



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2026 – 02:54 PM EDT

PDB ID : 9Z6A / pdb_00009z6a
Title : RT XFEL structure of the two-flash state of Photosystem II (2F, S3 rich) at 1.93 Angstrom obtained from conventional data at 9.5 keV
Authors : Bhowmick, A.; Kern, J.; Yano, J.; Yachandra, V.K.; Minnetian, N.M.; Zhang, M.
Deposited on : 2025-11-14
Resolution : 1.93 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

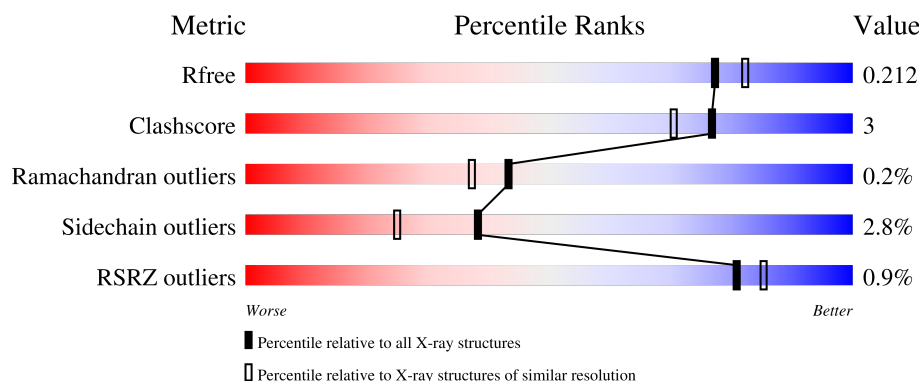
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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.



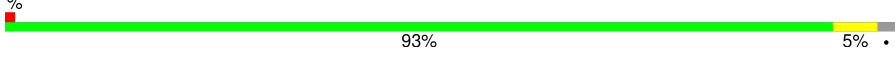
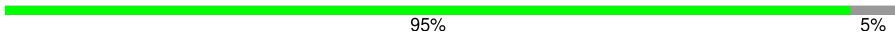
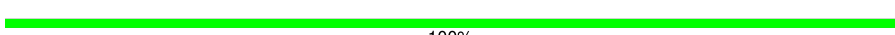
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	92% 6% .
1	a	344	89% 7% ..
2	B	510	95% . .
2	b	510	% 95% 5% .

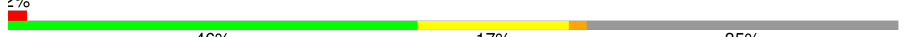
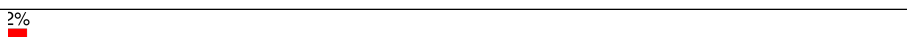
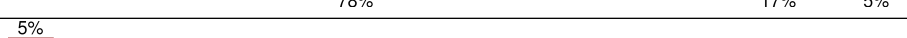
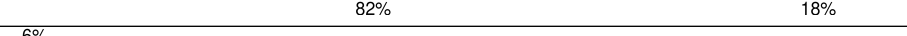
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Mol	Chain	Length	Quality of chain
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	

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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 107900 atoms, of which 53180 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	H	N	O	S	0	72	0
			6074	2055	2922	520	558	19			
1	a	334	Total	C	H	N	O	S	0	72	0
			6062	2052	2913	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	H	N	O	S	0	7	0
			7903	2637	3887	670	696	13			
2	b	505	Total	C	H	N	O	S	0	1	0
			7826	2614	3842	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	H	N	O	S	0	14	0
			6925	2302	3416	586	607	14			
3	c	451	Total	C	H	N	O	S	0	14	0
			7070	2343	3487	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	H	N	O	S	0	11	0
			5509	1859	2704	456	478	12			
4	d	341	Total	C	H	N	O	S	0	12	0
			5521	1863	2710	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	H	N	O	0	1	0
			1317	436	651	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1312	434	648	108	122			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	H	N	O	0	0	0
			557	187	282	45	42			
6	f	34	Total	C	H	N	O	0	0	0
			557	187	282	45	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	H	N	O	0	0	0
			1033	335	528	82	85			
7	h	63	Total	C	H	N	O	0	0	0
			1007	327	514	80	83			

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	H	N	O	0	0	0
			607	200	311	46	49			
8	i	36	Total	C	H	N	O	0	0	0
			607	200	311	46	49			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	H	N	O	0	0	0
			525	174	268	40	42			
9	j	36	Total	C	H	N	O	0	0	0
			525	174	268	40	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			
10	k	37	Total	C	H	N	O	0	0	0
			598	204	305	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	H	N	O	S	0	0	0
			620	202	316	48	53	1			
11	l	36	Total	C	H	N	O		0	0	0
			600	197	304	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	H	N	O	S	0	0	0
			523	171	267	37	47	1			
12	m	32	Total	C	H	N	O	S	0	0	0
			518	168	267	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	H	N	O	S	0	1	0
			3700	1168	1830	313	385	4			
13	o	244	Total	C	H	N	O	S	0	0	0
			3720	1170	1846	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	H	N	O	S	0	0	0
			519	181	261	36	39	2			
14	t	30	Total	C	H	N	O	S	0	0	0
			512	180	256	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	H	N	O	0	0	0
			1547	491	773	129	154			
15	u	97	Total	C	H	N	O	0	0	0
			1547	491	773	129	154			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
16	V	137	Total	C	H	N	O	S	0	0	0
			2135	675	1071	177	208	4			
16	v	137	Total	C	H	N	O	S	0	0	0
			2135	675	1071	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	H	N	O	S	0	0	0
			413	128	217	35	30	3			
17	y	30	Total	C	H	N	O	S	0	0	0
			459	144	241	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	H	N	O	0	0	0
			593	188	312	45	48			
18	x	39	Total	C	H	N	O	0	0	0
			602	191	316	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	H	N	O	S	0	0	0
			995	328	516	72	77	2			
19	z	62	Total	C	H	N	O	S	0	0	0
			986	326	509	72	77	2			

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

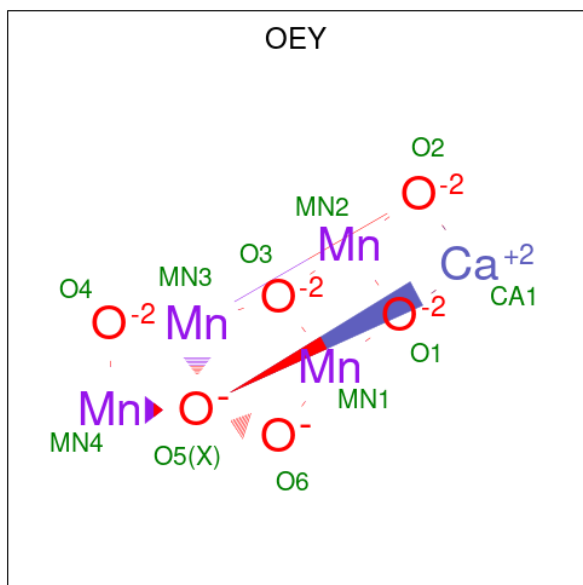
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	28	Total	C	H	N	O	0	0	0
			459	151	238	38	32			

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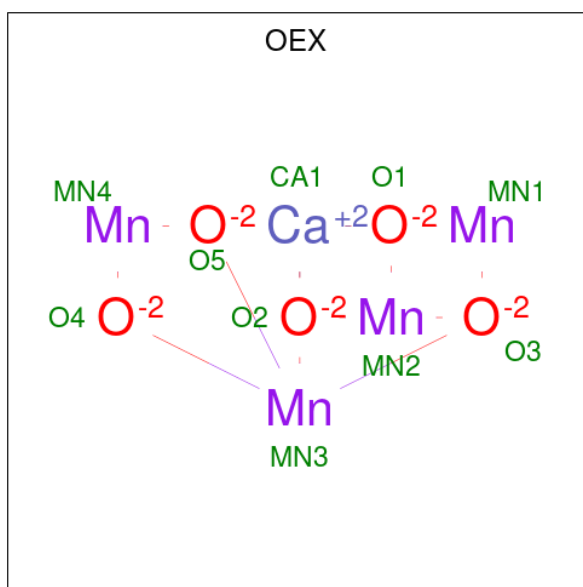
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	r	28	Total	C	H	N	O	0	0	0
			459	151	238	38	32			

- 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		

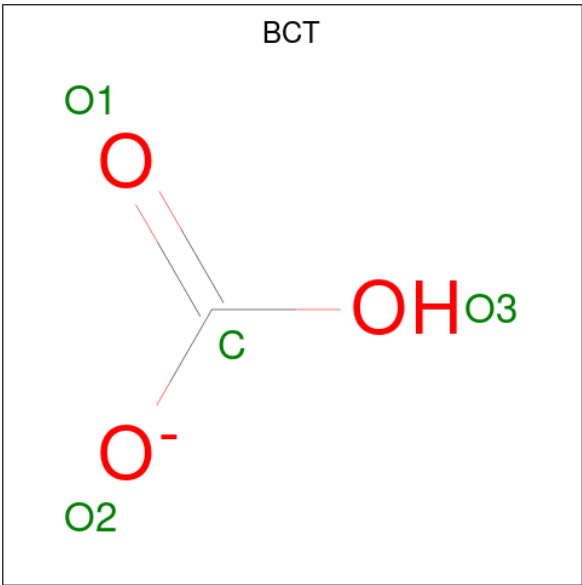
- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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).

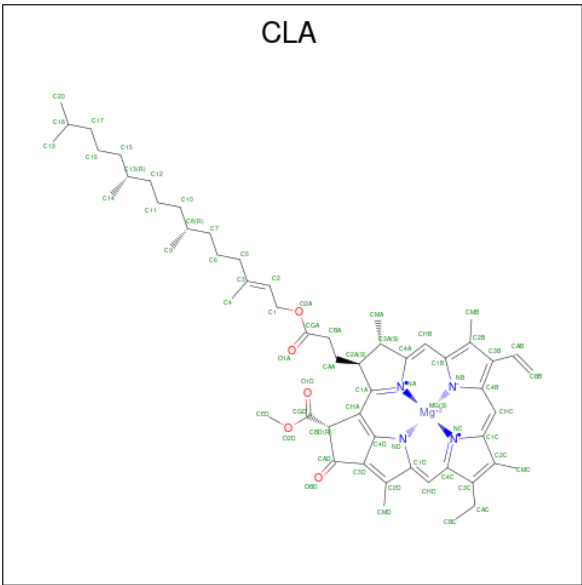
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	2	Total	Cl	0	0
			2	2		
24	a	2	Total	Cl	0	0
			2	2		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	H	O	0	0
			5	1	1	3		
25	a	1	Total	C	H	O	0	0
			5	1	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	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
26	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
26	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
26	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
26	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
26	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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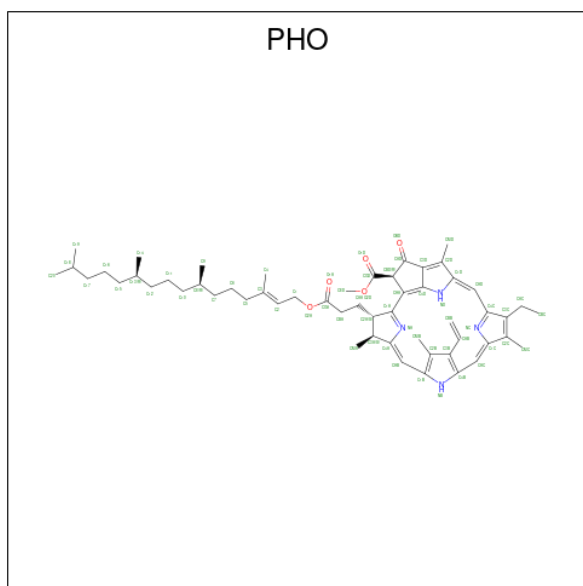
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
26	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
26	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	c	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
26	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	c	1	Total	C	H	Mg	N	O	0	0
			132	54	68	1	4	5		
26	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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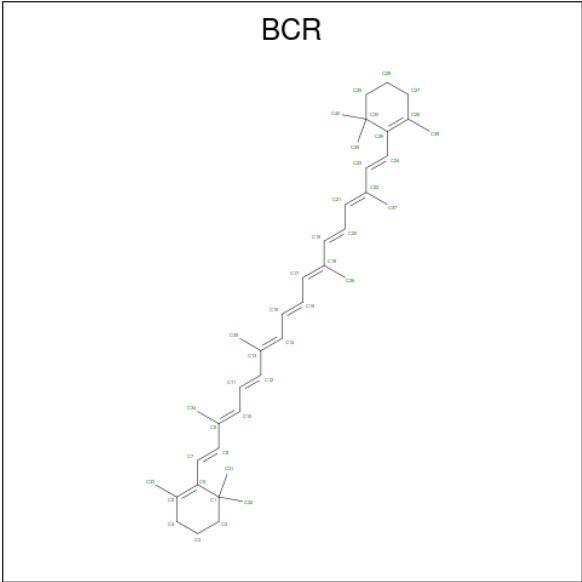
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
26	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- 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	H	N	O	0	0
			138	55	74	4	5		
27	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
27	a	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
27	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

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



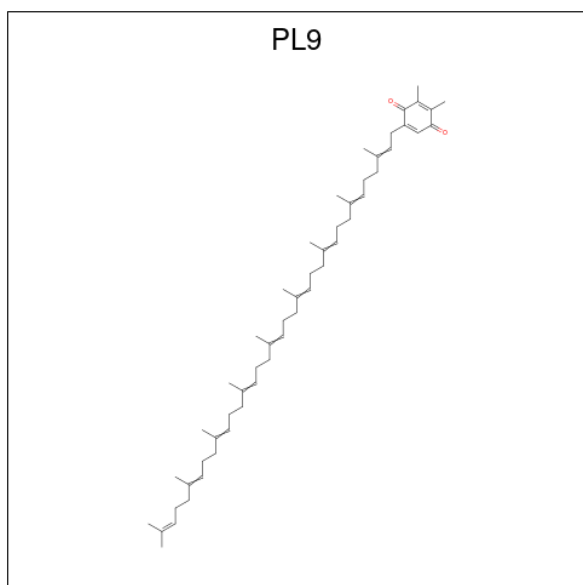
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	H	0	0
			96	40	56		
28	B	1	Total	C	H	0	0
			96	40	56		
28	B	1	Total	C	H	0	0
			96	40	56		
28	B	1	Total	C	H	0	0
			96	40	56		
28	C	1	Total	C	H	0	0
			96	40	56		
28	C	1	Total	C	H	0	0
			96	40	56		
28	D	1	Total	C	H	0	0
			96	40	56		
28	H	1	Total	C	H	0	0
			96	40	56		
28	K	1	Total	C	H	0	0
			96	40	56		
28	T	1	Total	C	H	0	0
			96	40	56		
28	Z	1	Total	C	H	0	0
			96	40	56		
28	a	1	Total	C	H	0	0
			96	40	56		
28	b	1	Total	C	H	0	0
			96	40	56		
28	b	1	Total	C	H	0	0
			96	40	56		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	b	1	Total	C	H	0	0
			96	40	56		
28	c	1	Total	C	H	0	0
			96	40	56		
28	c	1	Total	C	H	0	0
			96	40	56		
28	d	1	Total	C	H	0	0
			96	40	56		
28	k	1	Total	C	H	0	0
			96	40	56		
28	k	1	Total	C	H	0	0
			96	40	56		
28	t	1	Total	C	H	0	0
			96	40	56		
28	x	1	Total	C	H	0	0
			96	40	56		

- 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).



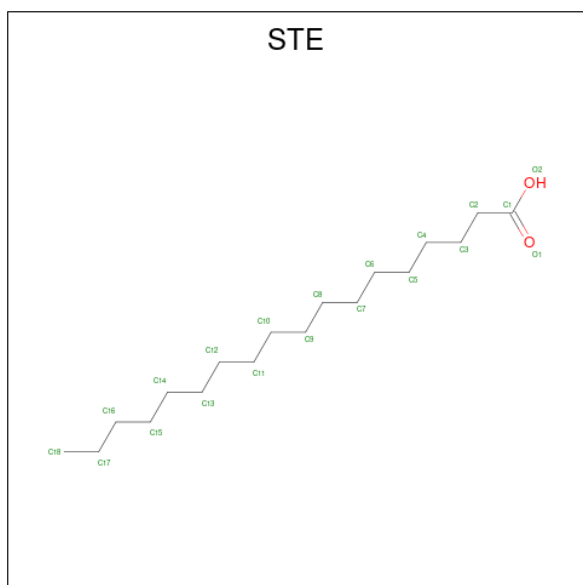
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			135	53	80	2		
29	D	1	Total	C	H	O	0	0
			135	53	80	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	a	1	Total	C	H	O	0	0
			135	53	80	2		
29	d	1	Total	C	H	O	0	0
			135	53	80	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	H		0	0
			23	9	14			
30	A	1	Total	C	H		0	0
			23	8	15			
30	A	1	Total	C	H		0	0
			50	17	33			
30	A	1	Total	C	H		0	0
			32	11	21			
30	B	1	Total	C	H	O	0	0
			43	15	26	2		
30	B	1	Total	C	H	O	0	0
			34	12	20	2		
30	B	1	Total	C	H	O	0	0
			46	16	28	2		
30	B	1	Total	C	H	O	0	0
			28	10	16	2		
30	B	1	Total	C	H		0	0
			41	15	26			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	C	1	Total C H O 34 12 20 2	0	0
30	C	1	Total C H 11 5 6	0	0
30	C	1	Total C H 17 7 10	0	0
30	C	1	Total C H 26 10 16	0	0
30	C	1	Total C H O 28 10 16 2	0	0
30	C	1	Total C H 47 16 31	0	0
30	C	1	Total C H 41 14 27	0	0
30	D	1	Total C H O 55 18 35 2	0	0
30	E	1	Total C H O 28 10 16 2	0	0
30	E	1	Total C H 35 12 23	0	0
30	E	1	Total C H O 55 18 35 2	0	0
30	H	1	Total C H 53 18 35	0	0
30	H	1	Total C H 26 9 17	0	0
30	I	1	Total C H O 43 15 26 2	0	0
30	I	1	Total C H O 37 13 22 2	0	0
30	J	1	Total C H O 28 10 16 2	0	0
30	K	1	Total C H 41 14 27	0	0
30	M	1	Total C H O 37 13 22 2	0	0
30	M	1	Total C H 26 10 16	0	0
30	T	1	Total C H 47 16 31	0	0
30	T	1	Total C H 44 15 29	0	0

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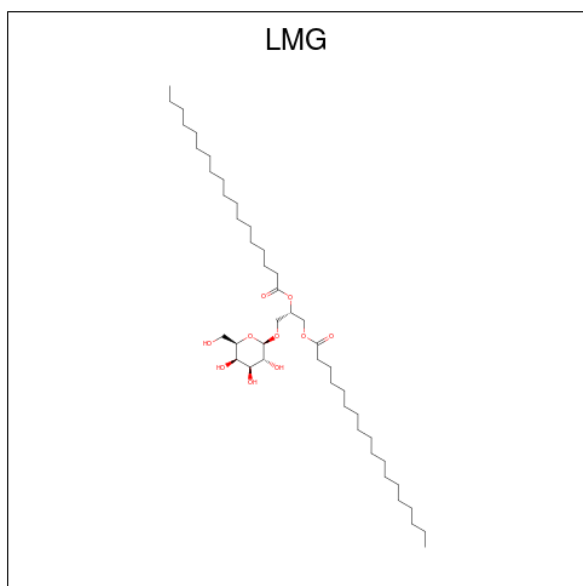
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	Z	1	Total C H 50 17 33	0	0
30	a	1	Total C H O 28 10 16 2	0	0
30	b	1	Total C H O 55 18 35 2	0	0
30	b	1	Total C H O 40 14 24 2	0	0
30	b	1	Total C H 26 10 16	0	0
30	b	1	Total C H 32 11 21	0	0
30	c	1	Total C H 53 18 35	0	0
30	d	1	Total C H O 55 18 35 2	0	0
30	d	1	Total C H O 55 18 35 2	0	0
30	d	1	Total C H O 55 18 35 2	0	0
30	e	1	Total C H 26 9 17	0	0
30	e	1	Total C H 23 8 15	0	0
30	e	1	Total C H 26 9 17	0	0
30	e	1	Total C H O 31 11 18 2	0	0
30	h	1	Total C H 29 10 19	0	0
30	i	1	Total C H O 28 10 16 2	0	0
30	i	1	Total C H 14 6 8	0	0
30	j	1	Total C H O 28 10 16 2	0	0
30	j	1	Total C H 47 16 31	0	0
30	k	1	Total C H O 34 12 20 2	0	0
30	m	1	Total C H O 28 10 16 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	m	1	Total	C	H	0	0
			53	18	35		
30	t	1	Total	C	H	0	0
			26	10	16		
30	z	1	Total	C	H	0	0
			35	13	22		
30	z	1	Total	C	H	0	0
			23	9	14		

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



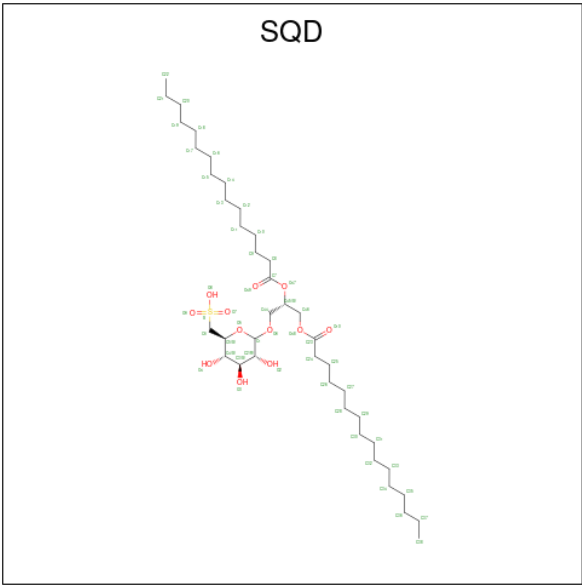
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	H	O	0	0
			114	38	66	10		
31	B	1	Total	C	H	O	0	0
			105	35	60	10		
31	C	1	Total	C	H	O	0	0
			76	26	40	10		
31	C	1	Total	C	H	O	0	0
			114	38	66	10		
31	D	1	Total	C	H	O	0	0
			120	40	70	10		
31	D	1	Total	C	H	O	0	0
			123	41	72	10		
31	M	1	Total	C	H	O	0	0
			123	41	72	10		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	a	1	Total	C	H	O	0	0
			141	45	86	10		
31	a	1	Total	C	H	O	0	0
			117	39	68	10		
31	b	1	Total	C	H	O	0	0
			141	45	86	10		
31	c	1	Total	C	H	O	0	0
			71	25	41	5		
31	c	1	Total	C	H	O	0	0
			108	36	62	10		
31	c	1	Total	C	H	O	0	0
			117	38	69	10		
31	d	1	Total	C	H	O	0	0
			102	34	58	10		
31	m	1	Total	C	H	O	0	0
			123	41	72	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).



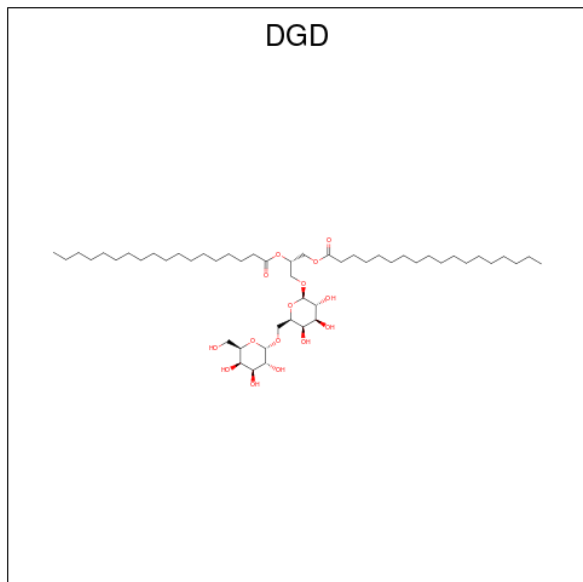
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
32	A	1	Total	C	H	O	S	0	0
			95	30	52	12	1		
32	B	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
32	D	1	Total	C	H	O	S	0	0
			122	39	70	12	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
32	F	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
32	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
32	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
32	b	1	Total	C	H	O	S	0	0
			113	36	64	12	1		
32	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



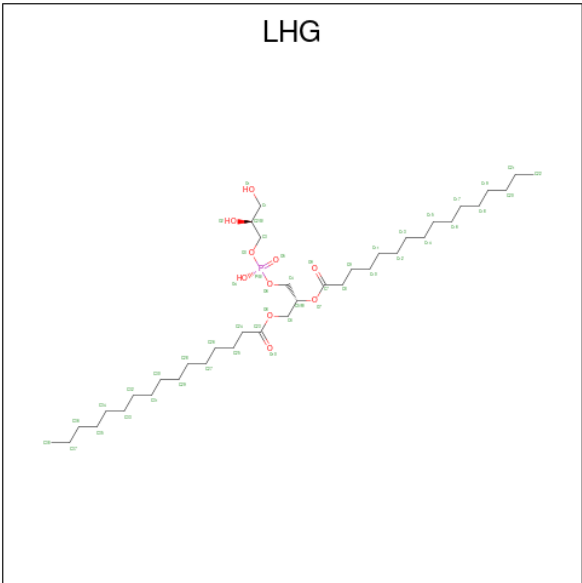
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	A	1	Total	C	H	O	0	0
			150	51	84	15		
33	C	1	Total	C	H	O	0	0
			132	47	70	15		
33	C	1	Total	C	H	O	0	0
			132	47	70	15		
33	C	1	Total	C	H	O	0	0
			132	47	70	15		
33	H	1	Total	C	H	O	0	0
			132	47	70	15		
33	c	1	Total	C	H	O	0	0
			132	47	70	15		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	c	1	Total	C	H	O	0	0
			132	47	70	15		
33	c	1	Total	C	H	O	0	0
			132	47	70	15		
33	h	1	Total	C	H	O	0	0
			132	47	70	15		

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



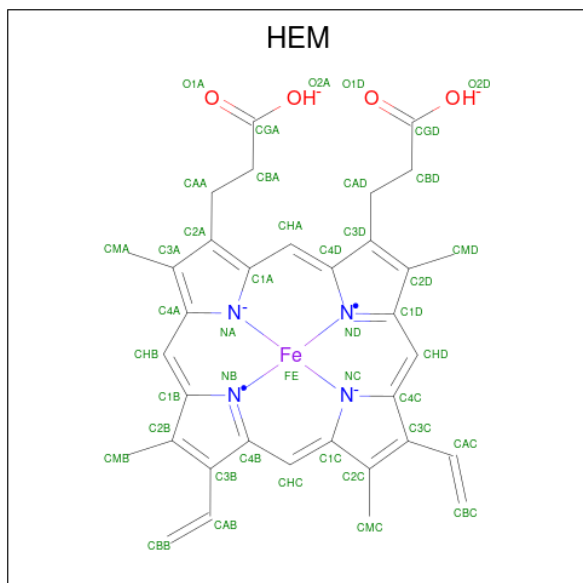
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
34	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
34	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
34	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
34	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
34	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
34	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
34	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
34	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		

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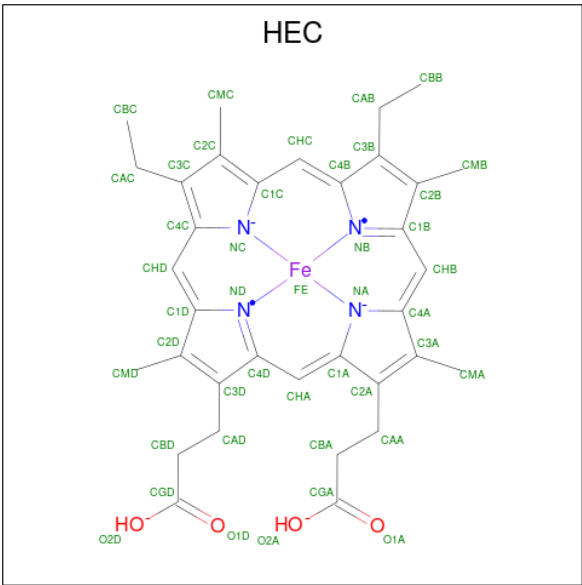
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
34	e	1	Total	C	H	O	P	0	0
			99	31	57	10	1		
34	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	F	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
35	f	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
36	V	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
36	v	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	178	Total	O	0	4
			182	182		
37	B	319	Total	O	0	0
			319	319		
37	C	254	Total	O	0	0
			254	254		
37	D	159	Total	O	0	0
			159	159		
37	E	42	Total	O	0	0
			42	42		
37	F	20	Total	O	0	0
			20	20		
37	H	41	Total	O	0	0
			41	41		
37	I	17	Total	O	0	0
			17	17		
37	J	11	Total	O	0	0
			11	11		
37	K	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	L	11	Total 11	O 11	0	0
37	M	13	Total 13	O 13	0	0
37	O	149	Total 149	O 149	0	0
37	T	13	Total 13	O 13	0	0
37	U	67	Total 67	O 67	0	0
37	V	96	Total 96	O 96	0	0
37	Y	9	Total 9	O 9	0	0
37	X	14	Total 14	O 14	0	0
37	Z	8	Total 8	O 8	0	0
37	R	1	Total 1	O 1	0	0
37	a	144	Total 148	O 148	0	4
37	b	280	Total 280	O 280	0	0
37	c	228	Total 228	O 228	0	0
37	d	171	Total 171	O 171	0	0
37	e	25	Total 25	O 25	0	0
37	f	14	Total 14	O 14	0	0
37	h	33	Total 33	O 33	0	0
37	i	12	Total 12	O 12	0	0
37	j	8	Total 8	O 8	0	0
37	k	11	Total 11	O 11	0	0
37	l	14	Total 14	O 14	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	m	17	Total 17	O 17	0	0
37	o	159	Total 159	O 159	0	0
37	t	16	Total 16	O 16	0	0
37	u	89	Total 89	O 89	0	0
37	v	77	Total 77	O 77	0	0
37	y	6	Total 6	O 6	0	0
37	x	11	Total 11	O 11	0	0
37	z	8	Total 8	O 8	0	0
37	r	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

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

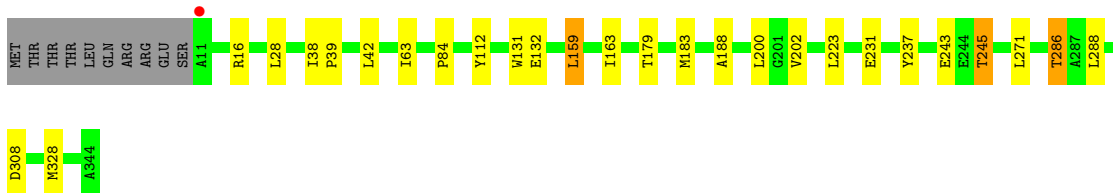
- Molecule 1: Photosystem II protein D1 1

Chain A: 

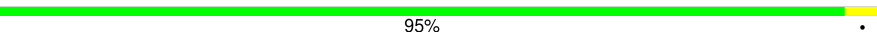


- Molecule 1: Photosystem II protein D1 1

Chain a: 

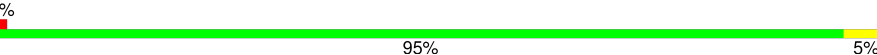


- Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 



- Molecule 2: Photosystem II CP47 reaction center protein

Chain b: 



- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 



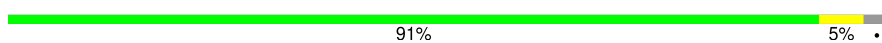
D473

- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  93% 5%

MET VAL THR LEU SER SER ASN SER ILE PHE A23 T24 L42 L72 L95 V99 V124 L125 L134 L165 G169 I170 M180 L240 L279 A286 E308 K315 L318 T335 E354 F361 S406 E413 S416 V420 D473

- Molecule 4: Photosystem II D2 protein

Chain D:  91% 5%

MET THR ILE ALA ILE GLY ARG ALA PRO ILE ALA GLU R12 Y42 I123 V136 A148 P149 A170 P171 S172 A177 N194 L209 I213 Y244 W253 K264 L267 L272 L279 S295 L352

- Molecule 4: Photosystem II D2 protein

Chain d:  89% 8%

MET THR ILE ALA ILE GLY ARG ALA PRO ILE ALA GLU R12 R24 Y42 L45 L90 R103 M126 A143 A148 P149 S172 A177 I178 F179 L182 Q186 W191 T192 L193 N194 L209 L210 L213 L259 L267 L272 L289 A290 L291 R292

L293 R294 S295 E307 L321 L352

- Molecule 5: Cytochrome b559 subunit alpha

Chain E:  87% 11%

MET ALA G3 V17 R18 V21 I22 I27 P28 Q60 D68 A72 F79 K84

- Molecule 5: Cytochrome b559 subunit alpha

Chain e:  89% 8%

MET ALA G3 L30 R61 S62 I63 V66 T67 D68 A72 F79 L83 K84

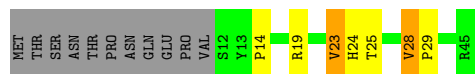
- Molecule 6: Cytochrome b559 subunit beta

Chain F:  67% 9% 24%

MET THR SER ASN PRO THR ASN GLN PRO VAL S12 A22 T25 V28 P29 R45

- Molecule 6: Cytochrome b559 subunit beta

Chain f:  60% 11% 24%



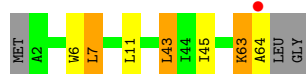
- Molecule 7: Photosystem II reaction center protein H

Chain H:  91% 8%



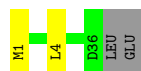
- Molecule 7: Photosystem II reaction center protein H

Chain h:  2% 85% 6% 5% 5%

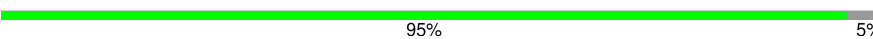


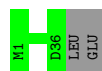
- Molecule 8: Photosystem II reaction center protein I

Chain I:  89% 5% 5%



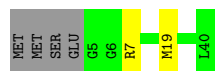
- Molecule 8: Photosystem II reaction center protein I

Chain i:  95% 5%



- Molecule 9: Photosystem II reaction center protein J

Chain J:  85% 5% 10%



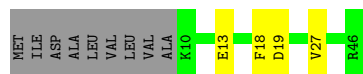
- Molecule 9: Photosystem II reaction center protein J

Chain j:  2% 80% 10% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain K:  72% 9% 20%

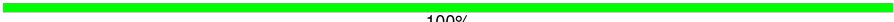


- Molecule 10: Photosystem II reaction center protein K

Chain k:  63% 17% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  100%

There are no outlier residues recorded for this chain.

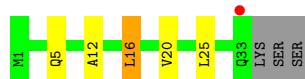
- Molecule 11: Photosystem II reaction center protein L

Chain l:  86% 11% •



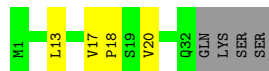
- Molecule 12: Photosystem II reaction center protein M

Chain M:  3% 78% 11% • 8%



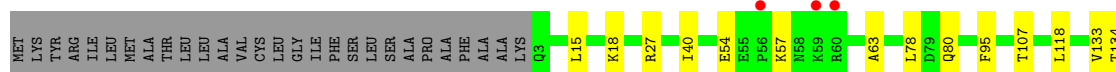
- Molecule 12: Photosystem II reaction center protein M

Chain m:  78% 11% 11%



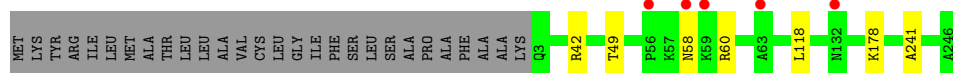
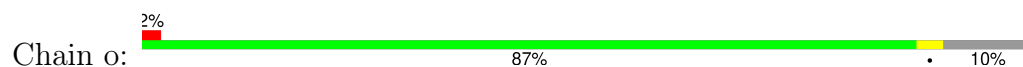
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  83% 7% 10%

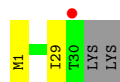
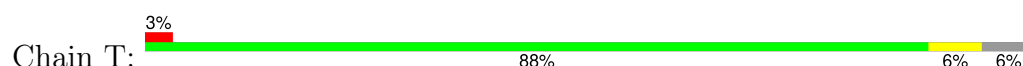




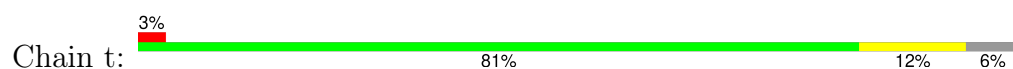
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



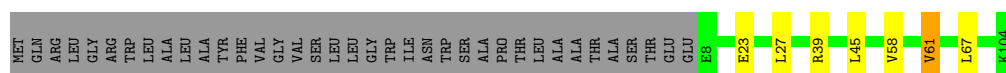
- Molecule 14: Photosystem II reaction center protein T



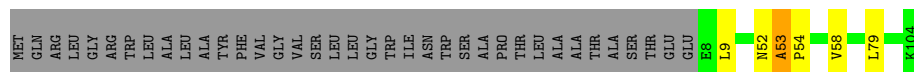
- Molecule 14: Photosystem II reaction center protein T



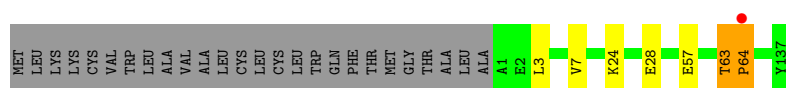
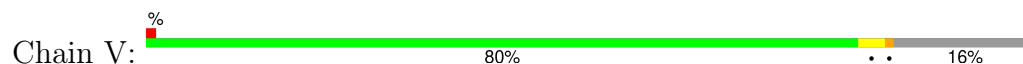
- Molecule 15: Photosystem II 12 kDa extrinsic protein



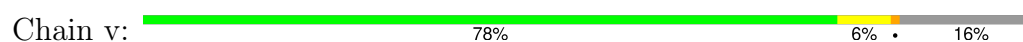
- Molecule 15: Photosystem II 12 kDa extrinsic protein

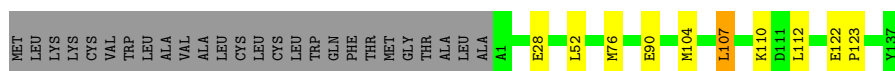


- Molecule 16: Cytochrome c-550

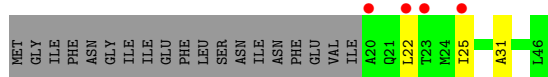


- Molecule 16: Cytochrome c-550

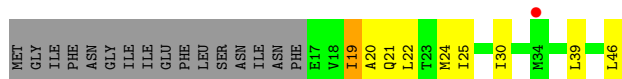




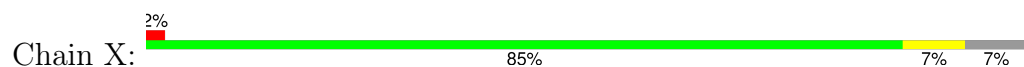
- Molecule 17: Photosystem II reaction center protein Ycf12



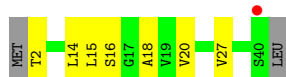
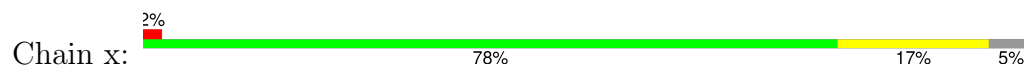
- Molecule 17: Photosystem II reaction center protein Ycf12



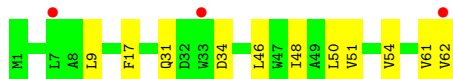
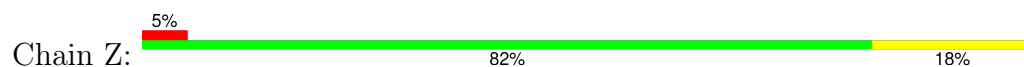
- Molecule 18: Photosystem II reaction center X protein



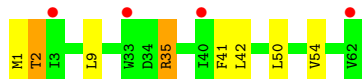
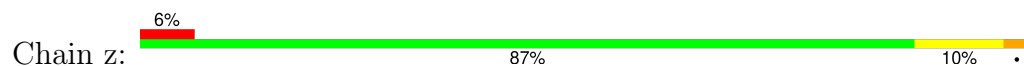
- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Z



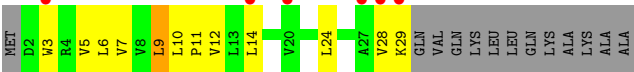
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



● Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.53Å 222.82Å 308.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.83 – 1.93 33.83 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.4 (33.83-1.93) 86.0 (33.83-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.39 (at 1.94Å)	Xtriage
Refinement program	PHENIX 2.0_5848	Depositor
R, R_{free}	0.175 , 0.212 0.175 , 0.212	Depositor DCC
R_{free} test set	5354 reflections (0.85%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	107900	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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: BCT, LMG, DGD, PHO, HEC, PL9, FME, CLA, OEX, BCR, STE, OEY, HEM, LHG, FE2, CL, SQD

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	0.21	0/3275	0.43	0/4462
1	a	0.20	0/3272	0.44	0/4458
2	B	0.20	0/4179	0.42	0/5693
2	b	0.20	0/4127	0.41	0/5623
3	C	0.20	0/3647	0.41	0/4965
3	c	0.18	0/3719	0.39	0/5061
4	D	0.22	0/2910	0.44	0/3962
4	d	0.19	0/2919	0.43	0/3974
5	E	0.18	0/688	0.37	0/940
5	e	0.16	0/683	0.36	0/932
6	F	0.19	0/284	0.37	0/387
6	f	0.17	0/284	0.41	0/387
7	H	0.19	0/517	0.40	0/705
7	h	0.17	0/505	0.38	0/689
8	I	0.18	0/293	0.40	0/396
8	i	0.19	0/293	0.34	0/396
9	J	0.16	0/263	0.34	0/356
9	j	0.15	0/263	0.35	0/356
10	K	0.16	0/303	0.35	0/416
10	k	0.15	0/303	0.36	0/416
11	L	0.22	0/311	0.39	0/422
11	l	0.20	0/303	0.41	0/412
12	M	0.20	0/249	0.43	0/341
12	m	0.21	0/244	0.42	0/334
13	O	0.21	0/1904	0.44	0/2585
13	o	0.20	0/1905	0.42	0/2583
14	T	0.20	0/257	0.45	0/349
14	t	0.21	0/255	0.45	0/346
15	U	0.19	0/785	0.39	0/1064
15	u	0.19	0/785	0.41	0/1064
16	V	0.20	0/1085	0.43	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.18	0/1085	0.36	0/1473
17	Y	0.17	0/197	0.31	0/264
17	y	0.15	0/219	0.36	0/294
18	X	0.16	0/284	0.32	0/384
18	x	0.15	0/289	0.30	0/391
19	Z	0.13	0/490	0.32	0/669
19	z	0.13	0/488	0.31	0/666
20	R	0.12	0/227	0.29	0/313
20	r	0.12	0/227	0.32	0/313
All	All	0.19	0/44316	0.41	0/60314

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3152	2922	2992	13	0
1	a	3149	2913	2983	17	0
2	B	4016	3887	3871	11	0
2	b	3984	3842	3842	19	0
3	C	3509	3416	3409	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3583	3487	3492	9	0
4	D	2805	2704	2692	14	0
4	d	2811	2710	2698	17	0
5	E	666	651	651	6	0
5	e	664	648	648	5	0
6	F	275	282	282	6	0
6	f	275	282	282	5	0
7	H	505	528	528	3	0
7	h	493	514	514	4	0
8	I	296	311	311	0	0
8	i	296	311	311	0	0
9	J	257	268	268	0	0
9	j	257	268	268	1	0
10	K	293	305	305	3	0
10	k	293	305	305	6	0
11	L	304	316	316	0	0
11	l	296	304	304	0	0
12	M	256	267	269	2	0
12	m	251	267	267	2	0
13	O	1870	1830	1830	11	0
13	o	1874	1846	1846	1	0
14	T	258	261	261	0	0
14	t	256	256	256	3	0
15	U	774	773	773	3	0
15	u	774	773	773	4	0
16	V	1064	1071	1073	4	0
16	v	1064	1071	1073	4	0
17	Y	196	217	217	3	0
17	y	218	241	241	8	0
18	X	281	312	312	4	0
18	x	286	316	314	4	0
19	Z	479	516	516	6	0
19	z	477	509	509	5	0
20	R	221	238	238	1	0
20	r	221	238	238	5	0
21	A	11	0	0	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	2	0	0	0	0
25	A	4	1	1	0	0
25	a	4	1	1	0	0
26	A	249	264	264	7	0
26	B	1035	1139	1139	18	0
26	C	839	922	922	11	0
26	D	130	144	144	0	0
26	a	260	288	288	4	0
26	b	1035	1139	1139	14	0
26	c	839	919	919	7	0
26	d	130	144	144	6	0
27	A	64	74	74	1	0
27	D	64	74	74	2	0
27	a	64	74	74	0	0
27	d	64	74	74	0	0
28	A	40	56	56	1	0
28	B	120	168	168	4	0
28	C	80	112	112	1	0
28	D	40	56	56	1	0
28	H	40	56	56	2	0
28	K	40	56	56	0	0
28	T	40	56	56	3	0
28	Z	40	56	56	2	0
28	a	40	56	56	2	0
28	b	120	168	168	3	0
28	c	80	112	112	0	0
28	d	40	56	56	0	0
28	k	80	112	112	4	0
28	t	40	56	56	5	0
28	x	40	56	56	3	0
29	A	55	80	80	2	0
29	D	55	80	80	0	0
29	a	55	80	80	3	0
29	d	55	80	80	0	0
30	A	45	83	83	1	0
30	B	76	116	116	0	0
30	C	78	126	126	2	0
30	D	20	35	35	3	0
30	E	44	74	74	1	0
30	H	27	52	52	3	0
30	I	32	48	48	2	0
30	J	12	16	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	K	14	27	27	1	0
30	M	25	38	38	0	0
30	T	31	60	60	0	0
30	Z	17	33	33	1	0
30	a	12	16	16	0	0
30	b	57	96	96	1	0
30	c	18	35	35	1	0
30	d	60	105	105	1	0
30	e	39	67	67	0	0
30	h	10	19	19	0	0
30	i	18	24	24	0	0
30	j	28	47	47	0	0
30	k	14	20	20	0	0
30	m	30	51	51	0	0
30	t	10	16	16	0	0
30	z	22	36	36	0	0
31	A	48	66	66	0	0
31	B	45	60	60	1	0
31	C	84	106	106	2	0
31	D	101	142	142	0	0
31	M	51	72	72	1	0
31	a	104	154	154	1	0
31	b	55	86	86	0	0
31	c	124	172	172	1	0
31	d	44	58	58	0	0
31	m	51	72	72	0	0
32	A	43	52	53	0	0
32	B	54	77	78	2	0
32	D	52	70	71	1	0
32	F	36	45	46	2	0
32	a	108	154	156	0	0
32	b	49	64	65	2	0
32	f	41	48	49	1	0
33	A	66	84	96	4	0
33	C	186	210	246	5	0
33	H	62	70	82	1	0
33	c	186	210	246	0	0
33	h	62	70	82	0	0
34	B	49	74	74	3	0
34	D	145	215	215	3	0
34	E	49	74	74	0	0
34	d	137	199	199	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	e	42	57	57	1	0
34	l	49	74	74	0	0
35	F	43	30	30	4	0
35	f	43	30	30	4	0
36	V	43	30	30	0	0
36	v	43	30	30	1	0
37	A	182	0	0	2	0
37	B	319	0	0	4	0
37	C	254	0	0	4	0
37	D	159	0	0	2	0
37	E	42	0	0	3	0
37	F	20	0	0	3	0
37	H	41	0	0	1	0
37	I	17	0	0	1	0
37	J	11	0	0	1	0
37	K	4	0	0	0	0
37	L	11	0	0	0	0
37	M	13	0	0	0	0
37	O	149	0	0	2	0
37	R	1	0	0	0	0
37	T	13	0	0	0	0
37	U	67	0	0	0	0
37	V	96	0	0	1	0
37	X	14	0	0	1	0
37	Y	9	0	0	1	0
37	Z	8	0	0	0	0
37	a	148	0	0	2	0
37	b	280	0	0	12	0
37	c	228	0	0	1	0
37	d	171	0	0	2	0
37	e	25	0	0	0	0
37	f	14	0	0	1	0
37	h	33	0	0	0	0
37	i	12	0	0	1	0
37	j	8	0	0	0	0
37	k	11	0	0	2	0
37	l	14	0	0	0	0
37	m	17	0	0	0	0
37	o	159	0	0	0	0
37	r	1	0	0	0	0
37	t	16	0	0	3	0
37	u	89	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	v	77	0	0	0	0
37	x	11	0	0	0	0
37	y	6	0	0	2	0
37	z	8	0	0	0	0
All	All	54720	53180	53398	305	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 3.

All (305) 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)
28:t:101:BCR:H363	37:t:201:HOH:O	1.70	0.91
28:t:101:BCR:HC8	28:t:101:BCR:H311	1.58	0.85
2:B:96:VAL:HG13	37:B:715:HOH:O	1.78	0.82
3:C:87:ILE:HD11	37:C:731:HOH:O	1.79	0.82
26:B:601:CLA:H41	30:H:103:STE:H183	1.62	0.81
28:B:618:BCR:H343	37:B:998:HOH:O	1.79	0.80
15:u:53:ALA:HB1	15:u:54:PRO:HD2	1.63	0.80
28:D:404:BCR:H392	28:D:404:BCR:H23C	1.67	0.76
35:F:101:HEM:HBC2	35:F:101:HEM:HHD	1.68	0.76
26:b:602:CLA:H43	7:h:45:ILE:HG22	1.67	0.75
30:H:103:STE:H181	37:H:241:HOH:O	1.86	0.74
21:a:601[B]:OEY:O6	21:a:601[B]:OEY:O5	2.06	0.74
33:A:617:DGD:HAG1	37:A:877:HOH:O	1.87	0.73
21:A:601[B]:OEY:O5	21:A:601[B]:OEY:O6	2.06	0.73
19:Z:17:PHE:CE2	28:Z:101:BCR:H322	2.25	0.71
26:B:601:CLA:H92	26:B:601:CLA:H42	1.74	0.70
26:B:604:CLA:H43	26:B:605:CLA:H2	1.74	0.70
2:b:278:SER:C	37:b:701:HOH:O	2.34	0.69
28:t:101:BCR:H23C	28:t:101:BCR:H382	1.75	0.69
28:Z:101:BCR:H321	28:Z:101:BCR:HC8	1.74	0.68
34:B:622:LHG:H383	31:M:101:LMG:C43	2.25	0.68
28:T:101:BCR:H382	28:T:101:BCR:H23C	1.75	0.67
35:f:101:HEM:HHD	35:f:101:HEM:HBC2	1.77	0.67
26:C:513:CLA:H201	30:C:519:STE:C2	2.23	0.67
5:e:30:LEU:HD23	20:r:12:VAL:HG12	1.76	0.67
16:V:63:THR:HG22	16:V:64:PRO:HD2	1.78	0.65
5:e:30:LEU:HD11	35:f:101:HEM:CBB	2.27	0.65
17:y:20:ALA:HB3	37:y:102:HOH:O	1.96	0.65
2:b:278:SER:O	37:b:701:HOH:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:58:VAL:O	15:U:61:VAL:HG22	1.96	0.64
10:k:22:VAL:HG12	10:k:22:VAL:O	1.98	0.63
16:v:76:MET:HE3	36:v:201:HEC:HBB3	1.79	0.63
26:C:509:CLA:HBB1	26:C:509:CLA:HMB1	1.81	0.62
26:B:601:CLA:C4	30:H:103:STE:H183	2.30	0.62
33:C:522:DGD:HA61	33:C:522:DGD:HAW1	1.81	0.62
6:f:24:HIS:O	6:f:28:VAL:HG13	1.99	0.62
4:d:267:LEU:C	4:d:267:LEU:HD23	2.26	0.61
10:k:22:VAL:C	37:k:201:HOH:O	2.43	0.61
26:c:505:CLA:H142	37:i:211:HOH:O	2.01	0.60
15:u:53:ALA:HB1	15:u:54:PRO:CD	2.31	0.60
17:y:39:LEU:HB3	17:y:46:LEU:HD21	1.84	0.60
1:a:237:TYR:HB2	1:a:245:THR:HG21	1.84	0.60
29:A:612:PL9:H361	6:F:25:THR:HG21	1.82	0.59
6:F:22:ALA:C	37:F:201:HOH:O	2.45	0.59
6:F:25:THR:HB	37:F:201:HOH:O	2.02	0.59
30:I:102:STE:H22	26:b:606:CLA:H192	1.85	0.59
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.85	0.59
26:C:502:CLA:H61	26:C:512:CLA:H42	1.86	0.58
5:E:18:ARG:C	37:E:201:HOH:O	2.45	0.58
2:b:281:GLN:HB3	37:b:701:HOH:O	2.04	0.57
35:f:101:HEM:HHC	35:f:101:HEM:HBB2	1.87	0.57
4:D:42:TYR:CE1	6:F:25:THR:HG22	2.39	0.57
26:C:508:CLA:H192	33:C:522:DGD:HAT2	1.86	0.57
26:b:613:CLA:H192	34:d:407:LHG:H211	1.85	0.57
2:b:281:GLN:N	37:b:701:HOH:O	2.37	0.57
1:a:245:THR:HG22	37:a:741:HOH:O	2.04	0.56
28:k:101:BCR:H321	28:k:101:BCR:HC8	1.88	0.56
5:E:17:VAL:HG12	37:J:204:HOH:O	2.05	0.56
3:c:42:LEU:HD21	26:c:511:CLA:H2A	1.88	0.56
2:b:313:ASP:HA	37:b:729:HOH:O	2.05	0.55
2:B:193:TYR:O	7:H:65:LEU:HD23	2.07	0.55
10:k:26:PRO:HD3	37:k:201:HOH:O	2.07	0.55
30:D:412:STE:H22	18:X:12:ILE:HD13	1.88	0.55
1:a:271:LEU:HD21	29:a:612:PL9:HC71	1.89	0.55
37:A:787:HOH:O	13:O:107:THR:HG21	2.06	0.54
15:u:52:ASN:C	37:u:202:HOH:O	2.50	0.54
2:b:36:SER:OG	28:b:618:BCR:H362	2.08	0.53
3:c:318:LEU:C	3:c:318:LEU:HD23	2.33	0.53
2:b:280:PHE:HB2	37:b:729:HOH:O	2.09	0.53
16:V:63:THR:HG22	16:V:64:PRO:CD	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:501:CLA:H192	26:c:507:CLA:HBB1	1.90	0.53
3:c:180:MET:HE1	31:c:522:LMG:HC72	1.91	0.53
32:F:102:SQD:H262	18:X:31:ILE:HD13	1.91	0.52
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.91	0.52
18:x:16:SER:O	18:x:20:VAL:HG23	2.10	0.52
10:k:21:LEU:HD13	17:y:24:MET:HE2	1.90	0.52
26:c:509:CLA:H43	26:c:509:CLA:O1A	2.09	0.52
16:V:28:GLU:HG2	37:V:349:HOH:O	2.10	0.52
10:k:18:PHE:CE2	19:z:9:LEU:HD23	2.45	0.52
3:C:406:SER:HA	3:C:420:VAL:HG23	1.91	0.52
27:D:401:PHO:HBC2	27:D:401:PHO:HHD	1.91	0.52
31:a:616:LMG:C10	31:a:616:LMG:O8	2.58	0.52
26:b:613:CLA:H192	34:d:407:LHG:C21	2.39	0.52
26:b:613:CLA:H192	34:d:407:LHG:C22	2.40	0.52
14:t:12:CYS:N	37:t:201:HOH:O	2.42	0.52
26:B:606:CLA:H11	37:B:715:HOH:O	2.10	0.51
17:y:19:ILE:HD13	17:y:20:ALA:N	2.25	0.51
19:z:50:LEU:O	19:z:54:VAL:HG23	2.11	0.51
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.92	0.51
4:D:272:LEU:C	4:D:272:LEU:HD23	2.35	0.51
26:A:607:CLA:H191	34:D:408:LHG:H161	1.93	0.51
33:A:617:DGD:HBW2	33:A:617:DGD:HB82	1.93	0.51
19:Z:51:VAL:O	19:Z:54:VAL:O	2.29	0.51
4:d:272:LEU:C	4:d:272:LEU:HD23	2.36	0.51
4:d:186:GLN:HB2	26:d:402:CLA:HBC1	1.93	0.50
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.46	0.50
16:v:76:MET:HE2	16:v:112:LEU:HD22	1.91	0.50
28:T:101:BCR:H311	28:T:101:BCR:HC8	1.93	0.50
13:O:15:LEU:HD23	13:O:18:LYS:HD2	1.93	0.50
9:j:18:GLY:O	9:j:21:VAL:HG22	2.12	0.50
30:C:527:STE:H181	37:I:201:HOH:O	2.11	0.50
4:D:123:ILE:HD11	33:H:102:DGD:HAW2	1.94	0.49
26:A:607:CLA:HBB1	26:A:607:CLA:HMB3	1.93	0.49
26:d:403:CLA:H92	18:x:18:ALA:HB2	1.95	0.49
4:d:148:ALA:HB3	4:d:149:PRO:HD3	1.95	0.49
13:O:54:GLU:O	13:O:63:ALA:HB1	2.12	0.49
26:d:403:CLA:H42	7:h:43:LEU:HD21	1.95	0.49
26:C:505:CLA:HBC2	28:C:515:BCR:H341	1.95	0.49
4:D:279:LEU:HD22	27:D:401:PHO:HBC3	1.95	0.49
5:E:18:ARG:O	5:E:18:ARG:HG2	2.13	0.49
17:Y:31:ALA:HB2	37:Y:101:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:613:CLA:H192	34:d:407:LHG:H223	1.94	0.49
1:A:200:LEU:HD11	33:C:523:DGD:HBW1	1.94	0.48
3:C:63:TRP:HZ2	37:C:731:HOH:O	1.96	0.48
5:e:30:LEU:HD11	35:f:101:HEM:HBB2	1.95	0.48
27:A:609:PHO:HBC2	27:A:609:PHO:HHD	1.95	0.48
7:h:63:LYS:O	7:h:64:ALA:HB2	2.13	0.48
4:D:194:ASN:HA	4:D:295:SER:OG	2.13	0.48
30:D:412:STE:C2	18:X:12:ILE:HD13	2.44	0.48
13:O:27:ARG:NH1	37:O:303:HOH:O	2.47	0.48
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.96	0.48
33:C:522:DGD:HAW1	33:C:522:DGD:C6A	2.42	0.48
29:a:612:PL9:H251	34:e:102:LHG:H211	1.95	0.48
26:d:403:CLA:H93	18:x:14:LEU:HD22	1.94	0.48
6:f:19:ARG:O	6:f:23:VAL:HG13	2.13	0.48
16:v:104:MET:HA	16:v:107:LEU:HD22	1.96	0.48
3:C:203:THR:O	3:C:235:GLY:HA3	2.13	0.48
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.96	0.48
15:U:27:LEU:HD13	15:U:61:VAL:CG1	2.43	0.48
14:t:11:ALA:HB3	37:t:201:HOH:O	2.13	0.47
28:x:101:BCR:H331	28:x:101:BCR:C8	2.44	0.47
26:C:512:CLA:C12	26:C:512:CLA:H91	2.44	0.47
28:T:101:BCR:C8	28:T:101:BCR:H321	2.43	0.47
28:b:619:BCR:H331	28:b:619:BCR:C8	2.43	0.47
1:A:188[A]:ALA:HB2	1:A:328[A]:MET:HB2	1.95	0.47
6:f:14:PRO:HB2	37:f:201:HOH:O	2.15	0.47
12:m:17:VAL:HB	12:m:18:PRO:HD3	1.96	0.47
28:x:101:BCR:H331	28:x:101:BCR:HC8	1.96	0.47
26:A:607:CLA:H191	34:D:408:LHG:C16	2.44	0.47
13:O:27:ARG:O	13:O:27:ARG:HG2	2.15	0.47
5:e:68:ASP:O	5:e:72:ALA:HB2	2.14	0.47
19:z:1:MET:O	19:z:2:THR:CB	2.62	0.47
3:C:318:LEU:C	3:C:318:LEU:HD23	2.40	0.47
20:R:10:LEU:HB3	20:R:11:PRO:HD3	1.96	0.47
26:B:602:CLA:HBB1	26:B:602:CLA:HMB3	1.96	0.47
1:a:286:THR:HG23	26:a:607:CLA:HED3	1.97	0.47
2:b:264:PRO:HG2	2:b:267:LEU:HD22	1.95	0.47
3:C:204:LEU:HD11	31:C:517:LMG:O2	2.14	0.46
5:E:68:ASP:O	5:E:72:ALA:HB2	2.16	0.46
19:Z:48:ILE:HD11	30:Z:102:STE:H132	1.98	0.46
30:E:104:STE:H181	37:E:237:HOH:O	2.16	0.46
3:C:443:TRP:CE2	26:C:508:CLA:HMD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:k:22:VAL:O	10:k:22:VAL:CG1	2.63	0.46
2:B:12:LEU:HB2	26:B:612:CLA:HMC2	1.98	0.46
34:B:622:LHG:HC5	34:B:622:LHG:O10	2.16	0.46
4:D:209:LEU:HD23	4:D:209:LEU:C	2.41	0.46
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.51	0.46
7:H:6:TRP:CZ2	7:H:10:ILE:HD11	2.50	0.46
2:b:413:ASP:HB2	37:b:719:HOH:O	2.16	0.46
28:k:101:BCR:H321	28:k:101:BCR:C8	2.46	0.46
4:d:179:PHE:HA	4:d:182:LEU:HD22	1.97	0.45
19:z:35:ARG:H	19:z:35:ARG:HE	1.64	0.45
5:E:21:VAL:HB	37:E:201:HOH:O	2.15	0.45
32:f:102:SQD:H312	18:x:27:VAL:HG11	1.98	0.45
17:y:19:ILE:HD13	17:y:19:ILE:C	2.42	0.45
2:B:36:SER:OG	28:B:618:BCR:H362	2.16	0.45
2:B:491:VAL:HG12	4:D:136:VAL:HG13	1.99	0.45
1:a:159[A]:LEU:O	1:a:163[A]:ILE:HG12	2.17	0.45
29:A:612:PL9:H502	32:F:102:SQD:H381	1.99	0.45
26:B:613:CLA:HBB1	26:B:613:CLA:HMB1	1.99	0.45
6:F:25:THR:N	37:F:201:HOH:O	2.49	0.45
1:a:84:PRO:HA	1:a:112:TYR:CG	2.52	0.45
26:B:611:CLA:H141	34:B:622:LHG:H382	1.98	0.45
30:D:412:STE:H42	18:X:12:ILE:HG21	1.99	0.45
26:c:513:CLA:H191	30:c:516:STE:C1	2.47	0.45
26:B:602:CLA:HMB3	37:B:721:HOH:O	2.15	0.44
29:a:612:PL9:H302	4:d:45:LEU:HD22	1.98	0.44
26:B:612:CLA:HBB1	26:B:612:CLA:HMB1	2.00	0.44
31:C:524:LMG:H172	17:Y:25:ILE:HD12	1.99	0.44
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	2.00	0.44
4:d:209:LEU:HD23	4:d:209:LEU:C	2.43	0.44
1:A:84:PRO:HA	1:A:112:TYR:CG	2.53	0.44
20:r:24:LEU:HD13	20:r:24:LEU:C	2.43	0.44
3:C:42:LEU:HD21	26:C:511:CLA:H2A	2.00	0.44
33:C:522:DGD:HAW1	33:C:522:DGD:C7A	2.47	0.44
4:D:267:LEU:C	4:D:267:LEU:HD23	2.42	0.44
3:c:95:LEU:HD21	26:c:501:CLA:OBD	2.18	0.44
16:v:122:GLU:N	16:v:123:PRO:HD2	2.33	0.44
26:B:614:CLA:H43	32:B:623:SQD:H132	2.00	0.44
19:Z:61:VAL:HG23	19:Z:62:VAL:N	2.32	0.44
1:a:183[A]:MET:HA	26:a:607:CLA:HMD1	1.98	0.44
26:b:601:CLA:H41	37:b:973:HOH:O	2.17	0.43
4:d:194:ASN:HA	4:d:295:SER:OG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:y:21:GLN:O	17:y:25:ILE:HG22	2.19	0.43
33:A:617:DGD:HD5	2:b:75:TRP:HB3	2.00	0.43
26:B:615:CLA:H93	26:B:615:CLA:H62	1.92	0.43
2:b:12:LEU:HB2	26:b:612:CLA:HMC2	2.01	0.43
2:b:29:LEU:HD23	32:b:620:SQD:H201	2.01	0.43
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.54	0.43
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.01	0.43
4:D:170:ALA:HB1	4:D:171:PRO:HD2	2.00	0.43
28:H:101:BCR:H331	28:H:101:BCR:C8	2.48	0.43
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	2.00	0.43
28:b:618:BCR:H24C	28:b:618:BCR:H371	1.82	0.43
28:k:101:BCR:C16	37:y:101:HOH:O	2.65	0.43
1:A:183[B]:MET:HA	26:A:607:CLA:HMD1	2.01	0.43
2:B:230:ARG:NH2	31:B:620:LMG:HC5	2.33	0.43
1:A:63[A]:ILE:HB	3:C:335:THR:HG21	2.00	0.42
1:A:283:VAL:HA	1:A:286:THR:HG22	2.01	0.42
35:F:101:HEM:HBB2	35:F:101:HEM:HMB1	2.01	0.42
12:M:20:VAL:HG11	12:m:20:VAL:CG2	2.49	0.42
3:c:169:GLY:HA3	37:c:603:HOH:O	2.20	0.42
35:F:101:HEM:HBB2	35:F:101:HEM:CMB	2.50	0.42
10:K:18:PHE:CE2	19:Z:9:LEU:HD21	2.55	0.42
28:k:101:BCR:H333	28:k:102:BCR:C12	2.50	0.42
20:r:10:LEU:HB3	20:r:11:PRO:HD3	2.00	0.42
1:A:227:THR:HB	1:A:231:GLU:HG3	2.02	0.42
28:B:617:BCR:H24C	28:B:617:BCR:H371	1.85	0.42
3:C:462:GLU:HG2	37:C:819:HOH:O	2.20	0.42
37:a:795:HOH:O	5:e:61:ARG:HA	2.19	0.42
3:c:286:ALA:HB2	26:c:502:CLA:HMD2	2.00	0.42
1:A:202:VAL:HG11	26:A:608:CLA:C3D	2.49	0.42
2:b:445:THR:HA	37:b:703:HOH:O	2.19	0.42
4:d:126:MET:HE3	4:d:143:ALA:O	2.18	0.42
26:b:613:CLA:HBB1	26:b:613:CLA:HMB1	2.01	0.42
28:t:101:BCR:H382	28:t:101:BCR:C23	2.47	0.42
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.01	0.42
12:M:12:ALA:O	12:M:16:LEU:HB2	2.20	0.42
6:f:28:VAL:N	6:f:29:PRO:CD	2.83	0.42
13:o:42:ARG:O	13:o:241:ALA:HA	2.19	0.42
30:A:618:STE:H181	37:b:977:HOH:O	2.20	0.42
26:B:603:CLA:H193	7:H:38:PHE:HD2	1.85	0.42
26:B:606:CLA:H141	26:B:606:CLA:H171	2.02	0.42
1:a:131:TRP:CE3	1:a:132:GLU:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:202:VAL:HG11	26:a:608:CLA:C3D	2.50	0.42
1:a:271:LEU:HD13	1:a:271:LEU:C	2.45	0.42
28:a:611:BCR:H24C	28:a:611:BCR:H371	1.93	0.42
2:b:70:GLY:HA2	2:b:178:VAL:HG21	2.01	0.42
2:b:277:SER:O	2:b:278:SER:C	2.63	0.42
3:c:406:SER:HA	3:c:420:VAL:HG23	2.02	0.42
26:A:608:CLA:HBB1	26:A:608:CLA:HMB3	2.02	0.41
13:O:133:VAL:C	13:O:135:SER:H	2.28	0.41
28:B:618:BCR:H331	28:B:618:BCR:C8	2.49	0.41
13:O:133:VAL:C	13:O:134:THR:HG23	2.45	0.41
15:U:27:LEU:HD13	15:U:61:VAL:HG13	2.02	0.41
4:d:42:TYR:CE1	6:f:25:THR:HG22	2.54	0.41
7:h:7:LEU:HD22	7:h:11:LEU:CD1	2.50	0.41
2:b:246:PHE:CD1	2:b:246:PHE:C	2.98	0.41
26:d:403:CLA:HMB1	26:d:403:CLA:HBB1	2.02	0.41
28:t:101:BCR:H24C	28:t:101:BCR:H371	1.93	0.41
28:x:101:BCR:H20C	28:x:101:BCR:H361	1.81	0.41
1:A:234:ASN:HD21	34:D:411:LHG:HC11	1.85	0.41
37:b:731:HOH:O	30:d:406:STE:H22	2.20	0.41
3:C:279:LEU:HD12	26:C:509:CLA:HED2	2.02	0.41
2:b:149:LEU:HD11	26:b:604:CLA:H111	2.01	0.41
1:A:161[B]:TYR:HB3	1:A:162[B]:PRO:HD3	2.02	0.41
3:C:50:LEU:O	3:C:54:VAL:HG23	2.20	0.41
4:D:170:ALA:HB1	4:D:171:PRO:CD	2.50	0.41
2:B:237:VAL:CG2	26:B:610:CLA:HBC2	2.50	0.41
26:B:601:CLA:H191	37:X:109:HOH:O	2.21	0.41
32:B:623:SQD:H442	14:t:23:PHE:CD1	2.55	0.41
26:C:506:CLA:H91	26:C:506:CLA:H111	1.90	0.41
16:V:57:GLU:CD	16:V:57:GLU:H	2.28	0.41
1:a:183[B]:MET:HA	26:a:607:CLA:HMD1	2.01	0.41
19:z:1:MET:O	19:z:2:THR:HB	2.19	0.41
20:r:28:VAL:HG12	20:r:28:VAL:O	2.20	0.41
1:A:121:LEU:HD11	26:C:505:CLA:H121	2.03	0.41
10:K:27:VAL:O	10:K:27:VAL:HG12	2.19	0.41
13:O:107:THR:HG23	37:O:354:HOH:O	2.19	0.41
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	2.03	0.41
32:b:620:SQD:H462	32:b:620:SQD:H1	2.03	0.41
1:A:183[A]:MET:HA	26:A:607:CLA:HMD1	2.02	0.41
28:A:611:BCR:H24C	28:A:611:BCR:H371	1.83	0.41
37:C:798:HOH:O	13:O:80:GLN:HG3	2.19	0.41
35:F:101:HEM:HBC2	35:F:101:HEM:CHD	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:H:101:BCR:H24C	28:H:101:BCR:H371	1.91	0.41
1:a:38:ILE:HB	1:a:39:PRO:HD3	2.03	0.41
1:a:63[B]:ILE:HB	3:c:335:THR:HG21	2.02	0.41
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.56	0.41
4:d:192:THR:HG23	26:d:402:CLA:HBC2	2.03	0.41
4:d:267:LEU:C	4:d:267:LEU:CD2	2.94	0.41
17:y:22:LEU:HA	17:y:25:ILE:HG22	2.03	0.41
20:r:5:VAL:O	20:r:9:LEU:HD22	2.20	0.41
4:D:244:TYR:OH	4:D:264:LYS:HE3	2.20	0.41
1:a:308:ASP:OD1	1:a:308:ASP:C	2.64	0.41
4:d:24:ARG:NH1	37:d:513:HOH:O	2.54	0.41
4:d:307:GLU:HG3	37:d:536:HOH:O	2.21	0.41
2:B:237:VAL:HG22	26:B:610:CLA:HBC2	2.03	0.40
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	2.02	0.40
32:D:410:SQD:H442	37:D:501:HOH:O	2.20	0.40
13:O:40:ILE:HD13	13:O:95:PHE:CD1	2.56	0.40
4:d:210:LEU:HA	4:d:213:ILE:HG22	2.03	0.40
37:D:551:HOH:O	30:K:102:STE:C7	2.69	0.40
10:K:18:PHE:HE2	19:Z:9:LEU:HD21	1.85	0.40
2:b:458:PHE:HB3	26:b:604:CLA:HBC2	2.04	0.40
26:b:610:CLA:H202	26:b:610:CLA:H162	1.88	0.40
2:B:67:ALA:HA	2:B:71:VAL:O	2.21	0.40
28:a:611:BCR:H361	28:a:611:BCR:H20C	1.83	0.40
26:b:615:CLA:H143	26:b:616:CLA:HMA2	2.02	0.40
17:y:20:ALA:O	17:y:24:MET:HG2	2.21	0.40
33:A:617:DGD:HBH1	30:I:102:STE:H101	2.02	0.40
1:a:179[A]:THR:O	1:a:183[A]:MET:HG3	2.22	0.40
2:b:86:ILE:HD12	2:b:86:ILE:O	2.21	0.40
26:b:608:CLA:HBC3	26:b:609:CLA:H122	2.03	0.40
30:b:623:STE:C1	37:b:731:HOH:O	2.70	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	403/344 (117%)	398 (99%)	5 (1%)	0	100	100
1	a	403/344 (117%)	397 (98%)	6 (2%)	0	100	100
2	B	510/510 (100%)	502 (98%)	8 (2%)	0	100	100
2	b	504/510 (99%)	495 (98%)	9 (2%)	0	100	100
3	C	454/461 (98%)	445 (98%)	8 (2%)	1 (0%)	43	37
3	c	463/461 (100%)	451 (97%)	11 (2%)	1 (0%)	43	37
4	D	349/352 (99%)	340 (97%)	9 (3%)	0	100	100
4	d	350/352 (99%)	342 (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%)	2 (3%)	1 (2%)	7	1
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
9	J	34/40 (85%)	33 (97%)	0	1 (3%)	3	0
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	232 (96%)	10 (4%)	1 (0%)	30	22
13	o	242/272 (89%)	233 (96%)	9 (4%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
15	u	95/134 (71%)	92 (97%)	2 (2%)	1 (1%)	11	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	V	135/163 (83%)	132 (98%)	2 (2%)	1 (1%)	18	9
16	v	135/163 (83%)	132 (98%)	3 (2%)	0	100	100
17	Y	25/46 (54%)	25 (100%)	0	0	100	100
17	y	28/46 (61%)	28 (100%)	0	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
19	z	60/62 (97%)	56 (93%)	3 (5%)	1 (2%)	7	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	5420/5700 (95%)	5299 (98%)	113 (2%)	8 (0%)	43	41

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	V	64	PRO
3	c	416	SER
19	z	2	THR
3	C	416	SER
15	u	53	ALA
9	J	7	ARG
13	O	57	LYS
7	h	63	LYS

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	329/280 (118%)	326 (99%)	3 (1%)	70	67
1	a	328/280 (117%)	316 (96%)	12 (4%)	30	16
2	B	410/407 (101%)	404 (98%)	6 (2%)	57	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	403/407 (99%)	399 (99%)	4 (1%)	68	64
3	C	356/362 (98%)	351 (99%)	5 (1%)	59	52
3	c	364/362 (101%)	351 (96%)	13 (4%)	31	17
4	D	286/283 (101%)	286 (100%)	0	100	100
4	d	287/283 (101%)	281 (98%)	6 (2%)	47	37
5	E	72/73 (99%)	69 (96%)	3 (4%)	26	13
5	e	71/73 (97%)	68 (96%)	3 (4%)	26	13
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	26 (93%)	2 (7%)	13	3
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	40
7	h	53/55 (96%)	50 (94%)	3 (6%)	18	6
8	I	32/34 (94%)	31 (97%)	1 (3%)	35	21
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	13
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	2
10	K	30/37 (81%)	28 (93%)	2 (7%)	15	4
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	0
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	0
12	M	28/32 (88%)	25 (89%)	3 (11%)	6	1
12	m	28/32 (88%)	27 (96%)	1 (4%)	31	17
13	O	206/228 (90%)	202 (98%)	4 (2%)	50	40
13	o	207/228 (91%)	202 (98%)	5 (2%)	43	31
14	T	26/28 (93%)	25 (96%)	1 (4%)	29	15
14	t	25/28 (89%)	24 (96%)	1 (4%)	28	14
15	U	84/112 (75%)	79 (94%)	5 (6%)	17	5
15	u	84/112 (75%)	83 (99%)	1 (1%)	63	57
16	V	117/138 (85%)	114 (97%)	3 (3%)	40	28
16	v	117/138 (85%)	112 (96%)	5 (4%)	26	13
17	Y	19/37 (51%)	19 (100%)	0	100	100
17	y	22/37 (60%)	20 (91%)	2 (9%)	9	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	X	31/34 (91%)	30 (97%)	1 (3%)	34	20
18	x	31/34 (91%)	29 (94%)	2 (6%)	15	4
19	Z	52/52 (100%)	48 (92%)	4 (8%)	12	3
19	z	51/52 (98%)	48 (94%)	3 (6%)	18	6
20	R	22/33 (67%)	20 (91%)	2 (9%)	9	1
20	r	22/33 (67%)	16 (73%)	6 (27%)	0	0
All	All	4482/4654 (96%)	4358 (97%)	124 (3%)	38	25

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	205	VAL
1	A	243	GLU
2	B	76	SER
2	B	79	SER
2	B	86	ILE
2	B	362	PHE
2	B	371	THR
2	B	476	ARG
3	C	142	GLU
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
3	C	416	SER
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	60	GLN
7	H	20	LYS
8	I	4	LEU
9	J	19	MET
10	K	13	GLU
10	K	19	ASP
12	M	5	GLN
12	M	16	LEU
12	M	25	LEU
13	O	78	LEU
13	O	118	LEU
13	O	189	ARG
13	O	214	THR

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Mol	Chain	Res	Type
14	T	29	ILE
15	U	23	GLU
15	U	39	ARG
15	U	45	LEU
15	U	61	VAL
15	U	67	LEU
16	V	3	LEU
16	V	7	VAL
16	V	24	LYS
18	X	3	ILE
19	Z	31	GLN
19	Z	34	ASP
19	Z	46	LEU
19	Z	50	LEU
20	R	6	LEU
20	R	29	LYS
1	a	16	ARG
1	a	28	LEU
1	a	42	LEU
1	a	159[A]	LEU
1	a	159[B]	LEU
1	a	200	LEU
1	a	223	LEU
1	a	231	GLU
1	a	243	GLU
1	a	245	THR
1	a	286	THR
1	a	288	LEU
2	b	63	LEU
2	b	98	LEU
2	b	362	PHE
2	b	485	GLU
3	c	72	LEU
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	165	LEU
3	c	170	ILE
3	c	240	ILE
3	c	279	LEU
3	c	315	MET
3	c	354[A]	GLU

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Mol	Chain	Res	Type
3	c	354[B]	GLU
3	c	413[A]	GLU
3	c	413[B]	GLU
4	d	90	LEU
4	d	182	LEU
4	d	259	ILE
4	d	291	LEU
4	d	293	LEU
4	d	321	LEU
5	e	63	ILE
5	e	66	VAL
5	e	83	LEU
6	f	23	VAL
6	f	28	VAL
7	h	6	TRP
7	h	7	LEU
7	h	43	LEU
9	j	7	ARG
9	j	13	VAL
10	k	10	LYS
10	k	19	ASP
10	k	30	VAL
10	k	35	LEU
11	l	2	GLU
11	l	8	GLN
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
13	o	49	THR
13	o	58	ASN
13	o	60	ARG
13	o	118	LEU
13	o	178	LYS
14	t	25	GLU
15	u	9	LEU
16	v	28	GLU
16	v	52	LEU
16	v	90	GLU
16	v	107	LEU
16	v	110	LYS
17	y	19	ILE
17	y	30	ILE

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Mol	Chain	Res	Type
18	x	2	THR
18	x	15	LEU
19	z	35	ARG
19	z	41	PHE
19	z	42	LEU
20	r	3	TRP
20	r	6	LEU
20	r	7	VAL
20	r	9	LEU
20	r	14	LEU
20	r	29	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	ASN
2	B	394	GLN
2	B	497	GLN
3	C	155	ASN
3	C	415	ASN
4	D	61	HIS
12	M	5	GLN
13	O	155	ASN
13	O	231	HIS
18	X	38	GLN
20	R	22	ASN
1	a	19	ASN
2	b	338	GLN
2	b	409	GLN
2	b	497	GLN
3	c	201	ASN
3	c	311	GLN
3	c	322	GLN
4	d	61	HIS
4	d	255	GLN
4	d	350	ASN
5	e	82	GLN
6	f	44	GLN
7	h	59	ASN
11	l	8	GLN
12	m	5	GLN
13	o	36	GLN

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Mol	Chain	Res	Type
13	o	155	ASN
16	v	118	HIS
18	x	33	GLN
18	x	38	GLN
19	z	31	GLN
19	z	38	GLN
19	z	58	ASN

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	0.38	0	8,9,11	0.82	0
12	FME	M	1	12	8,9,10	0.39	0	8,9,11	0.89	0
14	FME	T	1	14	8,9,10	0.43	0	8,9,11	1.44	2 (25%)
14	FME	t	1	14	8,9,10	0.42	0	8,9,11	0.85	0
8	FME	I	1	8	8,9,10	0.35	0	8,9,11	0.94	1 (12%)
8	FME	i	1	8	8,9,10	0.38	0	8,9,11	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	m	1	12	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	CA-N-CN	2.53	126.72	122.82
14	T	1	FME	CG-CB-CA	2.29	119.86	112.87
8	I	1	FME	O-C-CA	-2.01	119.59	124.77

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [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$
26	CLA	C	511	3	69,73,73	1.29	8 (11%)	82,113,113	1.25	5 (6%)
26	CLA	C	504	37	63,67,73	1.26	7 (11%)	74,105,113	1.24	8 (10%)
30	STE	E	102	-	11,11,19	0.76	0	11,11,19	1.12	0
28	BCR	D	404	-	41,41,41	0.44	0	56,56,56	0.87	1 (1%)
31	LMG	C	517	-	35,35,55	0.55	0	43,43,63	1.22	5 (11%)
30	STE	b	624	-	9,9,19	0.35	0	8,8,19	0.73	0
26	CLA	a	613	37	69,73,73	1.22	8 (11%)	82,113,113	1.12	6 (7%)
26	CLA	B	602	2	69,73,73	1.20	8 (11%)	82,113,113	1.11	7 (8%)
30	STE	e	103	-	7,7,19	0.38	0	6,6,19	0.57	0
26	CLA	D	402	4	69,73,73	1.15	6 (8%)	82,113,113	1.21	6 (7%)
26	CLA	C	507	37	69,73,73	1.24	6 (8%)	82,113,113	1.28	7 (8%)
26	CLA	b	604	2	69,73,73	1.23	7 (10%)	82,113,113	1.38	11 (13%)
30	STE	C	527	-	13,13,19	0.35	0	12,12,19	0.73	0
28	BCR	c	515	-	41,41,41	0.41	0	56,56,56	0.70	1 (1%)
33	DGD	C	522	-	63,63,67	0.57	0	77,77,81	0.74	1 (1%)
26	CLA	C	505	3	69,73,73	1.21	7 (10%)	82,113,113	1.26	9 (10%)
26	CLA	C	501	3	69,73,73	1.35	8 (11%)	82,113,113	1.22	5 (6%)
30	STE	z	701	-	12,12,19	0.39	0	11,11,19	0.67	0
26	CLA	b	605	2	69,73,73	1.22	7 (10%)	82,113,113	1.28	8 (9%)
30	STE	i	102	-	5,5,19	0.37	0	4,4,19	0.53	0
26	CLA	c	502	3	69,73,73	1.16	7 (10%)	82,113,113	1.15	4 (4%)
30	STE	A	619	-	16,16,19	0.32	0	15,15,19	0.79	0
31	LMG	M	101	-	51,51,55	0.58	0	59,59,63	0.80	2 (3%)
36	HEC	V	201	16	50,50,50	1.64	4 (8%)	68,82,82	1.31	9 (13%)
26	CLA	a	610	1	69,73,73	1.25	7 (10%)	82,113,113	1.20	6 (7%)
34	LHG	d	409	-	38,38,48	0.60	0	41,44,54	0.61	1 (2%)
26	CLA	C	513	3	69,73,73	1.26	8 (11%)	82,113,113	1.20	7 (8%)
34	LHG	d	407	-	48,48,48	0.52	0	51,54,54	0.59	1 (1%)
30	STE	m	102	-	11,11,19	0.74	0	11,11,19	1.09	1 (9%)
30	STE	h	102	-	9,9,19	0.36	0	8,8,19	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMG	d	411	-	44,44,55	0.52	0	52,52,63	0.63	0
33	DGD	H	102	-	63,63,67	0.58	0	77,77,81	0.85	2 (2%)
28	BCR	T	101	-	41,41,41	0.50	0	56,56,56	0.87	0
26	CLA	b	610	37	69,73,73	1.23	7 (10%)	82,113,113	1.16	7 (8%)
33	DGD	c	520	-	63,63,67	0.54	0	77,77,81	0.74	1 (1%)
26	CLA	c	512	3	69,73,73	1.13	7 (10%)	82,113,113	1.30	6 (7%)
26	CLA	C	508	3	69,73,73	1.27	7 (10%)	82,113,113	1.27	6 (7%)
21	OEY	A	601[B]	3,37,1	0,16,16	-	-	-	-	-
30	STE	C	520	-	9,9,19	0.40	0	8,8,19	0.61	0
28	BCR	A	611	-	41,41,41	0.39	0	56,56,56	0.57	0
30	STE	I	101	-	16,16,19	0.63	0	16,16,19	1.03	0
26	CLA	D	403	4	69,73,73	1.20	8 (11%)	82,113,113	1.20	6 (7%)
31	LMG	B	620	-	45,45,55	0.51	0	53,53,63	0.71	2 (3%)
32	SQD	b	620	-	47,49,54	1.62	7 (14%)	57,60,65	1.64	10 (17%)
28	BCR	C	515	-	41,41,41	0.39	0	56,56,56	0.61	0
26	CLA	B	605	2	69,73,73	1.22	7 (10%)	82,113,113	1.27	9 (10%)
26	CLA	b	608	2	69,73,73	1.15	6 (8%)	82,113,113	1.27	6 (7%)
32	SQD	f	102	-	39,41,54	1.66	7 (17%)	49,52,65	1.65	10 (20%)
33	DGD	C	523	-	63,63,67	0.59	1 (1%)	77,77,81	0.69	0
26	CLA	c	506	3	69,73,73	1.24	6 (8%)	82,113,113	1.16	5 (6%)
33	DGD	A	617	-	67,67,67	0.54	0	81,81,81	0.85	4 (4%)
26	CLA	d	403	4	69,73,73	1.34	9 (13%)	82,113,113	1.07	6 (7%)
34	LHG	D	409	-	46,46,48	0.55	0	49,52,54	0.50	0
27	PHO	A	609	-	58,69,69	2.04	11 (18%)	55,99,99	1.70	7 (12%)
30	STE	C	526	-	15,15,19	0.34	0	14,14,19	0.79	0
30	STE	m	103	-	17,17,19	0.33	0	16,16,19	0.84	0
27	PHO	d	401	-	58,69,69	2.16	10 (17%)	55,99,99	1.69	10 (18%)
26	CLA	A	610	1	58,62,73	1.20	5 (8%)	68,99,113	1.32	7 (10%)
28	BCR	t	101	-	41,41,41	0.51	0	56,56,56	0.75	1 (1%)
30	STE	E	104	-	19,19,19	0.61	0	19,19,19	1.10	2 (10%)
30	STE	T	102	-	15,15,19	0.36	0	14,14,19	0.70	0
30	STE	d	410	-	19,19,19	0.60	0	19,19,19	0.94	0
30	STE	I	102	-	14,14,19	0.70	0	14,14,19	1.02	0
25	BCT	A	606	23	3,3,3	0.83	0	2,3,3	2.20	1 (50%)
34	LHG	d	408	-	48,48,48	0.52	0	51,54,54	0.67	0
28	BCR	b	618	-	41,41,41	0.44	0	56,56,56	0.75	1 (1%)
30	STE	A	620	-	10,10,19	0.35	0	9,9,19	0.74	0
26	CLA	B	604	2	69,73,73	1.42	8 (11%)	82,113,113	1.36	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	STE	b	623	-	15,15,19	0.62	0	15,15,19	1.18	2 (13%)
26	CLA	C	512	3	69,73,73	1.24	8 (11%)	82,113,113	1.24	8 (9%)
30	STE	b	625	-	10,10,19	0.31	0	9,9,19	0.82	0
30	STE	C	519	-	6,6,19	0.36	0	5,5,19	0.68	0
30	STE	C	516	-	13,13,19	0.73	0	13,13,19	1.02	1 (7%)
30	STE	B	621	-	16,16,19	0.61	0	16,16,19	1.17	0
28	BCR	a	611	-	41,41,41	0.42	0	56,56,56	0.67	0
35	HEM	F	101	6,5	50,50,50	1.41	6 (12%)	67,82,82	1.13	4 (5%)
31	LMG	D	406	-	50,50,55	0.51	0	58,58,63	1.14	5 (8%)
26	CLA	b	615	2	69,73,73	1.31	9 (13%)	82,113,113	1.25	4 (4%)
26	CLA	c	505	3	69,73,73	1.16	6 (8%)	82,113,113	1.23	5 (6%)
26	CLA	B	616	2	64,68,73	1.44	7 (10%)	76,107,113	1.25	6 (7%)
21	OEY	a	601[B]	3,37,1	0,16,16	-	-	-	-	-
26	CLA	C	503	3	69,73,73	1.36	7 (10%)	82,113,113	1.34	7 (8%)
30	STE	e	101	-	8,8,19	0.37	0	7,7,19	0.63	0
30	STE	A	613	-	8,8,19	0.35	0	7,7,19	0.63	0
26	CLA	a	608	37	69,73,73	1.30	8 (11%)	82,113,113	1.14	6 (7%)
22	OEX	a	602[A]	3,37,1	0,14,14	-	-	-	-	-
26	CLA	B	613	2	69,73,73	1.22	8 (11%)	82,113,113	1.25	5 (6%)
30	STE	B	625	-	17,17,19	0.62	0	17,17,19	1.05	0
26	CLA	B	610	37	69,73,73	1.21	6 (8%)	82,113,113	1.26	7 (8%)
26	CLA	C	502	3	69,73,73	1.31	8 (11%)	82,113,113	1.28	6 (7%)
27	PHO	a	609	-	58,69,69	2.07	12 (20%)	55,99,99	1.67	7 (12%)
28	BCR	Z	101	-	41,41,41	0.41	0	56,56,56	0.84	2 (3%)
26	CLA	b	601	37	69,73,73	1.19	6 (8%)	82,113,113	1.29	5 (6%)
26	CLA	b	613	2	69,73,73	1.19	7 (10%)	82,113,113	1.20	6 (7%)
32	SQD	a	615	-	52,54,54	1.59	8 (15%)	62,65,65	1.38	7 (11%)
33	DGD	C	521	-	63,63,67	0.62	1 (1%)	77,77,81	0.86	3 (3%)
26	CLA	B	609	2	69,73,73	1.25	5 (7%)	82,113,113	1.20	7 (8%)
30	STE	H	103	-	17,17,19	0.38	0	16,16,19	0.74	0
26	CLA	C	506	3	69,73,73	1.20	6 (8%)	82,113,113	1.10	5 (6%)
29	PL9	A	612	-	55,55,55	0.80	1 (1%)	68,69,69	1.40	8 (11%)
30	STE	k	103	-	13,13,19	0.67	0	13,13,19	1.09	0
25	BCT	a	606	23	3,3,3	0.85	0	2,3,3	1.82	1 (50%)
30	STE	e	104	-	8,8,19	0.36	0	7,7,19	0.63	0
28	BCR	C	514	-	41,41,41	0.36	0	56,56,56	0.59	0
30	STE	B	626	-	11,11,19	0.74	0	11,11,19	1.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	c	508	3	68,72,73	1.19	6 (8%)	80,111,113	1.20	7 (8%)
31	LMG	A	615	-	48,48,55	0.50	0	56,56,63	0.68	0
35	HEM	f	101	6,5	50,50,50	1.47	8 (16%)	67,82,82	1.33	8 (11%)
26	CLA	b	616	2	64,68,73	1.18	6 (9%)	76,107,113	1.40	7 (9%)
30	STE	J	101	-	11,11,19	0.69	0	11,11,19	1.06	0
26	CLA	b	611	2	69,73,73	1.19	7 (10%)	82,113,113	1.29	7 (8%)
31	LMG	a	617	-	49,49,55	0.57	1 (2%)	57,57,63	0.82	2 (3%)
30	STE	M	102	-	14,14,19	0.69	0	14,14,19	1.06	0
26	CLA	B	608	2	69,73,73	1.19	7 (10%)	82,113,113	1.30	7 (8%)
30	STE	B	627	-	14,14,19	0.34	0	13,13,19	0.77	0
30	STE	M	103	-	9,9,19	0.31	0	8,8,19	0.83	0
26	CLA	B	612	2	69,73,73	1.16	8 (11%)	82,113,113	1.23	6 (7%)
30	STE	E	103	-	11,11,19	0.34	0	10,10,19	0.77	0
30	STE	i	101	-	11,11,19	0.75	0	11,11,19	1.05	0
31	LMG	a	616	-	55,55,55	0.51	0	63,63,63	0.83	4 (6%)
31	LMG	c	522	-	48,48,55	0.53	0	56,56,63	0.80	1 (1%)
26	CLA	A	608	37	69,73,73	1.25	6 (8%)	82,113,113	1.11	4 (4%)
26	CLA	c	510	3	69,73,73	1.25	8 (11%)	82,113,113	1.20	5 (6%)
28	BCR	d	404	-	41,41,41	0.41	0	56,56,56	1.27	4 (7%)
31	LMG	c	521	-	46,46,55	0.51	0	54,54,63	0.63	0
22	OEX	A	602[A]	3,37,1	0,14,14	-	-	-	-	-
34	LHG	l	101	-	48,48,48	0.52	0	51,54,54	0.63	0
28	BCR	B	619	-	41,41,41	0.39	0	56,56,56	0.71	0
28	BCR	c	514	-	41,41,41	0.38	0	56,56,56	0.53	0
29	PL9	D	405	-	55,55,55	1.09	4 (7%)	68,69,69	1.45	13 (19%)
26	CLA	B	615	2	69,73,73	1.33	8 (11%)	82,113,113	1.33	5 (6%)
32	SQD	F	102	-	34,36,54	1.49	5 (14%)	42,45,65	1.80	12 (28%)
28	BCR	b	617	-	41,41,41	0.46	0	56,56,56	0.79	1 (1%)
32	SQD	D	410	-	50,52,54	1.59	6 (12%)	60,63,65	1.76	11 (18%)
28	BCR	K	101	-	41,41,41	0.40	0	56,56,56	0.80	1 (1%)
28	BCR	k	102	-	41,41,41	0.43	0	56,56,56	0.73	1 (1%)
30	STE	z	702	-	8,8,19	0.39	0	7,7,19	0.61	0
27	PHO	D	401	-	58,69,69	2.06	11 (18%)	55,99,99	1.55	10 (18%)
31	LMG	C	524	-	48,48,55	0.50	0	56,56,63	0.63	0
34	LHG	E	101	-	48,48,48	0.53	0	51,54,54	0.54	0
26	CLA	c	509	3	69,73,73	1.25	8 (11%)	82,113,113	1.28	6 (7%)
30	STE	C	525	-	11,11,19	0.75	0	11,11,19	1.19	1 (9%)
26	CLA	b	602	2	69,73,73	1.26	9 (13%)	82,113,113	1.22	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	STE	K	102	-	13,13,19	0.35	0	12,12,19	0.72	0
30	STE	T	103	-	14,14,19	0.34	0	13,13,19	0.86	0
30	STE	D	412	-	19,19,19	0.60	0	19,19,19	1.03	1 (5%)
29	PL9	d	405	-	55,55,55	0.99	4 (7%)	68,69,69	1.64	13 (19%)
26	CLA	c	504	37	64,68,73	1.27	8 (12%)	76,107,113	1.26	5 (6%)
26	CLA	c	513	3	69,73,73	1.13	7 (10%)	82,113,113	1.15	6 (7%)
30	STE	b	621	-	19,19,19	0.57	0	19,19,19	1.04	0
30	STE	e	105	-	12,12,19	0.67	0	12,12,19	1.25	2 (16%)
28	BCR	B	617	-	41,41,41	0.42	0	56,56,56	0.69	0
30	STE	a	618	-	11,11,19	0.75	0	11,11,19	1.00	0
33	DGD	h	101	-	63,63,67	0.57	0	77,77,81	0.83	5 (6%)
36	HEC	v	201	16	50,50,50	1.67	3 (6%)	68,82,82	1.19	5 (7%)
28	BCR	k	101	-	41,41,41	0.44	0	56,56,56	0.76	0
30	STE	t	102	-	9,9,19	0.42	0	8,8,19	0.63	0
32	SQD	a	614	-	52,54,54	1.59	7 (13%)	62,65,65	1.80	10 (16%)
26	CLA	B	603	2	69,73,73	1.23	7 (10%)	82,113,113	1.27	6 (7%)
26	CLA	b	614	2	69,73,73	1.19	6 (8%)	82,113,113	1.24	6 (7%)
26	CLA	B	611	2	69,73,73	1.18	6 (8%)	82,113,113	1.35	8 (9%)
28	BCR	H	101	-	41,41,41	0.43	0	56,56,56	0.82	1 (1%)
26	CLA	c	503	3	69,73,73	1.34	7 (10%)	82,113,113	1.32	6 (7%)
30	STE	Z	102	-	16,16,19	0.35	0	15,15,19	0.75	0
30	STE	d	406	-	19,19,19	0.61	0	19,19,19	1.00	1 (5%)
28	BCR	x	101	-	41,41,41	0.47	0	56,56,56	0.76	1 (1%)
30	STE	j	102	-	15,15,19	0.35	0	14,14,19	0.77	0
26	CLA	c	501	3	69,73,73	1.20	8 (11%)	82,113,113	1.28	5 (6%)
26	CLA	B	606	2	69,73,73	1.41	8 (11%)	82,113,113	1.34	6 (7%)
26	CLA	b	609	2	69,73,73	1.25	5 (7%)	82,113,113	1.25	8 (9%)
31	LMG	b	622	-	55,55,55	0.51	0	63,63,63	0.91	2 (3%)
26	CLA	A	614	37	69,73,73	1.21	9 (13%)	82,113,113	1.25	5 (6%)
33	DGD	c	519	-	63,63,67	0.57	1 (1%)	77,77,81	0.80	2 (2%)
26	CLA	b	607	37	69,73,73	1.30	6 (8%)	82,113,113	1.17	4 (4%)
34	LHG	B	622	-	48,48,48	0.52	0	51,54,54	0.74	1 (1%)
26	CLA	b	606	2	69,73,73	1.36	7 (10%)	82,113,113	1.34	6 (7%)
34	LHG	e	102	-	41,41,48	0.56	0	44,47,54	0.57	0
31	LMG	m	101	-	51,51,55	0.50	0	59,59,63	0.68	1 (1%)
26	CLA	b	612	2	69,73,73	1.14	8 (11%)	82,113,113	1.15	9 (10%)
32	SQD	A	616	-	41,43,54	1.77	8 (19%)	51,54,65	1.42	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	BCR	B	618	-	41,41,41	0.45	0	56,56,56	0.66	1 (1%)
26	CLA	C	509	3	69,73,73	1.18	8 (11%)	82,113,113	1.18	6 (7%)
26	CLA	B	607	37	69,73,73	1.14	7 (10%)	82,113,113	1.16	6 (7%)
32	SQD	B	623	-	52,54,54	1.55	7 (13%)	62,65,65	1.62	11 (17%)
26	CLA	c	507	37	69,73,73	1.16	7 (10%)	82,113,113	1.25	5 (6%)
30	STE	A	618	-	7,7,19	0.33	0	6,6,19	0.71	0
26	CLA	B	601	37	69,73,73	1.28	8 (11%)	82,113,113	1.31	6 (7%)
30	STE	H	104	-	8,8,19	0.32	0	7,7,19	0.76	0
26	CLA	C	510	3	69,73,73	1.21	7 (10%)	82,113,113	1.22	5 (6%)
26	CLA	b	603	2	69,73,73	1.23	8 (11%)	82,113,113	1.28	7 (8%)
33	DGD	c	518	-	63,63,67	0.55	0	77,77,81	0.80	2 (2%)
34	LHG	D	411	-	48,48,48	0.55	0	51,54,54	0.70	0
31	LMG	D	407	-	51,51,55	0.50	0	59,59,63	0.78	2 (3%)
26	CLA	a	607	1	69,73,73	1.24	7 (10%)	82,113,113	1.24	8 (9%)
29	PL9	a	612	-	55,55,55	0.80	2 (3%)	68,69,69	1.50	10 (14%)
30	STE	C	518	-	4,4,19	0.37	0	3,3,19	0.51	0
26	CLA	d	402	4	69,73,73	1.16	6 (8%)	82,113,113	1.16	7 (8%)
30	STE	j	101	-	11,11,19	0.77	0	11,11,19	1.09	1 (9%)
26	CLA	c	511	3	69,73,73	1.46	6 (8%)	82,113,113	1.22	5 (6%)
26	CLA	B	614	2	69,73,73	1.23	8 (11%)	82,113,113	1.22	6 (7%)
28	BCR	b	619	-	41,41,41	0.44	0	56,56,56	0.78	1 (1%)
31	LMG	c	517	-	29,29,55	0.46	0	31,31,63	0.58	0
34	LHG	D	408	-	48,48,48	0.55	0	51,54,54	0.57	1 (1%)
30	STE	d	412	-	19,19,19	0.60	0	19,19,19	0.98	0
26	CLA	A	607	1	69,73,73	1.34	7 (10%)	82,113,113	1.15	5 (6%)
30	STE	c	516	-	17,17,19	0.36	0	16,16,19	0.75	0
30	STE	B	624	-	13,13,19	0.64	0	13,13,19	1.15	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
26	CLA	C	511	3	-	3/39/115/115	-
26	CLA	C	504	37	-	8/32/108/115	-
30	STE	E	102	-	-	3/9/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	BCR	D	404	-	-	0/29/63/63	0/2/2/2
31	LMG	C	517	-	-	14/30/50/70	0/1/1/1
30	STE	b	624	-	-	5/7/7/17	-
26	CLA	a	613	37	-	4/39/115/115	-
26	CLA	B	602	2	-	5/39/115/115	-
30	STE	e	103	-	-	2/5/5/17	-
26	CLA	D	402	4	-	2/39/115/115	-
26	CLA	C	507	37	-	7/39/115/115	-
26	CLA	b	604	2	-	6/39/115/115	-
30	STE	C	527	-	-	6/11/11/17	-
28	BCR	c	515	-	-	0/29/63/63	0/2/2/2
33	DGD	C	522	-	-	19/51/91/95	0/2/2/2
26	CLA	C	505	3	-	9/39/115/115	-
26	CLA	C	501	3	-	6/39/115/115	-
30	STE	z	701	-	-	4/10/10/17	-
26	CLA	b	605	2	-	5/39/115/115	-
30	STE	i	102	-	-	1/3/3/17	-
26	CLA	c	502	3	-	6/39/115/115	-
30	STE	A	619	-	-	1/14/14/17	-
31	LMG	M	101	-	-	21/46/66/70	0/1/1/1
36	HEC	V	201	16	1/1/7/7	5/14/54/54	-
26	CLA	a	610	1	-	10/39/115/115	-
34	LHG	d	409	-	-	10/43/43/53	-
26	CLA	C	513	3	-	10/39/115/115	-
34	LHG	d	407	-	-	17/53/53/53	-
30	STE	m	102	-	-	6/9/9/17	-
30	STE	h	102	-	-	3/7/7/17	-
31	LMG	d	411	-	-	10/39/59/70	0/1/1/1
33	DGD	H	102	-	-	18/51/91/95	0/2/2/2
28	BCR	T	101	-	-	4/29/63/63	0/2/2/2
26	CLA	b	610	37	-	6/39/115/115	-
33	DGD	c	520	-	-	18/51/91/95	0/2/2/2
26	CLA	c	512	3	-	10/39/115/115	-
26	CLA	C	508	3	-	4/39/115/115	-
30	STE	C	520	-	-	5/7/7/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	BCR	A	611	-	-	0/29/63/63	0/2/2/2
30	STE	I	101	-	-	7/14/14/17	-
26	CLA	D	403	4	-	9/39/115/115	-
31	LMG	B	620	-	-	23/40/60/70	0/1/1/1
32	SQD	b	620	-	-	15/44/64/69	0/1/1/1
28	BCR	C	515	-	-	0/29/63/63	0/2/2/2
26	CLA	B	605	2	-	7/39/115/115	-
26	CLA	b	608	2	-	1/39/115/115	-
32	SQD	f	102	-	-	14/36/56/69	0/1/1/1
33	DGD	C	523	-	-	13/51/91/95	0/2/2/2
26	CLA	c	506	3	-	10/39/115/115	-
33	DGD	A	617	-	-	19/55/95/95	0/2/2/2
26	CLA	d	403	4	-	4/39/115/115	-
34	LHG	D	409	-	-	8/51/51/53	-
27	PHO	A	609	-	-	3/37/103/103	0/5/6/6
30	STE	C	526	-	-	4/13/13/17	-
30	STE	m	103	-	-	4/15/15/17	-
27	PHO	d	401	-	-	5/37/103/103	0/5/6/6
26	CLA	A	610	1	-	1/26/102/115	-
28	BCR	t	101	-	-	3/29/63/63	0/2/2/2
30	STE	E	104	-	-	8/17/17/17	-
30	STE	T	102	-	-	11/13/13/17	-
30	STE	d	410	-	-	5/17/17/17	-
30	STE	I	102	-	-	6/12/12/17	-
34	LHG	d	408	-	-	14/53/53/53	-
28	BCR	b	618	-	-	0/29/63/63	0/2/2/2
30	STE	A	620	-	-	6/8/8/17	-
26	CLA	B	604	2	-	10/39/115/115	-
30	STE	b	623	-	-	2/13/13/17	-
26	CLA	C	512	3	-	10/39/115/115	-
30	STE	b	625	-	-	3/8/8/17	-
30	STE	C	519	-	-	2/4/4/17	-
30	STE	C	516	-	-	4/11/11/17	-
30	STE	B	621	-	-	6/14/14/17	-
28	BCR	a	611	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HEM	F	101	6,5	-	3/14/54/54	-
31	LMG	D	406	-	-	24/45/65/70	0/1/1/1
26	CLA	b	615	2	-	6/39/115/115	-
26	CLA	c	505	3	-	7/39/115/115	-
26	CLA	B	616	2	-	7/33/109/115	-
26	CLA	C	503	3	-	3/39/115/115	-
30	STE	e	101	-	-	2/6/6/17	-
30	STE	A	613	-	-	3/6/6/17	-
26	CLA	a	608	37	-	5/39/115/115	-
26	CLA	B	613	2	-	12/39/115/115	-
30	STE	B	625	-	-	10/15/15/17	-
26	CLA	B	610	37	-	2/39/115/115	-
26	CLA	C	502	3	-	4/39/115/115	-
27	PHO	a	609	-	-	1/37/103/103	0/5/6/6
28	BCR	Z	101	-	-	5/29/63/63	0/2/2/2
26	CLA	b	601	37	-	11/39/115/115	-
26	CLA	b	613	2	-	4/39/115/115	-
32	SQD	a	615	-	-	18/49/69/69	0/1/1/1
33	DGD	C	521	-	-	20/51/91/95	0/2/2/2
26	CLA	B	609	2	-	4/39/115/115	-
30	STE	H	103	-	-	7/15/15/17	-
26	CLA	C	506	3	-	10/39/115/115	-
29	PL9	A	612	-	-	16/53/73/73	0/1/1/1
30	STE	k	103	-	-	5/11/11/17	-
30	STE	e	104	-	-	3/6/6/17	-
28	BCR	C	514	-	-	4/29/63/63	0/2/2/2
30	STE	B	626	-	-	4/9/9/17	-
26	CLA	c	508	3	-	8/38/114/115	-
31	LMG	A	615	-	-	15/43/63/70	0/1/1/1
35	HEM	f	101	6,5	-	2/14/54/54	-
26	CLA	b	616	2	-	5/33/109/115	-
30	STE	J	101	-	-	3/9/9/17	-
26	CLA	b	611	2	-	4/39/115/115	-
31	LMG	a	617	-	-	17/44/64/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	STE	M	102	-	-	8/12/12/17	-
26	CLA	B	608	2	-	4/39/115/115	-
30	STE	B	627	-	-	4/12/12/17	-
30	STE	M	103	-	-	4/7/7/17	-
26	CLA	B	612	2	-	8/39/115/115	-
30	STE	E	103	-	-	2/9/9/17	-
30	STE	i	101	-	-	6/9/9/17	-
31	LMG	a	616	-	-	24/50/70/70	0/1/1/1
31	LMG	c	522	-	-	18/43/63/70	0/1/1/1
26	CLA	A	608	37	-	2/39/115/115	-
26	CLA	c	510	3	-	4/39/115/115	-
28	BCR	d	404	-	-	2/29/63/63	0/2/2/2
31	LMG	c	521	-	-	17/41/61/70	0/1/1/1
34	LHG	l	101	-	-	12/53/53/53	-
28	BCR	B	619	-	-	1/29/63/63	0/2/2/2
28	BCR	c	514	-	-	1/29/63/63	0/2/2/2
29	PL9	D	405	-	-	5/53/73/73	0/1/1/1
26	CLA	B	615	2	-	13/39/115/115	-
32	SQD	F	102	-	-	11/28/48/69	0/1/1/1
28	BCR	b	617	-	-	2/29/63/63	0/2/2/2
32	SQD	D	410	-	-	16/47/67/69	0/1/1/1
28	BCR	K	101	-	-	3/29/63/63	0/2/2/2
28	BCR	k	102	-	-	3/29/63/63	0/2/2/2
30	STE	z	702	-	-	2/6/6/17	-
27	PHO	D	401	-	-	1/37/103/103	0/5/6/6
31	LMG	C	524	-	-	10/43/63/70	0/1/1/1
34	LHG	E	101	-	-	14/53/53/53	-
26	CLA	c	509	3	-	9/39/115/115	-
30	STE	C	525	-	-	3/9/9/17	-
26	CLA	b	602	2	-	7/39/115/115	-
30	STE	K	102	-	-	6/11/11/17	-
30	STE	T	103	-	-	7/12/12/17	-
30	STE	D	412	-	-	6/17/17/17	-
29	PL9	d	405	-	-	9/53/73/73	0/1/1/1
26	CLA	c	504	37	-	8/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	c	513	3	-	12/39/115/115	-
30	STE	b	621	-	-	7/17/17/17	-
30	STE	e	105	-	-	4/10/10/17	-
28	BCR	B	617	-	-	4/29/63/63	0/2/2/2
30	STE	a	618	-	-	6/9/9/17	-
33	DGD	h	101	-	-	12/51/91/95	0/2/2/2
36	HEC	v	201	16	1/1/7/7	4/14/54/54	-
28	BCR	k	101	-	-	4/29/63/63	0/2/2/2
30	STE	t	102	-	-	1/7/7/17	-
32	SQD	a	614	-	-	27/49/69/69	0/1/1/1
26	CLA	B	603	2	-	5/39/115/115	-
26	CLA	b	614	2	-	12/39/115/115	-
26	CLA	B	611	2	-	4/39/115/115	-
28	BCR	H	101	-	-	1/29/63/63	0/2/2/2
26	CLA	c	503	3	-	8/39/115/115	-
30	STE	Z	102	-	-	7/14/14/17	-
30	STE	d	406	-	-	9/17/17/17	-
28	BCR	x	101	-	-	1/29/63/63	0/2/2/2
30	STE	j	102	-	-	5/13/13/17	-
26	CLA	c	501	3	-	1/39/115/115	-
26	CLA	B	606	2	-	7/39/115/115	-
26	CLA	b	609	2	-	4/39/115/115	-
31	LMG	b	622	-	-	21/50/70/70	0/1/1/1
26	CLA	A	614	37	-	4/39/115/115	-
33	DGD	c	519	-	-	19/51/91/95	0/2/2/2
26	CLA	b	607	37	-	5/39/115/115	-
34	LHG	B	622	-	-	15/53/53/53	-
26	CLA	b	606	2	-	9/39/115/115	-
34	LHG	e	102	-	-	21/46/46/53	-
31	LMG	m	101	-	-	15/46/66/70	0/1/1/1
26	CLA	b	612	2	-	4/39/115/115	-
32	SQD	A	616	-	-	14/38/58/69	0/1/1/1
28	BCR	B	618	-	-	0/29/63/63	0/2/2/2
26	CLA	C	509	3	-	9/39/115/115	-
26	CLA	B	607	37	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	SQD	B	623	-	-	21/49/69/69	0/1/1/1
26	CLA	c	507	37	-	5/39/115/115	-
30	STE	A	618	-	-	2/5/5/17	-
26	CLA	B	601	37	-	22/39/115/115	-
30	STE	H	104	-	-	2/6/6/17	-
26	CLA	C	510	3	-	7/39/115/115	-
26	CLA	b	603	2	-	14/39/115/115	-
33	DGD	c	518	-	-	17/51/91/95	0/2/2/2
34	LHG	D	411	-	-	14/53/53/53	-
31	LMG	D	407	-	-	10/46/66/70	0/1/1/1
26	CLA	a	607	1	-	4/39/115/115	-
29	PL9	a	612	-	-	22/53/73/73	0/1/1/1
30	STE	C	518	-	-	1/2/2/17	-
26	CLA	d	402	4	-	6/39/115/115	-
30	STE	j	101	-	-	5/9/9/17	-
26	CLA	c	511	3	-	7/39/115/115	-
26	CLA	B	614	2	-	13/39/115/115	-
28	BCR	b	619	-	-	0/29/63/63	0/2/2/2
31	LMG	c	517	-	-	6/31/31/70	-
34	LHG	D	408	-	-	13/53/53/53	-
30	STE	d	412	-	-	9/17/17/17	-
26	CLA	A	607	1	-	4/39/115/115	-
30	STE	c	516	-	-	9/15/15/17	-
30	STE	B	624	-	-	4/11/11/17	-

All (634) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	401	PHO	C1B-C2B	9.66	1.50	1.39
27	a	609	PHO	C1B-C2B	9.01	1.49	1.39
27	D	401	PHO	C1B-C2B	9.00	1.49	1.39
27	d	401	PHO	C3B-C4B	8.75	1.50	1.41
27	A	609	PHO	C1B-C2B	8.62	1.49	1.39
27	D	401	PHO	C3B-C4B	8.30	1.49	1.41
27	A	609	PHO	C3B-C4B	7.91	1.49	1.41
36	v	201	HEC	C3D-C2D	7.74	1.53	1.36
27	a	609	PHO	C3B-C4B	7.68	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	511	CLA	MG-NA	7.50	2.24	2.06
36	V	201	HEC	C3D-C2D	7.38	1.52	1.36
26	b	606	CLA	MG-NA	6.65	2.22	2.06
26	B	604	CLA	MG-NA	6.56	2.21	2.06
26	B	606	CLA	MG-NA	6.27	2.21	2.06
26	C	503	CLA	MG-NA	6.17	2.20	2.06
26	B	616	CLA	MG-NA	5.99	2.20	2.06
26	d	403	CLA	MG-ND	-5.68	1.94	2.05
26	c	503	CLA	MG-NA	5.46	2.19	2.06
26	b	603	CLA	MG-NA	4.92	2.17	2.06
26	A	607	CLA	MG-NA	4.87	2.17	2.06
26	b	609	CLA	MG-NA	4.83	2.17	2.06
26	B	609	CLA	MG-NA	4.78	2.17	2.06
26	b	607	CLA	MG-NA	4.76	2.17	2.06
32	a	615	SQD	O48-C23	4.75	1.47	1.33
32	D	410	SQD	O48-C23	4.72	1.47	1.33
32	A	616	SQD	O48-C23	4.70	1.47	1.33
32	a	614	SQD	O48-C23	4.69	1.47	1.33
32	b	620	SQD	O48-C23	4.69	1.47	1.33
26	A	608	CLA	MG-NA	4.68	2.17	2.06
26	C	511	CLA	MG-NA	4.63	2.17	2.06
26	c	510	CLA	MG-NA	4.58	2.17	2.06
26	B	601	CLA	MG-NA	4.55	2.17	2.06
32	B	623	SQD	O48-C23	4.55	1.46	1.33
26	C	502	CLA	MG-NA	4.53	2.17	2.06
32	F	102	SQD	O48-C23	4.53	1.46	1.33
32	f	102	SQD	O48-C23	4.53	1.46	1.33
36	V	201	HEC	FE-ND	4.52	2.08	1.94
26	C	501	CLA	MG-NA	4.48	2.16	2.06
35	F	101	HEM	FE-NC	4.45	2.09	1.95
35	f	101	HEM	FE-NA	4.44	2.09	1.95
26	B	615	CLA	MG-NA	4.44	2.16	2.06
36	v	201	HEC	FE-ND	4.30	2.08	1.94
26	b	610	CLA	MG-NB	-4.29	1.97	2.05
26	a	608	CLA	MG-ND	-4.29	1.97	2.05
27	d	401	PHO	C1D-C2D	4.25	1.44	1.39
26	C	501	CLA	MG-ND	-4.23	1.97	2.05
27	A	609	PHO	C1D-C2D	4.21	1.44	1.39
27	D	401	PHO	C1D-C2D	4.19	1.44	1.39
26	b	615	CLA	MG-NB	4.16	2.14	2.05
26	b	605	CLA	MG-NA	4.15	2.16	2.06
26	B	605	CLA	MG-ND	4.06	2.13	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	609	PHO	C1D-C2D	4.02	1.44	1.39
26	B	603	CLA	MG-NA	3.96	2.15	2.06
26	a	610	CLA	C1D-ND	3.89	1.43	1.37
26	C	505	CLA	MG-NA	3.86	2.15	2.06
26	C	507	CLA	MG-NA	3.84	2.15	2.06
32	D	410	SQD	O47-C45	-3.82	1.37	1.46
29	D	405	PL9	C3-C4	-3.82	1.43	1.49
26	a	610	CLA	MG-ND	-3.77	1.98	2.05
26	B	616	CLA	C1D-ND	3.76	1.42	1.37
26	B	615	CLA	C1D-ND	3.73	1.42	1.37
32	A	616	SQD	O5-C1	3.70	1.51	1.41
26	b	604	CLA	MG-NA	3.68	2.15	2.06
26	B	613	CLA	MG-NA	3.68	2.15	2.06
32	a	614	SQD	O47-C45	-3.68	1.37	1.46
26	b	602	CLA	MG-ND	-3.68	1.98	2.05
26	b	604	CLA	C1D-ND	3.66	1.42	1.37
26	c	510	CLA	C1D-ND	3.65	1.42	1.37
26	B	604	CLA	C1D-ND	3.64	1.42	1.37
32	a	615	SQD	O5-C1	3.62	1.51	1.41
26	b	607	CLA	C1D-ND	3.62	1.42	1.37
26	B	610	CLA	C1D-ND	3.62	1.42	1.37
26	B	602	CLA	C1D-ND	3.61	1.42	1.37
26	b	610	CLA	C1D-ND	3.60	1.42	1.37
26	B	611	CLA	C1D-ND	3.59	1.42	1.37
32	A	616	SQD	O47-C45	-3.58	1.38	1.46
32	a	615	SQD	O47-C45	-3.58	1.38	1.46
26	A	607	CLA	C1D-ND	3.58	1.42	1.37
26	C	506	CLA	MG-NA	3.58	2.14	2.06
26	C	502	CLA	C1D-ND	3.57	1.42	1.37
26	b	614	CLA	C1D-ND	3.55	1.42	1.37
26	b	601	CLA	C1D-ND	3.54	1.42	1.37
32	B	623	SQD	O47-C45	-3.53	1.38	1.46
26	b	602	CLA	C1D-ND	3.53	1.42	1.37
26	C	510	CLA	C1D-ND	3.53	1.42	1.37
26	C	512	CLA	MG-NA	3.53	2.14	2.06
26	c	509	CLA	C1D-ND	3.52	1.42	1.37
26	d	402	CLA	C1D-ND	3.52	1.42	1.37
26	b	615	CLA	C1D-ND	3.52	1.42	1.37
26	b	613	CLA	C1D-ND	3.50	1.42	1.37
32	b	620	SQD	O5-C1	3.50	1.50	1.41
26	b	616	CLA	C1D-ND	3.50	1.42	1.37
26	C	504	CLA	MG-NA	3.49	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	511	CLA	C1D-ND	3.49	1.42	1.37
26	C	512	CLA	C1D-ND	3.49	1.42	1.37
26	c	509	CLA	MG-ND	-3.48	1.98	2.05
32	f	102	SQD	O47-C7	3.47	1.44	1.34
26	D	403	CLA	C1D-ND	3.47	1.42	1.37
26	C	506	CLA	C1D-ND	3.47	1.42	1.37
26	c	507	CLA	C1D-ND	3.46	1.42	1.37
26	c	506	CLA	MG-ND	-3.45	1.98	2.05
26	C	508	CLA	MG-NA	3.45	2.14	2.06
32	f	102	SQD	O47-C45	-3.44	1.38	1.46
32	A	616	SQD	O47-C7	3.43	1.44	1.34
32	b	620	SQD	O47-C45	-3.43	1.38	1.46
26	B	603	CLA	C1D-ND	3.43	1.42	1.37
26	c	502	CLA	C1D-ND	3.42	1.42	1.37
26	c	503	CLA	C1D-ND	3.41	1.42	1.37
26	C	505	CLA	C1D-ND	3.41	1.42	1.37
26	a	607	CLA	C1D-ND	3.41	1.42	1.37
26	C	507	CLA	C1D-ND	3.40	1.42	1.37
26	d	403	CLA	C1D-ND	3.40	1.42	1.37
36	v	201	HEC	FE-NA	3.39	2.06	1.95
26	c	501	CLA	C1D-ND	3.39	1.42	1.37
26	B	601	CLA	C1D-ND	3.38	1.42	1.37
32	a	614	SQD	O47-C7	3.38	1.43	1.34
26	B	606	CLA	C1D-ND	3.37	1.42	1.37
35	f	101	HEM	FE-NB	3.37	2.05	1.94
26	A	608	CLA	C1D-ND	3.37	1.42	1.37
26	C	501	CLA	C1D-ND	3.36	1.42	1.37
26	c	506	CLA	C1D-ND	3.36	1.42	1.37
26	B	614	CLA	C1D-ND	3.35	1.42	1.37
26	a	613	CLA	C1D-ND	3.35	1.42	1.37
32	D	410	SQD	O5-C1	3.34	1.50	1.41
26	b	612	CLA	C1D-ND	3.34	1.42	1.37
32	a	614	SQD	O5-C1	3.34	1.50	1.41
26	A	614	CLA	C1D-ND	3.33	1.42	1.37
26	c	511	CLA	C1D-ND	3.33	1.42	1.37
26	c	513	CLA	C1D-ND	3.32	1.42	1.37
26	C	508	CLA	MG-ND	3.32	2.12	2.05
32	b	620	SQD	O47-C7	3.32	1.43	1.34
27	a	609	PHO	C4D-CHA	3.31	1.44	1.39
27	d	401	PHO	C4D-CHA	3.30	1.44	1.39
26	B	612	CLA	MG-NA	3.29	2.14	2.06
26	b	612	CLA	MG-ND	-3.29	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	610	CLA	C1D-ND	3.29	1.42	1.37
26	B	609	CLA	C1D-ND	3.27	1.42	1.37
26	B	615	CLA	C4B-NB	3.26	1.42	1.37
26	b	613	CLA	C4B-NB	3.26	1.42	1.37
26	b	607	CLA	MG-ND	-3.26	1.99	2.05
26	C	501	CLA	C4B-NB	3.26	1.42	1.37
26	c	505	CLA	C1D-ND	3.26	1.42	1.37
26	a	608	CLA	C4B-NB	3.25	1.42	1.37
26	C	507	CLA	MG-ND	-3.24	1.99	2.05
26	c	512	CLA	C1D-ND	3.23	1.42	1.37
32	a	615	SQD	O47-C7	3.23	1.43	1.34
36	V	201	HEC	FE-NB	3.23	2.04	1.94
26	C	513	CLA	C1D-ND	3.22	1.42	1.37
26	a	608	CLA	C1D-ND	3.21	1.42	1.37
26	B	610	CLA	C4B-NB	3.21	1.42	1.37
26	a	613	CLA	MG-NA	3.20	2.13	2.06
26	D	402	CLA	C1D-ND	3.20	1.42	1.37
26	C	504	CLA	C1D-ND	3.19	1.42	1.37
26	b	602	CLA	C4B-NB	3.19	1.42	1.37
26	B	608	CLA	C1D-ND	3.19	1.42	1.37
26	C	502	CLA	C4B-NB	3.19	1.42	1.37
26	B	615	CLA	MG-NC	3.19	2.13	2.06
27	A	609	PHO	C4D-CHA	3.18	1.44	1.39
26	b	609	CLA	C1D-ND	3.18	1.42	1.37
26	B	601	CLA	C4B-NB	3.18	1.42	1.37
26	B	614	CLA	C4B-NB	3.17	1.42	1.37
26	C	513	CLA	MG-ND	3.17	2.12	2.05
26	b	615	CLA	MG-NA	3.17	2.13	2.06
26	C	504	CLA	C4B-NB	3.17	1.42	1.37
26	C	509	CLA	C1D-ND	3.16	1.42	1.37
32	B	623	SQD	O47-C7	3.15	1.43	1.34
26	c	511	CLA	C4B-NB	3.15	1.42	1.37
26	b	606	CLA	C1D-ND	3.13	1.42	1.37
32	a	614	SQD	C24-C23	3.13	1.59	1.50
26	A	607	CLA	C1B-C2B	3.12	1.50	1.43
26	a	610	CLA	C4B-NB	3.12	1.42	1.37
26	B	613	CLA	C4B-NB	3.11	1.42	1.37
26	b	605	CLA	C4B-NB	3.11	1.41	1.37
26	b	608	CLA	C1D-ND	3.11	1.41	1.37
26	B	608	CLA	MG-NC	3.11	2.13	2.06
26	C	508	CLA	C1D-ND	3.10	1.41	1.37
26	b	601	CLA	C1B-C2B	3.10	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	620	SQD	C24-C23	3.10	1.59	1.50
32	F	102	SQD	C24-C23	3.09	1.59	1.50
26	c	508	CLA	C1D-ND	3.09	1.41	1.37
32	A	616	SQD	C24-C23	3.09	1.59	1.50
26	B	604	CLA	C4B-NB	3.09	1.41	1.37
26	B	613	CLA	C1D-ND	3.08	1.41	1.37
26	b	601	CLA	C4B-NB	3.08	1.41	1.37
26	b	603	CLA	C1D-ND	3.08	1.41	1.37
32	f	102	SQD	C24-C23	3.08	1.59	1.50
26	c	509	CLA	MG-NC	3.08	2.13	2.06
32	a	615	SQD	C24-C23	3.07	1.59	1.50
26	b	614	CLA	C4B-NB	3.07	1.41	1.37
26	B	605	CLA	C4B-NB	3.07	1.41	1.37
32	D	410	SQD	O47-C7	3.07	1.42	1.34
26	c	504	CLA	C4B-NB	3.06	1.41	1.37
26	b	603	CLA	C4B-NB	3.06	1.41	1.37
26	B	603	CLA	C4B-NB	3.05	1.41	1.37
26	c	508	CLA	C4B-NB	3.05	1.41	1.37
26	b	605	CLA	C1D-ND	3.05	1.41	1.37
26	b	606	CLA	C4B-NB	3.04	1.41	1.37
26	c	503	CLA	C4B-NB	3.04	1.41	1.37
26	c	503	CLA	C1B-C2B	3.04	1.50	1.43
26	C	503	CLA	C1D-ND	3.04	1.41	1.37
29	D	405	PL9	C6-C1	-3.04	1.43	1.48
26	b	604	CLA	C4B-NB	3.03	1.41	1.37
26	c	504	CLA	MG-NA	3.03	2.13	2.06
26	B	607	CLA	C1B-C2B	3.02	1.50	1.43
26	B	615	CLA	C1B-C2B	3.02	1.50	1.43
26	B	612	CLA	C1B-C2B	3.02	1.50	1.43
32	F	102	SQD	O5-C1	3.01	1.49	1.41
26	B	606	CLA	MG-NB	3.01	2.11	2.05
26	A	607	CLA	MG-NB	3.01	2.11	2.05
35	F	101	HEM	FE-NB	3.01	2.04	1.94
26	B	606	CLA	C1B-C2B	3.00	1.50	1.43
32	B	623	SQD	C24-C23	3.00	1.59	1.50
26	b	611	CLA	C1D-ND	3.00	1.41	1.37
26	C	513	CLA	MG-NB	-2.99	1.99	2.05
26	C	511	CLA	C1B-C2B	2.99	1.50	1.43
26	C	511	CLA	C4B-NB	2.99	1.41	1.37
26	B	612	CLA	C4B-NB	2.98	1.41	1.37
32	B	623	SQD	O5-C1	2.98	1.49	1.41
26	B	610	CLA	MG-NA	2.97	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	507	CLA	C1B-C2B	2.97	1.50	1.43
26	C	512	CLA	C4B-NB	2.97	1.41	1.37
26	B	611	CLA	C1B-C2B	2.96	1.50	1.43
26	b	615	CLA	C4B-NB	2.96	1.41	1.37
26	c	504	CLA	C1D-ND	2.96	1.41	1.37
26	c	509	CLA	C4B-NB	2.96	1.41	1.37
32	D	410	SQD	C24-C23	2.96	1.59	1.50
26	a	610	CLA	C1B-C2B	2.95	1.50	1.43
26	D	402	CLA	MG-NA	2.95	2.13	2.06
32	f	102	SQD	O5-C1	2.94	1.49	1.41
26	B	612	CLA	C1D-ND	2.94	1.41	1.37
26	b	611	CLA	C1B-C2B	2.93	1.50	1.43
26	C	507	CLA	C4B-NB	2.93	1.41	1.37
29	d	405	PL9	C6-C1	-2.93	1.43	1.48
26	C	508	CLA	C4B-NB	2.92	1.41	1.37
26	C	508	CLA	C1B-C2B	2.92	1.50	1.43
26	C	510	CLA	C1B-C2B	2.92	1.50	1.43
26	c	508	CLA	C1B-C2B	2.92	1.50	1.43
26	C	513	CLA	C1B-C2B	2.92	1.50	1.43
26	b	606	CLA	C1B-C2B	2.92	1.50	1.43
26	c	506	CLA	C4B-NB	2.91	1.41	1.37
35	f	101	HEM	CAC-C3C	2.91	1.55	1.47
26	c	510	CLA	C1B-C2B	2.90	1.49	1.43
26	A	614	CLA	C4B-NB	2.90	1.41	1.37
26	D	402	CLA	C1B-C2B	2.90	1.49	1.43
26	C	510	CLA	C4B-NB	2.89	1.41	1.37
26	B	602	CLA	C1B-C2B	2.89	1.49	1.43
26	a	607	CLA	C1B-C2B	2.89	1.49	1.43
26	c	501	CLA	C1B-C2B	2.89	1.49	1.43
26	c	509	CLA	C1B-C2B	2.89	1.49	1.43
26	c	513	CLA	C4B-NB	2.89	1.41	1.37
26	B	602	CLA	C4B-NB	2.88	1.41	1.37
26	c	501	CLA	C4B-NB	2.88	1.41	1.37
26	a	613	CLA	C4B-NB	2.88	1.41	1.37
26	a	607	CLA	MG-NB	2.87	2.11	2.05
26	c	507	CLA	C4B-NB	2.87	1.41	1.37
26	B	607	CLA	C1D-ND	2.87	1.41	1.37
26	d	403	CLA	C4B-NB	2.87	1.41	1.37
26	B	605	CLA	C1D-ND	2.87	1.41	1.37
26	C	506	CLA	C4B-NB	2.87	1.41	1.37
35	F	101	HEM	CAB-C3B	2.87	1.55	1.47
26	a	607	CLA	C4B-NB	2.87	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	609	PHO	CBD-CGD	-2.86	1.48	1.52
26	A	608	CLA	C4B-NB	2.86	1.41	1.37
26	b	607	CLA	C4B-NB	2.86	1.41	1.37
26	B	605	CLA	C1B-C2B	2.85	1.49	1.43
26	B	613	CLA	C1B-C2B	2.85	1.49	1.43
26	C	505	CLA	C1B-C2B	2.85	1.49	1.43
26	B	616	CLA	MG-NB	-2.85	2.00	2.05
26	A	608	CLA	C1B-C2B	2.84	1.49	1.43
27	a	609	PHO	C3D-C4D	2.84	1.45	1.41
26	b	611	CLA	MG-NA	2.84	2.13	2.06
26	c	501	CLA	MG-NA	2.84	2.13	2.06
26	C	503	CLA	C1B-C2B	2.84	1.49	1.43
26	c	505	CLA	C4B-NB	2.84	1.41	1.37
26	C	507	CLA	C1B-C2B	2.84	1.49	1.43
26	B	616	CLA	C1B-C2B	2.84	1.49	1.43
26	C	509	CLA	C1B-C2B	2.84	1.49	1.43
26	B	607	CLA	C4B-NB	2.83	1.41	1.37
26	b	613	CLA	MG-NA	2.83	2.13	2.06
26	d	403	CLA	C1B-C2B	2.83	1.49	1.43
26	C	509	CLA	C4B-NB	2.83	1.41	1.37
26	a	607	CLA	MG-NA	2.82	2.13	2.06
26	D	402	CLA	C4B-NB	2.82	1.41	1.37
26	b	615	CLA	C1B-C2B	2.82	1.49	1.43
26	b	605	CLA	C1B-C2B	2.81	1.49	1.43
26	b	604	CLA	C1B-C2B	2.81	1.49	1.43
26	b	612	CLA	C4B-NB	2.81	1.41	1.37
26	C	505	CLA	C4B-NB	2.79	1.41	1.37
26	b	611	CLA	C4B-NB	2.79	1.41	1.37
35	f	101	HEM	CAB-C3B	2.79	1.54	1.47
26	b	614	CLA	MG-NA	2.79	2.12	2.06
26	B	606	CLA	C4B-NB	2.79	1.41	1.37
26	c	502	CLA	C1B-C2B	2.79	1.49	1.43
26	B	611	CLA	MG-NA	2.78	2.12	2.06
26	C	513	CLA	MG-NA	2.78	2.12	2.06
26	b	613	CLA	C1B-C2B	2.77	1.49	1.43
26	d	402	CLA	C1B-C2B	2.77	1.49	1.43
26	C	502	CLA	C1B-C2B	2.77	1.49	1.43
26	B	608	CLA	C4B-NB	2.77	1.41	1.37
26	B	611	CLA	C4B-NB	2.77	1.41	1.37
26	b	608	CLA	C4B-NB	2.77	1.41	1.37
26	c	510	CLA	C4B-NB	2.76	1.41	1.37
26	B	603	CLA	C1B-C2B	2.76	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	513	CLA	C1B-C2B	2.76	1.49	1.43
26	b	609	CLA	C4B-NB	2.76	1.41	1.37
26	C	501	CLA	C1B-C2B	2.76	1.49	1.43
27	A	609	PHO	C3D-C4D	2.76	1.45	1.41
29	a	612	PL9	C53-C6	-2.75	1.45	1.50
26	a	613	CLA	MG-NC	2.75	2.12	2.06
26	C	513	CLA	C4B-NB	2.75	1.41	1.37
26	D	403	CLA	C1B-C2B	2.75	1.49	1.43
26	c	504	CLA	C1B-C2B	2.75	1.49	1.43
27	A	609	PHO	CBD-CGD	-2.74	1.49	1.52
26	b	614	CLA	C1B-C2B	2.74	1.49	1.43
26	A	610	CLA	C1B-C2B	2.74	1.49	1.43
26	b	607	CLA	C1B-C2B	2.73	1.49	1.43
26	c	506	CLA	C1B-C2B	2.73	1.49	1.43
26	B	601	CLA	C1B-C2B	2.73	1.49	1.43
26	b	616	CLA	C1B-C2B	2.73	1.49	1.43
26	b	602	CLA	C1B-C2B	2.72	1.49	1.43
27	D	401	PHO	C4D-CHA	2.72	1.43	1.39
26	A	614	CLA	MG-NA	2.72	2.12	2.06
26	B	608	CLA	MG-NA	2.72	2.12	2.06
26	c	512	CLA	C4B-NB	2.72	1.41	1.37
35	F	101	HEM	CAC-C3C	2.72	1.54	1.47
29	d	405	PL9	C3-C4	-2.72	1.45	1.49
26	b	608	CLA	MG-NA	2.71	2.12	2.06
26	C	508	CLA	C3B-C4B	2.71	1.50	1.42
26	A	610	CLA	C4B-NB	2.71	1.41	1.37
26	c	512	CLA	C1B-C2B	2.69	1.49	1.43
26	c	502	CLA	C4B-NB	2.69	1.41	1.37
26	c	511	CLA	C1B-C2B	2.69	1.49	1.43
26	B	609	CLA	C4B-NB	2.69	1.41	1.37
26	C	512	CLA	C1B-C2B	2.68	1.49	1.43
26	A	614	CLA	C3B-C4B	2.68	1.50	1.42
26	b	610	CLA	C4B-NB	2.68	1.41	1.37
26	b	603	CLA	C1B-C2B	2.67	1.49	1.43
26	b	610	CLA	C1B-C2B	2.67	1.49	1.43
26	C	503	CLA	C4B-NB	2.66	1.41	1.37
26	b	616	CLA	C4B-NB	2.66	1.41	1.37
26	B	616	CLA	C4B-NB	2.66	1.41	1.37
27	D	401	PHO	C4D-ND	-2.65	1.34	1.38
27	a	609	PHO	CMC-C2C	-2.65	1.46	1.50
26	b	615	CLA	C3B-C4B	2.65	1.50	1.42
26	B	607	CLA	MG-NA	2.65	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	610	CLA	C1B-C2B	2.65	1.49	1.43
26	B	604	CLA	C1B-C2B	2.64	1.49	1.43
26	D	403	CLA	C4B-NB	2.64	1.41	1.37
26	C	506	CLA	C1B-C2B	2.63	1.49	1.43
29	D	405	PL9	C52-C5	-2.63	1.45	1.50
26	A	607	CLA	C4B-NB	2.63	1.41	1.37
26	B	609	CLA	C1B-C2B	2.63	1.49	1.43
26	c	504	CLA	MG-NB	2.63	2.11	2.05
26	b	609	CLA	C1B-C2B	2.62	1.49	1.43
26	B	614	CLA	C1B-C2B	2.62	1.49	1.43
26	b	608	CLA	CHC-C1C	2.62	1.43	1.38
26	A	614	CLA	CHC-C1C	2.61	1.43	1.38
26	A	614	CLA	C1B-C2B	2.60	1.49	1.43
26	b	602	CLA	MG-NC	2.60	2.12	2.06
26	C	510	CLA	CHC-C1C	2.59	1.43	1.38
26	B	605	CLA	C3B-C4B	2.59	1.50	1.42
26	B	614	CLA	MG-NA	2.59	2.12	2.06
26	C	504	CLA	C1B-C2B	2.59	1.49	1.43
26	a	613	CLA	C1B-C2B	2.58	1.49	1.43
27	A	609	PHO	CMD-C2D	-2.58	1.46	1.51
26	C	509	CLA	MG-NB	-2.58	2.00	2.05
26	d	402	CLA	C4B-NB	2.57	1.41	1.37
26	C	510	CLA	C3B-C4B	2.57	1.50	1.42
26	c	513	CLA	C3B-C4B	2.56	1.50	1.42
26	c	505	CLA	C1B-C2B	2.56	1.49	1.43
26	c	508	CLA	CHC-C1C	2.55	1.43	1.38
26	c	508	CLA	C3B-C4B	2.55	1.50	1.42
26	a	610	CLA	MG-NA	2.55	2.12	2.06
26	A	607	CLA	C3B-C4B	2.55	1.50	1.42
26	b	611	CLA	C3B-C4B	2.55	1.50	1.42
27	D	401	PHO	CMC-C2C	-2.55	1.46	1.50
26	C	512	CLA	MG-NC	2.54	2.12	2.06
26	B	610	CLA	C3B-C4B	2.54	1.50	1.42
27	D	401	PHO	CMB-C2B	-2.54	1.46	1.51
27	a	609	PHO	CMB-C2B	-2.54	1.46	1.51
26	B	614	CLA	CHC-C1C	2.53	1.43	1.38
26	a	608	CLA	CHC-C1C	2.53	1.43	1.38
27	d	401	PHO	C4D-ND	-2.53	1.34	1.38
27	d	401	PHO	CMC-C2C	-2.53	1.46	1.50
26	C	509	CLA	MG-NA	2.52	2.12	2.06
26	b	612	CLA	C1B-C2B	2.52	1.49	1.43
26	a	608	CLA	C1B-C2B	2.50	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	512	CLA	CHC-C1C	2.49	1.43	1.38
26	C	512	CLA	C3B-C4B	2.49	1.50	1.42
26	b	608	CLA	C1B-C2B	2.48	1.49	1.43
26	b	608	CLA	C3B-C4B	2.48	1.50	1.42
26	a	607	CLA	C3B-C4B	2.48	1.49	1.42
35	f	101	HEM	FE-ND	2.48	2.02	1.94
27	D	401	PHO	CMD-C2D	-2.47	1.46	1.51
26	B	614	CLA	MG-ND	-2.47	2.00	2.05
26	B	602	CLA	MG-NC	2.47	2.12	2.06
26	b	605	CLA	C3B-C4B	2.47	1.49	1.42
26	a	608	CLA	C3B-C4B	2.47	1.49	1.42
26	b	614	CLA	C3B-C4B	2.47	1.49	1.42
26	c	501	CLA	MG-NB	-2.46	2.00	2.05
26	c	505	CLA	C3B-C4B	2.45	1.49	1.42
26	C	508	CLA	CHC-C1C	2.45	1.43	1.38
27	a	609	PHO	CMD-C2D	-2.45	1.46	1.51
26	b	613	CLA	C3B-C4B	2.45	1.49	1.42
26	c	505	CLA	CHC-C1C	2.45	1.43	1.38
26	B	604	CLA	MG-ND	-2.44	2.00	2.05
26	b	614	CLA	CHC-C1C	2.44	1.43	1.38
26	a	613	CLA	C3B-C4B	2.44	1.49	1.42
27	A	609	PHO	C4D-ND	-2.44	1.34	1.38
29	A	612	PL9	C53-C6	-2.42	1.45	1.50
26	A	607	CLA	CHC-C1C	2.41	1.43	1.38
26	c	502	CLA	MG-NA	2.41	2.12	2.06
27	A	609	PHO	CMC-C2C	-2.41	1.46	1.50
26	A	608	CLA	C3B-C4B	2.41	1.49	1.42
35	f	101	HEM	FE-NC	2.40	2.03	1.95
26	c	512	CLA	C3B-C4B	2.40	1.49	1.42
26	b	613	CLA	CHC-C1C	2.40	1.43	1.38
27	d	401	PHO	CMD-C2D	-2.40	1.46	1.51
26	C	504	CLA	C3B-C4B	2.39	1.49	1.42
26	b	611	CLA	CHC-C1C	2.39	1.43	1.38
26	b	604	CLA	C3B-C4B	2.39	1.49	1.42
26	d	402	CLA	MG-NA	2.39	2.11	2.06
27	a	609	PHO	CAC-C3C	-2.38	1.47	1.51
26	c	511	CLA	CHC-C1C	2.38	1.43	1.38
26	C	510	CLA	MG-NC	2.38	2.11	2.06
26	c	511	CLA	C3B-C4B	2.38	1.49	1.42
32	A	616	SQD	O7-S	2.37	1.51	1.45
32	a	615	SQD	O9-S	2.37	1.51	1.45
26	C	511	CLA	C3B-C4B	2.37	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	615	SQD	O7-S	2.37	1.51	1.45
32	A	616	SQD	O9-S	2.37	1.51	1.45
26	C	501	CLA	C3B-C4B	2.36	1.49	1.42
26	B	608	CLA	C1B-C2B	2.36	1.48	1.43
26	B	602	CLA	C3B-C4B	2.36	1.49	1.42
26	B	604	CLA	C3B-C4B	2.35	1.49	1.42
27	a	609	PHO	C4D-ND	-2.35	1.35	1.38
26	d	403	CLA	C3B-C4B	2.34	1.49	1.42
26	C	504	CLA	CHC-C1C	2.34	1.43	1.38
26	B	603	CLA	C3B-C4B	2.34	1.49	1.42
27	d	401	PHO	CMB-C2B	-2.34	1.47	1.51
26	d	403	CLA	MG-NA	2.33	2.11	2.06
32	A	616	SQD	O5-C5	2.32	1.50	1.44
26	a	608	CLA	MG-NB	2.32	2.10	2.05
26	B	613	CLA	CHC-C1C	2.32	1.43	1.38
32	b	620	SQD	O9-S	2.32	1.51	1.45
26	C	506	CLA	C3B-C4B	2.32	1.49	1.42
26	C	502	CLA	MG-ND	-2.31	2.01	2.05
26	A	610	CLA	MG-NB	-2.30	2.01	2.05
26	a	607	CLA	CHC-C1C	2.30	1.43	1.38
26	C	506	CLA	CHC-C1C	2.30	1.43	1.38
26	D	402	CLA	CMD-C2D	-2.30	1.46	1.50
26	D	403	CLA	MG-ND	-2.30	2.01	2.05
26	A	608	CLA	CHC-C1C	2.29	1.43	1.38
32	f	102	SQD	O9-S	2.29	1.51	1.45
26	B	613	CLA	C3B-C4B	2.29	1.49	1.42
26	c	502	CLA	C3B-C4B	2.29	1.49	1.42
26	C	512	CLA	CHC-C1C	2.29	1.43	1.38
26	B	605	CLA	CHC-C1C	2.29	1.43	1.38
27	d	401	PHO	C3D-C4D	2.29	1.44	1.41
26	B	610	CLA	CHC-C1C	2.29	1.43	1.38
26	b	606	CLA	C3B-C4B	2.28	1.49	1.42
26	c	506	CLA	CHC-C1C	2.27	1.43	1.38
26	B	606	CLA	C3B-C4B	2.27	1.49	1.42
27	D	401	PHO	CAC-C3C	-2.27	1.47	1.51
26	c	503	CLA	CHC-C1C	2.27	1.43	1.38
29	a	612	PL9	C3-C4	-2.27	1.46	1.49
26	b	601	CLA	C3B-C4B	2.26	1.49	1.42
32	B	623	SQD	O9-S	2.26	1.51	1.45
26	C	505	CLA	C3B-C4B	2.25	1.49	1.42
26	C	501	CLA	CHC-C1C	2.24	1.43	1.38
26	C	501	CLA	CMD-C2D	-2.24	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	513	CLA	CHC-C1C	2.24	1.43	1.38
26	b	612	CLA	C3B-C4B	2.24	1.49	1.42
26	b	603	CLA	C3B-C4B	2.24	1.49	1.42
26	B	611	CLA	C3B-C4B	2.23	1.49	1.42
26	C	509	CLA	C3B-C4B	2.23	1.49	1.42
26	d	403	CLA	CMD-C2D	-2.23	1.46	1.50
26	b	605	CLA	CHC-C1C	2.23	1.43	1.38
26	c	503	CLA	C3B-C4B	2.23	1.49	1.42
26	C	504	CLA	CMB-C2B	-2.23	1.46	1.50
26	b	609	CLA	C3B-C4B	2.23	1.49	1.42
26	b	601	CLA	CHC-C1C	2.23	1.43	1.38
26	B	612	CLA	C3B-C4B	2.23	1.49	1.42
26	c	507	CLA	MG-NB	-2.23	2.01	2.05
26	D	403	CLA	MG-NA	2.23	2.11	2.06
26	c	504	CLA	C3B-C4B	2.23	1.49	1.42
26	a	608	CLA	CMB-C2B	-2.22	1.46	1.50
32	a	614	SQD	O9-S	2.21	1.51	1.45
32	a	614	SQD	O7-S	2.21	1.51	1.45
26	B	616	CLA	C3B-C4B	2.21	1.49	1.42
26	c	504	CLA	CMB-C2B	-2.21	1.46	1.50
26	C	511	CLA	CHC-C1C	2.21	1.42	1.38
26	C	503	CLA	C3B-C4B	2.21	1.49	1.42
26	C	502	CLA	C3B-C4B	2.20	1.49	1.42
26	d	402	CLA	CMB-C2B	-2.20	1.46	1.50
26	c	506	CLA	C3B-C4B	2.20	1.49	1.42
26	c	510	CLA	CHC-C1C	2.20	1.42	1.38
26	C	513	CLA	C3B-C4B	2.20	1.49	1.42
27	D	401	PHO	C3D-C4D	2.19	1.44	1.41
26	b	616	CLA	MG-NC	2.19	2.11	2.06
26	c	504	CLA	CHC-C1C	2.19	1.42	1.38
29	d	405	PL9	C53-C6	-2.19	1.46	1.50
26	B	613	CLA	CMD-C2D	-2.19	1.46	1.50
26	b	602	CLA	C3B-C4B	2.18	1.49	1.42
35	F	101	HEM	FE-NA	2.18	2.02	1.95
26	d	402	CLA	C3B-C4B	2.18	1.49	1.42
26	b	606	CLA	CHC-C1C	2.18	1.42	1.38
26	B	601	CLA	C3B-C4B	2.18	1.49	1.42
26	C	502	CLA	CHC-C1C	2.18	1.42	1.38
26	b	611	CLA	CMD-C2D	-2.17	1.46	1.50
26	B	606	CLA	CHC-C1C	2.17	1.42	1.38
26	c	512	CLA	CMD-C2D	-2.17	1.46	1.50
26	B	607	CLA	CMD-C2D	-2.17	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	604	CLA	MG-NC	2.17	2.11	2.06
27	A	609	PHO	CAC-C3C	-2.17	1.47	1.51
26	C	503	CLA	CHC-C1C	2.16	1.42	1.38
26	a	610	CLA	CMB-C2B	-2.16	1.46	1.50
26	b	610	CLA	CMB-C2B	-2.16	1.46	1.50
26	B	601	CLA	CMB-C2B	-2.16	1.46	1.50
26	B	603	CLA	CMD-C2D	-2.16	1.46	1.50
26	B	614	CLA	C3B-C4B	2.16	1.49	1.42
26	B	616	CLA	CHC-C1C	2.16	1.42	1.38
26	B	611	CLA	CMB-C2B	-2.16	1.46	1.50
26	b	615	CLA	CHC-C1C	2.16	1.42	1.38
26	c	510	CLA	CMB-C2B	-2.15	1.46	1.50
32	D	410	SQD	O9-S	2.15	1.51	1.45
26	c	505	CLA	CMB-C2B	-2.15	1.46	1.50
32	f	102	SQD	O7-S	2.15	1.51	1.45
26	b	604	CLA	CHC-C1C	2.15	1.42	1.38
26	C	502	CLA	CMB-C2B	-2.15	1.46	1.50
27	A	609	PHO	CMB-C2B	-2.15	1.47	1.51
26	b	607	CLA	C3B-C4B	2.14	1.49	1.42
26	B	615	CLA	CMB-C2B	-2.14	1.46	1.50
32	b	620	SQD	O7-S	2.14	1.51	1.45
26	c	510	CLA	C3B-C4B	2.14	1.49	1.42
26	C	505	CLA	CMB-C2B	-2.14	1.46	1.50
26	b	602	CLA	CMB-C2B	-2.14	1.46	1.50
26	B	608	CLA	C3B-C4B	2.14	1.49	1.42
26	c	502	CLA	CHC-C1C	2.14	1.42	1.38
26	B	602	CLA	MG-NA	2.13	2.11	2.06
32	F	102	SQD	O9-S	2.13	1.51	1.45
26	b	603	CLA	CHC-C1C	2.13	1.42	1.38
26	b	610	CLA	CMD-C2D	-2.13	1.46	1.50
36	V	201	HEC	CMB-C2B	2.13	1.55	1.50
33	C	521	DGD	O3G-C3G	-2.13	1.40	1.43
26	A	614	CLA	MG-NB	2.13	2.10	2.05
26	B	607	CLA	C3B-C4B	2.12	1.48	1.42
32	B	623	SQD	O7-S	2.12	1.51	1.45
27	d	401	PHO	C3B-C2B	-2.12	1.37	1.40
26	b	602	CLA	CHC-C1C	2.12	1.42	1.38
26	B	602	CLA	CHC-C1C	2.12	1.42	1.38
26	B	601	CLA	CMC-C2C	-2.12	1.46	1.50
26	B	612	CLA	CMC-C2C	-2.11	1.46	1.50
26	c	513	CLA	CMB-C2B	-2.11	1.46	1.50
29	d	405	PL9	C52-C5	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	604	CLA	CHC-C1C	2.11	1.42	1.38
26	d	403	CLA	MG-NB	2.11	2.10	2.05
26	c	502	CLA	CMD-C2D	-2.11	1.46	1.50
26	b	612	CLA	CMC-C2C	-2.11	1.46	1.50
26	D	403	CLA	CMD-C2D	-2.11	1.46	1.50
26	c	501	CLA	C3B-C4B	2.10	1.48	1.42
27	D	401	PHO	C3B-C2B	-2.10	1.37	1.40
26	D	402	CLA	C3B-C4B	2.09	1.48	1.42
29	D	405	PL9	C7-C8	-2.09	1.47	1.50
26	C	510	CLA	CMD-C2D	-2.09	1.46	1.50
26	C	505	CLA	CHC-C1C	2.09	1.42	1.38
26	c	509	CLA	CMB-C2B	-2.09	1.46	1.50
26	b	603	CLA	CMB-C2B	-2.09	1.46	1.50
26	C	511	CLA	CMD-C2D	-2.09	1.46	1.50
33	c	519	DGD	O3G-C3G	-2.09	1.40	1.43
26	B	602	CLA	CMB-C2B	-2.08	1.46	1.50
26	B	612	CLA	CMB-C2B	-2.08	1.46	1.50
26	b	604	CLA	C3D-C4D	2.08	1.48	1.44
26	C	509	CLA	CMB-C2B	-2.08	1.46	1.50
26	B	607	CLA	CMB-C2B	-2.07	1.46	1.50
26	c	509	CLA	C3B-C4B	2.07	1.48	1.42
35	f	101	HEM	C2A-C3A	-2.07	1.33	1.38
26	B	609	CLA	CMD-C2D	-2.07	1.46	1.50
26	A	614	CLA	CMD-C2D	-2.06	1.46	1.50
26	D	403	CLA	CMB-C2B	-2.06	1.46	1.50
26	a	610	CLA	CMC-C2C	-2.06	1.46	1.50
26	b	601	CLA	MG-NA	2.06	2.11	2.06
26	A	614	CLA	CMB-C2B	-2.06	1.46	1.50
26	c	507	CLA	C3B-C4B	2.06	1.48	1.42
26	b	603	CLA	CMD-C2D	-2.06	1.46	1.50
26	C	507	CLA	CMB-C2B	-2.06	1.46	1.50
26	c	512	CLA	CMB-C2B	-2.06	1.46	1.50
26	B	601	CLA	CHC-C1C	2.05	1.42	1.38
26	C	513	CLA	CMB-C2B	-2.05	1.46	1.50
26	C	511	CLA	CMB-C2B	-2.05	1.46	1.50
26	B	608	CLA	CHC-C1C	2.05	1.42	1.38
26	b	615	CLA	CMD-C2D	-2.05	1.46	1.50
26	b	613	CLA	CMD-C2D	-2.05	1.46	1.50
26	c	503	CLA	CMB-C2B	-2.05	1.46	1.50
32	F	102	SQD	O7-S	2.05	1.50	1.45
26	a	613	CLA	CMB-C2B	-2.05	1.46	1.50
26	c	501	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	612	CLA	CHC-C1C	2.04	1.42	1.38
26	b	602	CLA	CMD-C2D	-2.04	1.46	1.50
26	b	605	CLA	CMB-C2B	-2.04	1.46	1.50
26	B	615	CLA	CMD-C2D	-2.04	1.46	1.50
26	B	612	CLA	CHC-C1C	2.04	1.42	1.38
26	c	510	CLA	CMC-C2C	-2.04	1.46	1.50
26	b	612	CLA	CMB-C2B	-2.04	1.46	1.50
33	C	523	DGD	O3G-C3G	-2.04	1.40	1.43
26	D	403	CLA	MG-NC	2.04	2.11	2.06
26	B	614	CLA	CMB-C2B	-2.04	1.46	1.50
35	f	101	HEM	CMC-C2C	2.03	1.54	1.50
26	B	603	CLA	MG-NC	2.03	2.11	2.06
26	A	610	CLA	CMD-C2D	-2.03	1.46	1.50
32	a	615	SQD	O5-C5	2.03	1.49	1.44
31	a	617	LMG	O1-C7	-2.03	1.40	1.43
26	d	403	CLA	CHC-C1C	2.03	1.42	1.38
26	c	501	CLA	CMB-C2B	-2.02	1.46	1.50
26	c	508	CLA	CMC-C2C	-2.02	1.46	1.50
26	B	613	CLA	CMB-C2B	-2.02	1.46	1.50
26	c	507	CLA	CMC-C2C	-2.02	1.46	1.50
26	b	616	CLA	CMB-C2B	-2.02	1.46	1.50
26	b	610	CLA	C3B-C4B	2.02	1.48	1.42
26	C	509	CLA	CMD-C2D	-2.02	1.46	1.50
26	B	605	CLA	CMB-C2B	-2.02	1.46	1.50
35	F	101	HEM	CMC-C2C	2.02	1.54	1.50
26	C	512	CLA	CMB-C2B	-2.02	1.46	1.50
26	c	507	CLA	CMD-C2D	-2.02	1.46	1.50
26	C	503	CLA	CMD-C2D	-2.01	1.46	1.50
26	c	513	CLA	CMD-C2D	-2.01	1.46	1.50
26	c	509	CLA	CMD-C2D	-2.01	1.46	1.50
26	b	615	CLA	CMB-C2B	-2.01	1.46	1.50
26	B	615	CLA	CHC-C1C	2.01	1.42	1.38
26	a	613	CLA	CHC-C1C	2.01	1.42	1.38
26	b	616	CLA	C3B-C4B	2.00	1.48	1.42
26	b	606	CLA	CMD-C2D	-2.00	1.46	1.50
27	a	609	PHO	C3B-C2B	-2.00	1.37	1.40
26	B	606	CLA	CMB-C2B	-2.00	1.46	1.50

All (702) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	609	PHO	C4D-CHA-CBD	-8.56	104.35	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	615	CLA	C4A-NA-C1A	8.21	110.42	106.68
27	a	609	PHO	C4D-CHA-CBD	-7.90	104.66	108.45
26	b	606	CLA	C4A-NA-C1A	7.50	110.10	106.68
26	b	601	CLA	C4A-NA-C1A	7.41	110.06	106.68
26	B	606	CLA	C4A-NA-C1A	7.34	110.03	106.68
26	C	511	CLA	C4A-NA-C1A	7.19	109.96	106.68
26	c	503	CLA	C4A-NA-C1A	7.12	109.93	106.68
26	c	501	CLA	C4A-NA-C1A	7.12	109.93	106.68
27	d	401	PHO	C4D-CHA-CBD	-7.09	105.05	108.45
26	c	509	CLA	C4A-NA-C1A	7.08	109.91	106.68
26	b	604	CLA	C4A-NA-C1A	7.01	109.88	106.68
26	B	611	CLA	C4A-NA-C1A	6.86	109.81	106.68
26	B	604	CLA	C4A-NA-C1A	6.81	109.78	106.68
26	C	502	CLA	C4A-NA-C1A	6.77	109.77	106.68
26	C	507	CLA	C4A-NA-C1A	6.67	109.72	106.68
26	c	507	CLA	C4A-NA-C1A	6.64	109.71	106.68
26	B	601	CLA	C4A-NA-C1A	6.51	109.65	106.68
26	A	614	CLA	C4A-NA-C1A	6.48	109.64	106.68
26	C	503	CLA	C4A-NA-C1A	6.40	109.60	106.68
26	C	508	CLA	C4A-NA-C1A	6.40	109.60	106.68
32	a	614	SQD	O6-C1-C2	6.36	117.93	108.27
26	C	510	CLA	C4A-NA-C1A	6.27	109.54	106.68
26	b	616	CLA	C4A-NA-C1A	6.23	109.52	106.68
26	B	613	CLA	C4A-NA-C1A	6.18	109.50	106.68
26	b	614	CLA	C4A-NA-C1A	6.15	109.48	106.68
26	a	607	CLA	C4A-NA-C1A	5.99	109.41	106.68
26	c	512	CLA	C4A-NA-C1A	5.98	109.41	106.68
29	a	612	PL9	C7-C3-C4	5.97	121.83	116.91
26	c	504	CLA	C4A-NA-C1A	5.97	109.40	106.68
26	B	608	CLA	C4A-NA-C1A	5.96	109.40	106.68
26	c	502	CLA	C4A-NA-C1A	5.94	109.39	106.68
27	D	401	PHO	C4D-CHA-CBD	-5.82	105.66	108.45
26	c	510	CLA	C4A-NA-C1A	5.82	109.33	106.68
26	b	615	CLA	C4A-NA-C1A	5.79	109.32	106.68
26	c	508	CLA	C4A-NA-C1A	5.74	109.30	106.68
32	D	410	SQD	O6-C1-C2	5.73	116.98	108.27
26	C	505	CLA	C4A-NA-C1A	5.68	109.27	106.68
26	B	612	CLA	C4A-NA-C1A	5.67	109.27	106.68
26	c	505	CLA	C4A-NA-C1A	5.65	109.26	106.68
26	C	509	CLA	C4A-NA-C1A	5.64	109.25	106.68
26	B	607	CLA	C4A-NA-C1A	5.59	109.23	106.68
26	b	609	CLA	C4A-NA-C1A	5.57	109.22	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	512	CLA	C4A-NA-C1A	5.52	109.20	106.68
26	B	616	CLA	C4A-NA-C1A	5.49	109.18	106.68
26	a	610	CLA	C4A-NA-C1A	5.49	109.18	106.68
26	d	402	CLA	C4A-NA-C1A	5.48	109.18	106.68
29	d	405	PL9	C7-C3-C4	5.47	121.42	116.91
26	b	611	CLA	C4A-NA-C1A	5.41	109.14	106.68
26	A	610	CLA	C4A-NA-C1A	5.40	109.14	106.68
28	d	404	BCR	C38-C26-C25	-5.35	118.65	124.48
26	D	402	CLA	C4A-NA-C1A	5.35	109.12	106.68
26	C	513	CLA	C4A-NA-C1A	5.32	109.11	106.68
32	a	614	SQD	C1-O5-C5	-5.29	103.39	113.72
26	c	511	CLA	C4A-NA-C1A	5.26	109.08	106.68
29	A	612	PL9	C7-C3-C4	5.26	121.24	116.91
26	B	610	CLA	C4A-NA-C1A	5.22	109.06	106.68
26	D	403	CLA	C4A-NA-C1A	5.20	109.05	106.68
32	D	410	SQD	C1-O5-C5	-5.15	103.66	113.72
26	C	504	CLA	C4A-NA-C1A	5.15	109.03	106.68
26	B	603	CLA	C4A-NA-C1A	5.12	109.02	106.68
26	b	605	CLA	C4A-NA-C1A	5.11	109.01	106.68
26	B	609	CLA	C4A-NA-C1A	5.02	108.97	106.68
36	V	201	HEC	C1D-ND-C4D	4.98	111.11	105.21
26	C	501	CLA	C4A-NA-C1A	4.93	108.93	106.68
26	c	506	CLA	C4A-NA-C1A	4.91	108.92	106.68
32	F	102	SQD	O6-C1-C2	4.84	115.63	108.27
26	c	513	CLA	C4A-NA-C1A	4.80	108.87	106.68
36	v	201	HEC	C1D-ND-C4D	4.79	110.88	105.21
26	b	607	CLA	C4A-NA-C1A	4.74	108.84	106.68
26	b	603	CLA	C4A-NA-C1A	4.71	108.83	106.68
26	B	605	CLA	C4A-NA-C1A	4.69	108.82	106.68
26	b	610	CLA	C4A-NA-C1A	4.65	108.80	106.68
26	B	614	CLA	C4A-NA-C1A	4.64	108.80	106.68
26	b	602	CLA	C4A-NA-C1A	4.63	108.79	106.68
26	A	607	CLA	C4A-NA-C1A	4.57	108.77	106.68
32	F	102	SQD	C1-O5-C5	-4.53	104.88	113.72
26	b	616	CLA	O2D-CGD-O1D	-4.50	115.09	123.85
27	d	401	PHO	O1D-CGD-CBD	4.48	131.52	124.72
26	b	613	CLA	C4A-NA-C1A	4.43	108.70	106.68
26	b	608	CLA	C4A-NA-C1A	4.41	108.69	106.68
26	C	506	CLA	C4A-NA-C1A	4.35	108.66	106.68
32	f	102	SQD	O9-S-O7	-4.35	99.68	113.82
32	b	620	SQD	O47-C7-C8	4.32	120.83	111.48
26	a	608	CLA	C4A-NA-C1A	4.30	108.64	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	623	SQD	C1-O5-C5	-4.23	105.46	113.72
29	a	612	PL9	C7-C3-C2	-4.22	118.42	123.39
32	D	410	SQD	O7-S-C6	4.20	113.02	106.76
26	A	608	CLA	C4A-NA-C1A	4.17	108.58	106.68
28	d	404	BCR	C30-C25-C26	-4.16	116.95	122.64
32	A	616	SQD	O7-S-C6	4.16	112.96	106.76
29	D	405	PL9	C7-C3-C4	4.14	120.32	116.91
32	f	102	SQD	O9-S-C6	4.13	112.93	106.76
26	b	603	CLA	O2D-CGD-O1D	-4.01	116.03	123.85
26	C	501	CLA	O2D-CGD-O1D	-3.98	116.10	123.85
31	D	406	LMG	O6-C5-C4	3.97	116.85	109.70
32	B	623	SQD	C3-C4-C5	3.92	117.34	110.23
27	a	609	PHO	CMA-C3A-C4A	-3.89	106.22	114.61
32	a	615	SQD	O7-S-C6	3.82	112.46	106.76
32	a	615	SQD	O47-C7-C8	3.80	119.71	111.48
32	a	615	SQD	O9-S-O7	-3.78	101.53	113.82
32	b	620	SQD	O6-C1-C2	3.78	114.01	108.27
26	B	610	CLA	O2D-CGD-O1D	-3.77	116.50	123.85
26	a	613	CLA	C4A-NA-C1A	3.77	108.40	106.68
32	A	616	SQD	O47-C7-C8	3.76	119.62	111.48
32	B	623	SQD	O7-S-C6	3.76	112.37	106.76
32	b	620	SQD	O9-S-O7	-3.75	101.63	113.82
26	b	608	CLA	C3B-C4B-NB	-3.75	107.19	110.53
26	B	610	CLA	C3B-C4B-NB	-3.72	107.21	110.53
26	b	611	CLA	O2D-CGD-O1D	-3.71	116.63	123.85
31	C	517	LMG	C7-O1-C1	3.70	121.72	113.80
29	d	405	PL9	C7-C3-C2	-3.69	119.03	123.39
26	b	603	CLA	C3B-C4B-NB	-3.69	107.23	110.53
26	b	612	CLA	C4A-NA-C1A	3.67	108.35	106.68
32	a	614	SQD	O47-C7-C8	3.65	119.38	111.48
26	B	614	CLA	O2D-CGD-O1D	-3.63	116.79	123.85
32	D	410	SQD	O47-C7-C8	3.61	119.29	111.48
26	B	611	CLA	O2D-CGD-O1D	-3.61	116.83	123.85
32	A	616	SQD	O9-S-O7	-3.58	102.17	113.82
32	f	102	SQD	C1-O5-C5	-3.58	106.73	113.72
32	D	410	SQD	O9-S-O7	-3.57	102.22	113.82
35	f	101	HEM	CBD-CAD-C3D	-3.57	102.67	112.53
26	b	605	CLA	C4-C3-C5	3.57	121.42	115.23
26	c	511	CLA	C3B-C4B-NB	-3.55	107.36	110.53
26	b	601	CLA	O2D-CGD-O1D	-3.54	116.96	123.85
27	D	401	PHO	O1D-CGD-CBD	3.53	130.08	124.72
26	b	608	CLA	O2D-CGD-O1D	-3.53	116.98	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	608	CLA	C3B-C4B-NB	-3.53	107.38	110.53
26	c	505	CLA	C3B-C4B-NB	-3.51	107.39	110.53
26	b	615	CLA	CHB-C4A-NA	3.50	129.46	124.40
32	D	410	SQD	C1-C2-C3	-3.50	102.65	110.01
35	F	101	HEM	CBD-CAD-C3D	-3.49	102.87	112.53
29	d	405	PL9	C42-C43-C44	-3.49	119.64	127.62
28	d	404	BCR	C27-C26-C25	-3.46	118.03	122.70
26	b	602	CLA	O2D-CGD-O1D	-3.45	117.12	123.85
27	A	609	PHO	CMA-C3A-C4A	-3.45	107.17	114.61
32	B	623	SQD	O9-S-O7	-3.45	102.61	113.82
26	c	501	CLA	O2D-CGD-O1D	-3.40	117.22	123.85
26	A	614	CLA	C3B-C4B-NB	-3.39	107.50	110.53
29	d	405	PL9	C40-C39-C41	3.39	121.12	115.23
26	b	608	CLA	CHB-C4A-NA	3.38	129.28	124.40
26	C	501	CLA	C3B-C4B-NB	-3.38	107.52	110.53
26	B	604	CLA	C3B-C4B-NB	-3.37	107.52	110.53
32	b	620	SQD	O9-S-C6	3.36	111.78	106.76
26	a	613	CLA	C3B-C4B-NB	-3.36	107.53	110.53
26	b	611	CLA	C3B-C4B-NB	-3.35	107.54	110.53
26	B	611	CLA	O2D-CGD-CBD	3.35	117.08	111.23
26	B	602	CLA	C4A-NA-C1A	3.33	108.20	106.68
31	c	522	LMG	C4-C3-C2	3.33	116.67	110.83
26	B	613	CLA	C3B-C4B-NB	-3.33	107.56	110.53
31	D	406	LMG	O6-C1-C2	-3.32	103.55	110.37
26	B	605	CLA	C4-C3-C5	3.31	120.98	115.23
26	d	403	CLA	C4A-NA-C1A	3.31	108.19	106.68
32	B	623	SQD	O47-C7-C8	3.28	118.59	111.48
26	A	614	CLA	O2D-CGD-O1D	-3.27	117.47	123.85
32	a	614	SQD	C1-C2-C3	-3.27	103.13	110.01
32	a	614	SQD	O48-C23-C24	3.26	121.79	111.83
29	A	612	PL9	C7-C3-C2	-3.26	119.55	123.39
26	B	612	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
26	C	513	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
26	b	610	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
26	B	613	CLA	C1-C2-C3	-3.25	120.88	126.20
32	b	620	SQD	O7-S-C6	3.24	111.60	106.76
31	D	406	LMG	C4-C3-C2	3.24	116.51	110.83
26	a	607	CLA	C3B-C4B-NB	-3.23	107.64	110.53
26	C	502	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
26	B	602	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
26	B	606	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
26	c	512	CLA	CHB-C4A-NA	3.23	129.06	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	512	CLA	C3B-C4B-NB	-3.21	107.67	110.53
26	b	615	CLA	C3B-C4B-NB	-3.20	107.67	110.53
26	B	608	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
27	A	609	PHO	CMB-C2B-C3B	3.20	131.08	124.68
26	B	614	CLA	C3B-C4B-NB	-3.19	107.69	110.53
26	B	616	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
26	C	512	CLA	C3B-C4B-NB	-3.16	107.71	110.53
27	d	401	PHO	O2D-CGD-O1D	-3.15	117.71	123.85
32	a	614	SQD	O9-S-O7	-3.15	103.59	113.82
26	C	510	CLA	C3B-C4B-NB	-3.14	107.72	110.53
26	C	508	CLA	C3B-C4B-NB	-3.14	107.73	110.53
26	b	613	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
28	b	618	BCR	C2-C1-C6	3.12	114.97	110.44
26	C	502	CLA	C3B-C4B-NB	-3.11	107.75	110.53
32	a	614	SQD	O8-S-C6	3.11	111.98	105.97
31	b	622	LMG	C3-C4-C5	-3.11	104.60	110.23
29	d	405	PL9	C37-C38-C39	-3.09	120.54	127.62
26	d	402	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
26	A	614	CLA	O2D-CGD-CBD	3.07	116.59	111.23
26	b	613	CLA	C3B-C4B-NB	-3.06	107.80	110.53
26	C	507	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
26	c	512	CLA	C1-C2-C3	-3.06	121.19	126.20
32	f	102	SQD	C3-C4-C5	3.06	115.78	110.23
26	C	508	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
27	D	401	PHO	C2B-C1B-NB	-3.04	107.23	109.43
26	b	613	CLA	CHB-C4A-NA	3.04	128.79	124.40
26	C	501	CLA	O2D-CGD-CBD	3.04	116.54	111.23
32	B	623	SQD	O48-C23-C24	3.03	121.06	111.83
26	B	612	CLA	CHB-C4A-NA	3.02	128.76	124.40
32	a	614	SQD	O5-C1-C2	-3.02	104.17	110.37
27	d	401	PHO	CBC-CAC-C3C	3.02	117.19	112.87
26	B	603	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
26	C	504	CLA	C3B-C4B-NB	-3.01	107.84	110.53
32	B	623	SQD	O5-C5-C4	3.01	115.12	109.70
26	b	606	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
26	b	612	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
32	A	616	SQD	O5-C5-C4	3.00	115.11	109.70
26	A	608	CLA	C3B-C4B-NB	-3.00	107.85	110.53
26	b	601	CLA	CHB-C4A-NA	2.99	128.72	124.40
32	F	102	SQD	O8-S-C6	2.99	111.75	105.97
27	a	609	PHO	C2B-C1B-NB	-2.99	107.27	109.43
26	A	610	CLA	C3B-C4B-NB	-2.98	107.87	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	608	CLA	C3B-C4B-NB	-2.97	107.88	110.53
26	b	609	CLA	O1D-CGD-CBD	2.97	130.37	124.52
26	c	505	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
32	a	614	SQD	O9-S-C6	2.96	111.17	106.76
32	F	102	SQD	O9-S-C6	2.96	111.17	106.76
28	b	619	BCR	C29-C30-C25	2.95	114.73	110.44
26	c	506	CLA	C3B-C4B-NB	-2.95	107.89	110.53
26	C	506	CLA	C3B-C4B-NB	-2.95	107.90	110.53
26	b	614	CLA	C3B-C4B-NB	-2.94	107.90	110.53
26	c	508	CLA	CHB-C4A-NA	2.94	128.64	124.40
28	k	102	BCR	C7-C8-C9	-2.94	121.89	126.23
26	c	511	CLA	O2D-CGD-O1D	-2.94	118.14	123.85
26	c	508	CLA	C3B-C4B-NB	-2.92	107.92	110.53
26	b	605	CLA	C3B-C4B-NB	-2.92	107.92	110.53
26	a	608	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
32	F	102	SQD	O48-C23-C24	2.92	120.74	111.83
26	B	611	CLA	CHB-C4A-NA	2.91	128.60	124.40
26	b	616	CLA	C3B-C4B-NB	-2.91	107.93	110.53
26	b	608	CLA	O2D-CGD-CBD	2.91	116.31	111.23
26	B	609	CLA	C3B-C4B-NB	-2.90	107.94	110.53
26	c	501	CLA	O2D-CGD-CBD	2.89	116.29	111.23
26	C	505	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
26	b	606	CLA	C3B-C4B-NB	-2.89	107.95	110.53
35	f	101	HEM	C3B-C4B-NB	-2.88	107.40	109.47
27	D	401	PHO	CMA-C3A-C4A	-2.88	108.40	114.61
26	B	601	CLA	O2A-CGA-O1A	-2.87	116.44	123.63
26	c	504	CLA	CHB-C4A-NA	2.87	128.54	124.40
26	c	512	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
26	A	610	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
26	b	616	CLA	O2D-CGD-CBD	2.86	116.23	111.23
26	a	607	CLA	CHB-C4A-NA	2.85	128.52	124.40
26	D	402	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
27	d	401	PHO	C2B-C1B-NB	-2.85	107.37	109.43
26	B	616	CLA	O2A-CGA-O1A	-2.85	116.51	123.63
26	B	601	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
26	c	513	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
31	D	406	LMG	O1-C1-C2	2.83	112.58	108.27
26	b	612	CLA	C3B-C4B-NB	-2.83	108.01	110.53
26	B	605	CLA	C3B-C4B-NB	-2.82	108.01	110.53
32	a	615	SQD	C3-C4-C5	2.82	115.35	110.23
26	C	510	CLA	CHB-C4A-NA	2.82	128.47	124.40
35	f	101	HEM	CHB-C1B-NB	2.81	127.85	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	401	PHO	CBC-CAC-C3C	2.81	116.90	112.87
26	c	509	CLA	O2A-CGA-O1A	-2.80	116.61	123.63
29	A	612	PL9	C22-C23-C24	-2.80	121.21	127.62
26	B	603	CLA	C3B-C4B-NB	-2.80	108.03	110.53
26	b	612	CLA	CHB-C4A-NA	2.80	128.44	124.40
27	D	401	PHO	O2D-CGD-O1D	-2.79	118.42	123.85
27	a	609	PHO	CMB-C2B-C3B	2.79	130.26	124.68
26	D	403	CLA	C1-C2-C3	-2.79	121.63	126.20
26	B	614	CLA	CHB-C4A-NA	2.79	128.43	124.40
26	D	403	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
26	C	509	CLA	CHB-C4A-NA	2.78	128.41	124.40
26	c	504	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
26	C	503	CLA	C3B-C4B-NB	-2.78	108.05	110.53
26	c	508	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
26	c	510	CLA	C3B-C4B-NB	-2.78	108.05	110.53
26	b	603	CLA	O2D-CGD-CBD	2.78	116.08	111.23
29	a	612	PL9	C40-C39-C41	2.77	120.04	115.23
35	F	101	HEM	CBA-CAA-C2A	-2.77	104.87	112.53
26	B	615	CLA	C3B-C4B-NB	-2.77	108.06	110.53
26	c	513	CLA	CHB-C4A-NA	2.77	128.40	124.40
26	B	606	CLA	C3B-C4B-NB	-2.77	108.06	110.53
26	C	502	CLA	O1D-CGD-CBD	2.77	129.97	124.52
36	V	201	HEC	CBD-CAD-C3D	-2.76	104.89	112.53
29	D	405	PL9	C7-C3-C2	-2.76	120.13	123.39
35	f	101	HEM	C3B-C2B-C1B	2.75	108.48	106.41
33	C	521	DGD	C6D-O5D-C1E	2.75	119.69	113.80
26	b	601	CLA	C3B-C4B-NB	-2.75	108.08	110.53
26	c	510	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
27	d	401	PHO	CMA-C3A-C4A	-2.74	108.70	114.61
26	A	607	CLA	CHB-C4A-NA	2.74	128.36	124.40
29	a	612	PL9	O1-C4-C3	-2.74	117.84	120.73
26	B	616	CLA	C3B-C4B-NB	-2.73	108.09	110.53
29	D	405	PL9	C27-C28-C29	-2.73	121.38	127.62
26	B	610	CLA	CHB-C4A-NA	2.73	128.34	124.40
26	b	616	CLA	CHB-C4A-NA	2.73	128.34	124.40
26	C	512	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
26	b	614	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
26	c	507	CLA	CHB-C4A-NA	2.71	128.32	124.40
26	d	403	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
26	c	513	CLA	C3B-C4B-NB	-2.71	108.11	110.53
31	C	517	LMG	O6-C5-C4	2.71	114.58	109.70
32	B	623	SQD	O6-C1-C2	2.70	112.38	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	608	CLA	CHB-C4A-NA	2.70	128.30	124.40
26	a	613	CLA	CMB-C2B-C1B	-2.69	121.32	125.42
26	B	610	CLA	O2A-CGA-O1A	-2.69	116.89	123.63
29	d	405	PL9	C27-C28-C29	-2.69	121.46	127.62
26	B	603	CLA	O2A-CGA-O1A	-2.68	116.92	123.63
26	c	503	CLA	C3B-C4B-NB	-2.68	108.14	110.53
29	d	405	PL9	C20-C19-C21	2.68	119.87	115.23
26	B	605	CLA	CHD-C1D-ND	-2.67	121.04	124.80
26	C	507	CLA	CHB-C4A-NA	2.67	128.25	124.40
26	A	614	CLA	CHB-C4A-NA	2.67	128.25	124.40
32	F	102	SQD	C1-C2-C3	-2.67	104.40	110.01
26	A	610	CLA	CHB-C4A-NA	2.66	128.25	124.40
32	f	102	SQD	O6-C1-C2	2.66	112.32	108.27
27	D	401	PHO	C1-C2-C3	-2.66	121.83	126.20
26	b	606	CLA	O2D-CGD-CBD	2.66	115.88	111.23
26	b	610	CLA	CHB-C4A-NA	2.66	128.23	124.40
32	b	620	SQD	O48-C23-C24	2.66	119.93	111.83
26	b	614	CLA	CHB-C4A-NA	2.65	128.23	124.40
26	B	602	CLA	CHB-C4A-NA	2.65	128.23	124.40
25	A	606	BCT	O2-C-O1	2.65	126.45	119.68
32	A	616	SQD	O48-C23-C24	2.64	119.89	111.83
26	c	503	CLA	C7-C6-C5	-2.64	106.22	113.26
26	B	605	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
26	a	610	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
26	C	506	CLA	CHB-C4A-NA	2.64	128.21	124.40
27	a	609	PHO	OBD-CAD-C3D	2.64	132.01	127.89
26	b	611	CLA	O2D-CGD-CBD	2.64	115.84	111.23
26	b	602	CLA	CHB-C4A-NA	2.64	128.21	124.40
26	C	511	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
26	B	601	CLA	C3B-C4B-NB	-2.64	108.18	110.53
26	b	607	CLA	C3B-C4B-NB	-2.63	108.18	110.53
26	b	605	CLA	C1-C2-C3	-2.63	121.89	126.20
33	c	519	DGD	O3G-C1D-C2D	-2.63	104.28	108.27
26	A	608	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
26	c	509	CLA	CHB-C4A-NA	2.62	128.19	124.40
26	B	609	CLA	CHC-C4B-NB	2.62	127.98	124.05
26	B	607	CLA	C3B-C4B-NB	-2.62	108.19	110.53
26	C	513	CLA	O2D-CGD-CBD	2.62	115.81	111.23
32	D	410	SQD	C3-C4-C5	2.62	114.97	110.23
26	C	505	CLA	O2D-CGD-CBD	2.61	115.80	111.23
29	D	405	PL9	C37-C38-C39	-2.61	121.66	127.62
26	b	604	CLA	C3B-C4B-NB	-2.60	108.21	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	402	CLA	CHB-C4A-NA	2.60	128.15	124.40
32	f	102	SQD	O7-S-C6	2.60	110.63	106.76
26	a	608	CLA	O2D-CGD-CBD	2.59	115.76	111.23
33	A	617	DGD	C3G-O3G-C1D	2.59	119.36	113.80
26	C	513	CLA	O2A-CGA-O1A	-2.59	117.14	123.63
26	c	506	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
32	D	410	SQD	O8-S-C6	2.58	110.96	105.97
26	B	608	CLA	CHB-C4A-NA	2.58	128.12	124.40
32	F	102	SQD	O5-C1-C2	-2.58	105.07	110.37
29	a	612	PL9	C37-C38-C39	-2.58	121.73	127.62
26	B	614	CLA	O2A-CGA-O1A	-2.58	117.19	123.63
26	C	508	CLA	CHD-C1D-ND	-2.57	121.19	124.80
26	B	601	CLA	C1-O2A-CGA	2.57	122.86	116.65
26	B	613	CLA	CHB-C4A-NA	2.57	128.10	124.40
32	f	102	SQD	O48-C23-C24	2.56	119.64	111.83
26	C	513	CLA	CHB-C4A-NA	2.56	128.09	124.40
32	F	102	SQD	O9-S-O7	-2.55	105.52	113.82
26	C	513	CLA	C3B-C4B-NB	-2.55	108.25	110.53
26	b	604	CLA	CHB-C4A-NA	2.55	128.08	124.40
26	c	507	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
26	B	604	CLA	O2D-CGD-CBD	2.54	115.67	111.23
26	C	506	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
26	b	614	CLA	C1-C2-C3	-2.54	122.04	126.20
26	c	504	CLA	C3B-C4B-NB	-2.54	108.27	110.53
26	c	506	CLA	O1D-CGD-CBD	2.54	129.52	124.52
26	c	510	CLA	CHB-C4A-NA	2.53	128.06	124.40
26	c	509	CLA	C3B-C4B-NB	-2.53	108.28	110.53
26	c	502	CLA	C3B-C4B-NB	-2.52	108.28	110.53
28	x	101	BCR	C2-C1-C6	2.52	114.10	110.44
27	d	401	PHO	C1-C2-C3	-2.52	122.07	126.20
26	B	611	CLA	C3B-C4B-NB	-2.52	108.28	110.53
26	D	402	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
26	c	511	CLA	CHB-C1B-NB	2.52	127.83	124.05
32	F	102	SQD	C3-C4-C5	2.51	114.79	110.23
31	a	616	LMG	C1-C2-C3	-2.51	104.73	110.01
29	d	405	PL9	C22-C23-C24	-2.51	121.88	127.62
35	f	101	HEM	CBA-CAA-C2A	-2.51	105.60	112.53
26	B	612	CLA	O1D-CGD-CBD	2.51	129.46	124.52
32	b	620	SQD	C1-C2-C3	-2.50	104.74	110.01
26	b	605	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
32	f	102	SQD	O5-C5-C4	2.50	114.21	109.70
26	c	503	CLA	O2D-CGD-O1D	-2.50	118.98	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	401	PHO	CMB-C2B-C3B	2.50	129.67	124.68
26	C	503	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
26	C	512	CLA	CHB-C4A-NA	2.50	128.00	124.40
28	H	101	BCR	C29-C30-C25	2.49	114.06	110.44
32	a	614	SQD	C3-C4-C5	2.49	114.75	110.23
27	D	401	PHO	CAA-C2A-C3A	-2.49	106.27	113.00
26	c	507	CLA	C3B-C4B-NB	-2.49	108.31	110.53
26	b	610	CLA	C3B-C4B-NB	-2.48	108.31	110.53
26	B	614	CLA	O2D-CGD-CBD	2.48	115.57	111.23
26	b	606	CLA	CHB-C4A-NA	2.48	127.98	124.40
27	d	401	PHO	CAA-C2A-C3A	-2.48	106.31	113.00
26	B	610	CLA	C1-C2-C3	-2.47	122.14	126.20
26	b	604	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
26	b	609	CLA	C3B-C4B-NB	-2.47	108.32	110.53
26	B	603	CLA	O2D-CGD-CBD	2.47	115.55	111.23
26	b	602	CLA	C3B-C4B-NB	-2.46	108.33	110.53
29	D	405	PL9	C7-C8-C9	-2.46	122.59	126.83
26	B	602	CLA	C3B-C4B-NB	-2.46	108.33	110.53
26	C	509	CLA	C3B-C4B-NB	-2.46	108.33	110.53
29	d	405	PL9	C7-C8-C9	-2.46	122.60	126.83
26	d	403	CLA	CHB-C4A-NA	2.45	127.94	124.40
33	c	518	DGD	C3D-C4D-C5D	-2.45	105.79	110.23
33	H	102	DGD	O6E-C5E-C4E	2.45	114.11	109.70
32	D	410	SQD	C44-O6-C1	-2.45	108.55	113.80
33	H	102	DGD	C3G-O3G-C1D	2.45	119.05	113.80
32	F	102	SQD	C46-C45-C44	-2.45	105.76	113.67
32	f	102	SQD	O47-C7-C8	2.45	119.92	110.93
29	a	612	PL9	O2-C1-C2	-2.45	116.26	121.83
29	a	612	PL9	C22-C23-C24	-2.45	122.02	127.62
26	C	511	CLA	C3B-C4B-NB	-2.45	108.35	110.53
26	B	606	CLA	CHB-C4A-NA	2.45	127.93	124.40
31	b	622	LMG	C1-O6-C5	-2.44	108.95	113.72
26	a	610	CLA	C4-C3-C5	2.44	119.47	115.23
26	b	603	CLA	O2A-CGA-O1A	-2.44	117.52	123.63
29	A	612	PL9	C40-C39-C41	2.44	119.46	115.23
26	b	607	CLA	C1-C2-C3	-2.44	122.21	126.20
26	b	602	CLA	O2D-CGD-CBD	2.43	115.48	111.23
26	A	610	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
26	b	611	CLA	CHB-C4A-NA	2.43	127.91	124.40
26	b	610	CLA	O1D-CGD-CBD	2.43	129.30	124.52
29	a	612	PL9	O2-C1-C6	2.42	124.34	120.48
28	Z	101	BCR	C1-C6-C5	-2.42	119.32	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	405	PL9	C32-C33-C34	-2.42	122.08	127.62
26	B	611	CLA	C1-C2-C3	-2.42	122.23	126.20
26	B	613	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
32	D	410	SQD	O9-S-C6	2.41	110.36	106.76
26	a	610	CLA	O2A-CGA-O1A	-2.41	117.59	123.63
32	b	620	SQD	O8-S-C6	2.41	110.63	105.97
31	M	101	LMG	C1-C2-C3	-2.41	104.94	110.01
26	C	504	CLA	CHB-C4A-NA	2.40	127.87	124.40
26	a	610	CLA	O2D-CGD-CBD	2.40	115.43	111.23
26	C	503	CLA	C7-C6-C5	-2.40	106.87	113.26
29	D	405	PL9	C42-C43-C44	-2.40	122.14	127.62
26	c	506	CLA	CHB-C4A-NA	2.40	127.86	124.40
26	C	503	CLA	CHD-C1D-ND	-2.40	121.43	124.80
32	a	615	SQD	O9-S-C6	2.39	110.33	106.76
31	a	616	LMG	O1-C1-C2	2.39	111.91	108.27
26	C	508	CLA	CHB-C4A-NA	2.39	127.85	124.40
26	d	402	CLA	CHB-C4A-NA	2.39	127.85	124.40
27	A	609	PHO	OBD-CAD-C3D	2.39	131.62	127.89
32	a	615	SQD	O48-C23-C24	2.39	119.12	111.83
26	B	605	CLA	O1D-CGD-CBD	2.38	129.22	124.52
26	b	605	CLA	CHD-C1D-ND	-2.38	121.45	124.80
29	D	405	PL9	C50-C49-C48	-2.38	115.53	122.66
26	B	603	CLA	CHB-C4A-NA	2.38	127.83	124.40
26	d	403	CLA	O2A-CGA-O1A	-2.37	117.69	123.63
33	c	518	DGD	C6D-O5D-C1E	2.37	118.87	113.80
29	A	612	PL9	O2-C1-C2	-2.37	116.45	121.83
34	D	408	LHG	O4-P-O5	2.36	123.44	112.44
33	A	617	DGD	C4E-C3E-C2E	-2.36	106.68	110.83
33	h	101	DGD	O4D-C4D-C5D	2.36	115.14	109.32
26	b	604	CLA	C1-C2-C3	-2.36	122.33	126.20
26	b	603	CLA	CHC-C4B-NB	2.36	127.58	124.05
29	a	612	PL9	C27-C28-C29	-2.35	122.24	127.62
26	B	604	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
32	F	102	SQD	C44-O6-C1	-2.35	109.66	113.68
26	B	606	CLA	C1-C2-C3	-2.35	122.35	126.20
26	a	613	CLA	CMB-C2B-C3B	2.34	132.06	126.55
26	c	507	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
29	D	405	PL9	C32-C33-C34	-2.34	122.26	127.62
26	B	602	CLA	C1-C2-C3	-2.34	122.36	126.20
29	D	405	PL9	C12-C13-C14	-2.34	122.27	127.62
26	C	508	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
26	c	508	CLA	O2A-CGA-O1A	-2.33	117.79	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	509	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
26	C	504	CLA	C4-C3-C5	2.33	119.28	115.23
29	A	612	PL9	O2-C1-C6	2.33	124.19	120.48
26	b	612	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
28	Z	101	BCR	C4-C5-C6	-2.33	119.56	122.70
26	c	511	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
26	b	604	CLA	C11-C12-C13	-2.33	108.23	115.97
28	D	404	BCR	C32-C1-C6	2.32	113.88	110.24
26	C	513	CLA	CHD-C1D-ND	-2.32	121.54	124.80
26	b	612	CLA	O1D-CGD-CBD	2.31	129.08	124.52
26	c	508	CLA	O2D-CGD-CBD	2.31	115.26	111.23
26	C	505	CLA	C3B-C4B-NB	-2.30	108.47	110.53
33	c	519	DGD	C3G-O3G-C1D	2.30	118.74	113.80
26	b	603	CLA	CHD-C1D-ND	-2.30	121.56	124.80
26	c	501	CLA	CHB-C4A-NA	2.30	127.72	124.40
30	e	105	STE	C3-C2-C1	-2.30	108.52	114.51
26	B	615	CLA	CHB-C4A-NA	2.30	127.71	124.40
26	B	604	CLA	O2D-CGD-O1D	-2.29	119.38	123.85
26	c	502	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
27	A	609	PHO	CAA-C2A-C3A	-2.29	106.81	113.00
26	C	511	CLA	CHB-C4A-NA	2.29	127.70	124.40
30	e	105	STE	O2-C1-C2	2.29	121.23	114.00
27	a	609	PHO	O1D-CGD-CBD	2.29	128.19	124.72
26	B	602	CLA	O2D-CGD-CBD	2.29	115.22	111.23
27	D	401	PHO	C3D-C4D-ND	2.28	110.64	107.71
26	C	504	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
32	b	620	SQD	O5-C5-C4	2.28	113.81	109.70
26	c	505	CLA	C1-C2-C3	-2.28	122.46	126.20
26	a	607	CLA	O1D-CGD-CBD	2.28	129.01	124.52
26	A	610	CLA	CHC-C4B-NB	2.28	127.47	124.05
26	B	607	CLA	CHB-C4A-NA	2.27	127.68	124.40
36	V	201	HEC	C2A-C1A-NA	-2.27	108.13	110.32
26	d	403	CLA	CHA-C1A-NA	-2.27	121.25	126.39
26	B	609	CLA	CHA-C1A-NA	-2.26	121.27	126.39
28	B	618	BCR	C2-C1-C6	2.26	113.72	110.44
26	d	402	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
26	b	601	CLA	O2D-CGD-CBD	2.26	115.17	111.23
26	A	607	CLA	C3B-C4B-NB	-2.25	108.52	110.53
26	c	510	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
26	b	604	CLA	C6-C5-C3	-2.25	107.98	113.47
26	C	505	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
26	C	504	CLA	CMB-C2B-C1B	-2.25	121.99	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	615	CLA	CHC-C4B-NB	2.25	127.42	124.05
32	D	410	SQD	O48-C23-C24	2.25	118.69	111.83
32	b	620	SQD	O5-C1-C2	-2.25	105.75	110.37
31	D	407	LMG	C3-C4-C5	-2.25	106.16	110.23
26	c	513	CLA	CHD-C1D-ND	-2.25	121.64	124.80
28	c	515	BCR	C2-C1-C6	2.24	113.70	110.44
26	c	508	CLA	CHD-C1D-ND	-2.24	121.64	124.80
26	c	509	CLA	C16-C15-C13	-2.24	108.51	115.97
26	c	502	CLA	CHB-C4A-NA	2.24	127.64	124.40
26	B	604	CLA	CHB-C1B-NB	2.24	127.41	124.05
25	a	606	BCT	O2-C-O1	2.24	125.41	119.68
26	B	612	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
29	D	405	PL9	C40-C39-C41	2.24	119.11	115.23
33	C	522	DGD	C3E-C4E-C5E	-2.24	106.18	110.23
36	V	201	HEC	CAD-CBD-CGD	-2.23	107.74	113.67
26	B	612	CLA	C3B-C4B-NB	-2.23	108.54	110.53
30	E	104	STE	O2-C1-C2	2.23	121.05	114.00
26	D	403	CLA	CHB-C4A-NA	2.23	127.62	124.40
31	a	617	LMG	O1-C7-C8	-2.23	105.39	110.82
30	C	525	STE	O2-C1-C2	2.23	121.05	114.00
26	D	402	CLA	O2D-CGD-CBD	2.23	115.13	111.23
36	v	201	HEC	CBD-CAD-C3D	-2.23	106.37	112.53
26	b	611	CLA	C1-C2-C3	-2.22	122.56	126.20
31	D	407	LMG	O3-C3-C4	2.22	115.61	110.38
26	C	507	CLA	C3B-C4B-NB	-2.22	108.55	110.53
26	D	402	CLA	C3B-C4B-NB	-2.22	108.55	110.53
26	a	607	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
29	D	405	PL9	O1-C4-C3	-2.22	118.39	120.73
26	b	609	CLA	CHB-C4A-NA	2.22	127.60	124.40
27	a	609	PHO	OBD-CAD-CBD	-2.22	122.57	125.82
31	C	517	LMG	O3-C3-C2	-2.22	105.15	110.38
31	M	101	LMG	C7-O1-C1	-2.22	109.05	113.80
30	b	623	STE	C3-C2-C1	-2.21	108.73	114.51
36	v	201	HEC	CBA-CAA-C2A	-2.21	106.42	112.53
26	B	606	CLA	O2D-CGD-CBD	2.21	115.10	111.23
26	A	608	CLA	CHB-C4A-NA	2.21	127.59	124.40
26	B	608	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
29	A	612	PL9	C20-C19-C21	2.21	119.07	115.23
26	C	503	CLA	O1D-CGD-CBD	2.21	128.88	124.52
33	h	101	DGD	C3E-C4E-C5E	-2.21	106.23	110.23
26	b	616	CLA	CHC-C4B-NB	2.21	127.36	124.05
26	B	607	CLA	CHC-C4B-NB	2.21	127.36	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	613	CLA	O1D-CGD-CBD	2.21	128.87	124.52
26	b	602	CLA	O2A-CGA-O1A	-2.20	118.11	123.63
26	B	610	CLA	O1D-CGD-CBD	2.20	128.86	124.52
26	C	501	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
26	a	608	CLA	CHB-C1B-NB	2.20	127.35	124.05
32	B	623	SQD	O8-S-C6	2.20	110.22	105.97
26	B	609	CLA	CHB-C4A-NA	2.20	127.58	124.40
26	c	501	CLA	C3B-C4B-NB	-2.20	108.57	110.53
29	d	405	PL9	C8-C7-C3	2.20	117.71	112.03
36	V	201	HEC	CHD-C4C-NC	2.20	127.84	123.86
33	h	101	DGD	C3D-C4D-C5D	-2.20	106.25	110.23
32	B	623	SQD	C44-O6-C1	-2.19	109.09	113.80
26	B	601	CLA	CHB-C1B-NB	2.19	127.34	124.05
26	b	605	CLA	CHB-C1B-NB	2.19	127.34	124.05
26	B	609	CLA	O1D-CGD-CBD	2.19	128.83	124.52
26	c	513	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
26	A	610	CLA	O2D-CGD-CBD	2.18	115.05	111.23
35	F	101	HEM	C3B-C2B-C1B	2.18	108.05	106.41
26	b	609	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
31	a	616	LMG	O6-C1-C2	-2.18	105.90	110.37
32	B	623	SQD	C1-C2-C3	-2.18	105.43	110.01
36	V	201	HEC	CHB-C4A-NA	2.17	126.82	124.45
32	F	102	SQD	O5-C5-C4	2.17	113.62	109.70
26	a	610	CLA	CHC-C4B-NB	2.17	127.30	124.05
26	B	605	CLA	CHD-C4C-NC	2.16	127.58	124.23
27	d	401	PHO	CMB-C2B-C3B	2.16	129.00	124.68
34	B	622	LHG	O7-C5-C4	-2.16	100.60	108.34
26	a	613	CLA	O2D-CGD-CBD	2.16	115.00	111.23
26	B	602	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
26	c	505	CLA	CHB-C4A-NA	2.15	127.51	124.40
29	d	405	PL9	C12-C13-C14	-2.15	122.69	127.62
26	b	609	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
28	b	617	BCR	C29-C30-C25	2.15	113.56	110.44
33	h	101	DGD	O3D-C3D-C2D	-2.15	105.32	110.38
26	B	604	CLA	C1-O2A-CGA	-2.15	111.46	116.65
26	B	608	CLA	CMB-C2B-C3B	2.14	131.59	126.55
26	b	614	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
26	B	605	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
31	C	517	LMG	O4-C4-C5	2.14	114.60	109.32
28	d	404	BCR	C38-C26-C27	-2.14	109.03	113.60
31	m	101	LMG	O1-C7-C8	-2.14	105.61	110.82
33	C	521	DGD	O3G-C1D-C2D	-2.13	105.03	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	405	PL9	C22-C23-C24	-2.13	122.75	127.62
26	C	503	CLA	CHD-C1D-C2D	2.13	129.92	125.49
26	b	604	CLA	O2D-CGD-CBD	2.13	114.95	111.23
29	A	612	PL9	C30-C29-C28	-2.12	118.17	123.63
26	B	608	CLA	O2D-CGD-CBD	2.12	114.94	111.23
36	v	201	HEC	C1D-C2D-C3D	-2.12	104.75	106.98
36	V	201	HEC	CMD-C2D-C1D	2.12	128.35	125.03
32	A	616	SQD	O9-S-C6	2.12	109.92	106.76
26	b	604	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
26	C	504	CLA	O2D-CGD-O1D	-2.12	119.73	123.85
26	D	403	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
26	d	403	CLA	C3B-C4B-NB	-2.11	108.64	110.53
26	b	616	CLA	O1D-CGD-CBD	2.11	128.68	124.52
26	b	610	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
26	C	504	CLA	CHB-C1B-NB	2.11	127.22	124.05
26	B	604	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
34	d	407	LHG	O4-P-O5	2.11	122.25	112.44
27	A	609	PHO	C1-C2-C3	-2.11	122.75	126.20
26	C	510	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
30	d	406	STE	O2-C1-C2	2.10	120.64	114.00
35	f	101	HEM	C1B-NB-C4B	2.10	107.69	105.21
30	b	623	STE	O2-C1-C2	2.10	120.64	114.00
26	C	512	CLA	C1-C2-C3	-2.10	122.76	126.20
26	C	511	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
26	C	505	CLA	CHB-C4A-NA	2.10	127.43	124.40
26	c	504	CLA	CHD-C1D-ND	-2.09	121.86	124.80
35	f	101	HEM	CAB-C3B-C2B	-2.09	121.63	128.43
26	b	608	CLA	C6-C7-C8	-2.09	109.02	115.97
31	B	620	LMG	O1-C1-C2	2.09	111.44	108.27
26	b	606	CLA	CHB-C1B-NB	2.09	127.18	124.05
31	a	616	LMG	O3-C3-C4	2.09	115.29	110.38
26	b	611	CLA	CHD-C1D-ND	-2.09	121.87	124.80
26	b	609	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
26	a	613	CLA	CHB-C4A-NA	2.08	127.41	124.40
26	C	509	CLA	C1-C2-C3	-2.08	122.79	126.20
35	f	101	HEM	CHC-C1C-NC	2.08	126.72	124.45
26	B	615	CLA	C2A-C3A-C4A	2.08	105.23	101.87
26	c	512	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
26	b	615	CLA	O2D-CGD-O1D	-2.08	119.81	123.85
27	A	609	PHO	OBD-CAD-CBD	-2.07	122.78	125.82
26	C	507	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
32	f	102	SQD	O5-C1-C2	-2.07	106.11	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	t	101	BCR	C2-C1-C6	2.07	113.45	110.44
36	v	201	HEC	CHB-C1B-NB	2.07	126.65	124.42
26	C	505	CLA	C11-C10-C8	-2.07	109.09	115.97
26	B	609	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
26	b	613	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
32	a	615	SQD	O5-C5-C4	2.07	113.42	109.70
26	C	510	CLA	O2D-CGD-O1D	-2.07	119.83	123.85
26	B	607	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
26	a	607	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
31	D	406	LMG	C1-C2-C3	-2.06	105.67	110.01
33	c	520	DGD	C3G-O3G-C1D	2.06	118.21	113.80
28	K	101	BCR	C29-C30-C25	2.06	113.43	110.44
27	d	401	PHO	CMA-C3A-C2A	-2.06	106.18	114.13
31	B	620	LMG	C8-O7-C10	2.06	122.72	117.80
26	B	611	CLA	C11-C12-C13	-2.06	109.13	115.97
35	F	101	HEM	CHC-C1C-NC	2.06	126.69	124.45
26	c	503	CLA	CHD-C1D-ND	-2.06	121.91	124.80
26	d	402	CLA	C4-C3-C5	2.06	118.80	115.23
26	c	503	CLA	O1D-CGD-CBD	2.06	128.57	124.52
26	d	402	CLA	CMB-C2B-C3B	2.05	131.38	126.55
26	B	604	CLA	CHA-C1A-NA	-2.05	121.74	126.39
26	C	502	CLA	CHA-C1A-NA	-2.05	121.74	126.39
26	A	607	CLA	CAC-C3C-C4C	2.05	127.46	124.79
26	b	612	CLA	CMB-C2B-C1B	-2.05	122.29	125.42
26	C	512	CLA	C6-C5-C3	-2.05	108.47	113.47
29	D	405	PL9	C8-C7-C3	2.05	117.33	112.03
30	D	412	STE	O2-C1-C2	2.05	120.48	114.00
26	C	509	CLA	O2D-CGD-O1D	-2.05	119.86	123.85
30	C	516	STE	O2-C1-C2	2.05	120.47	114.00
26	C	505	CLA	CHA-C1A-NA	-2.05	121.75	126.39
26	b	612	CLA	C1-C2-C3	-2.05	122.84	126.20
26	D	403	CLA	CHC-C4B-NB	2.05	127.12	124.05
26	B	607	CLA	C1-C2-C3	-2.04	122.85	126.20
26	B	616	CLA	CHC-C4B-NB	2.04	127.11	124.05
26	B	616	CLA	CHB-C4A-NA	2.04	127.35	124.40
26	b	610	CLA	CHC-C4B-NB	2.04	127.11	124.05
30	E	104	STE	C3-C2-C1	-2.04	109.18	114.51
26	C	509	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
30	m	102	STE	O2-C1-C2	2.04	120.44	114.00
26	C	505	CLA	C1-C2-C3	-2.04	122.86	126.20
26	b	604	CLA	C6-C7-C8	-2.04	109.19	115.97
26	C	512	CLA	CMB-C2B-C1B	-2.04	122.32	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	609	CLA	CMB-C2B-C3B	2.04	131.34	126.55
26	b	612	CLA	CMB-C2B-C3B	2.04	131.34	126.55
31	a	617	LMG	C3-C4-C5	-2.04	106.54	110.23
30	j	101	STE	O2-C1-C2	2.03	120.43	114.00
31	C	517	LMG	C4-C3-C2	2.03	114.40	110.83
26	A	607	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
33	C	521	DGD	C3G-C2G-C1G	-2.03	107.05	111.78
36	V	201	HEC	CHA-C4D-ND	2.03	126.61	124.42
26	C	506	CLA	O1D-CGD-CBD	2.03	128.52	124.52
33	A	617	DGD	O4E-C4E-C5E	2.03	114.32	109.32
26	C	507	CLA	O2D-CGD-CBD	2.03	114.78	111.23
29	d	405	PL9	C40-C39-C38	-2.03	118.42	123.63
26	C	507	CLA	C2A-C1A-CHA	2.03	127.38	123.87
26	B	611	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
29	a	612	PL9	C42-C43-C44	-2.02	122.99	127.62
36	V	201	HEC	CBA-CAA-C2A	-2.02	106.94	112.53
33	A	617	DGD	C2G-O2G-C1B	2.02	122.63	117.80
26	C	502	CLA	CHB-C1B-NB	2.02	127.08	124.05
26	a	607	CLA	C2A-C1A-CHA	2.02	127.37	123.87
26	b	604	CLA	C3A-C2A-C1A	2.02	104.36	101.34
26	b	605	CLA	O1D-CGD-CBD	2.02	128.50	124.52
26	B	605	CLA	CHB-C4A-NA	2.02	127.31	124.40
26	a	607	CLA	CMB-C2B-C3B	2.01	131.28	126.55
34	d	409	LHG	O4-P-O5	2.01	121.79	112.44
26	b	607	CLA	CHB-C1B-NB	2.01	127.06	124.05
26	d	402	CLA	C3B-C4B-NB	-2.01	108.74	110.53
26	B	604	CLA	CHB-C4A-NA	2.01	127.29	124.40
26	C	512	CLA	CMB-C2B-C3B	2.00	131.26	126.55
33	h	101	DGD	C6D-C5D-C4D	2.00	116.27	112.07

All (2) chirality outliers are listed below:

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

All (1520) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	B	601	CLA	C1A-C2A-CAA-CBA
26	B	601	CLA	CBA-CGA-O2A-C1
26	B	601	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	B	614	CLA	CAD-CBD-CGD-O1D
26	B	614	CLA	CAD-CBD-CGD-O2D
26	C	504	CLA	C2B-C3B-CAB-CBB
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	b	614	CLA	CAD-CBD-CGD-O1D
26	b	614	CLA	CAD-CBD-CGD-O2D
26	b	614	CLA	C6-C7-C8-C9
26	c	507	CLA	CHA-CBD-CGD-O1D
26	c	507	CLA	CHA-CBD-CGD-O2D
26	c	513	CLA	CBD-CGD-O2D-CED
28	K	101	BCR	C7-C8-C9-C10
28	K	101	BCR	C7-C8-C9-C34
28	T	101	BCR	C23-C24-C25-C26
28	Z	101	BCR	C5-C6-C7-C8
28	Z	101	BCR	C21-C22-C23-C24
28	d	404	BCR	C23-C24-C25-C30
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	102	BCR	C7-C8-C9-C10
28	k	102	BCR	C7-C8-C9-C34
29	A	612	PL9	C27-C28-C29-C31
29	A	612	PL9	C29-C31-C32-C33
29	A	612	PL9	C32-C33-C34-C35
29	A	612	PL9	C32-C33-C34-C36
29	A	612	PL9	C37-C38-C39-C41
29	D	405	PL9	C32-C33-C34-C36
29	a	612	PL9	C17-C18-C19-C21
29	a	612	PL9	C22-C23-C24-C25
29	a	612	PL9	C22-C23-C24-C26
29	a	612	PL9	C32-C33-C34-C35
29	a	612	PL9	C47-C48-C49-C50
29	d	405	PL9	C32-C33-C34-C36
29	d	405	PL9	C42-C43-C44-C45
31	A	615	LMG	C11-C10-O7-C8
31	B	620	LMG	C2-C1-O1-C7
31	B	620	LMG	O6-C1-O1-C7
31	C	517	LMG	C2-C1-O1-C7
31	D	406	LMG	C2-C1-O1-C7
31	D	406	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
31	D	406	LMG	C11-C10-O7-C8
31	M	101	LMG	C11-C10-O7-C8
31	a	617	LMG	O6-C1-O1-C7
32	A	616	SQD	C5-C6-S-O7
32	A	616	SQD	C5-C6-S-O8
32	A	616	SQD	C5-C6-S-O9
32	B	623	SQD	C2-C1-O6-C44
32	B	623	SQD	O5-C1-O6-C44
32	B	623	SQD	O6-C44-C45-O47
32	B	623	SQD	O49-C7-O47-C45
32	F	102	SQD	C2-C1-O6-C44
32	F	102	SQD	O5-C1-O6-C44
32	F	102	SQD	O10-C23-O48-C46
32	F	102	SQD	C24-C23-O48-C46
32	a	614	SQD	O47-C45-C46-O48
32	a	614	SQD	C5-C6-S-O7
32	a	614	SQD	C5-C6-S-O8
32	a	615	SQD	O6-C44-C45-O47
32	a	615	SQD	O5-C5-C6-S
32	a	615	SQD	C5-C6-S-O7
32	a	615	SQD	C5-C6-S-O8
32	b	620	SQD	C46-C45-O47-C7
32	b	620	SQD	C8-C7-O47-C45
34	B	622	LHG	C4-O6-P-O3
34	B	622	LHG	C4-O6-P-O4
34	B	622	LHG	C4-O6-P-O5
34	D	408	LHG	O2-C2-C3-O3
34	D	408	LHG	C3-O3-P-O4
34	D	408	LHG	C3-O3-P-O6
34	D	408	LHG	C4-O6-P-O4
34	D	411	LHG	O1-C1-C2-C3
34	E	101	LHG	C3-O3-P-O5
34	E	101	LHG	C3-O3-P-O6
34	d	408	LHG	C3-O3-P-O4
34	d	408	LHG	C3-O3-P-O6
34	d	408	LHG	C4-O6-P-O3
34	d	408	LHG	C4-O6-P-O4
34	e	102	LHG	C3-O3-P-O4
34	e	102	LHG	C3-O3-P-O5
34	e	102	LHG	C3-O3-P-O6
34	l	101	LHG	C4-O6-P-O3
34	l	101	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
34	l	101	LHG	C4-O6-P-O5
26	b	601	CLA	O1D-CGD-O2D-CED
26	b	601	CLA	CBD-CGD-O2D-CED
31	B	620	LMG	O10-C28-O8-C9
29	A	612	PL9	C47-C48-C49-C51
31	B	620	LMG	C29-C28-O8-C9
31	M	101	LMG	O10-C28-O8-C9
26	c	513	CLA	O1D-CGD-O2D-CED
31	A	615	LMG	O9-C10-O7-C8
31	D	406	LMG	O9-C10-O7-C8
31	M	101	LMG	O9-C10-O7-C8
29	a	612	PL9	C47-C48-C49-C51
26	B	615	CLA	C3-C5-C6-C7
26	b	614	CLA	C3-C5-C6-C7
26	c	512	CLA	C3-C5-C6-C7
26	B	616	CLA	CBA-CGA-O2A-C1
31	M	101	LMG	C29-C28-O8-C9
31	a	616	LMG	C29-C28-O8-C9
32	B	623	SQD	C8-C7-O47-C45
26	B	614	CLA	C4-C3-C5-C6
26	C	504	CLA	C4-C3-C5-C6
26	B	614	CLA	C2-C3-C5-C6
26	C	504	CLA	C2-C3-C5-C6
29	A	612	PL9	C28-C29-C31-C32
26	c	511	CLA	CBD-CGD-O2D-CED
32	B	623	SQD	C45-C46-O48-C23
26	b	601	CLA	CBA-CGA-O2A-C1
31	a	616	LMG	O10-C28-O8-C9
32	b	620	SQD	O49-C7-O47-C45
32	B	623	SQD	C24-C23-O48-C46
32	f	102	SQD	C24-C23-O48-C46
31	b	622	LMG	O6-C5-C6-O5
26	B	616	CLA	O1A-CGA-O2A-C1
27	d	401	PHO	CBD-CGD-O2D-CED
31	c	522	LMG	C11-C10-O7-C8
31	C	517	LMG	C29-C28-O8-C9
26	B	605	CLA	C4-C3-C5-C6
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	605	CLA	C2-C3-C5-C6
26	a	610	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	b	603	CLA	C2-C3-C5-C6
26	b	605	CLA	C2-C3-C5-C6
26	b	601	CLA	O1A-CGA-O2A-C1
32	B	623	SQD	O10-C23-O48-C46
29	a	612	PL9	C24-C26-C27-C28
29	a	612	PL9	C44-C46-C47-C48
31	C	517	LMG	O10-C28-O8-C9
32	f	102	SQD	O10-C23-O48-C46
26	B	607	CLA	C3-C5-C6-C7
31	A	615	LMG	O6-C1-O1-C7
31	M	101	LMG	O6-C1-O1-C7
33	H	102	DGD	O6E-C5E-C6E-O5E
34	e	102	LHG	C24-C23-O8-C6
29	A	612	PL9	C27-C28-C29-C30
29	a	612	PL9	C17-C18-C19-C20
26	b	603	CLA	CBD-CGD-O2D-CED
26	c	504	CLA	CBD-CGD-O2D-CED
29	D	405	PL9	C47-C48-C49-C51
34	e	102	LHG	O10-C23-O8-C6
31	c	522	LMG	O9-C10-O7-C8
34	D	408	LHG	C1-C2-C3-O3
26	c	506	CLA	CBA-CGA-O2A-C1
26	c	512	CLA	CBA-CGA-O2A-C1
26	B	606	CLA	C14-C13-C15-C16
26	B	613	CLA	C11-C12-C13-C14
26	B	614	CLA	C6-C7-C8-C9
26	B	615	CLA	C6-C7-C8-C9
26	C	509	CLA	C11-C10-C8-C9
26	C	512	CLA	C11-C10-C8-C9
26	b	606	CLA	C14-C13-C15-C16
31	M	101	LMG	C2-C1-O1-C7
31	a	617	LMG	C2-C1-O1-C7
30	i	101	STE	C1-C2-C3-C4
28	C	514	BCR	C11-C12-C13-C35
28	Z	101	BCR	C37-C22-C23-C24
28	k	101	BCR	C36-C18-C19-C20
26	c	506	CLA	O1A-CGA-O2A-C1
33	H	102	DGD	C4E-C5E-C6E-O5E
31	b	622	LMG	C11-C10-O7-C8
26	B	615	CLA	C15-C16-C17-C18
31	a	617	LMG	C10-C11-C12-C13
26	B	601	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	a	612	PL9	C42-C43-C44-C45
29	d	405	PL9	C32-C33-C34-C35
26	b	615	CLA	C13-C15-C16-C17
26	c	512	CLA	C13-C15-C16-C17
29	A	612	PL9	C47-C48-C49-C50
34	e	102	LHG	C7-C8-C9-C10
26	C	508	CLA	C12-C13-C15-C16
26	b	611	CLA	C12-C13-C15-C16
36	V	201	HEC	C2C-C3C-CAC-CBC
31	m	101	LMG	C10-C11-C12-C13
29	A	612	PL9	C24-C26-C27-C28
29	A	612	PL9	C34-C36-C37-C38
34	D	411	LHG	C11-C12-C13-C14
26	C	503	CLA	C5-C6-C7-C8
26	b	614	CLA	C13-C15-C16-C17
30	a	618	STE	C1-C2-C3-C4
26	c	512	CLA	O1A-CGA-O2A-C1
26	b	606	CLA	C15-C16-C17-C18
26	b	610	CLA	C15-C16-C17-C18
26	c	503	CLA	C5-C6-C7-C8
26	c	509	CLA	C10-C11-C12-C13
31	b	622	LMG	C4-C5-C6-O5
30	m	102	STE	C1-C2-C3-C4
31	c	521	LMG	C28-C29-C30-C31
32	b	620	SQD	O5-C1-O6-C44
26	B	604	CLA	C10-C11-C12-C13
26	C	505	CLA	C13-C15-C16-C17
34	l	101	LHG	C7-C8-C9-C10
26	B	615	CLA	C5-C6-C7-C8
26	a	610	CLA	C5-C6-C7-C8
26	c	511	CLA	O1D-CGD-O2D-CED
26	C	505	CLA	C15-C16-C17-C18
36	v	201	HEC	C2C-C3C-CAC-CBC
26	B	603	CLA	C8-C10-C11-C12
26	C	506	CLA	C13-C15-C16-C17
26	C	512	CLA	C10-C11-C12-C13
31	b	622	LMG	C29-C28-O8-C9
30	H	103	STE	C14-C15-C16-C17
33	c	518	DGD	C7A-C8A-C9A-CAA
26	B	613	CLA	C8-C10-C11-C12
31	c	517	LMG	C28-C29-C30-C31
31	b	622	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
26	b	606	CLA	C2A-CAA-CBA-CGA
33	A	617	DGD	C2A-C1A-O1G-C1G
26	B	601	CLA	C5-C6-C7-C8
26	B	611	CLA	C8-C10-C11-C12
26	a	608	CLA	C15-C16-C17-C18
26	b	611	CLA	C8-C10-C11-C12
26	c	503	CLA	C15-C16-C17-C18
26	c	508	CLA	C8-C10-C11-C12
34	d	409	LHG	C24-C25-C26-C27
26	B	611	CLA	C15-C16-C17-C18
26	B	614	CLA	C8-C10-C11-C12
26	b	601	CLA	C5-C6-C7-C8
26	b	607	CLA	C10-C11-C12-C13
26	b	614	CLA	C5-C6-C7-C8
27	d	401	PHO	O1D-CGD-O2D-CED
27	D	401	PHO	C2C-C3C-CAC-CBC
34	e	102	LHG	O2-C2-C3-O3
36	V	201	HEC	C4C-C3C-CAC-CBC
26	B	616	CLA	C11-C12-C13-C15
26	D	403	CLA	C10-C11-C12-C13
26	C	509	CLA	C10-C11-C12-C13
28	B	617	BCR	C36-C18-C19-C20
33	C	521	DGD	O6E-C5E-C6E-O5E
26	B	606	CLA	C2A-CAA-CBA-CGA
26	b	613	CLA	C13-C15-C16-C17
26	c	508	CLA	C10-C11-C12-C13
26	c	513	CLA	C13-C15-C16-C17
34	d	409	LHG	O1-C1-C2-C3
34	d	409	LHG	C23-C24-C25-C26
29	D	405	PL9	C47-C48-C49-C50
26	b	609	CLA	C13-C15-C16-C17
31	m	101	LMG	C38-C39-C40-C41
33	A	617	DGD	O1B-C1B-O2G-C2G
32	a	614	SQD	C8-C7-O47-C45
33	A	617	DGD	C2B-C1B-O2G-C2G
31	D	406	LMG	C29-C28-O8-C9
34	d	409	LHG	C32-C33-C34-C35
26	B	601	CLA	C16-C17-C18-C20
26	B	606	CLA	C16-C17-C18-C20
26	B	616	CLA	C11-C12-C13-C14
31	b	622	LMG	O10-C28-O8-C9
36	v	201	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
30	C	526	STE	C4-C5-C6-C7
31	a	617	LMG	C16-C17-C18-C19
32	F	102	SQD	C24-C25-C26-C27
33	c	520	DGD	C9B-CAB-CBB-CCB
33	h	101	DGD	C7B-C8B-C9B-CAB
31	a	617	LMG	C38-C39-C40-C41
32	a	614	SQD	C18-C19-C20-C21
33	C	523	DGD	C5A-C6A-C7A-C8A
26	c	503	CLA	C8-C10-C11-C12
26	c	505	CLA	C10-C11-C12-C13
30	M	102	STE	C4-C5-C6-C7
30	a	618	STE	C6-C7-C8-C9
30	e	101	STE	C13-C14-C15-C16
30	j	101	STE	C2-C3-C4-C5
32	B	623	SQD	C33-C34-C35-C36
33	H	102	DGD	C4B-C5B-C6B-C7B
34	e	102	LHG	C25-C26-C27-C28
30	I	101	STE	C2-C3-C4-C5
30	k	103	STE	C4-C5-C6-C7
31	C	524	LMG	C15-C16-C17-C18
32	A	616	SQD	C11-C12-C13-C14
32	B	623	SQD	C13-C14-C15-C16
33	A	617	DGD	C2B-C3B-C4B-C5B
33	C	523	DGD	C6A-C7A-C8A-C9A
33	H	102	DGD	C7A-C8A-C9A-CAA
33	c	518	DGD	CAB-CBB-CCB-CDB
34	B	622	LHG	C17-C18-C19-C20
34	D	408	LHG	C15-C16-C17-C18
34	D	411	LHG	C29-C30-C31-C32
34	d	409	LHG	C29-C30-C31-C32
34	D	411	LHG	O1-C1-C2-O2
30	m	103	STE	C4-C5-C6-C7
31	a	617	LMG	C37-C38-C39-C40
32	a	615	SQD	C9-C10-C11-C12
26	A	607	CLA	C15-C16-C17-C18
26	b	602	CLA	C13-C15-C16-C17
26	c	512	CLA	C4B-C3B-CAB-CBB
26	C	502	CLA	C16-C17-C18-C20
30	B	625	STE	C10-C11-C12-C13
30	J	101	STE	C6-C7-C8-C9
31	D	406	LMG	C32-C33-C34-C35
31	m	101	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
33	h	101	DGD	CAA-CBA-CCA-CDA
30	A	613	STE	C2-C3-C4-C5
30	J	101	STE	C5-C6-C7-C8
26	a	607	CLA	C2C-C3C-CAC-CBC
26	B	613	CLA	C11-C10-C8-C7
26	c	508	CLA	C11-C12-C13-C15
31	M	101	LMG	C39-C40-C41-C42
30	B	625	STE	C2-C3-C4-C5
32	a	615	SQD	C31-C32-C33-C34
33	A	617	DGD	C2A-C3A-C4A-C5A
31	a	616	LMG	C35-C36-C37-C38
33	c	520	DGD	C5B-C6B-C7B-C8B
26	C	513	CLA	CBD-CGD-O2D-CED
33	A	617	DGD	C6B-C7B-C8B-C9B
33	c	518	DGD	CAA-CBA-CCA-CDA
26	C	502	CLA	C16-C17-C18-C19
33	A	617	DGD	O1A-C1A-O1G-C1G
30	C	525	STE	C2-C3-C4-C5
33	c	520	DGD	C8A-C9A-CAA-CBA
26	B	615	CLA	CBD-CGD-O2D-CED
32	a	614	SQD	O49-C7-O47-C45
30	h	102	STE	C12-C13-C14-C15
30	z	702	STE	C2-C3-C4-C5
31	C	517	LMG	C16-C17-C18-C19
33	h	101	DGD	C2B-C3B-C4B-C5B
34	d	408	LHG	C13-C14-C15-C16
31	C	517	LMG	C7-C8-C9-O8
30	B	627	STE	C11-C12-C13-C14
30	M	102	STE	C3-C4-C5-C6
30	c	516	STE	C7-C8-C9-C10
30	e	104	STE	C14-C15-C16-C17
31	b	622	LMG	C29-C30-C31-C32
33	c	519	DGD	C9A-CAA-CBA-CCA
34	D	409	LHG	C34-C35-C36-C37
31	D	407	LMG	C10-C11-C12-C13
31	M	101	LMG	C28-C29-C30-C31
32	a	614	SQD	C23-C24-C25-C26
30	H	103	STE	C9-C10-C11-C12
30	I	101	STE	C9-C10-C11-C12
30	c	516	STE	C13-C14-C15-C16
30	k	103	STE	C3-C4-C5-C6
32	a	614	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
32	a	615	SQD	C17-C18-C19-C20
33	c	519	DGD	C7B-C8B-C9B-CAB
33	c	520	DGD	CCA-CDA-CEA-CFA
33	c	520	DGD	C4B-C5B-C6B-C7B
34	d	409	LHG	C25-C26-C27-C28
30	d	412	STE	C3-C4-C5-C6
30	k	103	STE	C6-C7-C8-C9
31	A	615	LMG	C16-C17-C18-C19
32	A	616	SQD	C15-C16-C17-C18
33	A	617	DGD	C9A-CAA-CBA-CCA
34	l	101	LHG	C11-C10-C9-C8
30	B	627	STE	C9-C10-C11-C12
30	b	621	STE	C4-C5-C6-C7
32	D	410	SQD	C13-C14-C15-C16
33	C	523	DGD	CCB-CDB-CEB-CFB
26	c	504	CLA	O1D-CGD-O2D-CED
30	B	625	STE	C9-C10-C11-C12
31	c	522	LMG	C36-C37-C38-C39
32	A	616	SQD	C10-C11-C12-C13
32	D	410	SQD	C11-C12-C13-C14
32	f	102	SQD	C25-C26-C27-C28
32	f	102	SQD	C32-C33-C34-C35
26	B	601	CLA	C16-C17-C18-C19
31	D	406	LMG	O10-C28-O8-C9
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	Z	101	BCR	C1-C6-C7-C8
28	d	404	BCR	C23-C24-C25-C26
28	t	101	BCR	C23-C24-C25-C26
31	C	524	LMG	C17-C18-C19-C20
31	D	406	LMG	C30-C31-C32-C33
33	C	522	DGD	C8B-C9B-CAB-CBB
33	c	518	DGD	C3A-C4A-C5A-C6A
26	B	604	CLA	CBD-CGD-O2D-CED
34	E	101	LHG	C8-C7-O7-C5
30	C	520	STE	C11-C10-C9-C8
30	i	101	STE	C5-C6-C7-C8
34	D	408	LHG	C11-C10-C9-C8
30	B	624	STE	C6-C7-C8-C9
30	Z	102	STE	C11-C12-C13-C14
32	b	620	SQD	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
30	e	105	STE	C5-C6-C7-C8
31	D	406	LMG	O6-C5-C6-O5
31	B	620	LMG	C14-C15-C16-C17
34	e	102	LHG	C14-C15-C16-C17
26	b	607	CLA	C8-C10-C11-C12
26	B	603	CLA	C2-C3-C5-C6
30	K	102	STE	C13-C14-C15-C16
30	d	412	STE	C7-C8-C9-C10
31	a	616	LMG	C29-C30-C31-C32
31	b	622	LMG	C15-C16-C17-C18
32	b	620	SQD	C13-C14-C15-C16
34	B	622	LHG	C25-C26-C27-C28
34	D	408	LHG	C12-C13-C14-C15
34	D	411	LHG	C27-C28-C29-C30
26	B	605	CLA	C6-C7-C8-C9
30	B	624	STE	C11-C10-C9-C8
30	K	102	STE	C7-C8-C9-C10
32	f	102	SQD	C27-C28-C29-C30
33	c	519	DGD	CBB-CCB-CDB-CEB
30	B	627	STE	C5-C6-C7-C8
30	K	102	STE	C9-C10-C11-C12
30	M	102	STE	C5-C6-C7-C8
31	M	101	LMG	C20-C21-C22-C23
31	m	101	LMG	C29-C30-C31-C32
33	C	521	DGD	CCA-CDA-CEA-CFA
33	C	522	DGD	CBB-CCB-CDB-CEB
33	c	519	DGD	C6A-C7A-C8A-C9A
34	e	102	LHG	C11-C12-C13-C14
31	D	406	LMG	C29-C30-C31-C32
31	a	616	LMG	C32-C33-C34-C35
33	C	521	DGD	C6A-C7A-C8A-C9A
34	e	102	LHG	C27-C28-C29-C30
33	A	617	DGD	O6E-C5E-C6E-O5E
26	b	613	CLA	C10-C11-C12-C13
26	c	508	CLA	C13-C15-C16-C17
30	z	701	STE	C7-C8-C9-C10
32	B	623	SQD	C25-C26-C27-C28
30	T	102	STE	C13-C14-C15-C16
30	T	103	STE	C5-C6-C7-C8
32	D	410	SQD	C33-C34-C35-C36
33	C	523	DGD	CBA-CCA-CDA-CEA
30	T	102	STE	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	c	522	LMG	C30-C31-C32-C33
33	C	522	DGD	C9B-CAB-CBB-CCB
34	d	408	LHG	C32-C33-C34-C35
30	A	613	STE	C5-C6-C7-C8
31	B	620	LMG	C11-C10-O7-C8
32	f	102	SQD	C8-C7-O47-C45
31	D	406	LMG	C10-C11-C12-C13
34	B	622	LHG	C5-C6-O8-C23
32	f	102	SQD	O49-C7-O47-C45
31	d	411	LMG	C37-C38-C39-C40
26	C	505	CLA	CBD-CGD-O2D-CED
26	D	403	CLA	CBD-CGD-O2D-CED
26	b	602	CLA	C10-C11-C12-C13
30	b	625	STE	C13-C14-C15-C16
31	A	615	LMG	C12-C13-C14-C15
32	a	614	SQD	C11-C12-C13-C14
33	C	522	DGD	C4B-C5B-C6B-C7B
30	C	526	STE	C5-C6-C7-C8
27	d	401	PHO	C2C-C3C-CAC-CBC
33	C	522	DGD	C5D-C6D-O5D-C1E
30	d	406	STE	C4-C5-C6-C7
26	B	606	CLA	C16-C17-C18-C19
26	B	609	CLA	C16-C17-C18-C20
26	B	614	CLA	C16-C17-C18-C20
26	C	507	CLA	C16-C17-C18-C19
26	d	402	CLA	C16-C17-C18-C19
26	d	402	CLA	C16-C17-C18-C20
26	B	603	CLA	C4-C3-C5-C6
29	a	612	PL9	C43-C44-C46-C47
31	b	622	LMG	C21-C22-C23-C24
33	h	101	DGD	C5B-C6B-C7B-C8B
34	D	409	LHG	C32-C33-C34-C35
26	C	512	CLA	C3-C5-C6-C7
26	A	608	CLA	C13-C15-C16-C17
26	B	603	CLA	C15-C16-C17-C18
30	j	101	STE	C5-C6-C7-C8
31	D	406	LMG	C31-C32-C33-C34
31	c	521	LMG	C12-C13-C14-C15
31	d	411	LMG	C39-C40-C41-C42
33	c	519	DGD	CBA-CCA-CDA-CEA
34	l	101	LHG	C29-C30-C31-C32
26	A	610	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
30	d	406	STE	C14-C15-C16-C17
31	d	411	LMG	C38-C39-C40-C41
33	h	101	DGD	C7A-C8A-C9A-CAA
26	c	504	CLA	C10-C11-C12-C13
35	F	101	HEM	C4C-C3C-CAC-CBC
30	e	104	STE	C13-C14-C15-C16
32	a	614	SQD	C28-C29-C30-C31
33	H	102	DGD	C8B-C9B-CAB-CBB
30	A	620	STE	C13-C14-C15-C16
30	b	623	STE	C7-C8-C9-C10
31	A	615	LMG	C33-C34-C35-C36
34	D	411	LHG	C31-C32-C33-C34
26	b	603	CLA	C10-C11-C12-C13
30	C	527	STE	C11-C12-C13-C14
30	T	103	STE	C11-C10-C9-C8
30	z	701	STE	C6-C7-C8-C9
31	B	620	LMG	C31-C32-C33-C34
32	A	616	SQD	O6-C44-C45-O47
30	B	625	STE	C5-C6-C7-C8
31	m	101	LMG	C29-C28-O8-C9
30	B	625	STE	C4-C5-C6-C7
30	D	412	STE	C9-C10-C11-C12
30	d	412	STE	C6-C7-C8-C9
31	c	521	LMG	C39-C40-C41-C42
33	H	102	DGD	C6B-C7B-C8B-C9B
26	b	616	CLA	C8-C10-C11-C12
33	C	521	DGD	CBA-CCA-CDA-CEA
33	c	520	DGD	C5A-C6A-C7A-C8A
34	D	411	LHG	C24-C25-C26-C27
30	I	102	STE	C5-C6-C7-C8
31	B	620	LMG	C15-C16-C17-C18
31	a	616	LMG	O6-C5-C6-O5
30	B	625	STE	C6-C7-C8-C9
30	E	104	STE	C4-C5-C6-C7
30	E	104	STE	C10-C11-C12-C13
31	D	407	LMG	C39-C40-C41-C42
30	d	406	STE	C1-C2-C3-C4
29	a	612	PL9	C18-C19-C21-C22
34	e	102	LHG	C1-C2-C3-O3
31	d	411	LMG	O6-C5-C6-O5
31	B	620	LMG	C29-C30-C31-C32
31	a	617	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
33	c	520	DGD	C4A-C5A-C6A-C7A
31	a	616	LMG	C31-C32-C33-C34
31	A	615	LMG	C34-C35-C36-C37
32	a	614	SQD	C11-C10-C9-C8
30	H	103	STE	C6-C7-C8-C9
32	f	102	SQD	C26-C27-C28-C29
31	c	522	LMG	C29-C30-C31-C32
26	c	511	CLA	C1A-C2A-CAA-CBA
31	c	521	LMG	O6-C5-C6-O5
30	e	105	STE	C3-C4-C5-C6
30	C	520	STE	C5-C6-C7-C8
31	c	522	LMG	C40-C41-C42-C43
30	B	621	STE	C3-C4-C5-C6
31	B	620	LMG	C30-C31-C32-C33
34	d	407	LHG	C10-C11-C12-C13
26	c	506	CLA	C13-C15-C16-C17
31	M	101	LMG	C18-C19-C20-C21
32	a	615	SQD	C33-C34-C35-C36
26	B	604	CLA	C12-C13-C15-C16
26	B	615	CLA	C11-C12-C13-C15
26	C	511	CLA	C6-C7-C8-C10
26	C	512	CLA	C11-C10-C8-C7
26	b	604	CLA	C12-C13-C15-C16
26	b	607	CLA	C6-C7-C8-C10
26	c	506	CLA	C11-C10-C8-C7
26	c	506	CLA	C11-C12-C13-C15
30	b	621	STE	C11-C10-C9-C8
31	c	521	LMG	C38-C39-C40-C41
34	B	622	LHG	C13-C14-C15-C16
34	D	411	LHG	C28-C29-C30-C31
34	l	101	LHG	C13-C14-C15-C16
26	C	507	CLA	C16-C17-C18-C20
31	m	101	LMG	C40-C41-C42-C43
30	B	621	STE	C1-C2-C3-C4
31	b	622	LMG	C28-C29-C30-C31
30	K	102	STE	C12-C13-C14-C15
30	T	103	STE	C14-C15-C16-C17
34	e	102	LHG	C16-C17-C18-C19
29	D	405	PL9	C45-C44-C46-C47
29	a	612	PL9	C45-C44-C46-C47
34	B	622	LHG	C11-C10-C9-C8
26	B	601	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
26	B	604	CLA	C14-C13-C15-C16
26	B	612	CLA	C14-C13-C15-C16
26	C	505	CLA	C11-C12-C13-C14
26	C	508	CLA	C11-C10-C8-C9
26	b	607	CLA	C6-C7-C8-C9
26	c	506	CLA	C11-C10-C8-C9
30	E	103	STE	C10-C11-C12-C13
30	H	103	STE	C2-C3-C4-C5
31	B	620	LMG	C34-C35-C36-C37
31	b	622	LMG	C16-C17-C18-C19
32	D	410	SQD	C15-C16-C17-C18
34	B	622	LHG	C29-C30-C31-C32
34	l	101	LHG	C27-C28-C29-C30
33	c	520	DGD	C1A-C2A-C3A-C4A
30	c	516	STE	C9-C10-C11-C12
26	B	602	CLA	C13-C15-C16-C17
34	E	101	LHG	C32-C33-C34-C35
34	E	101	LHG	O9-C7-O7-C5
33	C	523	DGD	CAA-CBA-CCA-CDA
31	B	620	LMG	O6-C5-C6-O5
33	c	518	DGD	O6E-C5E-C6E-O5E
29	A	612	PL9	C9-C11-C12-C13
32	A	616	SQD	O6-C44-C45-C46
32	B	623	SQD	O6-C44-C45-C46
33	A	617	DGD	C1G-C2G-C3G-O3G
31	c	522	LMG	C35-C36-C37-C38
33	C	522	DGD	CCB-CDB-CEB-CFB
34	d	407	LHG	C9-C10-C11-C12
34	d	409	LHG	C34-C35-C36-C37
30	I	102	STE	C2-C3-C4-C5
30	e	103	STE	C14-C15-C16-C17
31	a	617	LMG	C31-C32-C33-C34
33	C	521	DGD	C4A-C5A-C6A-C7A
26	B	611	CLA	C16-C17-C18-C20
26	C	509	CLA	C16-C17-C18-C20
33	C	522	DGD	C5B-C6B-C7B-C8B
31	M	101	LMG	C13-C14-C15-C16
31	D	407	LMG	O6-C5-C6-O5
26	b	603	CLA	O1D-CGD-O2D-CED
26	A	614	CLA	C13-C15-C16-C17
32	a	614	SQD	C10-C11-C12-C13
31	m	101	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
34	d	407	LHG	C18-C19-C20-C21
31	M	101	LMG	C15-C16-C17-C18
30	i	101	STE	C4-C5-C6-C7
31	B	620	LMG	C33-C34-C35-C36
26	C	506	CLA	C8-C10-C11-C12
30	T	103	STE	C9-C10-C11-C12
30	c	516	STE	C6-C7-C8-C9
31	c	522	LMG	O6-C5-C6-O5
31	A	615	LMG	C40-C41-C42-C43
30	E	104	STE	C12-C13-C14-C15
26	b	607	CLA	C5-C6-C7-C8
30	a	618	STE	C4-C5-C6-C7
30	i	102	STE	C11-C10-C9-C8
31	D	406	LMG	C34-C35-C36-C37
31	c	522	LMG	C32-C33-C34-C35
34	d	407	LHG	C24-C25-C26-C27
30	b	625	STE	C15-C16-C17-C18
34	D	411	LHG	C23-C24-C25-C26
30	k	103	STE	C11-C10-C9-C8
31	D	406	LMG	C17-C18-C19-C20
33	H	102	DGD	CAA-CBA-CCA-CDA
26	B	601	CLA	O1D-CGD-O2D-CED
26	C	512	CLA	O2A-C1-C2-C3
31	A	615	LMG	C9-C8-O7-C10
30	D	412	STE	C4-C5-C6-C7
30	m	102	STE	C6-C7-C8-C9
26	A	614	CLA	C15-C16-C17-C18
30	D	412	STE	C7-C8-C9-C10
30	T	102	STE	C6-C7-C8-C9
32	D	410	SQD	C25-C26-C27-C28
34	d	407	LHG	C25-C26-C27-C28
31	D	407	LMG	C13-C14-C15-C16
30	T	102	STE	C5-C6-C7-C8
30	m	103	STE	C6-C7-C8-C9
31	B	620	LMG	C32-C33-C34-C35
31	a	616	LMG	C21-C22-C23-C24
31	M	101	LMG	C40-C41-C42-C43
30	C	519	STE	C3-C4-C5-C6
30	E	104	STE	C3-C4-C5-C6
31	c	522	LMG	C39-C40-C41-C42
34	D	411	LHG	C13-C14-C15-C16
33	C	521	DGD	CDA-CEA-CFA-CGA

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Mol	Chain	Res	Type	Atoms
30	m	103	STE	C9-C10-C11-C12
31	c	522	LMG	C15-C16-C17-C18
32	D	410	SQD	C32-C33-C34-C35
34	D	409	LHG	C11-C12-C13-C14
30	C	520	STE	C7-C8-C9-C10
33	c	519	DGD	C8B-C9B-CAB-CBB
34	B	622	LHG	C11-C12-C13-C14
30	B	621	STE	C12-C13-C14-C15
31	m	101	LMG	C22-C23-C24-C25
34	d	408	LHG	C35-C36-C37-C38
31	m	101	LMG	O10-C28-O8-C9
26	B	608	CLA	C15-C16-C17-C18
30	d	412	STE	C5-C6-C7-C8
31	C	524	LMG	C18-C19-C20-C21
31	D	406	LMG	C13-C14-C15-C16
32	D	410	SQD	C11-C10-C9-C8
32	b	620	SQD	C28-C29-C30-C31
33	H	102	DGD	CBA-CCA-CDA-CEA
33	A	617	DGD	O2G-C2G-C3G-O3G
34	d	408	LHG	C11-C12-C13-C14
30	C	527	STE	C15-C16-C17-C18
30	b	625	STE	C11-C10-C9-C8
33	C	523	DGD	C3A-C4A-C5A-C6A
33	c	518	DGD	C6B-C7B-C8B-C9B
32	F	102	SQD	C27-C28-C29-C30
34	E	101	LHG	C14-C15-C16-C17
30	E	102	STE	C3-C4-C5-C6
32	F	102	SQD	C33-C34-C35-C36
30	b	623	STE	C11-C12-C13-C14
27	A	609	PHO	C2C-C3C-CAC-CBC
29	A	612	PL9	C39-C41-C42-C43
32	F	102	SQD	C30-C31-C32-C33
30	E	104	STE	C9-C10-C11-C12
30	Z	102	STE	C6-C7-C8-C9
34	d	407	LHG	C16-C17-C18-C19
30	h	102	STE	C9-C10-C11-C12
32	b	620	SQD	C10-C11-C12-C13
34	d	407	LHG	C11-C12-C13-C14
31	C	524	LMG	C11-C12-C13-C14
33	C	521	DGD	C5A-C6A-C7A-C8A
26	b	606	CLA	C10-C11-C12-C13
31	c	517	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
30	m	103	STE	C1-C2-C3-C4
32	a	615	SQD	C35-C36-C37-C38
31	C	517	LMG	C28-C29-C30-C31
31	d	411	LMG	C28-C29-C30-C31
26	b	614	CLA	C15-C16-C17-C18
26	d	403	CLA	C8-C10-C11-C12
26	C	509	CLA	C16-C17-C18-C19
31	a	617	LMG	C20-C21-C22-C23
30	I	102	STE	C6-C7-C8-C9
30	T	102	STE	C7-C8-C9-C10
33	c	519	DGD	C5B-C6B-C7B-C8B
34	D	409	LHG	C29-C30-C31-C32
26	c	513	CLA	CBA-CGA-O2A-C1
31	a	617	LMG	C29-C28-O8-C9
30	Z	102	STE	C2-C3-C4-C5
30	Z	102	STE	C10-C11-C12-C13
30	c	516	STE	C11-C10-C9-C8
31	C	524	LMG	C32-C33-C34-C35
30	I	101	STE	C4-C5-C6-C7
31	D	406	LMG	C16-C17-C18-C19
31	B	620	LMG	O9-C10-O7-C8
32	F	102	SQD	C45-C44-O6-C1
26	B	615	CLA	C11-C10-C8-C9
26	B	615	CLA	C11-C12-C13-C14
26	C	511	CLA	C6-C7-C8-C9
26	a	610	CLA	C14-C13-C15-C16
26	b	604	CLA	C14-C13-C15-C16
26	b	606	CLA	C11-C10-C8-C9
26	c	505	CLA	C6-C7-C8-C9
26	c	506	CLA	C6-C7-C8-C9
26	c	506	CLA	C11-C12-C13-C14
31	m	101	LMG	C31-C32-C33-C34
32	A	616	SQD	C11-C10-C9-C8
26	d	403	CLA	C5-C6-C7-C8
26	b	606	CLA	C4B-C3B-CAB-CBB
30	c	516	STE	C10-C11-C12-C13
26	C	501	CLA	CBD-CGD-O2D-CED
26	B	611	CLA	C16-C17-C18-C19
34	d	407	LHG	C28-C29-C30-C31
26	C	510	CLA	C10-C11-C12-C13
30	A	620	STE	C14-C15-C16-C17
31	c	521	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
30	j	101	STE	C7-C8-C9-C10
31	D	407	LMG	C22-C23-C24-C25
30	k	103	STE	C5-C6-C7-C8
31	a	617	LMG	C17-C18-C19-C20
33	C	522	DGD	CDA-CEA-CFA-CGA
26	B	601	CLA	C6-C7-C8-C10
26	B	602	CLA	C11-C12-C13-C15
26	B	612	CLA	C12-C13-C15-C16
26	B	613	CLA	C11-C12-C13-C15
26	B	614	CLA	C6-C7-C8-C10
26	B	614	CLA	C12-C13-C15-C16
26	C	505	CLA	C12-C13-C15-C16
26	C	508	CLA	C11-C10-C8-C7
26	C	513	CLA	C12-C13-C15-C16
26	a	610	CLA	C12-C13-C15-C16
26	b	606	CLA	C11-C10-C8-C7
26	b	614	CLA	C6-C7-C8-C10
26	c	505	CLA	C6-C7-C8-C10
26	c	505	CLA	C11-C12-C13-C15
26	c	506	CLA	C6-C7-C8-C10
30	C	516	STE	C9-C10-C11-C12
30	T	103	STE	C4-C5-C6-C7
34	E	101	LHG	C19-C20-C21-C22
31	M	101	LMG	C36-C37-C38-C39
31	c	522	LMG	C34-C35-C36-C37
32	a	614	SQD	C34-C35-C36-C37
30	C	527	STE	C13-C14-C15-C16
30	J	101	STE	C2-C3-C4-C5
26	B	601	CLA	C3A-C2A-CAA-CBA
26	C	510	CLA	C4-C3-C5-C6
29	A	612	PL9	C15-C14-C16-C17
30	d	412	STE	C10-C11-C12-C13
26	B	612	CLA	C10-C11-C12-C13
26	b	601	CLA	C10-C11-C12-C13
30	m	102	STE	C2-C3-C4-C5
30	C	527	STE	C7-C8-C9-C10
30	b	621	STE	C14-C15-C16-C17
31	D	407	LMG	C30-C31-C32-C33
33	C	521	DGD	CDB-CEB-CFB-CGB
26	c	503	CLA	C16-C17-C18-C20
34	B	622	LHG	C35-C36-C37-C38
33	A	617	DGD	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
33	c	518	DGD	CDA-CEA-CFA-CGA
31	a	617	LMG	C19-C20-C21-C22
30	A	618	STE	C13-C14-C15-C16
34	E	101	LHG	C33-C34-C35-C36
31	D	406	LMG	O1-C7-C8-C9
31	b	622	LMG	C7-C8-C9-O8
32	a	614	SQD	C44-C45-C46-O48
32	a	615	SQD	O6-C44-C45-C46
32	A	616	SQD	C9-C10-C11-C12
34	B	622	LHG	C24-C25-C26-C27
26	B	609	CLA	C16-C17-C18-C19
26	B	615	CLA	C16-C17-C18-C19
26	B	615	CLA	C16-C17-C18-C20
26	c	503	CLA	C16-C17-C18-C19
34	d	407	LHG	C26-C27-C28-C29
32	D	410	SQD	C9-C10-C11-C12
32	a	614	SQD	C13-C14-C15-C16
26	B	601	CLA	C8-C10-C11-C12
30	D	412	STE	C2-C3-C4-C5
32	a	615	SQD	C15-C16-C17-C18
31	D	407	LMG	C21-C22-C23-C24
31	b	622	LMG	C13-C14-C15-C16
30	M	102	STE	C10-C11-C12-C13
30	j	102	STE	C15-C16-C17-C18
33	A	617	DGD	C7B-C8B-C9B-CAB
33	c	519	DGD	CAB-CBB-CCB-CDB
33	C	521	DGD	O6D-C5D-C6D-O5D
31	A	615	LMG	C32-C33-C34-C35
33	C	521	DGD	C4B-C5B-C6B-C7B
33	c	519	DGD	CAA-CBA-CCA-CDA
28	b	617	BCR	C1-C6-C7-C8
32	a	614	SQD	C32-C33-C34-C35
26	B	606	CLA	C13-C15-C16-C17
26	C	511	CLA	C8-C10-C11-C12
34	d	409	LHG	C2-C3-O3-P
30	d	410	STE	C10-C11-C12-C13
26	B	603	CLA	C10-C11-C12-C13
26	C	509	CLA	C5-C6-C7-C8
26	b	605	CLA	C8-C10-C11-C12
31	c	522	LMG	C42-C43-C44-C45
30	z	701	STE	C3-C4-C5-C6
34	B	622	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
31	D	406	LMG	O7-C8-C9-O8
32	a	614	SQD	O6-C44-C45-O47
32	f	102	SQD	O6-C44-C45-O47
34	e	102	LHG	O7-C5-C6-O8
31	C	524	LMG	C40-C41-C42-C43
32	a	615	SQD	C11-C12-C13-C14
29	a	612	PL9	C4-C3-C7-C8
30	A	620	STE	C12-C13-C14-C15
31	M	101	LMG	C30-C31-C32-C33
30	E	103	STE	C9-C10-C11-C12
30	T	102	STE	C9-C10-C11-C12
34	d	408	LHG	C15-C16-C17-C18
26	C	510	CLA	C2-C3-C5-C6
30	e	105	STE	C7-C8-C9-C10
32	a	614	SQD	C31-C32-C33-C34
33	c	520	DGD	C6A-C7A-C8A-C9A
34	D	411	LHG	C17-C18-C19-C20
30	B	621	STE	C9-C10-C11-C12
30	B	627	STE	C11-C10-C9-C8
26	a	607	CLA	C4C-C3C-CAC-CBC
30	j	101	STE	C1-C2-C3-C4
32	a	614	SQD	C24-C23-O48-C46
31	A	615	LMG	C17-C18-C19-C20
34	E	101	LHG	C10-C11-C12-C13
26	B	601	CLA	C14-C13-C15-C16
26	B	602	CLA	C11-C12-C13-C14
26	B	614	CLA	C14-C13-C15-C16
26	b	603	CLA	C6-C7-C8-C9
26	b	615	CLA	C11-C12-C13-C14
33	A	617	DGD	CCB-CDB-CEB-CFB
32	b	620	SQD	C25-C26-C27-C28
31	M	101	LMG	C37-C38-C39-C40
33	A	617	DGD	C1B-C2B-C3B-C4B
26	b	616	CLA	C3-C5-C6-C7
31	B	620	LMG	C20-C21-C22-C23
33	C	523	DGD	C2B-C3B-C4B-C5B
29	a	612	PL9	C39-C41-C42-C43
31	d	411	LMG	C15-C16-C17-C18
30	B	626	STE	C2-C3-C4-C5
30	C	527	STE	C9-C10-C11-C12
30	T	102	STE	C11-C10-C9-C8
30	e	104	STE	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
30	e	105	STE	C4-C5-C6-C7
30	H	103	STE	C1-C2-C3-C4
34	d	407	LHG	O1-C1-C2-O2
31	C	524	LMG	C29-C28-O8-C9
33	h	101	DGD	O2G-C1B-C2B-C3B
30	C	520	STE	C3-C4-C5-C6
31	M	101	LMG	C33-C34-C35-C36
26	a	607	CLA	C15-C16-C17-C18
31	C	517	LMG	C10-C11-C12-C13
30	C	525	STE	C4-C5-C6-C7
33	C	522	DGD	C3A-C4A-C5A-C6A
30	b	621	STE	C12-C13-C14-C15
30	j	101	STE	C4-C5-C6-C7
30	z	701	STE	C5-C6-C7-C8
31	a	617	LMG	C18-C19-C20-C21
34	d	409	LHG	C30-C31-C32-C33
32	a	615	SQD	C11-C10-C9-C8
26	B	614	CLA	C16-C17-C18-C19
29	a	612	PL9	C21-C22-C23-C24
32	a	614	SQD	O10-C23-O48-C46
26	B	605	CLA	C8-C10-C11-C12
26	b	603	CLA	C13-C15-C16-C17
26	B	604	CLA	C11-C12-C13-C15
26	B	613	CLA	C12-C13-C15-C16
26	C	509	CLA	C12-C13-C15-C16
26	D	403	CLA	C6-C7-C8-C10
26	b	603	CLA	C6-C7-C8-C10
26	b	614	CLA	C11-C12-C13-C15
26	b	615	CLA	C11-C12-C13-C15
26	c	513	CLA	C12-C13-C15-C16
26	a	613	CLA	C2C-C3C-CAC-CBC
30	h	102	STE	C11-C12-C13-C14
30	M	103	STE	C1-C2-C3-C4
30	A	620	STE	C11-C10-C9-C8
30	e	103	STE	C15-C16-C17-C18
28	B	617	BCR	C17-C18-C19-C20
28	C	514	BCR	C11-C12-C13-C14
31	a	616	LMG	C8-C7-O1-C1
32	B	623	SQD	C45-C44-O6-C1
33	C	522	DGD	C2G-C3G-O3G-C1D
33	c	519	DGD	C2G-C3G-O3G-C1D
33	c	519	DGD	C5D-C6D-O5D-C1E

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Mol	Chain	Res	Type	Atoms
33	C	522	DGD	C9A-CAA-CBA-CCA
26	B	615	CLA	O1D-CGD-O2D-CED
26	C	510	CLA	C16-C17-C18-C20
33	c	518	DGD	C2B-C3B-C4B-C5B
29	a	612	PL9	C15-C14-C16-C17
33	H	102	DGD	O2G-C1B-C2B-C3B
26	c	513	CLA	O1A-CGA-O2A-C1
29	A	612	PL9	C13-C14-C16-C17
29	D	405	PL9	C43-C44-C46-C47
30	K	102	STE	C6-C7-C8-C9
30	M	102	STE	C2-C3-C4-C5
32	D	410	SQD	C12-C13-C14-C15
31	D	406	LMG	C37-C38-C39-C40
34	d	408	LHG	C30-C31-C32-C33
32	f	102	SQD	C46-C45-O47-C7
34	D	408	LHG	C33-C34-C35-C36
31	a	617	LMG	O10-C28-O8-C9
26	c	507	CLA	C5-C6-C7-C8
26	D	403	CLA	O1D-CGD-O2D-CED
32	b	620	SQD	C44-C45-C46-O48
34	e	102	LHG	C4-C5-C6-O8
26	b	601	CLA	C16-C17-C18-C20
31	c	521	LMG	C31-C32-C33-C34
30	m	102	STE	C3-C4-C5-C6
31	A	615	LMG	O7-C8-C9-O8
31	b	622	LMG	O7-C8-C9-O8
32	f	102	SQD	O47-C45-C46-O48
26	C	505	CLA	C14-C13-C15-C16
26	C	509	CLA	C14-C13-C15-C16
26	b	615	CLA	C6-C7-C8-C9
26	c	503	CLA	C11-C12-C13-C14
26	b	603	CLA	C16-C17-C18-C20
33	c	518	DGD	O6D-C5D-C6D-O5D
30	m	102	STE	C4-C5-C6-C7
31	A	615	LMG	C31-C32-C33-C34
31	c	522	LMG	C12-C13-C14-C15
33	H	102	DGD	C5B-C6B-C7B-C8B
31	C	524	LMG	O10-C28-O8-C9
34	l	101	LHG	C26-C27-C28-C29
31	b	622	LMG	C22-C23-C24-C25
30	C	520	STE	C6-C7-C8-C9
30	H	103	STE	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
34	D	411	LHG	C18-C19-C20-C21
33	C	521	DGD	C4D-C5D-C6D-O5D
31	d	411	LMG	C32-C33-C34-C35
34	D	408	LHG	C32-C33-C34-C35
26	B	616	CLA	C2-C1-O2A-CGA
33	c	519	DGD	C2E-C1E-O5D-C6D
26	c	504	CLA	C11-C12-C13-C14
30	A	620	STE	C15-C16-C17-C18
31	d	411	LMG	C10-C11-C12-C13
33	A	617	DGD	CBA-CCA-CDA-CEA
30	b	621	STE	C3-C4-C5-C6
26	a	613	CLA	C13-C15-C16-C17
26	c	509	CLA	C8-C10-C11-C12
26	D	403	CLA	C16-C17-C18-C20
33	H	102	DGD	CDA-CEA-CFA-CGA
30	M	102	STE	C6-C7-C8-C9
33	c	519	DGD	C9B-CAB-CBB-CCB
26	b	610	CLA	C8-C10-C11-C12
30	d	410	STE	C11-C12-C13-C14
31	m	101	LMG	O9-C10-O7-C8
26	C	513	CLA	O1D-CGD-O2D-CED
26	C	501	CLA	C4B-C3B-CAB-CBB
26	a	608	CLA	C4B-C3B-CAB-CBB
26	C	505	CLA	O1D-CGD-O2D-CED
32	a	615	SQD	C10-C11-C12-C13
34	E	101	LHG	C25-C26-C27-C28
34	d	408	LHG	C9-C10-C11-C12
26	c	509	CLA	C4-C3-C5-C6
33	C	521	DGD	C2A-C3A-C4A-C5A
34	d	408	LHG	C12-C13-C14-C15
33	c	518	DGD	CCB-CDB-CEB-CFB
34	l	101	LHG	C34-C35-C36-C37
26	C	510	CLA	C16-C17-C18-C19
26	d	402	CLA	C3-C5-C6-C7
34	B	622	LHG	C28-C29-C30-C31
32	a	615	SQD	C5-C6-S-O9
33	C	522	DGD	C6A-C7A-C8A-C9A
26	B	601	CLA	C12-C13-C15-C16
26	B	616	CLA	C6-C7-C8-C10
26	C	504	CLA	C11-C10-C8-C7
26	C	505	CLA	C6-C7-C8-C10
26	C	510	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
26	C	513	CLA	C11-C10-C8-C7
26	b	606	CLA	C12-C13-C15-C16
26	c	507	CLA	C12-C13-C15-C16
26	C	506	CLA	C16-C17-C18-C20
26	b	603	CLA	C16-C17-C18-C19
30	C	516	STE	C5-C6-C7-C8
33	C	521	DGD	C8B-C9B-CAB-CBB
34	d	409	LHG	C27-C28-C29-C30
32	B	623	SQD	C10-C11-C12-C13
33	h	101	DGD	CDB-CEB-CFB-CGB
30	H	104	STE	C11-C12-C13-C14
31	c	517	LMG	C32-C33-C34-C35
33	C	522	DGD	CCA-CDA-CEA-CFA
26	c	513	CLA	C8-C10-C11-C12
26	C	503	CLA	C10-C11-C12-C13
26	B	604	CLA	C11-C12-C13-C14
26	B	613	CLA	C14-C13-C15-C16
26	D	403	CLA	C6-C7-C8-C9
26	b	611	CLA	C14-C13-C15-C16
26	b	614	CLA	C11-C12-C13-C14
26	c	507	CLA	C14-C13-C15-C16
26	c	513	CLA	C14-C13-C15-C16
31	b	622	LMG	C32-C33-C34-C35
33	C	521	DGD	C3B-C4B-C5B-C6B
28	H	101	BCR	C9-C10-C11-C12
33	c	519	DGD	C5A-C6A-C7A-C8A
26	B	604	CLA	O1D-CGD-O2D-CED
26	c	510	CLA	C10-C11-C12-C13
30	d	406	STE	C7-C8-C9-C10
33	c	518	DGD	C8B-C9B-CAB-CBB
33	A	617	DGD	CCA-CDA-CEA-CFA
31	C	517	LMG	O7-C8-C9-O8
31	a	616	LMG	O7-C8-C9-O8
30	j	102	STE	C10-C11-C12-C13
34	D	409	LHG	C27-C28-C29-C30
30	I	102	STE	C9-C10-C11-C12
31	C	517	LMG	C12-C13-C14-C15
31	D	407	LMG	C14-C15-C16-C17
32	f	102	SQD	C44-C45-C46-O48
29	d	405	PL9	C45-C44-C46-C47
32	b	620	SQD	C16-C17-C18-C19
26	B	615	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	b	622	LMG	C10-C11-C12-C13
26	C	502	CLA	CAD-CBD-CGD-O2D
26	C	504	CLA	CAD-CBD-CGD-O2D
26	c	502	CLA	CAD-CBD-CGD-O2D
26	c	504	CLA	CAD-CBD-CGD-O2D
26	b	608	CLA	C13-C15-C16-C17
32	a	615	SQD	C32-C33-C34-C35
30	Z	102	STE	C5-C6-C7-C8
33	c	518	DGD	CBA-CCA-CDA-CEA
30	b	624	STE	C7-C8-C9-C10
30	T	103	STE	C13-C14-C15-C16
29	a	612	PL9	C32-C33-C34-C36
33	c	520	DGD	C6B-C7B-C8B-C9B
26	B	601	CLA	CAD-CBD-CGD-O1D
26	C	502	CLA	CAD-CBD-CGD-O1D
26	C	504	CLA	CAD-CBD-CGD-O1D
26	b	616	CLA	CHA-CBD-CGD-O1D
26	b	616	CLA	CHA-CBD-CGD-O2D
26	c	502	CLA	CAD-CBD-CGD-O1D
26	c	504	CLA	CAD-CBD-CGD-O1D
26	c	509	CLA	CHA-CBD-CGD-O1D
26	c	509	CLA	CHA-CBD-CGD-O2D
28	C	514	BCR	C9-C10-C11-C12
28	C	514	BCR	C13-C14-C15-C16
28	T	101	BCR	C13-C14-C15-C16
28	c	514	BCR	C13-C14-C15-C16
28	x	101	BCR	C9-C10-C11-C12
34	d	408	LHG	C4-O6-P-O5
26	c	511	CLA	C16-C17-C18-C19
34	d	407	LHG	C7-C8-C9-C10
26	a	608	CLA	C2B-C3B-CAB-CBB
28	T	101	BCR	C23-C24-C25-C30
31	a	617	LMG	C35-C36-C37-C38
34	D	409	LHG	C2-C3-O3-P
34	e	102	LHG	C2-C3-O3-P
26	B	613	CLA	C16-C17-C18-C19
26	D	403	CLA	C16-C17-C18-C19
33	c	518	DGD	C4D-C5D-C6D-O5D
33	H	102	DGD	C8A-C9A-CAA-CBA
34	D	411	LHG	C32-C33-C34-C35
31	b	622	LMG	C36-C37-C38-C39
30	c	516	STE	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
29	A	612	PL9	C4-C3-C7-C8
30	a	618	STE	C3-C4-C5-C6
31	C	517	LMG	C7-C8-O7-C10
26	B	604	CLA	C16-C17-C18-C20
26	C	506	CLA	C16-C17-C18-C19
26	C	513	CLA	C8-C10-C11-C12
30	T	103	STE	C10-C11-C12-C13
32	D	410	SQD	C35-C36-C37-C38
33	h	101	DGD	C6B-C7B-C8B-C9B
30	t	102	STE	C7-C8-C9-C10
26	C	503	CLA	C11-C10-C8-C9
26	C	505	CLA	C6-C7-C8-C9
26	b	603	CLA	C11-C12-C13-C14
26	b	605	CLA	C6-C7-C8-C9
26	c	505	CLA	C11-C12-C13-C14
26	B	615	CLA	C6-C7-C8-C10
26	C	507	CLA	C11-C12-C13-C15
26	C	509	CLA	C11-C10-C8-C7
26	c	513	CLA	C11-C10-C8-C7
30	B	621	STE	C5-C6-C7-C8
33	c	520	DGD	CBB-CCB-CDB-CEB
30	B	625	STE	C1-C2-C3-C4
31	a	616	LMG	C30-C31-C32-C33
31	a	616	LMG	O6-C1-O1-C7
26	c	504	CLA	C11-C12-C13-C15
29	a	612	PL9	C20-C19-C21-C22
26	c	509	CLA	C2-C3-C5-C6
26	B	612	CLA	C16-C17-C18-C19
26	c	511	CLA	C16-C17-C18-C20
26	B	614	CLA	C13-C15-C16-C17
31	D	407	LMG	C35-C36-C37-C38
31	D	406	LMG	O1-C7-C8-O7
32	b	620	SQD	O47-C45-C46-O48
26	a	613	CLA	C4C-C3C-CAC-CBC
30	b	621	STE	C9-C10-C11-C12
30	d	406	STE	C6-C7-C8-C9
34	B	622	LHG	C10-C11-C12-C13
26	B	604	CLA	C16-C17-C18-C19
31	b	622	LMG	C11-C12-C13-C14
34	E	101	LHG	C24-C25-C26-C27
31	c	521	LMG	C29-C30-C31-C32
26	c	509	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
33	C	523	DGD	C7B-C8B-C9B-CAB
31	D	406	LMG	C35-C36-C37-C38
31	c	522	LMG	C31-C32-C33-C34
31	c	521	LMG	C34-C35-C36-C37
28	T	101	BCR	C37-C22-C23-C24
33	H	102	DGD	C9B-CAB-CBB-CCB
32	a	614	SQD	C35-C36-C37-C38
26	A	614	CLA	C16-C17-C18-C19
26	B	613	CLA	C16-C17-C18-C20
26	b	612	CLA	C13-C15-C16-C17
34	d	407	LHG	C27-C28-C29-C30
26	c	511	CLA	CBA-CGA-O2A-C1
33	C	521	DGD	C3A-C4A-C5A-C6A
30	C	526	STE	C9-C10-C11-C12
26	b	604	CLA	C15-C16-C17-C18
26	C	510	CLA	C11-C10-C8-C9
26	C	513	CLA	C11-C10-C8-C9
26	C	513	CLA	C14-C13-C15-C16
26	c	508	CLA	C11-C12-C13-C14
30	m	102	STE	C5-C6-C7-C8
31	m	101	LMG	C35-C36-C37-C38
33	C	523	DGD	O6D-C5D-C6D-O5D
26	b	610	CLA	C16-C17-C18-C20
26	B	605	CLA	C13-C15-C16-C17
31	C	517	LMG	C11-C12-C13-C14
26	C	509	CLA	C3-C5-C6-C7
34	D	411	LHG	C25-C26-C27-C28
26	A	614	CLA	C16-C17-C18-C20
30	B	625	STE	C13-C14-C15-C16
26	B	604	CLA	C2C-C3C-CAC-CBC
33	c	520	DGD	CDA-CEA-CFA-CGA
32	D	410	SQD	C29-C30-C31-C32
26	C	506	CLA	C11-C12-C13-C15
26	c	510	CLA	C12-C13-C15-C16
30	Z	102	STE	C13-C14-C15-C16
26	c	511	CLA	O1A-CGA-O2A-C1
34	l	101	LHG	C16-C17-C18-C19
34	e	102	LHG	C15-C16-C17-C18
33	C	523	DGD	C9B-CAB-CBB-CCB
30	C	519	STE	C4-C5-C6-C7
34	D	408	LHG	C25-C26-C27-C28
34	d	407	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
33	C	521	DGD	CBB-CCB-CDB-CEB
26	C	507	CLA	C5-C6-C7-C8
26	b	614	CLA	C10-C11-C12-C13
30	M	103	STE	C7-C8-C9-C10
30	A	620	STE	C10-C11-C12-C13
30	e	101	STE	C11-C12-C13-C14
34	e	102	LHG	C12-C13-C14-C15
28	t	101	BCR	C13-C14-C15-C16
31	c	521	LMG	C15-C16-C17-C18
26	C	506	CLA	C15-C16-C17-C18
30	j	102	STE	C13-C14-C15-C16
33	A	617	DGD	CDB-CEB-CFB-CGB
31	a	616	LMG	C41-C42-C43-C44
30	B	625	STE	O2-C1-C2-C3
26	c	508	CLA	C16-C17-C18-C19
26	B	601	CLA	C4-C3-C5-C6
26	C	506	CLA	C4-C3-C5-C6
26	c	512	CLA	C4-C3-C5-C6
29	d	405	PL9	C47-C48-C49-C51
26	b	615	CLA	C8-C10-C11-C12
31	A	615	LMG	C7-C8-C9-O8
31	a	616	LMG	C7-C8-C9-O8
32	a	614	SQD	O6-C44-C45-C46
30	T	102	STE	C14-C15-C16-C17
33	h	101	DGD	CBA-CCA-CDA-CEA
31	M	101	LMG	C34-C35-C36-C37
29	d	405	PL9	C47-C48-C49-C50
26	B	602	CLA	C6-C7-C8-C9
26	C	504	CLA	C11-C10-C8-C9
26	C	506	CLA	C11-C12-C13-C14
26	a	610	CLA	C11-C12-C13-C14
26	b	601	CLA	C11-C10-C8-C9
26	b	610	CLA	C14-C13-C15-C16
26	c	512	CLA	C11-C12-C13-C14
31	M	101	LMG	C12-C13-C14-C15
31	m	101	LMG	C14-C15-C16-C17
31	a	616	LMG	C7-C8-O7-C10
31	a	616	LMG	C9-C8-O7-C10
31	A	615	LMG	C35-C36-C37-C38
30	I	101	STE	C5-C6-C7-C8
26	B	601	CLA	C2-C3-C5-C6
30	d	406	STE	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
26	c	508	CLA	C1A-C2A-CAA-CBA
33	A	617	DGD	CEA-CFA-CGA-CHA
33	c	519	DGD	CDB-CEB-CFB-CGB
26	b	601	CLA	C16-C17-C18-C19
26	b	602	CLA	C16-C17-C18-C19
30	B	625	STE	O1-C1-C2-C3
36	V	201	HEC	CAD-CBD-CGD-O1D
32	D	410	SQD	C28-C29-C30-C31
33	H	102	DGD	CCB-CDB-CEB-CFB
26	C	501	CLA	C2B-C3B-CAB-CBB
28	b	617	BCR	C5-C6-C7-C8
32	b	620	SQD	C23-C24-C25-C26
33	H	102	DGD	C1A-C2A-C3A-C4A
30	I	101	STE	O2-C1-C2-C3
35	F	101	HEM	CAD-CBD-CGD-O1D
26	a	610	CLA	C15-C16-C17-C18
31	M	101	LMG	C32-C33-C34-C35
31	a	616	LMG	C33-C34-C35-C36
33	C	522	DGD	C8A-C9A-CAA-CBA
26	b	610	CLA	C16-C17-C18-C19
26	a	610	CLA	C13-C15-C16-C17
36	V	201	HEC	CAD-CBD-CGD-O2D
29	a	612	PL9	C30-C29-C31-C32
26	C	506	CLA	C2-C3-C5-C6
32	b	620	SQD	C19-C20-C21-C22
31	d	411	LMG	C33-C34-C35-C36
26	A	607	CLA	C2C-C3C-CAC-CBC
26	B	606	CLA	C12-C13-C15-C16
26	B	608	CLA	C6-C7-C8-C10
26	C	512	CLA	C11-C12-C13-C15
26	C	512	CLA	C12-C13-C15-C16
26	b	602	CLA	C12-C13-C15-C16
26	c	509	CLA	C12-C13-C15-C16
30	M	103	STE	C6-C7-C8-C9
34	D	408	LHG	C11-C12-C13-C14
31	B	620	LMG	O7-C8-C9-O8
32	D	410	SQD	O6-C44-C45-O47
35	f	101	HEM	CAD-CBD-CGD-O1D
36	v	201	HEC	CAD-CBD-CGD-O1D
32	F	102	SQD	C44-C45-C46-O48
30	K	102	STE	C15-C16-C17-C18
30	D	412	STE	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	c	522	LMG	C38-C39-C40-C41
32	D	410	SQD	C34-C35-C36-C37
26	B	612	CLA	C16-C17-C18-C20
30	B	621	STE	C7-C8-C9-C10
26	b	605	CLA	C5-C6-C7-C8
26	c	512	CLA	C2-C3-C5-C6
29	a	612	PL9	C13-C14-C16-C17
32	a	615	SQD	C18-C19-C20-C21
34	l	101	LHG	C5-C6-O8-C23
31	c	521	LMG	C29-C28-O8-C9
30	j	102	STE	C6-C7-C8-C9
30	I	101	STE	C6-C7-C8-C9
30	i	101	STE	O2-C1-C2-C3
36	v	201	HEC	CAD-CBD-CGD-O2D
26	a	610	CLA	C6-C7-C8-C9
34	D	409	LHG	C12-C13-C14-C15
26	B	610	CLA	C16-C17-C18-C19
30	C	527	STE	C11-C10-C9-C8
30	d	412	STE	O1-C1-C2-C3
30	d	412	STE	O2-C1-C2-C3
34	e	102	LHG	C18-C19-C20-C21
30	I	101	STE	O1-C1-C2-C3
30	C	518	STE	C2-C3-C4-C5
30	E	104	STE	O1-C1-C2-C3
31	b	622	LMG	C12-C13-C14-C15
32	b	620	SQD	O48-C23-C24-C25
30	A	618	STE	C15-C16-C17-C18
31	B	620	LMG	O1-C7-C8-C9
31	B	620	LMG	C7-C8-C9-O8
32	f	102	SQD	O6-C44-C45-C46
30	T	102	STE	C3-C4-C5-C6
35	F	101	HEM	CAD-CBD-CGD-O2D
30	D	412	STE	C12-C13-C14-C15
33	C	523	DGD	C3B-C4B-C5B-C6B
26	D	403	CLA	O1A-CGA-O2A-C1
26	B	610	CLA	C2A-CAA-CBA-CGA
26	C	501	CLA	C2A-CAA-CBA-CGA
26	b	614	CLA	C2A-CAA-CBA-CGA
26	D	402	CLA	C2C-C3C-CAC-CBC
34	e	102	LHG	O9-C7-O7-C5
26	b	604	CLA	C8-C10-C11-C12
26	B	609	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	B	620	LMG	C13-C14-C15-C16
32	B	623	SQD	C29-C30-C31-C32
31	c	521	LMG	O10-C28-O8-C9
34	D	409	LHG	C17-C18-C19-C20
32	D	410	SQD	C31-C32-C33-C34
30	B	624	STE	O2-C1-C2-C3
26	b	615	CLA	C16-C17-C18-C19
34	d	407	LHG	C1-C2-C3-O3
33	c	519	DGD	C3A-C4A-C5A-C6A
33	c	519	DGD	C8A-C9A-CAA-CBA
27	d	401	PHO	CHA-CBD-CGD-O1D
27	d	401	PHO	CHA-CBD-CGD-O2D
26	C	512	CLA	O1A-CGA-O2A-C1
30	B	626	STE	O2-C1-C2-C3
30	d	406	STE	O2-C1-C2-C3
33	c	519	DGD	O6E-C1E-O5D-C6D
32	a	614	SQD	C25-C26-C27-C28
35	f	101	HEM	CAD-CBD-CGD-O2D
30	H	103	STE	C7-C8-C9-C10
30	I	102	STE	C4-C5-C6-C7
33	C	521	DGD	C9B-CAB-CBB-CCB
31	a	616	LMG	C40-C41-C42-C43
33	h	101	DGD	CCA-CDA-CEA-CFA
30	i	101	STE	O1-C1-C2-C3
26	a	608	CLA	C6-C7-C8-C9
26	b	603	CLA	C11-C10-C8-C9
26	c	502	CLA	C11-C12-C13-C14
33	c	520	DGD	CAB-CBB-CCB-CDB
26	B	602	CLA	C15-C16-C17-C18
33	C	521	DGD	C5D-C6D-O5D-C1E
32	B	623	SQD	C15-C16-C17-C18
33	c	520	DGD	C3A-C4A-C5A-C6A
26	b	603	CLA	C2A-CAA-CBA-CGA
26	b	610	CLA	C2A-CAA-CBA-CGA
26	c	501	CLA	C2A-CAA-CBA-CGA
26	B	613	CLA	C2-C1-O2A-CGA
30	i	101	STE	C6-C7-C8-C9
26	c	513	CLA	C4-C3-C5-C6
32	f	102	SQD	C33-C34-C35-C36
31	m	101	LMG	C39-C40-C41-C42
26	C	501	CLA	O1D-CGD-O2D-CED
30	I	102	STE	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
26	A	607	CLA	C16-C17-C18-C19
30	C	525	STE	C7-C8-C9-C10
33	C	522	DGD	C2E-C1E-O5D-C6D
26	C	513	CLA	O2A-C1-C2-C3
30	B	626	STE	O1-C1-C2-C3
30	b	624	STE	C2-C3-C4-C5
31	M	101	LMG	C21-C22-C23-C24
31	c	517	LMG	O8-C28-C29-C30
30	a	618	STE	O2-C1-C2-C3
32	B	623	SQD	C34-C35-C36-C37
30	B	624	STE	O1-C1-C2-C3
26	B	609	CLA	C2-C3-C5-C6
31	a	616	LMG	C38-C39-C40-C41
33	c	518	DGD	C7B-C8B-C9B-CAB
30	d	406	STE	C13-C14-C15-C16
26	C	512	CLA	CBA-CGA-O2A-C1
30	C	516	STE	O2-C1-C2-C3
31	D	406	LMG	C7-C8-C9-O8
34	E	101	LHG	C4-C5-C6-O8
26	b	604	CLA	C5-C6-C7-C8
31	a	616	LMG	C18-C19-C20-C21
32	a	614	SQD	C14-C15-C16-C17
31	C	517	LMG	C14-C15-C16-C17
26	D	403	CLA	CBA-CGA-O2A-C1
29	d	405	PL9	C20-C19-C21-C22
29	d	405	PL9	C38-C39-C41-C42
31	c	521	LMG	C11-C12-C13-C14
30	d	406	STE	C11-C10-C9-C8
30	j	102	STE	C9-C10-C11-C12
34	E	101	LHG	O7-C5-C6-O8
30	A	619	STE	C11-C10-C9-C8
30	d	410	STE	O1-C1-C2-C3
26	B	616	CLA	C6-C7-C8-C9
26	C	507	CLA	C11-C12-C13-C14
26	C	508	CLA	C14-C13-C15-C16
26	c	505	CLA	C14-C13-C15-C16
26	B	612	CLA	CAA-CBA-CGA-O2A
31	B	620	LMG	O7-C10-C11-C12
33	H	102	DGD	O1B-C1B-C2B-C3B
30	a	618	STE	O1-C1-C2-C3
32	B	623	SQD	C28-C29-C30-C31
31	c	517	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
32	a	614	SQD	O47-C7-C8-C9
30	d	410	STE	O2-C1-C2-C3
26	B	605	CLA	C11-C10-C8-C7
26	B	607	CLA	C12-C13-C15-C16
26	a	608	CLA	C6-C7-C8-C10
26	a	610	CLA	C6-C7-C8-C10
26	b	602	CLA	C11-C10-C8-C7
26	b	603	CLA	C11-C10-C8-C7
26	c	502	CLA	C11-C12-C13-C15
26	c	503	CLA	C11-C10-C8-C7
26	c	508	CLA	C11-C10-C8-C7
26	d	403	CLA	C11-C12-C13-C15
31	C	524	LMG	C12-C13-C14-C15
30	H	104	STE	C12-C13-C14-C15
33	H	102	DGD	C3B-C4B-C5B-C6B
36	V	201	HEC	C2B-C3B-CAB-CBB
26	b	606	CLA	C2B-C3B-CAB-CBB
28	Z	101	BCR	C23-C24-C25-C30
31	c	522	LMG	C33-C34-C35-C36
30	T	102	STE	C12-C13-C14-C15
31	a	617	LMG	C13-C14-C15-C16
31	d	411	LMG	C36-C37-C38-C39
26	D	402	CLA	C2-C1-O2A-CGA
26	c	506	CLA	C2-C1-O2A-CGA
32	A	616	SQD	C18-C19-C20-C21
30	E	104	STE	O2-C1-C2-C3
30	b	624	STE	C6-C7-C8-C9
26	B	607	CLA	CBA-CGA-O2A-C1
30	Z	102	STE	C11-C10-C9-C8
26	b	609	CLA	C4-C3-C5-C6
26	B	613	CLA	CAA-CBA-CGA-O2A
26	b	609	CLA	C2-C3-C5-C6
31	a	616	LMG	O9-C10-O7-C8
26	c	505	CLA	C13-C15-C16-C17
30	c	516	STE	C14-C15-C16-C17
31	a	616	LMG	C11-C10-O7-C8
30	C	516	STE	O1-C1-C2-C3
26	B	607	CLA	O1A-CGA-O2A-C1
26	B	608	CLA	C3-C5-C6-C7
30	d	412	STE	C2-C3-C4-C5
31	c	522	LMG	C16-C17-C18-C19
30	b	624	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
33	c	520	DGD	CAA-CBA-CCA-CDA
32	B	623	SQD	C11-C10-C9-C8
33	C	522	DGD	C5A-C6A-C7A-C8A
34	d	407	LHG	C33-C34-C35-C36
30	M	103	STE	C4-C5-C6-C7
30	z	702	STE	C3-C4-C5-C6
26	b	602	CLA	C16-C17-C18-C20
33	H	102	DGD	C2B-C3B-C4B-C5B
29	a	612	PL9	C28-C29-C31-C32
34	e	102	LHG	C8-C7-O7-C5
26	c	502	CLA	O1A-CGA-O2A-C1
26	b	612	CLA	CAA-CBA-CGA-O2A
33	c	520	DGD	C2A-C1A-O1G-C1G
33	h	101	DGD	O1B-C1B-C2B-C3B
26	A	608	CLA	C15-C16-C17-C18
33	C	522	DGD	CDB-CEB-CFB-CGB
30	b	624	STE	C1-C2-C3-C4
26	B	605	CLA	C11-C10-C8-C9
26	B	608	CLA	C6-C7-C8-C9
26	C	512	CLA	C14-C13-C15-C16
26	c	513	CLA	C11-C10-C8-C9
32	A	616	SQD	C16-C17-C18-C19
26	c	512	CLA	C8-C10-C11-C12
26	B	601	CLA	C4B-C3B-CAB-CBB
26	b	601	CLA	C4B-C3B-CAB-CBB
33	c	520	DGD	O6D-C5D-C6D-O5D
30	M	102	STE	O2-C1-C2-C3
26	A	607	CLA	C4C-C3C-CAC-CBC
33	C	522	DGD	O6E-C1E-O5D-C6D
27	A	609	PHO	C2-C3-C5-C6
31	a	617	LMG	O7-C8-C9-O8
30	M	102	STE	O1-C1-C2-C3
28	B	619	BCR	C7-C8-C9-C10
28	K	101	BCR	C17-C18-C19-C20
28	t	101	BCR	C11-C12-C13-C14
31	a	616	LMG	O7-C10-C11-C12
32	B	623	SQD	O47-C7-C8-C9
26	B	614	CLA	C2A-CAA-CBA-CGA
34	d	407	LHG	C19-C20-C21-C22
33	C	523	DGD	C7A-C8A-C9A-CAA
34	d	407	LHG	C12-C13-C14-C15
26	B	607	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
26	c	510	CLA	CAA-CBA-CGA-O2A
33	c	518	DGD	O2G-C1B-C2B-C3B
31	c	521	LMG	C13-C14-C15-C16
32	a	614	SQD	C5-C6-S-O9
26	b	612	CLA	C10-C11-C12-C13
27	A	609	PHO	C4-C3-C5-C6
26	b	601	CLA	C2-C1-O2A-CGA
26	d	402	CLA	C2-C1-O2A-CGA
32	a	615	SQD	C16-C17-C18-C19
26	C	501	CLA	C11-C12-C13-C15
26	b	604	CLA	C11-C12-C13-C15
26	b	611	CLA	C6-C7-C8-C10
26	d	402	CLA	C6-C7-C8-C10
26	d	402	CLA	C11-C12-C13-C15
34	E	101	LHG	C23-C24-C25-C26
31	B	620	LMG	C18-C19-C20-C21
31	C	517	LMG	O7-C10-C11-C12
33	C	522	DGD	C3B-C4B-C5B-C6B
28	k	102	BCR	C9-C10-C11-C12
26	B	601	CLA	C2A-CAA-CBA-CGA
32	F	102	SQD	C34-C35-C36-C37
30	A	613	STE	C3-C4-C5-C6
34	d	408	LHG	C26-C27-C28-C29
32	A	616	SQD	C12-C13-C14-C15
33	h	101	DGD	CDA-CEA-CFA-CGA
31	c	521	LMG	C30-C31-C32-C33
26	a	613	CLA	C15-C16-C17-C18
30	d	412	STE	C11-C12-C13-C14
31	D	407	LMG	C31-C32-C33-C34
29	d	405	PL9	C46-C47-C48-C49
30	T	102	STE	C15-C16-C17-C18
26	b	609	CLA	C15-C16-C17-C18
26	B	613	CLA	C11-C10-C8-C9
26	b	602	CLA	C14-C13-C15-C16
26	c	503	CLA	C11-C10-C8-C9
26	c	509	CLA	C14-C13-C15-C16
26	d	403	CLA	C11-C12-C13-C14
31	m	101	LMG	O8-C28-C29-C30
31	C	517	LMG	O9-C10-C11-C12
30	E	104	STE	C11-C12-C13-C14
26	b	616	CLA	C10-C11-C12-C13
26	B	613	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
31	B	620	LMG	O9-C10-C11-C12
33	C	523	DGD	C9A-CAA-CBA-CCA
32	a	614	SQD	O49-C7-C8-C9
30	C	526	STE	C3-C4-C5-C6
31	D	406	LMG	C11-C12-C13-C14
31	b	622	LMG	C17-C18-C19-C20
26	B	601	CLA	C13-C15-C16-C17
26	B	612	CLA	CAA-CBA-CGA-O1A
31	c	517	LMG	O9-C10-C11-C12
33	c	518	DGD	O1B-C1B-C2B-C3B
31	c	521	LMG	O7-C10-C11-C12
33	c	518	DGD	O1G-C1A-C2A-C3A
30	c	516	STE	C12-C13-C14-C15
26	C	513	CLA	C4-C3-C5-C6
26	B	601	CLA	C15-C16-C17-C18
26	B	606	CLA	C5-C6-C7-C8
26	B	612	CLA	C13-C15-C16-C17
26	b	613	CLA	C15-C16-C17-C18
30	B	626	STE	C7-C8-C9-C10
31	D	406	LMG	C21-C22-C23-C24
26	c	502	CLA	CBA-CGA-O2A-C1
32	D	410	SQD	C30-C31-C32-C33
26	B	601	CLA	CAD-CBD-CGD-O2D
26	B	607	CLA	CAD-CBD-CGD-O2D
26	C	513	CLA	CAD-CBD-CGD-O2D
26	c	513	CLA	CAD-CBD-CGD-O2D
27	a	609	PHO	CAD-CBD-CGD-O2D
30	E	102	STE	O2-C1-C2-C3
26	c	510	CLA	CAA-CBA-CGA-O1A
26	c	504	CLA	C8-C10-C11-C12
31	C	524	LMG	C35-C36-C37-C38
26	C	506	CLA	C2-C1-O2A-CGA
26	b	612	CLA	CAA-CBA-CGA-O1A
31	a	616	LMG	O9-C10-C11-C12
26	b	613	CLA	CAA-CBA-CGA-O2A
32	A	616	SQD	O47-C7-C8-C9
33	C	521	DGD	O2G-C1B-C2B-C3B
30	b	621	STE	C15-C16-C17-C18
31	c	521	LMG	C33-C34-C35-C36
30	E	102	STE	O1-C1-C2-C3
33	c	519	DGD	O6D-C5D-C6D-O5D
33	c	520	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
26	a	607	CLA	C16-C17-C18-C19
33	C	521	DGD	O1B-C1B-C2B-C3B
30	d	410	STE	C5-C6-C7-C8
34	D	408	LHG	C10-C11-C12-C13
32	B	623	SQD	O49-C7-C8-C9

There are no ring outliers.

100 monomers are involved in 150 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	C	511	CLA	1	0
28	D	404	BCR	1	0
31	C	517	LMG	1	0
26	B	602	CLA	2	0
26	b	604	CLA	2	0
30	C	527	STE	1	0
33	C	522	DGD	4	0
26	C	505	CLA	2	0
26	c	502	CLA	1	0
31	M	101	LMG	1	0
26	C	513	CLA	1	0
34	d	407	LHG	4	0
33	H	102	DGD	1	0
28	T	101	BCR	3	0
26	b	610	CLA	1	0
26	C	508	CLA	2	0
21	A	601[B]	OEY	1	0
28	A	611	BCR	1	0
31	B	620	LMG	1	0
32	b	620	SQD	2	0
28	C	515	BCR	1	0
26	B	605	CLA	1	0
26	b	608	CLA	1	0
32	f	102	SQD	1	0
33	C	523	DGD	1	0
33	A	617	DGD	4	0
26	d	403	CLA	4	0
27	A	609	PHO	1	0
28	t	101	BCR	5	0
30	E	104	STE	1	0
30	I	102	STE	2	0
28	b	618	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	604	CLA	1	0
30	b	623	STE	1	0
26	C	512	CLA	2	0
30	C	519	STE	1	0
28	a	611	BCR	2	0
35	F	101	HEM	4	0
26	b	615	CLA	1	0
26	c	505	CLA	1	0
21	a	601[B]	OEY	1	0
26	a	608	CLA	1	0
26	B	613	CLA	1	0
26	B	610	CLA	2	0
26	C	502	CLA	1	0
28	Z	101	BCR	2	0
26	b	601	CLA	1	0
26	b	613	CLA	5	0
30	H	103	STE	3	0
26	C	506	CLA	1	0
29	A	612	PL9	2	0
35	f	101	HEM	4	0
26	b	616	CLA	1	0
26	B	612	CLA	2	0
31	a	616	LMG	1	0
31	c	522	LMG	1	0
26	A	608	CLA	2	0
26	B	615	CLA	1	0
32	F	102	SQD	2	0
32	D	410	SQD	1	0
28	k	102	BCR	1	0
27	D	401	PHO	2	0
31	C	524	LMG	1	0
26	c	509	CLA	1	0
26	b	602	CLA	1	0
30	K	102	STE	1	0
30	D	412	STE	3	0
26	c	513	CLA	1	0
28	B	617	BCR	1	0
36	v	201	HEC	1	0
28	k	101	BCR	4	0
26	B	603	CLA	1	0
26	B	611	CLA	1	0
28	H	101	BCR	2	0

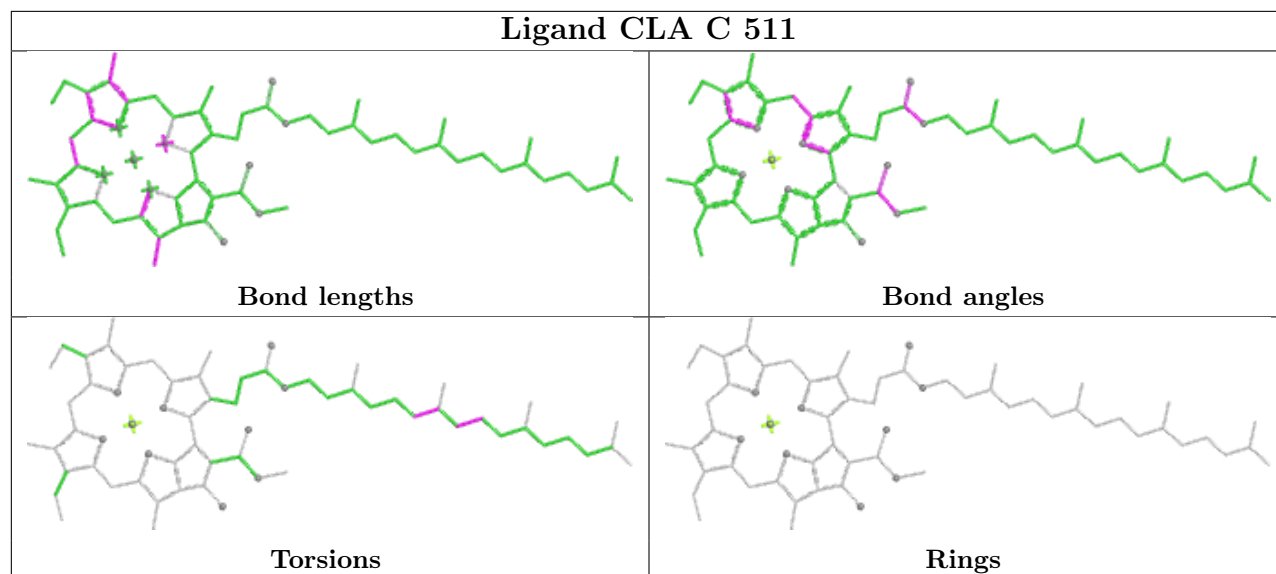
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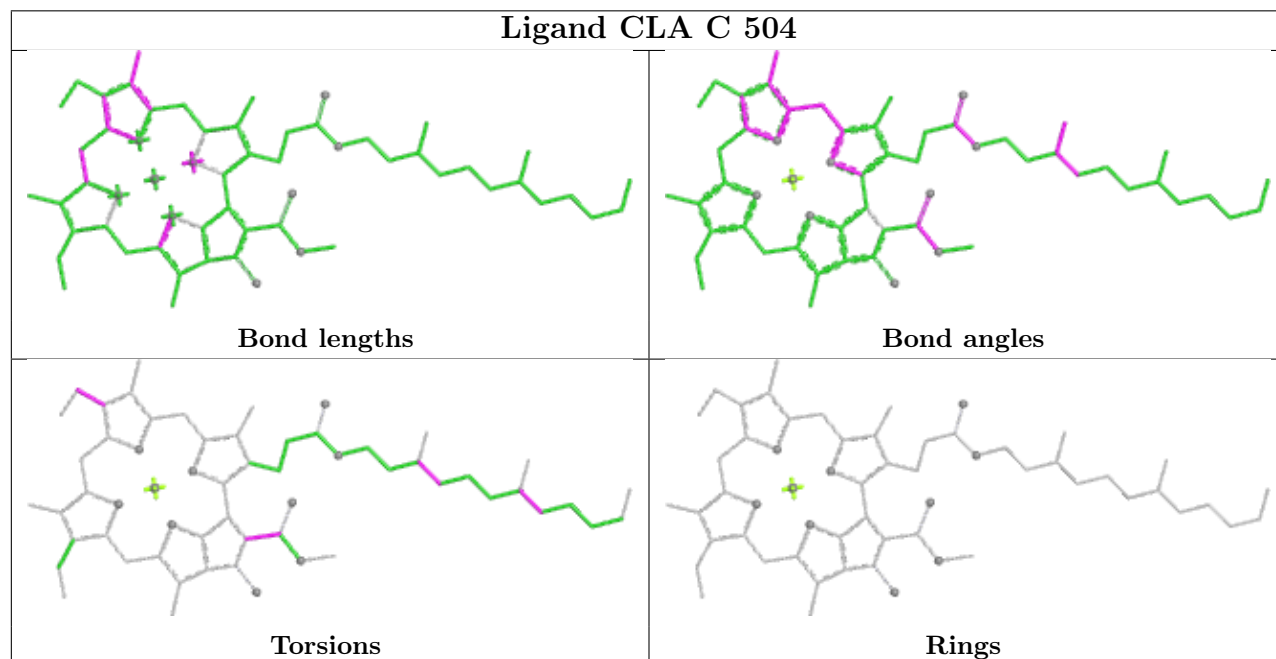
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	Z	102	STE	1	0
30	d	406	STE	1	0
28	x	101	BCR	3	0
26	c	501	CLA	2	0
26	B	606	CLA	2	0
26	b	609	CLA	1	0
34	B	622	LHG	3	0
26	b	606	CLA	1	0
34	e	102	LHG	1	0
26	b	612	CLA	1	0
28	B	618	BCR	3	0
26	C	509	CLA	2	0
32	B	623	SQD	2	0
26	c	507	CLA	1	0
30	A	618	STE	1	0
26	B	601	CLA	4	0
34	D	411	LHG	1	0
26	a	607	CLA	3	0
29	a	612	PL9	3	0
26	d	402	CLA	2	0
26	c	511	CLA	1	0
26	B	614	CLA	1	0
28	b	619	BCR	1	0
34	D	408	LHG	2	0
26	A	607	CLA	5	0
30	c	516	STE	1	0

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

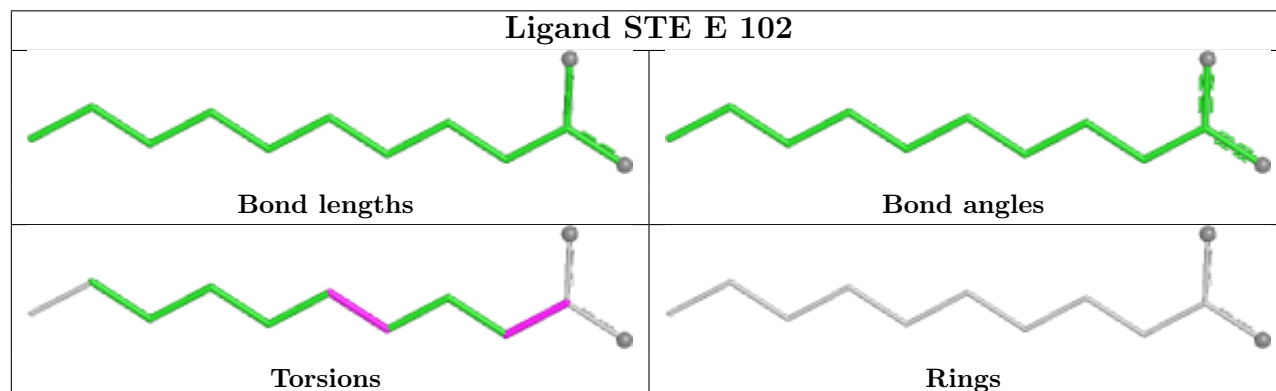
Ligand CLA C 511

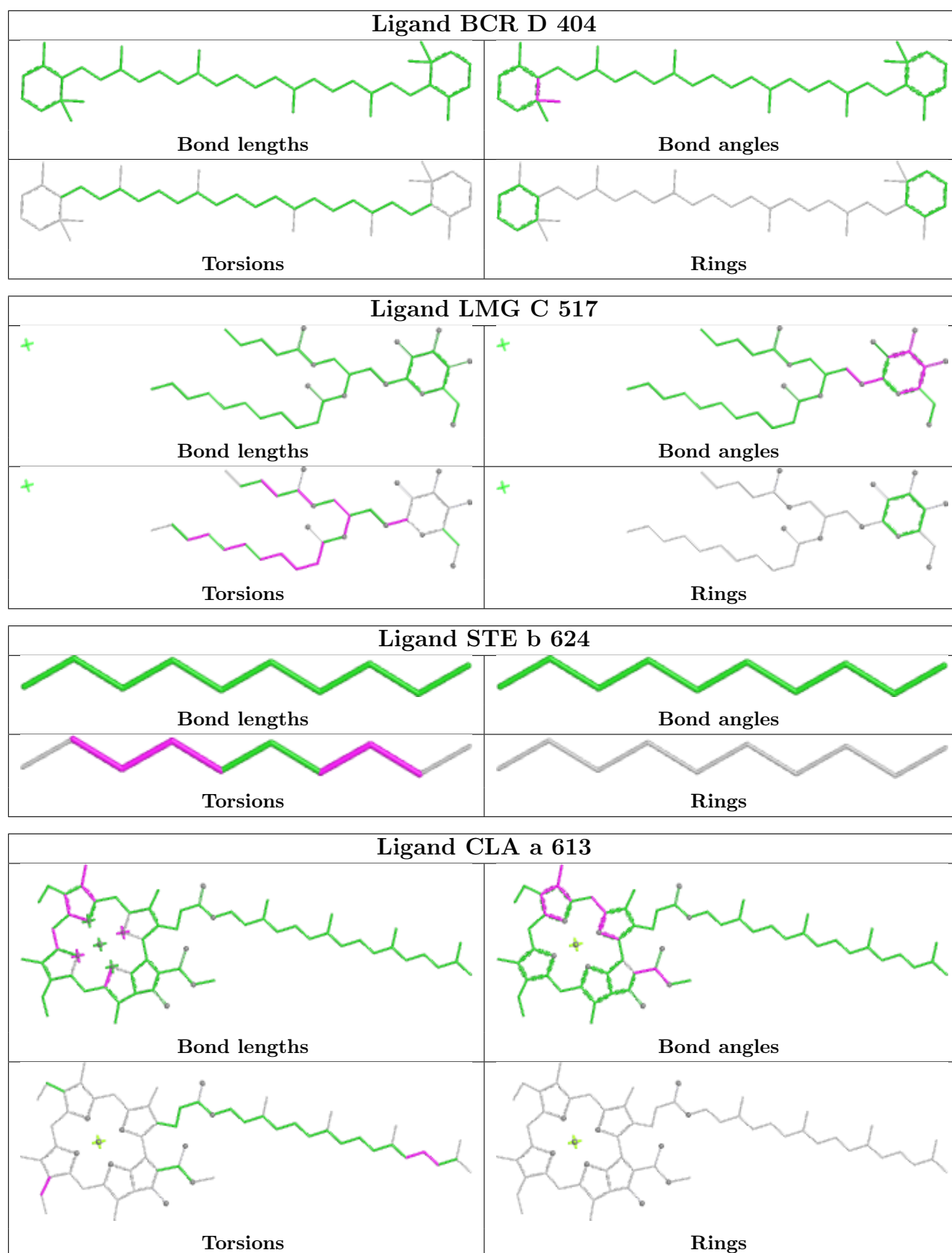


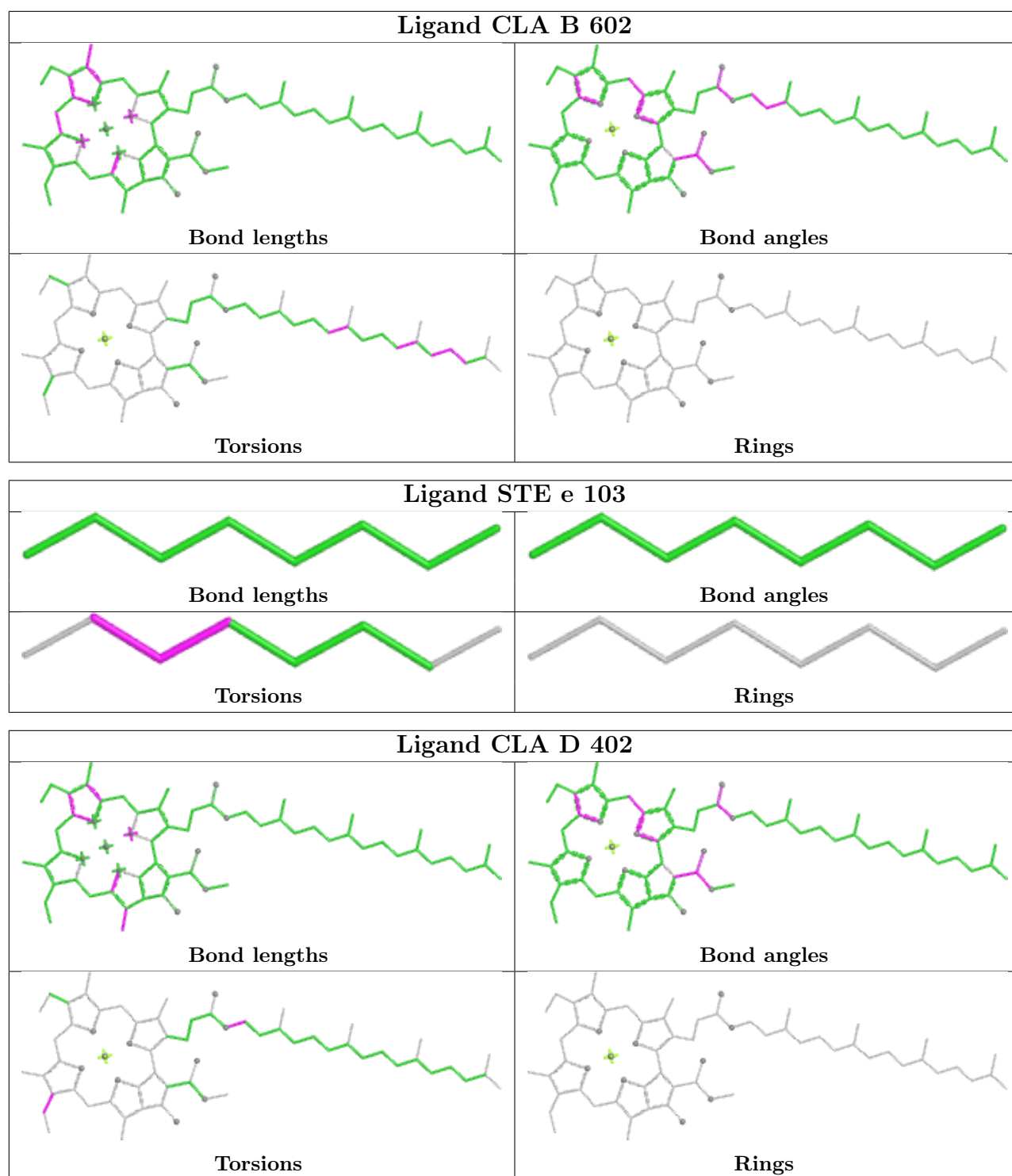
Ligand CLA C 504

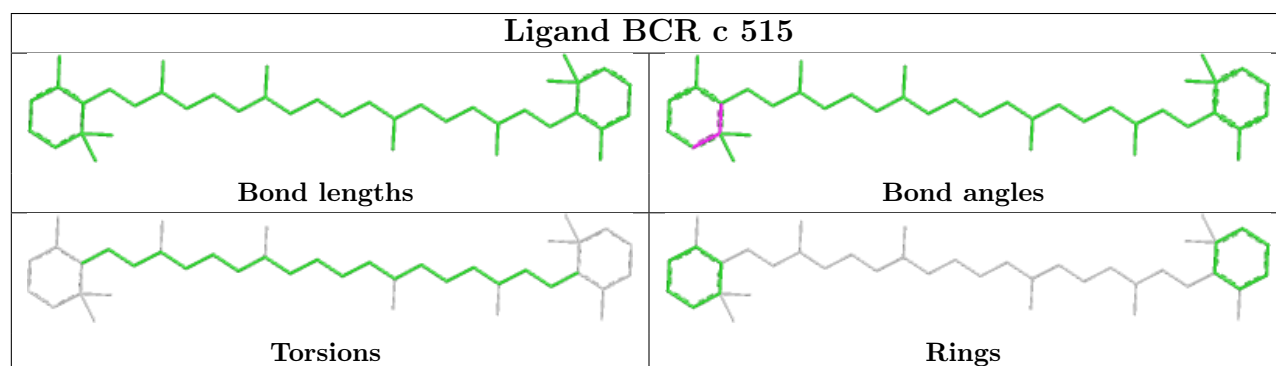
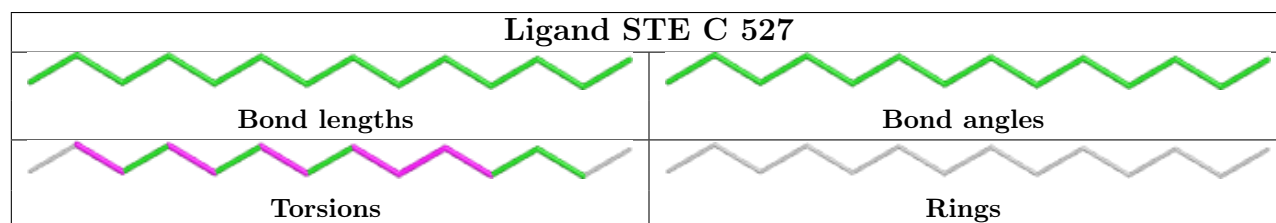
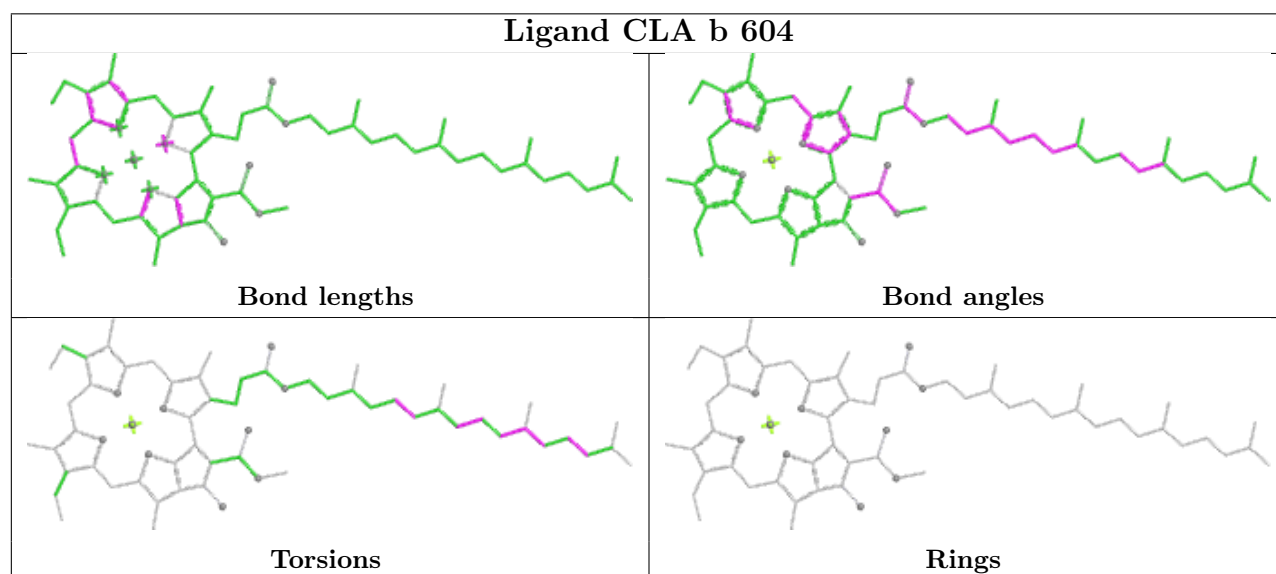
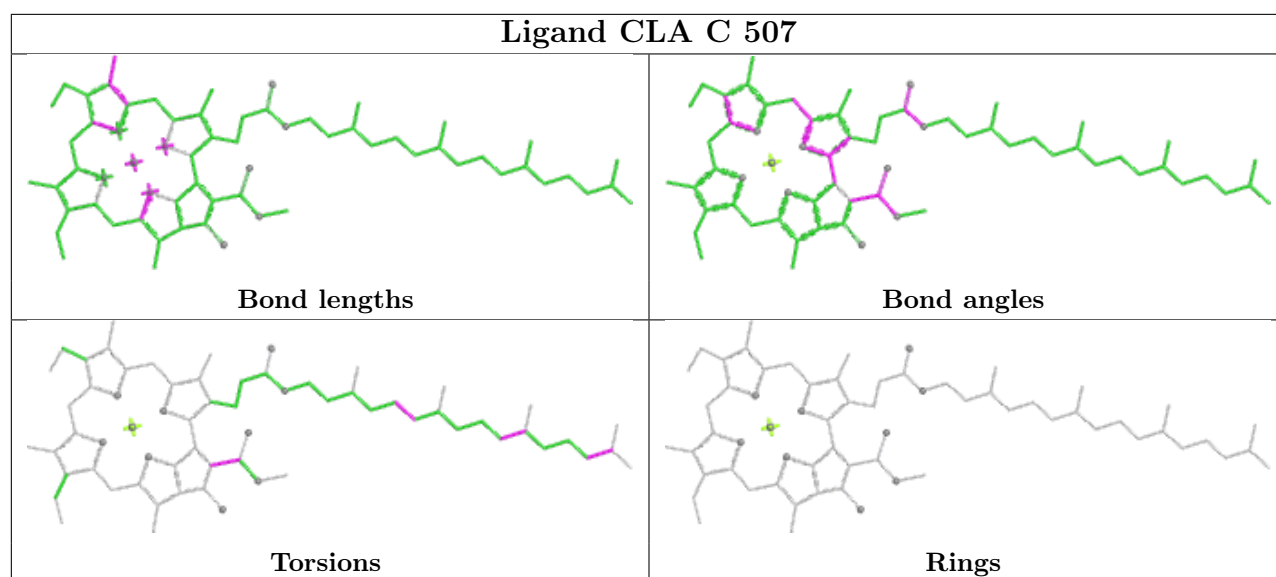


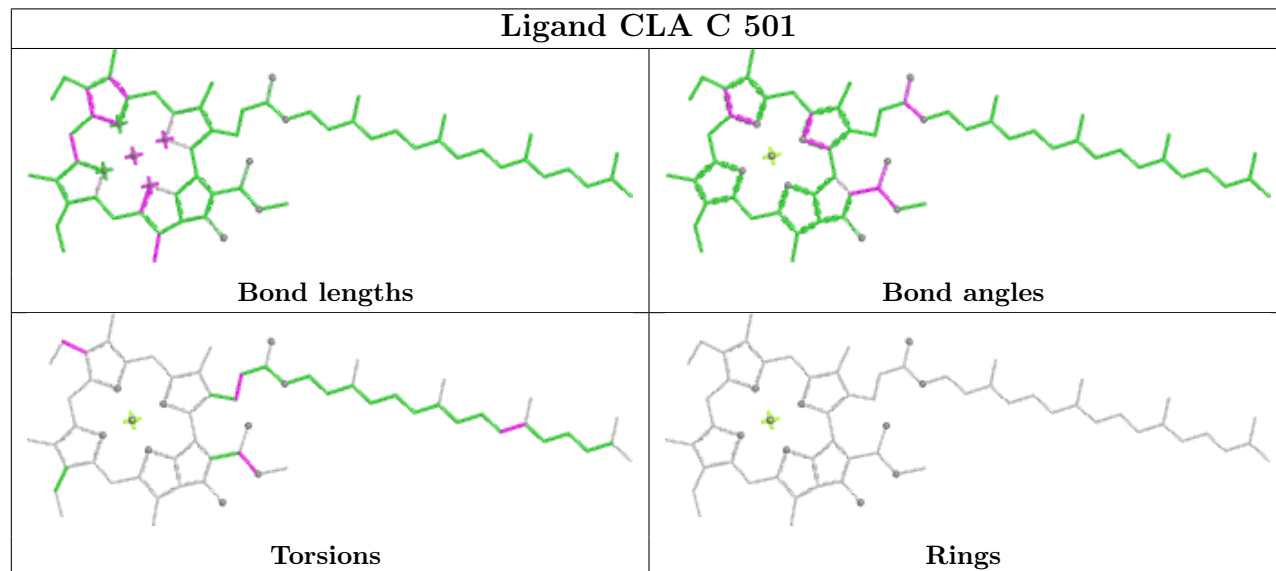
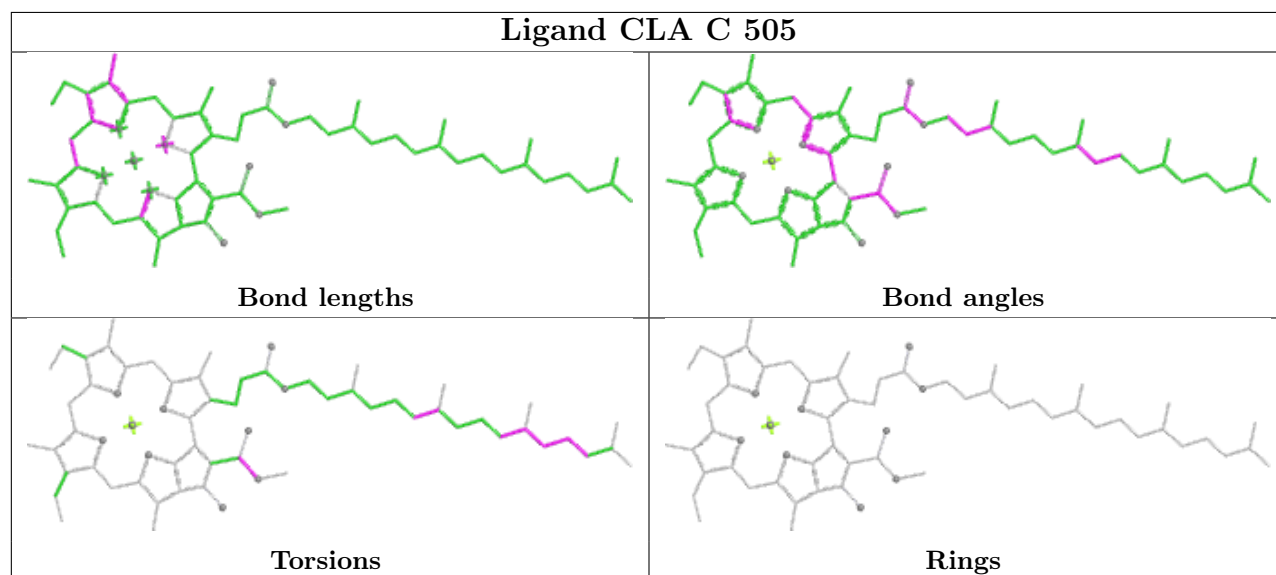
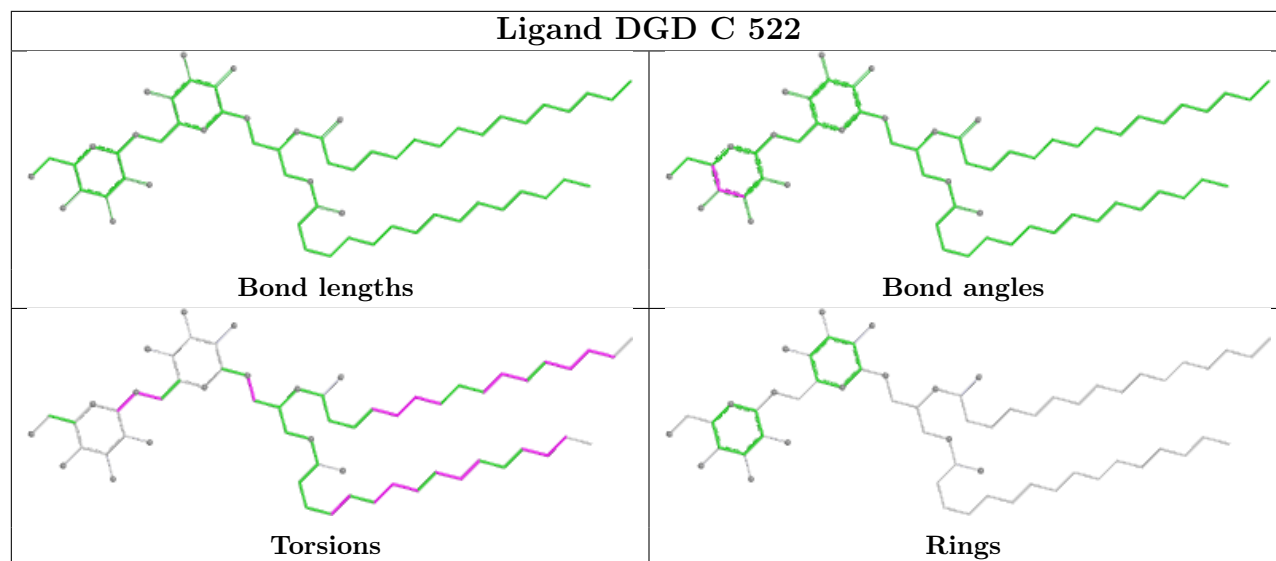
Ligand STE E 102

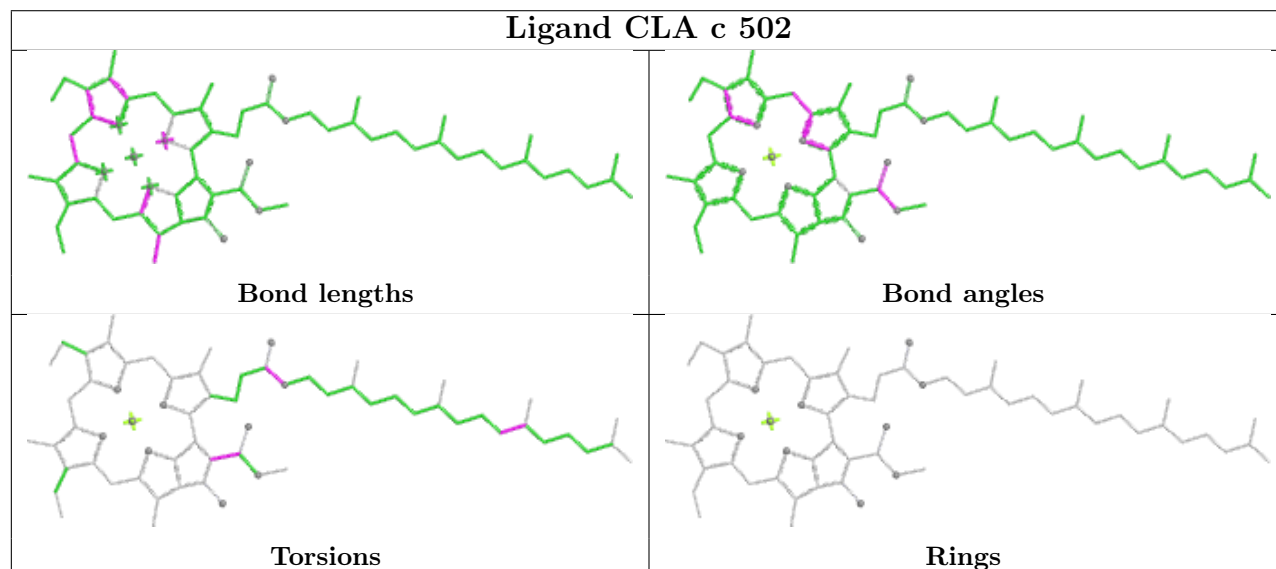
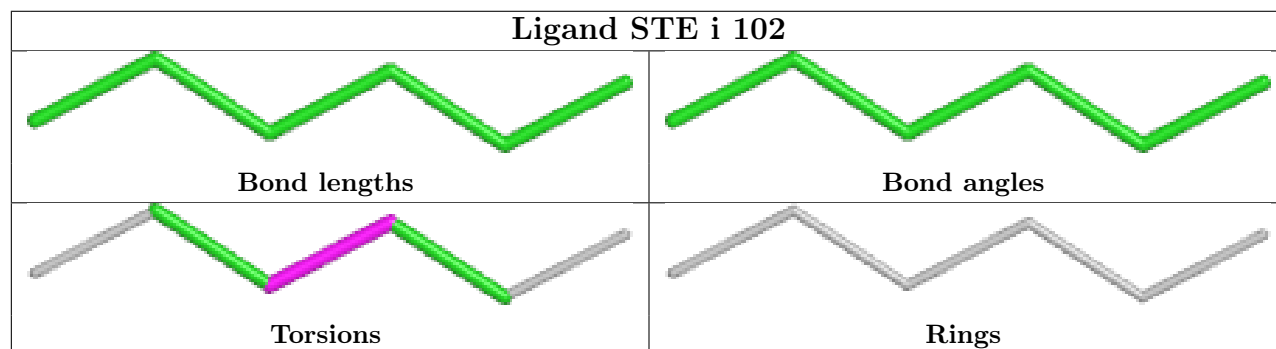
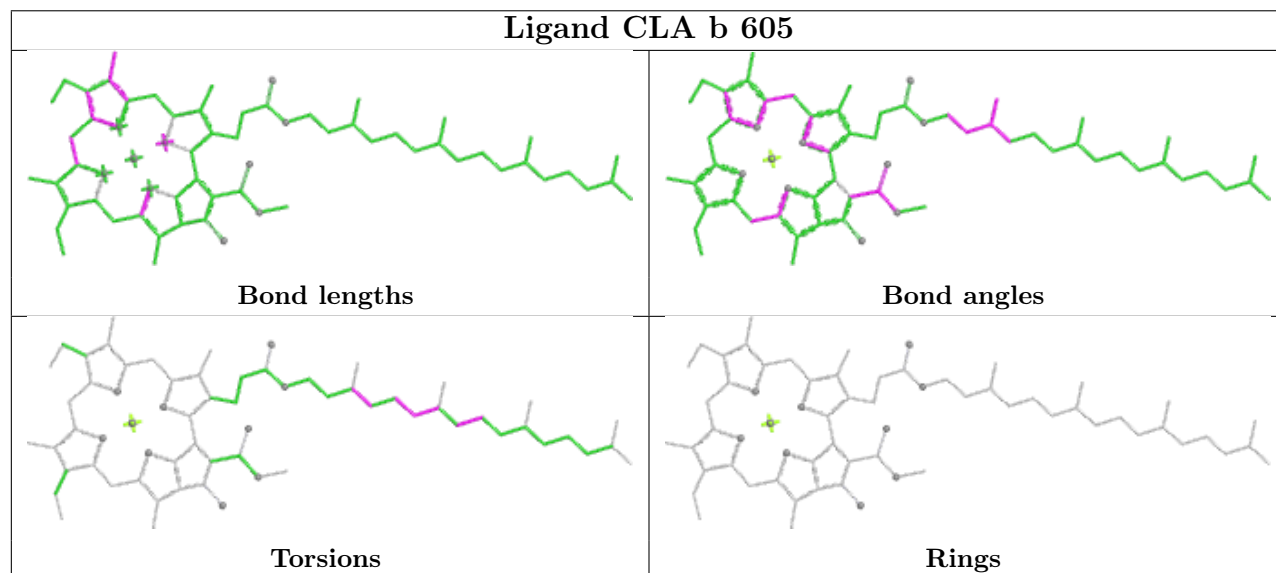
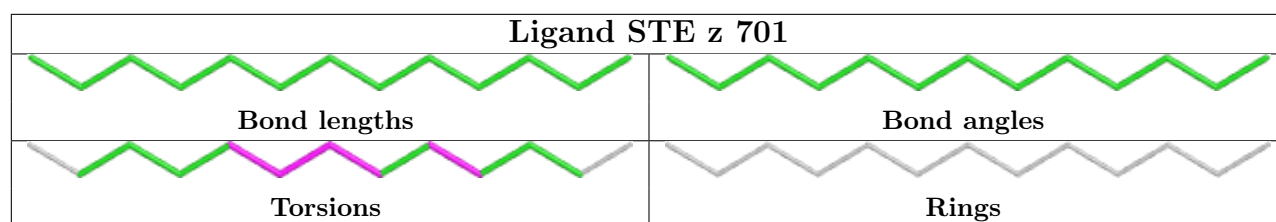


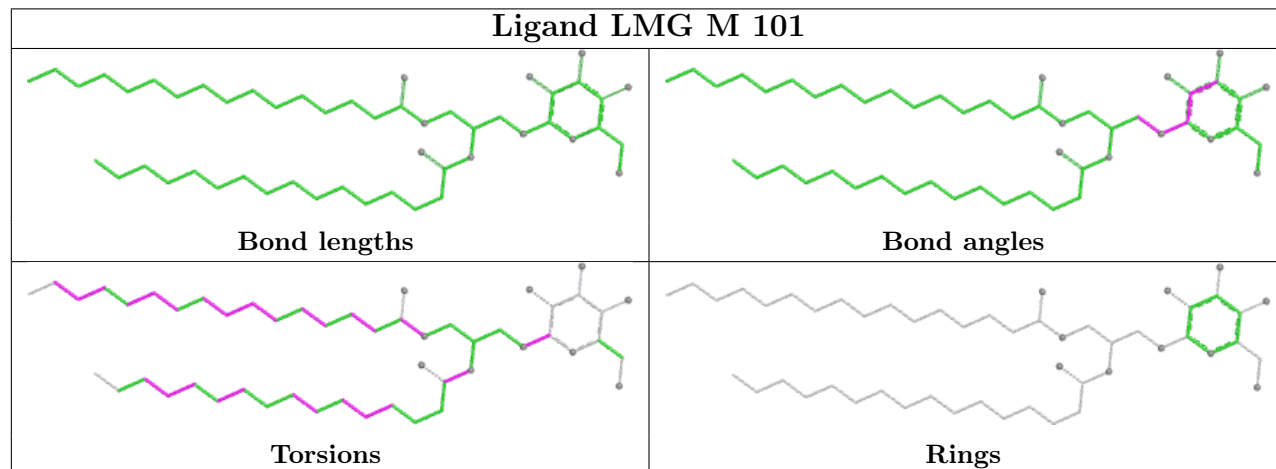
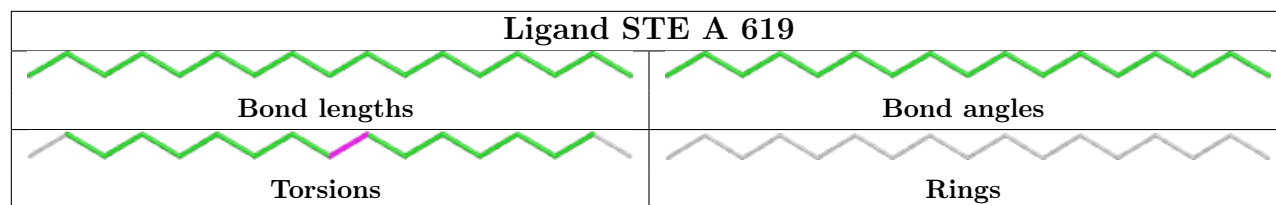




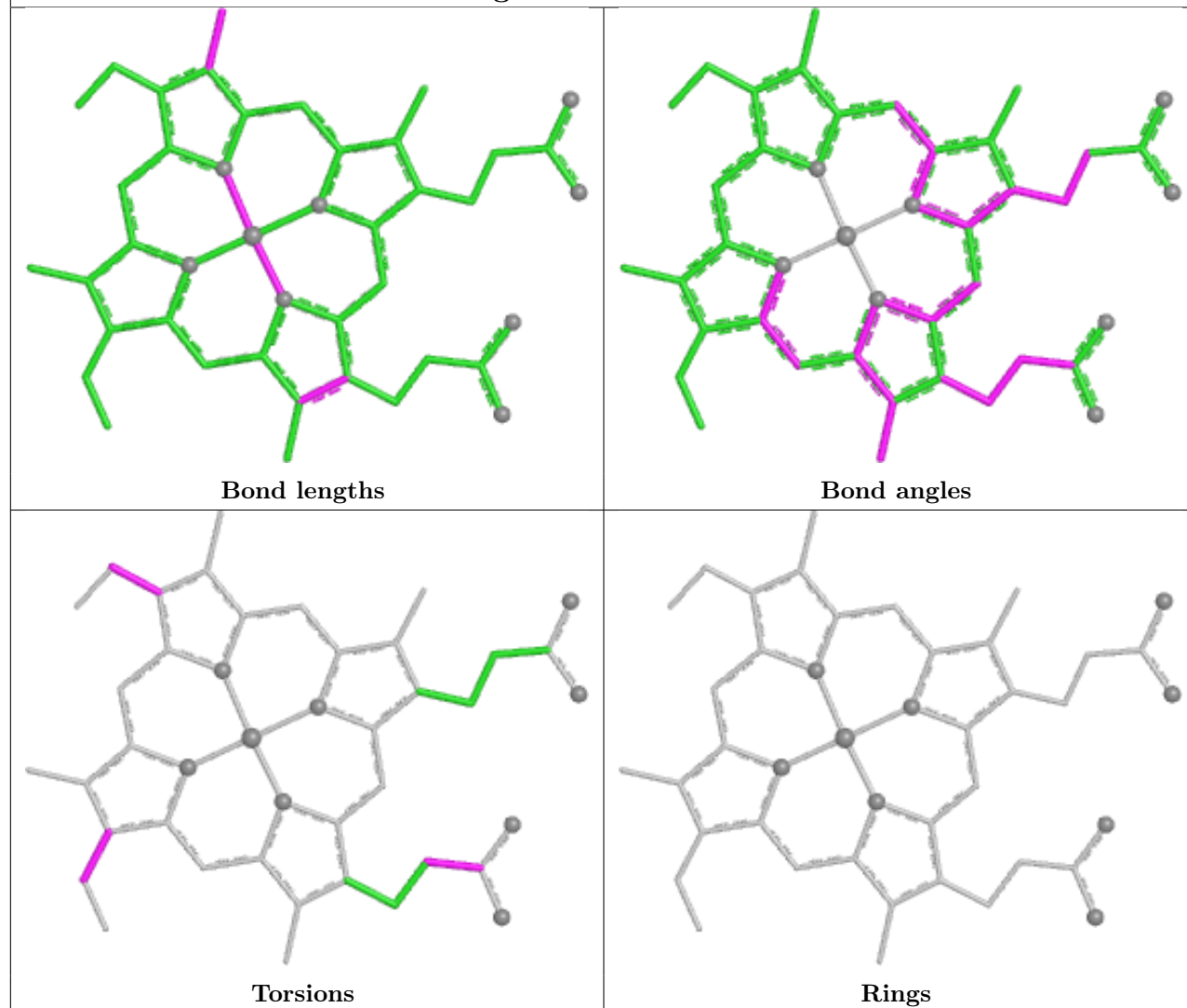




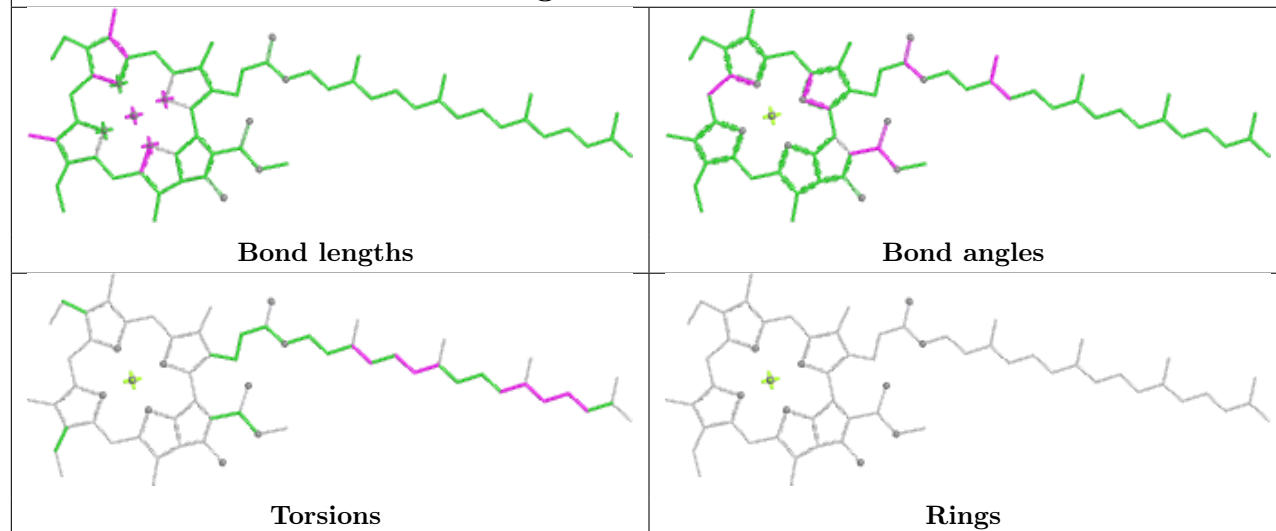


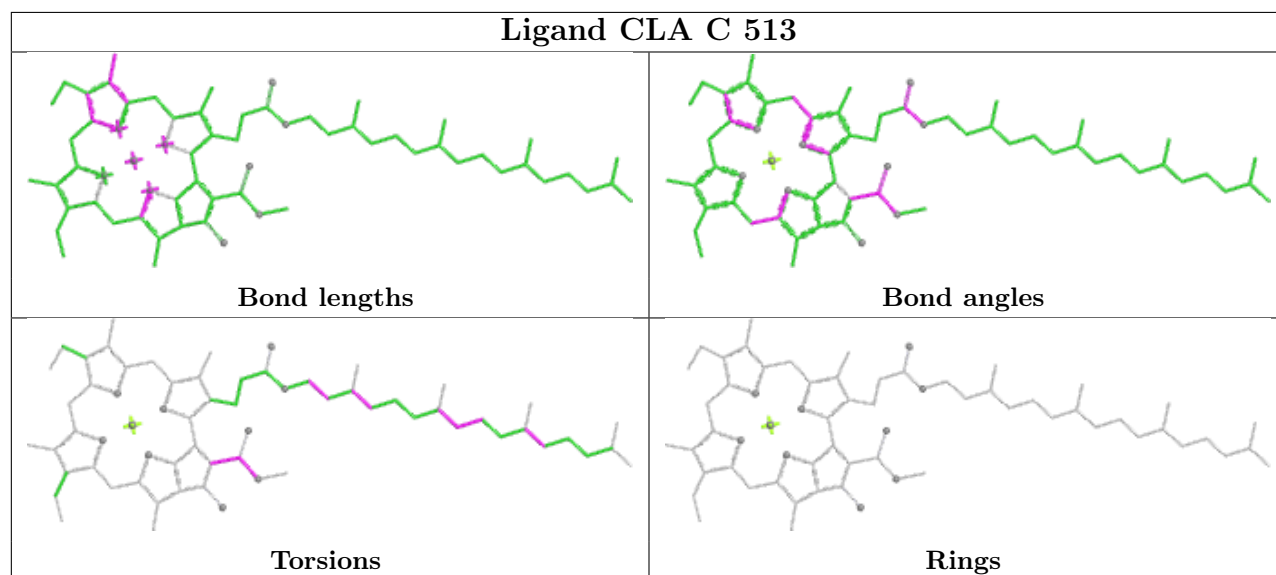
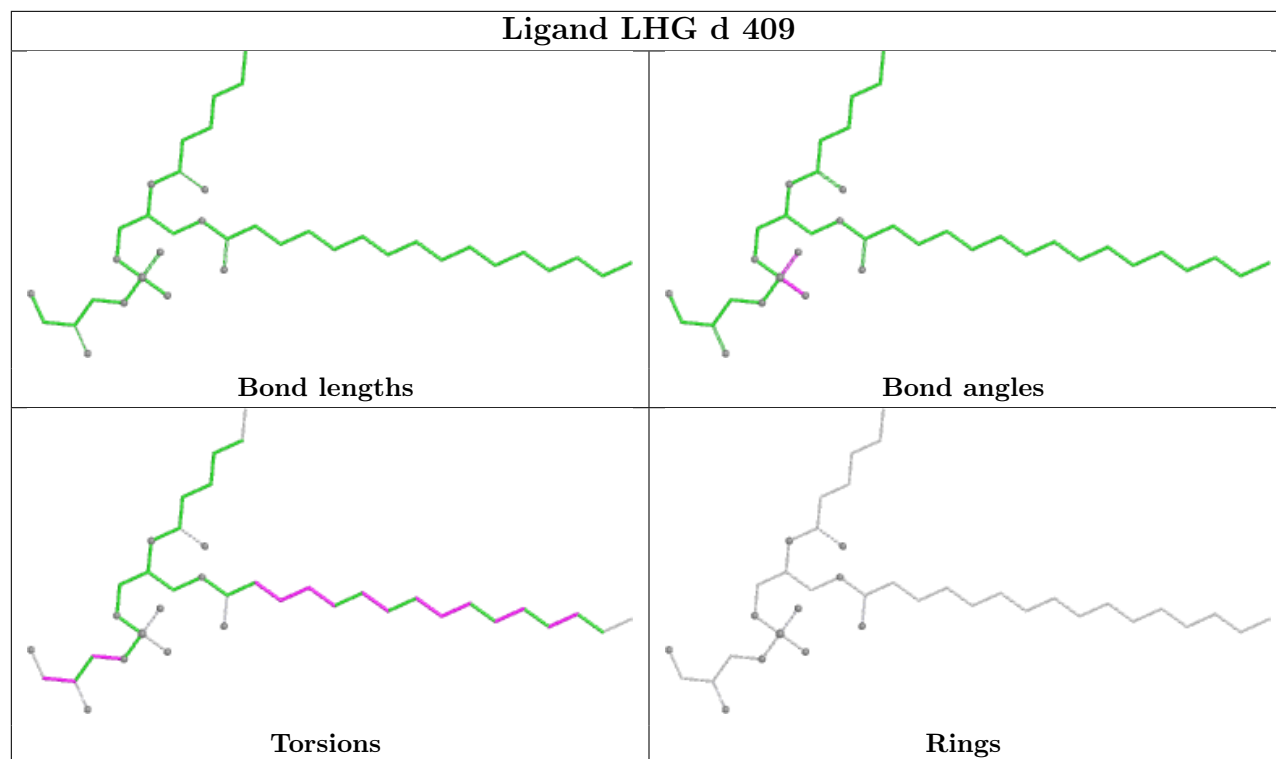


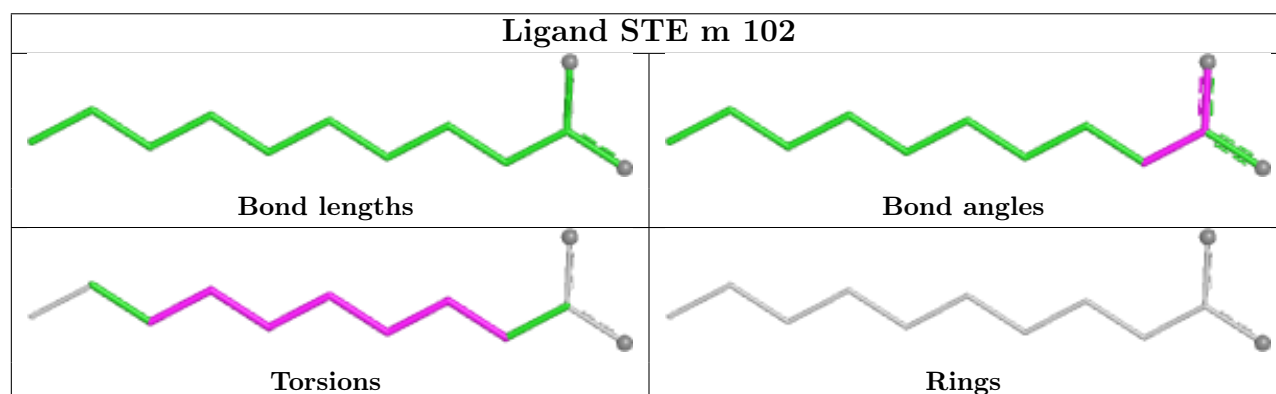
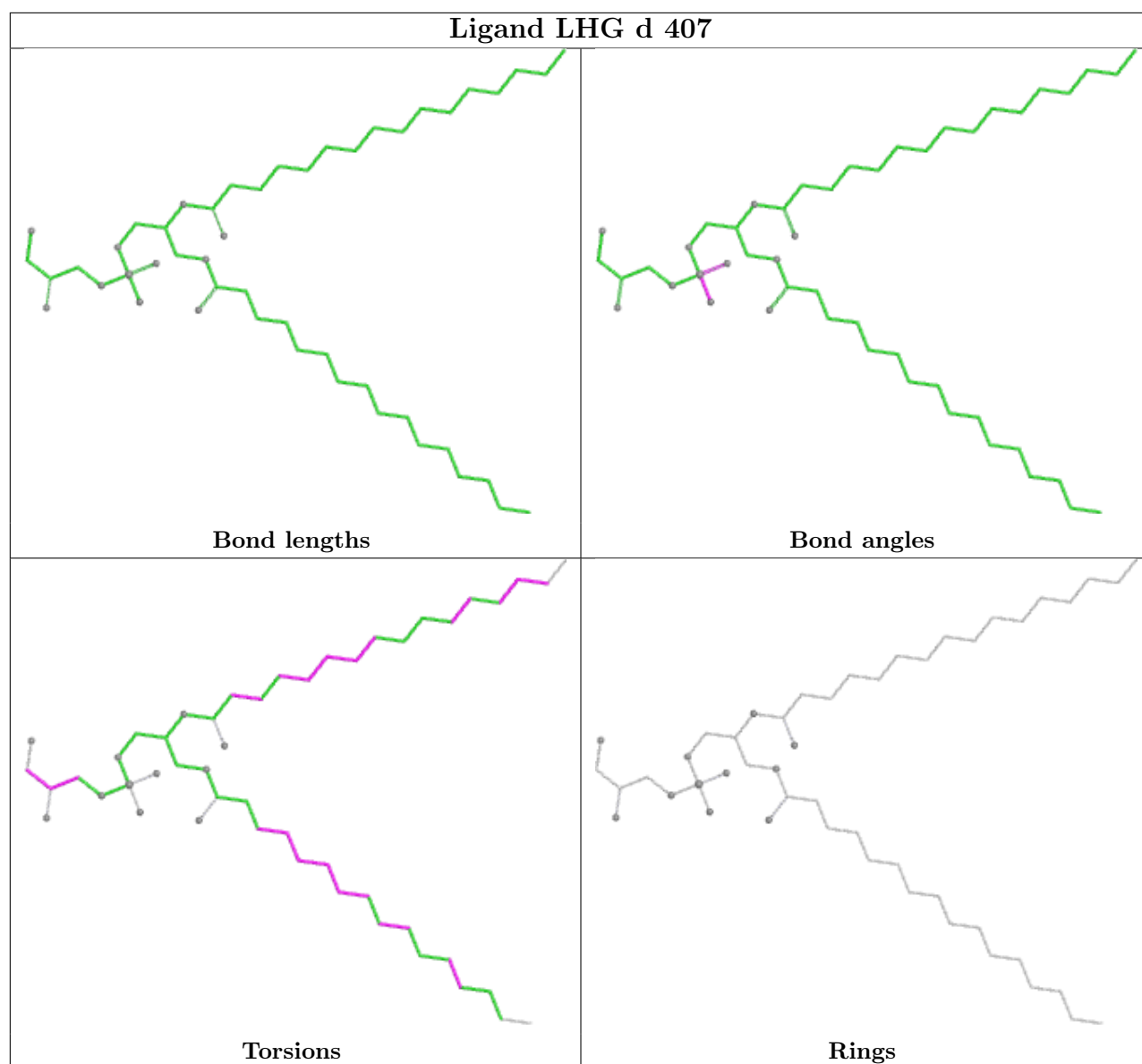
Ligand HEC V 201

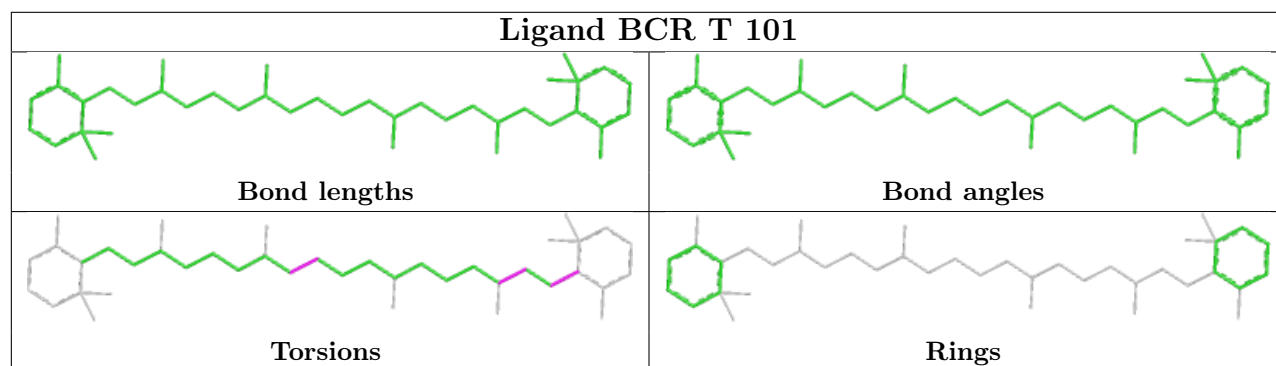
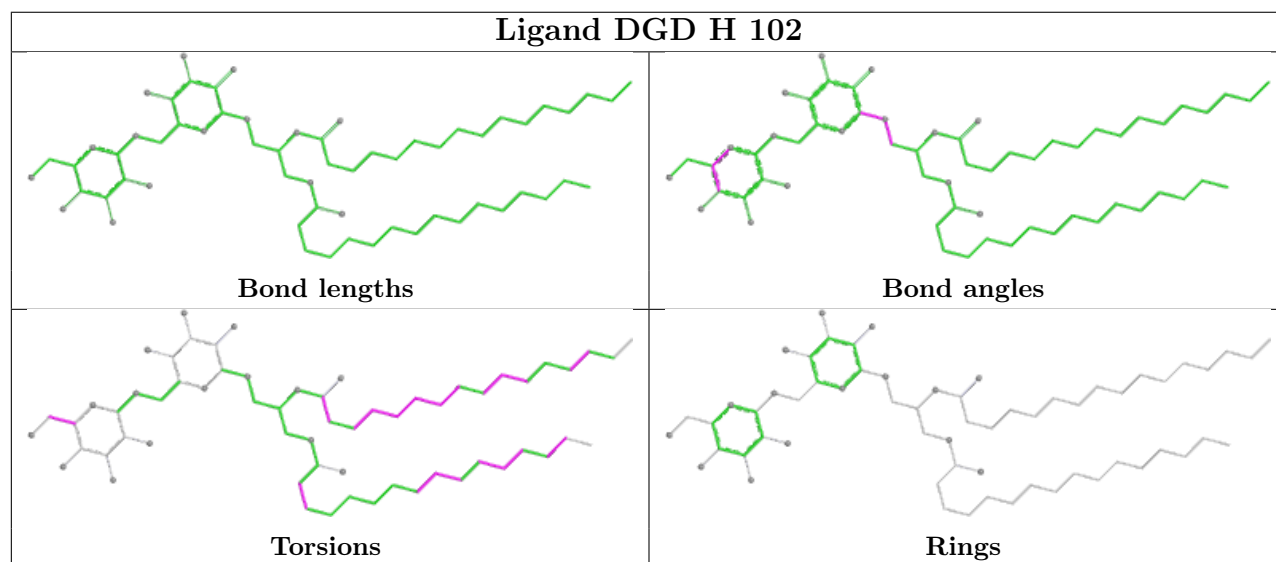
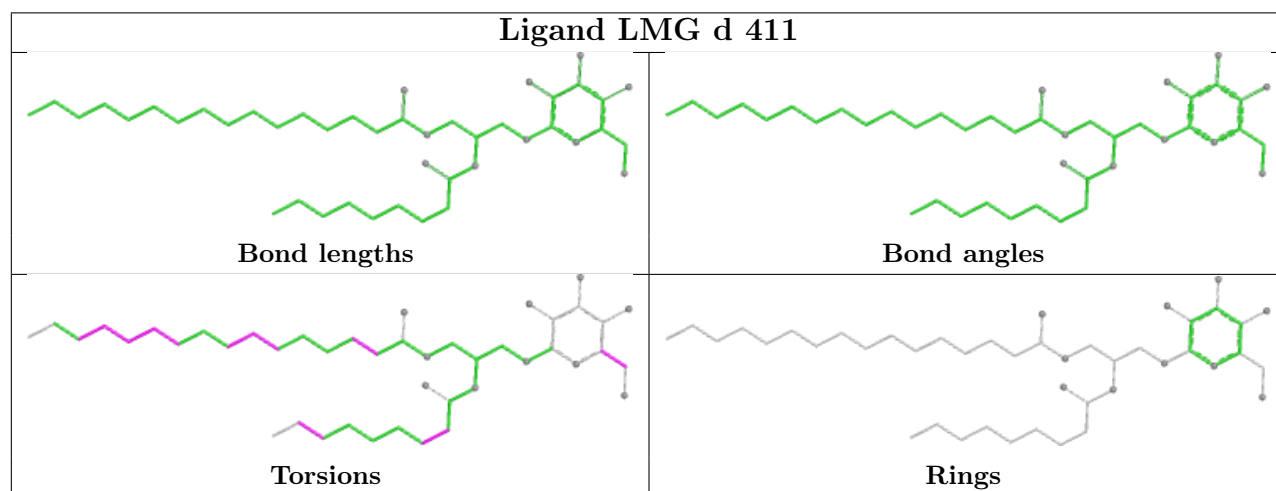
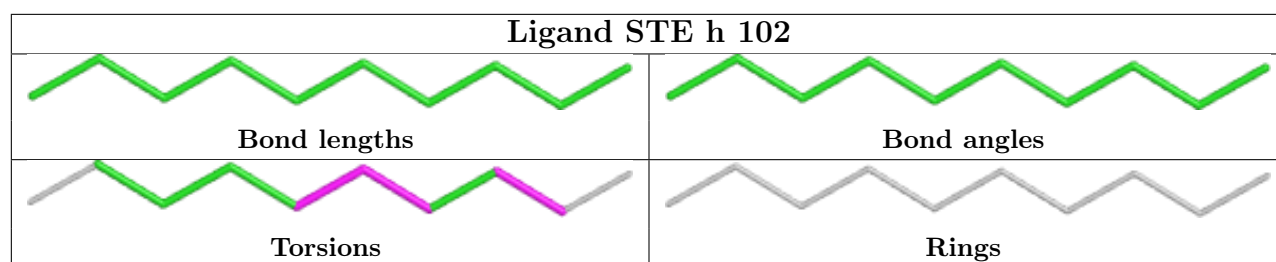


Ligand CLA a 610

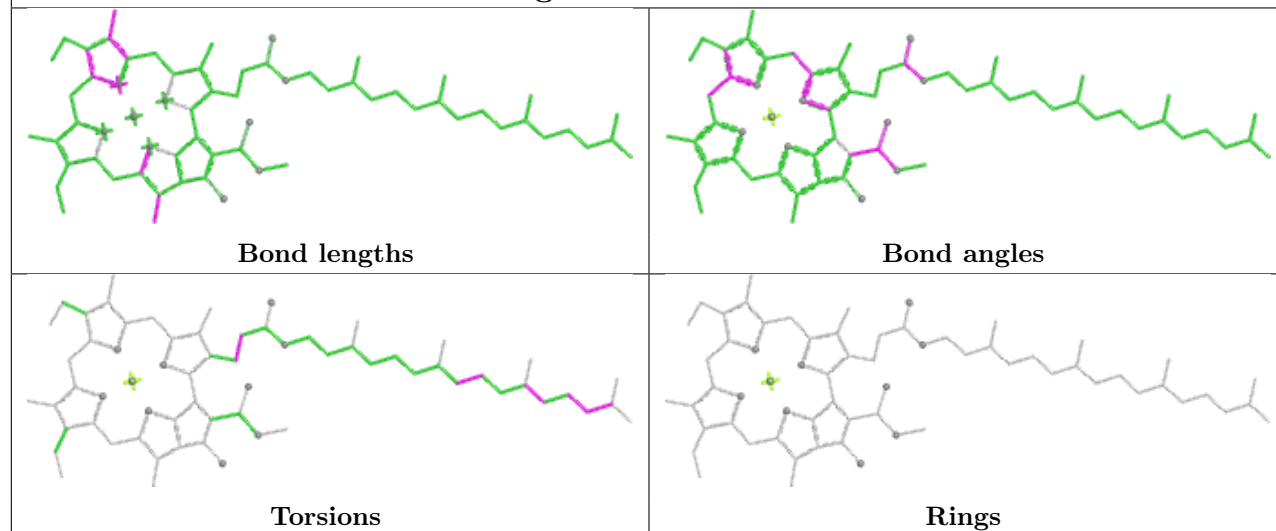




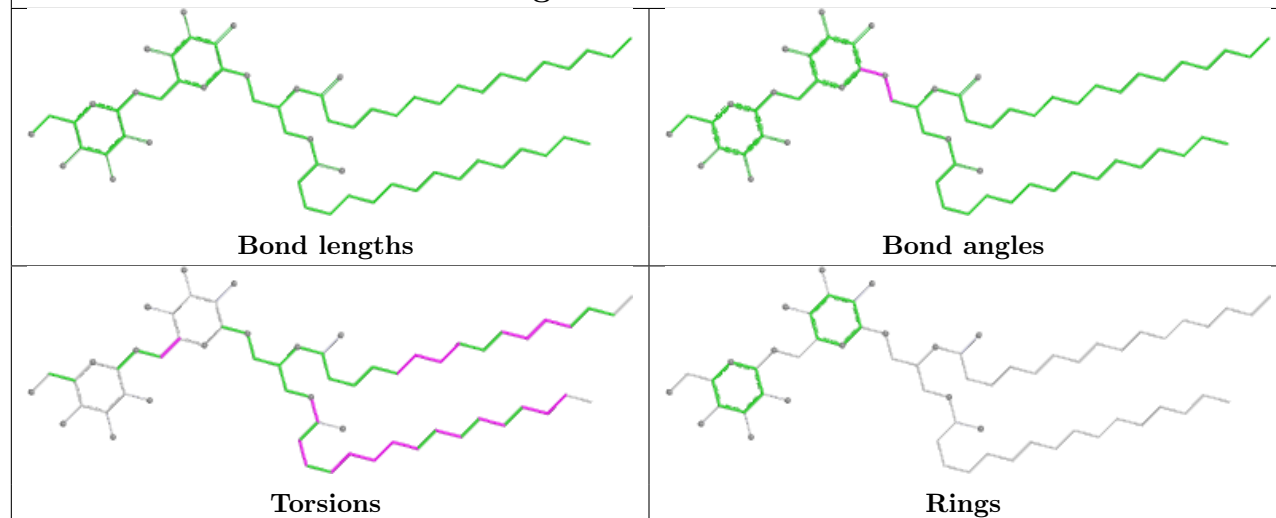




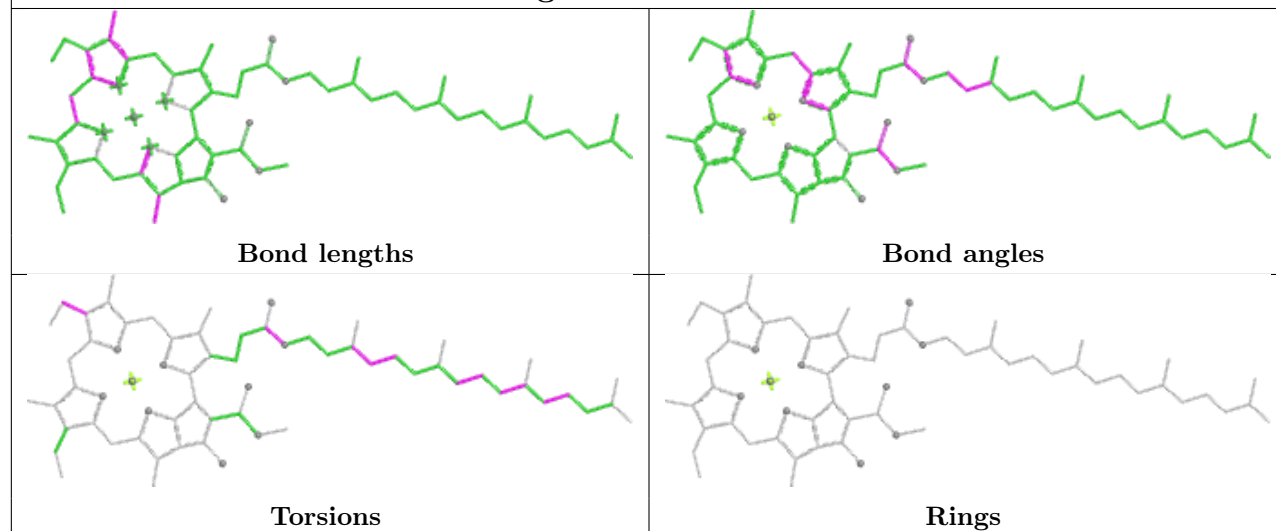
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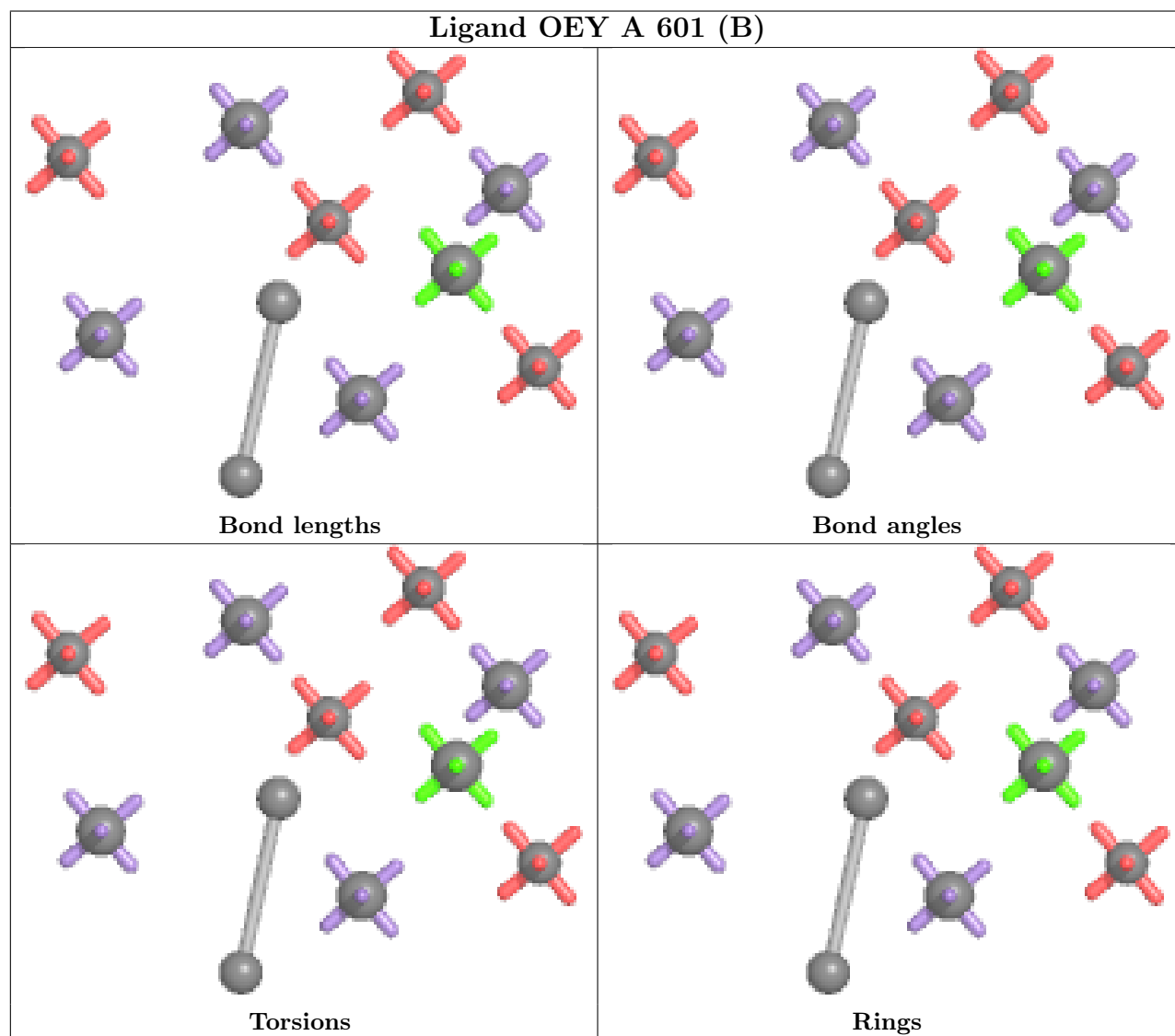
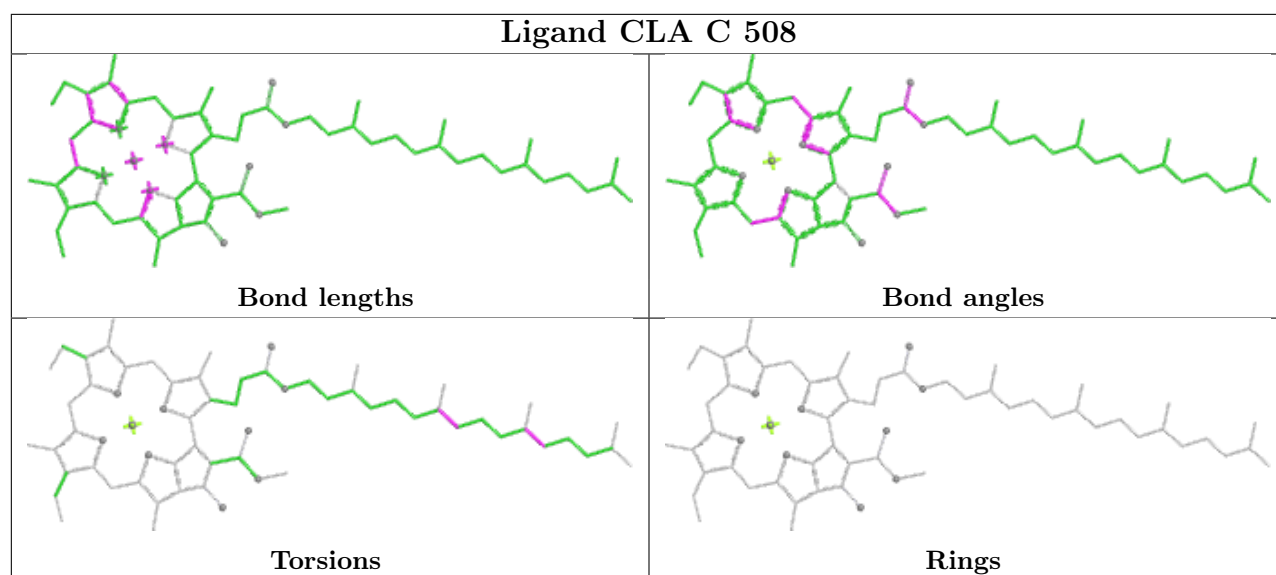


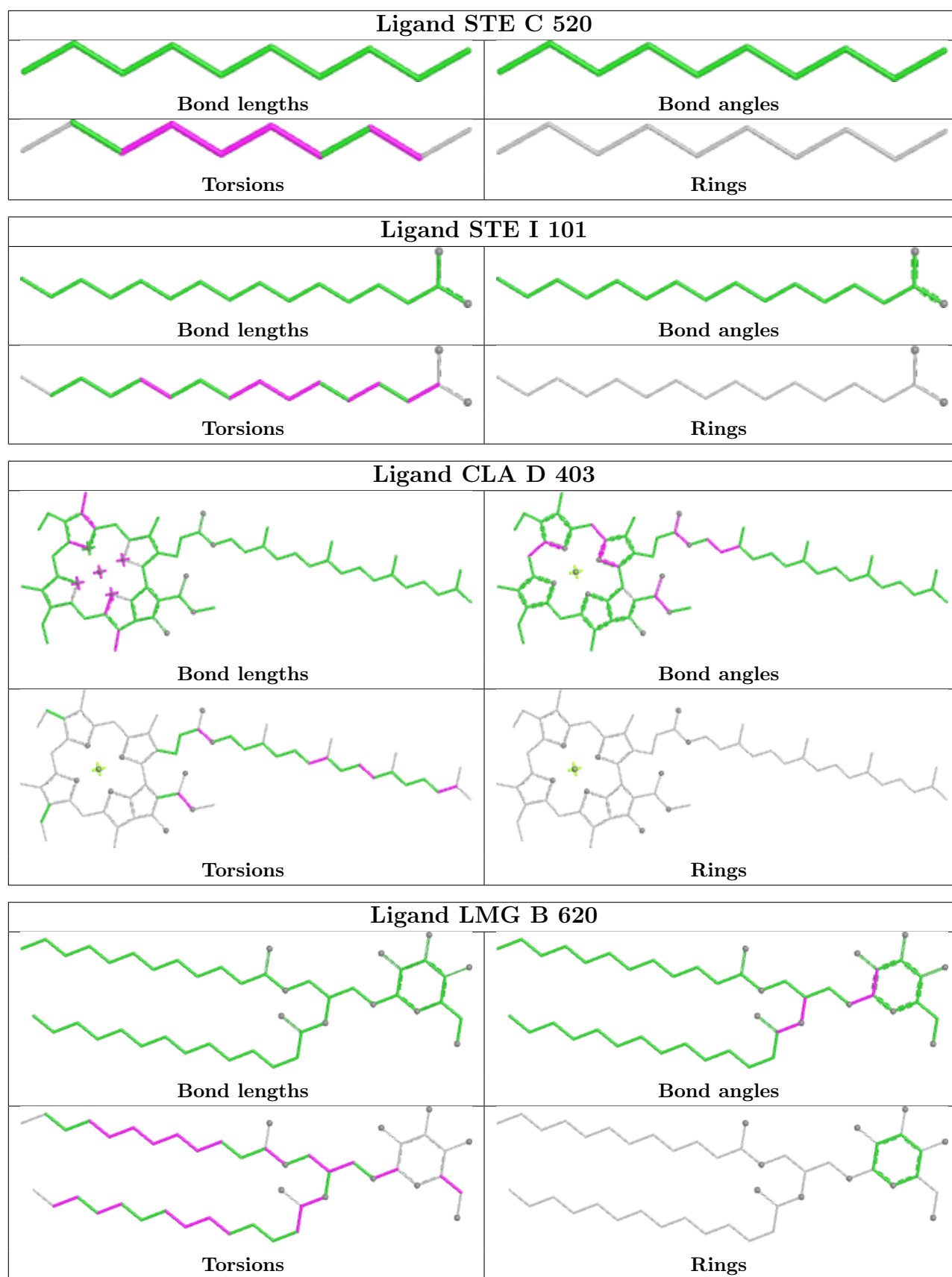
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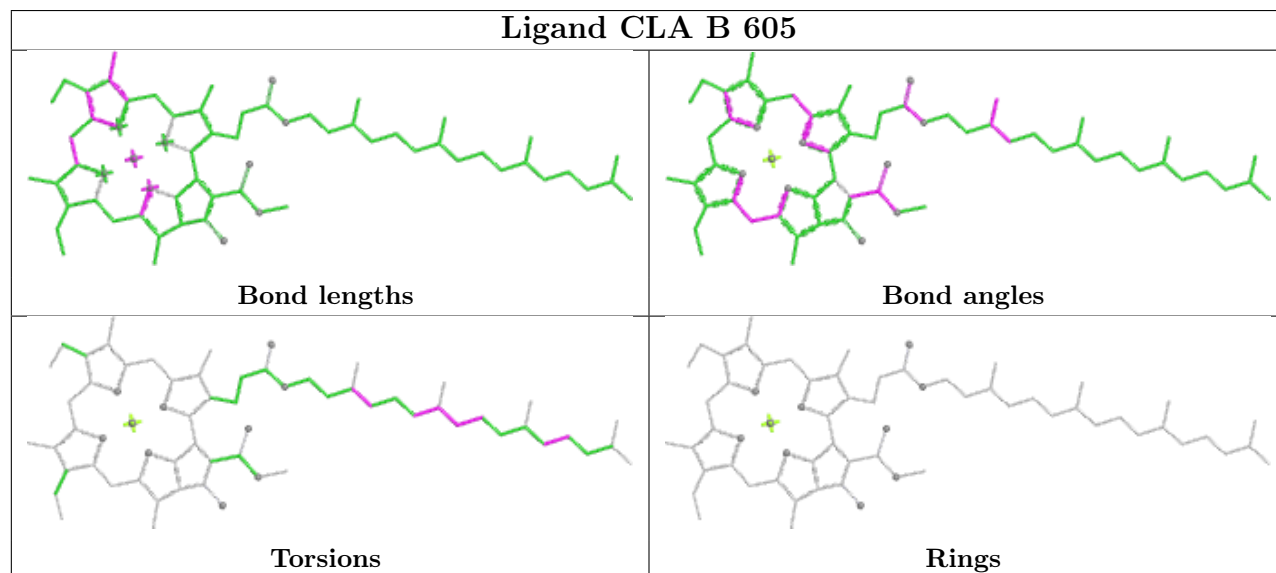
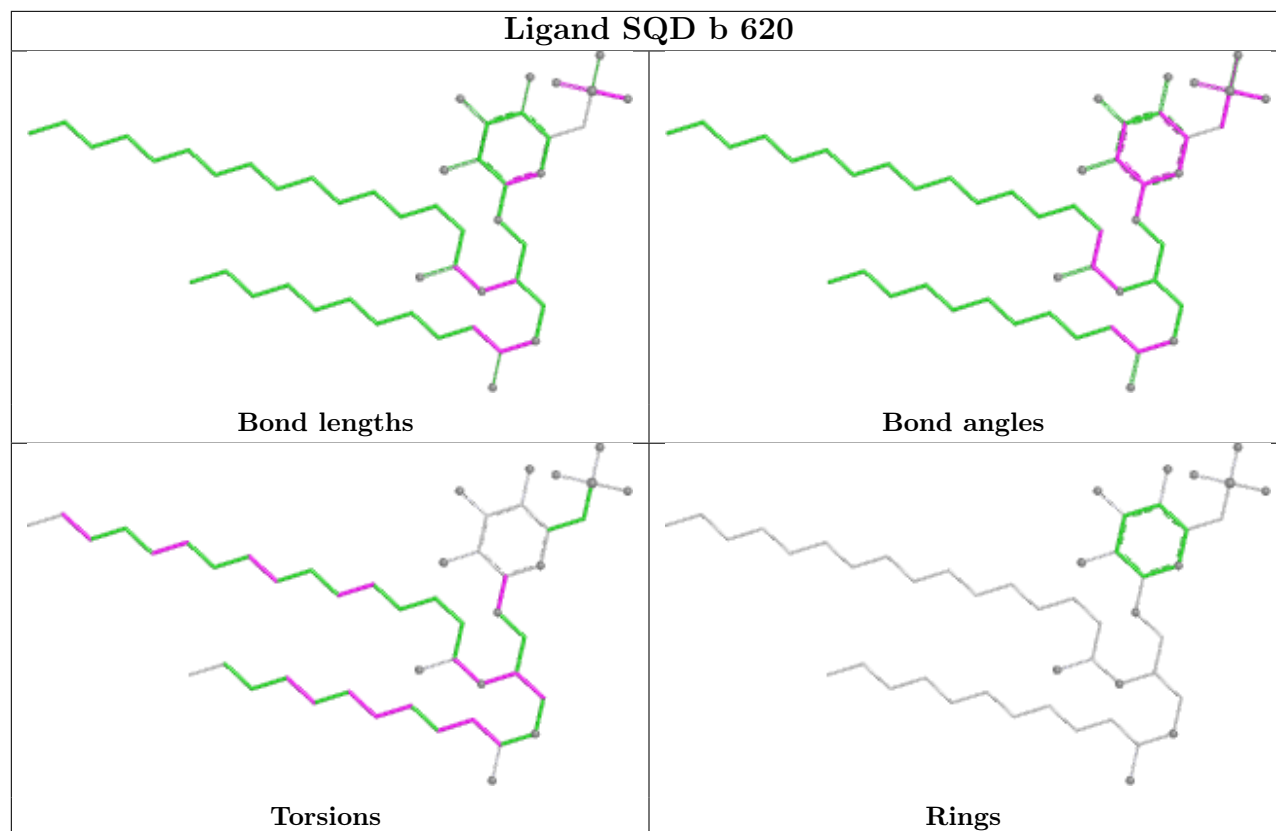


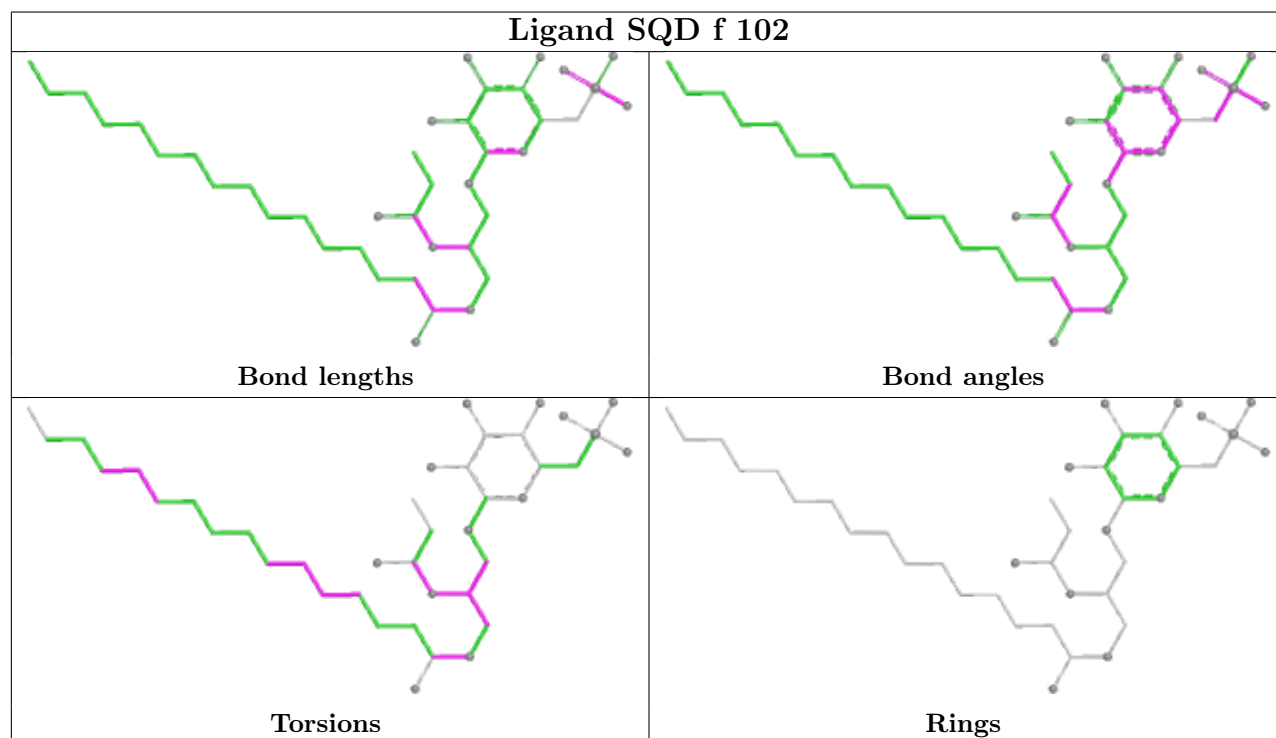
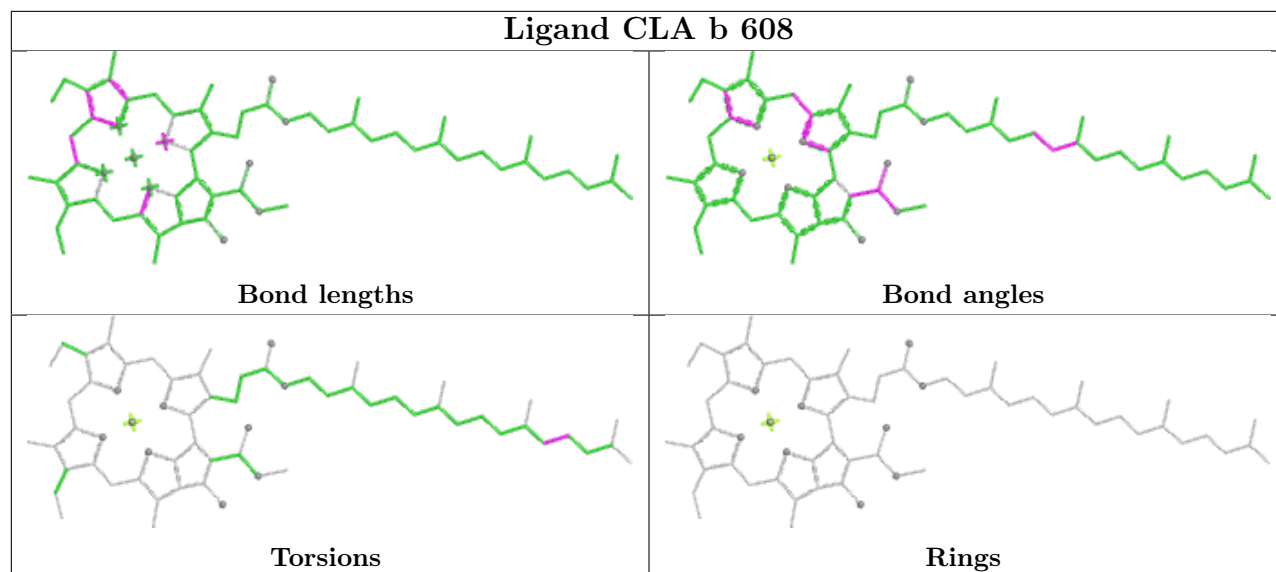
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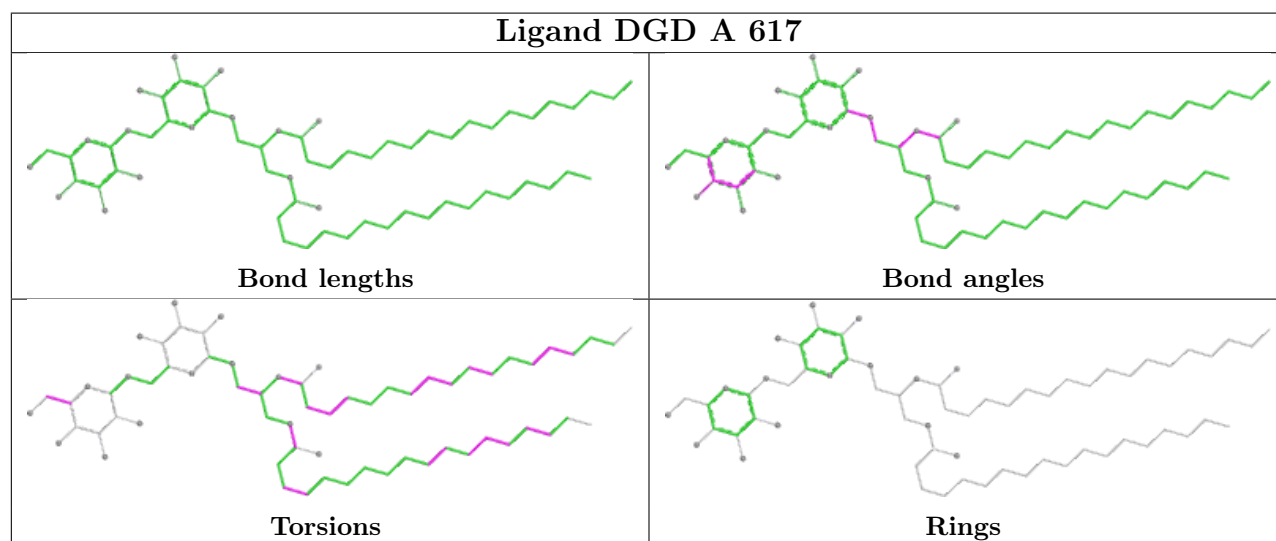
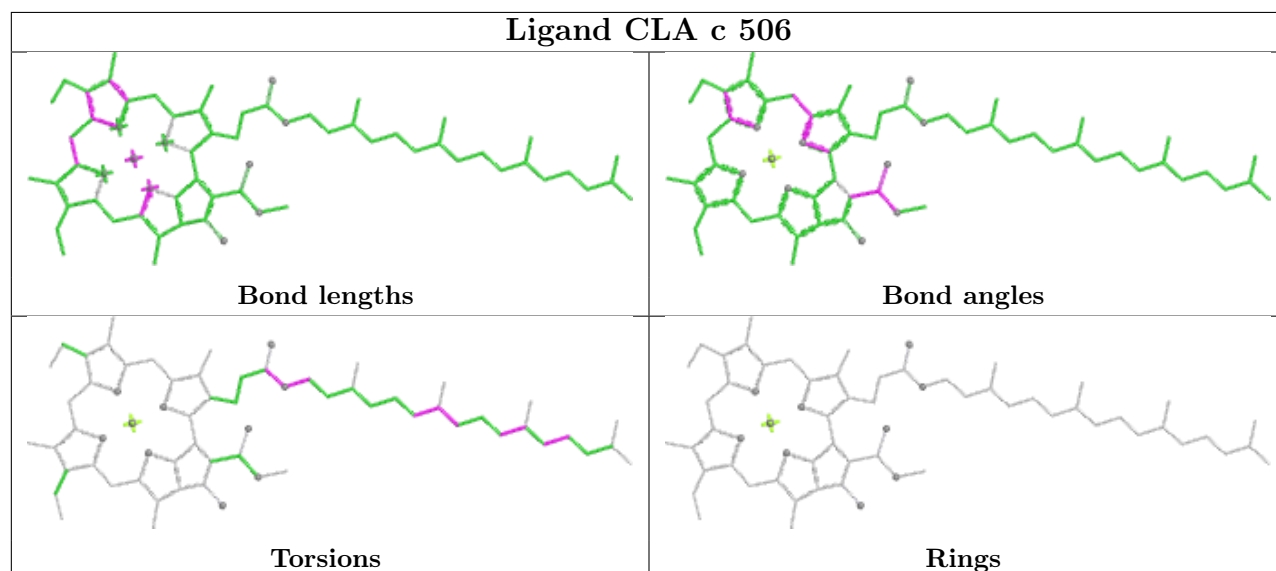
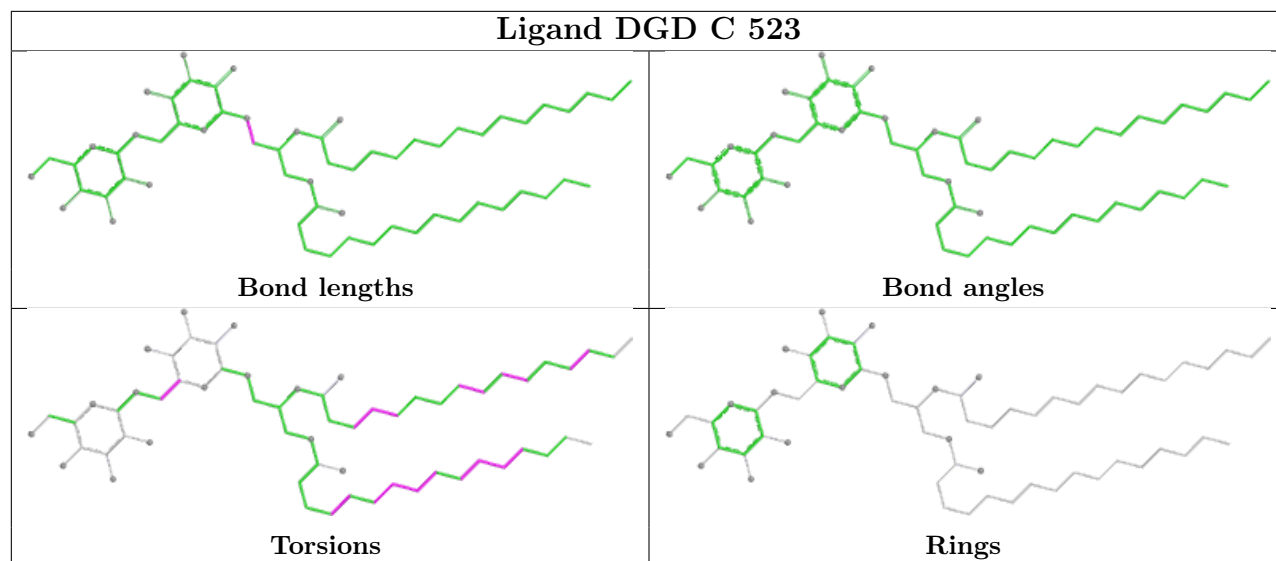




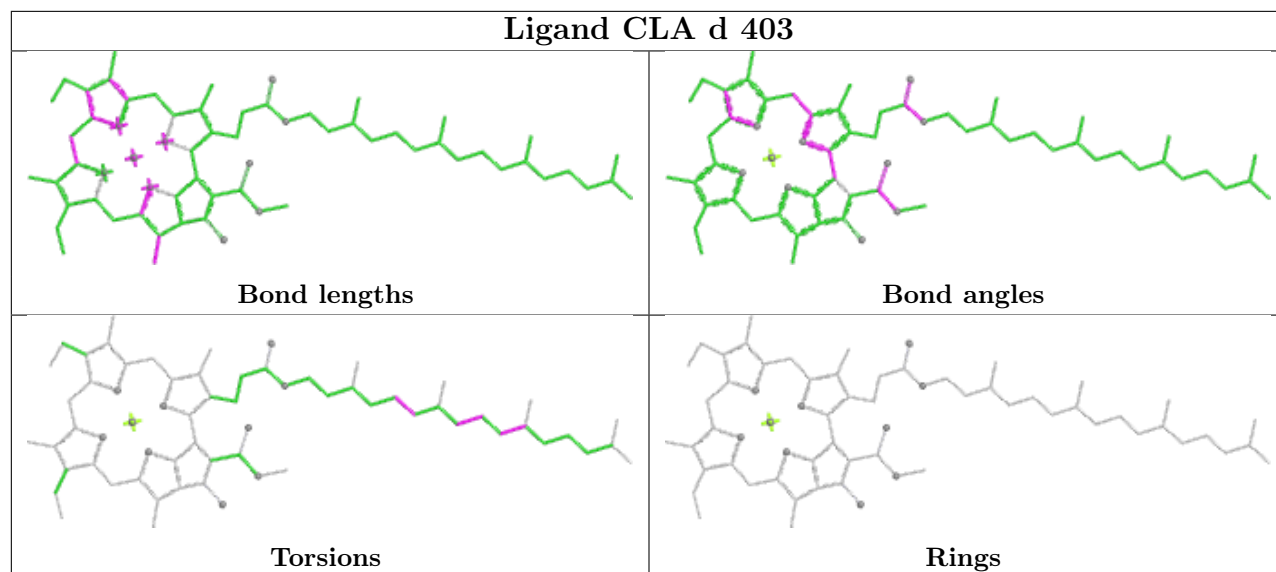




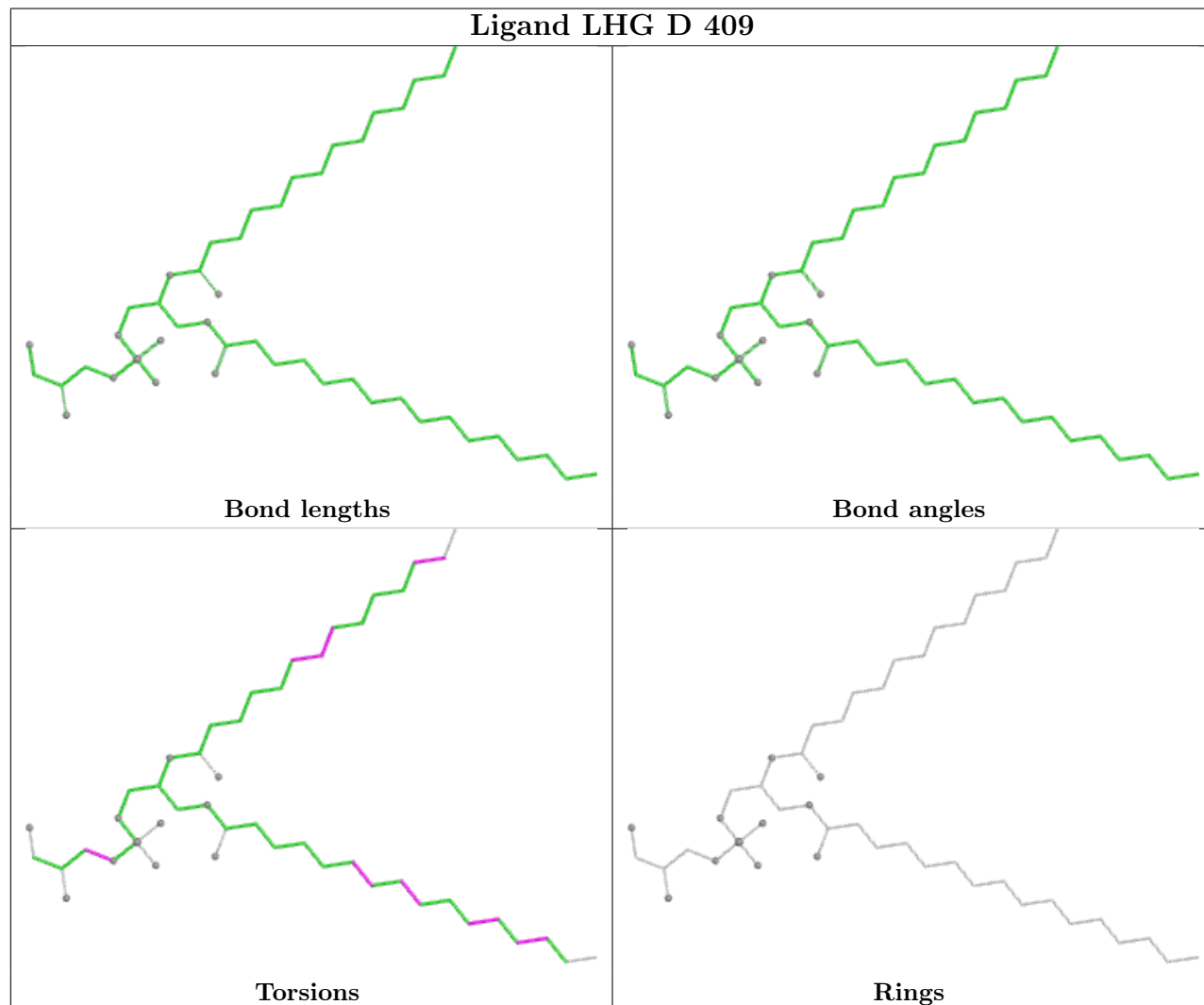


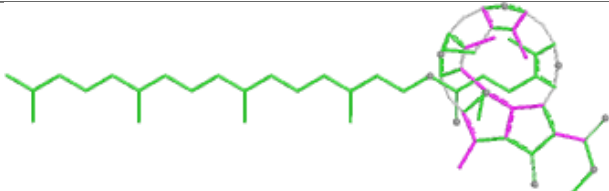
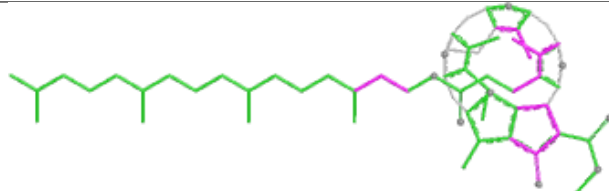
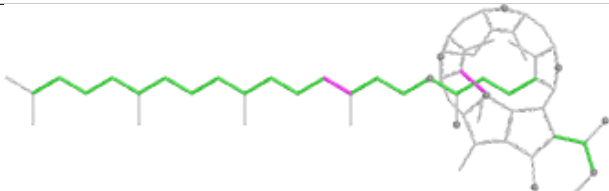
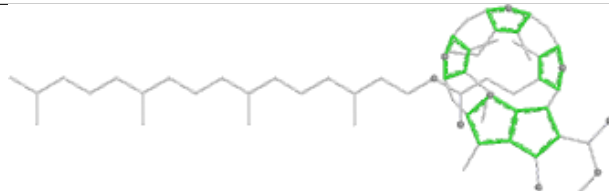


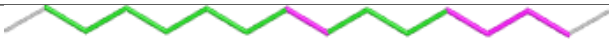
Ligand CLA d 403



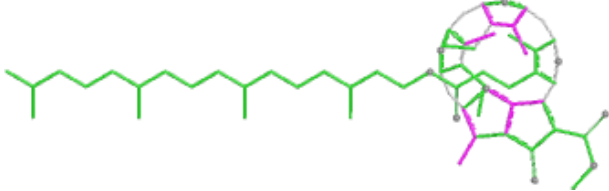
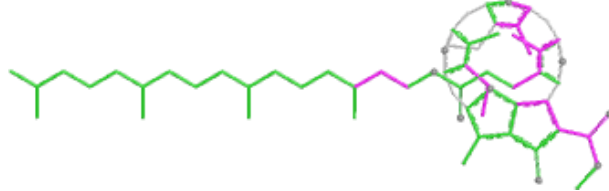
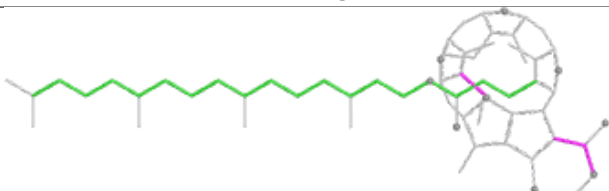
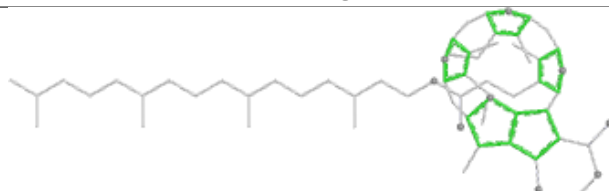
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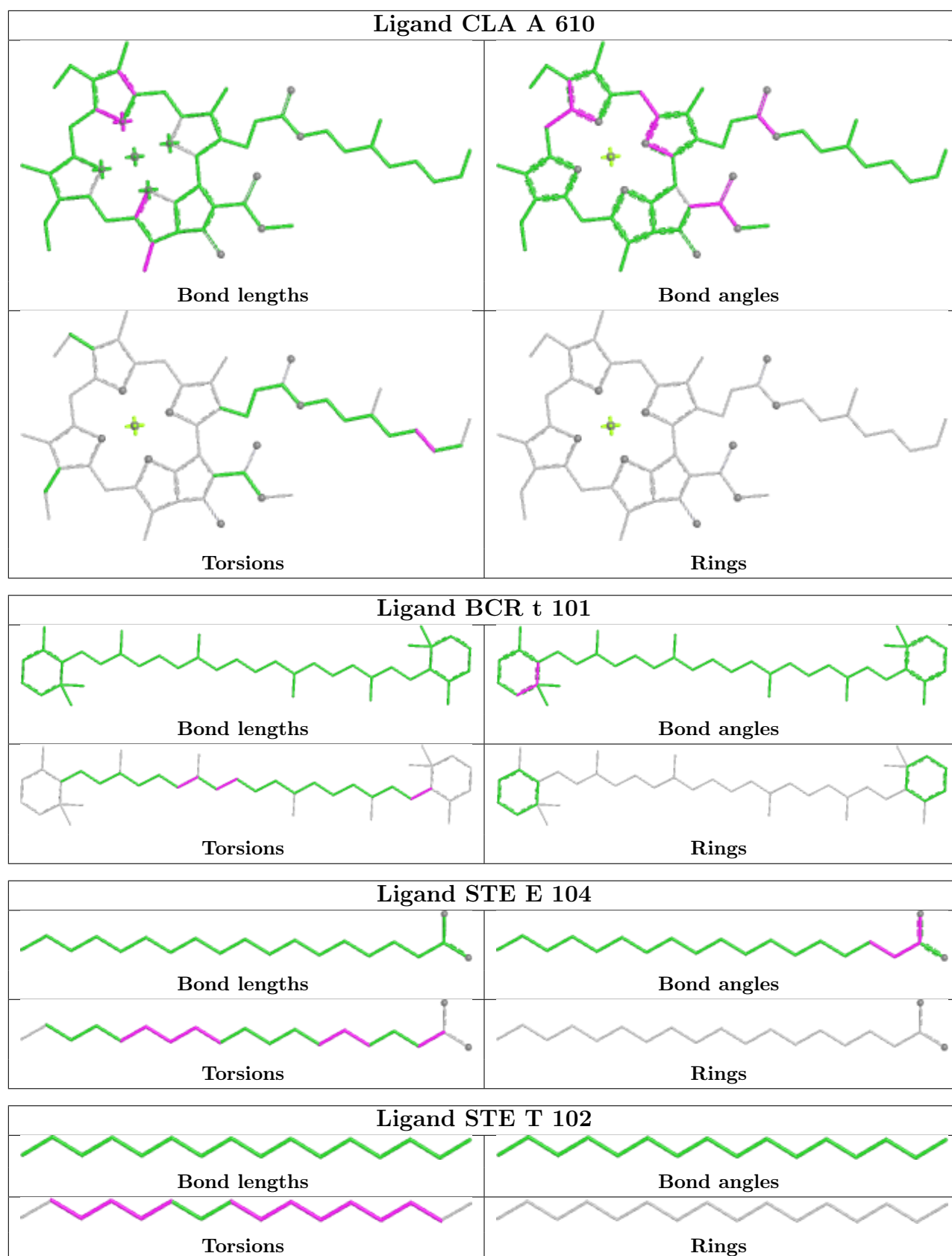


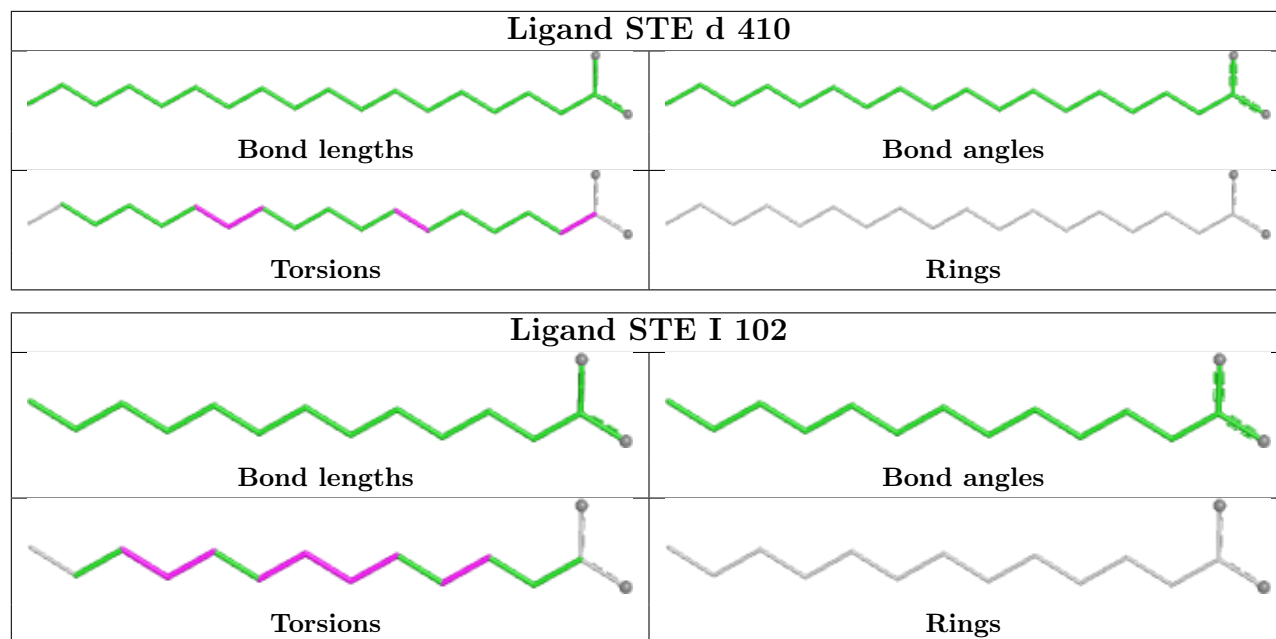
Ligand PHO A 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE C 526	
	
Bond lengths	Bond angles
	
Torsions	Rings

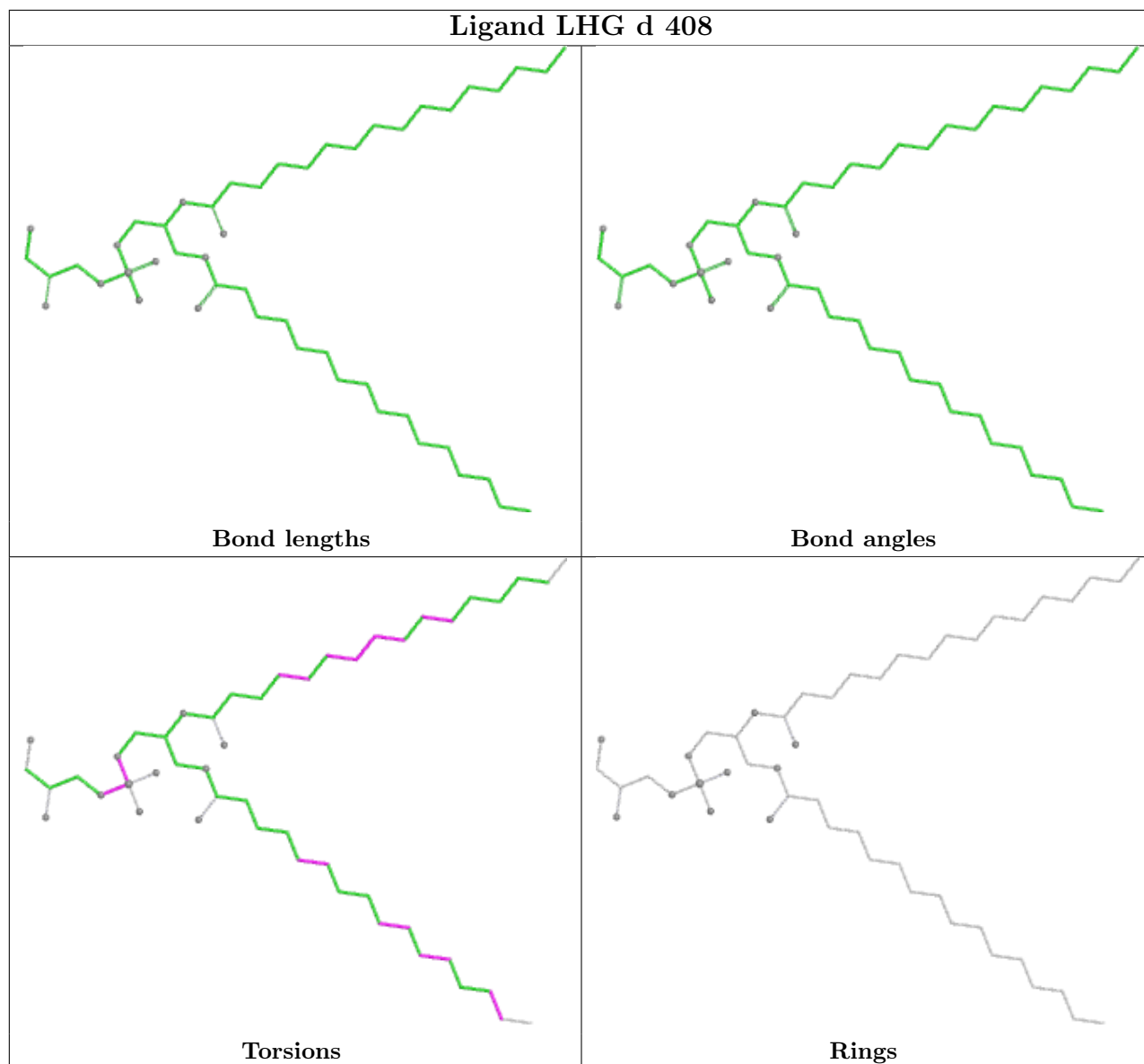
Ligand STE m 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PHO d 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

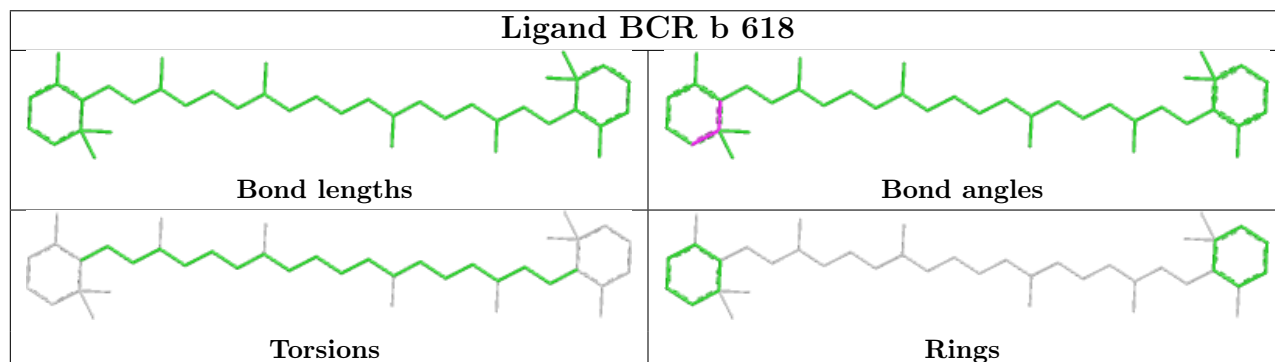


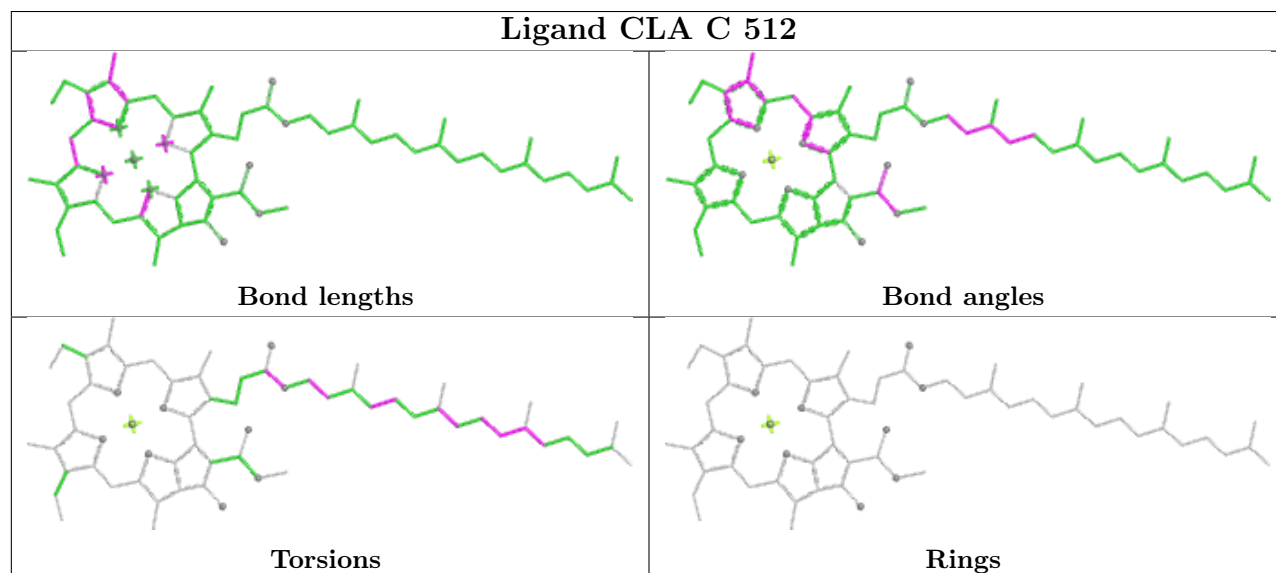
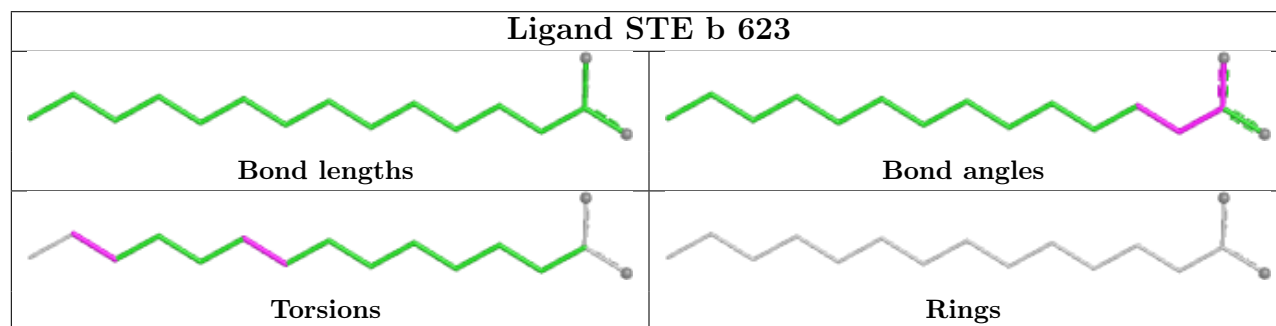
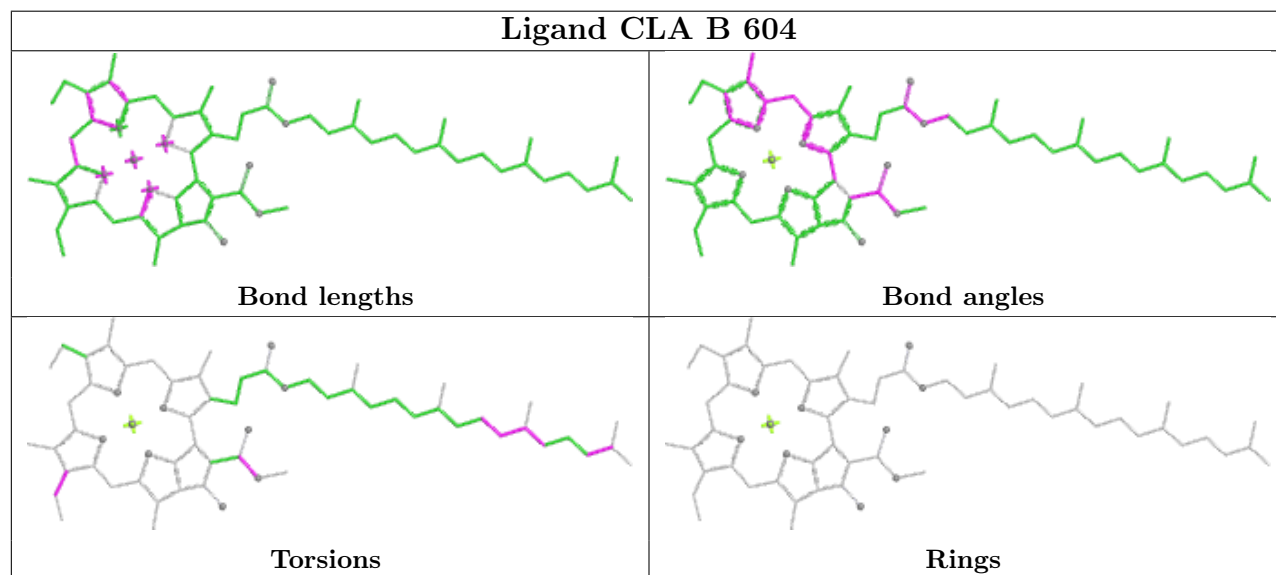
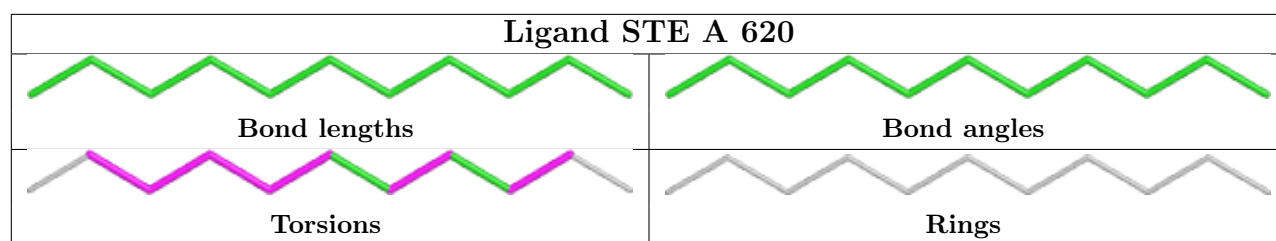


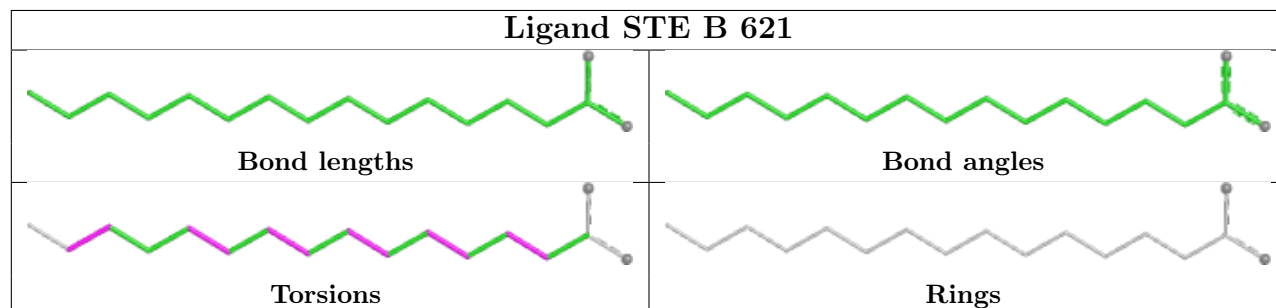
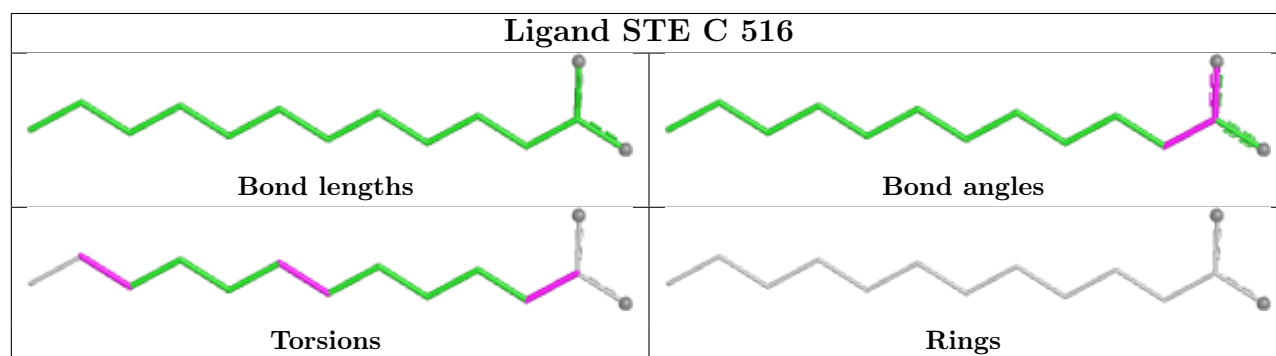
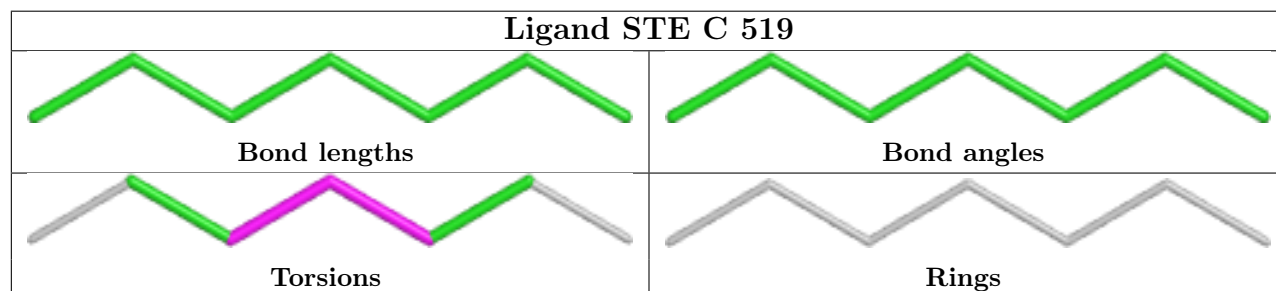
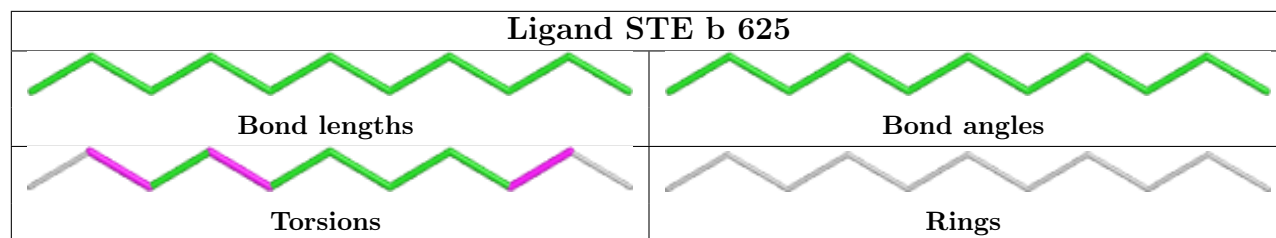
Ligand LHG d 408

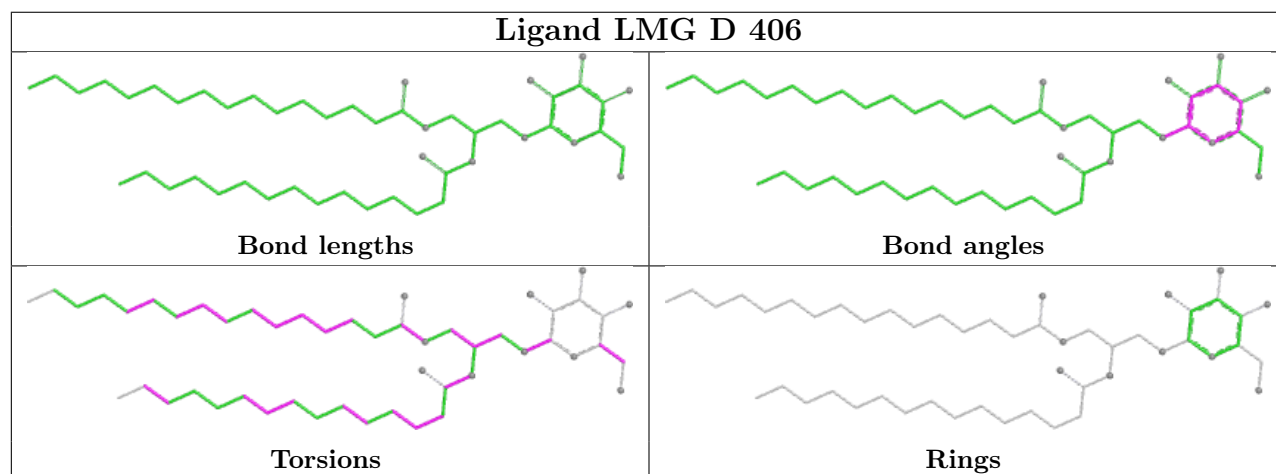
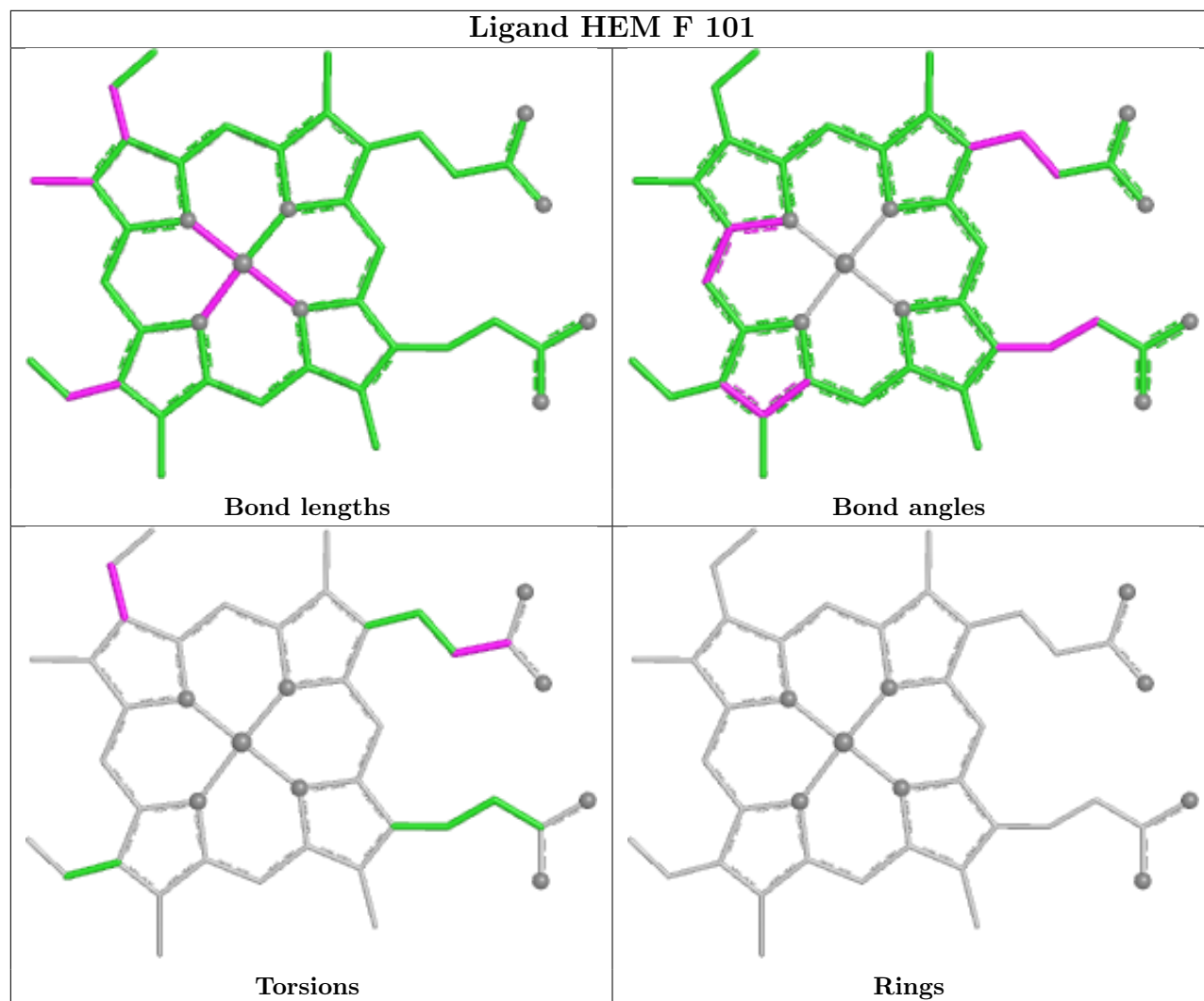


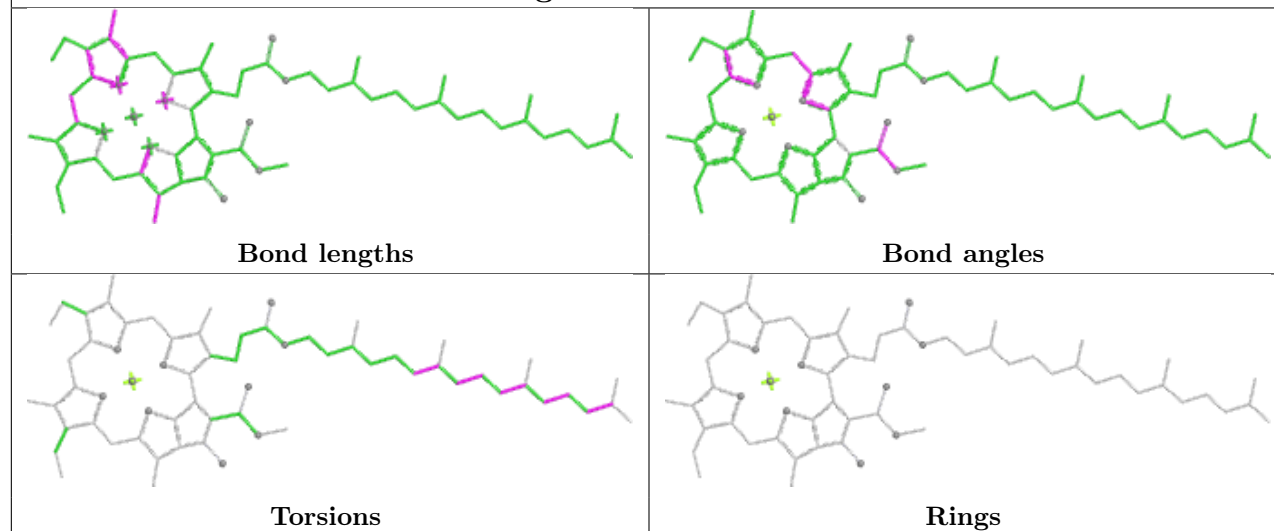
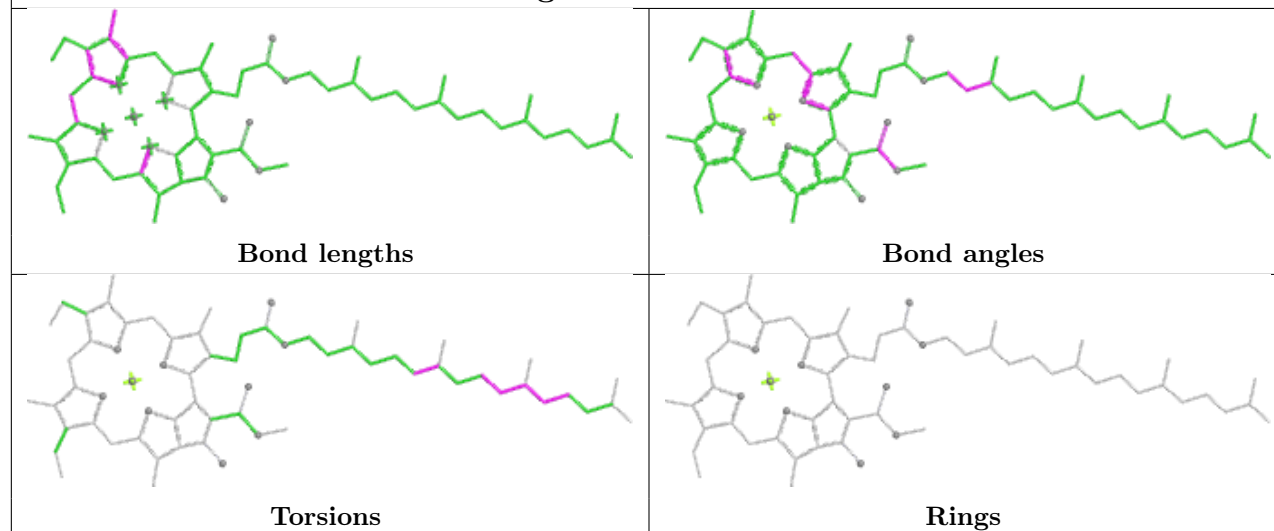
Ligand BCR b 618



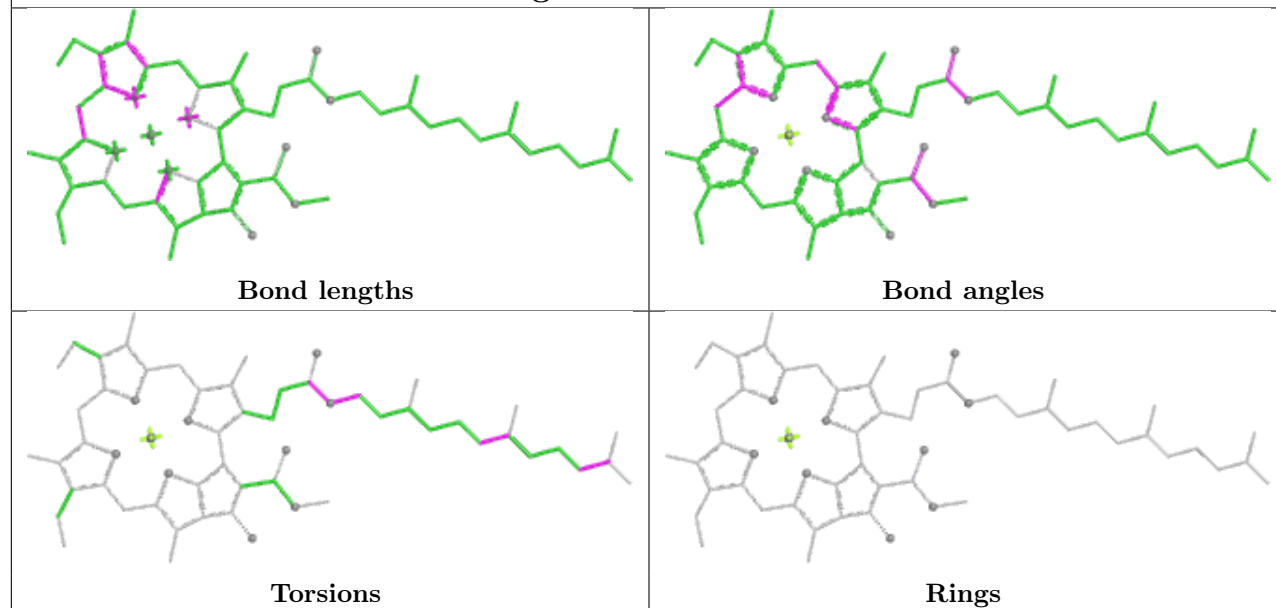




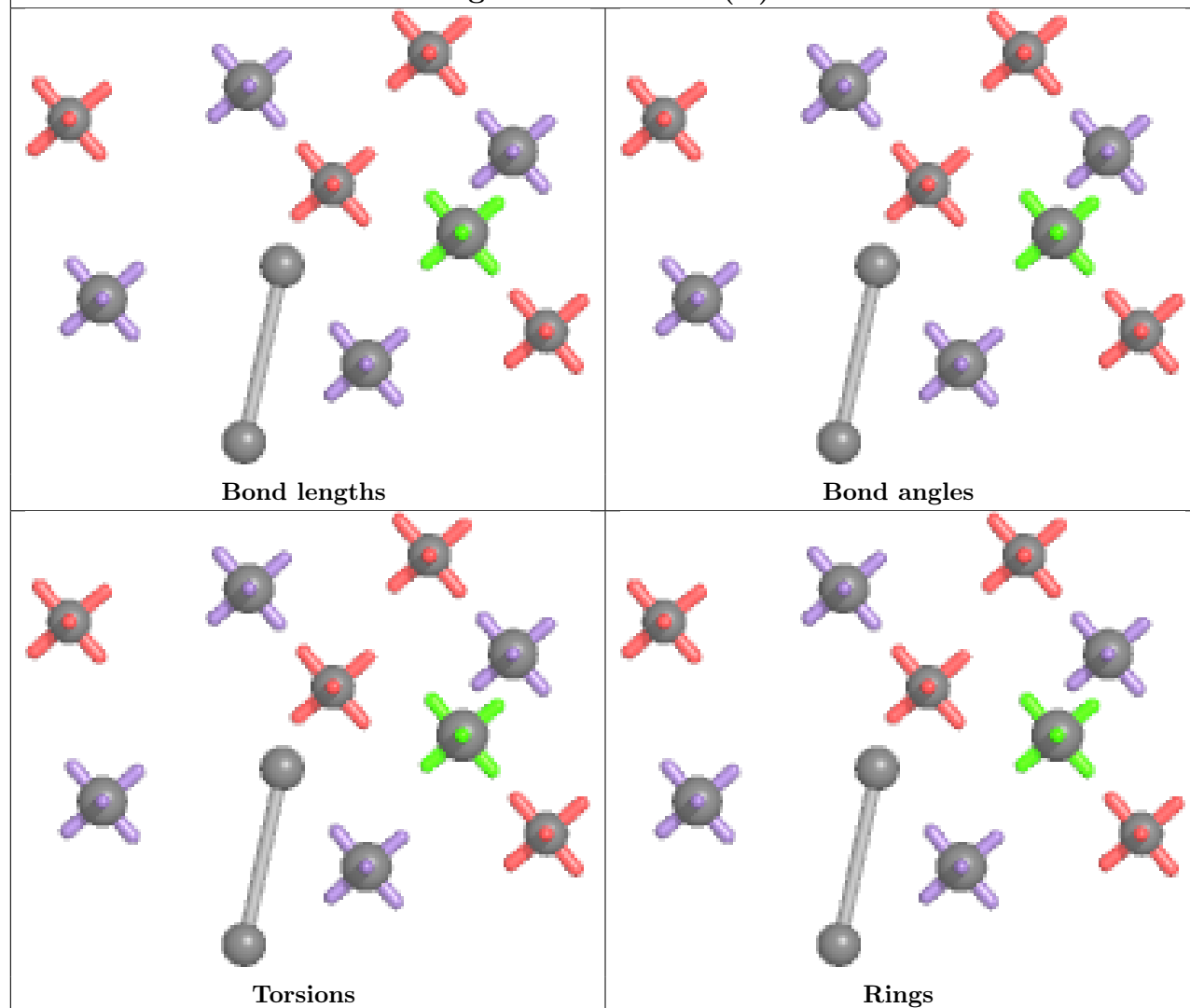


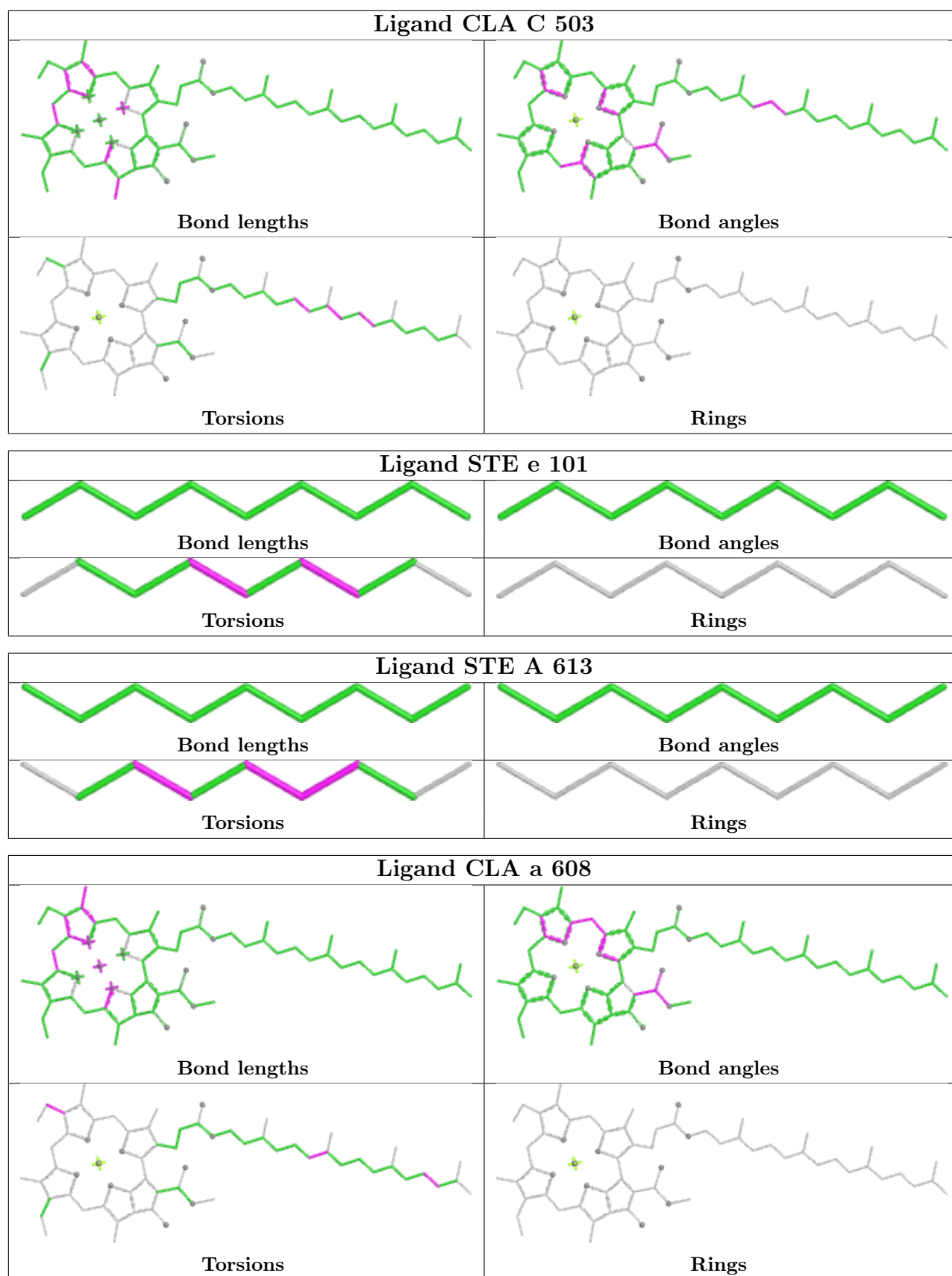
Ligand CLA b 615**Ligand CLA c 505**

Ligand CLA B 616

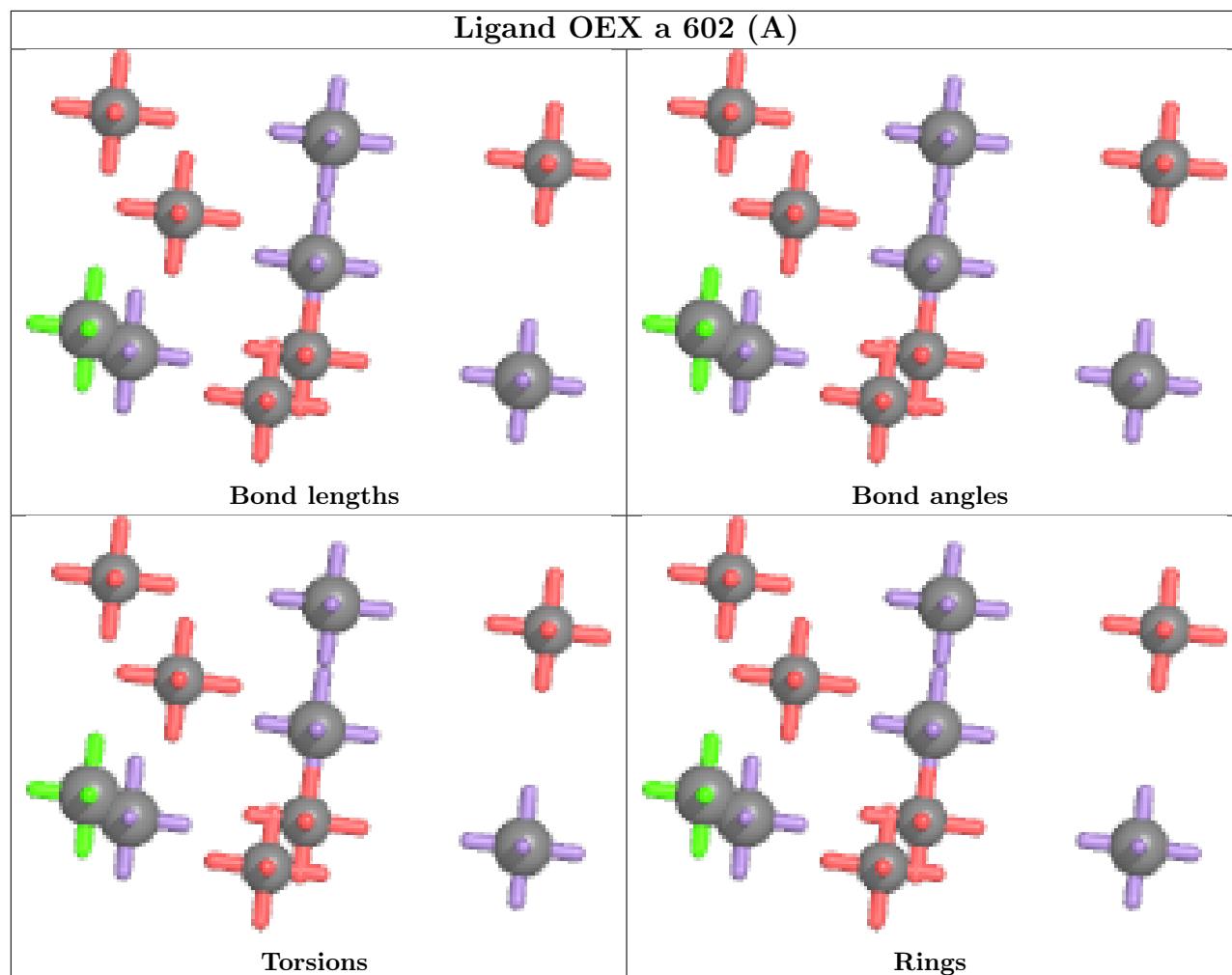


Ligand OEY a 601 (B)

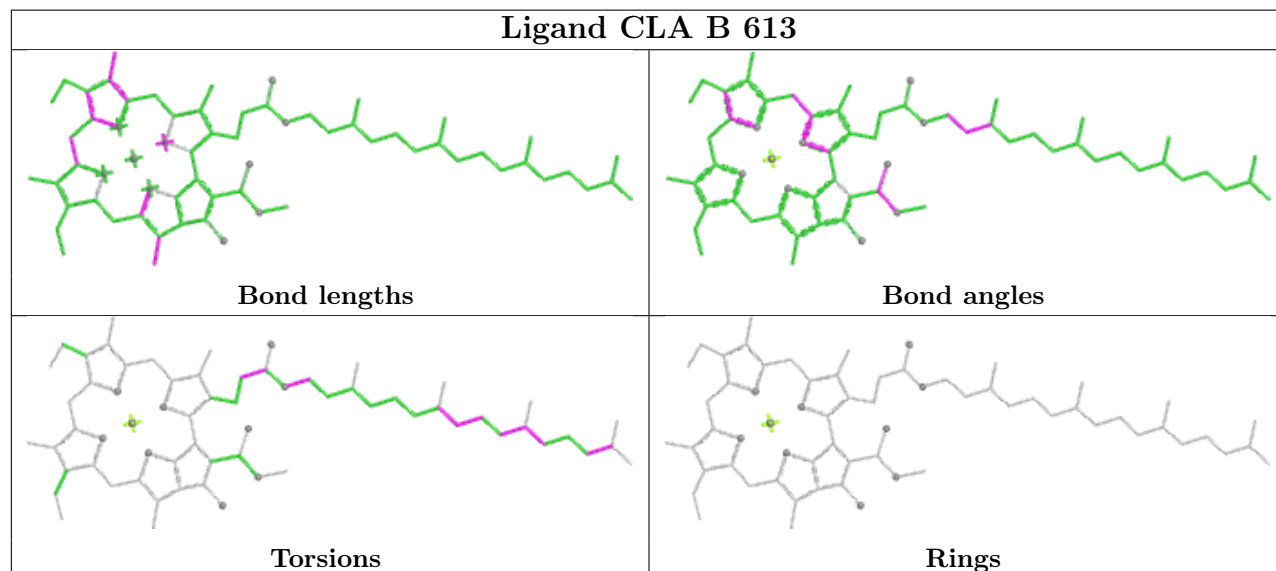


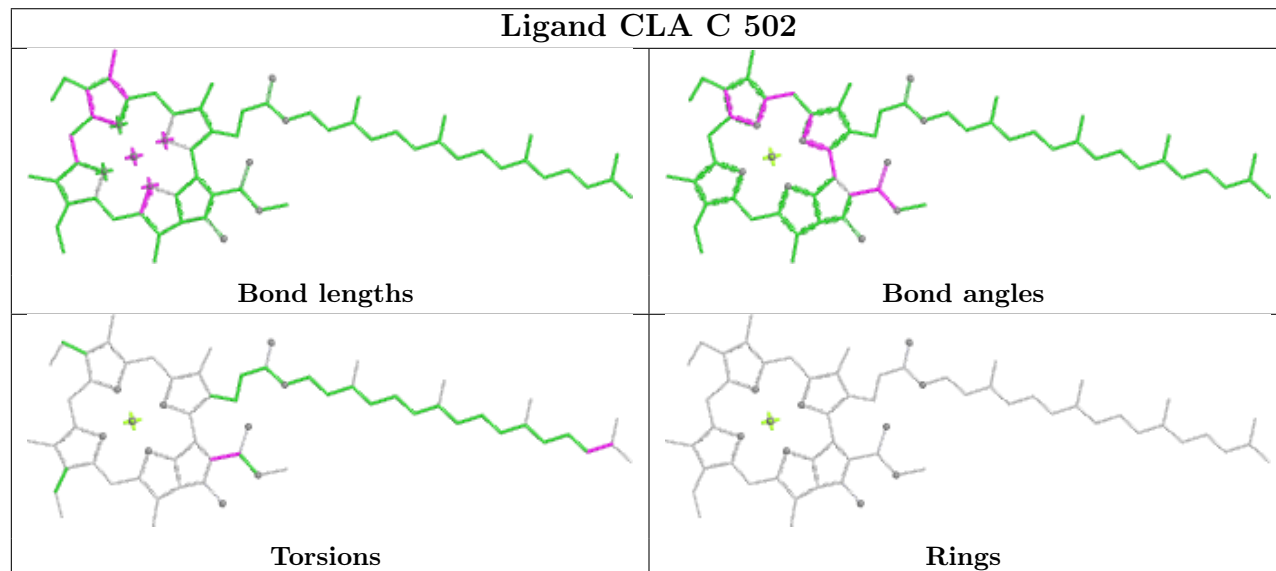
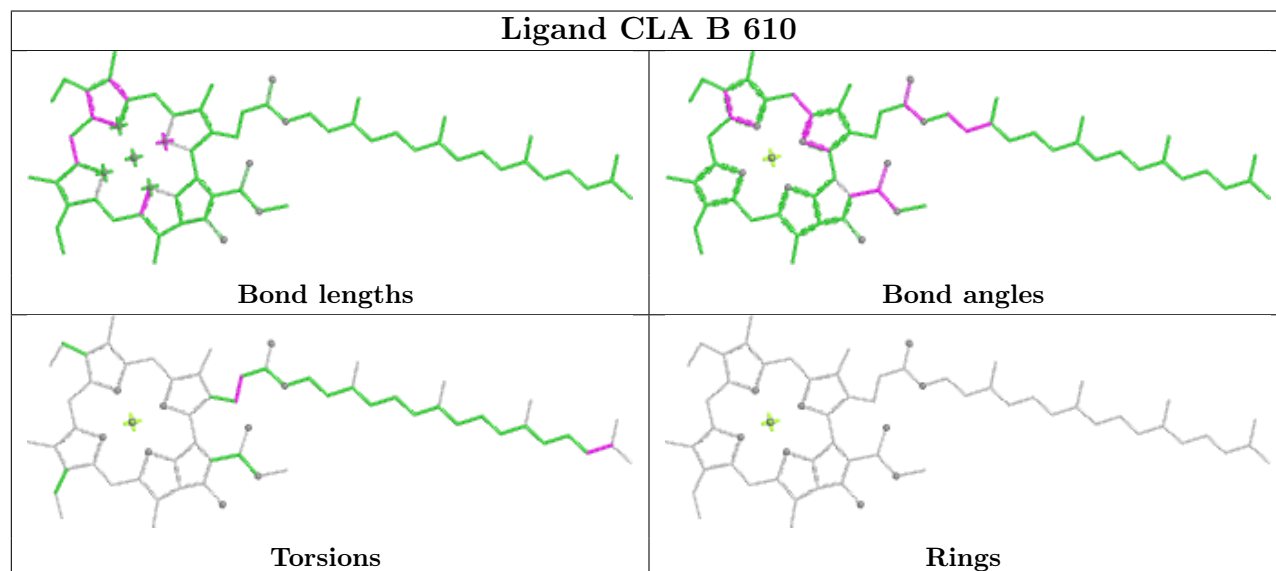
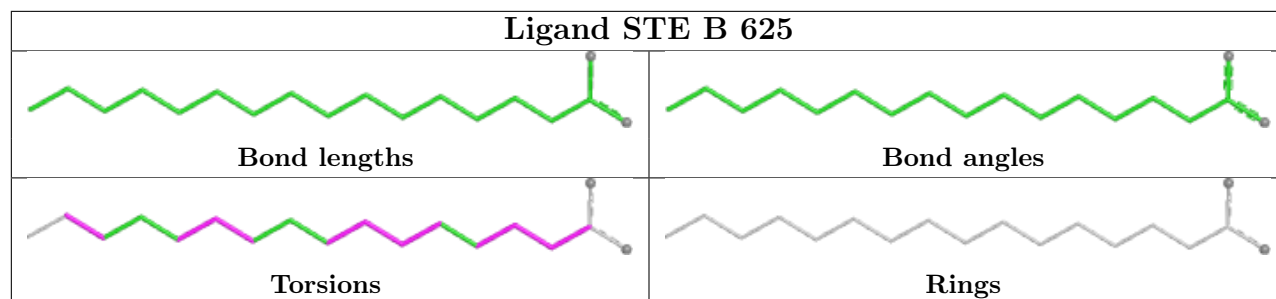


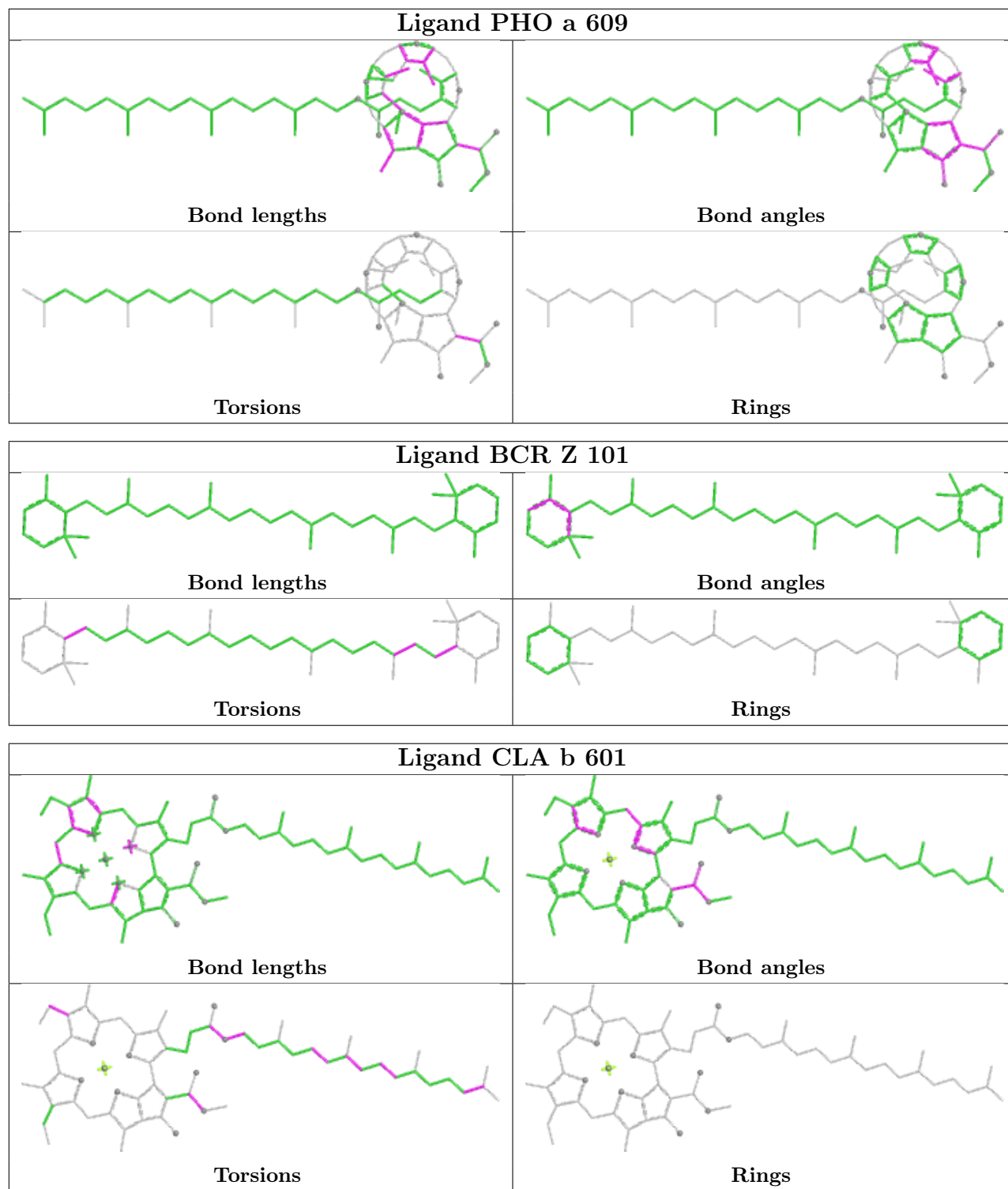
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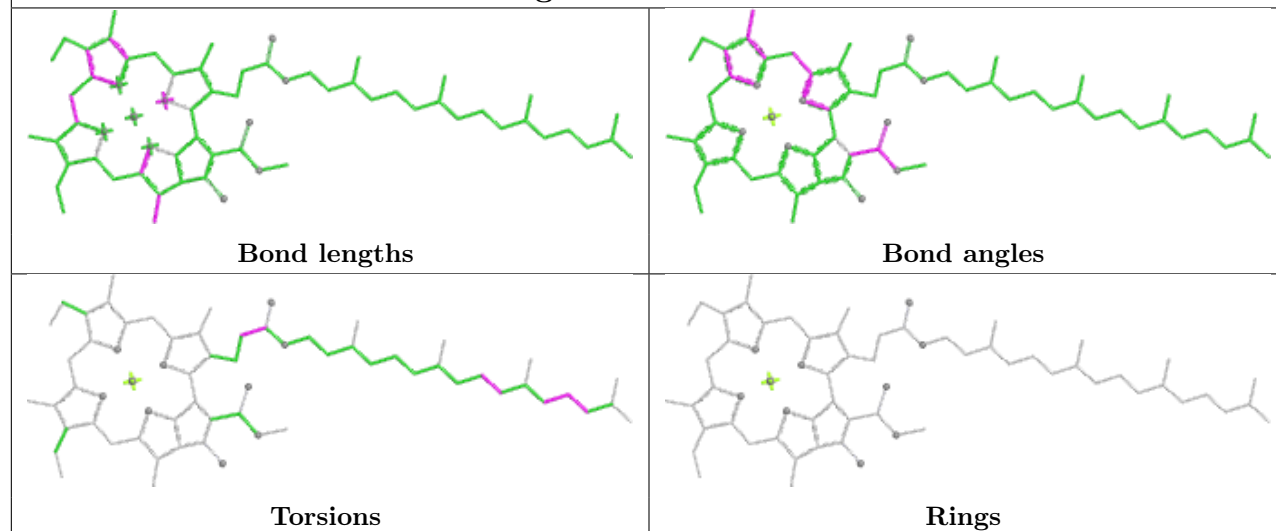
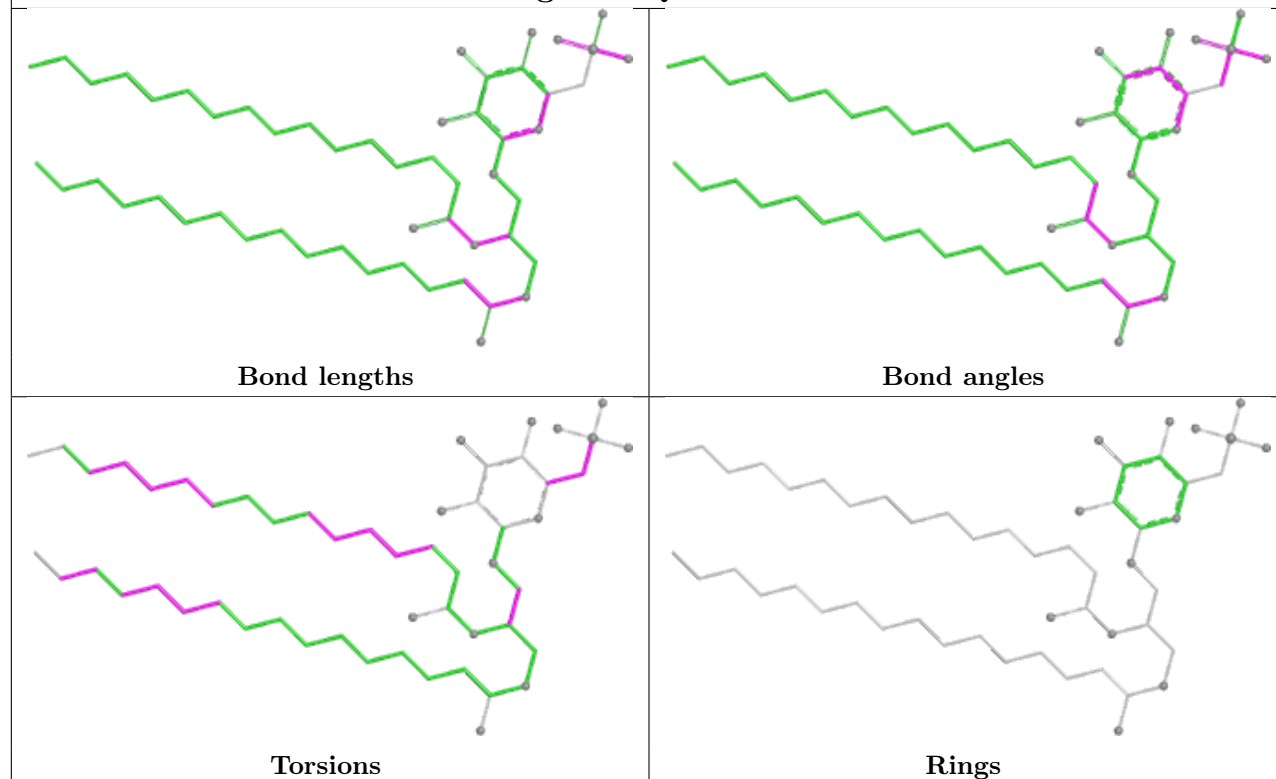


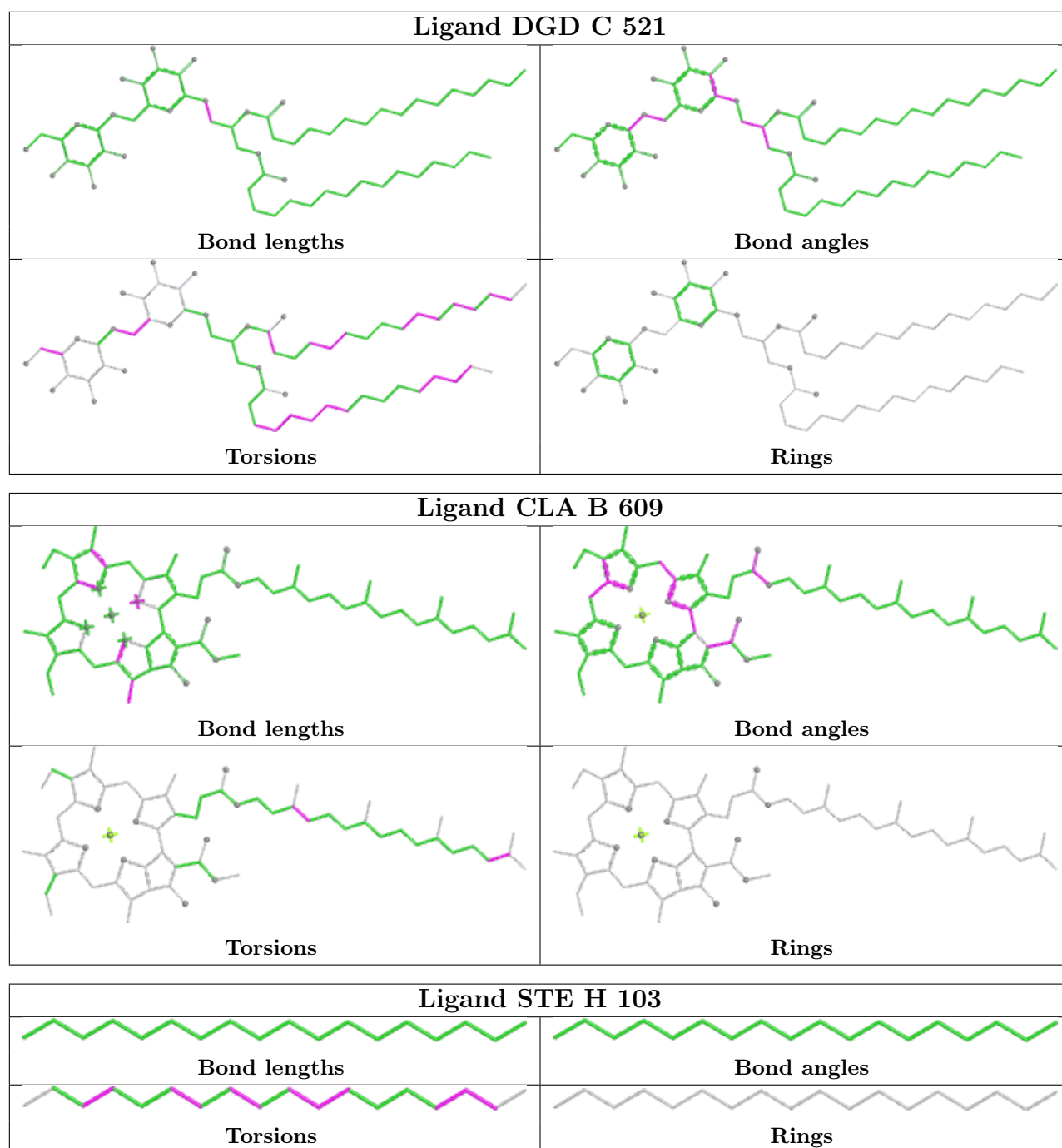
Ligand CLA B 613

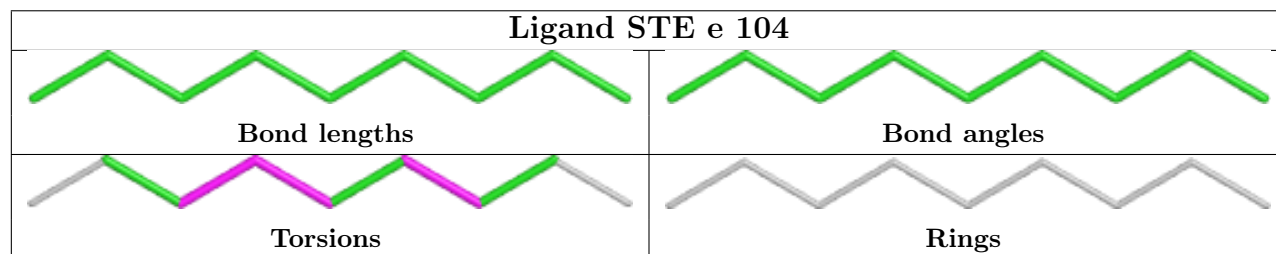
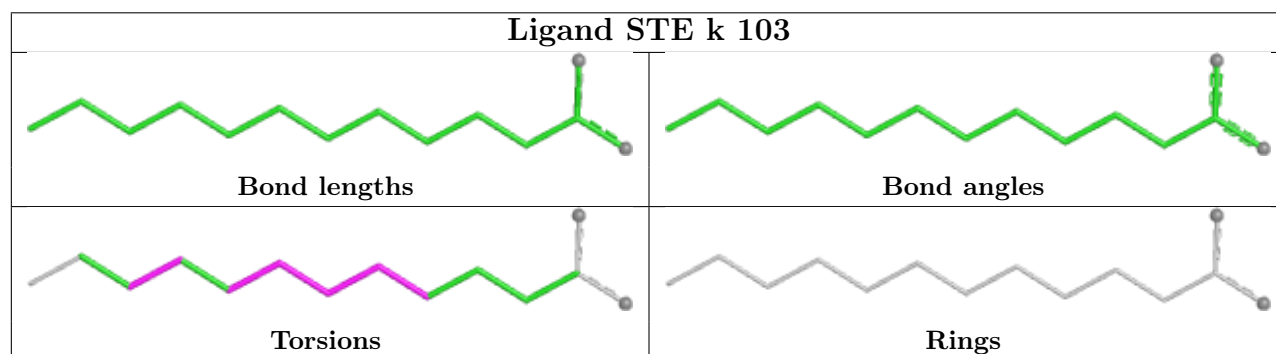
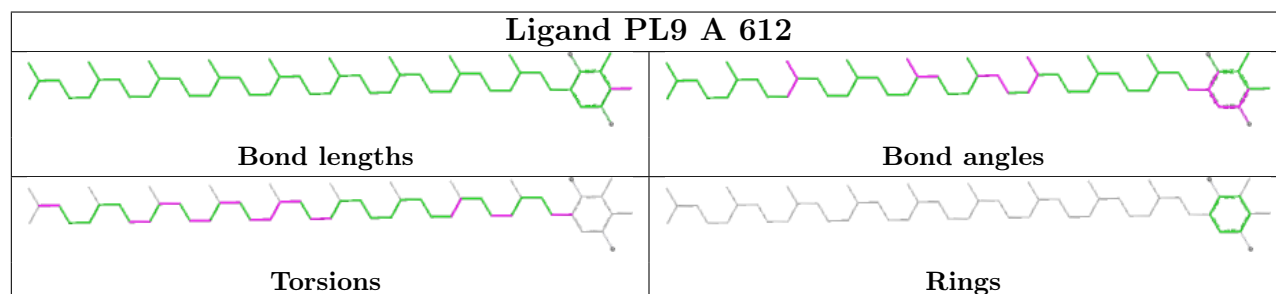
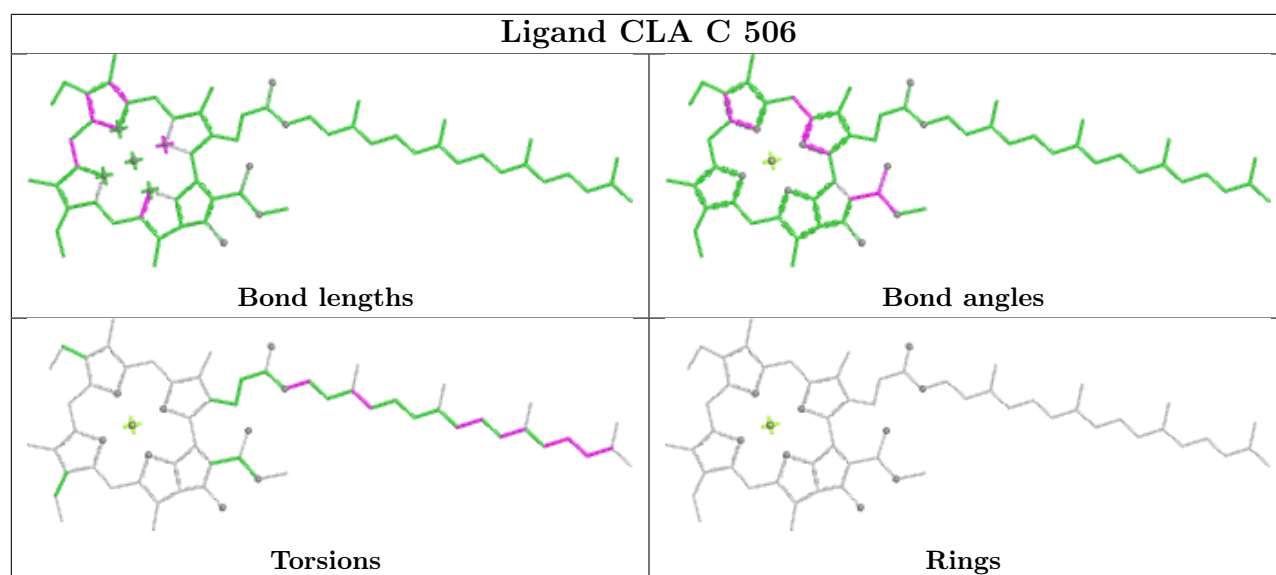


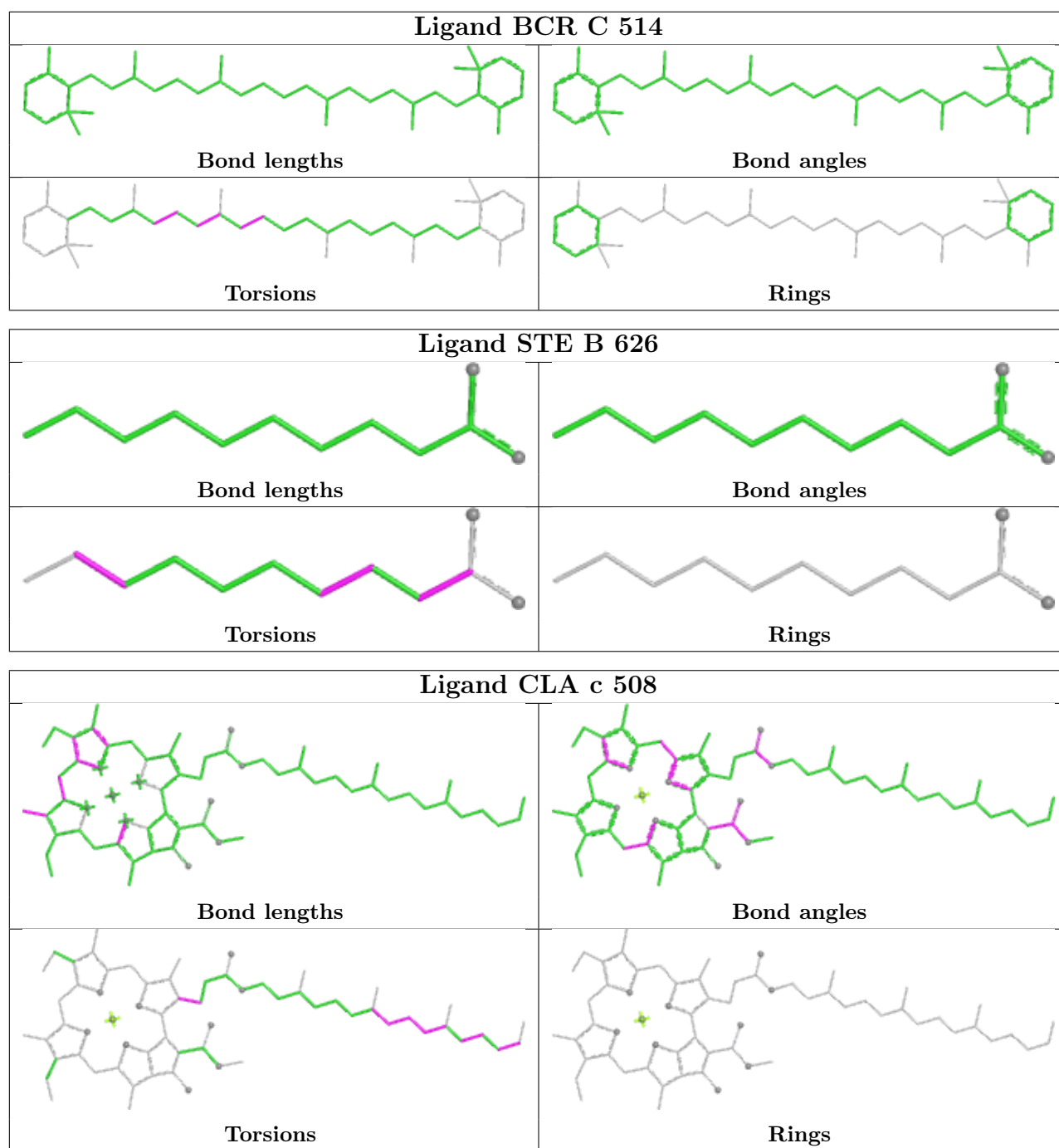


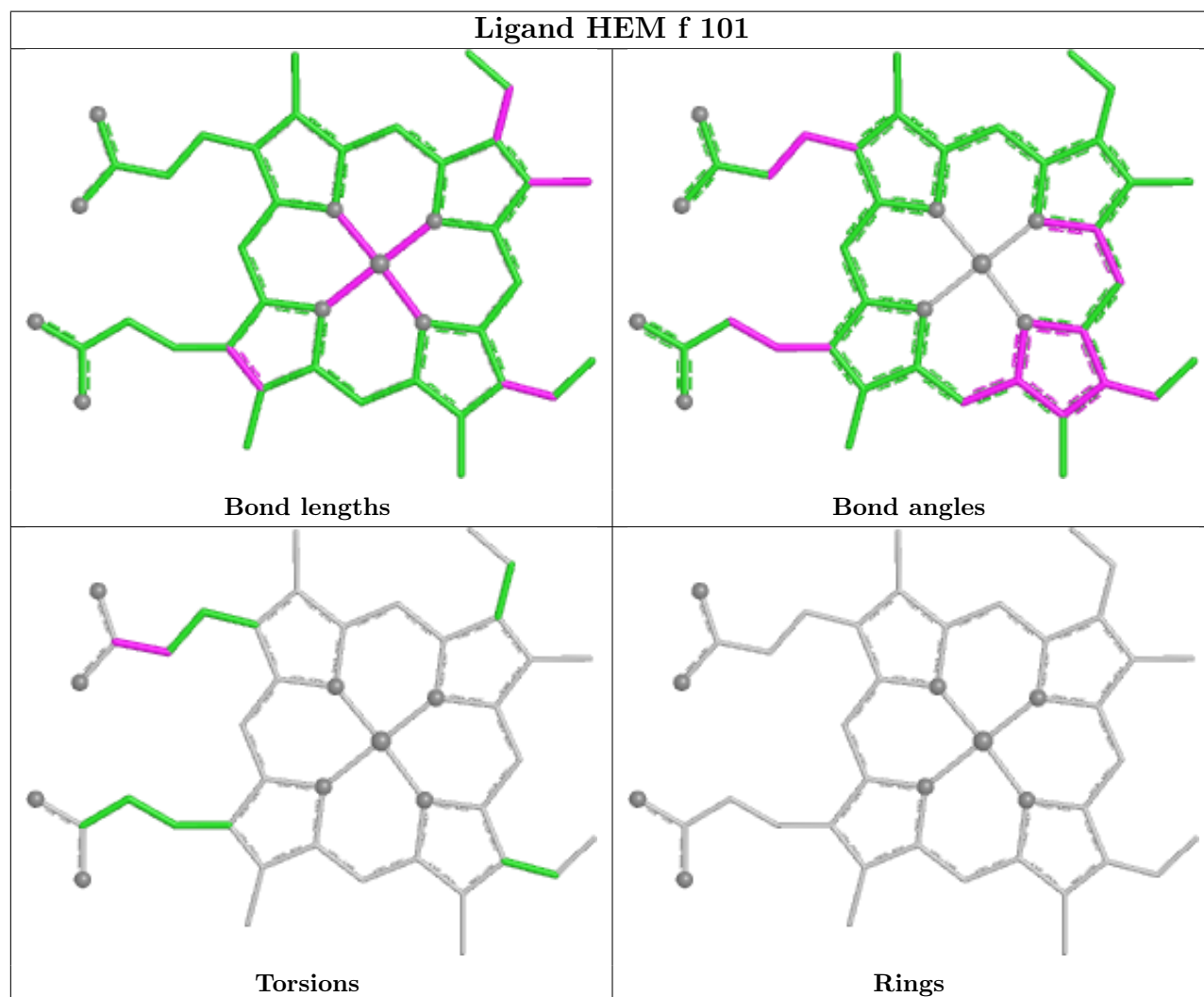
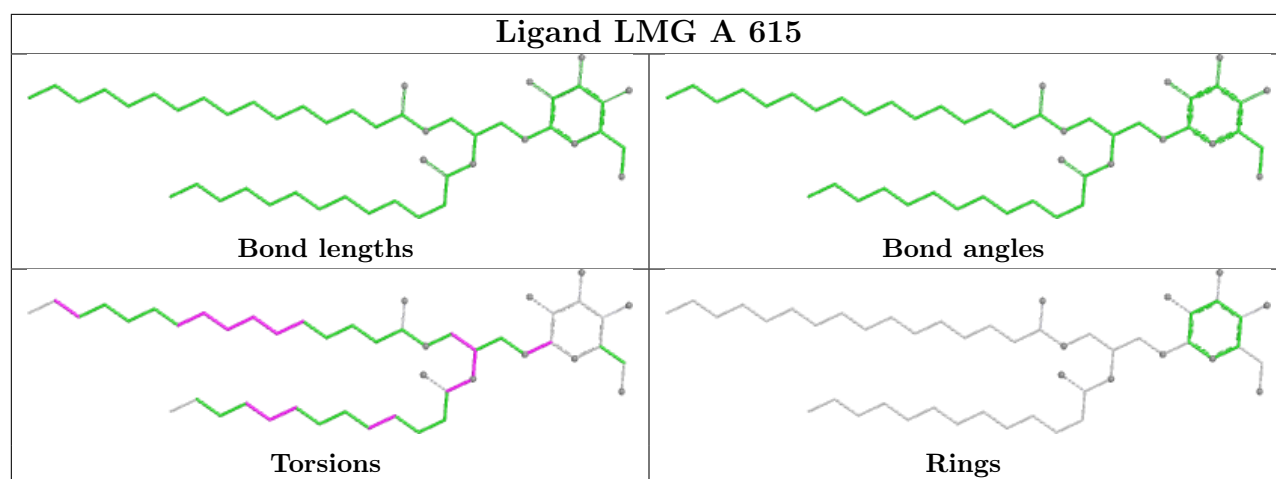


Ligand CLA b 613**Ligand SQD a 615**

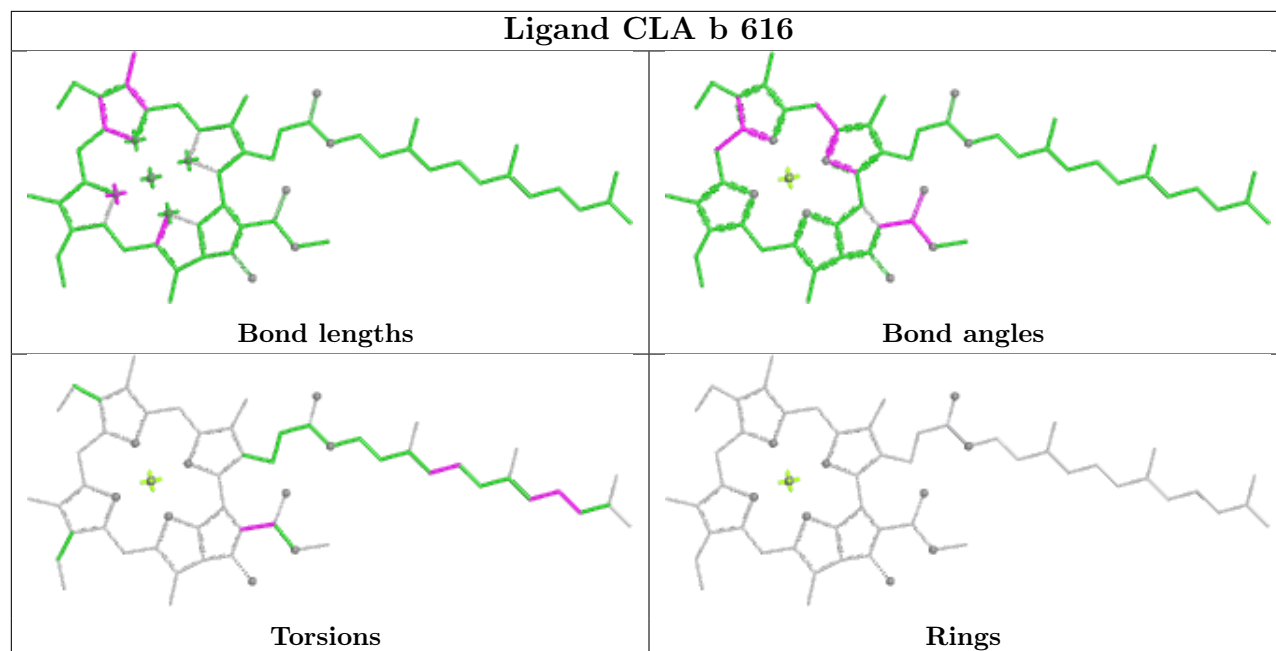




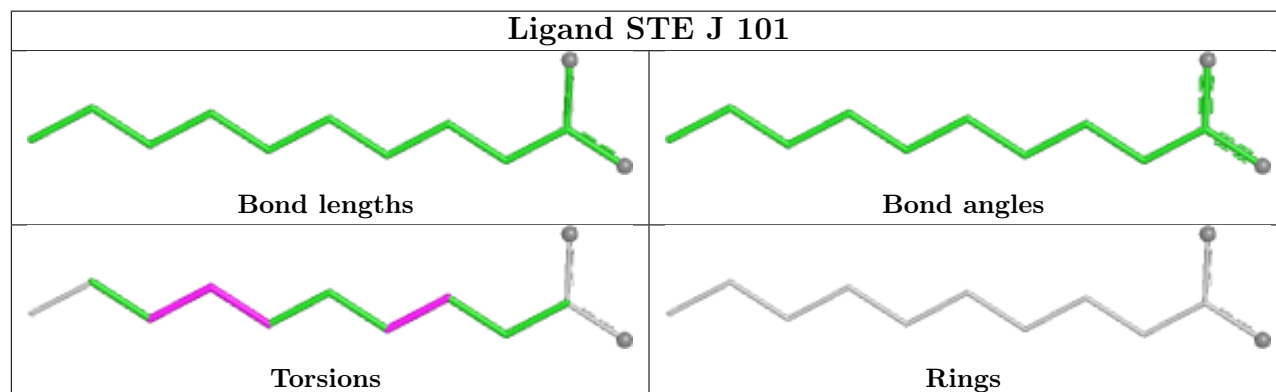




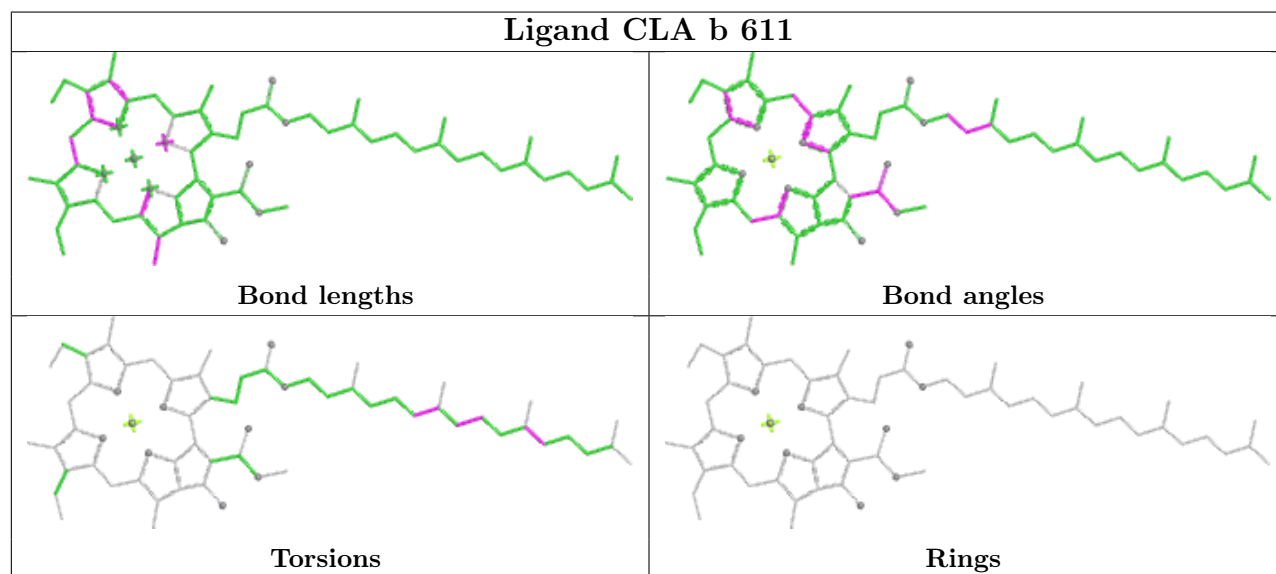
Ligand CLA b 616

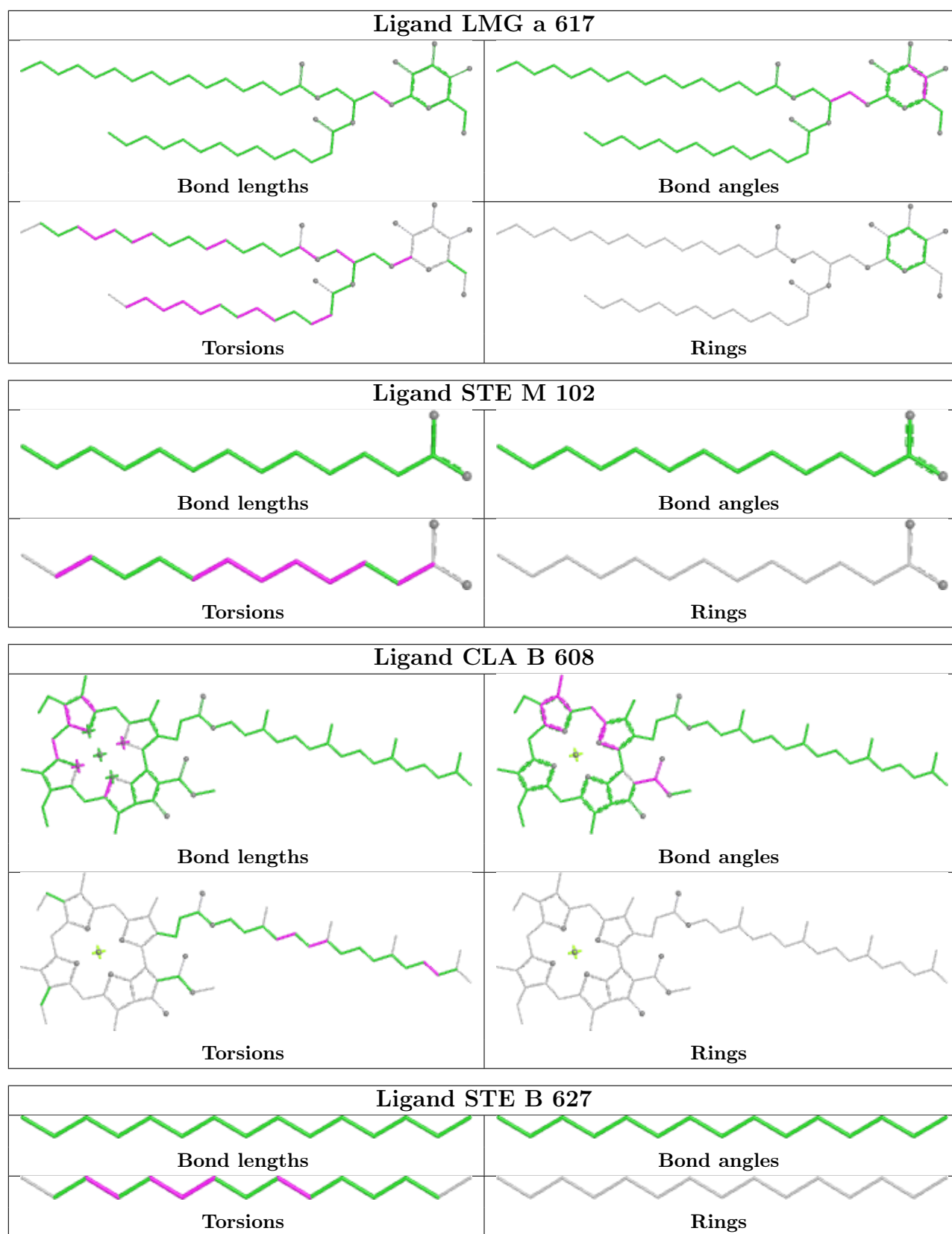


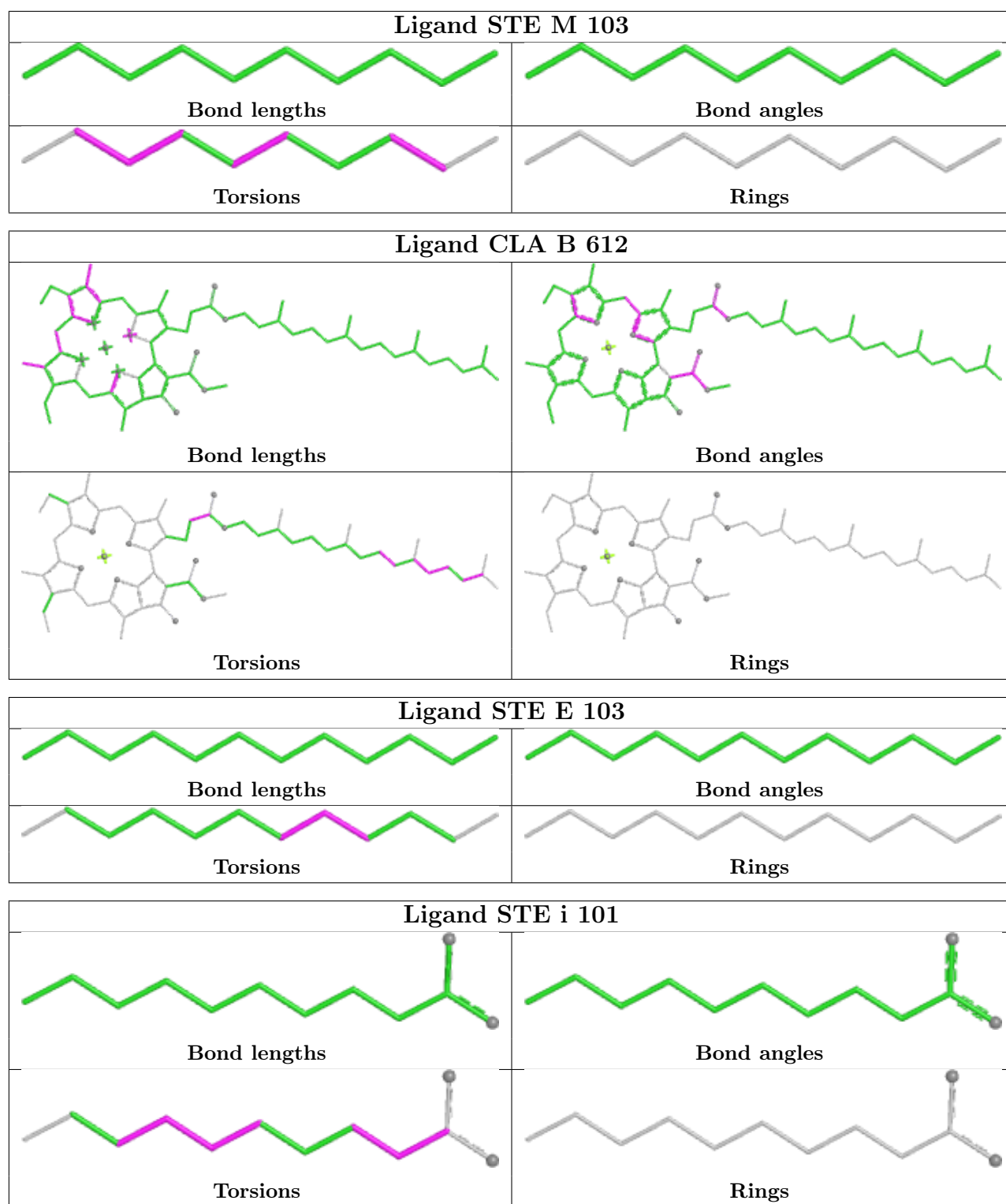
Ligand STE J 101

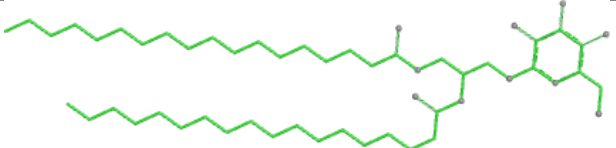
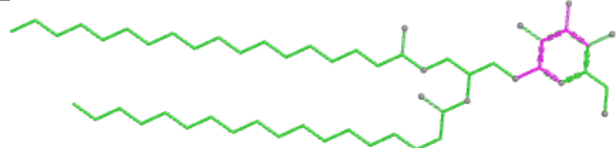
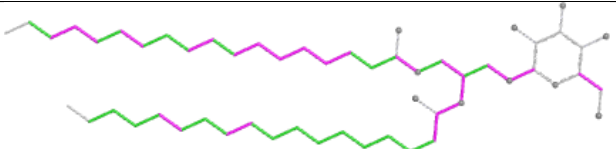
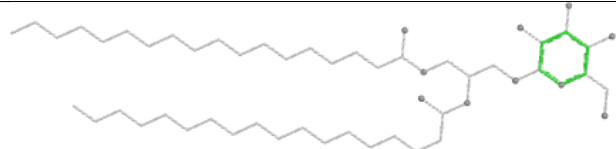


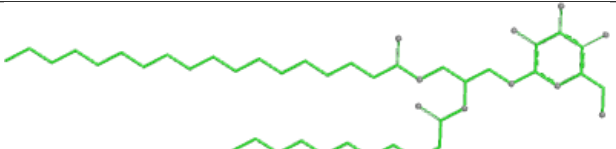
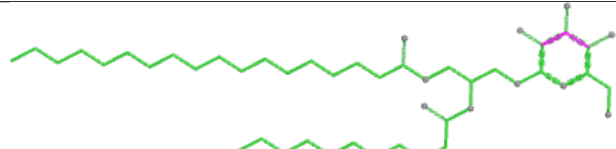
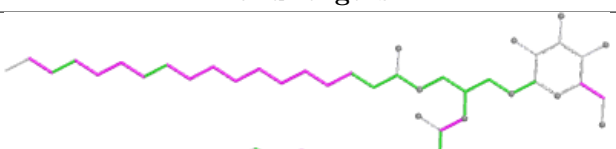
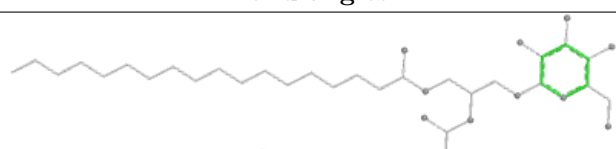
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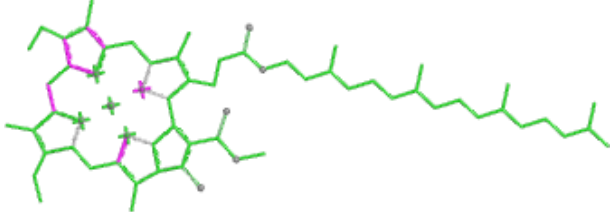
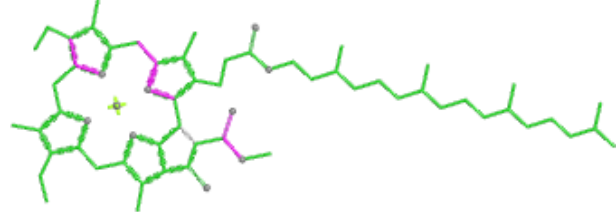
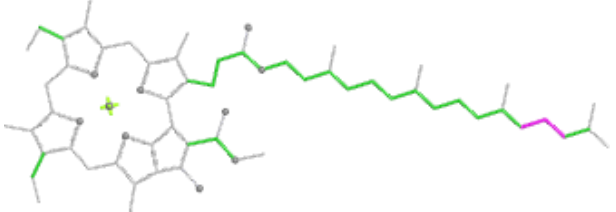
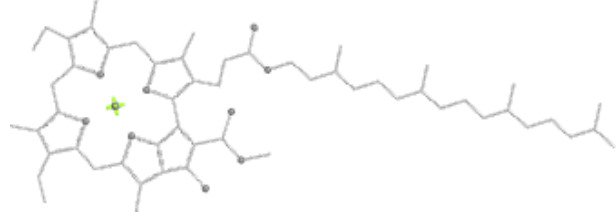


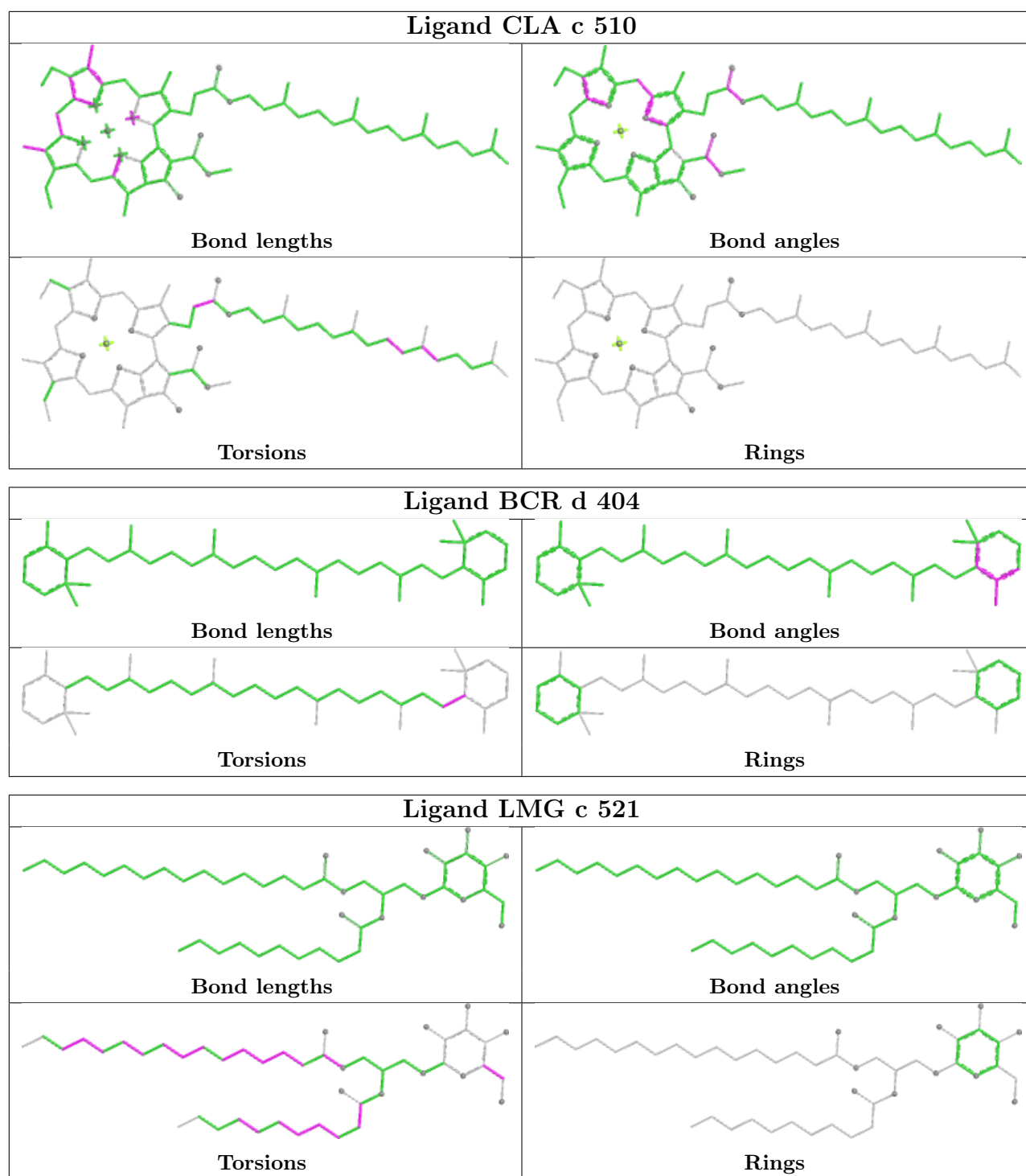




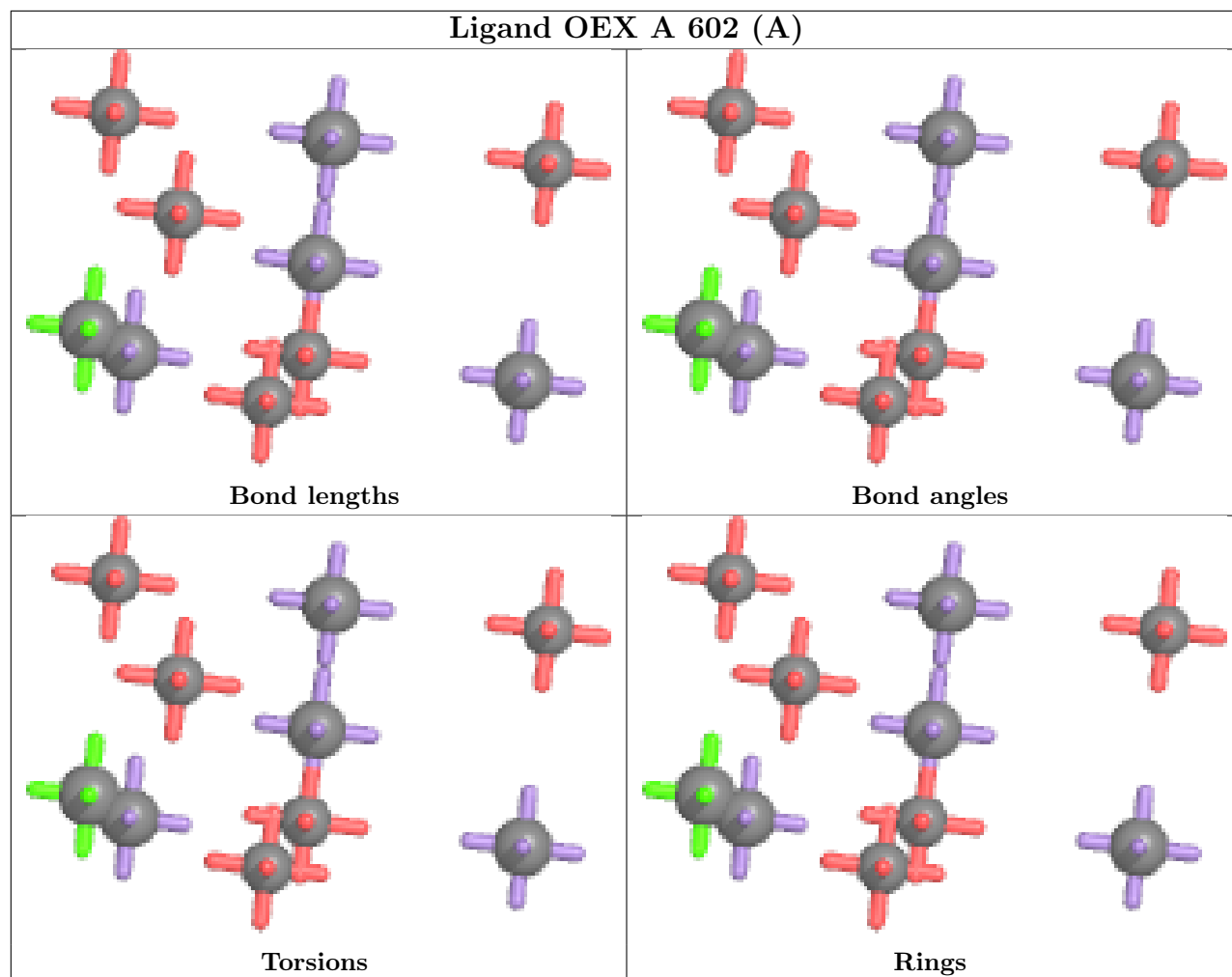
Ligand LMG a 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

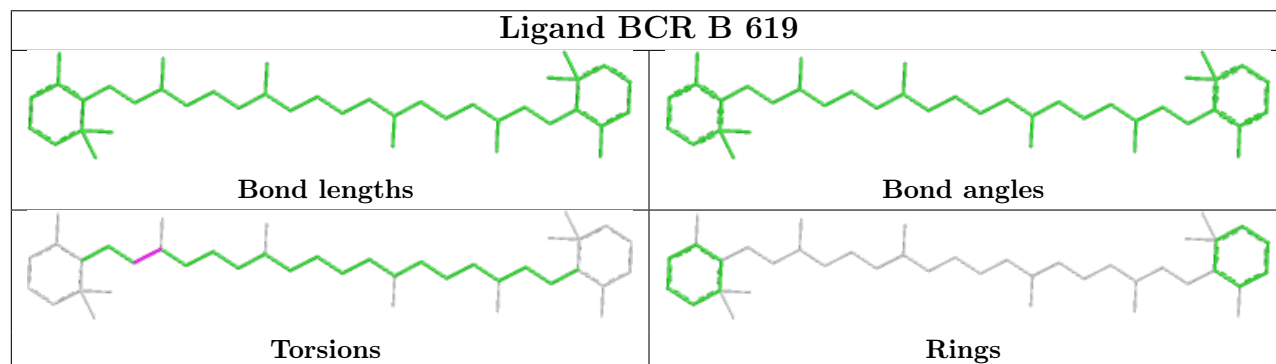
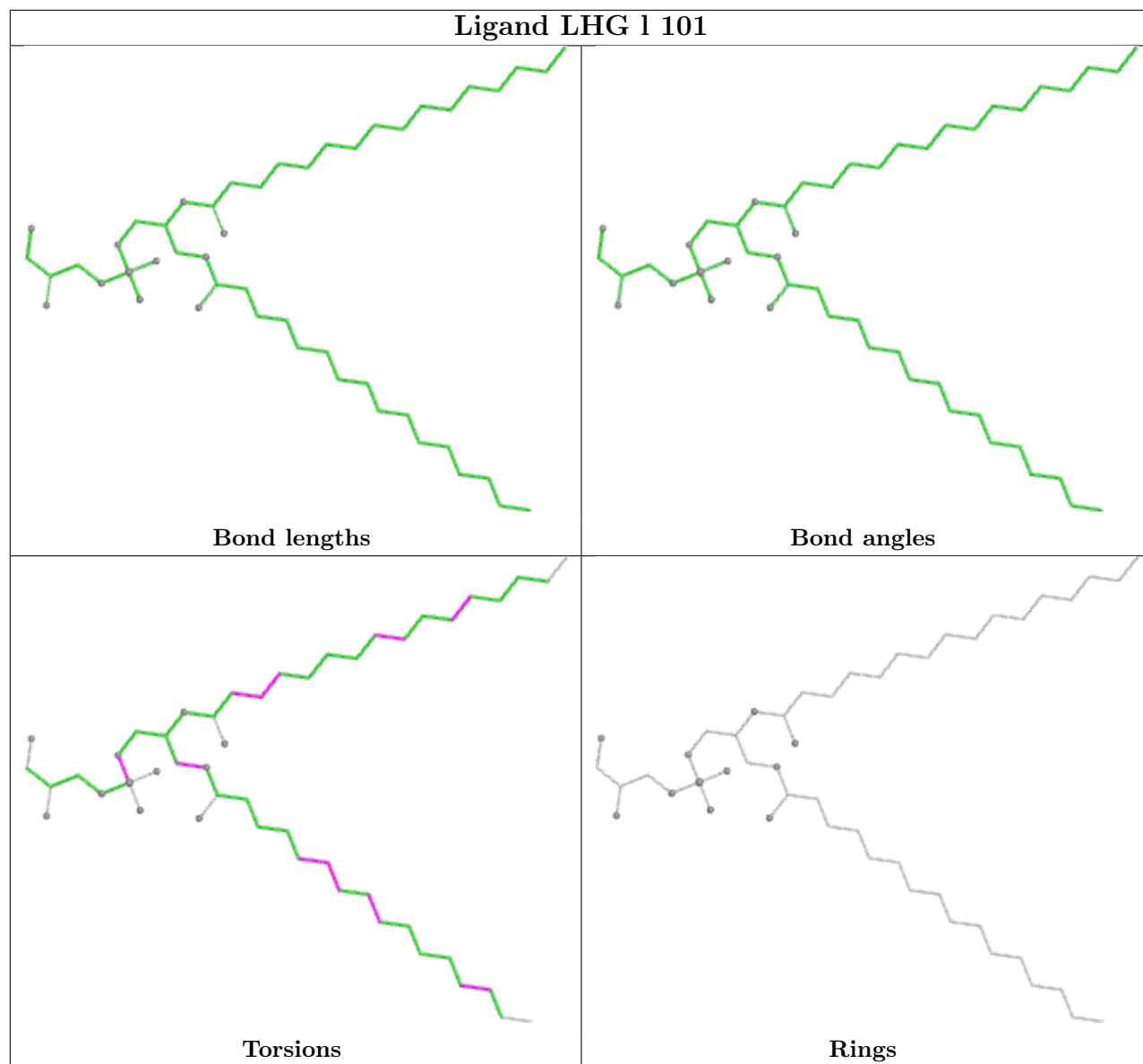
Ligand LMG c 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

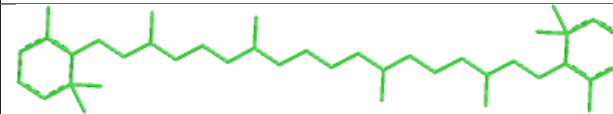
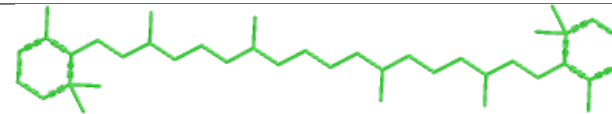
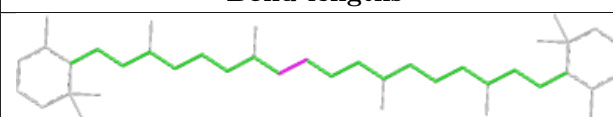
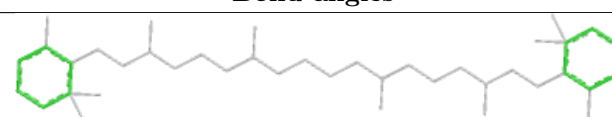
Ligand CLA A 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

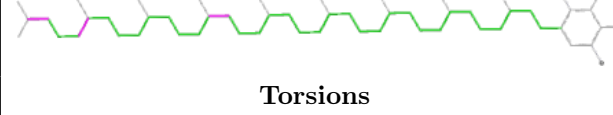


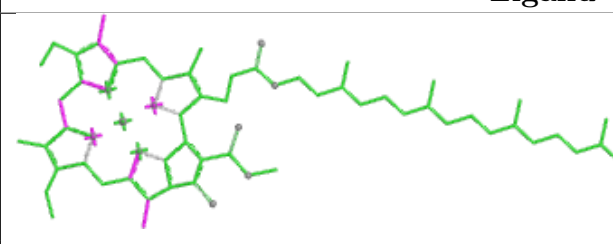
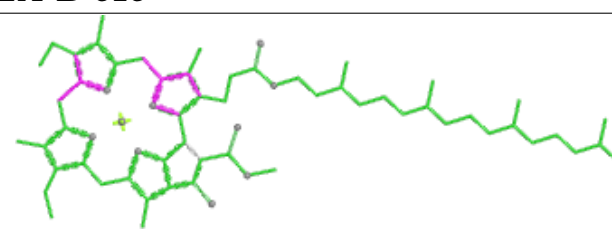
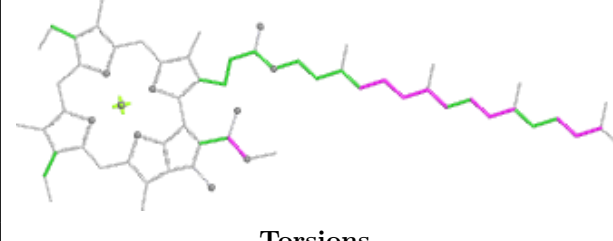
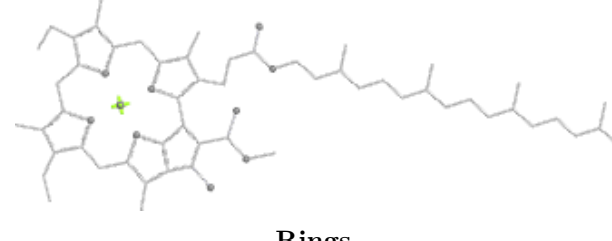
Ligand OEX A 602 (A)

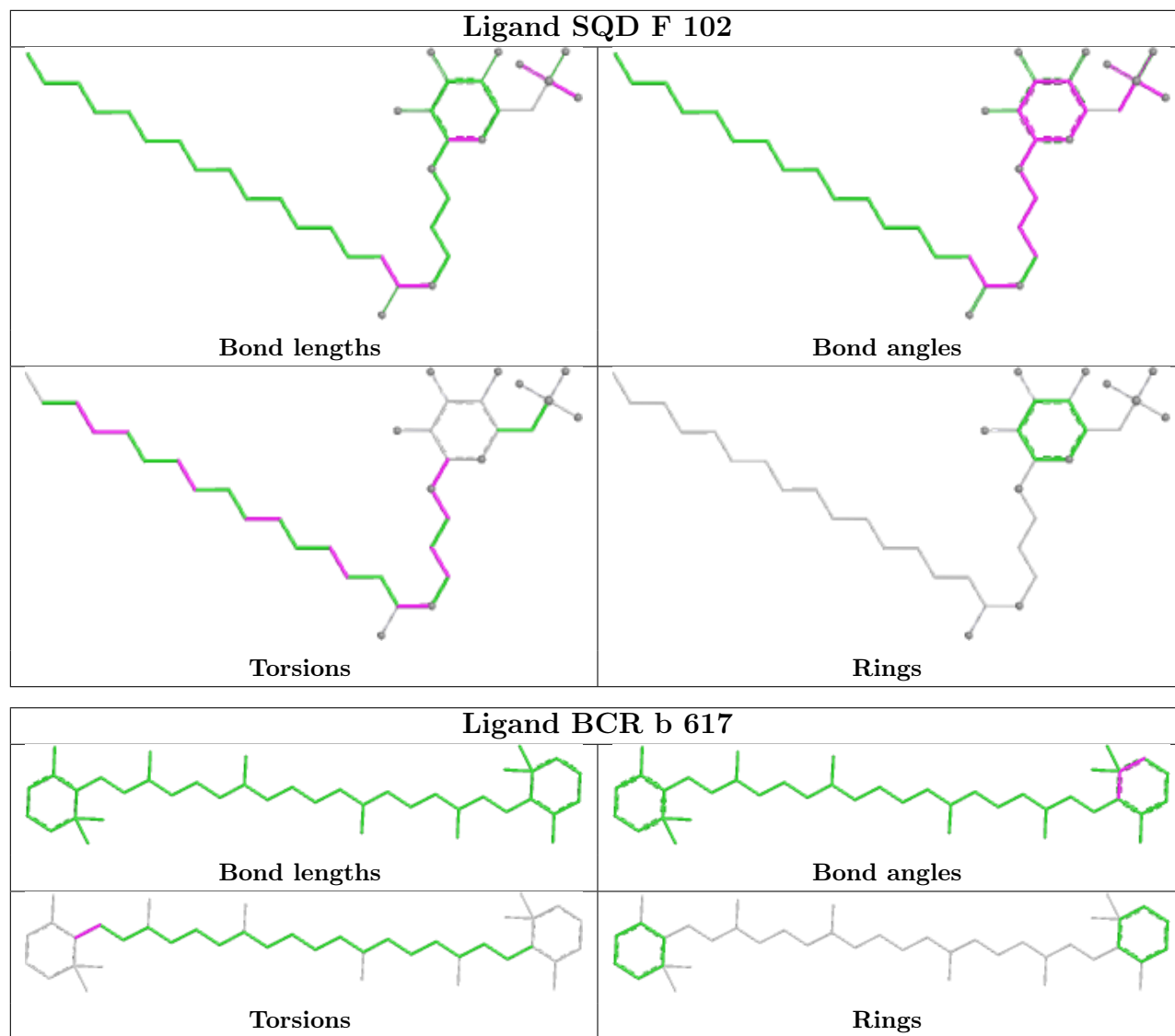


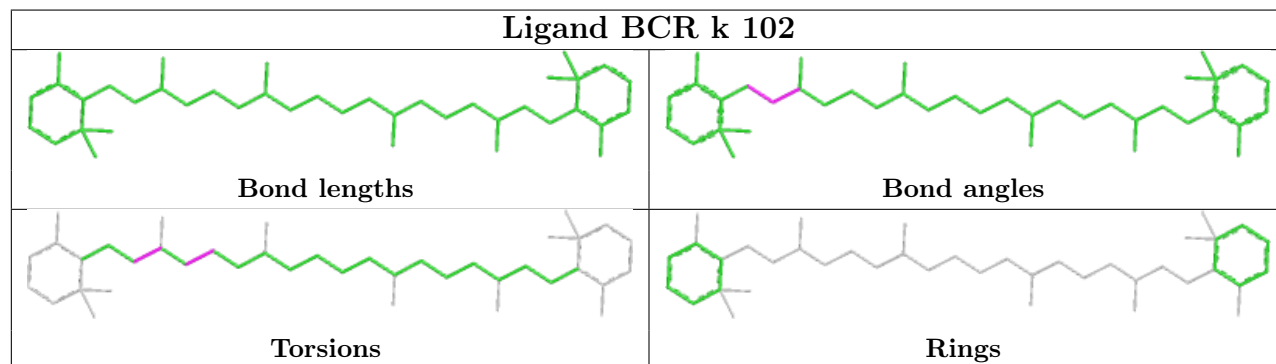
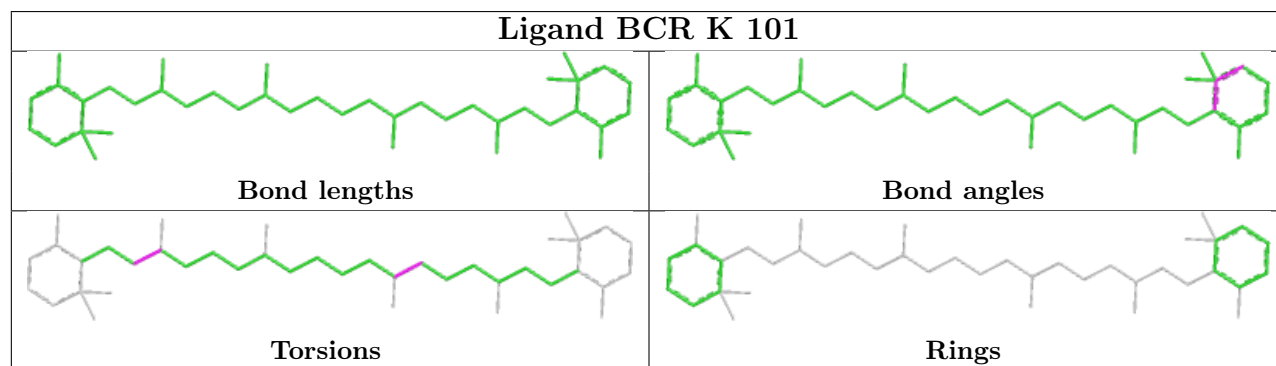
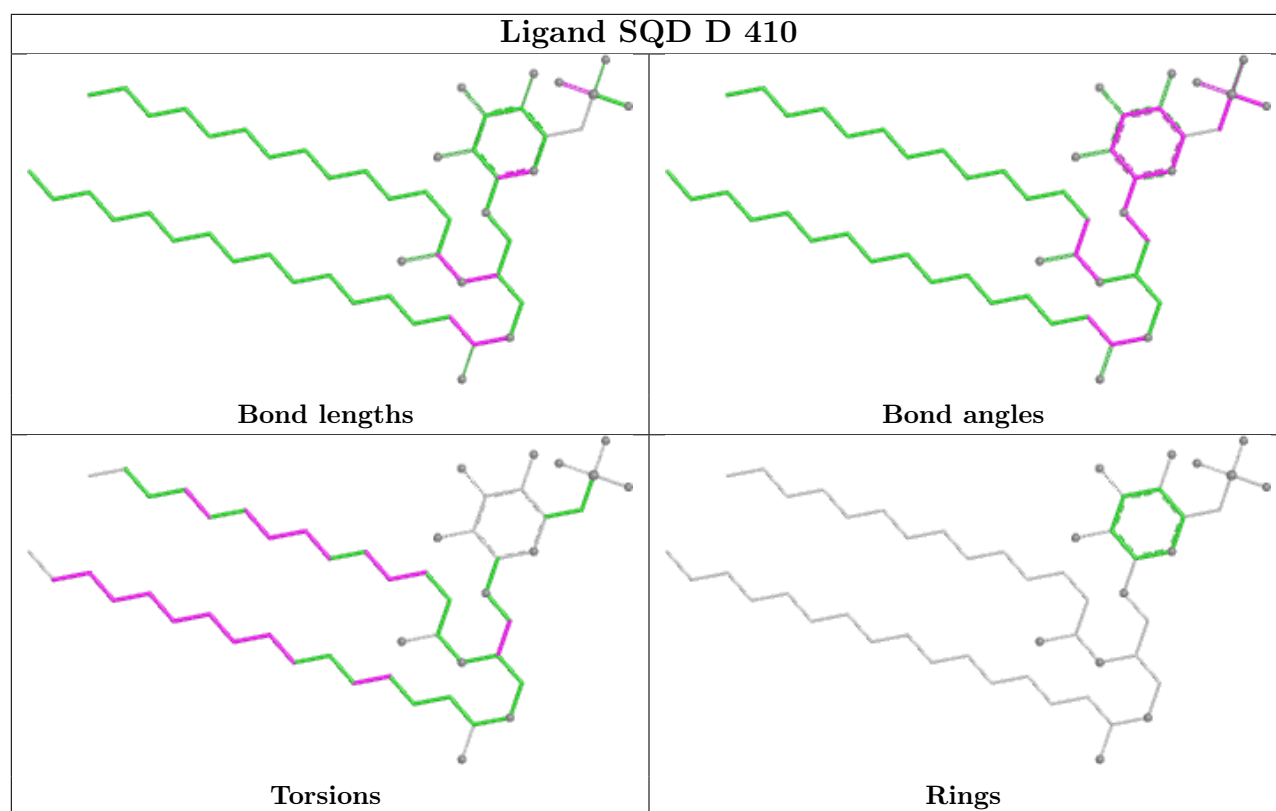


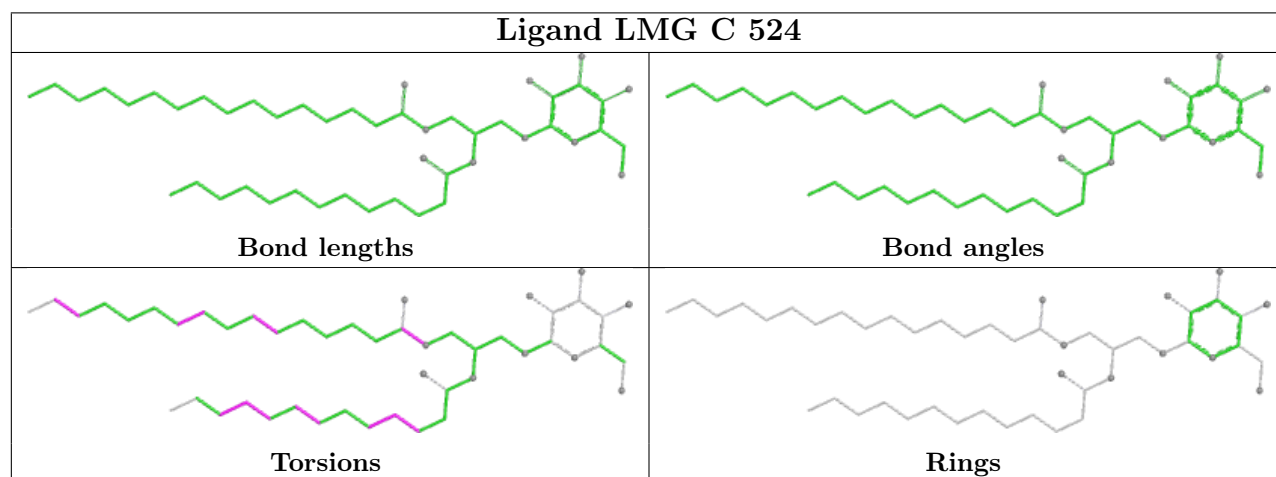
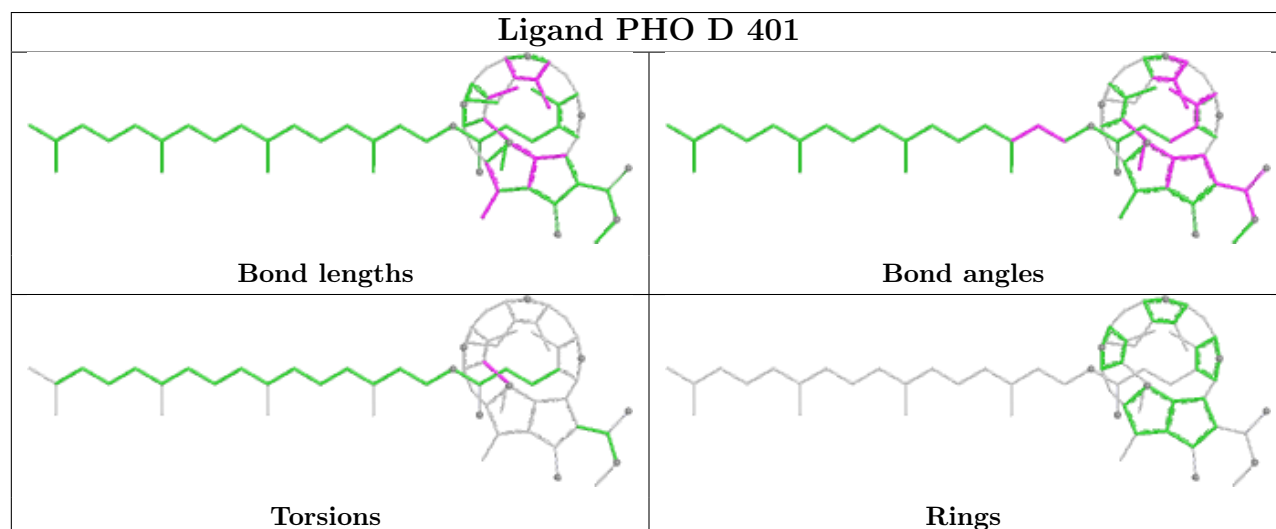
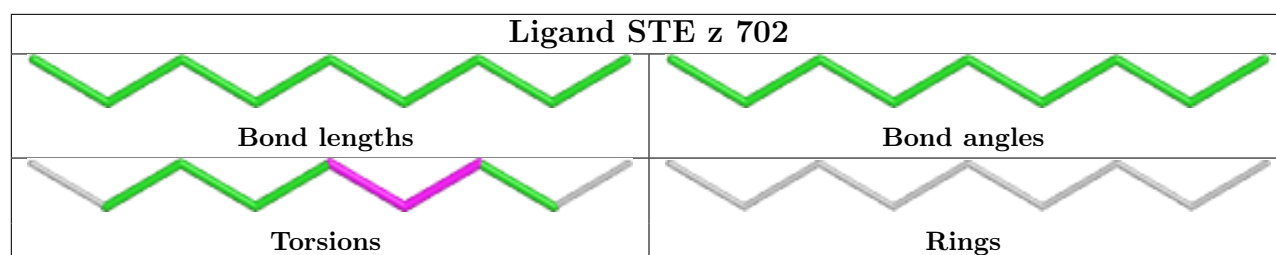
Ligand BCR c 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

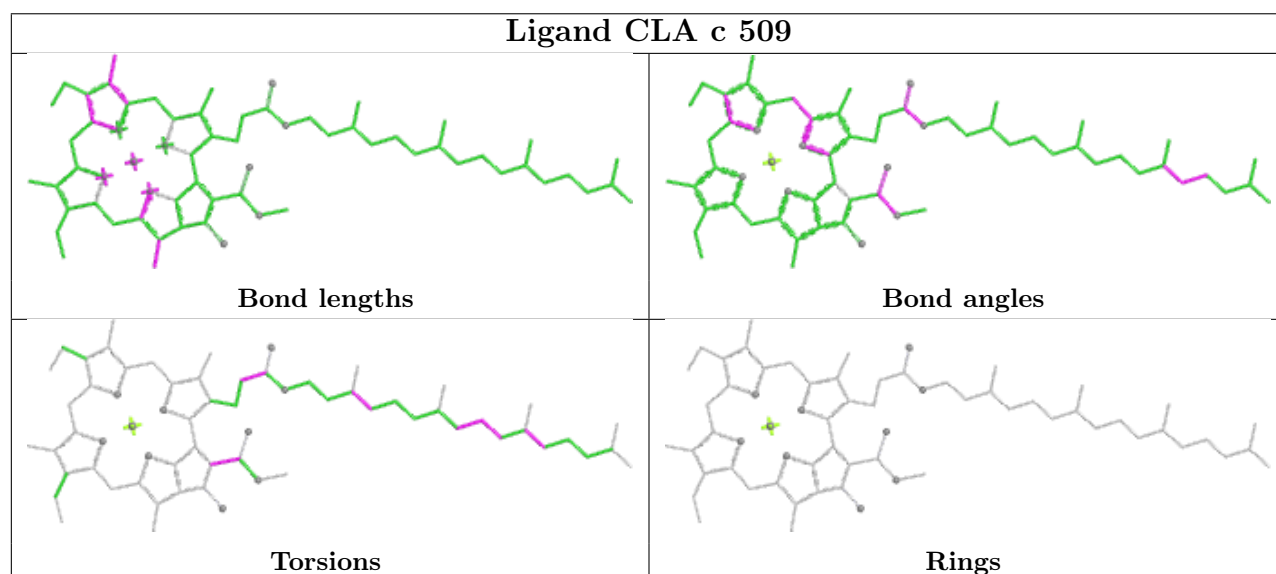
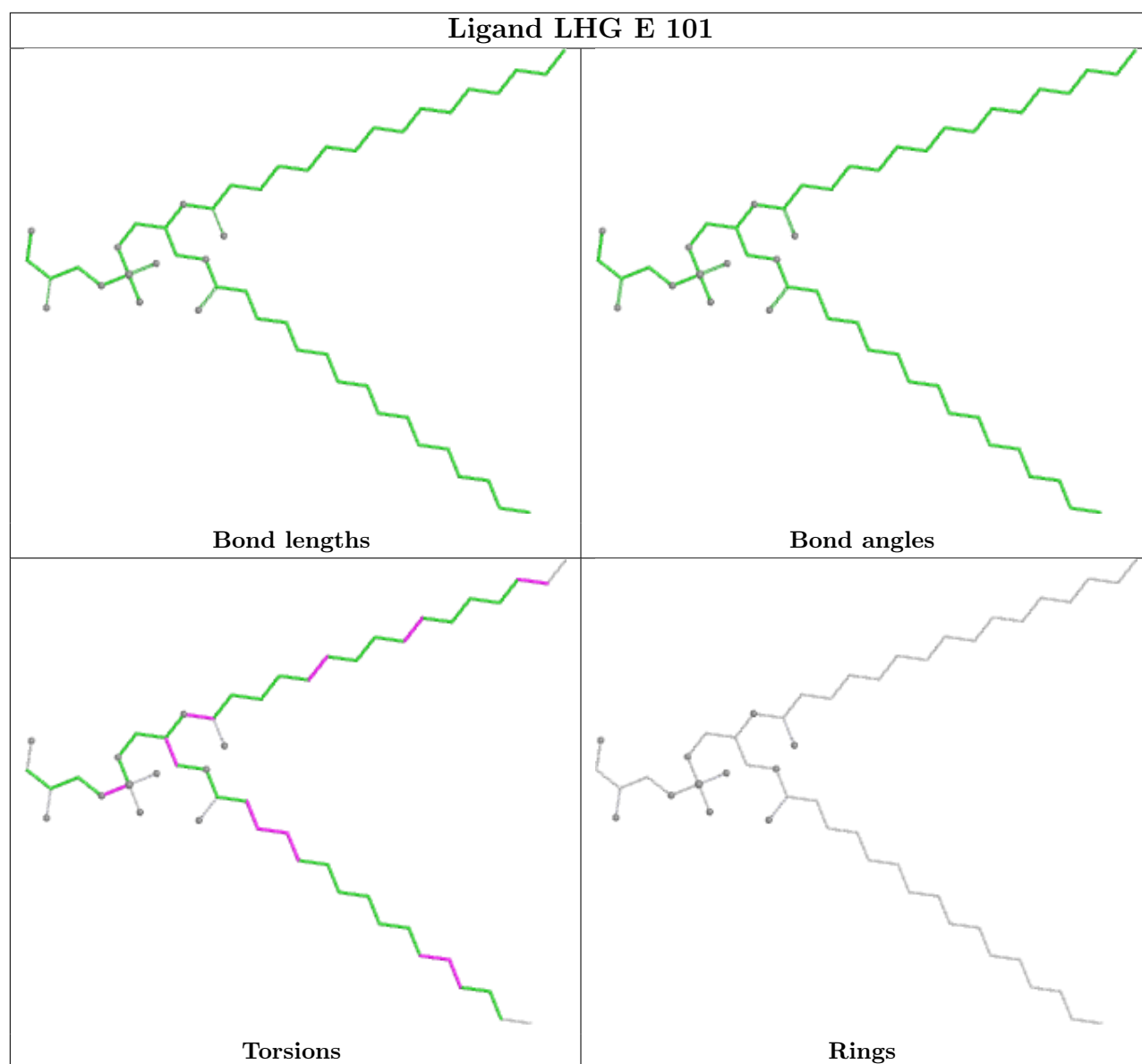
Ligand PL9 D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

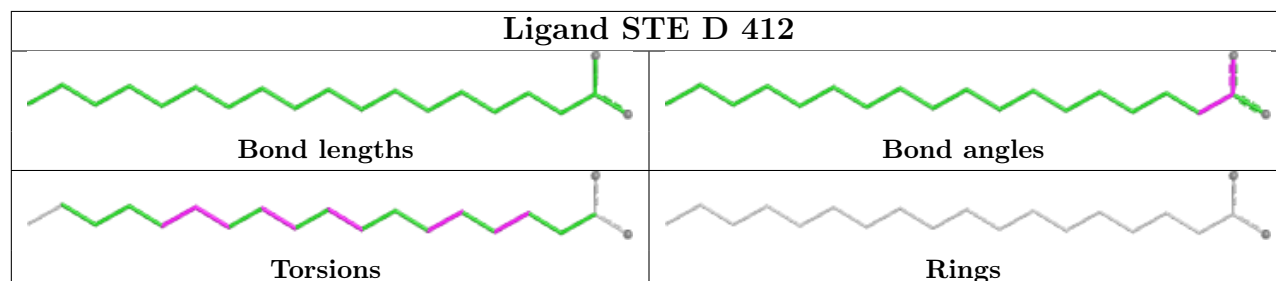
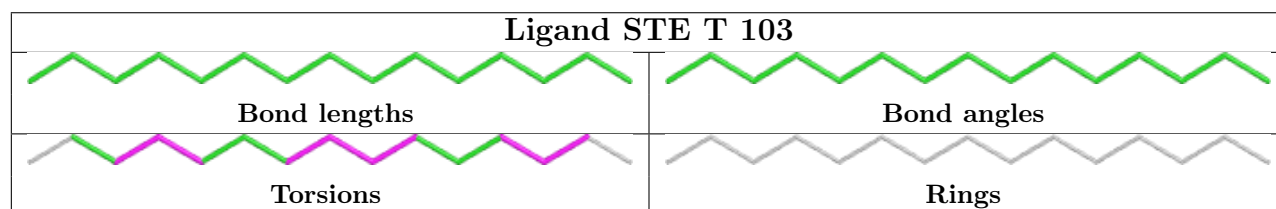
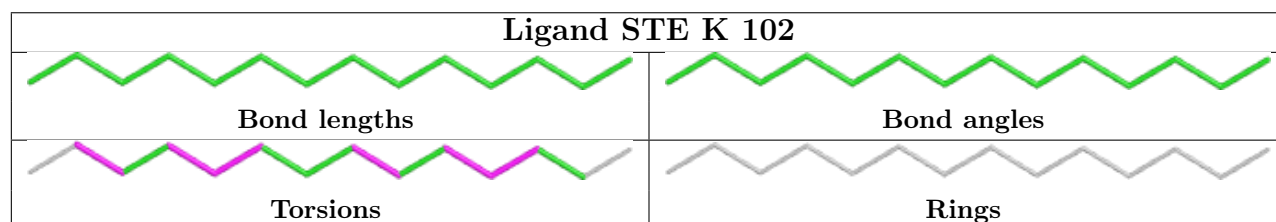
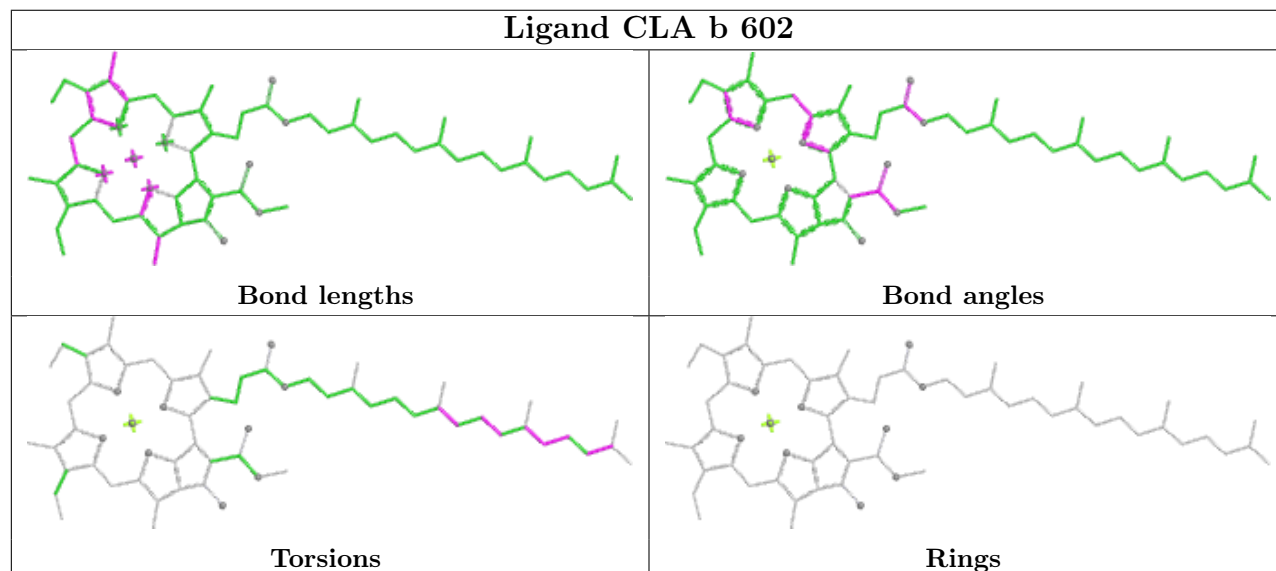
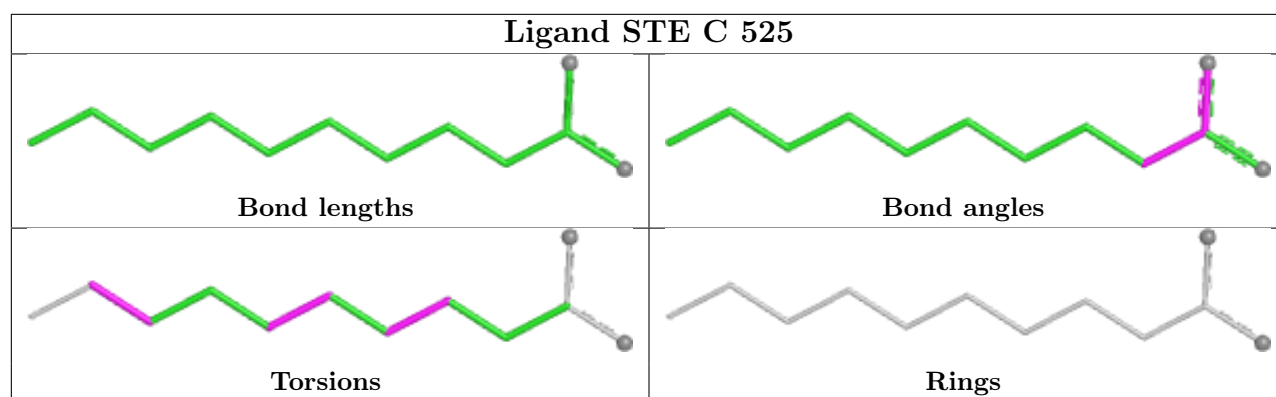
Ligand CLA B 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

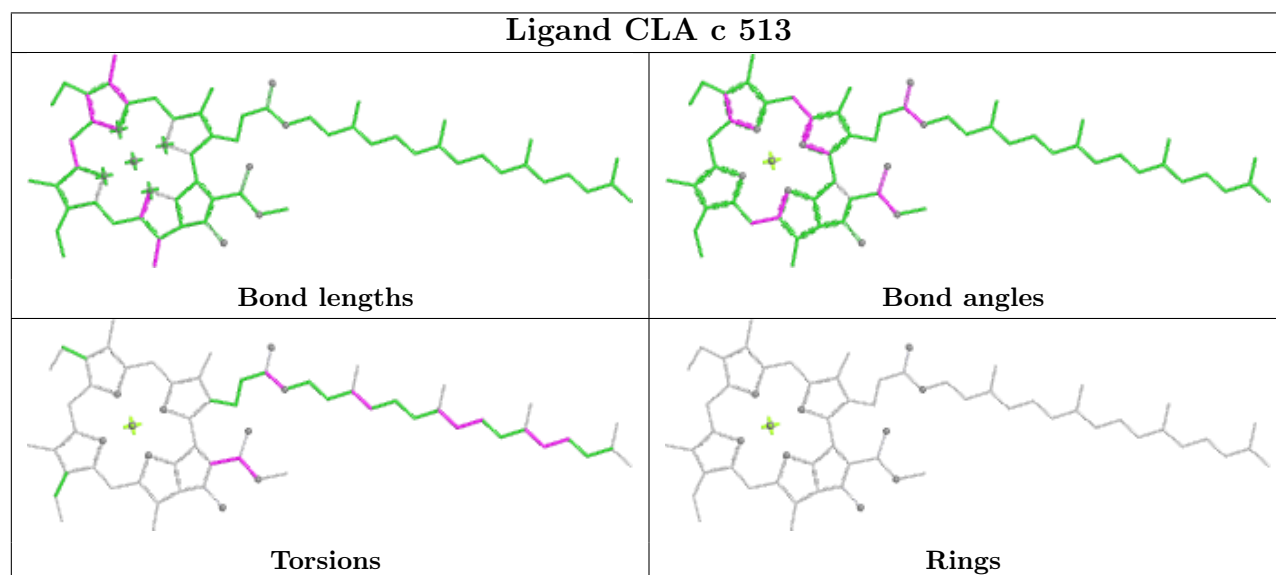
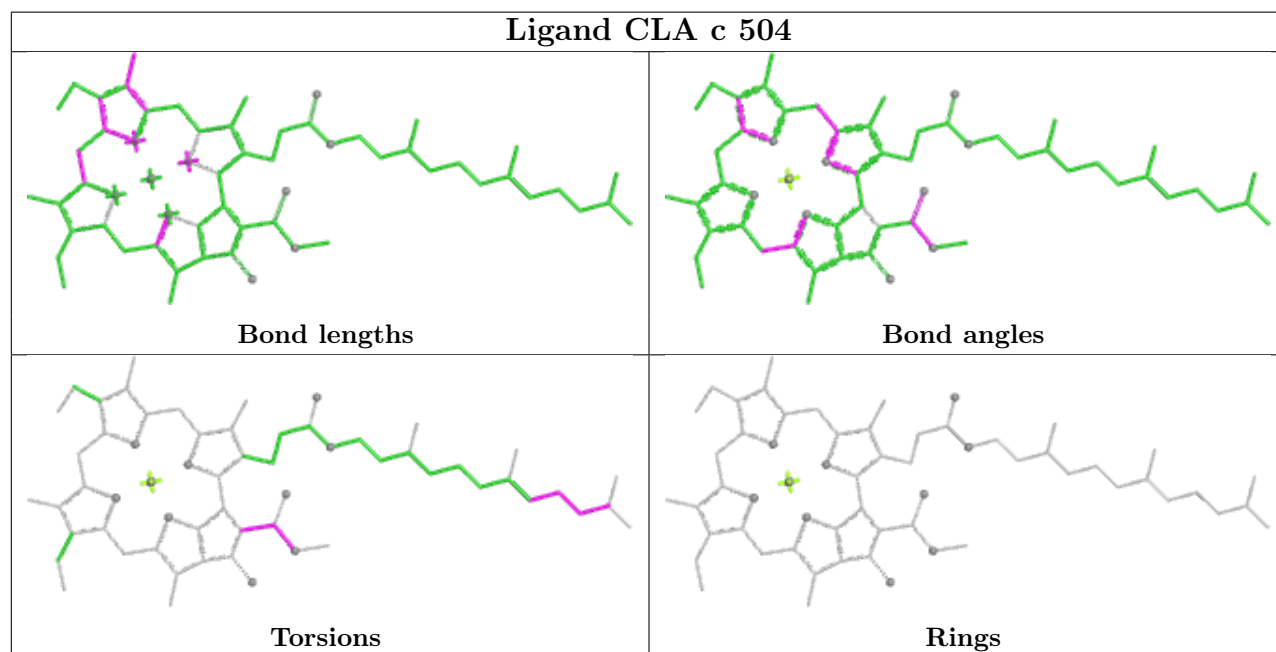
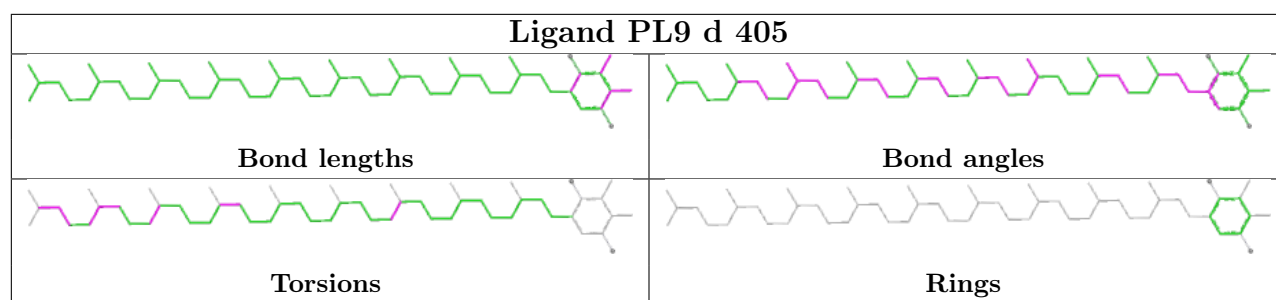


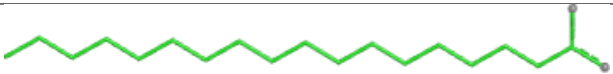
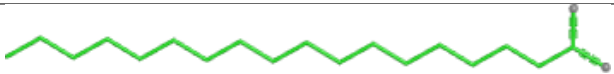


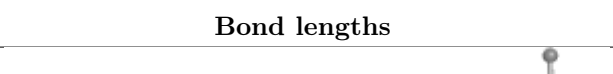
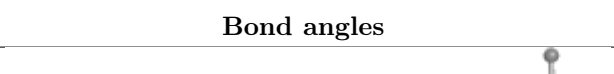


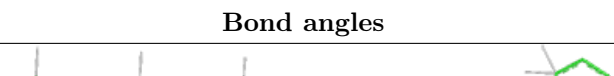




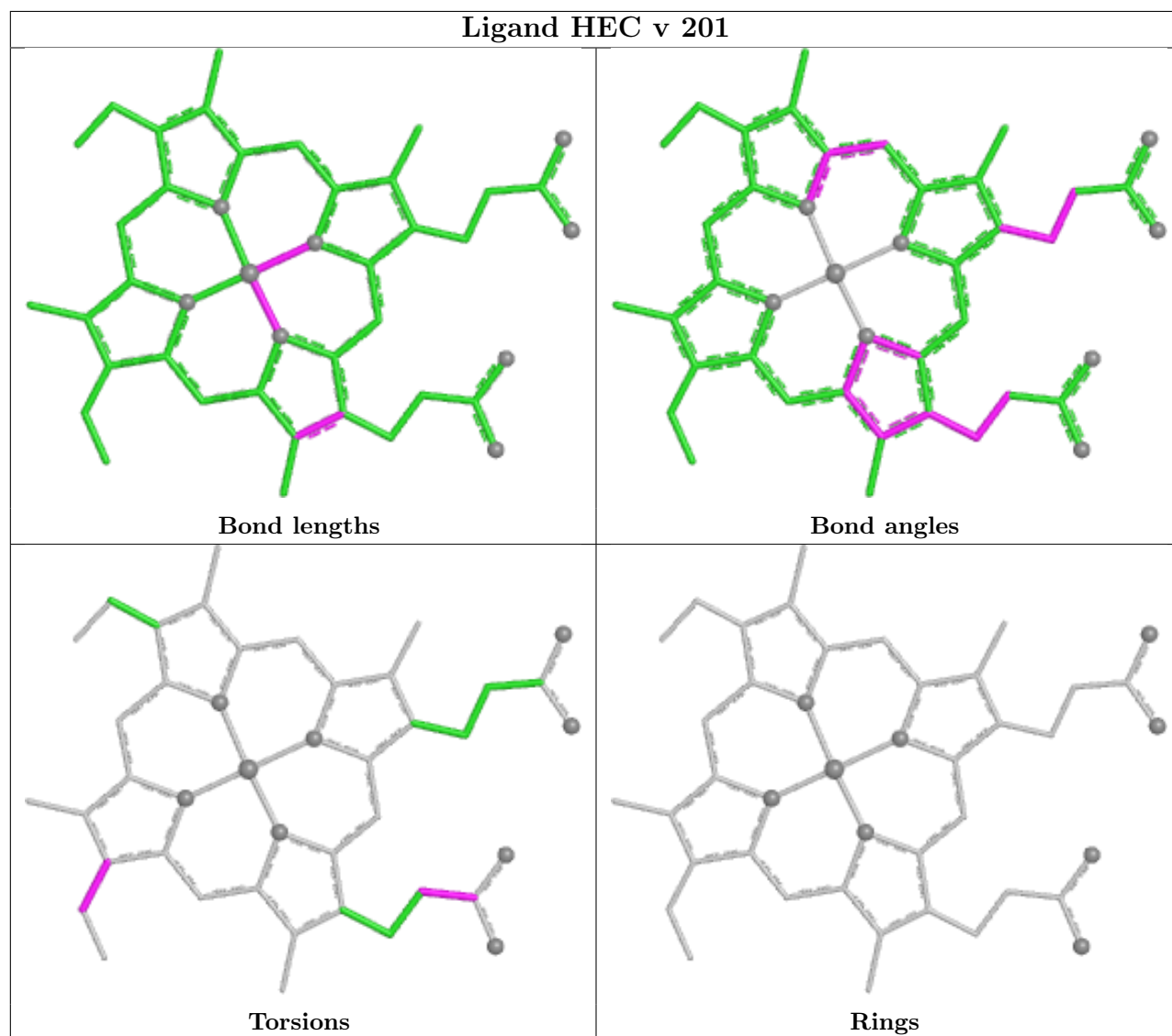
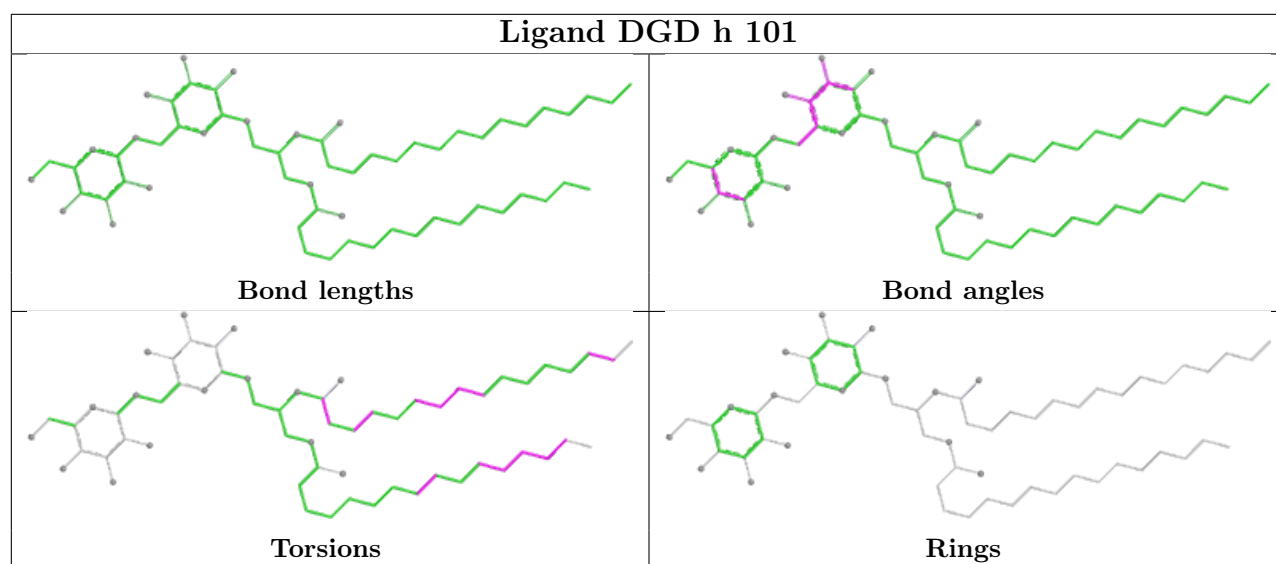


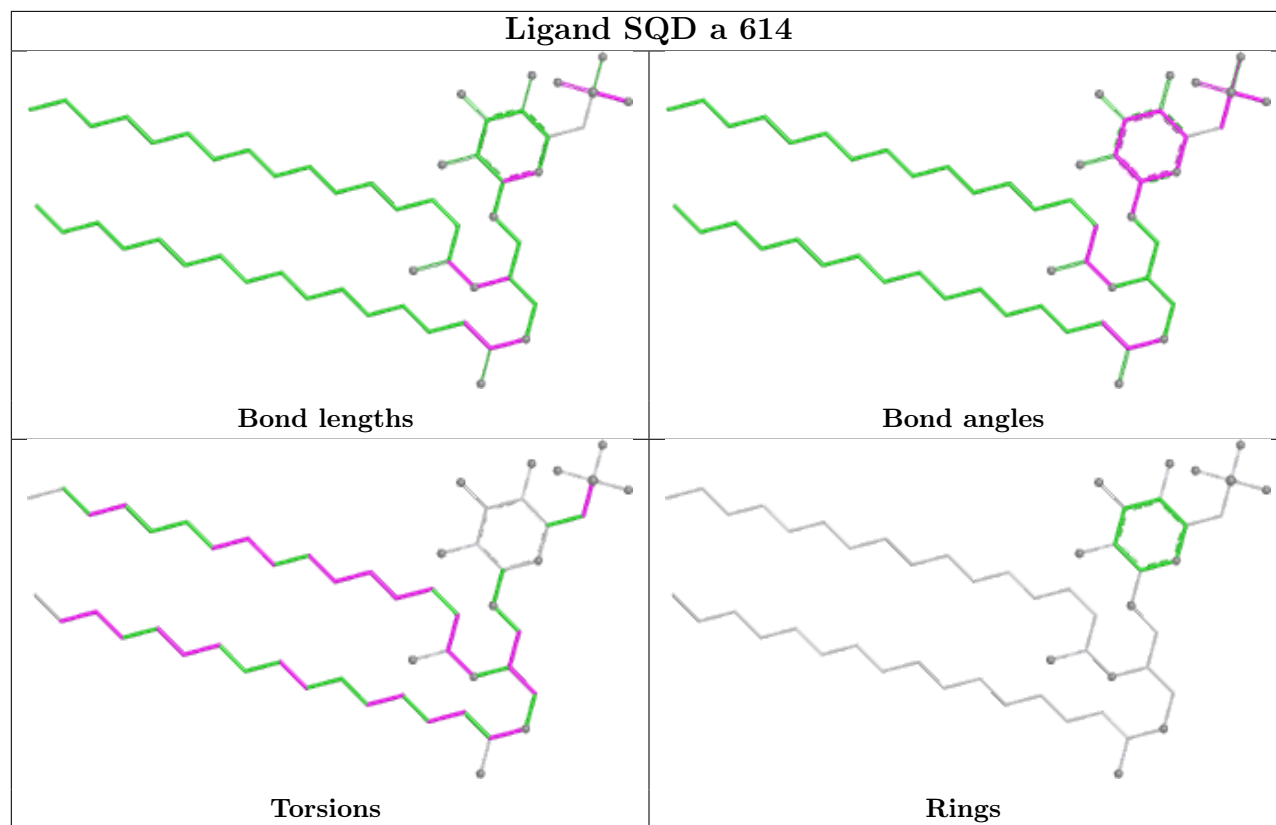
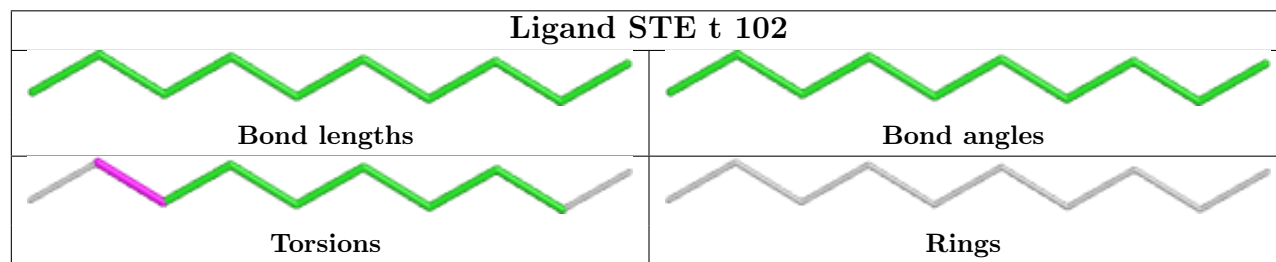
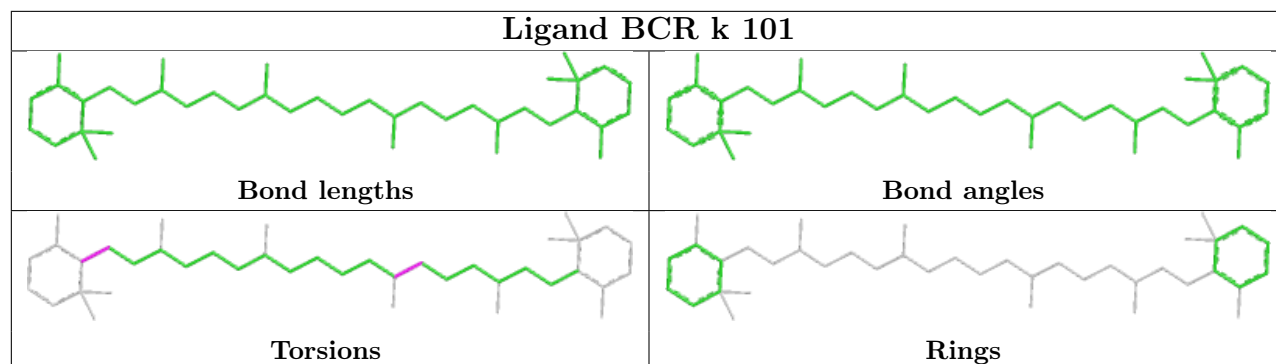
Ligand STE b 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE e 105	
 Bond lengths	 Bond angles
 Torsions	 Rings

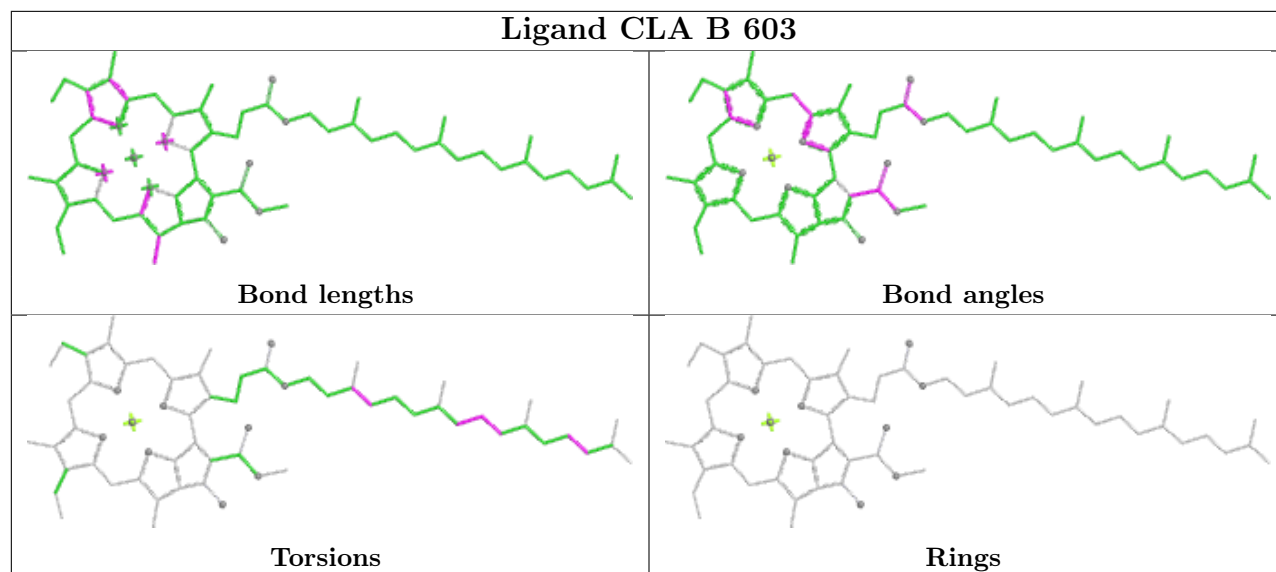
Ligand BCR B 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE a 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

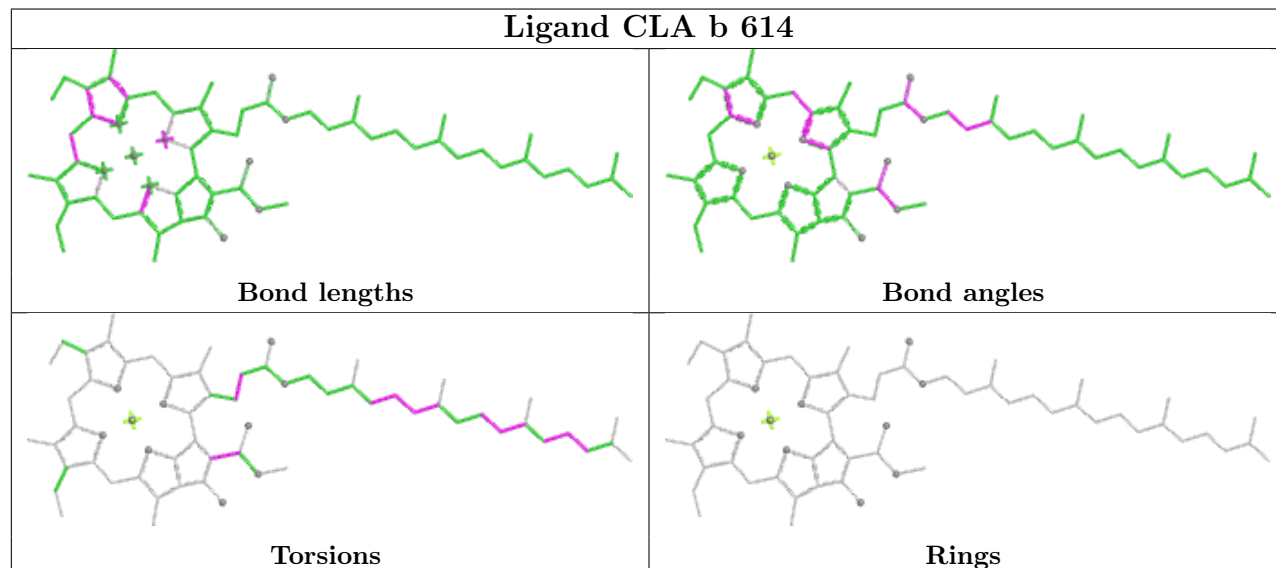




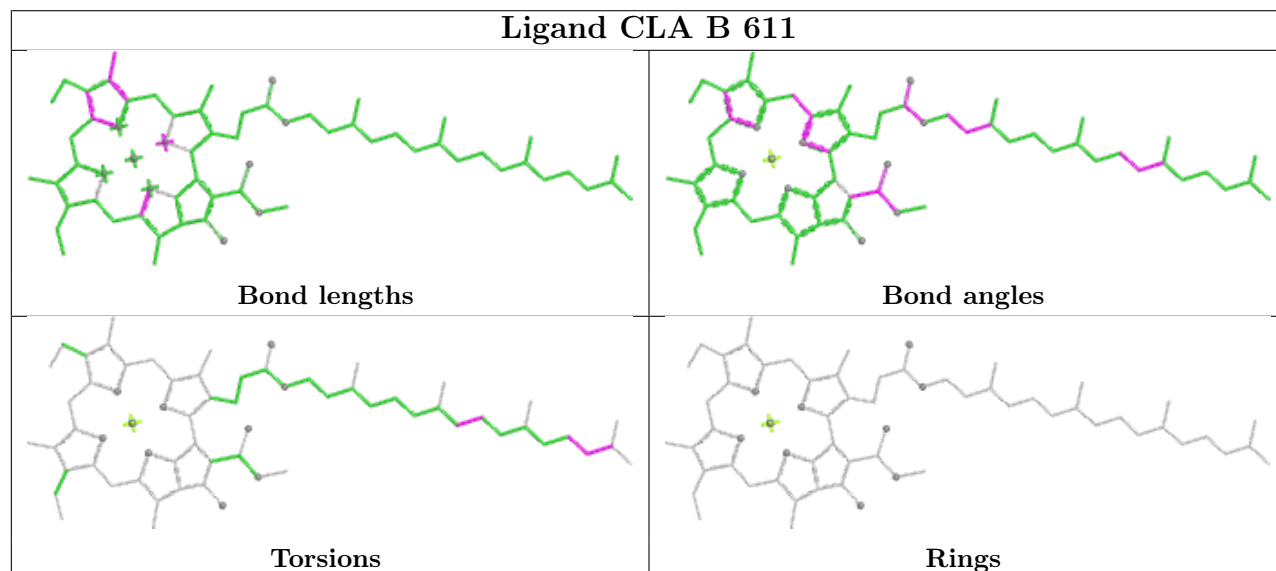
Ligand CLA B 603

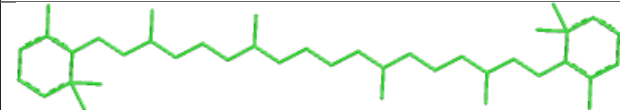
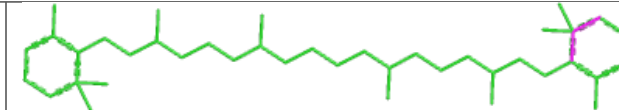
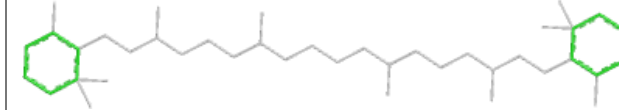


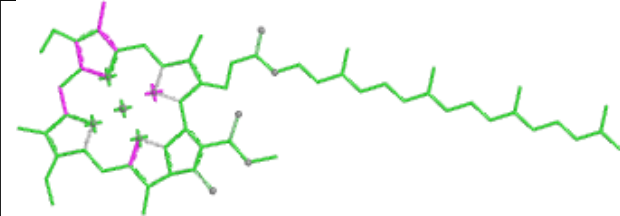
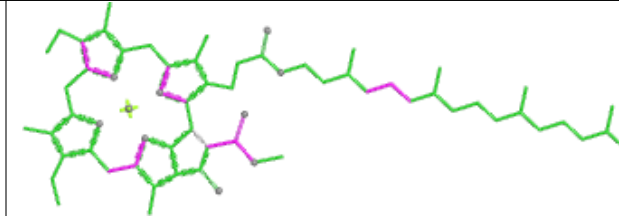
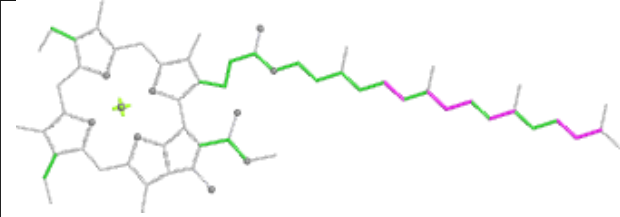
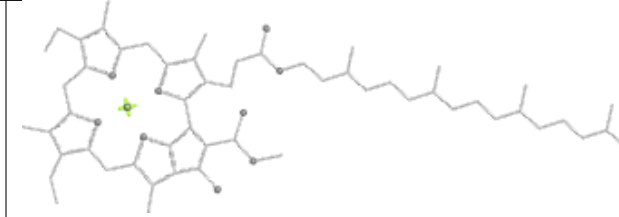
Ligand CLA b 614

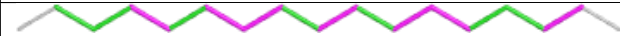


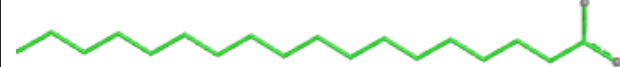
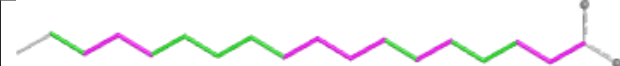
Ligand CLA B 611

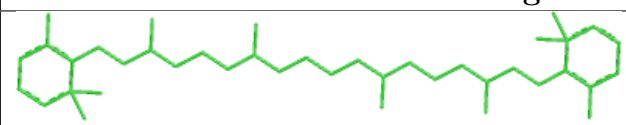
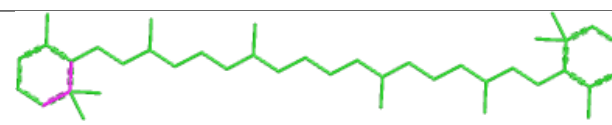
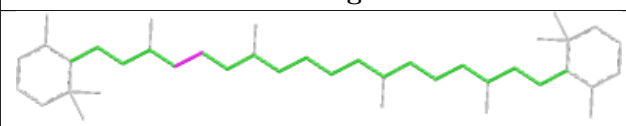
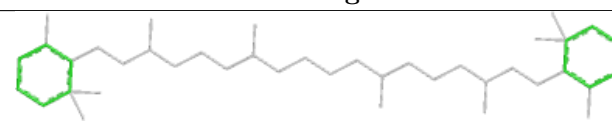


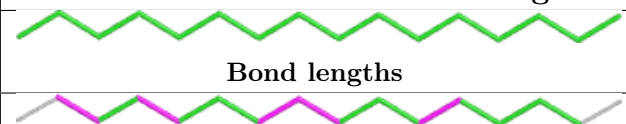
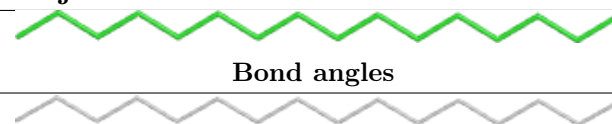
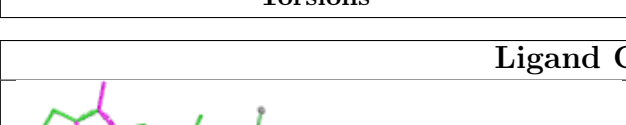
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

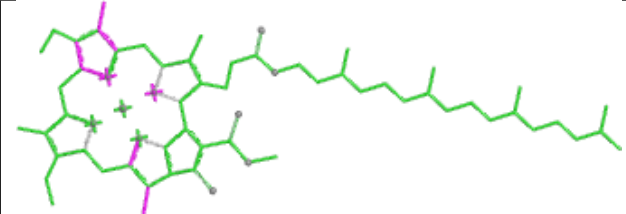
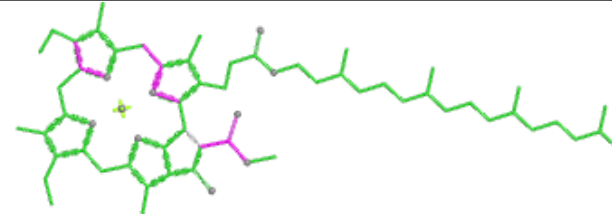
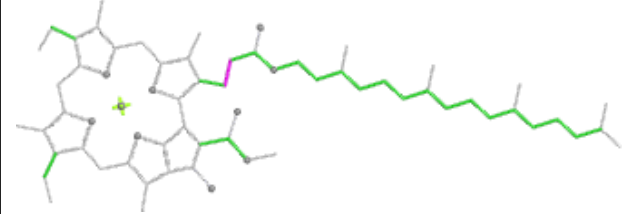
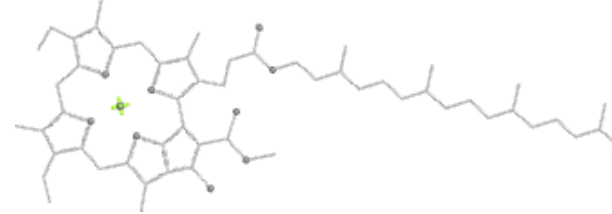
Ligand CLA c 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

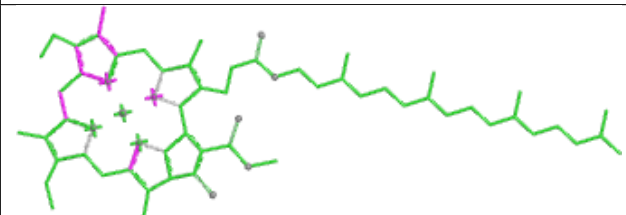
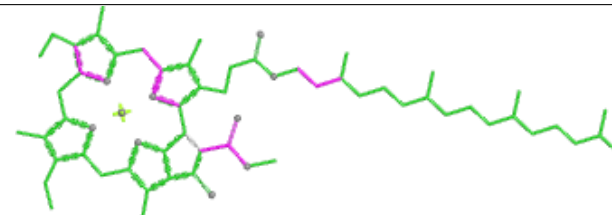
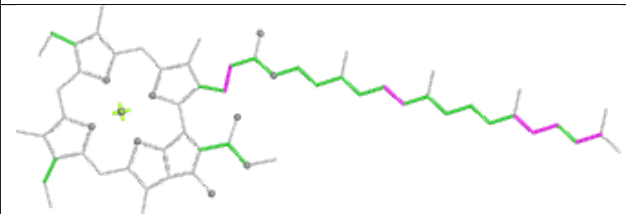
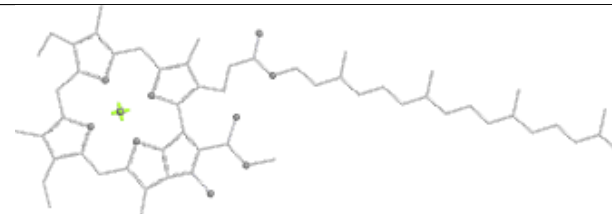
Ligand STE Z 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE d 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

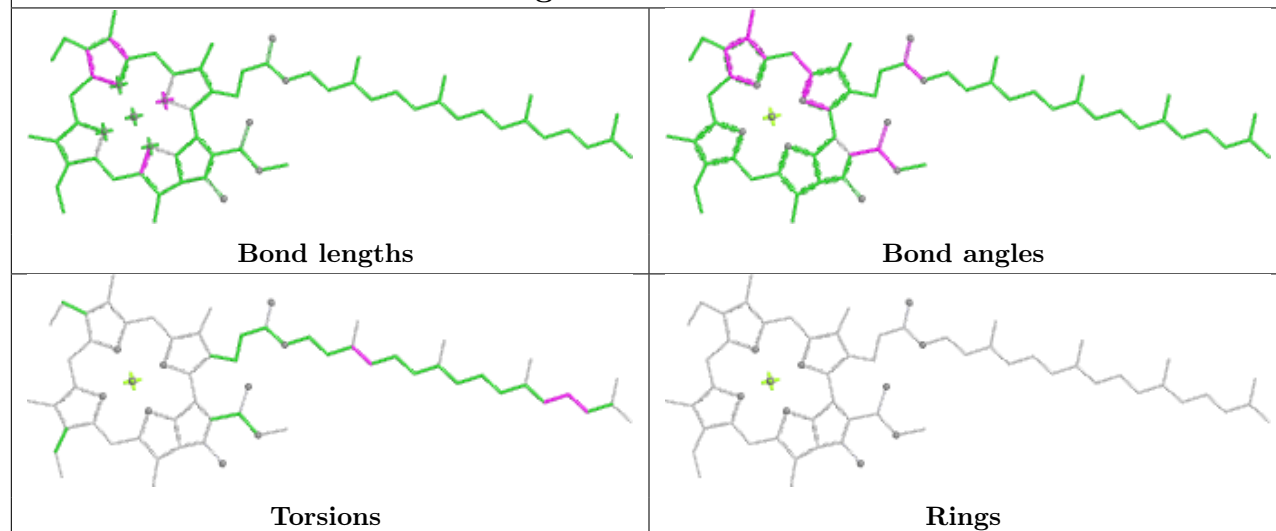
Ligand BCR x 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE j 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

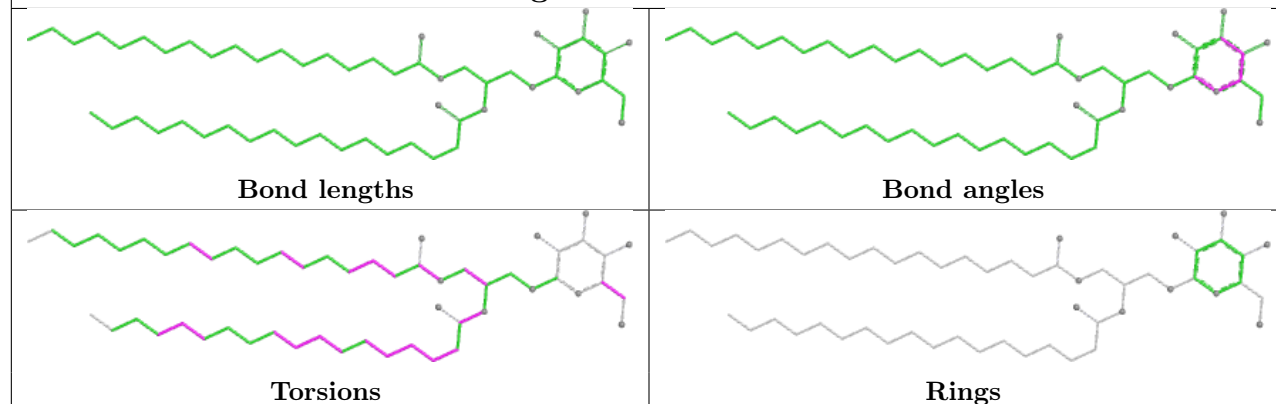
Ligand CLA c 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

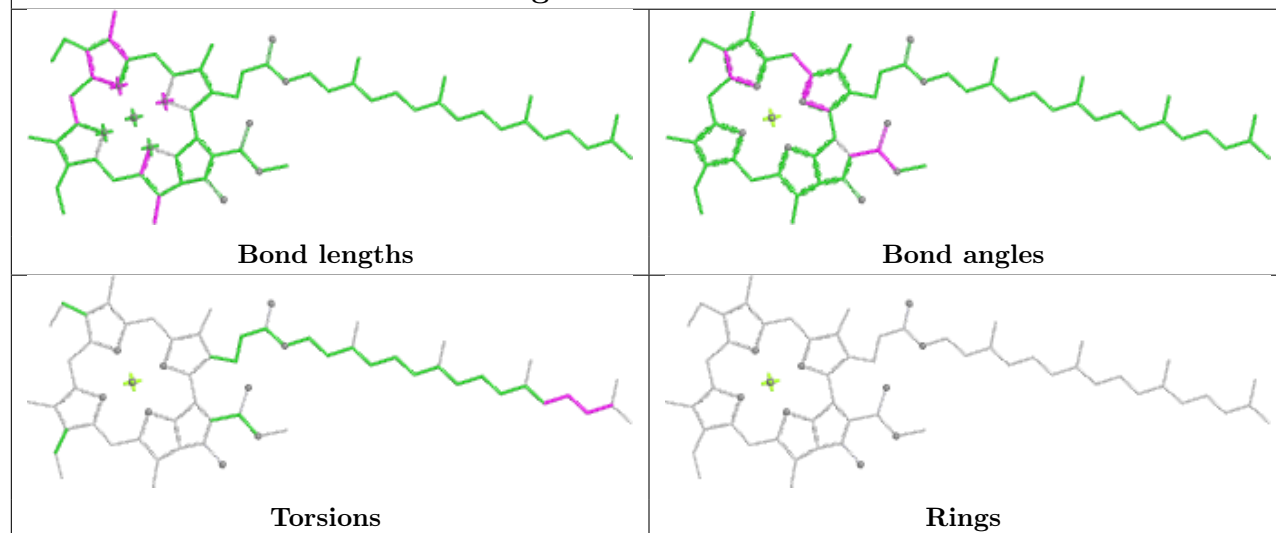
Ligand CLA b 609

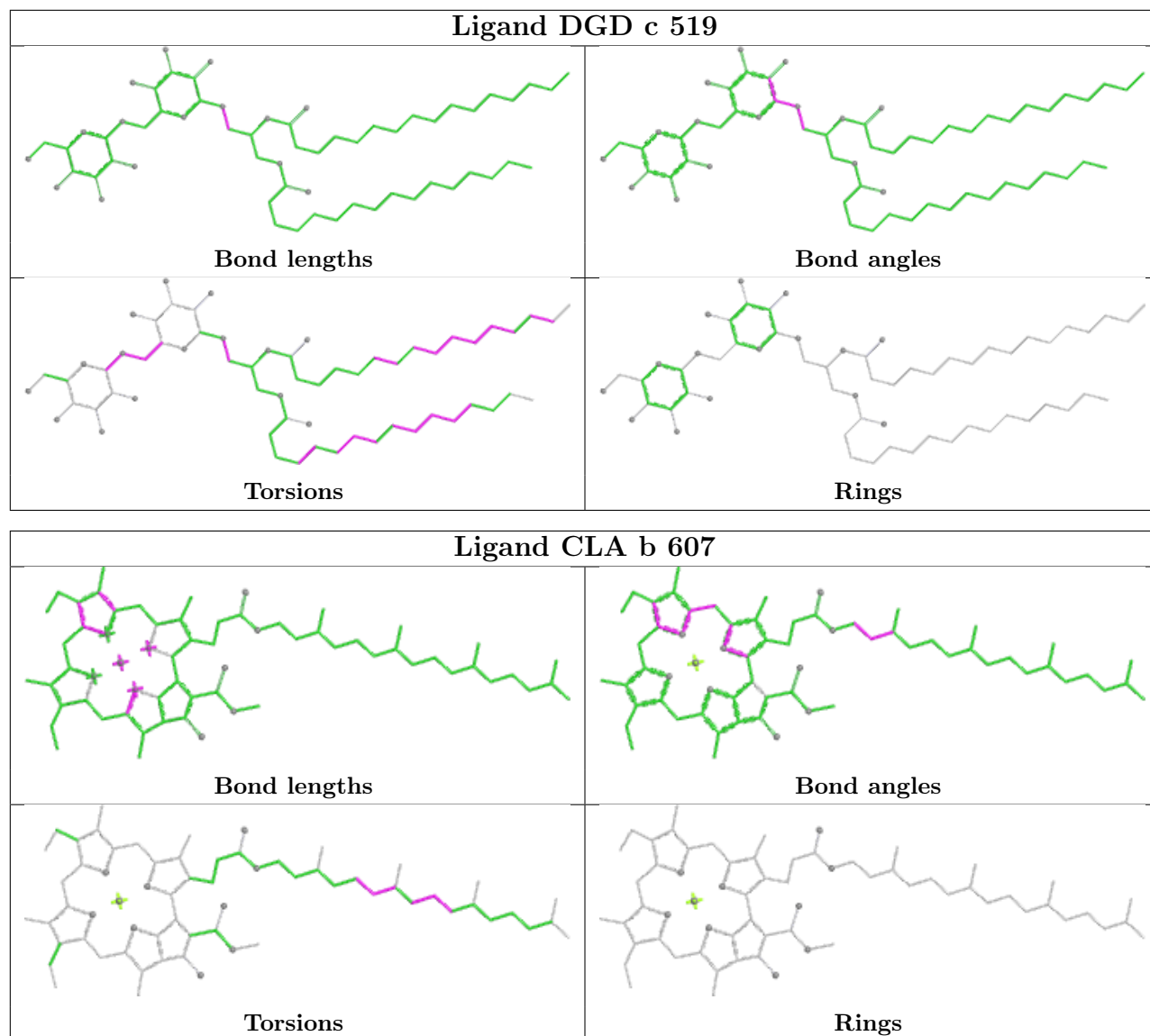


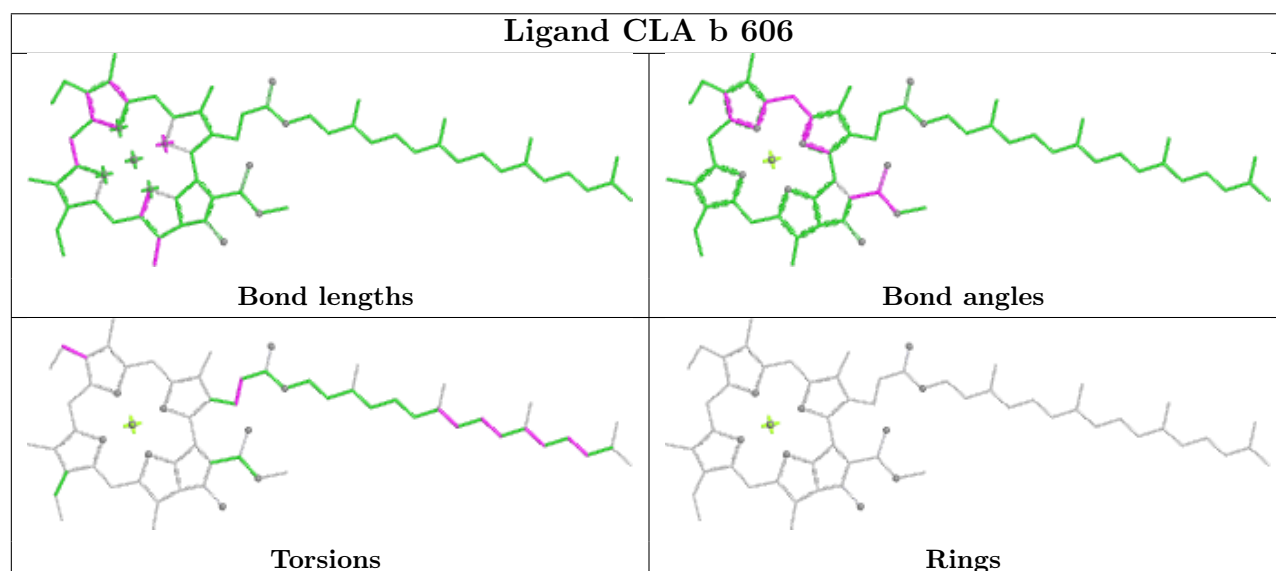
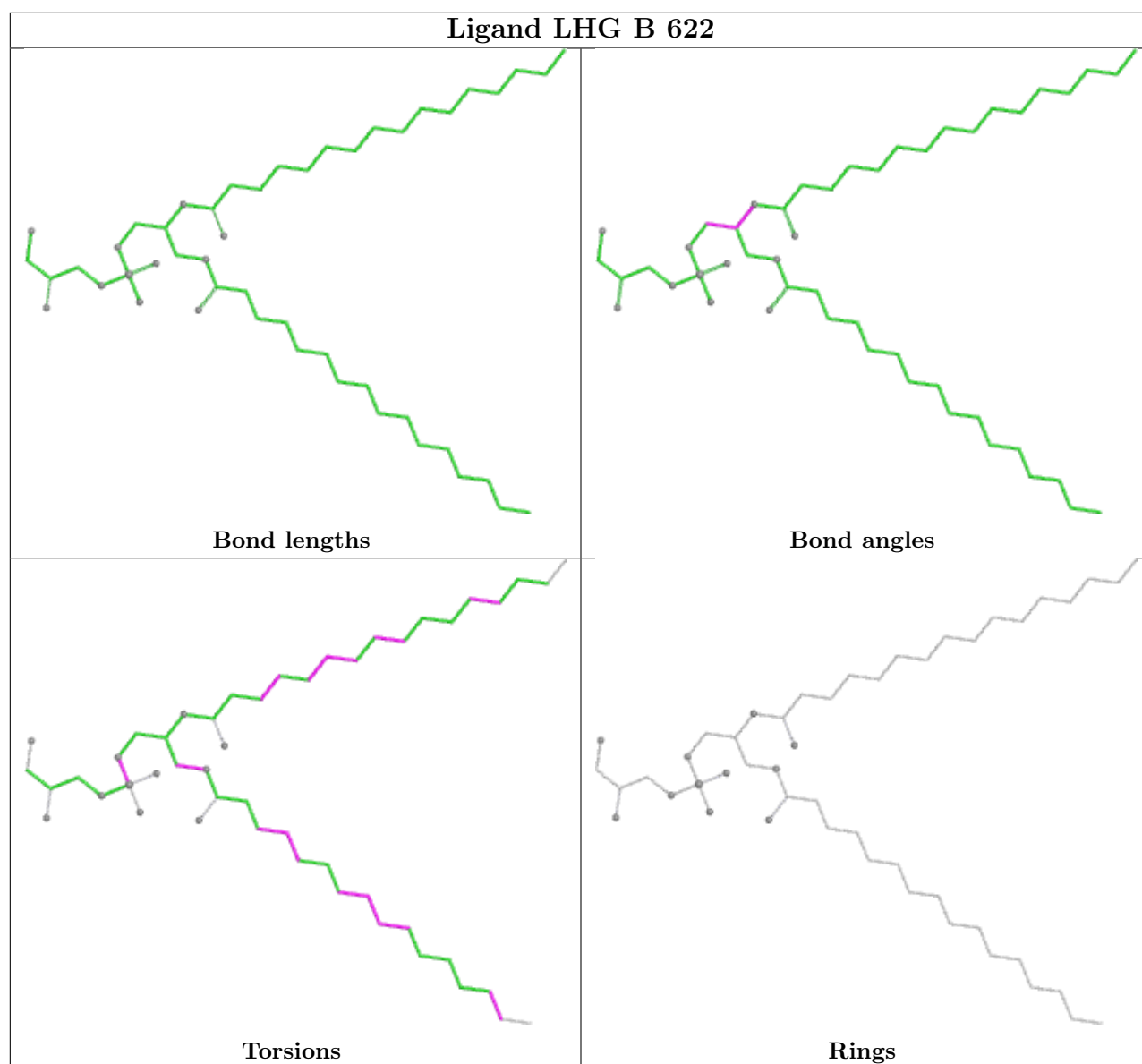
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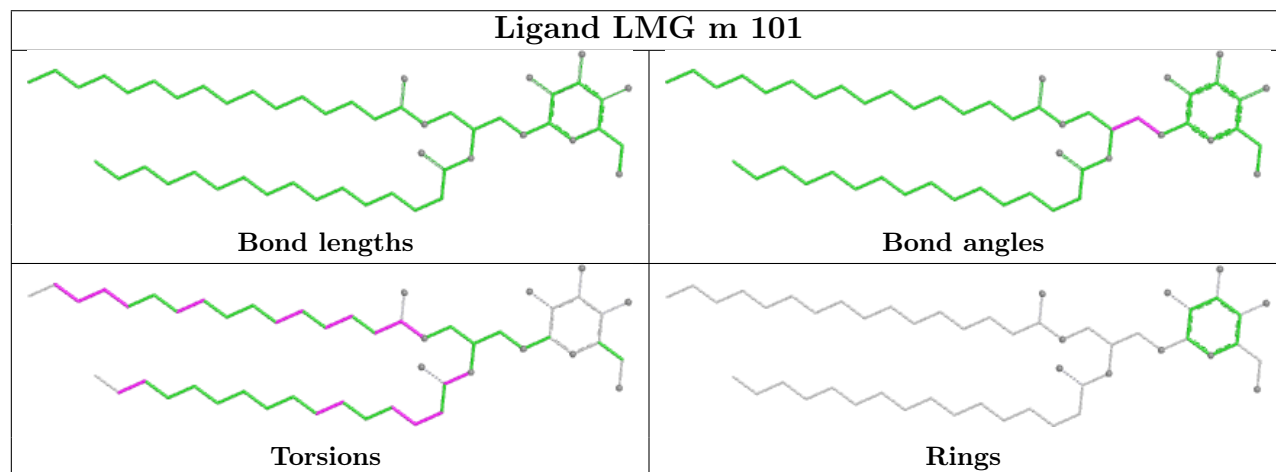
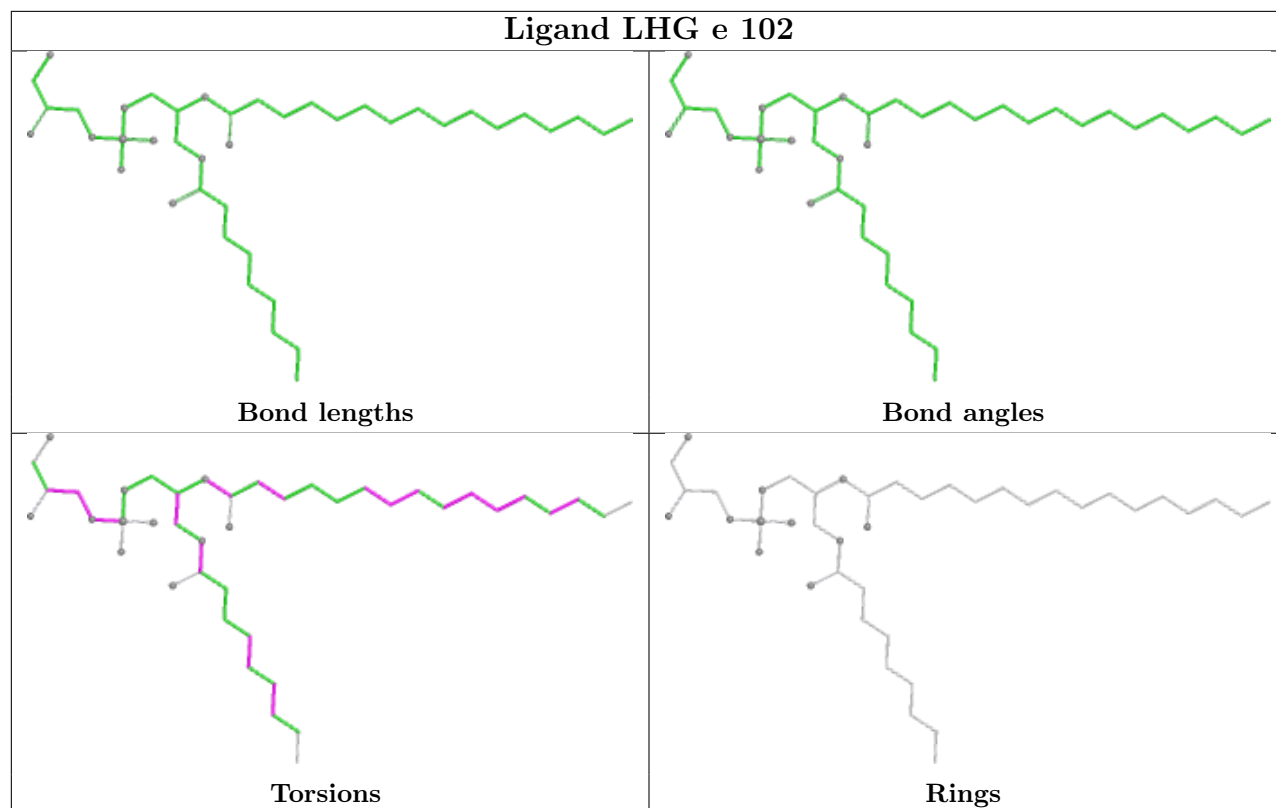


Ligand CLA A 614

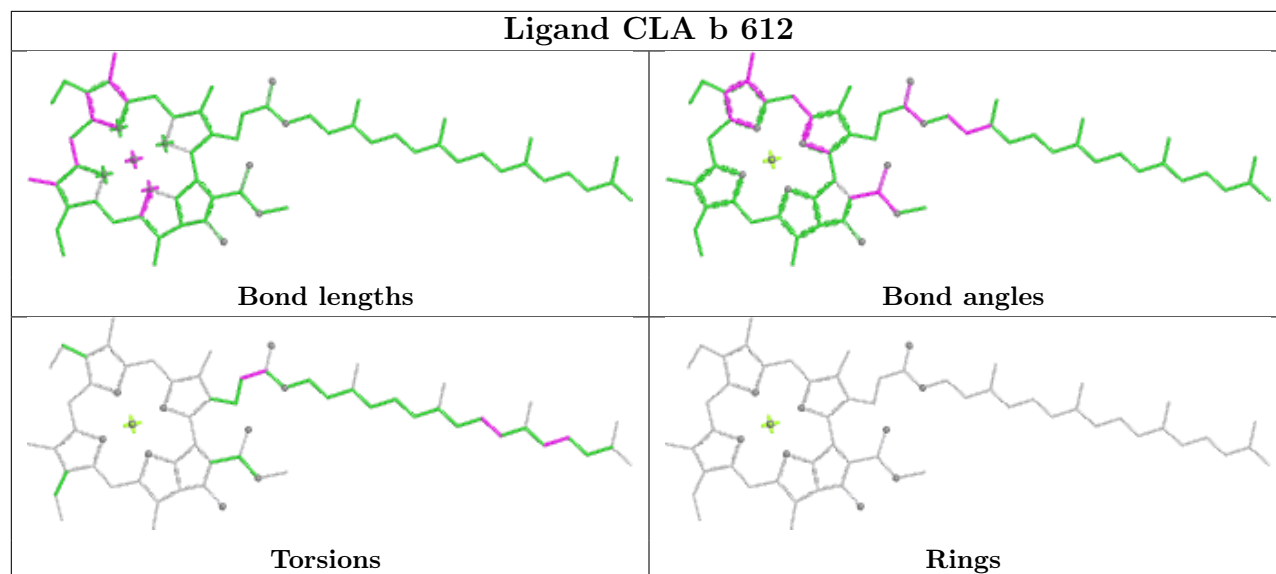




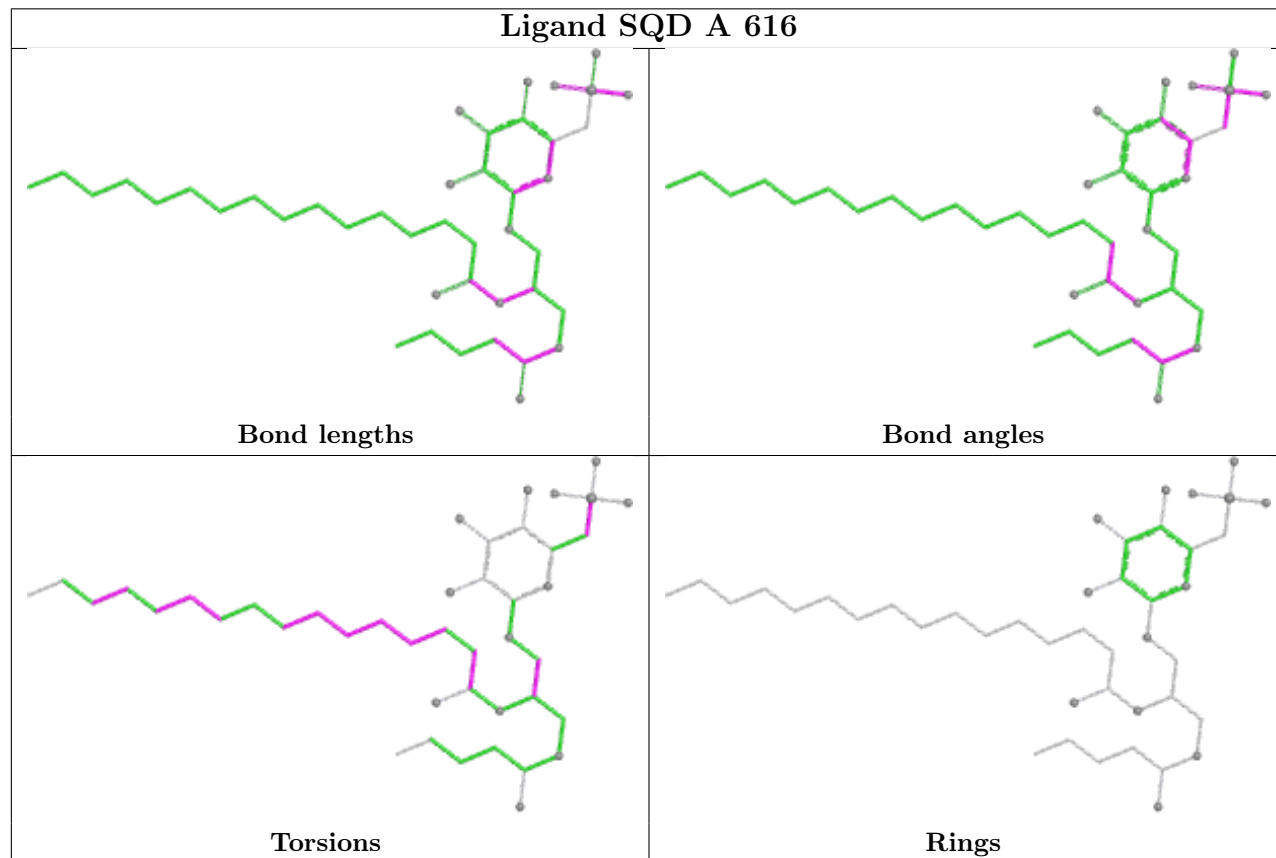


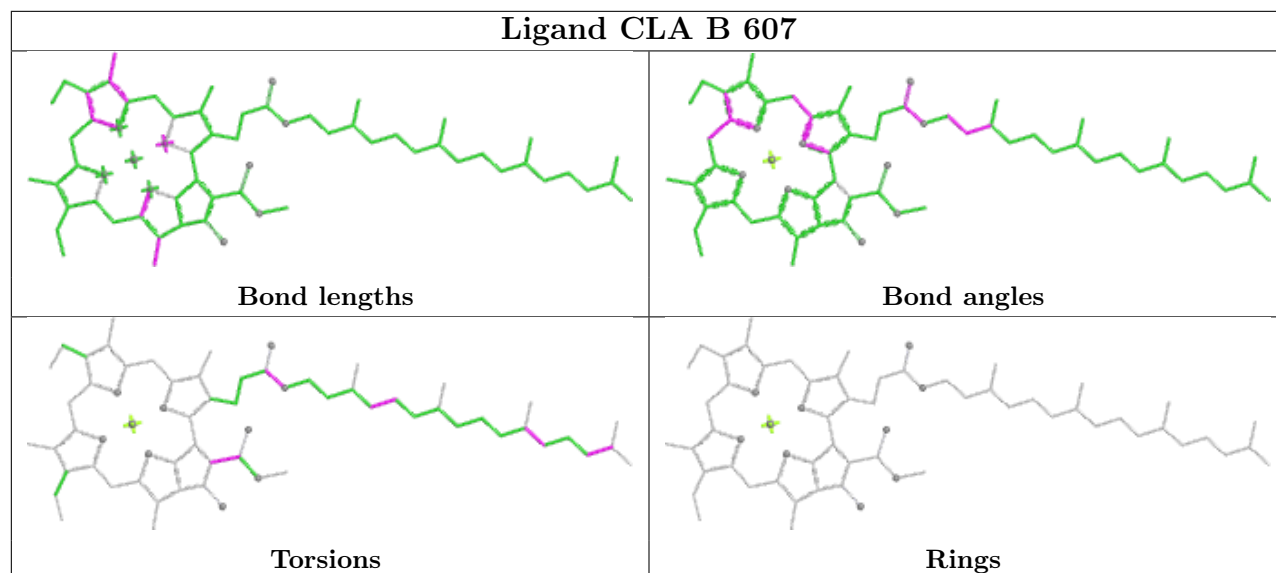
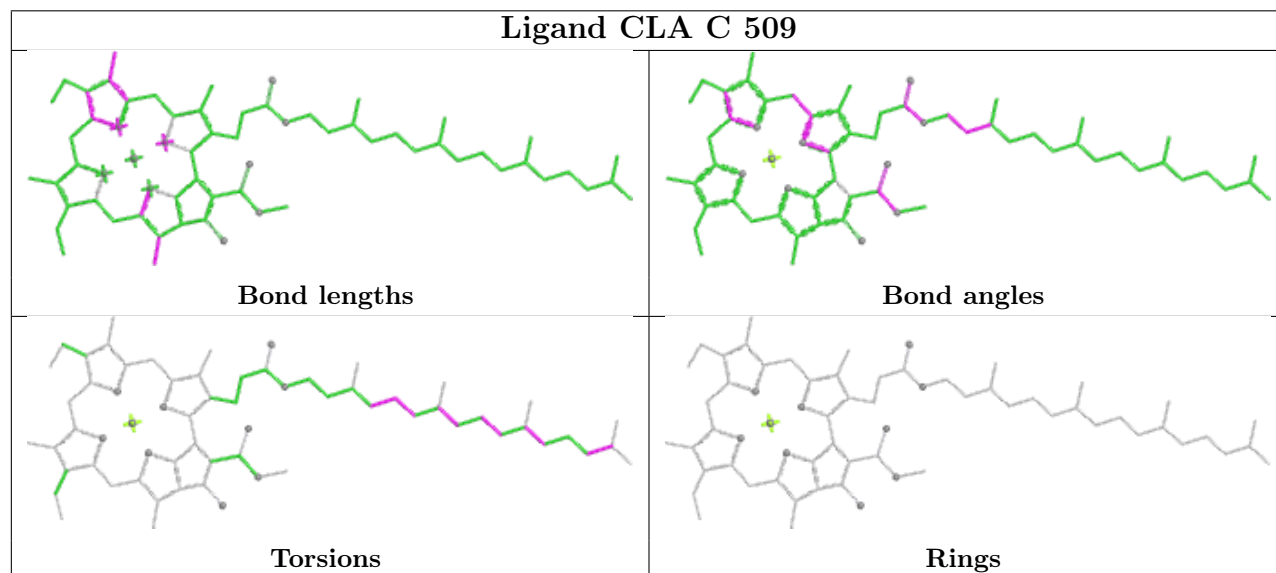
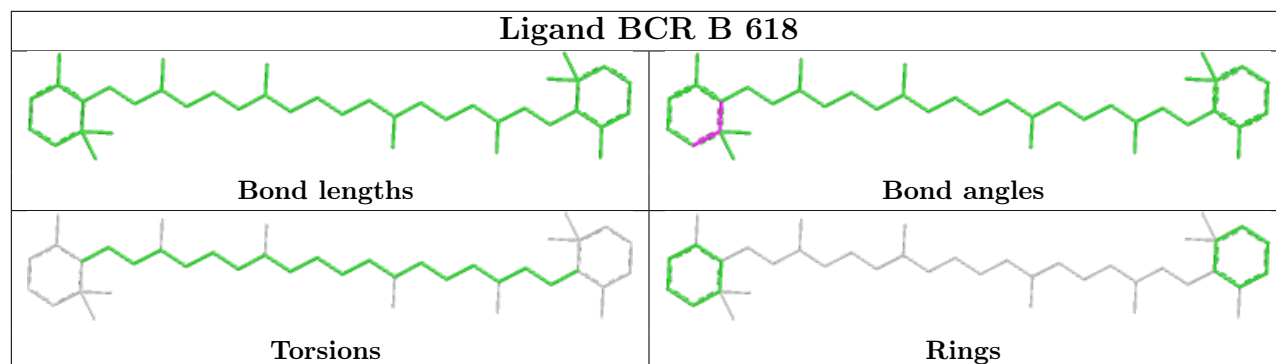


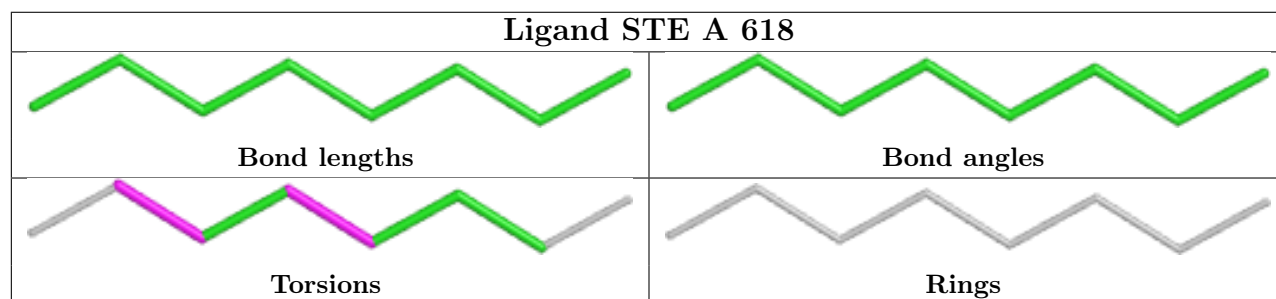
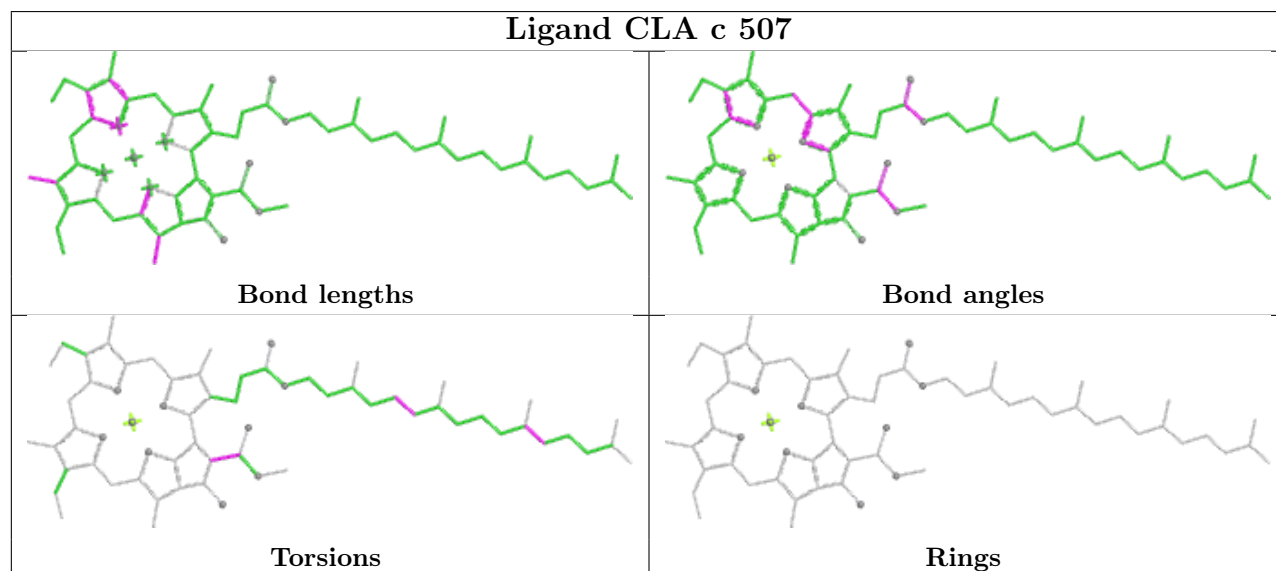
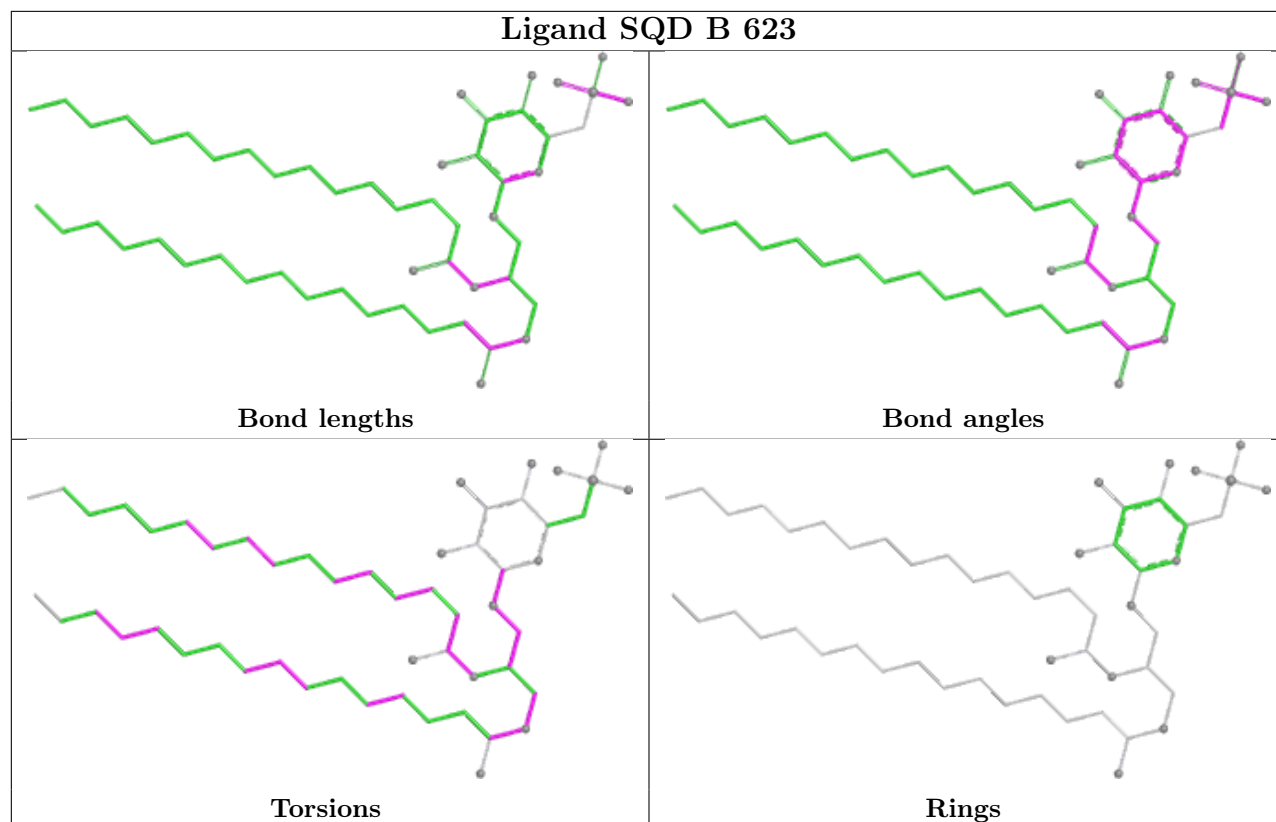
Ligand CLA b 612



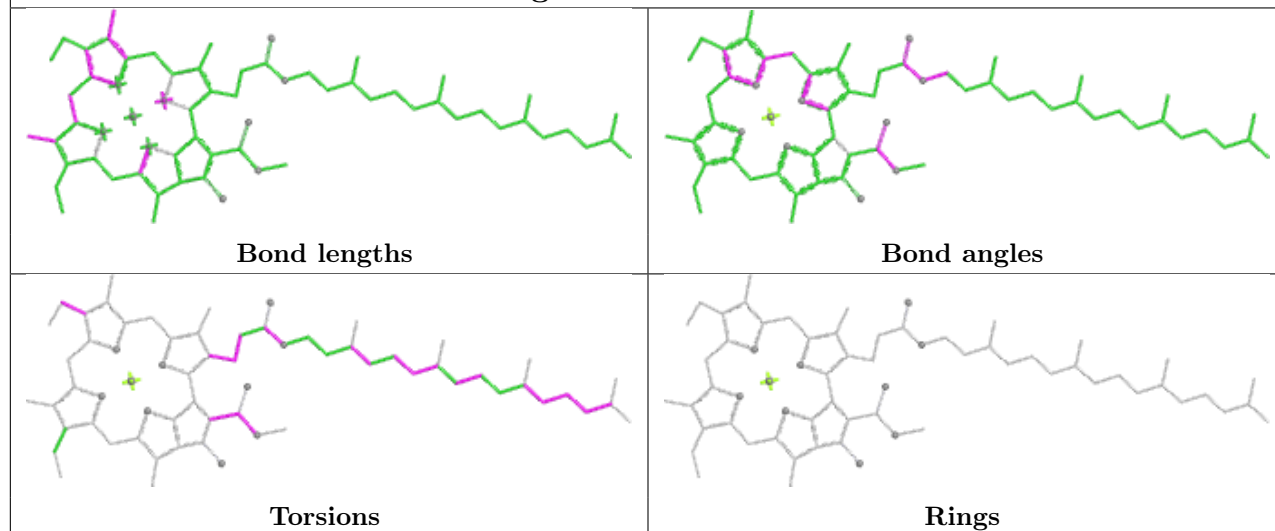
Ligand SQD A 616



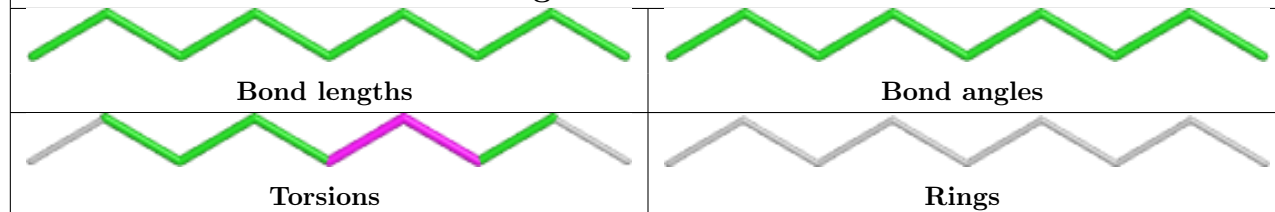




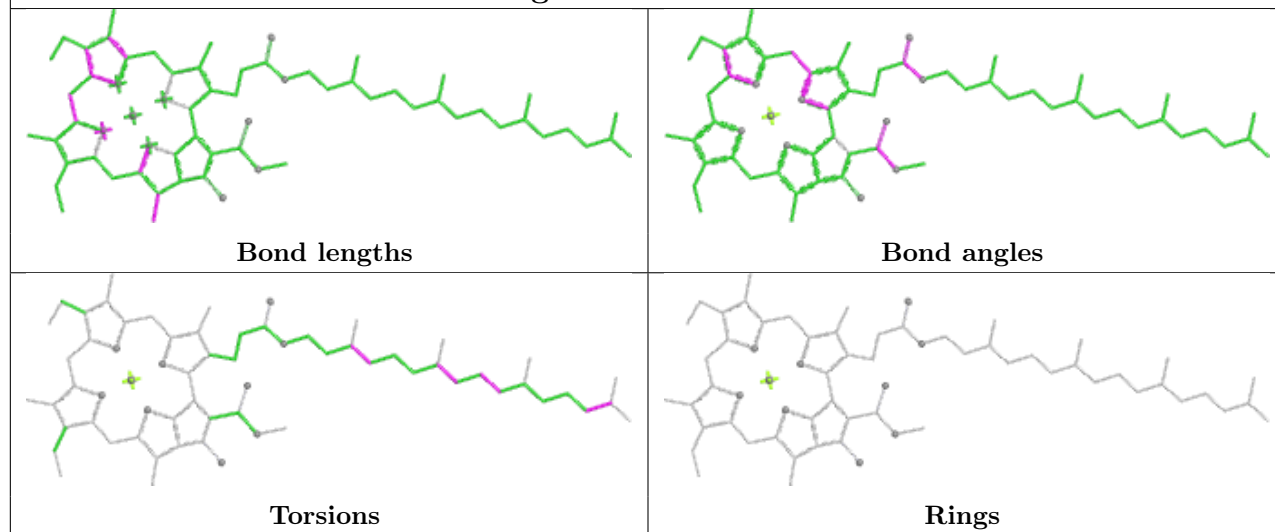
Ligand CLA B 601



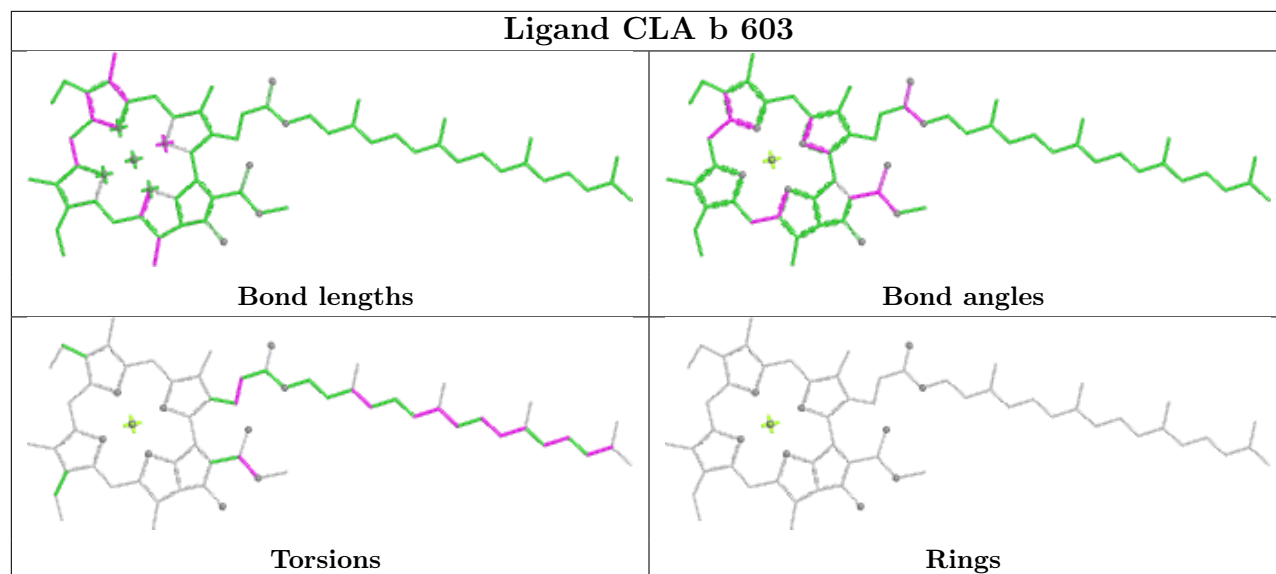
Ligand STE H 104



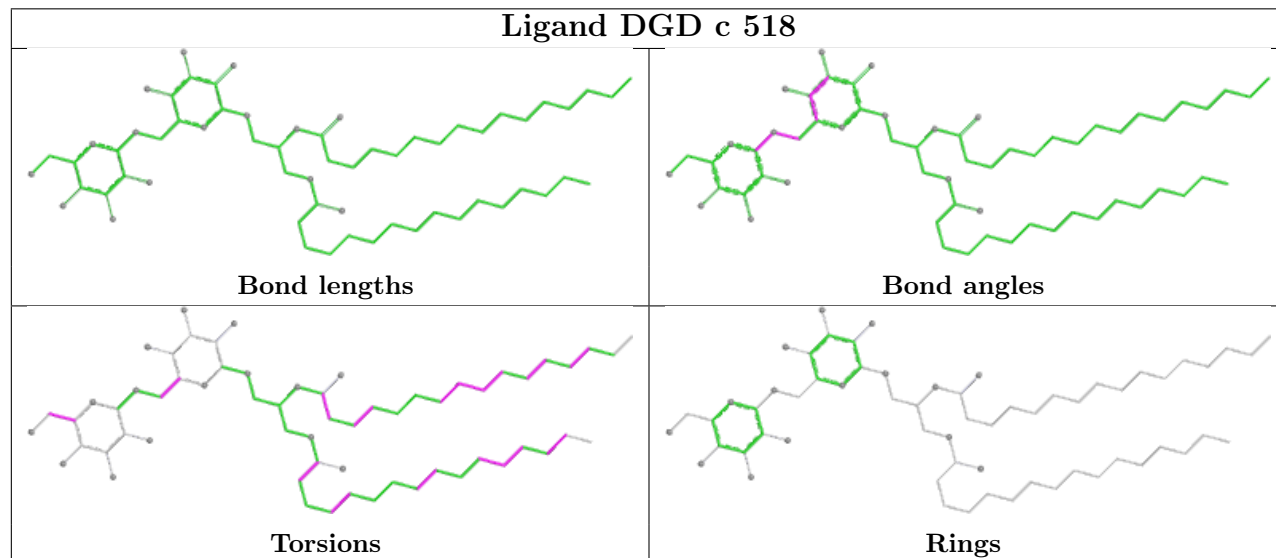
Ligand CLA C 510

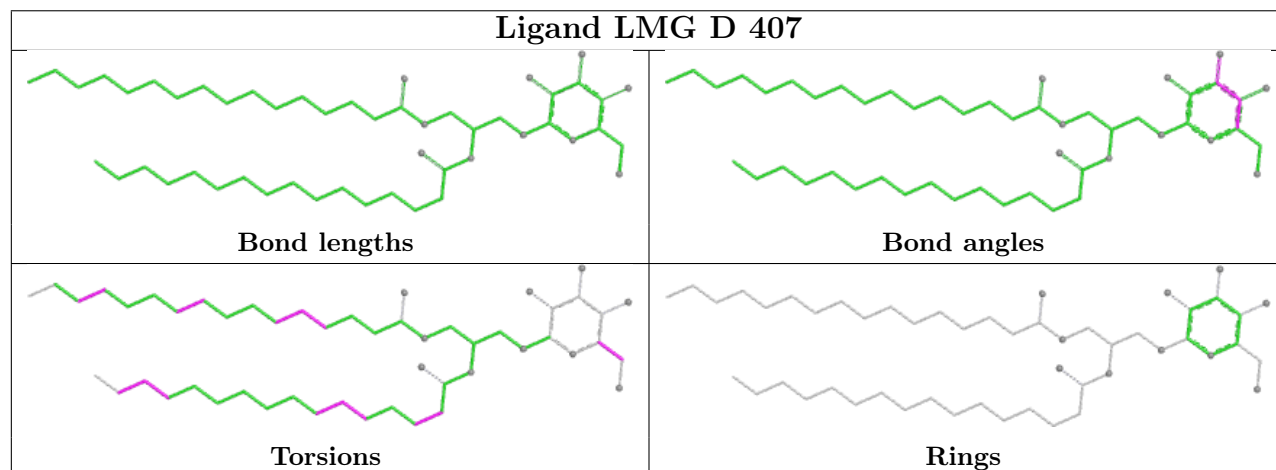
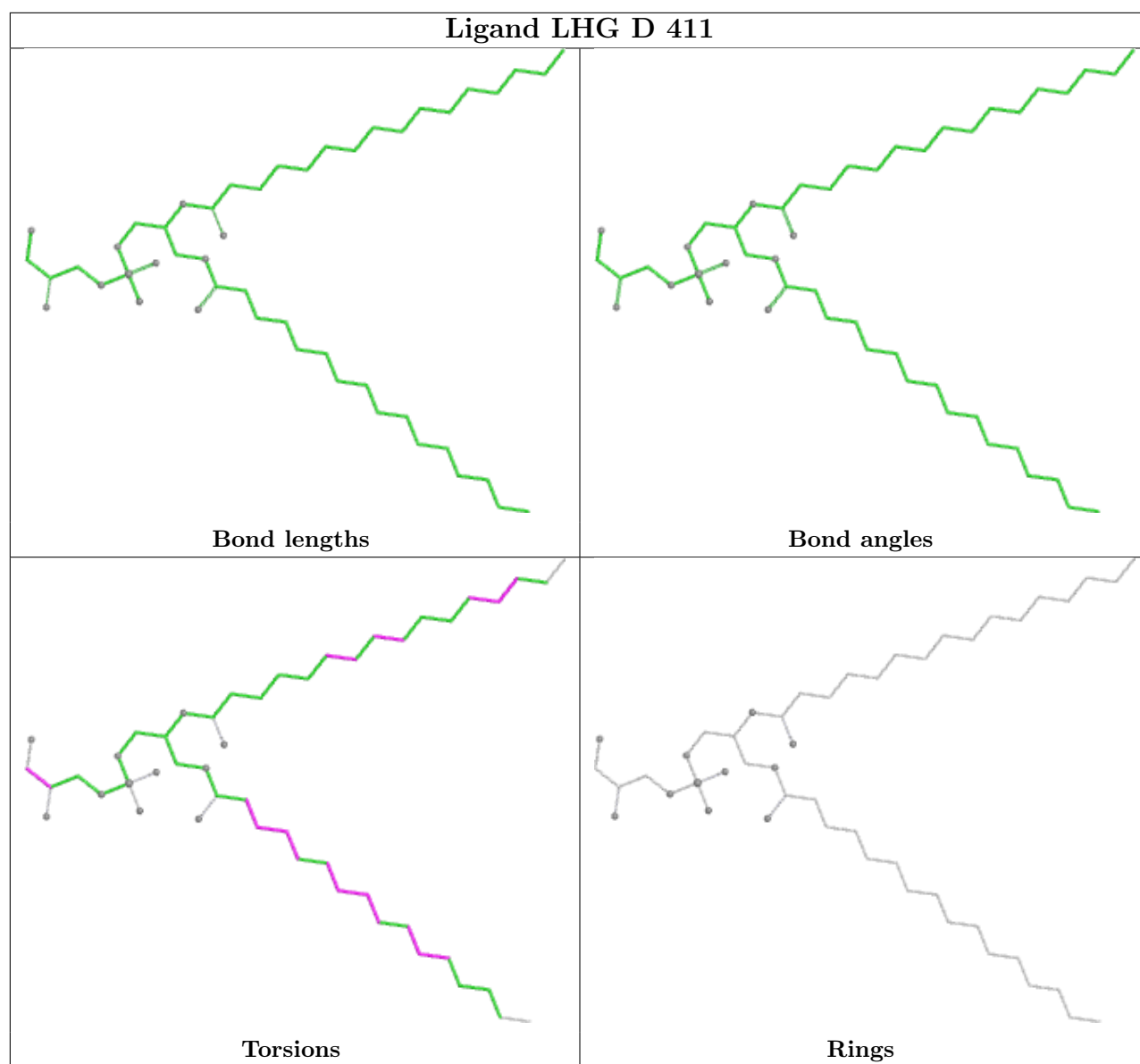


Ligand CLA b 603

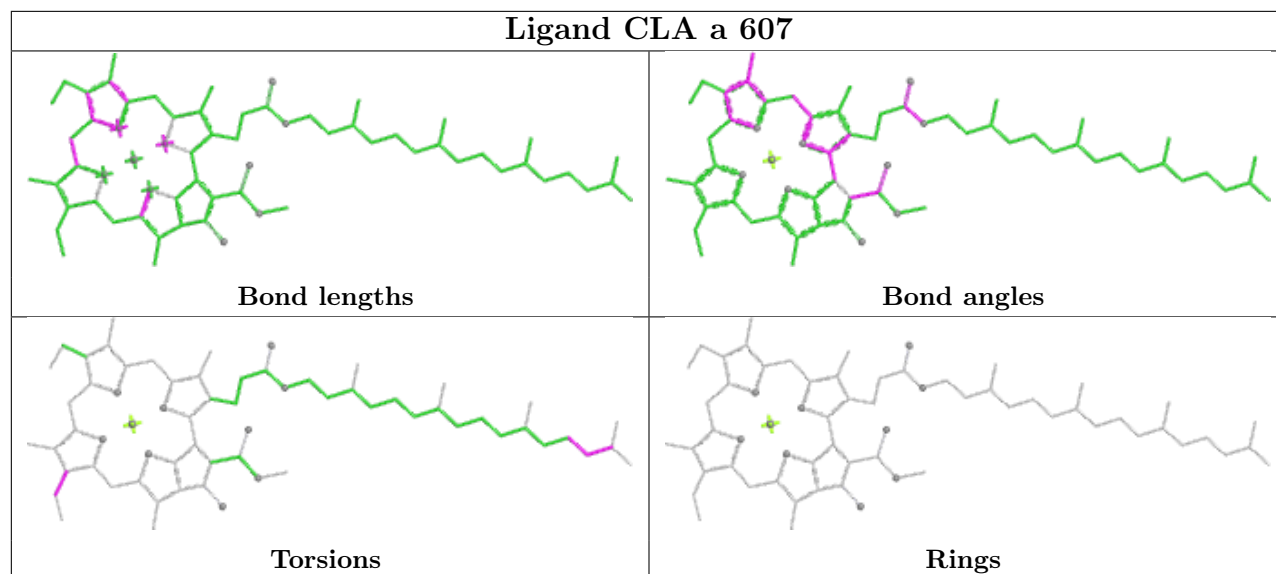


Ligand DGD c 518

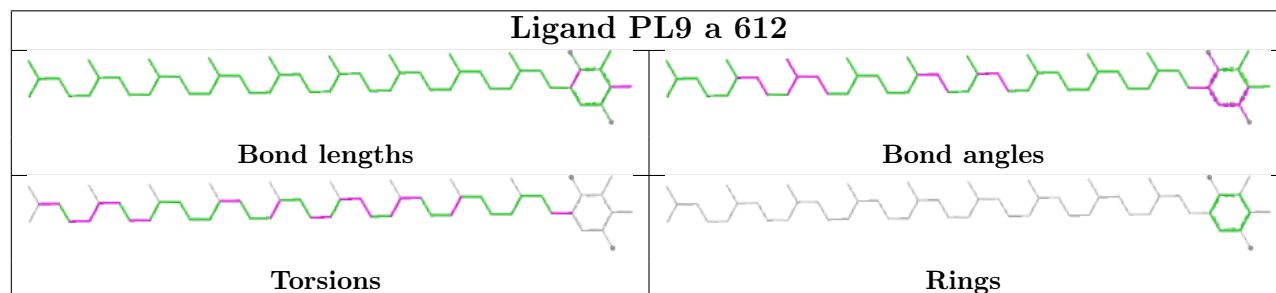




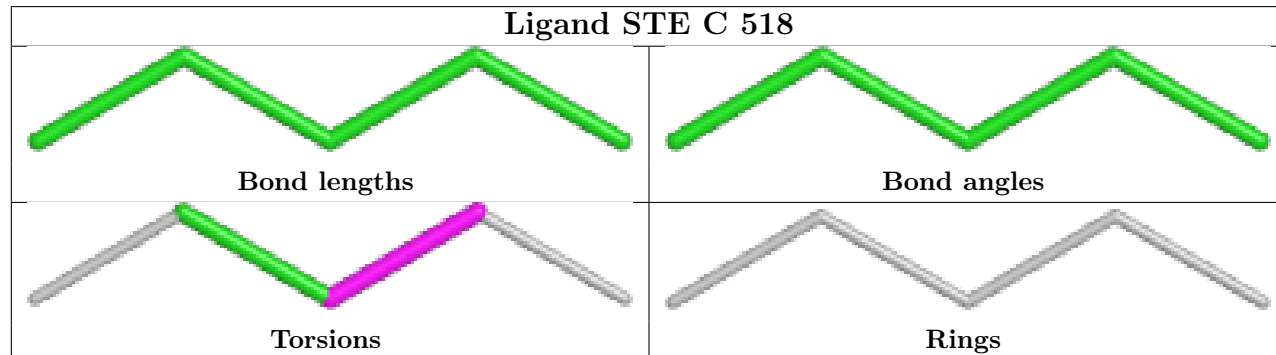
Ligand CLA a 607



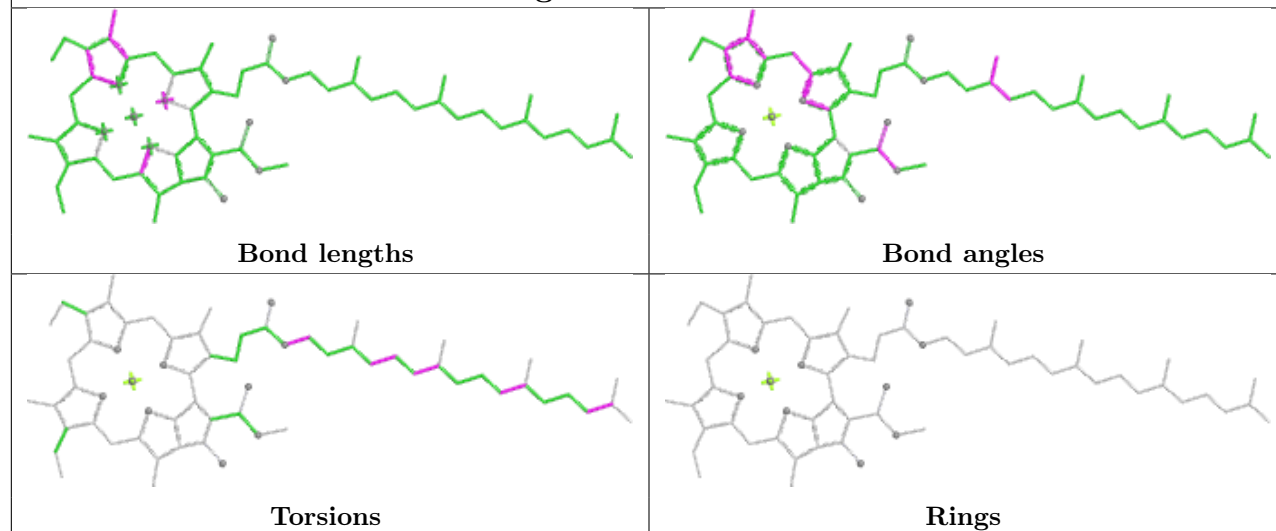
Ligand PL9 a 612



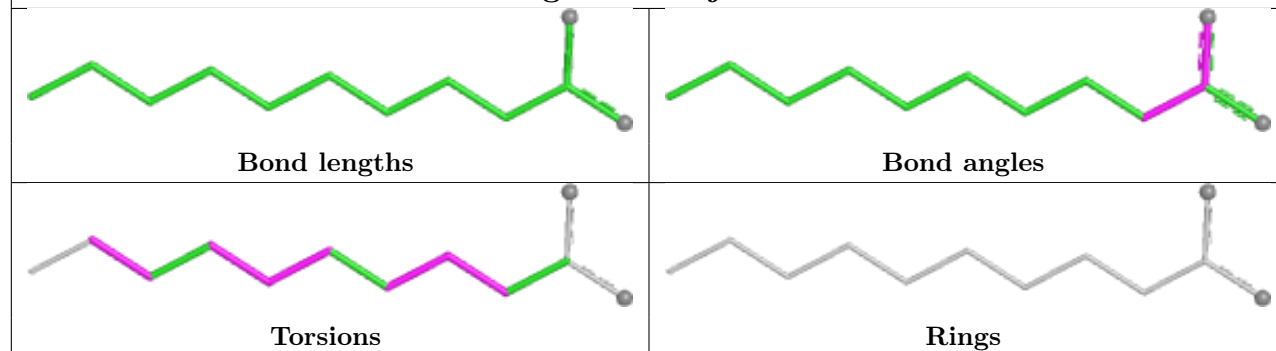
Ligand STE C 518



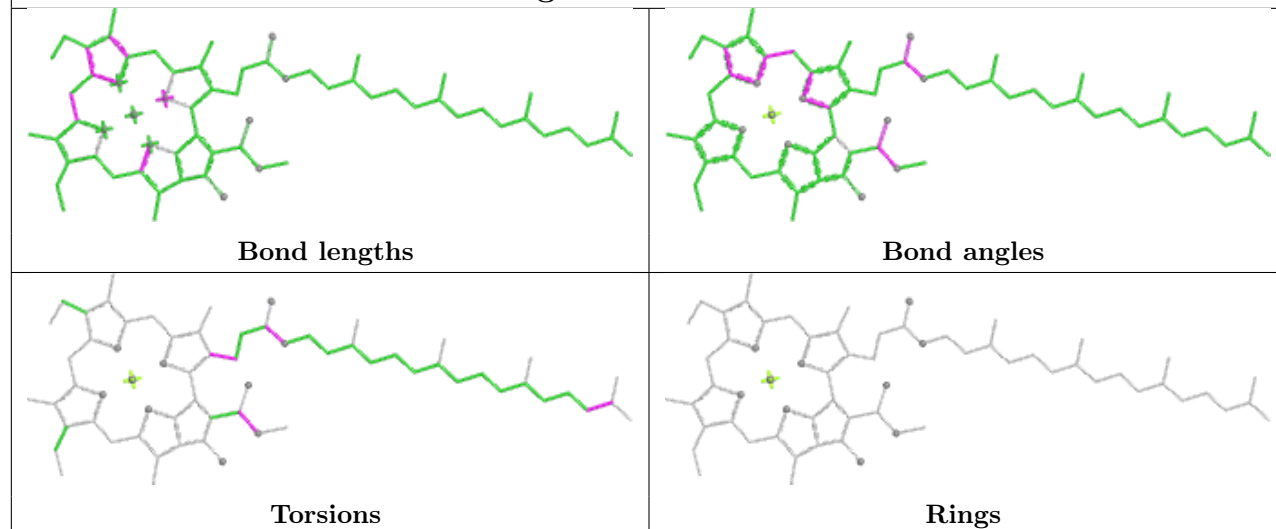
Ligand CLA d 402

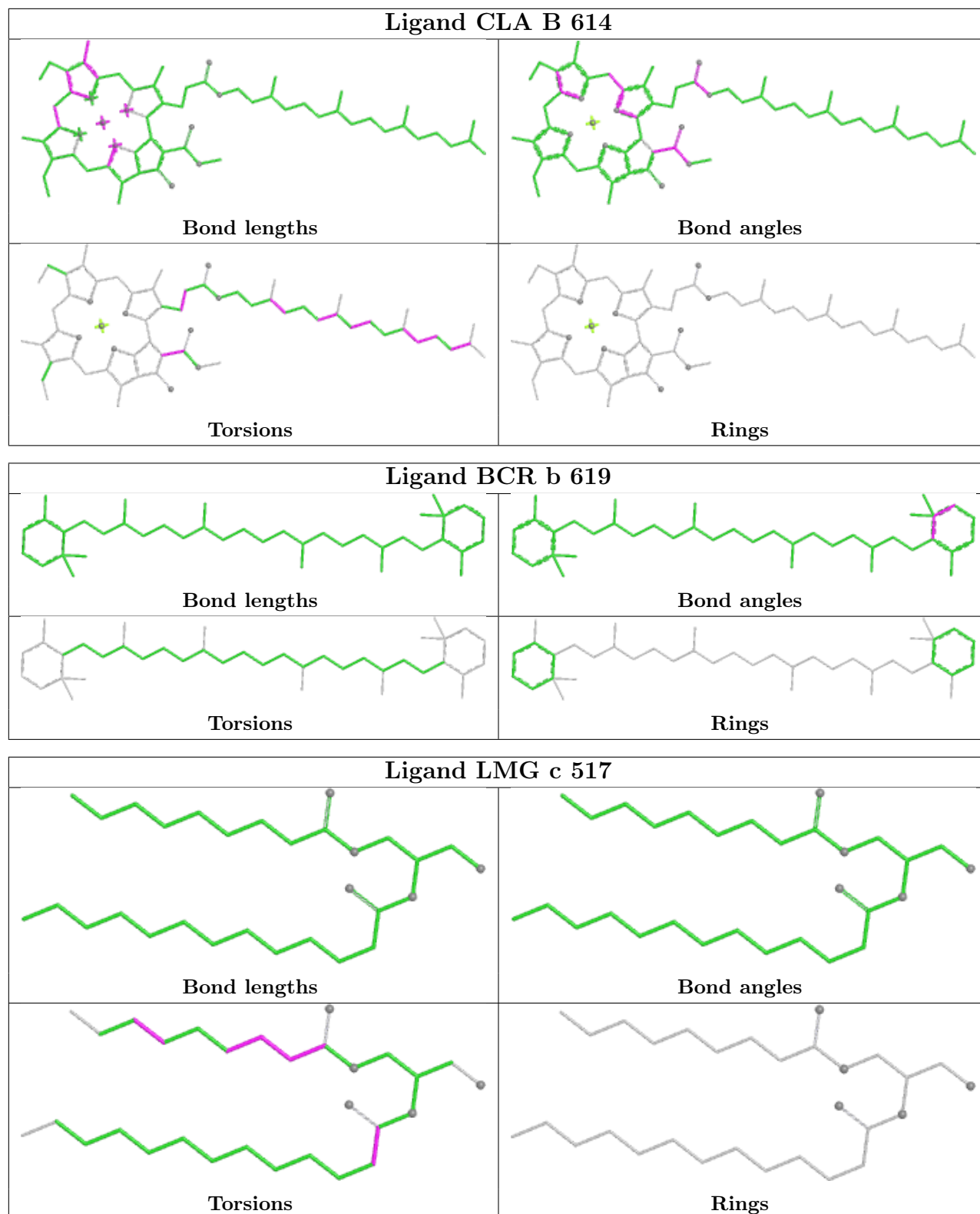


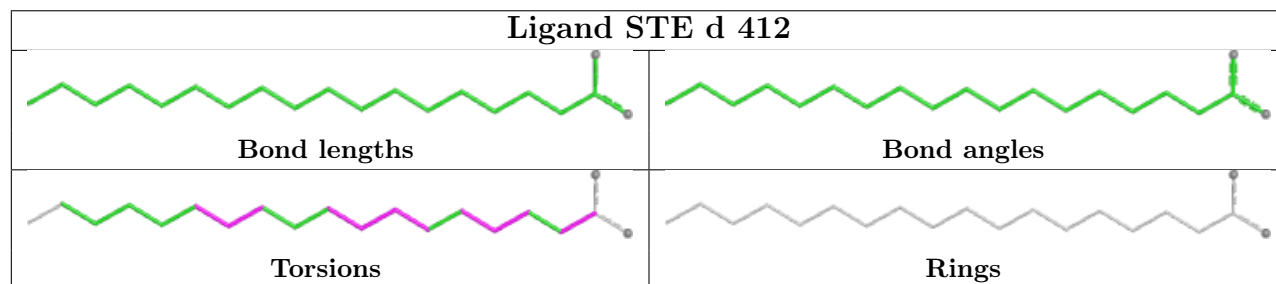
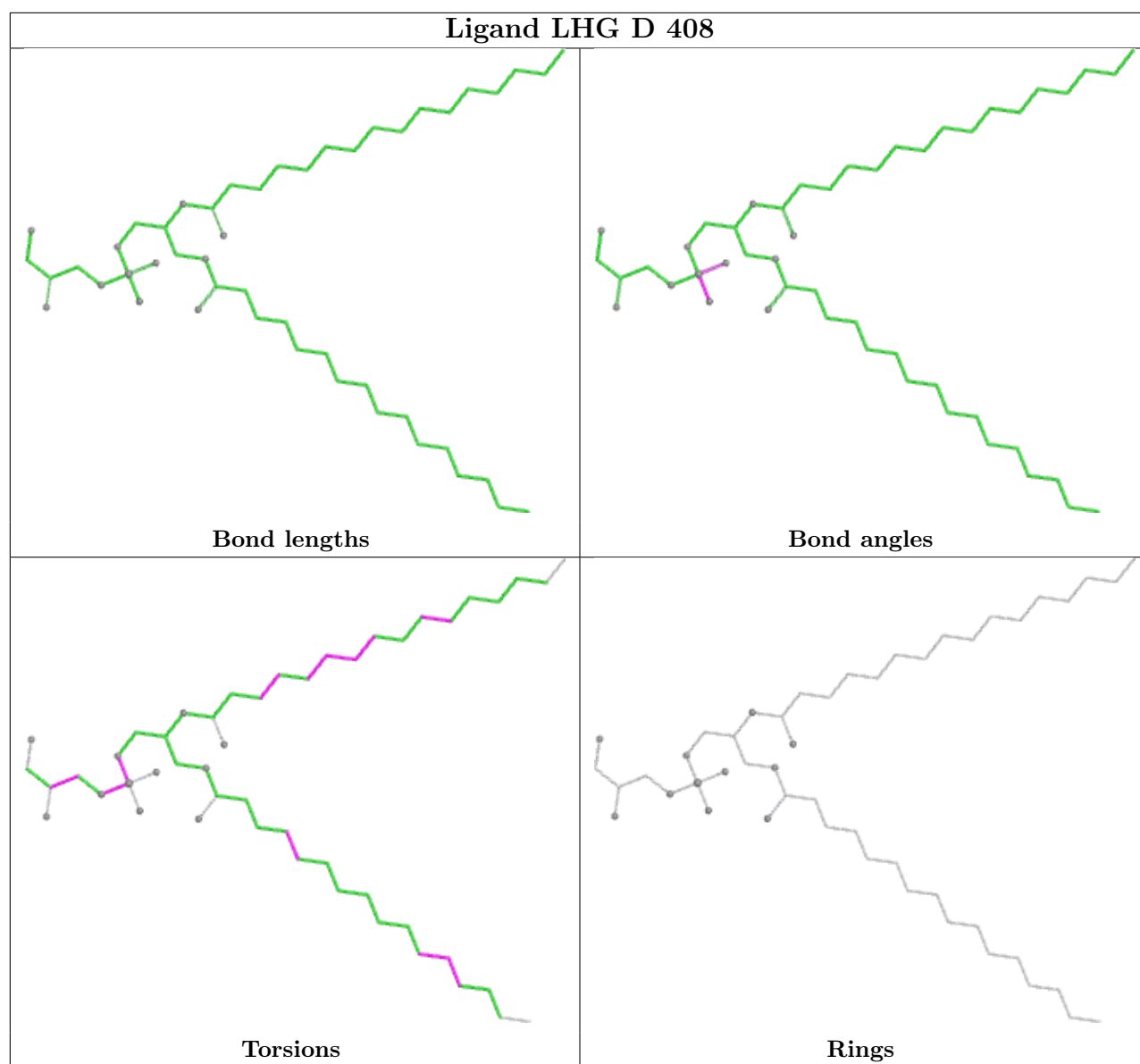
Ligand STE j 101

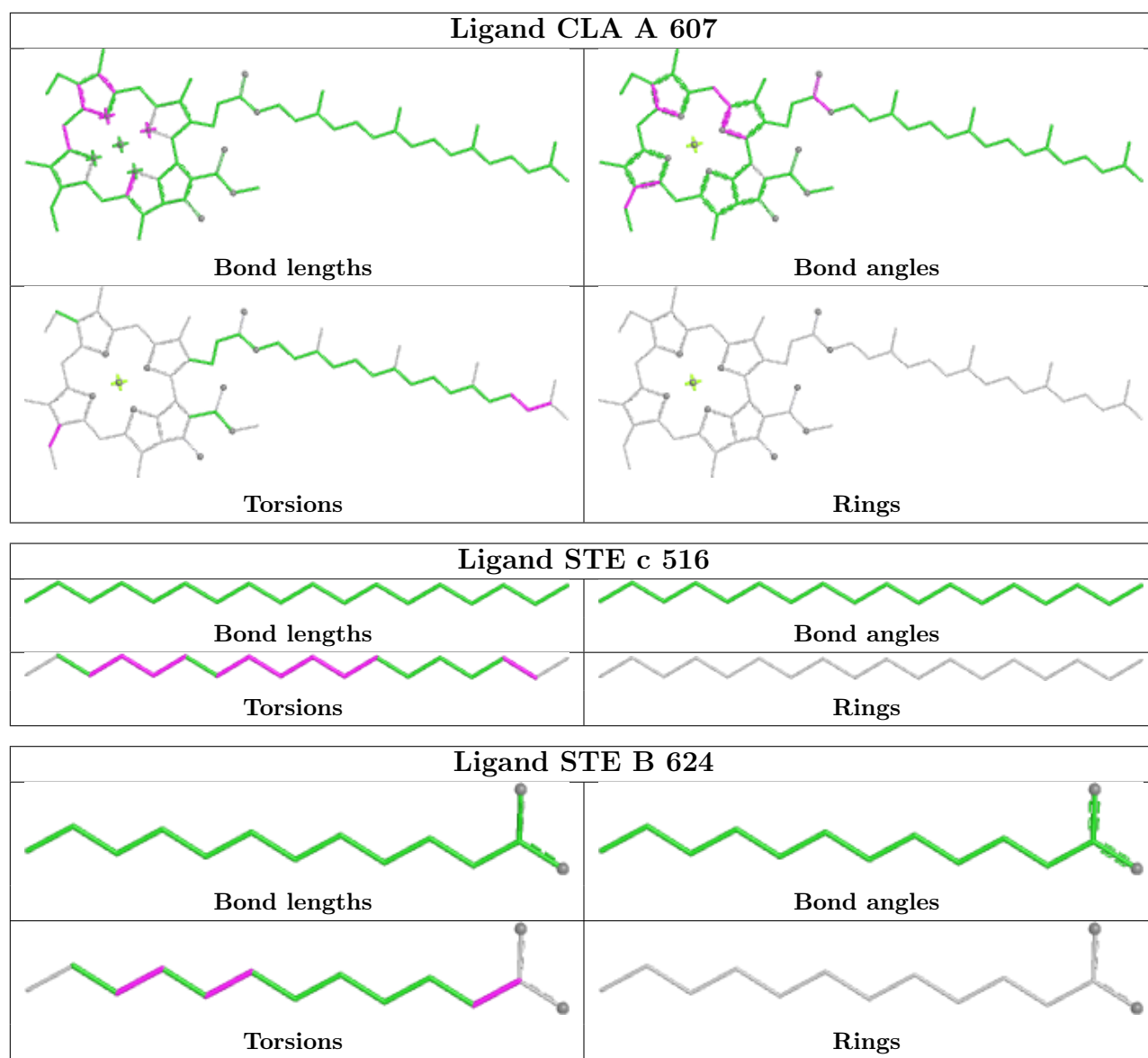


Ligand CLA c 511









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.57	0 100 100	13, 30, 53, 84	69 (20%)
1	a	334/344 (97%)	-0.48	1 (0%) 90 93	13, 33, 58, 82	69 (20%)
2	B	505/510 (99%)	-0.43	2 (0%) 88 92	18, 35, 63, 100	5 (0%)
2	b	505/510 (99%)	-0.27	4 (0%) 82 87	28, 40, 73, 113	1 (0%)
3	C	442/461 (95%)	-0.39	0 100 100	14, 39, 56, 87	11 (2%)
3	c	451/461 (97%)	-0.25	3 (0%) 84 88	14, 43, 64, 101	12 (2%)
4	D	341/352 (96%)	-0.62	0 100 100	14, 33, 50, 85	10 (2%)
4	d	341/352 (96%)	-0.42	1 (0%) 90 93	14, 37, 60, 81	11 (3%)
5	E	82/84 (97%)	0.23	2 (2%) 59 67	31, 52, 72, 86	1 (1%)
5	e	82/84 (97%)	0.33	2 (2%) 59 67	40, 62, 78, 94	0
6	F	34/45 (75%)	-0.07	0 100 100	38, 46, 64, 88	0
6	f	34/45 (75%)	0.08	0 100 100	44, 52, 79, 96	0
7	H	65/66 (98%)	-0.25	0 100 100	32, 42, 66, 76	0
7	h	63/66 (95%)	0.05	1 (1%) 70 77	39, 51, 67, 74	0
8	I	35/38 (92%)	-0.38	0 100 100	34, 42, 75, 88	0
8	i	35/38 (92%)	-0.27	0 100 100	35, 45, 81, 92	0
9	J	36/40 (90%)	-0.01	0 100 100	38, 53, 77, 102	0
9	j	36/40 (90%)	0.17	1 (2%) 55 62	42, 58, 95, 97	0
10	K	37/46 (80%)	0.04	0 100 100	45, 55, 76, 82	0
10	k	37/46 (80%)	0.21	0 100 100	48, 58, 75, 87	0
11	L	37/37 (100%)	-0.47	0 100 100	27, 33, 67, 75	0
11	l	36/37 (97%)	-0.58	0 100 100	29, 35, 73, 84	0
12	M	32/36 (88%)	-0.26	1 (3%) 51 57	30, 36, 61, 78	0
12	m	31/36 (86%)	-0.36	0 100 100	31, 37, 54, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.15	3 (1%) 76 81	27, 45, 87, 137	1 (0%)
13	o	244/272 (89%)	-0.11	5 (2%) 65 72	26, 45, 86, 136	0
14	T	29/32 (90%)	-0.46	1 (3%) 48 54	28, 35, 65, 85	0
14	t	29/32 (90%)	-0.39	1 (3%) 48 54	30, 35, 78, 83	0
15	U	97/134 (72%)	-0.17	0 100 100	33, 46, 76, 103	0
15	u	97/134 (72%)	-0.26	0 100 100	34, 44, 60, 92	0
16	V	137/163 (84%)	-0.31	1 (0%) 84 88	30, 43, 61, 77	0
16	v	137/163 (84%)	-0.12	0 100 100	34, 50, 73, 88	0
17	Y	27/46 (58%)	1.10	4 (14%) 5 6	57, 79, 104, 107	0
17	y	30/46 (65%)	0.74	1 (3%) 49 55	65, 75, 93, 110	0
18	X	38/41 (92%)	0.04	1 (2%) 57 64	40, 52, 76, 86	0
18	x	39/41 (95%)	0.21	1 (2%) 57 64	47, 60, 82, 102	0
19	Z	62/62 (100%)	0.74	3 (4%) 35 40	56, 72, 119, 127	0
19	z	62/62 (100%)	0.82	4 (6%) 25 28	59, 75, 115, 132	0
20	R	28/41 (68%)	0.61	1 (3%) 46 52	60, 71, 85, 98	0
20	r	28/41 (68%)	1.09	6 (21%) 2 2	68, 86, 100, 110	0
All	All	5293/5700 (92%)	-0.26	50 (0%) 81 85	13, 41, 77, 137	190 (3%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	5.7
19	z	33	TRP	4.0
2	b	495	PHE	3.9
17	Y	25	ILE	3.7
3	c	24	THR	3.6
7	h	64	ALA	3.2
19	Z	62	VAL	3.2
14	t	30	THR	3.2
17	Y	22	LEU	3.2
13	O	60	ARG	3.1
17	Y	20	ALA	3.1
20	r	27	ALA	3.0
2	b	499	VAL	2.9
13	o	59	LYS	2.9
2	B	495	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
3	c	23	ALA	2.8
19	Z	33	TRP	2.8
19	z	62	VAL	2.8
5	E	79	PHE	2.8
18	x	40	SER	2.7
13	O	56	PRO	2.7
20	r	20	VAL	2.7
5	E	84	LYS	2.7
1	a	11	ALA	2.6
5	e	3	GLY	2.5
5	e	79	PHE	2.5
14	T	30	THR	2.5
20	r	28	VAL	2.4
9	j	5	GLY	2.4
19	z	40	ILE	2.4
19	z	3	ILE	2.4
12	M	33	GLN	2.3
13	o	63	ALA	2.3
17	y	34	MET	2.3
2	b	488	PRO	2.3
13	O	59	LYS	2.3
13	o	56	PRO	2.3
18	X	2	THR	2.2
20	r	29	LYS	2.2
20	R	7	VAL	2.2
17	Y	23	THR	2.2
16	V	64	PRO	2.2
13	o	132	ASN	2.1
20	r	14	LEU	2.1
2	B	479[A]	PHE	2.1
2	b	84	THR	2.1
3	c	134	ILE	2.1
19	Z	7	LEU	2.0
20	r	3	TRP	2.0
4	d	103	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	FME	T	1	10/11	0.94	0.08	29,46,73,73	0
14	FME	t	1	10/11	0.94	0.08	32,47,68,68	0
8	FME	I	1	10/11	0.96	0.07	40,50,59,63	0
12	FME	M	1	10/11	0.96	0.09	42,50,70,80	0
12	FME	m	1	10/11	0.97	0.07	36,47,75,82	0
8	FME	i	1	10/11	0.97	0.07	39,47,59,62	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	C	520	10/20	0.57	0.20	46,73,90,91	0
30	STE	i	101	12/20	0.62	0.14	66,91,107,110	0
30	STE	K	102	14/20	0.66	0.16	60,75,96,98	0
30	STE	C	527	14/20	0.67	0.17	58,84,120,123	0
30	STE	A	620	11/20	0.68	0.18	51,70,96,98	0
30	STE	H	103	18/20	0.70	0.18	48,75,90,90	0
30	STE	e	101	9/20	0.71	0.22	56,81,97,97	0
30	STE	i	102	6/20	0.71	0.22	49,75,83,83	0
30	STE	j	102	16/20	0.71	0.17	56,80,100,102	0
30	STE	e	103	8/20	0.73	0.19	53,66,79,86	0
30	STE	I	101	17/20	0.74	0.15	53,71,83,86	0
30	STE	E	104	20/20	0.74	0.15	52,73,91,93	0
30	STE	a	618	12/20	0.74	0.14	49,72,82,93	0
30	STE	E	103	12/20	0.74	0.15	57,76,107,107	0
30	STE	h	102	10/20	0.75	0.17	59,76,89,91	0
30	STE	C	518	5/20	0.76	0.17	48,61,73,73	0
30	STE	A	619	17/20	0.76	0.14	55,77,95,97	0
30	STE	C	516	14/20	0.76	0.16	52,70,81,86	0
30	STE	t	102	10/20	0.76	0.17	44,65,76,77	0
30	STE	c	516	18/20	0.77	0.16	62,85,102,105	0
30	STE	Z	102	17/20	0.77	0.18	50,80,102,103	0
31	LMG	D	406	50/55	0.77	0.16	42,66,117,137	0
31	LMG	c	517	30/55	0.77	0.14	40,79,117,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	PL9	a	612	55/55	0.78	0.16	45,70,89,96	0
34	LHG	e	102	42/49	0.78	0.15	53,86,122,141	0
31	LMG	b	622	55/55	0.79	0.16	53,74,100,104	0
31	LMG	C	517	36/55	0.79	0.15	42,60,84,94	0
31	LMG	a	616	55/55	0.79	0.14	38,64,87,99	0
30	STE	e	104	9/20	0.80	0.17	60,75,91,92	0
33	DGD	A	617	66/66	0.80	0.14	48,68,97,105	0
29	PL9	A	612	55/55	0.80	0.16	39,69,86,90	0
30	STE	k	103	14/20	0.81	0.12	59,74,87,88	0
31	LMG	c	522	48/55	0.81	0.14	50,78,99,110	0
30	STE	e	105	13/20	0.82	0.16	67,85,93,100	0
34	LHG	E	101	49/49	0.82	0.14	48,77,111,120	0
30	STE	z	701	13/20	0.82	0.14	59,75,85,87	0
30	STE	z	702	9/20	0.83	0.20	55,71,79,84	0
30	STE	d	410	20/20	0.83	0.12	51,68,89,90	0
30	STE	B	627	15/20	0.83	0.18	35,64,74,86	0
30	STE	B	626	12/20	0.83	0.14	43,65,79,81	0
30	STE	C	526	16/20	0.83	0.12	40,56,68,72	0
30	STE	C	519	7/20	0.84	0.13	50,64,74,74	0
30	STE	A	613	9/20	0.84	0.16	49,71,82,83	0
30	STE	b	624	10/20	0.85	0.12	40,58,78,86	0
30	STE	T	103	15/20	0.85	0.15	46,62,92,94	0
30	STE	E	102	12/20	0.85	0.14	53,74,88,89	0
30	STE	T	102	16/20	0.85	0.17	38,54,107,111	0
30	STE	C	525	12/20	0.86	0.13	34,47,58,59	0
31	LMG	B	620	45/55	0.86	0.13	37,59,107,132	0
32	SQD	a	615	54/54	0.86	0.12	43,67,104,119	0
30	STE	b	625	11/20	0.87	0.13	54,67,71,75	0
31	LMG	A	615	48/55	0.87	0.12	40,60,81,90	0
30	STE	I	102	15/20	0.87	0.12	42,56,77,81	0
32	SQD	A	616	43/54	0.87	0.11	41,61,101,108	0
30	STE	A	618	8/20	0.88	0.12	50,61,74,74	0
30	STE	B	625	18/20	0.88	0.11	44,58,83,88	0
30	STE	j	101	12/20	0.88	0.11	49,59,71,71	0
31	LMG	c	521	46/55	0.88	0.11	41,68,82,83	0
30	STE	b	623	16/20	0.88	0.13	49,63,78,79	0
30	STE	H	104	9/20	0.89	0.12	51,64,74,76	0
32	SQD	B	623	54/54	0.89	0.10	38,60,90,96	0
30	STE	b	621	20/20	0.89	0.09	36,57,76,77	0
32	SQD	b	620	49/54	0.89	0.10	42,58,84,95	0
32	SQD	f	102	41/54	0.89	0.12	52,78,95,97	0
30	STE	J	101	12/20	0.89	0.11	45,58,68,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	LMG	C	524	48/55	0.89	0.12	44,73,97,104	0
30	STE	B	624	14/20	0.89	0.10	38,53,61,65	0
30	STE	B	621	17/20	0.90	0.10	37,54,67,67	0
31	LMG	a	617	49/55	0.90	0.10	37,61,86,100	0
31	LMG	m	101	51/55	0.90	0.10	37,53,72,81	0
30	STE	d	412	20/20	0.90	0.10	39,55,71,72	0
31	LMG	M	101	51/55	0.90	0.10	31,53,73,79	0
32	SQD	a	614	54/54	0.90	0.11	43,67,94,96	0
26	CLA	b	601	65/65	0.91	0.10	42,65,91,113	0
30	STE	D	412	20/20	0.91	0.10	34,50,65,73	0
30	STE	d	406	20/20	0.91	0.09	40,55,72,74	0
30	STE	m	102	12/20	0.91	0.11	46,59,77,77	0
30	STE	m	103	18/20	0.91	0.10	37,50,77,81	0
28	BCR	c	514	40/40	0.92	0.10	51,64,73,77	0
32	SQD	D	410	52/54	0.92	0.10	31,63,98,105	0
26	CLA	c	513	65/65	0.92	0.11	46,70,103,111	0
28	BCR	d	404	40/40	0.93	0.08	36,52,85,86	0
28	BCR	k	101	40/40	0.93	0.09	45,59,70,73	0
32	SQD	F	102	36/54	0.93	0.10	43,70,88,92	0
30	STE	M	102	15/20	0.93	0.09	39,51,59,71	0
30	STE	M	103	10/20	0.93	0.09	40,50,57,62	0
26	CLA	c	512	65/65	0.93	0.09	42,60,93,99	0
26	CLA	C	513	65/65	0.93	0.09	43,66,99,107	0
28	BCR	C	514	40/40	0.93	0.09	43,58,68,70	0
33	DGD	C	522	62/66	0.93	0.09	33,50,94,108	0
28	BCR	Z	101	40/40	0.93	0.08	38,55,73,75	0
26	CLA	B	601	65/65	0.93	0.10	27,54,87,92	0
26	CLA	c	503	65/65	0.94	0.07	33,46,55,63	0
28	BCR	b	618	40/40	0.94	0.07	28,41,55,61	0
28	BCR	B	618	40/40	0.94	0.07	26,40,52,54	0
28	BCR	c	515	40/40	0.94	0.09	30,45,60,68	0
26	CLA	C	503	65/65	0.94	0.07	32,43,52,55	0
28	BCR	H	101	40/40	0.94	0.07	29,42,56,59	0
31	LMG	D	407	51/55	0.94	0.10	30,58,94,98	0
33	DGD	H	102	62/66	0.94	0.08	28,42,55,59	0
33	DGD	c	519	62/66	0.94	0.08	34,50,90,94	0
33	DGD	h	101	62/66	0.94	0.08	31,48,59,61	0
34	LHG	D	411	49/49	0.94	0.10	30,46,70,79	0
28	BCR	k	102	40/40	0.94	0.09	44,56,66,80	0
34	LHG	d	407	49/49	0.94	0.09	32,52,78,83	0
28	BCR	x	101	40/40	0.94	0.07	37,49,62,65	0
28	BCR	T	101	40/40	0.95	0.06	26,40,54,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	CLA	b	616	60/65	0.95	0.08	29,46,91,94	0
28	BCR	b	617	40/40	0.95	0.06	30,42,51,53	0
26	CLA	C	510	65/65	0.95	0.07	32,46,67,77	0
28	BCR	b	619	40/40	0.95	0.07	30,48,64,66	0
26	CLA	c	508	64/65	0.95	0.08	34,45,101,124	0
26	CLA	c	509	65/65	0.95	0.09	33,49,66,69	0
26	CLA	c	511	65/65	0.95	0.08	40,55,71,73	0
26	CLA	C	511	65/65	0.95	0.08	36,51,67,69	0
26	CLA	C	512	65/65	0.95	0.09	37,55,90,100	0
28	BCR	t	101	40/40	0.95	0.06	30,41,52,56	0
27	PHO	d	401	64/64	0.95	0.07	29,38,47,52	0
28	BCR	A	611	40/40	0.95	0.06	27,38,45,46	0
33	DGD	C	523	62/66	0.95	0.08	29,46,80,96	0
26	CLA	C	506	65/65	0.95	0.08	27,42,89,107	0
28	BCR	B	619	40/40	0.95	0.07	27,42,58,66	0
33	DGD	c	520	62/66	0.95	0.08	30,50,73,95	0
26	CLA	C	509	65/65	0.95	0.08	29,45,65,68	0
34	LHG	D	409	47/49	0.95	0.09	29,48,82,98	0
28	BCR	C	515	40/40	0.95	0.07	27,40,54,61	0
28	BCR	D	404	40/40	0.95	0.08	30,46,92,105	0
26	CLA	b	606	65/65	0.95	0.07	29,40,73,81	0
34	LHG	d	409	39/49	0.95	0.09	33,46,74,83	0
28	BCR	K	101	40/40	0.95	0.08	40,52,66,71	0
27	PHO	A	609	64/64	0.96	0.06	20,30,39,44	0
27	PHO	D	401	64/64	0.96	0.06	23,33,43,46	0
27	PHO	a	609	64/64	0.96	0.06	22,33,39,43	0
26	CLA	b	602	65/65	0.96	0.07	27,41,60,66	0
26	CLA	B	610	65/65	0.96	0.07	23,34,44,47	0
28	BCR	B	617	40/40	0.96	0.06	27,40,52,56	0
26	CLA	b	608	65/65	0.96	0.06	27,42,62,63	0
26	CLA	b	609	65/65	0.96	0.07	30,44,61,71	0
31	LMG	d	411	44/55	0.96	0.08	34,53,82,93	0
26	CLA	b	610	65/65	0.96	0.08	27,39,53,56	0
26	CLA	b	611	65/65	0.96	0.07	25,35,53,56	0
26	CLA	b	614	65/65	0.96	0.07	26,41,78,84	0
26	CLA	b	615	65/65	0.96	0.07	27,40,65,75	0
26	CLA	C	502	65/65	0.96	0.06	29,42,57,68	0
26	CLA	c	501	65/65	0.96	0.07	29,41,53,62	0
26	CLA	c	502	65/65	0.96	0.06	30,43,64,69	0
28	BCR	a	611	40/40	0.96	0.06	26,36,46,50	0
25	BCT	a	606	4/4	0.96	0.07	36,39,46,56	0
26	CLA	c	504	60/65	0.96	0.07	30,45,82,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	DGD	C	521	62/66	0.96	0.08	26,42,75,90	0
26	CLA	c	505	65/65	0.96	0.07	31,42,69,72	0
26	CLA	c	506	65/65	0.96	0.09	32,49,105,112	0
26	CLA	c	507	65/65	0.96	0.07	31,45,58,63	0
33	DGD	c	518	62/66	0.96	0.08	24,40,76,80	0
26	CLA	C	504	59/65	0.96	0.07	29,41,94,100	0
26	CLA	C	505	65/65	0.96	0.08	28,39,68,74	0
26	CLA	c	510	65/65	0.96	0.07	32,47,64,75	0
26	CLA	a	608	65/65	0.96	0.08	27,39,100,110	0
26	CLA	a	610	65/65	0.96	0.08	21,37,90,100	0
26	CLA	B	606	65/65	0.96	0.07	23,36,72,82	0
29	PL9	D	405	55/55	0.96	0.06	22,34,45,46	0
26	CLA	d	403	65/65	0.96	0.08	31,49,89,100	0
29	PL9	d	405	55/55	0.96	0.06	24,36,46,53	0
34	LHG	l	101	49/49	0.96	0.08	32,47,61,75	0
26	CLA	B	612	65/65	0.97	0.06	22,33,46,55	0
26	CLA	B	613	65/65	0.97	0.06	22,32,75,85	0
26	CLA	b	603	65/65	0.97	0.06	25,37,66,70	0
26	CLA	b	604	65/65	0.97	0.07	25,35,79,99	0
26	CLA	b	605	65/65	0.97	0.06	25,37,52,57	0
26	CLA	B	614	65/65	0.97	0.08	23,38,80,89	0
26	CLA	b	607	65/65	0.97	0.08	22,38,75,86	0
26	CLA	B	615	65/65	0.97	0.07	24,38,67,74	0
26	CLA	B	616	60/65	0.97	0.08	26,40,92,106	0
26	CLA	C	501	65/65	0.97	0.06	25,37,49,55	0
26	CLA	A	610	54/65	0.97	0.06	22,35,67,71	0
26	CLA	b	612	65/65	0.97	0.07	23,38,50,60	0
26	CLA	b	613	65/65	0.97	0.07	20,35,80,89	0
26	CLA	A	614	65/65	0.97	0.06	21,29,52,69	0
25	BCT	A	606	4/4	0.97	0.08	25,30,35,42	0
26	CLA	B	602	65/65	0.97	0.06	25,34,59,65	0
26	CLA	B	603	65/65	0.97	0.06	22,32,58,58	0
26	CLA	C	507	65/65	0.97	0.06	26,42,56,61	0
26	CLA	C	508	65/65	0.97	0.07	29,42,121,129	0
26	CLA	B	604	65/65	0.97	0.07	21,32,77,83	0
26	CLA	B	605	65/65	0.97	0.06	22,33,49,53	0
26	CLA	A	607	65/65	0.97	0.06	19,29,49,59	0
26	CLA	B	607	65/65	0.97	0.06	21,35,64,75	0
26	CLA	B	608	65/65	0.97	0.06	21,35,52,64	0
34	LHG	B	622	49/49	0.97	0.07	28,43,56,68	0
34	LHG	D	408	49/49	0.97	0.06	27,41,50,58	0
26	CLA	D	402	65/65	0.97	0.06	20,31,57,62	0

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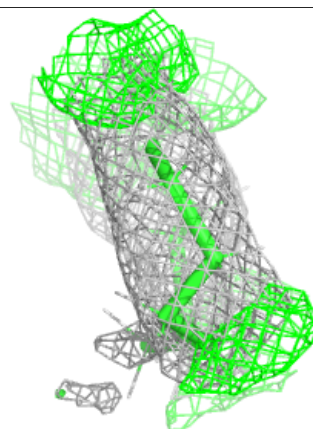
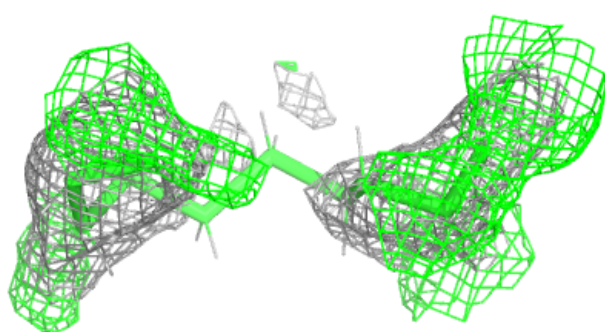
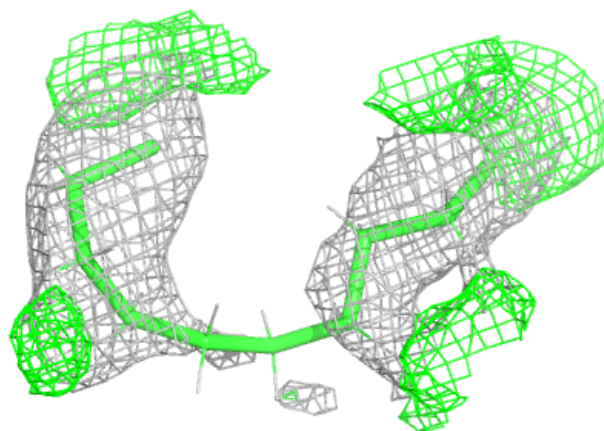
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	CLA	D	403	65/65	0.97	0.07	25,40,119,132	0
26	CLA	a	607	65/65	0.97	0.06	20,31,49,61	0
26	CLA	B	609	65/65	0.97	0.06	25,37,56,64	0
34	LHG	d	408	49/49	0.97	0.07	26,44,58,69	0
26	CLA	A	608	65/65	0.97	0.09	24,35,102,111	0
26	CLA	d	402	65/65	0.97	0.06	23,33,61,69	0
26	CLA	a	613	65/65	0.97	0.06	22,31,49,54	0
35	HEM	F	101	43/43	0.97	0.07	35,46,61,68	0
35	HEM	f	101	43/43	0.97	0.08	44,56,71,73	0
26	CLA	B	611	65/65	0.98	0.05	20,32,51,55	0
24	CL	A	605	1/1	0.99	0.07	26,26,26,26	0
24	CL	a	604	1/1	0.99	0.04	26,26,26,26	0
21	OEY	A	601[B]	11/11	0.99	0.03	22,26,29,30	11
22	OEX	A	602[A]	10/10	0.99	0.03	26,27,30,30	10
22	OEX	a	602[A]	10/10	0.99	0.02	25,27,31,31	10
23	FE2	a	603	1/1	0.99	0.02	35,35,35,35	0
24	CL	A	604	1/1	0.99	0.02	27,27,27,27	0
36	HEC	V	201	43/43	0.99	0.05	26,33,41,42	0
36	HEC	v	201	43/43	0.99	0.05	29,38,47,47	0
24	CL	a	605	1/1	1.00	0.06	29,29,29,29	0
21	OEY	a	601[B]	11/11	1.00	0.02	23,27,30,30	11
23	FE2	A	603	1/1	1.00	0.01	28,28,28,28	0

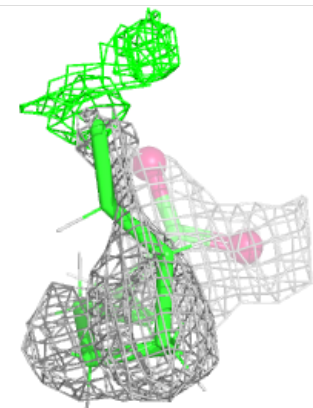
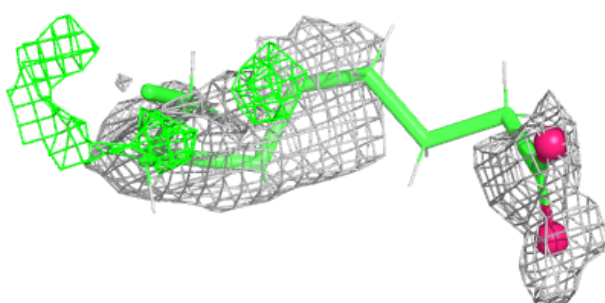
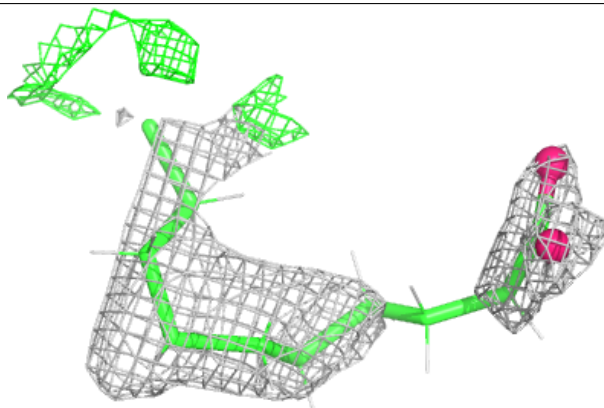
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE 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)

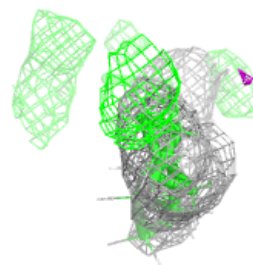
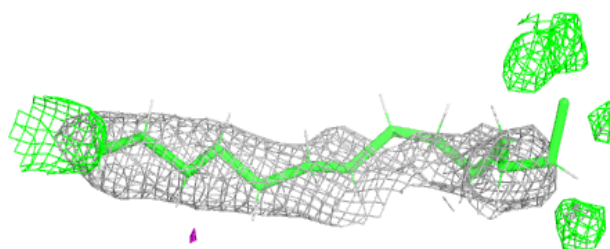
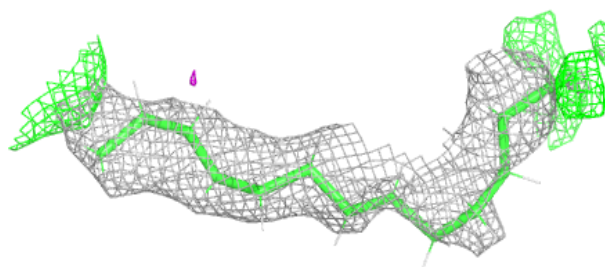
**Electron density around STE i 101:**

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

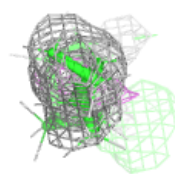
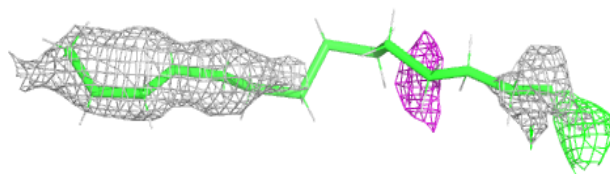
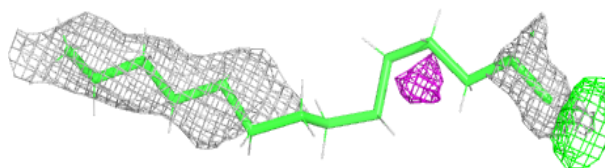


Electron density around STE K 102:

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

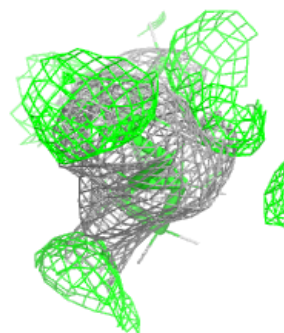
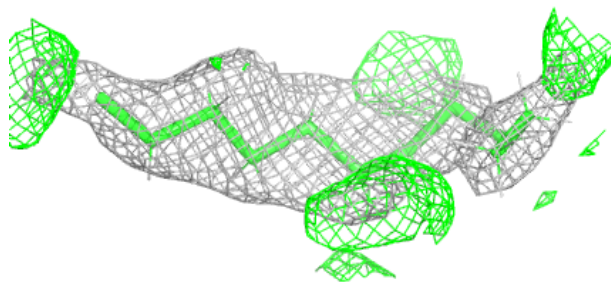
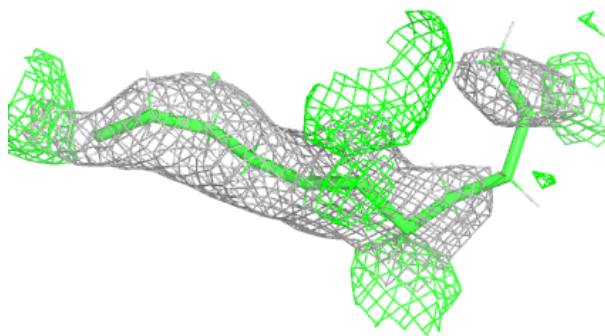
**Electron density around STE C 527:**

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

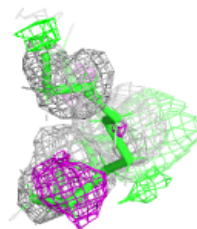
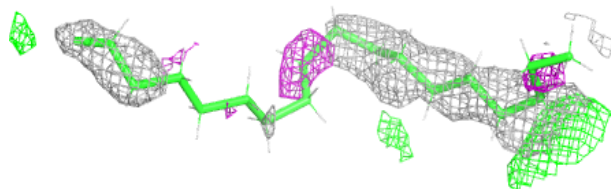
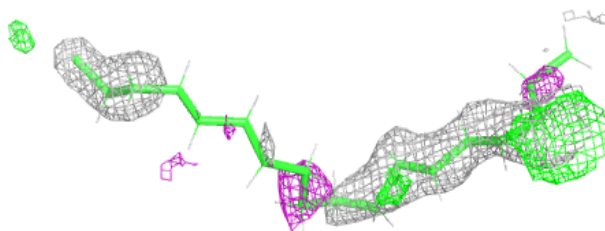


Electron density around STE A 620:

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

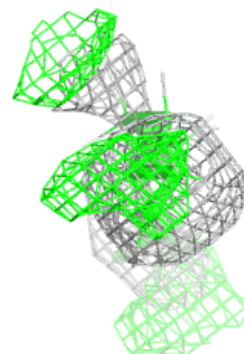
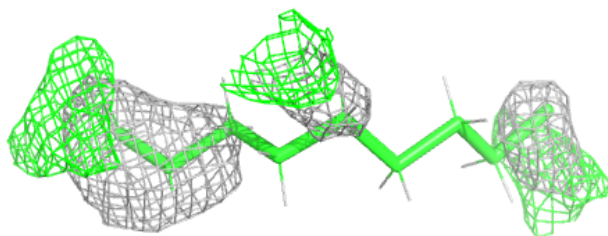
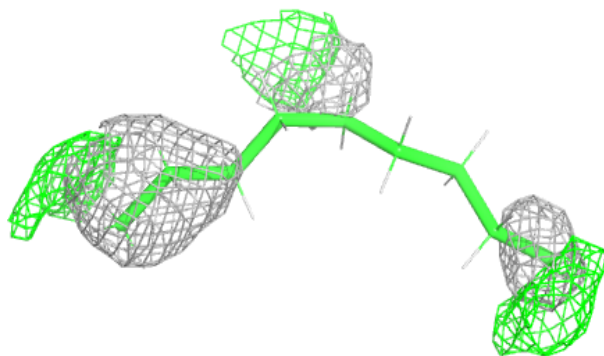
**Electron density around STE H 103:**

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

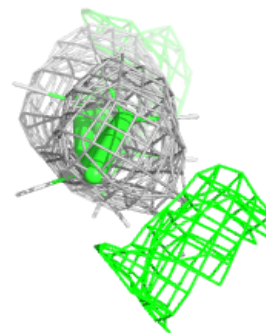
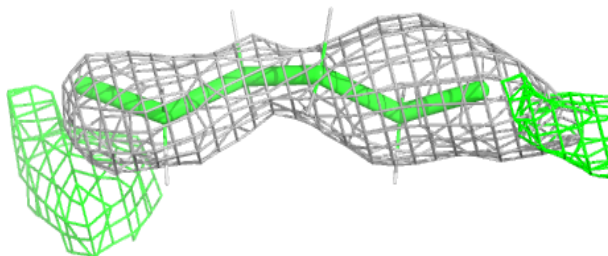
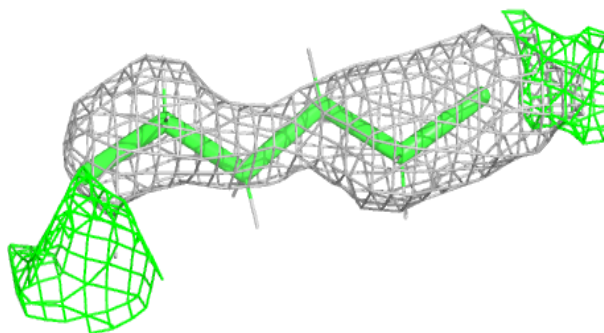


Electron density around STE e 101:

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

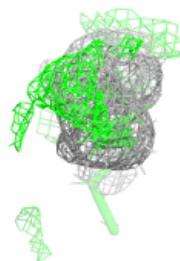
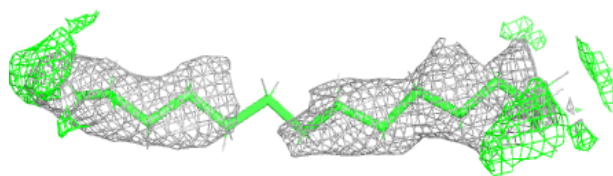
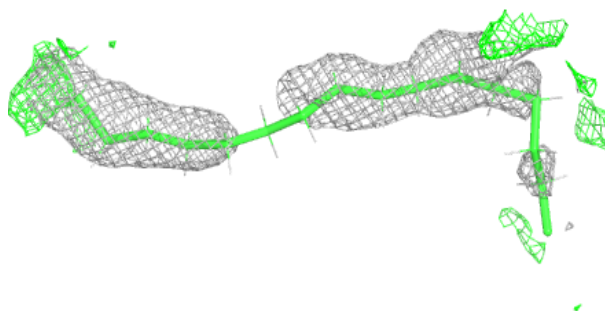
**Electron density around STE i 102:**

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

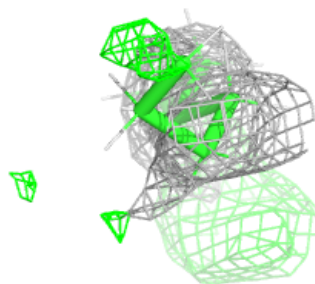
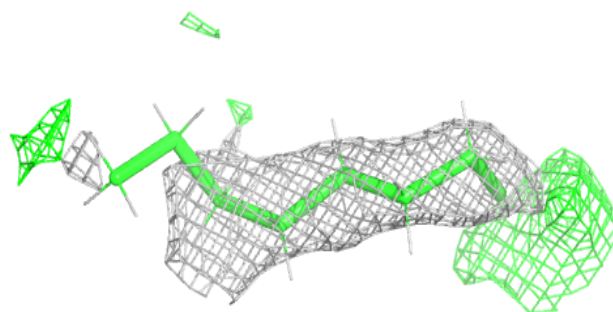
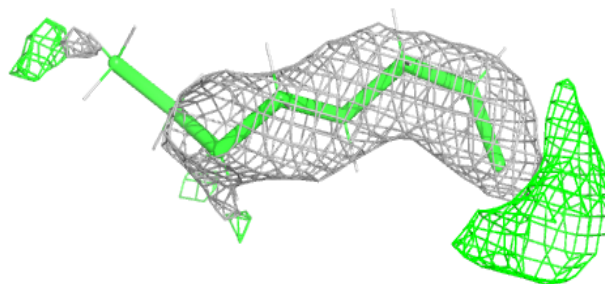


Electron density around STE j 102:

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

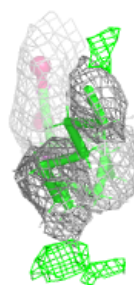
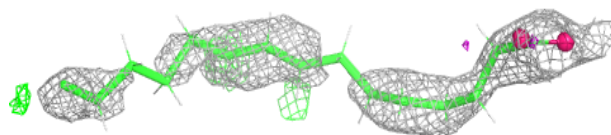
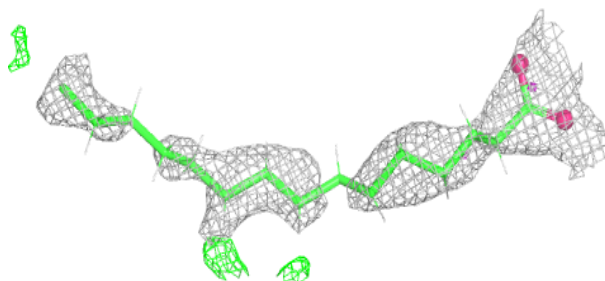
**Electron density around STE e 103:**

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

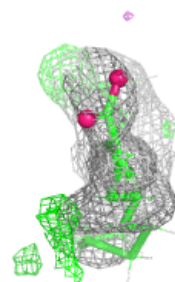
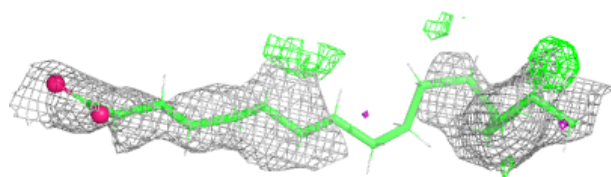
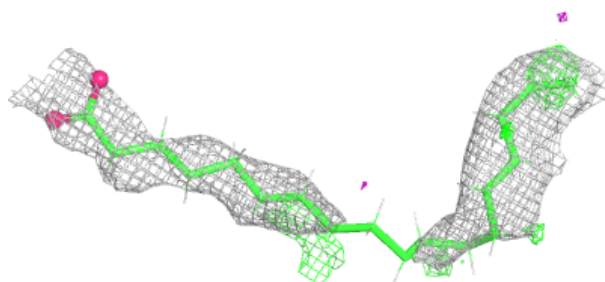


Electron density around STE I 101:

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

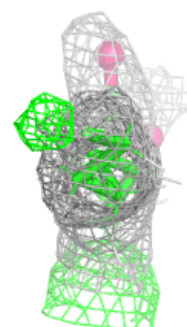
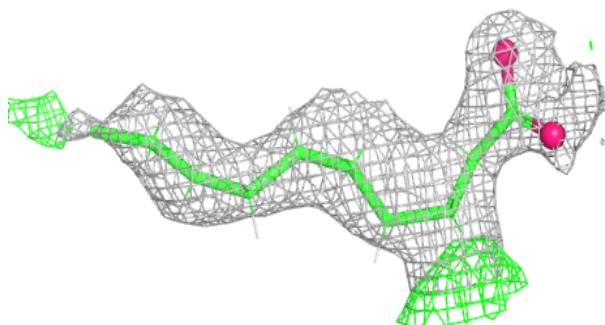
**Electron density around STE E 104:**

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

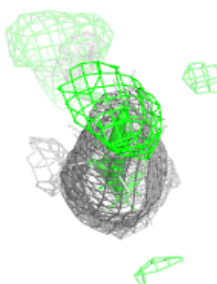
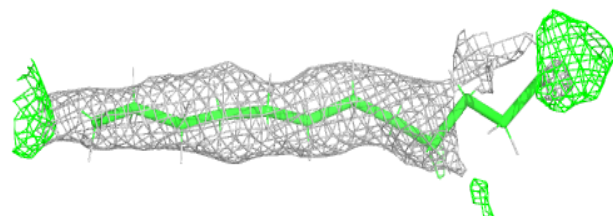
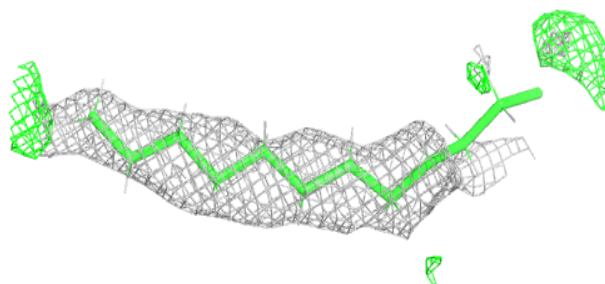


Electron density around STE a 618:

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

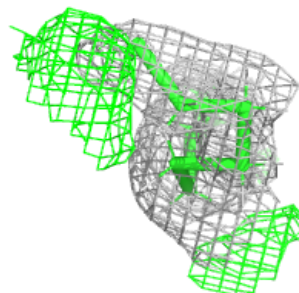
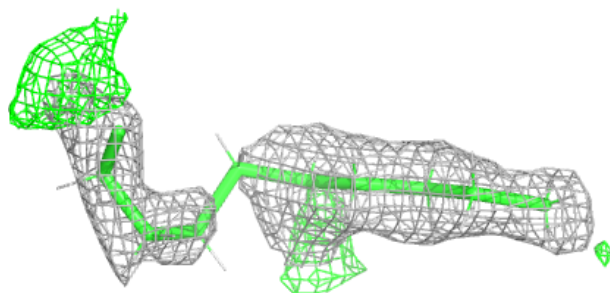
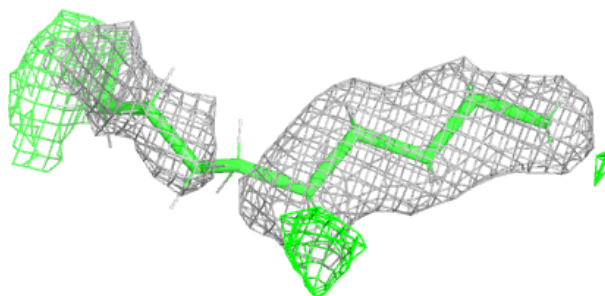
**Electron density around STE E 103:**

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

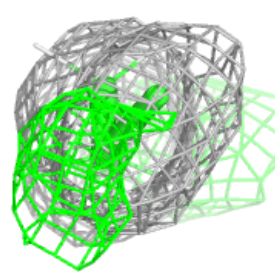
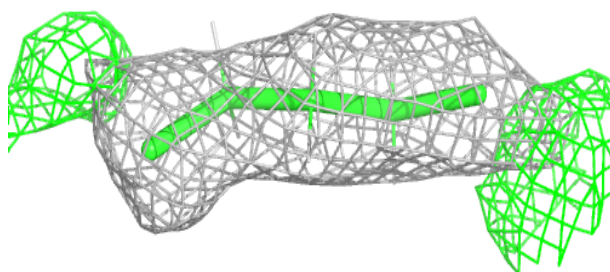
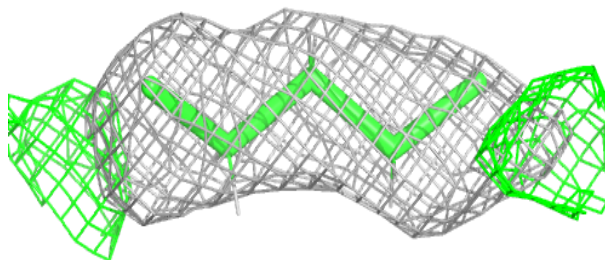


Electron density around STE h 102:

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

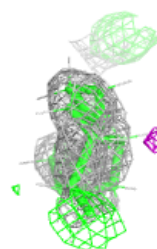
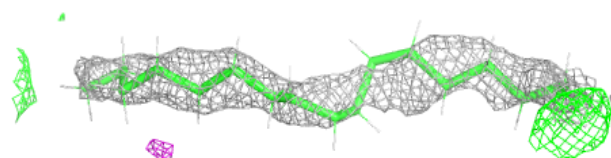
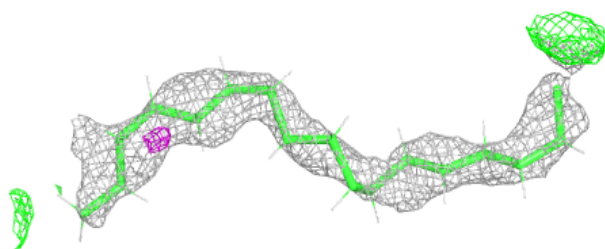
**Electron density around STE C 518:**

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

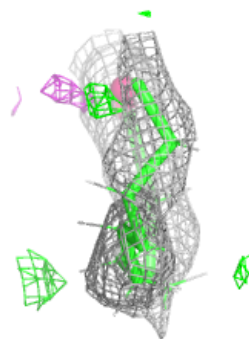
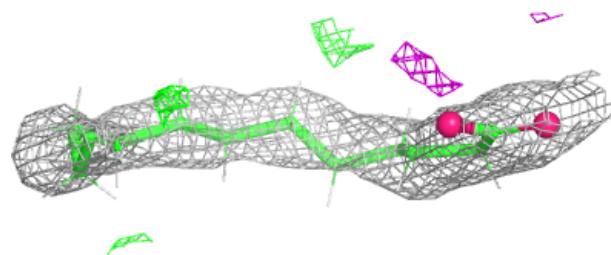
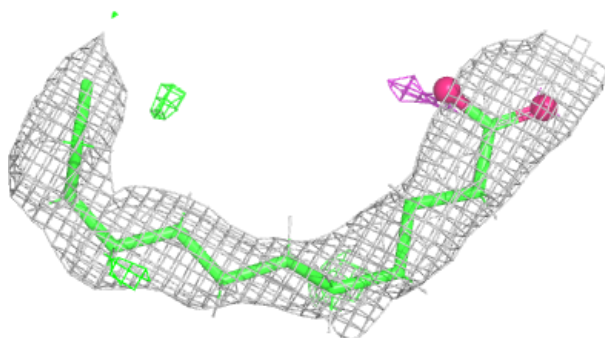


Electron density around STE A 619:

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

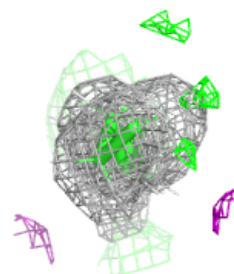
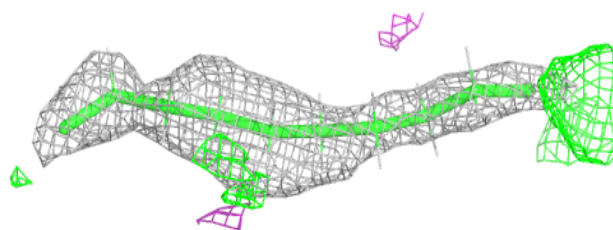
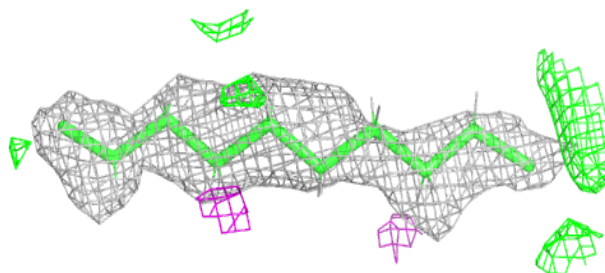
**Electron density around STE C 516:**

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

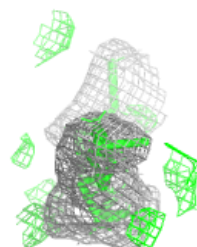
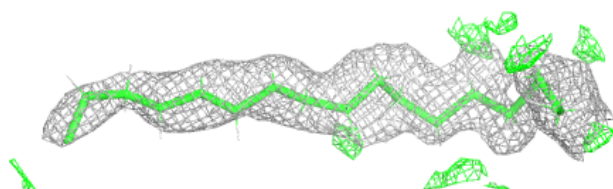
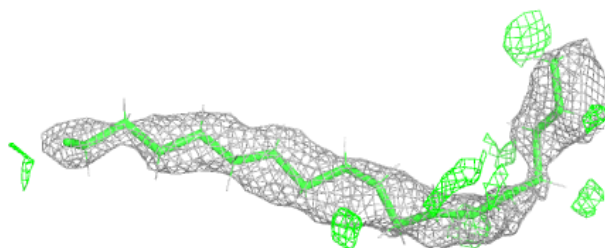


Electron density around STE t 102:

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

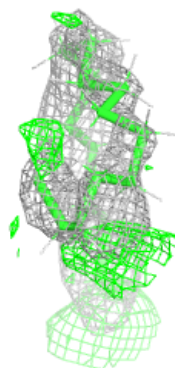
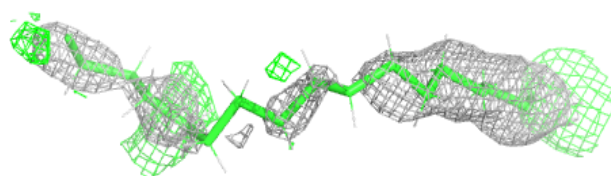
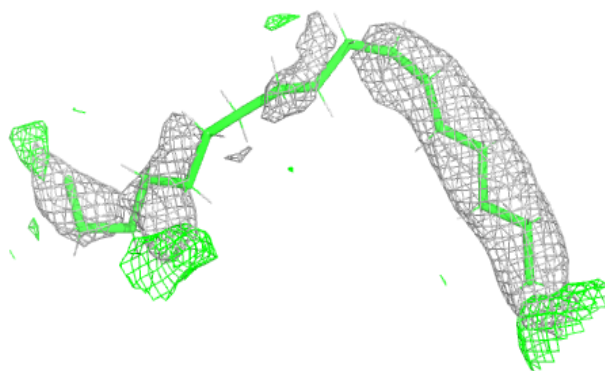
**Electron density around STE c 516:**

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

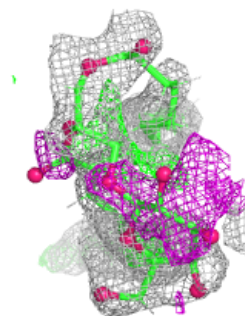
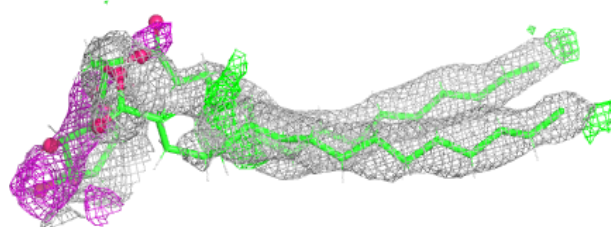
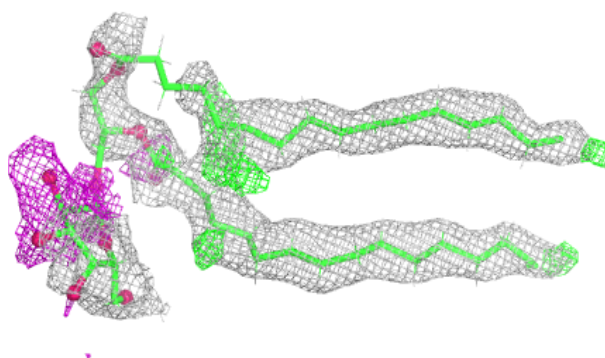


Electron density around STE Z 102:

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

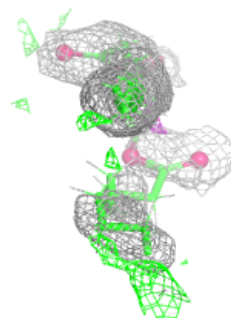
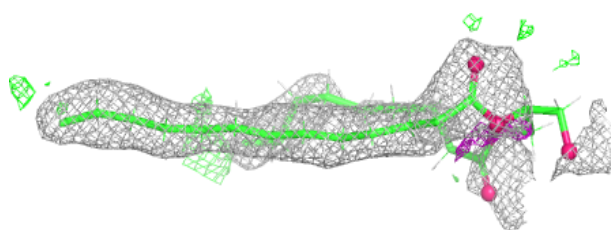
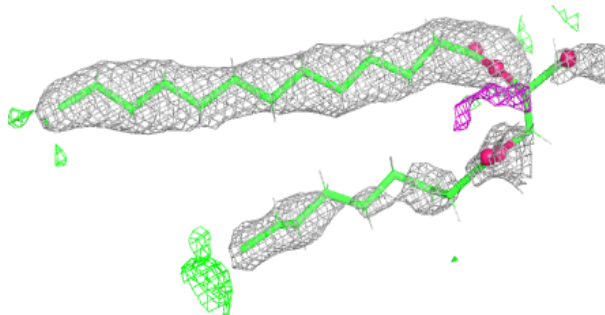
**Electron density around LMG D 406:**

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

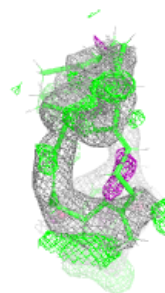
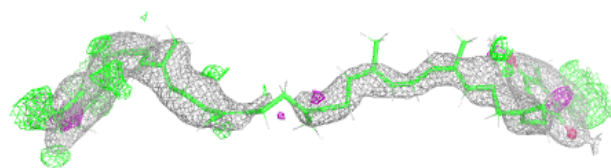
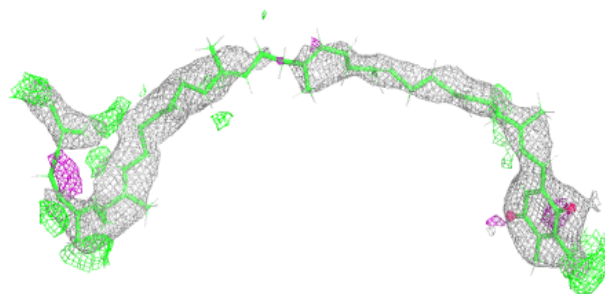


Electron density around LMG c 517:

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

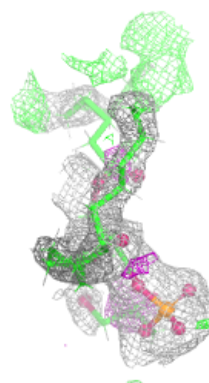
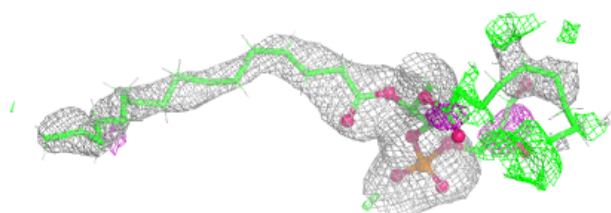
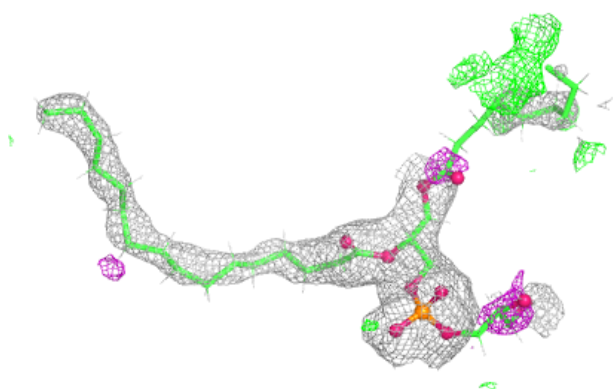
**Electron density around PL9 a 612:**

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

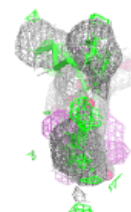
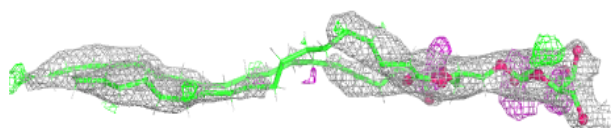
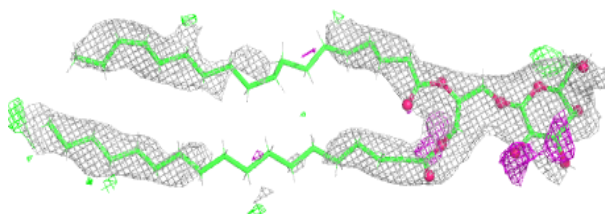


Electron density around LHG e 102:

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

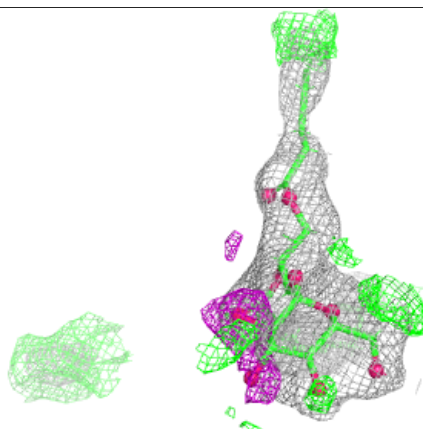
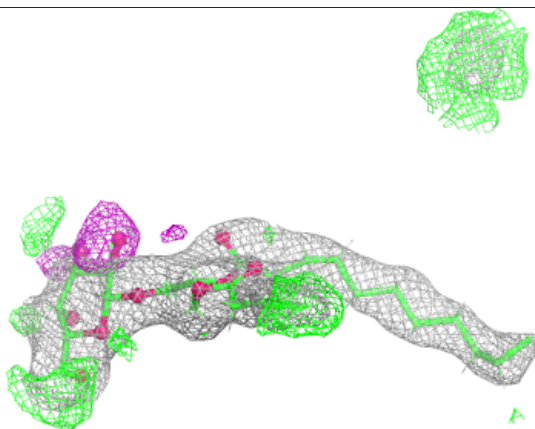
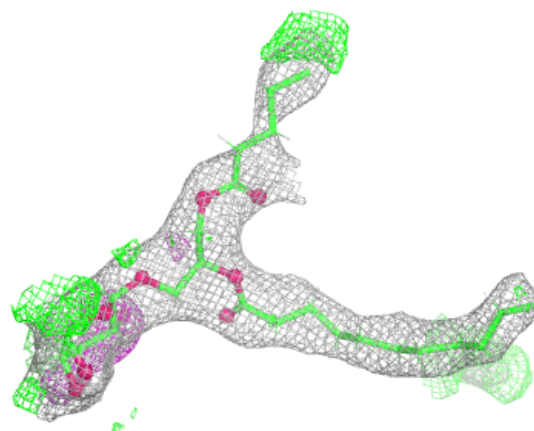
**Electron density around LMG b 622:**

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



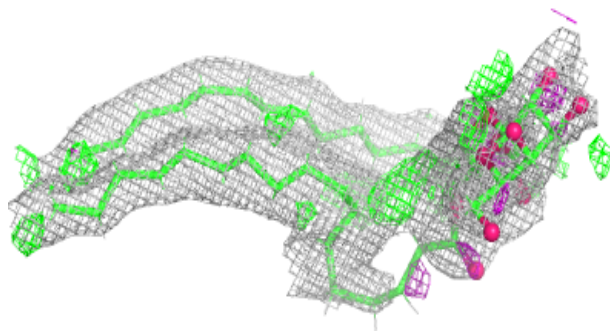
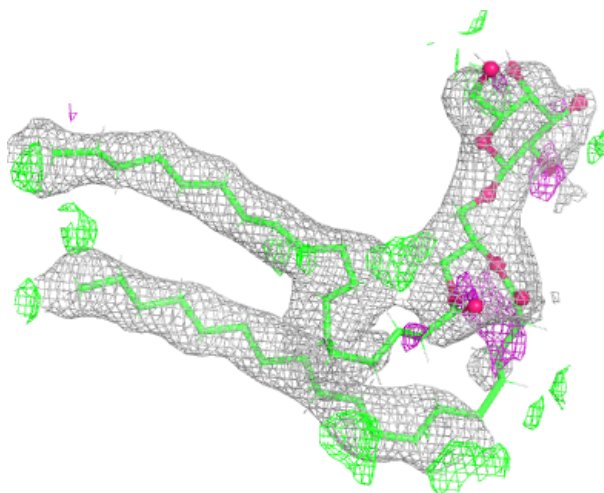
Electron density around LMG C 517:

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



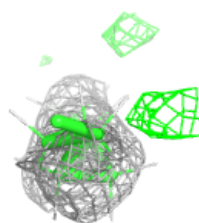
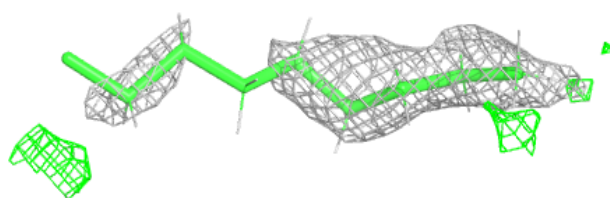
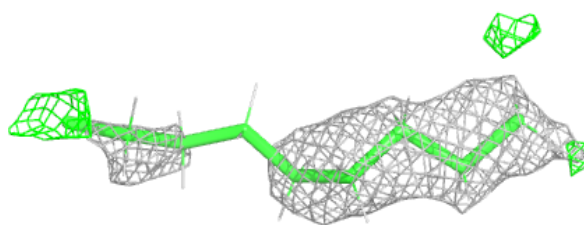
Electron density around LMG a 616:

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

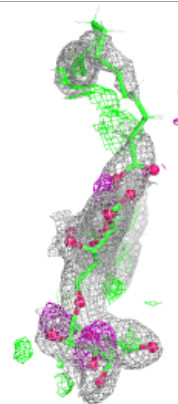
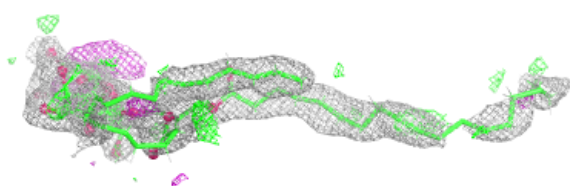
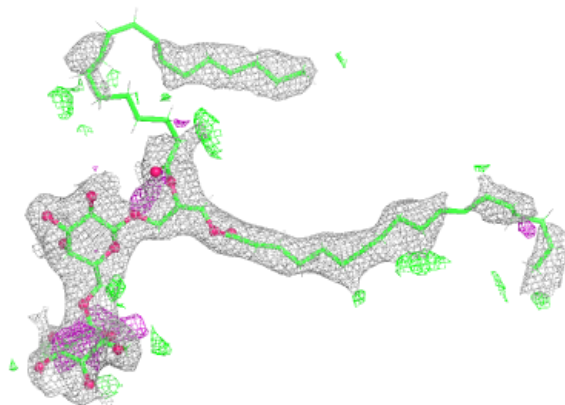


Electron density around STE e 104:

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

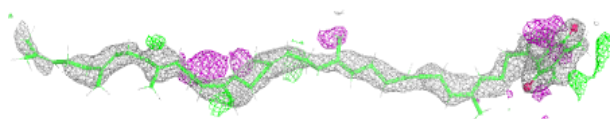
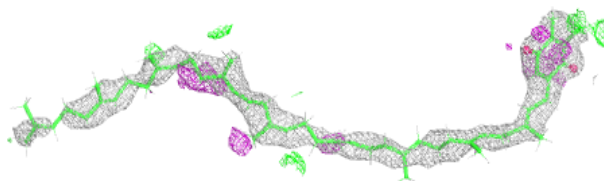
**Electron density around DGD A 617:**

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

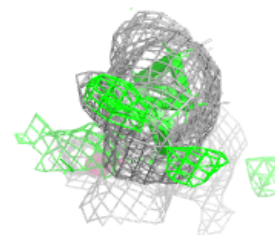
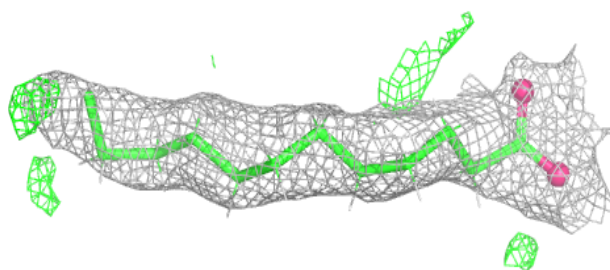
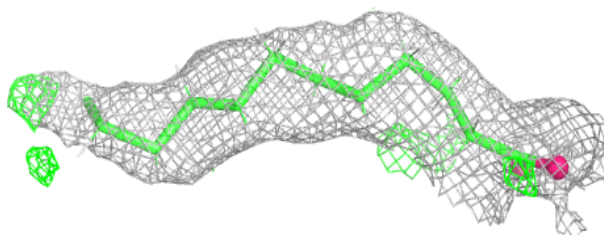


Electron density around PL9 A 612:

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

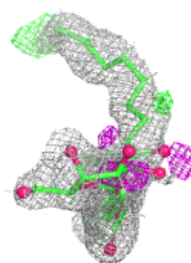
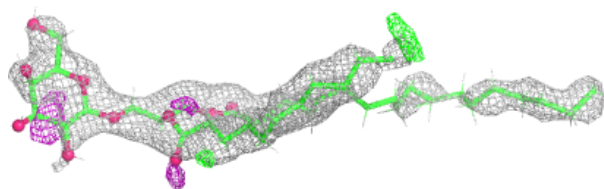
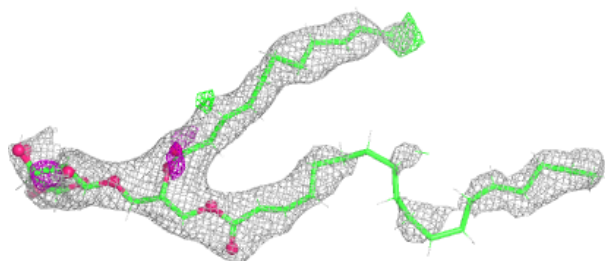
**Electron density around STE k 103:**

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

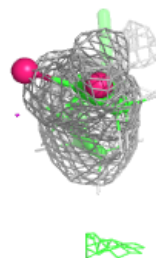
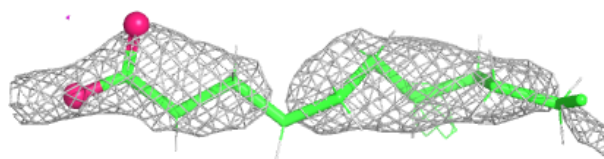
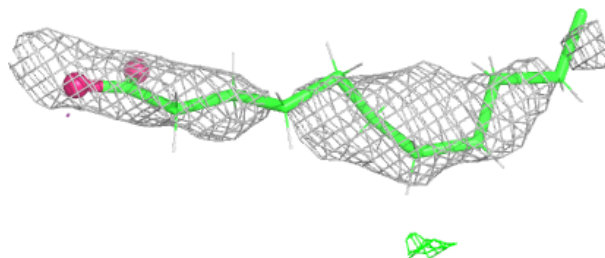


Electron density around LMG c 522:

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

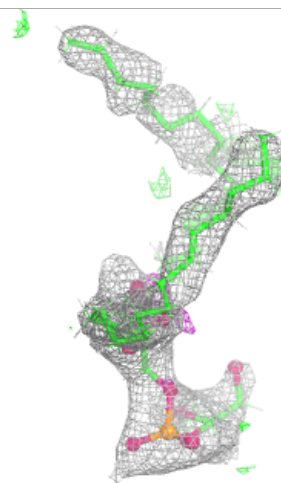
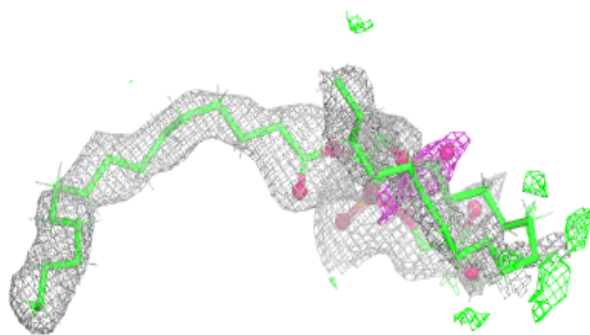
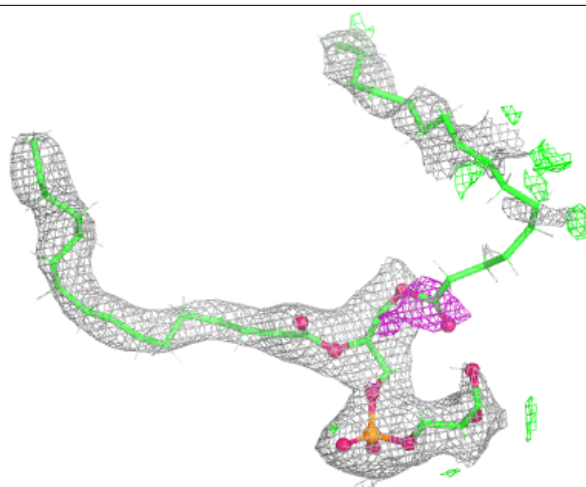
**Electron density around STE e 105:**

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



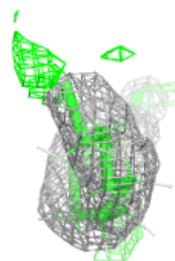
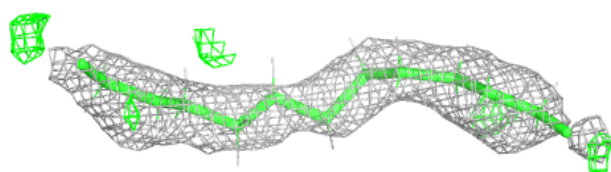
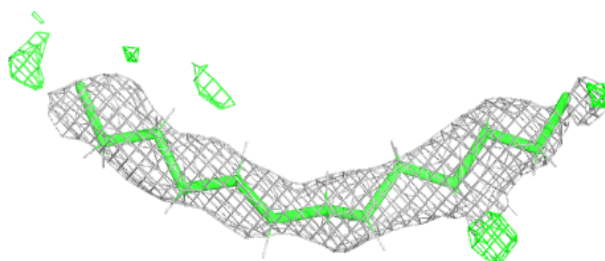
Electron density around LHG E 101:

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

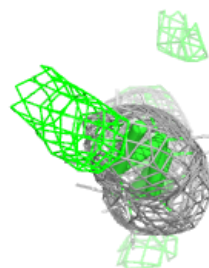
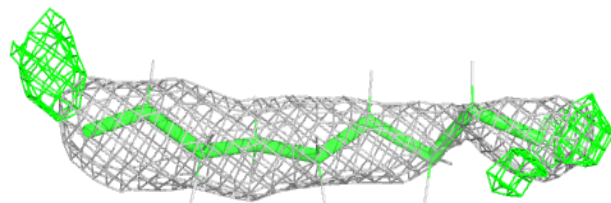
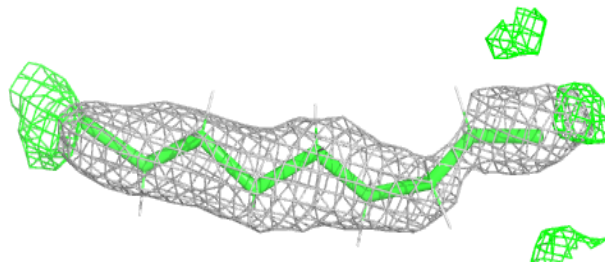


Electron density around STE z 701:

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

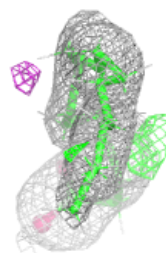
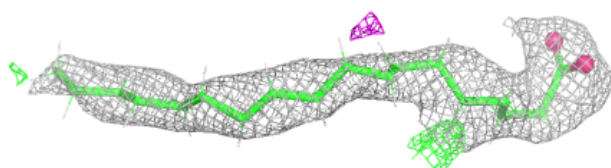
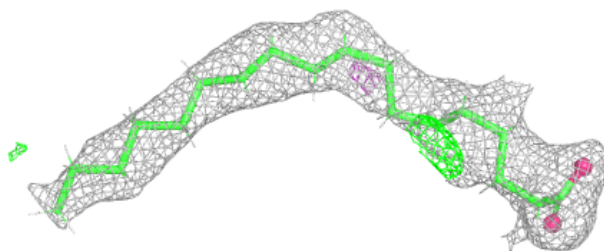
**Electron density around STE z 702:**

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

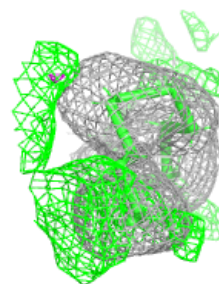
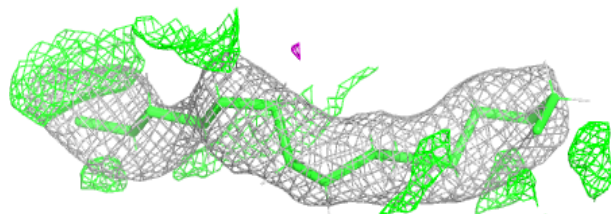
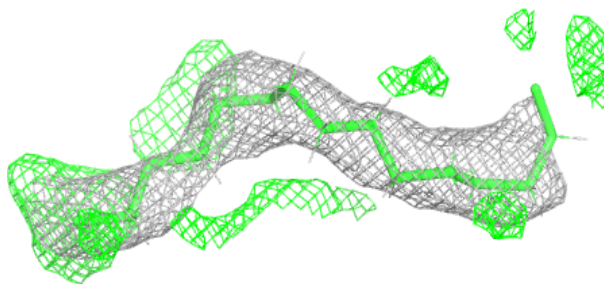


Electron density around STE d 410:

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

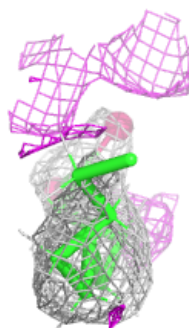
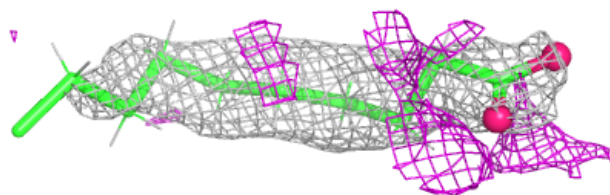
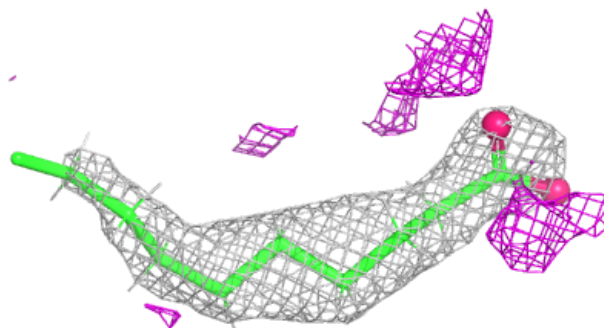
**Electron density around STE B 627:**

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

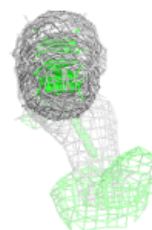
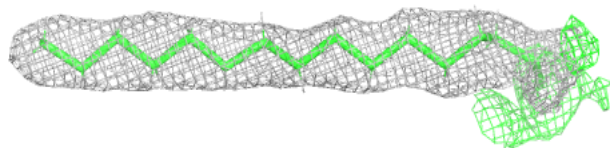
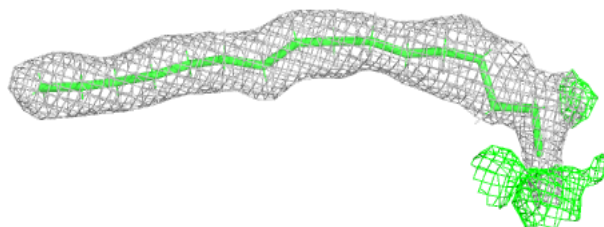


Electron density around STE B 626:

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

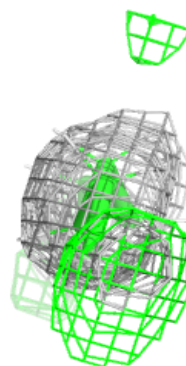
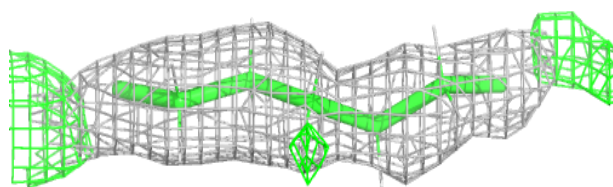
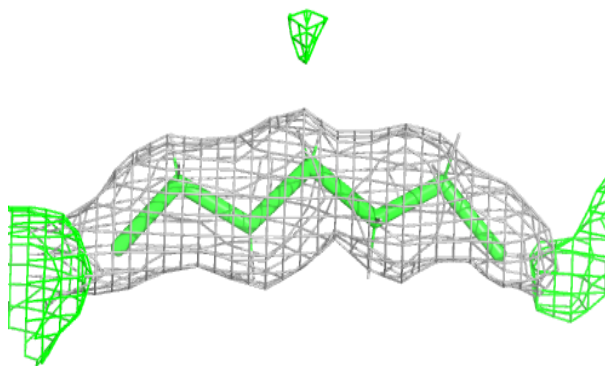
**Electron density around STE C 526:**

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

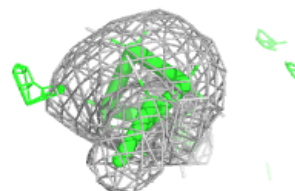
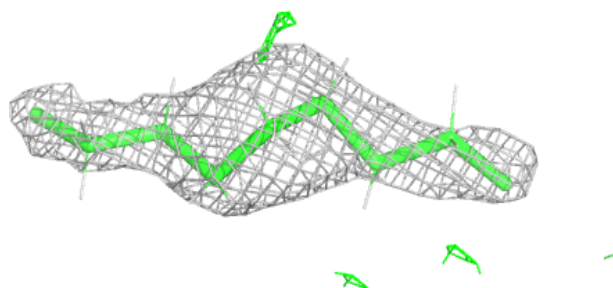
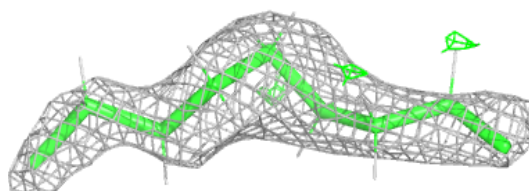


Electron density around STE C 519:

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

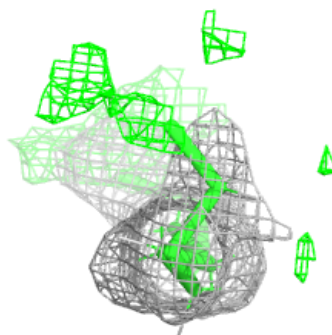
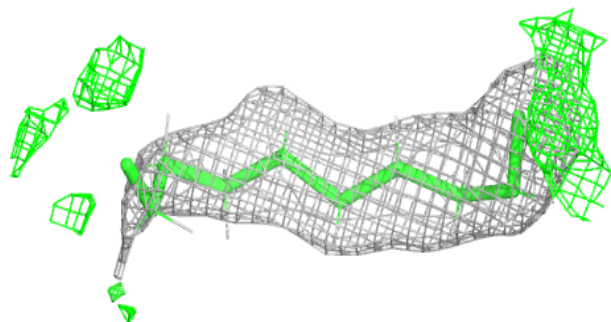
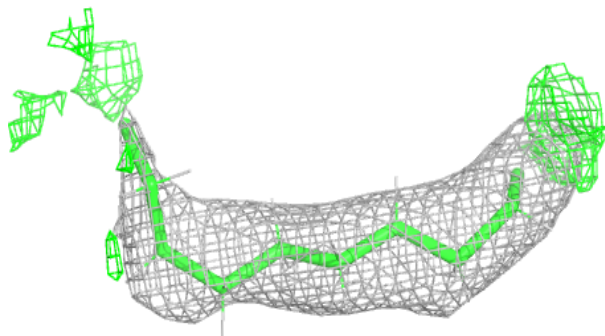
**Electron density around STE A 613:**

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

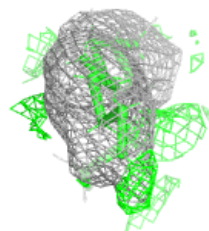
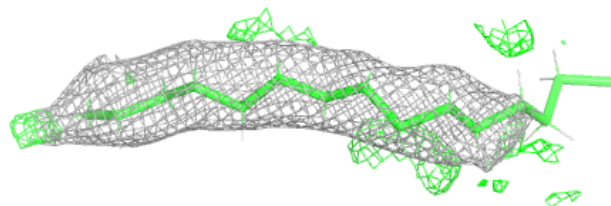
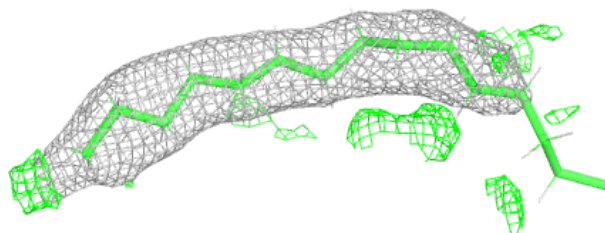


Electron density around STE b 624:

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

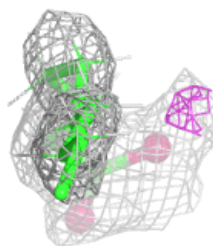
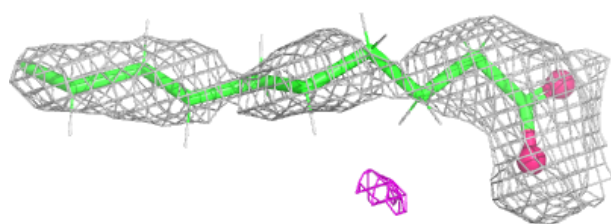
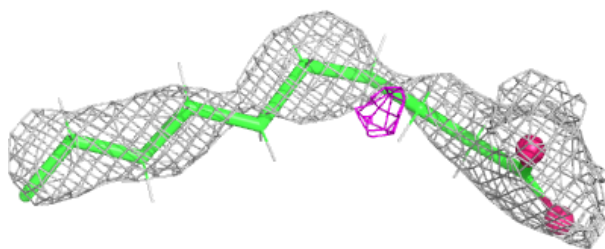
**Electron density around STE T 103:**

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

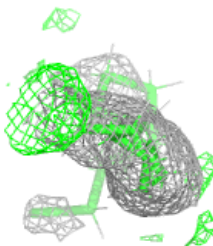
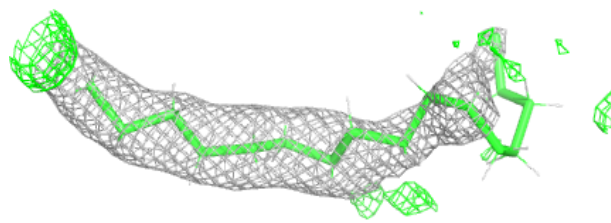
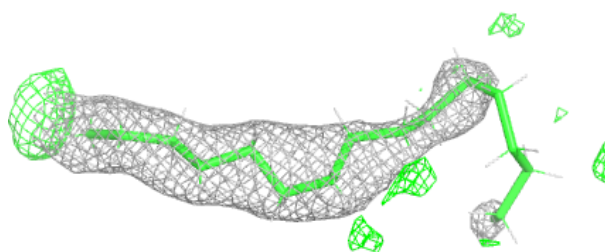


Electron density around STE E 102:

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

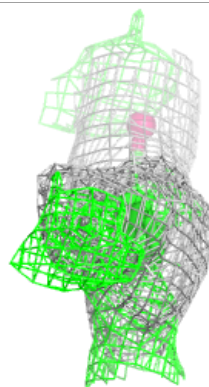
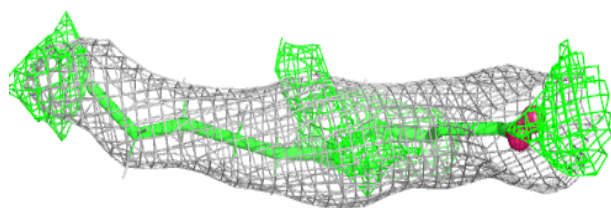
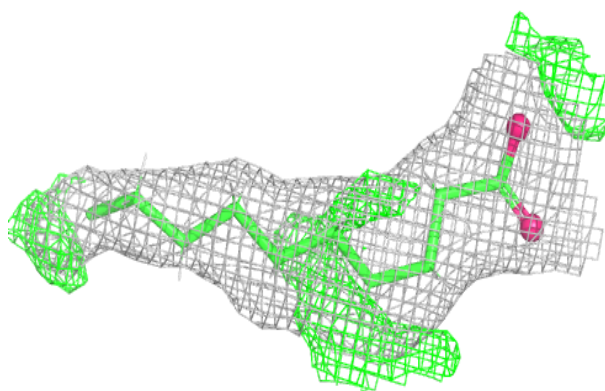
**Electron density around STE T 102:**

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

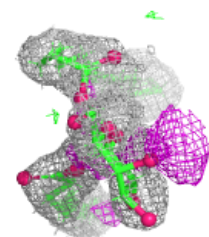
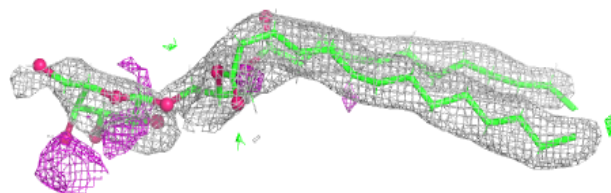
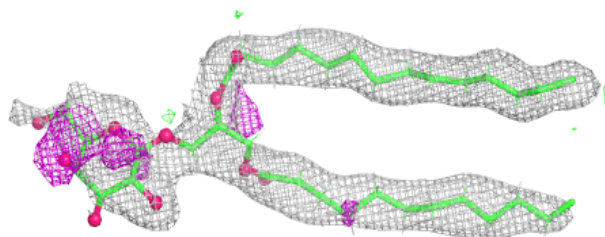


Electron density around STE C 525:

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

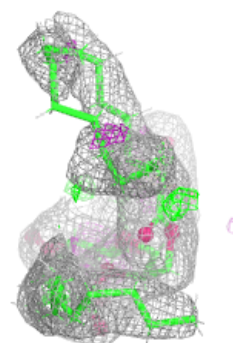
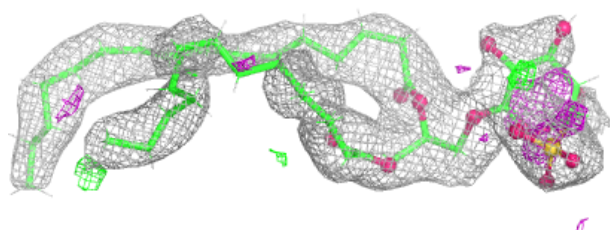
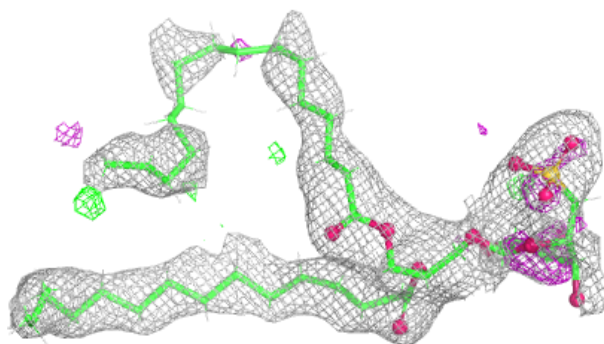
**Electron density around LMG B 620:**

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

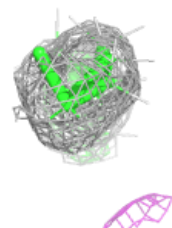
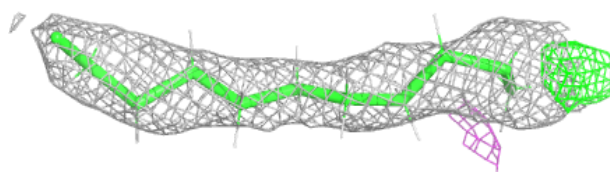
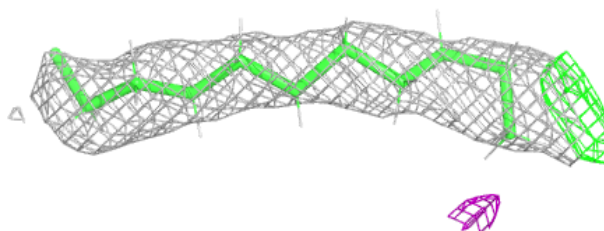


Electron density around SQD a 615:

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

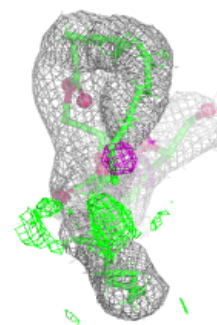
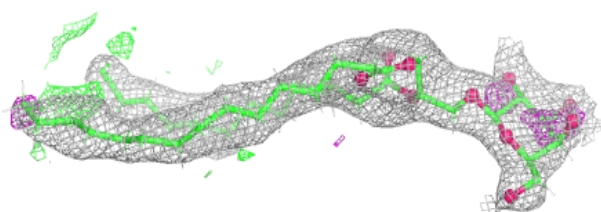
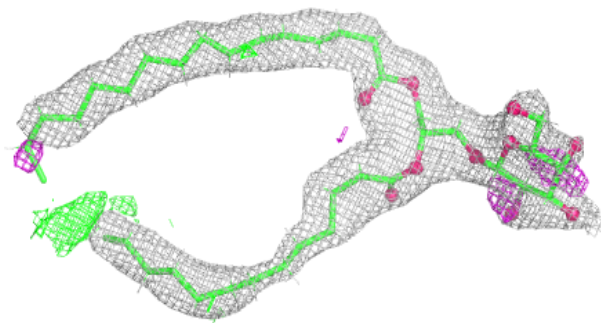
**Electron density around STE b 625:**

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

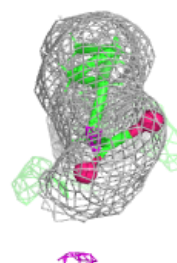
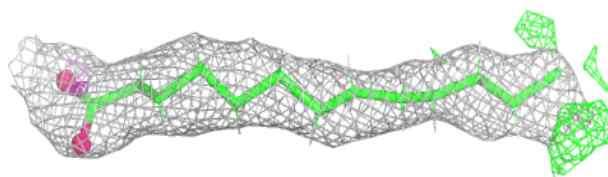
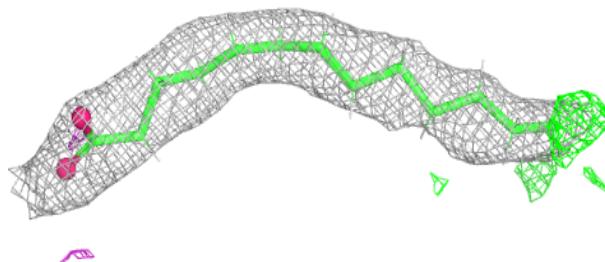


Electron density around LMG A 615:

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

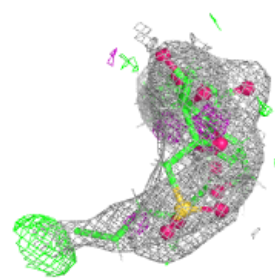
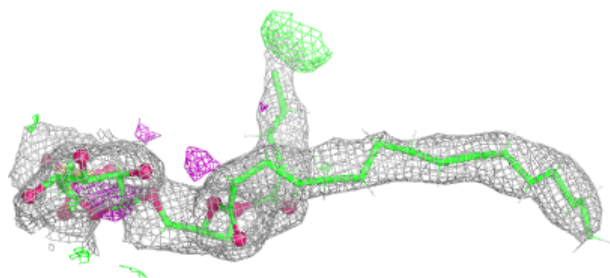
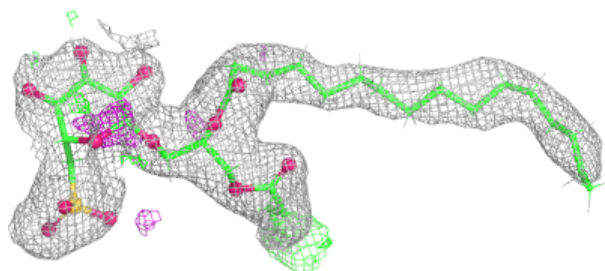
**Electron density around STE I 102:**

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

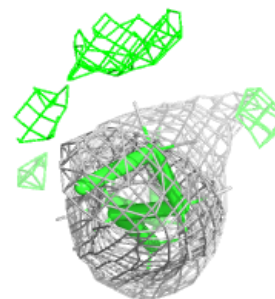
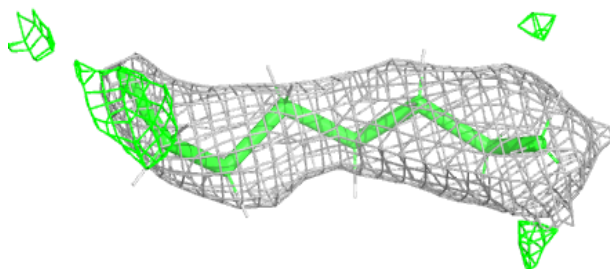
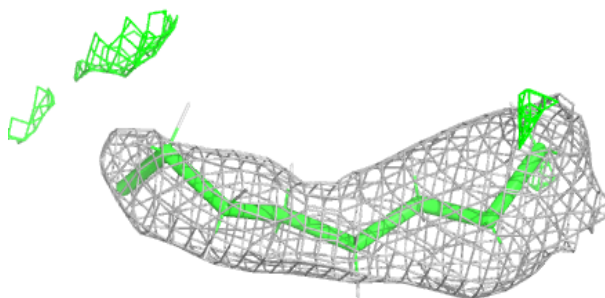


Electron density around SQD A 616:

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

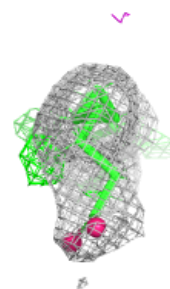
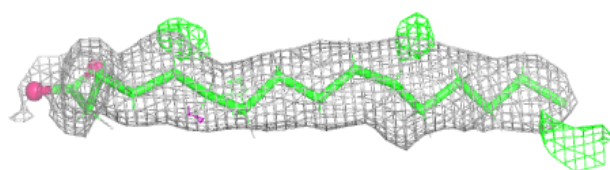
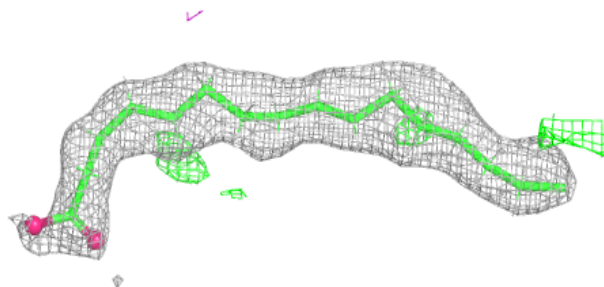
**Electron density around STE A 618:**

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

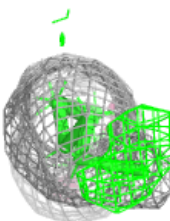
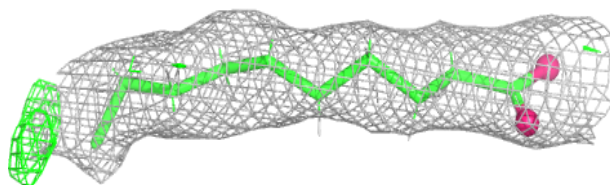
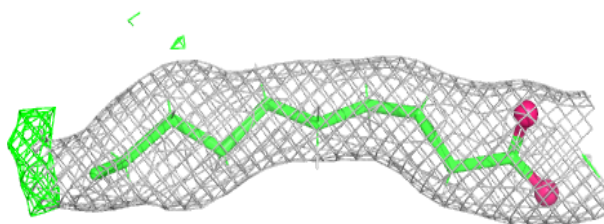


Electron density around STE B 625:

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

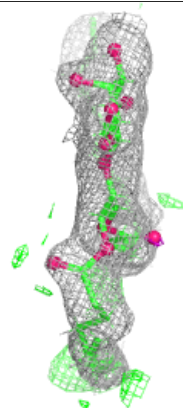
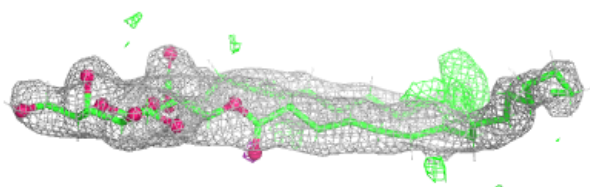
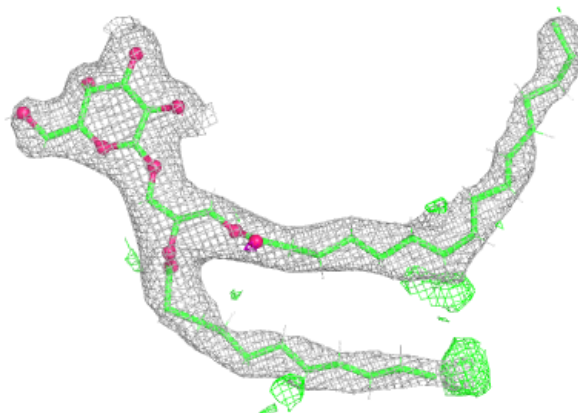
**Electron density around STE j 101:**

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

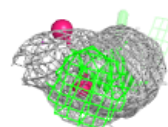
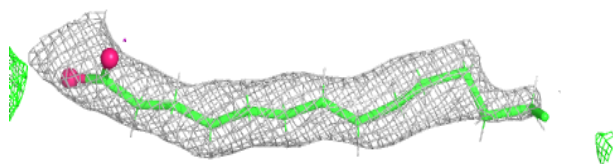
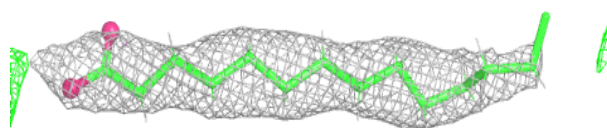


Electron density around LMG c 521:

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

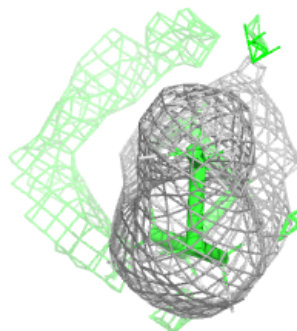
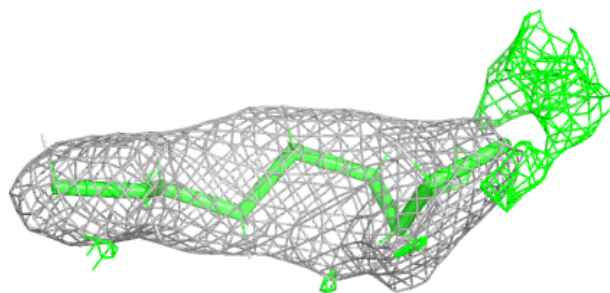
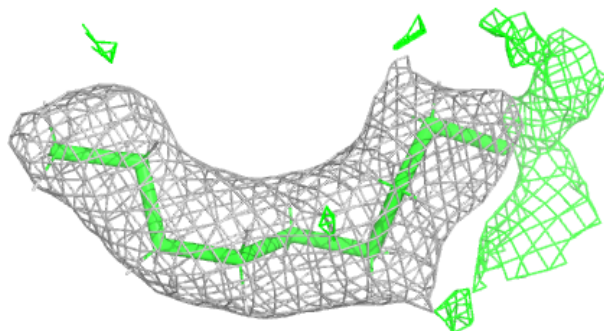
**Electron density around STE b 623:**

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

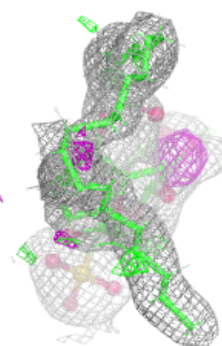
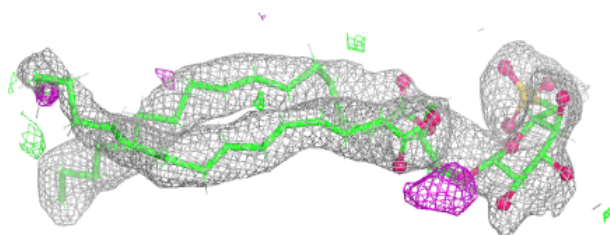
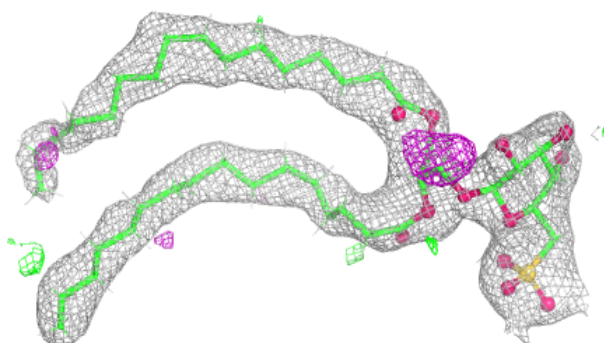


Electron density around STE H 104:

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

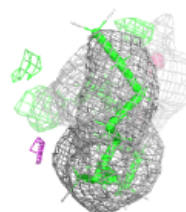
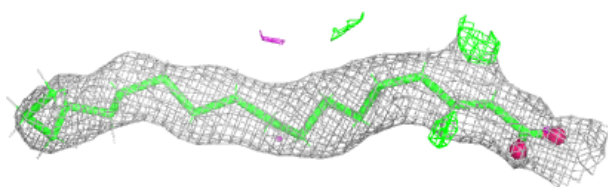
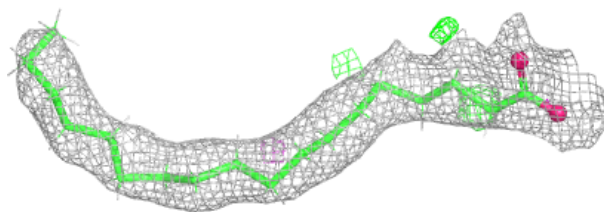
**Electron density around SQD B 623:**

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

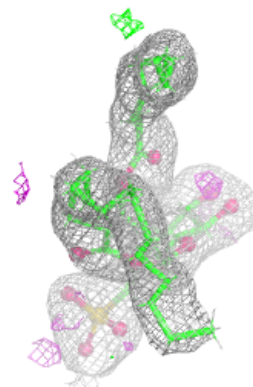
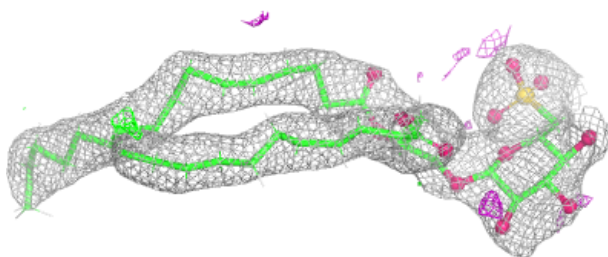
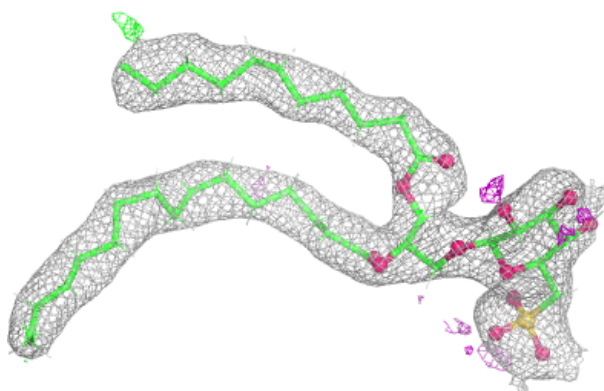


Electron density around STE b 621:

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

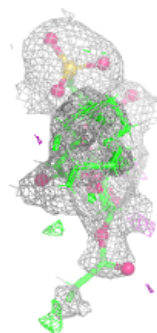
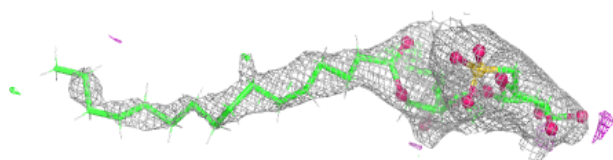
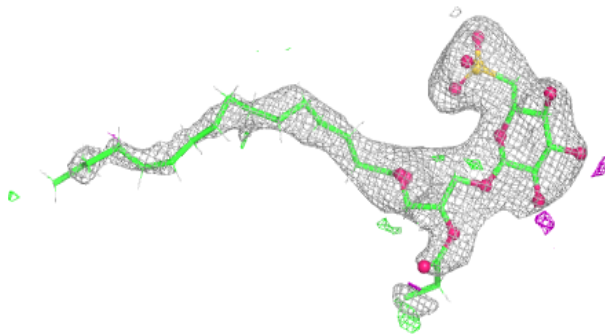
**Electron density around SQD b 620:**

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

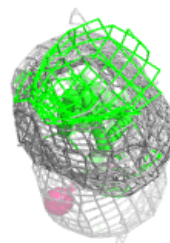
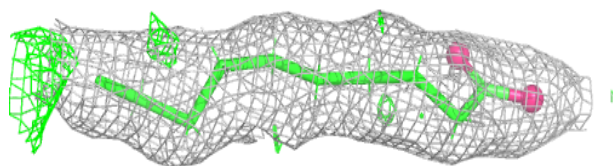
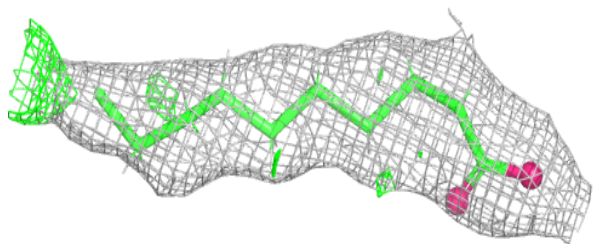


Electron density around SQD f 102:

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

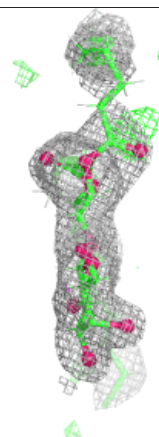
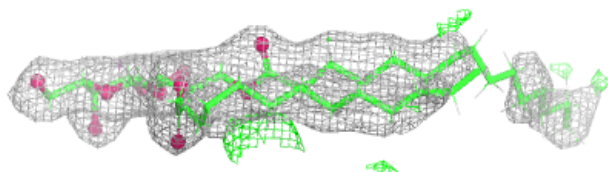
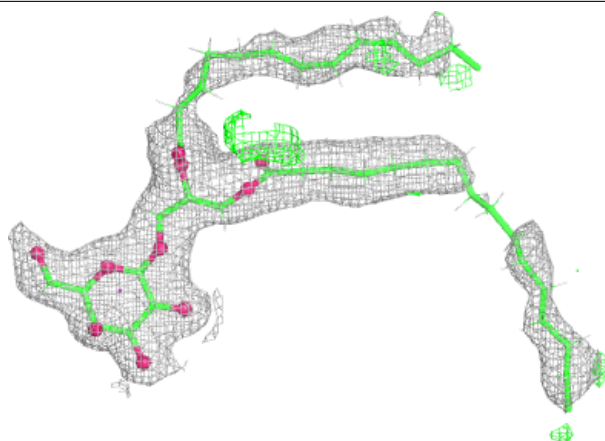
**Electron density around STE J 101:**

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

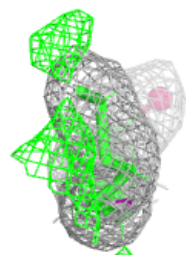
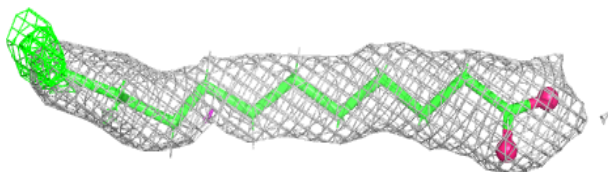
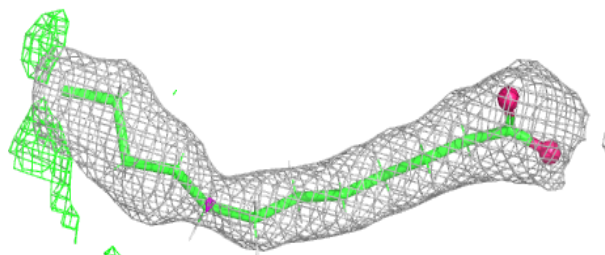


Electron density around LMG C 524:

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

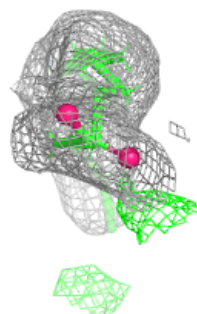
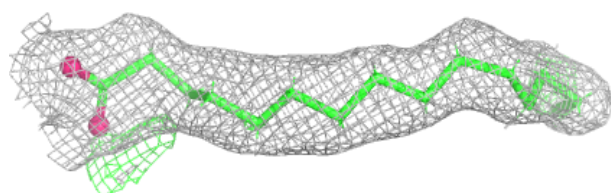
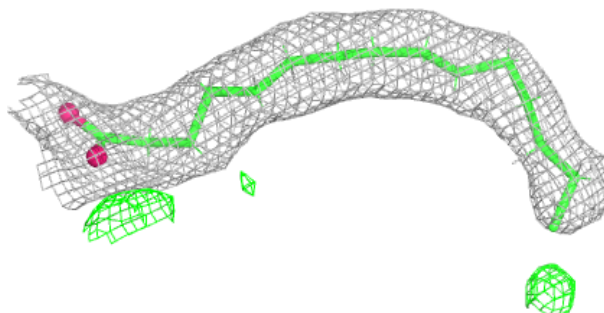
**Electron density around STE B 624:**

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

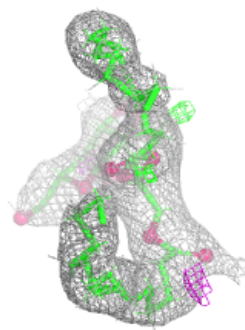
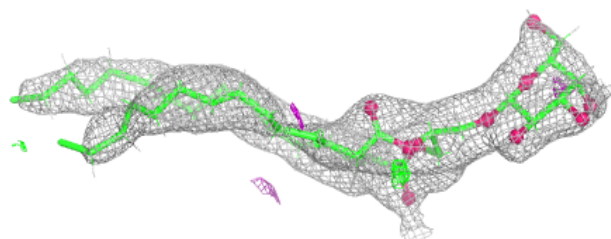
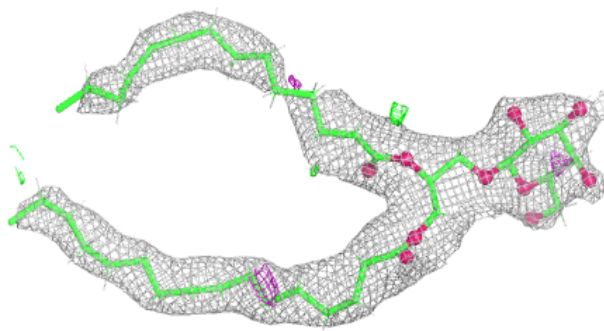


Electron density around STE B 621:

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

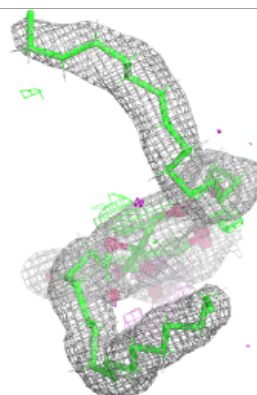
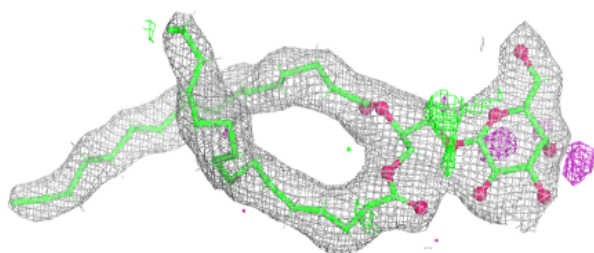
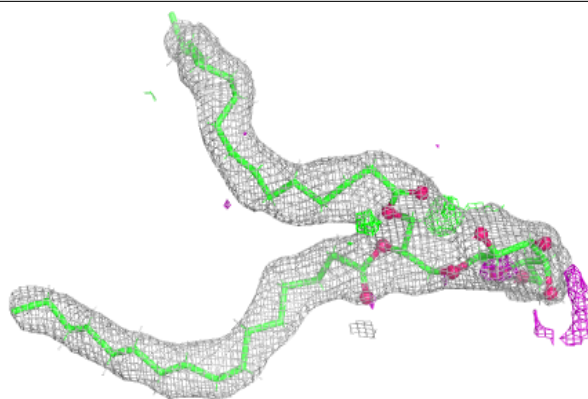
**Electron density around LMG a 617:**

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

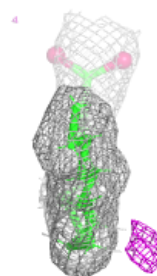
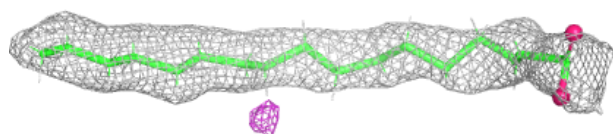
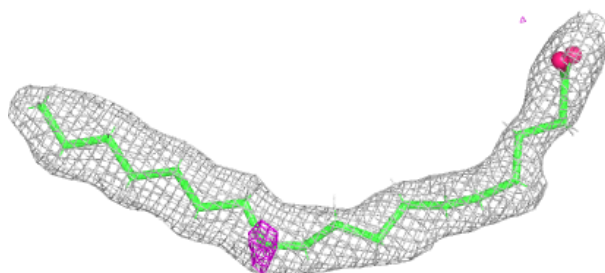


Electron density around LMG m 101:

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

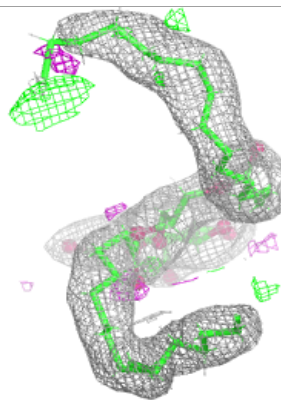
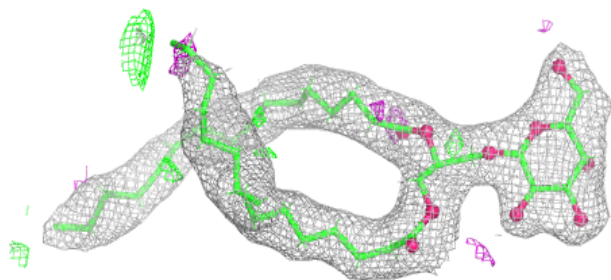
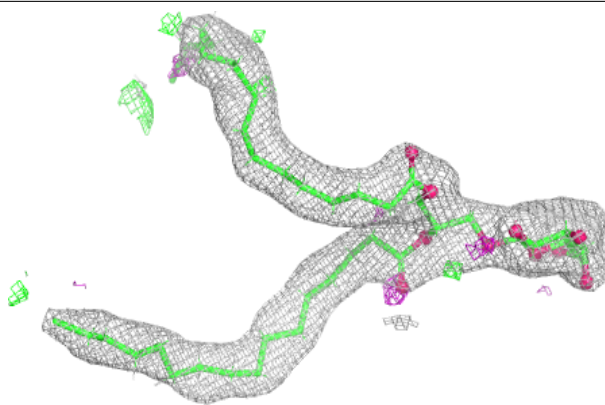
**Electron density around STE d 412:**

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



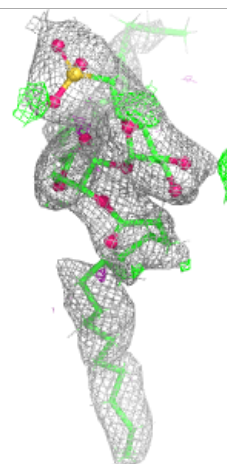
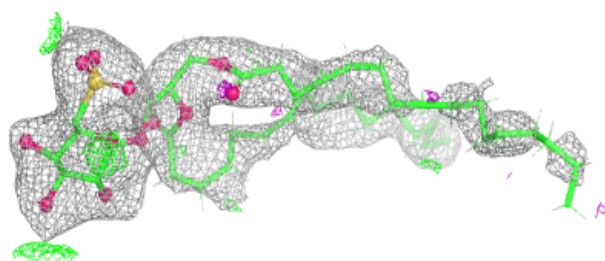
Electron density around LMG M 101:

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



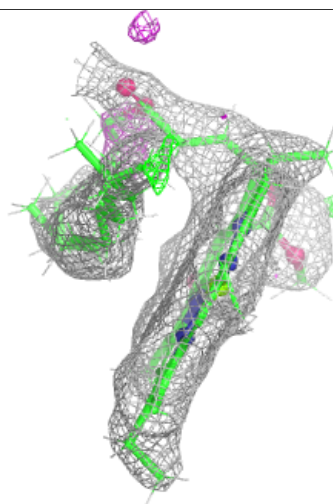
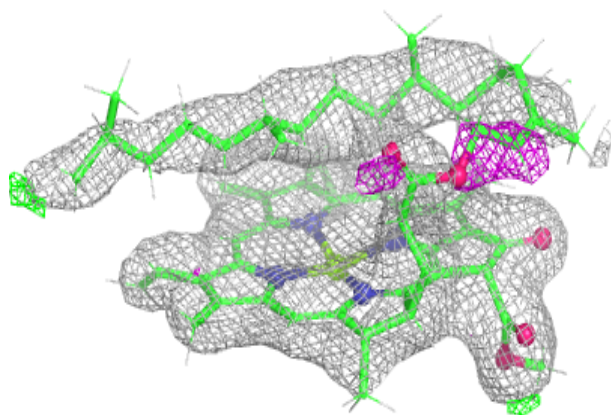
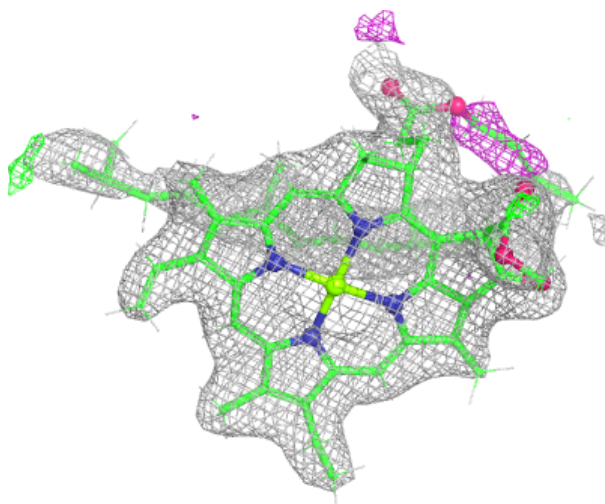
Electron density around SQD a 614:

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



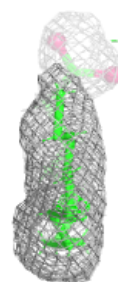
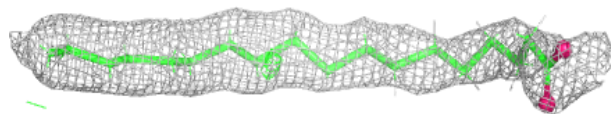
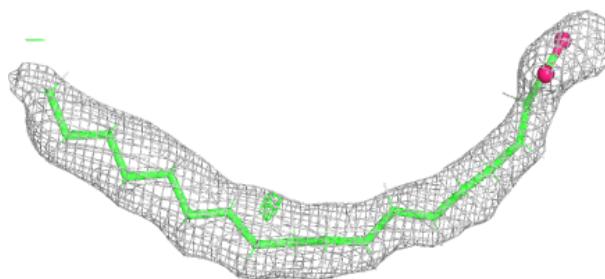
Electron density around CLA b 601:

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

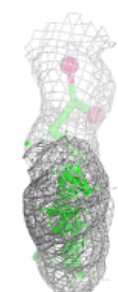
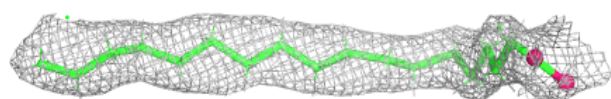
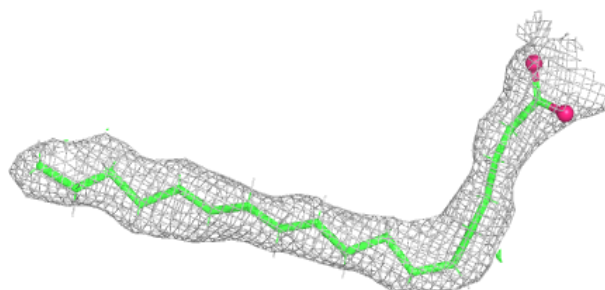


Electron density around STE D 412:

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

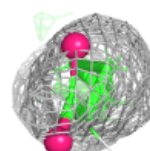
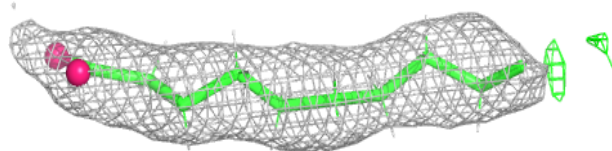
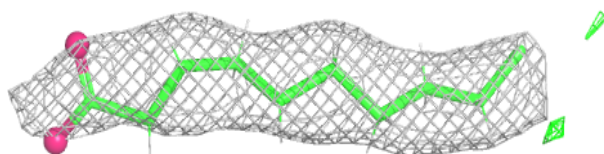
**Electron density around STE d 406:**

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

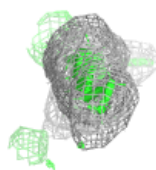
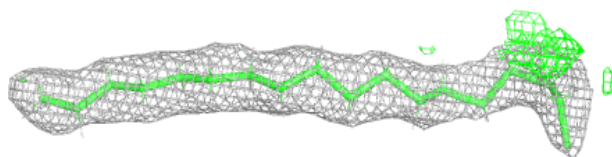
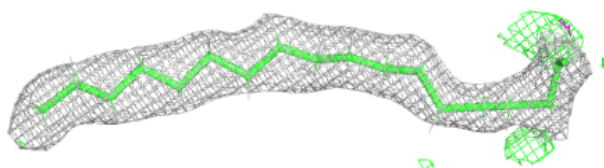


Electron density around STE m 102:

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

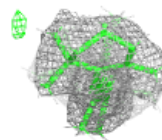
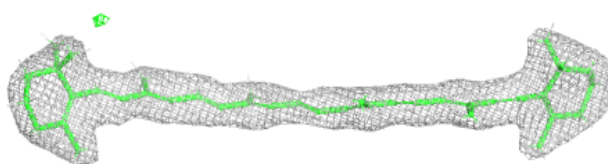
**Electron density around STE m 103:**

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



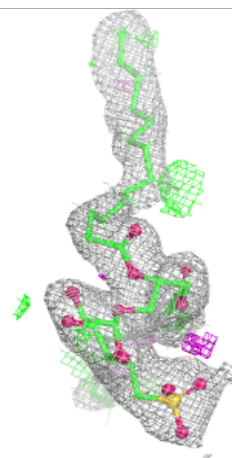
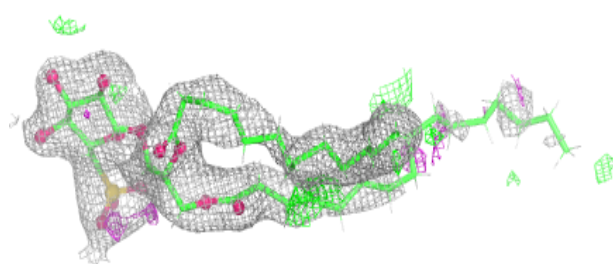
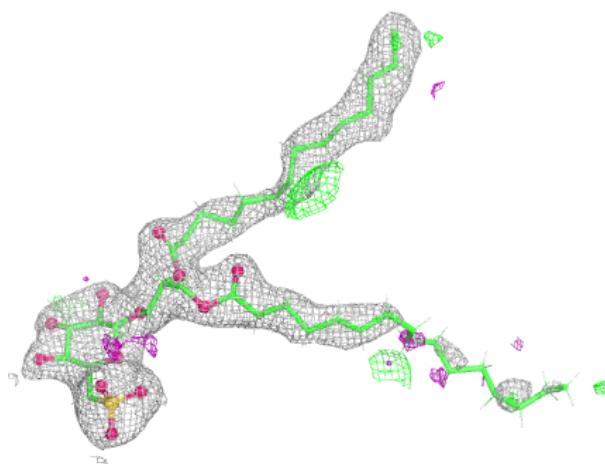
Electron density around BCR c 514:

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



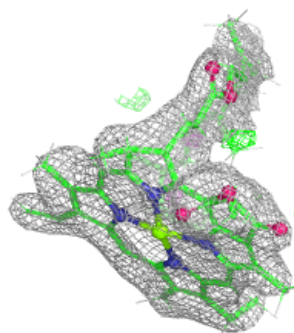
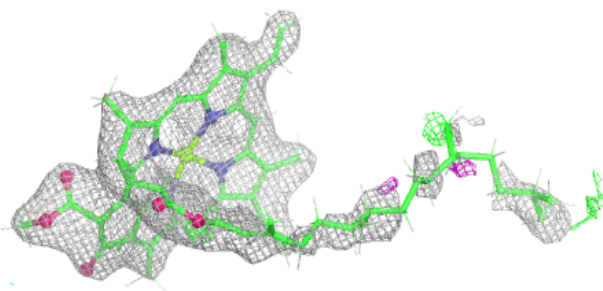
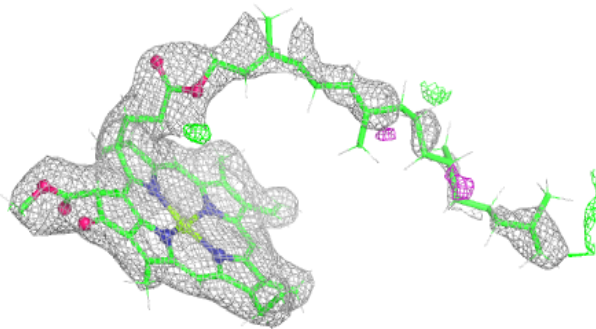
Electron density around SQD D 410:

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

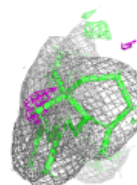
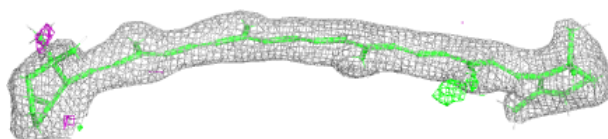
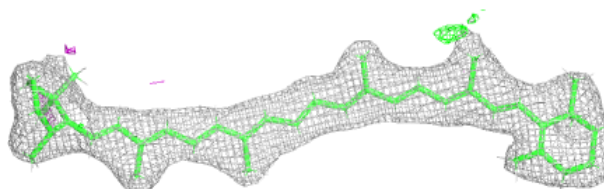


Electron density around CLA c 513:

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

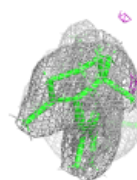
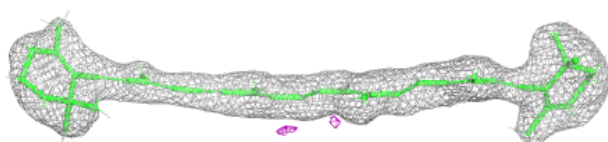
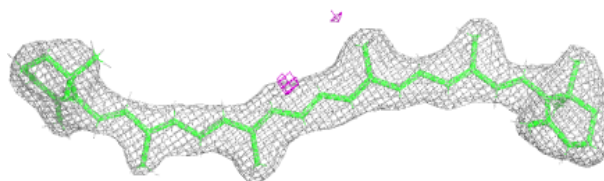
**Electron density around BCR d 404:**

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

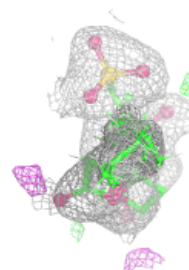
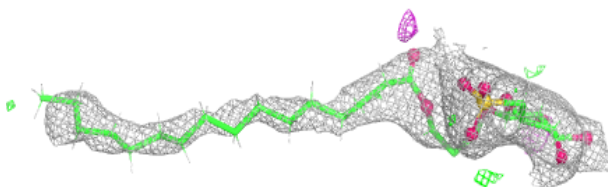
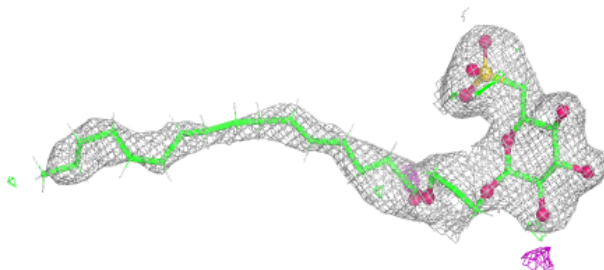


Electron density around BCR k 101:

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

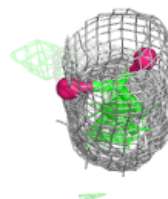
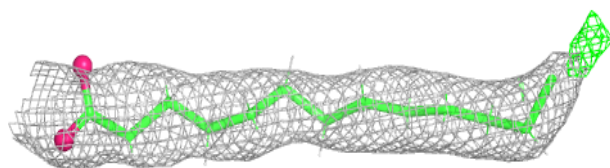
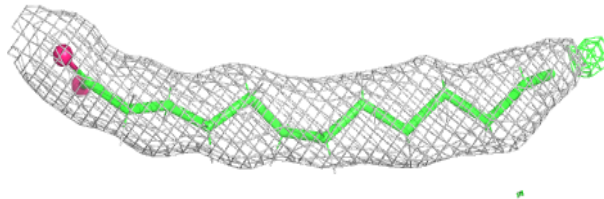
**Electron density around SQD F 102:**

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

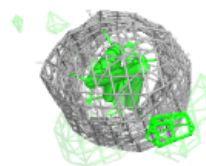
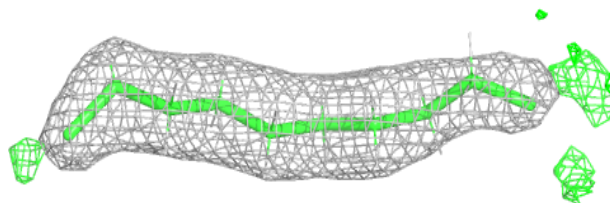
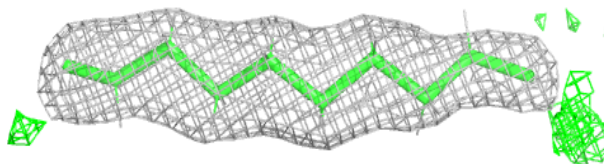


Electron density around STE M 102:

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

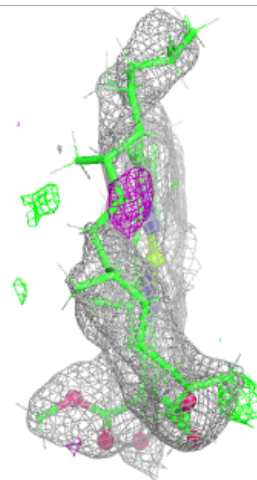
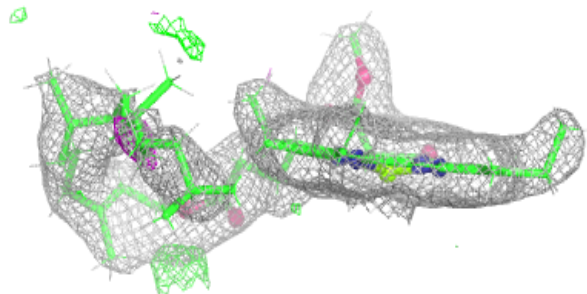
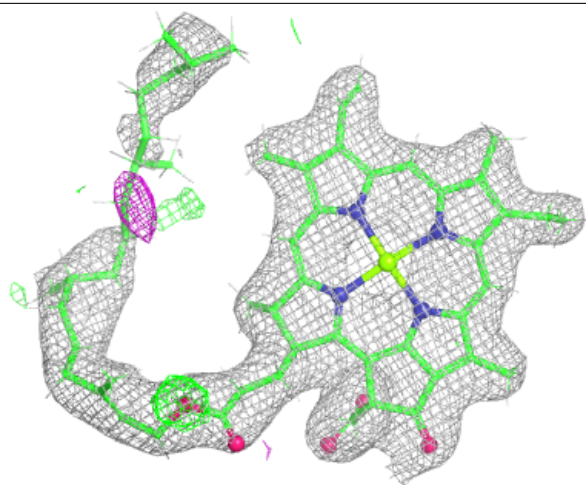
**Electron density around STE M 103:**

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



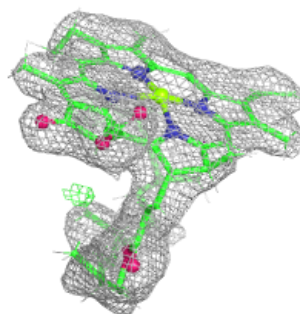
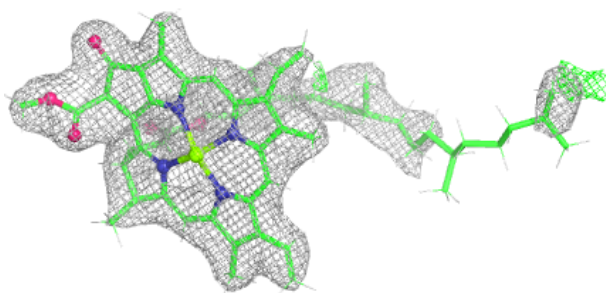
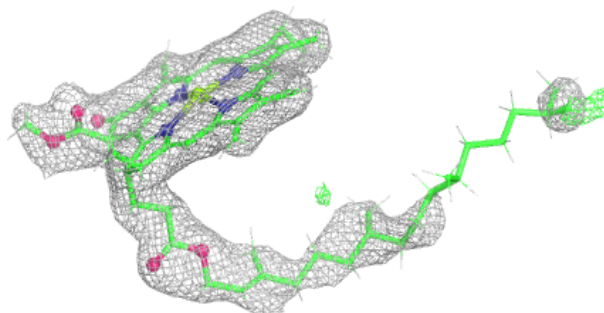
Electron density around CLA c 512:

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

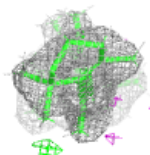
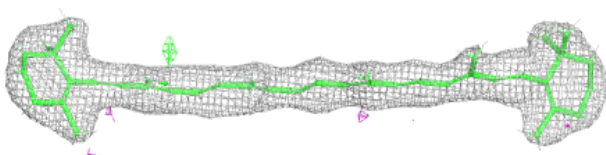


Electron density around CLA C 513:

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

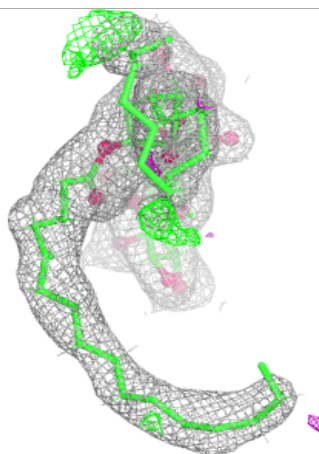
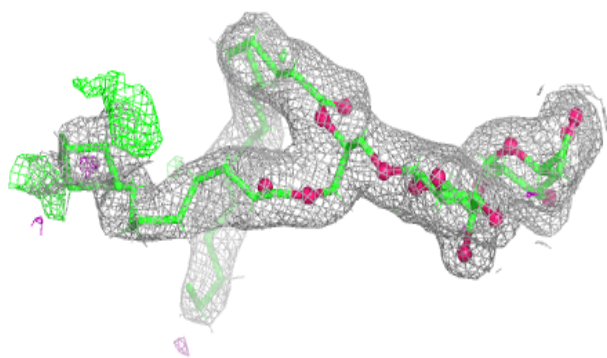
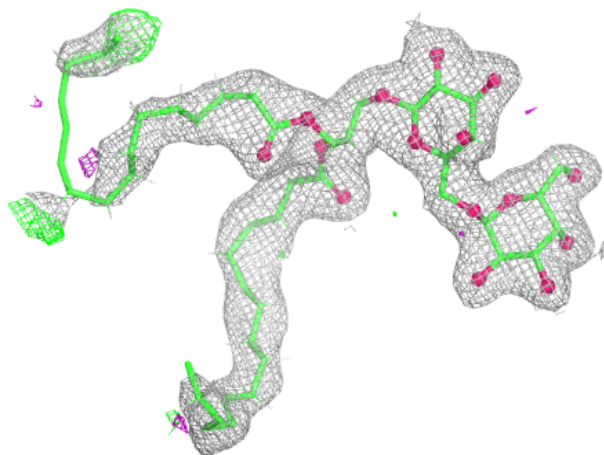
**Electron density around BCR C 514:**

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



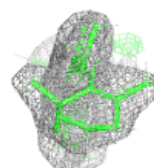
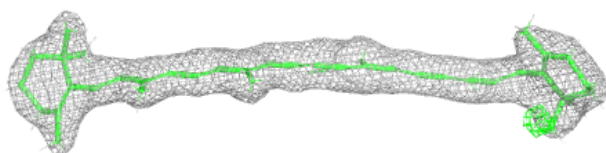
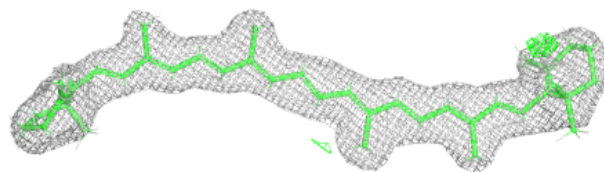
Electron density around DGD C 522:

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

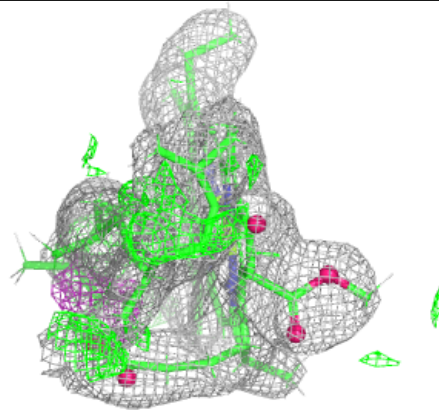
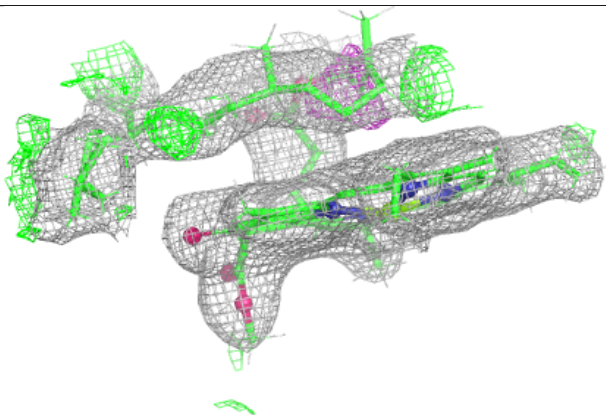
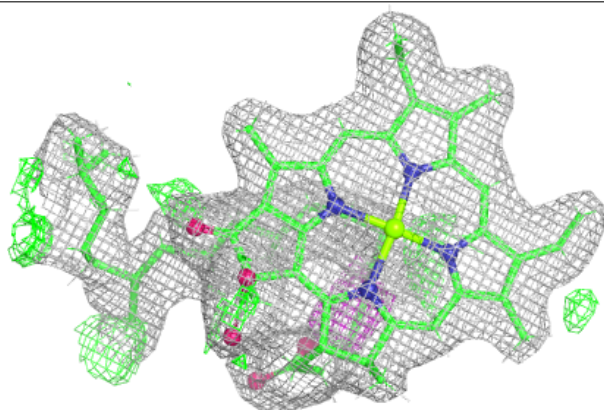


Electron density around BCR Z 101:

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

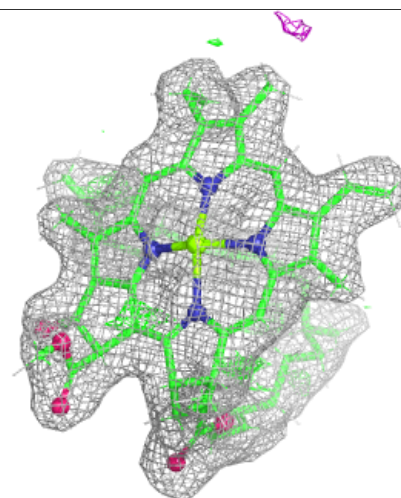
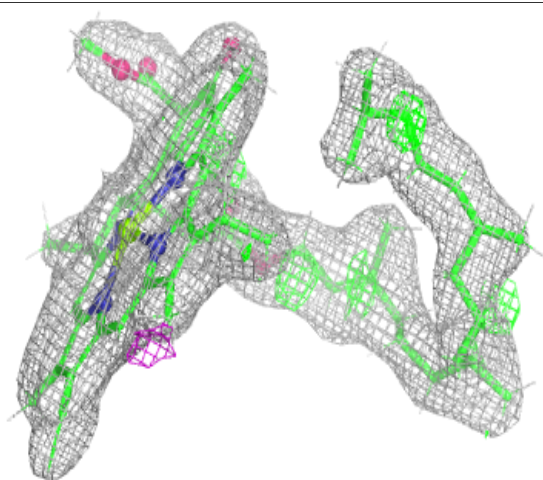
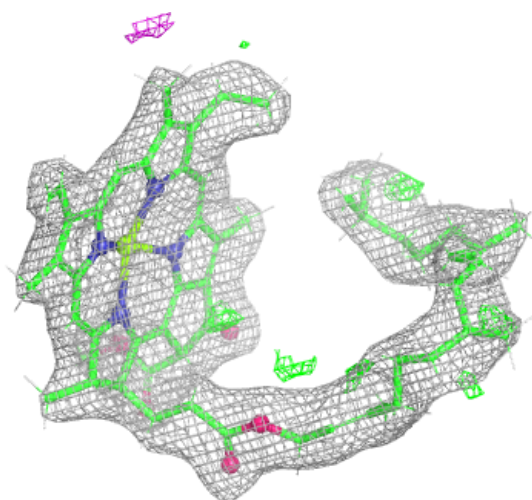
**Electron density around CLA B 601:**

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



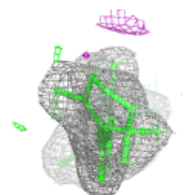
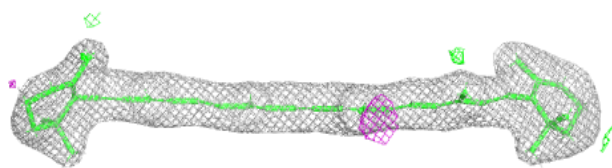
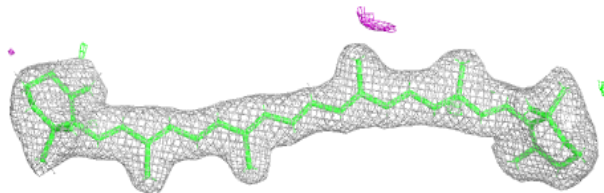
Electron density around CLA c 503:

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

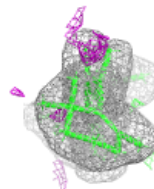
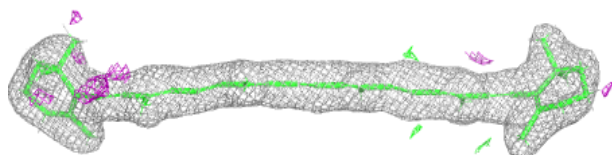
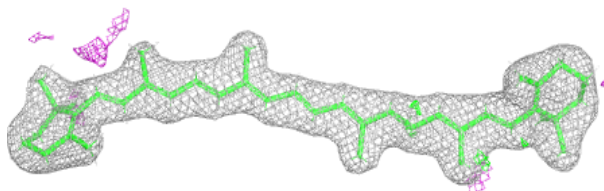


Electron density around BCR b 618:

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

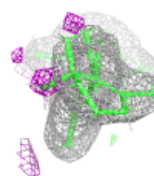
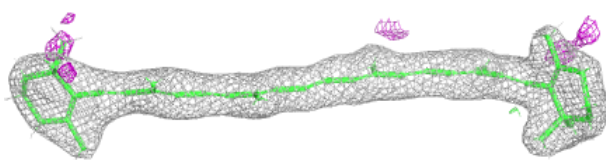
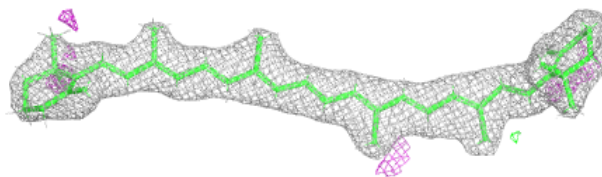
**Electron density around BCR B 618:**

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

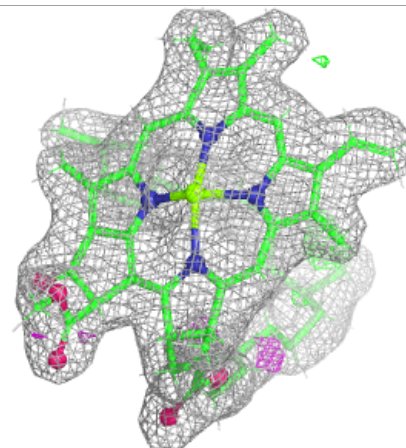
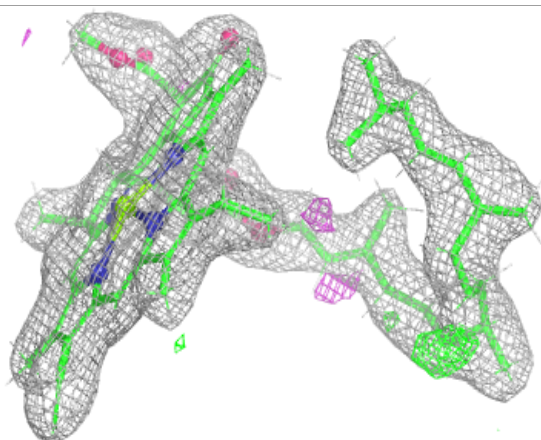
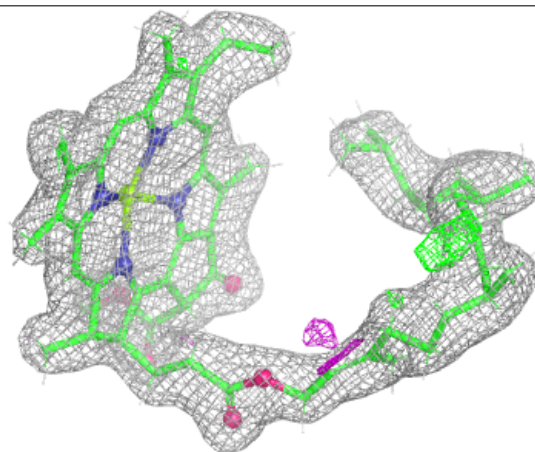


Electron density around BCR c 515:

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

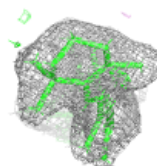
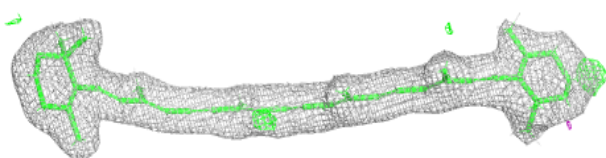
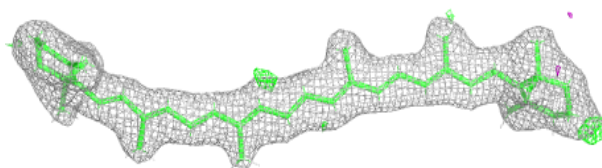
**Electron density around CLA C 503:**

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

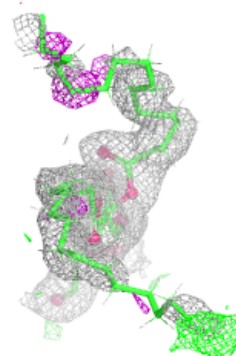
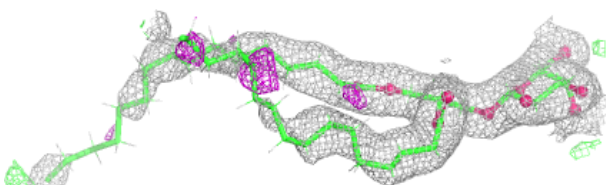
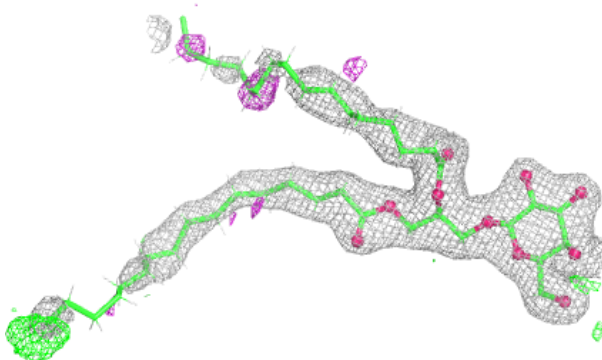


Electron density around BCR H 101:

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

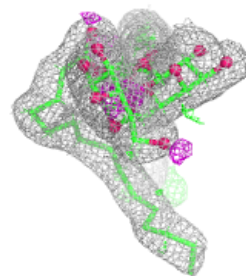
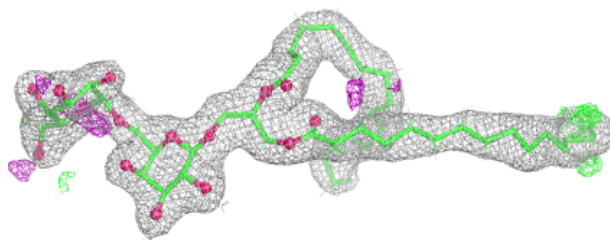
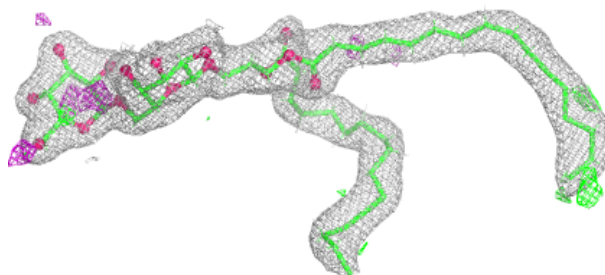
**Electron density around LMG D 407:**

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

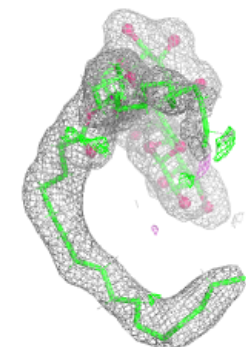
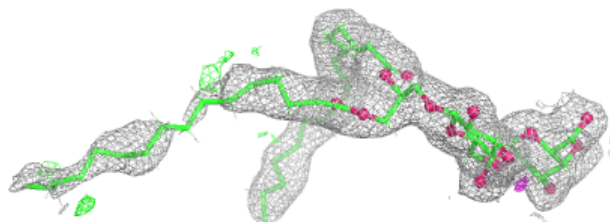
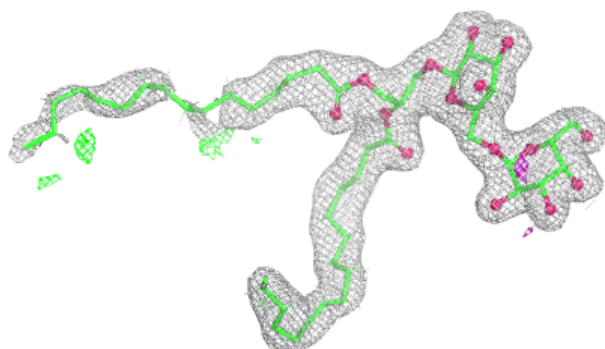


Electron density around DGD H 102:

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

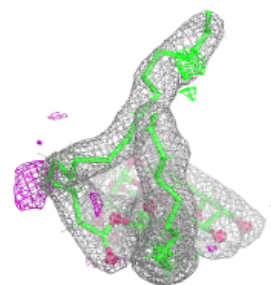
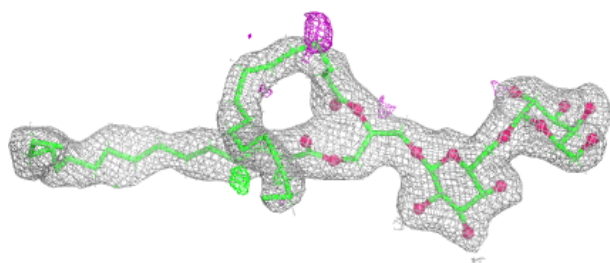
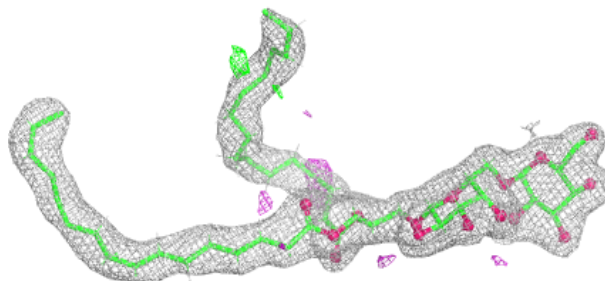
**Electron density around DGD c 519:**

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

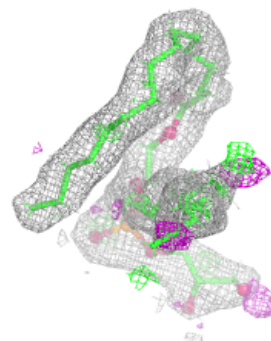
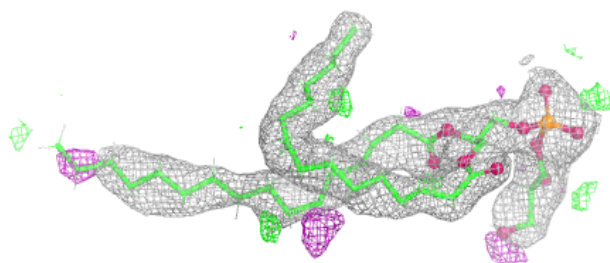
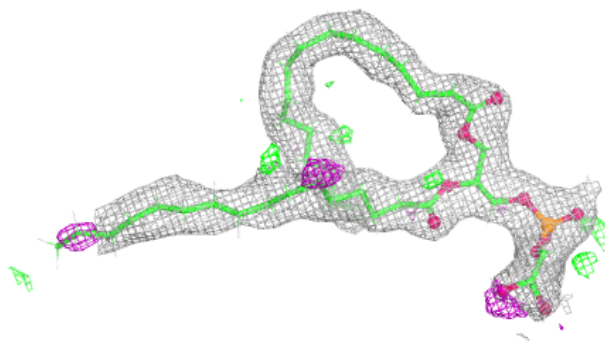


Electron density around DGD h 101:

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

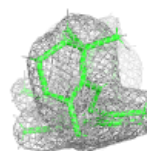
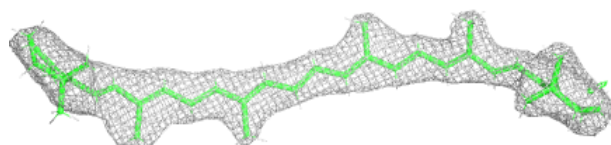
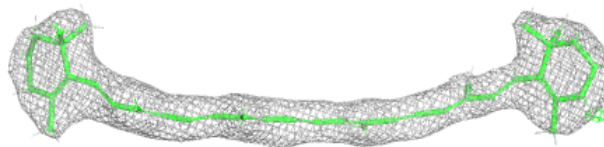
**Electron density around LHG D 411:**

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

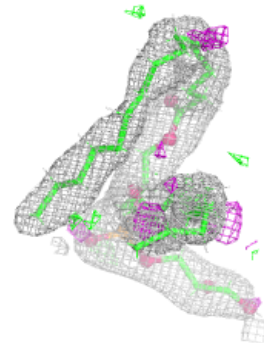
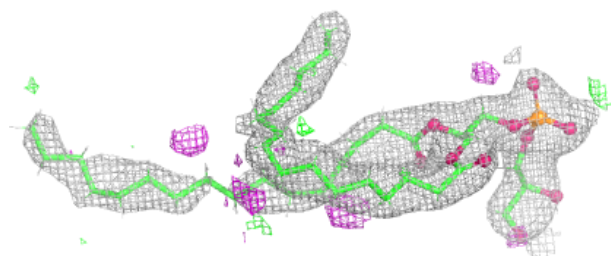
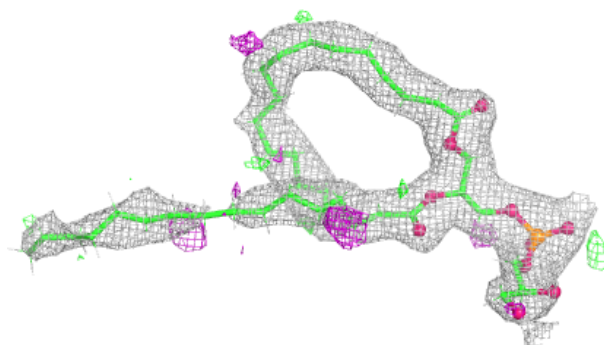


Electron density around BCR k 102:

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

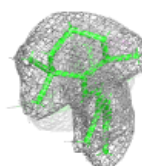
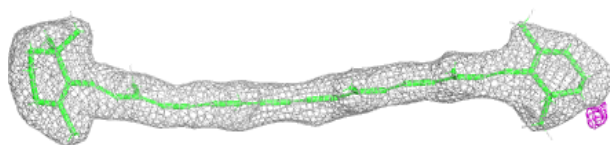
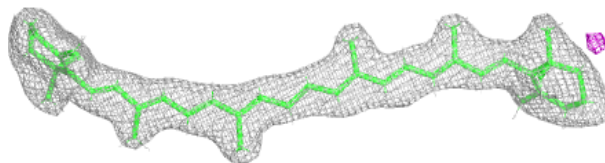
**Electron density around LHG d 407:**

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

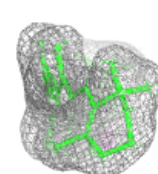
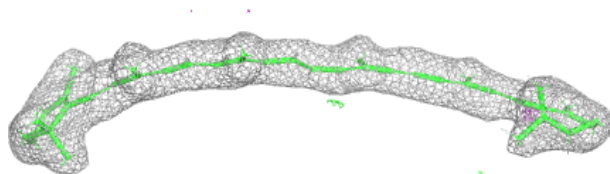
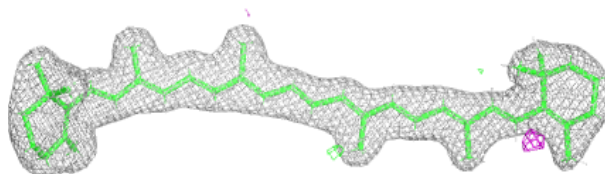


Electron density around BCR x 101:

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

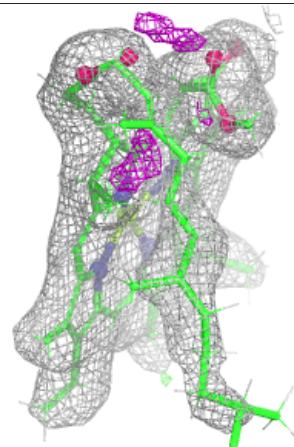
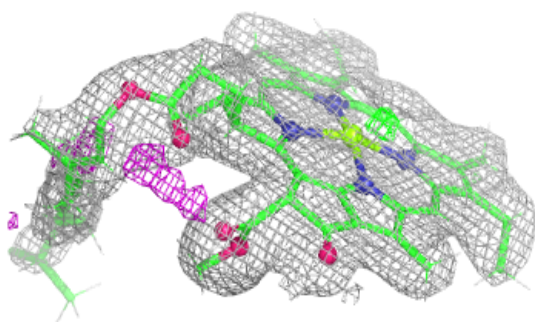
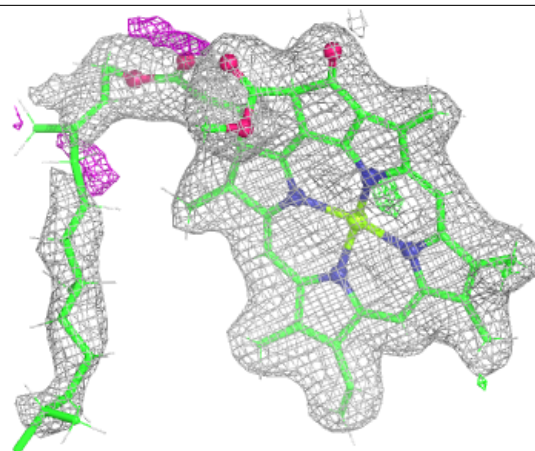
**Electron density around BCR T 101:**

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

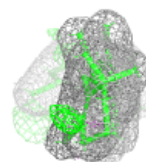
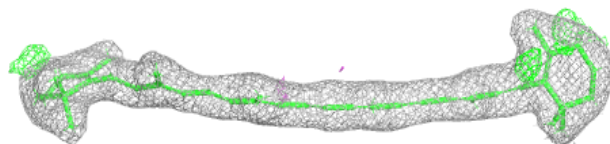
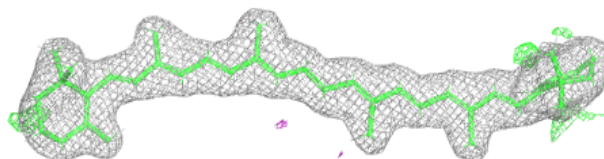


Electron density around CLA b 616:

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

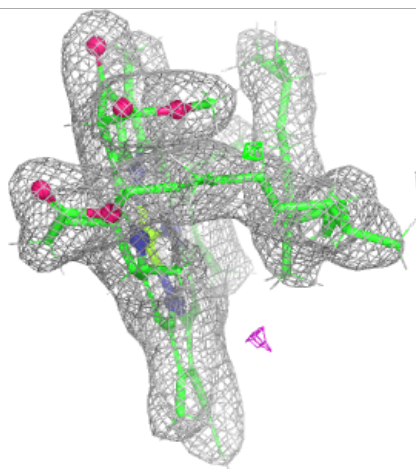
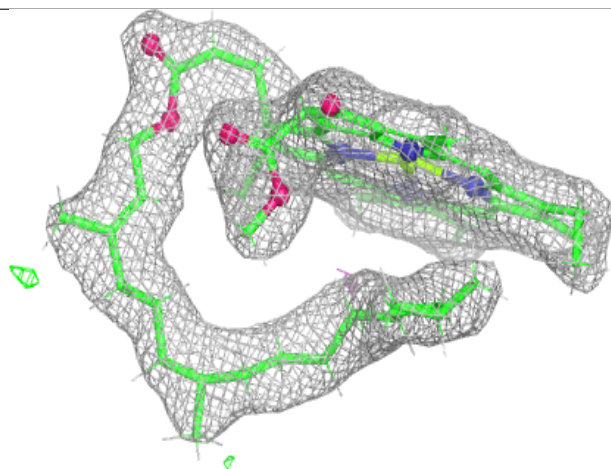
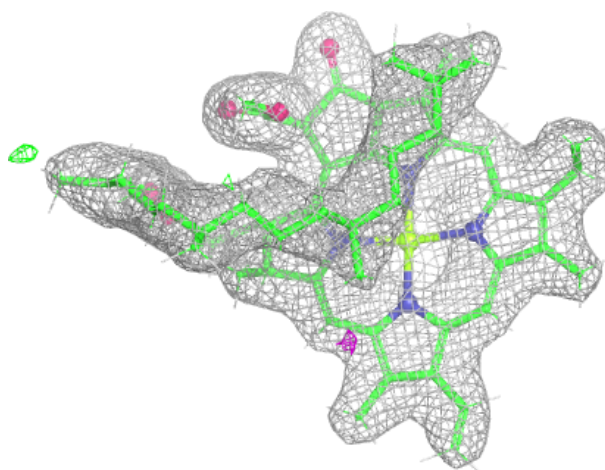
**Electron density around BCR b 617:**

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



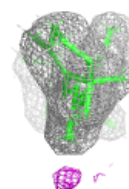
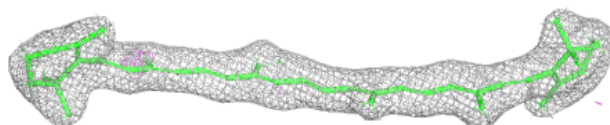
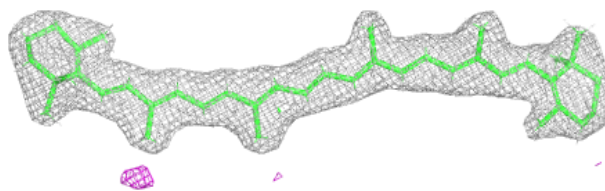
Electron density around CLA C 510:

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

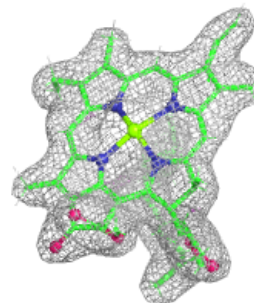
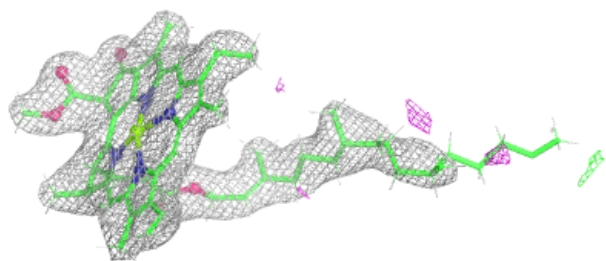
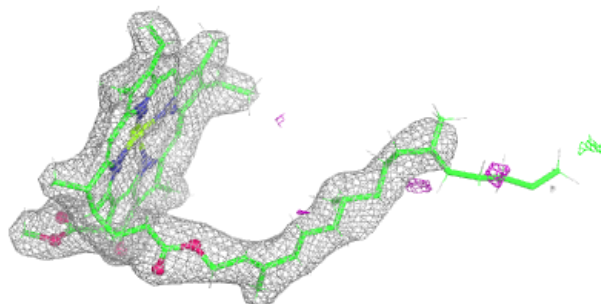


Electron density around BCR b 619:

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

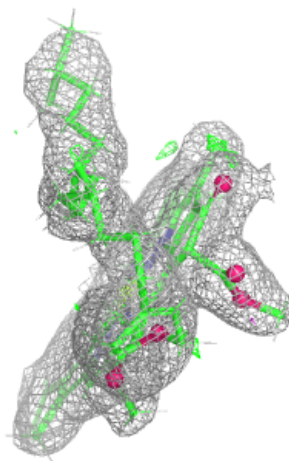
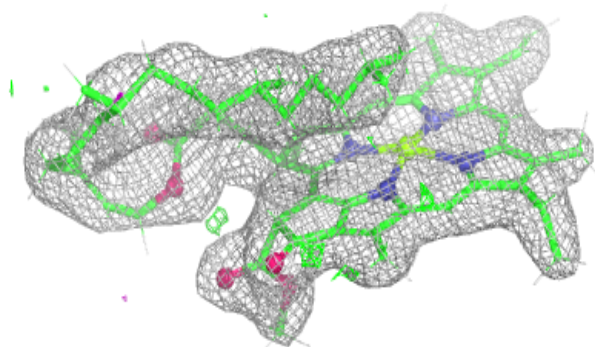
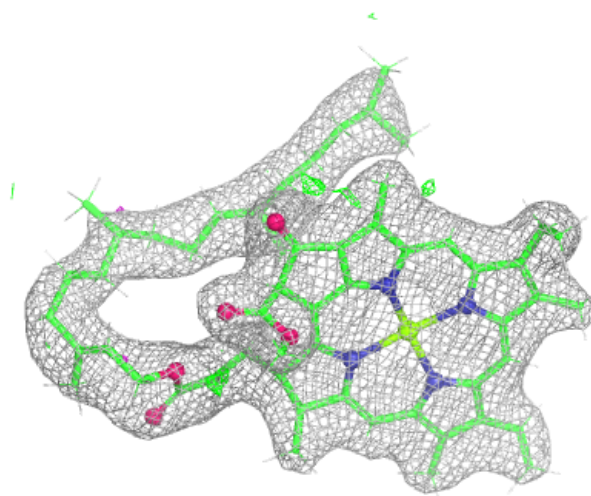
**Electron density around CLA c 508:**

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



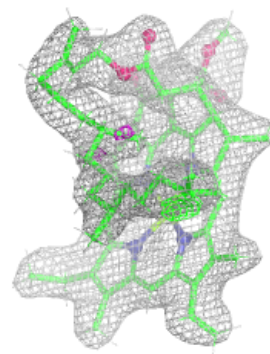
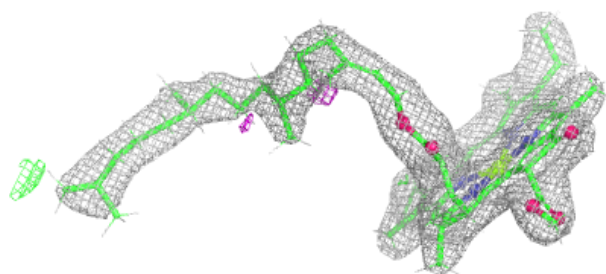
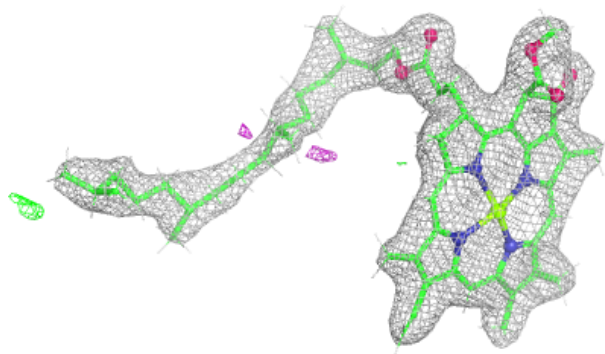
Electron density around CLA c 509:

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

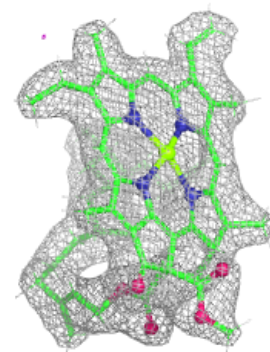
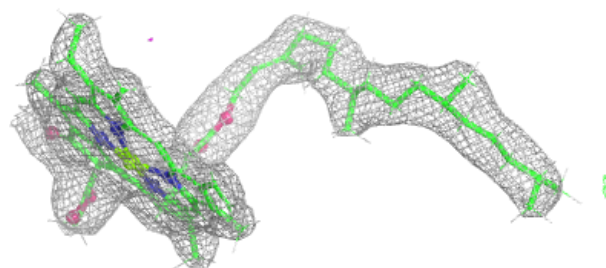
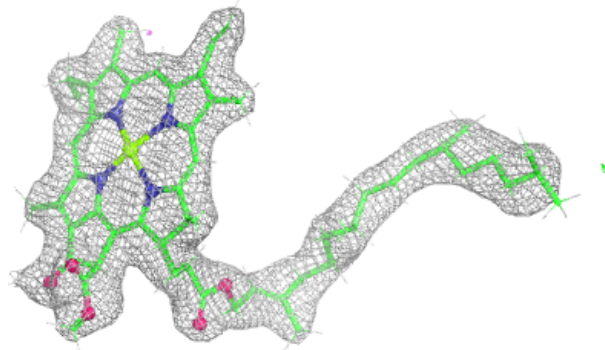


Electron density around CLA c 511:

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

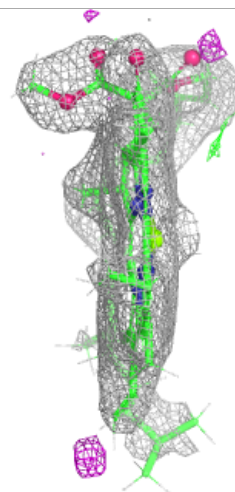
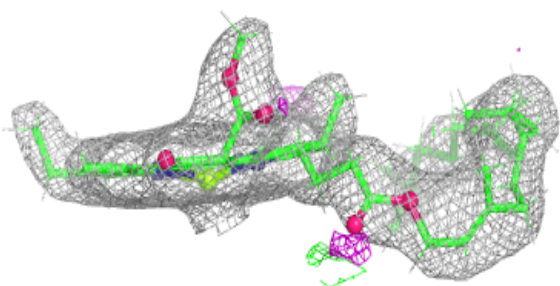
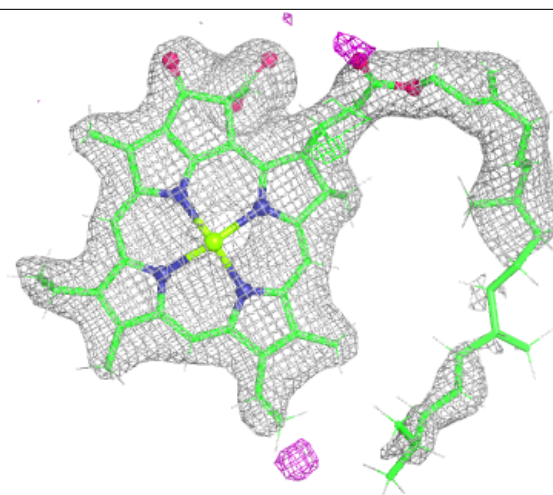
**Electron density around CLA C 511:**

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



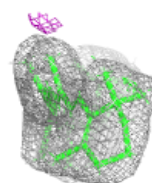
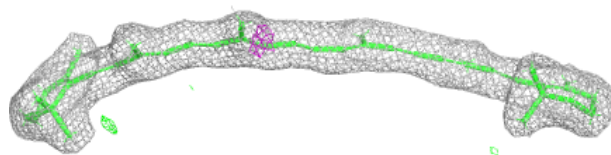
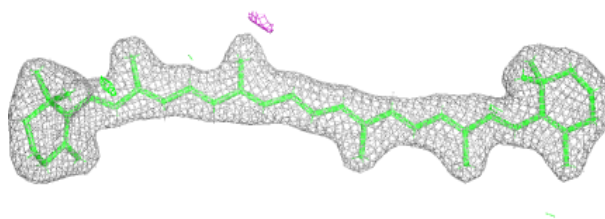
Electron density around CLA C 512:

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

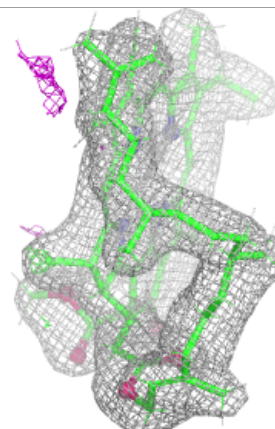
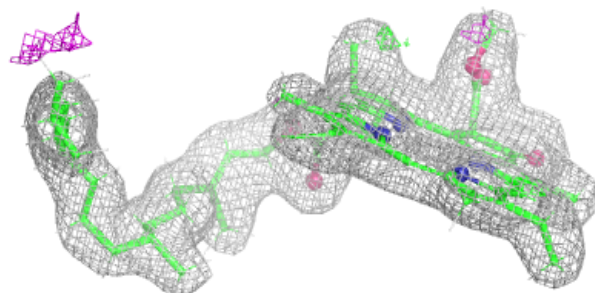
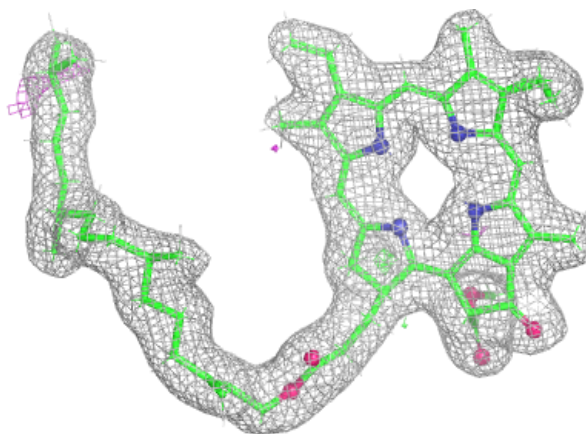


Electron density around BCR t 101:

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

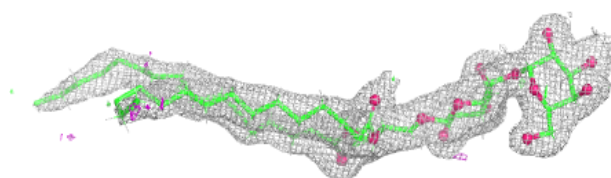
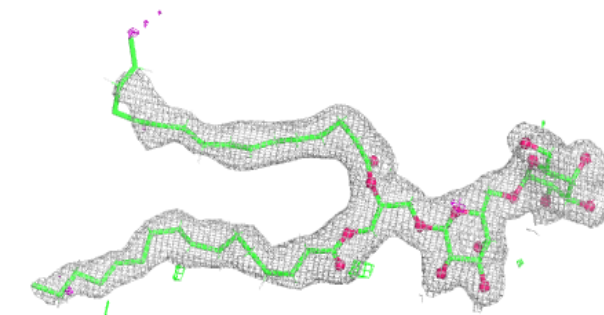
**Electron density around PHO d 401:**

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

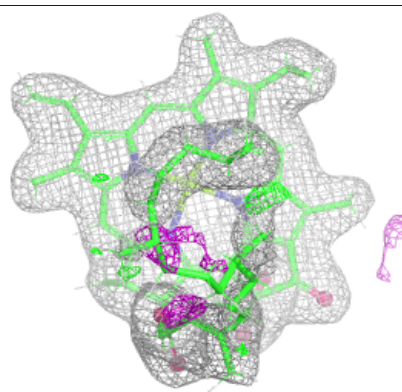
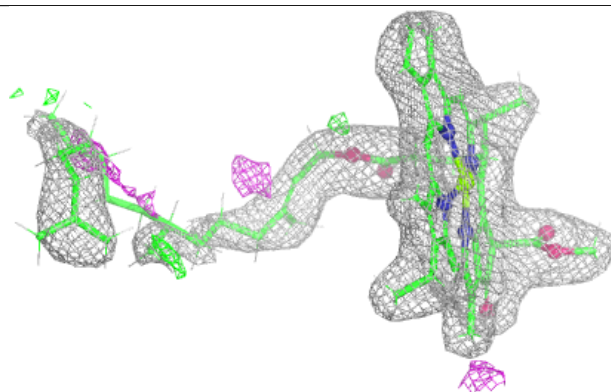
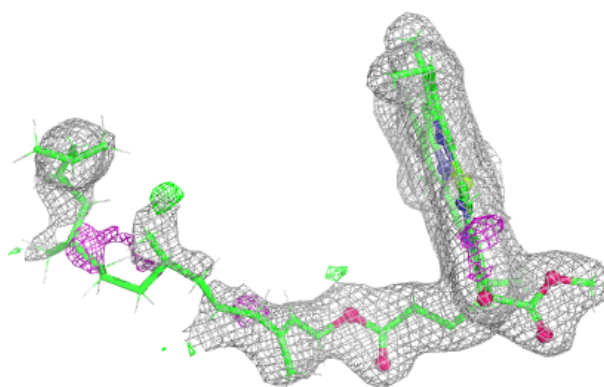


Electron density around DGD C 523:

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

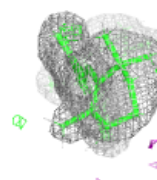
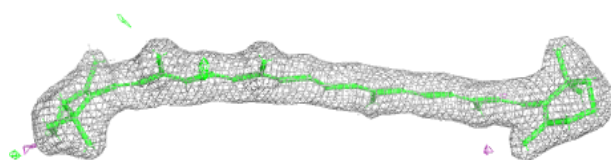
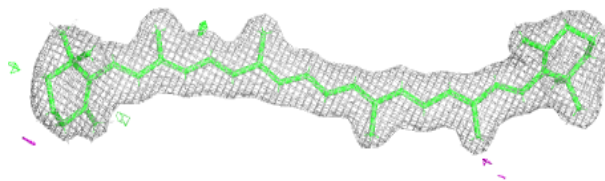
**Electron density around CLA C 506:**

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

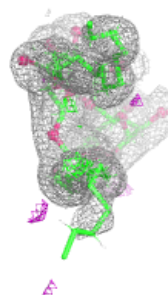
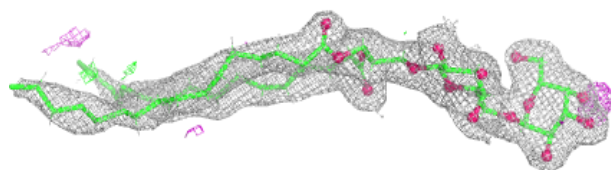
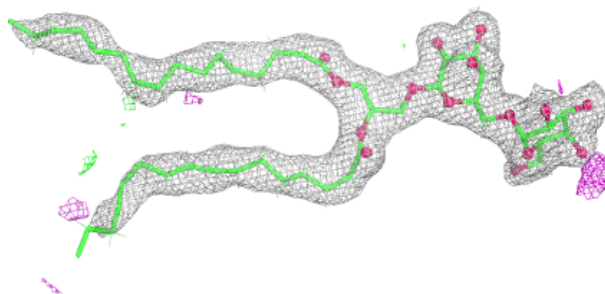


Electron density around BCR B 619:

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

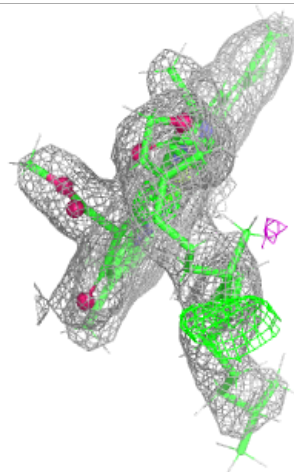
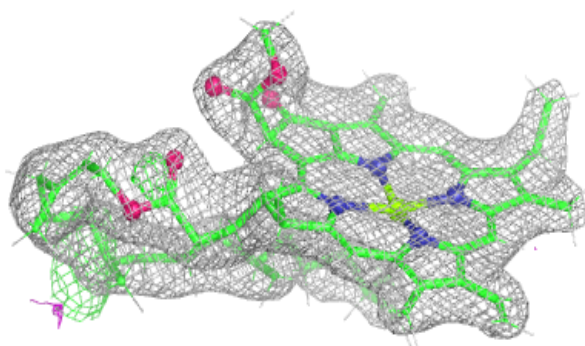
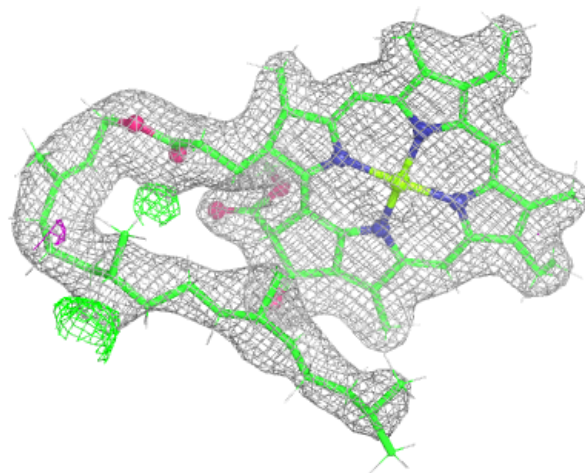
**Electron density around DGD c 520:**

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



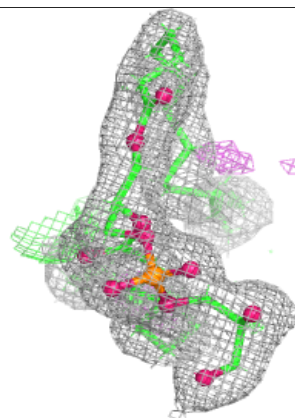
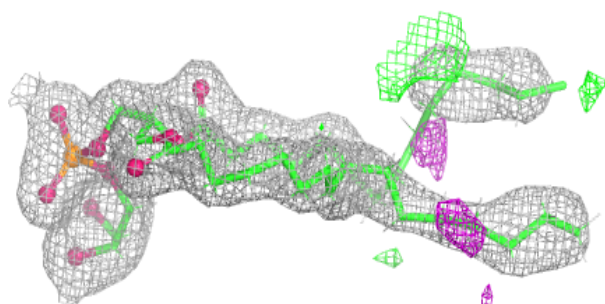
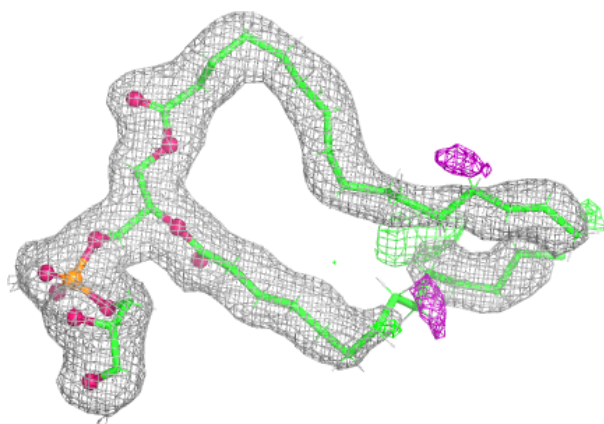
Electron density around CLA C 509:

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

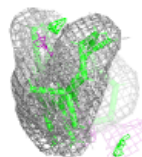
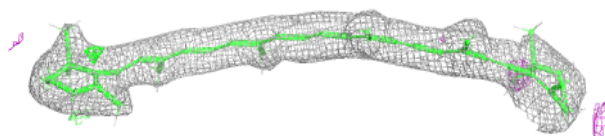
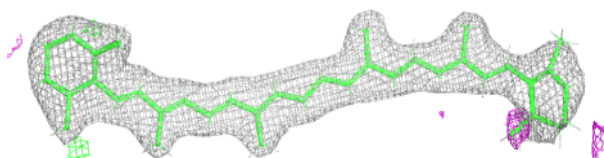


Electron density around LHG D 409:

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

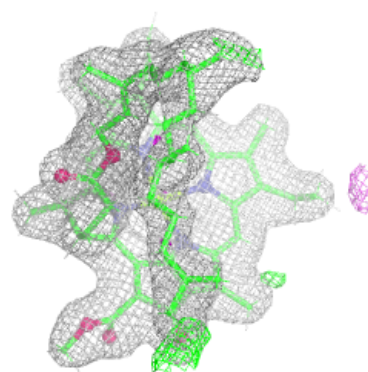
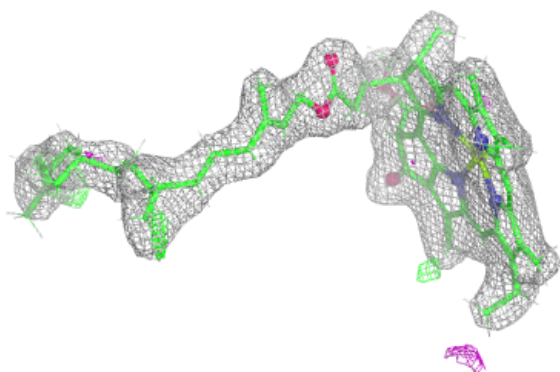
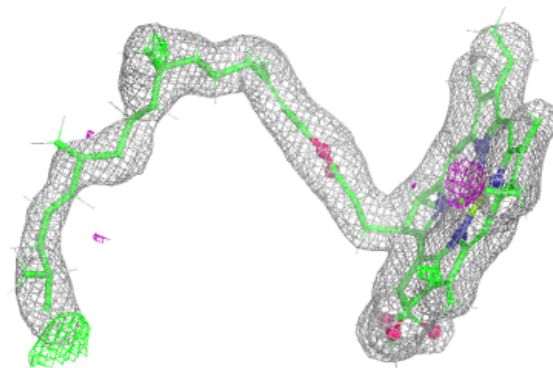
**Electron density around BCR D 404:**

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

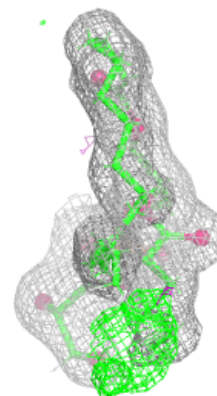
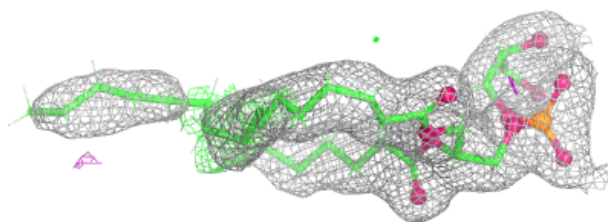
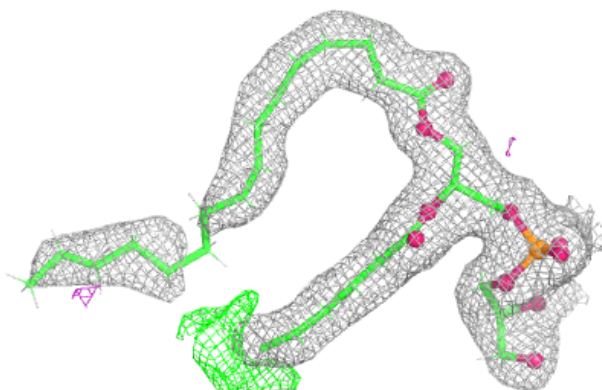


Electron density around CLA b 606:

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

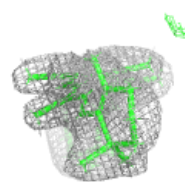
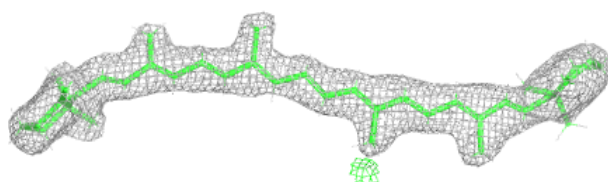
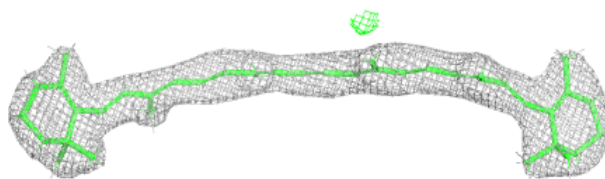
**Electron density around LHG d 409:**

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

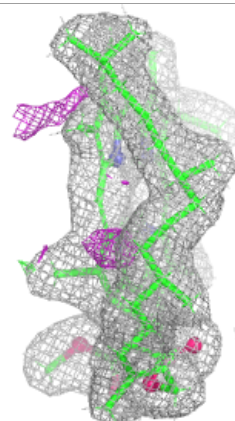
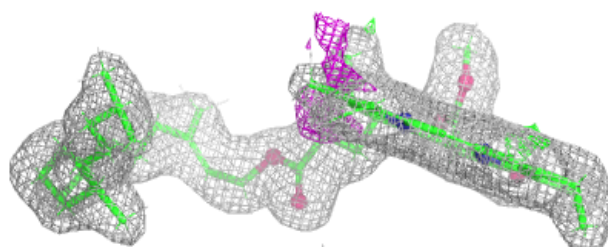
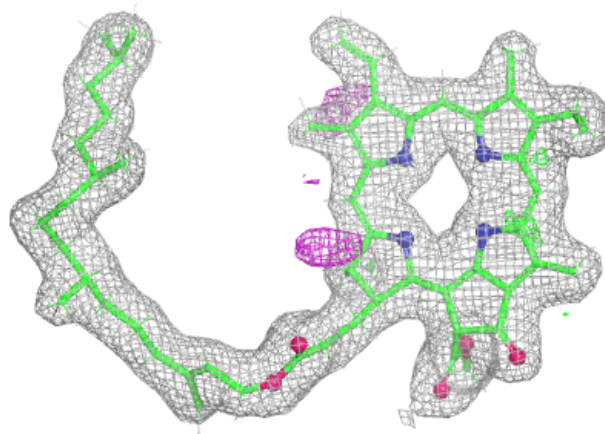


Electron density around BCR K 101:

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

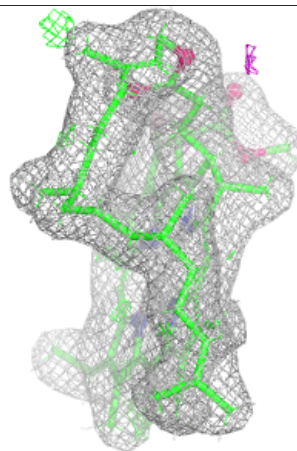
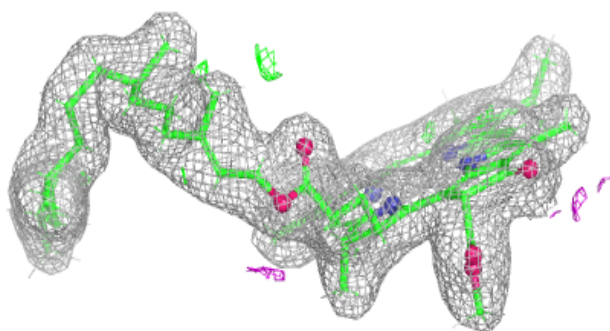
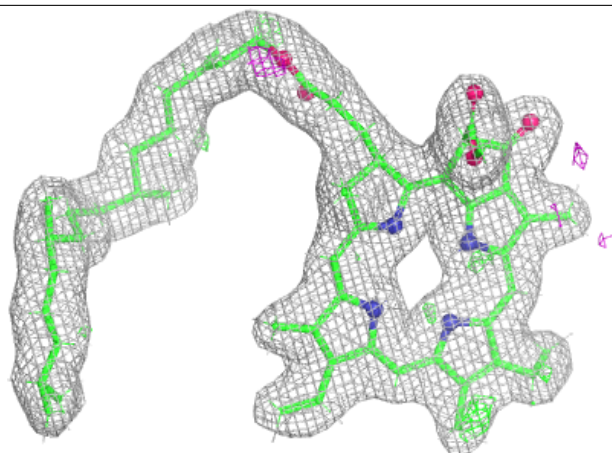
**Electron density around PHO A 609:**

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



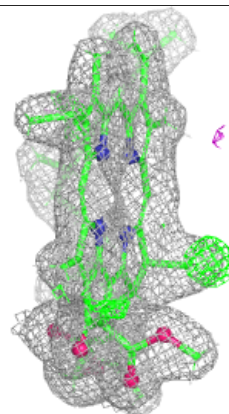
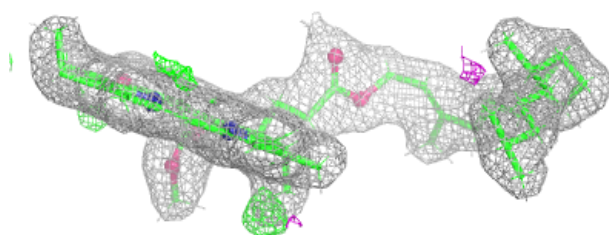
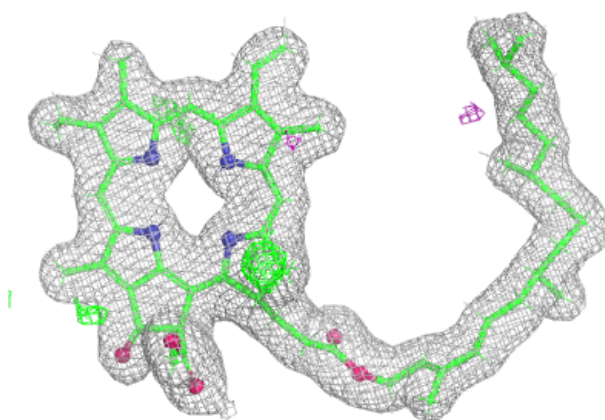
Electron density around PHO D 401:

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

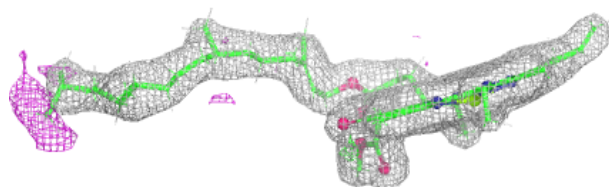
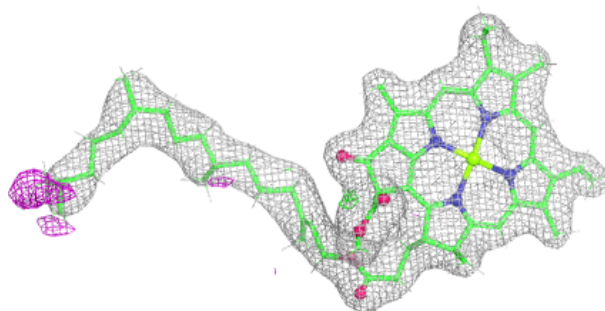


Electron density around PHO a 609:

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

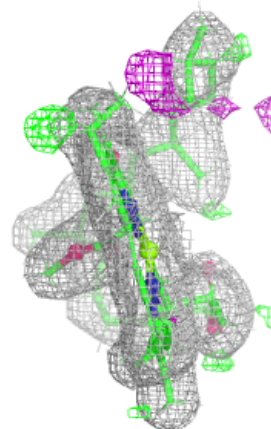
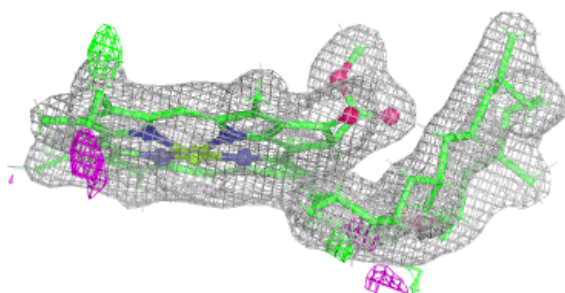
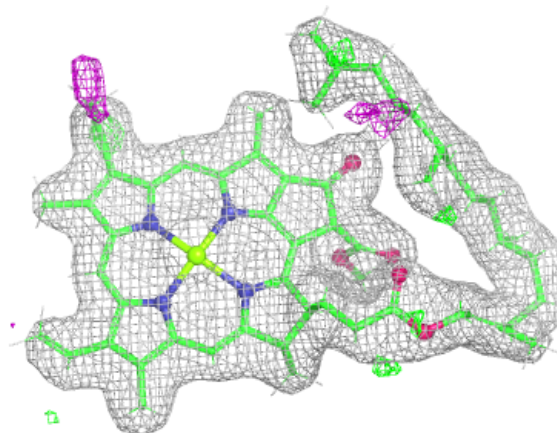
**Electron density around CLA b 602:**

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

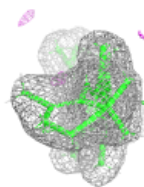
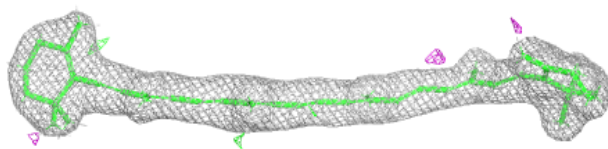
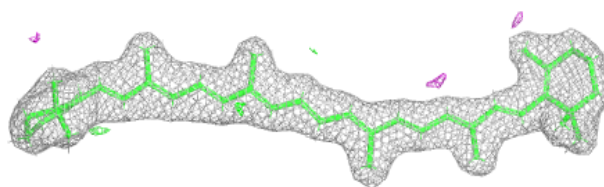


Electron density around CLA B 610:

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

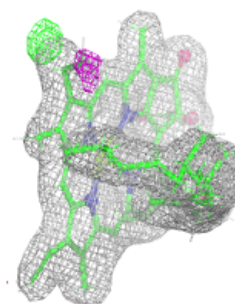
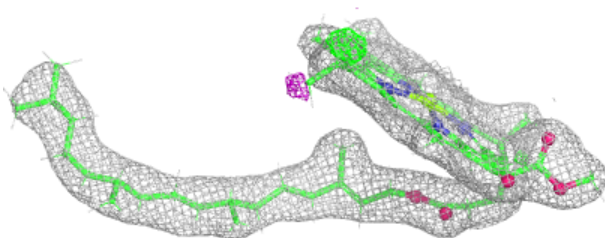
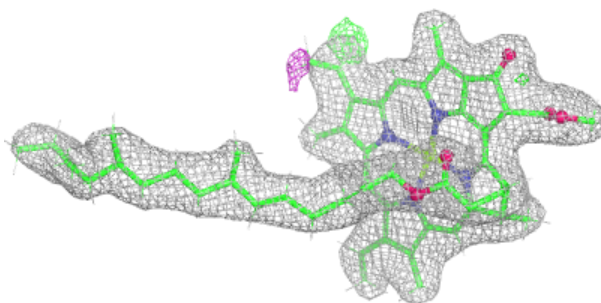
**Electron density around BCR B 617:**

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

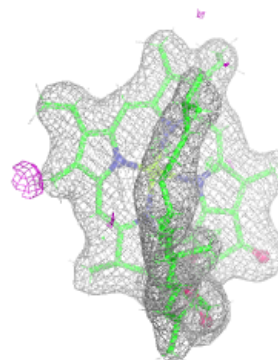
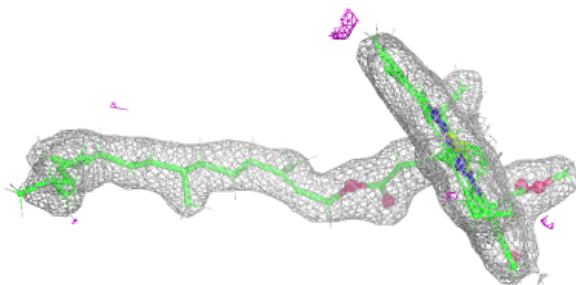
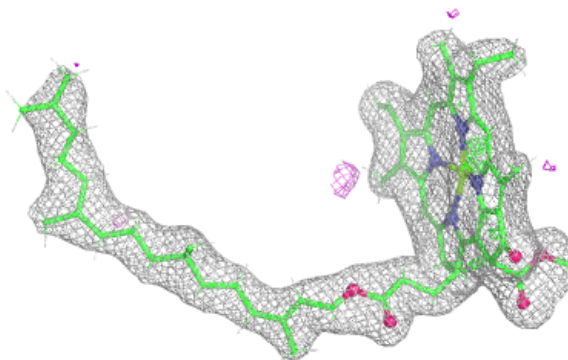


Electron density around CLA b 608:

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

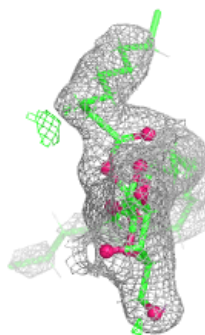
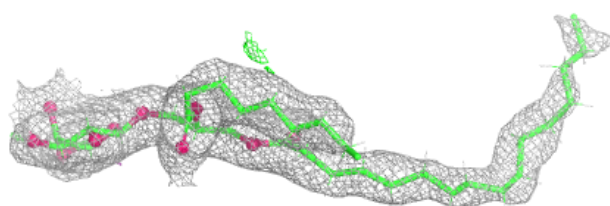
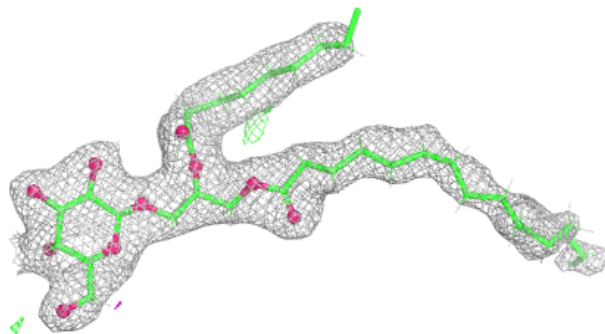
**Electron density around CLA b 609:**

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

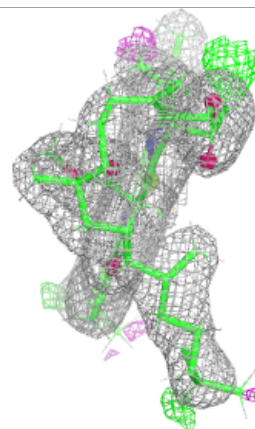
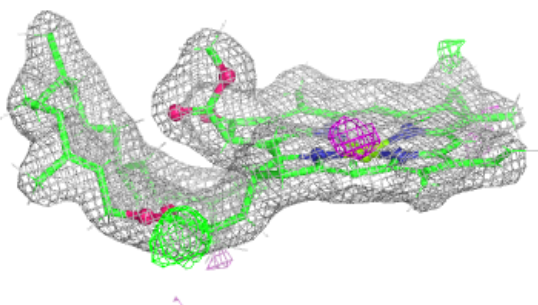
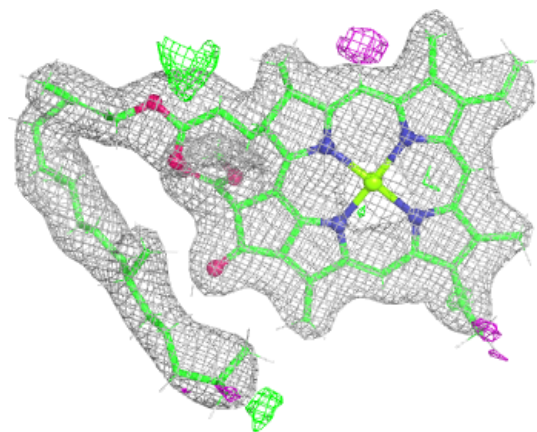


Electron density around LMG d 411:

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

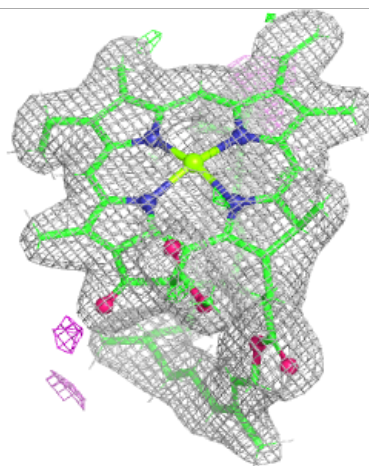
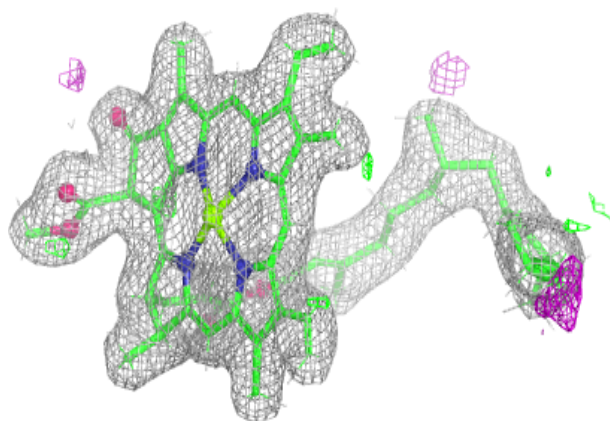
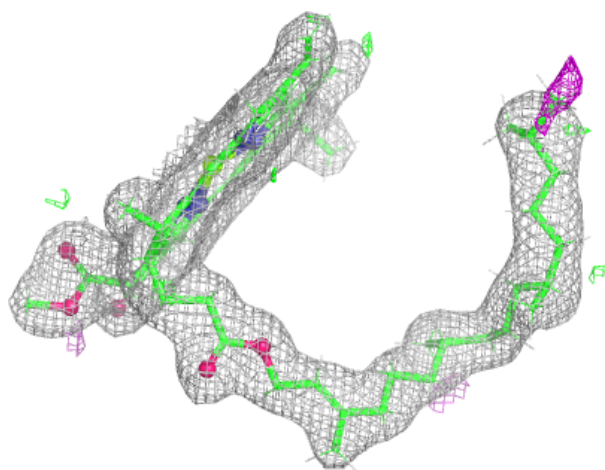
**Electron density around CLA b 610:**

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



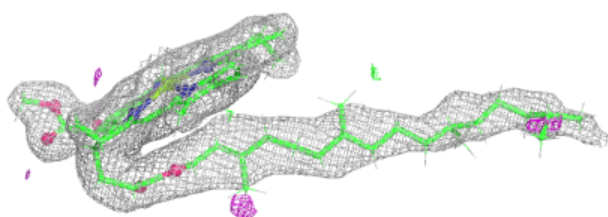
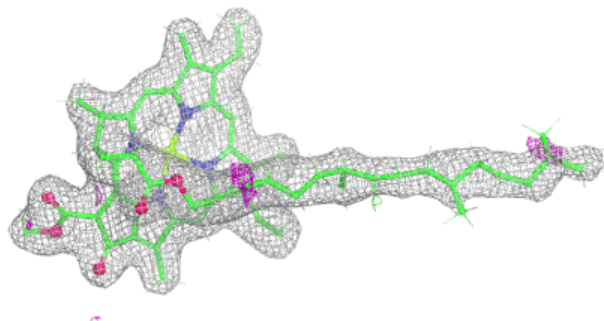
Electron density around CLA b 611:

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



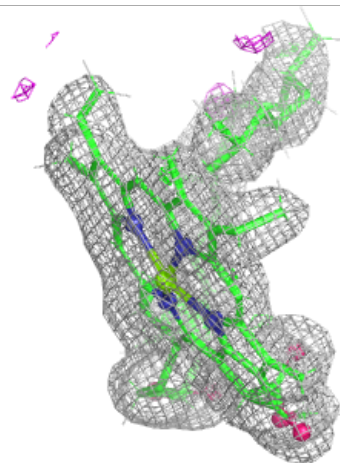
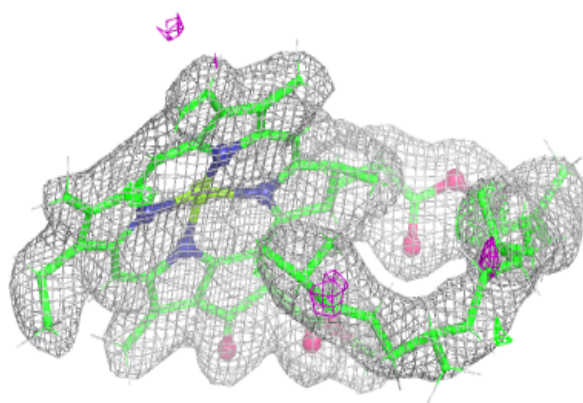
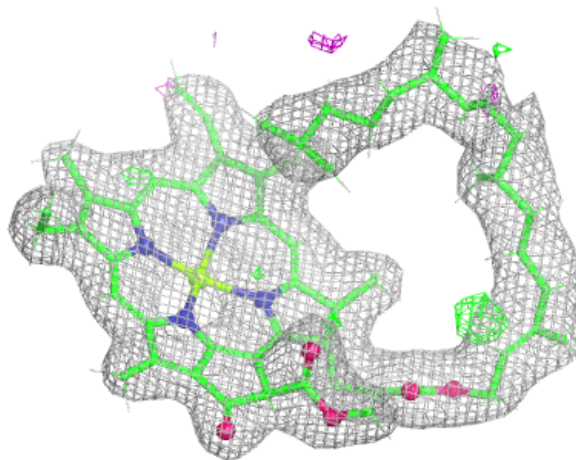
Electron density around CLA b 614:

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



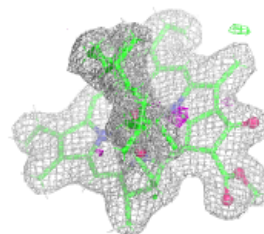
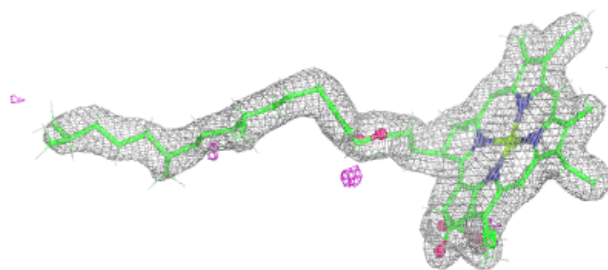
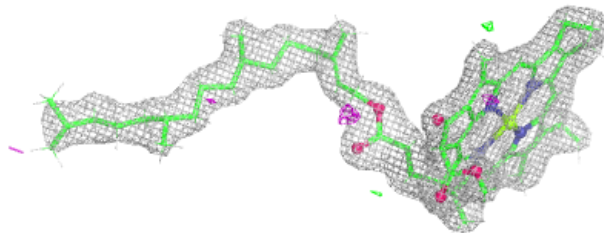
Electron density around CLA b 615:

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

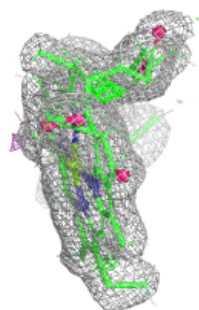
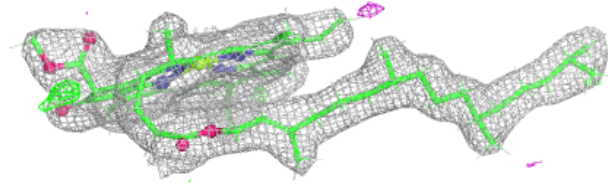
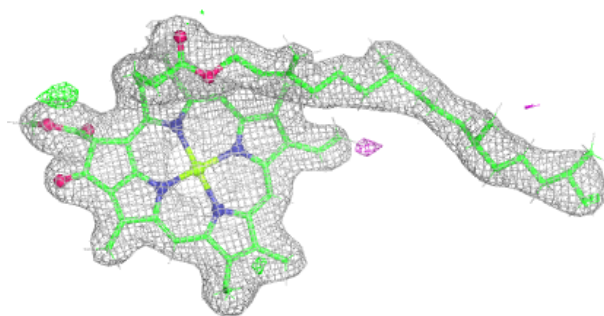


Electron density around CLA C 502:

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

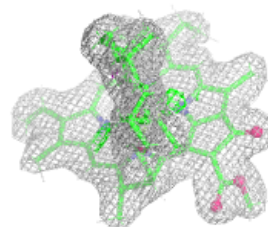
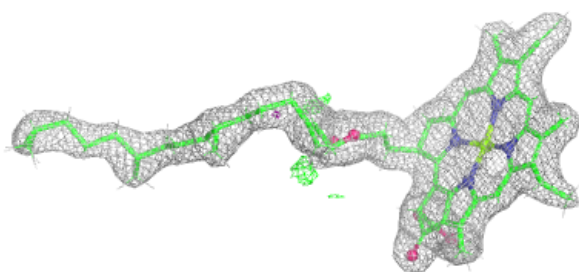
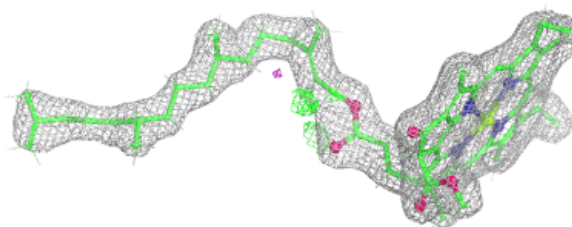
**Electron density around CLA c 501:**

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

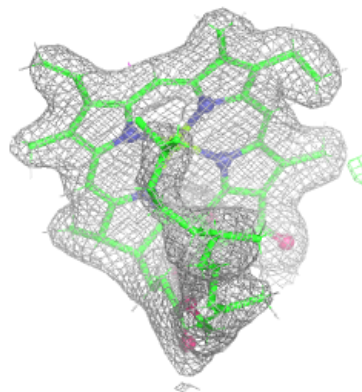
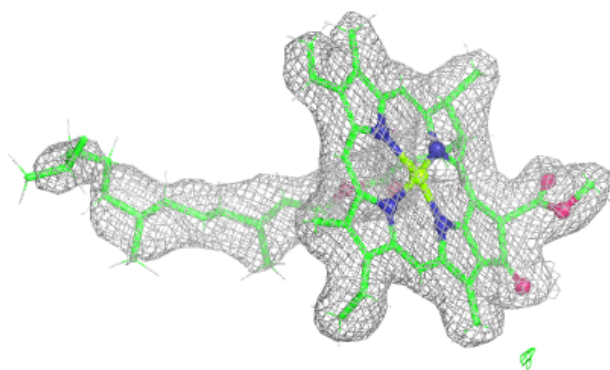
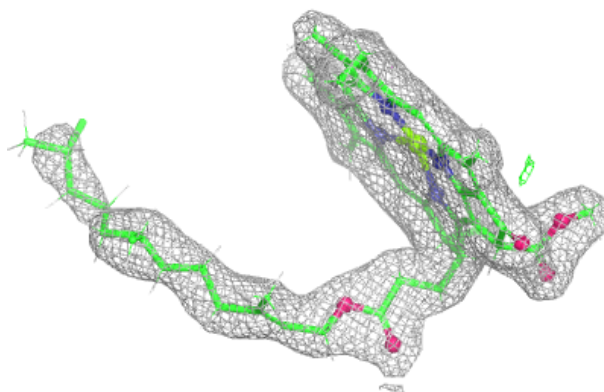


Electron density around CLA c 502:

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

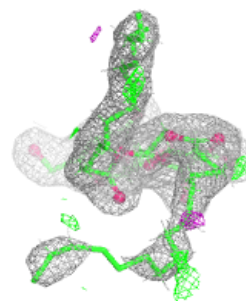
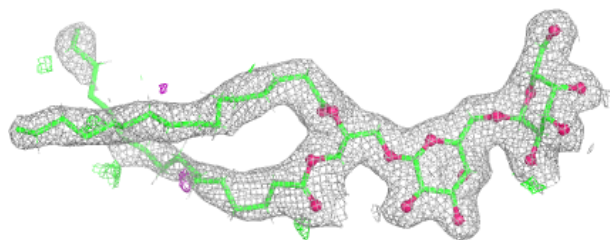
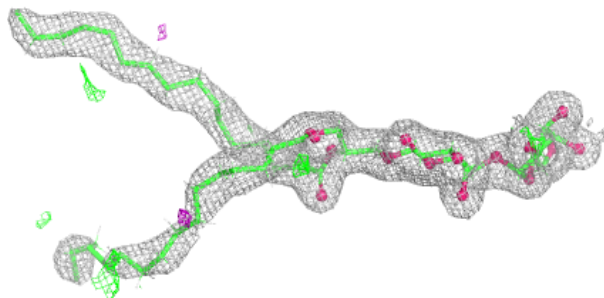
**Electron density around CLA c 504:**

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

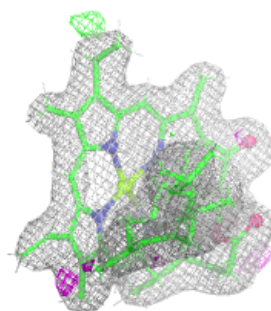
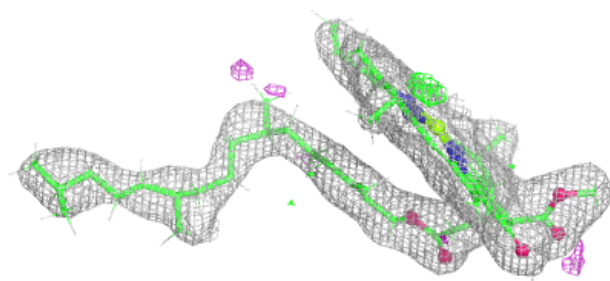
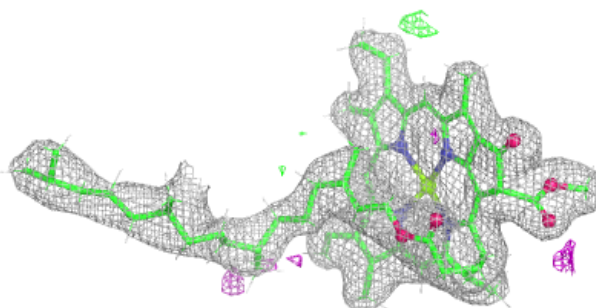


Electron density around DGD C 521:

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

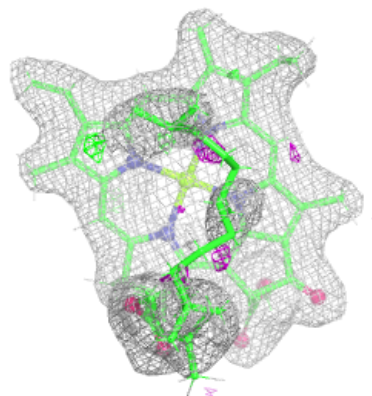
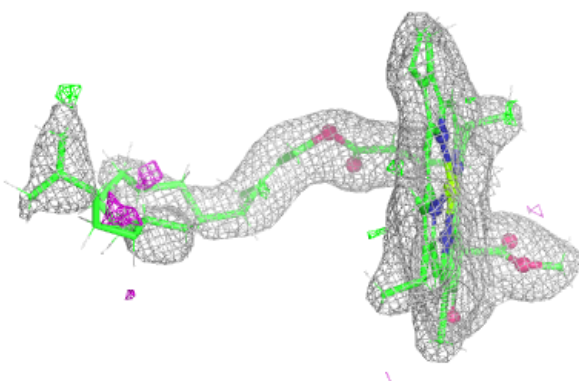
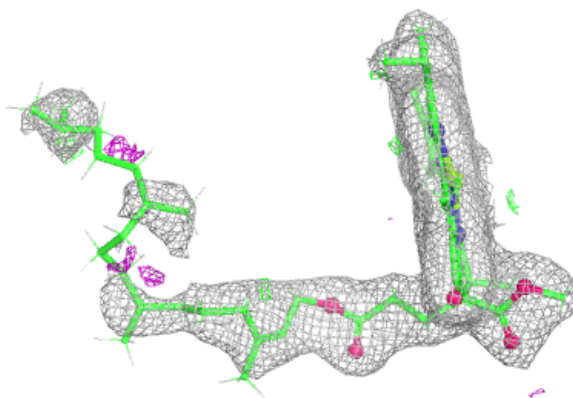
**Electron density around CLA c 505:**

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



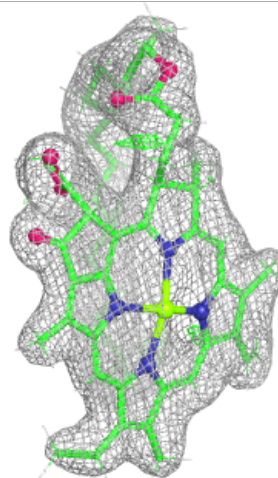
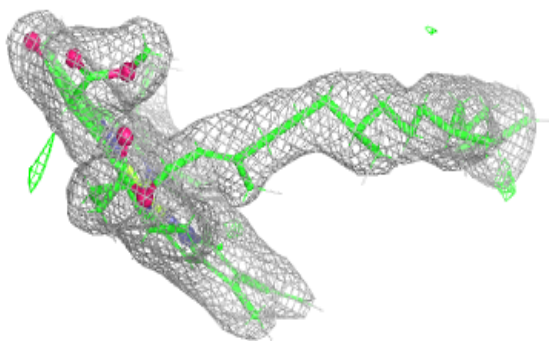
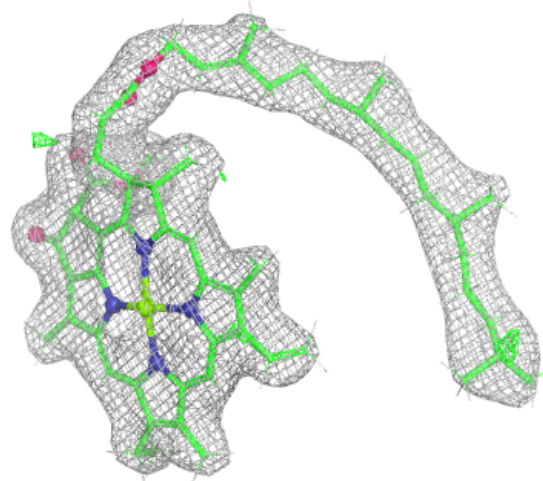
Electron density around CLA c 506:

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



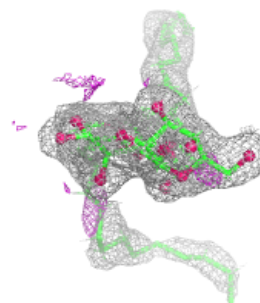
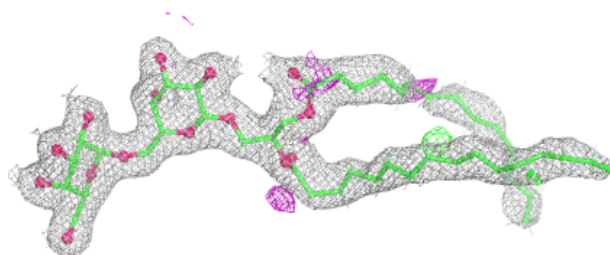
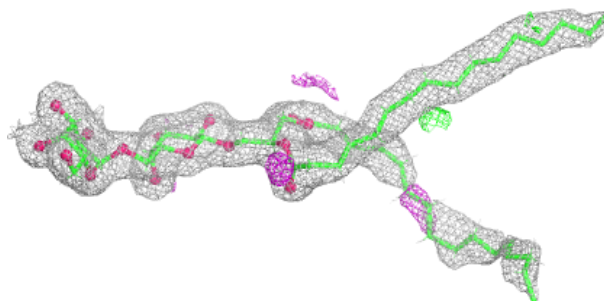
Electron density around CLA c 507:

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

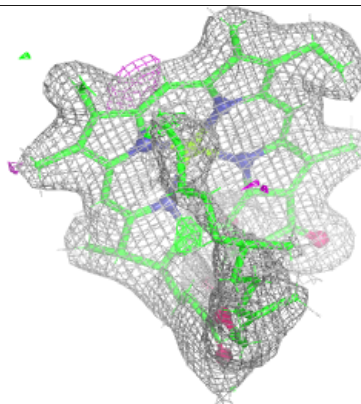
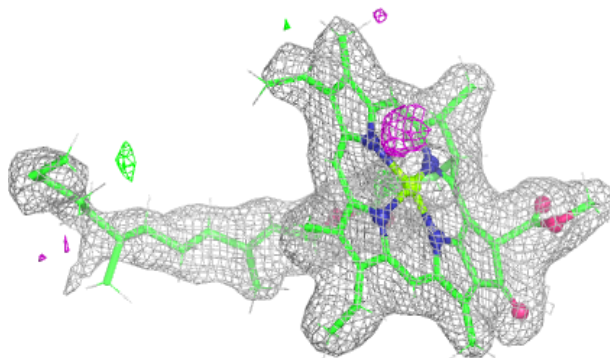
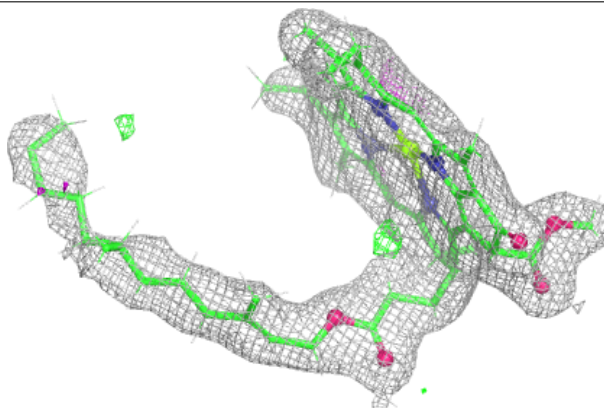


Electron density around DGD c 518:

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

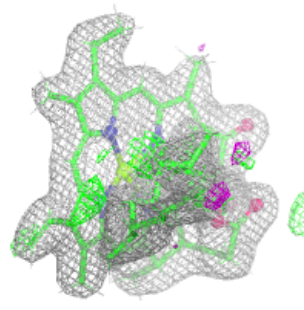
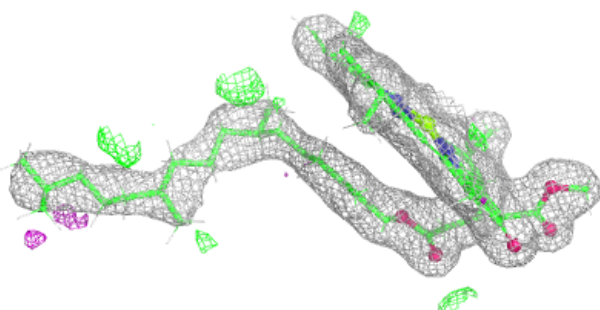
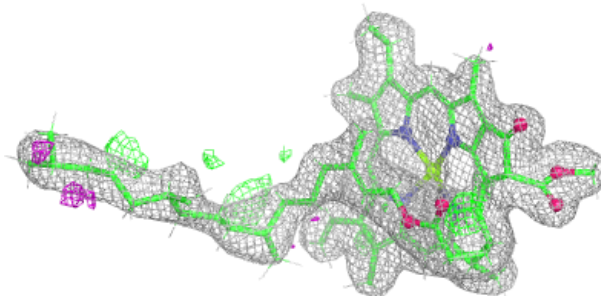
**Electron density around CLA C 504:**

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

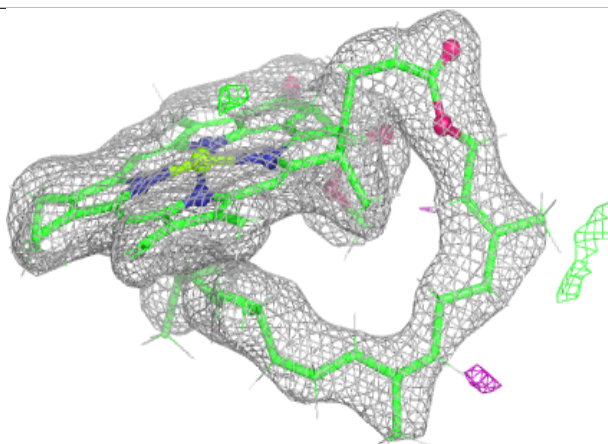
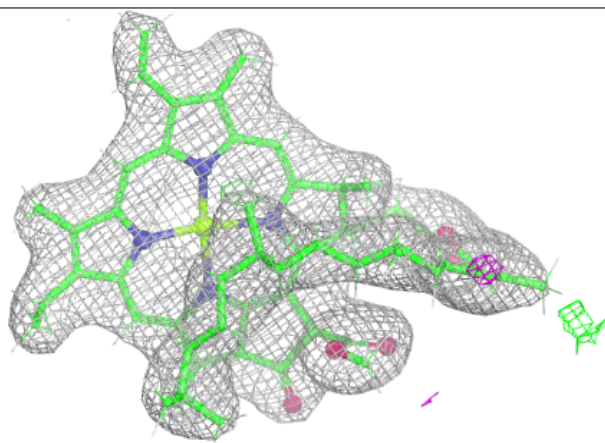


Electron density around CLA C 505:

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

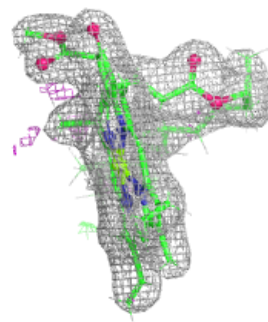
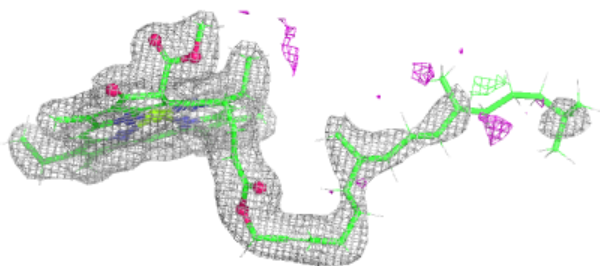
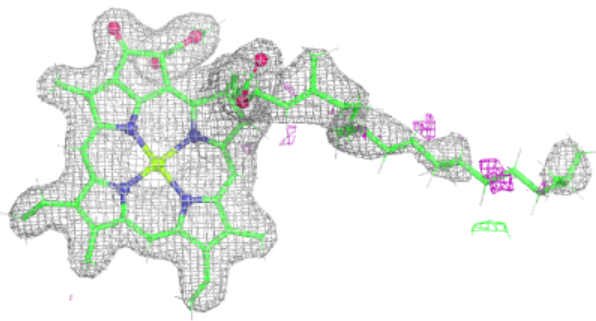
**Electron density around CLA c 510:**

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

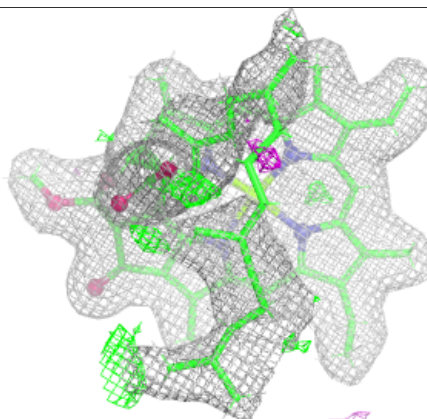
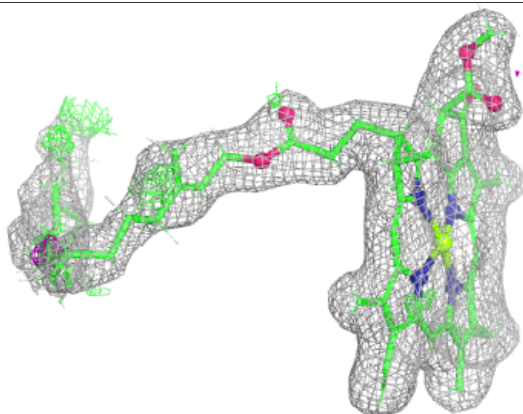
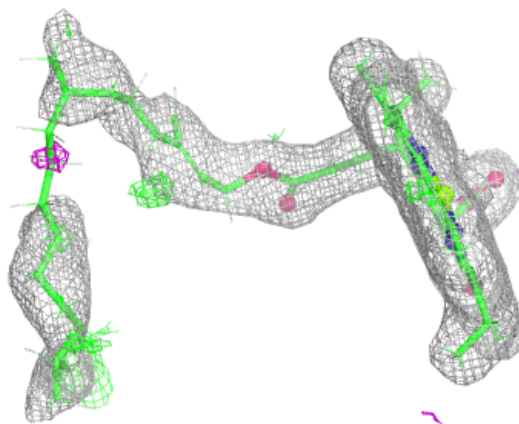


Electron density around CLA a 608:

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

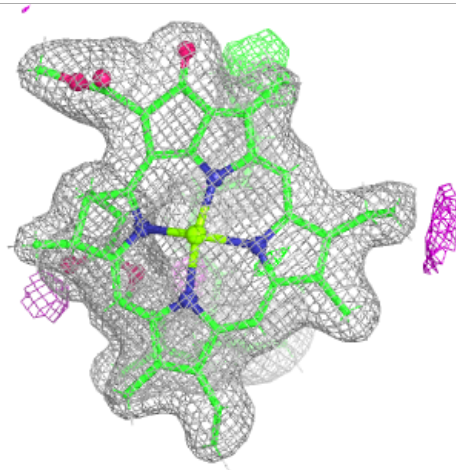
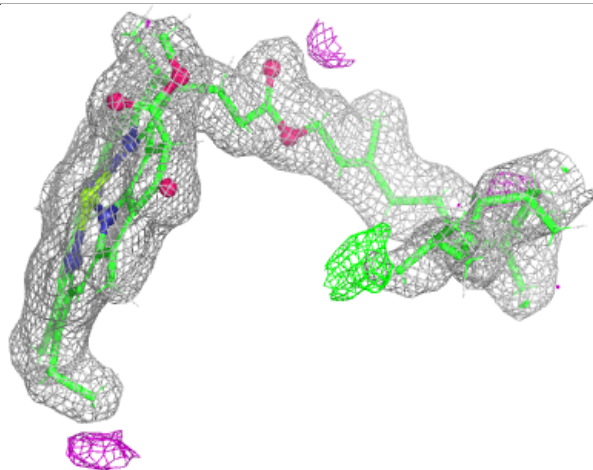
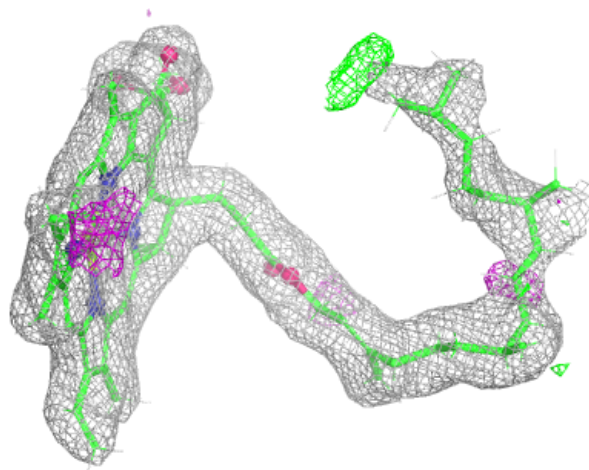
**Electron density around CLA a 610:**

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



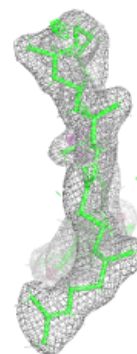
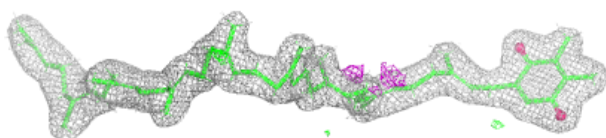
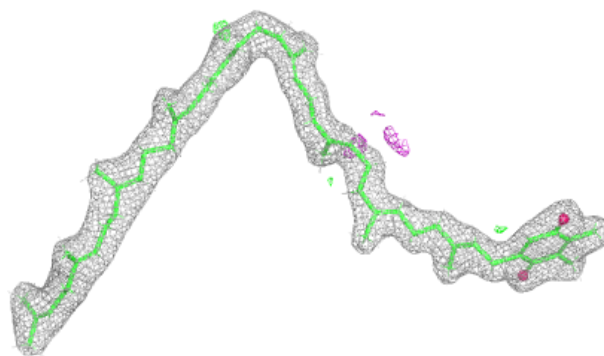
Electron density around CLA B 606:

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

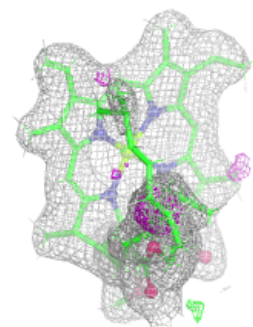
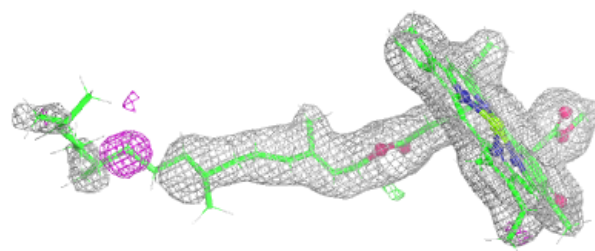
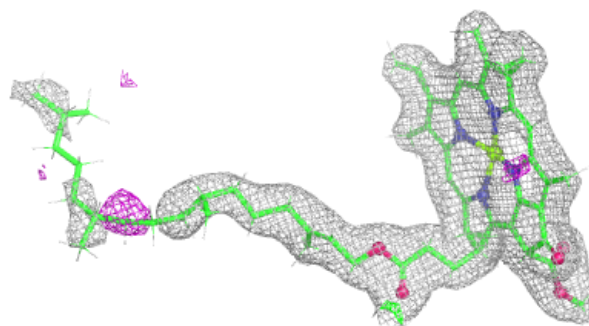


Electron density around PL9 D 405:

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

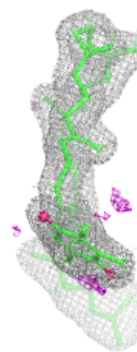
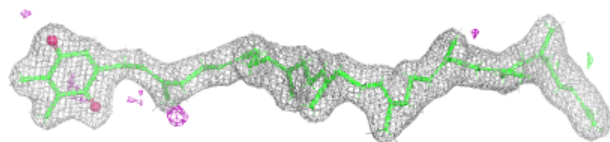
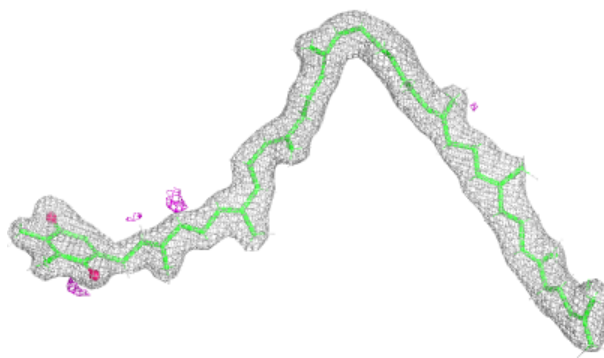
**Electron density around CLA d 403:**

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



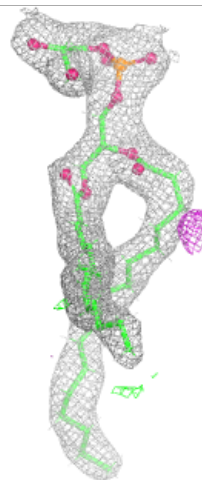
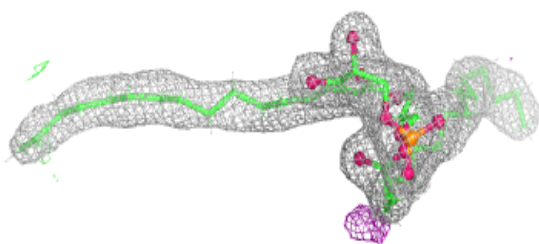
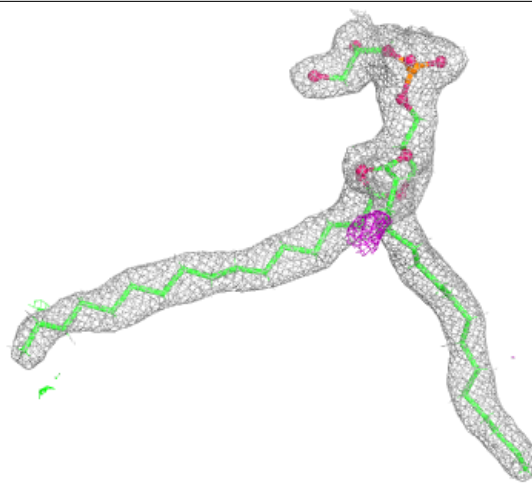
Electron density around PL9 d 405:

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



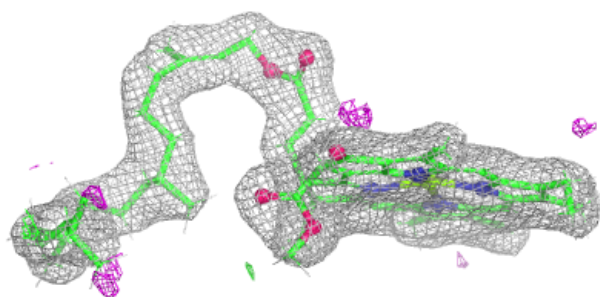
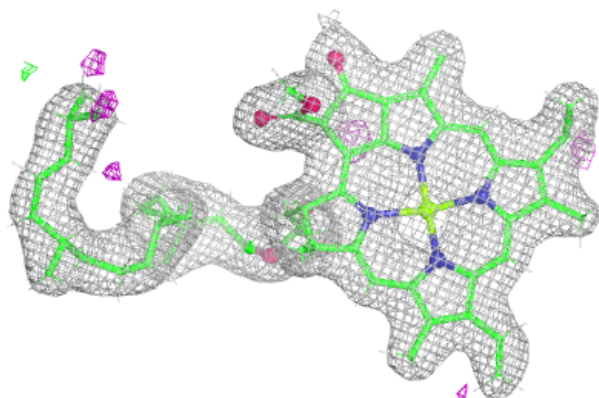
Electron density around LHG 1 101:

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



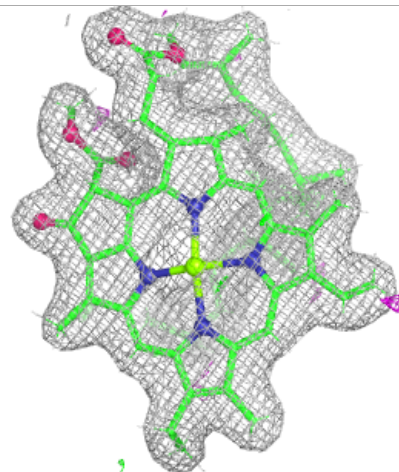
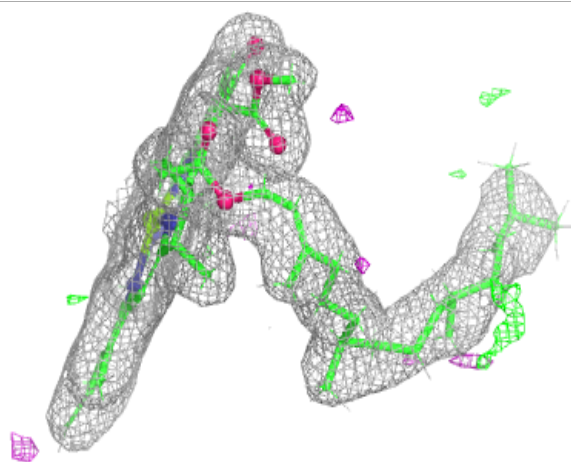
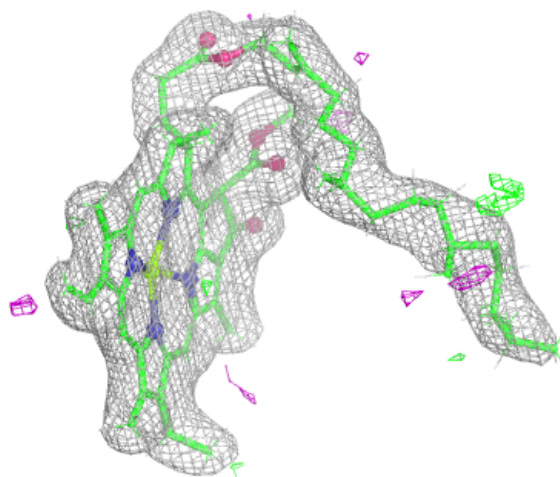
Electron density around CLA B 612:

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



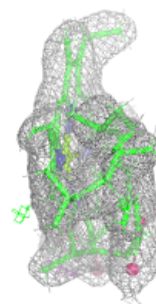
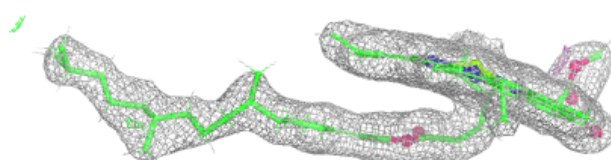
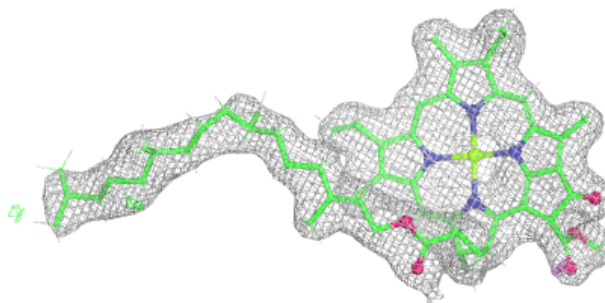
Electron density around CLA B 613:

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

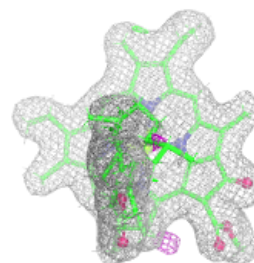
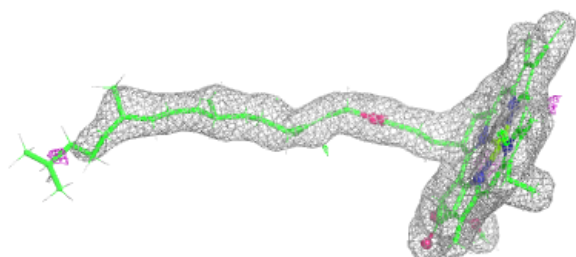
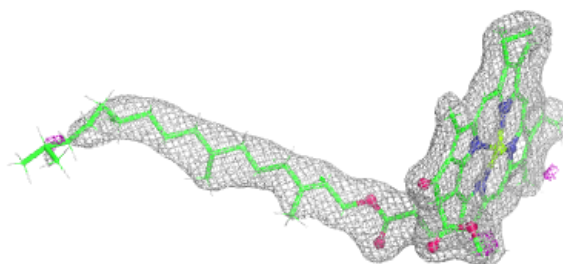


Electron density around CLA b 603:

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

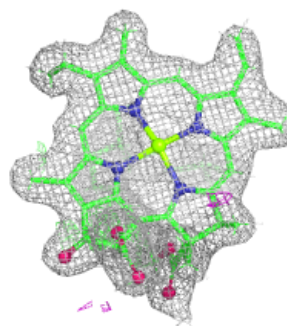
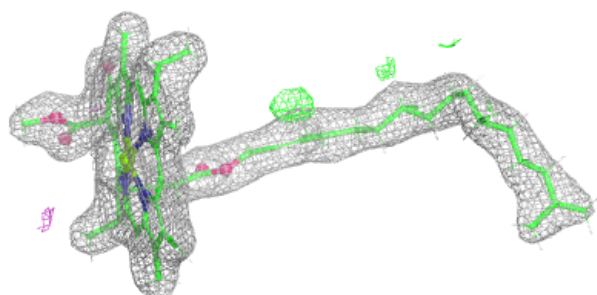
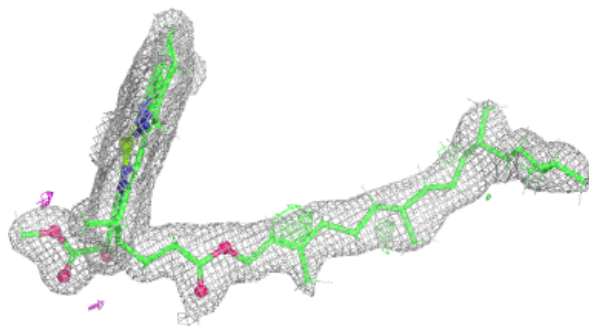
**Electron density around CLA b 604:**

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

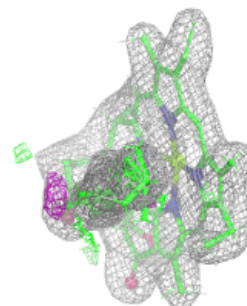
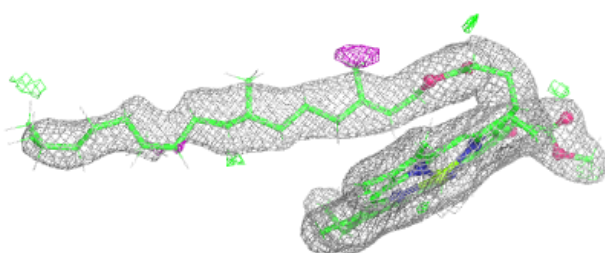
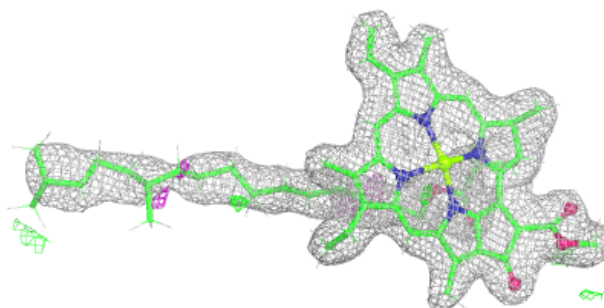


Electron density around CLA b 605:

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

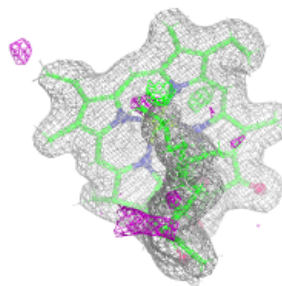
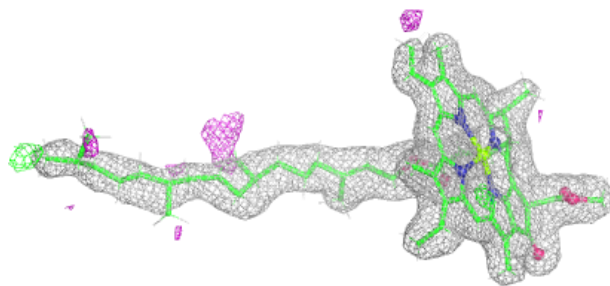
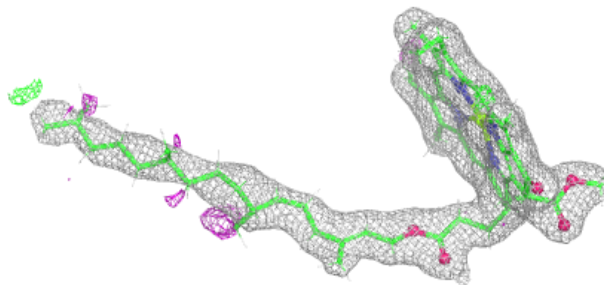
**Electron density around CLA B 614:**

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



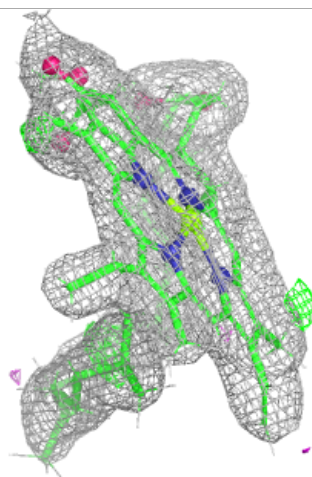
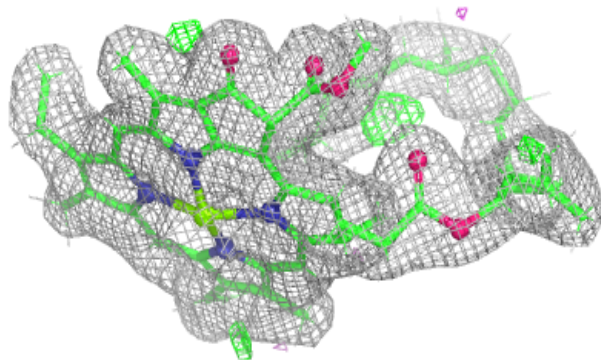
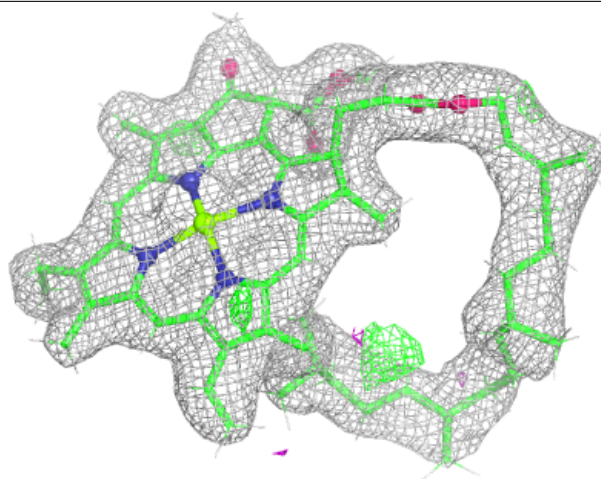
Electron density around CLA b 607:

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



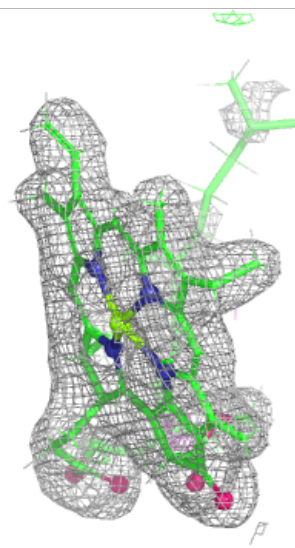
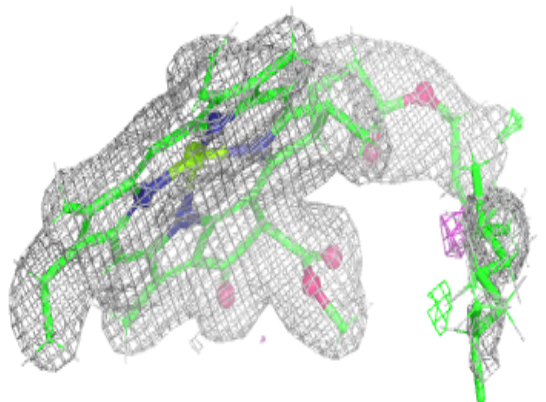
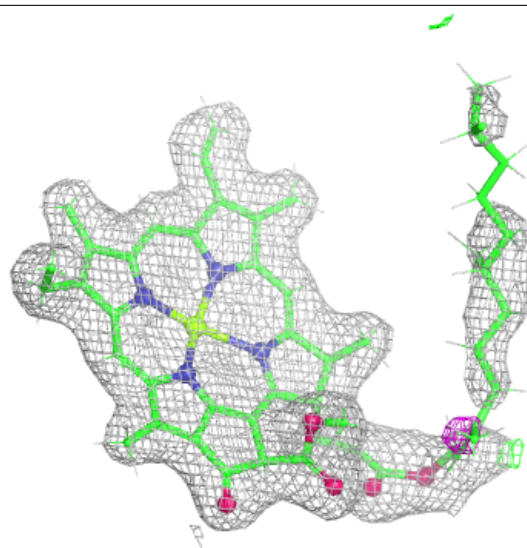
Electron density around CLA B 615:

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



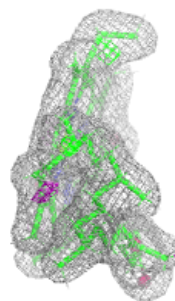
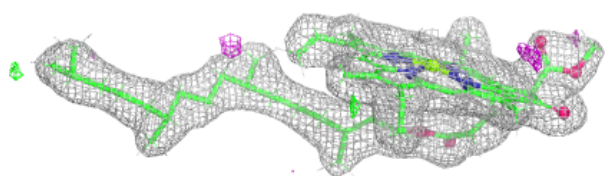
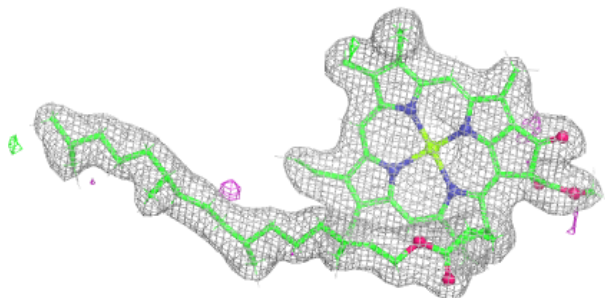
Electron density around CLA B 616:

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

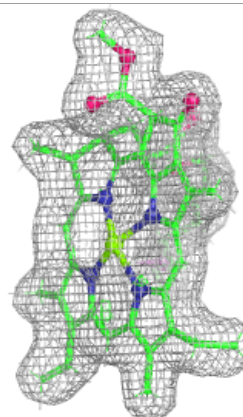
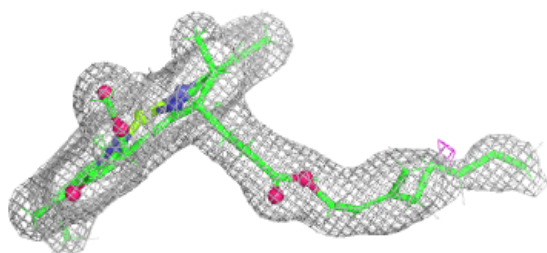
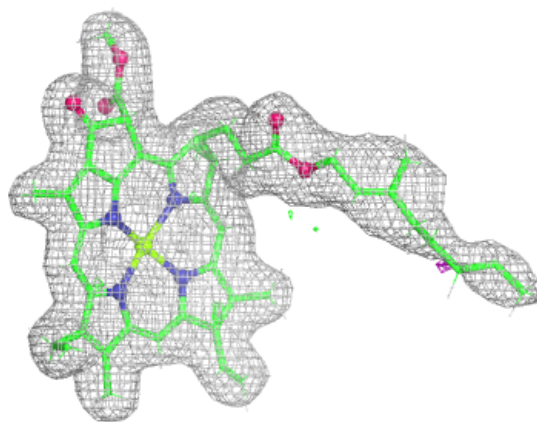


Electron density around CLA C 501:

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

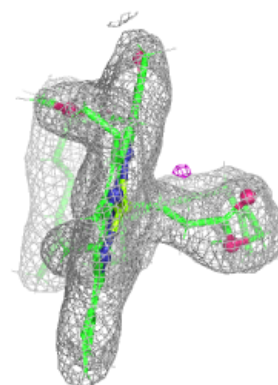
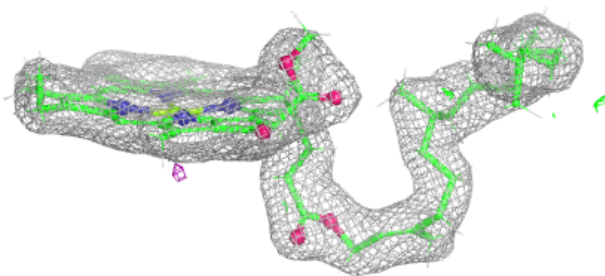
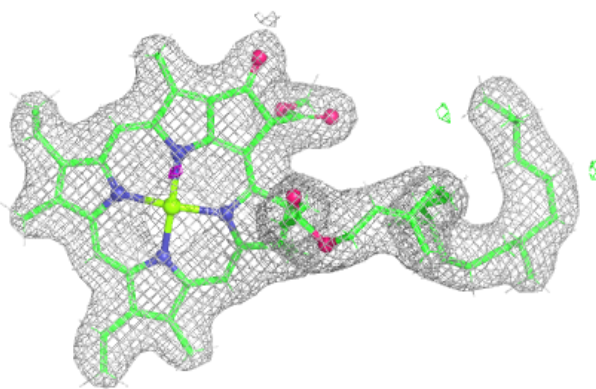
**Electron density around CLA A 610:**

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



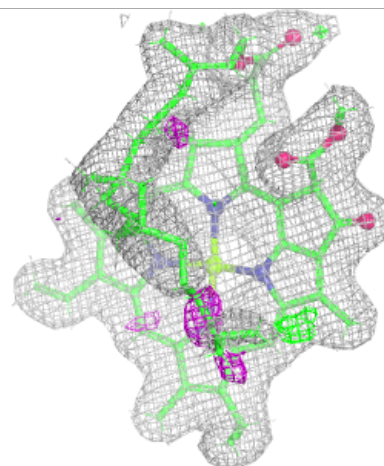
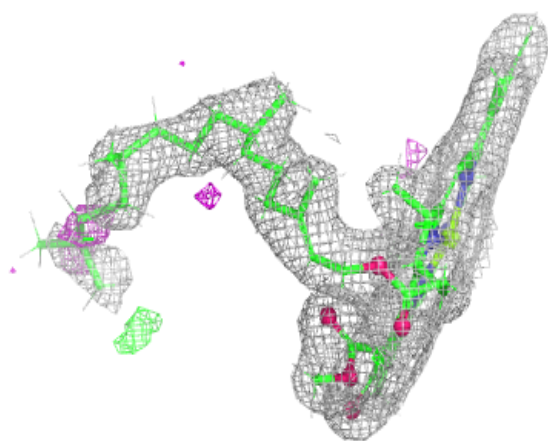
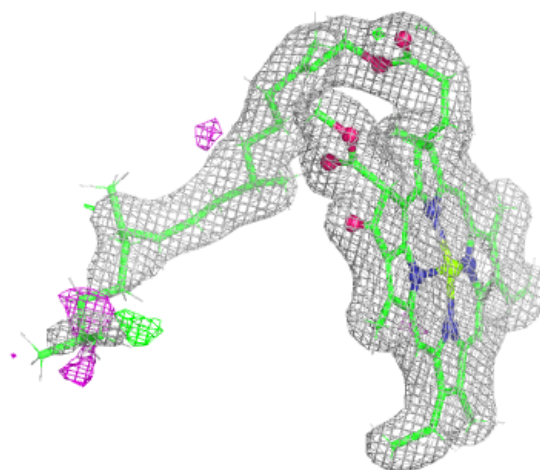
Electron density around CLA b 612:

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



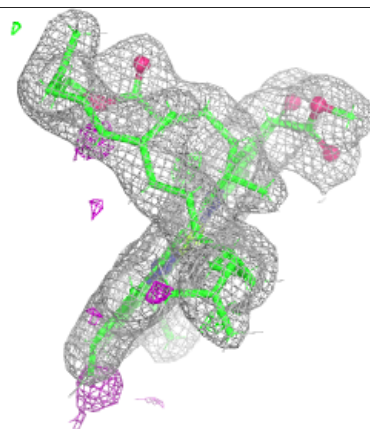
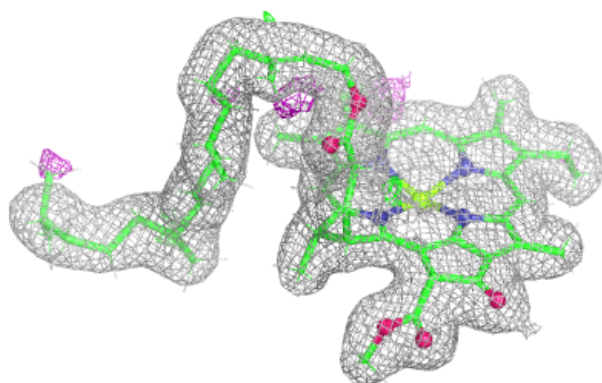
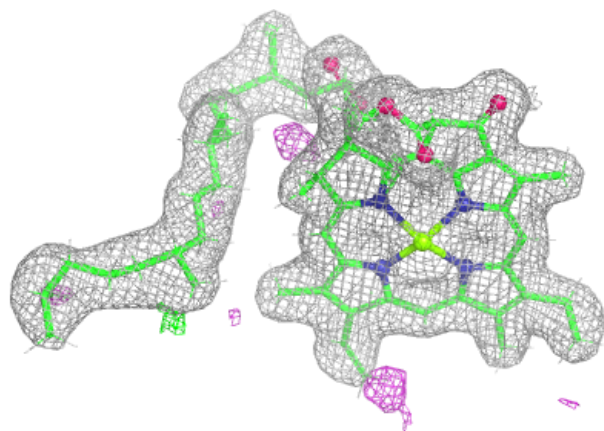
Electron density around CLA b 613:

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

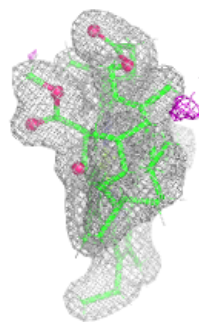
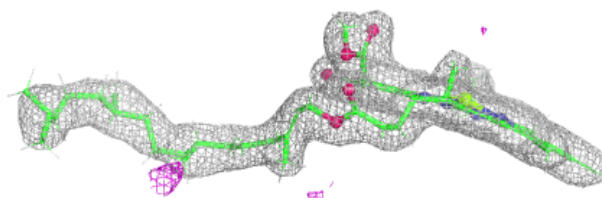
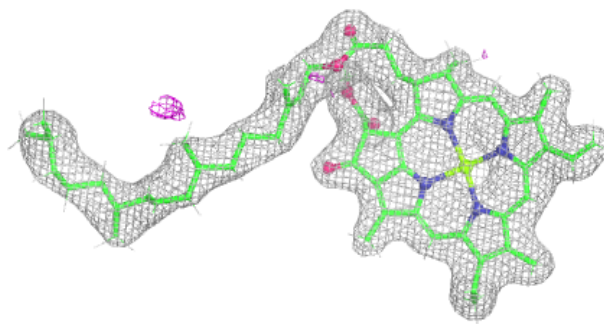


Electron density around CLA A 614:

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

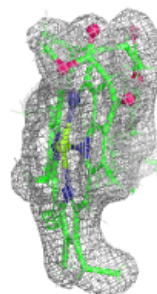
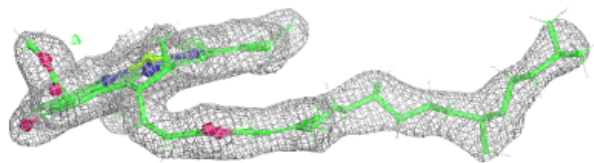
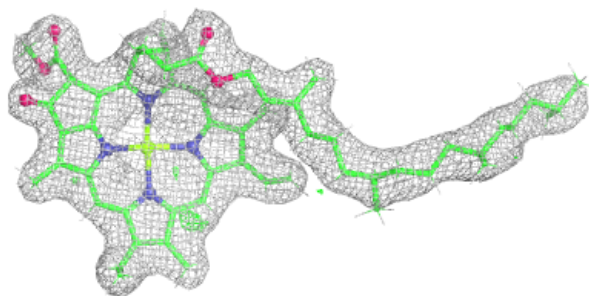
**Electron density around CLA B 602:**

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



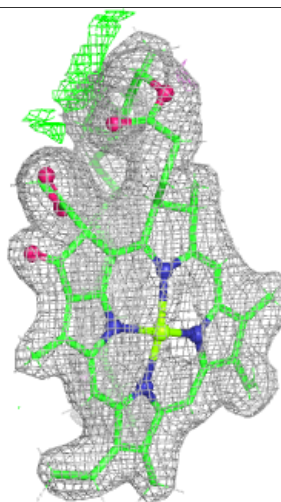
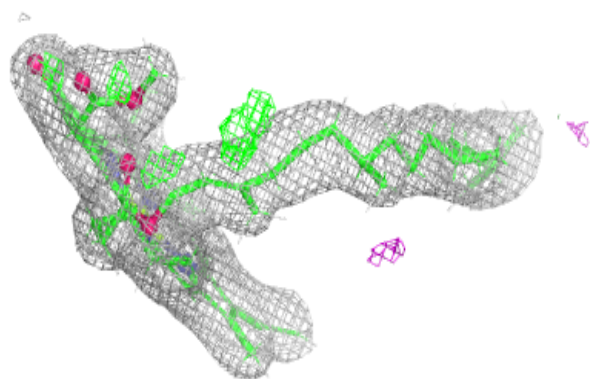
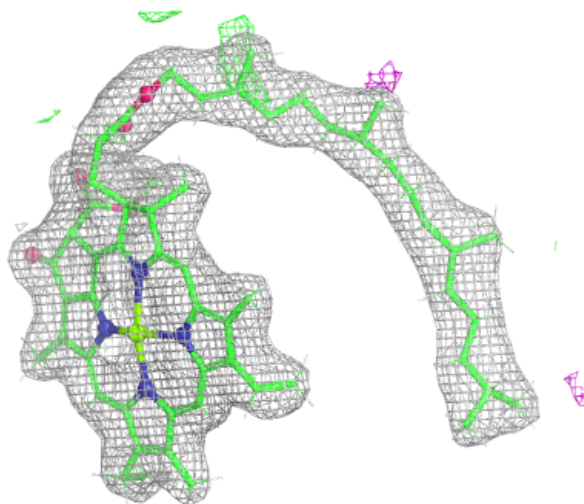
Electron density around CLA B 603:

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



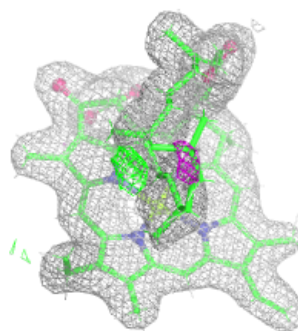
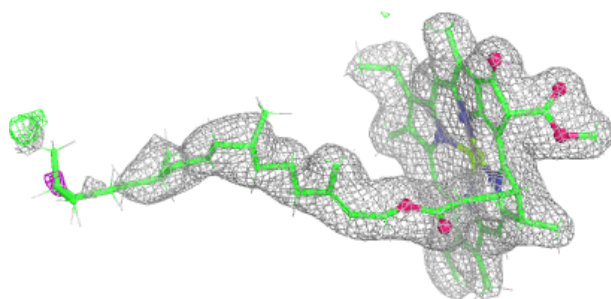
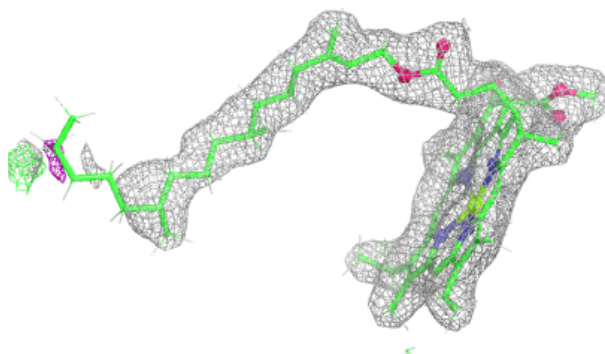
Electron density around CLA C 507:

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

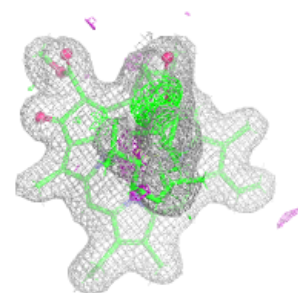
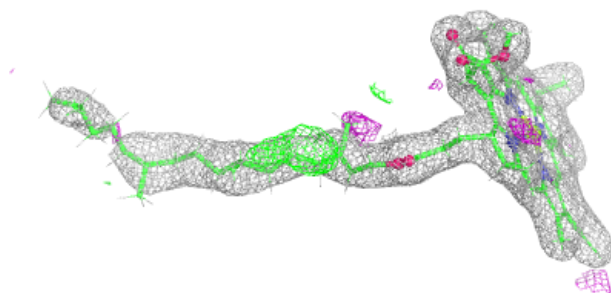
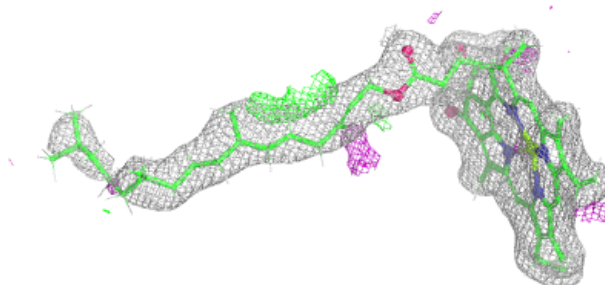


Electron density around CLA C 508:

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

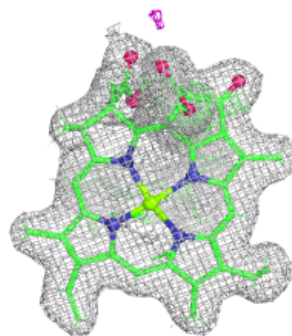
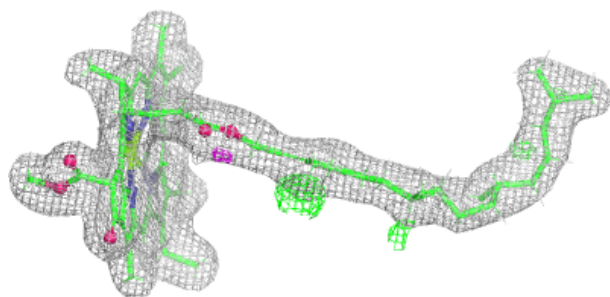
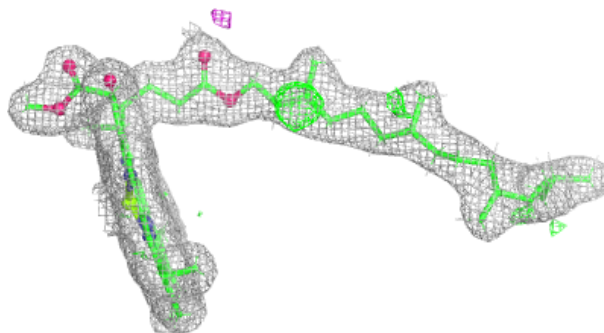
**Electron density around CLA B 604:**

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

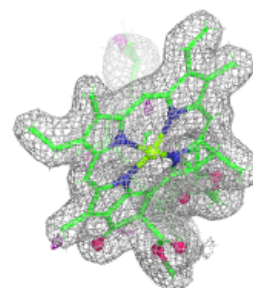
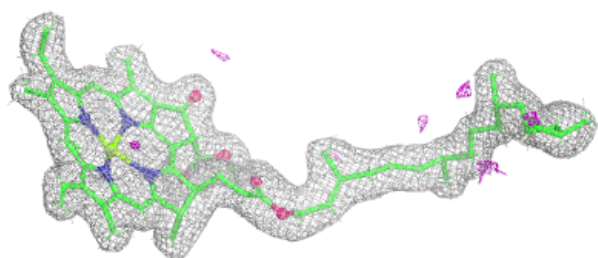
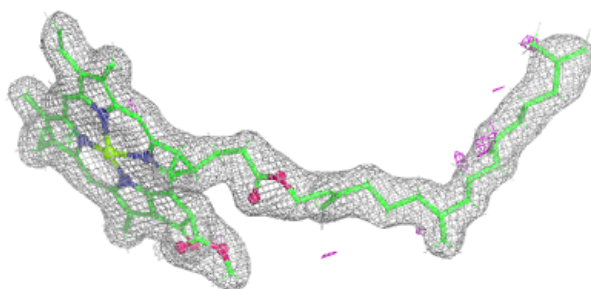


Electron density around CLA B 605:

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

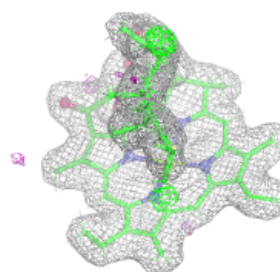
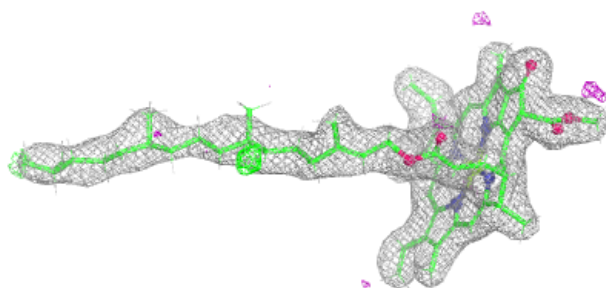
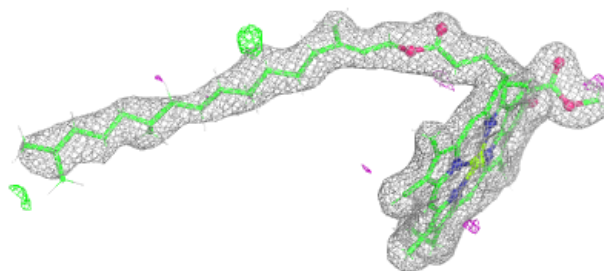
**Electron density around CLA A 607:**

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

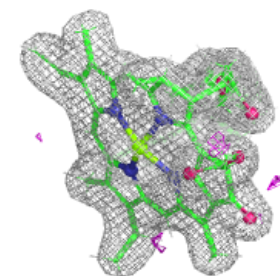
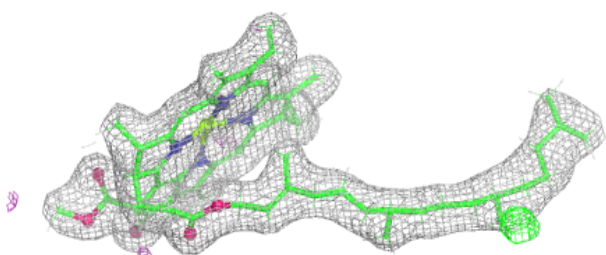
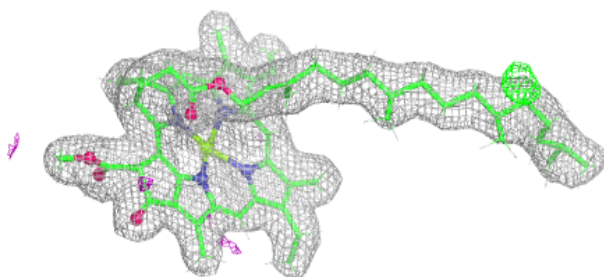


Electron density around CLA B 607:

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

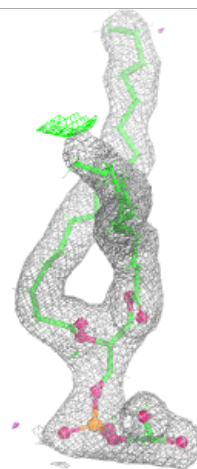
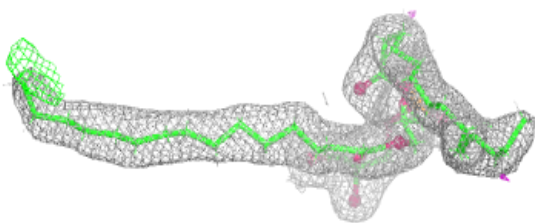
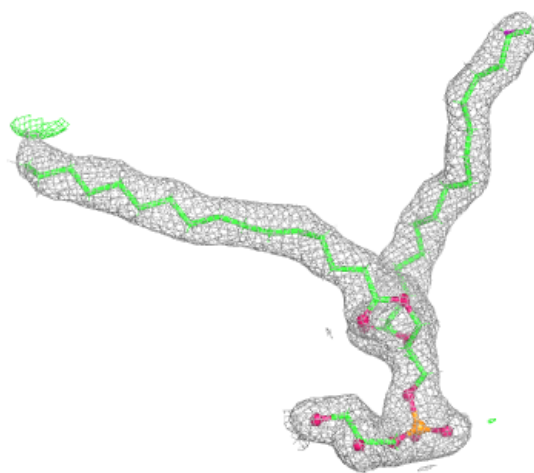
**Electron density around CLA B 608:**

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



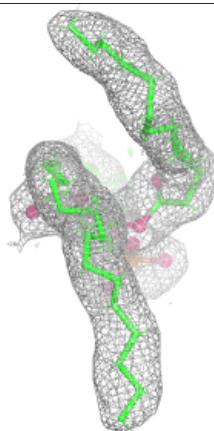
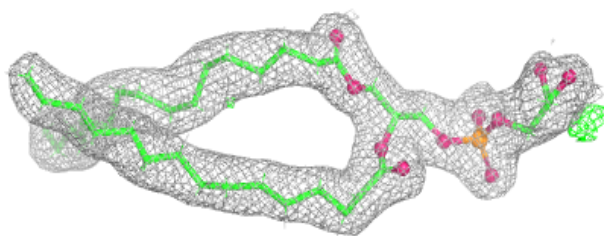
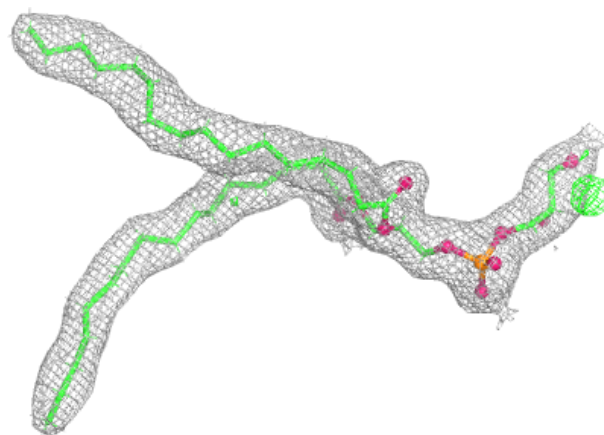
Electron density around LHG B 622:

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



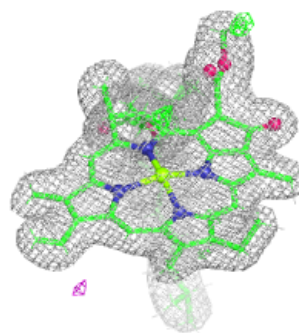
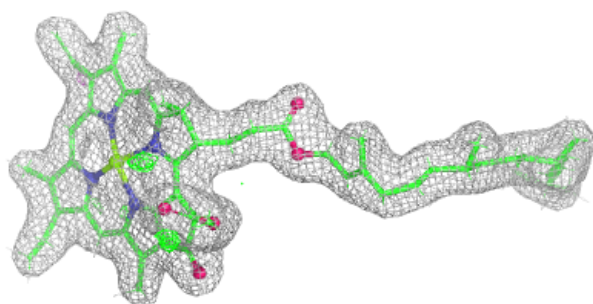
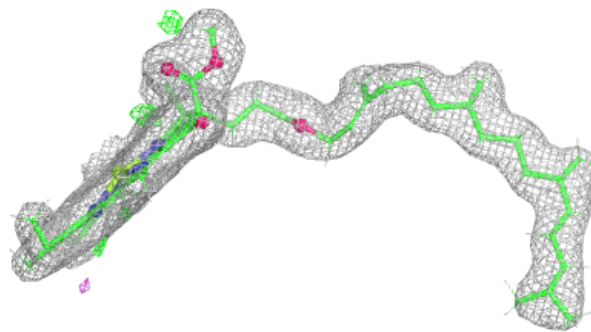
Electron density around LHG D 408:

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

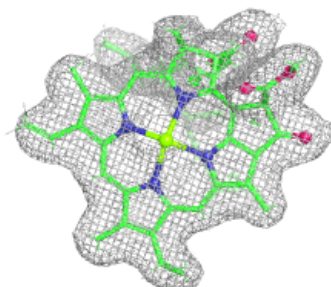
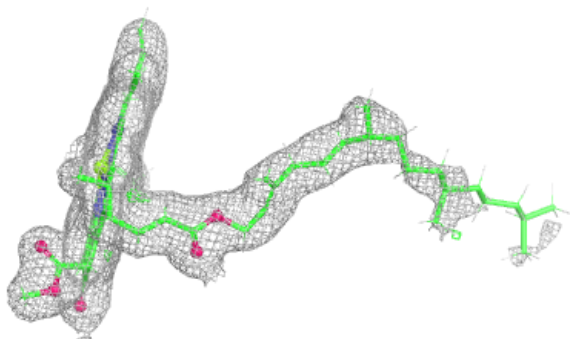
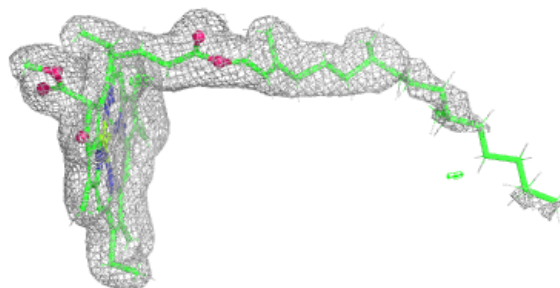


Electron density around CLA D 402:

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

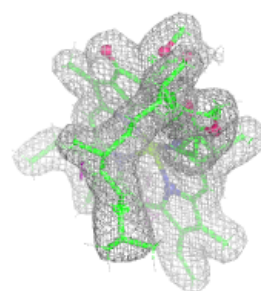
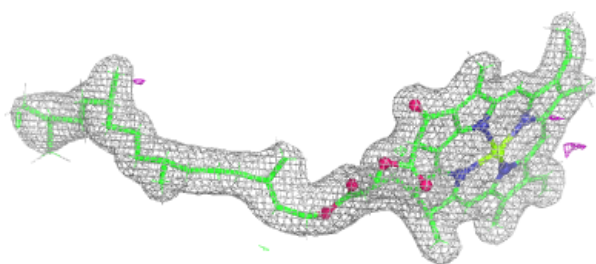
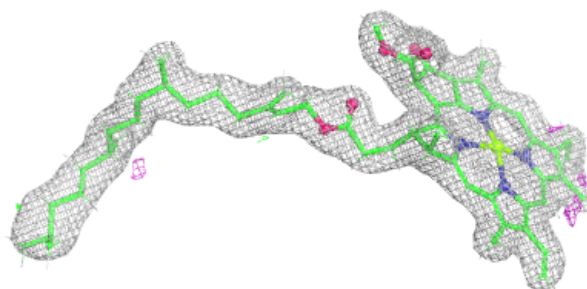
**Electron density around CLA D 403:**

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

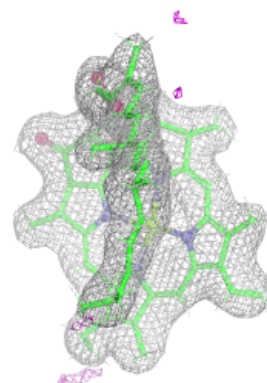
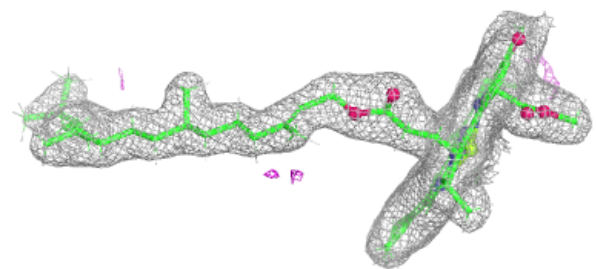
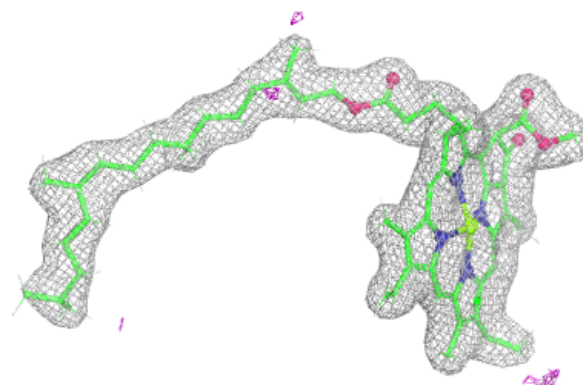


Electron density around CLA a 607:

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

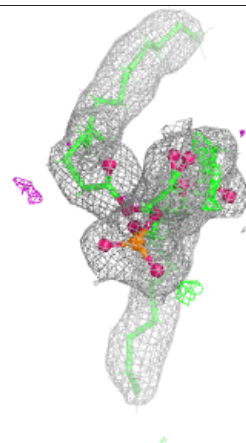
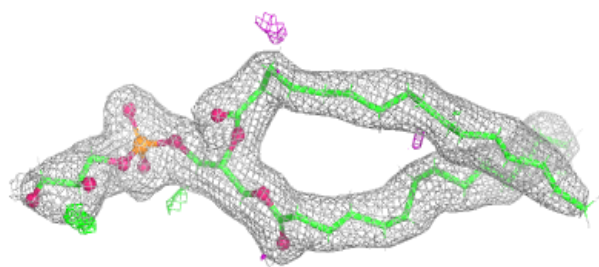
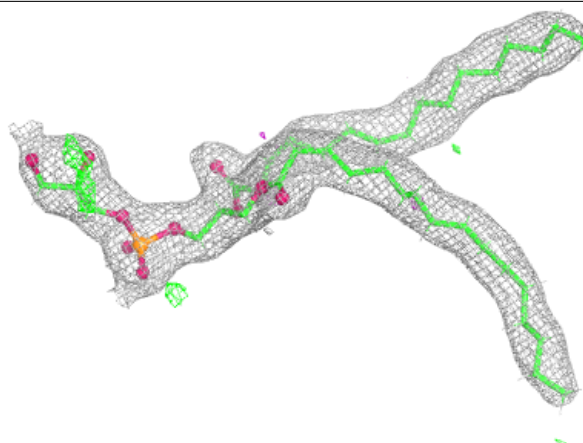
**Electron density around CLA B 609:**

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

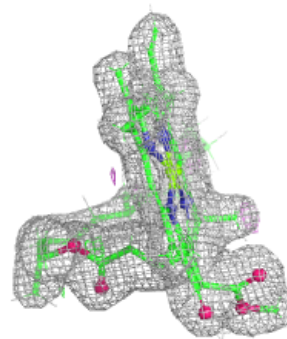
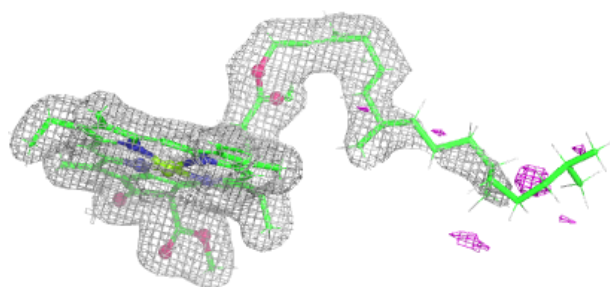
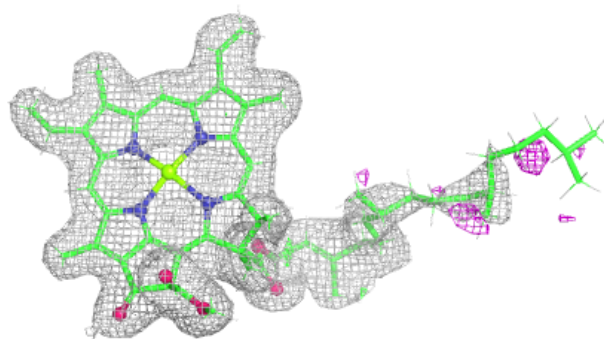


Electron density around LHG d 408:

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

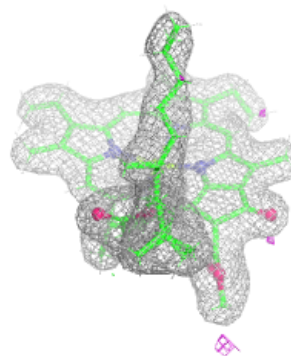
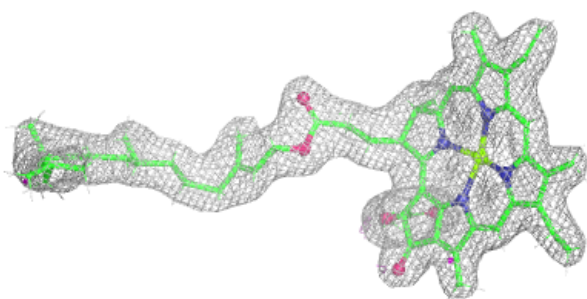
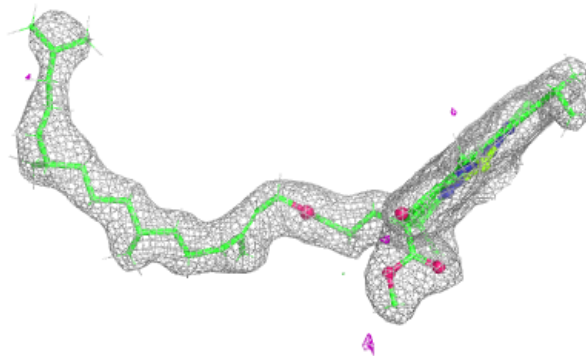
**Electron density around CLA A 608:**

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

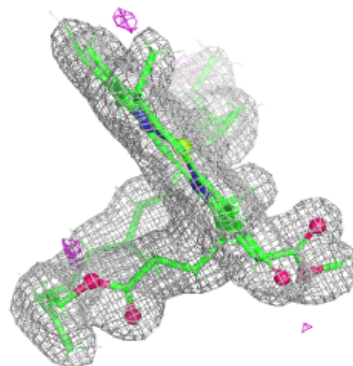
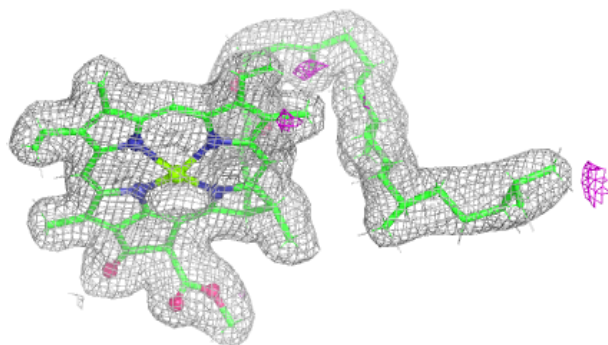
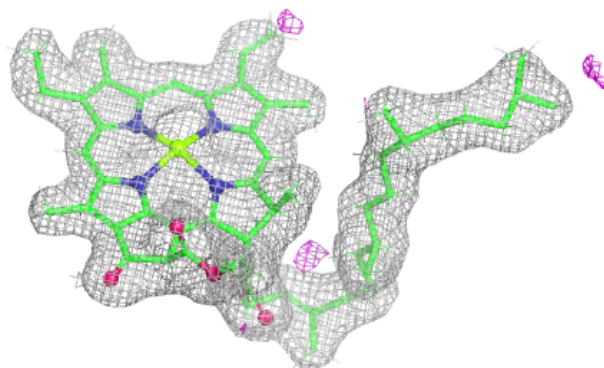


Electron density around CLA d 402:

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

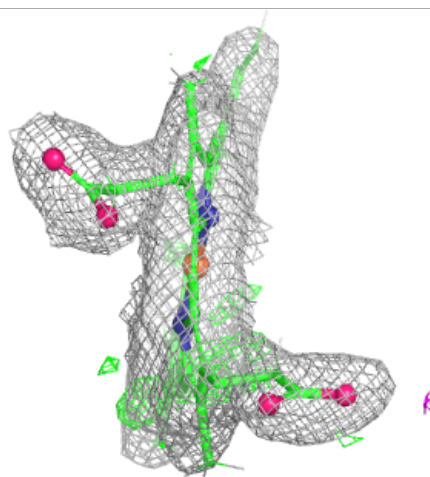
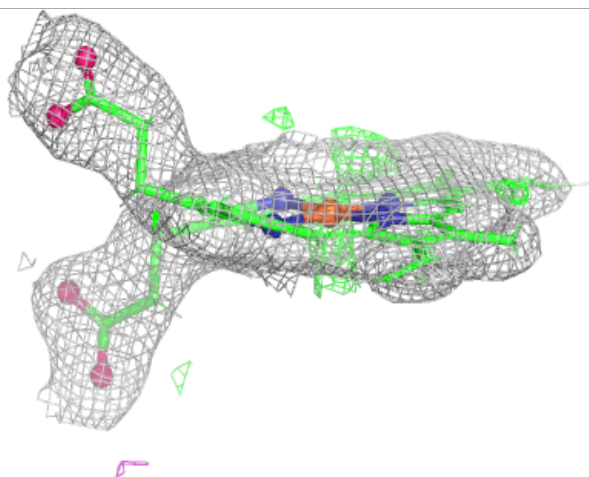
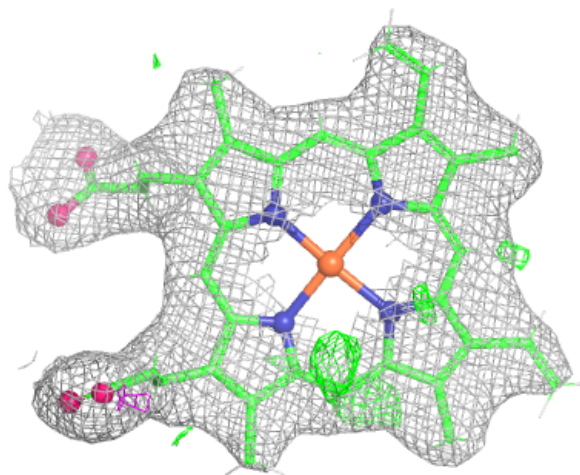
**Electron density around CLA a 613:**

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



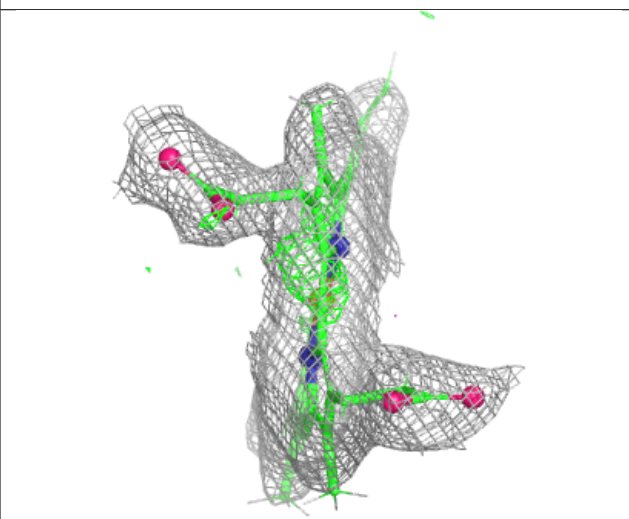
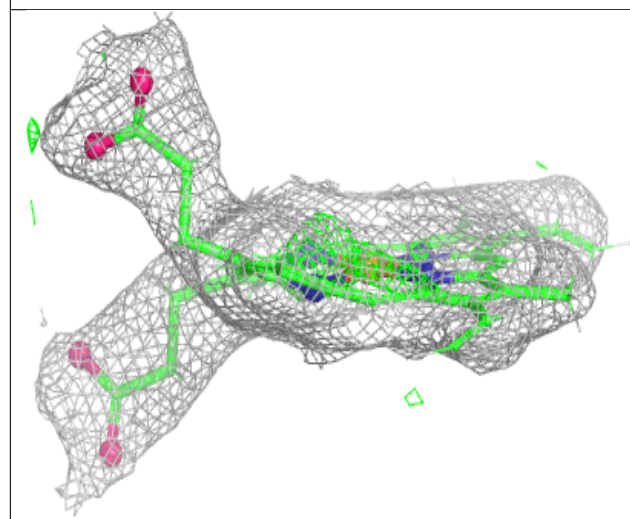
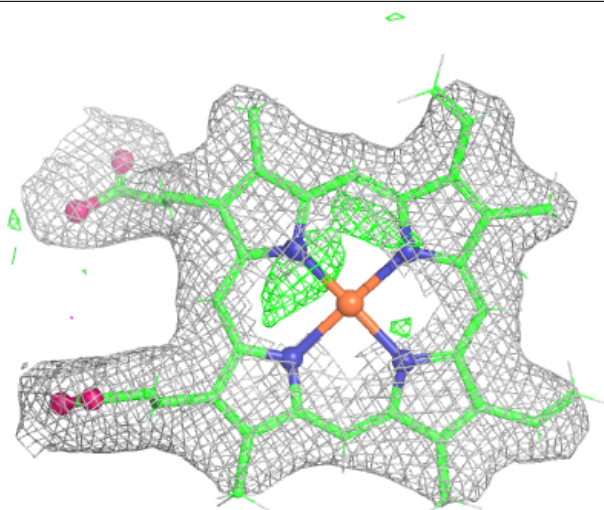
Electron density around HEM F 101:

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



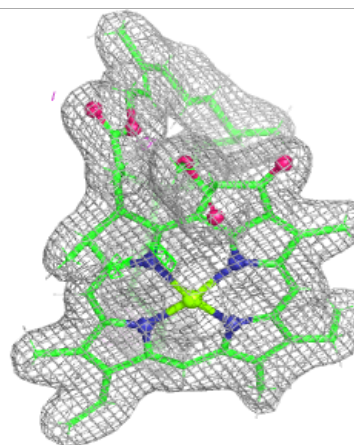
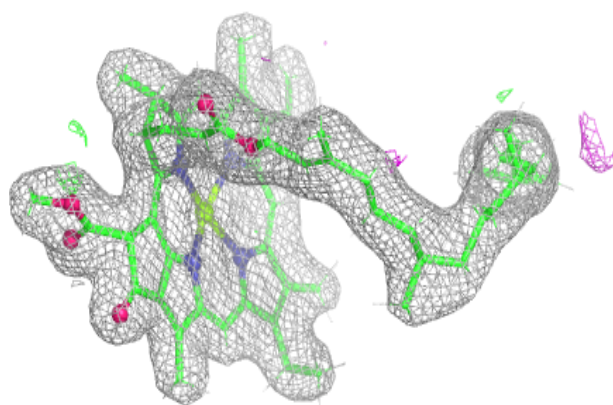
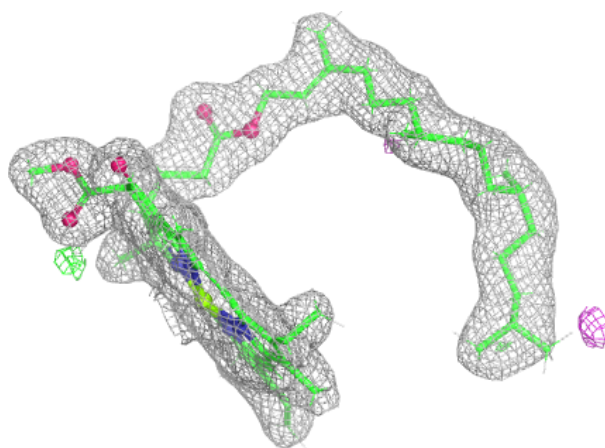
Electron density around HEM f 101:

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



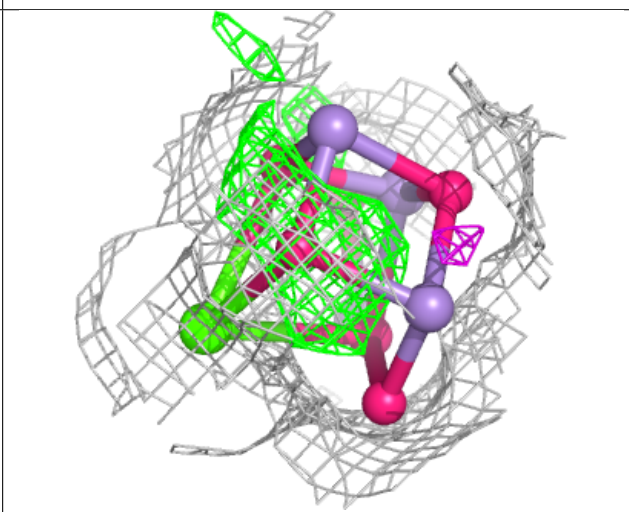
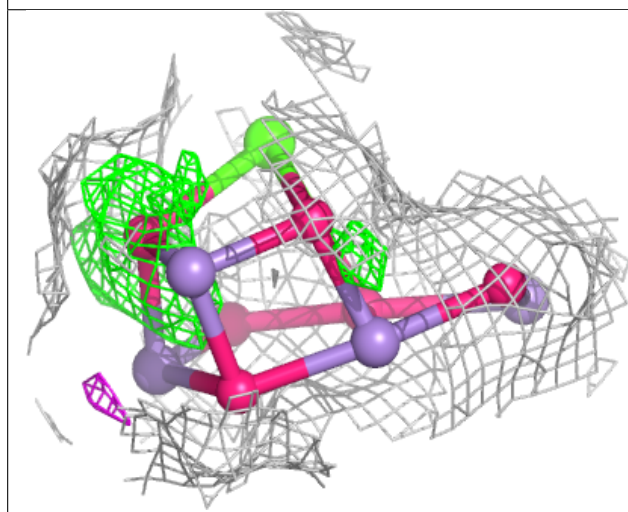
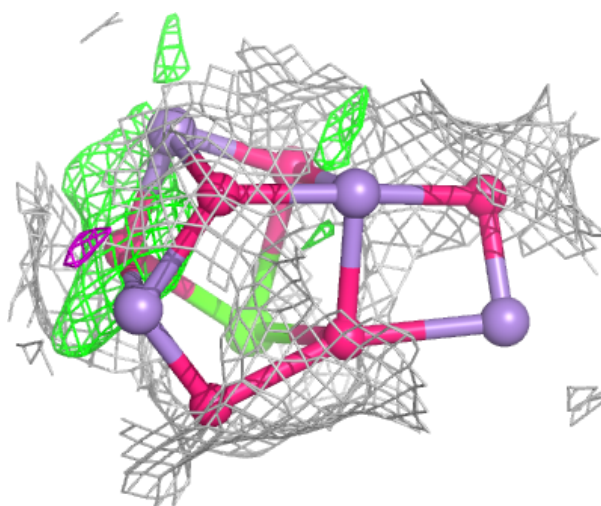
Electron density around CLA B 611:

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



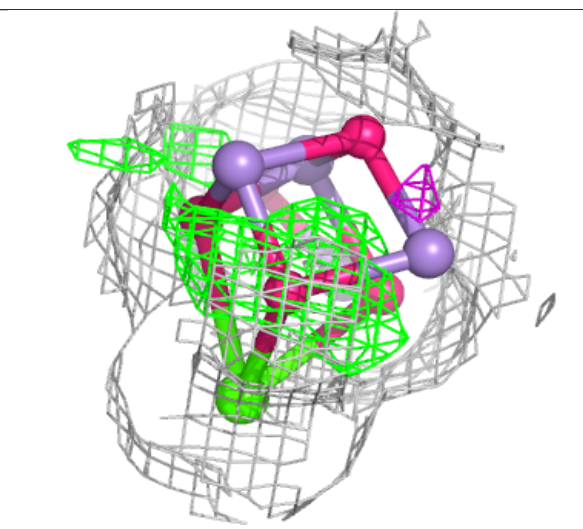
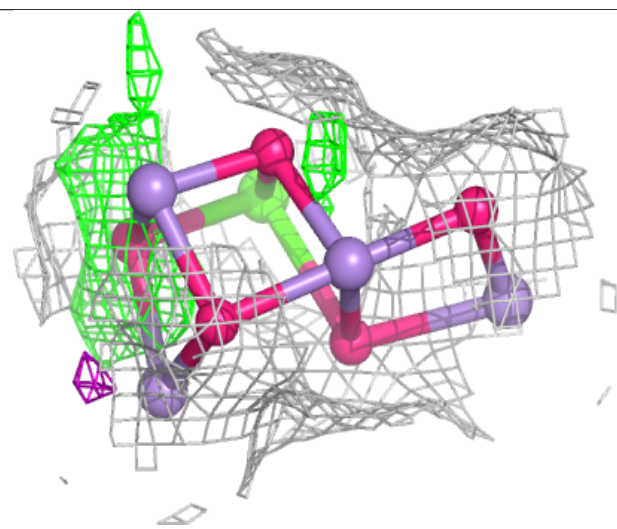
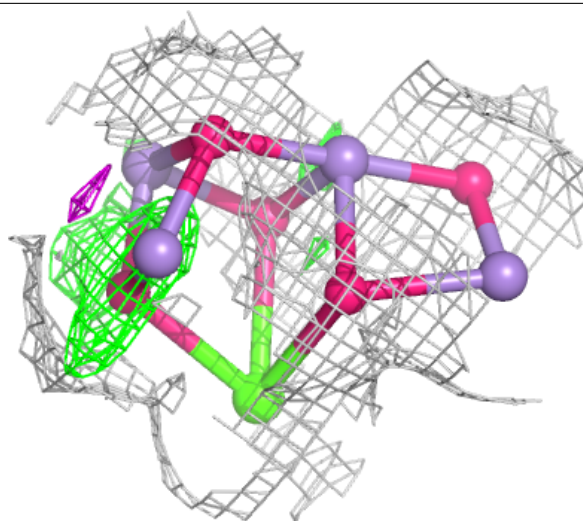
Electron density around OEY A 601 (B):

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



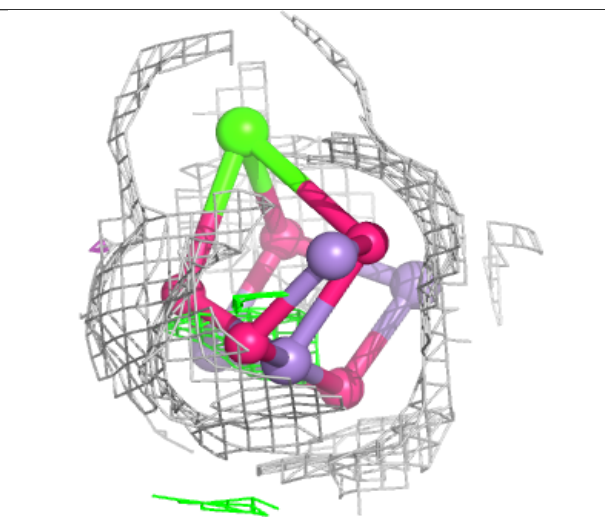
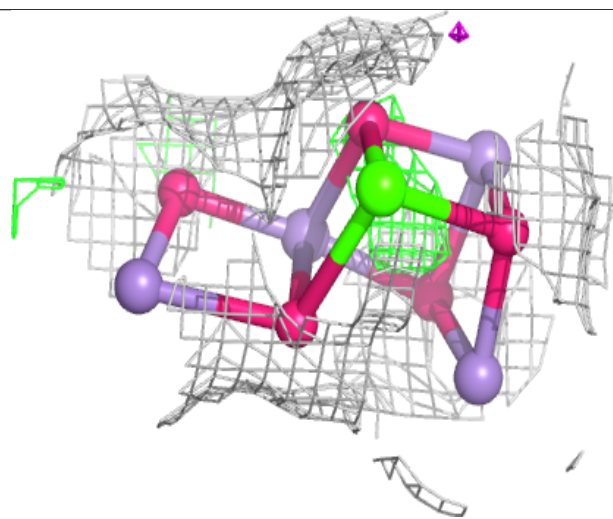
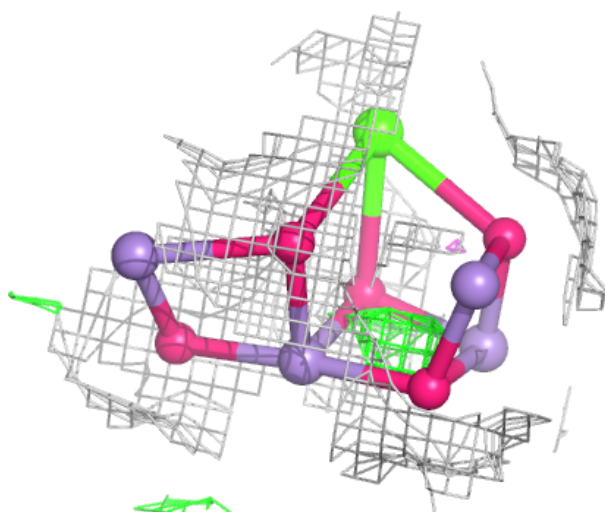
Electron density around OEX A 602 (A):

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



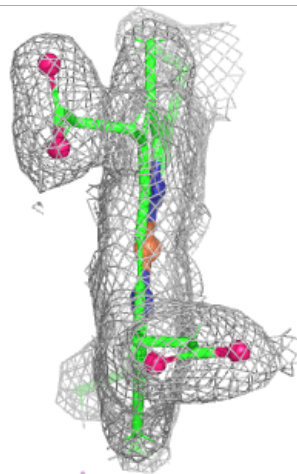
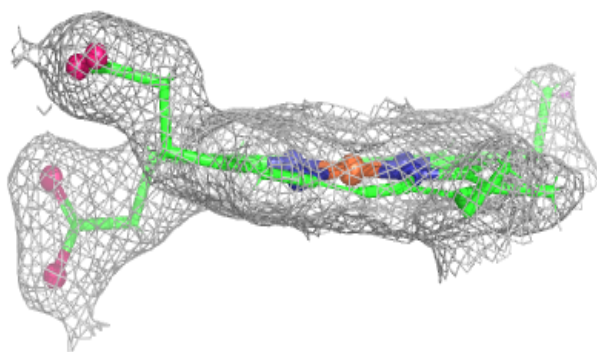
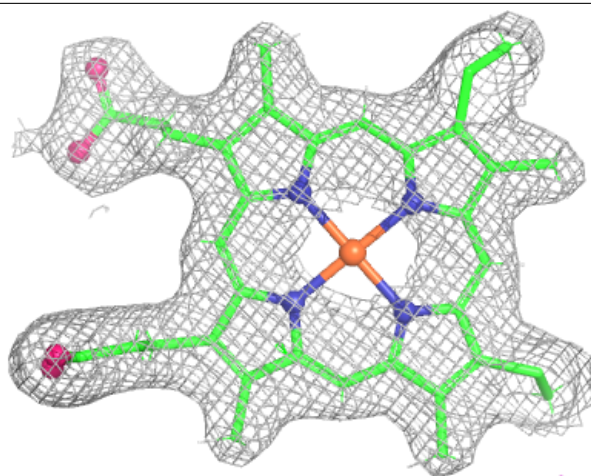
Electron density around OEX a 602 (A):

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



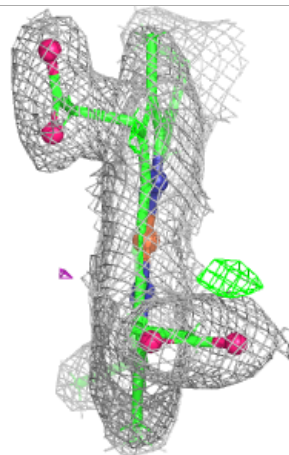
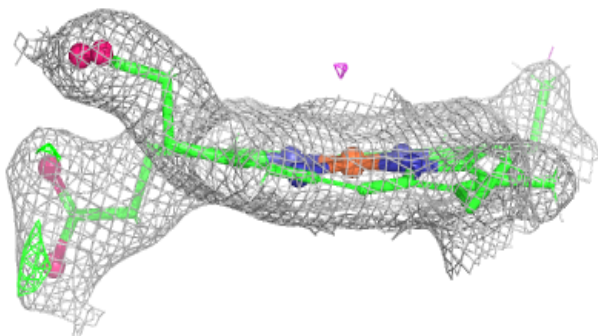
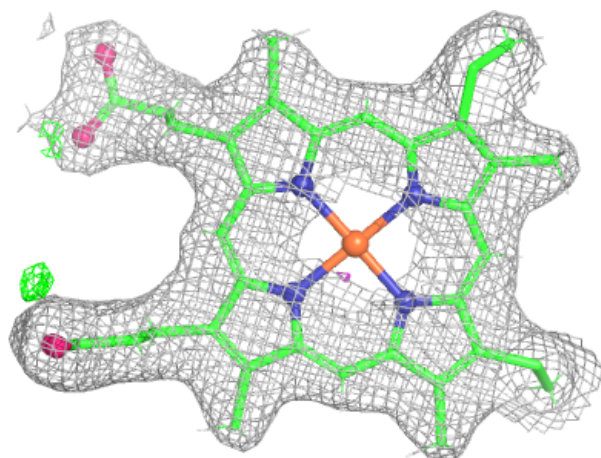
Electron density around HEC V 201:

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



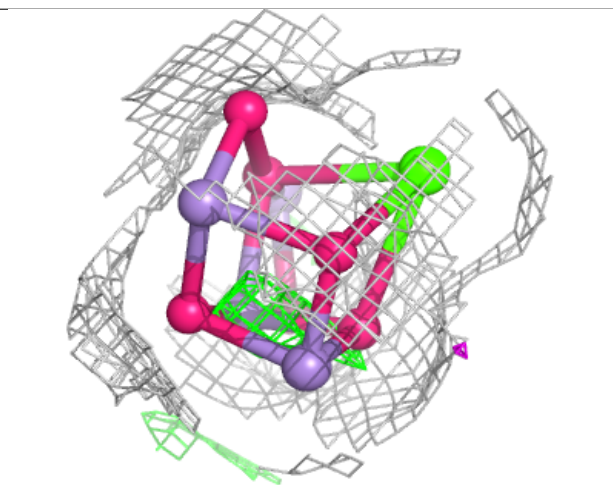
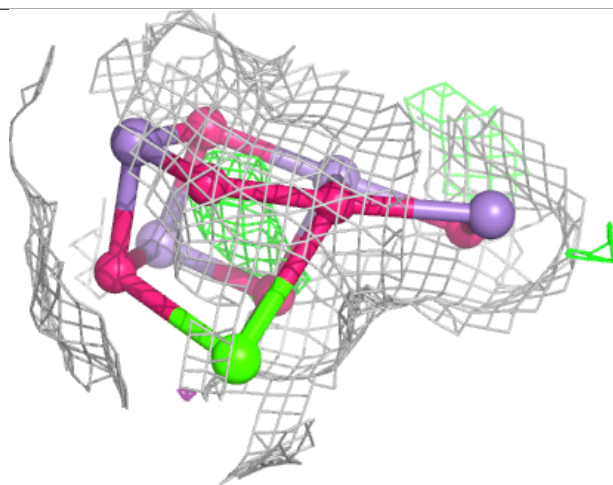
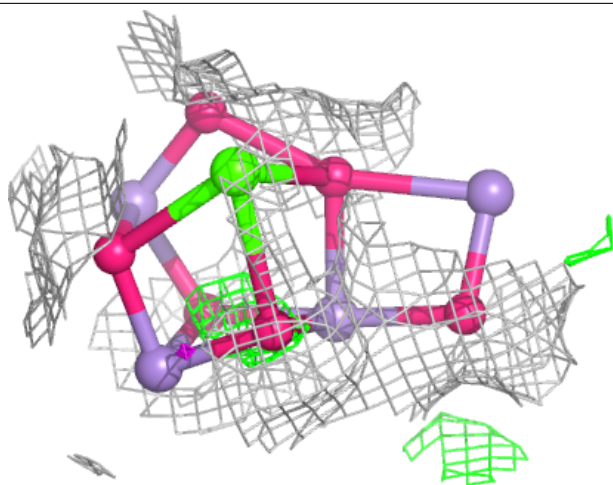
Electron density around HEC v 201:

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



Electron density around 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.