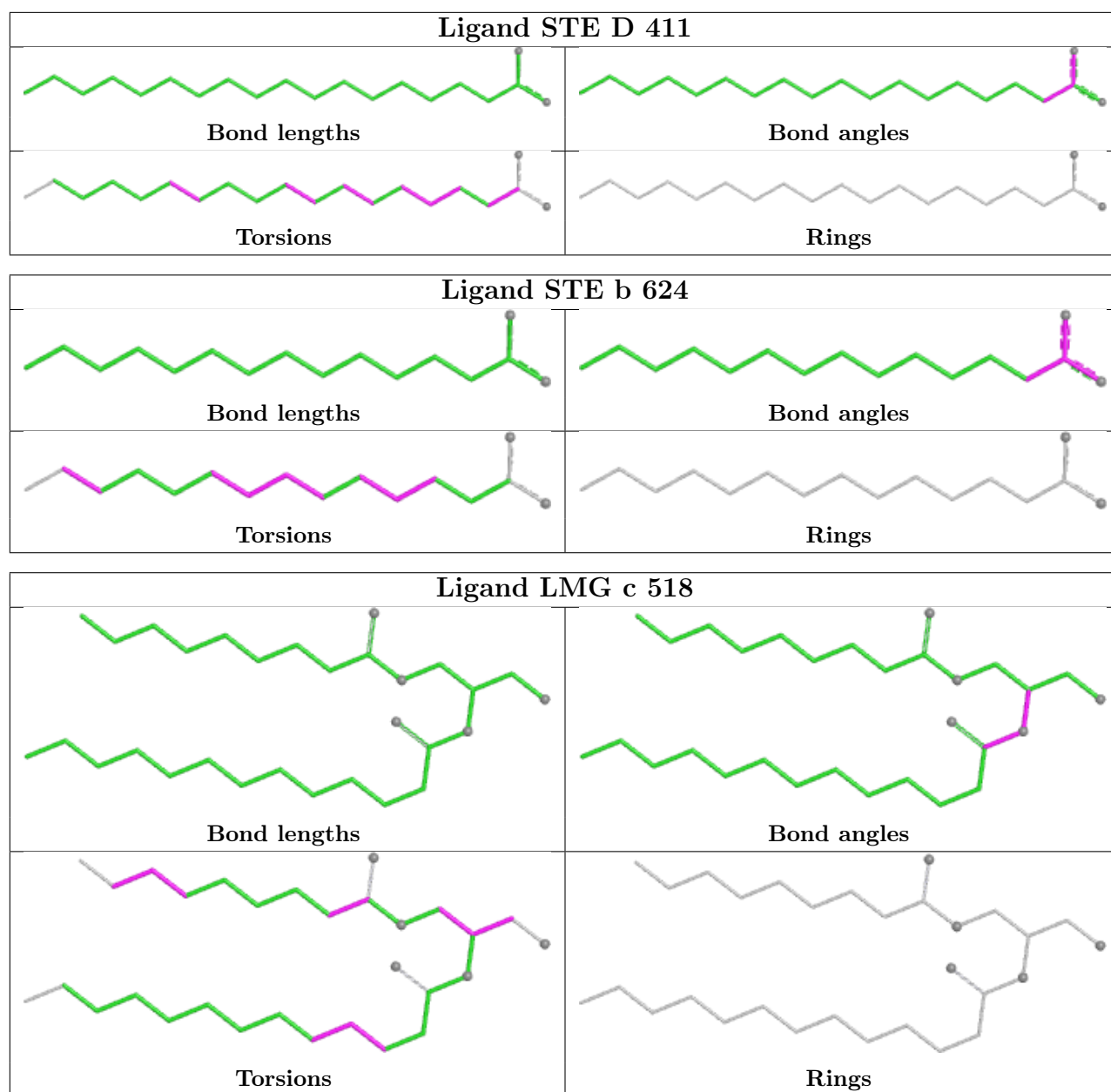
Ligand OEY a 601 (B)



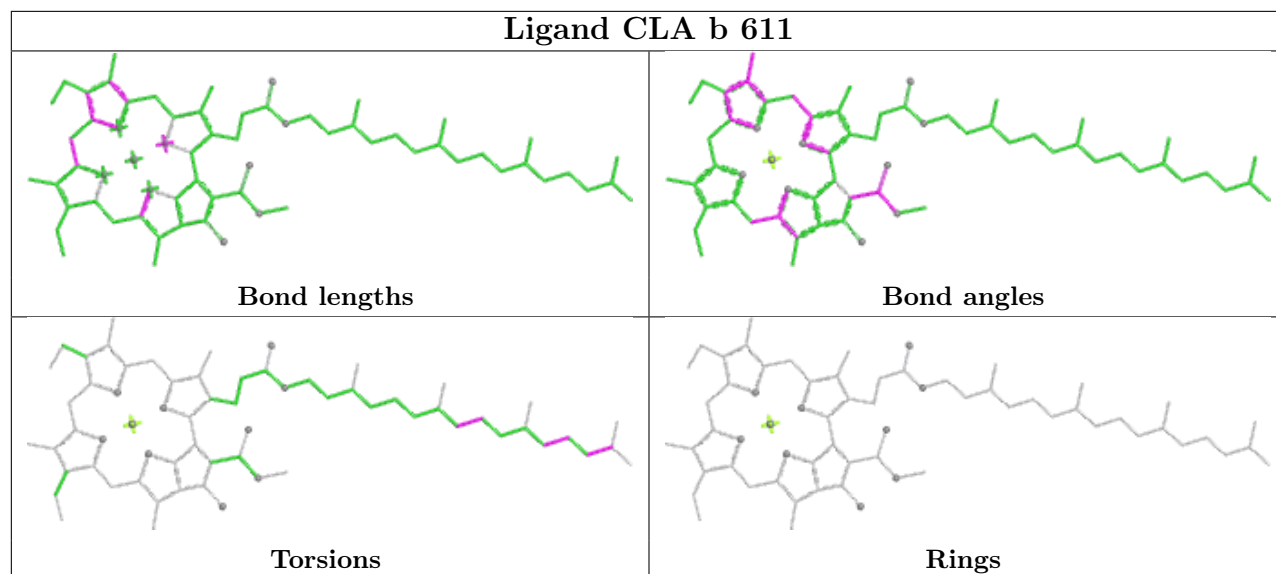
Ligand STE i 101



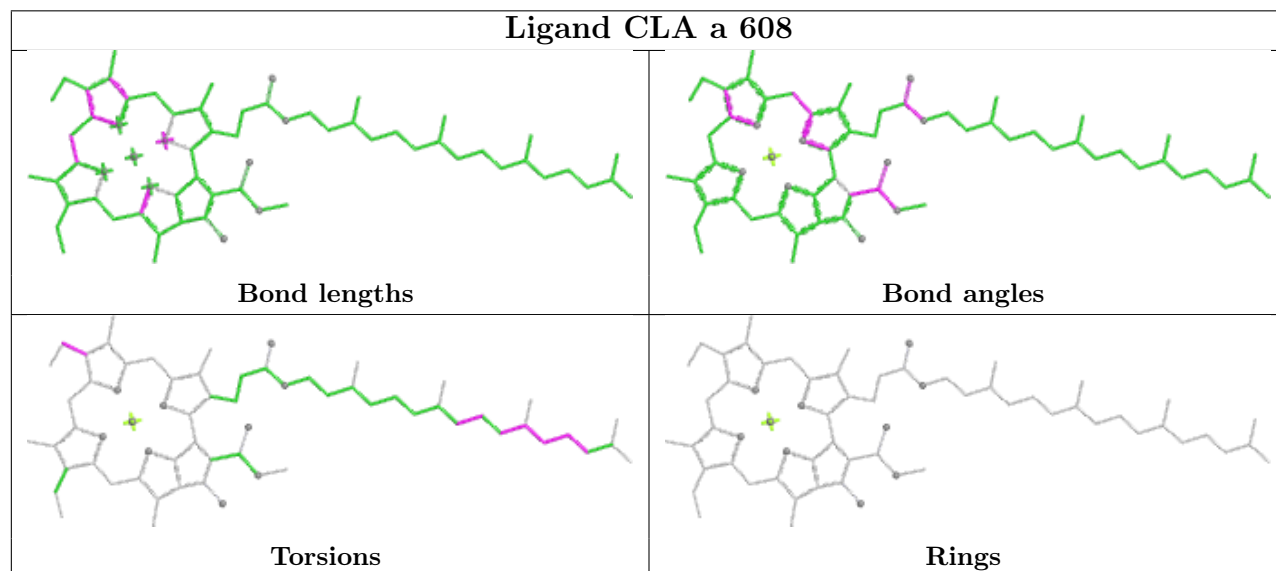




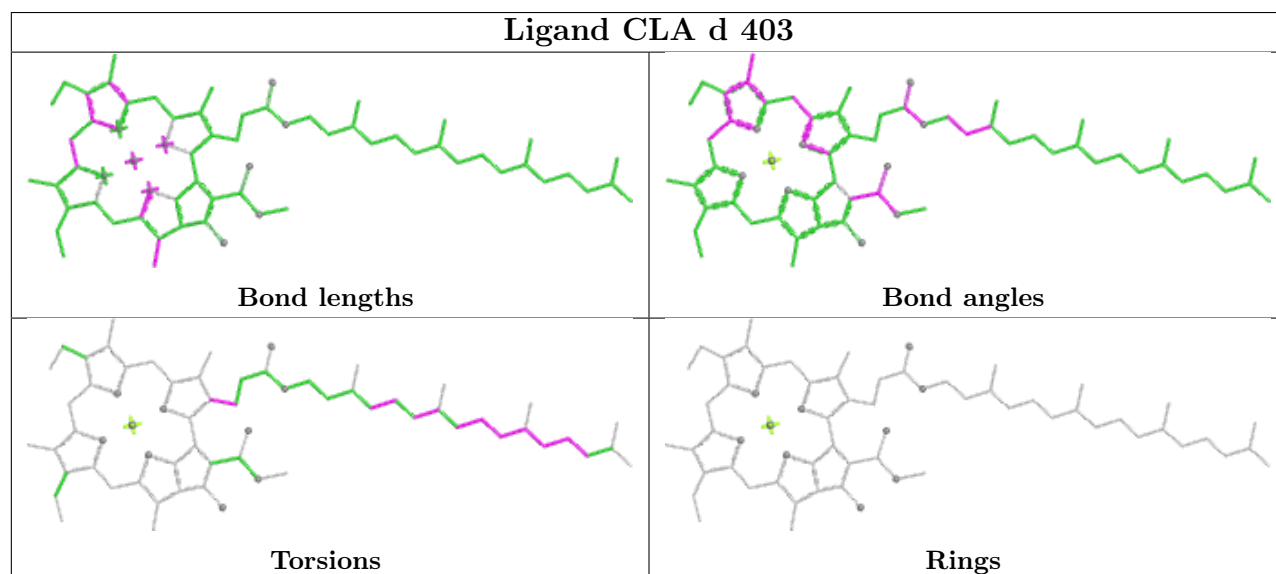
Ligand CLA b 611

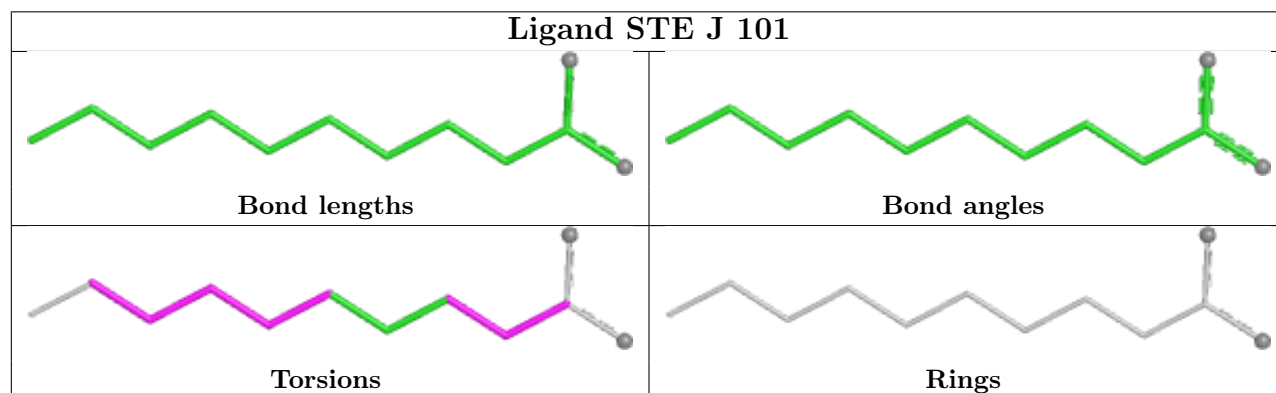
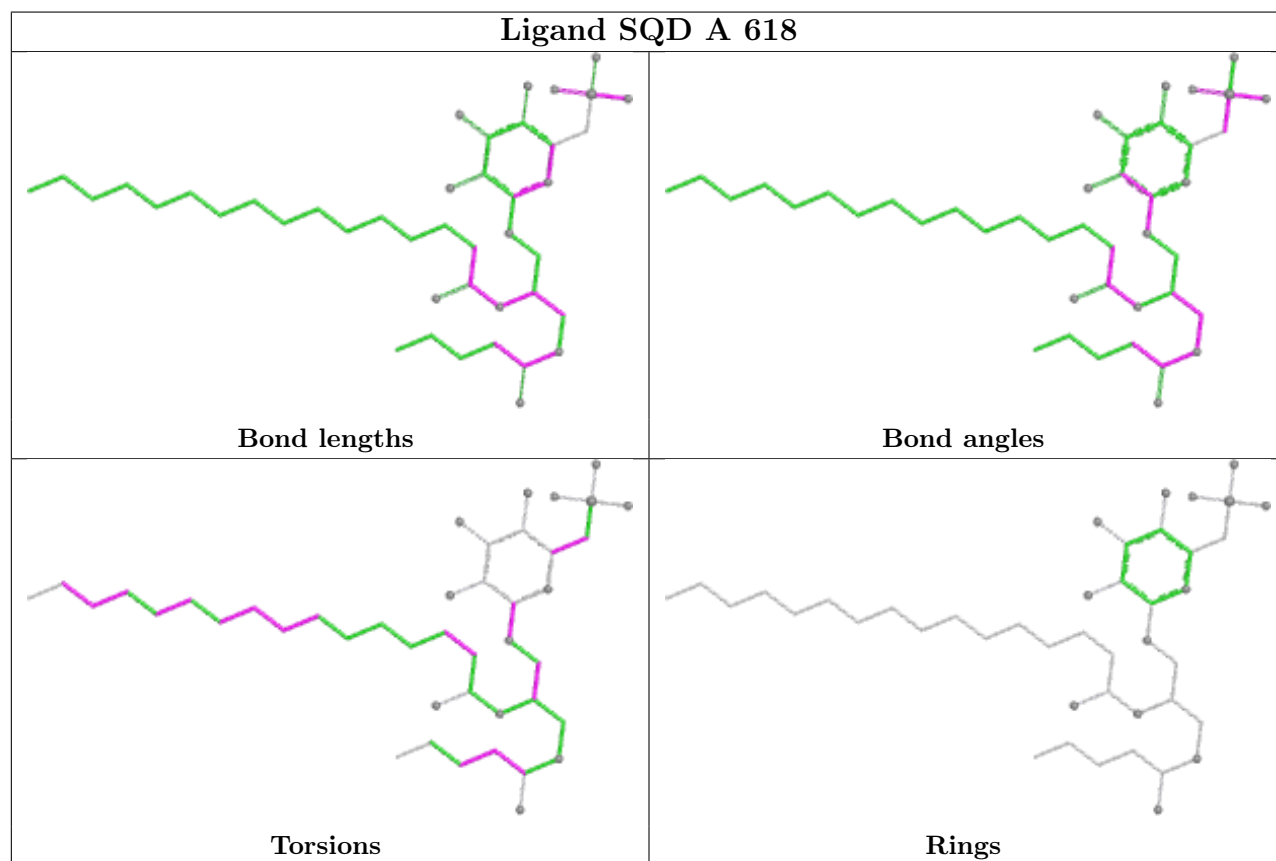
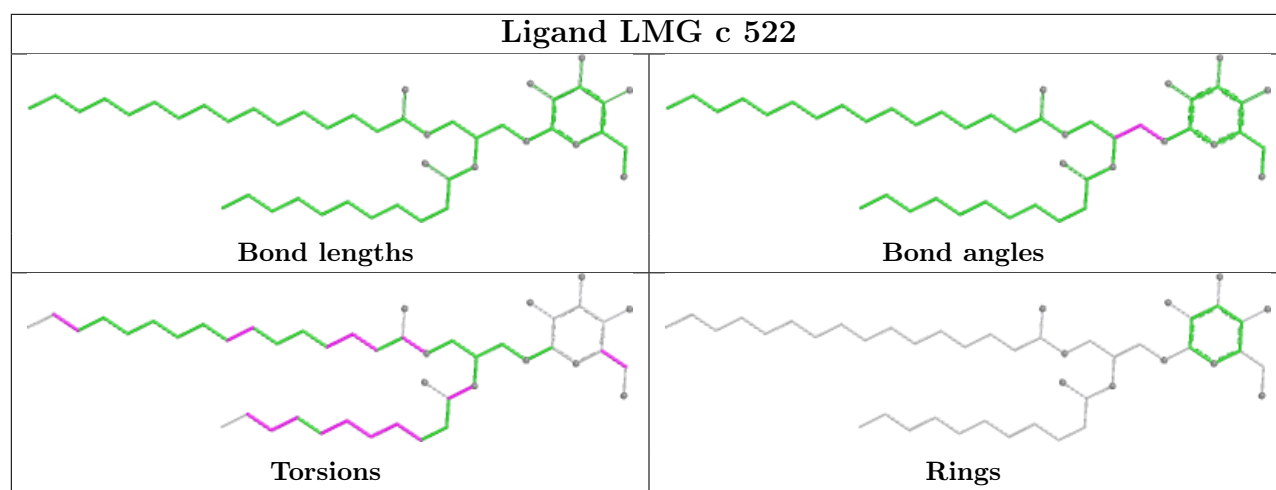


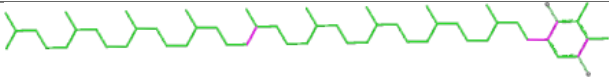
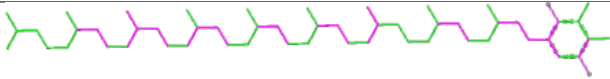
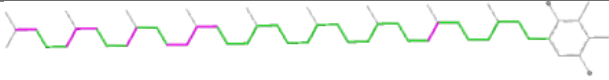
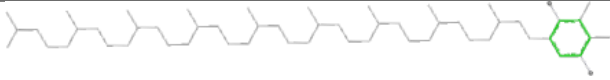
Ligand CLA a 608

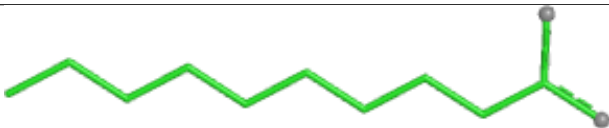
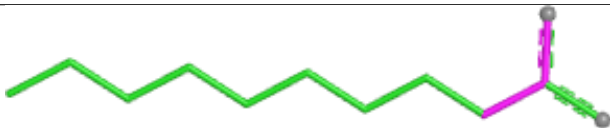
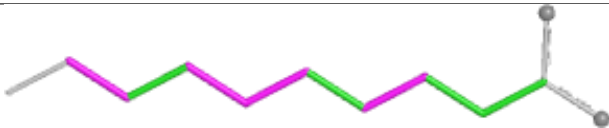
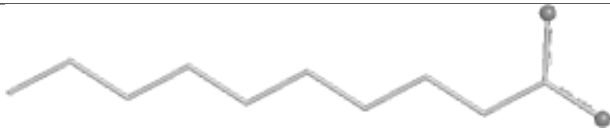


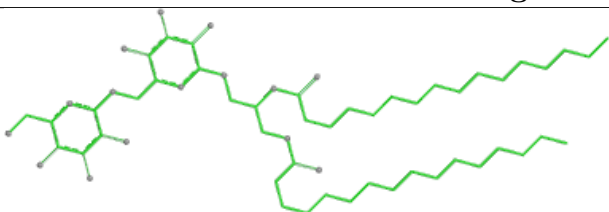
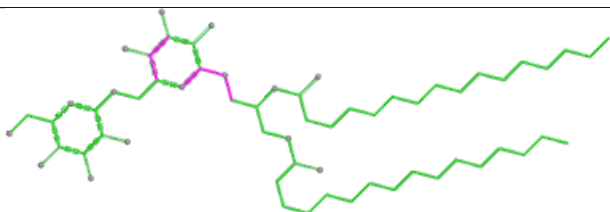
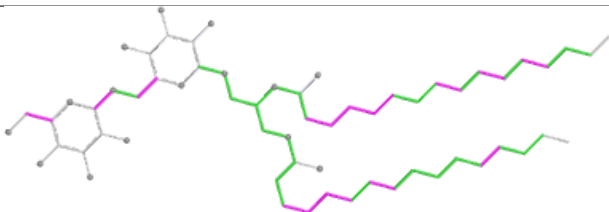
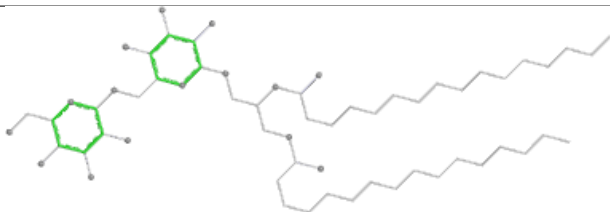
Ligand CLA d 403

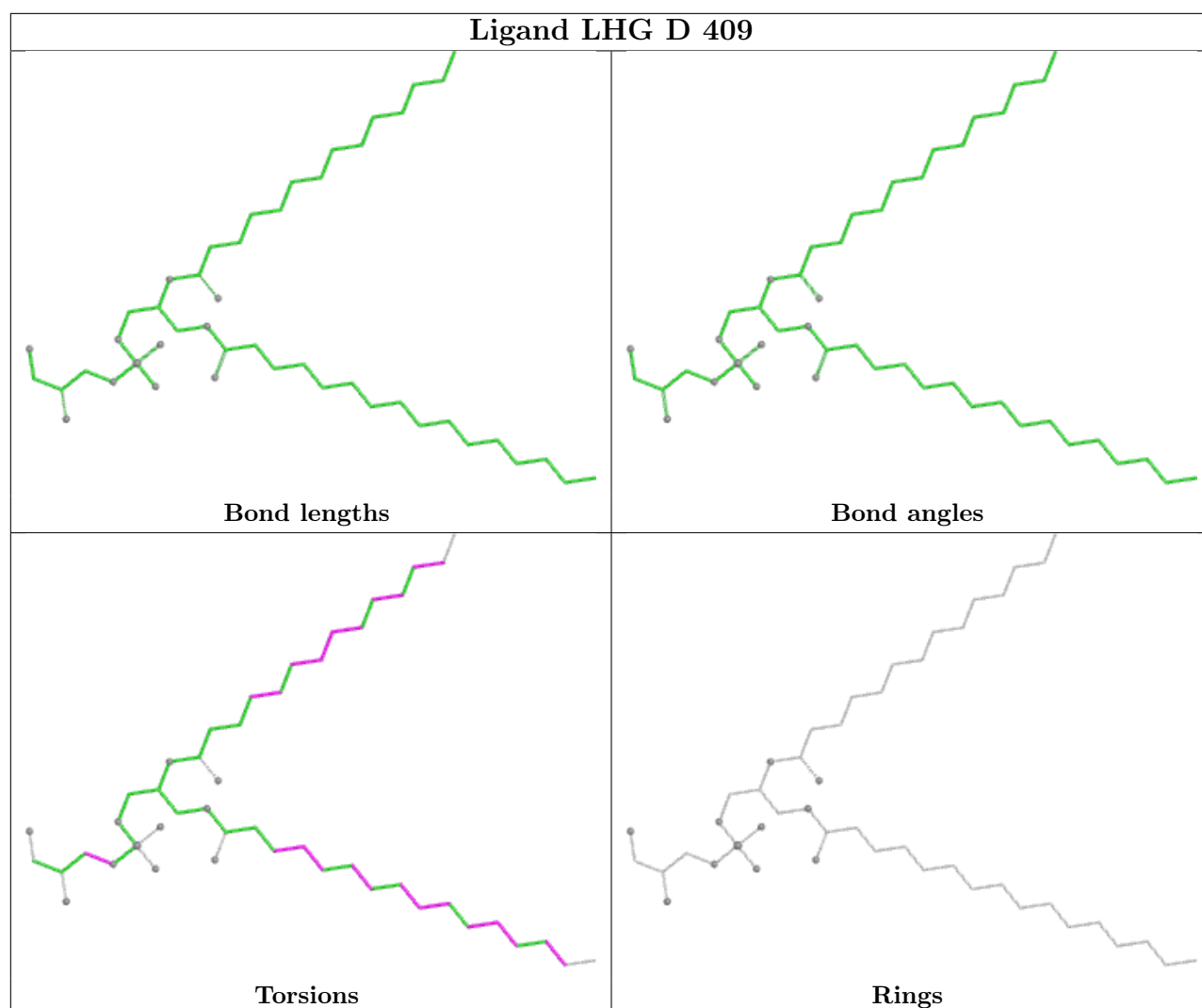




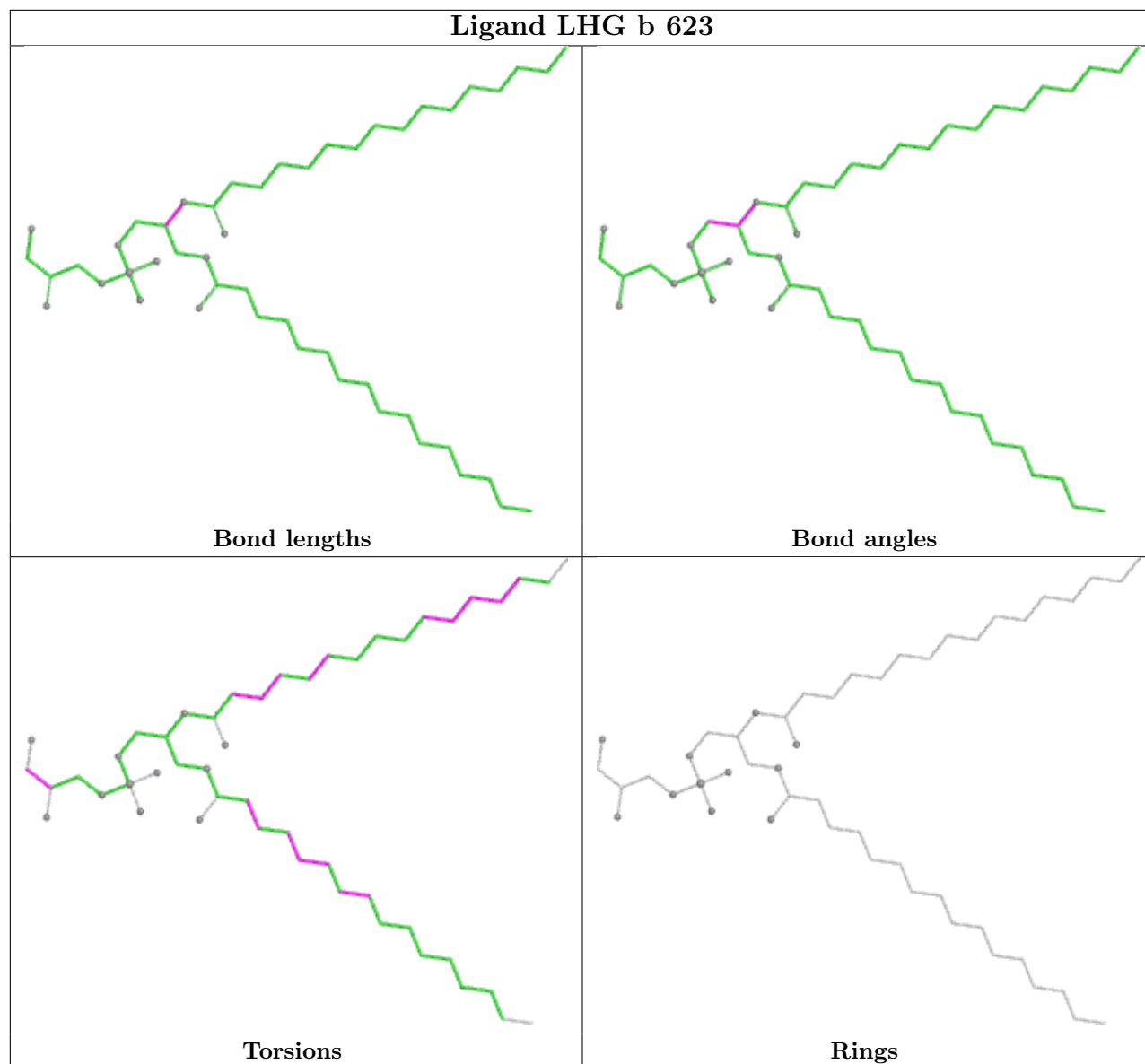
Ligand PL9 d 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE j 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

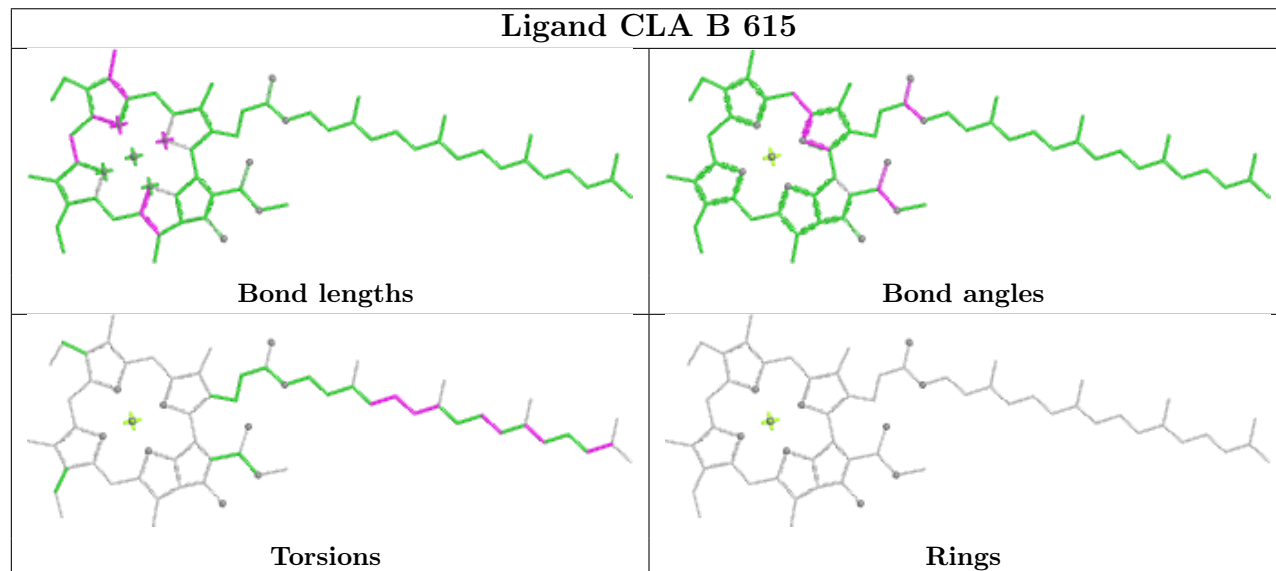
Ligand DGD c 519	
 Bond lengths	 Bond angles
 Torsions	 Rings

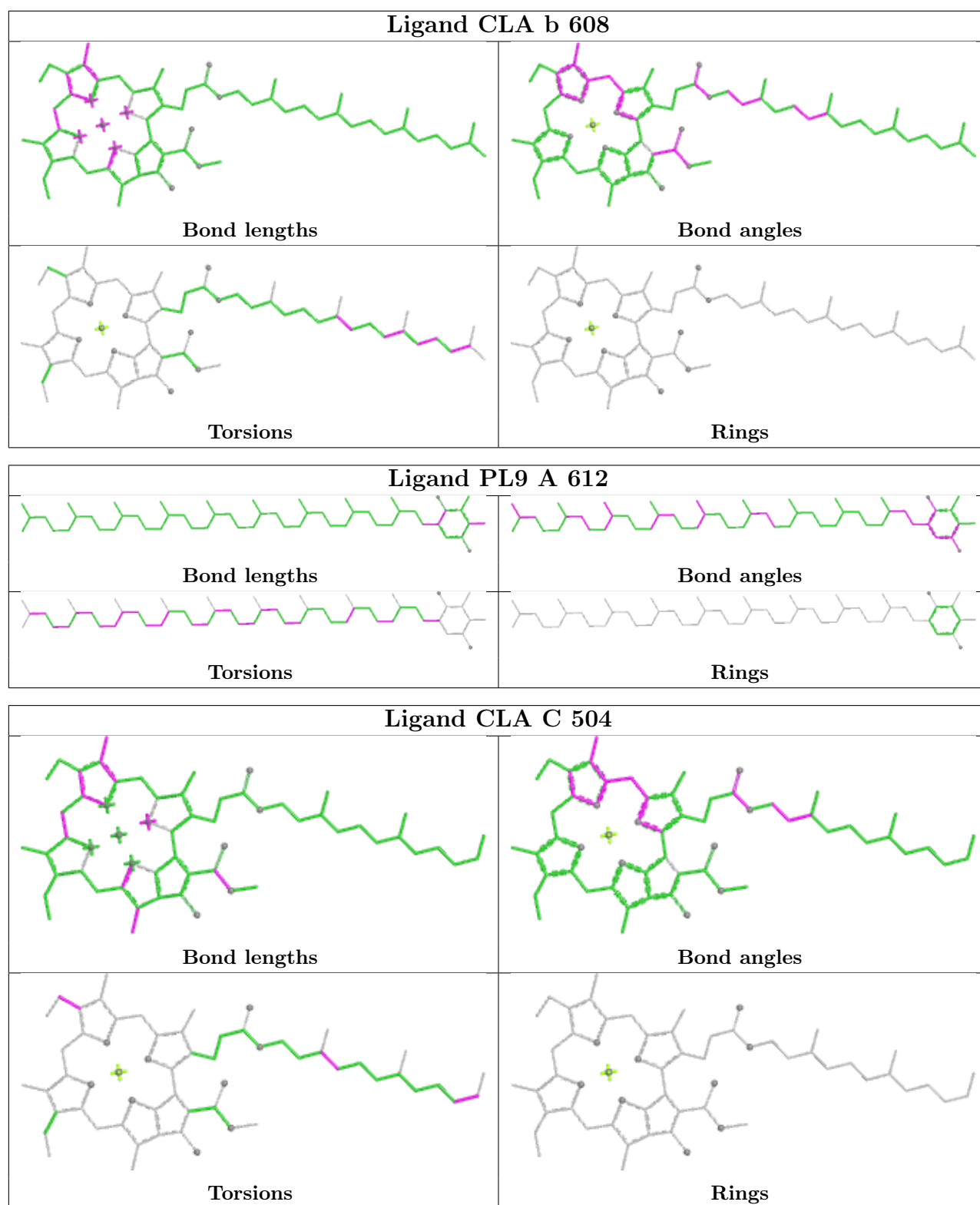


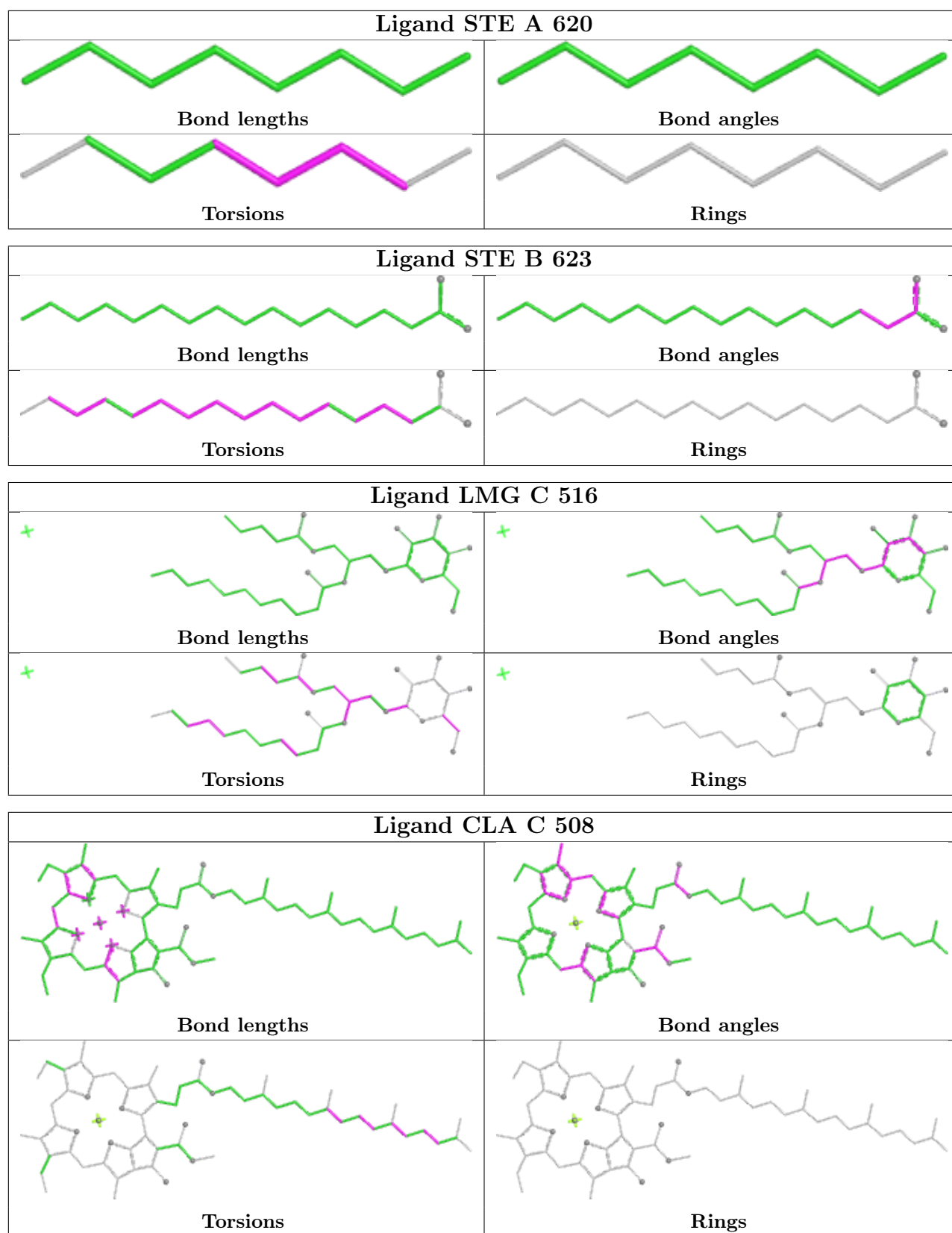
Ligand LHG b 623

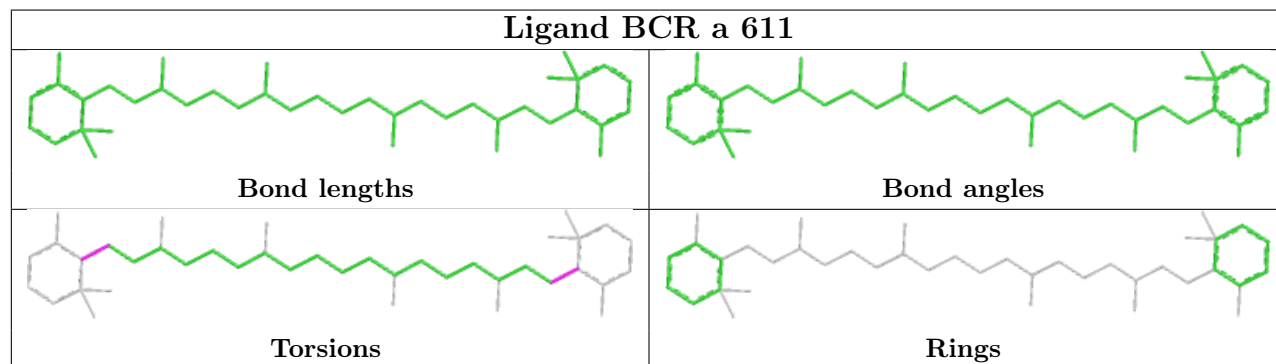
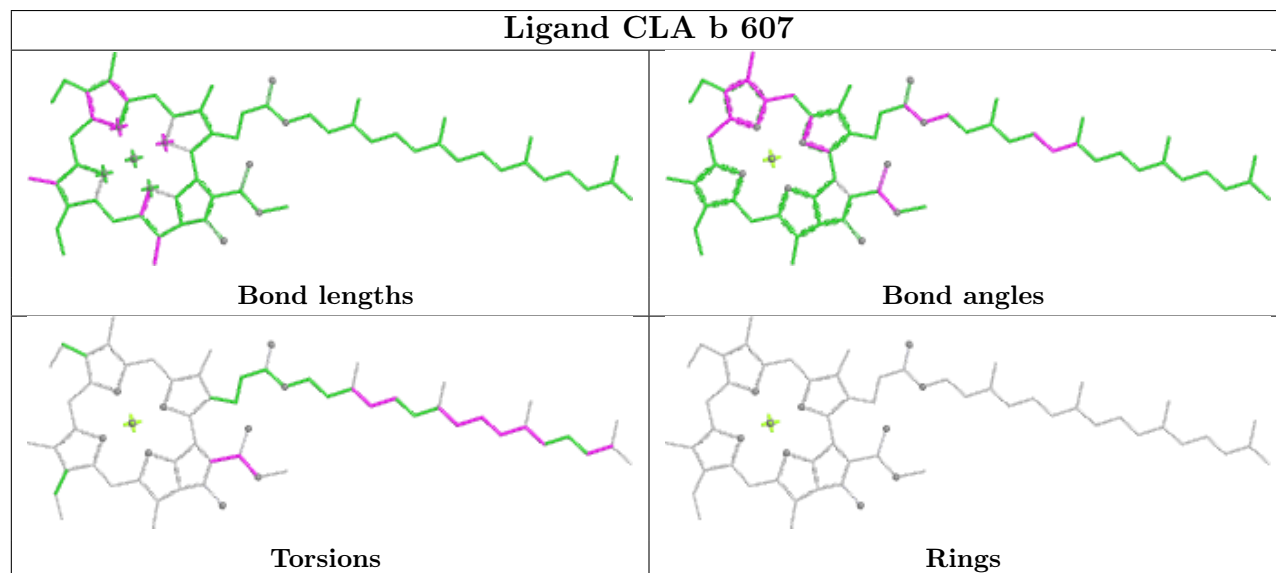
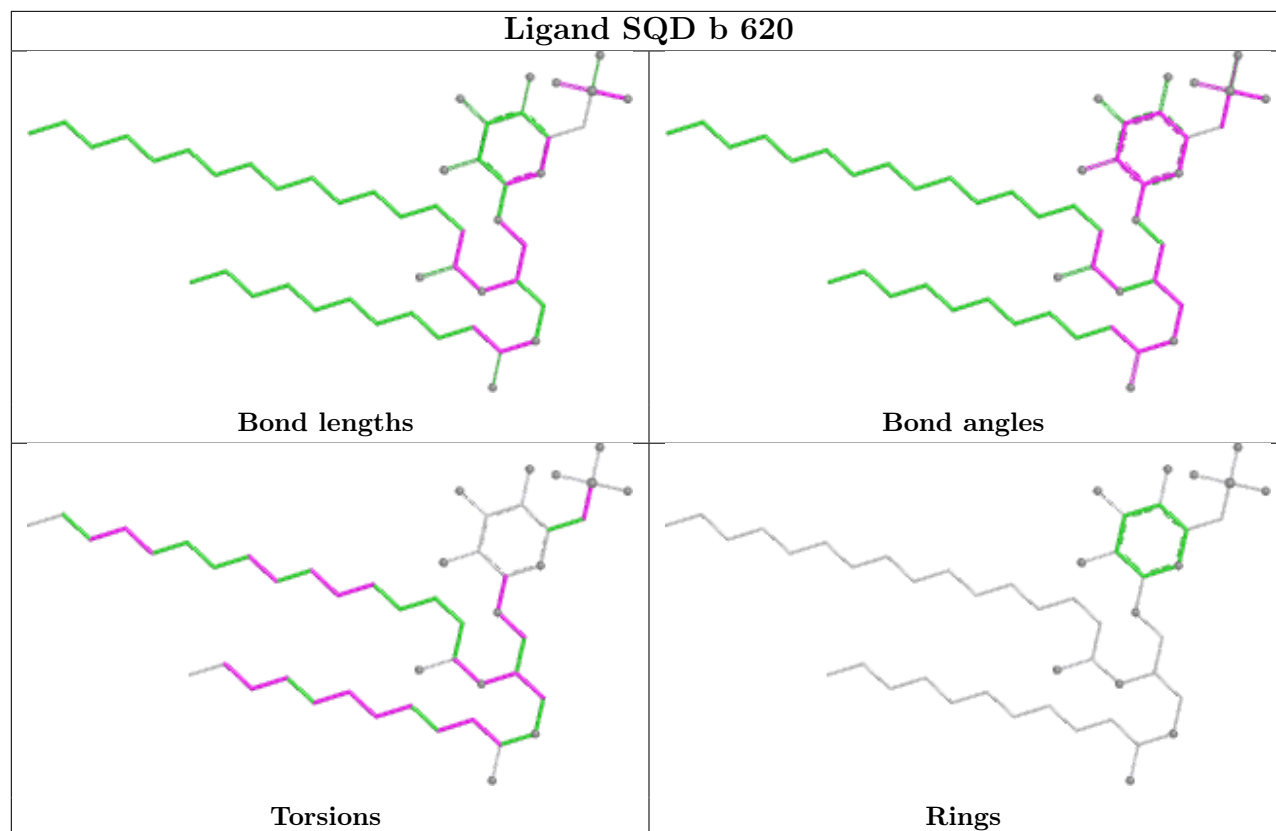


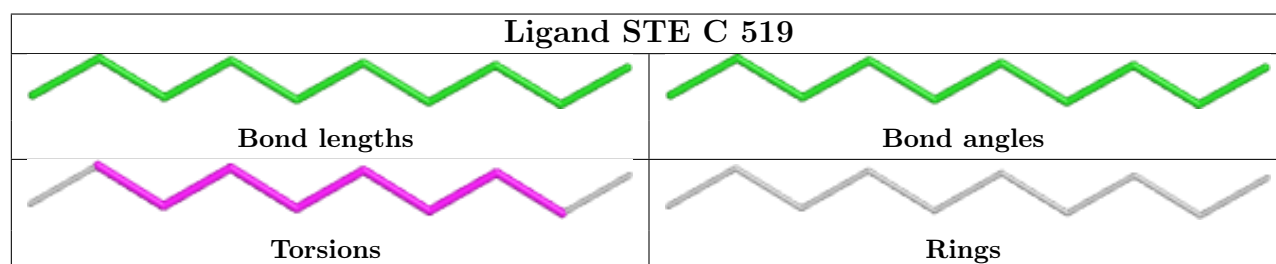
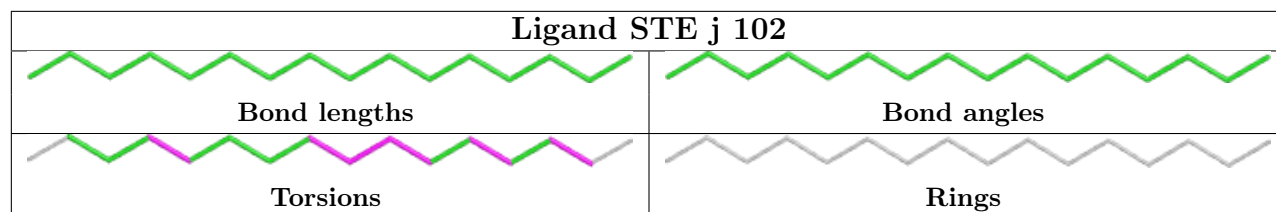
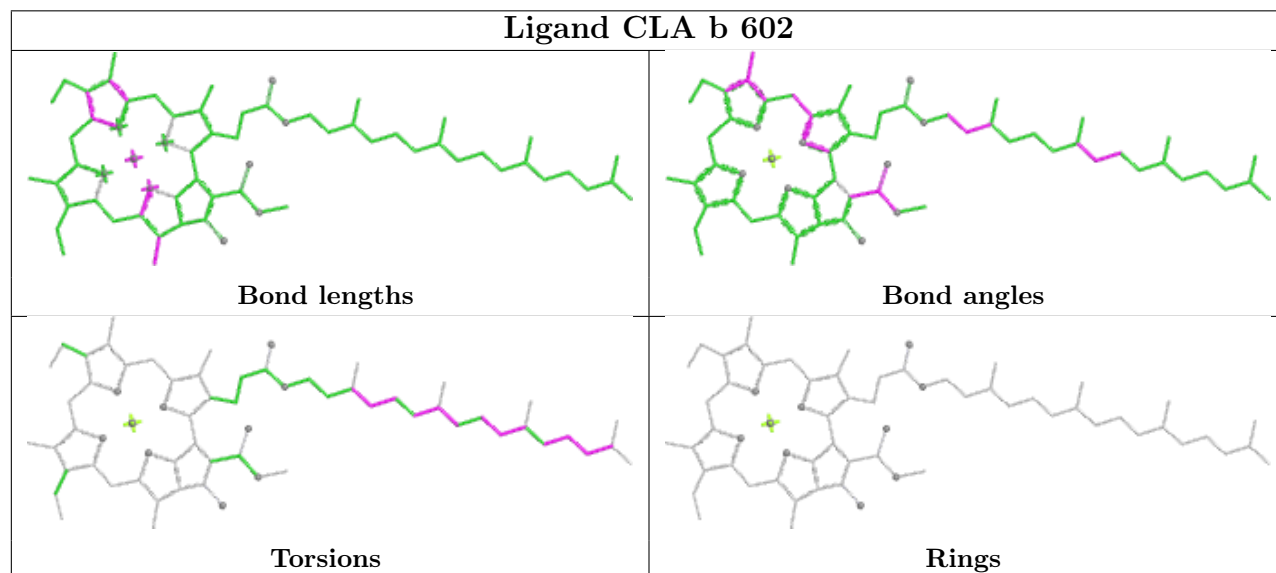
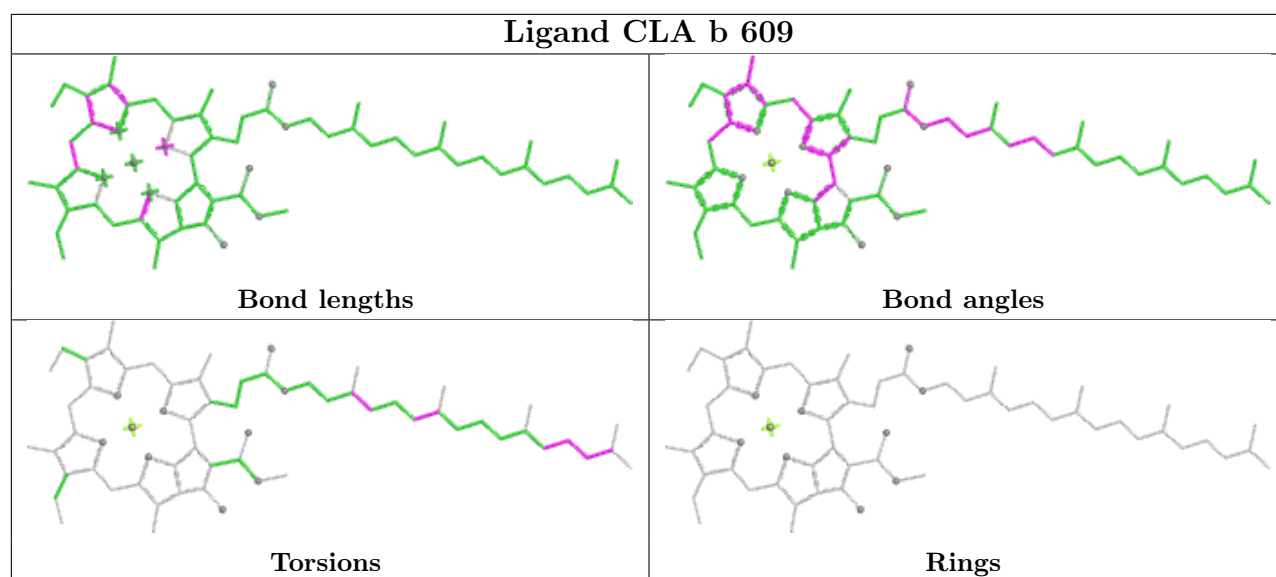
Ligand CLA B 615

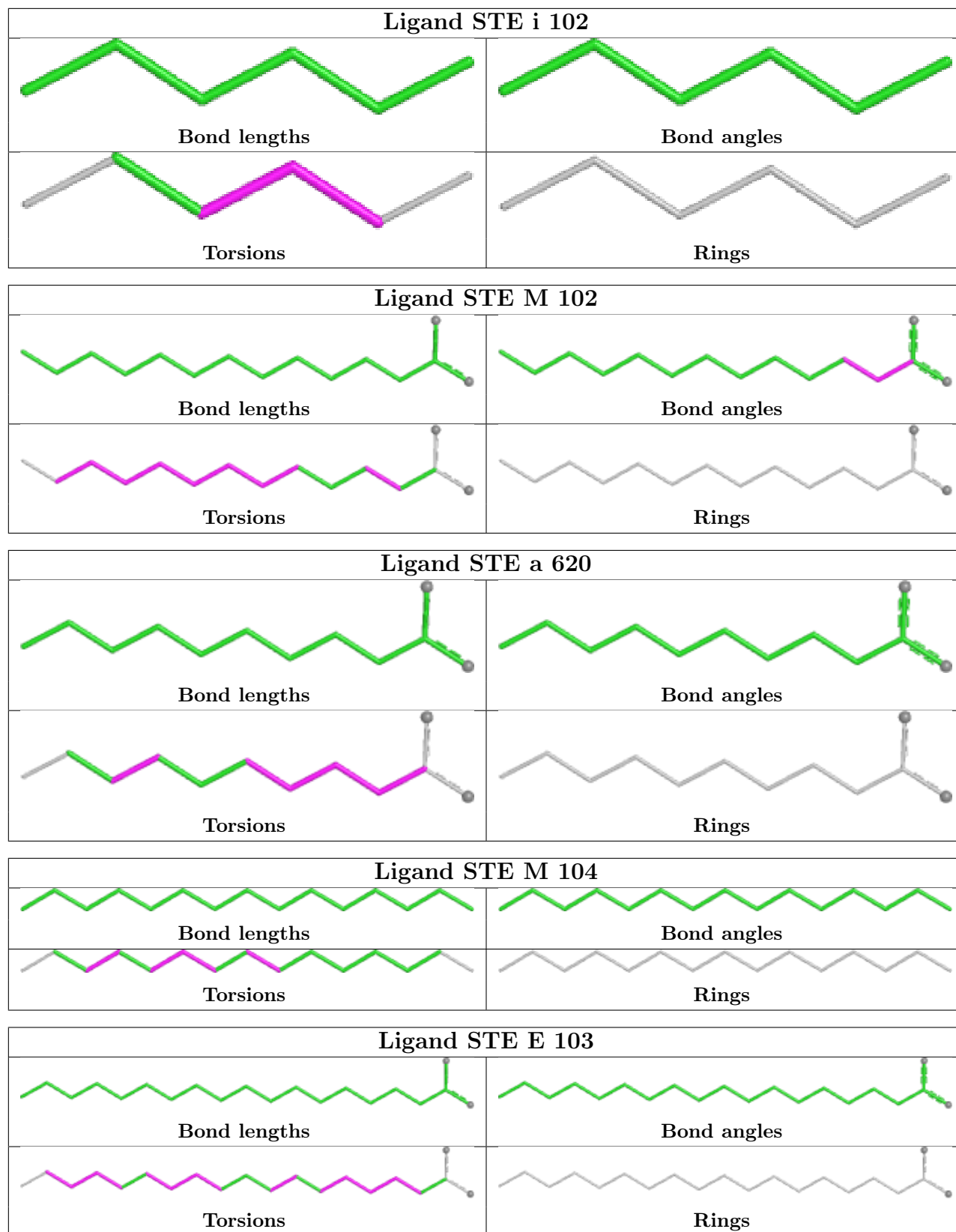


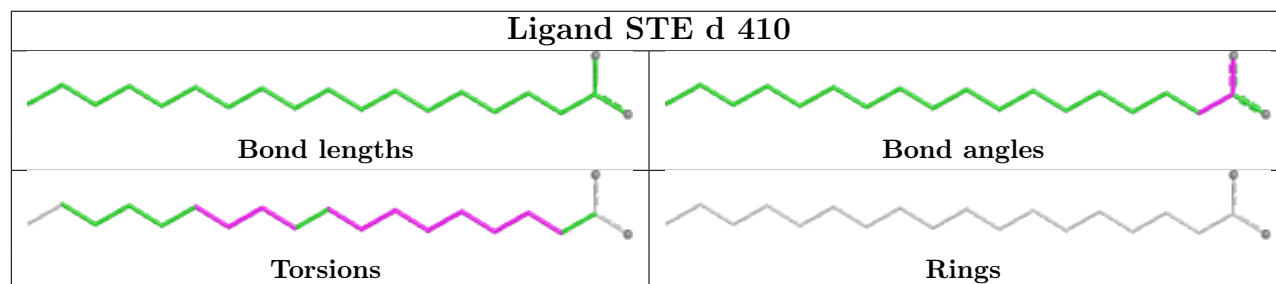
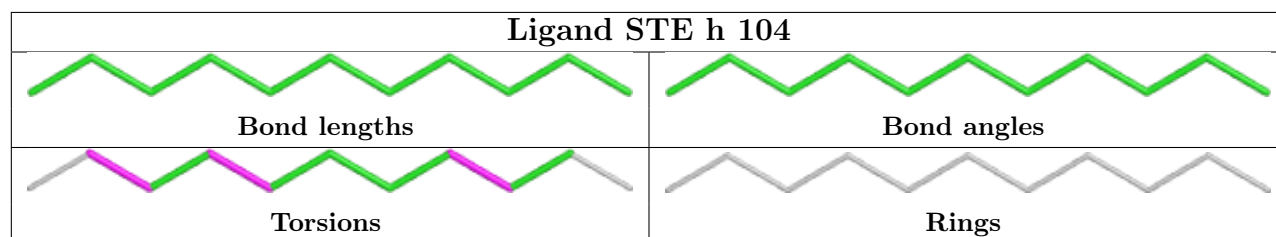
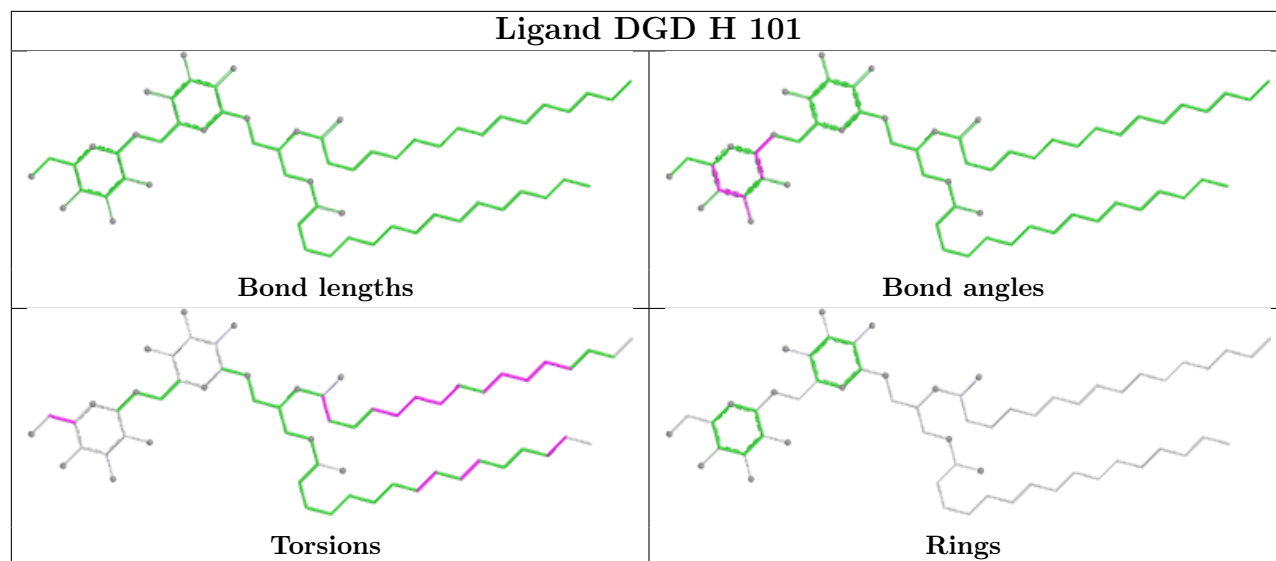




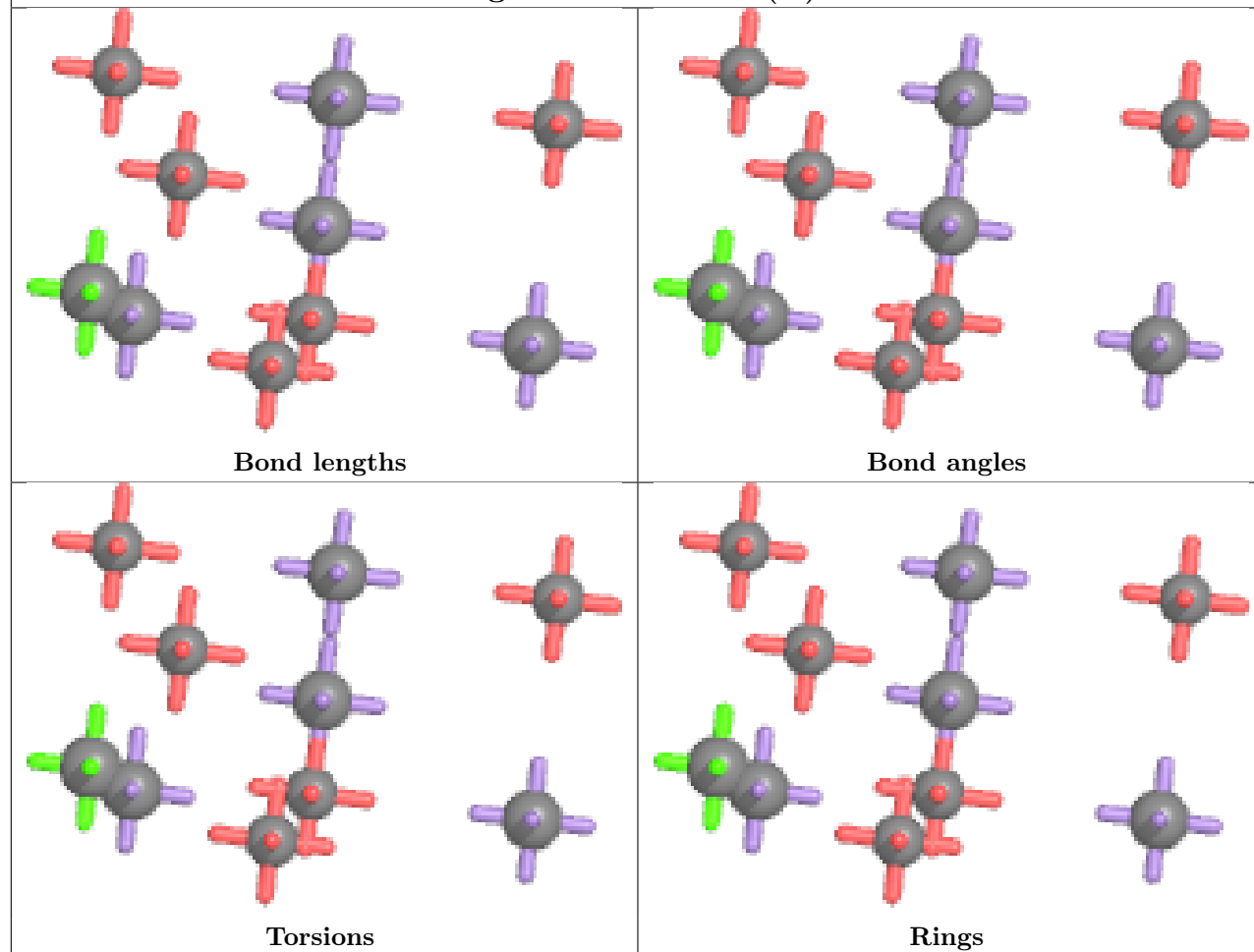




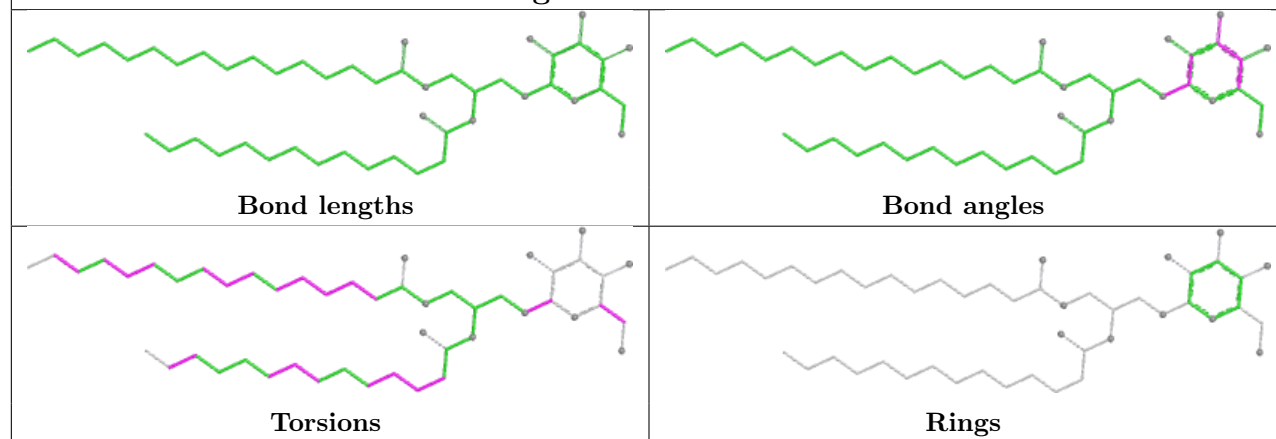


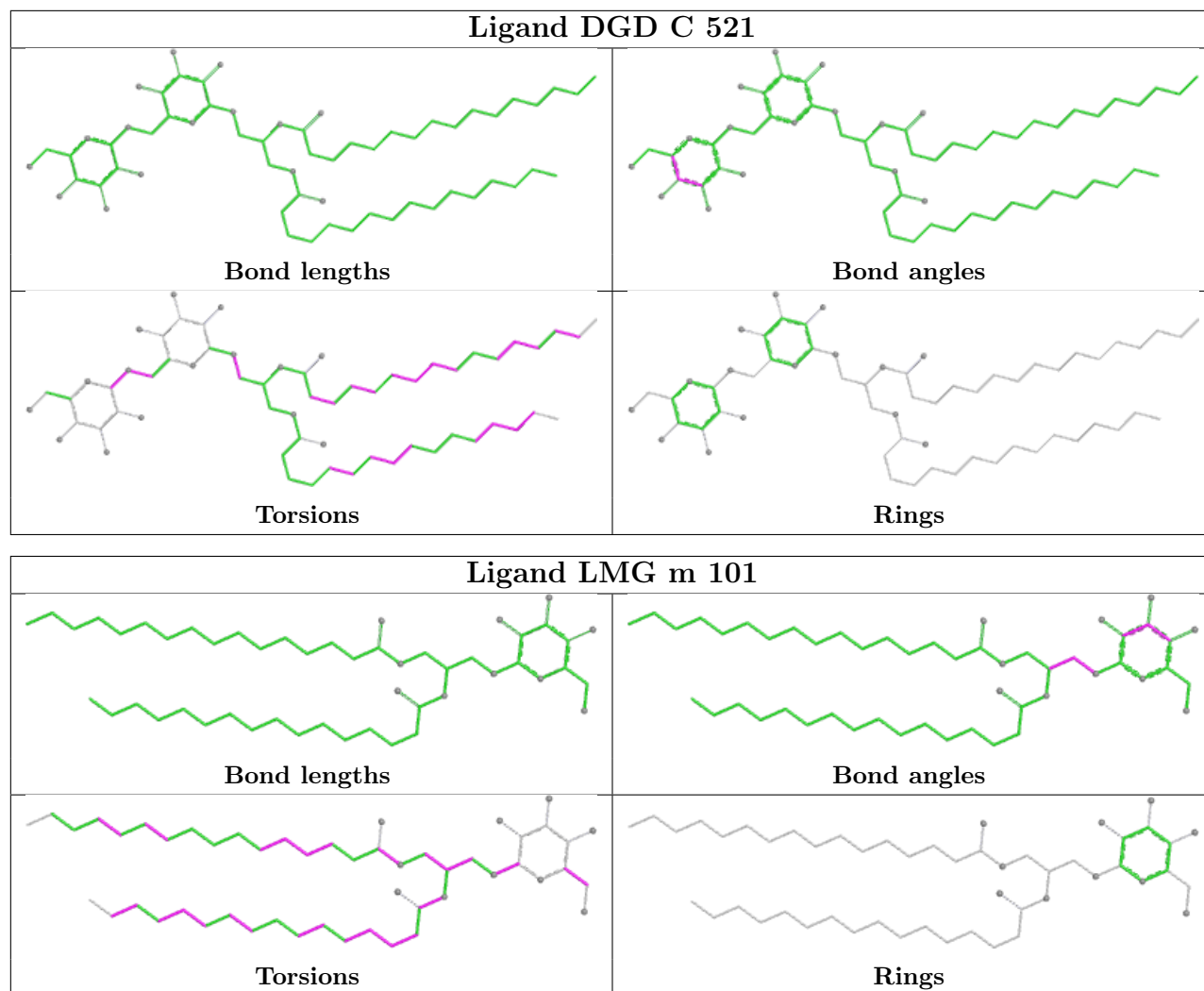


Ligand OEX A 602 (A)

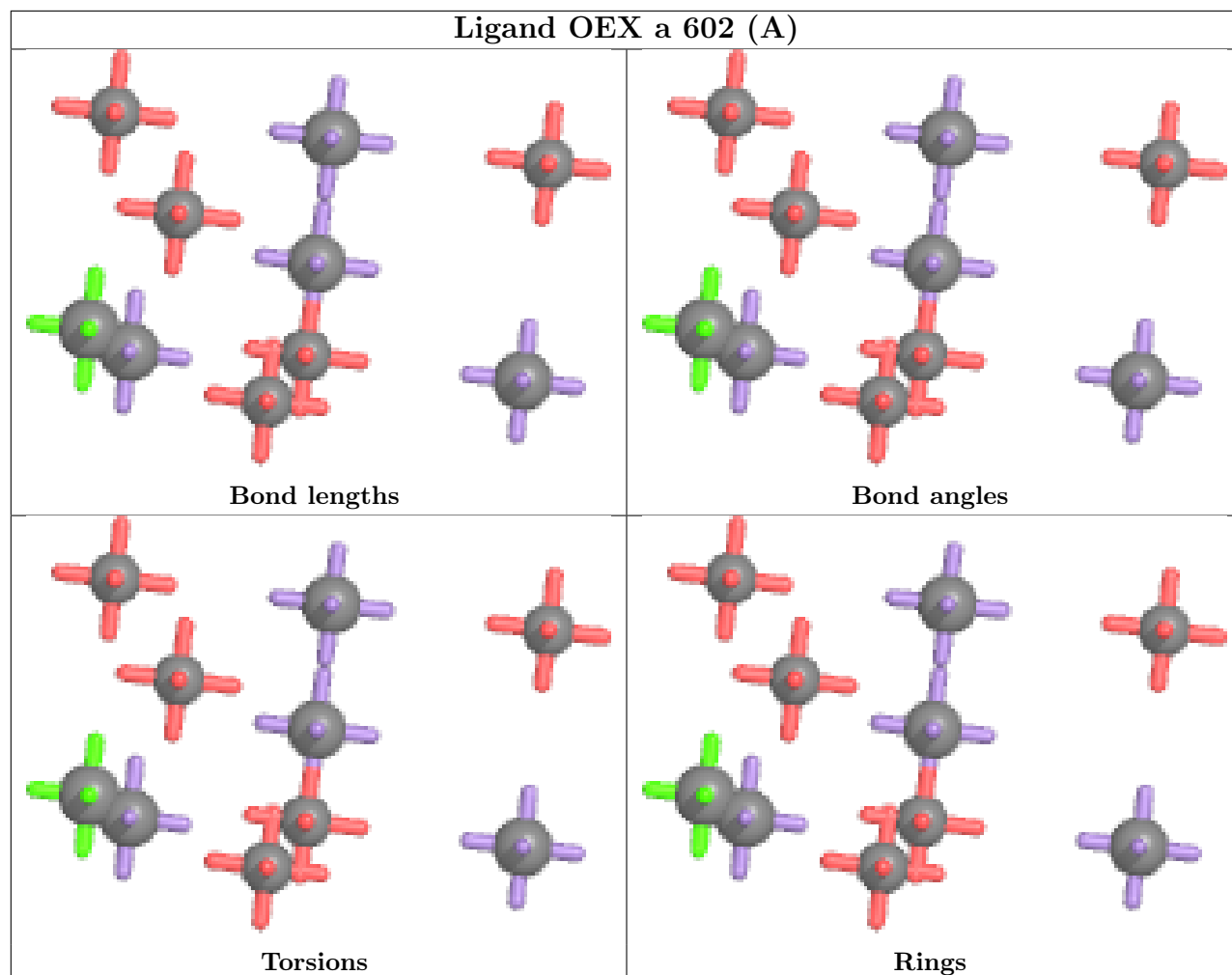


Ligand LMG c 524

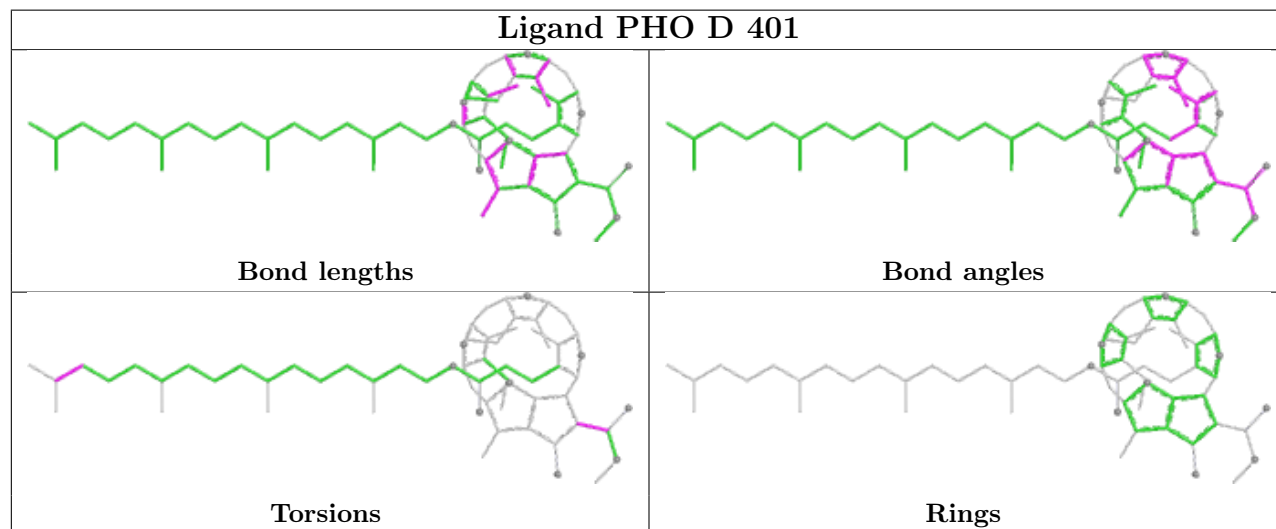


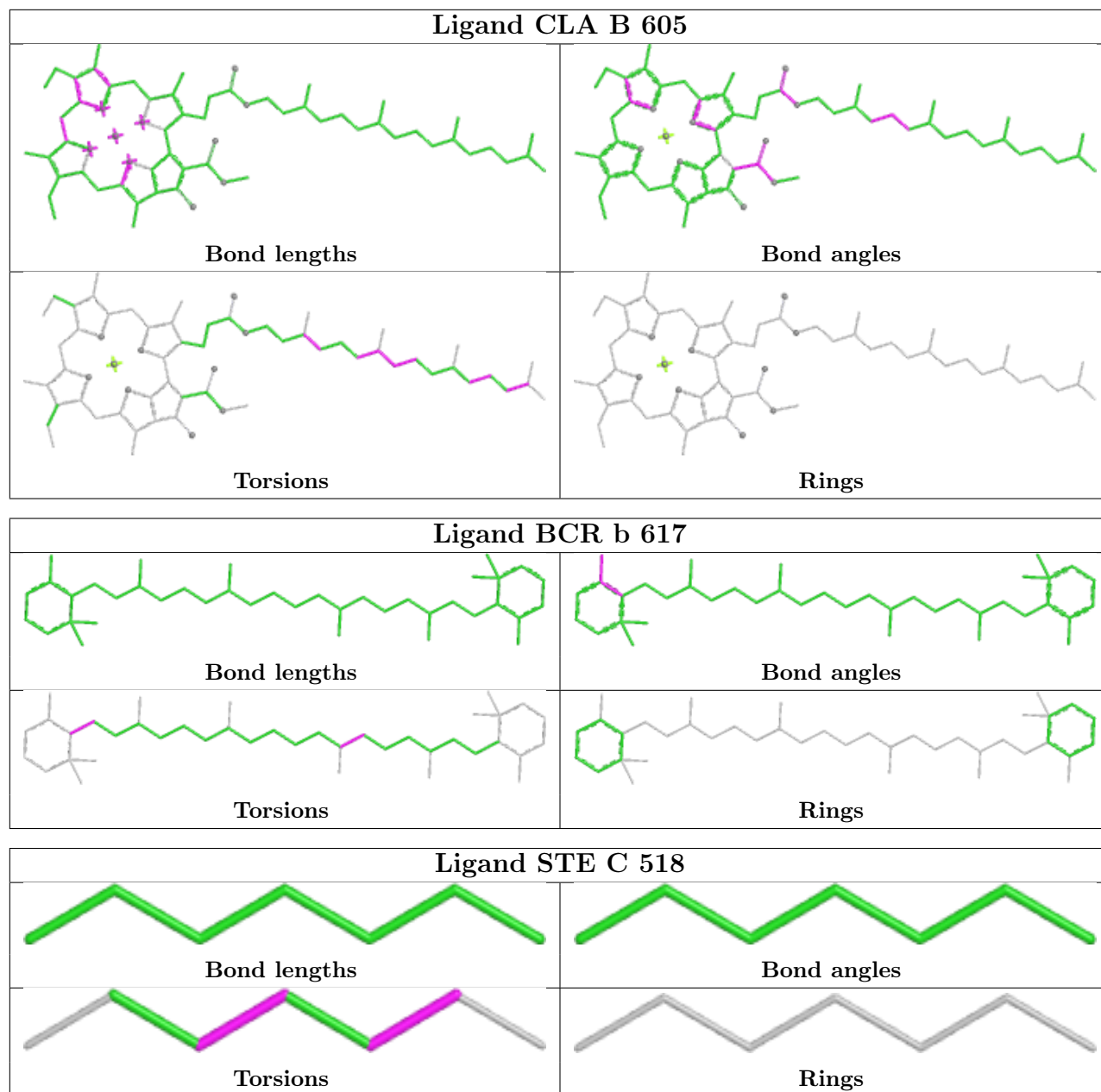


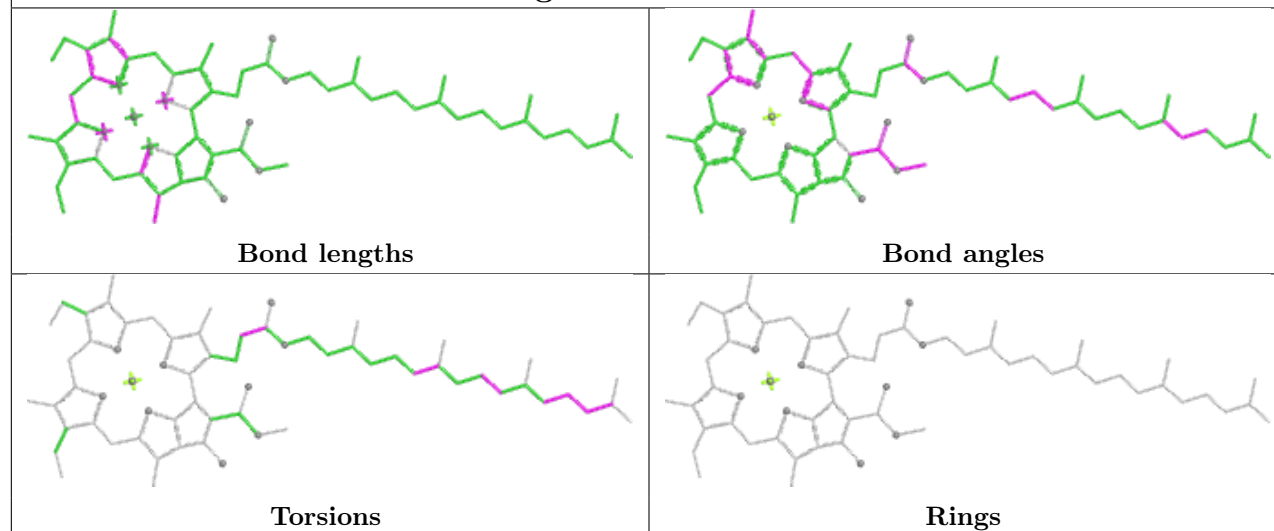
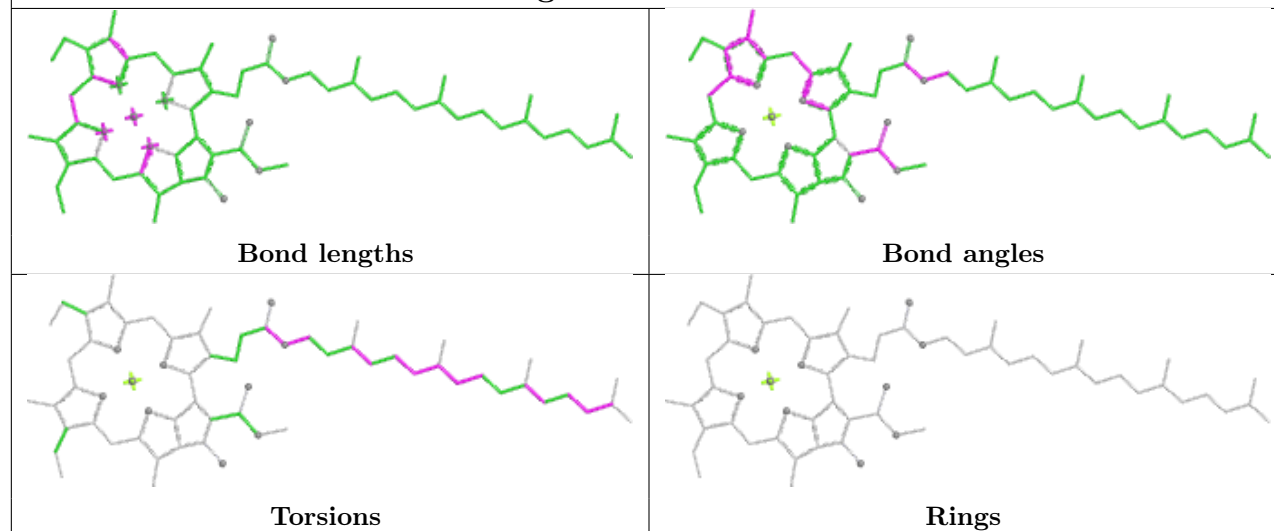
Ligand OEX a 602 (A)



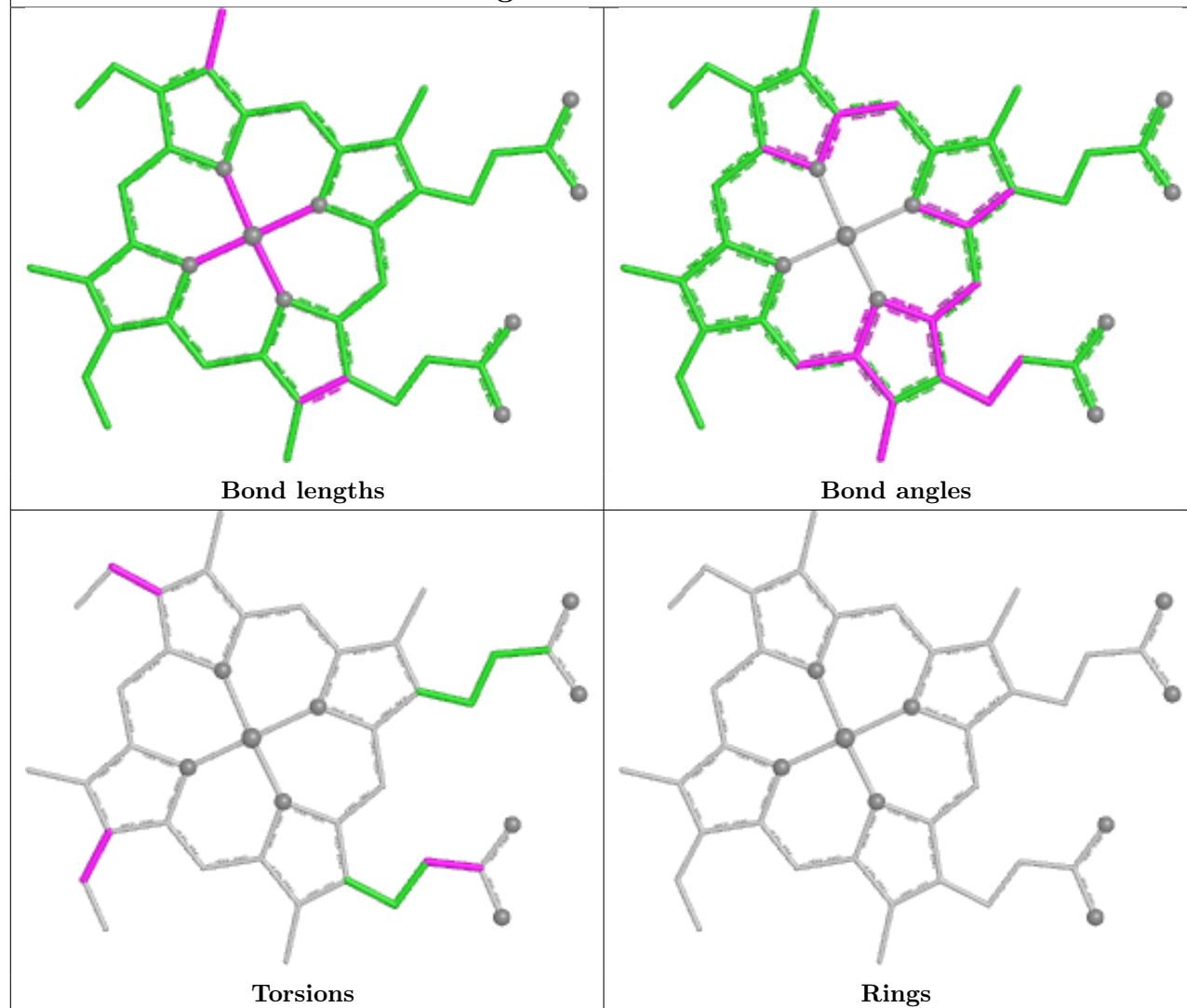
Ligand PHO D 401



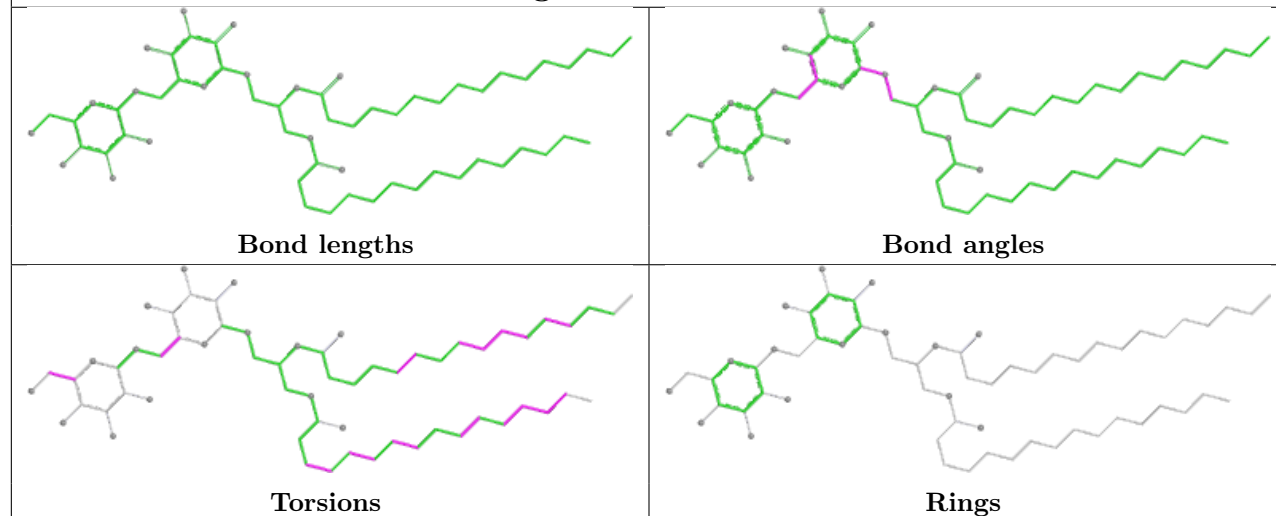


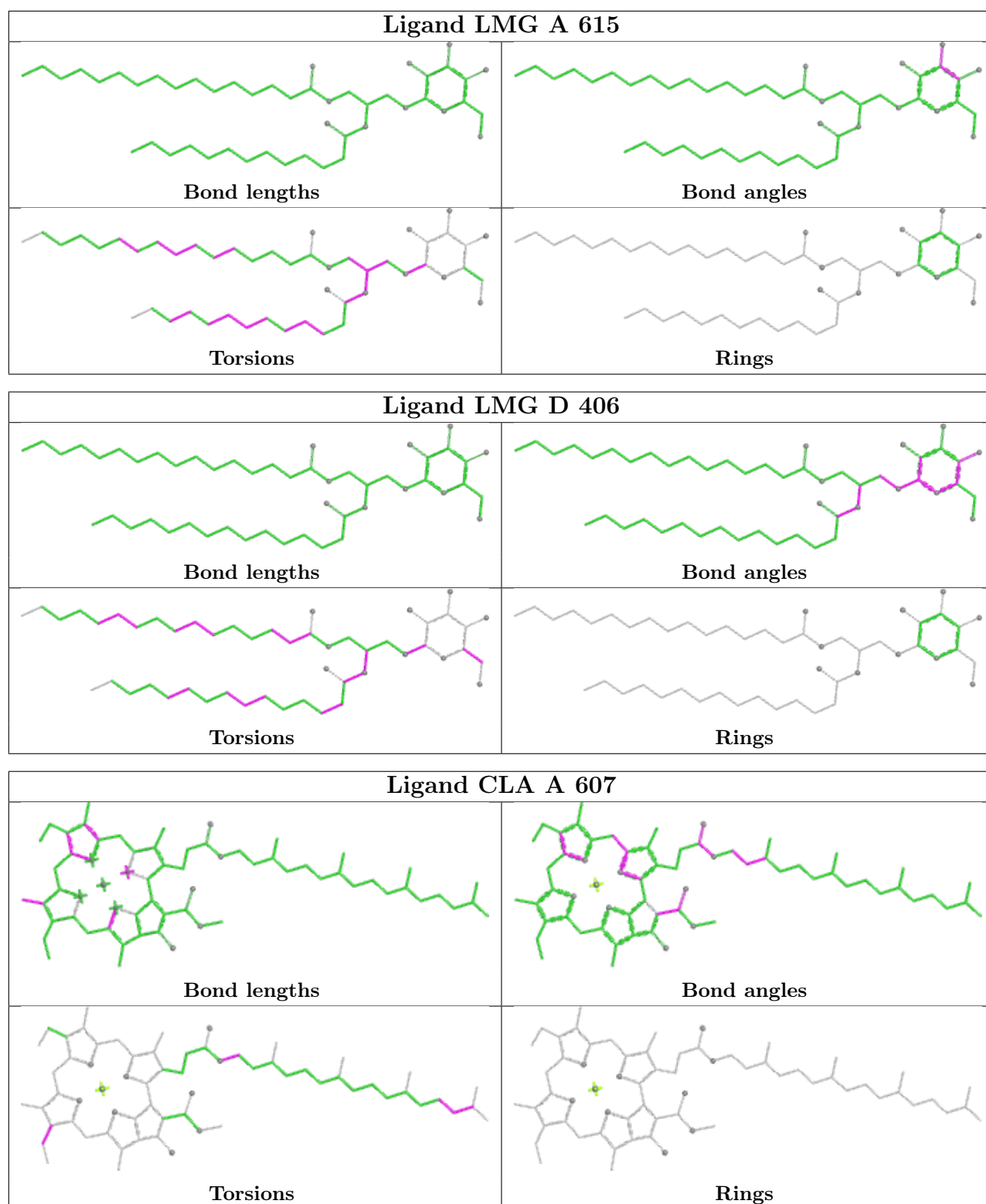
Ligand CLA b 613**Ligand CLA c 506**

Ligand HEC v 201

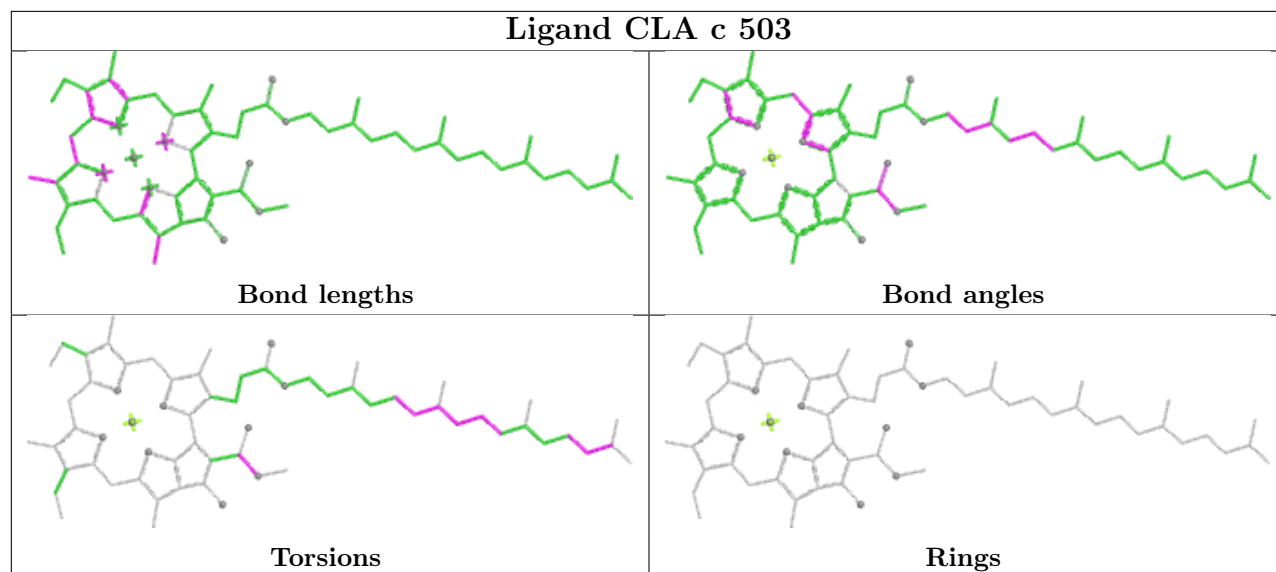


Ligand DGD c 521

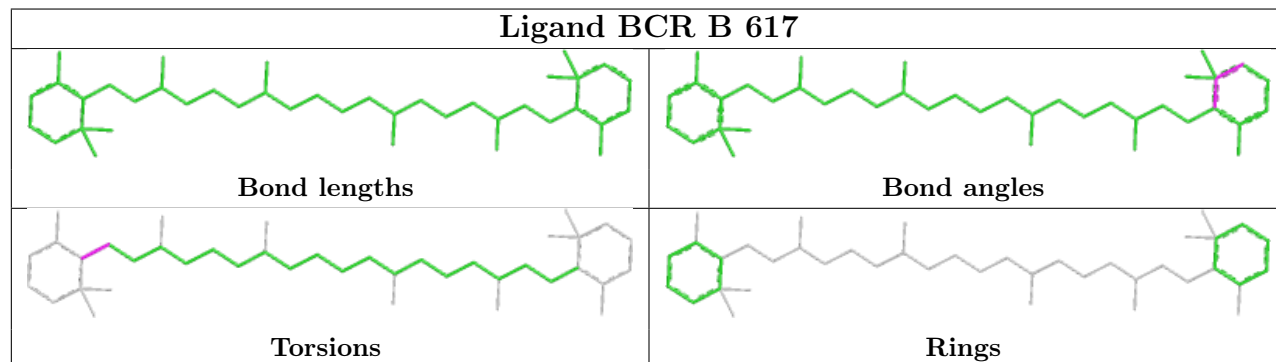




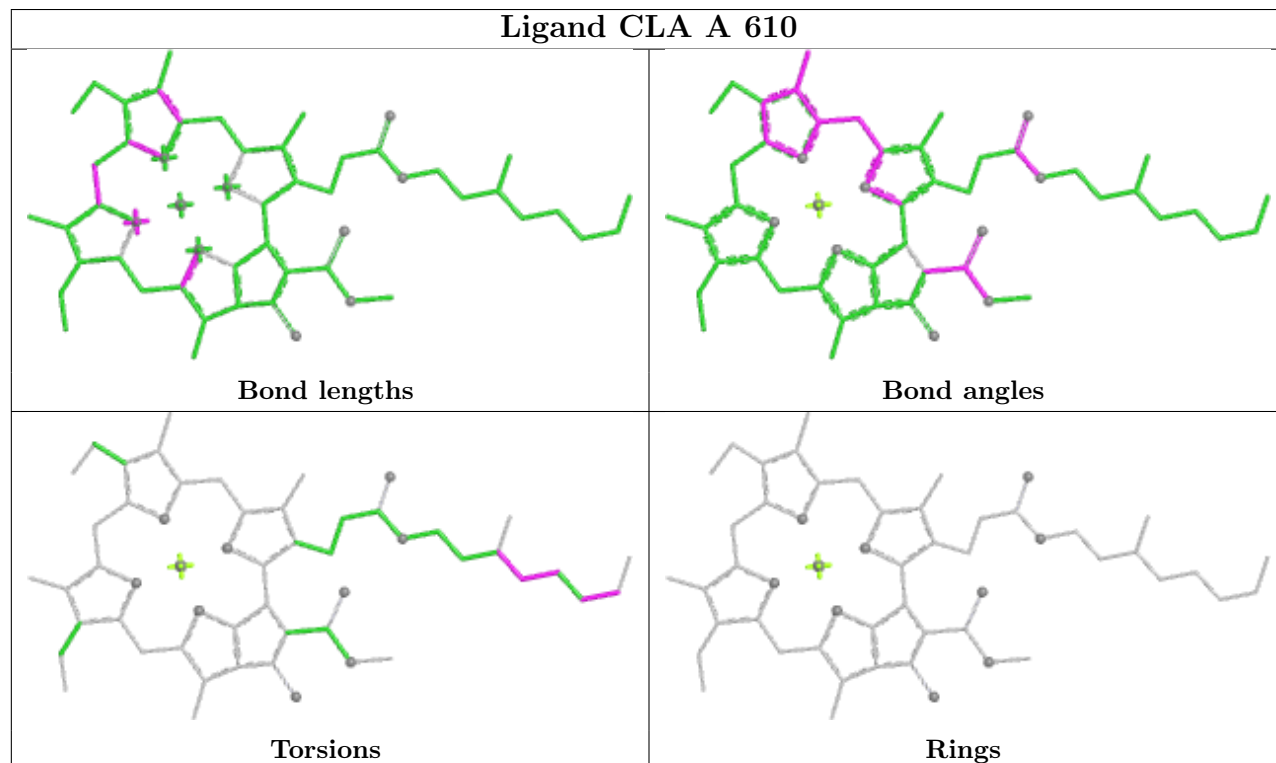
Ligand CLA c 503

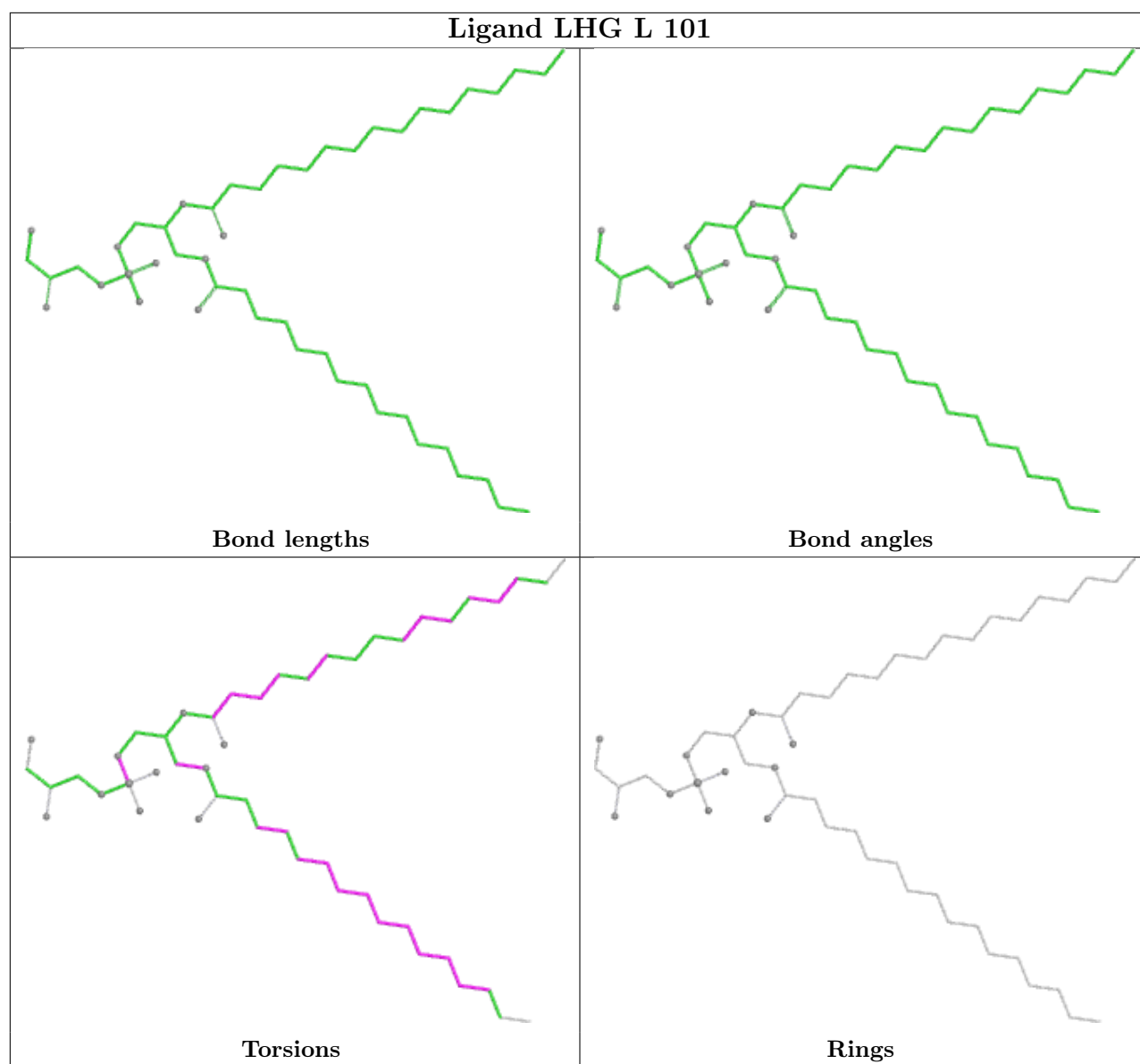


Ligand BCR B 617

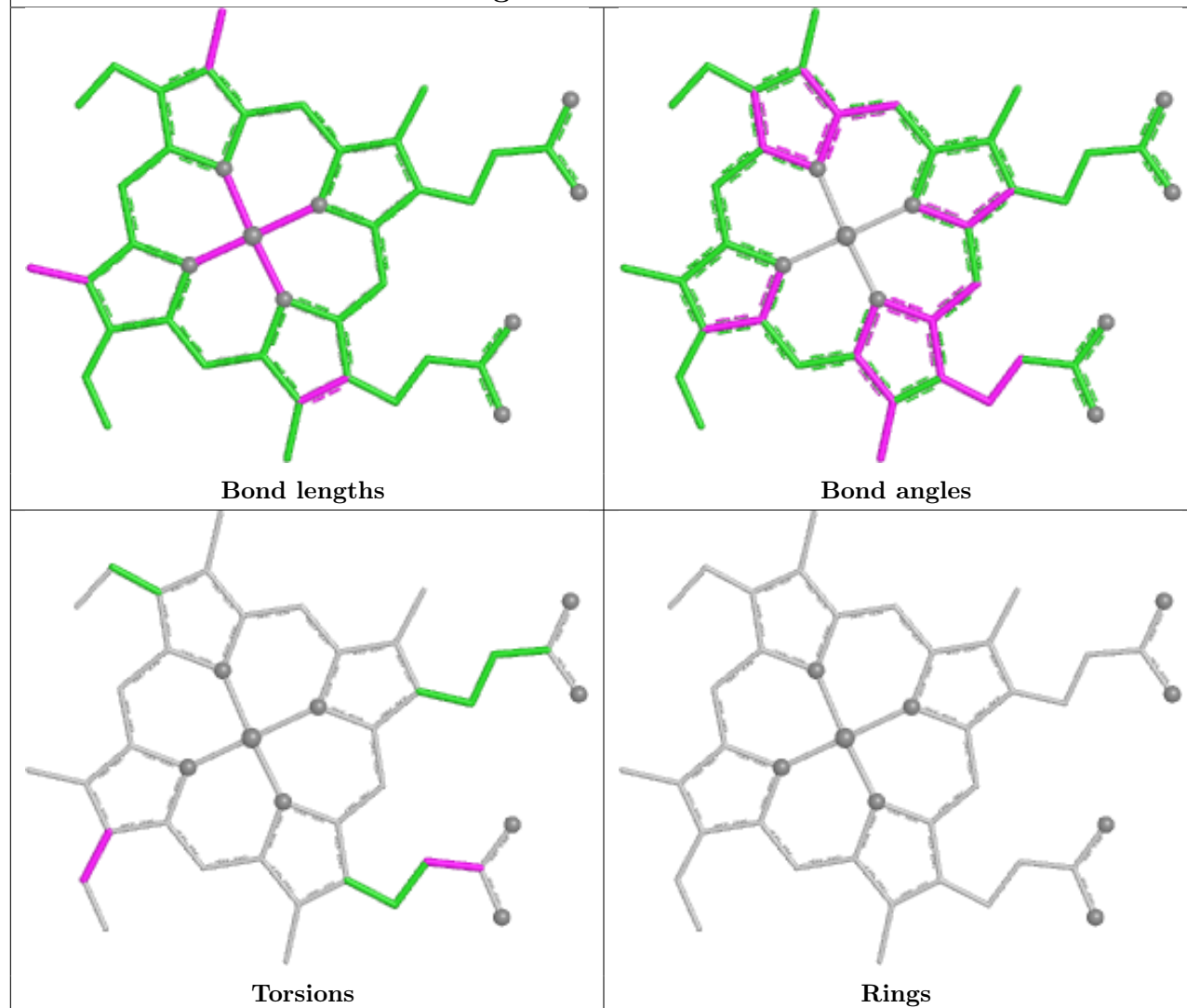


Ligand CLA A 610

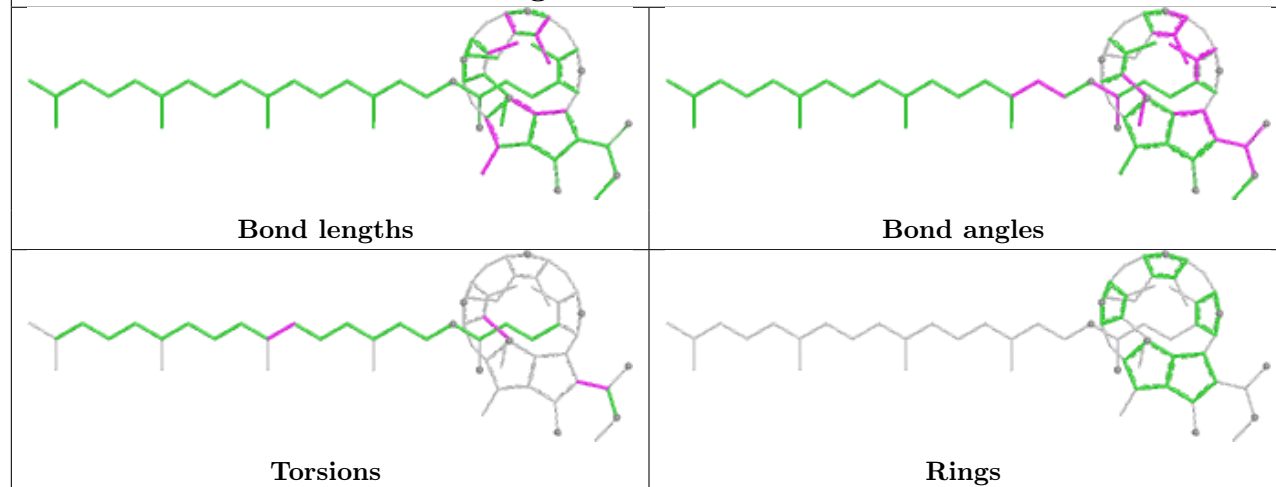


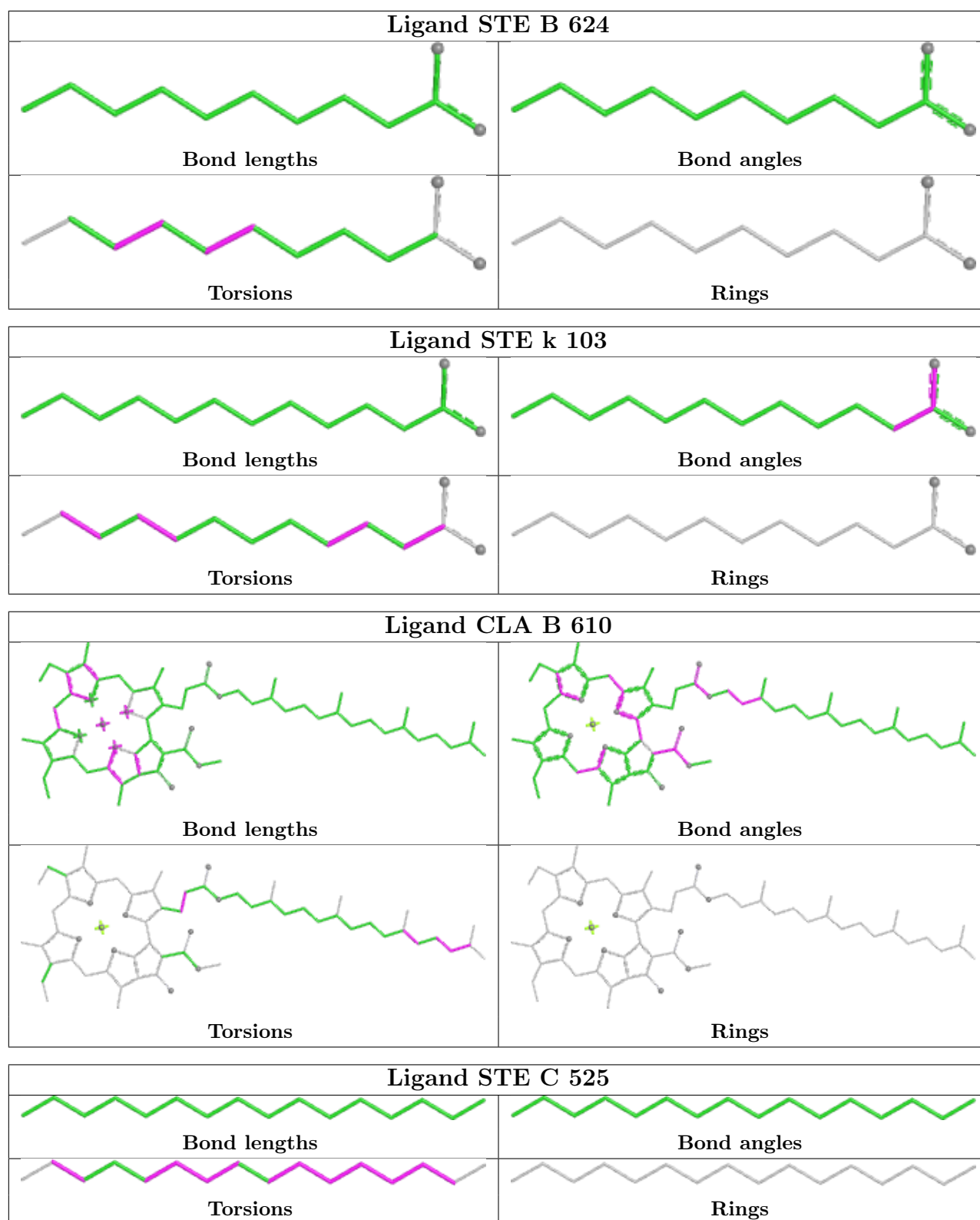


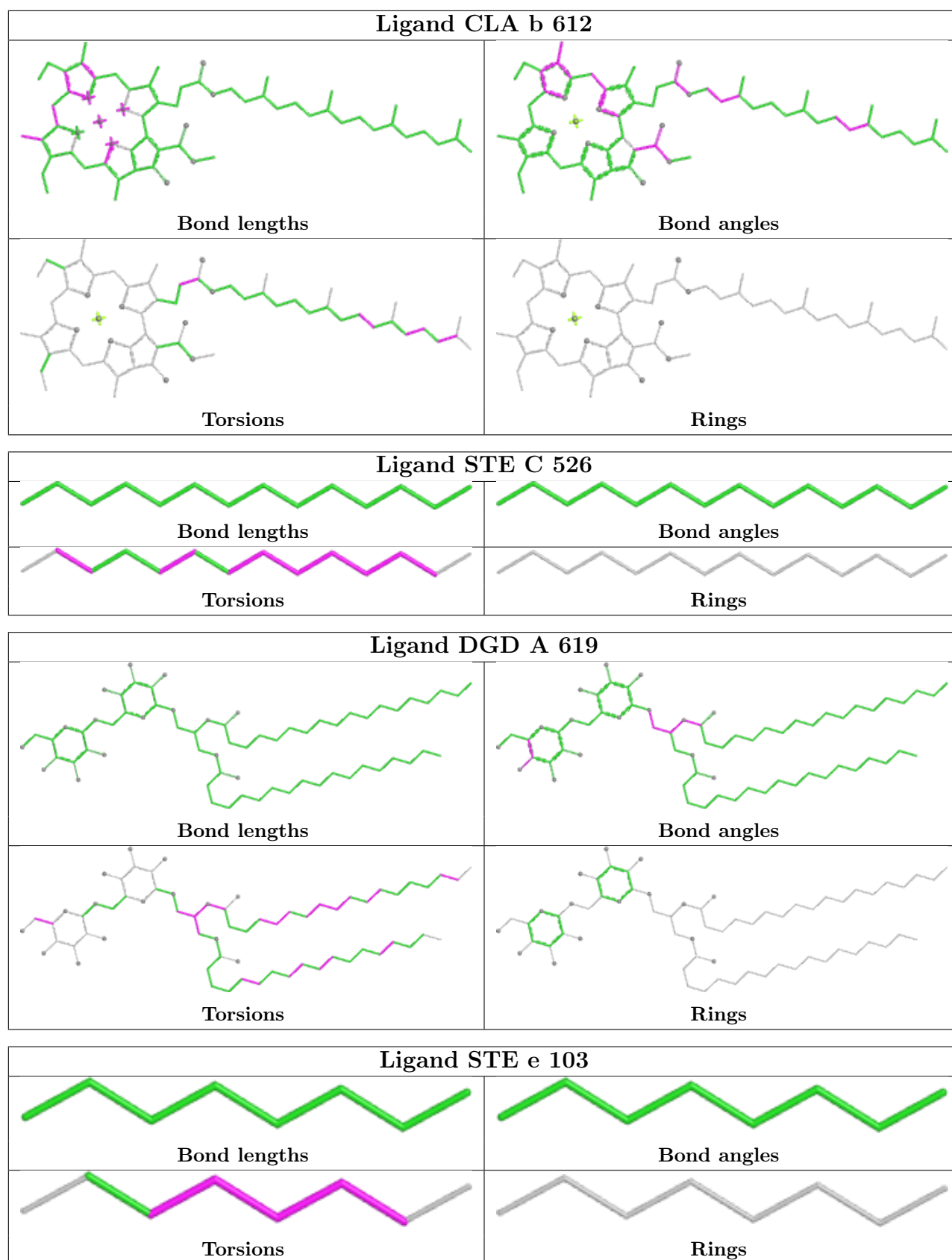
Ligand HEC V 201

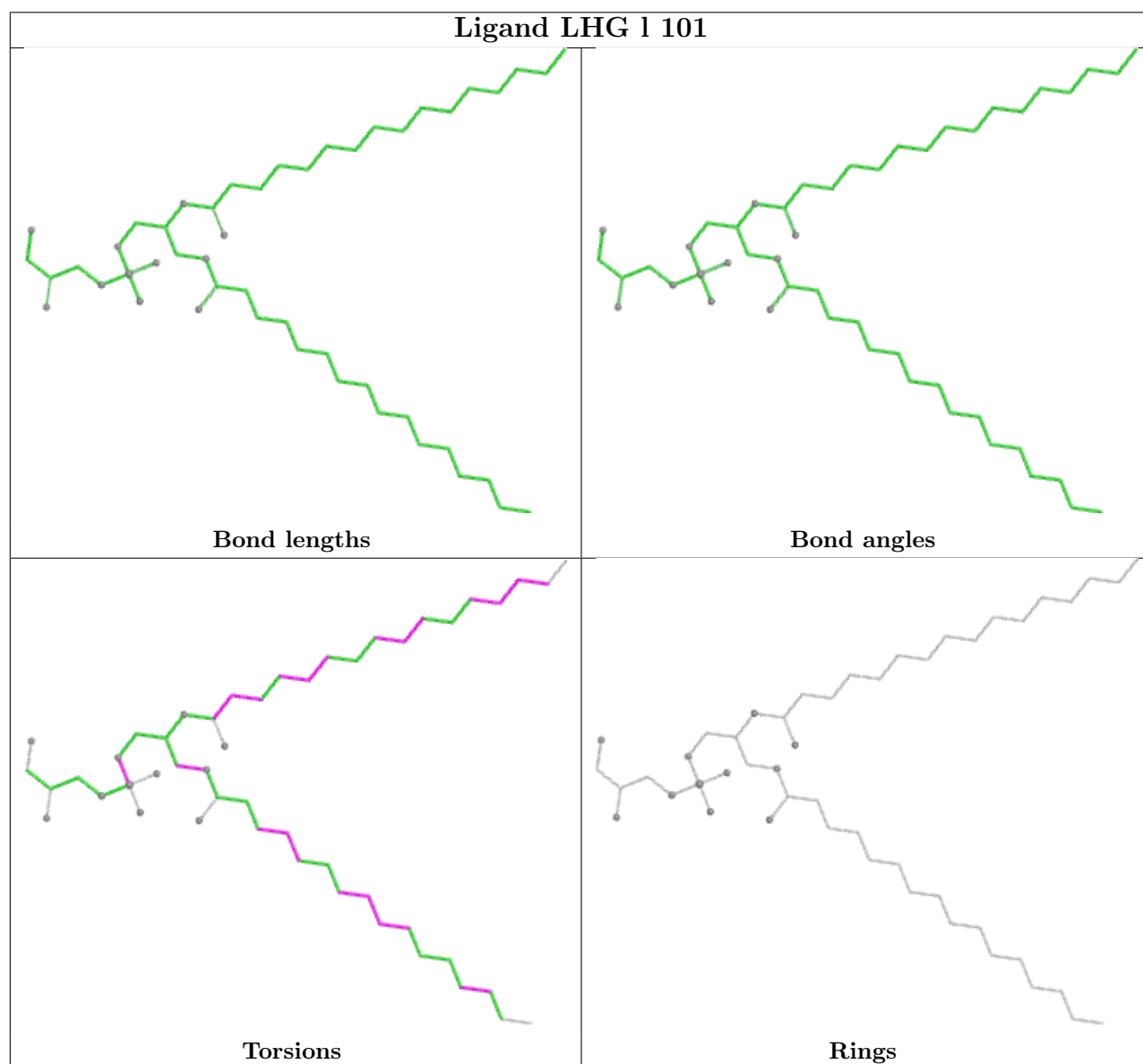
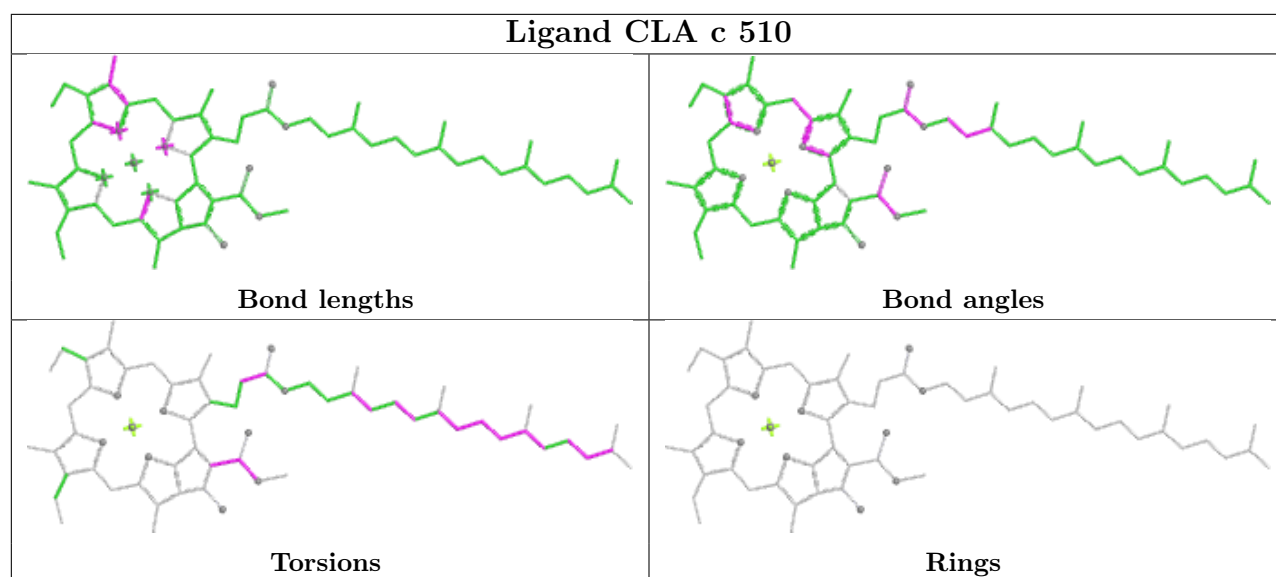


Ligand PHO A 609

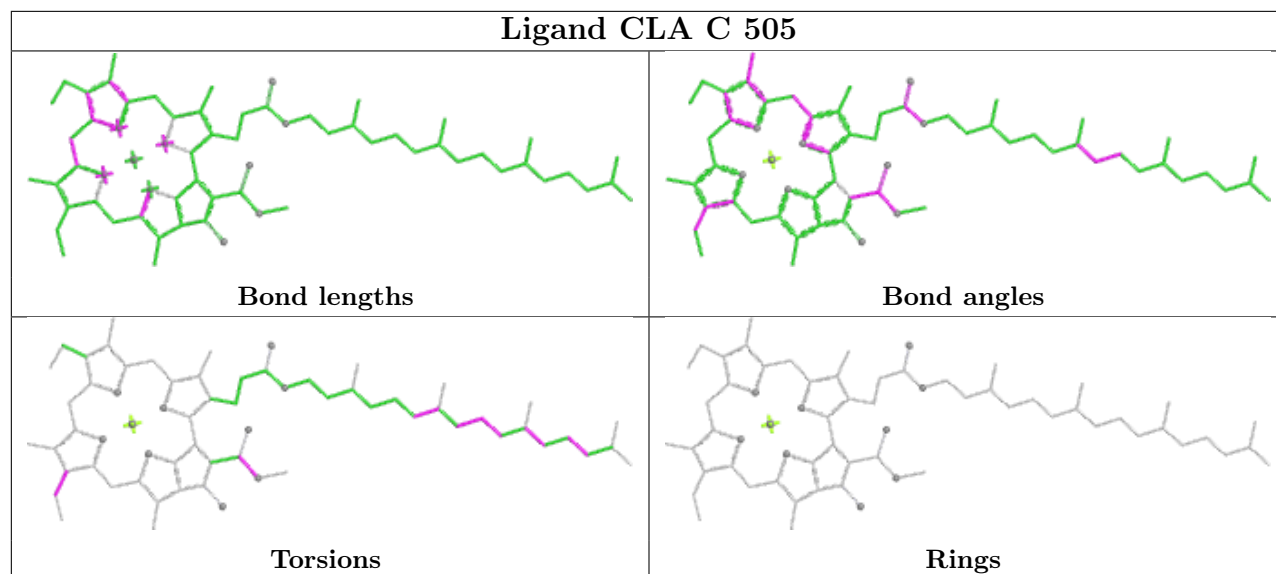




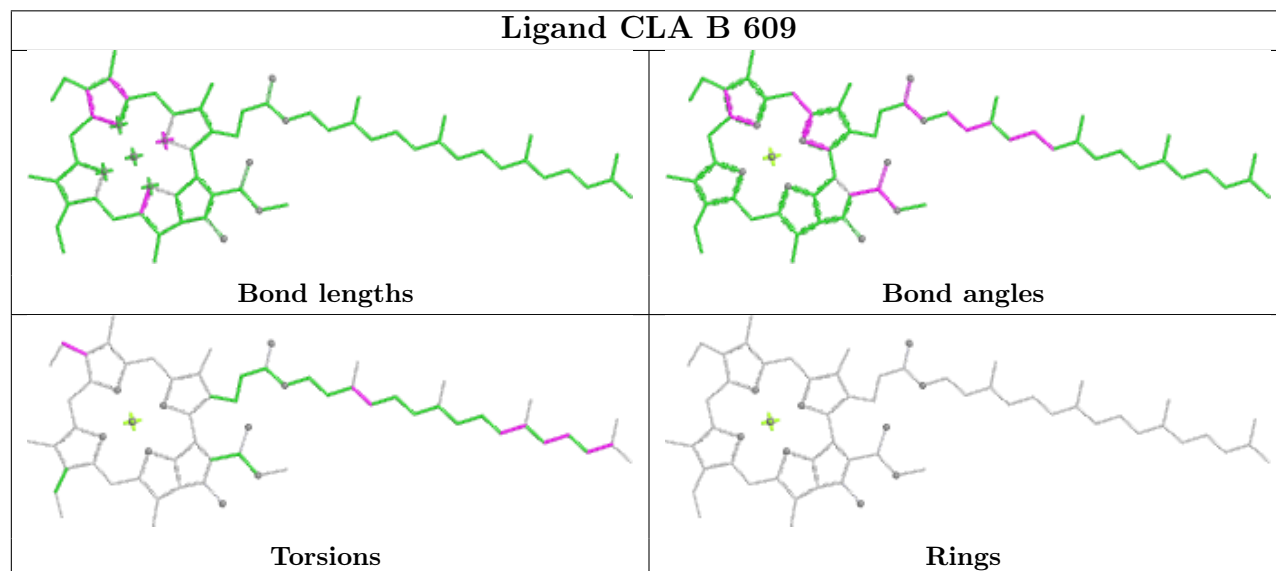




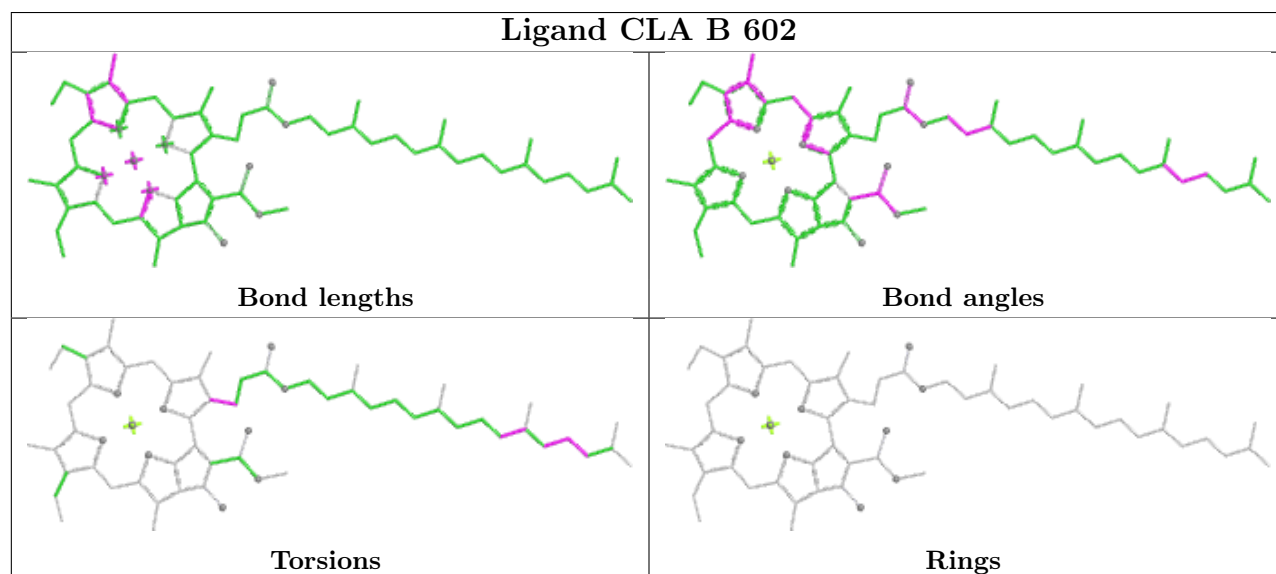
Ligand CLA C 505

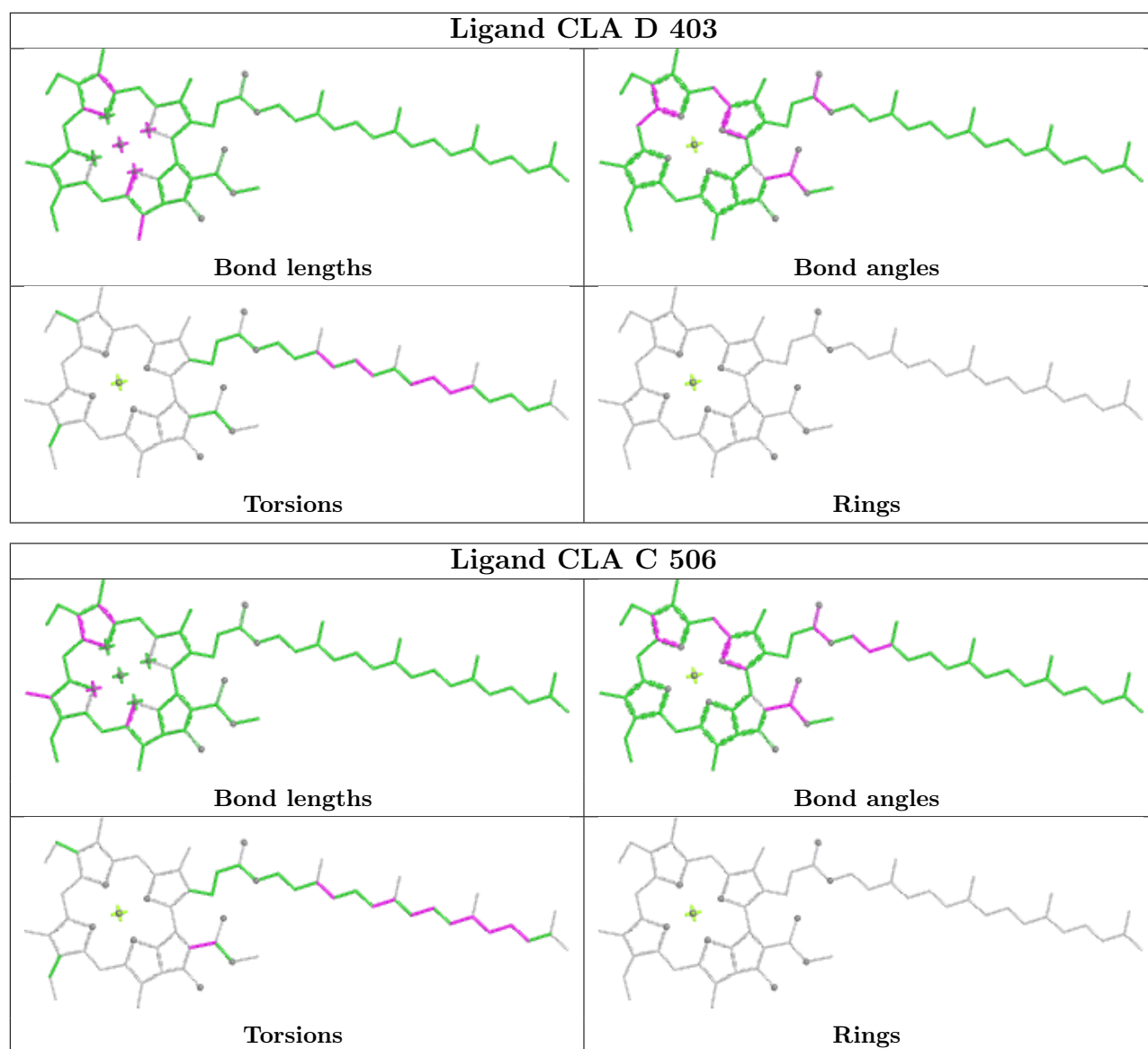


Ligand CLA B 609



Ligand CLA B 602





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%)	-0.30	1 (0%) 90 91	12, 29, 50, 76	69 (20%)
1	a	334/344 (97%)	-0.18	2 (0%) 85 87	12, 31, 55, 75	69 (20%)
2	B	505/510 (99%)	-0.19	4 (0%) 82 85	19, 33, 61, 90	5 (0%)
2	b	505/510 (99%)	-0.02	3 (0%) 85 87	26, 37, 69, 96	1 (0%)
3	C	442/461 (95%)	-0.09	0 100 100	14, 37, 53, 78	11 (2%)
3	c	451/461 (97%)	0.03	3 (0%) 84 86	14, 40, 59, 95	12 (2%)
4	D	341/352 (96%)	-0.33	0 100 100	14, 31, 49, 75	10 (2%)
4	d	341/352 (96%)	-0.15	2 (0%) 85 87	13, 35, 56, 75	11 (3%)
5	E	82/84 (97%)	0.54	3 (3%) 45 48	35, 52, 68, 85	1 (1%)
5	e	82/84 (97%)	0.63	2 (2%) 59 62	39, 58, 75, 84	0
6	F	34/45 (75%)	0.26	1 (2%) 53 56	37, 45, 60, 89	0
6	f	34/45 (75%)	0.32	0 100 100	40, 50, 75, 86	0
7	H	65/66 (98%)	0.11	1 (1%) 72 74	33, 40, 57, 72	0
7	h	63/66 (95%)	0.39	2 (3%) 50 53	40, 49, 62, 65	0
8	I	35/38 (92%)	0.05	1 (2%) 53 56	34, 39, 64, 82	0
8	i	35/38 (92%)	0.08	1 (2%) 53 56	32, 40, 66, 88	0
9	J	36/40 (90%)	0.33	1 (2%) 55 58	37, 51, 74, 88	0
9	j	36/40 (90%)	0.67	1 (2%) 55 58	39, 56, 81, 83	0
10	K	37/46 (80%)	0.39	0 100 100	45, 53, 69, 78	0
10	k	37/46 (80%)	0.47	0 100 100	47, 55, 70, 81	0
11	L	37/37 (100%)	-0.27	0 100 100	25, 30, 56, 66	0
11	l	36/37 (97%)	-0.42	0 100 100	27, 31, 62, 79	0
12	M	32/36 (88%)	-0.26	0 100 100	29, 33, 57, 73	0
12	m	31/36 (86%)	-0.35	0 100 100	30, 33, 50, 60	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	0.06	2 (0%) 82 85	26, 42, 73, 120	1 (0%)
13	o	244/272 (89%)	0.14	4 (1%) 70 73	26, 40, 76, 119	0
14	T	29/32 (90%)	-0.25	2 (6%) 23 25	26, 31, 52, 72	0
14	t	29/32 (90%)	-0.09	2 (6%) 23 25	29, 33, 66, 76	0
15	U	97/134 (72%)	0.04	0 100 100	33, 42, 65, 87	0
15	u	97/134 (72%)	-0.05	0 100 100	31, 40, 57, 85	0
16	V	137/163 (84%)	-0.06	0 100 100	31, 40, 56, 72	0
16	v	137/163 (84%)	0.17	0 100 100	35, 47, 65, 84	0
17	Y	27/46 (58%)	1.40	6 (22%) 2 2	53, 71, 107, 111	0
17	y	30/46 (65%)	0.93	2 (6%) 24 26	57, 74, 91, 99	0
18	X	38/41 (92%)	0.32	2 (5%) 32 35	42, 51, 67, 75	0
18	x	39/41 (95%)	0.40	0 100 100	48, 57, 76, 93	0
19	Z	62/62 (100%)	1.17	9 (14%) 6 6	54, 66, 105, 116	0
19	z	62/62 (100%)	1.03	3 (4%) 35 38	59, 71, 116, 132	0
20	R	28/41 (68%)	0.94	1 (3%) 46 49	60, 70, 83, 88	0
20	r	28/41 (68%)	1.54	8 (28%) 1 1	69, 82, 101, 103	0
All	All	5293/5700 (92%)	0.01	69 (1%) 75 77	12, 38, 71, 132	190 (3%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	z	33	TRP	4.5
19	Z	62	VAL	4.2
13	o	58	ASN	4.1
2	b	495	PHE	3.7
3	c	24	THR	3.6
14	t	30	THR	3.5
17	Y	25	ILE	3.5
19	Z	33	TRP	3.4
3	c	23	ALA	3.4
17	Y	24	MET	3.3
9	J	5	GLY	3.1
13	o	63	ALA	3.0
20	r	28	VAL	3.0
9	j	6	GLY	2.9
5	E	79	PHE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	Z	30	PRO	2.9
13	O	56	PRO	2.7
17	Y	20	ALA	2.7
20	r	14	LEU	2.7
13	o	59	LYS	2.7
2	B	479[A]	PHE	2.6
7	H	65	LEU	2.6
18	X	2	THR	2.6
14	t	29	ILE	2.6
19	z	40	ILE	2.6
2	B	495	PHE	2.6
20	r	29	LYS	2.6
19	Z	40	ILE	2.5
2	b	127	ARG	2.5
17	Y	41	VAL	2.5
14	T	30	THR	2.5
19	z	39	LEU	2.5
20	r	3	TRP	2.5
1	A	11	ALA	2.5
7	h	64	ALA	2.5
1	a	11	ALA	2.4
17	Y	22	LEU	2.4
3	c	147	PHE	2.4
5	e	79	PHE	2.4
17	Y	23	THR	2.4
5	E	3	GLY	2.4
13	O	57	LYS	2.4
19	Z	27	TYR	2.3
2	b	289	GLN	2.3
1	a	265	PHE	2.3
4	d	237	PRO	2.3
19	Z	2	THR	2.3
17	y	18	VAL	2.3
5	E	29	ALA	2.3
19	Z	41	PHE	2.2
19	Z	3	ILE	2.2
6	F	12	SER	2.2
8	I	34	ARG	2.2
14	T	29	ILE	2.2
18	X	3	ILE	2.2
17	y	22	LEU	2.2
13	o	56	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	r	12	VAL	2.2
7	h	6	TRP	2.1
2	B	505	ARG	2.1
20	r	9	LEU	2.1
20	r	26	TYR	2.1
19	Z	17	PHE	2.1
4	d	28	VAL	2.1
2	B	293	ALA	2.1
20	r	15	ALA	2.1
8	i	36	ASP	2.1
5	e	22	ILE	2.1
20	R	28	VAL	2.1

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	0.09	31,37,48,65	0
14	FME	T	1	10/11	0.92	0.10	29,36,52,68	0
12	FME	M	1	10/11	0.92	0.11	37,46,56,63	0
12	FME	m	1	10/11	0.95	0.07	32,44,56,64	0
8	FME	i	1	10/11	0.96	0.08	38,43,48,51	0
8	FME	I	1	10/11	0.97	0.07	40,45,51,54	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($\text{\AA}^2$)	Q<0.9
30	STE	i	101	12/20	0.61	0.16	61,83,99,99	0
30	STE	I	101	17/20	0.63	0.18	60,67,74,75	0
30	STE	C	519	10/20	0.63	0.22	55,65,70,74	0
30	STE	C	526	14/20	0.67	0.21	59,73,81,81	0
30	STE	E	103	20/20	0.67	0.20	51,65,72,73	0
31	LMG	D	406	50/55	0.67	0.19	37,63,88,91	0
30	STE	i	102	6/20	0.68	0.18	57,63,68,69	0
30	STE	e	104	9/20	0.69	0.20	60,65,71,74	0
30	STE	E	102	12/20	0.70	0.24	55,73,94,96	0
33	LHG	a	616	42/49	0.70	0.19	53,81,93,103	0
30	STE	A	621	17/20	0.71	0.15	55,61,67,69	0
30	STE	j	102	16/20	0.71	0.22	61,72,88,88	0
30	STE	H	102	18/20	0.72	0.18	50,64,72,74	0
30	STE	e	101	9/20	0.72	0.26	56,72,83,85	0
30	STE	C	518	7/20	0.73	0.19	51,57,60,61	0
30	STE	A	613	9/20	0.75	0.15	52,57,63,64	0
30	STE	K	104	14/20	0.75	0.17	57,63,75,77	0
30	STE	h	103	10/20	0.75	0.21	59,71,77,78	0
30	STE	c	517	18/20	0.75	0.20	62,76,83,83	0
30	STE	a	620	12/20	0.76	0.13	51,60,76,76	0
30	STE	e	105	13/20	0.76	0.19	67,73,83,83	0
30	STE	A	622	11/20	0.76	0.18	51,59,70,71	0
31	LMG	c	518	30/55	0.76	0.17	44,79,95,98	0
33	LHG	A	617	49/49	0.76	0.17	49,70,94,100	0
30	STE	a	619	10/20	0.76	0.14	43,48,55,57	0
30	STE	C	517	5/20	0.77	0.20	56,60,63,65	0
30	STE	C	515	14/20	0.78	0.17	52,60,66,69	0
31	LMG	c	523	48/55	0.78	0.17	52,69,82,85	0
31	LMG	a	618	55/55	0.78	0.15	36,57,67,70	0
31	LMG	b	622	55/55	0.78	0.17	48,65,79,85	0
34	DGD	A	619	66/66	0.78	0.15	46,57,79,86	0
30	STE	b	625	10/20	0.79	0.15	47,53,66,67	0
30	STE	k	103	14/20	0.79	0.14	54,67,77,79	0
29	PL9	A	612	55/55	0.80	0.18	40,62,78,79	0
30	STE	B	624	12/20	0.80	0.14	42,53,66,66	0
29	PL9	a	612	55/55	0.80	0.18	47,63,74,78	0
31	LMG	B	620	45/55	0.80	0.16	37,54,77,80	0
30	STE	d	410	20/20	0.81	0.13	41,50,64,79	0
31	LMG	C	516	36/55	0.81	0.14	45,59,71,75	0
32	SQD	a	617	54/54	0.81	0.14	40,58,88,97	0
30	STE	j	101	12/20	0.81	0.15	48,59,66,67	0
30	STE	C	524	12/20	0.81	0.16	38,48,51,54	0
30	STE	Z	101	17/20	0.81	0.21	55,69,88,92	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	STE	c	516	13/20	0.82	0.19	63,67,73,74	0
30	STE	E	101	12/20	0.82	0.17	59,66,76,81	0
30	STE	B	623	18/20	0.82	0.14	40,51,73,74	0
30	STE	I	102	15/20	0.82	0.15	42,49,61,63	0
30	STE	e	103	8/20	0.82	0.19	55,61,63,72	0
30	STE	B	625	15/20	0.82	0.20	39,53,68,70	0
30	STE	H	103	9/20	0.83	0.14	46,54,63,63	0
26	CLA	b	601	65/65	0.83	0.13	41,62,86,89	0
30	STE	M	104	15/20	0.83	0.17	45,54,75,75	0
31	LMG	A	615	48/55	0.83	0.13	40,55,68,77	0
30	STE	d	408	20/20	0.83	0.14	53,64,84,88	0
30	STE	b	624	16/20	0.84	0.15	47,57,71,73	0
30	STE	T	102	16/20	0.84	0.17	38,46,71,71	0
30	STE	h	104	11/20	0.85	0.18	58,60,64,65	0
31	LMG	c	522	46/55	0.85	0.14	47,65,75,79	0
30	STE	A	620	8/20	0.85	0.15	41,50,51,58	0
32	SQD	A	618	43/54	0.85	0.11	37,51,80,89	0
30	STE	B	621	17/20	0.86	0.14	39,48,62,64	0
30	STE	J	101	12/20	0.86	0.15	52,58,64,69	0
30	STE	b	621	20/20	0.86	0.13	40,51,67,67	0
31	LMG	c	524	49/55	0.86	0.13	39,54,70,73	0
31	LMG	C	523	48/55	0.86	0.14	44,64,75,78	0
30	STE	D	411	20/20	0.86	0.13	34,50,65,75	0
32	SQD	b	620	49/54	0.86	0.11	39,52,69,74	0
31	LMG	M	101	51/55	0.86	0.12	30,47,61,66	0
30	STE	m	102	12/20	0.86	0.11	39,45,64,69	0
30	STE	t	102	14/20	0.86	0.11	35,43,53,53	0
32	SQD	B	622	54/54	0.87	0.11	38,54,71,74	0
31	LMG	m	101	51/55	0.87	0.11	35,47,61,64	0
30	STE	M	103	10/20	0.87	0.13	33,42,49,53	0
30	STE	d	406	20/20	0.88	0.12	44,50,74,79	0
30	STE	M	102	15/20	0.88	0.12	38,42,59,69	0
30	STE	C	525	16/20	0.88	0.15	41,49,59,60	0
26	CLA	C	513	65/65	0.88	0.12	46,57,78,83	0
30	STE	z	101	9/20	0.88	0.19	52,62,63,64	0
28	BCR	k	101	40/40	0.89	0.12	47,57,64,65	0
32	SQD	a	615	54/54	0.89	0.12	40,59,73,75	0
32	SQD	f	101	41/54	0.89	0.13	51,71,79,84	0
32	SQD	F	102	36/54	0.90	0.12	49,66,75,77	0
26	CLA	B	601	65/65	0.90	0.11	34,51,76,82	0
26	CLA	c	512	65/65	0.90	0.11	44,53,71,79	0
28	BCR	K	102	40/40	0.90	0.10	44,51,57,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	BCR	c	514	40/40	0.90	0.12	53,56,63,65	0
32	SQD	A	616	52/54	0.90	0.11	33,51,70,71	0
28	BCR	d	404	40/40	0.90	0.11	38,46,76,83	0
28	BCR	h	101	40/40	0.90	0.11	38,51,59,62	0
34	DGD	c	520	62/66	0.90	0.11	37,47,73,77	0
30	STE	m	103	18/20	0.91	0.11	34,41,65,66	0
28	BCR	X	101	40/40	0.91	0.09	33,44,55,56	0
26	CLA	c	513	65/65	0.91	0.12	47,61,78,83	0
28	BCR	D	404	40/40	0.91	0.12	35,42,76,84	0
28	BCR	K	101	40/40	0.91	0.12	45,53,57,59	0
26	CLA	c	503	65/65	0.91	0.10	37,43,47,52	0
34	DGD	C	521	62/66	0.91	0.11	39,47,83,94	0
28	BCR	k	102	40/40	0.91	0.12	44,51,59,63	0
26	CLA	C	503	65/65	0.92	0.09	36,41,47,53	0
26	CLA	C	511	65/65	0.92	0.10	37,48,61,63	0
28	BCR	K	103	40/40	0.92	0.10	40,48,60,64	0
28	BCR	T	101	40/40	0.92	0.09	28,36,45,48	0
33	LHG	b	623	49/49	0.92	0.11	33,44,60,62	0
28	BCR	B	619	40/40	0.92	0.09	29,39,49,51	0
26	CLA	C	512	65/65	0.92	0.10	38,49,76,85	0
34	DGD	H	101	62/66	0.92	0.10	32,41,48,52	0
31	LMG	D	407	51/55	0.92	0.12	34,48,71,79	0
34	DGD	h	102	62/66	0.92	0.10	32,44,52,56	0
26	CLA	c	504	60/65	0.93	0.09	30,41,68,75	0
26	CLA	c	507	65/65	0.93	0.09	33,42,50,52	0
26	CLA	c	509	65/65	0.93	0.10	35,44,52,60	0
26	CLA	c	511	65/65	0.93	0.10	36,51,61,65	0
28	BCR	b	619	40/40	0.93	0.09	33,41,51,53	0
26	CLA	C	510	65/65	0.93	0.09	26,40,51,60	0
28	BCR	c	515	40/40	0.93	0.10	33,43,48,51	0
26	CLA	a	607	65/65	0.93	0.07	20,29,35,46	0
28	BCR	A	611	40/40	0.93	0.08	27,34,38,42	0
26	CLA	C	502	65/65	0.93	0.09	32,37,49,56	0
28	BCR	C	514	40/40	0.93	0.09	29,39,51,51	0
28	BCR	t	101	40/40	0.93	0.08	27,35,43,47	0
31	LMG	d	409	44/55	0.93	0.10	34,47,68,71	0
26	CLA	b	606	65/65	0.93	0.09	30,36,59,68	0
26	CLA	C	508	65/65	0.93	0.10	32,37,78,89	0
26	CLA	c	506	65/65	0.94	0.09	35,42,71,76	0
26	CLA	C	504	59/65	0.94	0.08	32,40,65,74	0
26	CLA	c	508	64/65	0.94	0.09	34,41,84,96	0
25	BCT	a	606	4/4	0.94	0.07	36,38,44,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	CLA	b	610	65/65	0.94	0.08	28,35,42,45	0
28	BCR	a	611	40/40	0.94	0.07	21,32,38,40	0
28	BCR	b	617	40/40	0.94	0.07	29,39,42,45	0
28	BCR	b	618	40/40	0.94	0.07	26,36,44,46	0
26	CLA	b	614	65/65	0.94	0.09	25,35,63,70	0
26	CLA	b	616	60/65	0.94	0.09	28,40,78,84	0
26	CLA	d	403	65/65	0.94	0.09	30,38,69,75	0
27	PHO	A	609	64/64	0.94	0.07	26,31,36,38	0
27	PHO	a	609	64/64	0.94	0.07	25,29,34,38	0
27	PHO	d	401	64/64	0.94	0.07	30,35,42,47	0
33	LHG	D	409	47/49	0.94	0.10	30,39,67,73	0
33	LHG	D	410	49/49	0.94	0.10	29,39,54,56	0
33	LHG	a	614	39/49	0.94	0.10	32,42,60,60	0
26	CLA	c	502	65/65	0.94	0.08	35,40,50,56	0
28	BCR	B	617	40/40	0.94	0.07	25,35,41,42	0
33	LHG	l	101	49/49	0.94	0.09	31,40,47,53	0
28	BCR	B	618	40/40	0.94	0.07	27,35,44,46	0
34	DGD	C	520	62/66	0.94	0.09	26,36,65,70	0
29	PL9	D	405	55/55	0.94	0.07	24,31,36,39	0
34	DGD	C	522	62/66	0.94	0.10	32,42,66,76	0
26	CLA	C	509	65/65	0.94	0.09	32,40,55,58	0
34	DGD	c	519	62/66	0.94	0.10	29,36,62,68	0
26	CLA	B	606	65/65	0.94	0.08	25,34,54,61	0
34	DGD	c	521	62/66	0.94	0.09	33,47,70,82	0
26	CLA	c	505	65/65	0.94	0.09	30,40,53,59	0
26	CLA	B	602	65/65	0.95	0.07	26,33,48,52	0
25	BCT	A	606	4/4	0.95	0.07	33,34,38,39	0
26	CLA	B	610	65/65	0.95	0.08	24,30,38,42	0
26	CLA	a	608	65/65	0.95	0.09	26,35,79,83	0
26	CLA	a	610	65/65	0.95	0.09	21,28,69,79	0
26	CLA	a	613	65/65	0.95	0.07	18,29,42,45	0
26	CLA	C	505	65/65	0.95	0.08	27,35,51,59	0
26	CLA	c	510	65/65	0.95	0.08	33,43,52,57	0
26	CLA	b	602	65/65	0.95	0.08	31,38,50,56	0
26	CLA	b	603	65/65	0.95	0.08	24,32,56,58	0
33	LHG	L	101	49/49	0.95	0.08	31,37,45,51	0
26	CLA	b	605	65/65	0.95	0.07	24,32,41,43	0
26	CLA	d	402	65/65	0.95	0.07	23,29,47,52	0
26	CLA	C	506	65/65	0.95	0.09	32,40,76,81	0
26	CLA	b	608	65/65	0.95	0.07	27,39,51,57	0
27	PHO	D	401	64/64	0.95	0.07	19,28,33,38	0
26	CLA	b	609	65/65	0.95	0.08	33,41,54,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
26	CLA	B	611	65/65	0.95	0.07	23,28,41,45	0
26	CLA	B	614	65/65	0.95	0.09	23,32,59,67	0
26	CLA	b	615	65/65	0.95	0.08	28,37,52,61	0
26	CLA	B	616	60/65	0.95	0.08	27,32,74,80	0
29	PL9	d	405	55/55	0.95	0.07	25,32,37,41	0
26	CLA	c	501	65/65	0.95	0.07	29,36,47,50	0
26	CLA	C	501	65/65	0.95	0.08	27,33,45,48	0
26	CLA	B	612	65/65	0.96	0.07	23,28,36,43	0
26	CLA	B	603	65/65	0.96	0.07	22,27,48,54	0
26	CLA	b	607	65/65	0.96	0.07	24,31,52,63	0
33	LHG	D	408	49/49	0.96	0.07	29,35,45,48	0
26	CLA	B	615	65/65	0.96	0.07	24,32,53,56	0
26	CLA	B	604	65/65	0.96	0.08	22,28,59,66	0
26	CLA	B	605	65/65	0.96	0.07	22,28,39,41	0
26	CLA	b	611	65/65	0.96	0.07	28,31,42,49	0
26	CLA	b	612	65/65	0.96	0.07	25,33,40,44	0
26	CLA	b	613	65/65	0.96	0.08	23,30,59,66	0
33	LHG	d	407	49/49	0.96	0.08	30,36,45,52	0
26	CLA	D	402	65/65	0.96	0.06	22,27,44,50	0
26	CLA	D	403	65/65	0.96	0.09	27,34,86,93	0
26	CLA	A	614	65/65	0.96	0.06	22,27,40,43	0
26	CLA	B	607	65/65	0.96	0.07	20,29,49,52	0
26	CLA	B	608	65/65	0.96	0.07	26,31,45,50	0
26	CLA	B	609	65/65	0.96	0.07	26,34,49,55	0
26	CLA	A	607	65/65	0.96	0.07	22,26,37,44	0
26	CLA	C	507	65/65	0.96	0.07	28,36,48,55	0
26	CLA	A	608	65/65	0.96	0.08	24,31,78,89	0
26	CLA	b	604	65/65	0.96	0.08	25,31,59,70	0
35	HEM	F	101	43/43	0.96	0.09	44,48,58,63	0
35	HEM	e	102	43/43	0.96	0.09	48,56,67,73	0
26	CLA	A	610	54/65	0.97	0.07	22,28,57,58	0
26	CLA	B	613	65/65	0.97	0.06	22,28,54,58	0
24	CL	A	605	1/1	0.98	0.05	31,31,31,31	0
22	OEX	a	602[A]	10/10	0.98	0.04	26,33,35,39	10
36	HEC	V	201	43/43	0.98	0.06	25,31,37,44	0
36	HEC	v	201	43/43	0.98	0.06	31,35,42,48	0
22	OEX	A	602[A]	10/10	0.99	0.03	28,34,35,38	10
21	OEY	A	601[B]	11/11	0.99	0.04	25,28,32,33	11
23	FE2	A	603	1/1	0.99	0.04	37,37,37,37	0
23	FE2	a	603	1/1	0.99	0.03	40,40,40,40	0
24	CL	A	604	1/1	0.99	0.03	29,29,29,29	0
21	OEY	a	601[B]	11/11	0.99	0.04	25,29,31,32	11

Continued on next page...

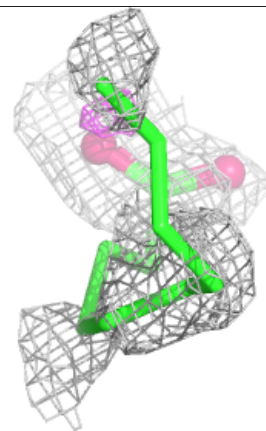
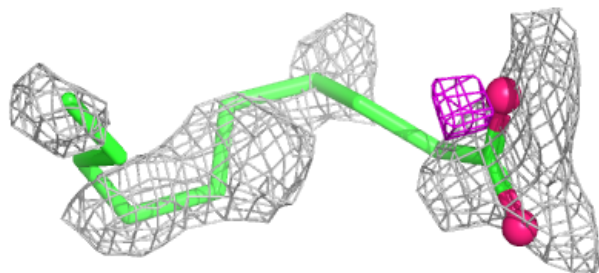
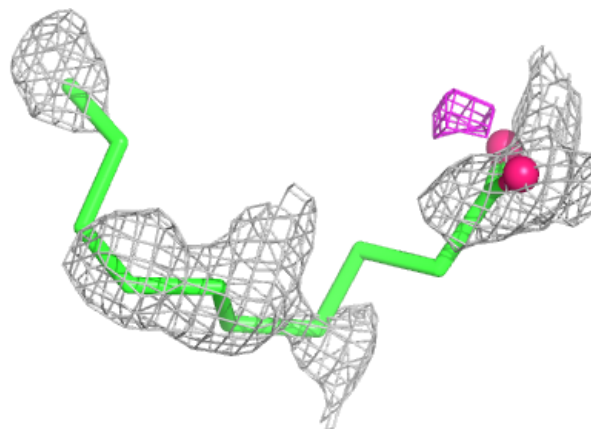
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CL	a	605	1/1	0.99	0.05	29,29,29,29	0
24	CL	a	604	1/1	1.00	0.05	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.

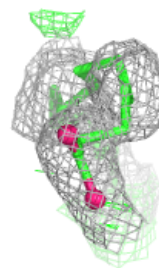
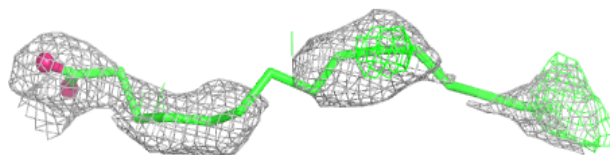
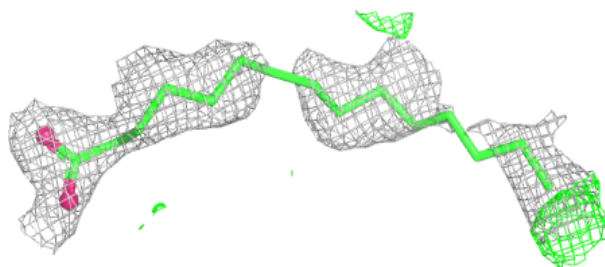
Electron density around STE i 101:

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



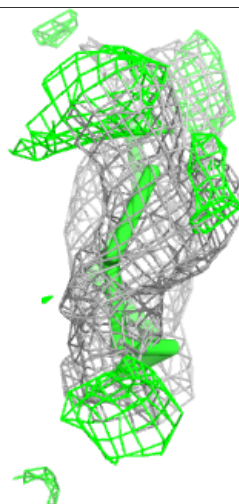
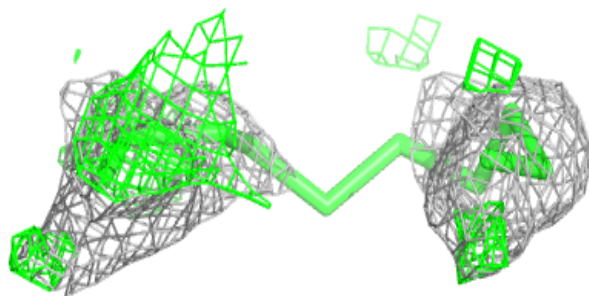
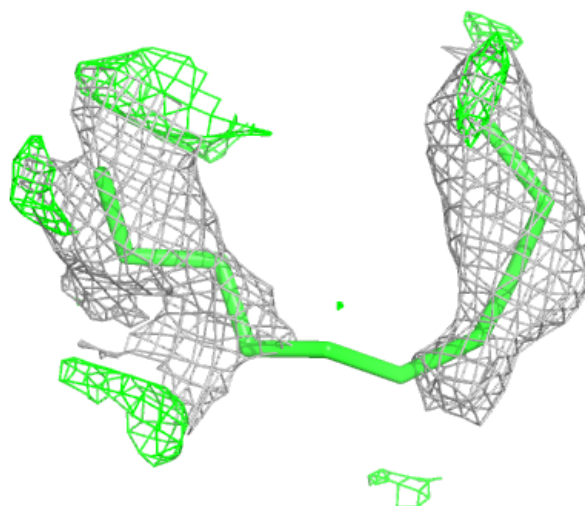
Electron density around STE I 101:

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



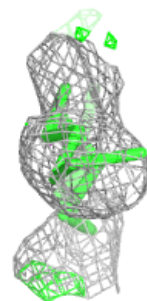
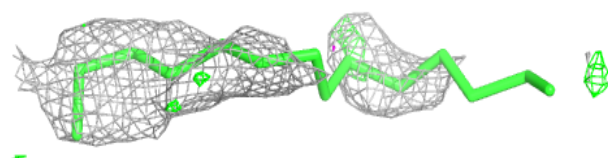
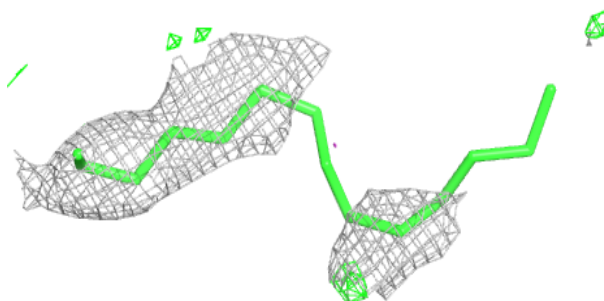
Electron density around STE C 519:

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

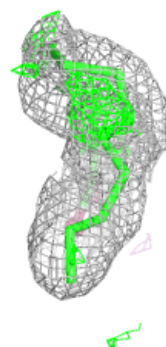
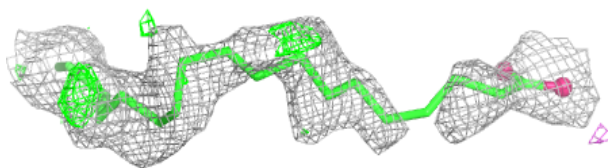
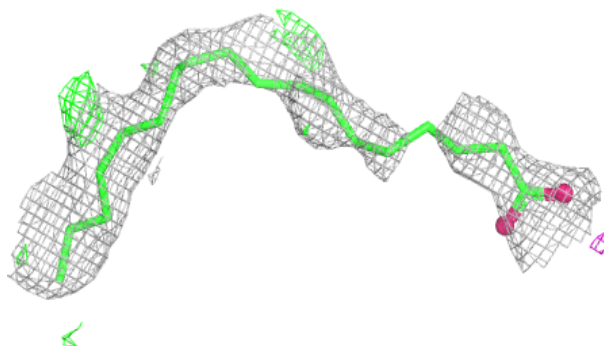


Electron density around STE C 526:

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

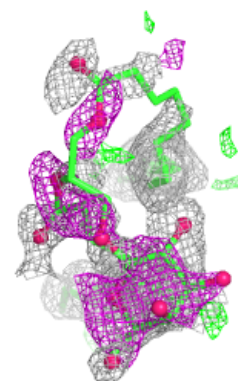
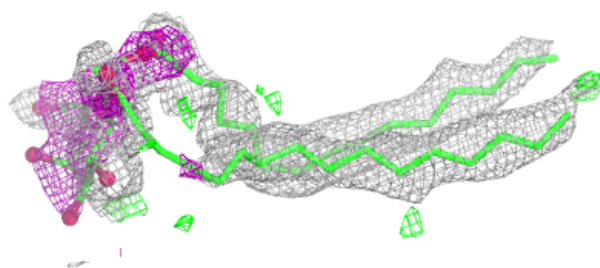
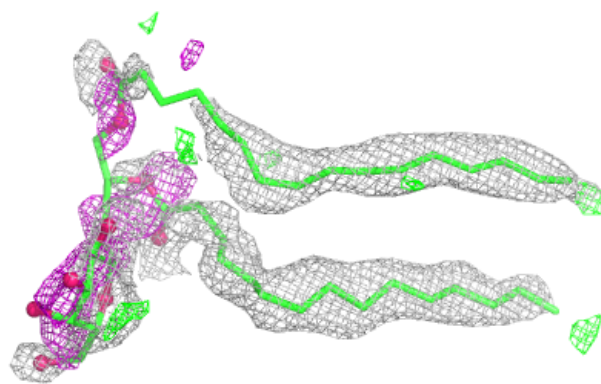
**Electron density around STE E 103:**

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

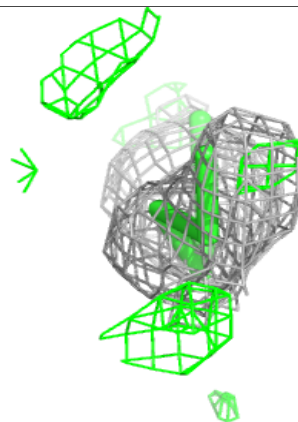
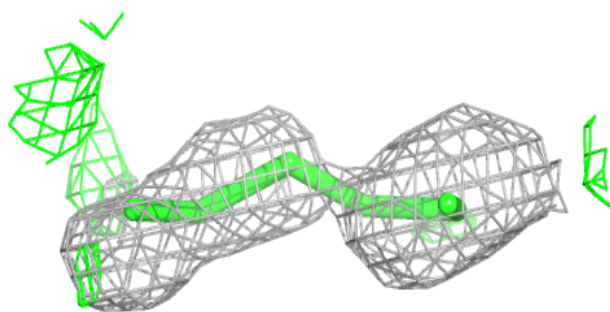
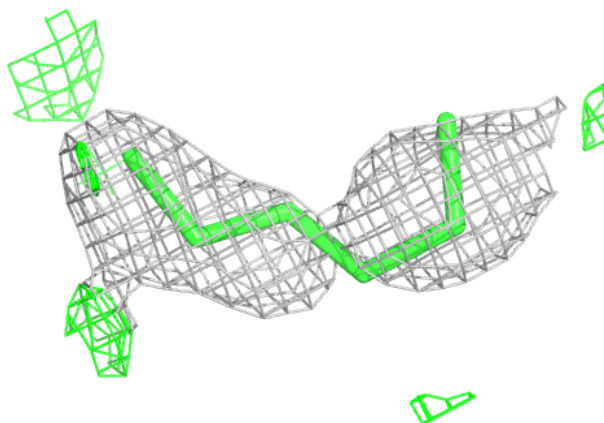


Electron density around LMG D 406:

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

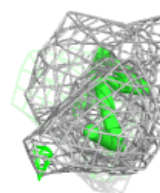
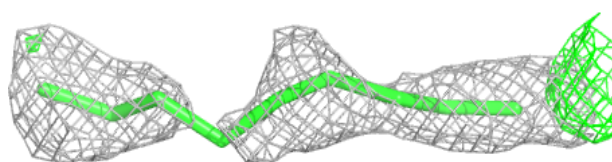
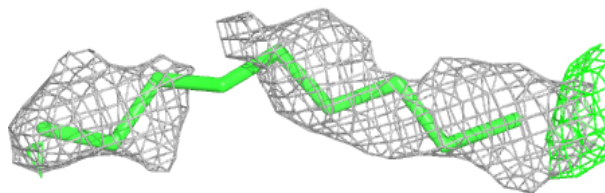
**Electron density around STE i 102:**

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

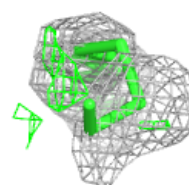
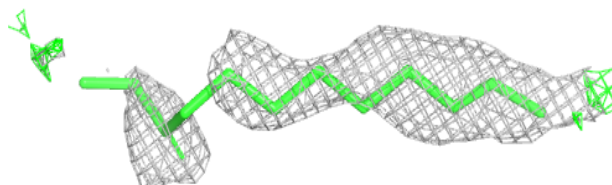
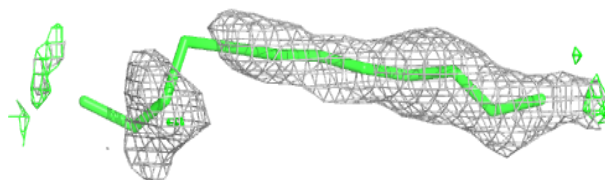


Electron density around STE e 104:

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

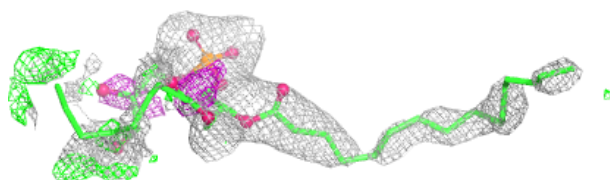
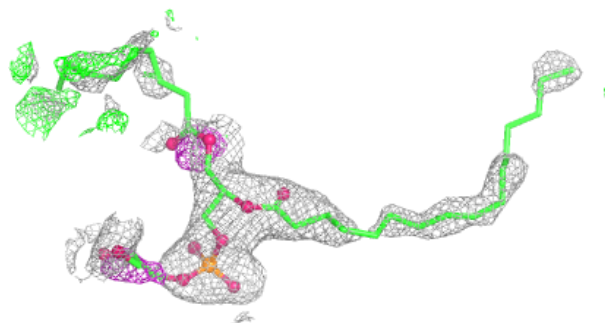
**Electron density around STE E 102:**

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

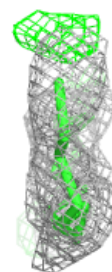
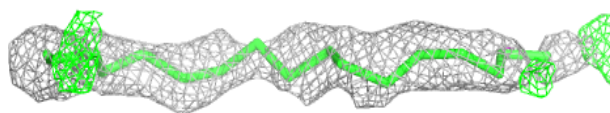
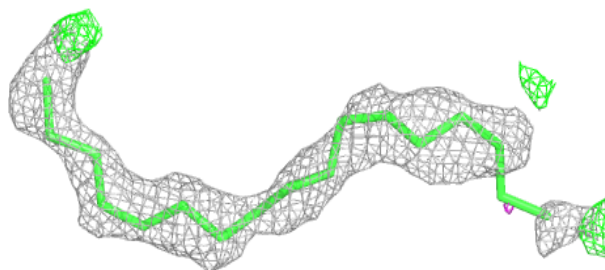


Electron density around LHG a 616:

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

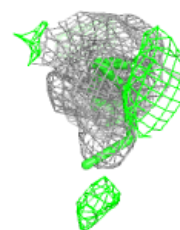
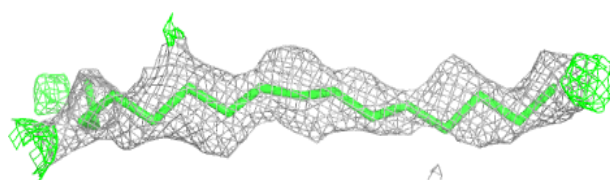
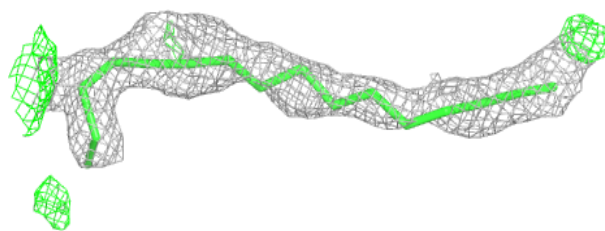
**Electron density around STE A 621:**

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

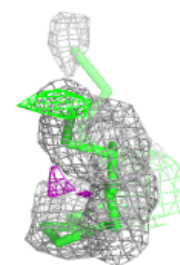
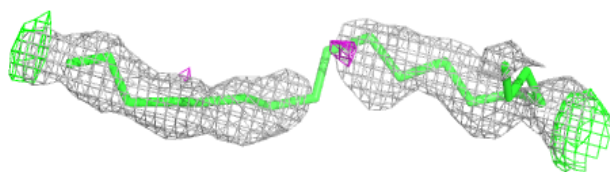
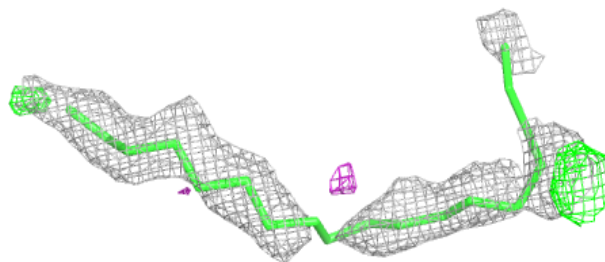


Electron density around STE j 102:

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

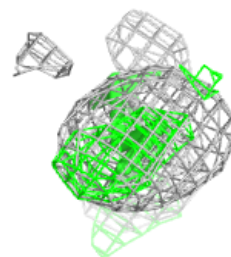
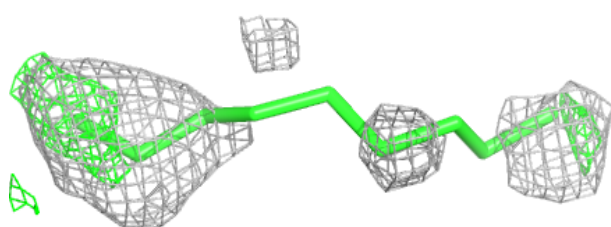
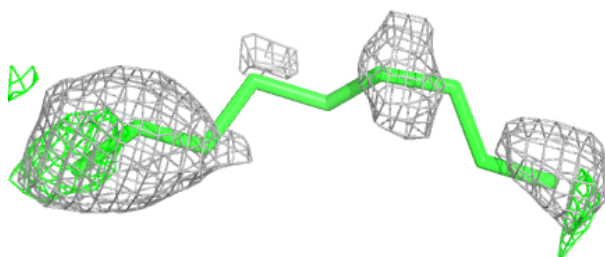
**Electron density around STE H 102:**

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

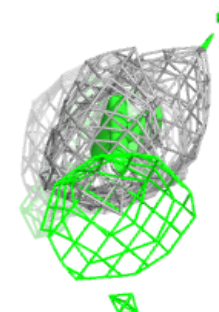
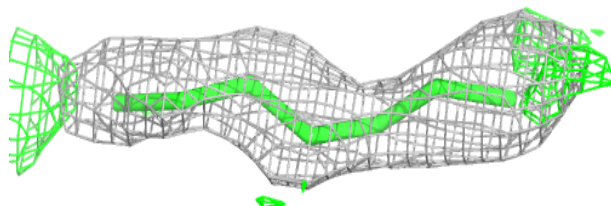
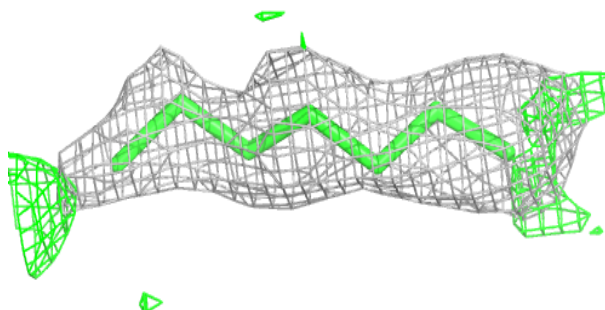


Electron density around STE e 101:

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

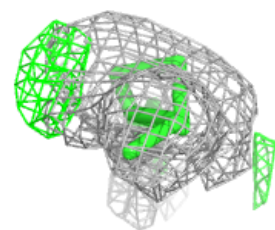
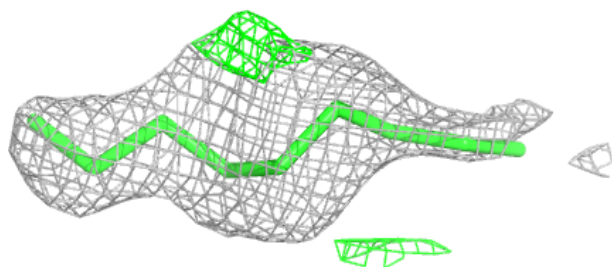
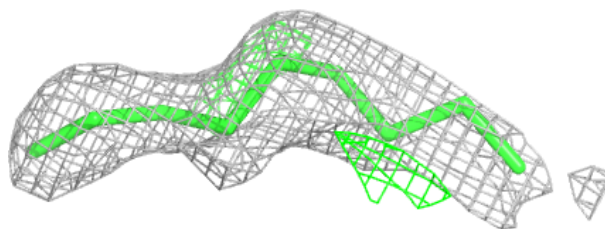
**Electron density around STE C 518:**

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

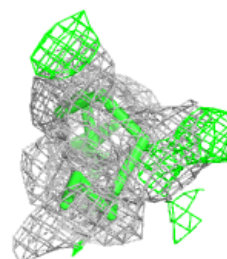
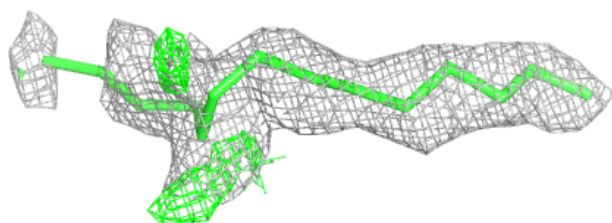
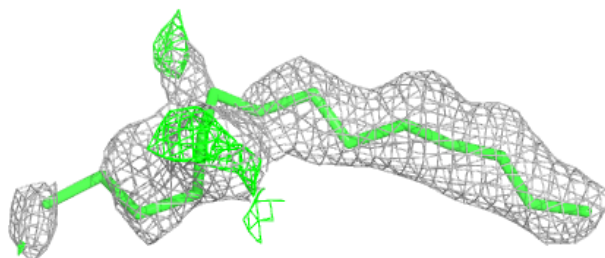


Electron density around STE A 613:

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

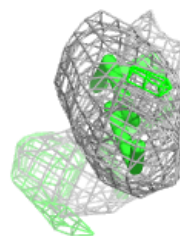
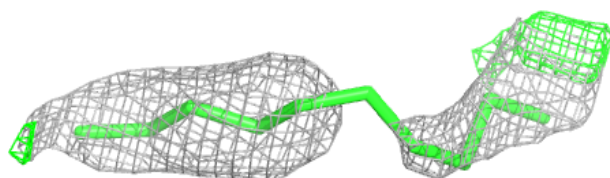
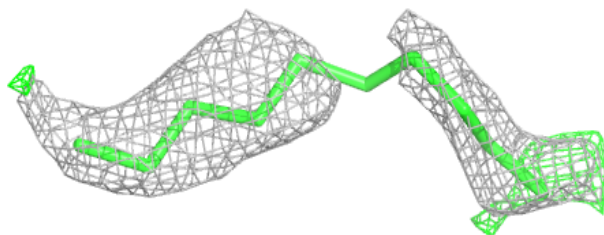
**Electron density around STE K 104:**

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

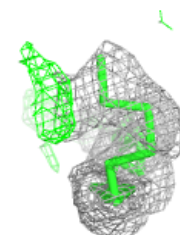
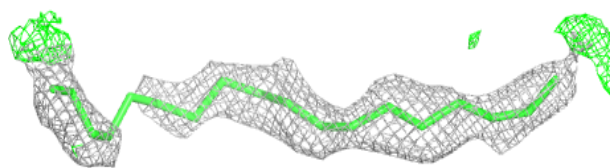
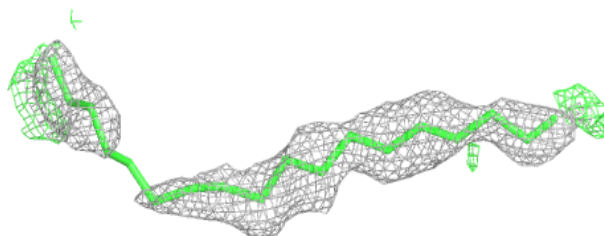


Electron density around STE h 103:

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

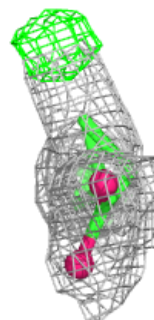
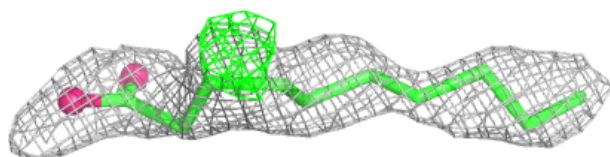
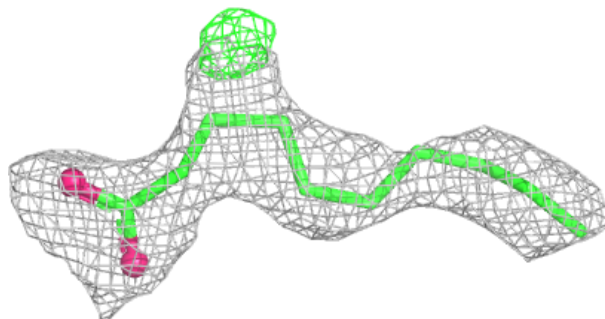
**Electron density around STE c 517:**

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

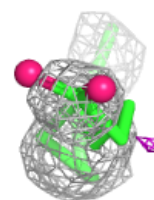
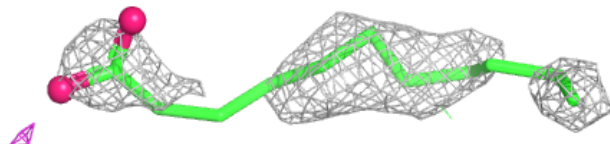
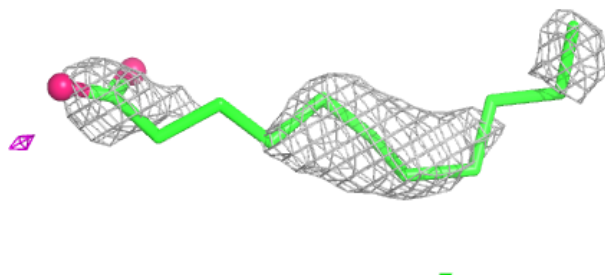


Electron density around STE a 620:

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

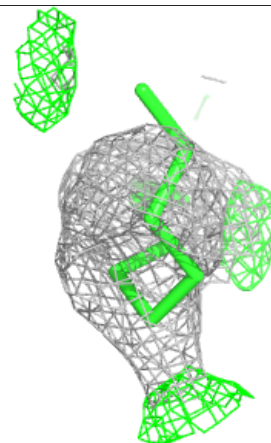
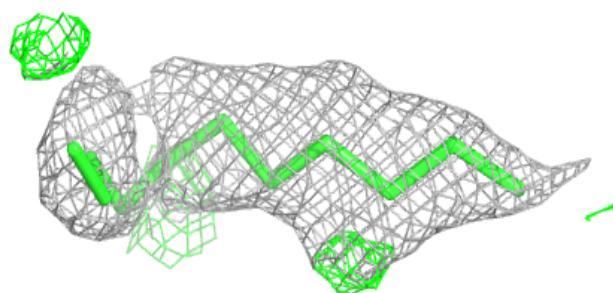
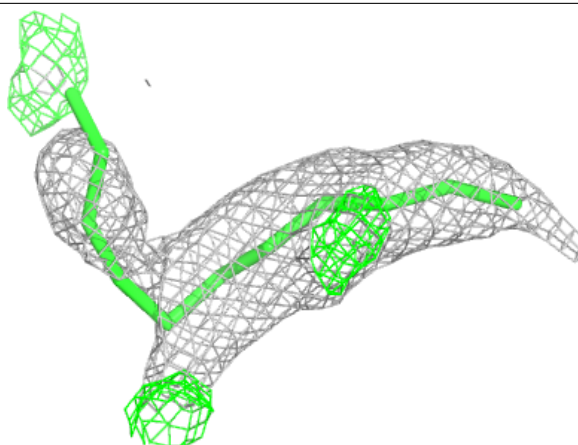
**Electron density around STE e 105:**

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

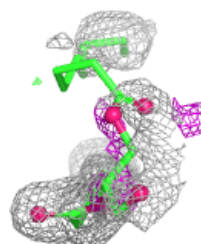
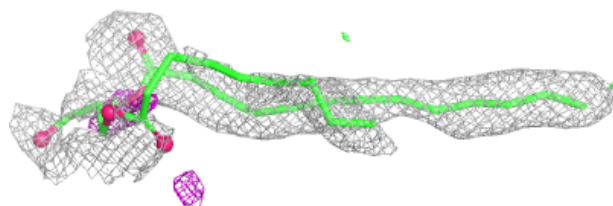
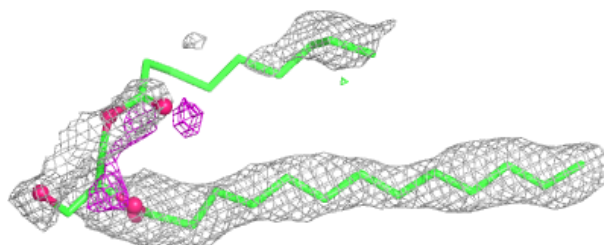


Electron density around STE A 622:

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

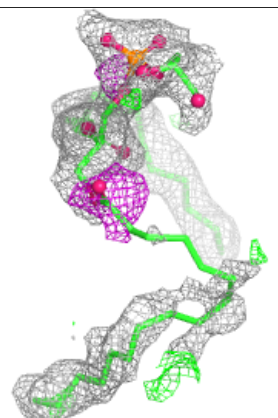
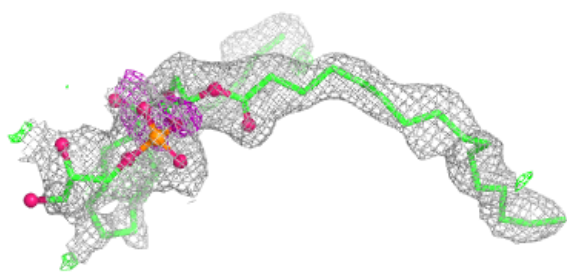
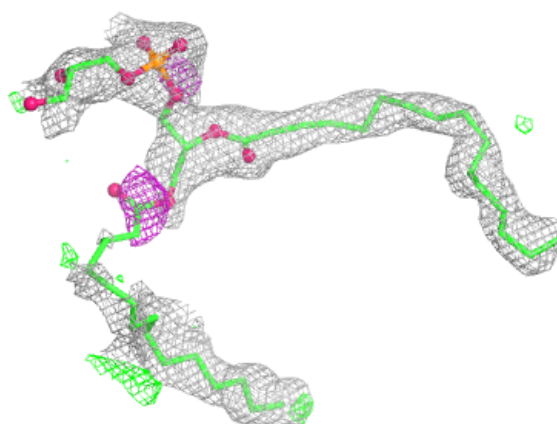
**Electron density around LMG c 518:**

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

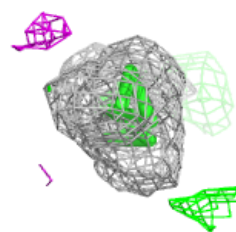
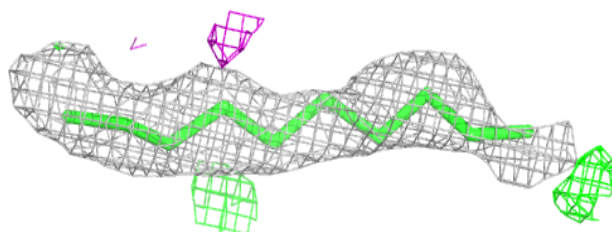
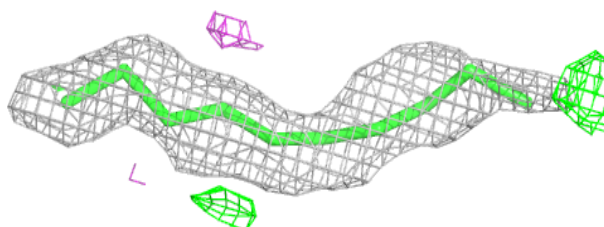


Electron density around LHG A 617:

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

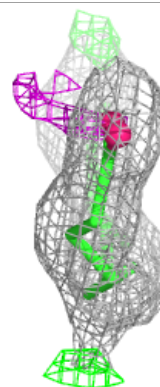
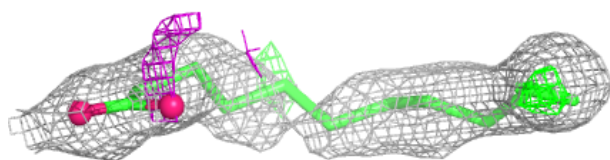
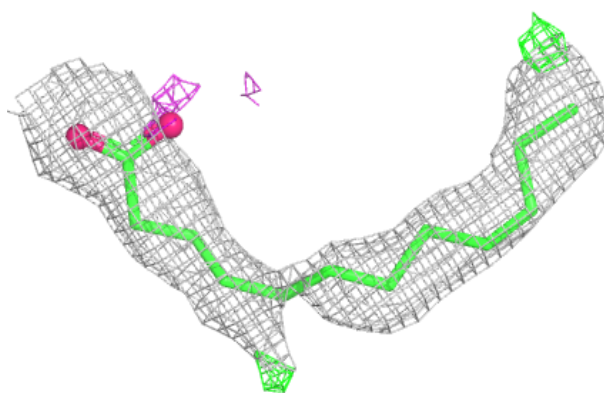
**Electron density around STE a 619:**

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

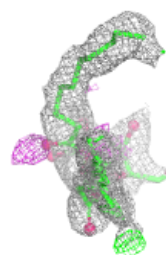
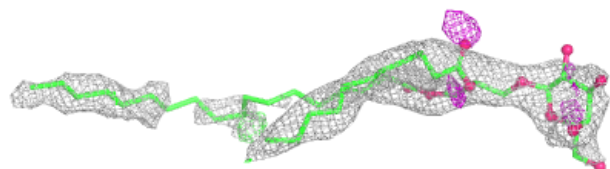
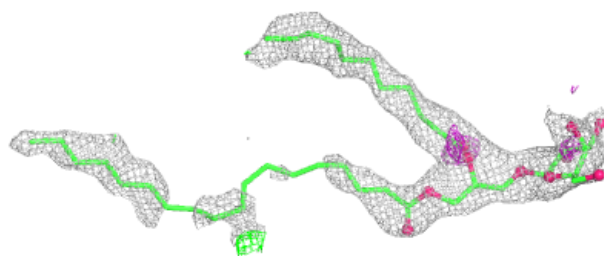


Electron density around STE C 515:

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

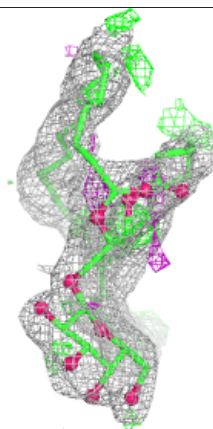
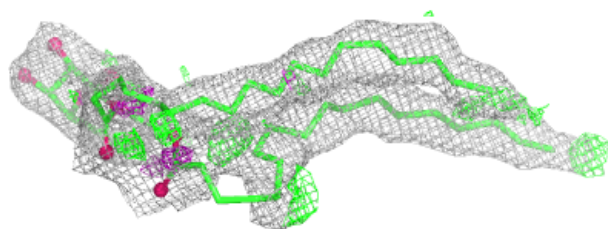
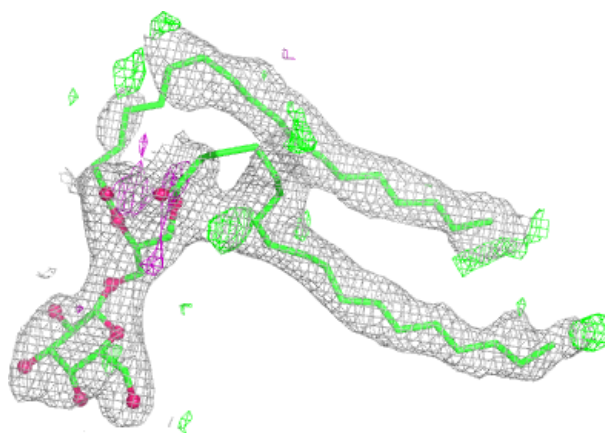
**Electron density around LMG c 523:**

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

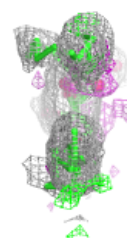
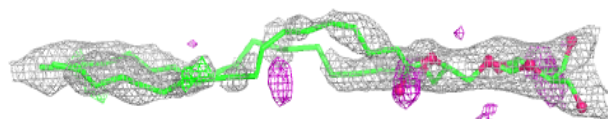
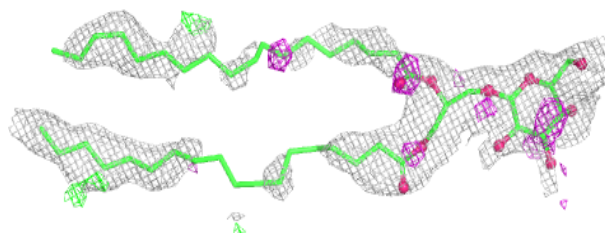


Electron density around LMG a 618:

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

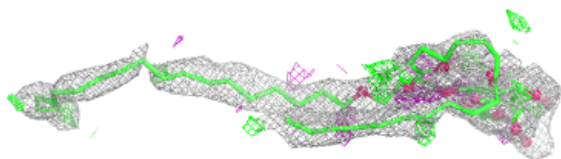
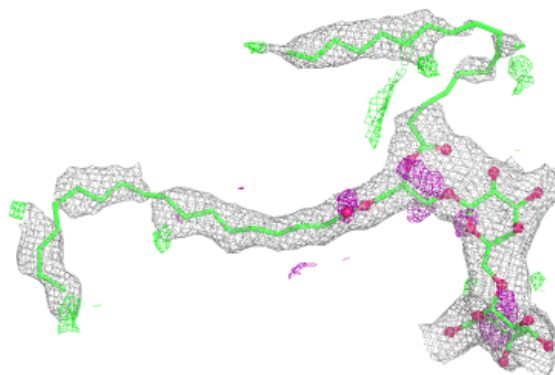
**Electron density around LMG b 622:**

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

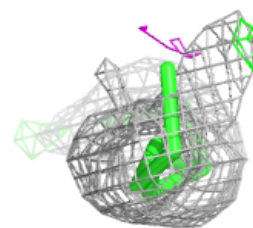
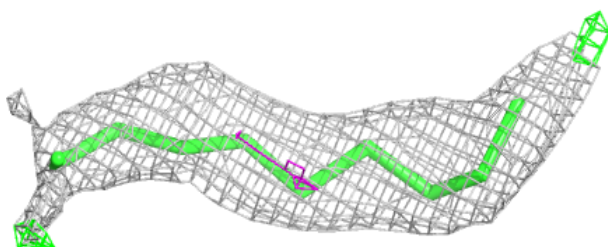
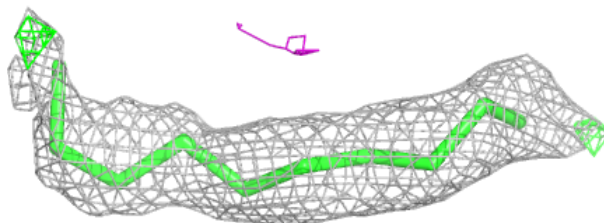


Electron density around DGD A 619:

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

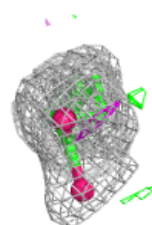
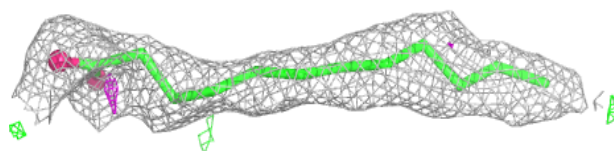
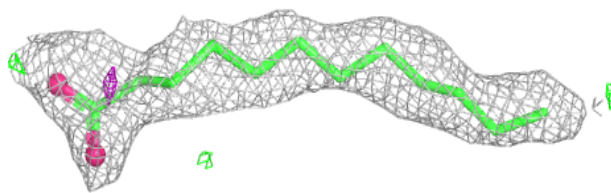
**Electron density around STE b 625:**

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

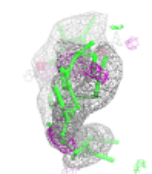
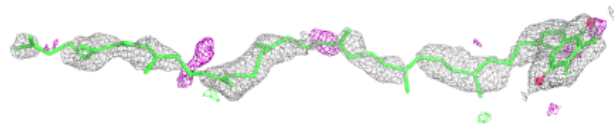
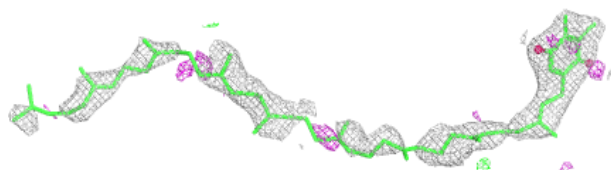


Electron density around STE k 103:

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

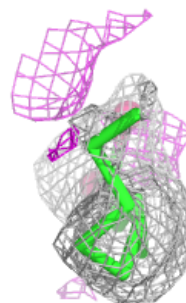
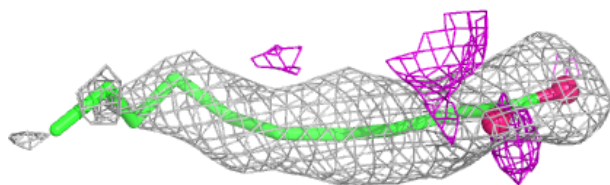
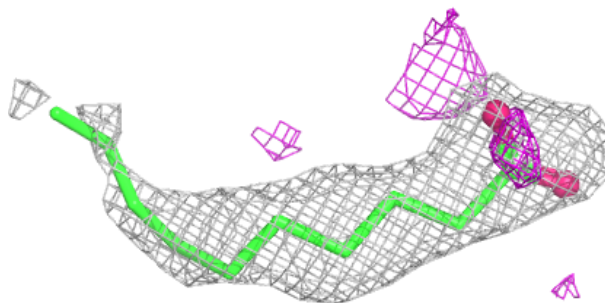
**Electron density around PL9 A 612:**

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

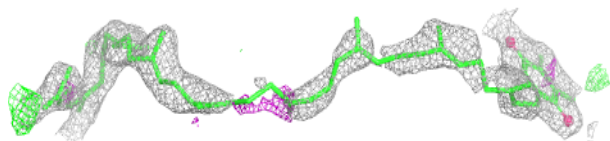
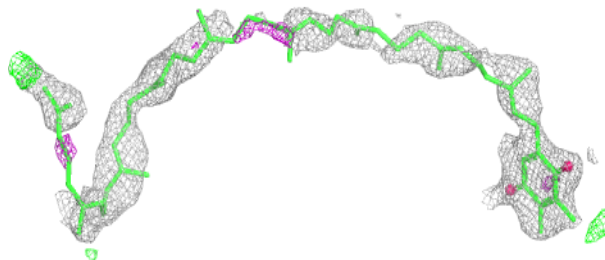


Electron density around STE B 624:

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

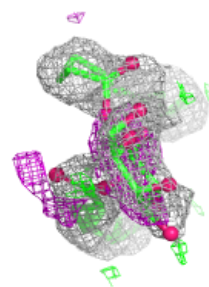
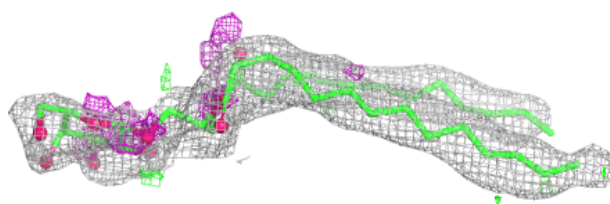
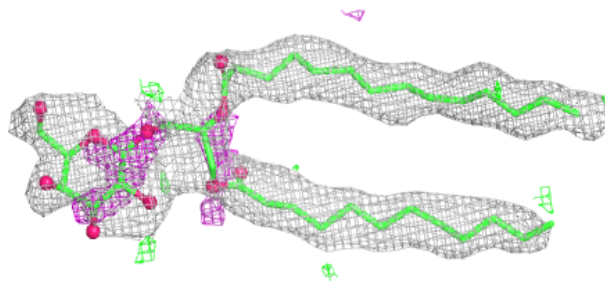
**Electron density around PL9 a 612:**

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

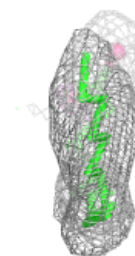
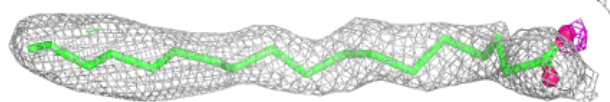
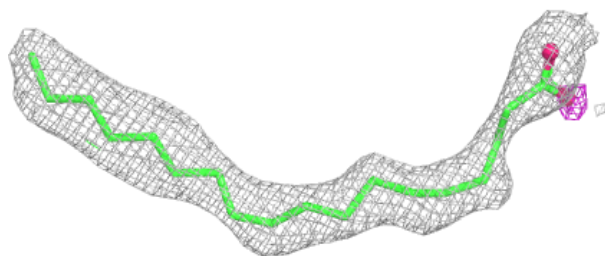


Electron density around LMG B 620:

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

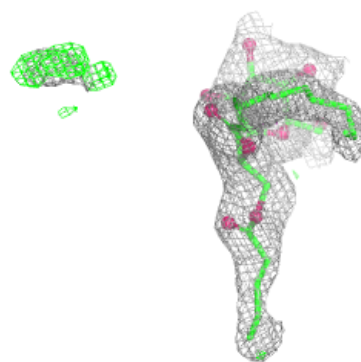
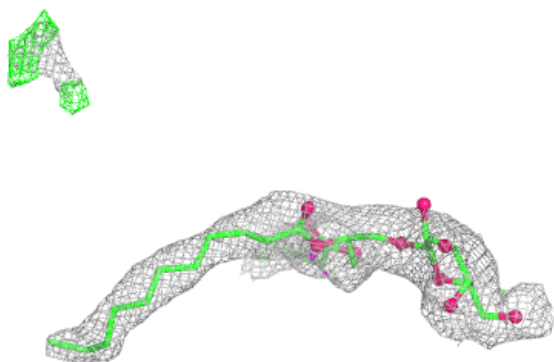
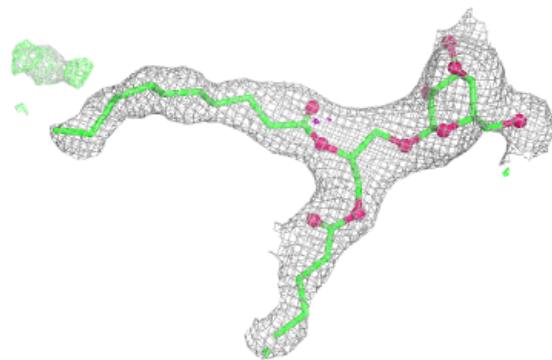
**Electron density around STE d 410:**

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

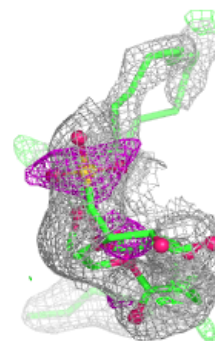
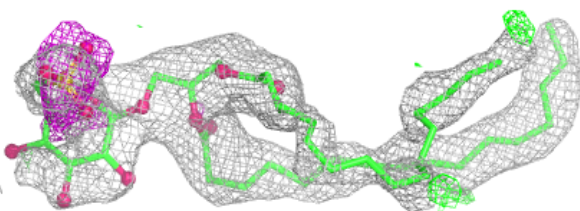
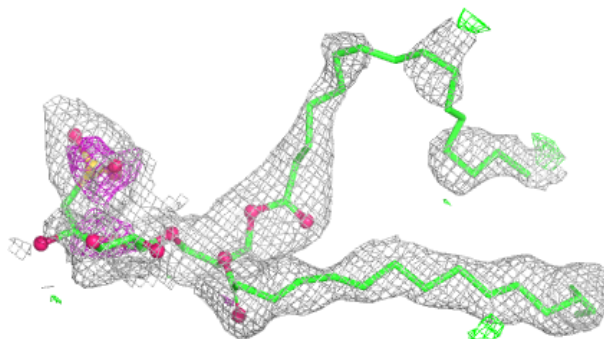


Electron density around LMG C 516:

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

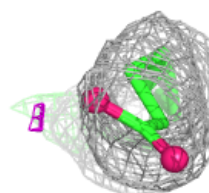
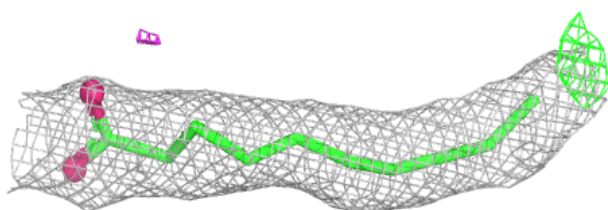
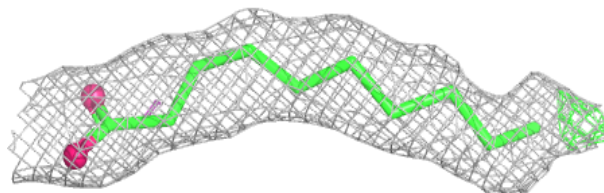
**Electron density around SQD a 617:**

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

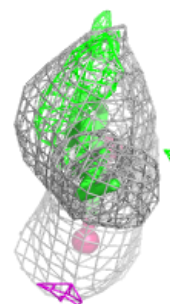
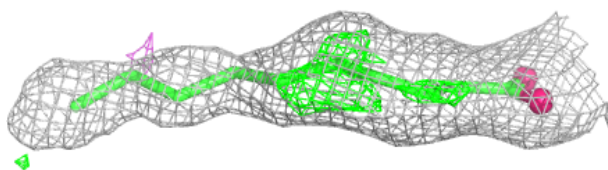
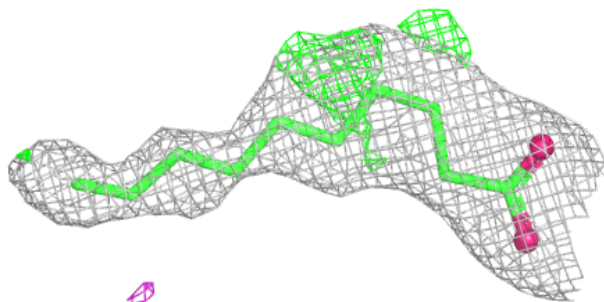


Electron density around STE j 101:

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

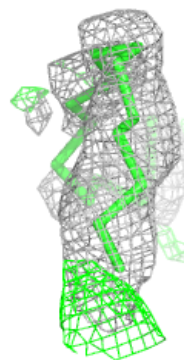
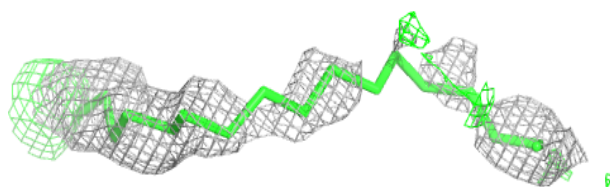
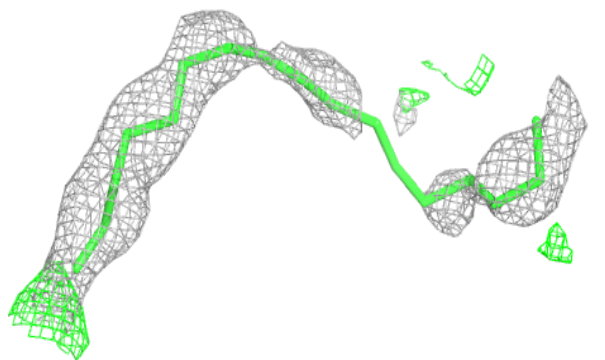
**Electron density around STE C 524:**

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

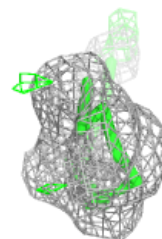
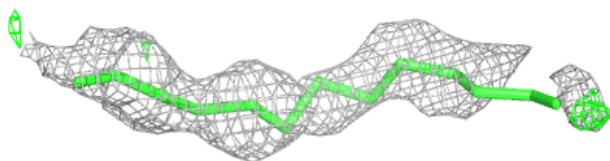
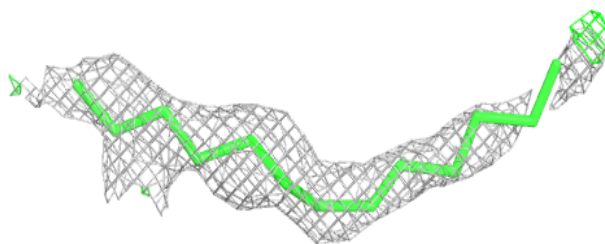


Electron density around STE Z 101:

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

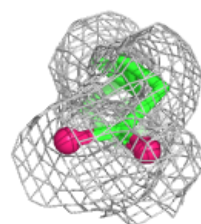
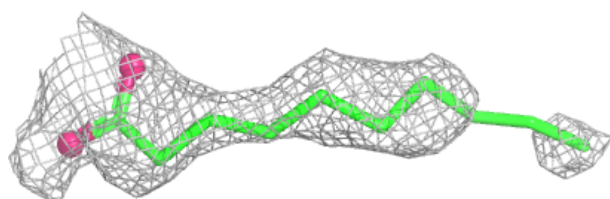
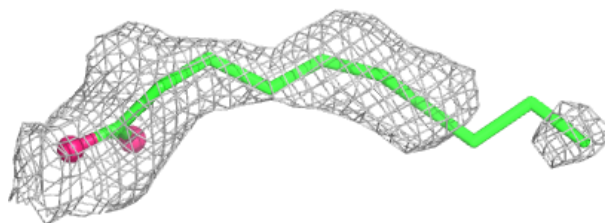
**Electron density around STE c 516:**

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

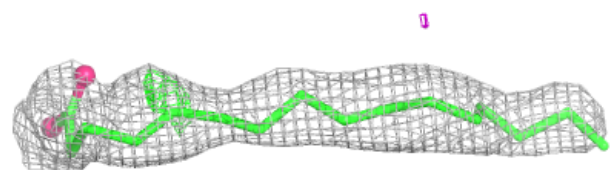
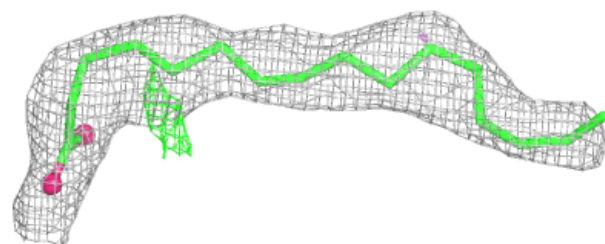


Electron density around STE E 101:

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

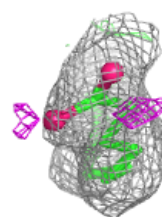
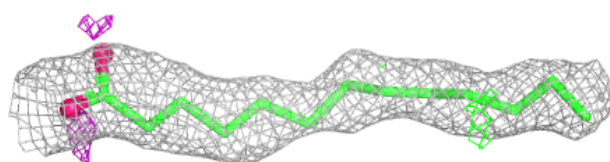
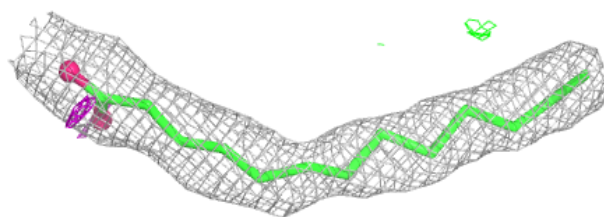
**Electron density around STE B 623:**

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

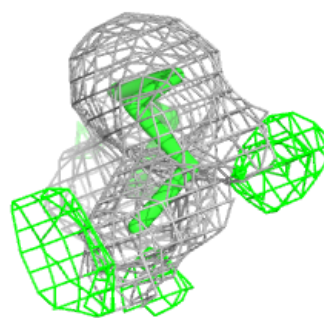
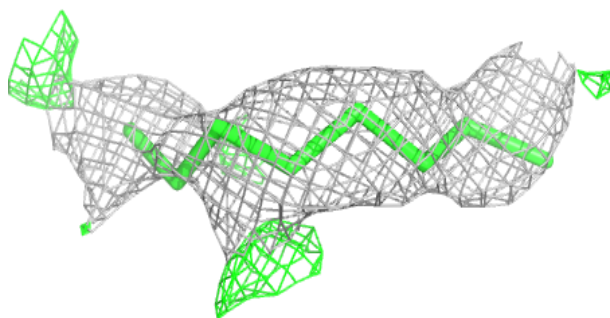
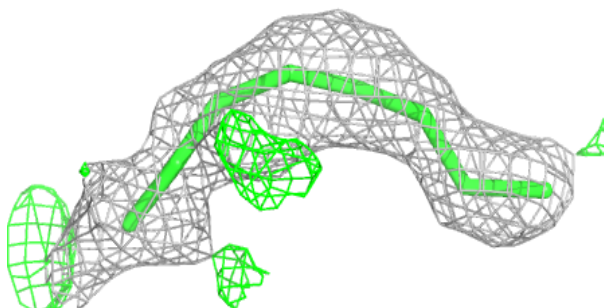


Electron density around STE I 102:

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

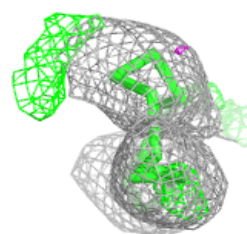
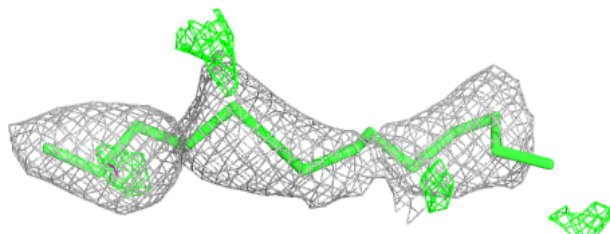
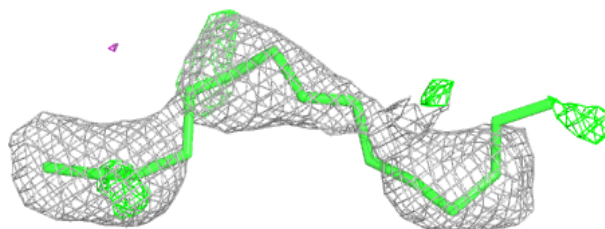
**Electron density around STE e 103:**

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

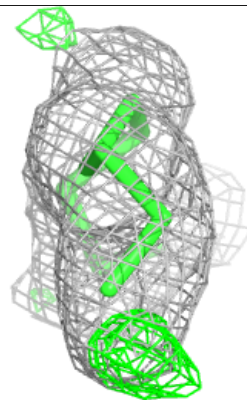
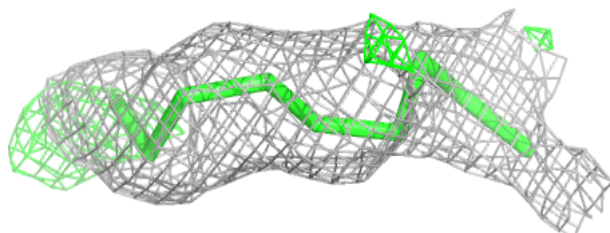
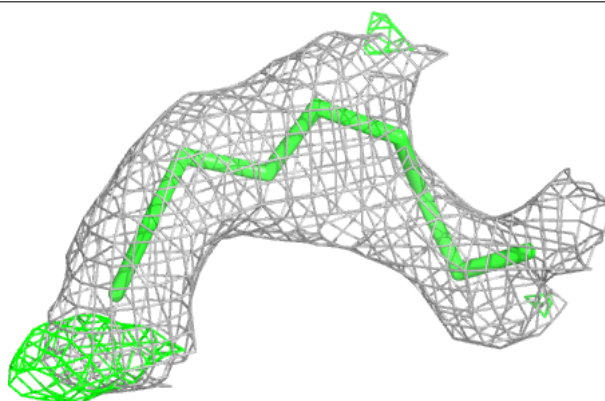


Electron density around STE B 625:

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

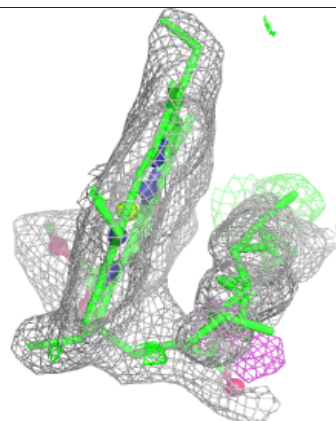
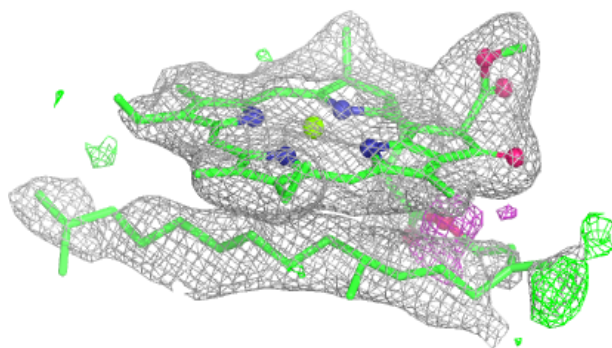
**Electron density around STE H 103:**

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

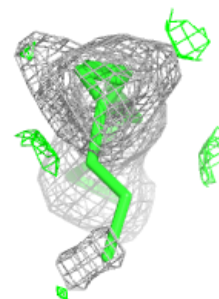
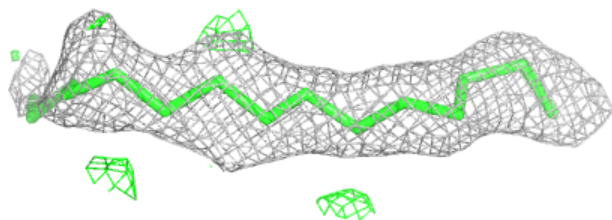
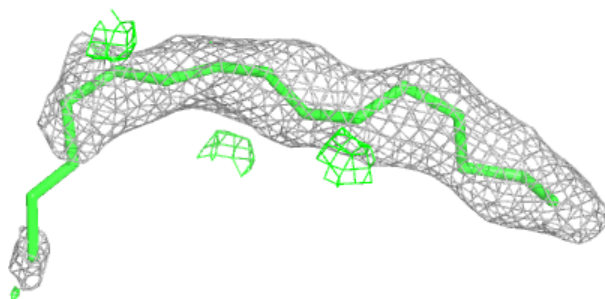


Electron density around CLA b 601:

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

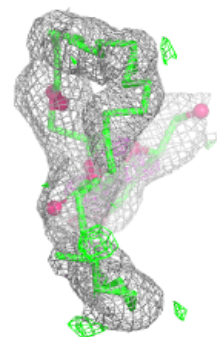
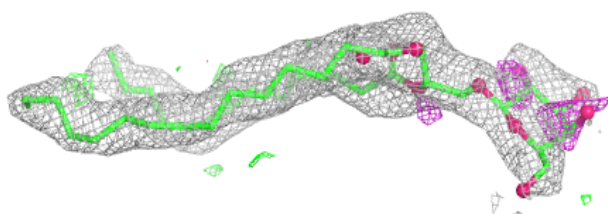
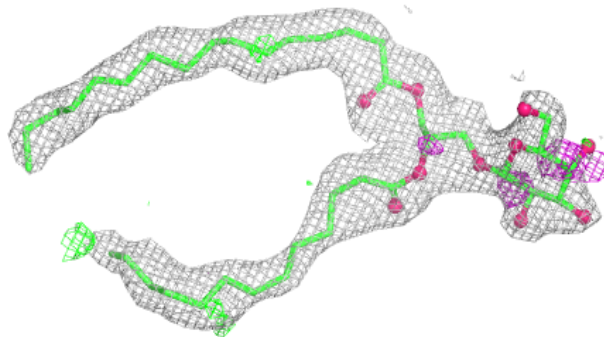
**Electron density around STE M 104:**

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

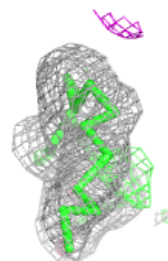
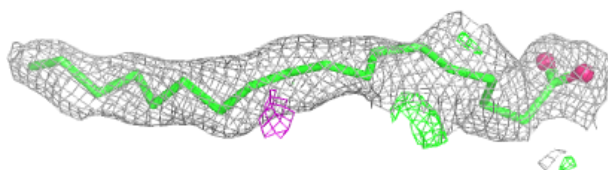
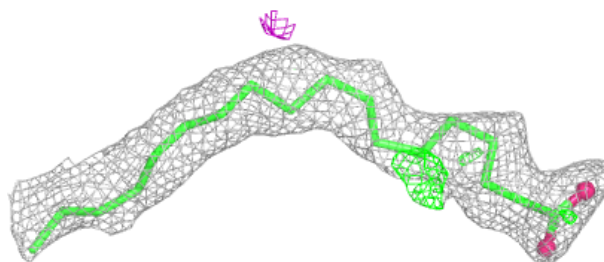


Electron density around LMG A 615:

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

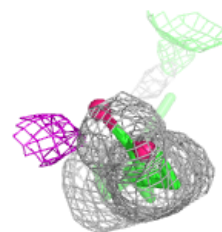
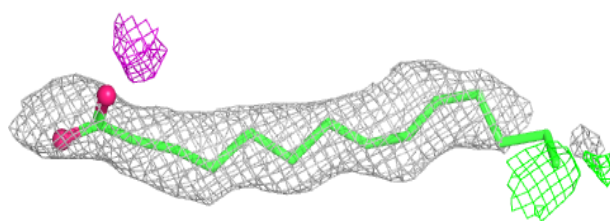
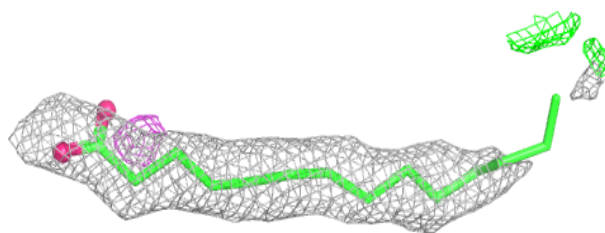
**Electron density around STE d 408:**

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

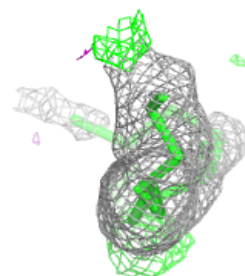
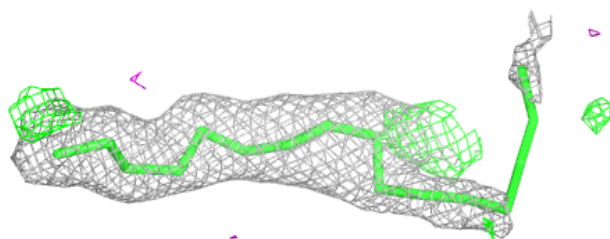
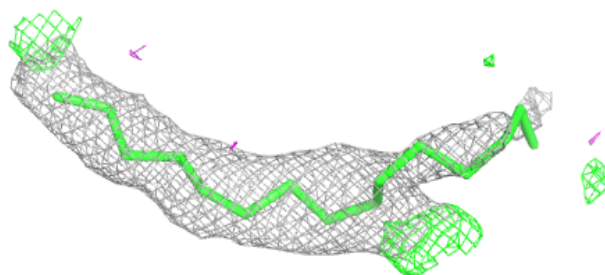


Electron density around STE b 624:

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

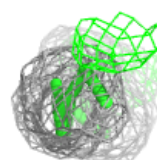
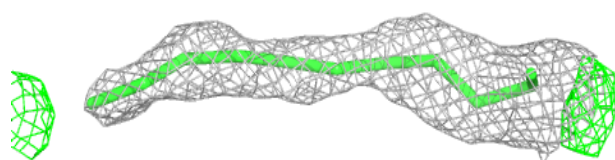
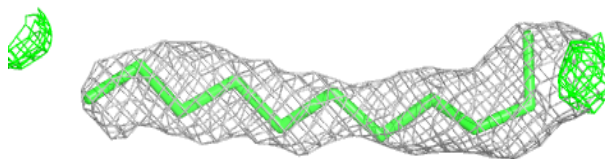
**Electron density around STE T 102:**

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

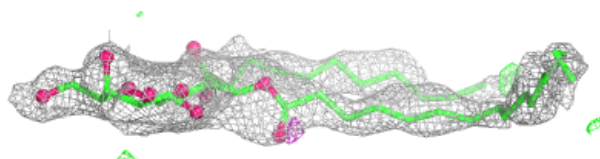
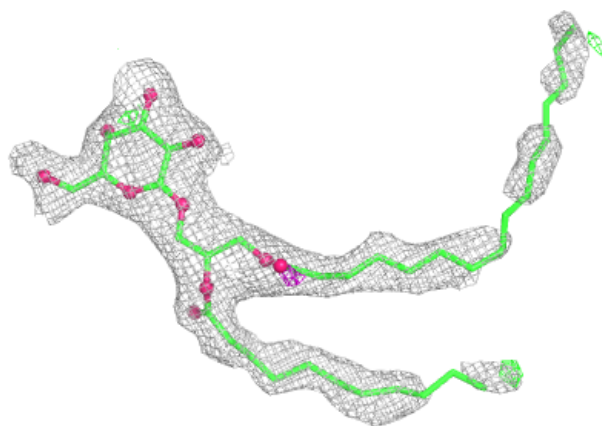


Electron density around STE h 104:

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

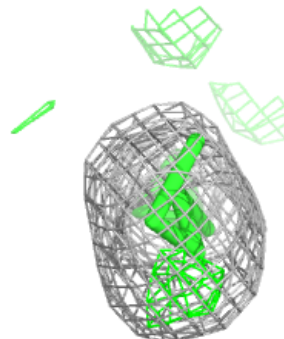
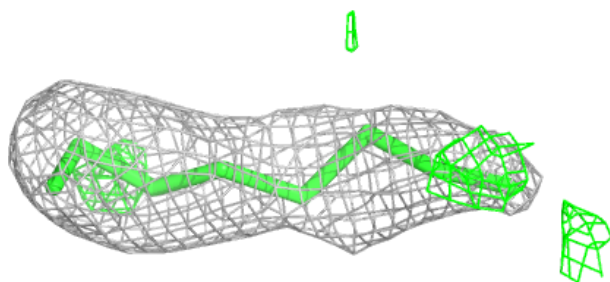
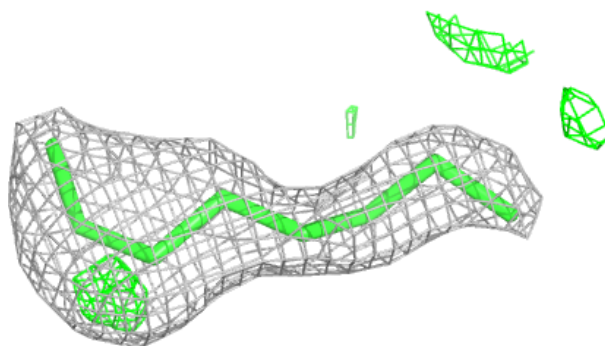
**Electron density around LMG c 522:**

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

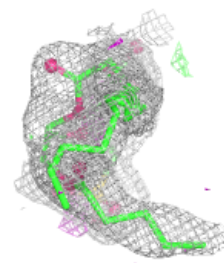
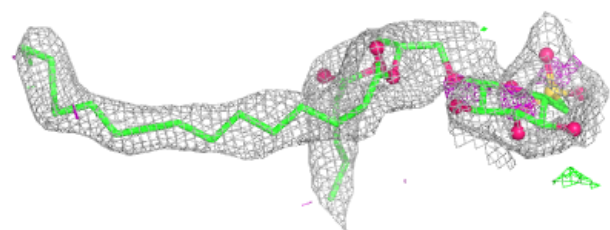
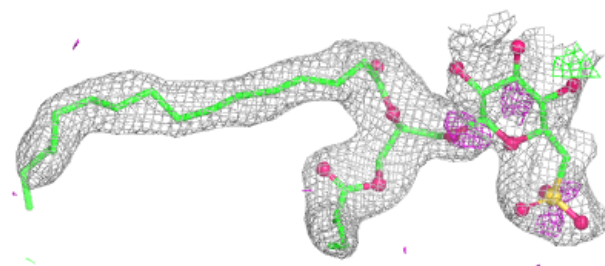


Electron density around STE A 620:

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

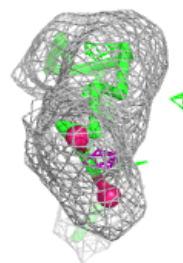
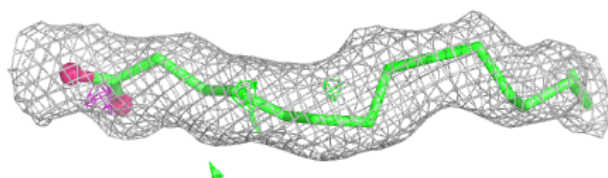
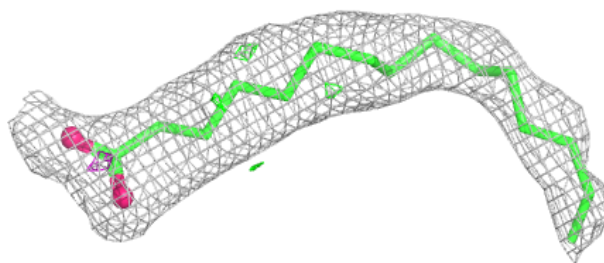
**Electron density around SQD A 618:**

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

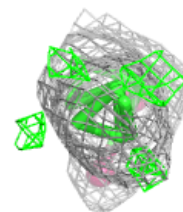
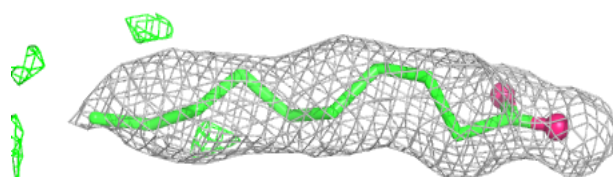
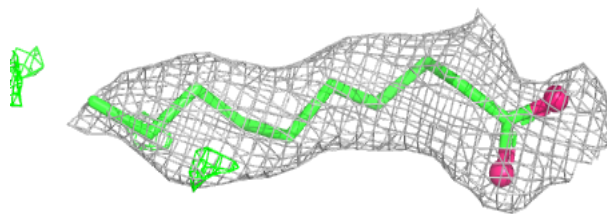


Electron density around STE B 621:

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

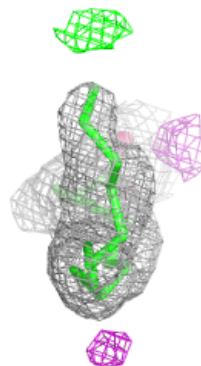
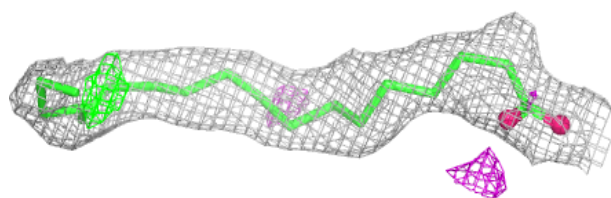
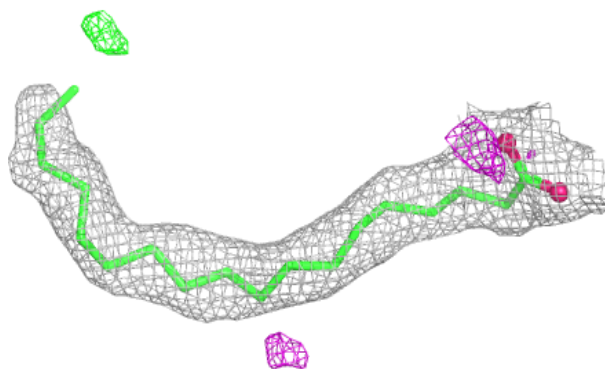
**Electron density around STE J 101:**

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

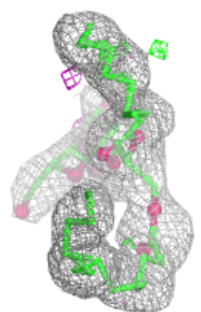
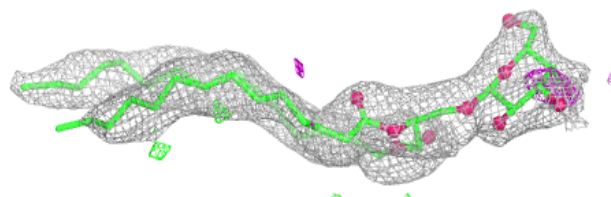
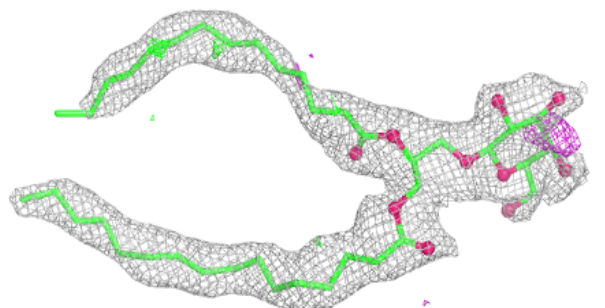


Electron density around STE b 621:

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

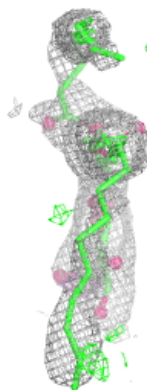
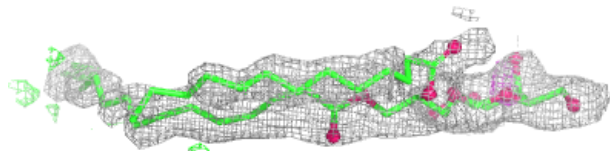
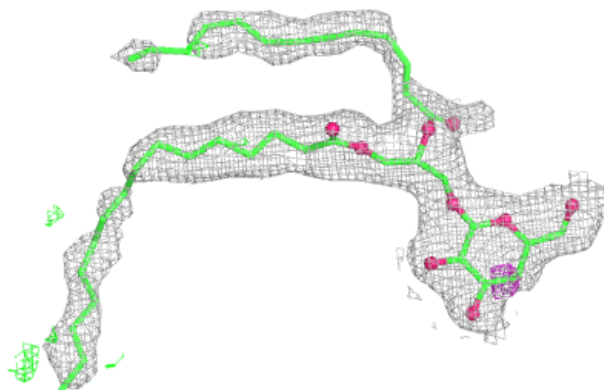
**Electron density around LMG c 524:**

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

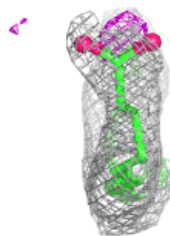
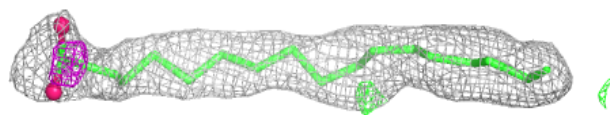
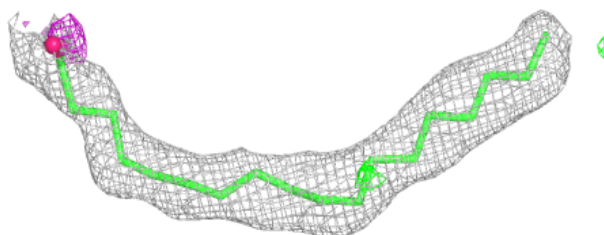


Electron density around LMG C 523:

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

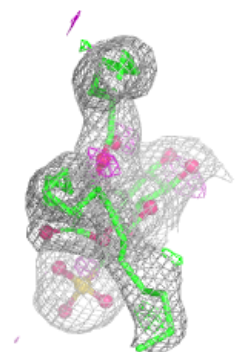
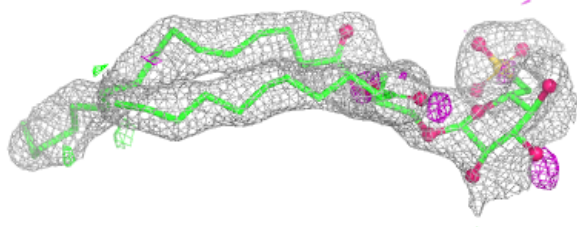
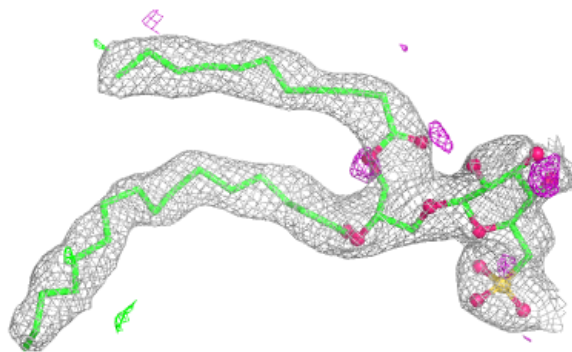
**Electron density around STE D 411:**

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

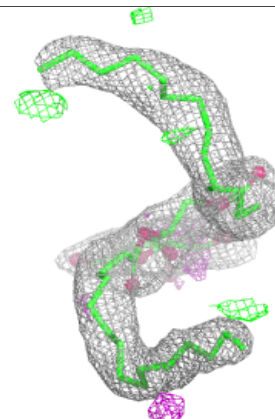
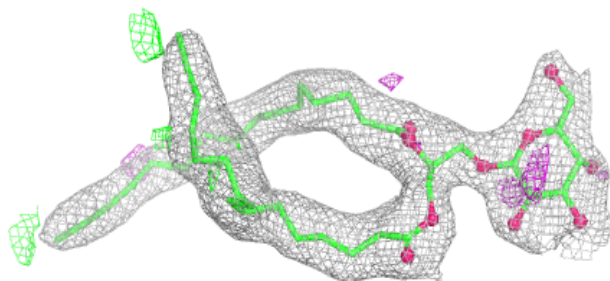
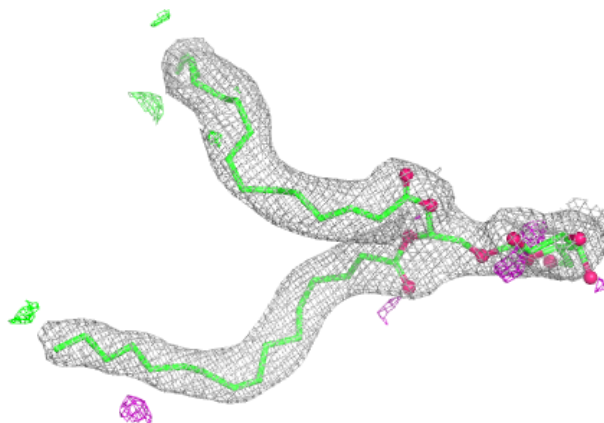


Electron density around SQD b 620:

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

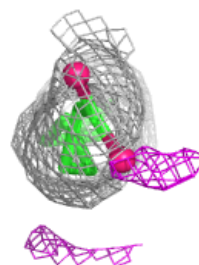
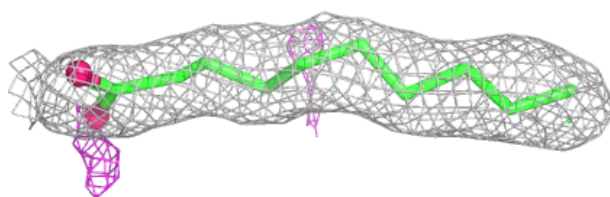
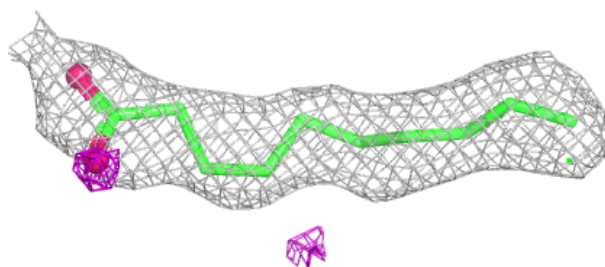
**Electron density around LMG M 101:**

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

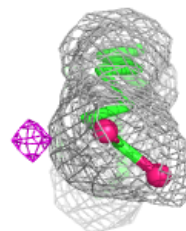
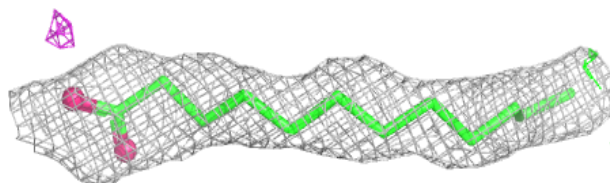
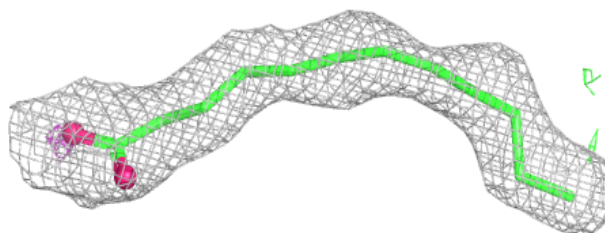


Electron density around STE m 102:

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

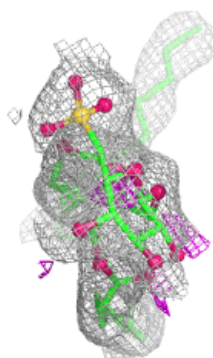
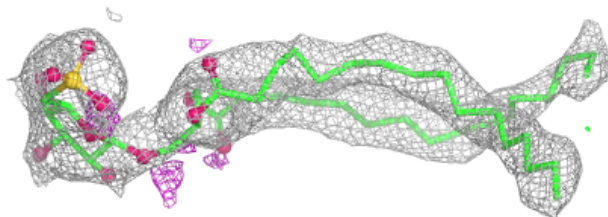
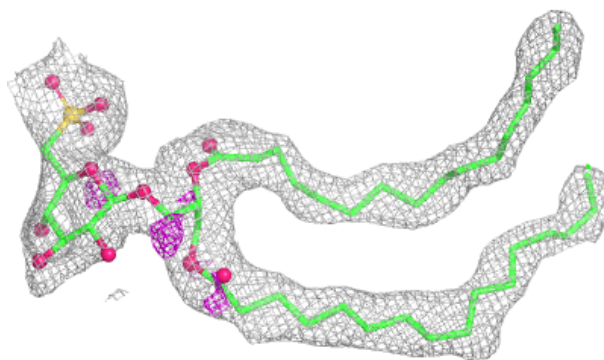
**Electron density around STE t 102:**

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

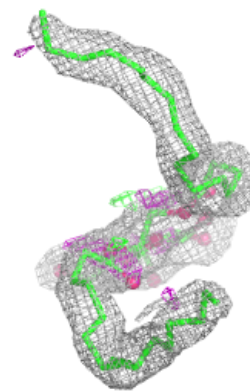
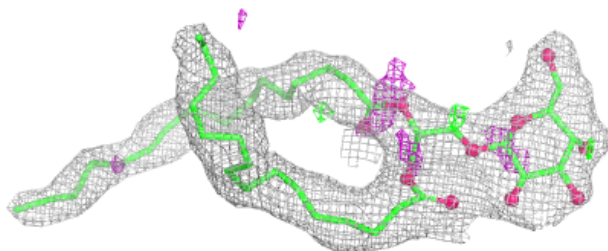
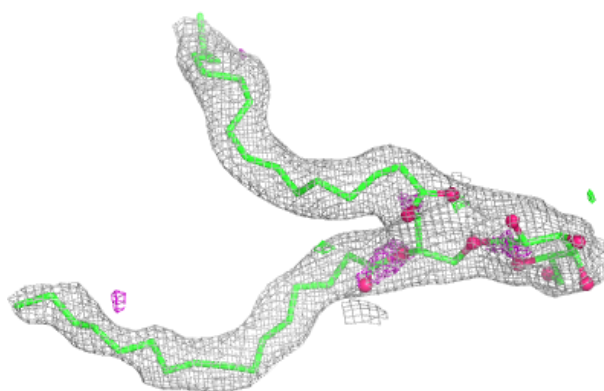


Electron density around SQD B 622:

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

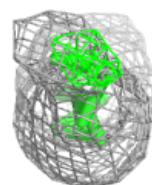
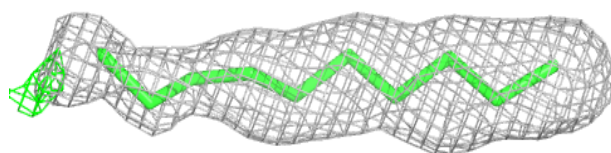
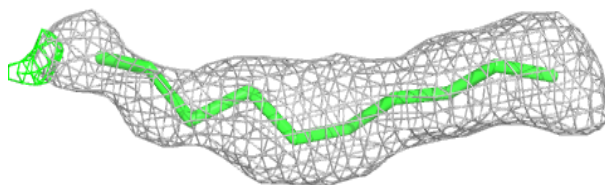
**Electron density around LMG m 101:**

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

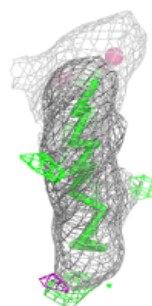
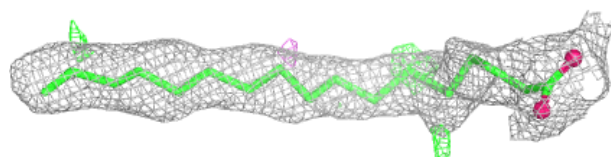
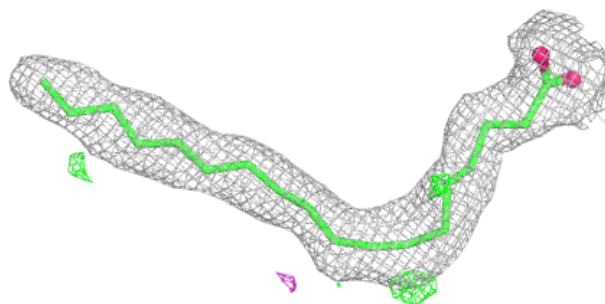


Electron density around STE M 103:

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

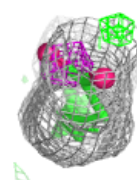
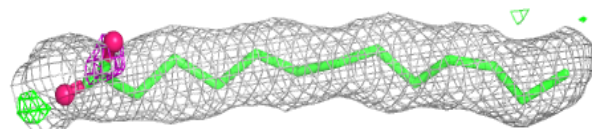
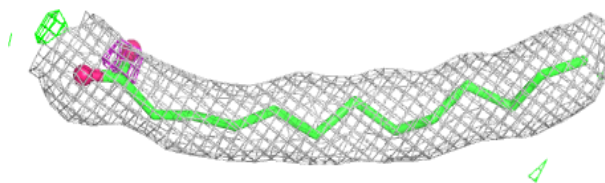
**Electron density around STE d 406:**

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

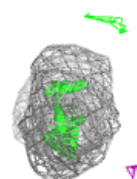
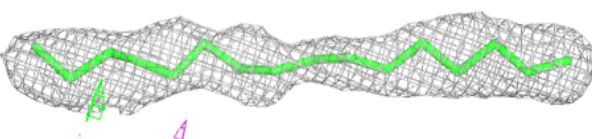
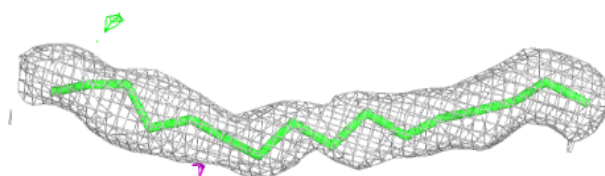


Electron density around STE M 102:

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

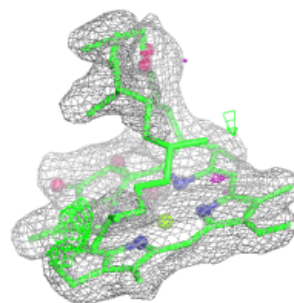
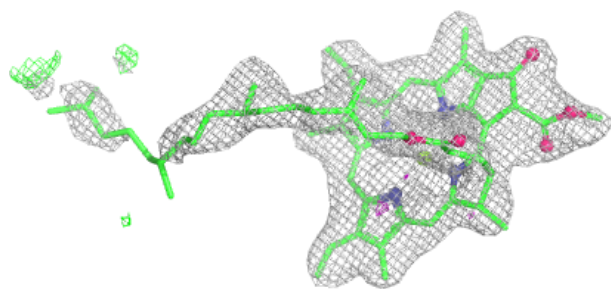
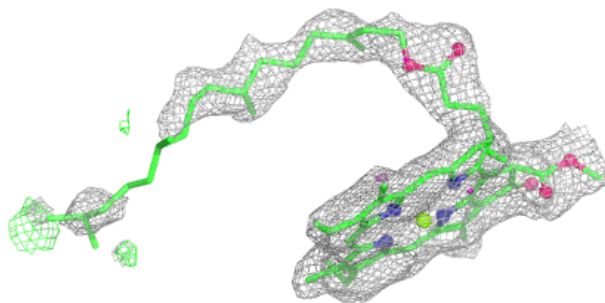
**Electron density around STE C 525:**

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

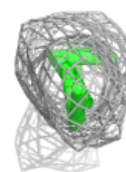
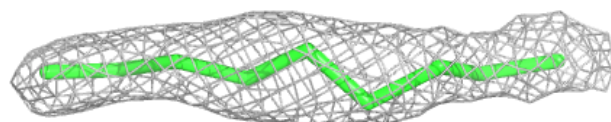
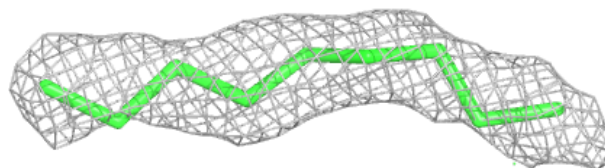


Electron density around CLA C 513:

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

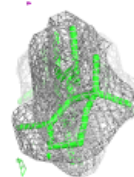
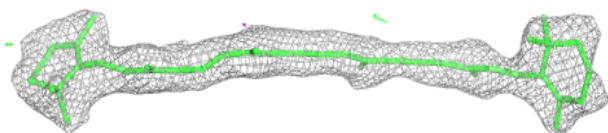
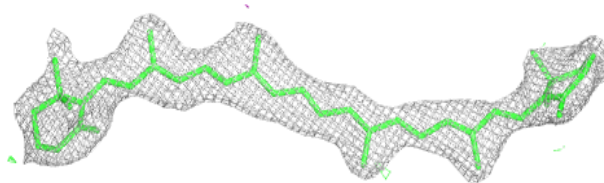
**Electron density around STE z 101:**

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

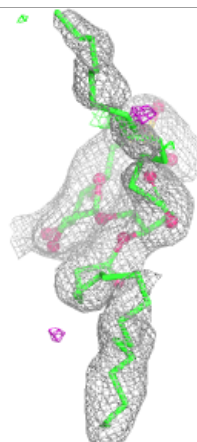
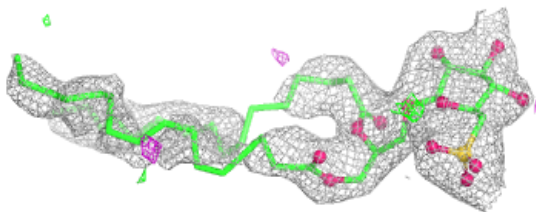
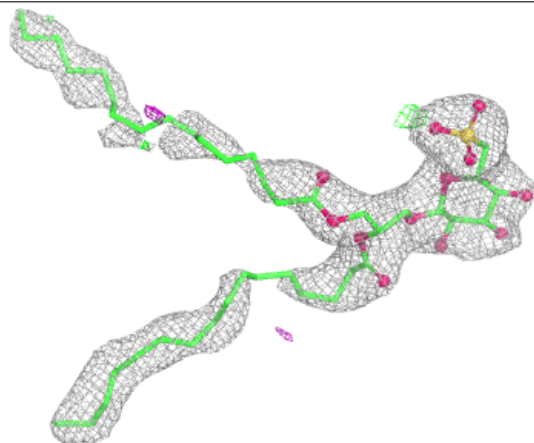


Electron density around BCR k 101:

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

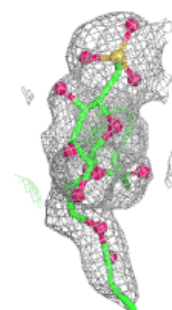
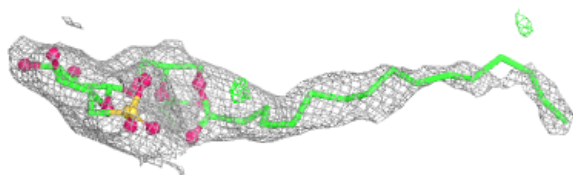
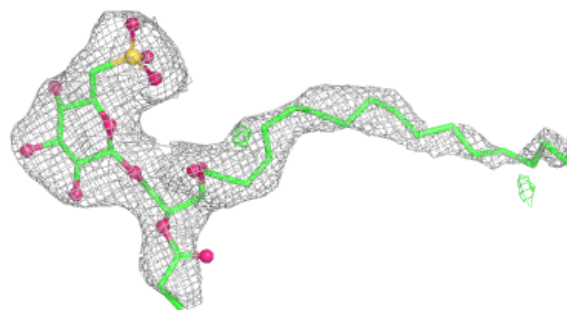
**Electron density around SQD a 615:**

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

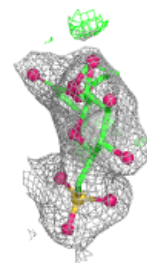
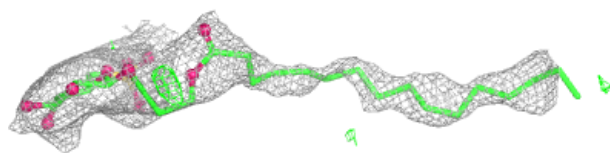
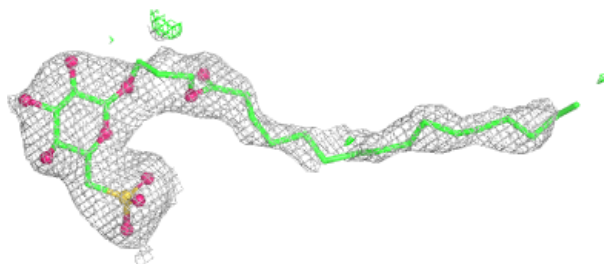


Electron density around SQD f 101:

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

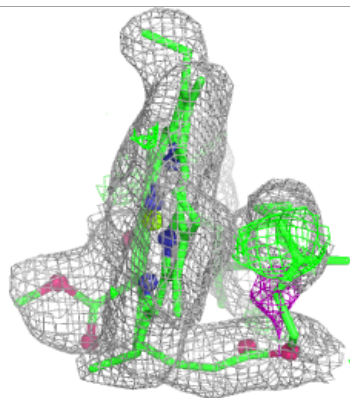
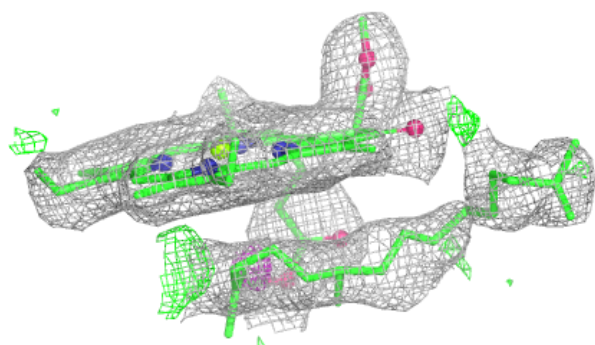
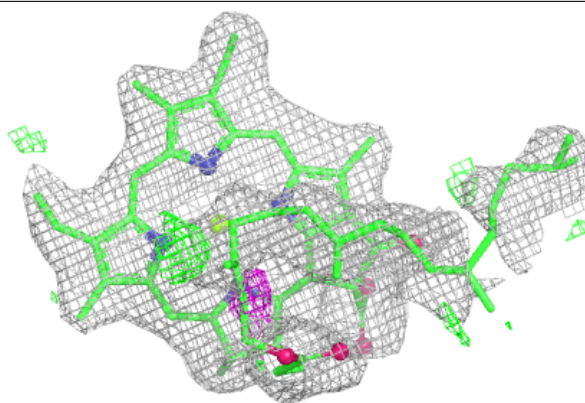
**Electron density around SQD F 102:**

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



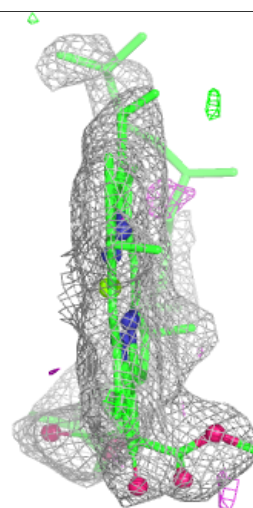
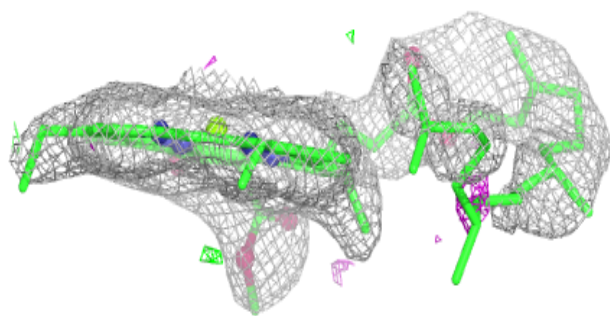
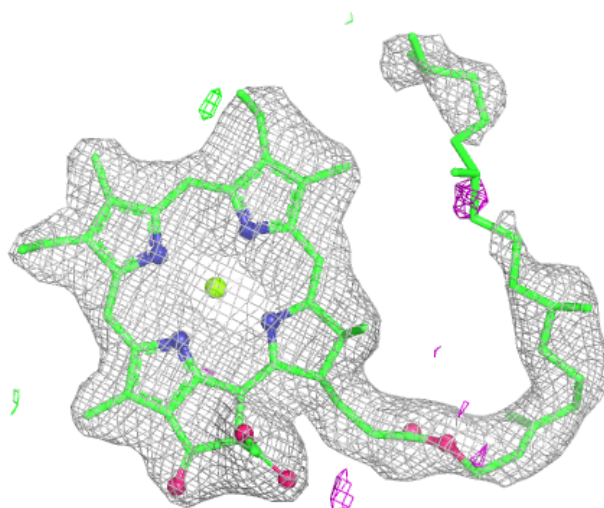
Electron density around CLA B 601:

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



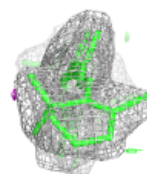
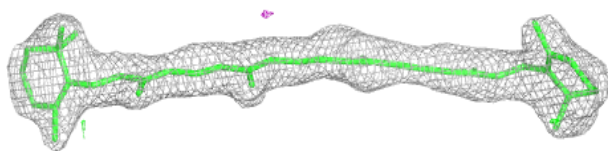
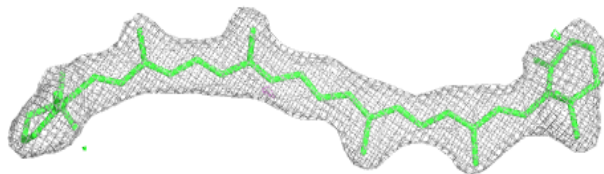
Electron density around CLA c 512:

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

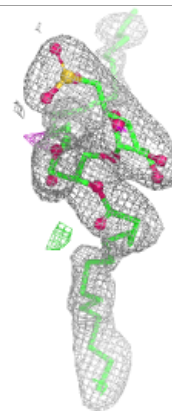
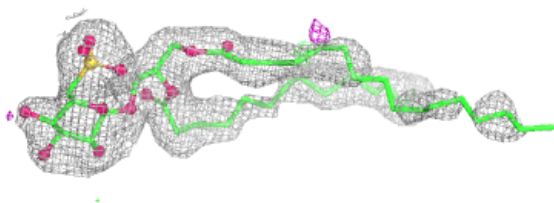
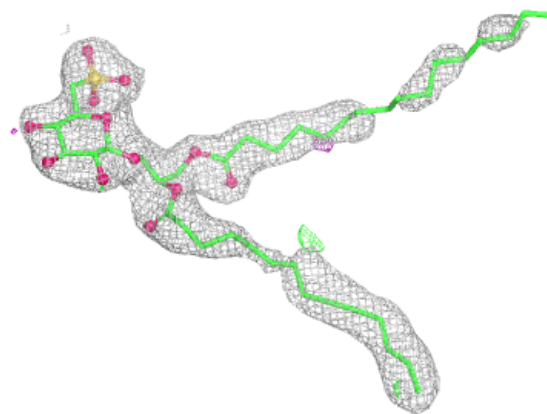


Electron density around BCR K 102:

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

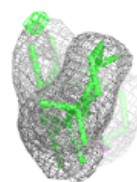
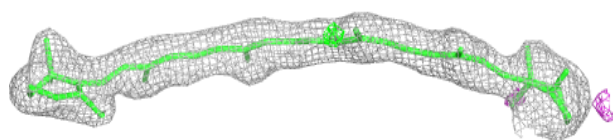
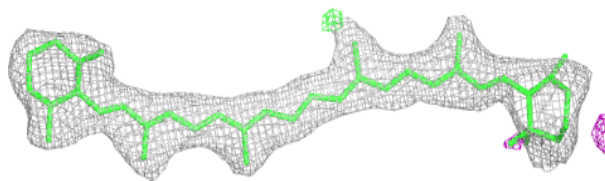
**Electron density around SQD A 616:**

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

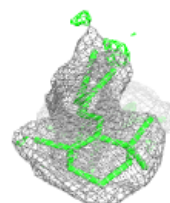
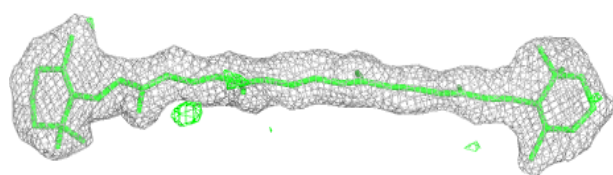
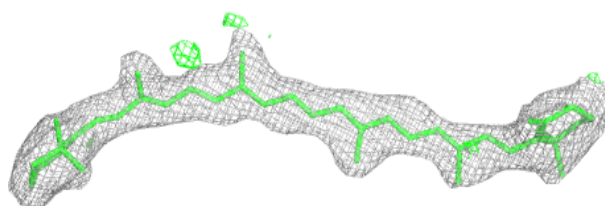


Electron density around BCR d 404:

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

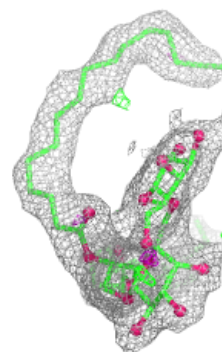
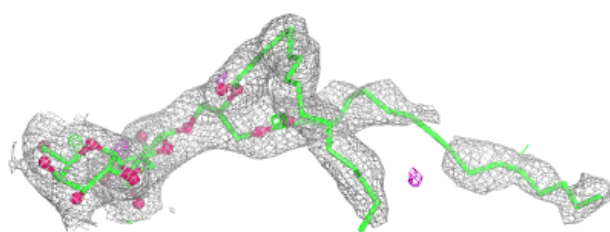
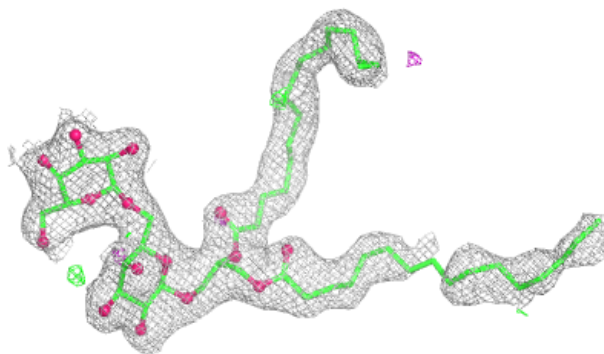
**Electron density around BCR h 101:**

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

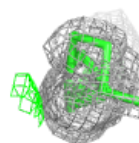
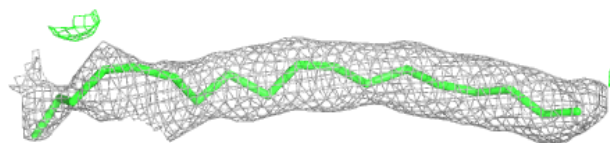
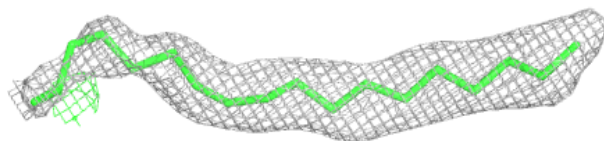


Electron density around DGD c 520:

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

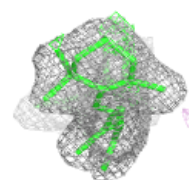
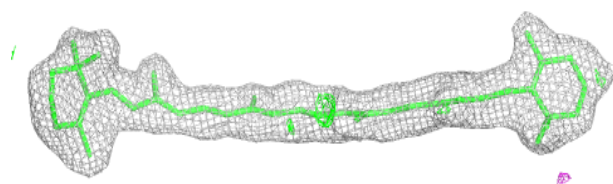
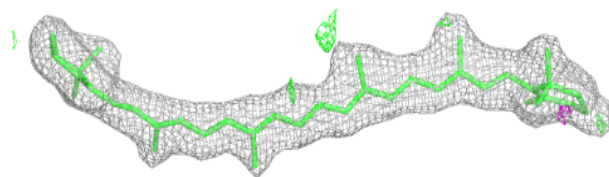
**Electron density around STE m 103:**

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

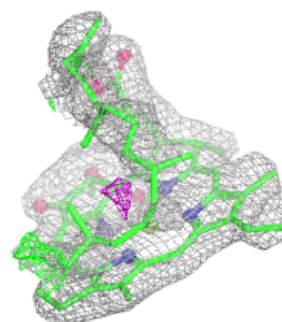
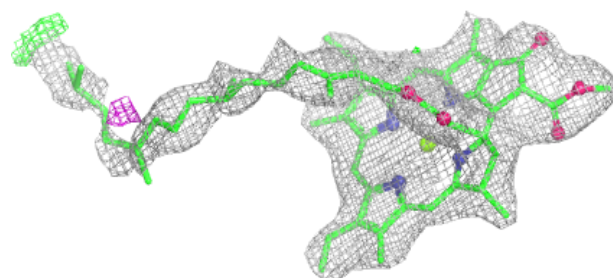
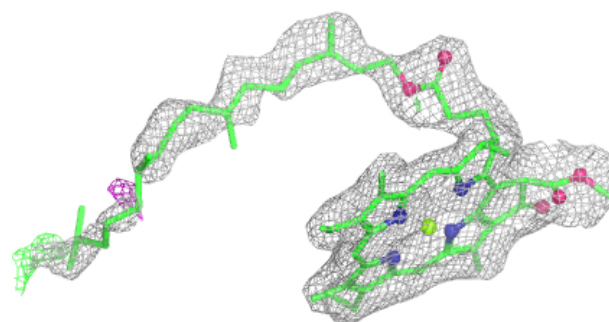


Electron density around BCR X 101:

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

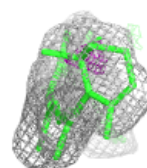
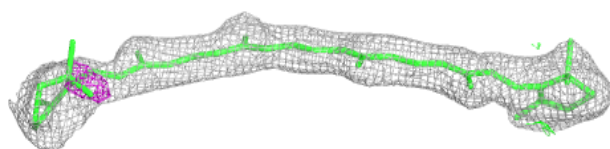
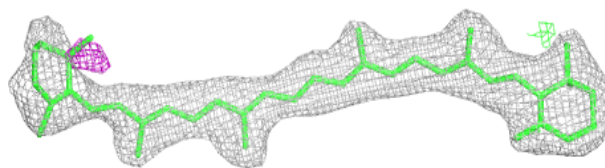
**Electron density around CLA c 513:**

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

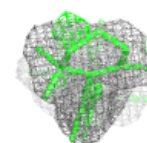
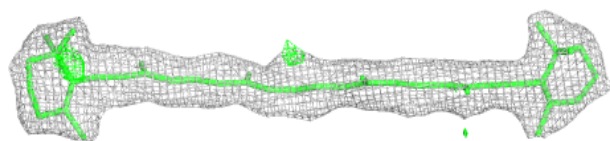
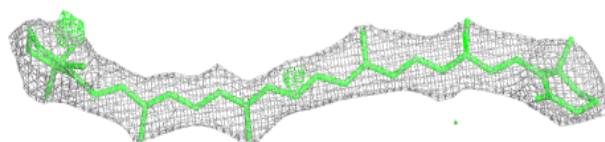


Electron density around BCR D 404:

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

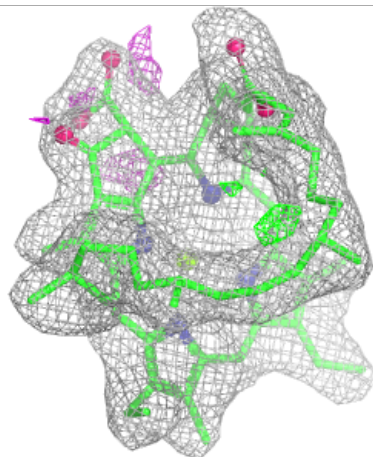
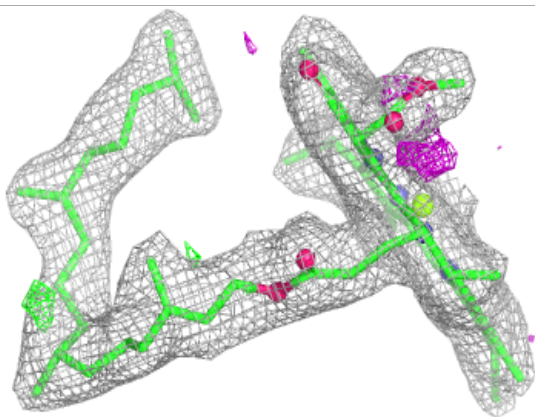
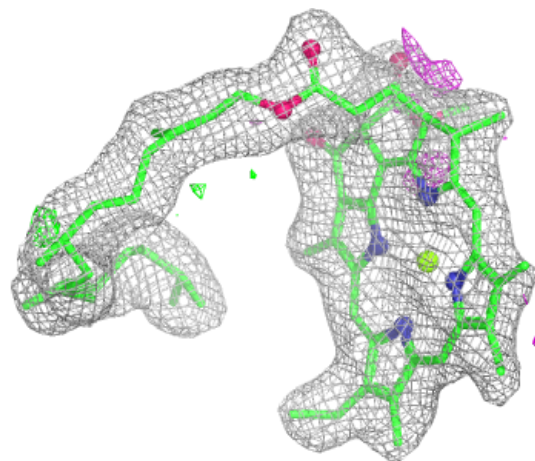
**Electron density around BCR K 101:**

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



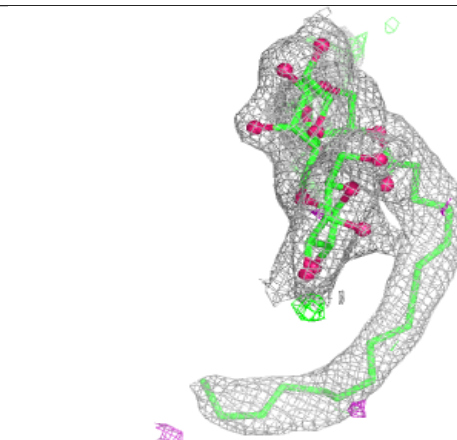
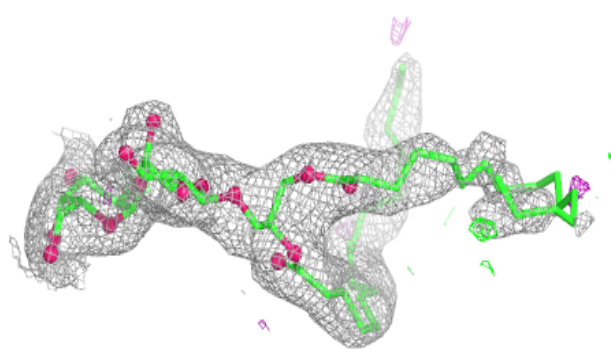
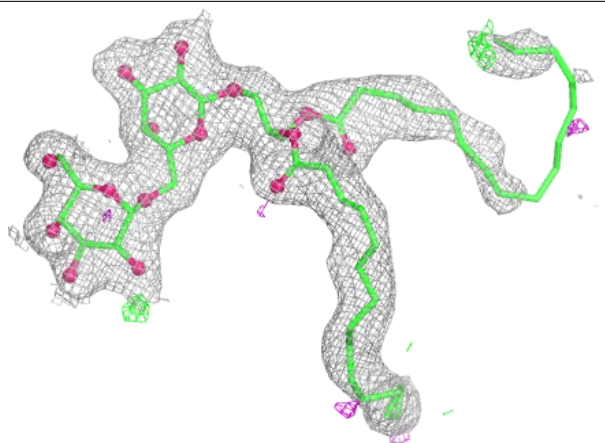
Electron density around CLA c 503:

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

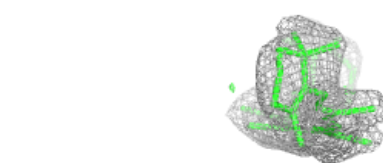
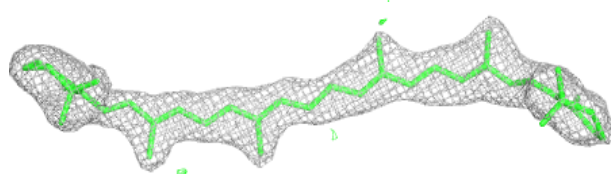
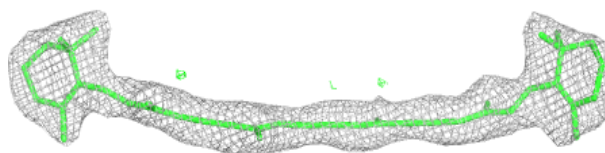


Electron density around DGD C 521:

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

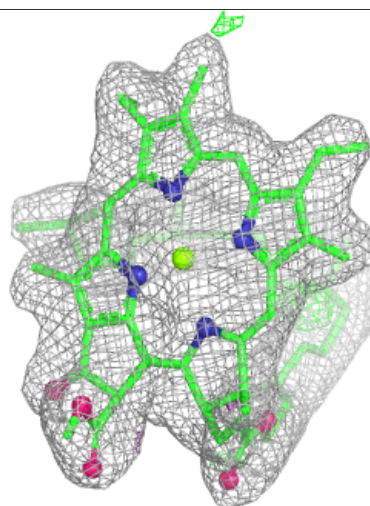
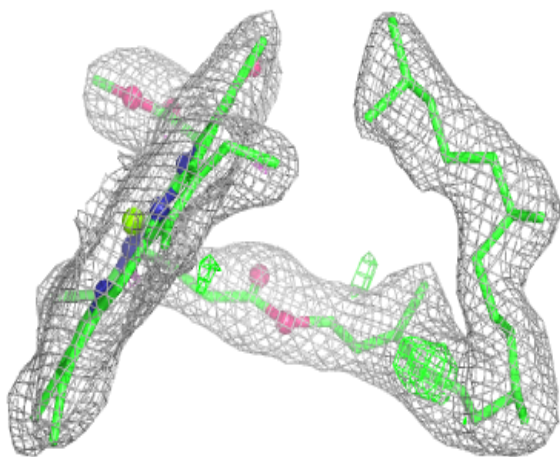
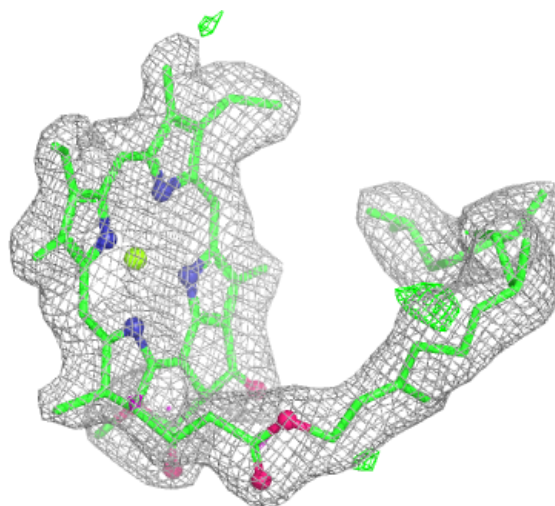
**Electron density around BCR k 102:**

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



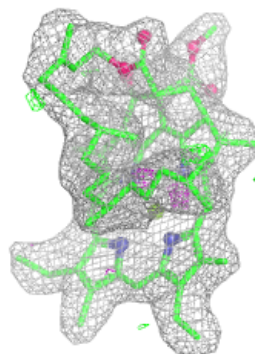
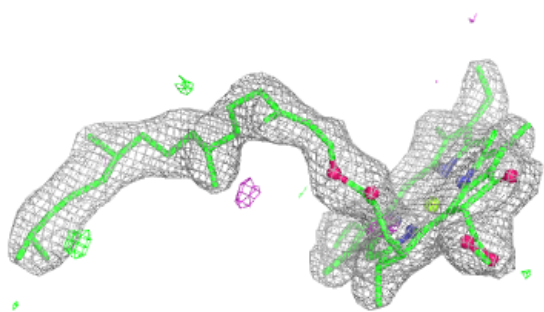
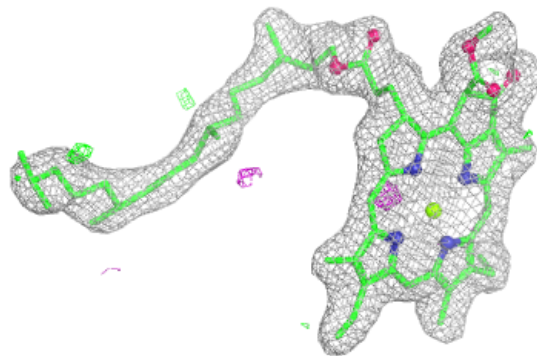
Electron density around CLA C 503:

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

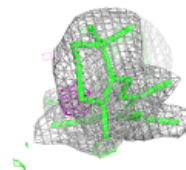
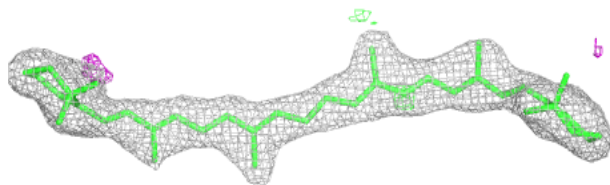
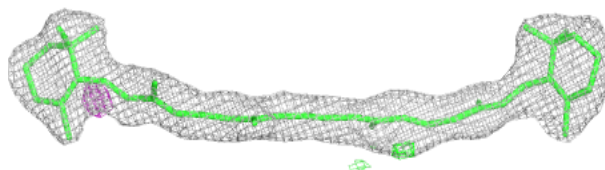


Electron density around CLA C 511:

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

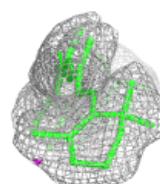
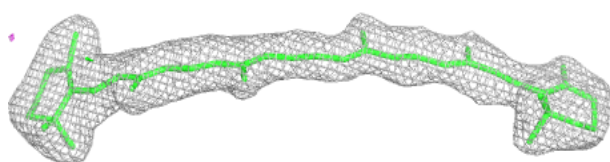
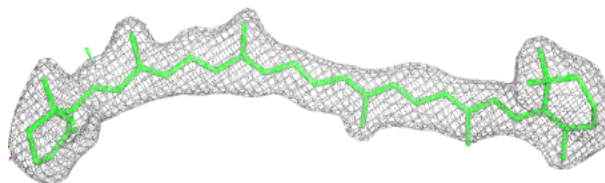
**Electron density around BCR K 103:**

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

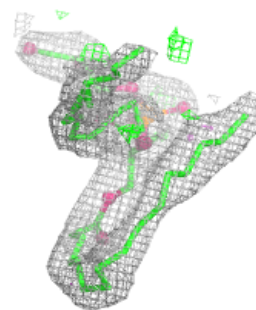
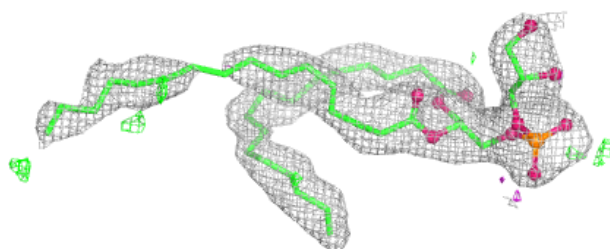
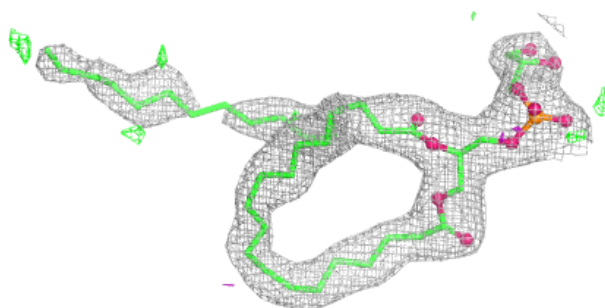


Electron density around BCR T 101:

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

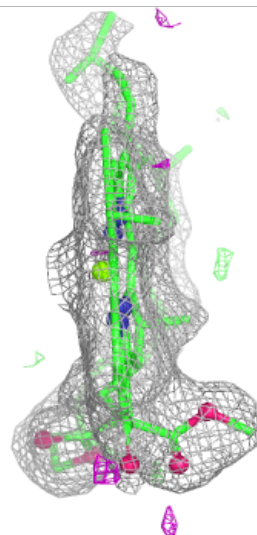
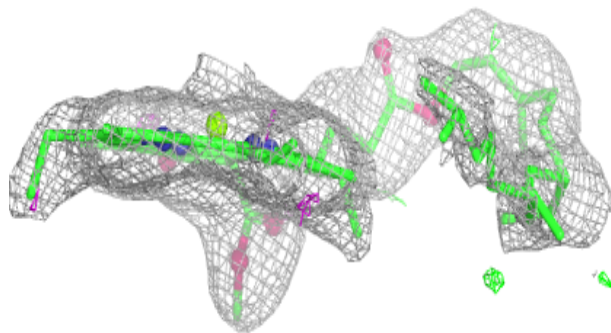
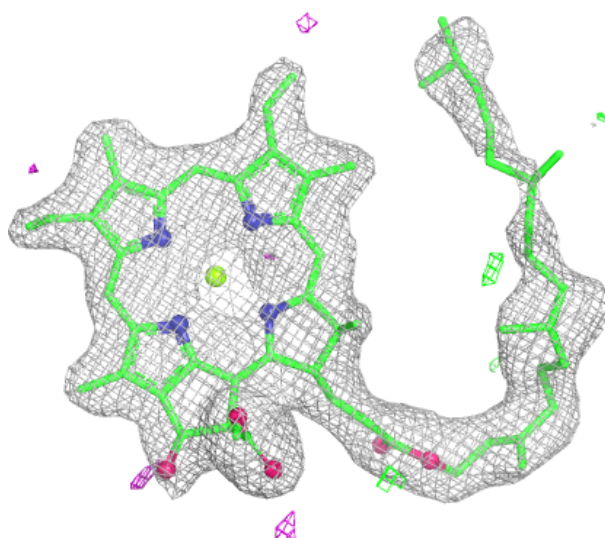
**Electron density around LHG b 623:**

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



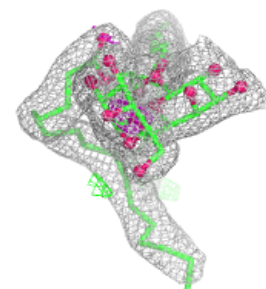
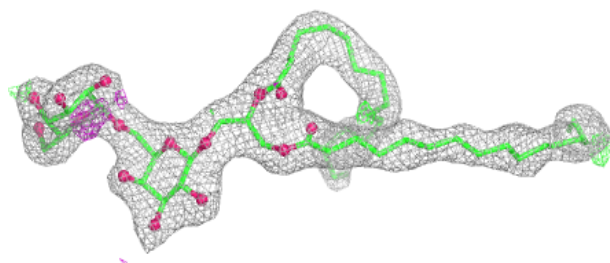
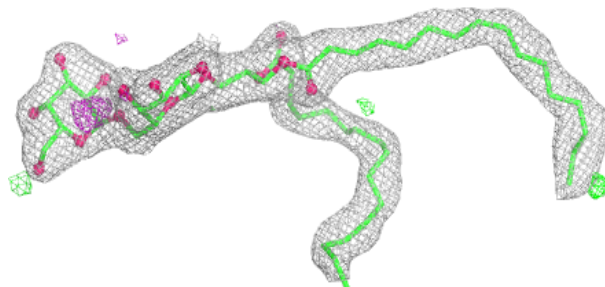
Electron density around CLA C 512:

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

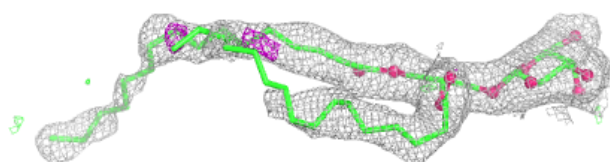
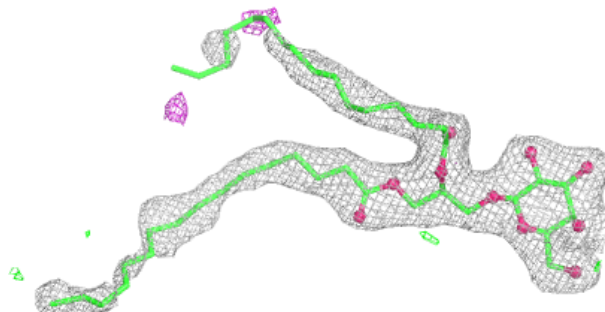


Electron density around DGD H 101:

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

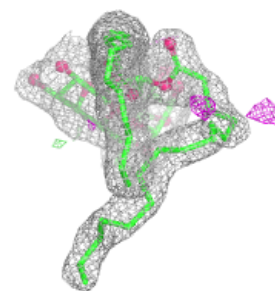
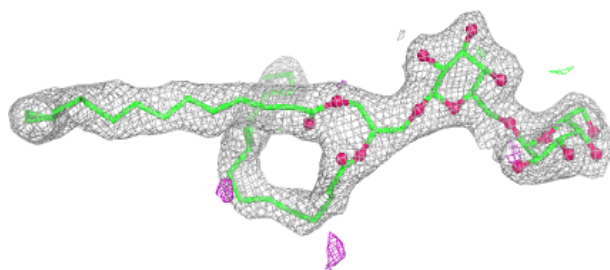
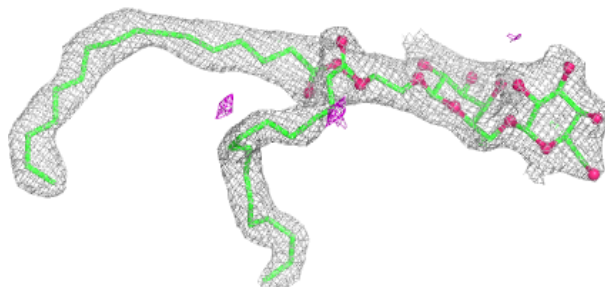
**Electron density around LMG D 407:**

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

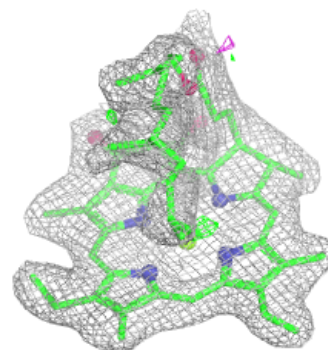
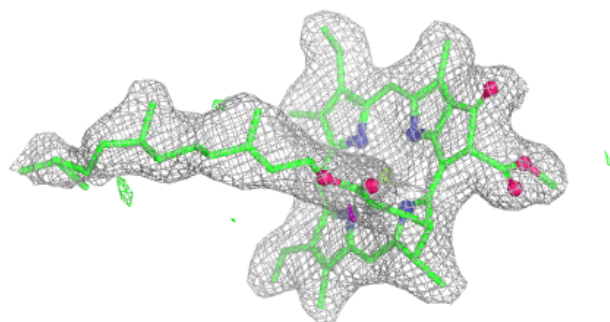
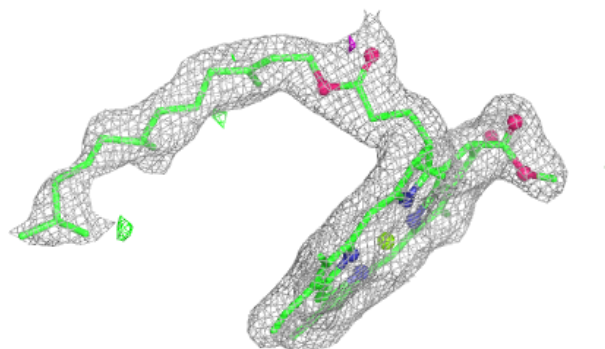


Electron density around DGD h 102:

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

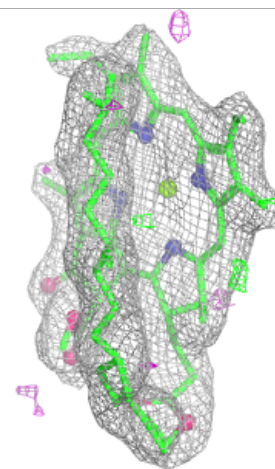
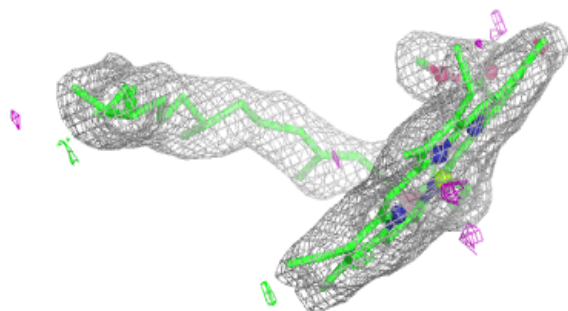
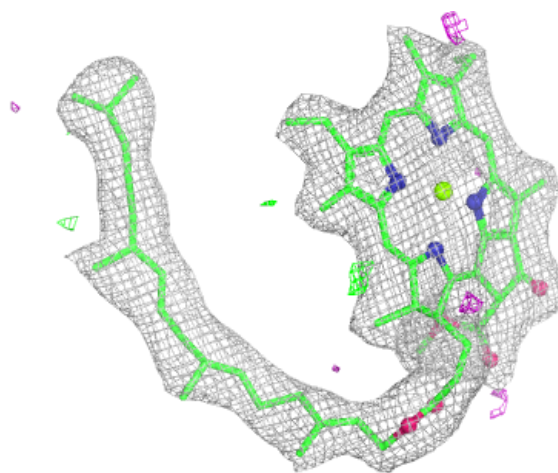
**Electron density around CLA c 504:**

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



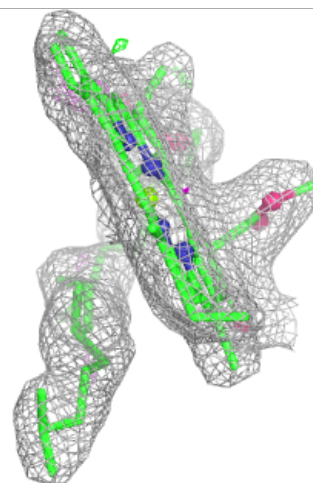
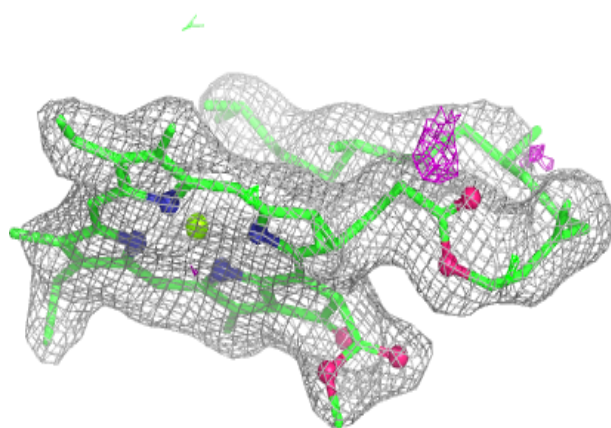
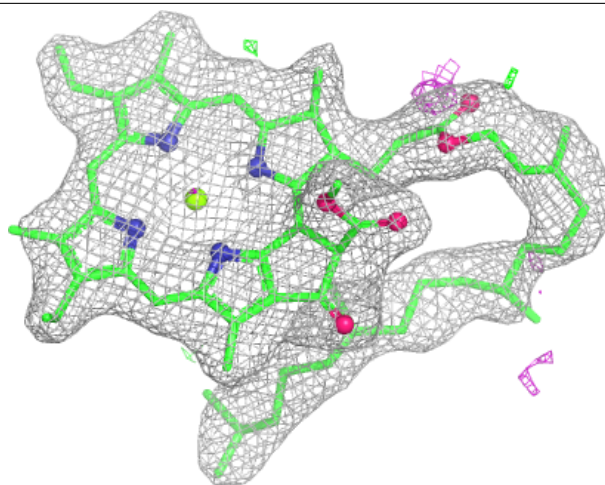
Electron density around CLA c 507:

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



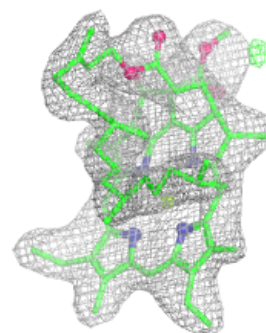
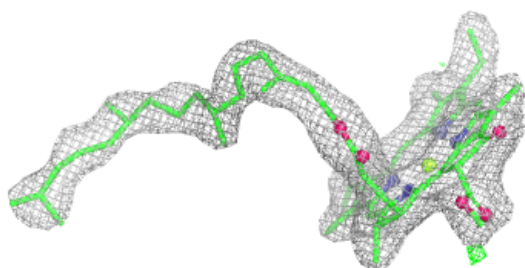
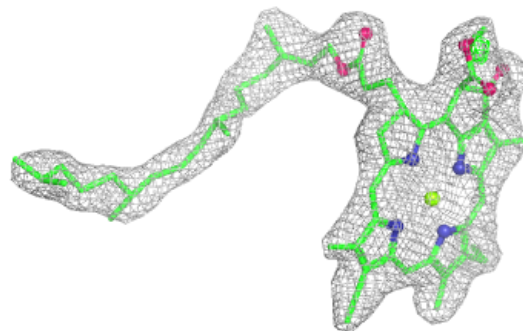
Electron density around CLA c 509:

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

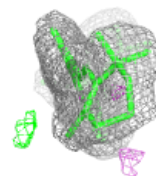
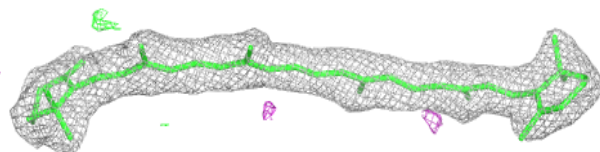
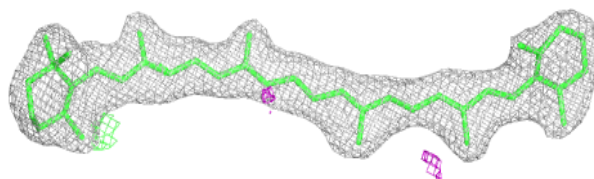


Electron density around CLA c 511:

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

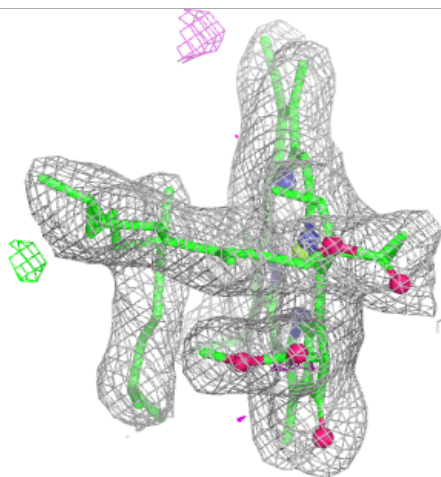
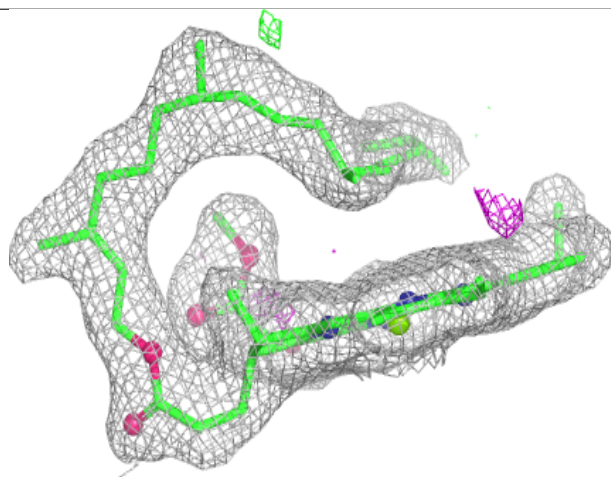
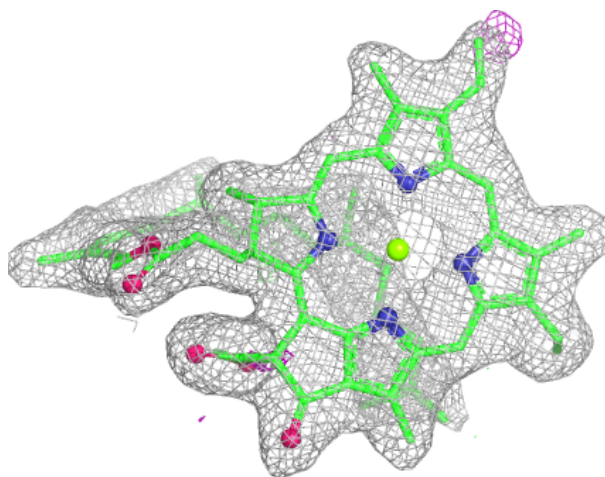
**Electron density around BCR b 619:**

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



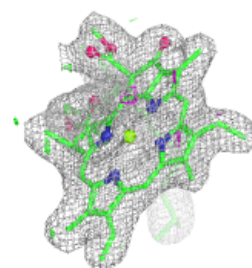
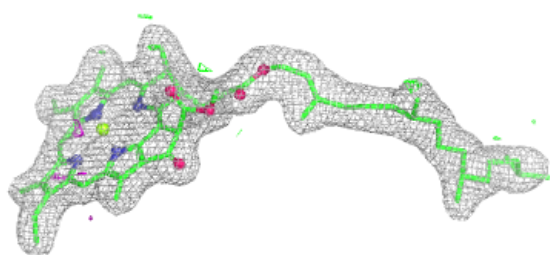
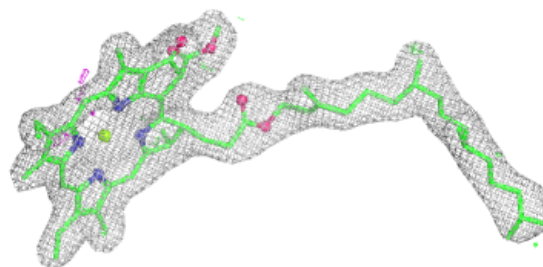
Electron density around CLA C 510:

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

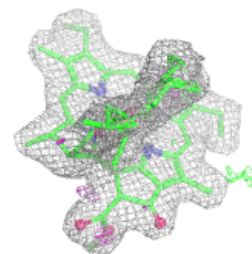
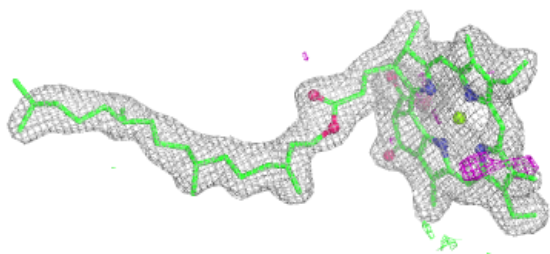
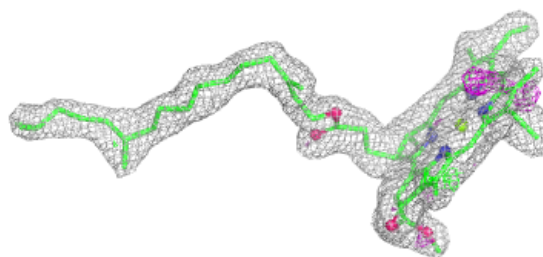


Electron density around CLA a 607:

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

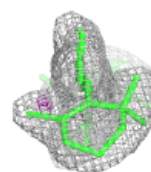
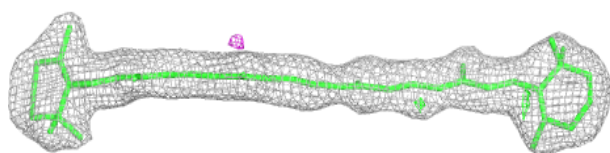
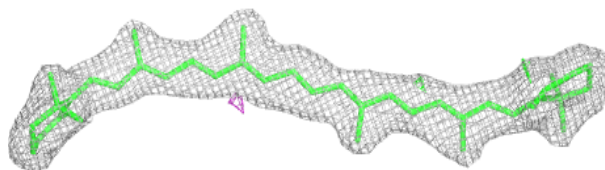
**Electron density around CLA C 502:**

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

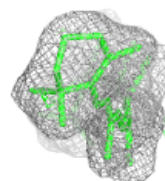
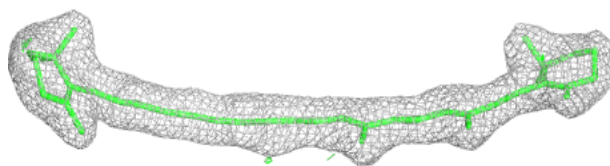
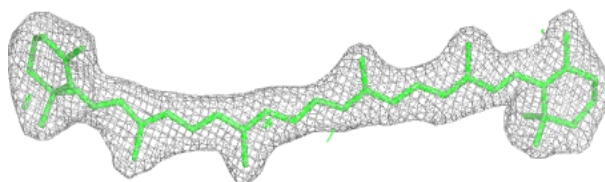


Electron density around BCR C 514:

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

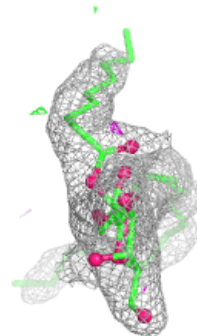
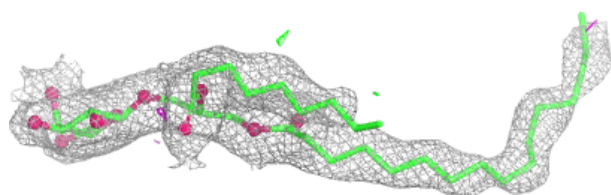
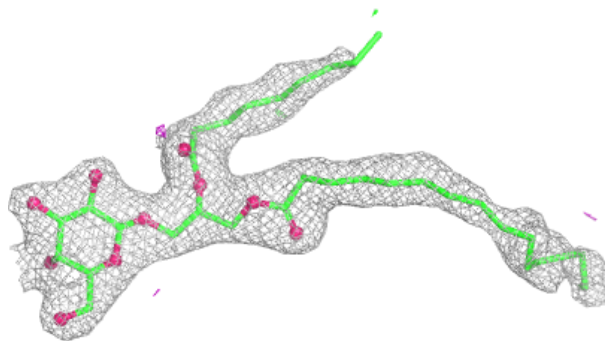
**Electron density around BCR t 101:**

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

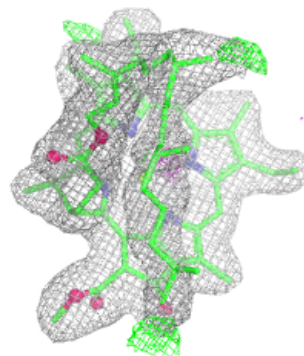
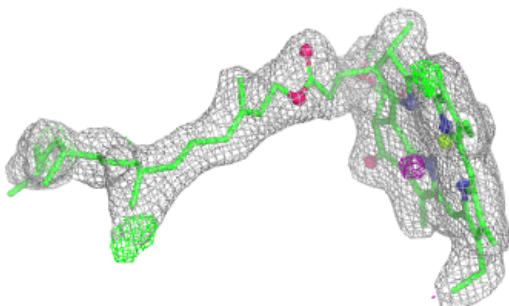
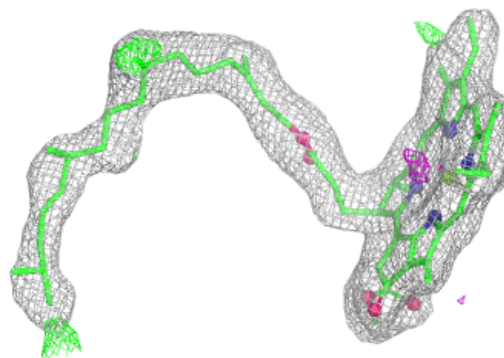


Electron density around LMG d 409:

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

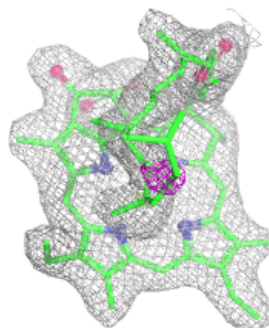
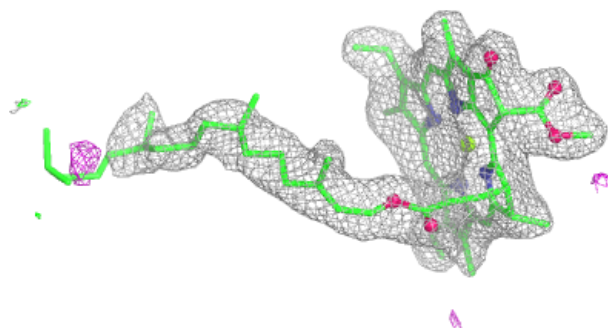
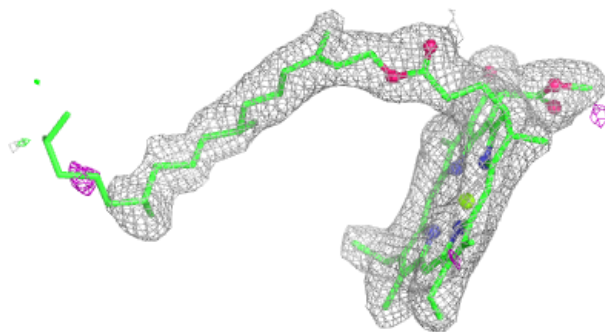
**Electron density around CLA b 606:**

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

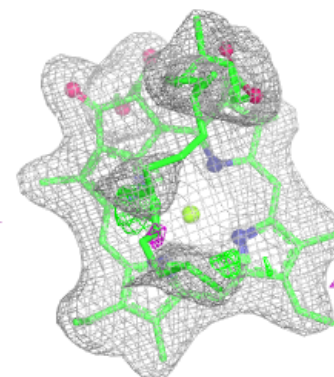
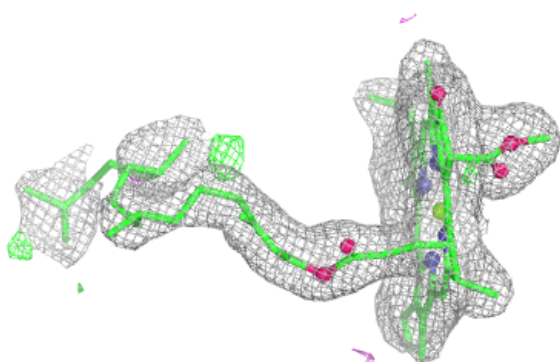
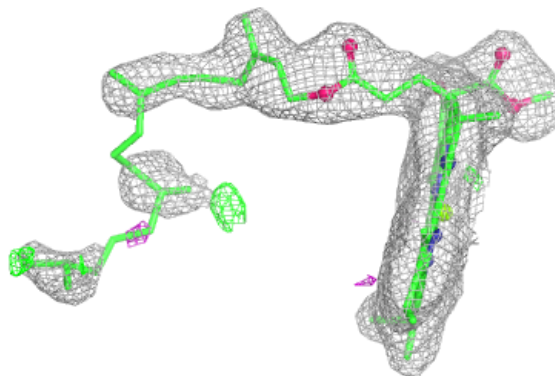


Electron density around CLA C 508:

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

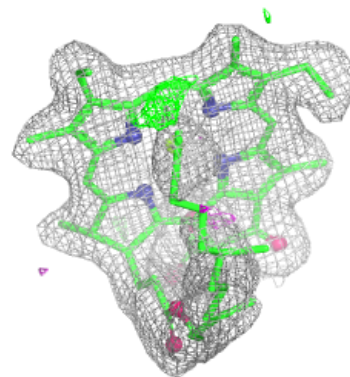
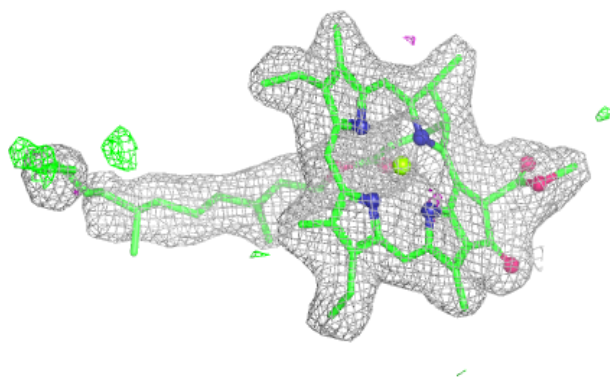
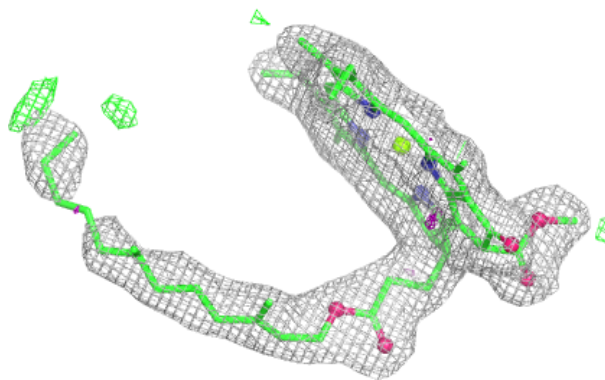
**Electron density around CLA c 506:**

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

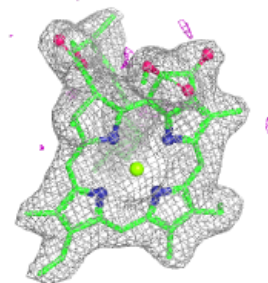
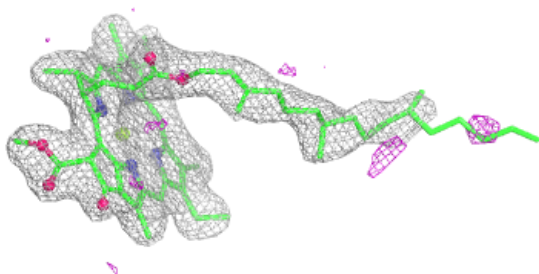
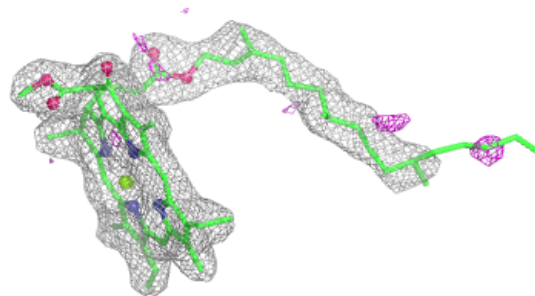


Electron density around CLA C 504:

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

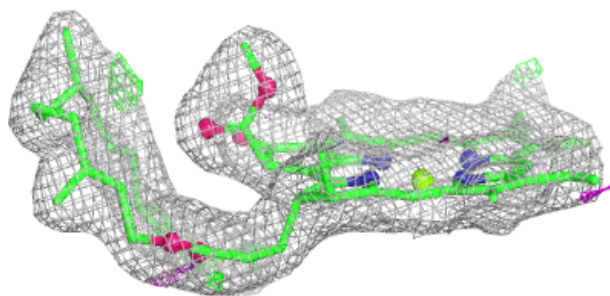
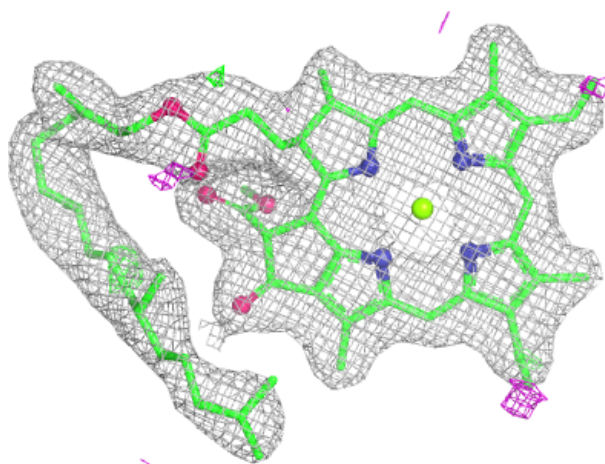
**Electron density around CLA c 508:**

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



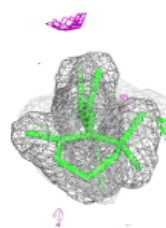
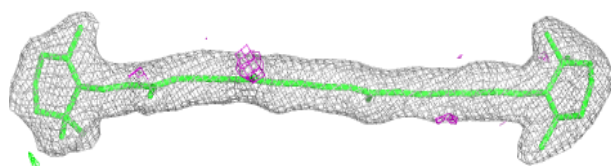
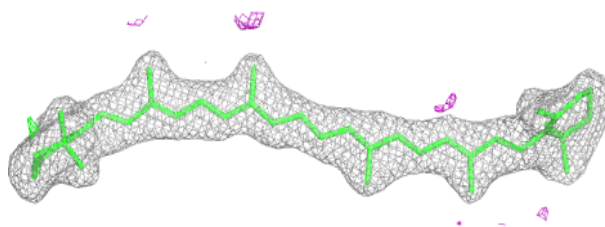
Electron density around CLA b 610:

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

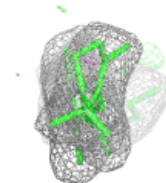
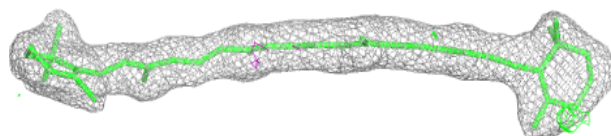
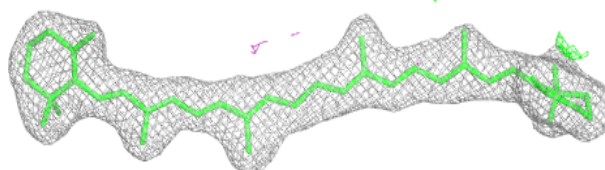


Electron density around BCR a 611:

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

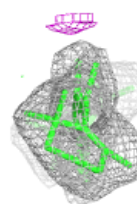
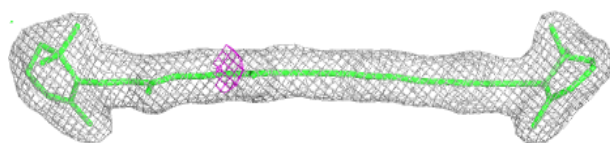
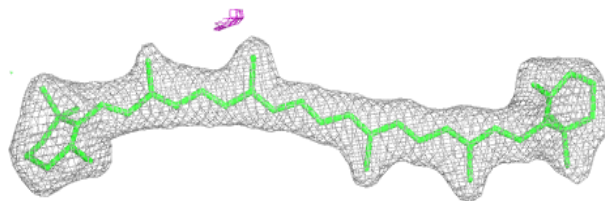
**Electron density around BCR b 617:**

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

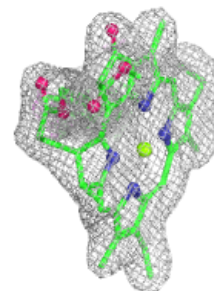
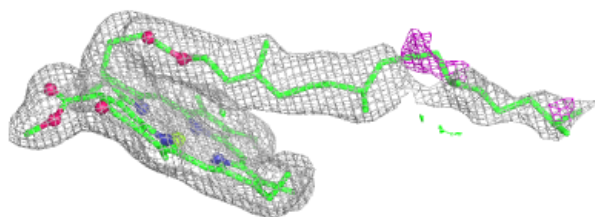
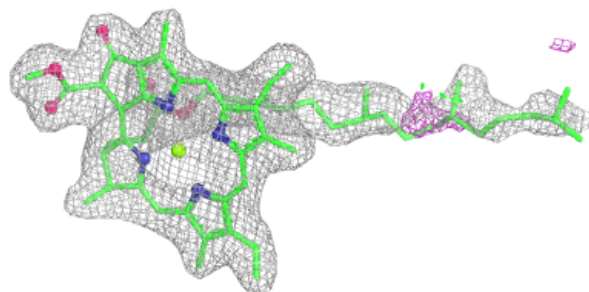


Electron density around BCR b 618:

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

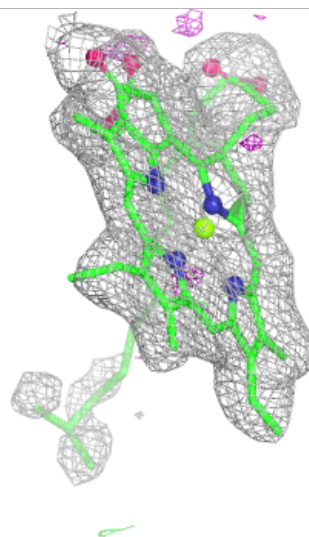
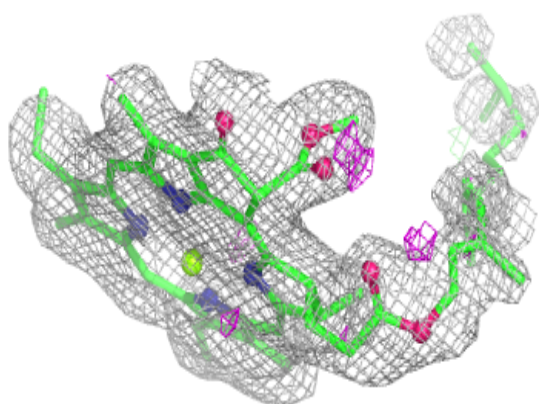
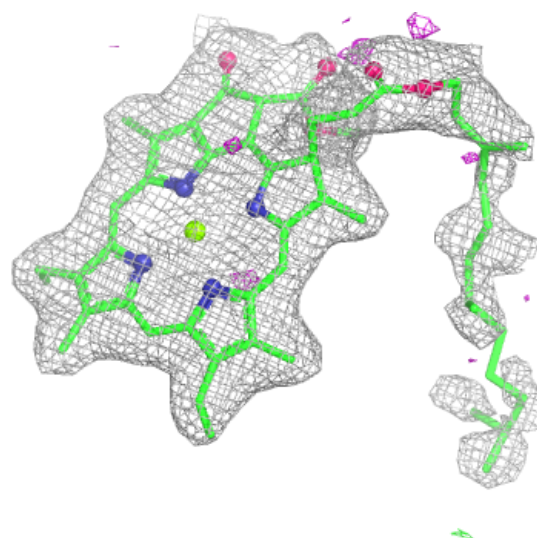
**Electron density around CLA b 614:**

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



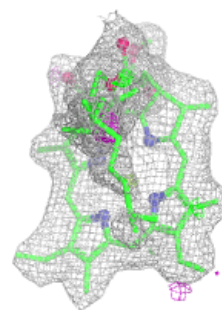
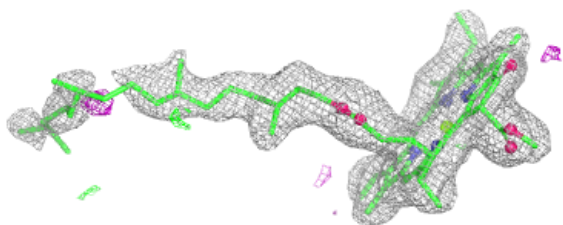
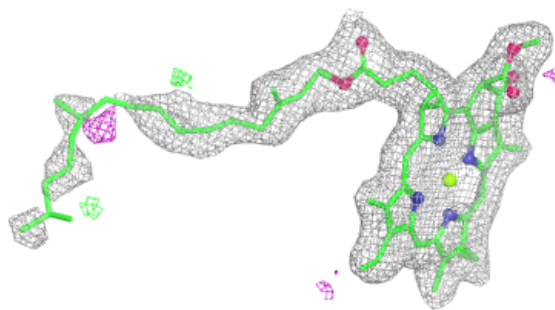
Electron density around CLA b 616:

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



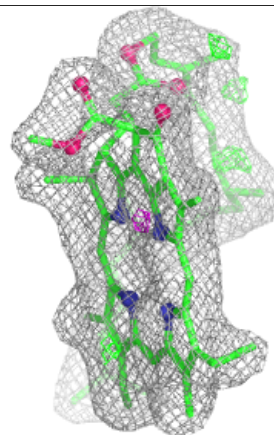
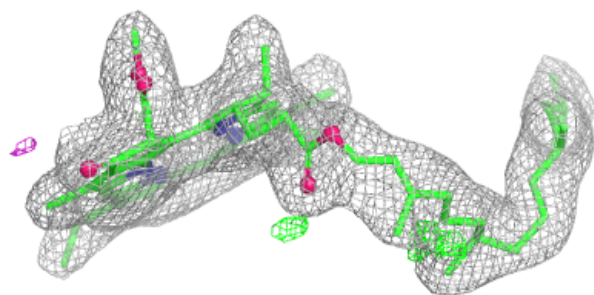
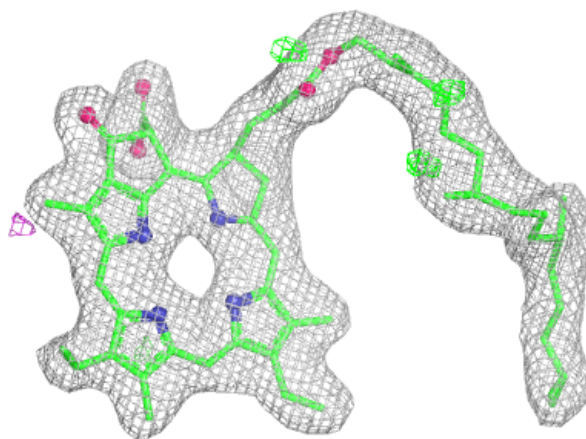
Electron density around CLA d 403:

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



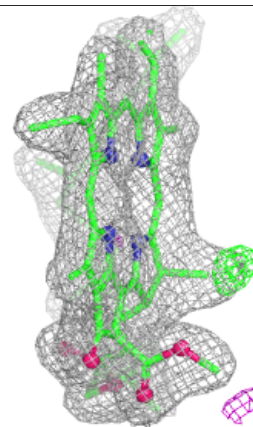
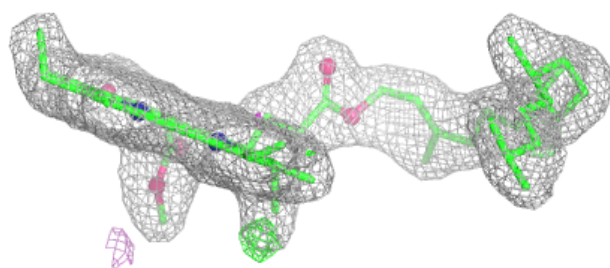
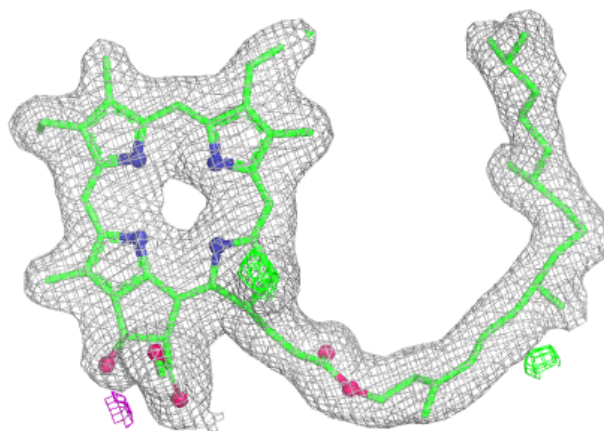
Electron density around PHO A 609:

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

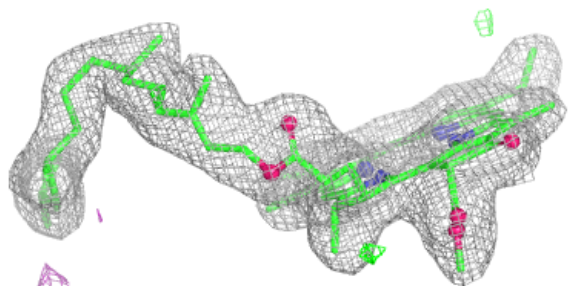
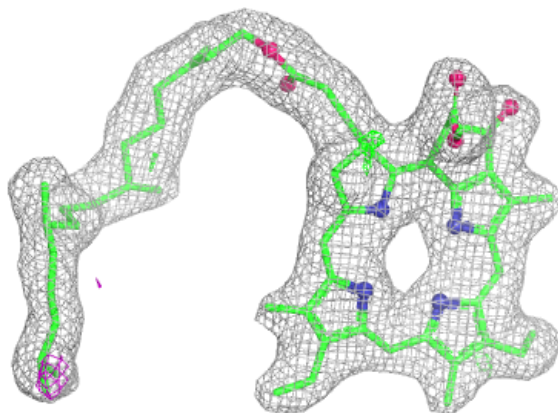


Electron density around PHO a 609:

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

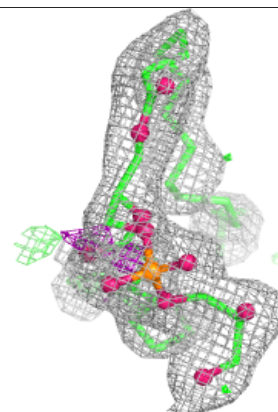
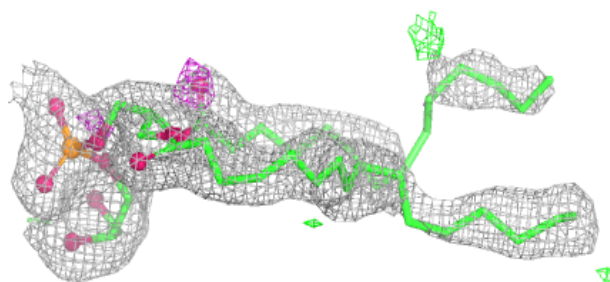
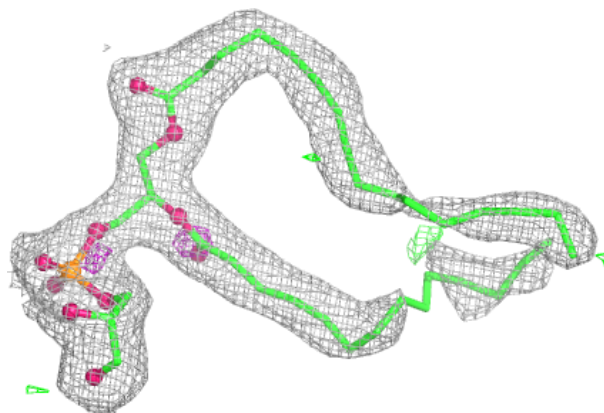
**Electron density around PHO d 401:**

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

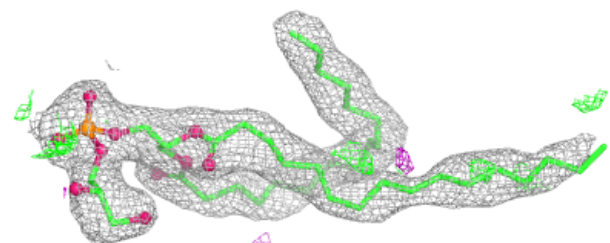
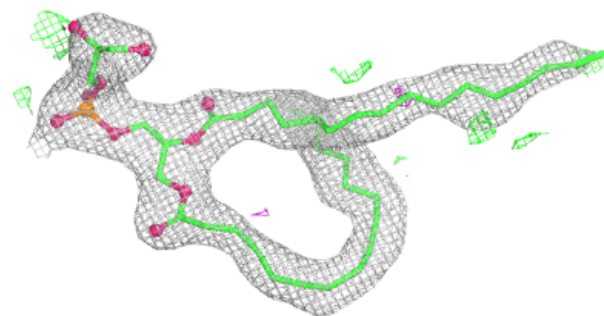


Electron density around LHG D 409:

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

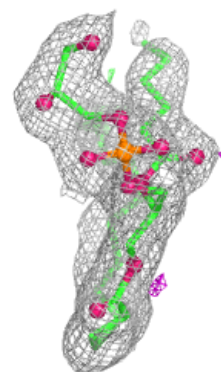
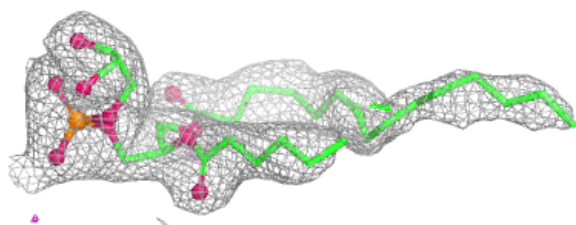
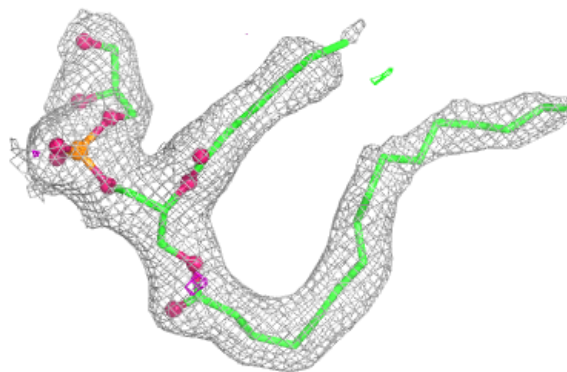
**Electron density around LHG D 410:**

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

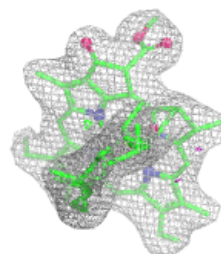
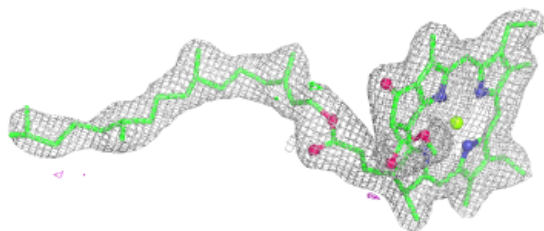
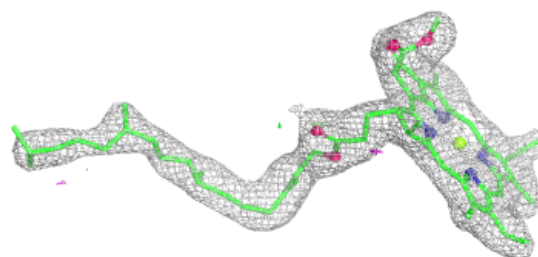


Electron density around LHG a 614:

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

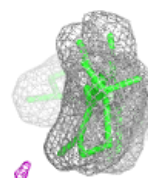
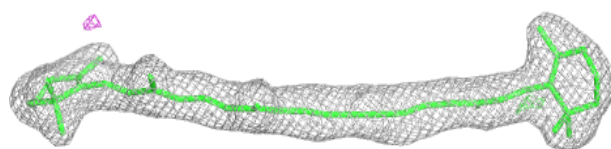
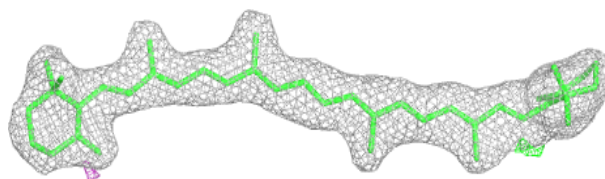
**Electron density around CLA c 502:**

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



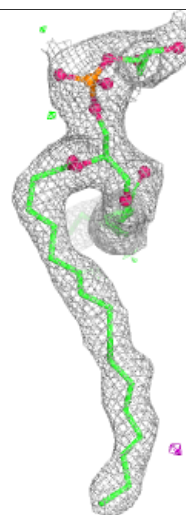
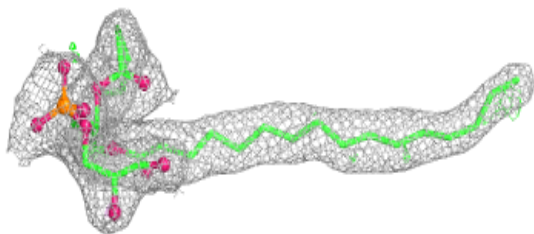
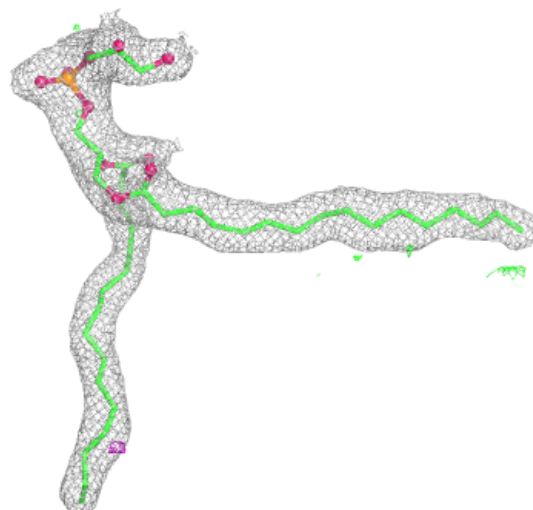
Electron density around BCR B 617:

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



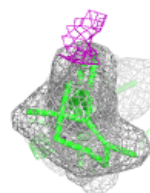
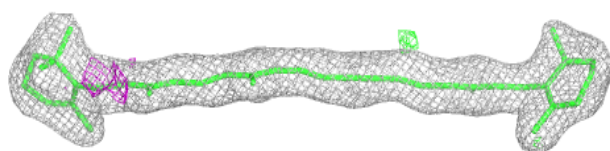
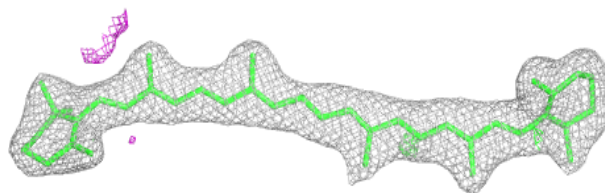
Electron density around LHG 1 101:

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

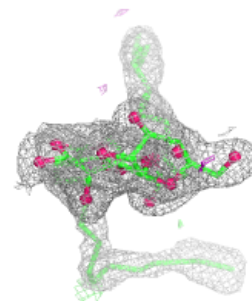
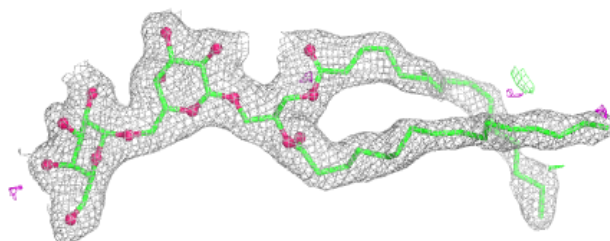
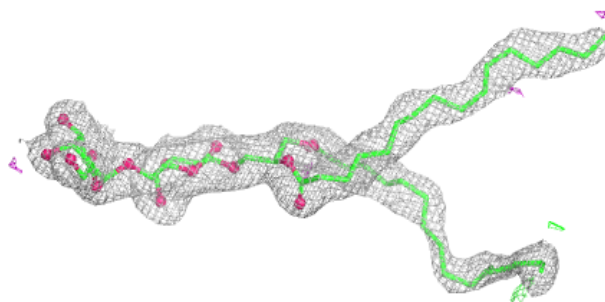


Electron density around BCR B 618:

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

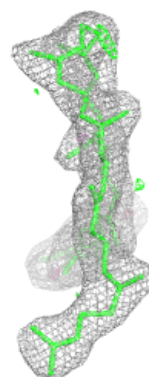
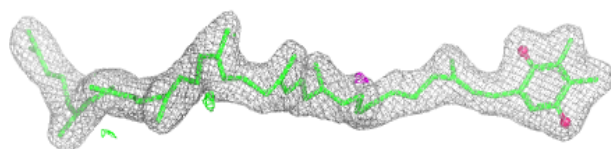
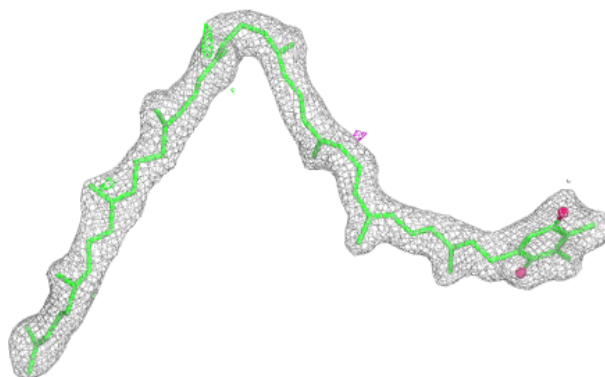
**Electron density around DGD C 520:**

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

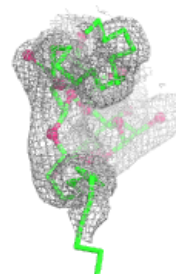
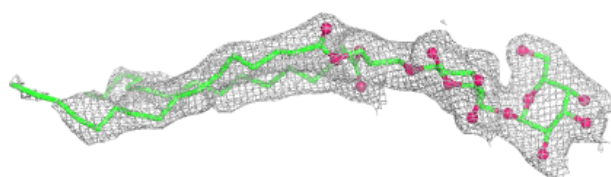
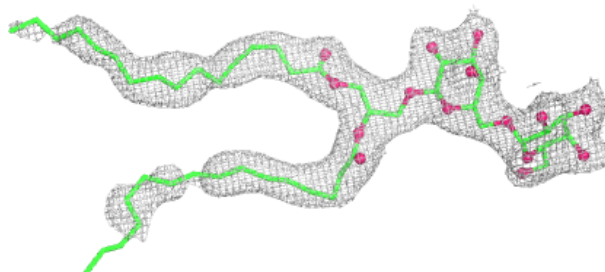


Electron density around PL9 D 405:

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

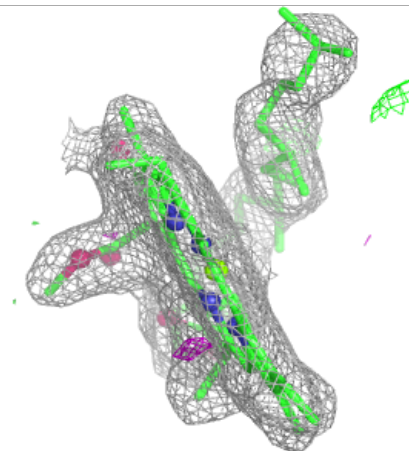
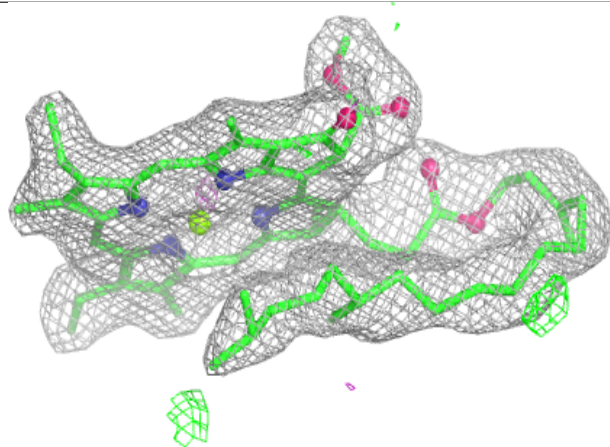
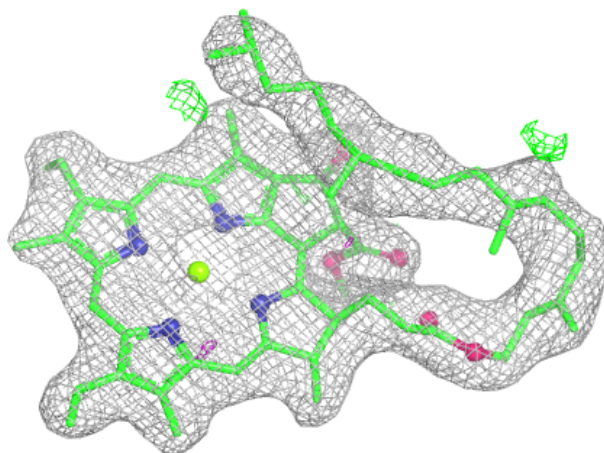
**Electron density around DGD C 522:**

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



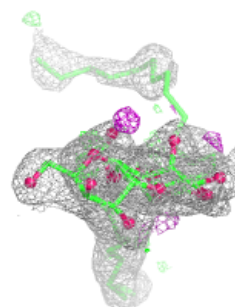
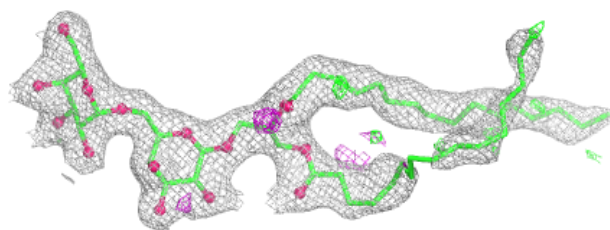
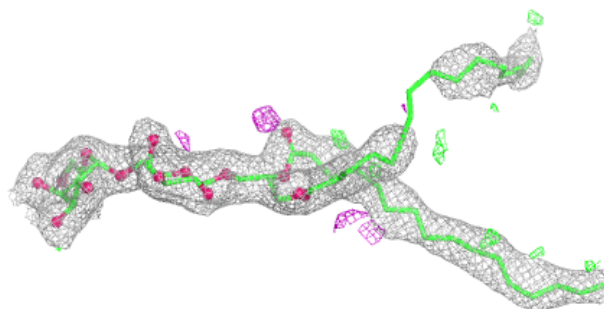
Electron density around CLA C 509:

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

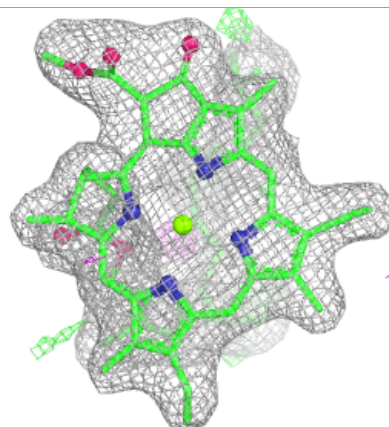
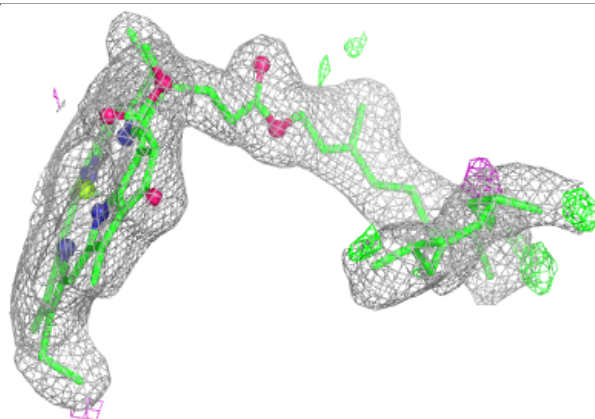
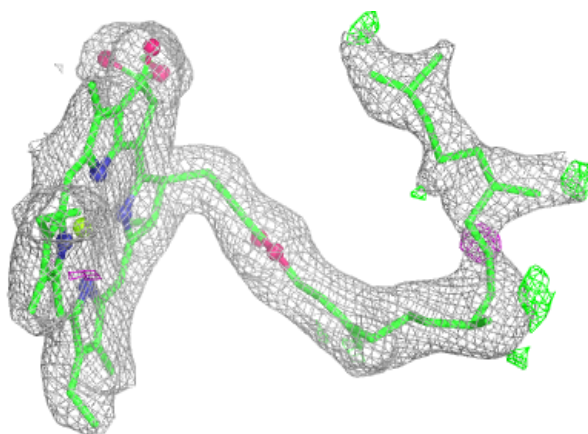


Electron density around DGD c 519:

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

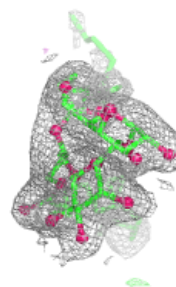
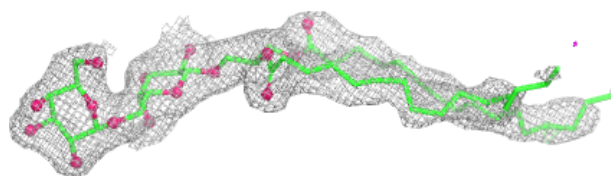
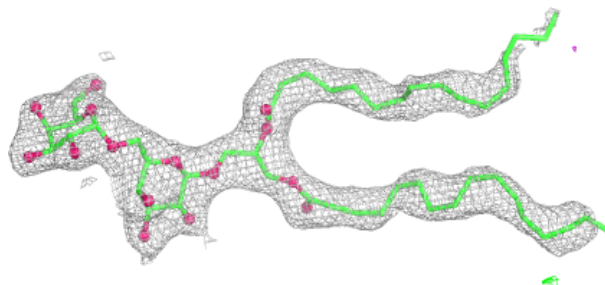
**Electron density around CLA B 606:**

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

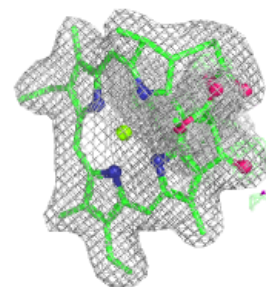
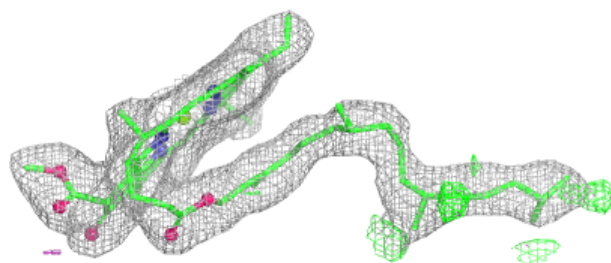
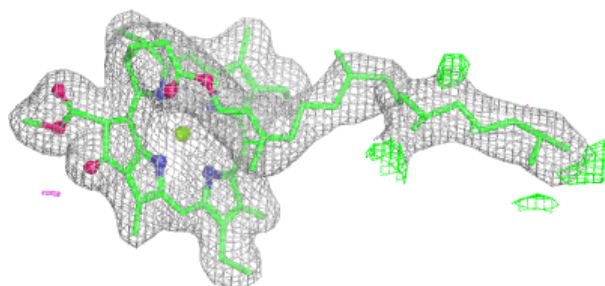


Electron density around DGD c 521:

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

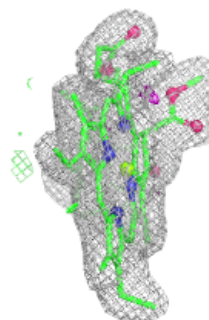
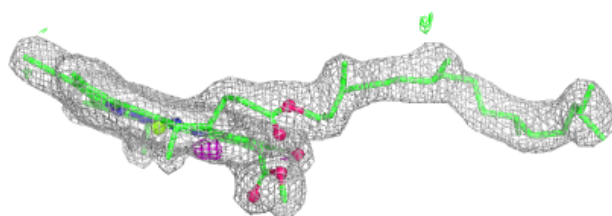
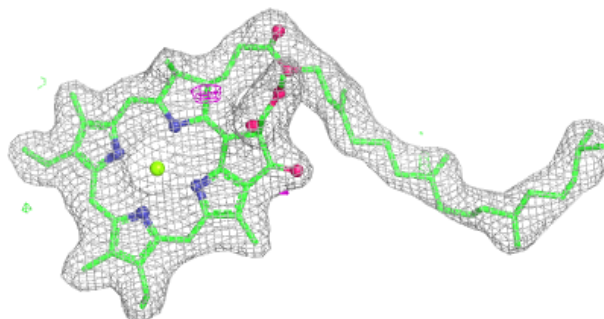
**Electron density around CLA c 505:**

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

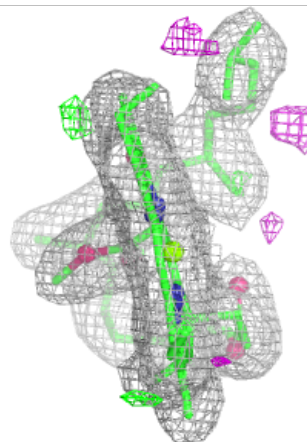
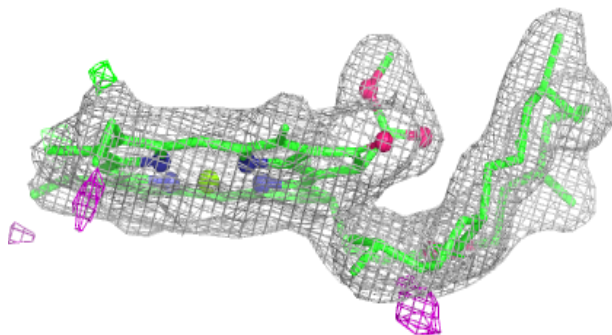
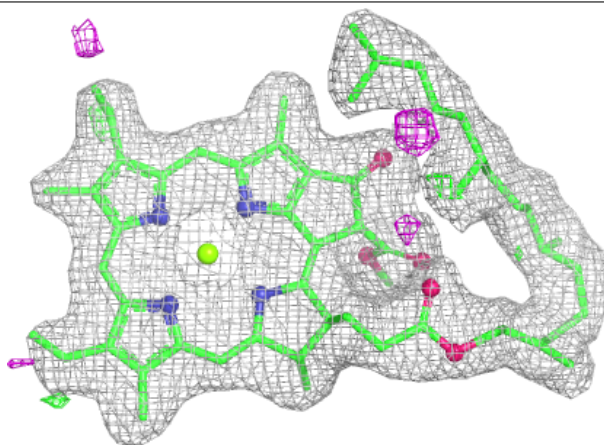


Electron density around CLA B 602:

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

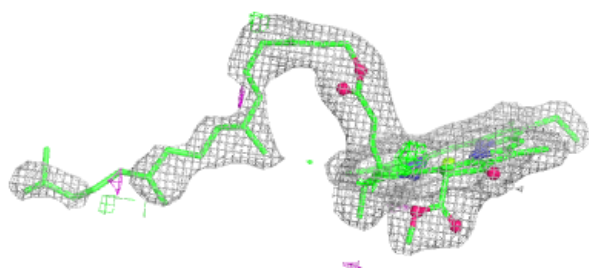
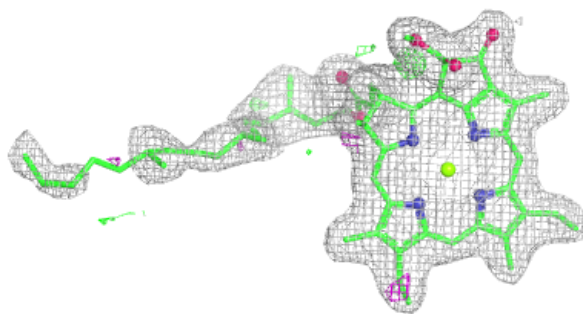
**Electron density around CLA B 610:**

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



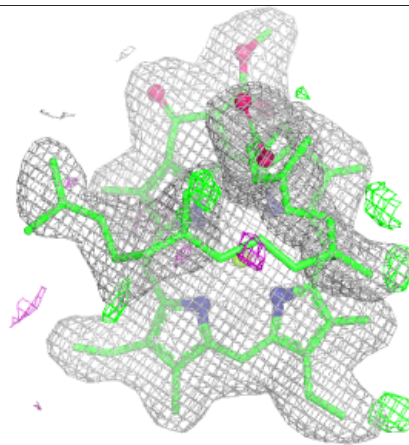
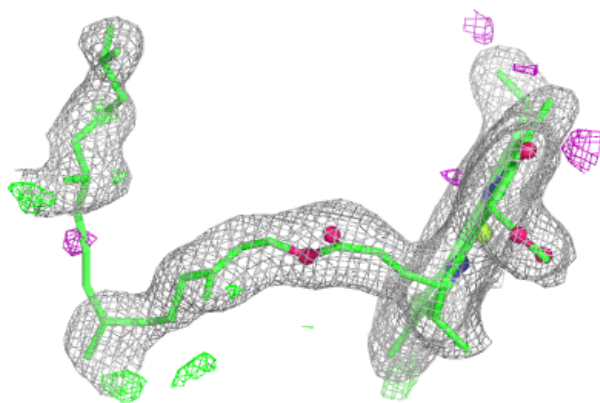
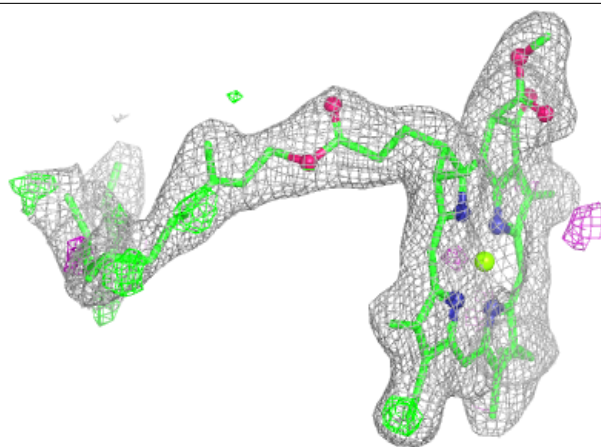
Electron density around CLA a 608:

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



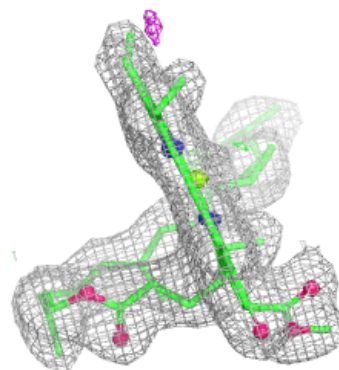
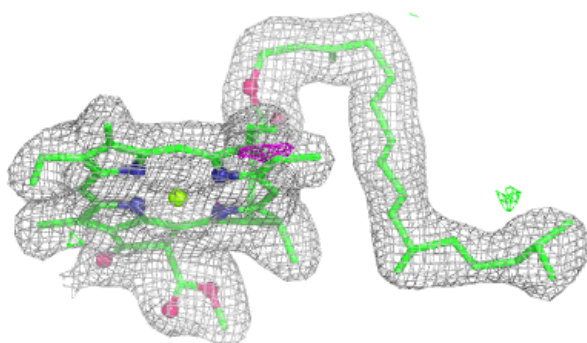
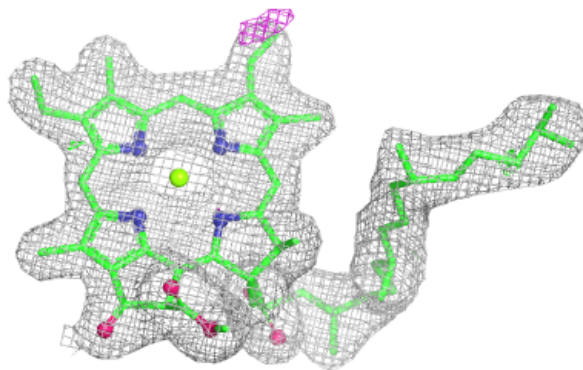
Electron density around CLA a 610:

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

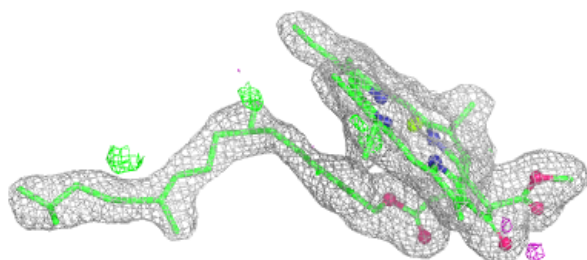
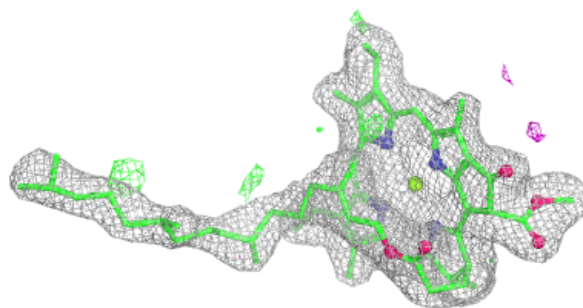


Electron density around CLA a 613:

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

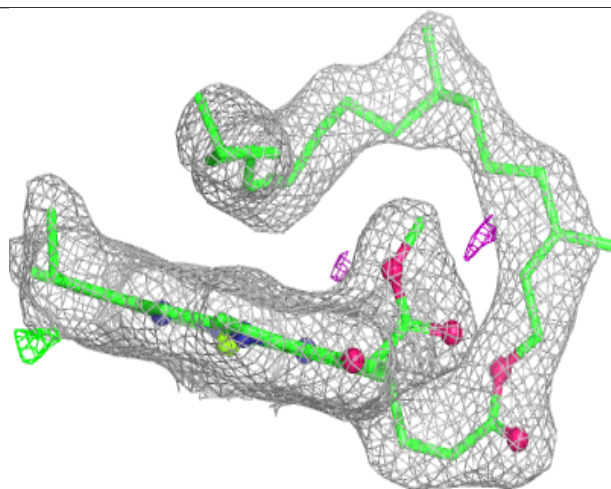
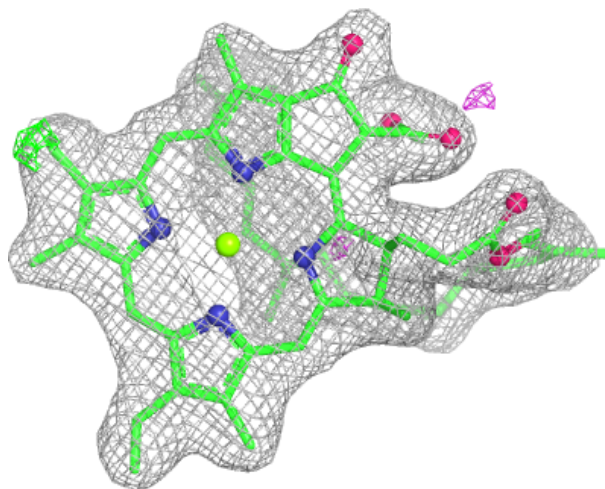
**Electron density around CLA C 505:**

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



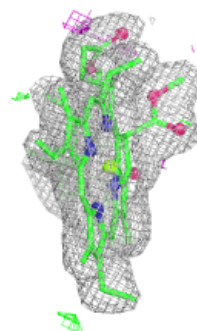
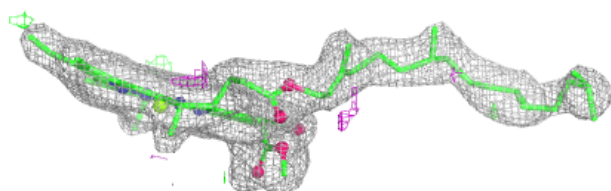
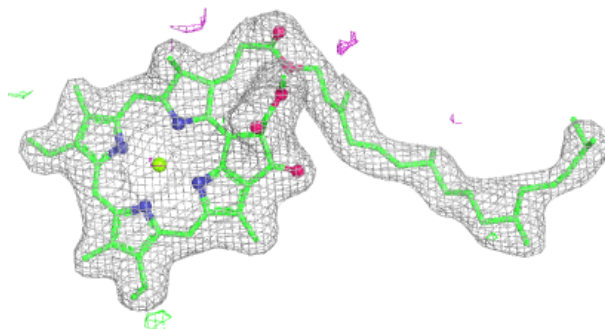
Electron density around CLA c 510:

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

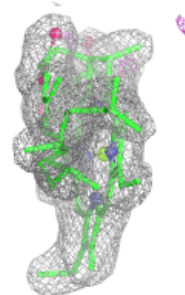
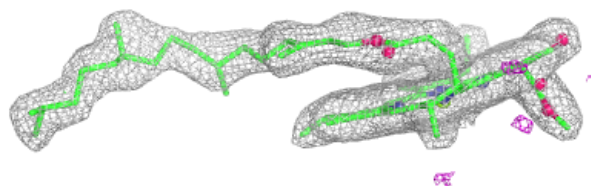
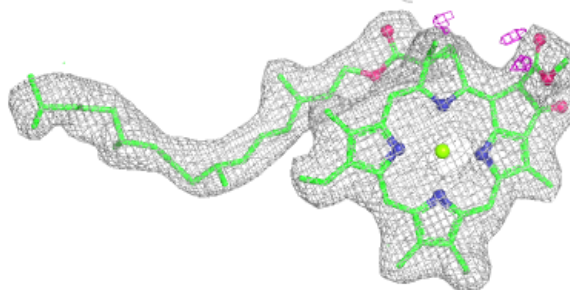


Electron density around CLA b 602:

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

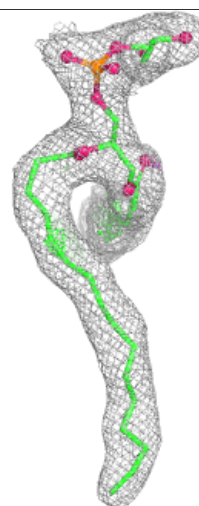
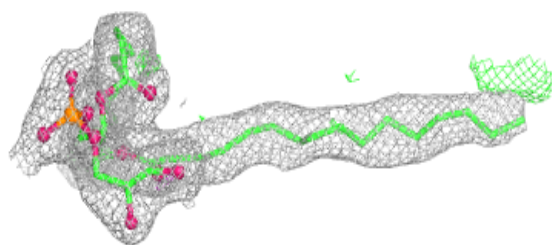
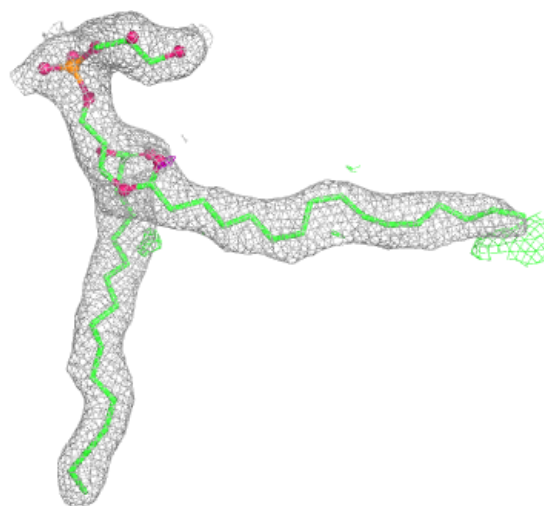
**Electron density around CLA b 603:**

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



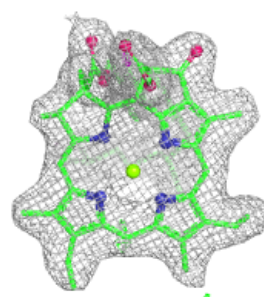
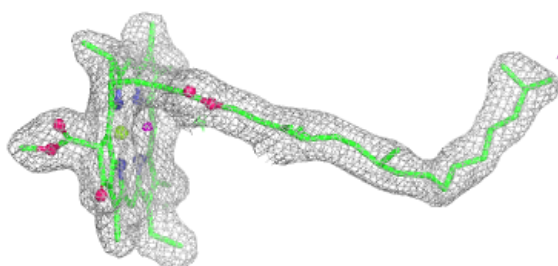
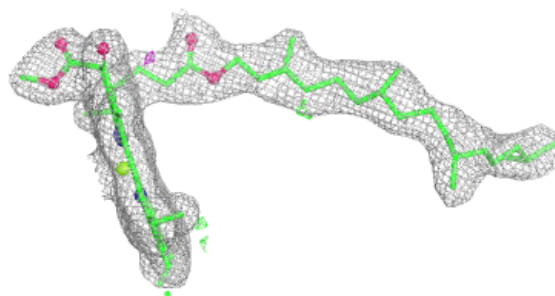
Electron density around LHG L 101:

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

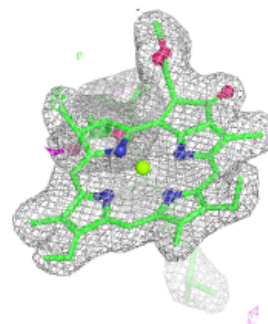
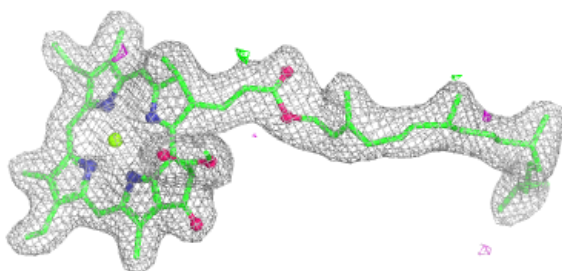
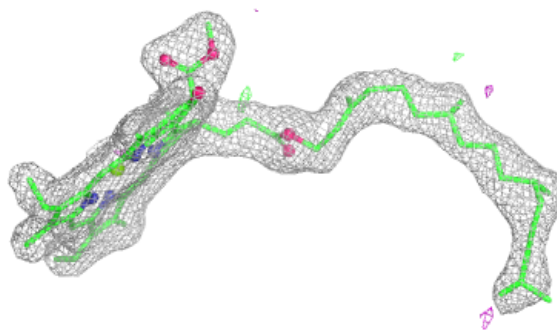


Electron density around CLA b 605:

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

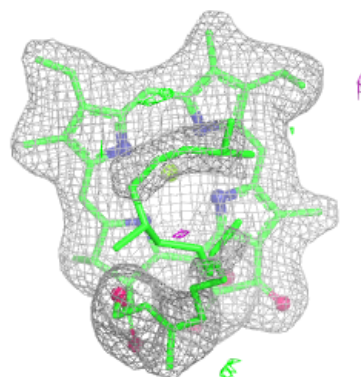
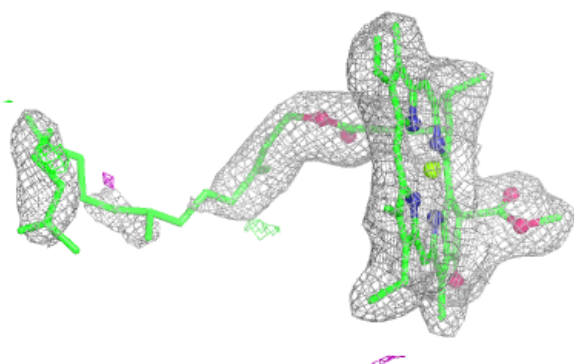
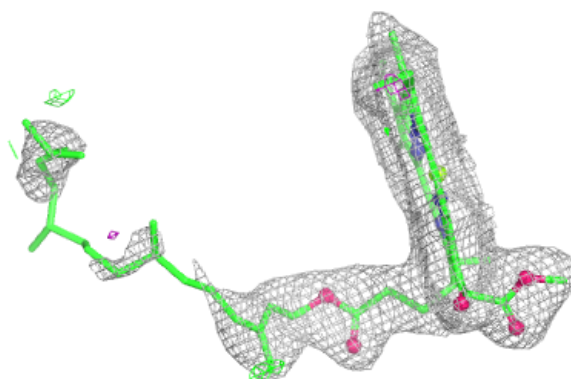
**Electron density around CLA d 402:**

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

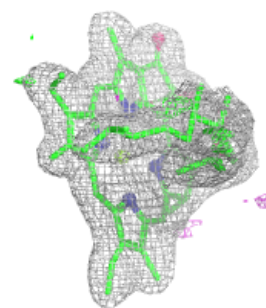
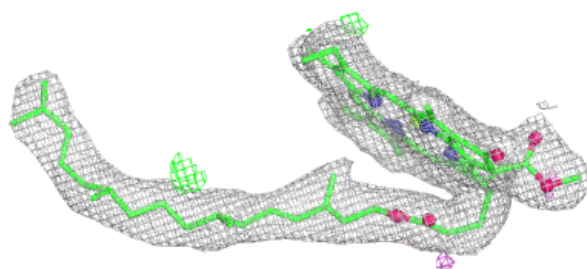
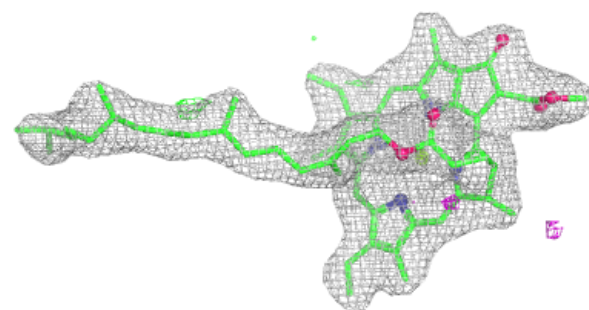


Electron density around CLA C 506:

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

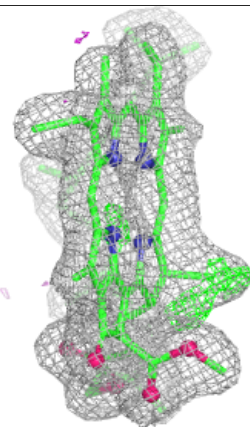
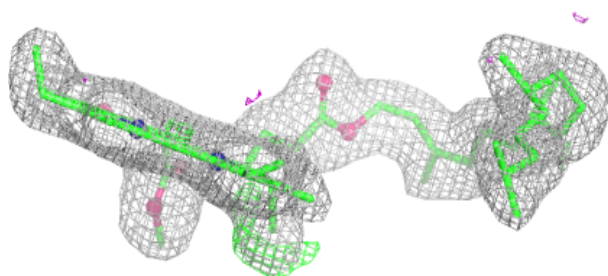
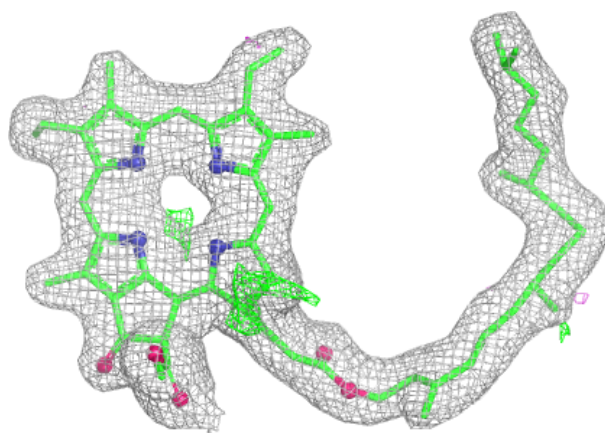
**Electron density around CLA b 608:**

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

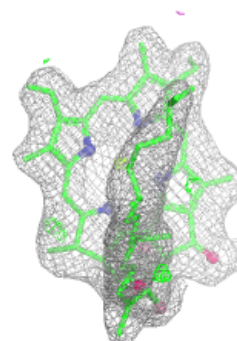
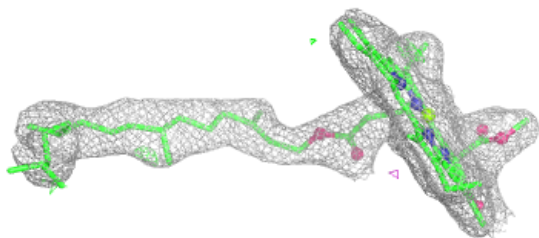
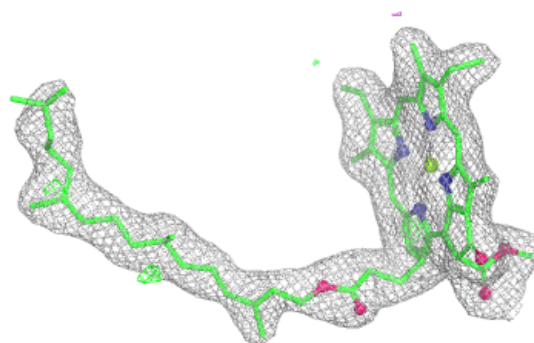


Electron density around PHO D 401:

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

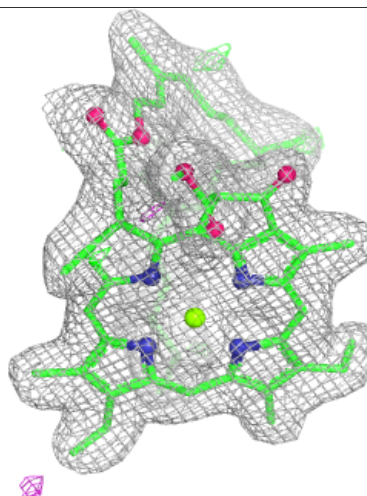
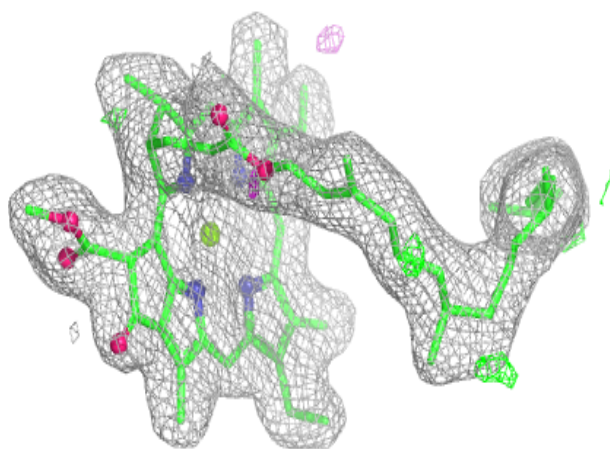
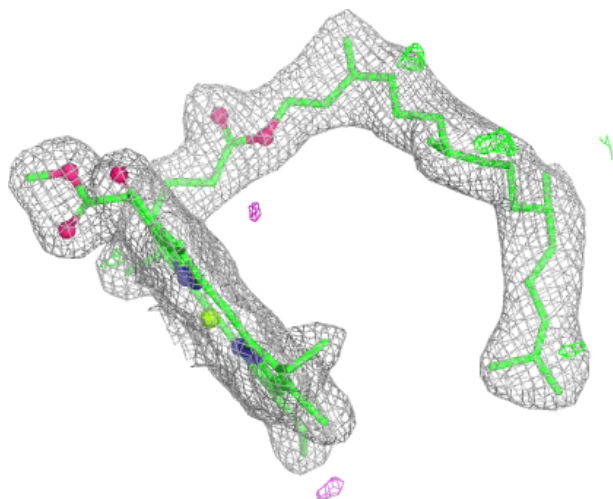
**Electron density around CLA b 609:**

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



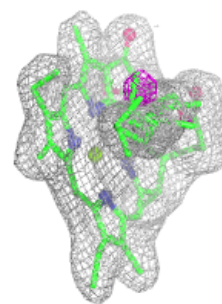
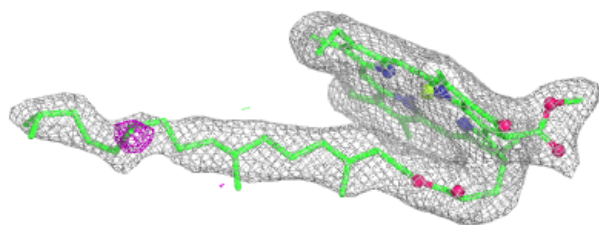
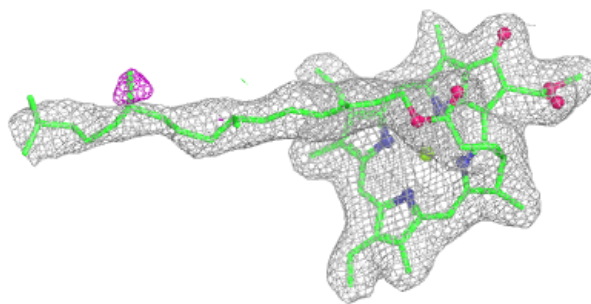
Electron density around CLA B 611:

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



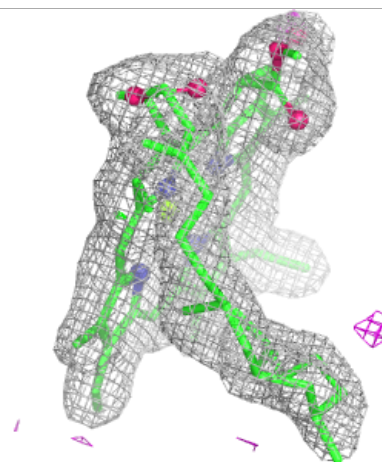
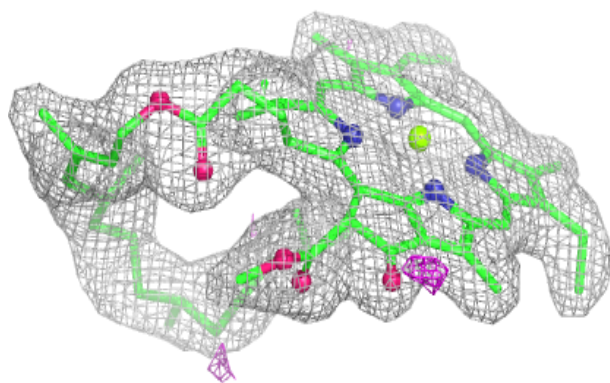
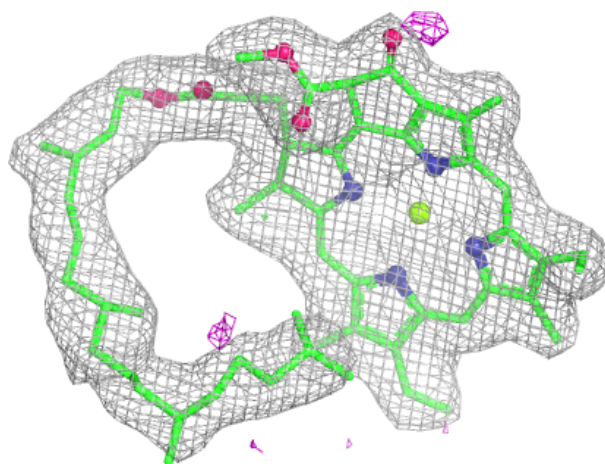
Electron density around CLA B 614:

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



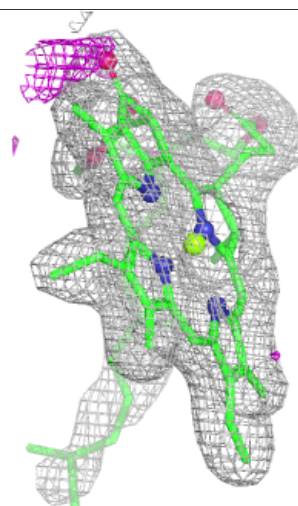
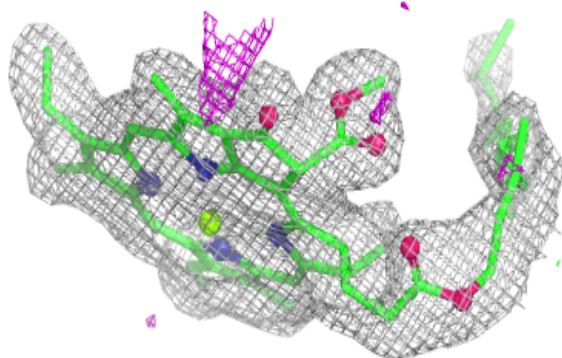
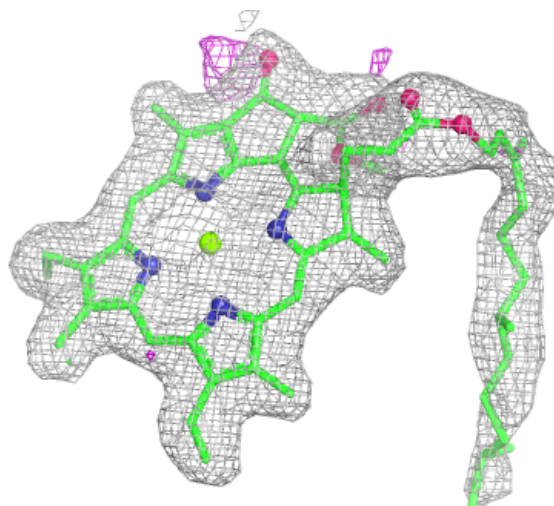
Electron density around CLA b 615:

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



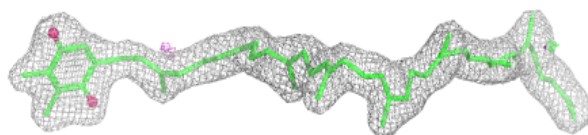
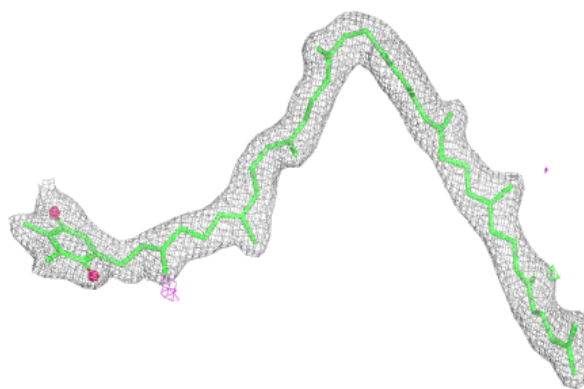
Electron density around CLA B 616:

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

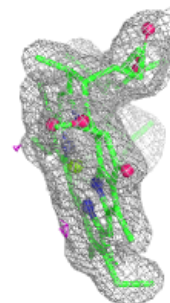
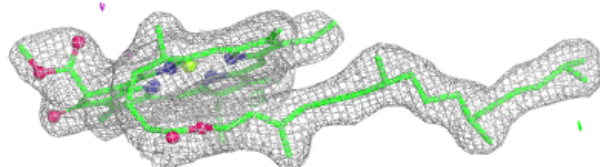
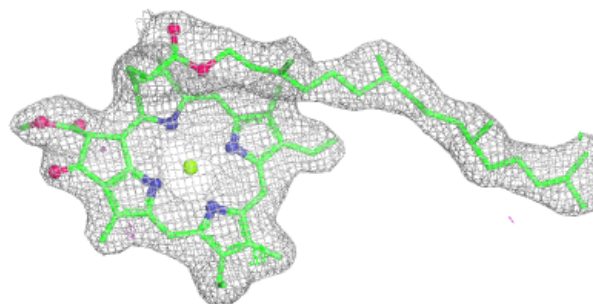


Electron density around PL9 d 405:

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

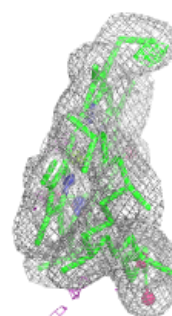
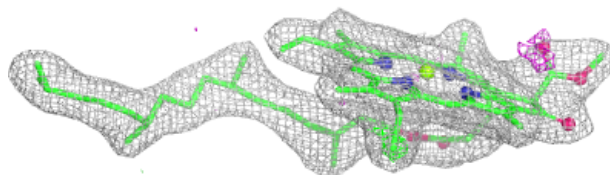
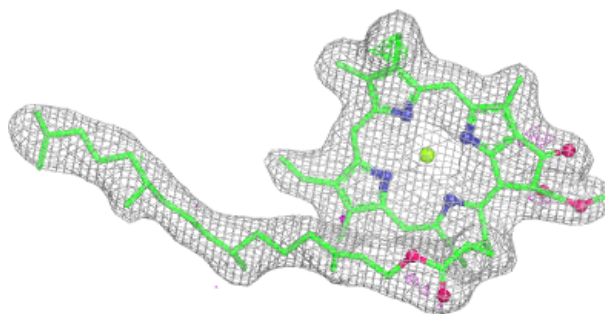
**Electron density around CLA c 501:**

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

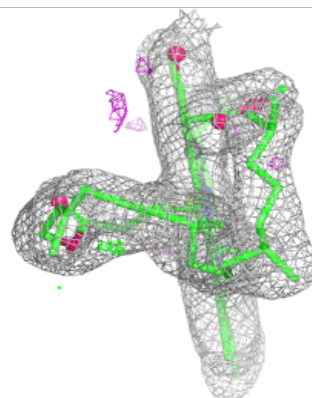
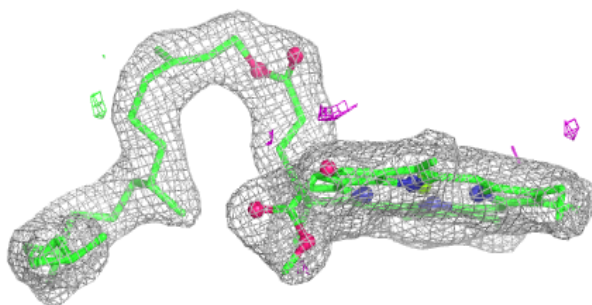
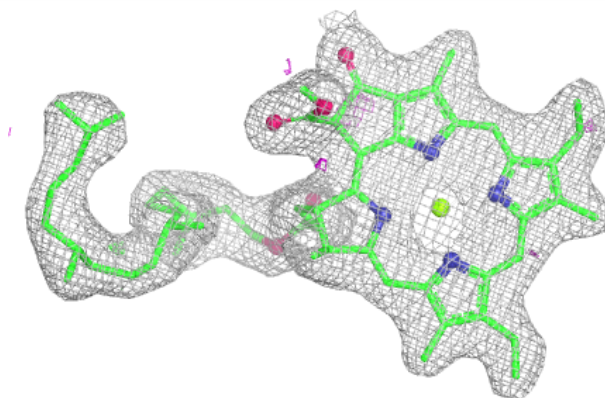


Electron density around CLA C 501:

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

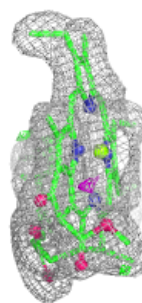
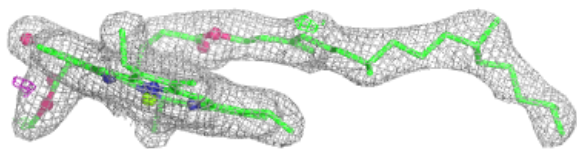
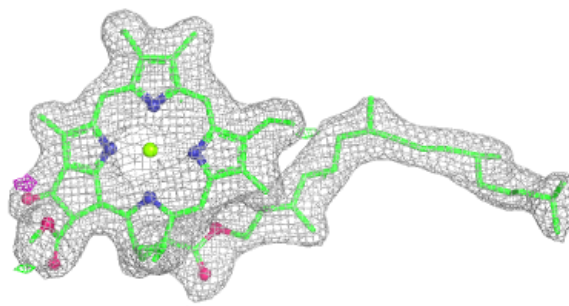
**Electron density around CLA B 612:**

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

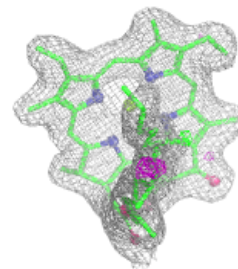
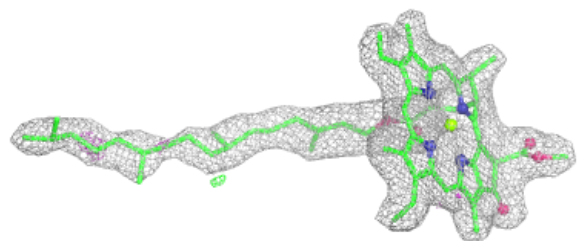
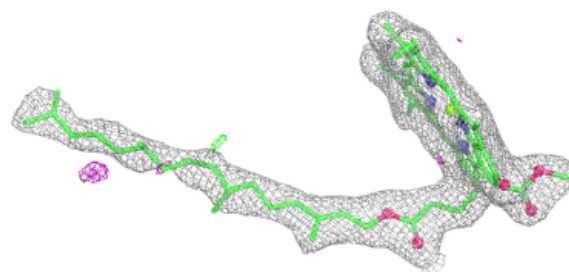


Electron density around CLA B 603:

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

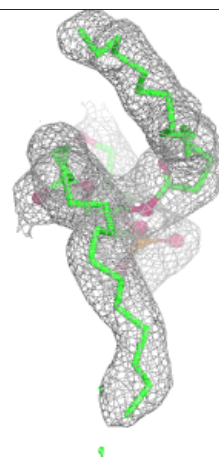
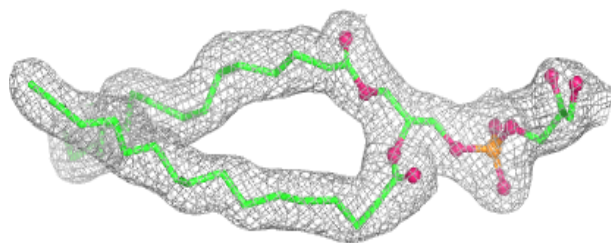
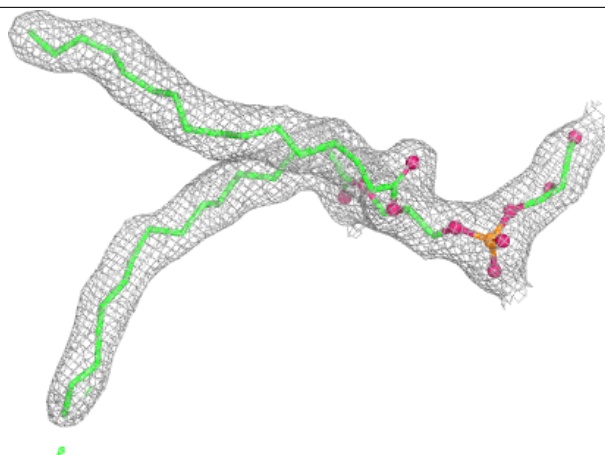
**Electron density around CLA b 607:**

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



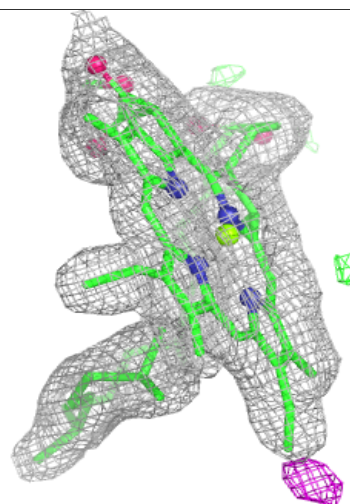
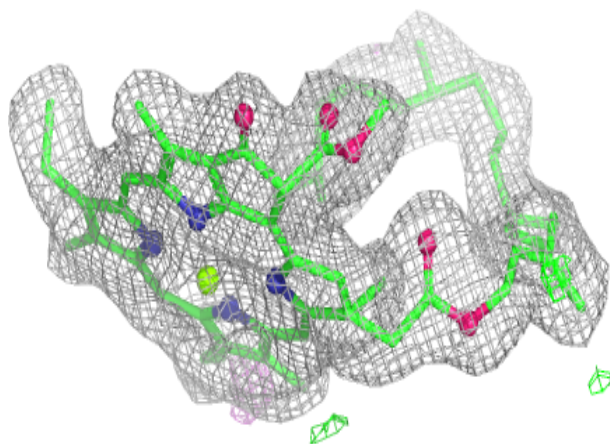
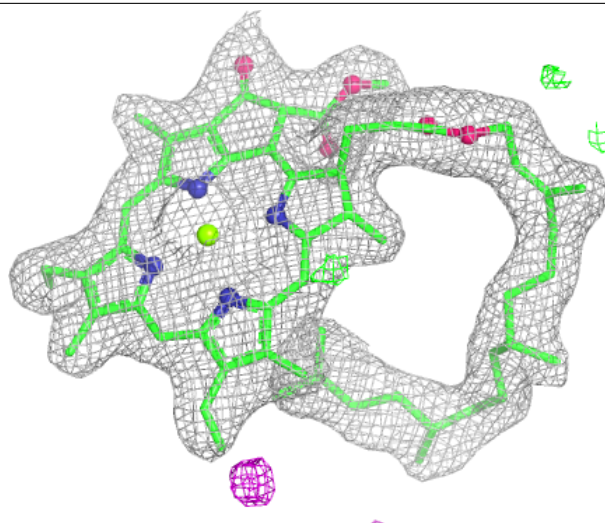
Electron density around LHG D 408:

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



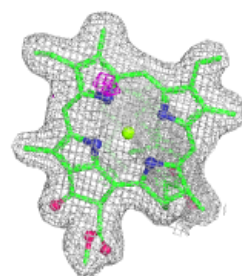
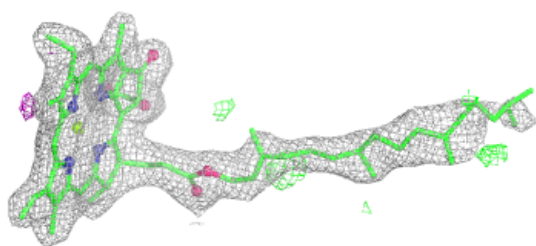
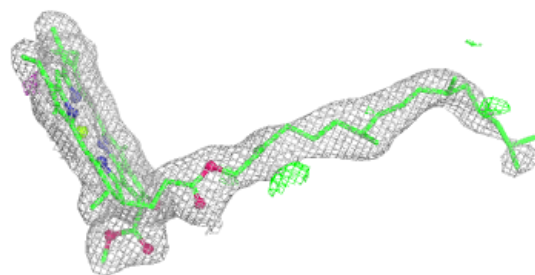
Electron density around CLA B 615:

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

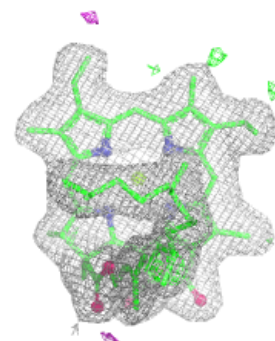
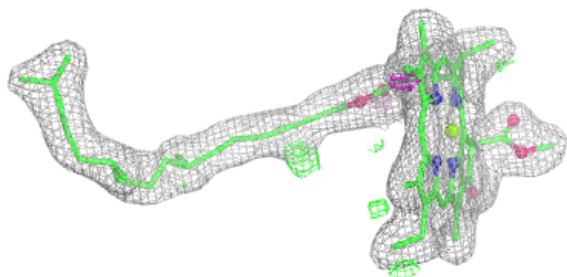
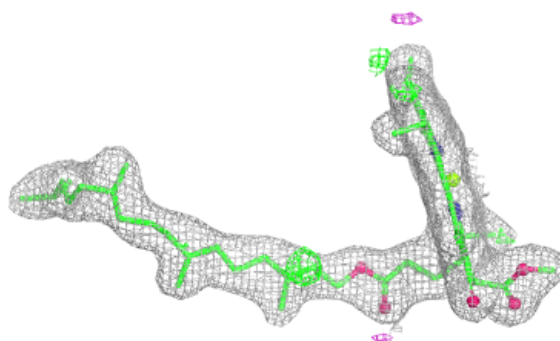


Electron density around CLA B 604:

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

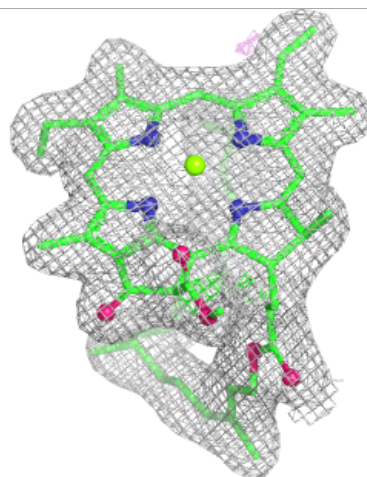
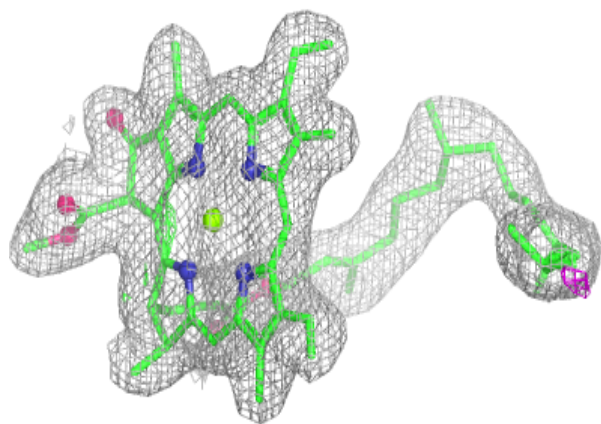
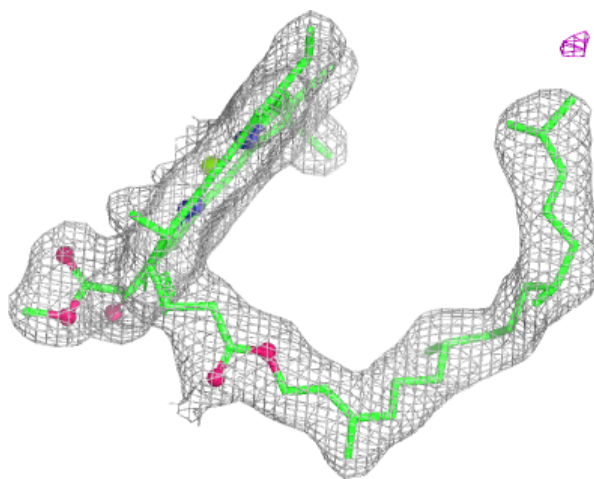
**Electron density around CLA B 605:**

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



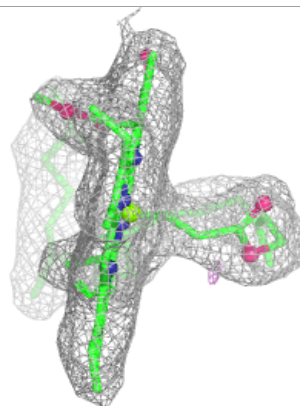
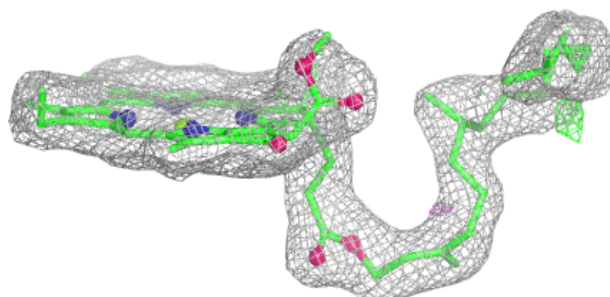
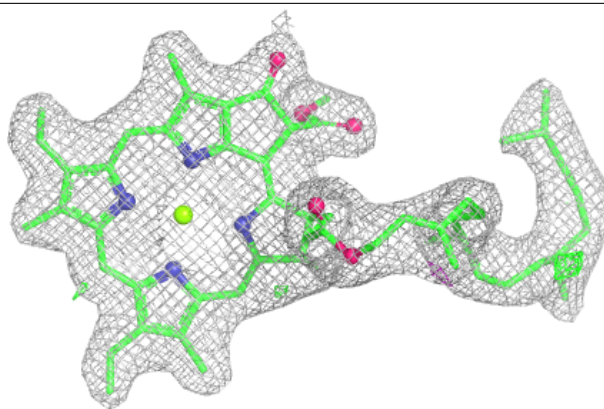
Electron density around CLA b 611:

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



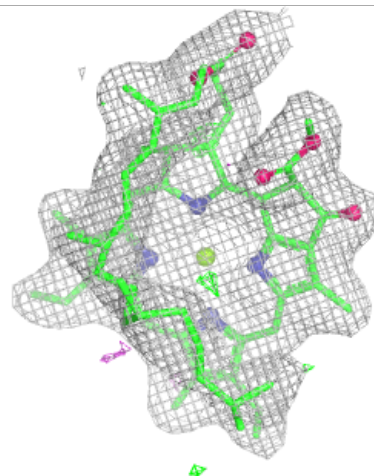
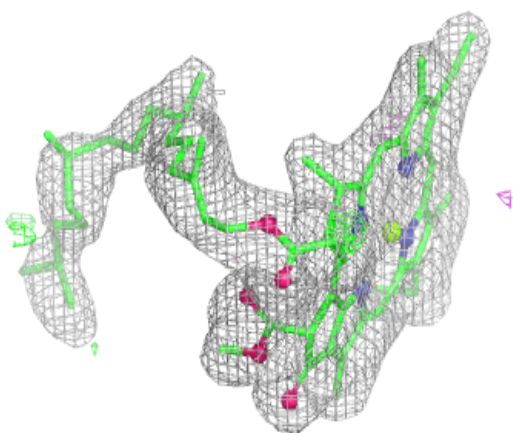
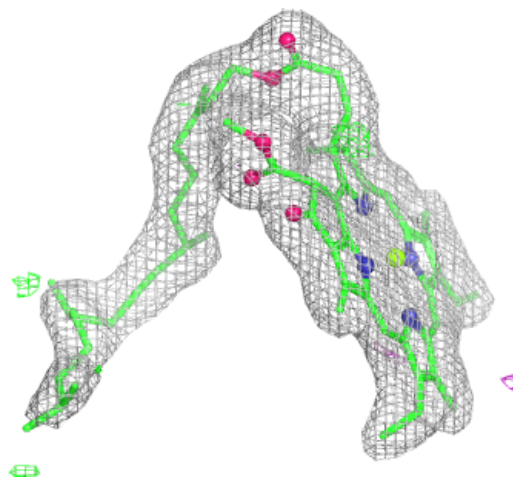
Electron density around CLA b 612:

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



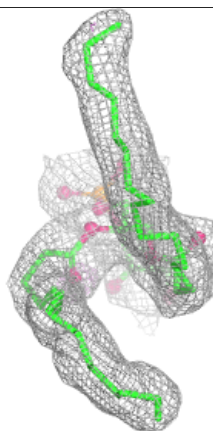
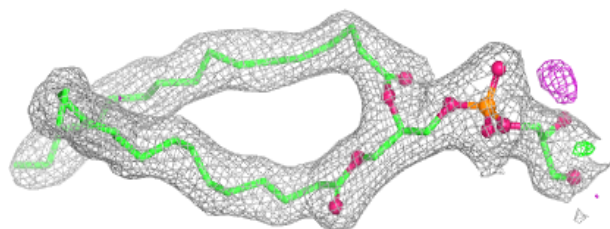
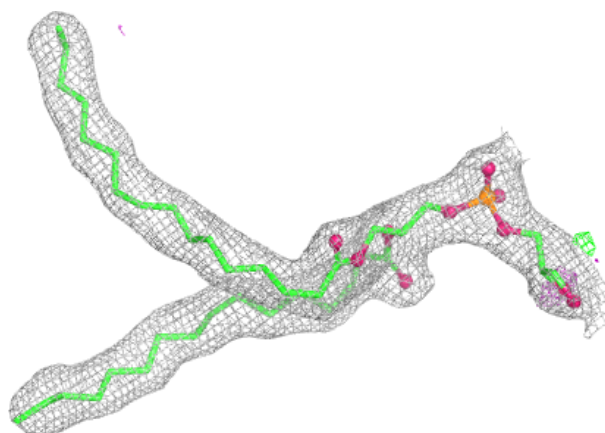
Electron density around CLA b 613:

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

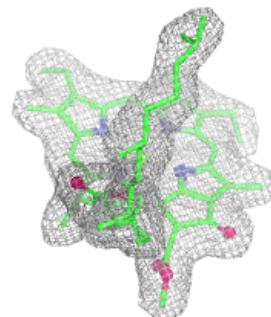
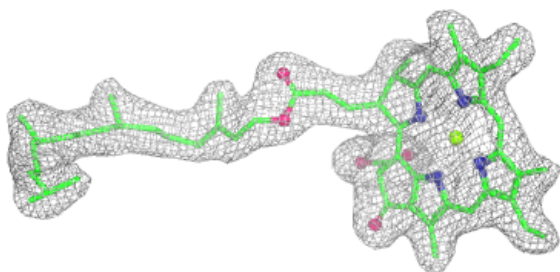
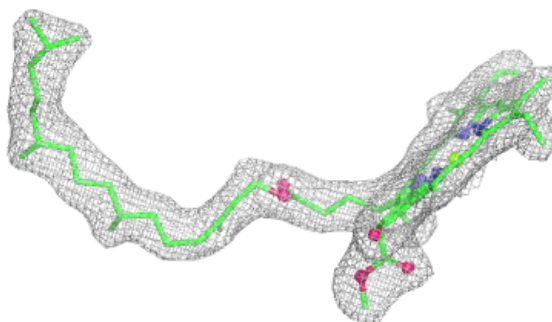


Electron density around LHG d 407:

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

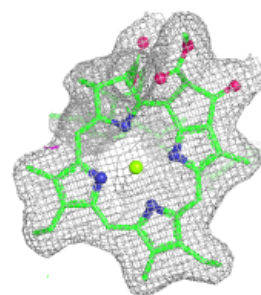
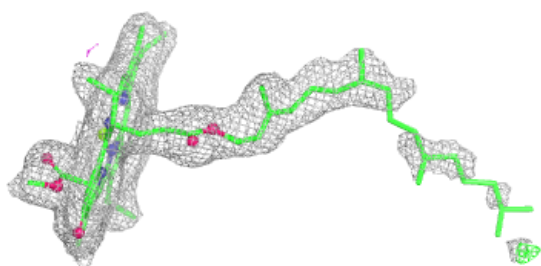
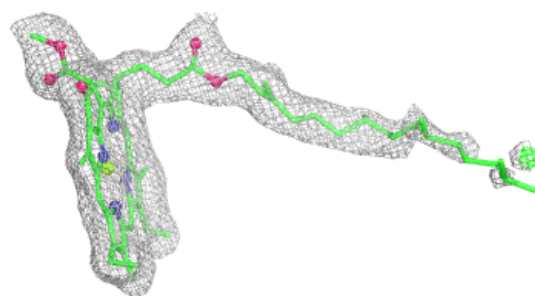
**Electron density around CLA D 402:**

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

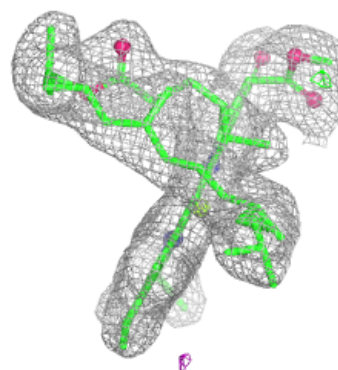
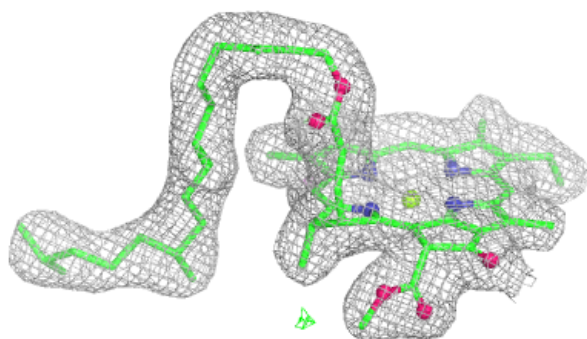
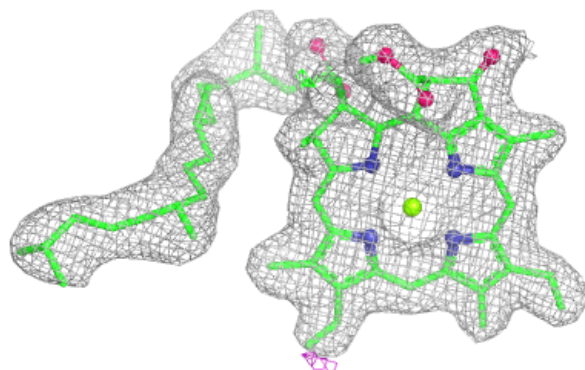


Electron density around CLA D 403:

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

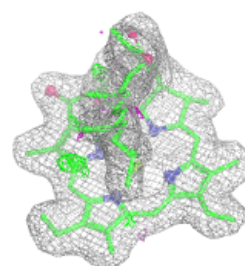
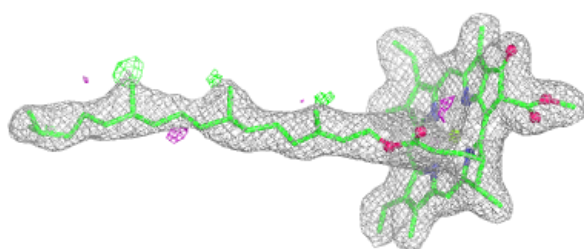
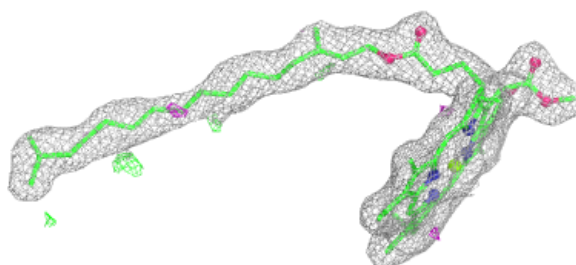
**Electron density around CLA A 614:**

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

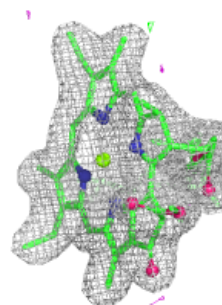
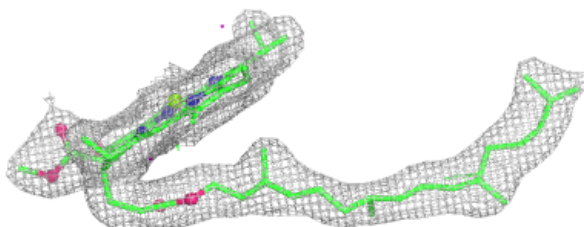
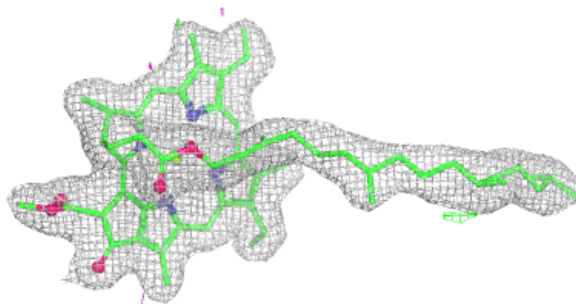


Electron density around CLA B 607:

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

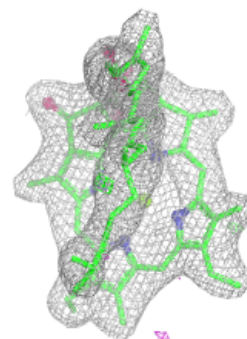
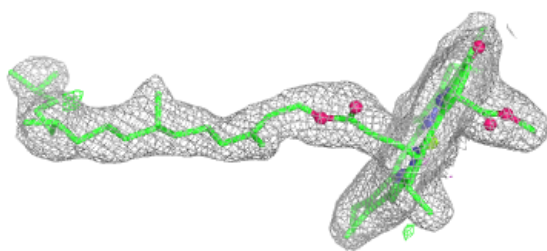
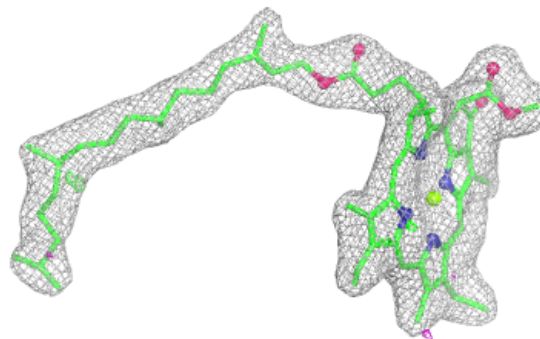
**Electron density around CLA B 608:**

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

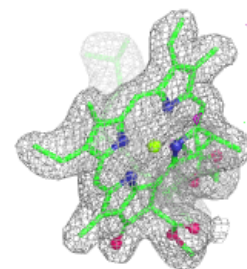
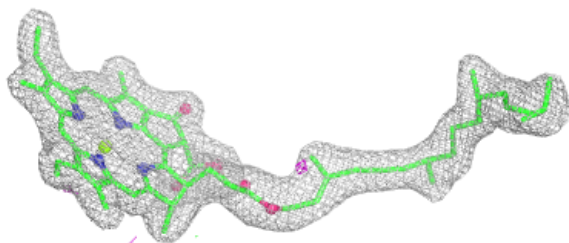
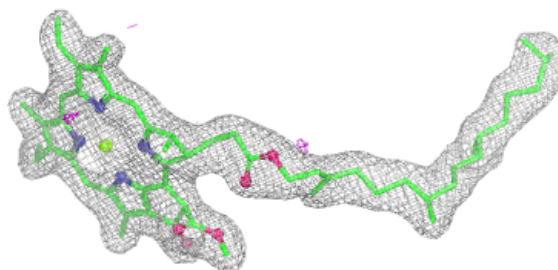


Electron density around CLA B 609:

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

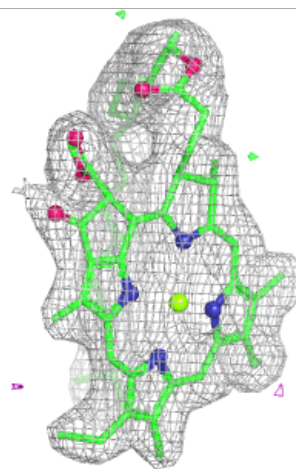
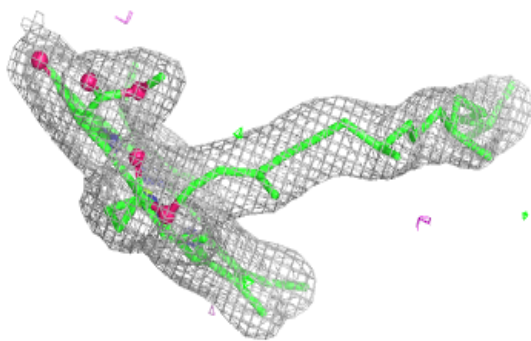
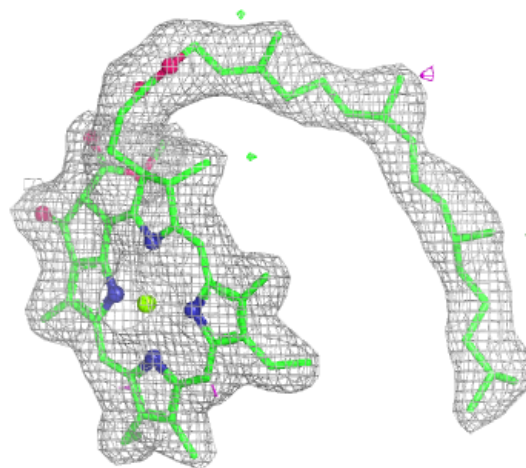
**Electron density around CLA A 607:**

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



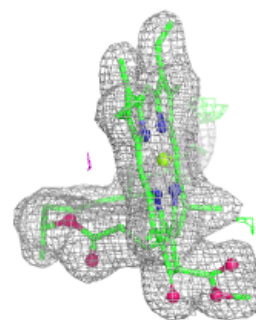
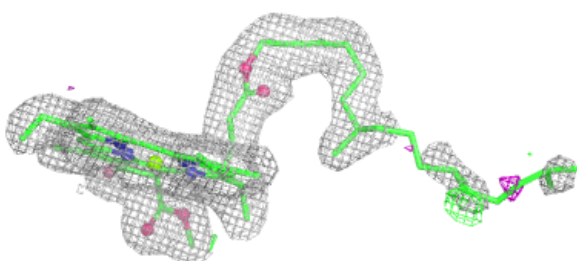
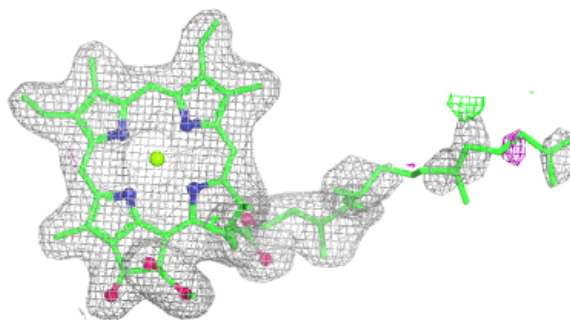
Electron density around CLA C 507:

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

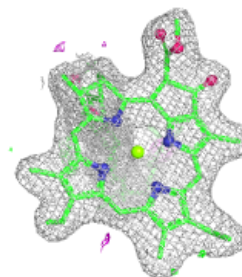
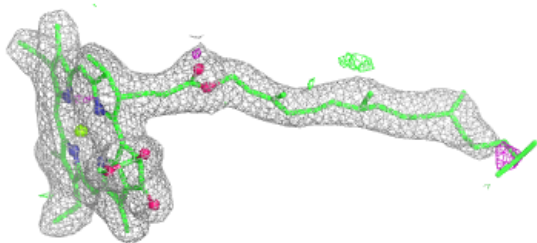
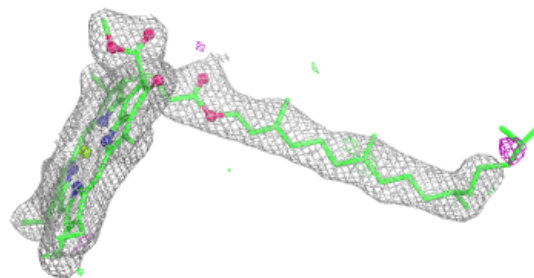


Electron density around CLA A 608:

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

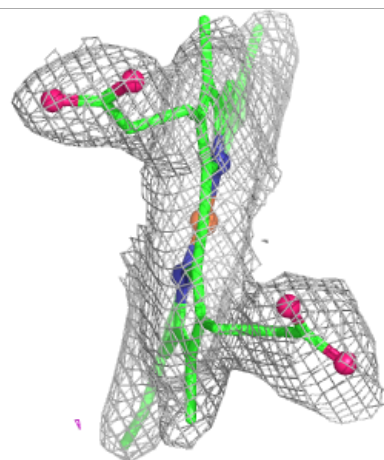
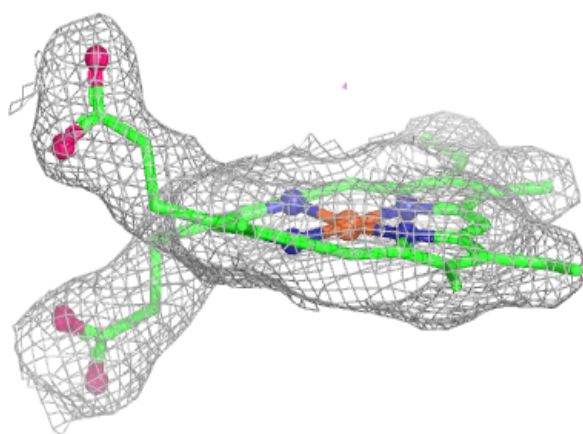
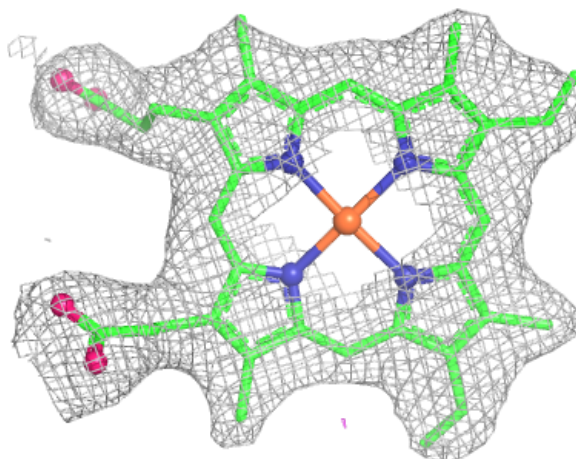
**Electron density around CLA b 604:**

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



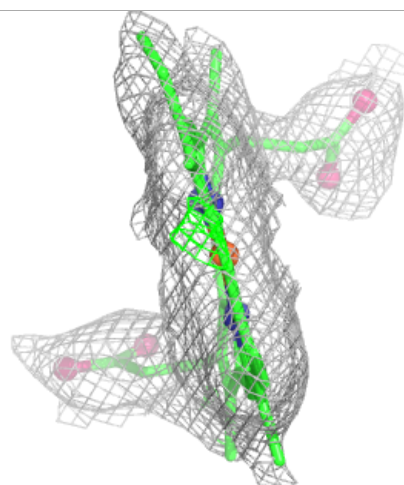
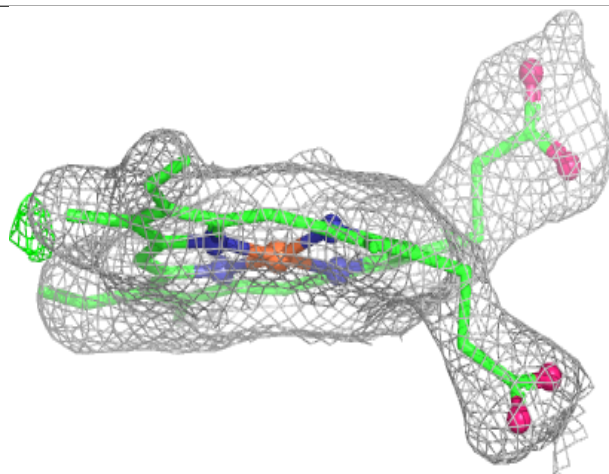
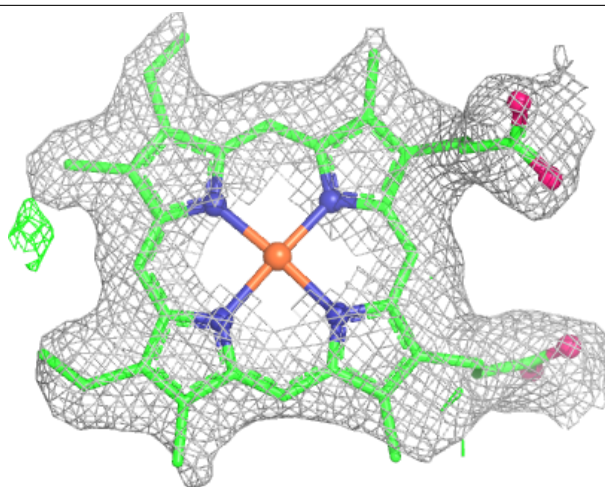
Electron density around HEM F 101:

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



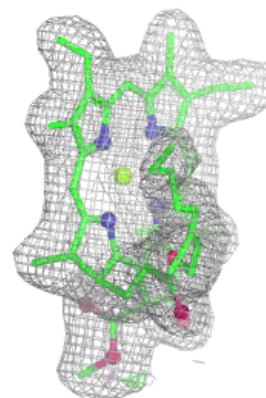
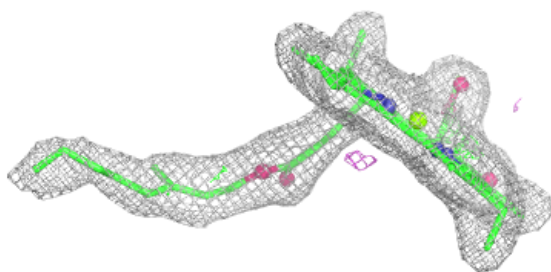
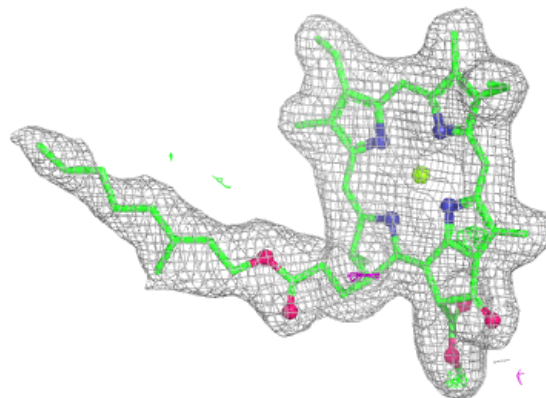
Electron density around HEM e 102:

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



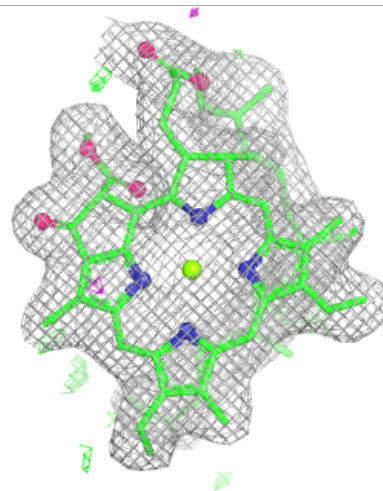
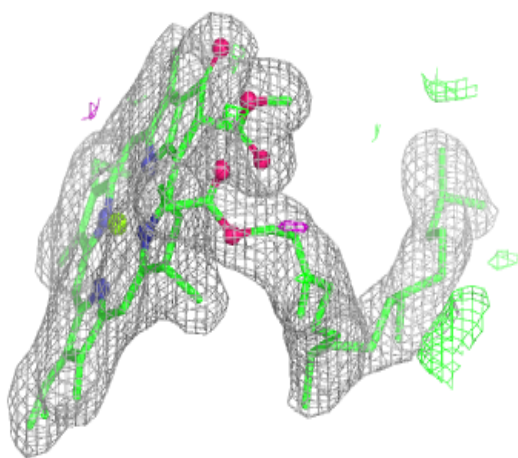
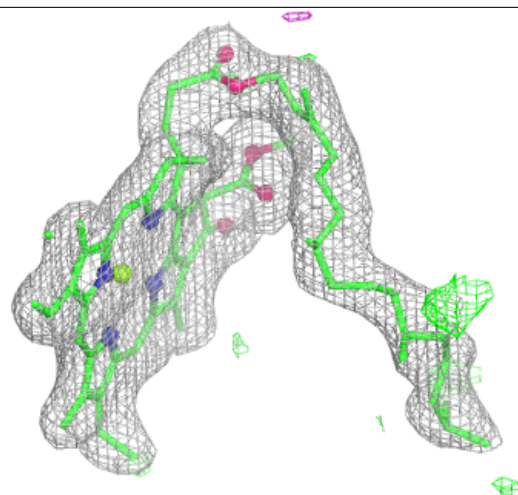
Electron density around CLA A 610:

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



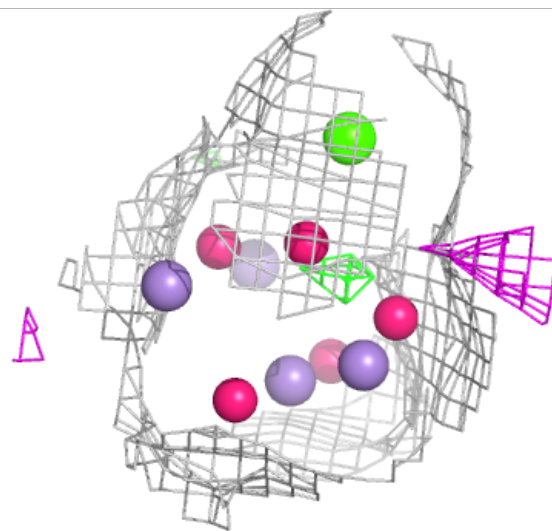
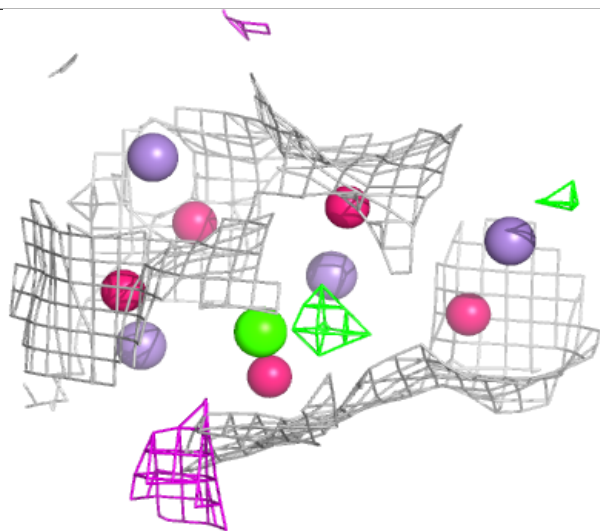
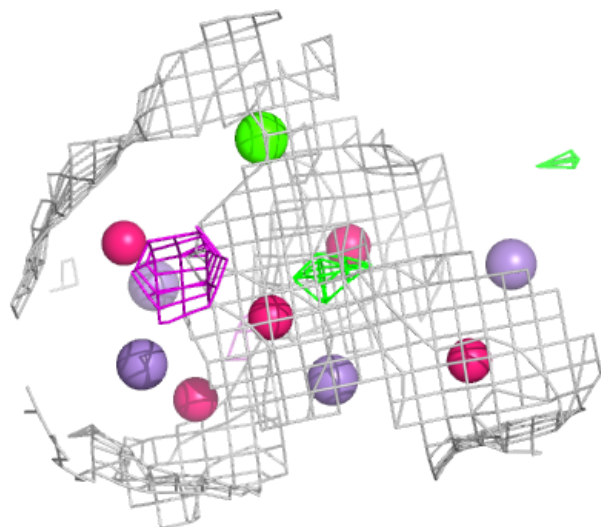
Electron density around CLA B 613:

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



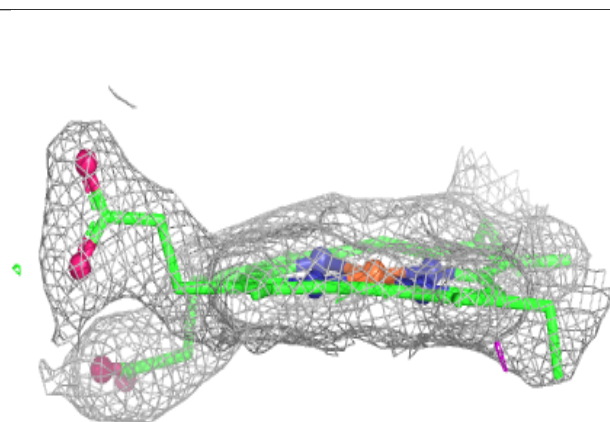
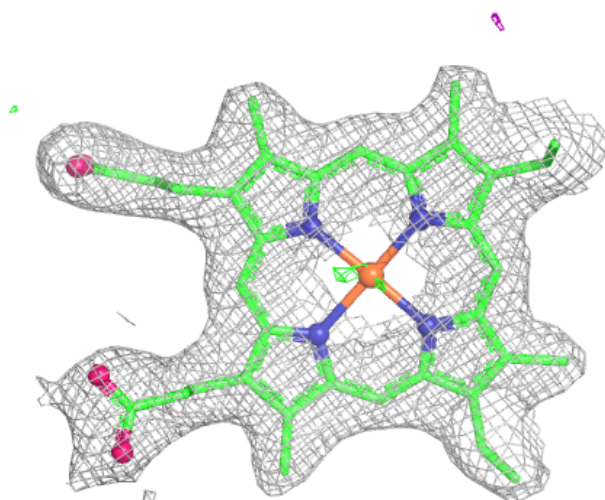
Electron density around OEX a 602 (A):

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



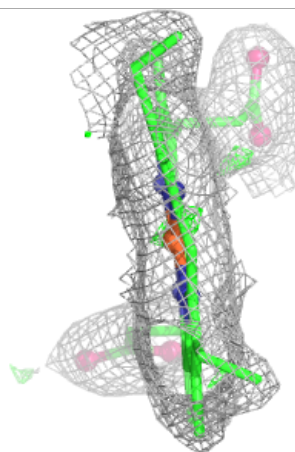
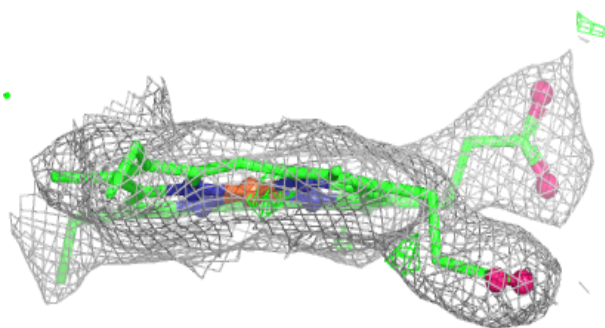
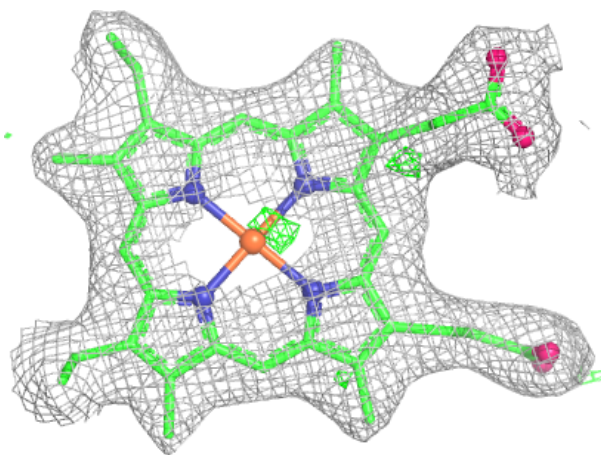
Electron density around HEC V 201:

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



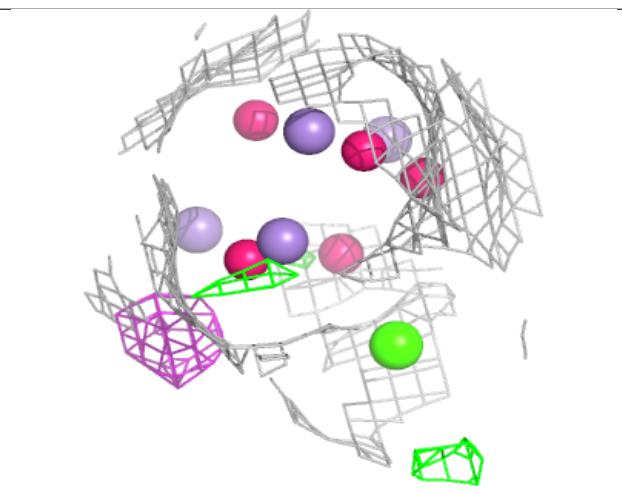
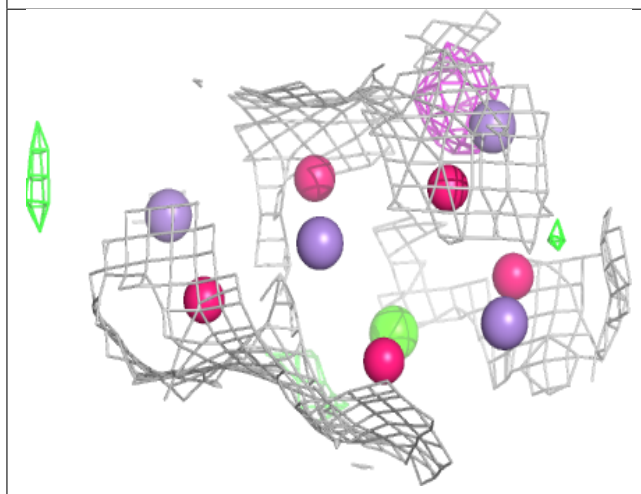
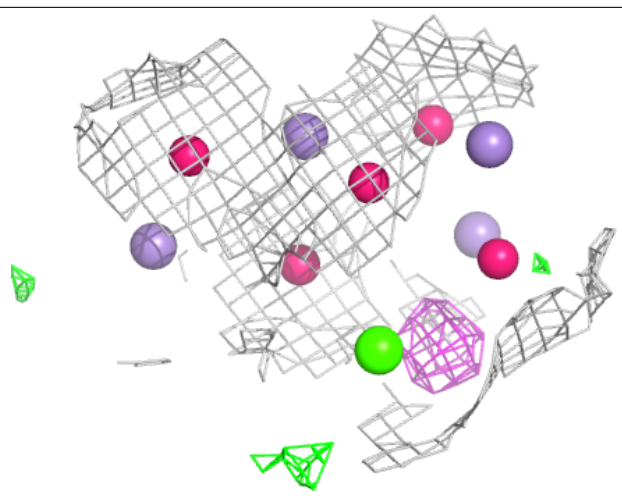
Electron density around HEC v 201:

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



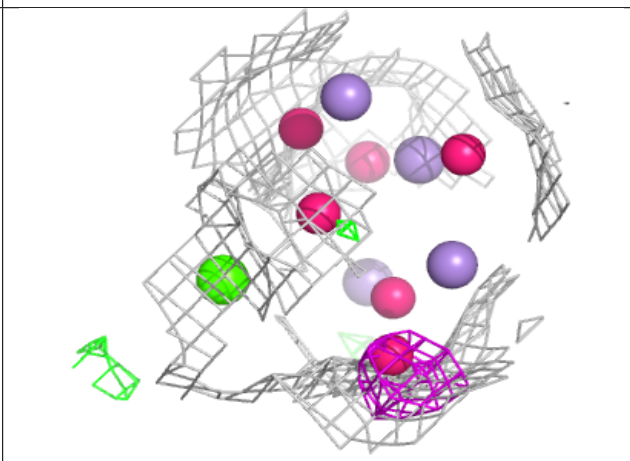
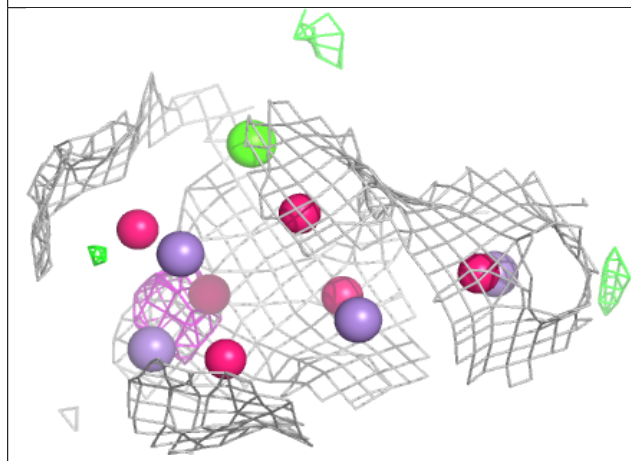
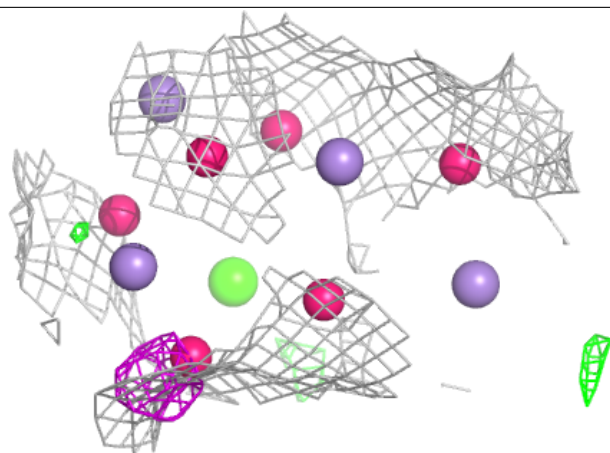
Electron density around OEX A 602 (A):

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



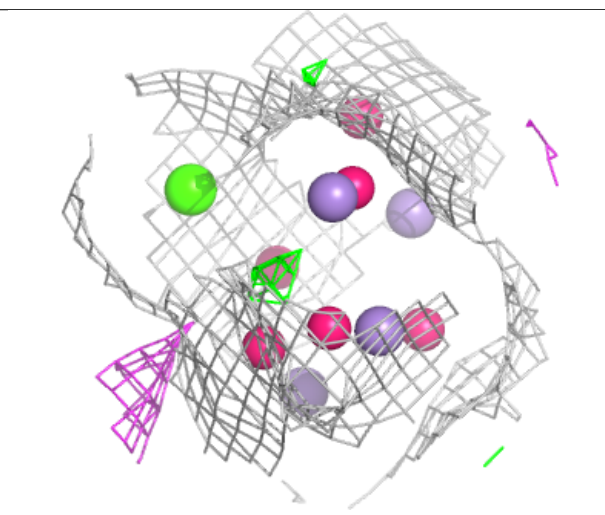
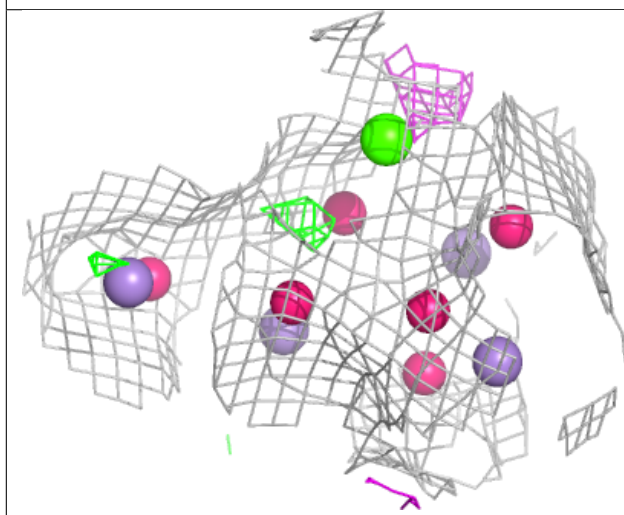
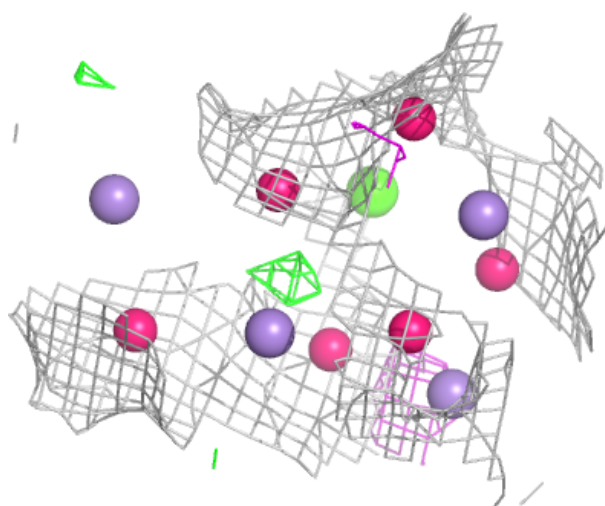
Electron density around OEY A 601 (B):

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



Electron density around OEY a 601 (B):

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



6.5 Other polymers [i](#)

There are no such residues in this entry.